Full wwPDB EM Validation Report (i)

Jul 10, 2024 – 12:23 PM JST

PDB ID	:	7XNS
EMDB ID	:	EMD-33325
Title	:	SARS-CoV-2 Omicron BA.2.12.1 variant spike
Authors	:	Wang, X.; Wang, L.
Deposited on	:	2022-04-29
Resolution	:	3.48 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/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:

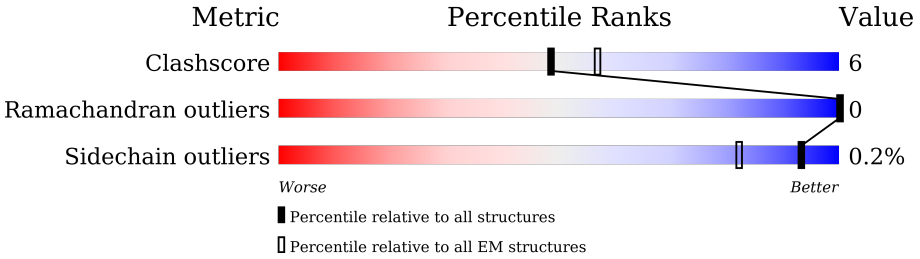
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (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:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.48 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	A	1270	23% 73% 13% 14%
1	B	1270	23% 74% 12% 14%
1	C	1270	23% 73% 13% 14%
2	D	2	100% 100%
2	E	2	50% 50% 50%
2	F	2	100%
2	G	2	50% 100%
2	H	2	50% 50% 50%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	I	2	50% 100%
2	J	2	100% 50% 50%
2	K	2	50% 50% 50%
2	L	2	100%
2	M	2	50% 100%
2	N	2	50% 50% 50%
2	O	2	50% 100%
2	P	2	100% 100%
2	Q	2	50% 50% 50%
2	R	2	100%
2	S	2	50% 100%
2	T	2	50% 50% 50%
2	U	2	50% 100%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 26595 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1095	8557	5471	1425	1623	38	0	0
1	B	1095	8557	5471	1425	1623	38	0	0
1	C	1095	8557	5471	1425	1623	38	0	0

There are 123 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	ILE	THR	variant	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	27	SER	ALA	variant	UNP P0DTC2
A	142	ASP	GLY	variant	UNP P0DTC2
A	213	GLY	VAL	variant	UNP P0DTC2
A	339	ASP	GLY	variant	UNP P0DTC2
A	371	PHE	SER	variant	UNP P0DTC2
A	373	PRO	SER	variant	UNP P0DTC2
A	375	PHE	SER	variant	UNP P0DTC2
A	376	ALA	THR	variant	UNP P0DTC2
A	405	ASN	ASP	variant	UNP P0DTC2
A	408	SER	ARG	variant	UNP P0DTC2
A	417	ASN	LYS	variant	UNP P0DTC2
A	440	LYS	ASN	variant	UNP P0DTC2
A	452	GLN	LEU	variant	UNP P0DTC2
A	477	ASN	SER	variant	UNP P0DTC2
A	478	LYS	THR	variant	UNP P0DTC2
A	484	ALA	GLU	variant	UNP P0DTC2
A	493	ARG	GLN	variant	UNP P0DTC2
A	498	ARG	GLN	variant	UNP P0DTC2
A	501	TYR	ASN	variant	UNP P0DTC2
A	505	HIS	TYR	variant	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	614	GLY	ASP	variant	UNP P0DTC2
A	655	TYR	HIS	variant	UNP P0DTC2
A	679	TYR	ASN	variant	UNP P0DTC2
A	681	HIS	PRO	variant	UNP P0DTC2
A	683	ALA	ARG	variant	UNP P0DTC2
A	685	ALA	ARG	variant	UNP P0DTC2
A	704	LEU	SER	variant	UNP P0DTC2
A	764	LYS	ASN	variant	UNP P0DTC2
A	796	TYR	ASP	variant	UNP P0DTC2
A	817	PRO	PHE	variant	UNP P0DTC2
A	892	PRO	ALA	variant	UNP P0DTC2
A	899	PRO	ALA	variant	UNP P0DTC2
A	942	PRO	ALA	variant	UNP P0DTC2
A	954	HIS	GLN	variant	UNP P0DTC2
A	969	LYS	ASN	variant	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	22	ILE	THR	variant	UNP P0DTC2
B	?	-	LEU	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	27	SER	ALA	variant	UNP P0DTC2
B	142	ASP	GLY	variant	UNP P0DTC2
B	213	GLY	VAL	variant	UNP P0DTC2
B	339	ASP	GLY	variant	UNP P0DTC2
B	371	PHE	SER	variant	UNP P0DTC2
B	373	PRO	SER	variant	UNP P0DTC2
B	375	PHE	SER	variant	UNP P0DTC2
B	376	ALA	THR	variant	UNP P0DTC2
B	405	ASN	ASP	variant	UNP P0DTC2
B	408	SER	ARG	variant	UNP P0DTC2
B	417	ASN	LYS	variant	UNP P0DTC2
B	440	LYS	ASN	variant	UNP P0DTC2
B	452	GLN	LEU	variant	UNP P0DTC2
B	477	ASN	SER	variant	UNP P0DTC2
B	478	LYS	THR	variant	UNP P0DTC2
B	484	ALA	GLU	variant	UNP P0DTC2
B	493	ARG	GLN	variant	UNP P0DTC2
B	498	ARG	GLN	variant	UNP P0DTC2
B	501	TYR	ASN	variant	UNP P0DTC2
B	505	HIS	TYR	variant	UNP P0DTC2
B	614	GLY	ASP	variant	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	655	TYR	HIS	variant	UNP P0DTC2
B	679	TYR	ASN	variant	UNP P0DTC2
B	681	HIS	PRO	variant	UNP P0DTC2
B	683	ALA	ARG	variant	UNP P0DTC2
B	685	ALA	ARG	variant	UNP P0DTC2
B	704	LEU	SER	variant	UNP P0DTC2
B	764	LYS	ASN	variant	UNP P0DTC2
B	796	TYR	ASP	variant	UNP P0DTC2
B	817	PRO	PHE	variant	UNP P0DTC2
B	892	PRO	ALA	variant	UNP P0DTC2
B	899	PRO	ALA	variant	UNP P0DTC2
B	942	PRO	ALA	variant	UNP P0DTC2
B	954	HIS	GLN	variant	UNP P0DTC2
B	969	LYS	ASN	variant	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	22	ILE	THR	variant	UNP P0DTC2
C	?	-	LEU	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	27	SER	ALA	variant	UNP P0DTC2
C	142	ASP	GLY	variant	UNP P0DTC2
C	213	GLY	VAL	variant	UNP P0DTC2
C	339	ASP	GLY	variant	UNP P0DTC2
C	371	PHE	SER	variant	UNP P0DTC2
C	373	PRO	SER	variant	UNP P0DTC2
C	375	PHE	SER	variant	UNP P0DTC2
C	376	ALA	THR	variant	UNP P0DTC2
C	405	ASN	ASP	variant	UNP P0DTC2
C	408	SER	ARG	variant	UNP P0DTC2
C	417	ASN	LYS	variant	UNP P0DTC2
C	440	LYS	ASN	variant	UNP P0DTC2
C	452	GLN	LEU	variant	UNP P0DTC2
C	477	ASN	SER	variant	UNP P0DTC2
C	478	LYS	THR	variant	UNP P0DTC2
C	484	ALA	GLU	variant	UNP P0DTC2
C	493	ARG	GLN	variant	UNP P0DTC2
C	498	ARG	GLN	variant	UNP P0DTC2
C	501	TYR	ASN	variant	UNP P0DTC2
C	505	HIS	TYR	variant	UNP P0DTC2
C	614	GLY	ASP	variant	UNP P0DTC2
C	655	TYR	HIS	variant	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	679	TYR	ASN	variant	UNP P0DTC2
C	681	HIS	PRO	variant	UNP P0DTC2
C	683	ALA	ARG	variant	UNP P0DTC2
C	685	ALA	ARG	variant	UNP P0DTC2
C	704	LEU	SER	variant	UNP P0DTC2
C	764	LYS	ASN	variant	UNP P0DTC2
C	796	TYR	ASP	variant	UNP P0DTC2
C	817	PRO	PHE	variant	UNP P0DTC2
C	892	PRO	ALA	variant	UNP P0DTC2
C	899	PRO	ALA	variant	UNP P0DTC2
C	942	PRO	ALA	variant	UNP P0DTC2
C	954	HIS	GLN	variant	UNP P0DTC2
C	969	LYS	ASN	variant	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2

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

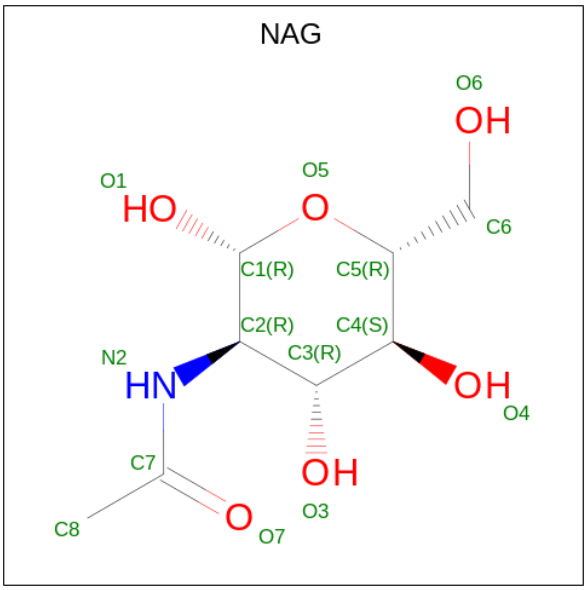
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	D	2	28	16	2	10	0	0
2	E	2	28	16	2	10	0	0
2	F	2	28	16	2	10	0	0
2	G	2	28	16	2	10	0	0
2	H	2	28	16	2	10	0	0
2	I	2	28	16	2	10	0	0
2	J	2	28	16	2	10	0	0
2	K	2	28	16	2	10	0	0
2	L	2	28	16	2	10	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	M	2	28	16	2	10	0	0
			Total	C	N	O		
2	N	2	28	16	2	10	0	0
			Total	C	N	O		
2	O	2	28	16	2	10	0	0
			Total	C	N	O		
2	P	2	28	16	2	10	0	0
			Total	C	N	O		
2	Q	2	28	16	2	10	0	0
			Total	C	N	O		
2	R	2	28	16	2	10	0	0
			Total	C	N	O		
2	S	2	28	16	2	10	0	0
			Total	C	N	O		
2	T	2	28	16	2	10	0	0
			Total	C	N	O		
2	U	2	28	16	2	10	0	0

- Molecule 3 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	
3	A	1	14	8	1	5	0
			Total	C	N	O	
3	A	1	14	8	1	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
3	A	1	14	8	1	5	0
3	A	1	14	8	1	5	0
3	A	1	14	8	1	5	0
3	A	1	14	8	1	5	0
3	A	1	14	8	1	5	0
3	A	1	14	8	1	5	0
3	A	1	14	8	1	5	0
3	A	1	14	8	1	5	0
3	B	1	14	8	1	5	0
3	B	1	14	8	1	5	0
3	B	1	14	8	1	5	0
3	B	1	14	8	1	5	0
3	B	1	14	8	1	5	0
3	B	1	14	8	1	5	0
3	B	1	14	8	1	5	0
3	B	1	14	8	1	5	0
3	B	1	14	8	1	5	0
3	B	1	14	8	1	5	0
3	C	1	14	8	1	5	0
3	C	1	14	8	1	5	0
3	C	1	14	8	1	5	0

Continued on next page...

Continued from previous page...

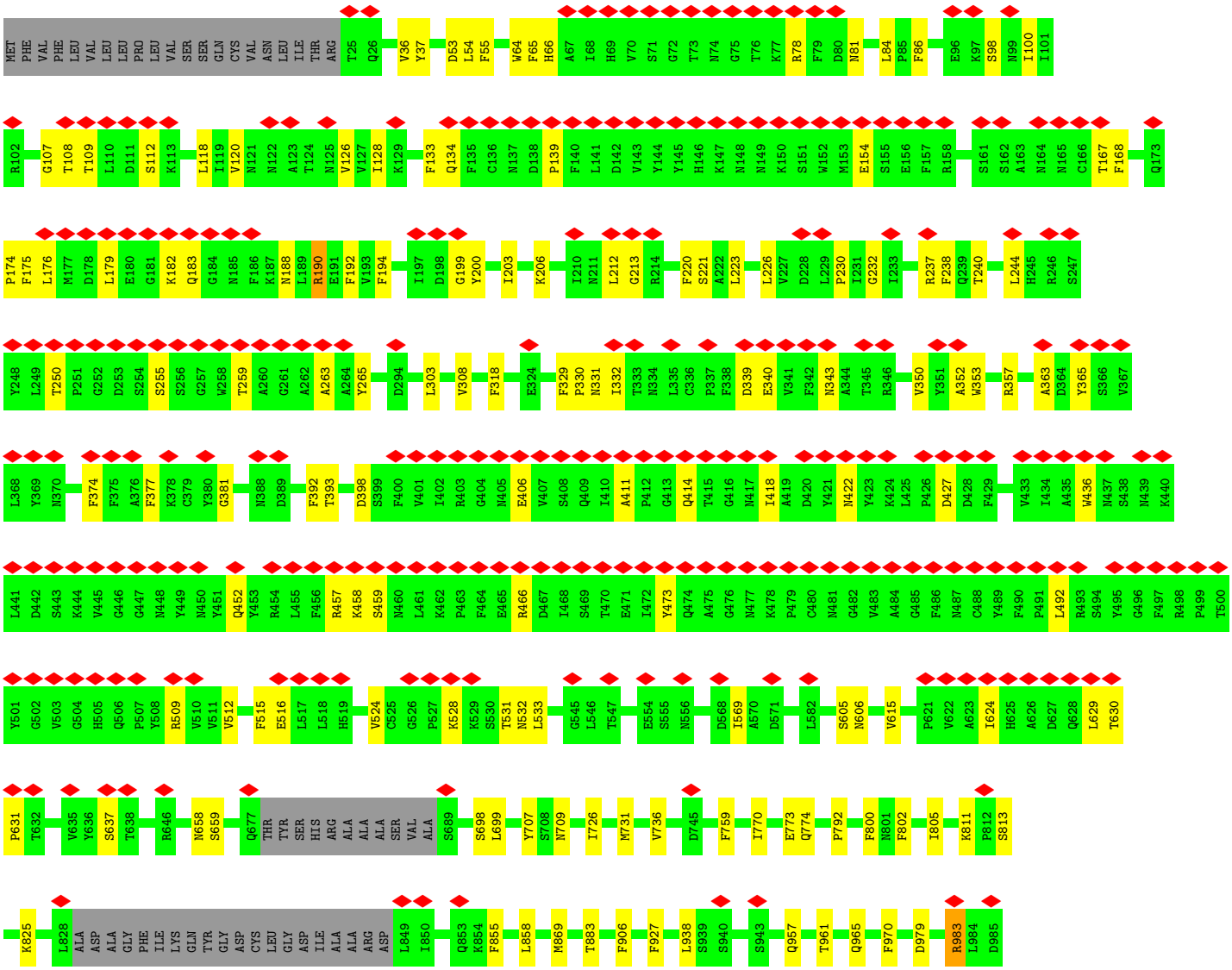
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
3	C	1	14	8	1	5	0
			Total	C	N	O	
3	C	1	14	8	1	5	0
			Total	C	N	O	
3	C	1	14	8	1	5	0
			Total	C	N	O	
3	C	1	14	8	1	5	0
			Total	C	N	O	
3	C	1	14	8	1	5	0
			Total	C	N	O	
3	C	1	14	8	1	5	0
			Total	C	N	O	
3	C	1	14	8	1	5	0

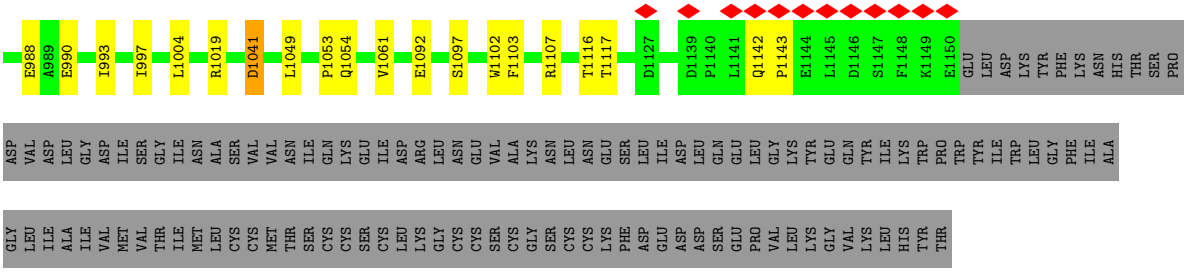
3 Residue-property plots (i)

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: Spike glycoprotein

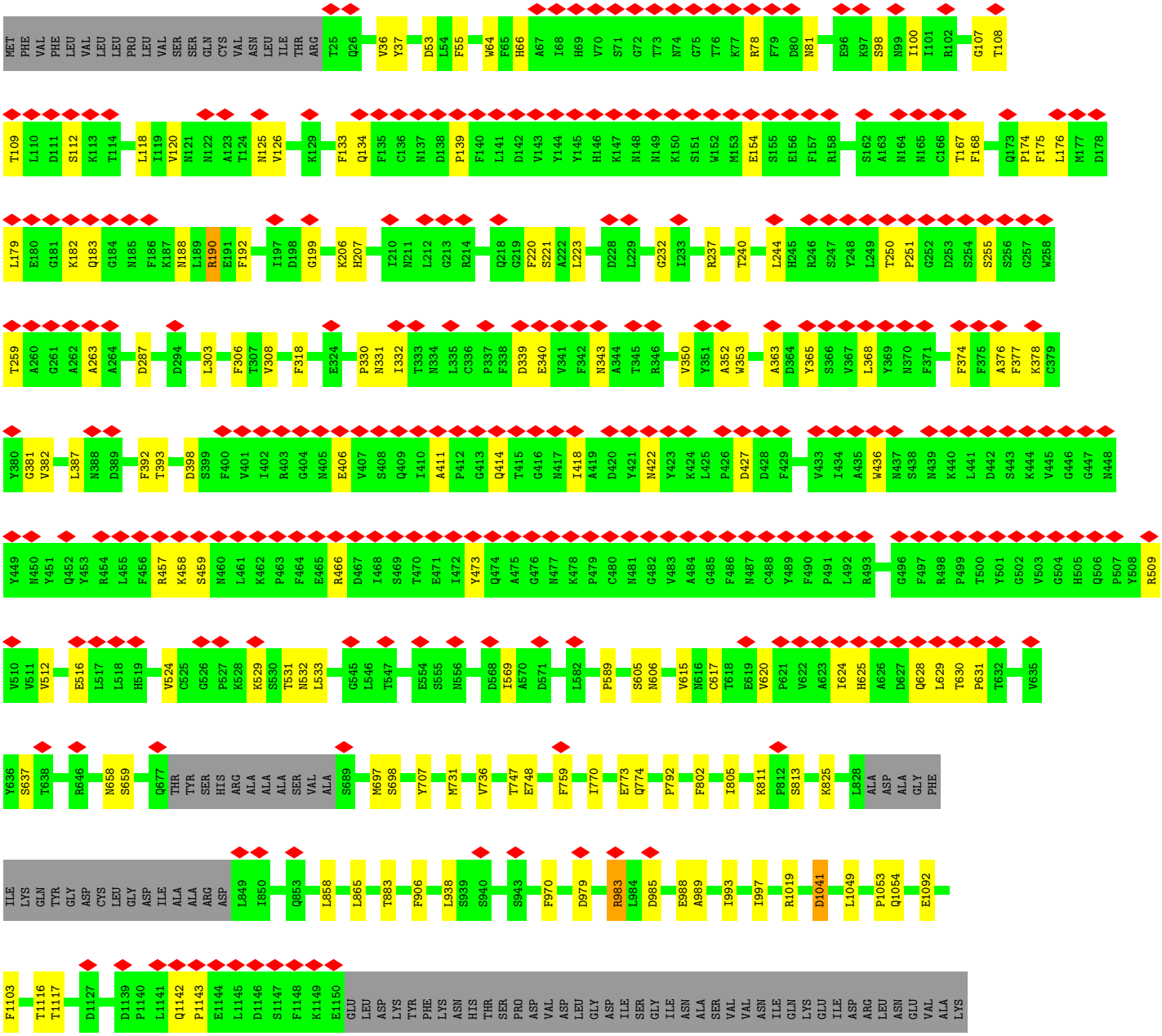
Chain A: 23% 73% 13% 14%

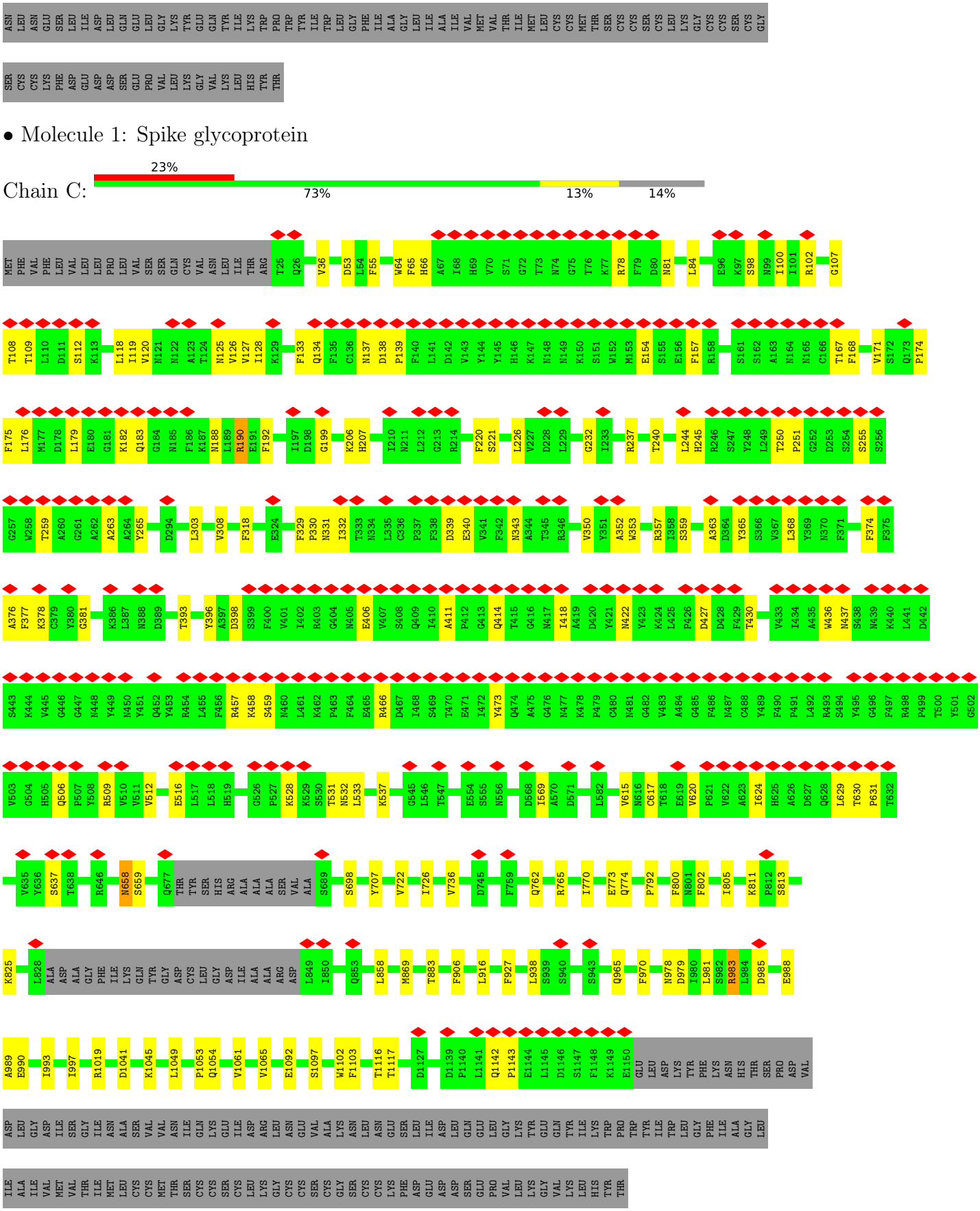




- Molecule 1: Spike glycoprotein

Chain B:




ASN LEU ASN GLU SER LEU ILE ASP LEU GLN GLU LEU GLY LYS TYR GLU GLN TYR ILE LYS TRP PRO TRP TYR ILE TRP LEU GLY PHE ILE ALA GLY LEU ILE ALA ILE VAL MET VAL THR ILE MET LEU CYS CYS MET THR SER CYS CYS SER CYS LEU LYS GLY CYS CYS SER CYS GLY
SER CYS CYS LYS PHE ASP GLU ASP ASP SER GLU PRO VAL LEU LYS GLY VAL LYS LEU HIS TYR THR
• Molecule 1: Spike glycoprotein
Chain C:
23%
73%
13%
14%
MET PHE VAL PHE LEU VAL LEU LEU PRO LEU VAL SER SER GLN CYS VAL ASN LEU ILE THR ARG T25 Q26 V36 D53 L54 F55 W64 F65 H66 A67 I68 H69 V70 S71 G72 T73 N74 G75 T76 K77 R78 F79 D80 N81 L84 E96 K97 S98 N99 I100 T101 R102 G107
T108 T109 L110 D111 S112 K113 L118 I119 V120 N121 N122 A123 T124 N125 V126 V127 I128 K129 F133 Q134 F135 C136 N137 D138 P139 F140 L141 D142 V143 Y144 Y145 H146 K147 N148 N149 K150 S151 W152 M153 E154 S155 E156 F157 R158 S161 S162 A163 N164 N165 C166 T167 F168 V171 S172 Q173 P174
F175 L176 M177 D178 L179 E180 G181 K182 Q183 G184 N185 F186 K187 N188 L189 R190 E191 F192 I197 D198 G199 K206 H207 I210 N211 L212 G213 R214 F220 S221 L226 V227 D228 L229 G232 I233 R237 T240 L244 H245 R246 S247 Y248 L249 T250 P251 G252 D253 S254 S255 S256
G257 W258 T259 A260 G261 A262 A263 A264 Y265 D294 L303 V308 F318 E324 F329 P330 N331 I332 T333 N334 L335 C336 P337 F338 D339 E340 V341 F342 N343 A344 T345 R346 V350 Y351 A352 W353 R357 I358 S359 A363 D364 Y365 S366 V367 L368 Y369 N370 F371 F374 F375
A376 F377 K378 C379 Y380 G381 K386 L387 N388 D389 T393 Y396 A397 D398 S399 F400 V401 I402 R403 G404 N405 E406 V407 S408 Q409 I410 A411 P412 G413 Q414 T415 G416 N417 I418 A419 D420 Y421 N422 Y423 K424 L425 P426 D427 D428 F429 T430 V433 I434 A435 W436 N437 S438 N439 K440 L441 D442
S443 K444 V445 G446 G447 N448 Y449 N450 Y451 Q452 Y453 R454 L455 F456 R457 K458 S459 N460 L461 K462 P463 F464 E465 R466 D467 I468 S469 T470 E471 I472 Y473 Q474 A475 G476 N477 K478 P479 C480 N481 G482 V483 A484 G485 F486 N487 C488 Y489 F490 P491 L492 R493 S494 Y495 G496 F497 R498 P499 T500 Y501 G502
V503 G504 H505 Q506 P507 Y508 R509 V510 V511 V512 E516 L517 L518 H519 G526 P527 K528 K529 S530 T531 N532 L533 K537 G545 L546 T547 E554 S555 N556 D568 I569 A570 D571 L582 V615 N616 C617 T618 E619 V620 P621 V622 A623 I624 H625 A626 D627 Q628 L629 T630 P631 T632
V635 Y636 S637 T638 R646 N658 S659 Q677 THR TYR SER HIS ARG ALA ALA ALA SER VAL ALA S689 S698 Y707 V722 I726 V736 D745 F759 Q762 R765 I770 E773 Q774 P792 F800 N801 F802 I805 K811 P812 S813
K825 L828 ALA ASP ALA GLY PHE ILE LYS GLN TYR GLY ASP CYS LEU GLY ASP ILE ALA ALA ARG ASP L849 I850 Q853 L858 M869 T883 F906 L916 F927 L938 S939 S940 S943 Q965 F970 N978 D979 I980 L981 S982 R983 L984 D985 E988
A989 E990 I993 I997 R1019 D1041 K1045 L1049 P1053 Q1054 V1061 V1065 E1092 S1097 W1102 F1103 T1116 T1117 D1127 D1139 P1140 L1141 Q1142 P1143 E1144 L1145 D1146 S1147 F1148 K1149 E1150 GLU LEU ASP LYS TYR PHE LYS ASN HIS THR SER PRO ASP VAL
ASP LEU GLY ASP ILE SER GLY ILE ASN ALA SER VAL VAL ASN ILE GLN LYS GLU ILE ASP ARG LEU ASN GLU VAL ALA LYS ASN LEU ASN GLU SER LEU ILE ASP LEU GLN GLU LEU GLY LYS TYR GLU GLN TYR ILE LYS TRP PRO TRP TYR ILE TRP LEU GLY PHE ILE ASN ALA GLY LEU
ILE ALA ILE VAL MET VAL THR ILE MET LEU CYS CYS MET THR SER CYS CYS SER CYS LEU LYS GLY CYS CYS SER CYS CYS GLY SER CYS CYS LYS PHE ASP GLU ASP ASP SER GLU PRO VAL LEU LYS GLY VAL LYS LEU HIS TYR THR

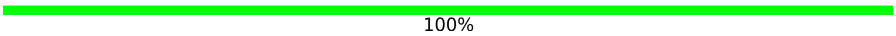
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:

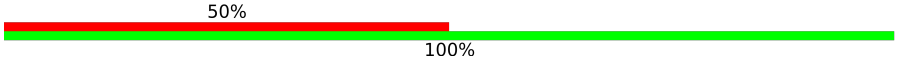
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:

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

Chain F: 

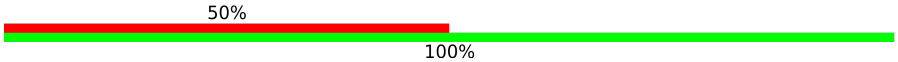
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G: 

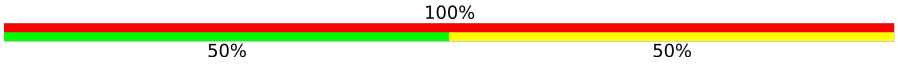
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:

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

Chain I: 

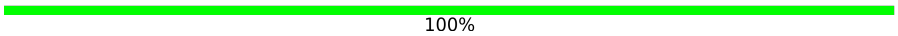
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J: 

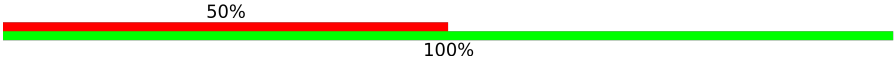
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:

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

Chain L: 

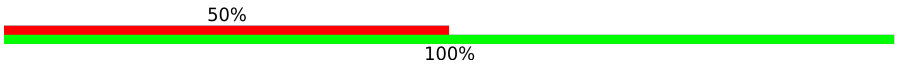
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M: 

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

Chain N:

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

Chain O: 

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

Chain P:

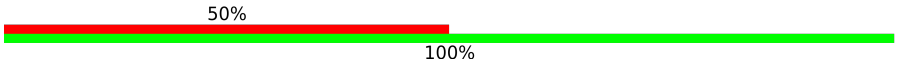
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:

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

Chain R:

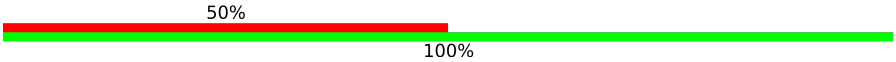
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S: 

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

Chain T:

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

Chain U: 

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	364517	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.075	Depositor
Minimum map value	-1.630	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.060	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	342.40002, 342.40002, 342.40002	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	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	A	0.29	0/8767	0.50	1/11941 (0.0%)
1	B	0.29	0/8767	0.49	1/11941 (0.0%)
1	C	0.28	0/8767	0.49	0/11941
All	All	0.28	0/26301	0.49	2/35823 (0.0%)

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	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1041	ASP	CB-CG-OD1	7.34	124.91	118.30
1	B	1041	ASP	CB-CG-OD1	5.62	123.36	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	515	PHE	Peptide

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	8557	0	8317	113	0
1	B	8557	0	8317	109	0
1	C	8557	0	8317	119	0
2	D	28	0	25	0	0
2	E	28	0	25	1	0
2	F	28	0	25	0	0
2	G	28	0	25	0	0
2	H	28	0	25	1	0
2	I	28	0	25	0	0
2	J	28	0	25	0	0
2	K	28	0	25	0	0
2	L	28	0	25	0	0
2	M	28	0	25	0	0
2	N	28	0	25	1	0
2	O	28	0	25	0	0
2	P	28	0	25	0	0
2	Q	28	0	25	0	0
2	R	28	0	25	0	0
2	S	28	0	25	0	0
2	T	28	0	25	1	0
2	U	28	0	25	0	0
3	A	140	0	130	3	0
3	B	140	0	130	3	0
3	C	140	0	130	3	0
All	All	26595	0	25791	327	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 6.

