Full wwPDB EM Validation Report ⓘ

Nov 6, 2022 – 12:42 PM EST

PDB ID	:	6CS1
EMDB ID	:	EMD-7579
Title	:	SARS Spike Glycoprotein, Trypsin-cleaved, Stabilized variant, two S1 CTDs in an upwards conformation
Authors	:	Kirchdoerfer, R.N.; Wang, N.; Pallesen, J.; Turner, H.L.; Cottrell, C.A.; McLellan, J.S.; Ward, A.B.
Deposited on	:	2018-03-19
Resolution	:	4.60 Å(reported)
Based on initial models	:	5I08, 2AJF, 5X4S

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 ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

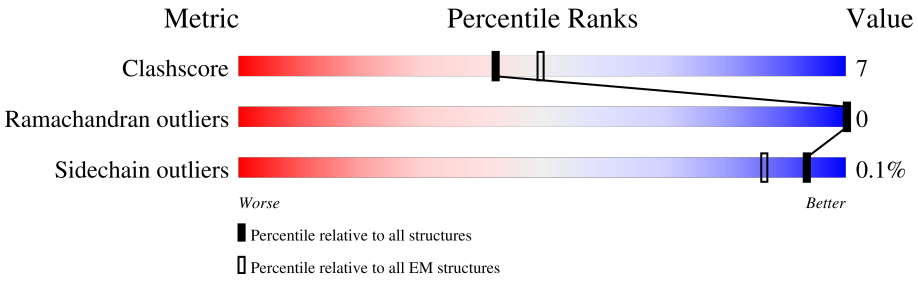
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance

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

The reported resolution of this entry is 4.60 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	A	1215	52% 71% 17% 12%
1	B	1215	44% 72% 16% 12%
1	C	1215	45% 70% 18% 12%
2	D	2	100% 50% 50%
2	F	2	100% 100%
2	I	2	100% 100%
2	J	2	100% 50% 50%
2	K	2	100% 100%

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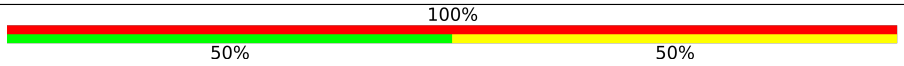
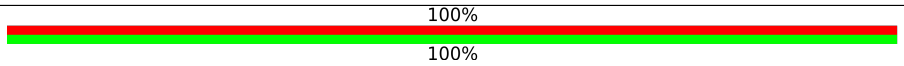
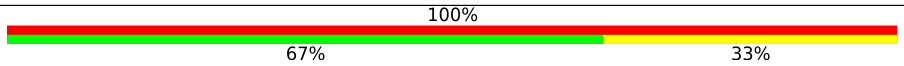
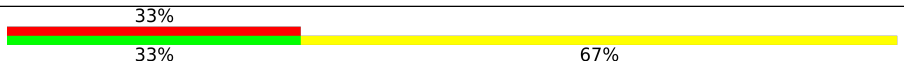
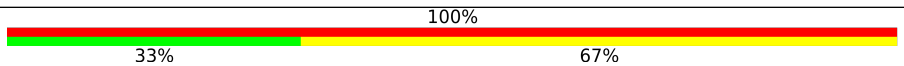
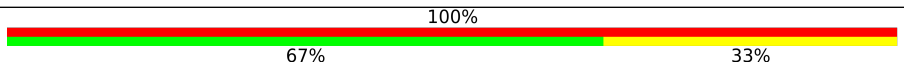
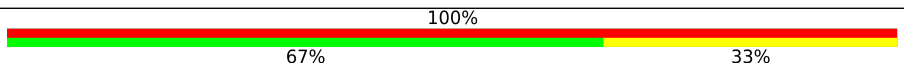
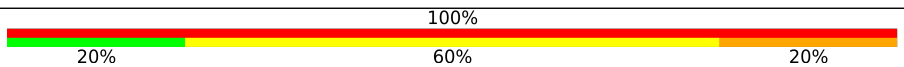
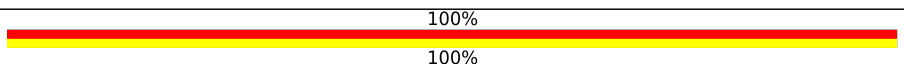
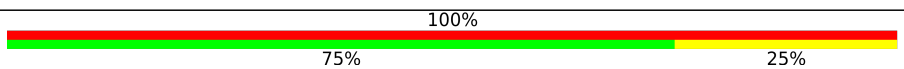
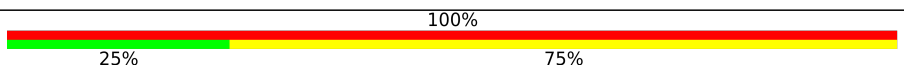
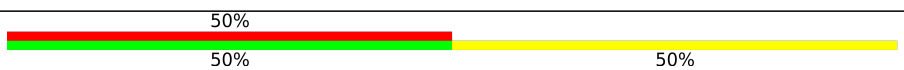
Mol	Chain	Length	Quality of chain
2	M	2	
2	R	2	
2	T	2	
2	W	2	
3	E	3	
3	L	3	
3	Q	3	
3	U	3	
3	V	3	
3	X	3	
4	G	5	
4	H	5	
4	S	5	
5	N	4	
5	O	4	
5	P	4	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 25995 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,Fibritin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	1068	Total	C	N	O	S	0	0
			8342	5331	1379	1586	46		
1	C	1068	Total	C	N	O	S	0	0
			8339	5328	1379	1586	46		
1	A	1066	Total	C	N	O	S	0	0
			8327	5320	1377	1584	46		

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	577	ALA	SER	conflict	UNP P59594
B	968	PRO	LYS	engineered mutation	UNP P59594
B	969	PRO	VAL	engineered mutation	UNP P59594
B	1191	GLY	-	linker	UNP P59594
B	1192	SER	ALA	linker	UNP D9IEJ2
B	1220	GLY	-	expression tag	UNP D9IEJ2
B	1221	ARG	-	expression tag	UNP D9IEJ2
B	1222	SER	-	expression tag	UNP D9IEJ2
B	1223	LEU	-	expression tag	UNP D9IEJ2
B	1224	GLU	-	expression tag	UNP D9IEJ2
B	1225	VAL	-	expression tag	UNP D9IEJ2
B	1226	LEU	-	expression tag	UNP D9IEJ2
B	1227	PHE	-	expression tag	UNP D9IEJ2
B	1228	GLN	-	expression tag	UNP D9IEJ2
C	577	ALA	SER	conflict	UNP P59594
C	968	PRO	LYS	engineered mutation	UNP P59594
C	969	PRO	VAL	engineered mutation	UNP P59594
C	1191	GLY	-	linker	UNP P59594
C	1192	SER	ALA	linker	UNP D9IEJ2
C	1220	GLY	-	expression tag	UNP D9IEJ2
C	1221	ARG	-	expression tag	UNP D9IEJ2
C	1222	SER	-	expression tag	UNP D9IEJ2
C	1223	LEU	-	expression tag	UNP D9IEJ2
C	1224	GLU	-	expression tag	UNP D9IEJ2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1225	VAL	-	expression tag	UNP D9IEJ2
C	1226	LEU	-	expression tag	UNP D9IEJ2
C	1227	PHE	-	expression tag	UNP D9IEJ2
C	1228	GLN	-	expression tag	UNP D9IEJ2
A	577	ALA	SER	conflict	UNP P59594
A	968	PRO	LYS	engineered mutation	UNP P59594
A	969	PRO	VAL	engineered mutation	UNP P59594
A	1191	GLY	-	linker	UNP P59594
A	1192	SER	ALA	linker	UNP D9IEJ2
A	1220	GLY	-	expression tag	UNP D9IEJ2
A	1221	ARG	-	expression tag	UNP D9IEJ2
A	1222	SER	-	expression tag	UNP D9IEJ2
A	1223	LEU	-	expression tag	UNP D9IEJ2
A	1224	GLU	-	expression tag	UNP D9IEJ2
A	1225	VAL	-	expression tag	UNP D9IEJ2
A	1226	LEU	-	expression tag	UNP D9IEJ2
A	1227	PHE	-	expression tag	UNP D9IEJ2
A	1228	GLN	-	expression tag	UNP D9IEJ2

- 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
2	D	2	Total	C	N	O	0	0
			28	16	2	10		
2	F	2	Total	C	N	O	0	0
			28	16	2	10		
2	I	2	Total	C	N	O	0	0
			28	16	2	10		
2	J	2	Total	C	N	O	0	0
			28	16	2	10		
2	K	2	Total	C	N	O	0	0
			28	16	2	10		
2	M	2	Total	C	N	O	0	0
			28	16	2	10		
2	R	2	Total	C	N	O	0	0
			28	16	2	10		

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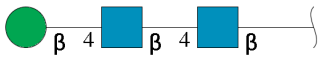
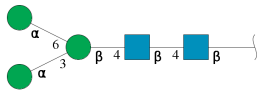
Mol	Chain	Residues	Atoms	AltConf	Trace
2	T	2	Total C N O 28 16 2 10	0	0
2	W	2	Total C N O 28 16 2 10	0	0

- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms	AltConf	Trace
3	E	3	Total C N O 39 22 2 15	0	0
3	L	3	Total C N O 39 22 2 15	0	0
3	Q	3	Total C N O 39 22 2 15	0	0
3	U	3	Total C N O 39 22 2 15	0	0
3	V	3	Total C N O 39 22 2 15	0	0
3	X	3	Total C N O 39 22 2 15	0	0

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

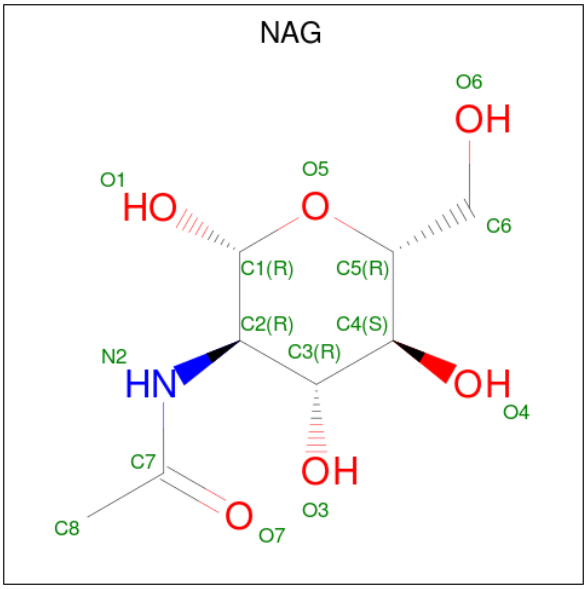


Mol	Chain	Residues	Atoms	AltConf	Trace
4	G	5	Total C N O 61 34 2 25	0	0
4	H	5	Total C N O 61 34 2 25	0	0
4	S	5	Total C N O 61 34 2 25	0	0

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	N	4	Total	C	N	O	0	0
			50	28	2	20		
5	O	4	Total	C	N	O	0	0
			50	28	2	20		
5	P	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
6	B	1	Total	C	N	O	0
			56	32	4	20	
6	B	1	Total	C	N	O	0
			56	32	4	20	
6	B	1	Total	C	N	O	0
			56	32	4	20	
6	B	1	Total	C	N	O	0
			56	32	4	20	

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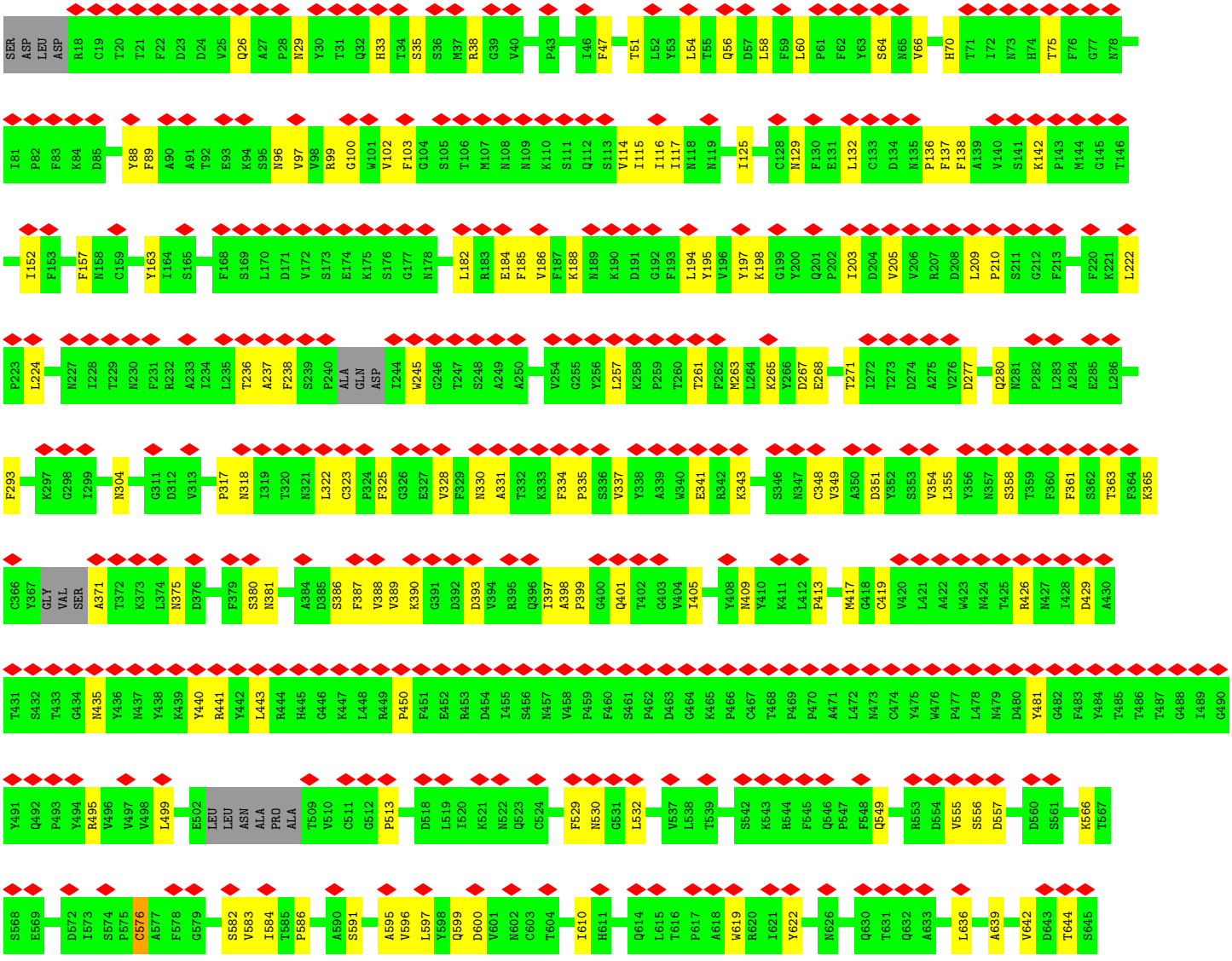
Mol	Chain	Residues	Atoms				AltConf
6	C	1	Total	C	N	O	0
			42	24	3	15	
6	C	1	Total	C	N	O	0
			42	24	3	15	
6	C	1	Total	C	N	O	0
			42	24	3	15	
6	A	1	Total	C	N	O	0
			70	40	5	25	
6	A	1	Total	C	N	O	0
			70	40	5	25	
6	A	1	Total	C	N	O	0
			70	40	5	25	
6	A	1	Total	C	N	O	0
			70	40	5	25	
6	A	1	Total	C	N	O	0
			70	40	5	25	

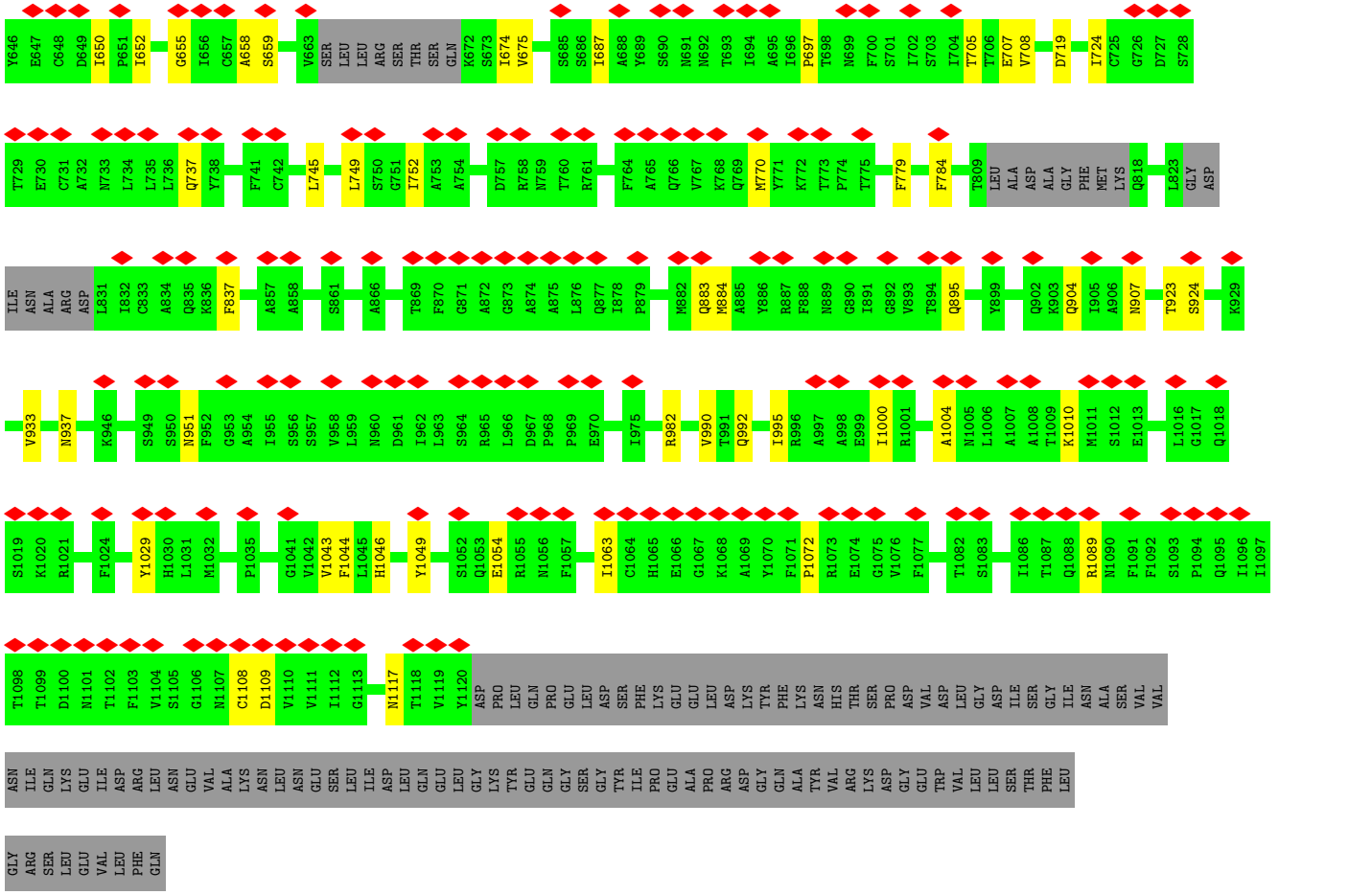
3 Residue-property plots (i)