All (327) 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:B:629:LEU:HG	1:B:631:PRO:HD2	1.59	0.84
1:C:629:LEU:HG	1:C:631:PRO:HD2	1.60	0.84
1:A:629:LEU:HG	1:A:631:PRO:HD2	1.59	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:979:ASP:O	1:C:983:ARG:HB2	1.80	0.82
1:C:659:SER:HB3	1:C:698:SER:HB2	1.64	0.80
1:B:979:ASP:O	1:B:983:ARG:HB2	1.82	0.79
1:A:979:ASP:O	1:A:983:ARG:HB2	1.83	0.79
1:A:659:SER:HB3	1:A:698:SER:HB2	1.64	0.79
1:B:659:SER:HB3	1:B:698:SER:HB2	1.66	0.77
1:B:167:THR:HG22	1:B:168:PHE:H	1.53	0.74
1:C:112:SER:HB3	1:C:134:GLN:HG3	1.71	0.73
1:A:167:THR:HG22	1:A:168:PHE:H	1.54	0.73
1:C:167:THR:HG22	1:C:168:PHE:H	1.53	0.73
1:C:624:ILE:HG13	1:C:637:SER:HA	1.73	0.71
1:A:112:SER:HB3	1:A:134:GLN:HG3	1.73	0.70
1:A:624:ILE:HG13	1:A:637:SER:HA	1.74	0.69
1:B:624:ILE:HG13	1:B:637:SER:HA	1.73	0.69
1:B:112:SER:HB3	1:B:134:GLN:HG3	1.77	0.66
1:C:66:HIS:NE2	1:C:250:THR:OG1	2.29	0.65
1:B:66:HIS:NE2	1:B:250:THR:OG1	2.29	0.65
1:B:353:TRP:O	1:B:466:ARG:NH2	2.30	0.64
1:C:569:ILE:H	1:C:569:ILE:HD12	1.62	0.64
1:B:118:LEU:HD11	1:B:120:VAL:HB	1.78	0.64
1:B:569:ILE:HD12	1:B:569:ILE:H	1.62	0.64
1:A:66:HIS:NE2	1:A:250:THR:OG1	2.29	0.64
1:A:731:MET:HG2	1:A:774:GLN:HE21	1.63	0.63
1:C:102:ARG:HH12	1:C:157:PHE:HE2	1.43	0.63
1:C:436:TRP:HE3	1:C:509:ARG:HD2	1.64	0.63
1:A:353:TRP:O	1:A:466:ARG:NH2	2.30	0.63
1:C:199:GLY:HA2	1:C:232:GLY:HA2	1.81	0.63
1:A:436:TRP:HE3	1:A:509:ARG:HD2	1.64	0.62
1:C:353:TRP:O	1:C:466:ARG:NH2	2.31	0.62
1:B:436:TRP:HE3	1:B:509:ARG:HD2	1.64	0.62
1:A:255:SER:HB3	1:A:259:THR:HG21	1.83	0.60
1:B:1053:PRO:O	1:B:1054:GLN:NE2	2.35	0.60
1:C:176:LEU:HD12	1:C:190:ARG:HH22	1.66	0.60
1:B:811:LYS:HD3	1:B:813:SER:H	1.66	0.60
1:A:811:LYS:HD3	1:A:813:SER:H	1.66	0.60
1:A:869:MET:HE1	1:B:697:MET:HB3	1.84	0.60
1:A:176:LEU:HD12	1:A:190:ARG:HH22	1.67	0.59
1:B:255:SER:HB3	1:B:259:THR:HG21	1.84	0.58
1:A:53:ASP:OD1	1:A:54:LEU:N	2.33	0.58
1:B:199:GLY:HA2	1:B:232:GLY:HA2	1.85	0.58
1:A:199:GLY:HA2	1:A:232:GLY:HA2	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:255:SER:HB3	1:C:259:THR:HG21	1.84	0.58
1:C:811:LYS:HD3	1:C:813:SER:H	1.68	0.58
1:B:759:PHE:HE1	1:C:965:GLN:HE21	1.52	0.58
1:C:1053:PRO:O	1:C:1054:GLN:NE2	2.36	0.57
1:C:773:GLU:OE2	1:C:1019:ARG:NE	2.30	0.57
1:A:773:GLU:OE2	1:A:1019:ARG:NE	2.30	0.57
1:A:1053:PRO:O	1:A:1054:GLN:NE2	2.36	0.57
1:C:658:ASN:ND2	1:C:659:SER:H	2.04	0.56
1:C:979:ASP:O	1:C:983:ARG:CB	2.52	0.56
1:B:825:LYS:NZ	1:B:938:LEU:O	2.29	0.56
3:B:1301:NAG:H3	3:B:1301:NAG:H83	1.88	0.56
1:B:376:ALA:HB1	1:B:378:LYS:HG3	1.88	0.55
1:B:989:ALA:O	1:B:993:ILE:HG12	2.05	0.55
1:B:770:ILE:O	1:B:774:GLN:HG2	2.06	0.55
3:C:1301:NAG:H83	3:C:1301:NAG:H3	1.88	0.55
1:C:107:GLY:O	1:C:237:ARG:HB2	2.06	0.55
1:C:330:PRO:HG2	1:C:332:ILE:HD11	1.89	0.55
1:B:773:GLU:OE1	1:B:1019:ARG:NE	2.40	0.55
1:B:176:LEU:HD12	1:B:190:ARG:HH22	1.72	0.55
1:A:993:ILE:O	1:A:997:ILE:HG12	2.08	0.54
1:A:381:GLY:O	1:C:983:ARG:NH1	2.41	0.54
1:A:731:MET:HG2	1:A:774:GLN:NE2	2.22	0.54
1:A:330:PRO:HG2	1:A:332:ILE:HD11	1.89	0.54
1:B:107:GLY:O	1:B:237:ARG:HB2	2.07	0.54
1:B:382:VAL:HG21	1:B:387:LEU:HD21	1.90	0.53
1:B:802:PHE:HD1	1:B:805:ILE:HD11	1.73	0.53
1:C:352:ALA:HA	1:C:466:ARG:HD3	1.90	0.53
1:C:376:ALA:HB1	1:C:378:LYS:HG3	1.88	0.53
3:A:1301:NAG:H83	3:A:1301:NAG:H3	1.88	0.53
1:A:352:ALA:HA	1:A:466:ARG:HD3	1.88	0.53
1:B:330:PRO:HG2	1:B:332:ILE:HD11	1.90	0.53
1:C:531:THR:HG22	1:C:532:ASN:H	1.74	0.53
1:A:957:GLN:HE21	1:C:765:ARG:CZ	2.22	0.53
1:A:770:ILE:O	1:A:774:GLN:HG2	2.09	0.52
1:A:883:THR:HG23	1:B:707:TYR:HB2	1.91	0.52
1:A:979:ASP:O	1:A:983:ARG:CB	2.56	0.52
1:A:107:GLY:O	1:A:237:ARG:HB2	2.10	0.52
1:A:707:TYR:HB2	1:C:883:THR:HG23	1.92	0.52
1:A:802:PHE:HD1	1:A:805:ILE:HD11	1.74	0.52
1:B:352:ALA:HA	1:B:466:ARG:HD3	1.90	0.52
1:A:175:PHE:HD1	1:A:226:LEU:HD23	1.74	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:VAL:HG11	1:B:175:PHE:HD2	1.74	0.52
1:C:339:ASP:OD1	1:C:340:GLU:N	2.43	0.52
1:B:906:PHE:HE1	1:B:1049:LEU:HD11	1.74	0.52
1:C:64:TRP:HB3	1:C:263:ALA:HB3	1.92	0.52
1:B:617:CYS:HA	1:B:620:VAL:HG23	1.92	0.52
1:C:118:LEU:HD11	1:C:120:VAL:HB	1.90	0.51
1:A:66:HIS:ND1	1:A:263:ALA:HA	2.25	0.51
1:A:339:ASP:OD1	1:A:340:GLU:N	2.42	0.51
1:B:993:ILE:O	1:B:997:ILE:HG12	2.11	0.51
1:A:118:LEU:HD11	1:A:120:VAL:HB	1.91	0.51
1:B:78:ARG:HH11	1:B:244:LEU:HD22	1.74	0.51
1:B:883:THR:HG23	1:C:707:TYR:HB2	1.90	0.51
1:B:66:HIS:ND1	1:B:263:ALA:HA	2.26	0.51
1:A:78:ARG:HH11	1:A:244:LEU:HD22	1.76	0.51
1:A:36:VAL:HG21	1:A:220:PHE:CZ	2.46	0.50
1:A:154:GLU:OE1	1:A:154:GLU:N	2.44	0.50
1:B:339:ASP:OD1	1:B:340:GLU:N	2.43	0.50
1:A:81:ASN:ND2	1:A:240:THR:O	2.44	0.50
1:B:179:LEU:HB2	1:B:188:ASN:HB3	1.93	0.50
1:C:179:LEU:HB2	1:C:188:ASN:HB3	1.93	0.50
1:A:179:LEU:HB2	1:A:188:ASN:HB3	1.93	0.50
1:A:906:PHE:HE1	1:A:1049:LEU:HD11	1.76	0.50
1:B:64:TRP:HB3	1:B:263:ALA:HB3	1.93	0.50
1:B:531:THR:HG22	1:B:532:ASN:H	1.76	0.50
1:B:318:PHE:HZ	1:B:615:VAL:HG11	1.77	0.50
1:C:65:PHE:HE2	1:C:84:LEU:HD21	1.77	0.50
1:C:206:LYS:NZ	1:C:221:SER:OG	2.45	0.50
1:C:190:ARG:HB3	1:C:192:PHE:CE1	2.47	0.49
1:C:139:PRO:HB2	1:C:244:LEU:HD12	1.93	0.49
1:C:802:PHE:HD1	1:C:805:ILE:HD11	1.76	0.49
1:C:993:ILE:O	1:C:997:ILE:HG12	2.13	0.49
1:C:303:LEU:HD12	1:C:308:VAL:HG12	1.94	0.49
1:A:531:THR:HG22	1:A:532:ASN:H	1.77	0.49
1:C:118:LEU:HB2	1:C:133:PHE:HE2	1.77	0.49
1:B:154:GLU:N	1:B:154:GLU:OE1	2.45	0.49
1:C:66:HIS:ND1	1:C:263:ALA:HA	2.27	0.49
1:C:154:GLU:OE1	1:C:154:GLU:N	2.45	0.49
1:A:427:ASP:N	1:A:427:ASP:OD1	2.46	0.49
1:A:1041:ASP:OD1	1:A:1041:ASP:O	2.31	0.49
1:C:437:ASN:OD1	1:C:506:GLN:NE2	2.46	0.49
1:B:1142:GLN:HB3	1:B:1143:PRO:HD3	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:TRP:HB3	1:A:263:ALA:HB3	1.94	0.48
1:A:126:VAL:HG13	1:A:174:PRO:HA	1.94	0.48
1:A:374:PHE:CE2	1:A:377:PHE:HB2	2.48	0.48
1:B:988:GLU:N	1:B:988:GLU:OE1	2.46	0.48
1:A:190:ARG:HB3	1:A:192:PHE:CE1	2.48	0.48
1:C:127:VAL:HG22	1:C:171:VAL:HG22	1.94	0.48
1:C:65:PHE:O	1:C:265:TYR:HB3	2.13	0.48
1:B:36:VAL:HG21	1:B:220:PHE:CZ	2.48	0.48
1:A:303:LEU:HD12	1:A:308:VAL:HG12	1.95	0.48
1:B:190:ARG:HB3	1:B:192:PHE:CE1	2.48	0.48
1:C:406:GLU:HG2	1:C:418:ILE:HG21	1.95	0.48
1:A:190:ARG:HB3	1:A:192:PHE:HE1	1.79	0.48
1:C:126:VAL:HG13	1:C:174:PRO:HA	1.95	0.48
1:A:983:ARG:NH1	1:B:381:GLY:O	2.46	0.48
1:B:190:ARG:HB3	1:B:192:PHE:HE1	1.79	0.48
1:C:427:ASP:OD1	1:C:427:ASP:N	2.46	0.48
1:A:658:ASN:OD1	1:A:659:SER:N	2.40	0.48
1:B:731:MET:HG2	1:B:774:GLN:NE2	2.29	0.48
1:C:175:PHE:HD1	1:C:226:LEU:HD23	1.78	0.48
1:C:374:PHE:CE2	1:C:377:PHE:HB2	2.49	0.48
1:A:825:LYS:NZ	1:A:938:LEU:O	2.29	0.48
1:B:374:PHE:CE2	1:B:377:PHE:HB2	2.49	0.48
1:C:64:TRP:HB3	1:C:263:ALA:CB	2.44	0.48
1:A:569:ILE:HD12	1:A:569:ILE:H	1.79	0.47
1:B:427:ASP:OD1	1:B:427:ASP:N	2.46	0.47
1:B:1041:ASP:OD1	1:B:1041:ASP:O	2.32	0.47
1:C:190:ARG:HB3	1:C:192:PHE:HE1	1.78	0.47
1:B:736:VAL:HG22	1:B:858:LEU:HD13	1.95	0.47
1:C:357:ARG:HH22	1:C:359:SER:HB3	1.79	0.47
1:A:118:LEU:HB2	1:A:133:PHE:HE2	1.79	0.47
1:A:1142:GLN:HB3	1:A:1143:PRO:HD3	1.96	0.47
1:C:1142:GLN:HB3	1:C:1143:PRO:HD3	1.95	0.47
1:C:825:LYS:NZ	1:C:938:LEU:O	2.30	0.47
1:B:411:ALA:HB3	1:B:414:GLN:HG3	1.97	0.47
1:C:65:PHE:CE2	1:C:84:LEU:HD21	2.50	0.47
1:A:64:TRP:HB3	1:A:263:ALA:CB	2.44	0.47
1:B:64:TRP:HB3	1:B:263:ALA:CB	2.44	0.47
1:B:658:ASN:OD1	1:B:659:SER:N	2.40	0.47
1:C:736:VAL:HG22	1:C:858:LEU:HD13	1.97	0.47
1:A:398:ASP:OD1	1:A:512:VAL:HB	2.15	0.47
1:A:736:VAL:HG22	1:A:858:LEU:HD13	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:965:GLN:NE2	1:A:970:PHE:HZ	2.12	0.47
1:A:411:ALA:HB3	1:A:414:GLN:HG3	1.96	0.46
1:B:125:ASN:HA	1:B:174:PRO:HD3	1.96	0.46
1:B:303:LEU:HD12	1:B:308:VAL:HG12	1.96	0.46
1:C:411:ALA:HB3	1:C:414:GLN:HG3	1.96	0.46
1:A:393:THR:OG1	1:A:516:GLU:O	2.32	0.46
1:A:350:VAL:HG11	1:A:422:ASN:HB3	1.97	0.46
1:A:406:GLU:HG2	1:A:418:ILE:HG21	1.98	0.46
1:C:78:ARG:HH11	1:C:244:LEU:HD22	1.80	0.46
1:A:126:VAL:HG22	1:A:174:PRO:HA	1.96	0.46
1:B:350:VAL:HG11	1:B:422:ASN:HB3	1.97	0.46
1:B:81:ASN:ND2	1:B:240:THR:O	2.49	0.46
1:B:118:LEU:HB2	1:B:133:PHE:HE2	1.80	0.46
1:B:393:THR:OG1	1:B:516:GLU:OE2	2.33	0.46
1:C:108:THR:HG23	1:C:109:THR:HG23	1.97	0.46
1:C:350:VAL:HG11	1:C:422:ASN:HB3	1.96	0.46
1:C:978:ASN:HA	1:C:981:LEU:HG	1.97	0.46
1:A:318:PHE:HZ	1:A:615:VAL:HG11	1.81	0.46
1:B:436:TRP:CE3	1:B:509:ARG:HD2	2.49	0.46
1:B:532:ASN:OD1	1:B:533:LEU:N	2.42	0.46
1:A:108:THR:HG23	1:A:109:THR:HG23	1.98	0.46
1:A:200:TYR:CE2	1:A:230:PRO:HG3	2.51	0.46
1:B:331:ASN:HB3	3:B:1309:NAG:C7	2.47	0.45
1:C:167:THR:HG22	1:C:168:PHE:N	2.28	0.45
1:C:393:THR:OG1	1:C:516:GLU:O	2.33	0.45
1:C:398:ASP:OD1	1:C:512:VAL:HB	2.16	0.45
1:A:128:ILE:HD11	1:A:175:PHE:CE2	2.52	0.45
1:C:81:ASN:ND2	1:C:240:THR:O	2.50	0.45
1:A:532:ASN:OD1	1:A:533:LEU:N	2.43	0.45
1:A:86:PHE:HB2	1:A:238:PHE:HD1	1.82	0.45
1:A:988:GLU:OE1	1:A:988:GLU:N	2.50	0.45
1:C:53:ASP:HB2	1:C:55:PHE:CE2	2.51	0.45
1:C:126:VAL:HG22	1:C:174:PRO:HA	1.98	0.45
1:C:331:ASN:HB3	3:C:1309:NAG:C7	2.46	0.45
1:A:343:ASN:HB3	3:A:1310:NAG:O5	2.17	0.45
1:B:98:SER:HB3	1:B:100:ILE:HG12	1.99	0.45
1:B:393:THR:OG1	1:B:516:GLU:O	2.30	0.45
1:B:406:GLU:HG2	1:B:418:ILE:HG21	1.99	0.45
1:B:747:THR:OG1	1:B:748:GLU:OE2	2.33	0.45
1:A:331:ASN:HB3	3:A:1309:NAG:C7	2.47	0.45
1:B:630:THR:HB	1:B:631:PRO:HD3	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:457:ARG:NH1	1:C:459:SER:O	2.35	0.45
1:B:126:VAL:HG22	1:B:174:PRO:HA	1.98	0.45
1:B:343:ASN:HB3	3:B:1310:NAG:O5	2.16	0.45
1:C:78:ARG:NH1	1:C:244:LEU:O	2.50	0.45
1:C:1041:ASP:OD2	1:C:1045:LYS:NZ	2.35	0.45
1:C:1092:GLU:OE2	1:C:1092:GLU:HA	2.16	0.45
1:C:1103:PHE:HZ	2:T:1:NAG:H61	1.82	0.45
1:B:108:THR:HG23	1:B:109:THR:HG23	1.99	0.44
1:B:37:TYR:HB3	1:B:223:LEU:HB2	1.99	0.44
1:C:157:PHE:HE1	1:C:245:HIS:HE1	1.64	0.44
1:C:988:GLU:N	1:C:988:GLU:OE2	2.50	0.44
1:A:182:LYS:HG3	1:A:183:GLN:HG2	2.00	0.44
1:B:457:ARG:NH1	1:B:459:SER:O	2.35	0.44
1:C:137:ASN:OD1	1:C:138:ASP:N	2.46	0.44
1:C:770:ILE:O	1:C:774:GLN:HG2	2.17	0.44
1:A:726:ILE:HG13	1:A:1061:VAL:HG22	2.00	0.44
1:B:983:ARG:NH1	1:C:381:GLY:O	2.50	0.44
1:B:182:LYS:HG3	1:B:183:GLN:HG2	1.99	0.44
1:B:398:ASP:OD1	1:B:512:VAL:HB	2.18	0.44
1:A:699:LEU:HD21	1:C:869:MET:HG2	1.99	0.44
1:B:458:LYS:HD2	1:B:473:TYR:HE1	1.83	0.44
1:B:206:LYS:NZ	1:B:221:SER:OG	2.49	0.43
1:B:759:PHE:HZ	1:C:970:PHE:HE2	1.66	0.43
1:C:343:ASN:HB3	3:C:1310:NAG:O5	2.16	0.43
1:A:212:LEU:HB3	1:A:213:GLY:H	1.55	0.43
1:A:707:TYR:HB3	1:C:792:PRO:HG2	2.01	0.43
1:C:617:CYS:HA	1:C:620:VAL:HG23	2.00	0.43
1:A:458:LYS:HD2	1:A:473:TYR:HE1	1.83	0.43
1:B:748:GLU:OE2	1:B:748:GLU:N	2.49	0.43
1:B:139:PRO:HB2	1:B:244:LEU:HD12	2.01	0.43
1:B:78:ARG:NH1	1:B:244:LEU:O	2.52	0.43
1:C:458:LYS:HD2	1:C:473:TYR:HE1	1.83	0.43
1:A:126:VAL:HG11	1:A:175:PHE:H	1.84	0.43
1:A:167:THR:HG22	1:A:168:PHE:N	2.28	0.43
1:A:353:TRP:H	1:A:466:ARG:HE	1.66	0.43
1:C:531:THR:HG22	1:C:532:ASN:N	2.34	0.43
1:C:630:THR:HB	1:C:631:PRO:HD3	1.99	0.43
1:A:37:TYR:HB3	1:A:223:LEU:HB2	2.00	0.43
1:C:906:PHE:CD2	1:C:916:LEU:HB2	2.54	0.43
1:B:287:ASP:HB3	1:B:306:PHE:HE2	1.84	0.42
1:A:65:PHE:CE2	1:A:84:LEU:HD21	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:759:PHE:HZ	1:B:970:PHE:HE2	1.68	0.42
1:B:529:LYS:HD2	1:B:529:LYS:HA	1.86	0.42
1:C:119:ILE:HG22	1:C:119:ILE:O	2.19	0.42
1:A:78:ARG:NH1	1:A:244:LEU:O	2.53	0.42
1:A:139:PRO:HB2	1:A:244:LEU:HD12	2.01	0.42
1:A:392:PHE:N	1:A:524:VAL:O	2.42	0.42
1:A:630:THR:HB	1:A:631:PRO:HD3	2.00	0.42
1:A:1116:THR:OG1	1:A:1117:THR:N	2.52	0.42
1:B:179:LEU:HD11	1:B:207:HIS:HB3	2.01	0.42
1:C:125:ASN:HA	1:C:174:PRO:HD3	2.00	0.42
1:C:532:ASN:OD1	1:C:533:LEU:N	2.38	0.42
1:A:329:PHE:HE2	1:A:528:LYS:HG2	1.84	0.42
1:C:182:LYS:HG3	1:C:183:GLN:HG2	2.01	0.42
1:C:318:PHE:HZ	1:C:615:VAL:HG11	1.84	0.42
1:C:989:ALA:O	1:C:993:ILE:HG12	2.19	0.42
1:A:128:ILE:HD11	1:A:175:PHE:HE2	1.85	0.42
1:C:906:PHE:HE1	1:C:1049:LEU:HD11	1.84	0.42
1:A:53:ASP:HB3	1:A:55:PHE:CE2	2.54	0.42
1:A:1092:GLU:OE1	1:A:1107:ARG:NH1	2.53	0.42
1:A:531:THR:HG22	1:A:532:ASN:N	2.35	0.42
1:B:605:SER:OG	1:B:606:ASN:N	2.51	0.42
1:C:985:ASP:OD1	1:C:985:ASP:N	2.47	0.42
1:A:65:PHE:O	1:A:265:TYR:HB3	2.20	0.42
1:B:53:ASP:HB3	1:B:55:PHE:CE2	2.55	0.42
1:B:363:ALA:HB1	1:B:365:TYR:HE1	1.85	0.42
1:C:1116:THR:OG1	1:C:1117:THR:N	2.53	0.42
1:B:353:TRP:H	1:B:466:ARG:HE	1.67	0.42
1:C:368:LEU:HD11	1:C:377:PHE:CE1	2.55	0.42
1:B:531:THR:HG22	1:B:532:ASN:N	2.34	0.41
1:B:1103:PHE:HZ	2:N:1:NAG:H61	1.85	0.41
1:C:1097:SER:HB2	1:C:1102:TRP:CD2	2.55	0.41
1:A:792:PRO:HG2	1:B:707:TYR:HB3	2.03	0.41
1:A:1103:PHE:HZ	2:H:1:NAG:H61	1.85	0.41
1:B:1092:GLU:OE1	1:B:1092:GLU:HA	2.21	0.41
1:C:436:TRP:CE3	1:C:509:ARG:HD2	2.49	0.41
1:A:194:PHE:HD1	1:A:203:ILE:HG12	1.85	0.41
1:B:167:THR:HG22	1:B:168:PHE:N	2.28	0.41
1:C:722:VAL:HG22	1:C:1065:VAL:HG22	2.02	0.41
1:C:374:PHE:HE2	1:C:377:PHE:HB2	1.85	0.41
1:C:726:ILE:HG13	1:C:1061:VAL:HG22	2.01	0.41
1:A:855:PHE:HD2	1:B:589:PRO:HG2	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:792:PRO:HG2	1:C:707:TYR:HB3	2.03	0.41
1:C:329:PHE:HE2	1:C:528:LYS:HG2	1.85	0.41
1:A:357:ARG:HH11	1:A:357:ARG:HG2	1.86	0.41
1:B:625:HIS:HB3	1:B:628:GLN:HB3	2.03	0.41
1:A:206:LYS:NZ	1:A:221:SER:OG	2.52	0.41
1:A:709:ASN:ND2	2:E:1:NAG:H62	2.36	0.41
1:A:990:GLU:HA	1:A:993:ILE:HG12	2.03	0.41
1:B:126:VAL:HG13	1:B:174:PRO:HA	2.02	0.41
1:B:392:PHE:N	1:B:524:VAL:O	2.48	0.41
1:B:979:ASP:O	1:B:983:ARG:CB	2.61	0.41
1:C:128:ILE:HD11	1:C:175:PHE:HE2	1.86	0.41
1:C:537:LYS:HE2	1:C:537:LYS:HB3	1.98	0.41
1:C:990:GLU:HA	1:C:993:ILE:HG12	2.02	0.41
1:A:98:SER:HB3	1:A:100:ILE:HG12	2.02	0.41
1:B:985:ASP:OD1	1:B:985:ASP:N	2.48	0.41
1:C:36:VAL:HG21	1:C:220:PHE:CE2	2.56	0.41
1:C:66:HIS:NE2	1:C:251:PRO:O	2.53	0.41
1:C:98:SER:HB3	1:C:100:ILE:HG12	2.02	0.41
1:C:179:LEU:HD11	1:C:207:HIS:HB3	2.02	0.41
1:C:353:TRP:H	1:C:466:ARG:HE	1.69	0.41
1:A:452:GLN:HG2	1:A:492:LEU:HD23	2.03	0.40
1:A:1004:LEU:HA	1:A:1004:LEU:HD23	1.90	0.40
1:A:800:PHE:HD2	1:A:927:PHE:CD2	2.39	0.40
1:B:368:LEU:HD11	1:B:377:PHE:CE2	2.55	0.40
1:C:430:THR:O	1:C:430:THR:HG23	2.21	0.40
1:A:457:ARG:NH1	1:A:459:SER:O	2.35	0.40
1:A:605:SER:OG	1:A:606:ASN:N	2.54	0.40
1:C:800:PHE:HD2	1:C:927:PHE:CD2	2.39	0.40
1:A:363:ALA:HB1	1:A:365:TYR:HE1	1.87	0.40
1:A:961:THR:HG21	1:C:762:GLN:NE2	2.35	0.40
1:A:1097:SER:HB2	1:A:1102:TRP:CD2	2.57	0.40
1:B:353:TRP:CH2	1:B:466:ARG:HB2	2.57	0.40
1:B:1116:THR:OG1	1:B:1117:THR:N	2.53	0.40
1:B:66:HIS:NE2	1:B:251:PRO:O	2.54	0.40
1:B:865:LEU:HD23	1:B:865:LEU:HA	1.96	0.40
1:C:357:ARG:HG3	1:C:396:TYR:CE1	2.57	0.40
1:C:363:ALA:HB1	1:C:365:TYR:HE1	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	A	1089/1270 (86%)	1035 (95%)	54 (5%)	0	100	100
1	B	1089/1270 (86%)	1037 (95%)	52 (5%)	0	100	100
1	C	1089/1270 (86%)	1038 (95%)	51 (5%)	0	100	100
All	All	3267/3810 (86%)	3110 (95%)	157 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	A	952/1109 (86%)	950 (100%)	2 (0%)	93	98
1	B	952/1109 (86%)	950 (100%)	2 (0%)	93	98
1	C	952/1109 (86%)	949 (100%)	3 (0%)	92	97
All	All	2856/3327 (86%)	2849 (100%)	7 (0%)	93	98

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	190	ARG
1	A	983	ARG
1	B	190	ARG
1	B	983	ARG
1	C	190	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	658	ASN
1	C	983	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	774	GLN
1	A	957	GLN
1	B	148	ASN
1	C	148	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)

36 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	NAG	D	1	2,1	14,14,15	0.22	0	17,19,21	0.51	0
2	NAG	D	2	2	14,14,15	0.21	0	17,19,21	0.40	0
2	NAG	E	1	2,1	14,14,15	0.34	0	17,19,21	1.30	1 (5%)
2	NAG	E	2	2	14,14,15	0.19	0	17,19,21	0.41	0
2	NAG	F	1	2,1	14,14,15	0.23	0	17,19,21	0.45	0
2	NAG	F	2	2	14,14,15	0.17	0	17,19,21	0.48	0
2	NAG	G	1	2,1	14,14,15	0.19	0	17,19,21	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	G	2	2	14,14,15	0.25	0	17,19,21	0.41	0
2	NAG	H	1	2,1	14,14,15	0.19	0	17,19,21	0.43	0
2	NAG	H	2	2	14,14,15	0.23	0	17,19,21	0.39	0
2	NAG	I	1	2,1	14,14,15	0.48	0	17,19,21	0.63	0
2	NAG	I	2	2	14,14,15	0.19	0	17,19,21	0.51	0
2	NAG	J	1	2,1	14,14,15	0.27	0	17,19,21	0.61	1 (5%)
2	NAG	J	2	2	14,14,15	0.20	0	17,19,21	0.42	0
2	NAG	K	1	2,1	14,14,15	0.35	0	17,19,21	1.30	1 (5%)
2	NAG	K	2	2	14,14,15	0.21	0	17,19,21	0.42	0
2	NAG	L	1	2,1	14,14,15	0.24	0	17,19,21	0.47	0
2	NAG	L	2	2	14,14,15	0.22	0	17,19,21	0.49	0
2	NAG	M	1	2,1	14,14,15	0.18	0	17,19,21	0.44	0
2	NAG	M	2	2	14,14,15	0.22	0	17,19,21	0.41	0
2	NAG	N	1	2,1	14,14,15	0.21	0	17,19,21	0.43	0
2	NAG	N	2	2	14,14,15	0.23	0	17,19,21	0.40	0
2	NAG	O	1	2,1	14,14,15	0.47	0	17,19,21	0.63	0
2	NAG	O	2	2	14,14,15	0.19	0	17,19,21	0.50	0
2	NAG	P	1	2,1	14,14,15	0.20	0	17,19,21	0.49	0
2	NAG	P	2	2	14,14,15	0.21	0	17,19,21	0.41	0
2	NAG	Q	1	2,1	14,14,15	0.35	0	17,19,21	1.29	1 (5%)
2	NAG	Q	2	2	14,14,15	0.21	0	17,19,21	0.42	0
2	NAG	R	1	2,1	14,14,15	0.24	0	17,19,21	0.46	0
2	NAG	R	2	2	14,14,15	0.18	0	17,19,21	0.49	0
2	NAG	S	1	2,1	14,14,15	0.18	0	17,19,21	0.45	0
2	NAG	S	2	2	14,14,15	0.23	0	17,19,21	0.40	0
2	NAG	T	1	2,1	14,14,15	0.18	0	17,19,21	0.44	0
2	NAG	T	2	2	14,14,15	0.24	0	17,19,21	0.39	0
2	NAG	U	1	2,1	14,14,15	0.45	0	17,19,21	0.64	0
2	NAG	U	2	2	14,14,15	0.18	0	17,19,21	0.51	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
2	NAG	D	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	NAG	E	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	E	2	2	-	4/6/23/26	0/1/1/1
2	NAG	F	1	2,1	-	2/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1
2	NAG	G	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	0/6/23/26	0/1/1/1
2	NAG	H	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	H	2	2	-	2/6/23/26	0/1/1/1
2	NAG	I	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	I	2	2	-	0/6/23/26	0/1/1/1
2	NAG	J	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	J	2	2	-	2/6/23/26	0/1/1/1
2	NAG	K	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	K	2	2	-	4/6/23/26	0/1/1/1
2	NAG	L	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	L	2	2	-	0/6/23/26	0/1/1/1
2	NAG	M	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	M	2	2	-	0/6/23/26	0/1/1/1
2	NAG	N	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	N	2	2	-	2/6/23/26	0/1/1/1
2	NAG	O	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	O	2	2	-	1/6/23/26	0/1/1/1
2	NAG	P	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	P	2	2	-	2/6/23/26	0/1/1/1
2	NAG	Q	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	Q	2	2	-	4/6/23/26	0/1/1/1
2	NAG	R	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	R	2	2	-	0/6/23/26	0/1/1/1
2	NAG	S	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	S	2	2	-	0/6/23/26	0/1/1/1
2	NAG	T	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	T	2	2	-	2/6/23/26	0/1/1/1
2	NAG	U	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	U	2	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	K	1	NAG	C1-O5-C5	4.80	118.70	112.19
2	E	1	NAG	C1-O5-C5	4.79	118.68	112.19
2	Q	1	NAG	C1-O5-C5	4.76	118.65	112.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	1	NAG	C1-O5-C5	2.05	114.97	112.19

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	N	2	NAG	C4-C5-C6-O6
2	T	2	NAG	C4-C5-C6-O6
2	H	2	NAG	C4-C5-C6-O6
2	O	1	NAG	O5-C5-C6-O6
2	U	1	NAG	O5-C5-C6-O6
2	I	1	NAG	O5-C5-C6-O6
2	N	2	NAG	O5-C5-C6-O6
2	T	2	NAG	O5-C5-C6-O6
2	H	2	NAG	O5-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	K	2	NAG	O5-C5-C6-O6
2	Q	2	NAG	O5-C5-C6-O6
2	U	1	NAG	C4-C5-C6-O6
2	I	1	NAG	C4-C5-C6-O6
2	O	1	NAG	C4-C5-C6-O6
2	R	1	NAG	O5-C5-C6-O6
2	F	1	NAG	O5-C5-C6-O6
2	J	2	NAG	O5-C5-C6-O6
2	L	1	NAG	O5-C5-C6-O6
2	P	2	NAG	O5-C5-C6-O6
2	E	2	NAG	C8-C7-N2-C2
2	E	2	NAG	O7-C7-N2-C2
2	K	2	NAG	C8-C7-N2-C2
2	K	2	NAG	O7-C7-N2-C2
2	Q	2	NAG	C8-C7-N2-C2
2	Q	2	NAG	O7-C7-N2-C2
2	D	2	NAG	O5-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	R	1	NAG	C4-C5-C6-O6
2	K	2	NAG	C4-C5-C6-O6
2	Q	2	NAG	C4-C5-C6-O6
2	F	1	NAG	C4-C5-C6-O6
2	J	2	NAG	C4-C5-C6-O6
2	P	2	NAG	C4-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	L	1	NAG	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	K	1	NAG	O5-C5-C6-O6
2	Q	1	NAG	O5-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
2	N	1	NAG	O5-C5-C6-O6
2	T	1	NAG	O5-C5-C6-O6
2	H	1	NAG	O5-C5-C6-O6
2	I	1	NAG	C3-C2-N2-C7
2	O	1	NAG	C3-C2-N2-C7
2	U	1	NAG	C3-C2-N2-C7
2	O	2	NAG	C4-C5-C6-O6

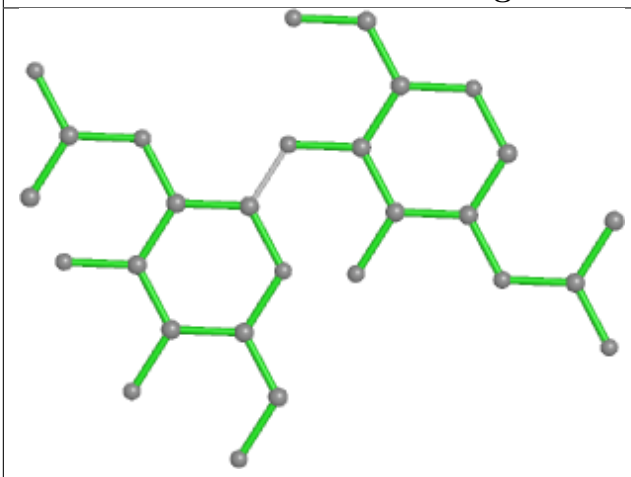
There are no ring outliers.

4 monomers are involved in 4 short contacts:

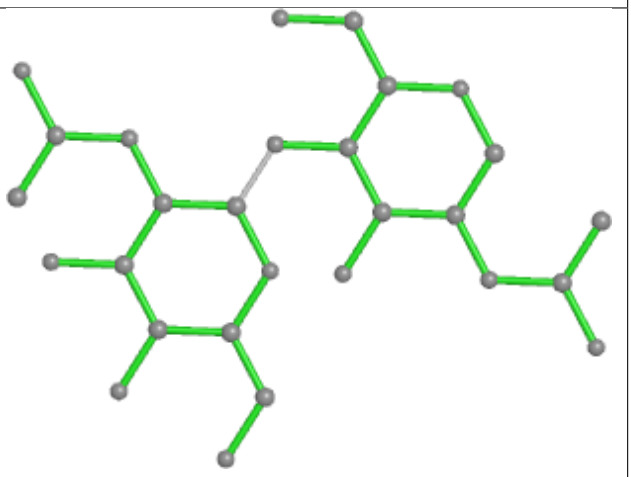
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1	NAG	1	0
2	H	1	NAG	1	0
2	N	1	NAG	1	0
2	T	1	NAG	1	0

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

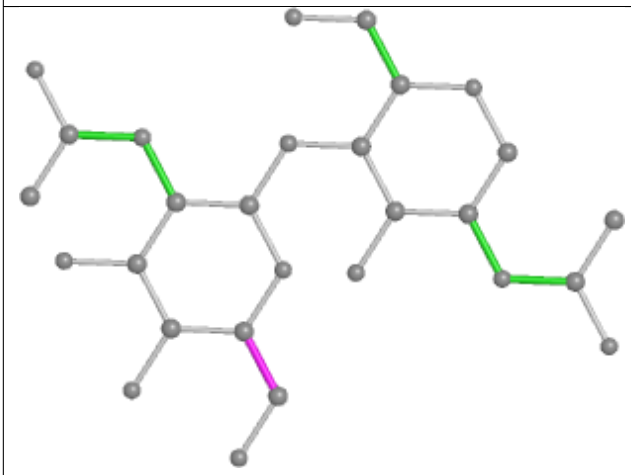
Oligosaccharide Chain D



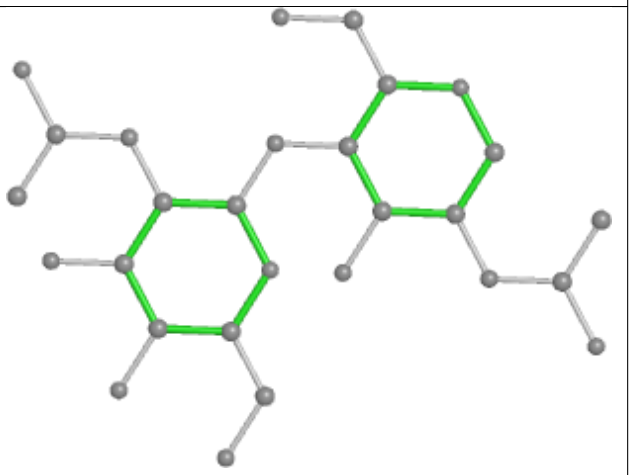
Bond lengths



Bond angles

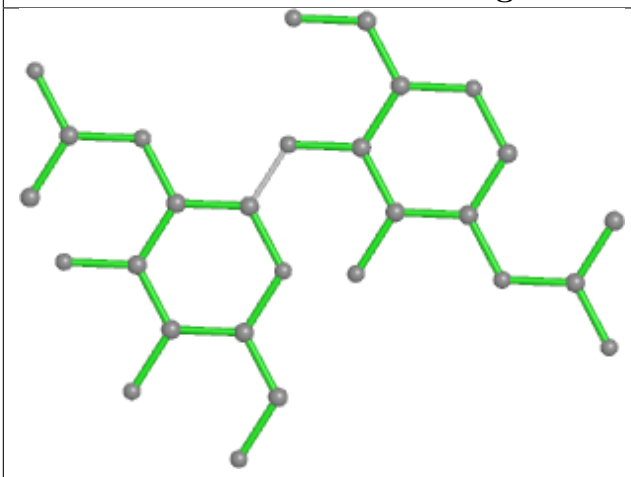


Torsions

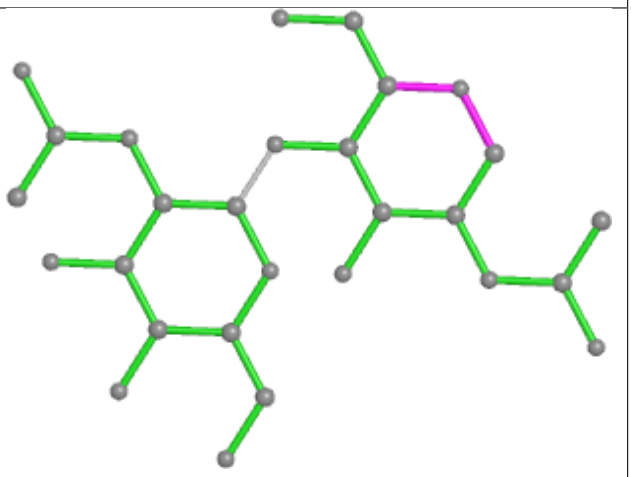


Rings

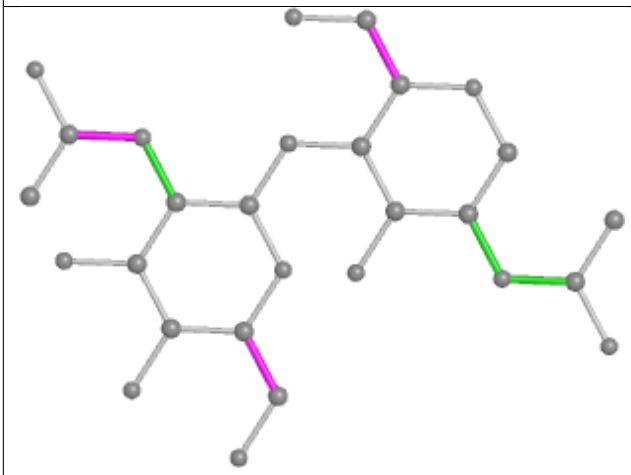
Oligosaccharide Chain E



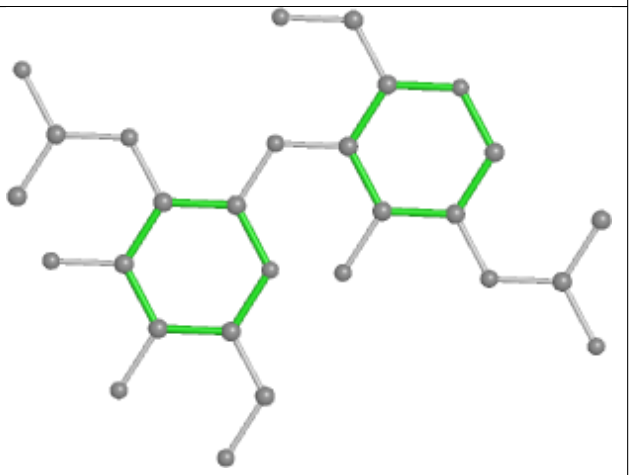
Bond lengths



Bond angles

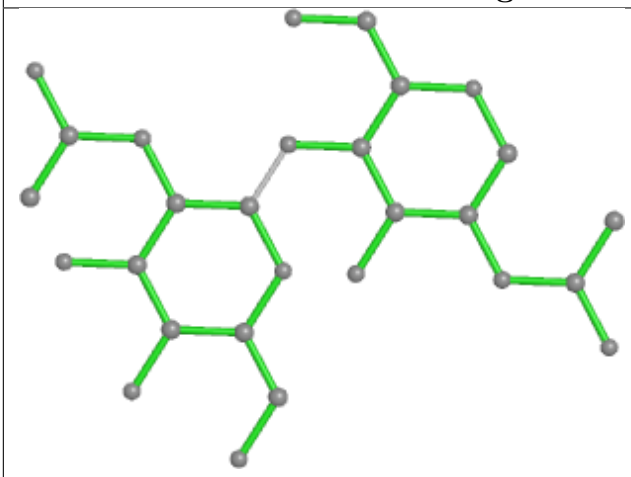


Torsions

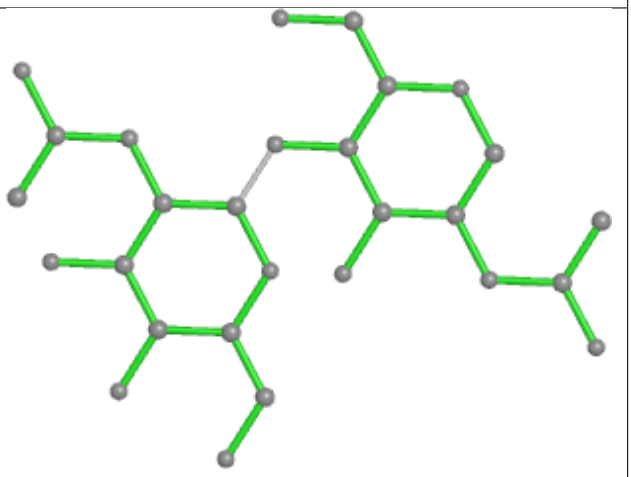


Rings

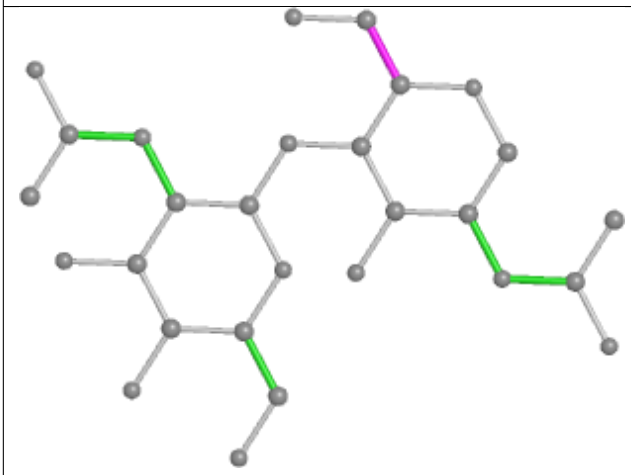
Oligosaccharide Chain F



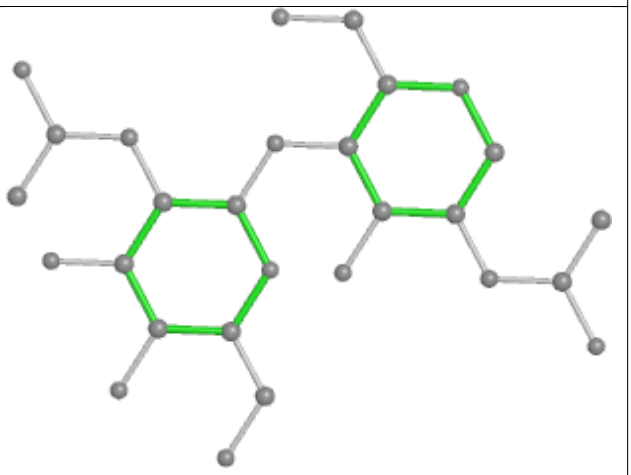
Bond lengths



Bond angles

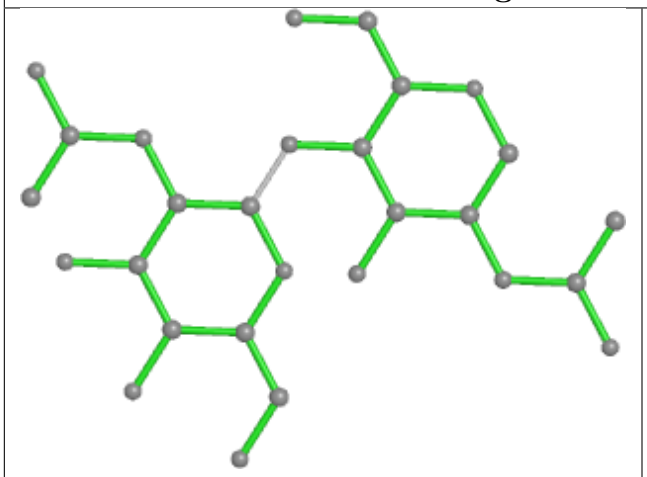


Torsions

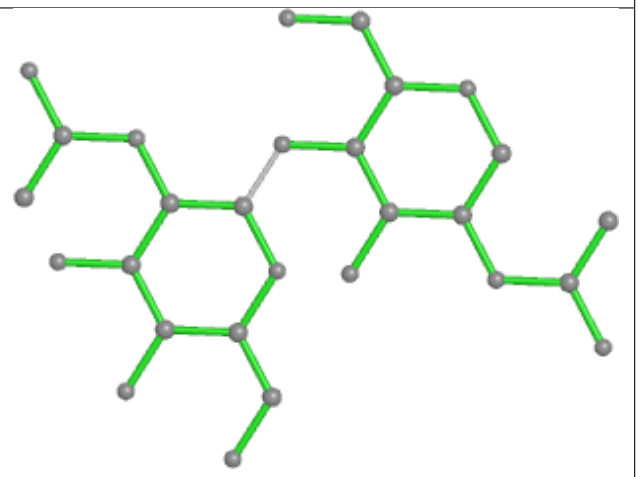


Rings

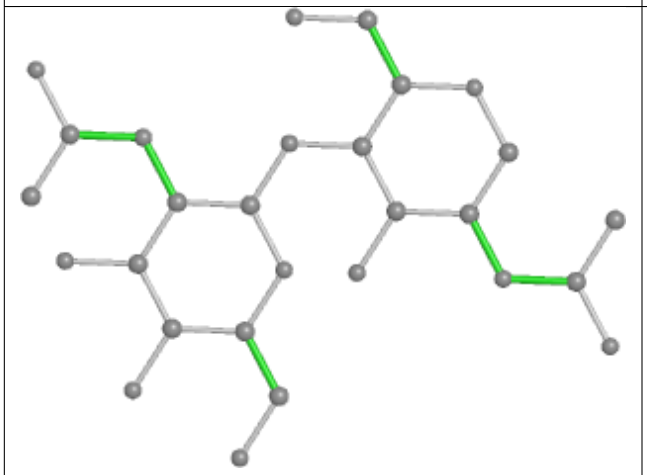
Oligosaccharide Chain G



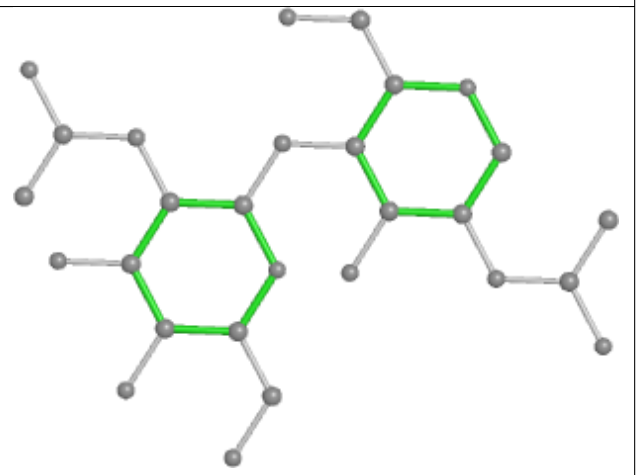
Bond lengths



Bond angles

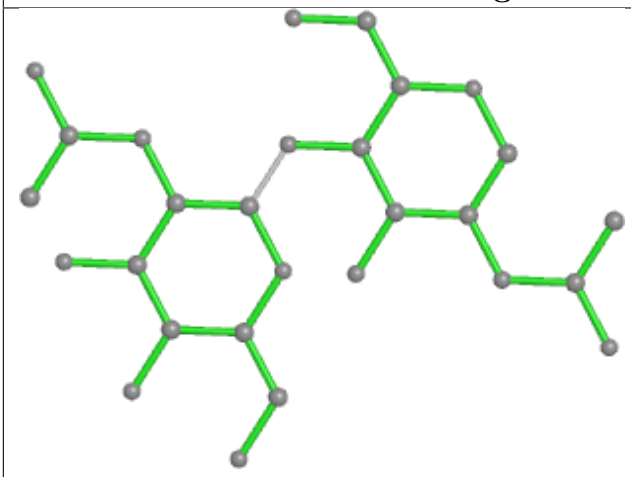


Torsions

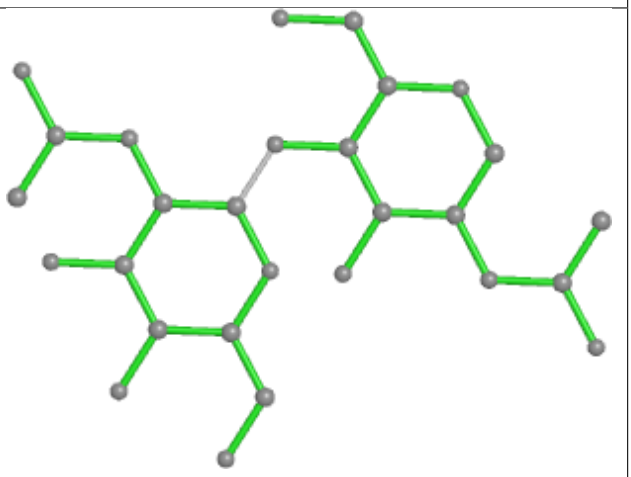


Rings

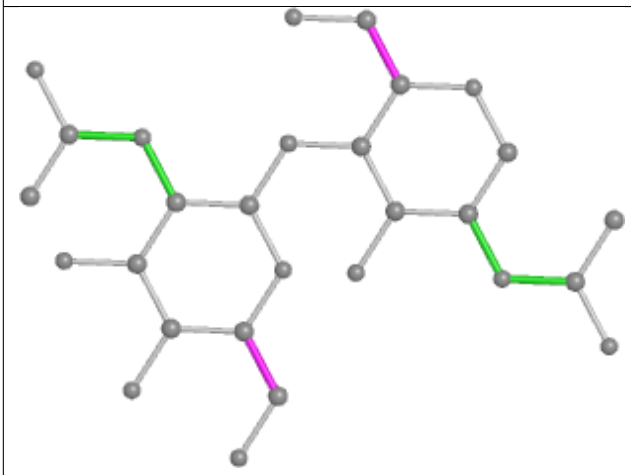
Oligosaccharide Chain H



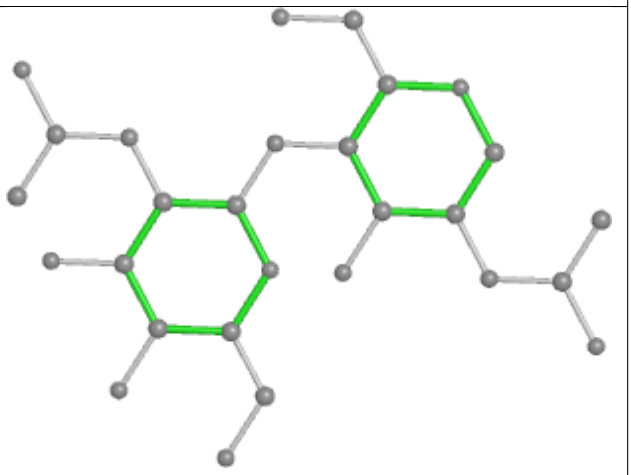
Bond lengths



Bond angles

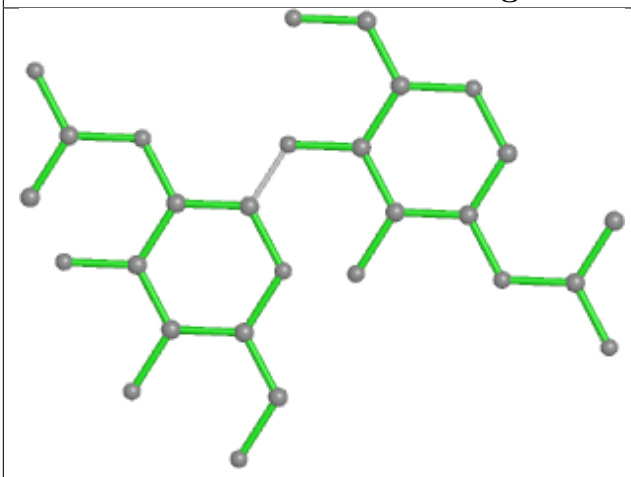


Torsions

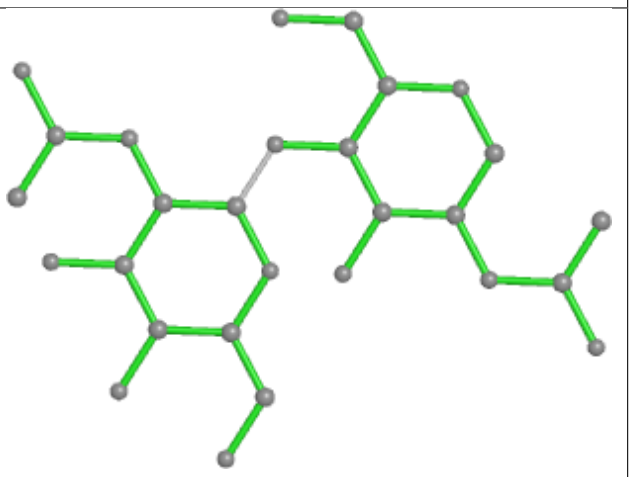


Rings