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,Fibritin

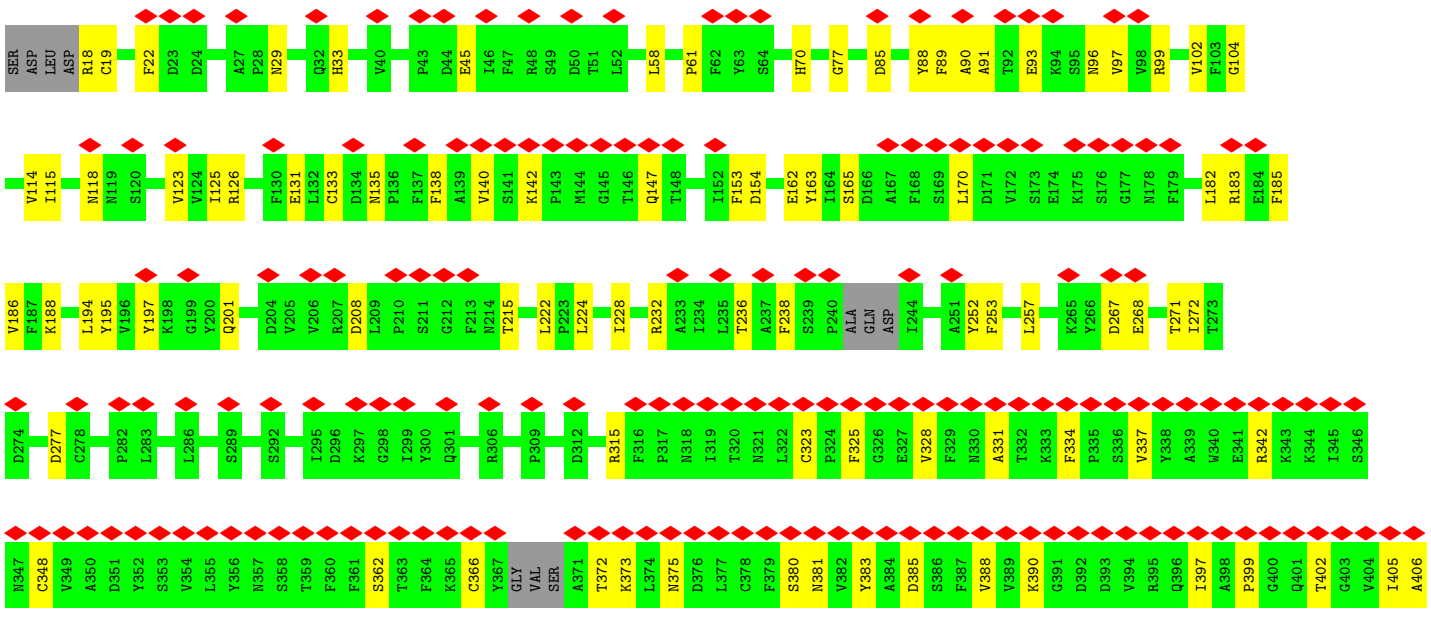
Chain B:

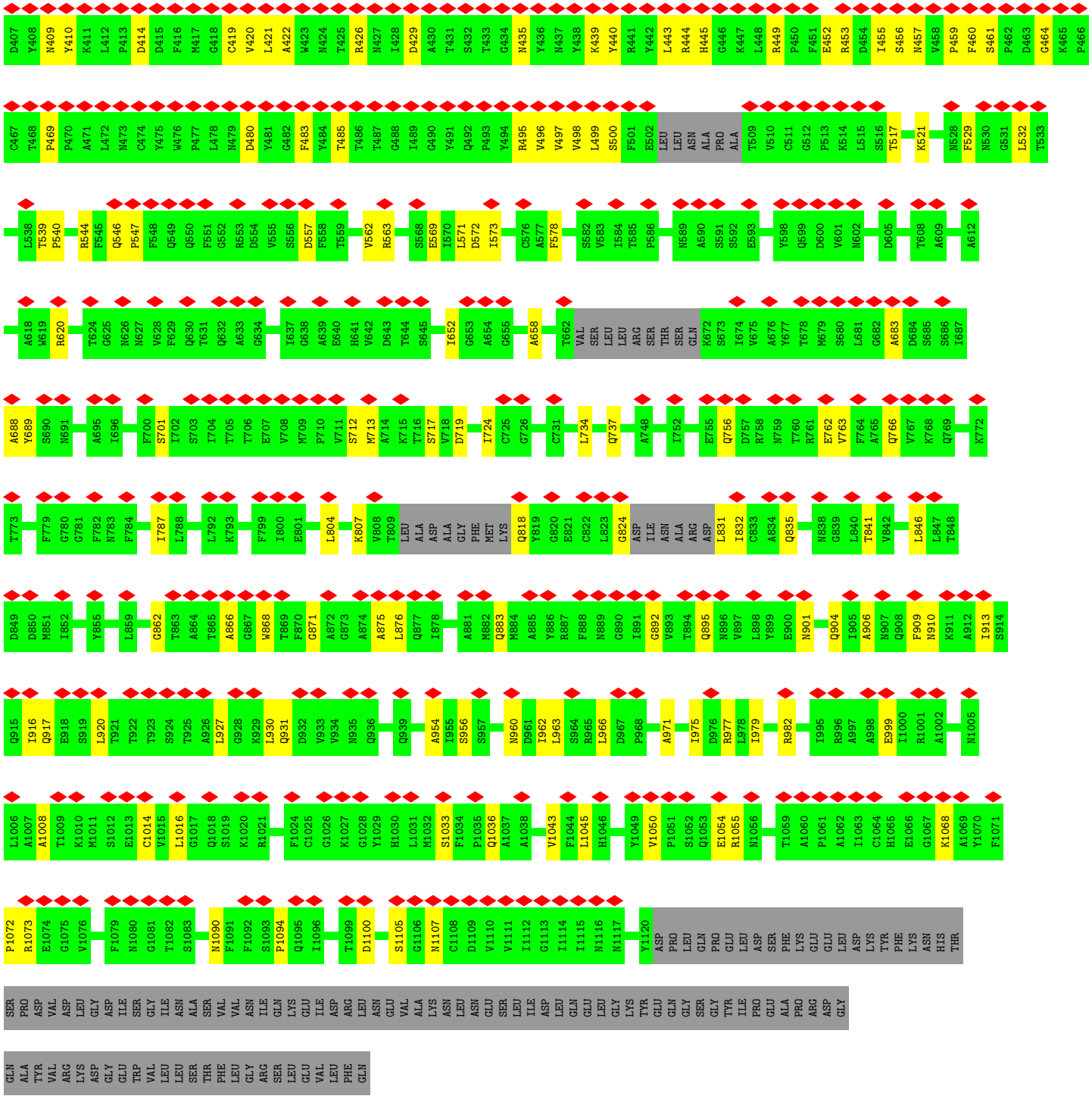




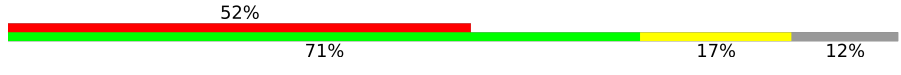
• Molecule 1: Spike glycoprotein,Fibritin

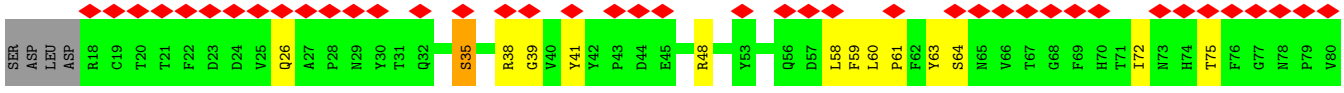
Chain C:

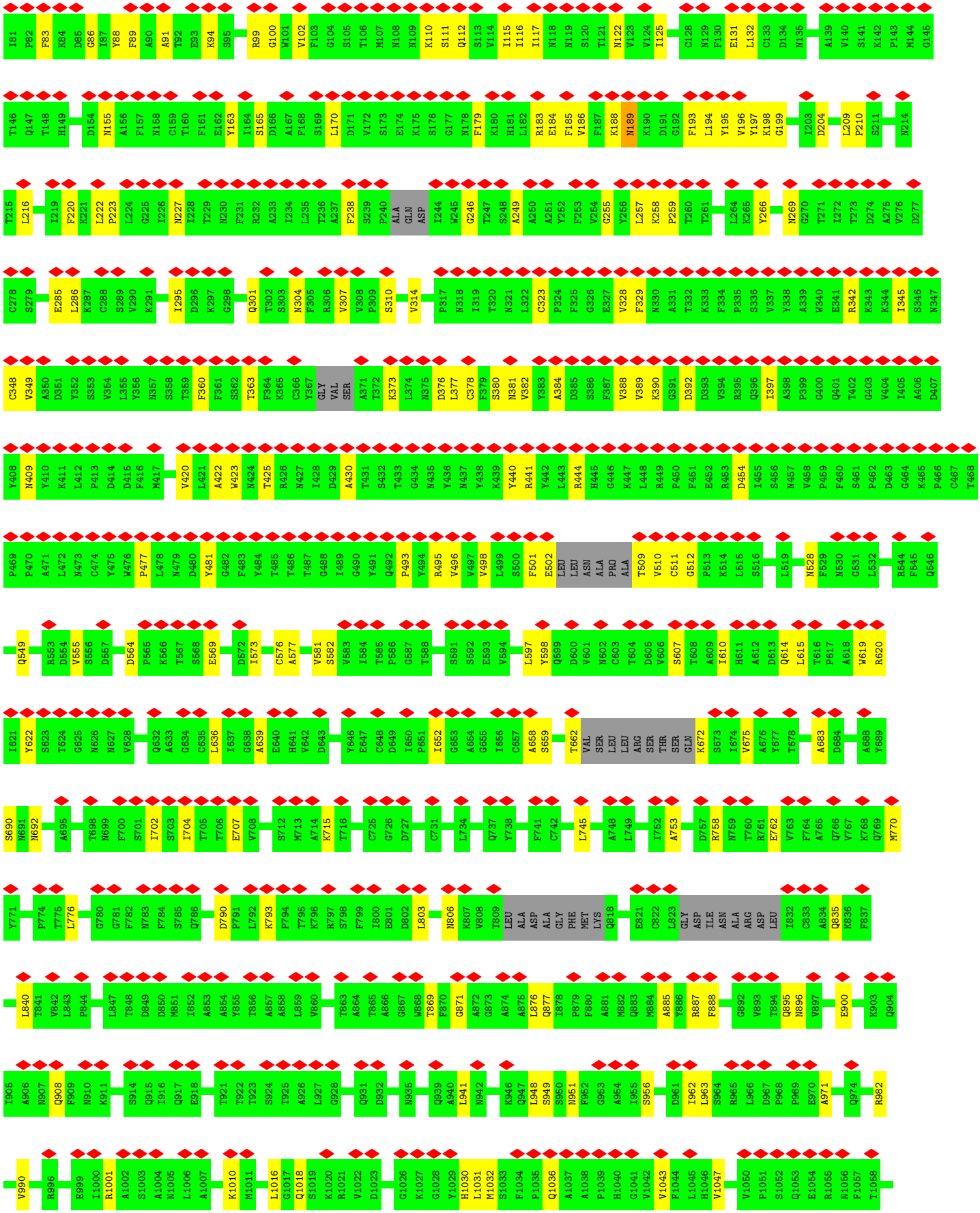


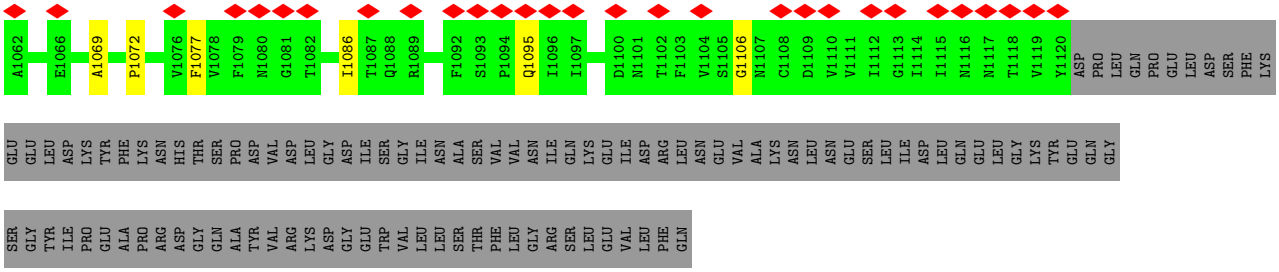


• Molecule 1: Spike glycoprotein,Fibritin



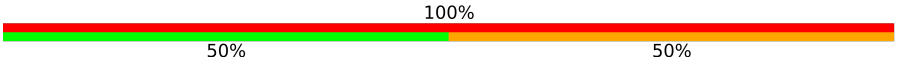



I81 P82 F83 K84 D85 G86 I87 Y88 F89 A90 A91 T92 E93 K94 S95 R99 G100 W101 V102 F103 G104 S105 T106 M107 N108 N109 K110 S111 Q112 S113 V114 I115 I116 I117 N118 N119 S120 T121 N122 V123 V124 I125 C128 N129 F130 E131 L132 C133 D134 N135 A139 V140 S141 K142 P143 M144 G145
T146 Q147 T148 H149 D154 N155 A156 F157 N158 C159 T160 F161 E162 Y163 I164 S165 D166 A167 F168 S169 L170 D171 V172 S173 E174 K175 S176 G177 N178 F179 K180 H181 L182 R183 E184 F185 V186 F187 K188 N189 K190 D191 G192 F193 L194 Y195 V196 Y197 K198 G199 T203 D204 L209 P210 S211 W214
T215 L216 T219 F220 K221 L222 P223 L224 G225 I226 N227 I228 T229 N230 F231 R232 A233 I234 L235 T236 A237 F238 S239 P240 ALA GLN ASP I244 W245 G246 T247 S248 A249 A250 A251 Y252 F253 V254 G255 Y256 L257 K258 P259 T260 T261 L264 K265 Y266 N269 G270 T271 I272 T273 D274 A275 V276 D277
C278 S279 E285 L286 K287 C288 S289 V290 K291 I295 D296 K297 G298 Q301 T302 S303 N304 F305 R306 V307 V308 P309 S310 V314 P317 N318 I319 T320 N321 L322 C323 P324 F325 G326 E327 V328 F329 N330 A331 T332 K333 F334 P335 S336 V337 Y338 A339 W340 E341 R342 K343 K344 I345 S346 N347
C348 V349 A350 D351 Y352 S353 V354 L355 Y356 N357 S358 T359 F360 F361 S362 T363 F364 K365 C366 Y367 GLY VAL SER A371 T372 K373 L374 N375 D376 L377 C378 F379 S380 N381 V382 Y383 A384 D385 S386 F387 V388 V389 K390 G391 D392 D393 V394 R395 Q396 I397 A398 P399 G400 Q401 T402 G403 V404 I405 A406 D407
Y408 N409 Y410 K411 L412 P413 D414 D415 F416 M417 V420 L421 A422 W423 N424 T425 R426 N427 I428 D429 A430 T431 S432 T433 G434 N435 Y436 N437 Y438 K439 Y440 R441 Y442 L443 R444 H445 G446 K447 L448 R449 P450 F451 E452 R453 D454 I455 S456 N457 V458 P459 F460 S461 P462 D463 G464 K465 P466 C467 T468
P469 P470 A471 L472 N473 C474 Y475 W476 P477 L478 N479 D480 Y481 G482 F483 Y484 T485 T486 T487 G488 I489 G490 Y491 Q492 P493 Y494 R495 V496 V497 V498 L499 S500 F501 E502 LEU LEU ASN ALA PRO ALA T509 V510 C511 G512 P513 K514 L515 S516 L519 N528 F529 N530 G531 L532 R544 F545 Q546
Q549 R553 D554 V555 S556 D557 D564 P565 K566 T567 S568 E569 D572 I573 C576 A577 V581 S582 V583 I584 T585 P586 G587 T588 S591 S592 E593 V594 L597 Y598 Q599 D600 V601 N602 C603 T604 D605 V606 S607 T608 A609 I610 H611 A612 D613 Q614 L615 T616 P617 A618 V619 R620
I621 Y622 S623 T624 G625 N626 N627 V628 Q632 A633 G634 C635 L636 I637 G638 A639 E640 H641 V642 D643 Y646 E647 C648 D649 I650 P651 I652 G653 A654 G655 I656 C657 A658 S659 T662 VAL SER LEU LEU ARG SER THR SER GLN K672 S673 I674 V675 A676 Y677 T678 A683 D684 A688 Y689
S690 N691 N692 A695 T698 N699 F700 S701 I702 S703 I704 T705 T706 E707 V708 S712 M713 A714 K715 T716 C725 G726 D727 C731 L734 Q737 Y738 F741 C742 L745 A748 L749 I752 A753 D757 R758 N759 T760 R761 E762 V763 F764 A765 Q766 V767 K768 Q769 M770
Y771 P774 T775 L776 G780 G781 F782 N783 F784 S785 Q786 D790 P791 L792 K793 P794 T795 K796 R797 S798 F799 I800 E801 D802 L803 N806 K807 V808 T809 LEU ALA ASP ALA GLY PHE MET LYS Q818 E821 C822 L823 GLY ASP ILE ASN ALA ARG ASP LEU I832 C833 A834 Q835 K836 F837
L840 T841 V842 L843 P844 L847 T848 D849 D850 M851 I852 A853 A854 Y855 T856 A857 A858 L859 V860 T863 A864 T865 A866 G867 V868 T869 F870 G871 A872 G873 A874 A875 L876 Q877 I878 P879 F880 A881 M882 Q883 M884 A885 Y886 R887 F888 G892 V893 T894 Q895 N896 V897 E900 K903 Q904
I905 A906 N907 Q908 F909 N910 K911 S914 Q915 I916 Q917 E918 T921 T922 T923 S924 T925 A926 L927 G928 Q931 D932 N935 Q939 A940 L941 N942 K946 Q947 L948 S949 S950 N951 F952 G953 A954 I955 S956 D961 I962 L963 S964 R965 L966 D967 P968 P969 E970 A971 Q974 R982
V990 R996 E999 I1000 R1001 A1002 S1003 A1004 N1005 L1006 A1007 K1010 M1011 L1016 G1017 Q1018 S1019 K1020 R1021 V1022 D1023 G1026 K1027 G1028 Y1029 H1030 L1031 M1032 S1033 F1034 P1035 Q1036 A1037 A1038 P1039 H1040 G1041 V1042 V1043 F1044 L1045 H1046 V1047 V1050 P1051 S1052 Q1053 E1054 R1055 N1056 F1057 T1058



• 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

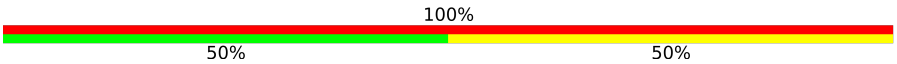
Chain F:

• 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

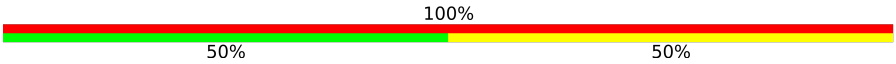
Chain M:

• 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 T:



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

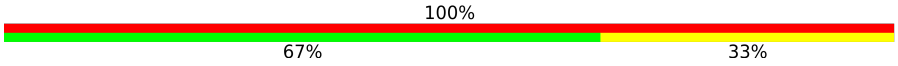
Chain W:

• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:

• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:

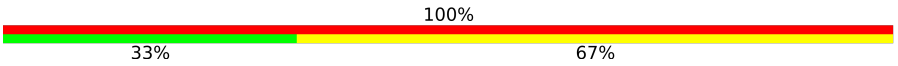


• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:

• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:



• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

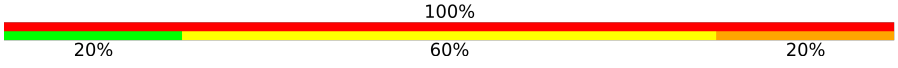
Chain V:

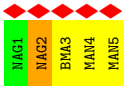
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:

• Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

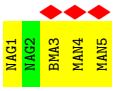
Chain G:





• Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:

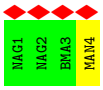


• Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:

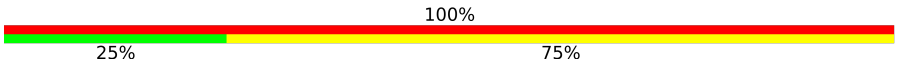
• Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

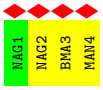
Chain N:



• Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:





• Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	15314	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 ($e^-/Å^2$)	65	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	29000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.131	Depositor
Minimum map value	-0.070	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.032	Depositor
Map size (Å)	329.59998, 329.59998, 329.59998	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.03, 1.03, 1.03	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, BMA, 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	0.32	0/8526	0.54	0/11601
1	B	0.33	0/8541	0.55	0/11622
1	C	0.32	0/8538	0.55	0/11617
All	All	0.32	0/25605	0.54	0/34840

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
1	B	0	1
1	C	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	35	SER	Peptide
1	B	576	CYS	Peptide
1	C	85	ASP	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	8327	0	8068	136	0
1	B	8342	0	8088	123	0
1	C	8339	0	8082	144	0
2	D	28	0	25	1	0
2	F	28	0	25	0	0
2	I	28	0	25	0	0
2	J	28	0	25	1	0
2	K	28	0	25	0	0
2	M	28	0	25	0	0
2	R	28	0	25	0	0
2	T	28	0	25	0	0
2	W	28	0	25	0	0
3	E	39	0	34	0	0
3	L	39	0	34	1	0
3	Q	39	0	34	1	0
3	U	39	0	34	0	0
3	V	39	0	34	0	0
3	X	39	0	34	0	0
4	G	61	0	52	1	0
4	H	61	0	52	0	0
4	S	61	0	52	2	0
5	N	50	0	43	0	0
5	O	50	0	43	1	0
5	P	50	0	43	0	0
6	A	70	0	65	0	0
6	B	56	0	52	0	0
6	C	42	0	39	1	0
All	All	25995	0	25108	369	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (369) 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:1089:ARG:HH21	1:C:876:LEU:HB2	1.57	0.68
1:A:188:LYS:HB2	1:A:195:TYR:HB2	1.76	0.67
1:A:390:LYS:HE3	1:A:392:ASP:HB2	1.75	0.66
1:C:93:GLU:HG3	1:C:183:ARG:HH21	1.59	0.66
1:C:131:GLU:HB2	1:C:154:ASP:HB2	1.77	0.65
1:B:341:GLU:HB3	1:B:386:SER:HB3	1.79	0.64
1:B:363:THR:HB	1:B:365:LYS:HG3	1.79	0.64
1:C:342:ARG:NH2	1:A:223:PRO:O	2.32	0.63
1:C:61:PRO:HB3	1:C:620:ARG:HH12	1.63	0.63
1:B:549:GLN:HA	1:C:45:GLU:HB2	1.81	0.63
1:C:901:ASN:HB3	1:C:904:GLN:HB3	1.81	0.62
1:C:366:CYS:HB2	1:C:373:LYS:HD2	1.81	0.62
1:B:582:SER:HB2	1:B:597:LEU:HB3	1.81	0.62
1:B:33:HIS:HB2	1:B:66:VAL:HB	1.80	0.61
1:C:449:ARG:NH2	1:A:189:ASN:O	2.34	0.61
1:B:390:LYS:HG3	1:B:481:TYR:HD1	1.64	0.61
1:B:1029:TYR:HB2	1:B:1049:TYR:HB3	1.83	0.61
1:A:636:LEU:HD21	1:A:639:ALA:HB3	1.83	0.61
1:A:745:LEU:HD22	1:A:990:VAL:HG21	1.81	0.61
1:C:91:ALA:HB3	1:C:183:ARG:HB2	1.83	0.60
1:C:529:PHE:HB2	1:C:532:LEU:HB2	1.83	0.60
1:C:547:PRO:HA	1:C:563:ARG:HH12	1.65	0.60
1:A:94:LYS:HB3	1:A:179:PHE:HA	1.82	0.60
1:B:555:VAL:HG11	1:C:818:GLN:HE22	1.67	0.60
1:C:421:LEU:HB3	1:C:497:VAL:HB	1.83	0.60
1:C:962:ILE:HG23	1:C:966:LEU:HD12	1.82	0.60
1:C:90:ALA:HB3	1:C:253:PHE:HB2	1.82	0.60
1:B:600:ASP:O	1:C:835:GLN:NE2	2.35	0.60
1:B:188:LYS:HB2	1:B:195:TYR:HB2	1.84	0.59
1:B:237:ALA:HB1	1:B:245:TRP:HB3	1.83	0.59
1:B:322:LEU:HD22	1:B:351:ASP:HB3	1.84	0.59
1:B:419:CYS:HB2	1:B:499:LEU:HB2	1.84	0.59
1:B:659:SER:O	1:B:675:VAL:HG22	2.02	0.59
1:B:707:GLU:OE1	1:B:1046:HIS:NE2	2.35	0.59
1:C:18:ARG:N	1:C:153:PHE:O	2.35	0.59
1:C:277:ASP:OD2	1:C:620:ARG:NH2	2.35	0.59
1:B:337:VAL:HG22	1:B:387:PHE:HB2	1.85	0.59
1:A:659:SER:OG	1:A:675:VAL:CG2	2.51	0.59
1:B:331:ALA:HB3	1:B:334:PHE:HE1	1.68	0.59
1:C:562:VAL:HG13	1:C:573:ILE:HD11	1.84	0.58
1:C:133:CYS:O	1:C:232:ARG:NH2	2.37	0.58
1:A:582:SER:HB2	1:A:597:LEU:HB3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:688:ALA:O	1:A:877:GLN:NE2	2.37	0.57
1:A:378:CYS:HA	1:A:511:CYS:HA	1.87	0.57
1:C:419:CYS:H	1:C:499:LEU:HB2	1.70	0.57
1:C:1105:SER:OG	1:A:896:ASN:ND2	2.37	0.57
1:A:102:VAL:HG22	1:A:115:ILE:HG12	1.85	0.57
1:A:100:GLY:HA3	1:A:117:ILE:HG22	1.86	0.57
1:C:456:SER:HB2	1:A:111:SER:HB3	1.87	0.57
1:A:690:SER:OG	1:A:692:ASN:OD1	2.23	0.57
1:C:96:ASN:O	1:C:99:ARG:NH1	2.37	0.57
1:C:578:PHE:H	1:A:835:GLN:HE22	1.53	0.57
1:A:382:VAL:HG22	1:A:501:PHE:HA	1.87	0.57
1:B:895:GLN:NE2	1:A:1072:PRO:O	2.38	0.57
1:A:704:ILE:HG12	1:A:1047:VAL:HG22	1.86	0.57
1:B:138:PHE:HB2	1:B:236:THR:HA	1.86	0.56
1:B:375:ASN:ND2	1:B:513:PRO:O	2.36	0.56
1:C:445:HIS:HA	1:C:464:GLY:HA2	1.87	0.56
1:A:186:VAL:HB	1:A:197:TYR:HB2	1.86	0.56
1:C:337:VAL:HG11	1:C:405:ILE:HD12	1.86	0.56
1:B:737:GLN:OE1	1:A:951:ASN:ND2	2.39	0.56
1:C:439:LYS:NZ	1:C:480:ASP:OD1	2.37	0.56
1:A:328:VAL:HG11	1:A:345:ILE:HD11	1.87	0.56
1:A:715:LYS:HD2	1:A:753:ALA:HB1	1.87	0.56
1:B:705:THR:HB	1:B:1046:HIS:HB2	1.87	0.56
1:A:38:ARG:NH1	1:A:184:GLU:OE2	2.38	0.56
1:C:114:VAL:HG21	1:C:224:LEU:HD13	1.87	0.56
1:C:429:ASP:OD1	1:C:495:ARG:NH2	2.38	0.56
1:A:314:VAL:HG22	1:A:528:ASN:HB3	1.88	0.56
1:C:892:GLY:O	1:C:1090:ASN:ND2	2.39	0.56
1:A:102:VAL:HG11	1:A:132:LEU:HD11	1.88	0.56
1:A:871:GLY:HA3	1:A:1016:LEU:HB3	1.87	0.55
1:B:745:LEU:HD22	1:B:990:VAL:HG21	1.89	0.55
1:A:91:ALA:HB3	1:A:183:ARG:HB2	1.87	0.55
1:A:348:CYS:HB3	1:A:510:VAL:HG12	1.89	0.55
1:C:268:GLU:HB2	3:L:1:NAG:H82	1.88	0.55
1:B:186:VAL:HB	1:B:197:TYR:HB2	1.89	0.54
1:B:636:LEU:HD21	1:B:639:ALA:HB3	1.88	0.54
1:C:29:ASN:HD22	1:C:70:HIS:HB2	1.72	0.54
1:A:885:ALA:HB1	1:A:895:GLN:HB2	1.90	0.54
1:A:1036:GLN:HB2	1:A:1043:VAL:HB	1.89	0.54
1:C:762:GLU:O	1:C:766:GLN:NE2	2.40	0.54
1:C:1072:PRO:O	1:A:895:GLN:NE2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:ARG:NH2	1:A:502:GLU:OE1	2.41	0.54
1:A:348:CYS:SG	1:A:349:VAL:N	2.81	0.54
1:B:610:ILE:HG23	1:B:622:TYR:HE2	1.72	0.54
1:C:807:LYS:O	1:C:931:GLN:NE2	2.41	0.54
1:C:960:ASN:HA	1:C:963:LEU:HB2	1.90	0.54
1:A:619:TRP:HB2	1:A:622:TYR:HB2	1.90	0.54
1:A:41:TYR:HB3	1:A:216:LEU:HB2	1.90	0.54
1:B:389:VAL:HG11	1:B:397:ILE:HD11	1.90	0.53
1:C:99:ARG:HB3	1:C:118:ASN:HB3	1.90	0.53
1:C:429:ASP:O	1:C:435:ASN:ND2	2.41	0.53
1:C:557:ASP:OD2	1:A:949:SER:OG	2.25	0.53
1:B:265:LYS:HD2	1:B:293:PHE:HE2	1.72	0.53
1:C:186:VAL:HB	1:C:197:TYR:HB2	1.91	0.53
1:C:325:PHE:HB3	1:C:328:VAL:HB	1.90	0.53
1:C:323:CYS:N	1:C:348:CYS:SG	2.81	0.53
1:A:285:GLU:HB2	1:A:619:TRP:HH2	1.73	0.53
1:B:136:PRO:HB3	1:B:152:ILE:HA	1.91	0.53
1:B:334:PHE:HB2	1:B:388:VAL:HG23	1.91	0.53
1:B:687:ILE:HD11	1:C:875:ALA:HB1	1.89	0.53
1:C:188:LYS:HB2	1:C:195:TYR:HB2	1.90	0.53
1:C:422:ALA:HB2	1:C:496:VAL:HG22	1.90	0.53
1:B:1072:PRO:O	1:C:895:GLN:NE2	2.42	0.53
1:C:832:ILE:HB	2:J:1:NAG:H83	1.91	0.53
1:B:26:GLN:HB2	1:B:75:THR:HA	1.91	0.53
1:B:719:ASP:OD1	1:A:304:ASN:ND2	2.41	0.53
1:C:804:LEU:HD13	1:C:1043:VAL:HG21	1.90	0.53
1:A:94:LYS:NZ	1:A:249:ALA:O	2.42	0.52
1:A:1018:GLN:HG3	1:A:1030:HIS:HD2	1.73	0.52
1:B:348:CYS:SG	1:B:349:VAL:N	2.82	0.52
1:C:1055:ARG:HA	6:C:1321:NAG:H82	1.91	0.52
1:A:409:ASN:HD21	1:A:440:TYR:HB2	1.73	0.52
1:C:449:ARG:N	1:C:452:GLU:OE1	2.42	0.52
1:B:413:PRO:HG3	1:B:450:PRO:HB3	1.92	0.52
1:B:724:ILE:O	1:B:982:ARG:NH1	2.40	0.52
1:A:1086:ILE:O	1:A:1095:GLN:N	2.42	0.52
1:B:58:LEU:HB3	1:B:257:LEU:HB3	1.90	0.52
1:B:114:VAL:HG21	1:B:224:LEU:HD13	1.92	0.52
1:B:194:LEU:HB3	1:B:222:LEU:HB2	1.92	0.52
1:B:330:ASN:HB2	1:B:354:VAL:HG21	1.92	0.52
1:A:61:PRO:HG2	1:A:258:LYS:HD2	1.92	0.52
1:C:963:LEU:HD23	1:C:971:ALA:HB1	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:ASN:OD1	1:A:509:THR:N	2.42	0.52
1:A:896:ASN:O	1:A:900:GLU:N	2.41	0.52
1:B:619:TRP:HB2	1:B:622:TYR:HB2	1.90	0.52
1:A:444:ARG:NE	1:A:454:ASP:OD2	2.35	0.52
1:C:1073:ARG:NH1	1:C:1100:ASP:O	2.43	0.51
1:A:840:LEU:HD21	1:A:941:LEU:HD22	1.91	0.51
1:B:331:ALA:HB3	1:B:334:PHE:CE1	2.46	0.51
1:C:138:PHE:HB2	1:C:236:THR:HA	1.92	0.51
1:C:712:SER:HG	1:C:756:GLN:HE21	1.54	0.51
1:C:956:SER:H	1:C:962:ILE:HD11	1.75	0.51
1:C:954:ALA:HB2	1:C:977:ARG:HD3	1.91	0.51
1:A:116:ILE:HG12	1:A:125:ILE:HG23	1.92	0.51
1:B:96:ASN:O	1:B:99:ARG:NH1	2.44	0.51
1:B:129:ASN:HB2	1:B:157:PHE:HB2	1.91	0.51
1:A:131:GLU:HB3	1:A:155:ASN:H	1.76	0.51
1:A:35:SER:OG	1:A:64:SER:N	2.42	0.51
1:B:56:GLN:HB2	1:B:261:THR:HG22	1.93	0.51
1:C:409:ASN:HD21	1:C:440:TYR:HB2	1.75	0.51
1:C:267:ASP:OD1	1:C:271:THR:N	2.42	0.51
1:A:389:VAL:HG11	1:A:397:ILE:HD11	1.93	0.51
1:A:390:LYS:HB2	1:A:481:TYR:HD1	1.75	0.50
1:C:544:ARG:HH12	4:S:2:NAG:H82	1.76	0.50
1:C:315:ARG:NH1	1:C:517:THR:O	2.42	0.50
1:A:193:PHE:HA	1:A:223:PRO:HA	1.92	0.50
1:B:770:MET:N	1:A:683:ALA:O	2.44	0.50
1:C:824:GLY:HA3	1:C:831:LEU:HA	1.93	0.50
1:C:975:ILE:O	1:C:979:ILE:N	2.41	0.50
1:A:662:THR:HA	1:A:672:LYS:HA	1.92	0.50
1:A:702:ILE:HB	1:A:908:GLN:HB3	1.94	0.50
1:B:142:LYS:HD3	1:B:238:PHE:HB3	1.94	0.50
1:B:707:GLU:HB3	1:B:1044:PHE:HB2	1.94	0.50
1:C:521:LYS:NZ	1:C:569:GLU:OE2	2.41	0.50