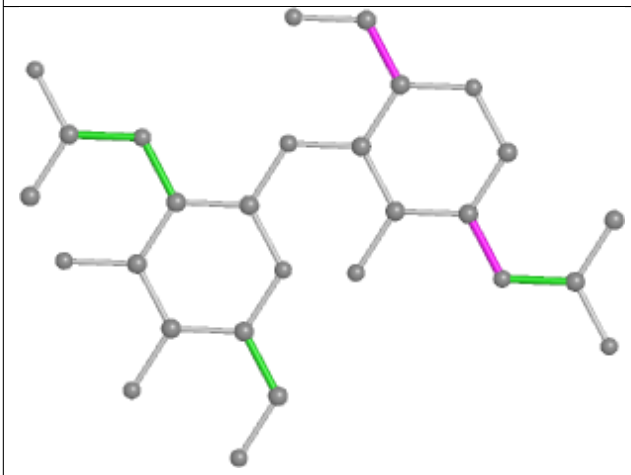
Oligosaccharide Chain I



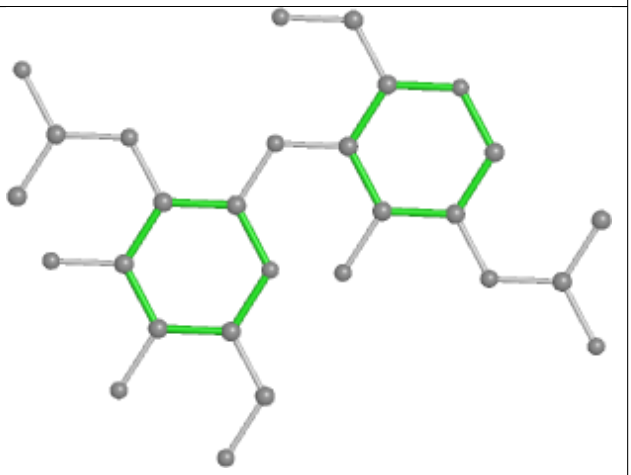
Bond lengths



Bond angles

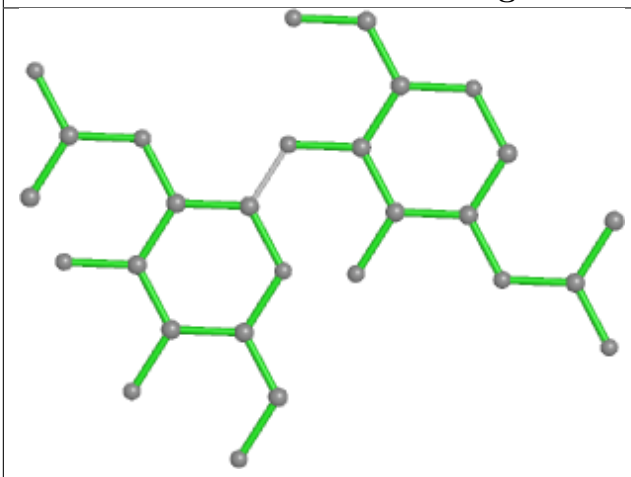


Torsions

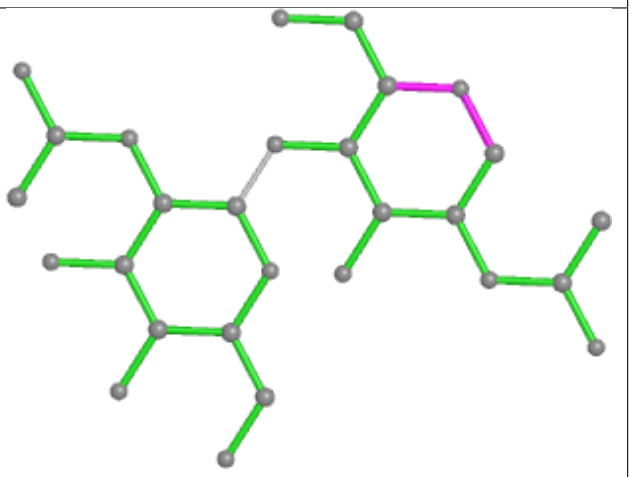


Rings

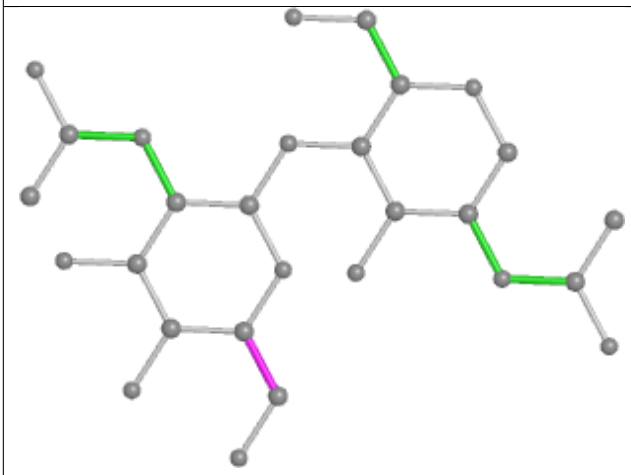
Oligosaccharide Chain J



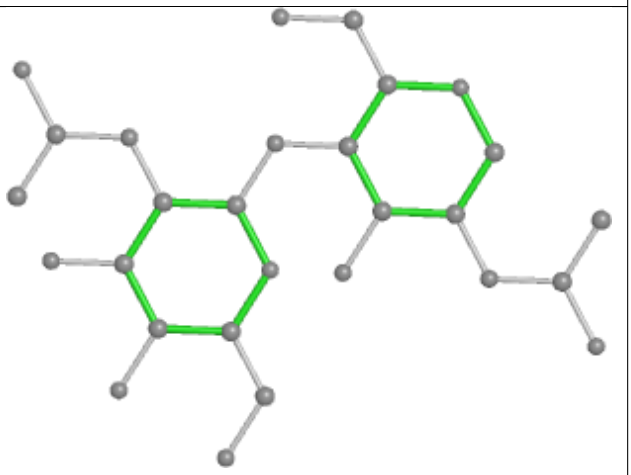
Bond lengths



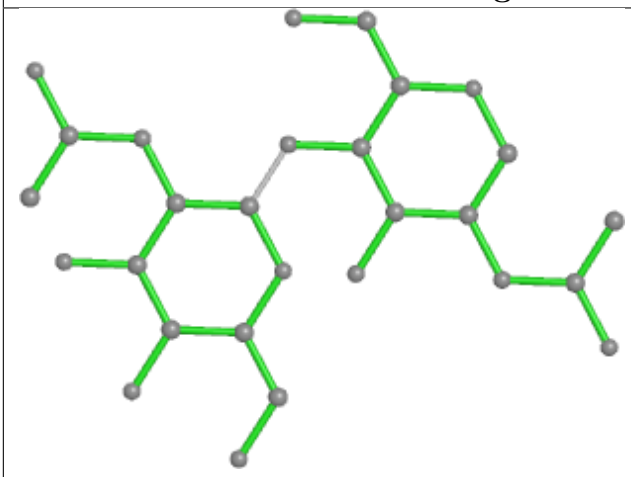
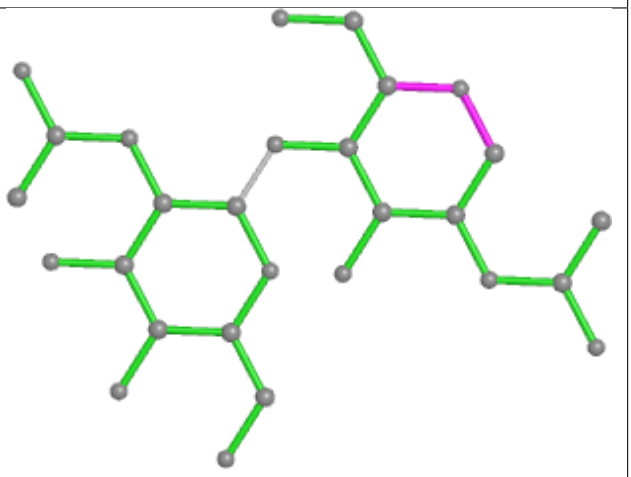
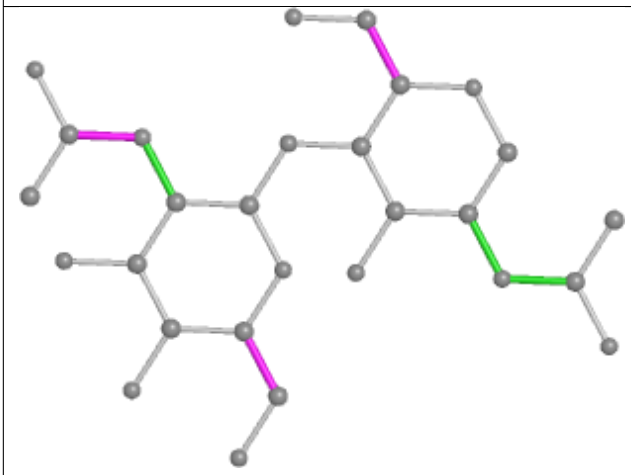
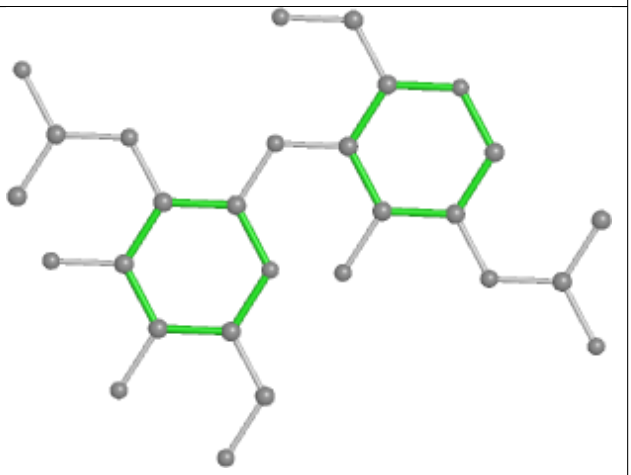
Bond angles

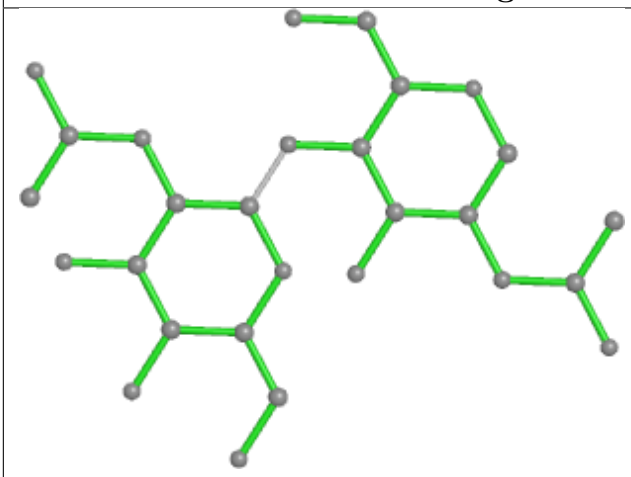
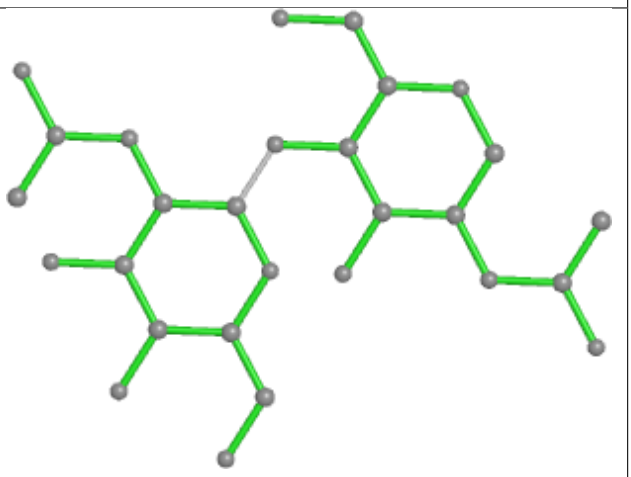
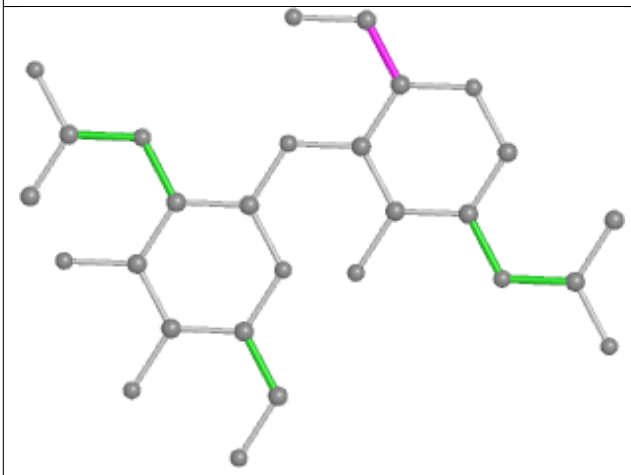
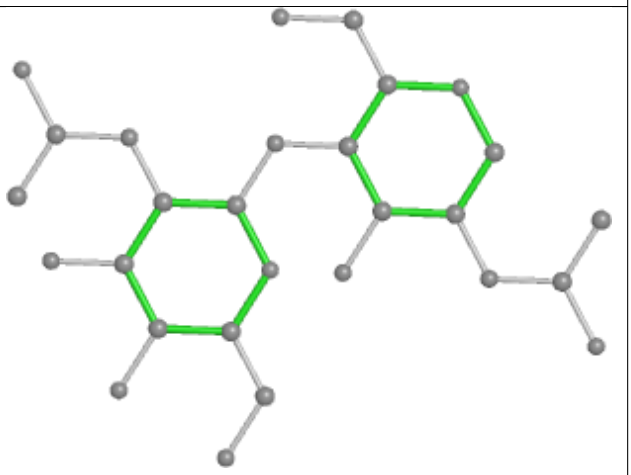


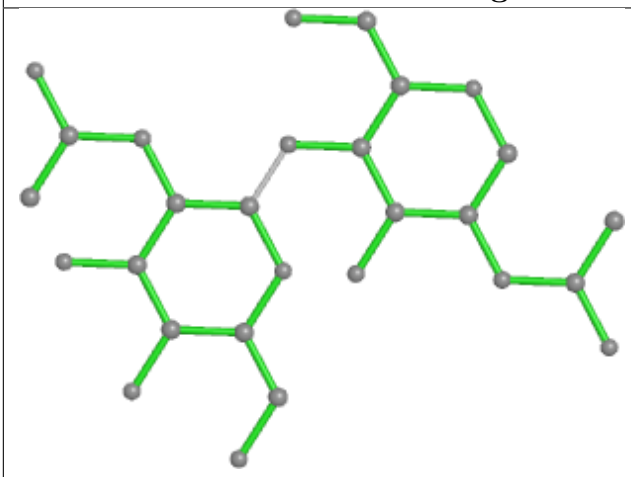
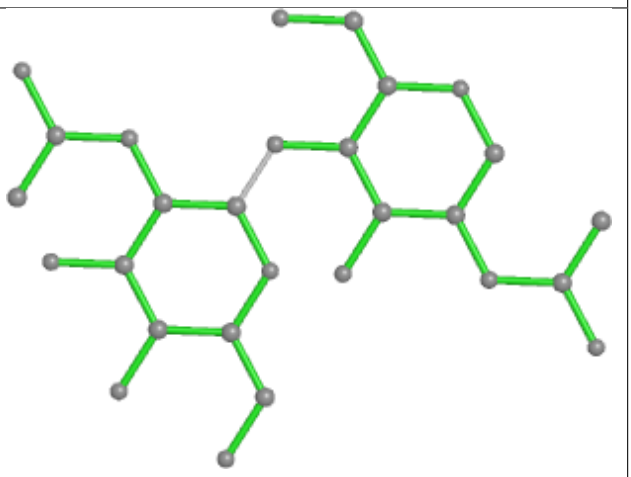
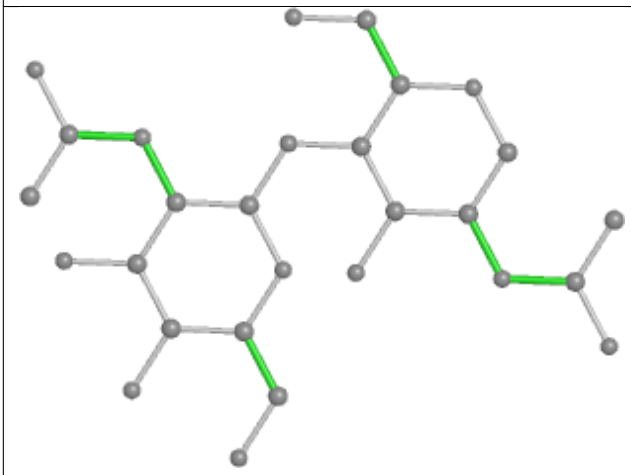
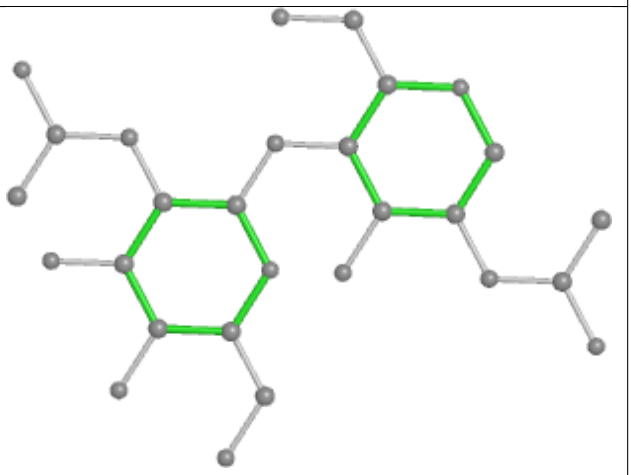
Torsions

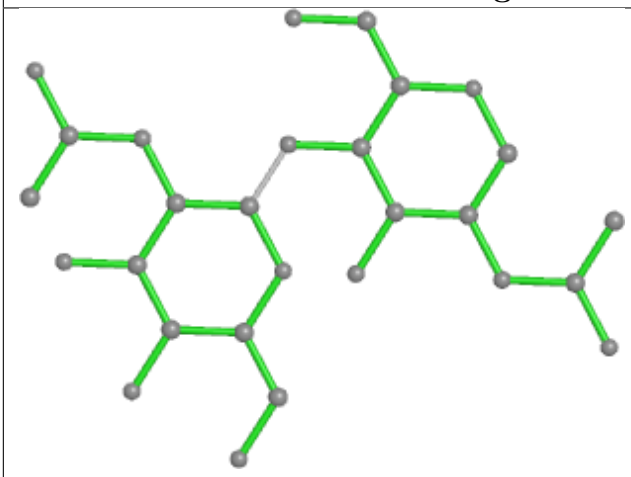
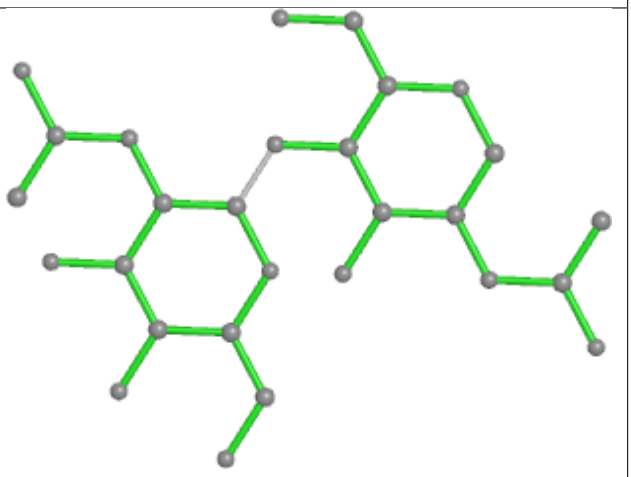
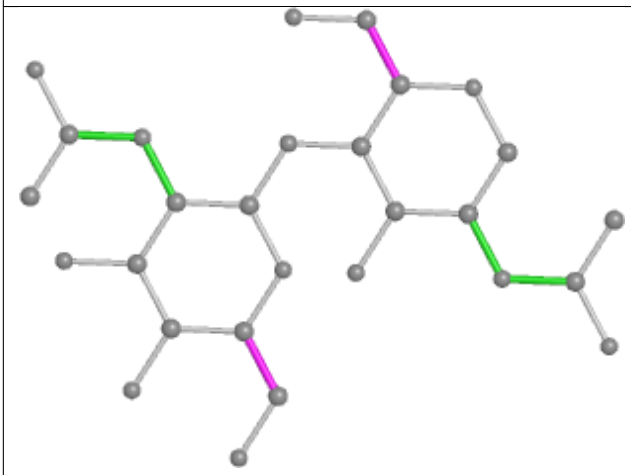
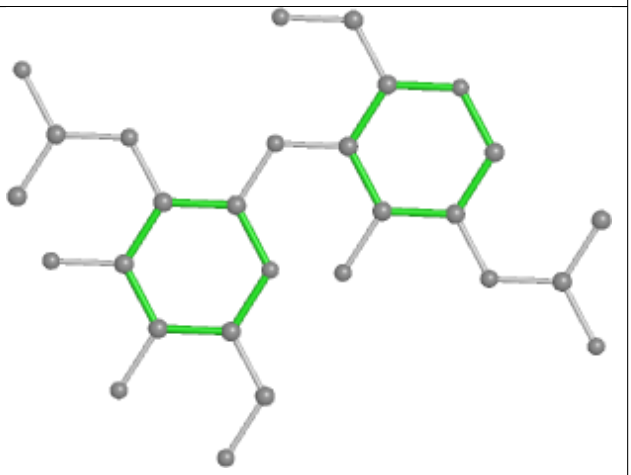


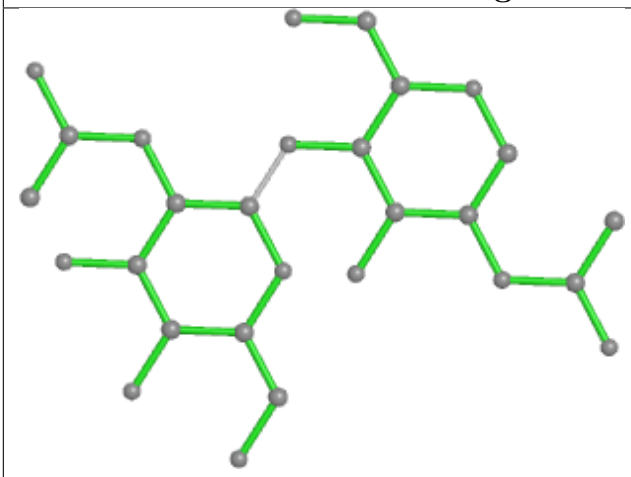
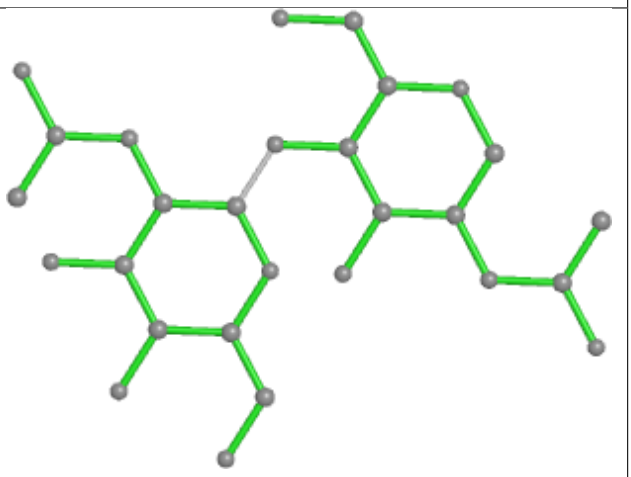
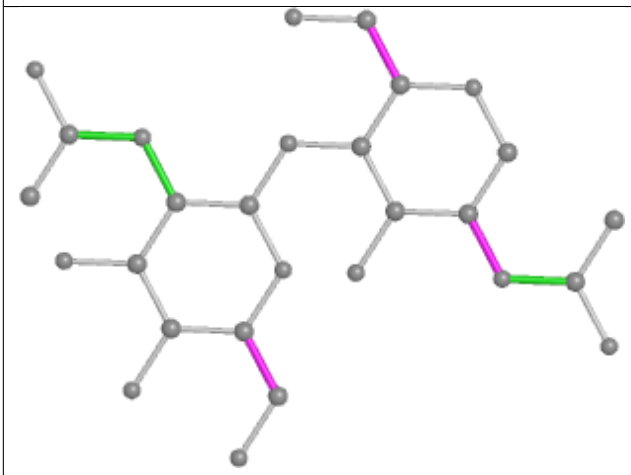
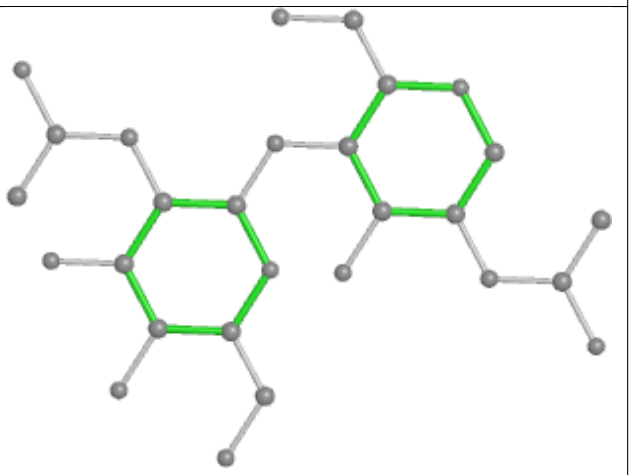
Rings

Oligosaccharide Chain K	
 Bond lengths	 Bond angles
 Torsions	 Rings

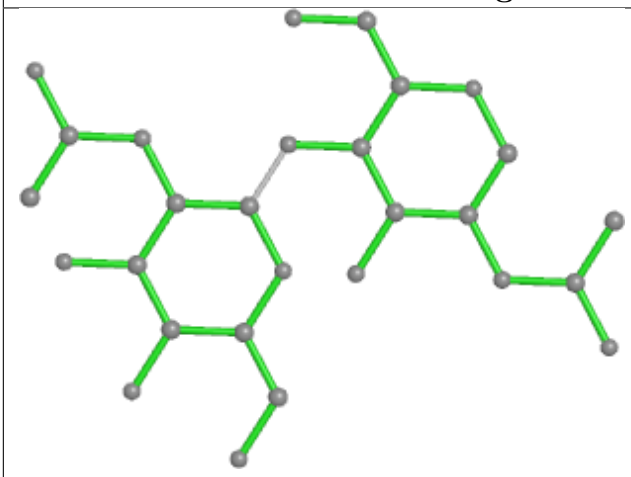
Oligosaccharide Chain L	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain M	
 Bond lengths	 Bond angles
 Torsions	 Rings