1:A:35:SER:HB2	1:A:60:LEU:HD21	1.92	0.50
1:C:397:ILE:HG21	1:C:496:VAL:HG11	1.94	0.50
1:B:582:SER:OG	1:B:599:GLN:NE2	2.39	0.50
1:A:26:GLN:HB3	1:A:75:THR:HA	1.94	0.50
1:A:196:VAL:HB	1:A:220:PHE:HB2	1.94	0.49
1:B:380:SER:OG	1:B:381:ASN:N	2.44	0.49
1:B:393:ASP:HB3	1:B:405:ILE:HD11	1.94	0.49
1:B:429:ASP:O	1:B:435:ASN:ND2	2.45	0.49
1:A:184:GLU:O	1:A:199:GLY:N	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:360:PHE:HB3	1:A:423:TRP:HB2	1.94	0.49
1:C:99:ARG:HE	1:C:170:LEU:HD23	1.77	0.49
1:C:724:ILE:O	1:C:982:ARG:NH1	2.40	0.49
1:C:904:GLN:HG3	5:O:2:NAG:H82	1.93	0.49
1:A:388:VAL:HG22	1:A:495:ARG:HG2	1.94	0.49
1:C:97:VAL:HA	1:C:236:THR:HB	1.94	0.49
1:C:734:LEU:HD12	1:C:975:ILE:HD11	1.94	0.49
1:C:906:ALA:O	1:C:910:ASN:ND2	2.42	0.49
1:B:35:SER:HB2	1:B:60:LEU:HD21	1.95	0.49
1:B:185:PHE:HE1	1:B:198:LYS:HG3	1.78	0.49
1:B:268:GLU:HB2	2:D:1:NAG:H82	1.94	0.49
1:C:1094:PRO:HB2	3:Q:1:NAG:H61	1.95	0.49
1:A:607:SER:HA	1:A:610:ILE:HD12	1.94	0.49
1:B:116:ILE:HG12	1:B:125:ILE:HG12	1.95	0.49
1:C:459:PRO:HG2	1:C:469:PRO:HG3	1.94	0.48
1:A:758:ARG:NH1	1:A:762:GLU:OE2	2.46	0.48
1:A:887:ARG:NH1	1:A:1031:LEU:O	2.46	0.48
1:A:329:PHE:HE1	1:A:384:ALA:HB1	1.78	0.48
1:B:182:LEU:HB2	1:B:203:ILE:HD13	1.96	0.48
1:C:701:SER:HB3	1:C:1050:VAL:HB	1.96	0.48
1:A:323:CYS:N	1:A:348:CYS:SG	2.86	0.48
1:A:1086:ILE:HB	1:A:1095:GLN:HB2	1.95	0.48
1:A:380:SER:OG	1:A:381:ASN:N	2.47	0.48
1:C:123:VAL:N	1:C:165:SER:OG	2.46	0.48
1:C:717:SER:HB3	1:C:841:THR:HG23	1.95	0.48
1:A:420:VAL:HA	1:A:498:VAL:HG22	1.94	0.48
1:B:97:VAL:HG22	1:B:238:PHE:HE2	1.78	0.48
1:A:204:ASP:OD1	1:A:204:ASP:N	2.47	0.48
1:A:301:GLN:NE2	1:A:581:VAL:O	2.46	0.48
1:B:904:GLN:HA	1:B:907:ASN:HB2	1.96	0.48
1:A:885:ALA:HA	1:A:888:PHE:HD2	1.78	0.48
1:B:102:VAL:HG11	1:B:132:LEU:HD11	1.95	0.47
1:C:383:TYR:HB2	1:C:500:SER:HB3	1.95	0.47
1:A:39:GLY:HA3	1:A:60:LEU:HB3	1.96	0.47
1:A:88:TYR:HB2	1:A:257:LEU:HD21	1.96	0.47
1:A:373:LYS:HB3	1:A:377:LEU:HB2	1.96	0.47
1:C:331:ALA:HB3	1:C:334:PHE:HE1	1.80	0.47
1:C:546:GLN:NE2	1:A:269:ASN:O	2.47	0.47
1:B:655:GLY:H	1:C:846:LEU:HD12	1.78	0.47
1:C:544:ARG:NH1	4:S:1:NAG:O6	2.46	0.47
1:B:51:THR:HB	1:A:555:VAL:HG12	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:584:ILE:HB	1:B:595:ALA:HB3	1.96	0.47
1:B:779:PHE:HB2	1:B:784:PHE:HE2	1.79	0.47
1:C:455:ILE:HD11	1:A:112:GLN:HE21	1.80	0.47
1:A:194:LEU:N	1:A:222:LEU:O	2.39	0.47
1:C:713:MET:O	1:C:756:GLN:NE2	2.48	0.47
1:C:917:GLN:HA	1:C:920:LEU:HB2	1.96	0.47
1:A:72:ILE:H	1:A:75:THR:HB	1.80	0.47
1:A:209:LEU:HD12	1:A:210:PRO:HD2	1.97	0.47
1:A:963:LEU:HD23	1:A:971:ALA:HB1	1.97	0.47
1:B:89:PHE:HB3	1:B:185:PHE:HB2	1.98	0.47
1:A:238:PHE:N	1:A:246:GLY:O	2.47	0.47
1:A:89:PHE:HB3	1:A:185:PHE:HB2	1.97	0.46
1:A:659:SER:OG	1:A:675:VAL:HG23	2.15	0.46
1:A:125:ILE:O	1:A:163:TYR:N	2.43	0.46
1:A:1032:MET:HG2	1:A:1047:VAL:HB	1.97	0.46
1:C:194:LEU:HD23	1:C:222:LEU:HD12	1.96	0.46
1:A:59:PHE:N	1:A:258:LYS:O	2.47	0.46
1:B:47:PHE:HD1	1:A:549:GLN:HE22	1.64	0.46
1:A:185:PHE:HE1	1:A:198:LYS:HG3	1.80	0.46
1:B:405:ILE:HA	1:B:409:ASN:HB2	1.98	0.46
1:C:372:THR:HA	1:C:375:ASN:HD22	1.80	0.46
1:C:390:LYS:HA	1:C:483:PHE:HE1	1.81	0.46
1:C:19:CYS:N	1:C:154:ASP:OD1	2.48	0.46
1:A:99:ARG:HH12	1:A:170:LEU:HD23	1.80	0.45
1:B:137:PHE:HB2	1:B:237:ALA:HB2	1.98	0.45
1:A:707:GLU:OE2	1:A:1010:LYS:NZ	2.49	0.45
1:B:103:PHE:HB2	1:B:114:VAL:HB	1.98	0.45
1:B:325:PHE:HA	1:B:328:VAL:HB	1.99	0.45
1:B:337:VAL:HG12	1:B:409:ASN:HB3	1.98	0.45
1:B:708:VAL:HG22	1:B:1043:VAL:HG22	1.99	0.45
1:A:83:PHE:O	1:A:86:GLY:N	2.42	0.45
1:A:790:ASP:OD2	1:A:793:LYS:N	2.46	0.45
1:B:337:VAL:HG21	1:B:389:VAL:HG12	1.98	0.45
1:B:583:VAL:HG22	1:B:596:VAL:HG12	1.98	0.45
1:C:182:LEU:HD23	1:C:201:GLN:HE21	1.80	0.45
1:B:586:PRO:HG2	1:B:591:SER:HB3	1.99	0.45
1:C:142:LYS:HG2	1:C:238:PHE:HB3	1.99	0.45
1:C:410:TYR:HE1	1:C:453:ARG:HD2	1.82	0.45
1:A:803:LEU:HA	1:A:806:ASN:HD22	1.82	0.45
1:B:318:ASN:HB2	1:B:566:LYS:HA	1.99	0.45
1:C:402:THR:HA	1:C:406:ALA:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:ASN:ND2	1:A:165:SER:O	2.49	0.45
1:B:652:ILE:HD11	1:B:658:ALA:HB2	1.98	0.45
1:B:1108:CYS:SG	1:B:1109:ASP:N	2.90	0.45
1:A:363:THR:OG1	1:A:420:VAL:O	2.34	0.45
1:B:440:TYR:HB3	1:B:481:TYR:CZ	2.51	0.45
1:B:267:ASP:OD1	1:B:271:THR:N	2.44	0.45
1:C:89:PHE:HB3	1:C:185:PHE:HB2	1.98	0.45
1:C:1014:CYS:O	1:C:1033:SER:OG	2.31	0.45
1:B:328:VAL:HG22	1:B:343:LYS:HD3	2.00	0.44
1:B:697:PRO:HA	1:B:1054:GLU:HA	1.98	0.44
1:A:307:VAL:HB	1:A:577:ALA:HB3	1.99	0.44
1:A:869:THR:HG21	1:A:876:LEU:HD12	2.00	0.44
1:A:441:ARG:HG3	1:A:477:PRO:HB2	1.98	0.44
1:C:405:ILE:HD13	1:C:409:ASN:HD22	1.82	0.44
1:C:444:ARG:HH21	1:A:227:ASN:HD21	1.64	0.44
1:C:22:PHE:H	1:C:135:ASN:HB2	1.81	0.44
1:C:956:SER:HB3	1:C:962:ILE:HG13	1.99	0.44
1:B:209:LEU:HD12	1:B:210:PRO:HD2	2.00	0.44
1:C:104:GLY:H	1:C:228:ILE:HG23	1.83	0.44
1:B:358:SER:HB3	1:B:361:PHE:HE2	1.83	0.44
1:A:286:LEU:HG	1:A:295:ILE:HD13	2.00	0.44
1:B:441:ARG:NH2	1:B:443:LEU:O	2.51	0.43
1:B:529:PHE:N	1:B:532:LEU:O	2.45	0.43
1:B:1072:PRO:HG2	1:C:895:GLN:HE21	1.82	0.43
1:C:385:ASP:HB2	1:C:498:VAL:HB	1.99	0.43
1:C:420:VAL:HG13	1:C:496:VAL:HG13	1.99	0.43
1:C:868:TRP:HZ3	1:C:883:GLN:HA	1.83	0.43
1:C:916:ILE:HD13	1:C:1045:LEU:HD22	2.00	0.43
1:A:63:TYR:O	1:A:620:ARG:NH2	2.51	0.43
1:C:61:PRO:HB3	1:C:620:ARG:NH1	2.29	0.43
1:C:652:ILE:HD11	1:C:658:ALA:HB2	1.99	0.43
1:C:1054:GLU:HG2	1:A:876:LEU:HD22	2.00	0.43
1:B:277:ASP:HB3	1:B:280:GLN:HG2	1.99	0.43
1:C:77:GLY:O	1:C:252:TYR:OH	2.28	0.43
1:B:38:ARG:NH1	1:B:184:GLU:OE2	2.50	0.43
1:C:362:SER:N	1:C:422:ALA:O	2.49	0.43
1:C:539:THR:HG23	1:C:572:ASP:HB2	2.01	0.43
1:A:125:ILE:HB	1:A:163:TYR:HB3	2.01	0.43
1:C:871:GLY:HA3	1:C:1016:LEU:HB3	2.00	0.43
1:A:307:VAL:HG22	1:A:615:LEU:HD23	2.01	0.43
1:B:388:VAL:HG22	1:B:495:ARG:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:707:GLU:OE2	1:B:1010:LYS:NZ	2.38	0.43
1:B:992:GLN:HA	1:B:995:ILE:HD12	2.00	0.43
1:C:33:HIS:ND1	1:C:208:ASP:OD1	2.51	0.43
1:C:88:TYR:HB2	1:C:257:LEU:HD21	2.01	0.43
1:C:909:PHE:O	1:C:913:ILE:N	2.51	0.43
1:C:763:VAL:HG22	1:C:1008:ALA:HB2	2.01	0.43
1:A:89:PHE:HE2	1:A:91:ALA:HB2	1.83	0.43
1:A:652:ILE:HD11	1:A:658:ALA:HB2	2.01	0.43
1:B:586:PRO:HD3	1:B:674:ILE:HD11	2.00	0.43
1:C:126:ARG:HA	1:C:162:GLU:HG2	2.00	0.43
1:B:323:CYS:N	1:B:348:CYS:SG	2.92	0.43
1:C:443:LEU:HG	1:C:460:PHE:HB2	2.01	0.43
1:A:58:LEU:HD23	1:A:259:PRO:HB3	2.00	0.43
1:C:125:ILE:HD12	1:C:163:TYR:HB3	2.01	0.42
1:C:140:VAL:HG22	1:C:147:GLN:HA	2.01	0.42
1:A:310:SER:HB2	1:A:614:GLN:HE22	1.84	0.42
1:B:304:ASN:ND2	1:C:719:ASP:OD1	2.52	0.42
1:B:317:PRO:HD3	1:B:530:ASN:HB2	2.01	0.42
1:B:837:PHE:HZ	1:A:573:ILE:HG22	1.85	0.42
1:B:883:GLN:NE2	1:B:884:MET:SD	2.92	0.42
1:C:1036:GLN:HB2	1:C:1043:VAL:HB	2.02	0.42
1:A:88:TYR:N	1:A:255:GLY:O	2.40	0.42
1:B:650:ILE:HB	1:B:658:ALA:HB3	2.00	0.42
1:C:862:GLY:O	1:C:866:ALA:N	2.49	0.42
1:A:94:LYS:HZ2	1:A:179:PHE:HE1	1.68	0.42
1:B:102:VAL:HG22	1:B:115:ILE:HG12	2.01	0.42
1:B:933:VAL:O	1:B:937:ASN:ND2	2.52	0.42
1:C:102:VAL:HG23	1:C:115:ILE:HG12	2.01	0.42
1:C:578:PHE:N	1:A:835:GLN:HE22	2.17	0.42
1:B:60:LEU:HB2	1:B:88:TYR:CE2	2.55	0.42
1:B:398:ALA:HB3	1:B:401:GLN:HG3	2.00	0.42
1:C:787:ILE:HG23	1:C:1036:GLN:HE22	1.83	0.42
1:C:1068:LYS:HG2	1:C:1107:ASN:HA	2.02	0.42
1:A:48:ARG:HB2	1:A:266:TYR:HD2	1.83	0.42
1:A:425:THR:HG21	1:A:495:ARG:HD2	2.01	0.42
1:B:399:PRO:HG3	1:B:417:MET:HG2	2.02	0.42
1:C:540:PRO:HA	1:C:571:LEU:HA	2.01	0.42
1:B:100:GLY:HA3	1:B:117:ILE:HG22	2.00	0.42
1:A:511:CYS:SG	1:A:512:GLY:N	2.90	0.42
1:B:355:LEU:HB3	1:B:371:ALA:HB1	2.02	0.41
1:A:430:ALA:HB2	1:A:493:PRO:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:999:GLU:OE2	1:A:1001:ARG:NH1	2.52	0.41
1:A:948:LEU:O	1:A:982:ARG:NH2	2.47	0.41
1:A:598:TYR:HH	1:A:622:TYR:HH	1.68	0.41
1:C:58:LEU:HD12	1:C:188:LYS:HE3	2.02	0.41
1:C:380:SER:OG	1:C:381:ASN:N	2.52	0.41
1:C:927:LEU:HD22	1:C:930:LEU:HD12	2.02	0.41
1:B:54:LEU:HD13	1:B:263:MET:HB2	2.01	0.41
1:B:904:GLN:HB2	4:G:2:NAG:H81	2.02	0.41
1:B:951:ASN:HD21	1:C:737:GLN:HB2	1.85	0.41
1:C:426:ARG:NH2	1:C:485:THR:O	2.47	0.41
1:A:390:LYS:HB2	1:A:481:TYR:CD1	2.55	0.41
1:B:35:SER:OG	1:B:64:SER:N	2.52	0.41
1:C:215:THR:HG23	1:C:272:ILE:HD12	2.03	0.41
1:B:1063:ILE:HG21	1:B:1117:ASN:HD22	1.86	0.41
1:C:334:PHE:HB2	1:C:388:VAL:HG23	2.02	0.41
1:A:1072:PRO:HD3	1:A:1077:PHE:CE2	2.56	0.41
1:C:445:HIS:CD2	1:C:461:SER:H	2.39	0.41
1:A:1069:ALA:N	1:A:1106:GLY:O	2.44	0.41
1:B:29:ASN:ND2	1:B:70:HIS:O	2.54	0.41
1:B:556:SER:OG	1:B:557:ASP:N	2.54	0.41
1:B:923:THR:OG1	1:B:924:SER:N	2.53	0.41
1:C:99:ARG:HB2	1:C:138:PHE:HE2	1.85	0.41
1:C:683:ALA:O	1:A:770:MET:N	2.54	0.41
1:A:373:LYS:HD3	1:A:376:ASP:HB2	2.03	0.41
1:A:441:ARG:HD3	1:A:444:ARG:HB2	2.03	0.41
1:A:564:ASP:HB3	1:A:569:GLU:H	1.86	0.41
1:B:125:ILE:HB	1:B:163:TYR:HB3	2.02	0.40
1:B:1000:ILE:O	1:B:1004:ALA:N	2.54	0.40
1:C:689:TYR:HB3	1:A:776:LEU:HD22	2.03	0.40
1:B:115:ILE:HD11	1:B:132:LEU:HD21	2.03	0.40
1:C:457:ASN:H	1:A:110:LYS:HB3	1.86	0.40
1:C:546:GLN:HA	1:C:547:PRO:HD3	1.93	0.40
1:A:422:ALA:HA	1:A:496:VAL:HG22	2.03	0.40
1:B:205:VAL:HG11	1:B:210:PRO:HG3	2.03	0.40
1:B:335:PRO:HG2	1:B:341:GLU:HB2	2.03	0.40
1:B:642:VAL:HG12	1:B:644:THR:HG23	2.03	0.40
1:B:749:LEU:HD23	1:B:752:ILE:HD12	2.04	0.40
1:A:956:SER:HB3	1:A:962:ILE:HG23	2.03	0.40
1:C:399:PRO:HB2	1:C:414:ASP:HA	2.03	0.40
1:A:220:PHE:HB3	1:A:222:LEU:HG	2.03	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	1052/1215 (87%)	979 (93%)	73 (7%)	0	100	100
1	B	1054/1215 (87%)	977 (93%)	77 (7%)	0	100	100
1	C	1054/1215 (87%)	977 (93%)	77 (7%)	0	100	100
All	All	3160/3645 (87%)	2933 (93%)	227 (7%)	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	925/1053 (88%)	923 (100%)	2 (0%)	93	96
1	B	927/1053 (88%)	925 (100%)	2 (0%)	93	96
1	C	926/1053 (88%)	926 (100%)	0	100	100
All	All	2778/3159 (88%)	2774 (100%)	4 (0%)	93	96