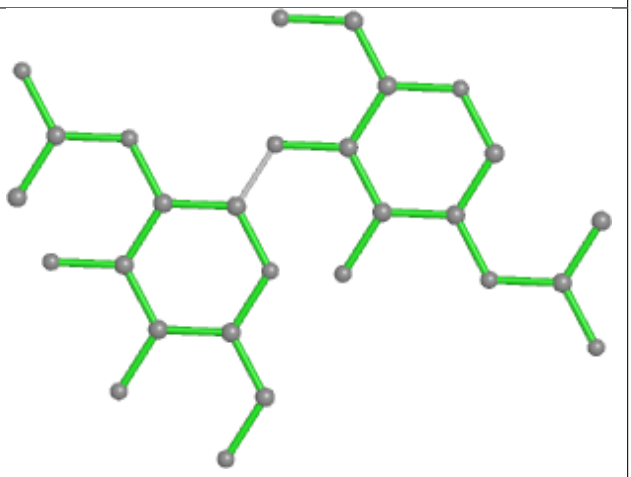
Oligosaccharide Chain N	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain O	
 Bond lengths	 Bond angles
 Torsions	 Rings

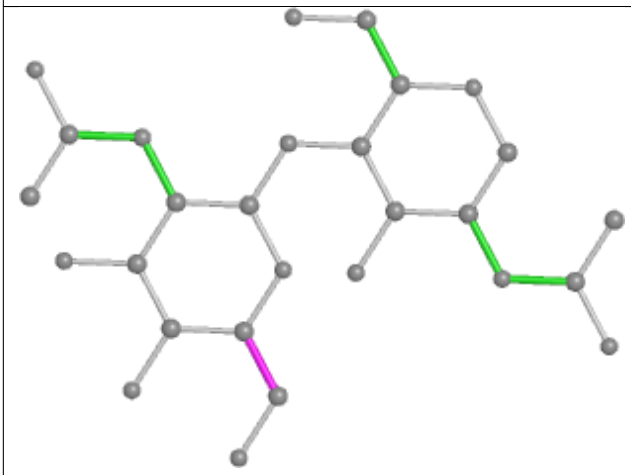
Oligosaccharide Chain P



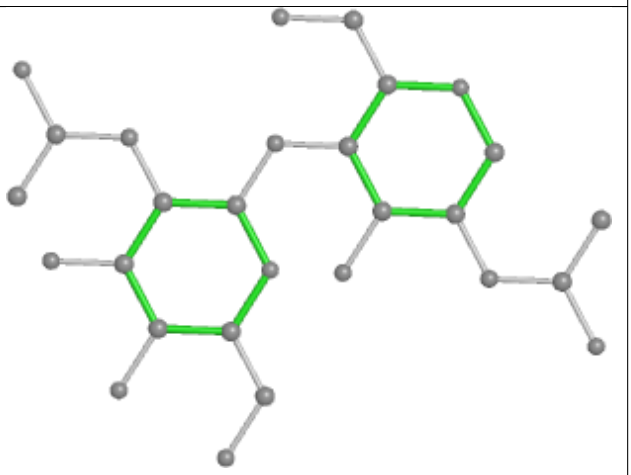
Bond lengths



Bond angles

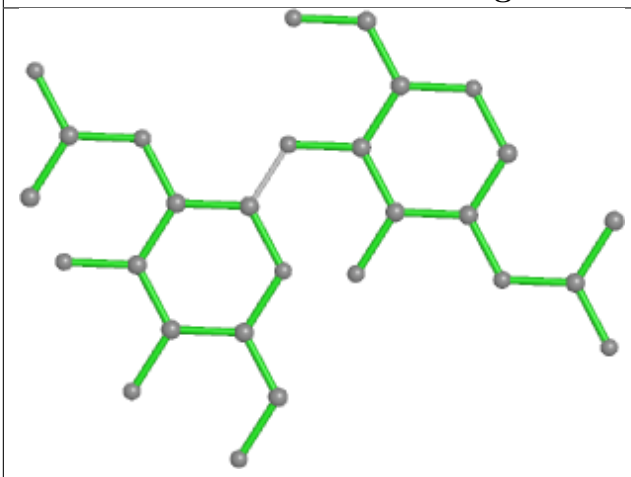


Torsions

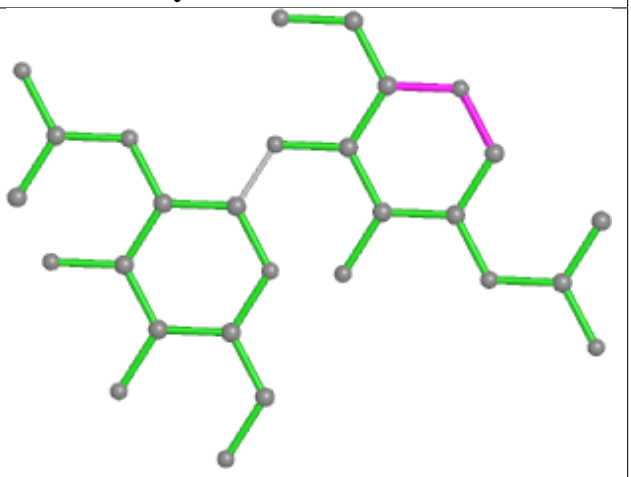


Rings

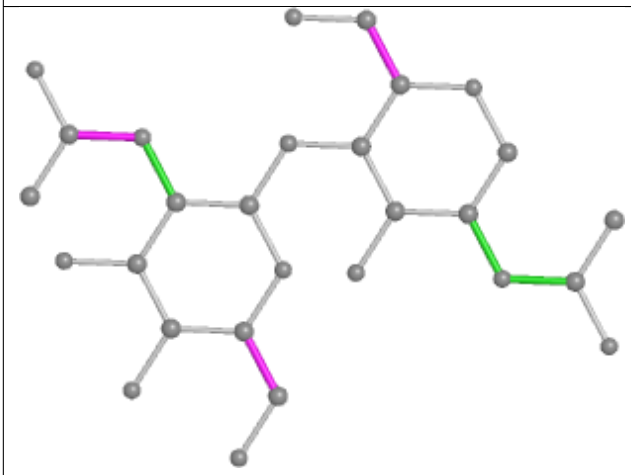
Oligosaccharide Chain Q



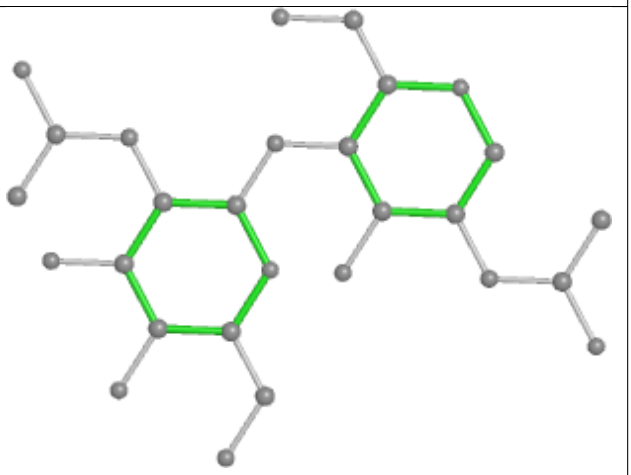
Bond lengths



Bond angles

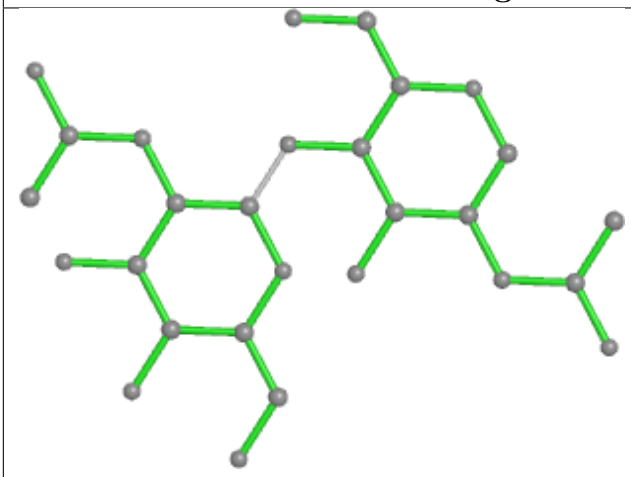


Torsions

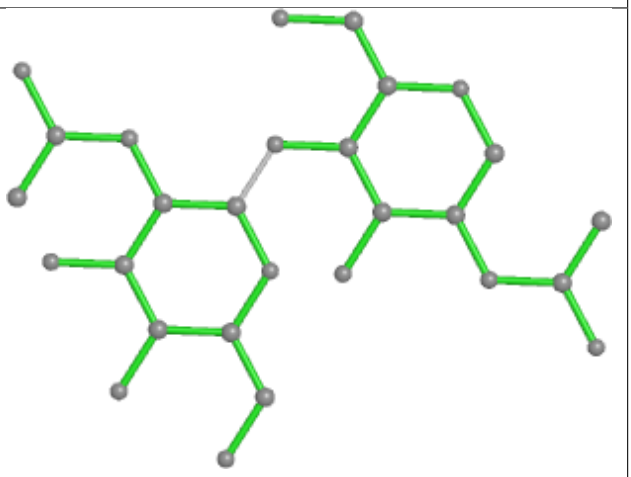


Rings

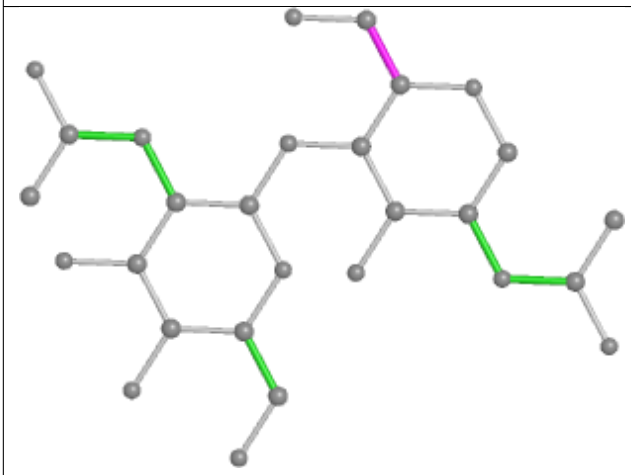
Oligosaccharide Chain R



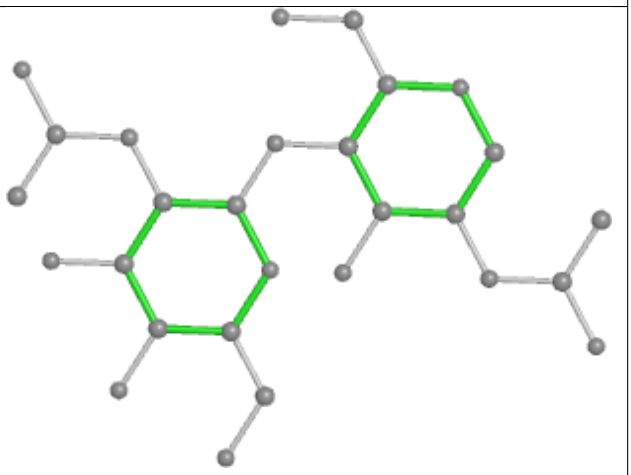
Bond lengths



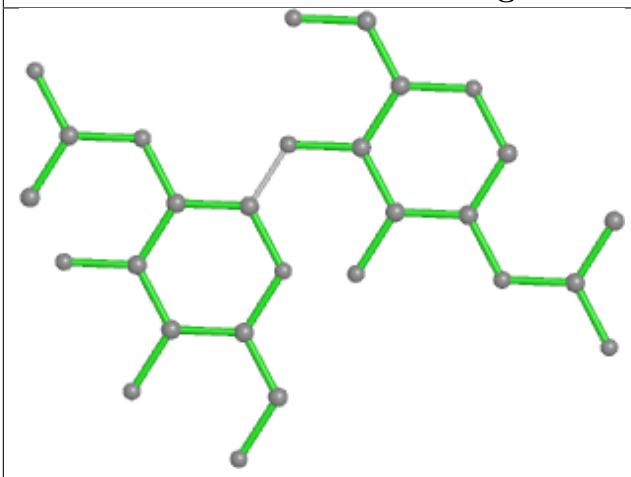
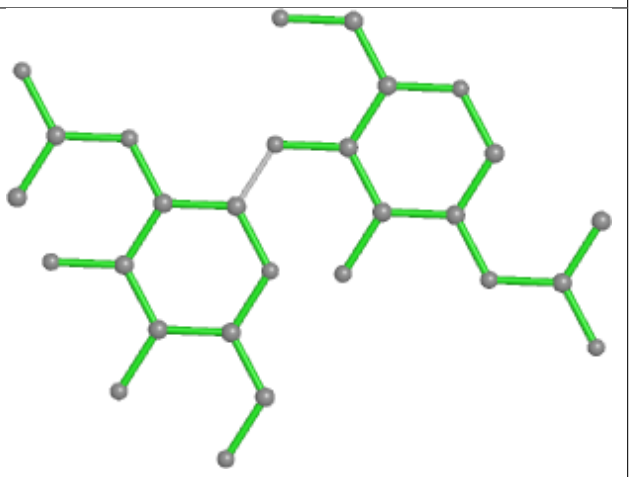
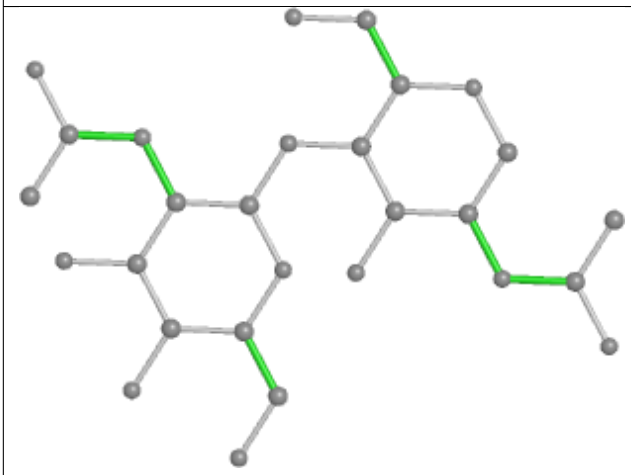
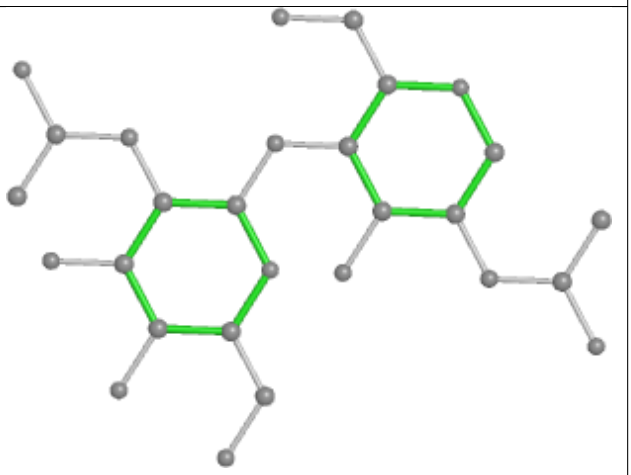
Bond angles



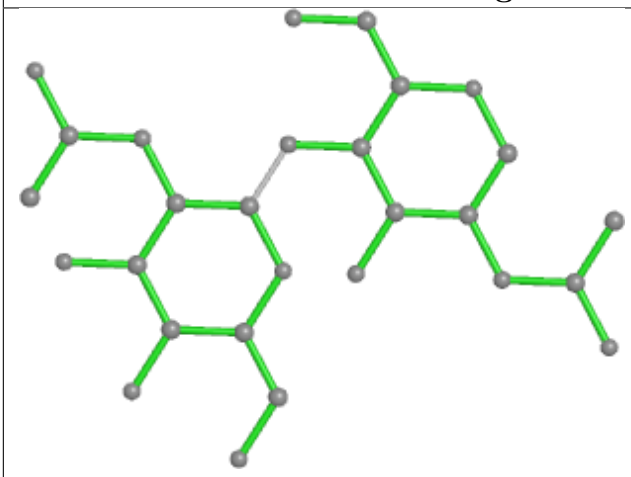
Torsions



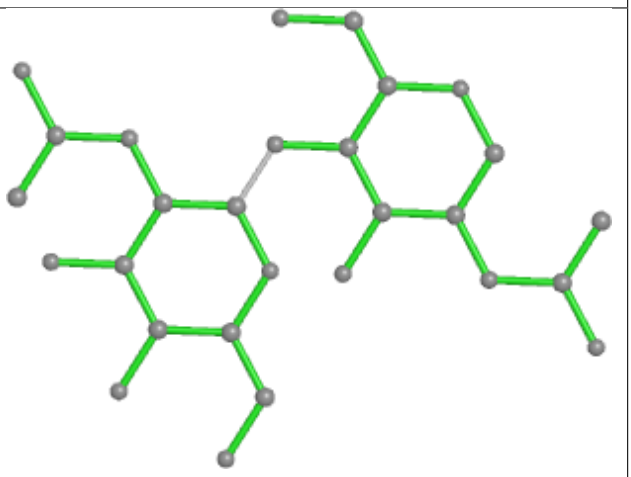
Rings

Oligosaccharide Chain S	
 Bond lengths	 Bond angles
 Torsions	 Rings

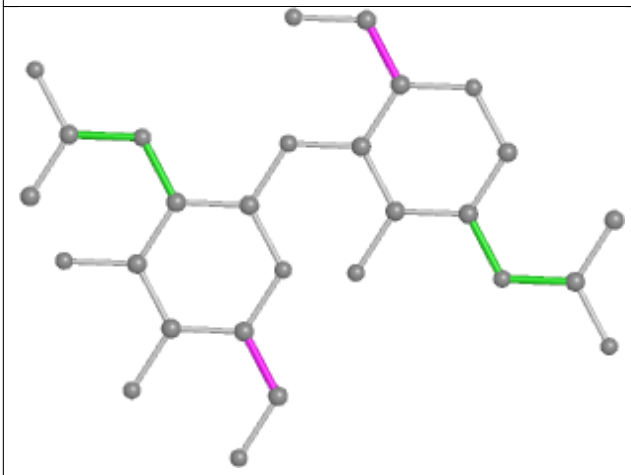
Oligosaccharide Chain T



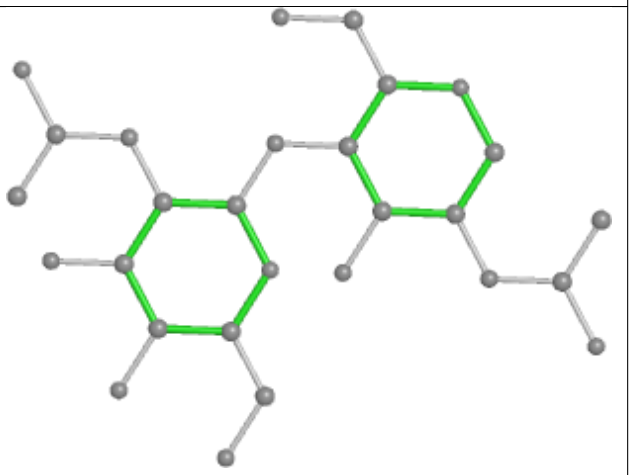
Bond lengths



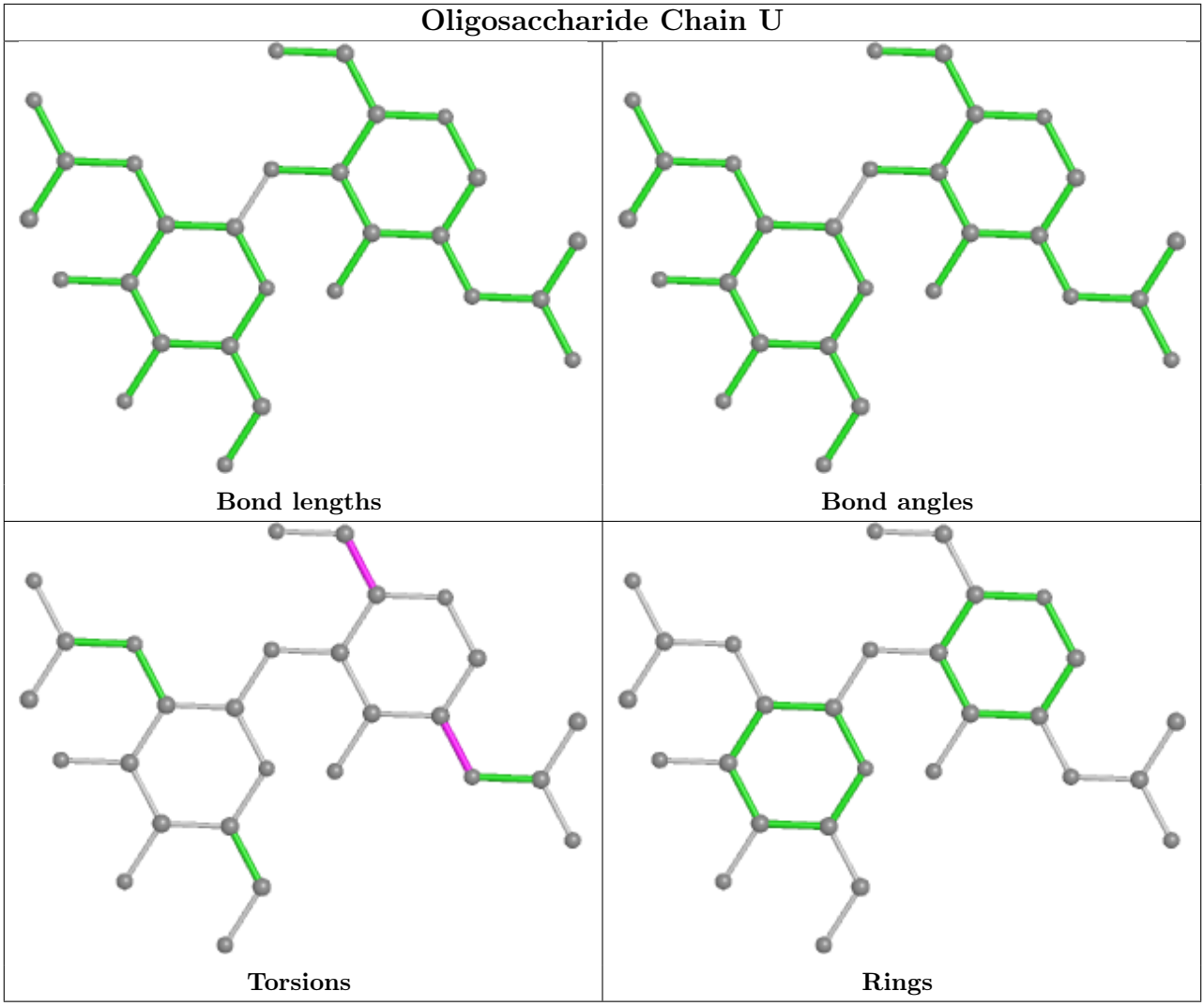
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

30 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	$\#\|Z\| > 2$
3	NAG	A	1307	1	14,14,15	0.17	0	17,19,21	0.53	0
3	NAG	B	1308	1	14,14,15	0.17	0	17,19,21	0.42	0
3	NAG	C	1305	1	14,14,15	0.30	0	17,19,21	0.50	0
3	NAG	B	1310	1	14,14,15	0.27	0	17,19,21	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	C	1303	1	14,14,15	0.22	0	17,19,21	0.46	0
3	NAG	B	1306	1	14,14,15	0.18	0	17,19,21	0.46	0
3	NAG	B	1302	1	14,14,15	0.17	0	17,19,21	0.43	0
3	NAG	C	1308	1	14,14,15	0.19	0	17,19,21	0.41	0
3	NAG	B	1303	1	14,14,15	0.20	0	17,19,21	0.46	0
3	NAG	A	1305	1	14,14,15	0.25	0	17,19,21	0.51	0
3	NAG	C	1302	1	14,14,15	0.17	0	17,19,21	0.43	0
3	NAG	C	1309	1	14,14,15	0.34	0	17,19,21	0.54	0
3	NAG	A	1301	1	14,14,15	0.43	0	17,19,21	1.23	1 (5%)
3	NAG	B	1304	1	14,14,15	0.21	0	17,19,21	0.41	0
3	NAG	C	1306	1	14,14,15	0.19	0	17,19,21	0.43	0
3	NAG	A	1310	1	14,14,15	0.28	0	17,19,21	0.43	0
3	NAG	A	1306	1	14,14,15	0.20	0	17,19,21	0.45	0
3	NAG	C	1307	1	14,14,15	0.16	0	17,19,21	0.55	0
3	NAG	C	1301	1	14,14,15	0.45	0	17,19,21	1.23	2 (11%)
3	NAG	B	1307	1	14,14,15	0.16	0	17,19,21	0.54	0
3	NAG	C	1310	1	14,14,15	0.27	0	17,19,21	0.42	0
3	NAG	A	1302	1	14,14,15	0.18	0	17,19,21	0.43	0
3	NAG	B	1309	1	14,14,15	0.35	0	17,19,21	0.55	0
3	NAG	A	1304	1	14,14,15	0.22	0	17,19,21	0.43	0
3	NAG	C	1304	1	14,14,15	0.17	0	17,19,21	0.41	0
3	NAG	B	1305	1	14,14,15	0.29	0	17,19,21	0.51	0
3	NAG	A	1308	1	14,14,15	0.18	0	17,19,21	0.41	0
3	NAG	A	1309	1	14,14,15	0.31	0	17,19,21	0.55	0
3	NAG	A	1303	1	14,14,15	0.20	0	17,19,21	0.45	0
3	NAG	B	1301	1	14,14,15	0.45	0	17,19,21	1.23	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	1307	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1308	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1305	1	-	1/6/23/26	0/1/1/1
3	NAG	B	1310	1	-	4/6/23/26	0/1/1/1
3	NAG	C	1303	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1306	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1302	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1308	1	-	2/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	1303	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1305	1	-	1/6/23/26	0/1/1/1
3	NAG	C	1302	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1309	1	-	3/6/23/26	0/1/1/1
3	NAG	A	1301	1	-	3/6/23/26	0/1/1/1
3	NAG	B	1304	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1306	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1310	1	-	4/6/23/26	0/1/1/1
3	NAG	A	1306	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1307	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1301	1	-	3/6/23/26	0/1/1/1
3	NAG	B	1307	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1310	1	-	4/6/23/26	0/1/1/1
3	NAG	A	1302	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1309	1	-	3/6/23/26	0/1/1/1
3	NAG	A	1304	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1304	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1305	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1308	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1309	1	-	3/6/23/26	0/1/1/1
3	NAG	A	1303	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1301	1	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1301	NAG	C2-N2-C7	4.30	129.02	122.90
3	A	1301	NAG	C2-N2-C7	4.28	129.00	122.90
3	C	1301	NAG	C2-N2-C7	4.27	128.98	122.90
3	C	1301	NAG	C1-C2-N2	2.02	113.94	110.49

There are no chirality outliers.

All (62) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1309	NAG	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	B	1309	NAG	C4-C5-C6-O6
3	C	1309	NAG	C4-C5-C6-O6
3	A	1308	NAG	O5-C5-C6-O6
3	A	1309	NAG	O5-C5-C6-O6
3	B	1308	NAG	O5-C5-C6-O6
3	C	1308	NAG	O5-C5-C6-O6
3	A	1310	NAG	O5-C5-C6-O6
3	A	1304	NAG	O5-C5-C6-O6
3	B	1304	NAG	O5-C5-C6-O6
3	B	1310	NAG	O5-C5-C6-O6
3	C	1304	NAG	O5-C5-C6-O6
3	C	1309	NAG	O5-C5-C6-O6
3	C	1310	NAG	O5-C5-C6-O6
3	B	1309	NAG	O5-C5-C6-O6
3	A	1308	NAG	C4-C5-C6-O6
3	B	1308	NAG	C4-C5-C6-O6
3	B	1310	NAG	C4-C5-C6-O6
3	C	1308	NAG	C4-C5-C6-O6
3	C	1310	NAG	C4-C5-C6-O6
3	A	1310	NAG	C4-C5-C6-O6
3	A	1301	NAG	C8-C7-N2-C2
3	A	1301	NAG	O7-C7-N2-C2
3	A	1302	NAG	C8-C7-N2-C2
3	A	1302	NAG	O7-C7-N2-C2
3	A	1310	NAG	C8-C7-N2-C2
3	A	1310	NAG	O7-C7-N2-C2
3	B	1301	NAG	C8-C7-N2-C2
3	B	1301	NAG	O7-C7-N2-C2
3	B	1302	NAG	C8-C7-N2-C2
3	B	1302	NAG	O7-C7-N2-C2
3	B	1310	NAG	C8-C7-N2-C2
3	B	1310	NAG	O7-C7-N2-C2
3	C	1301	NAG	C8-C7-N2-C2
3	C	1301	NAG	O7-C7-N2-C2
3	C	1302	NAG	C8-C7-N2-C2
3	C	1302	NAG	O7-C7-N2-C2
3	C	1310	NAG	C8-C7-N2-C2
3	C	1310	NAG	O7-C7-N2-C2
3	C	1304	NAG	C4-C5-C6-O6
3	B	1304	NAG	C4-C5-C6-O6
3	A	1304	NAG	C4-C5-C6-O6
3	B	1303	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	B	1303	NAG	C4-C5-C6-O6
3	C	1303	NAG	O5-C5-C6-O6
3	A	1303	NAG	O5-C5-C6-O6
3	C	1306	NAG	C4-C5-C6-O6
3	C	1303	NAG	C4-C5-C6-O6
3	A	1303	NAG	C4-C5-C6-O6
3	B	1306	NAG	C4-C5-C6-O6
3	A	1306	NAG	C4-C5-C6-O6
3	C	1306	NAG	O5-C5-C6-O6
3	B	1306	NAG	O5-C5-C6-O6
3	A	1306	NAG	O5-C5-C6-O6
3	A	1309	NAG	C3-C2-N2-C7
3	B	1309	NAG	C3-C2-N2-C7
3	C	1309	NAG	C3-C2-N2-C7
3	A	1305	NAG	O5-C5-C6-O6
3	C	1305	NAG	O5-C5-C6-O6
3	A	1301	NAG	C3-C2-N2-C7
3	B	1301	NAG	C3-C2-N2-C7
3	C	1301	NAG	C3-C2-N2-C7

There are no ring outliers.

9 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1310	NAG	1	0
3	C	1309	NAG	1	0
3	A	1301	NAG	1	0
3	A	1310	NAG	1	0
3	C	1301	NAG	1	0
3	C	1310	NAG	1	0
3	B	1309	NAG	1	0
3	A	1309	NAG	1	0
3	B	1301	NAG	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

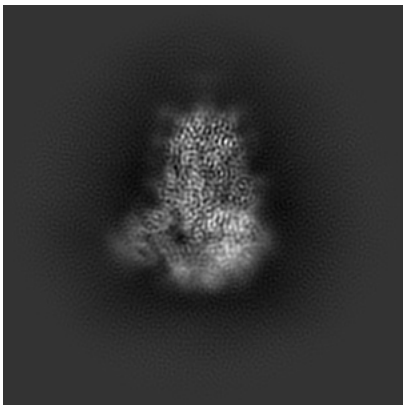
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-33325. These allow visual inspection of the internal detail of the map and identification of artifacts.

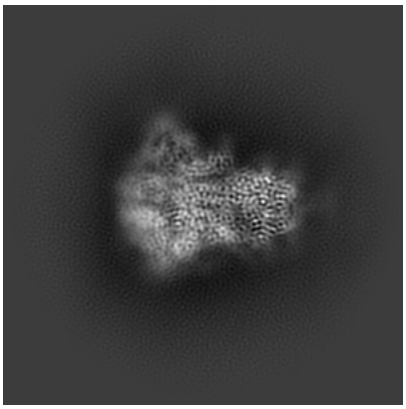
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

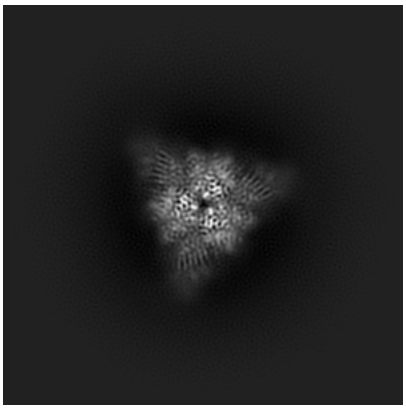
6.1.1 Primary map



X

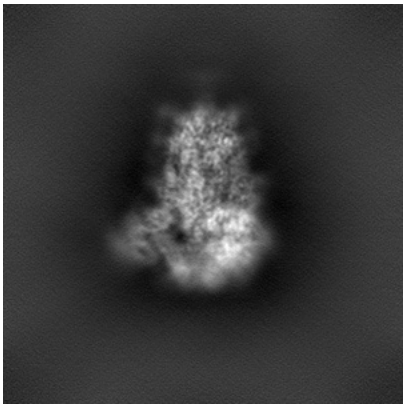


Y

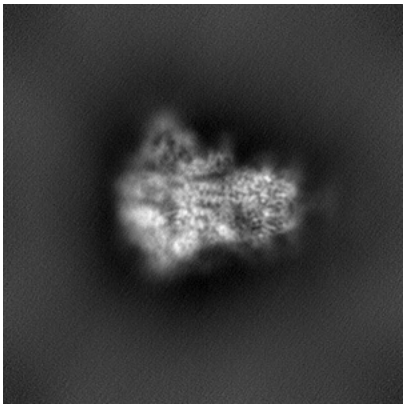


Z

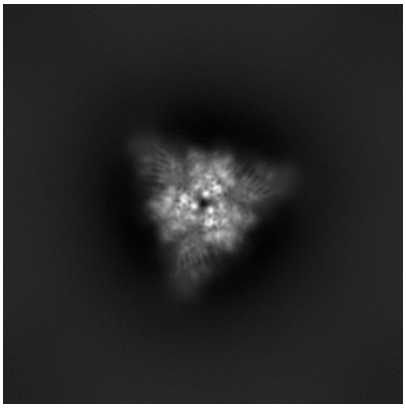
6.1.2 Raw map



X



Y

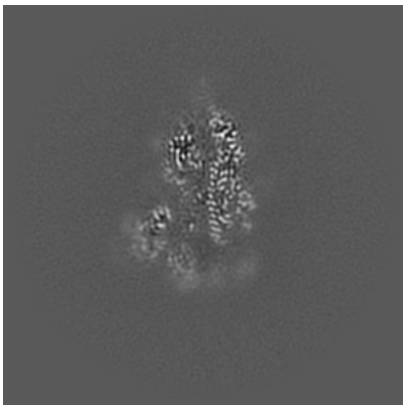


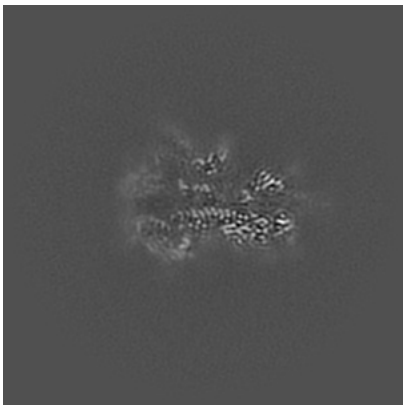
Z

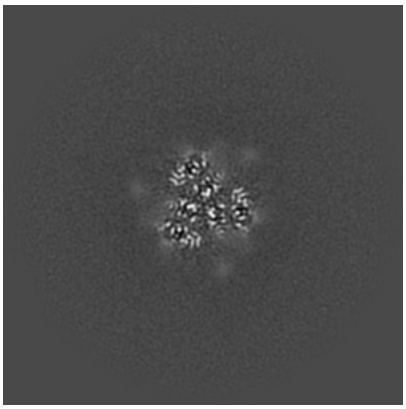
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

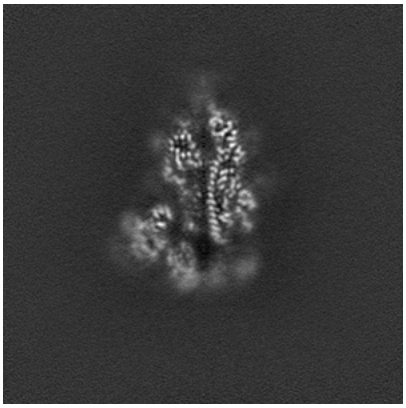
6.2.1 Primary map

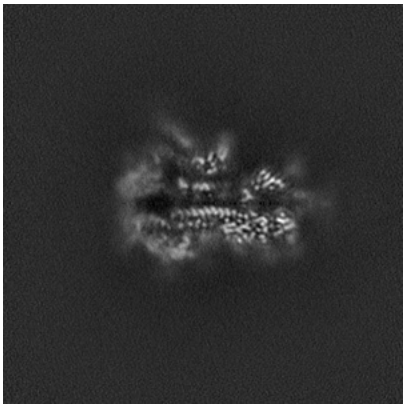

X Index: 160

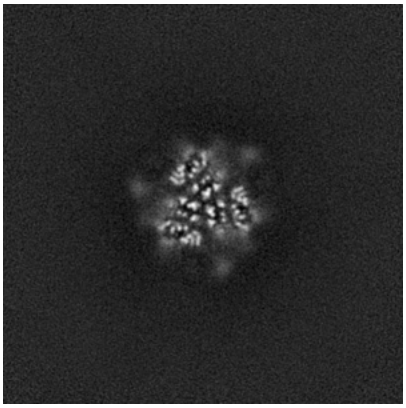

Y Index: 160


Z Index: 160

6.2.2 Raw map


X Index: 160

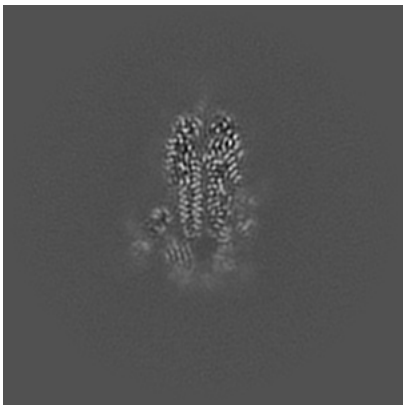

Y Index: 160

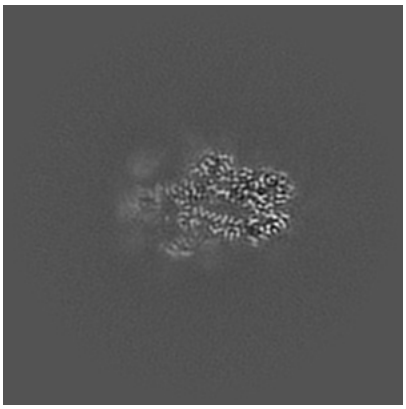

Z Index: 160

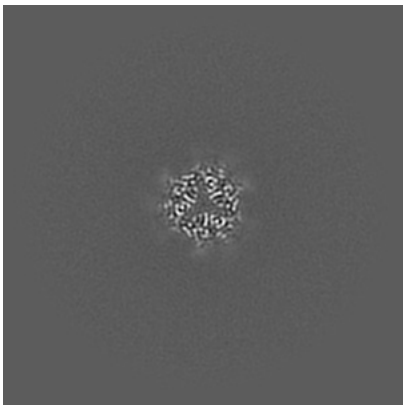
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

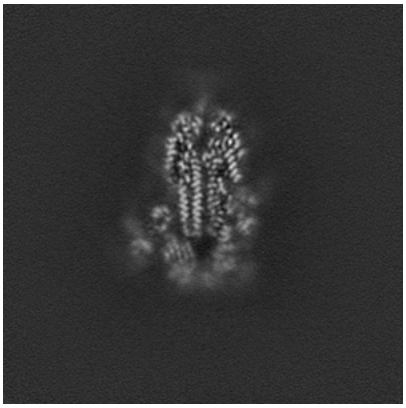
6.3.1 Primary map

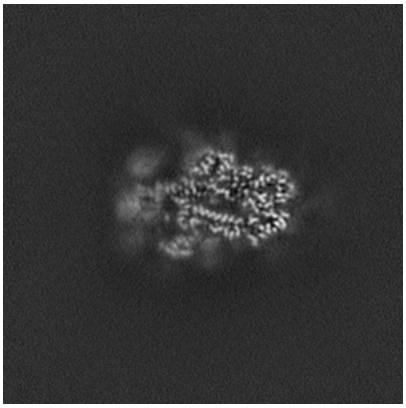

X Index: 165

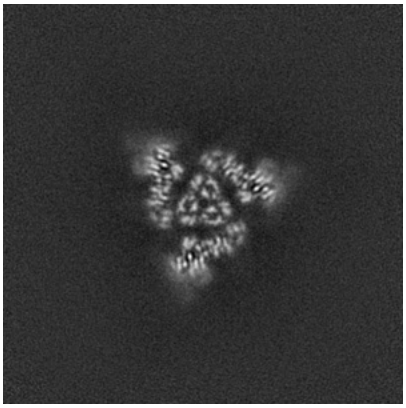

Y Index: 149


Z Index: 208

6.3.2 Raw map


X Index: 165

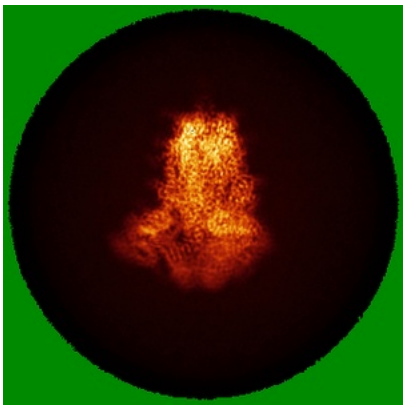

Y Index: 149

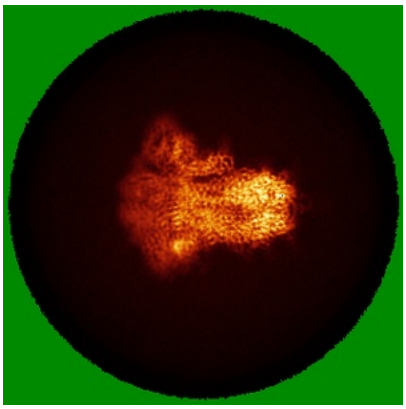

Z Index: 141

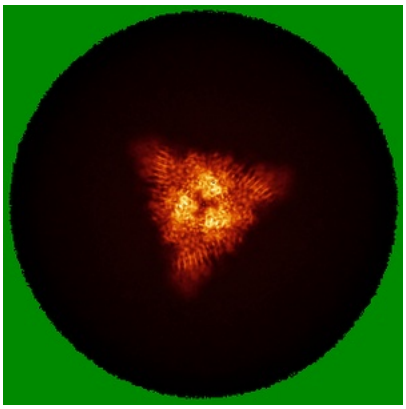
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

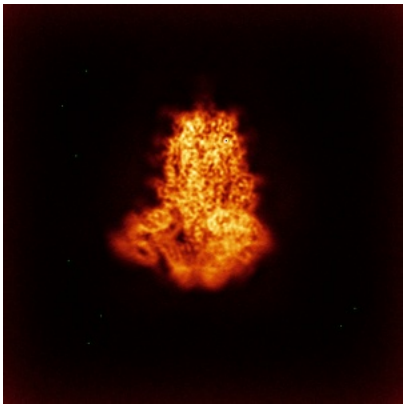
6.4.1 Primary map

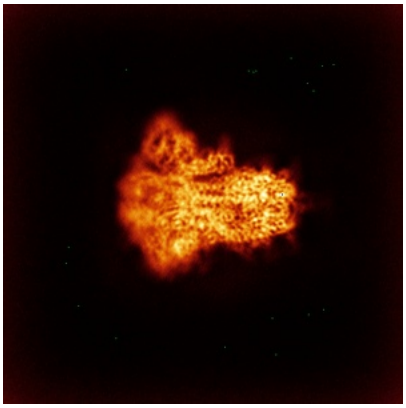

X

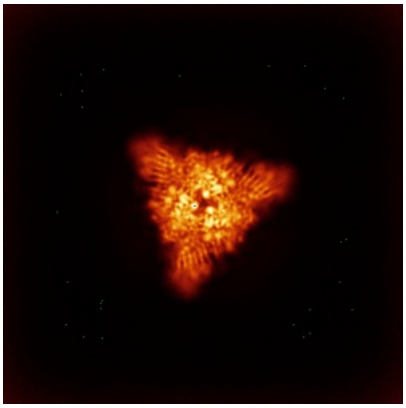

Y


Z

6.4.2 Raw map


X


Y


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

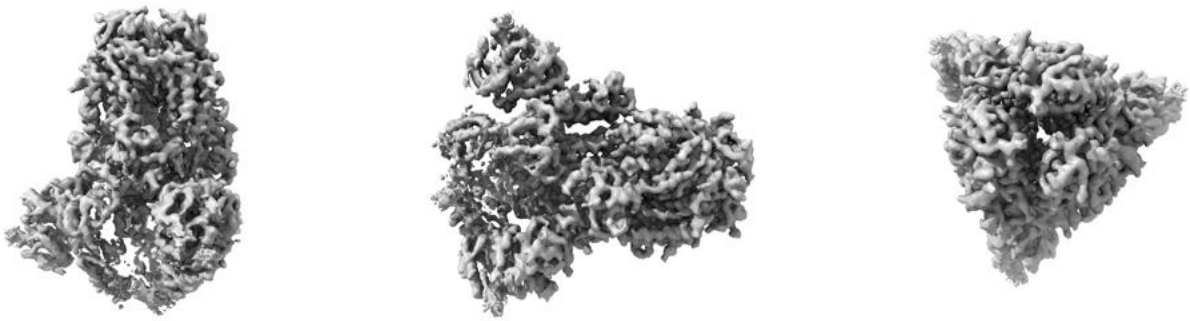
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