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	426	ARG
1	B	576	CYS
1	A	189	ASN
1	A	576	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	29	ASN
1	B	301	GLN
1	B	599	GLN
1	B	746	ASN
1	B	766	GLN
1	B	806	ASN
1	B	907	ASN
1	B	984	GLN
1	B	1036	GLN
1	C	29	ASN
1	C	158	ASN
1	C	201	GLN
1	C	357	ASN
1	C	375	ASN
1	C	599	GLN
1	C	721	ASN
1	C	759	ASN
1	C	766	GLN
1	C	818	GLN
1	C	917	GLN
1	C	931	GLN
1	C	935	ASN
1	C	937	ASN
1	C	984	GLN
1	C	993	GLN
1	C	1036	GLN
1	A	122	ASN
1	A	189	ASN
1	A	301	GLN
1	A	733	ASN
1	A	759	ASN
1	A	806	ASN
1	A	835	GLN
1	A	877	GLN
1	A	889	ASN
1	A	896	ASN
1	A	907	ASN
1	A	910	ASN
1	A	937	ASN
1	A	951	ASN
1	A	984	GLN

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Mol	Chain	Res	Type
1	A	1030	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

63 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	1,2	14,14,15	0.32	0	17,19,21	0.78	1 (5%)
2	NAG	D	2	2	14,14,15	0.25	0	17,19,21	0.56	0
3	NAG	E	1	1,3	14,14,15	0.52	0	17,19,21	0.62	0
3	NAG	E	2	3	14,14,15	0.20	0	17,19,21	0.58	0
3	BMA	E	3	3	11,11,12	0.71	0	15,15,17	0.88	1 (6%)
2	NAG	F	1	1,2	14,14,15	0.28	0	17,19,21	0.38	0
2	NAG	F	2	2	14,14,15	0.41	0	17,19,21	0.42	0
4	NAG	G	1	1,4	14,14,15	0.45	0	17,19,21	0.57	0
4	NAG	G	2	4	14,14,15	0.31	0	17,19,21	0.78	1 (5%)
4	BMA	G	3	4	11,11,12	1.56	2 (18%)	15,15,17	1.65	2 (13%)
4	MAN	G	4	4	11,11,12	0.79	1 (9%)	15,15,17	1.15	2 (13%)
4	MAN	G	5	4	11,11,12	0.75	0	15,15,17	1.24	2 (13%)
4	NAG	H	1	1,4	14,14,15	0.20	0	17,19,21	0.75	1 (5%)
4	NAG	H	2	4	14,14,15	0.43	0	17,19,21	0.71	0
4	BMA	H	3	4	11,11,12	0.73	0	15,15,17	1.05	1 (6%)
4	MAN	H	4	4	11,11,12	0.88	0	15,15,17	1.28	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	MAN	H	5	4	11,11,12	0.76	0	15,15,17	1.26	2 (13%)
2	NAG	I	1	1,2	14,14,15	0.33	0	17,19,21	0.36	0
2	NAG	I	2	2	14,14,15	0.37	0	17,19,21	0.55	0
2	NAG	J	1	1,2	14,14,15	0.23	0	17,19,21	0.62	0
2	NAG	J	2	2	14,14,15	0.28	0	17,19,21	0.42	0
2	NAG	K	1	1,2	14,14,15	0.23	0	17,19,21	0.54	0
2	NAG	K	2	2	14,14,15	0.21	0	17,19,21	0.56	0
3	NAG	L	1	1,3	14,14,15	0.32	0	17,19,21	0.55	0
3	NAG	L	2	3	14,14,15	0.24	0	17,19,21	0.62	0
3	BMA	L	3	3	11,11,12	0.86	0	15,15,17	0.78	0
2	NAG	M	1	1,2	14,14,15	0.32	0	17,19,21	0.67	0
2	NAG	M	2	2	14,14,15	0.50	0	17,19,21	0.36	0
5	NAG	N	1	1,5	14,14,15	0.26	0	17,19,21	0.67	0
5	NAG	N	2	5	14,14,15	0.39	0	17,19,21	0.58	0
5	BMA	N	3	5	11,11,12	0.87	0	15,15,17	0.80	0
5	MAN	N	4	5	11,11,12	0.93	1 (9%)	15,15,17	1.35	2 (13%)
5	NAG	O	1	1,5	14,14,15	0.49	0	17,19,21	0.56	0
5	NAG	O	2	5	14,14,15	0.23	0	17,19,21	0.64	0
5	BMA	O	3	5	11,11,12	0.76	0	15,15,17	1.28	1 (6%)
5	MAN	O	4	5	11,11,12	0.96	0	15,15,17	0.99	2 (13%)
5	NAG	P	1	1,5	14,14,15	0.41	0	17,19,21	0.59	0
5	NAG	P	2	5	14,14,15	0.22	0	17,19,21	0.53	0
5	BMA	P	3	5	11,11,12	0.71	0	15,15,17	1.05	1 (6%)
5	MAN	P	4	5	11,11,12	1.38	2 (18%)	15,15,17	1.94	4 (26%)
3	NAG	Q	1	1,3	14,14,15	0.31	0	17,19,21	0.37	0
3	NAG	Q	2	3	14,14,15	0.19	0	17,19,21	0.56	0
3	BMA	Q	3	3	11,11,12	0.81	0	15,15,17	1.00	1 (6%)
2	NAG	R	1	1,2	14,14,15	0.48	0	17,19,21	0.61	0
2	NAG	R	2	2	14,14,15	0.25	0	17,19,21	0.53	0
4	NAG	S	1	1,4	14,14,15	0.37	0	17,19,21	0.61	0
4	NAG	S	2	4	14,14,15	0.50	0	17,19,21	0.70	0
4	BMA	S	3	4	11,11,12	1.16	2 (18%)	15,15,17	1.07	0
4	MAN	S	4	4	11,11,12	0.83	1 (9%)	15,15,17	1.21	2 (13%)
4	MAN	S	5	4	11,11,12	0.88	1 (9%)	15,15,17	1.30	2 (13%)
2	NAG	T	1	1,2	14,14,15	0.69	1 (7%)	17,19,21	0.82	0
2	NAG	T	2	2	14,14,15	0.46	0	17,19,21	0.42	0
3	NAG	U	1	1,3	14,14,15	0.64	1 (7%)	17,19,21	0.71	0
3	NAG	U	2	3	14,14,15	0.29	0	17,19,21	0.44	0
3	BMA	U	3	3	11,11,12	0.81	0	15,15,17	1.04	1 (6%)
3	NAG	V	1	1,3	14,14,15	0.41	0	17,19,21	1.08	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	V	2	3	14,14,15	0.31	0	17,19,21	0.86	0
3	BMA	V	3	3	11,11,12	0.92	0	15,15,17	0.84	0
2	NAG	W	1	1,2	14,14,15	0.39	0	17,19,21	0.56	0
2	NAG	W	2	2	14,14,15	0.36	0	17,19,21	0.45	0
3	NAG	X	1	1,3	14,14,15	0.31	0	17,19,21	0.40	0
3	NAG	X	2	3	14,14,15	0.29	0	17,19,21	0.41	0
3	BMA	X	3	3	11,11,12	0.73	0	15,15,17	0.94	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	D	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
3	NAG	E	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	BMA	E	3	3	-	2/2/19/22	0/1/1/1
2	NAG	F	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1
4	NAG	G	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	1/6/23/26	0/1/1/1
4	BMA	G	3	4	-	0/2/19/22	0/1/1/1
4	MAN	G	4	4	-	2/2/19/22	0/1/1/1
4	MAN	G	5	4	-	2/2/19/22	0/1/1/1
4	NAG	H	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	H	2	4	-	2/6/23/26	0/1/1/1
4	BMA	H	3	4	-	2/2/19/22	0/1/1/1
4	MAN	H	4	4	-	0/2/19/22	0/1/1/1
4	MAN	H	5	4	-	0/2/19/22	0/1/1/1
2	NAG	I	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	I	2	2	-	2/6/23/26	0/1/1/1
2	NAG	J	1	1,2	-	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	1,2	-	0/6/23/26	0/1/1/1
2	NAG	K	2	2	-	2/6/23/26	0/1/1/1
3	NAG	L	1	1,3	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	L	2	3	-	2/6/23/26	0/1/1/1
3	BMA	L	3	3	-	0/2/19/22	0/1/1/1
2	NAG	M	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	M	2	2	-	2/6/23/26	0/1/1/1
5	NAG	N	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	N	2	5	-	2/6/23/26	0/1/1/1
5	BMA	N	3	5	-	0/2/19/22	0/1/1/1
5	MAN	N	4	5	-	0/2/19/22	0/1/1/1
5	NAG	O	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	O	2	5	-	0/6/23/26	0/1/1/1
5	BMA	O	3	5	-	0/2/19/22	0/1/1/1
5	MAN	O	4	5	-	0/2/19/22	0/1/1/1
5	NAG	P	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	P	2	5	-	2/6/23/26	0/1/1/1
5	BMA	P	3	5	-	2/2/19/22	0/1/1/1
5	MAN	P	4	5	-	2/2/19/22	0/1/1/1
3	NAG	Q	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	2/6/23/26	0/1/1/1
3	BMA	Q	3	3	-	1/2/19/22	0/1/1/1
2	NAG	R	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	R	2	2	-	0/6/23/26	0/1/1/1
4	NAG	S	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	S	2	4	-	2/6/23/26	0/1/1/1
4	BMA	S	3	4	-	2/2/19/22	0/1/1/1
4	MAN	S	4	4	-	0/2/19/22	0/1/1/1
4	MAN	S	5	4	-	0/2/19/22	0/1/1/1
2	NAG	T	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	T	2	2	-	1/6/23/26	0/1/1/1
3	NAG	U	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	U	2	3	-	2/6/23/26	0/1/1/1
3	BMA	U	3	3	-	1/2/19/22	0/1/1/1
3	NAG	V	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	V	2	3	-	0/6/23/26	0/1/1/1
3	BMA	V	3	3	-	1/2/19/22	0/1/1/1
2	NAG	W	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	W	2	2	-	2/6/23/26	0/1/1/1
3	NAG	X	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	X	2	3	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BMA	X	3	3	-	2/2/19/22	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	3	BMA	C2-C3	3.62	1.57	1.52
5	P	4	MAN	O5-C1	3.10	1.48	1.43
5	P	4	MAN	C1-C2	2.96	1.59	1.52
4	G	3	BMA	C4-C3	2.59	1.58	1.52
5	N	4	MAN	C1-C2	2.44	1.57	1.52
4	S	3	BMA	C4-C3	2.34	1.58	1.52
4	S	3	BMA	C2-C3	2.33	1.55	1.52
4	S	5	MAN	C1-C2	2.30	1.57	1.52
2	T	1	NAG	O5-C1	-2.26	1.40	1.43
3	U	1	NAG	O5-C1	-2.21	1.40	1.43
4	S	4	MAN	C1-C2	2.11	1.57	1.52
4	G	4	MAN	C1-C2	2.00	1.56	1.52

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	P	4	MAN	C1-O5-C5	5.86	120.14	112.19
4	G	3	BMA	C2-C3-C4	3.98	117.78	110.89
4	H	5	MAN	C1-O5-C5	3.81	117.36	112.19
5	N	4	MAN	C1-O5-C5	3.79	117.33	112.19
4	G	3	BMA	C1-C2-C3	3.77	114.30	109.67
4	H	4	MAN	C1-O5-C5	3.77	117.30	112.19
4	G	5	MAN	C1-O5-C5	3.63	117.11	112.19
4	S	5	MAN	C1-O5-C5	3.53	116.98	112.19
3	V	1	NAG	C1-O5-C5	3.53	116.97	112.19
5	O	3	BMA	C1-O5-C5	3.25	116.60	112.19
4	G	4	MAN	C1-O5-C5	3.06	116.33	112.19
4	S	4	MAN	C1-O5-C5	3.01	116.27	112.19
3	U	3	BMA	C1-O5-C5	2.77	115.94	112.19
4	G	2	NAG	C1-O5-C5	2.63	115.76	112.19
2	D	1	NAG	C1-O5-C5	2.56	115.66	112.19
5	P	4	MAN	C1-C2-C3	2.54	112.79	109.67
4	H	1	NAG	C1-O5-C5	2.54	115.63	112.19
3	X	3	BMA	C1-O5-C5	2.48	115.55	112.19
5	P	4	MAN	O2-C2-C3	-2.43	105.27	110.14
5	P	3	BMA	C1-O5-C5	2.43	115.48	112.19
4	G	4	MAN	O2-C2-C3	-2.38	105.36	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	5	MAN	O2-C2-C3	-2.36	105.41	110.14
5	N	4	MAN	O2-C2-C3	-2.36	105.42	110.14
5	O	4	MAN	C1-O5-C5	2.35	115.37	112.19
3	E	3	BMA	C1-O5-C5	2.27	115.27	112.19
4	S	4	MAN	O2-C2-C3	-2.24	105.66	110.14
4	S	5	MAN	O2-C2-C3	-2.23	105.67	110.14
4	H	5	MAN	O2-C2-C3	-2.21	105.70	110.14
4	H	3	BMA	C1-C2-C3	-2.21	106.95	109.67
5	O	4	MAN	O2-C2-C3	-2.13	105.87	110.14
5	P	4	MAN	O5-C1-C2	2.13	114.06	110.77
3	Q	3	BMA	C1-O5-C5	2.11	115.05	112.19
4	H	4	MAN	O2-C2-C3	-2.00	106.13	110.14

There are no chirality outliers.

All (82) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	4	MAN	O5-C5-C6-O6
2	W	1	NAG	O5-C5-C6-O6
2	W	2	NAG	O5-C5-C6-O6
2	M	1	NAG	O5-C5-C6-O6
2	J	2	NAG	O5-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
4	G	5	MAN	O5-C5-C6-O6
4	H	2	NAG	O5-C5-C6-O6
5	P	2	NAG	O5-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
3	L	1	NAG	O5-C5-C6-O6
3	L	2	NAG	O5-C5-C6-O6
4	S	3	BMA	O5-C5-C6-O6
5	P	4	MAN	O5-C5-C6-O6
2	J	2	NAG	C4-C5-C6-O6
4	H	2	NAG	C4-C5-C6-O6
3	E	3	BMA	O5-C5-C6-O6
5	P	1	NAG	O5-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
5	P	2	NAG	C4-C5-C6-O6
4	S	1	NAG	O5-C5-C6-O6
2	M	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	W	2	NAG	C4-C5-C6-O6
3	Q	2	NAG	O5-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	W	1	NAG	C4-C5-C6-O6
3	X	2	NAG	C4-C5-C6-O6
2	M	2	NAG	O5-C5-C6-O6
4	G	4	MAN	C4-C5-C6-O6
4	H	1	NAG	C4-C5-C6-O6
2	F	1	NAG	C4-C5-C6-O6
3	Q	1	NAG	C4-C5-C6-O6
4	G	5	MAN	C4-C5-C6-O6
5	P	3	BMA	O5-C5-C6-O6
2	M	2	NAG	C4-C5-C6-O6
3	E	3	BMA	C4-C5-C6-O6
4	S	3	BMA	C4-C5-C6-O6
5	P	1	NAG	C4-C5-C6-O6
2	K	2	NAG	O5-C5-C6-O6
2	I	1	NAG	C4-C5-C6-O6
3	X	2	NAG	O5-C5-C6-O6
5	N	2	NAG	C4-C5-C6-O6
3	U	2	NAG	O5-C5-C6-O6
3	L	2	NAG	C4-C5-C6-O6
3	Q	2	NAG	C4-C5-C6-O6
5	P	4	MAN	C4-C5-C6-O6
4	G	1	NAG	O5-C5-C6-O6
2	F	1	NAG	O5-C5-C6-O6
3	Q	1	NAG	O5-C5-C6-O6
4	H	1	NAG	O5-C5-C6-O6
3	X	3	BMA	O5-C5-C6-O6
4	S	2	NAG	O5-C5-C6-O6
3	L	1	NAG	C4-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
2	I	2	NAG	C4-C5-C6-O6
2	K	2	NAG	C4-C5-C6-O6
5	P	3	BMA	C4-C5-C6-O6
2	I	1	NAG	O5-C5-C6-O6
3	X	3	BMA	C4-C5-C6-O6
5	N	2	NAG	O5-C5-C6-O6
4	S	1	NAG	C4-C5-C6-O6
2	I	2	NAG	O5-C5-C6-O6
2	T	2	NAG	O5-C5-C6-O6
2	R	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	U	2	NAG	C4-C5-C6-O6
4	H	3	BMA	C4-C5-C6-O6
3	V	3	BMA	O5-C5-C6-O6
2	F	2	NAG	C4-C5-C6-O6
2	R	1	NAG	O5-C5-C6-O6
4	G	1	NAG	C4-C5-C6-O6
2	T	1	NAG	O5-C5-C6-O6
4	S	2	NAG	C4-C5-C6-O6
3	U	3	BMA	C4-C5-C6-O6
4	G	2	NAG	C4-C5-C6-O6
3	Q	3	BMA	C4-C5-C6-O6
5	N	1	NAG	C4-C5-C6-O6
4	H	3	BMA	O5-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6
3	X	1	NAG	O5-C5-C6-O6

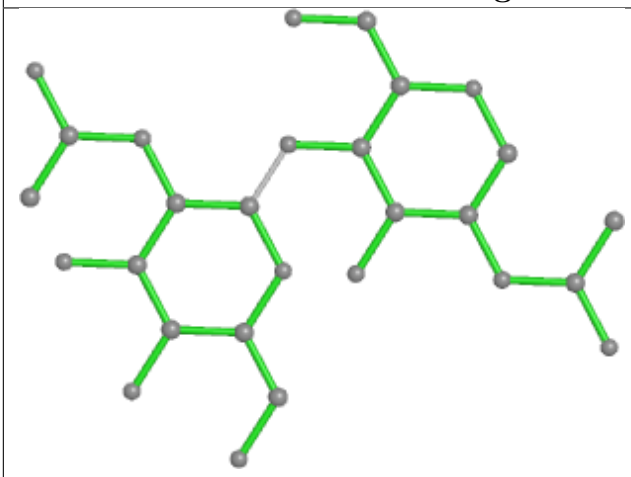
There are no ring outliers.

8 monomers are involved in 8 short contacts:

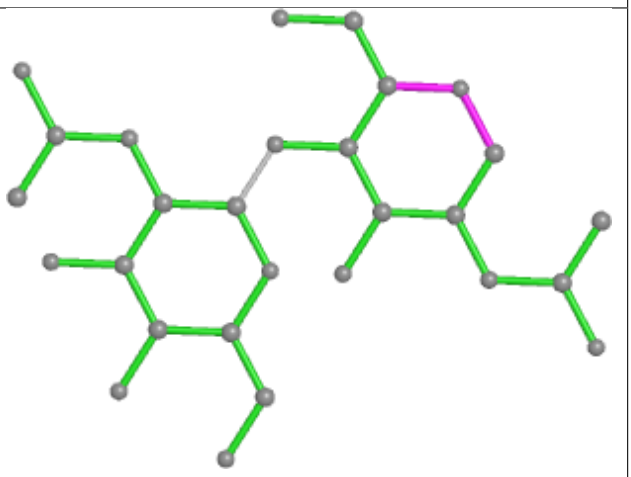
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	O	2	NAG	1	0
4	G	2	NAG	1	0
3	L	1	NAG	1	0
4	S	2	NAG	1	0
2	D	1	NAG	1	0
2	J	1	NAG	1	0
4	S	1	NAG	1	0
3	Q	1	NAG	1	0