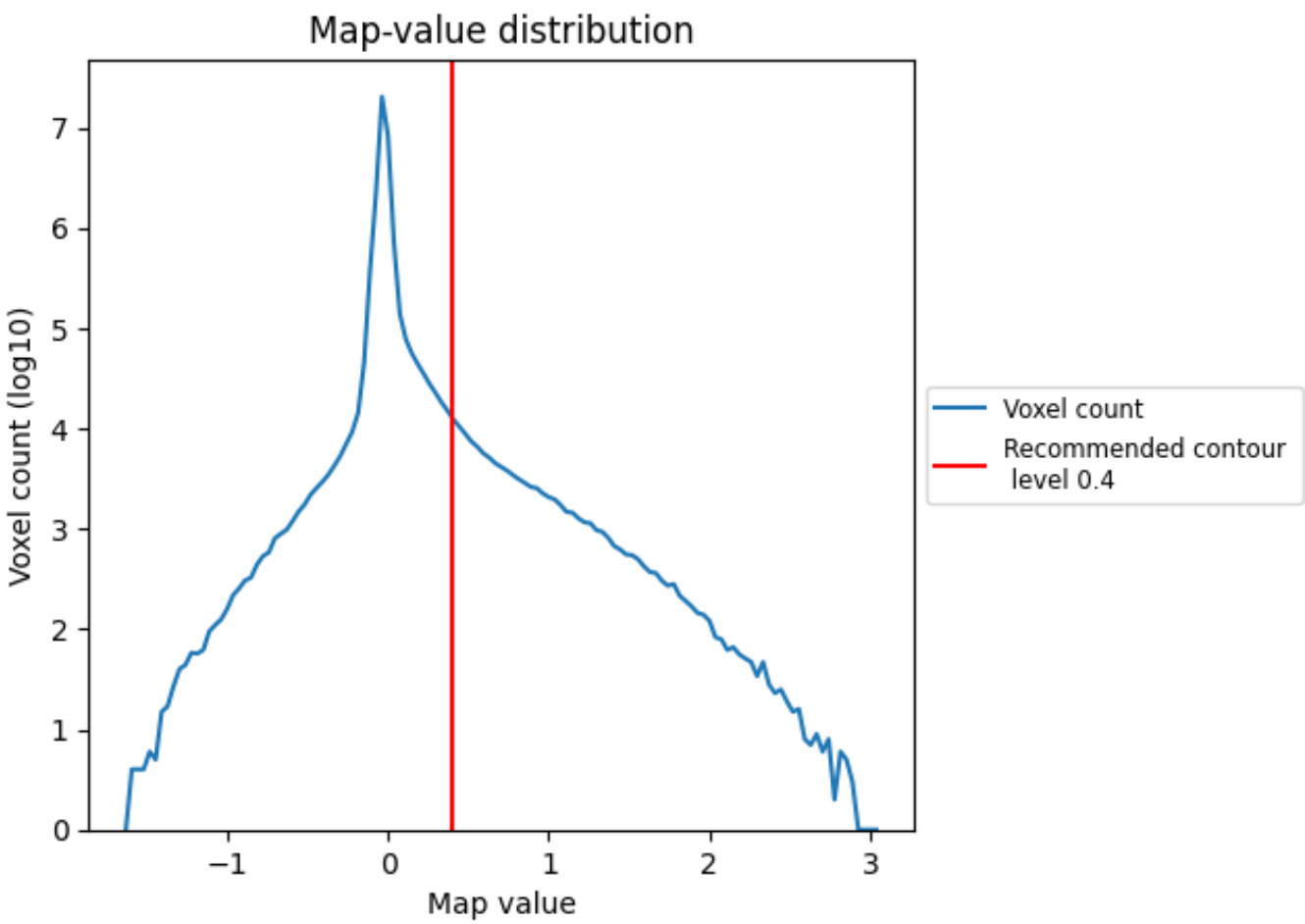
6.6 Mask visualisation (i)

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

7 Map analysis (i)

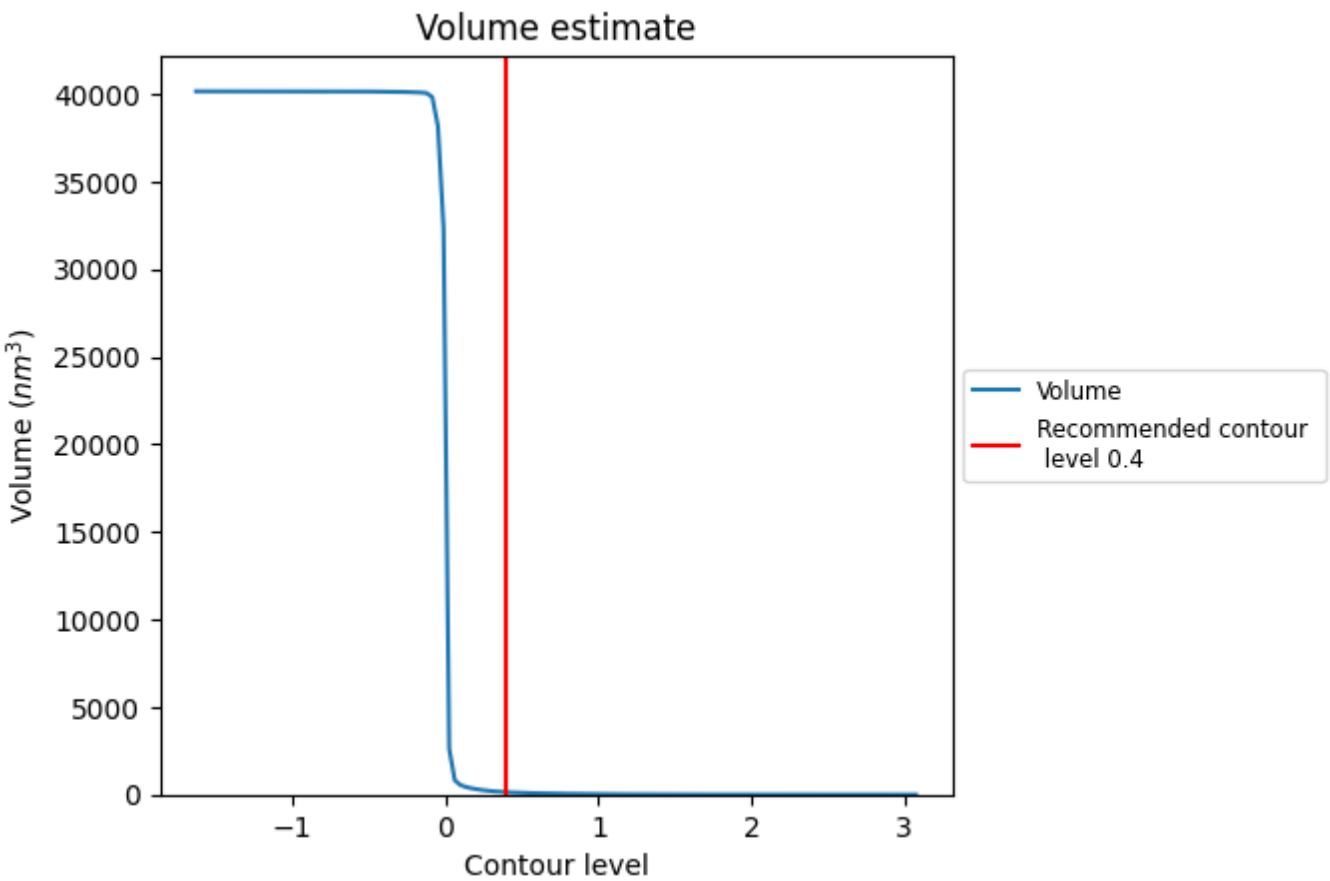
This section contains the results of statistical analysis of the map.

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.

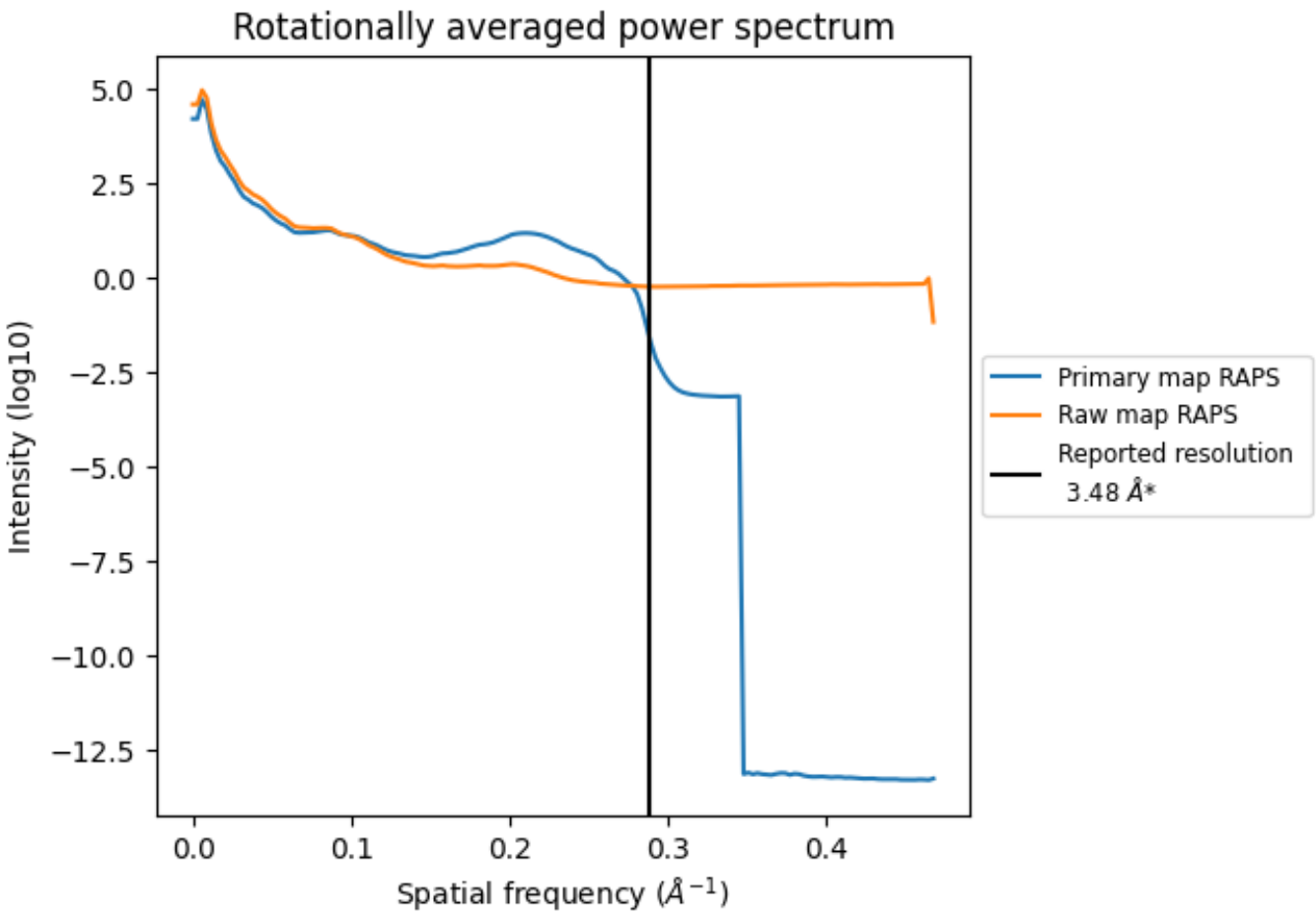
7.2 Volume estimate (i)



The volume at the recommended contour level is 135 nm^3; this corresponds to an approximate mass of 122 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)

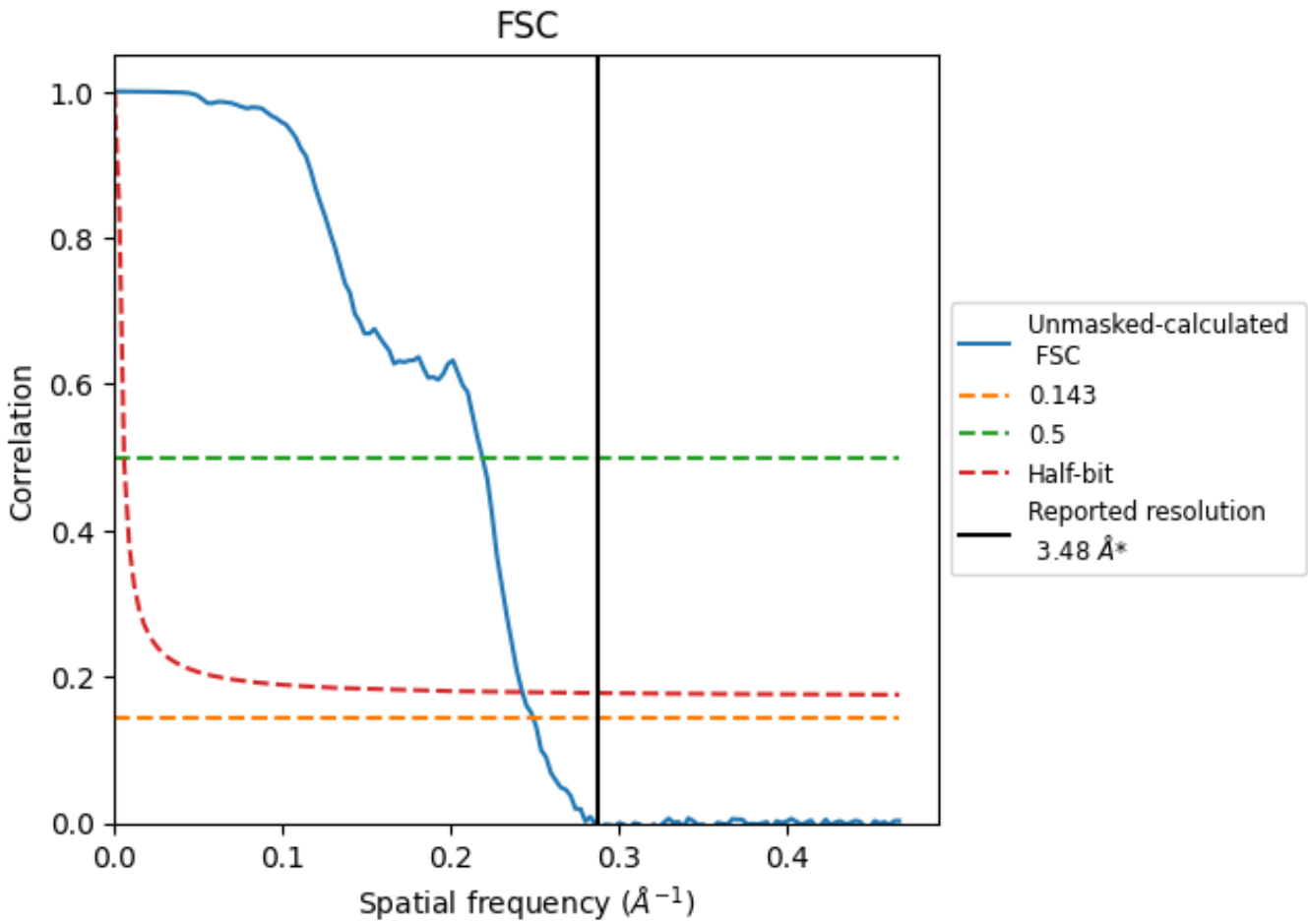


*Reported resolution corresponds to spatial frequency of 0.287 Å^{-1}

8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.287 Å^{-1}

8.2 Resolution estimates (i)

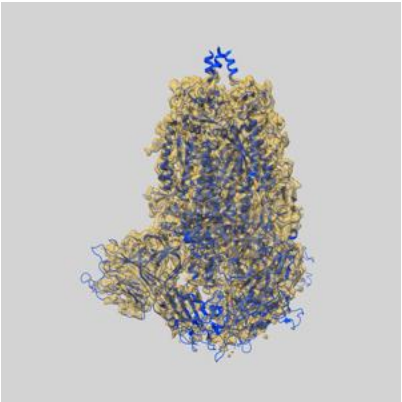
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.48	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.01	4.56	4.12

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.01 differs from the reported value 3.48 by more than 10 %

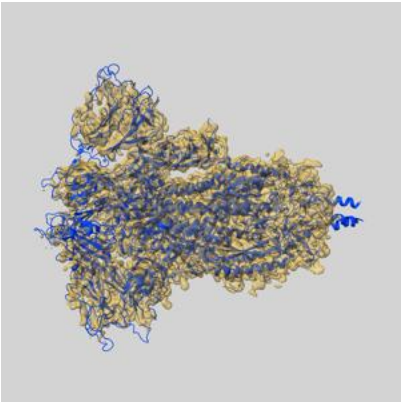
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-33325 and PDB model 7XNS. Per-residue inclusion information can be found in section 3 on page 11.

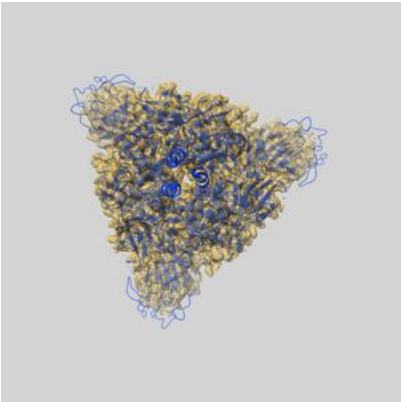
9.1 Map-model overlay (i)



X



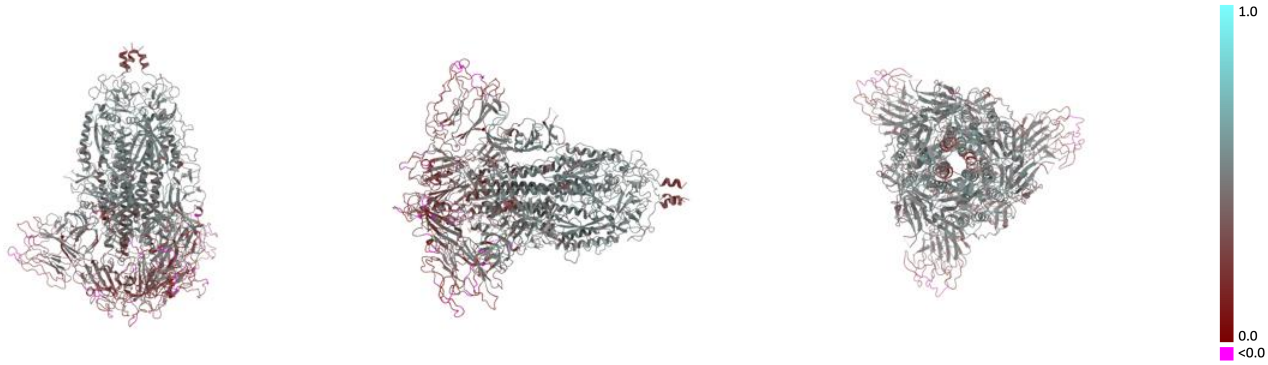
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.4 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.

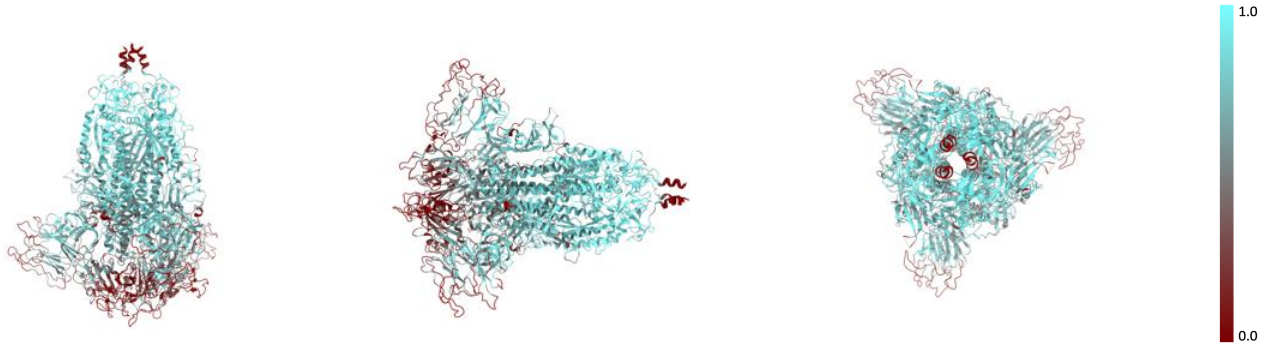
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

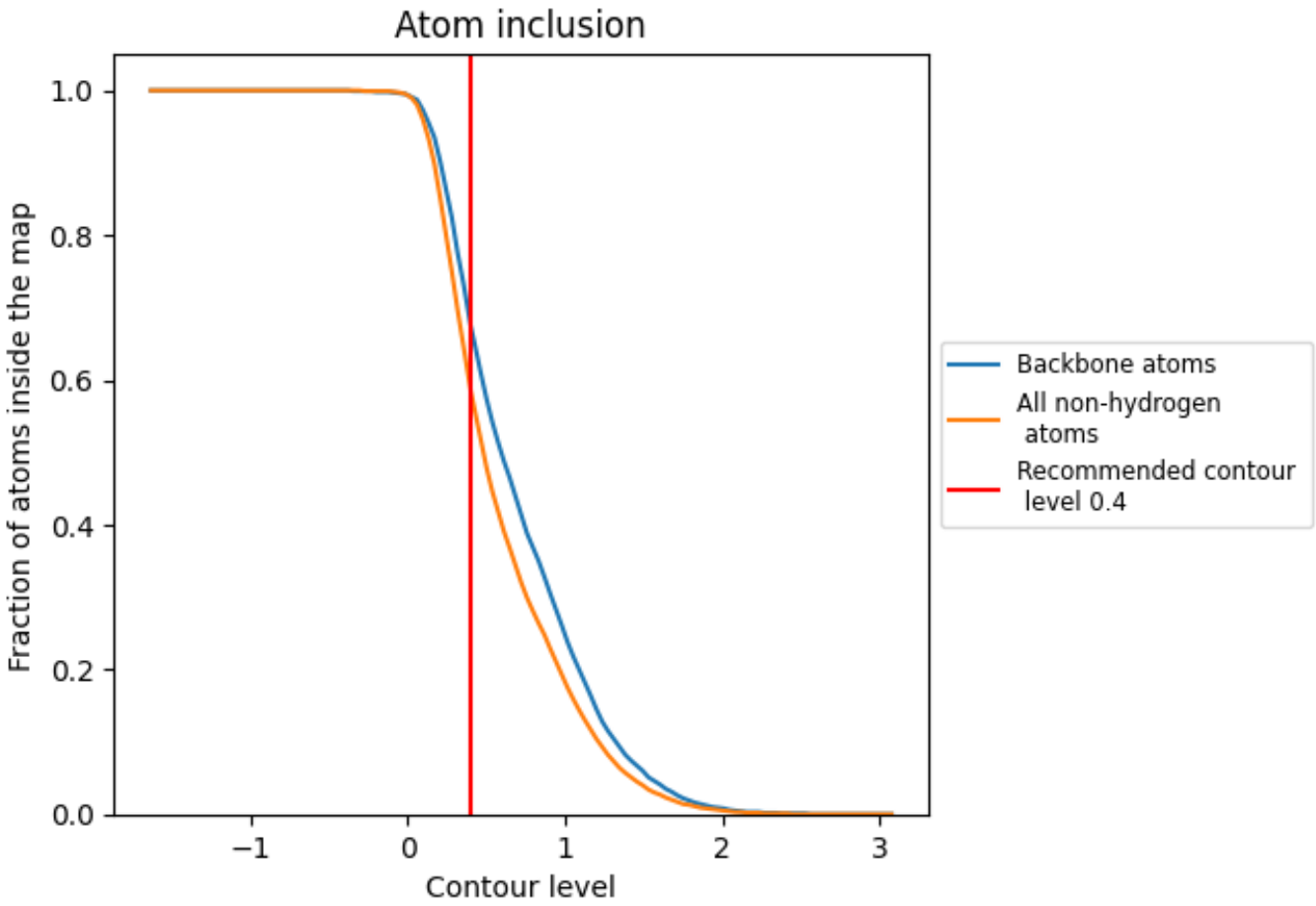
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.4).

9.4 Atom inclusion (i)



At the recommended contour level, 68% of all backbone atoms, 59% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5870	0.4020
A	0.5910	0.4040
B	0.5920	0.4040
C	0.5910	0.4040
D	0.1430	0.1490
E	0.2500	0.0810
F	0.7140	0.4630
G	0.5360	0.3610
H	0.3570	0.4030
I	0.2860	0.3060
J	0.1070	0.1780
K	0.2500	0.0950
L	0.7500	0.4730
M	0.5000	0.3580
N	0.3570	0.3960
O	0.2860	0.3050
P	0.1430	0.1700
Q	0.2500	0.0870
R	0.7140	0.4510
S	0.5360	0.3520
T	0.3570	0.3970
U	0.2860	0.2910