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

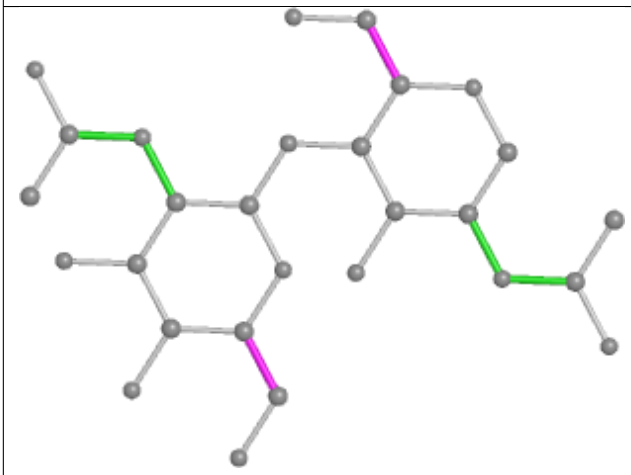
Oligosaccharide Chain D



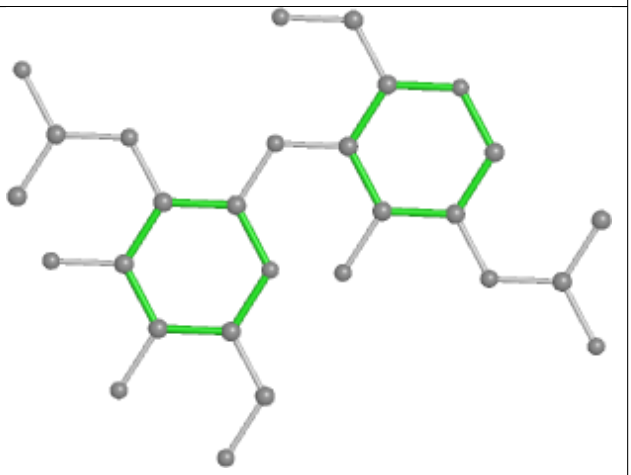
Bond lengths



Bond angles

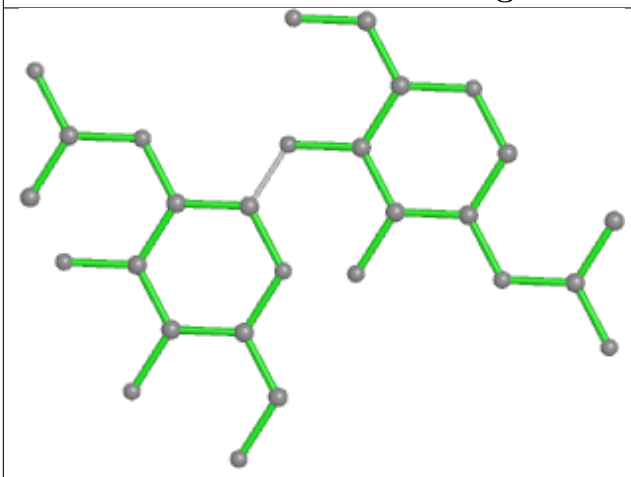


Torsions

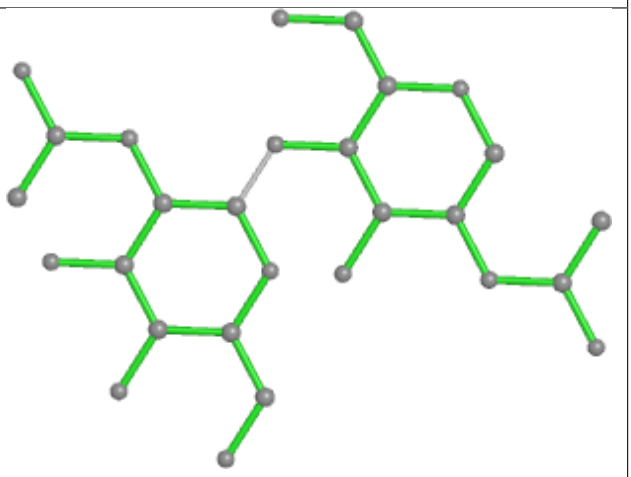


Rings

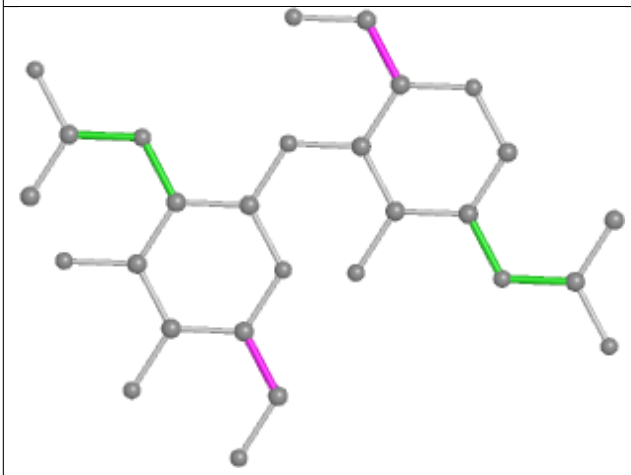
Oligosaccharide Chain F



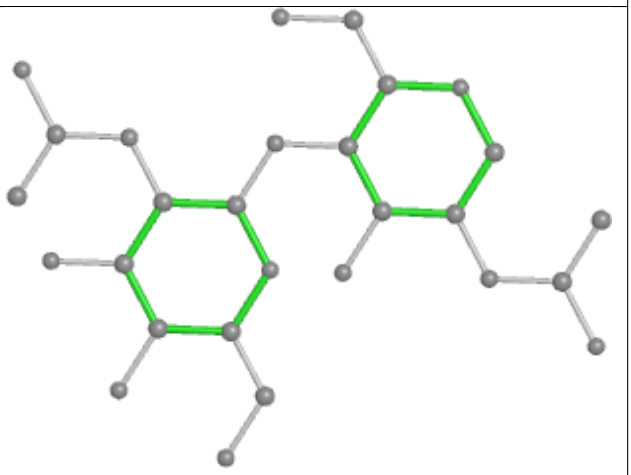
Bond lengths



Bond angles

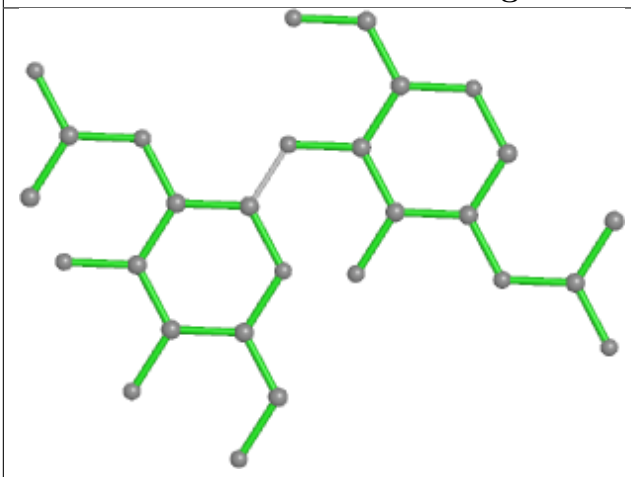


Torsions

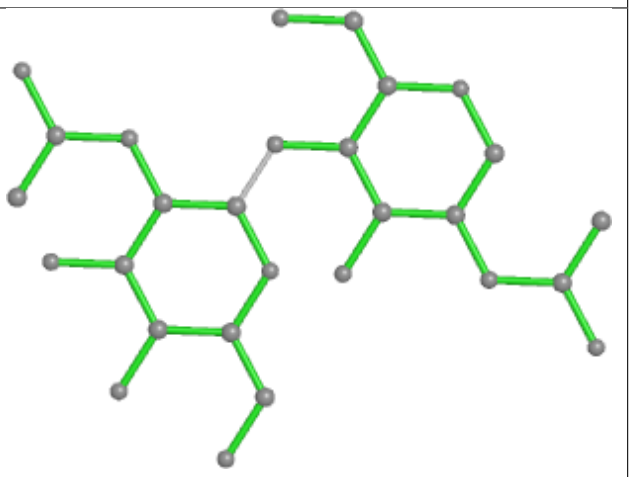


Rings

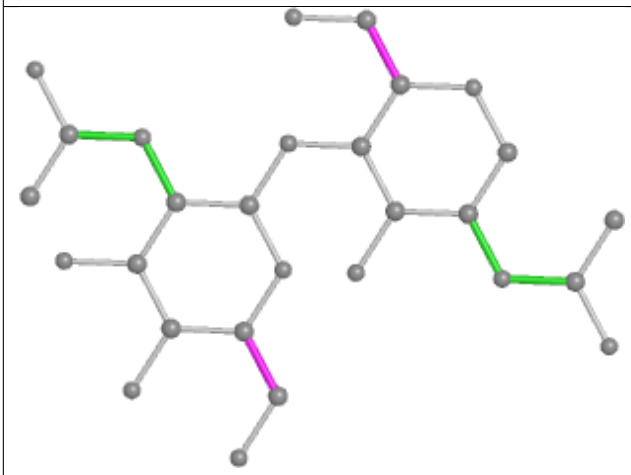
Oligosaccharide Chain I



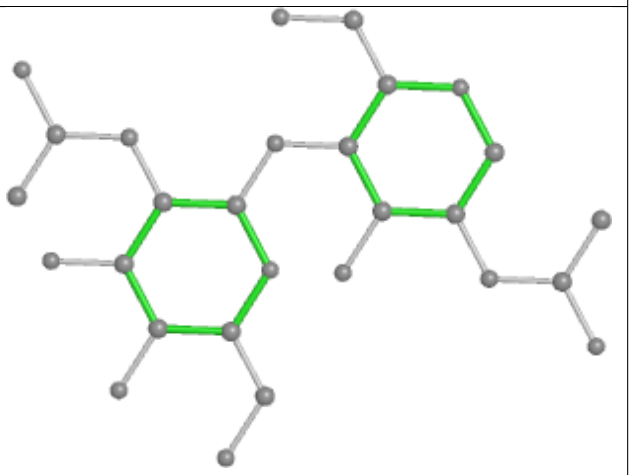
Bond lengths



Bond angles

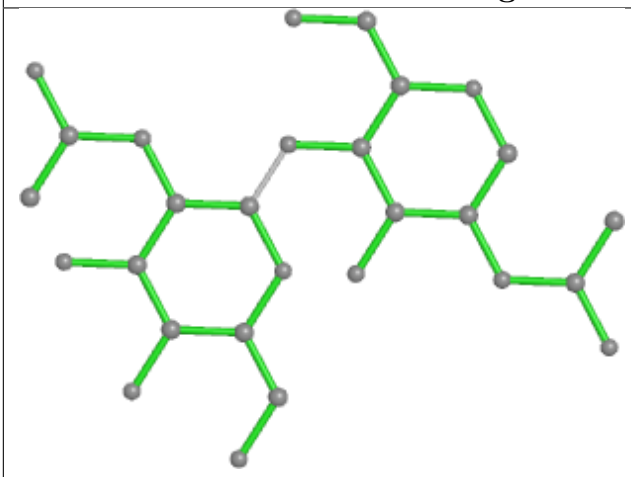


Torsions

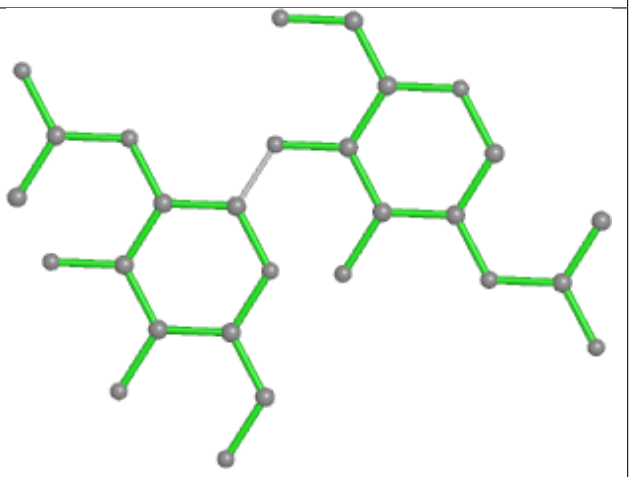


Rings

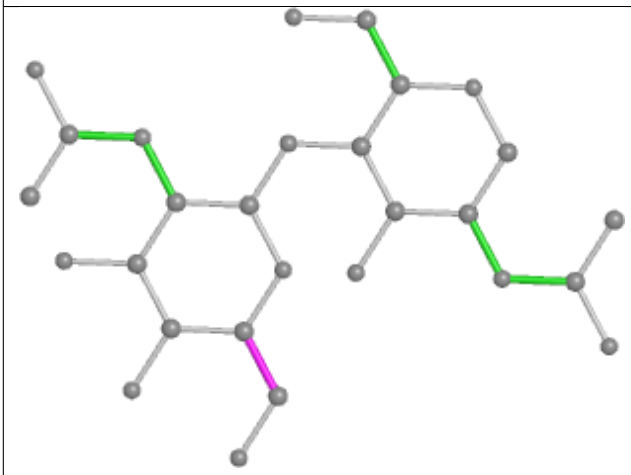
Oligosaccharide Chain J



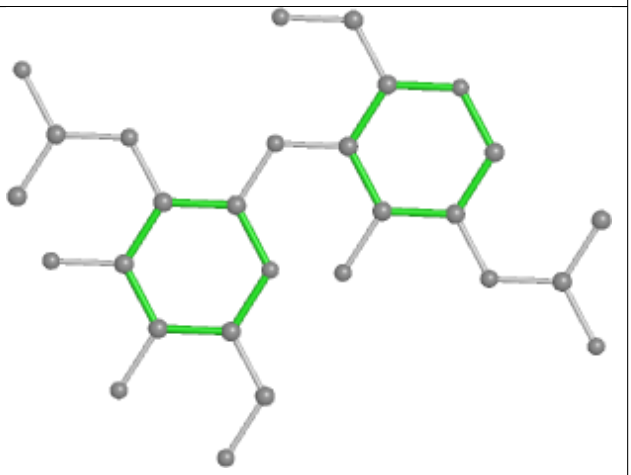
Bond lengths



Bond angles

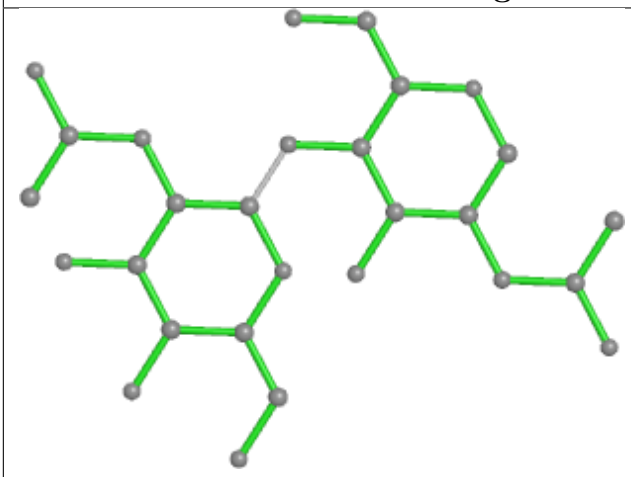


Torsions

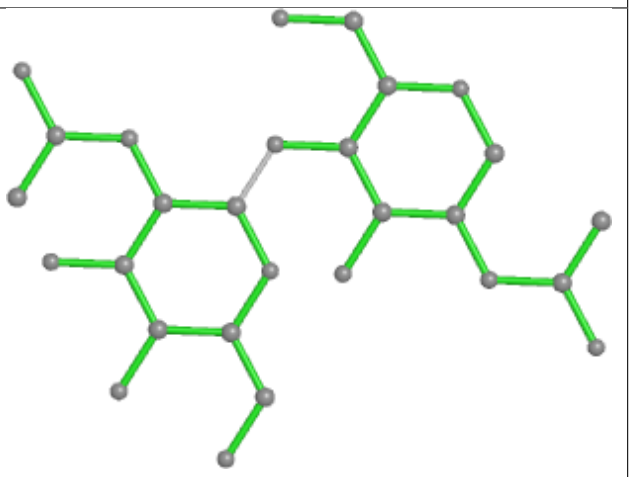


Rings

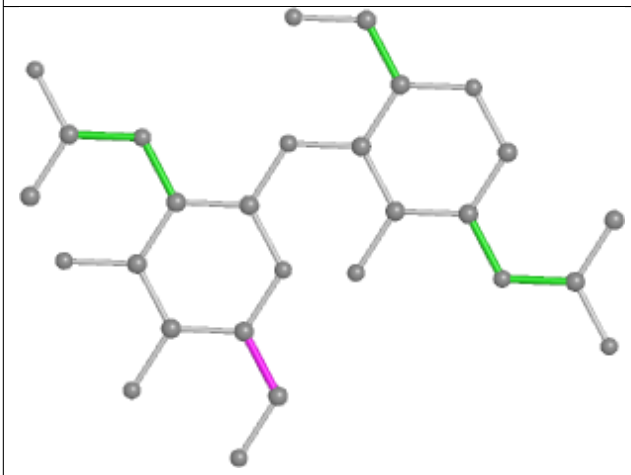
Oligosaccharide Chain K



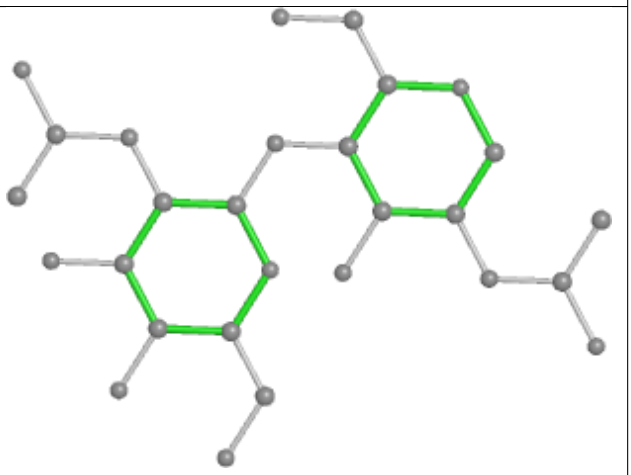
Bond lengths



Bond angles

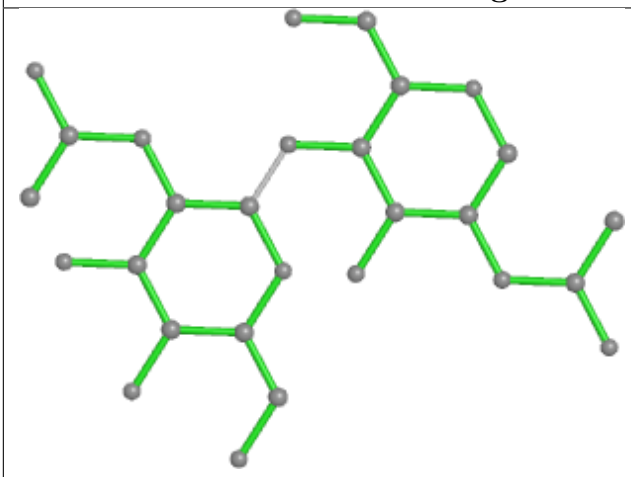


Torsions

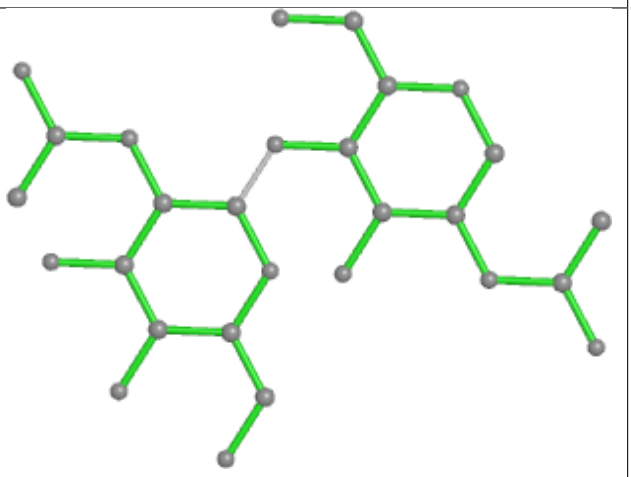


Rings

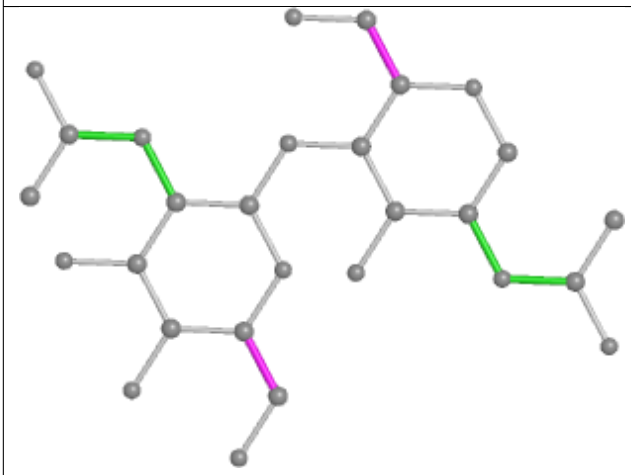
Oligosaccharide Chain M



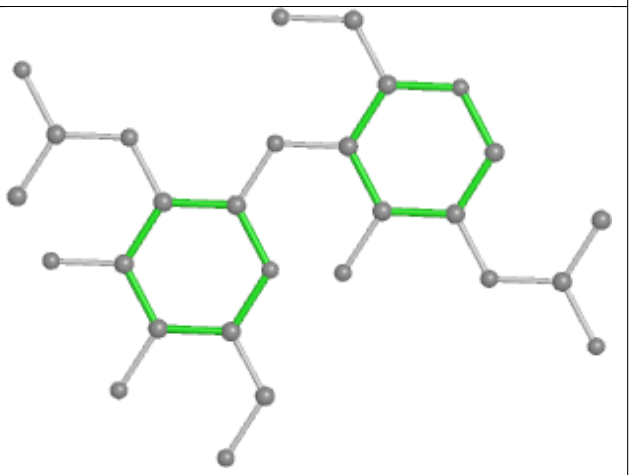
Bond lengths



Bond angles

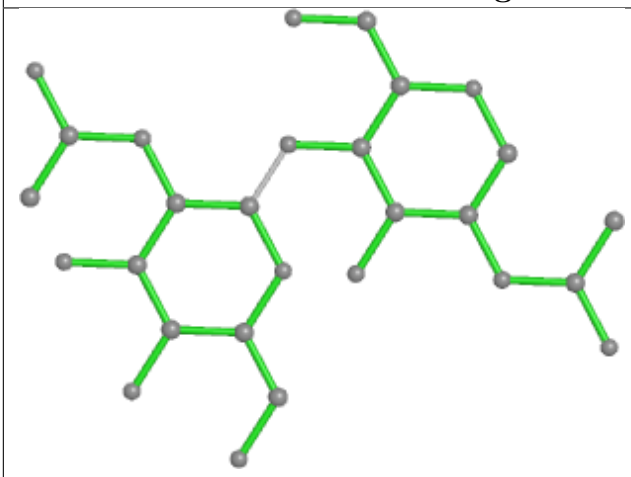


Torsions

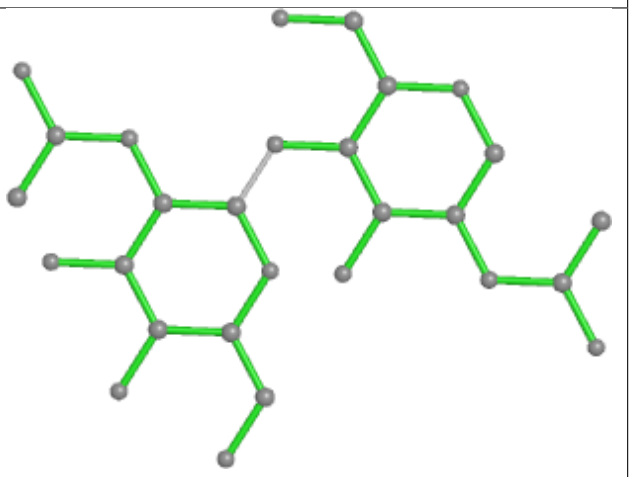


Rings

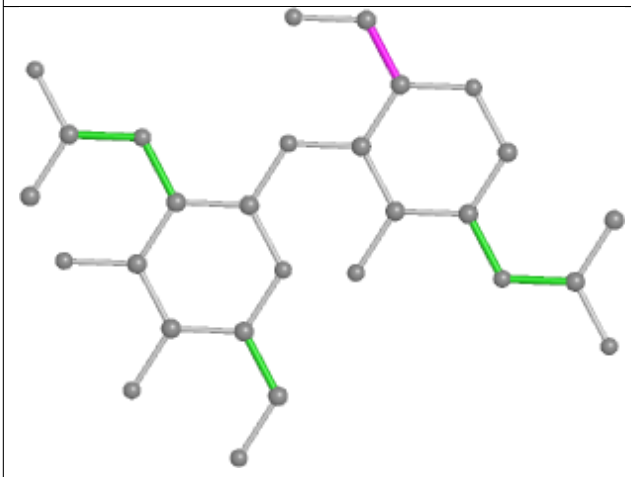
Oligosaccharide Chain R



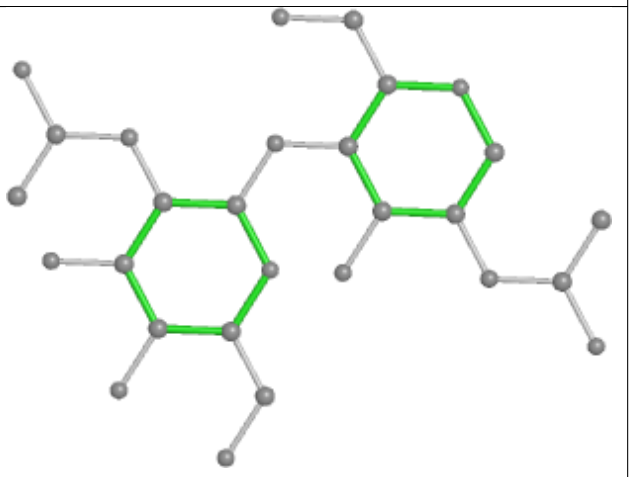
Bond lengths



Bond angles

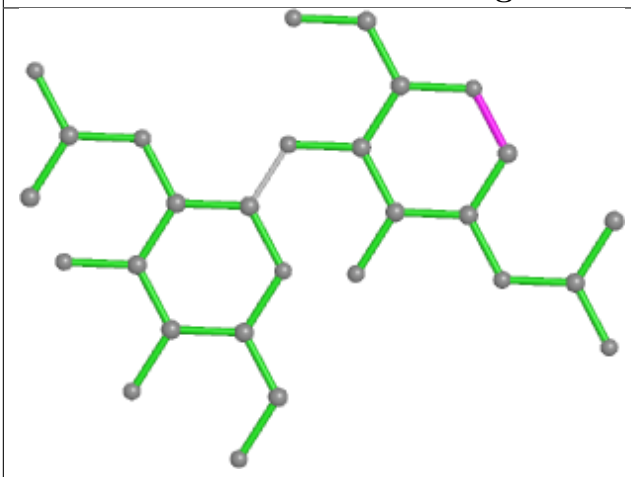


Torsions

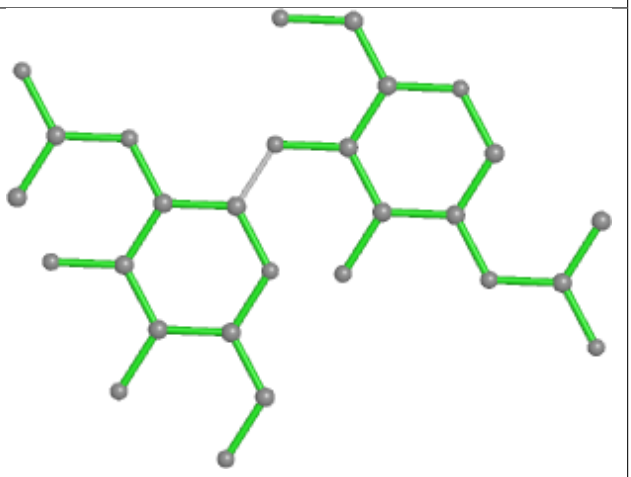


Rings

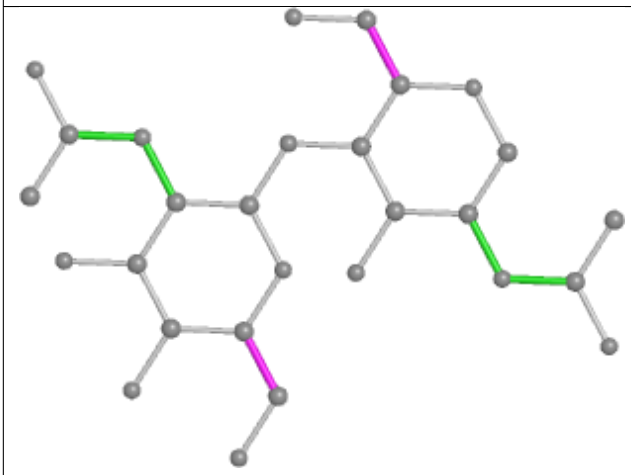
Oligosaccharide Chain T



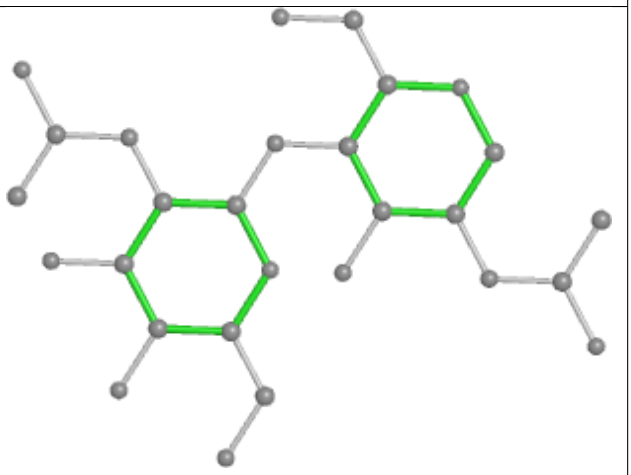
Bond lengths



Bond angles

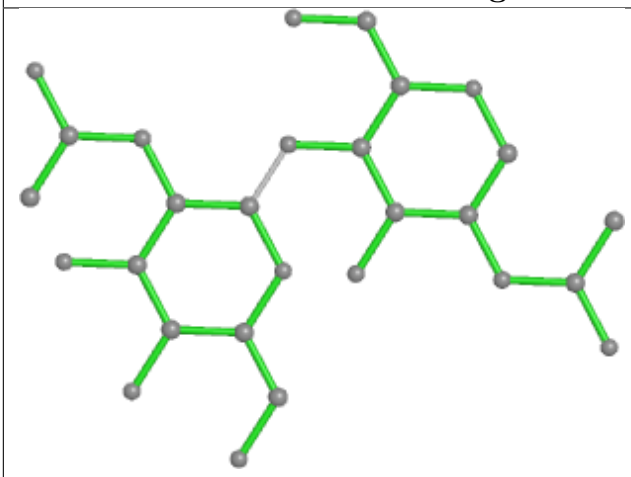


Torsions

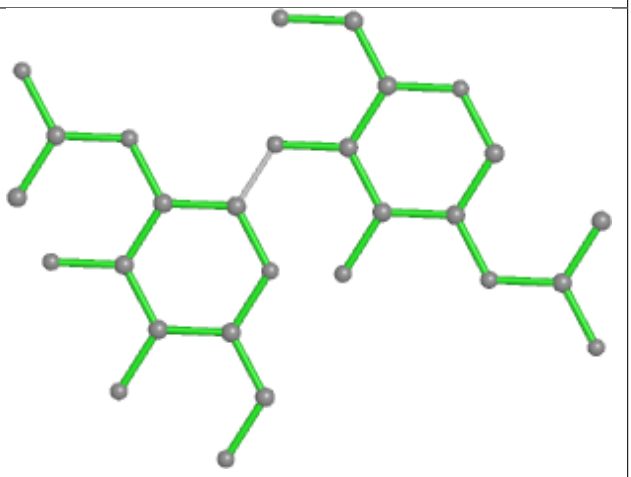


Rings

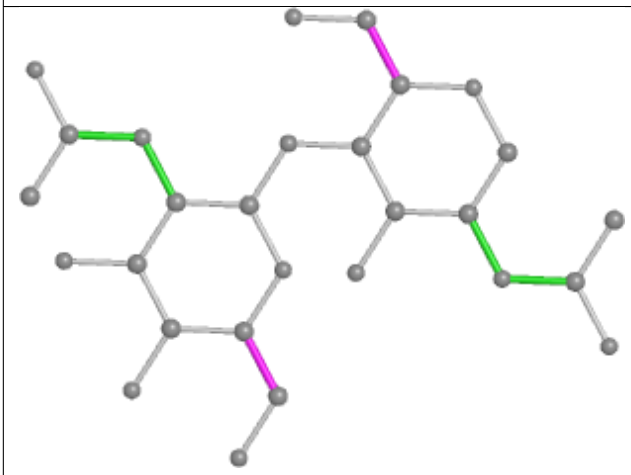
Oligosaccharide Chain W



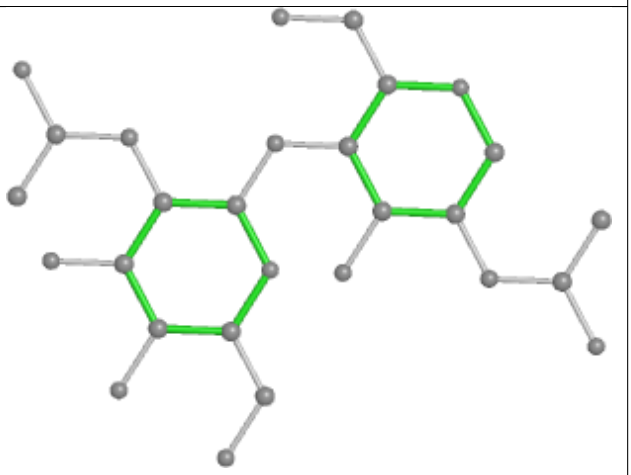
Bond lengths



Bond angles

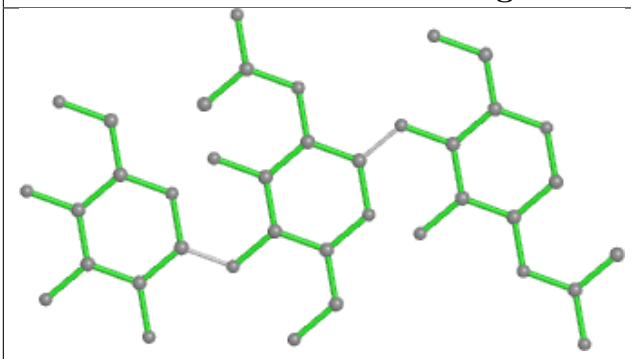


Torsions

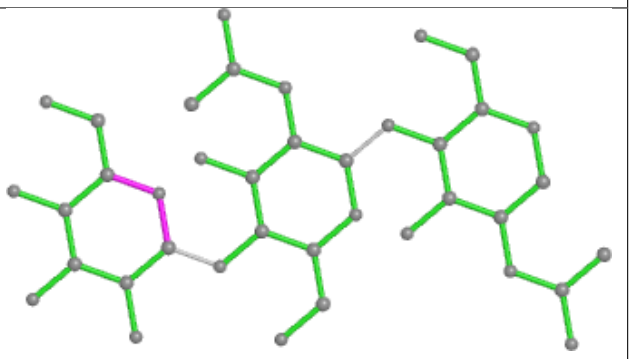


Rings

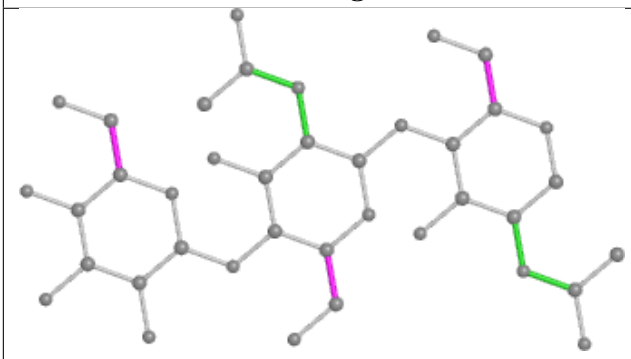
Oligosaccharide Chain E



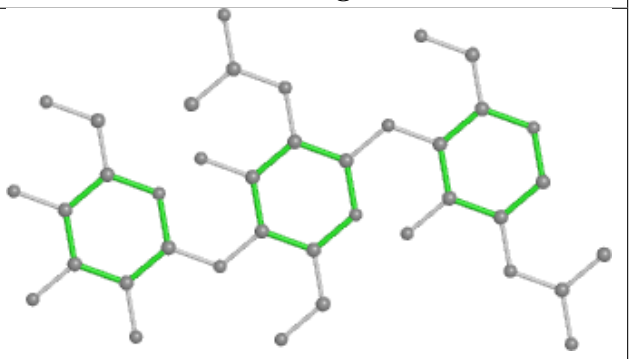
Bond lengths



Bond angles

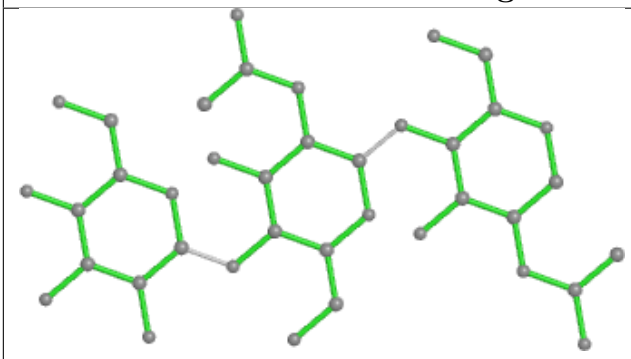


Torsions

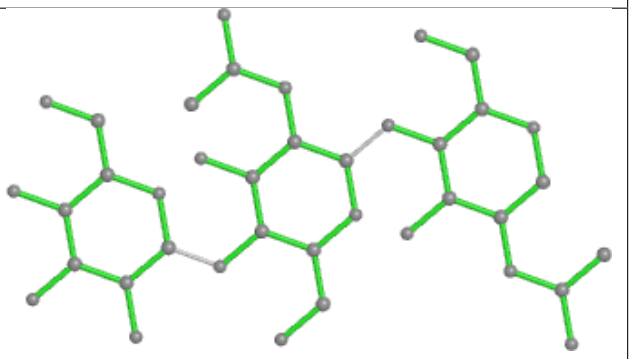


Rings

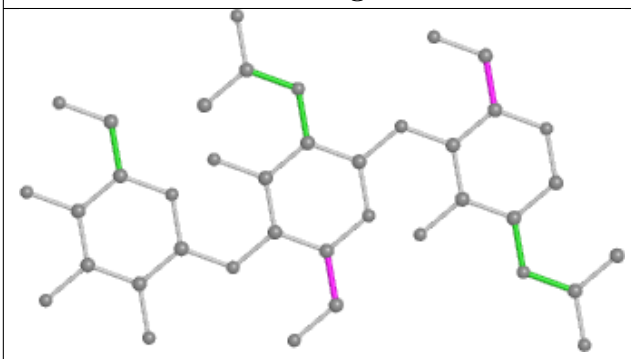
Oligosaccharide Chain L



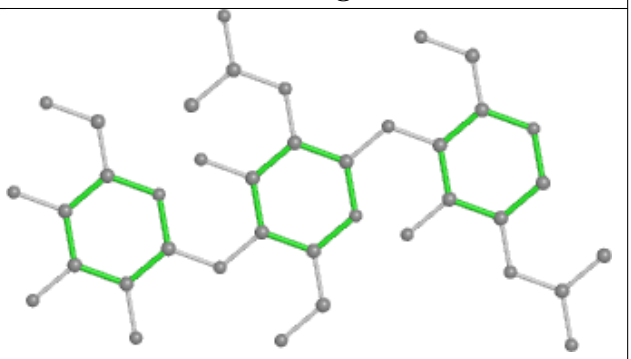
Bond lengths



Bond angles

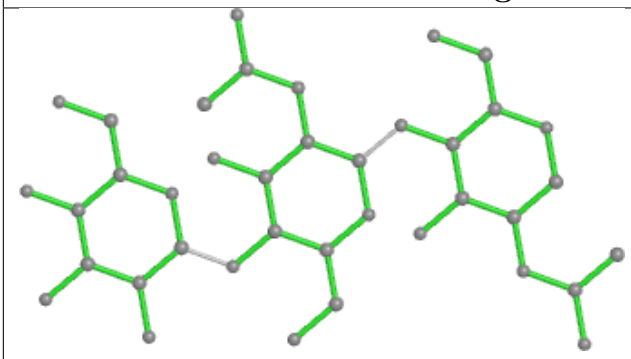


Torsions

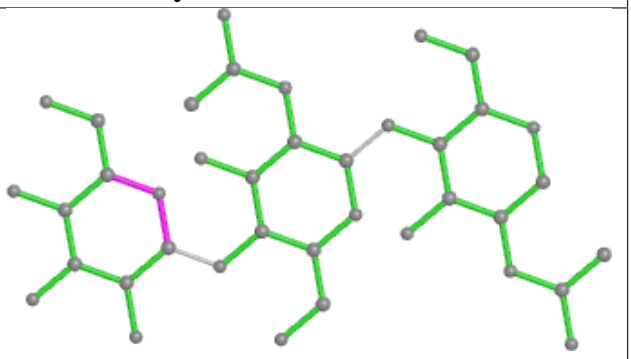


Rings

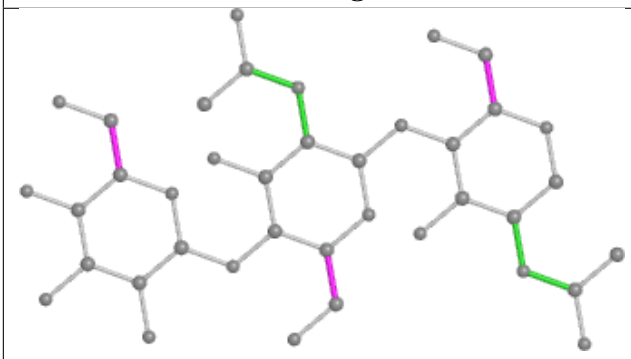
Oligosaccharide Chain Q



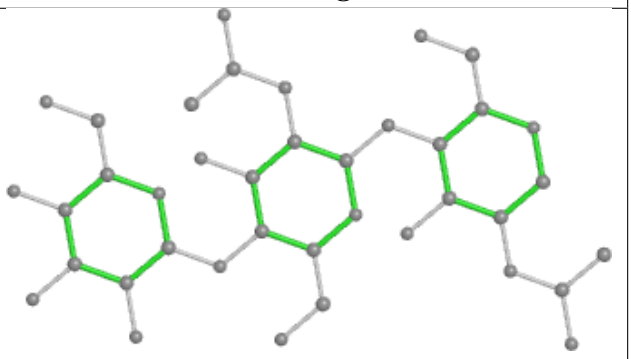
Bond lengths



Bond angles

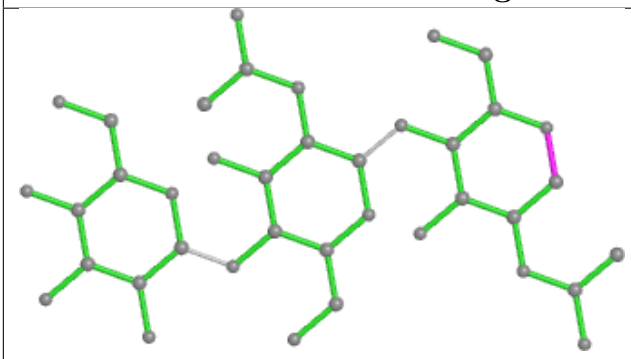


Torsions

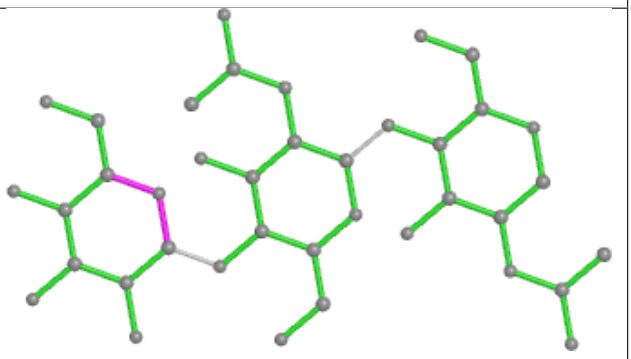


Rings

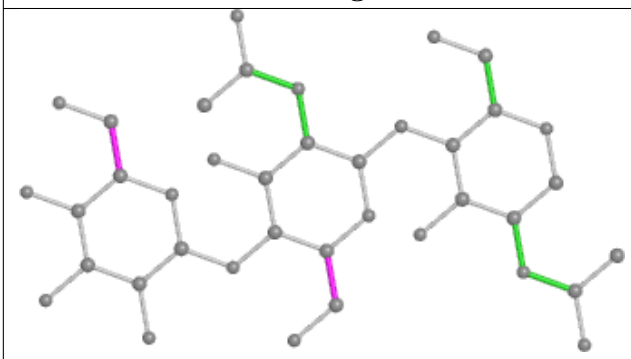
Oligosaccharide Chain U



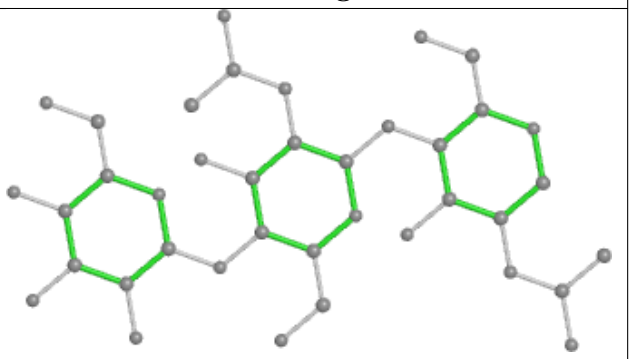
Bond lengths



Bond angles

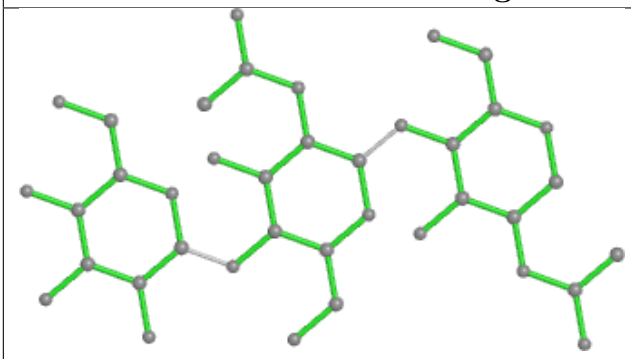


Torsions

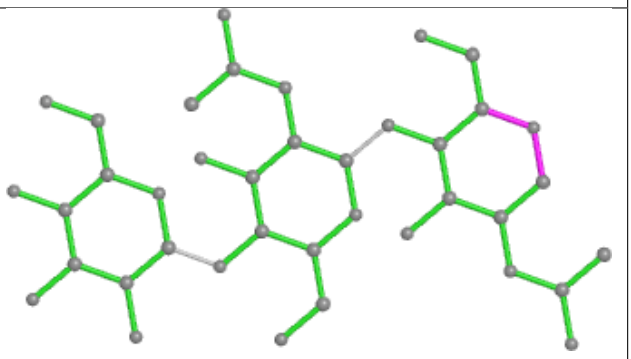


Rings

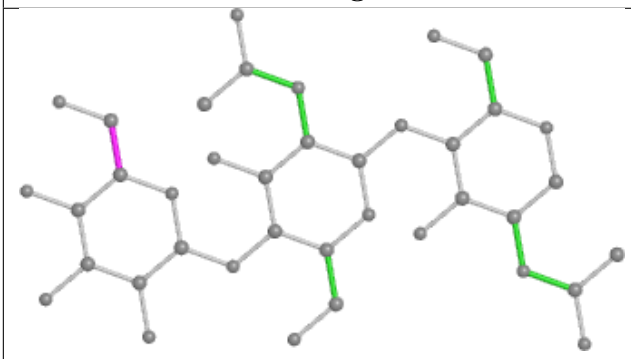
Oligosaccharide Chain V



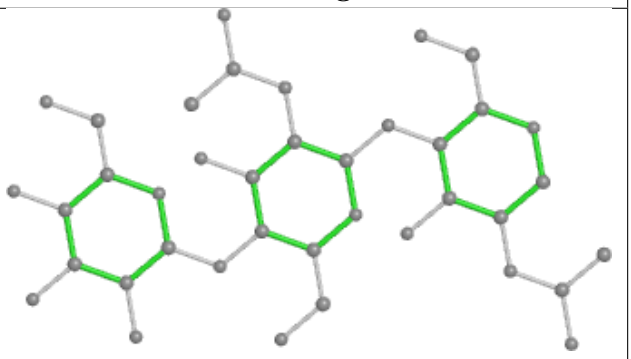
Bond lengths



Bond angles

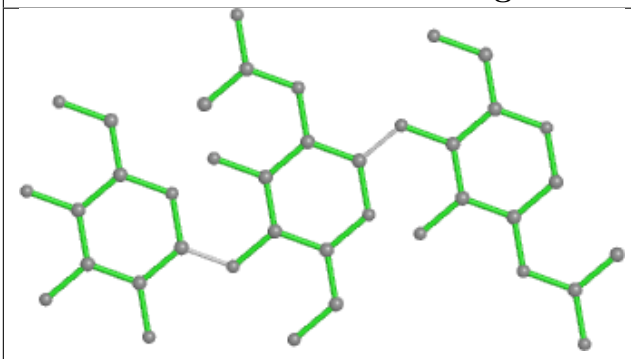


Torsions

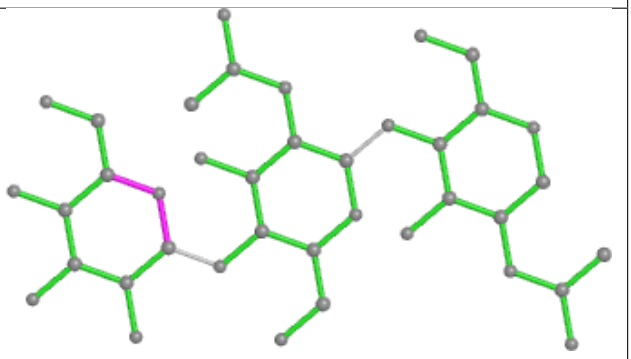


Rings

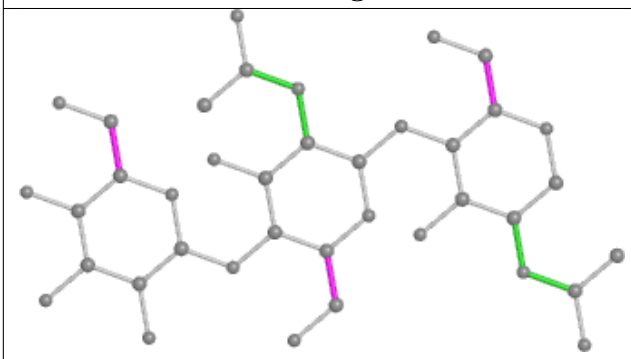
Oligosaccharide Chain X



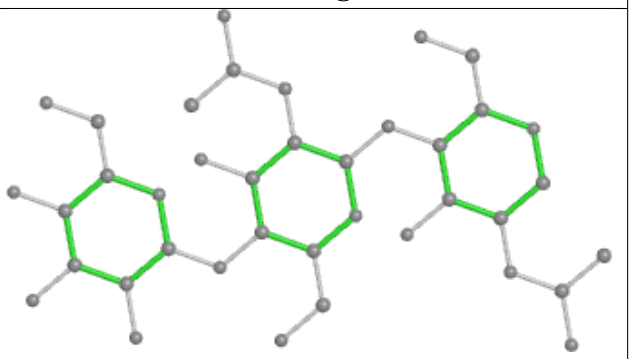
Bond lengths



Bond angles

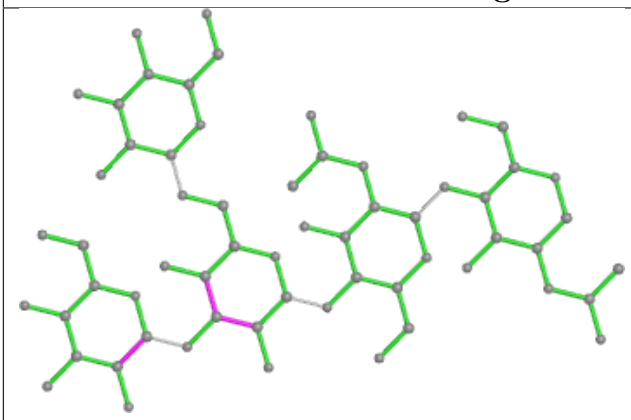


Torsions

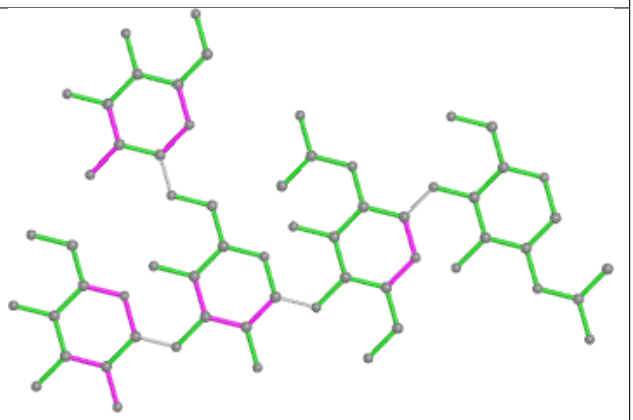


Rings

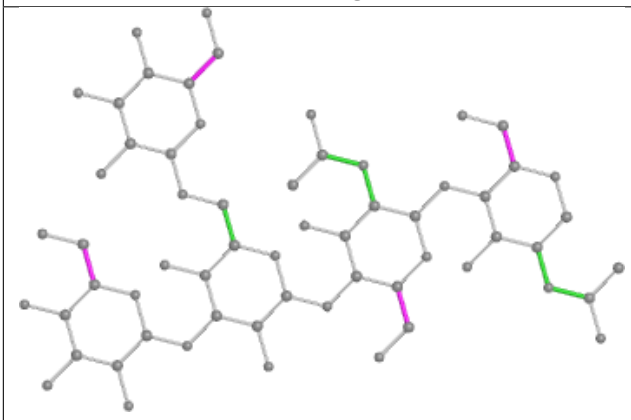
Oligosaccharide Chain G



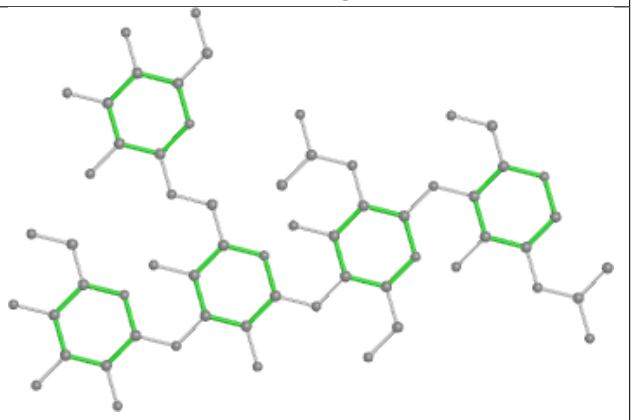
Bond lengths



Bond angles

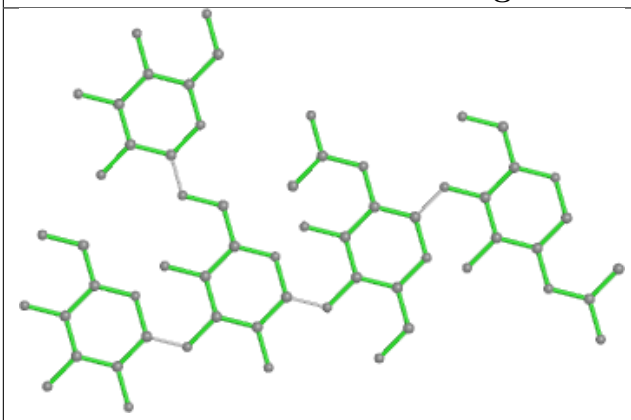


Torsions

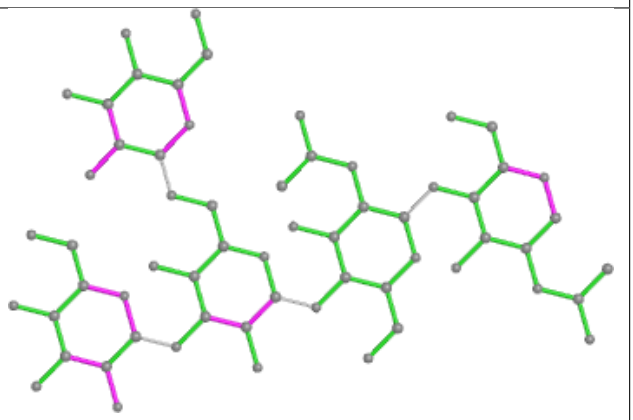


Rings

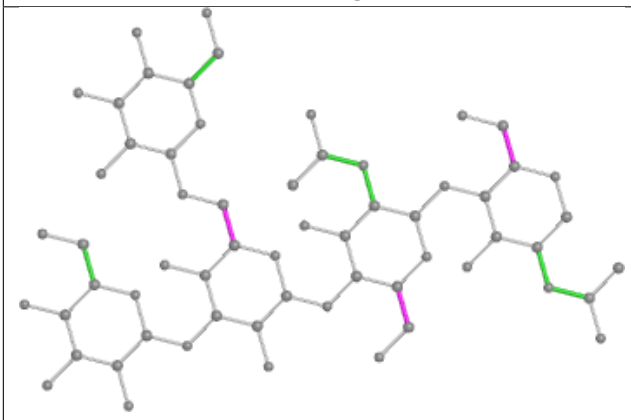
Oligosaccharide Chain H



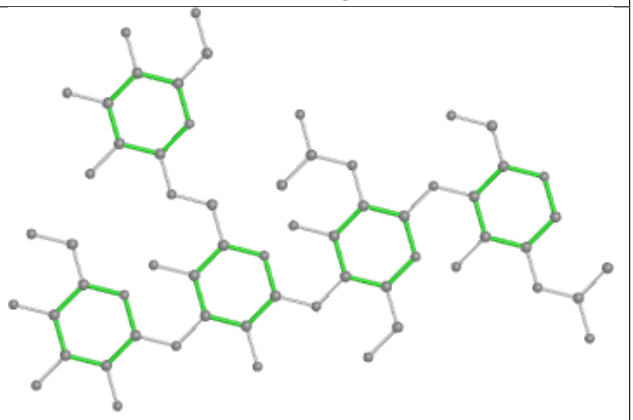
Bond lengths



Bond angles

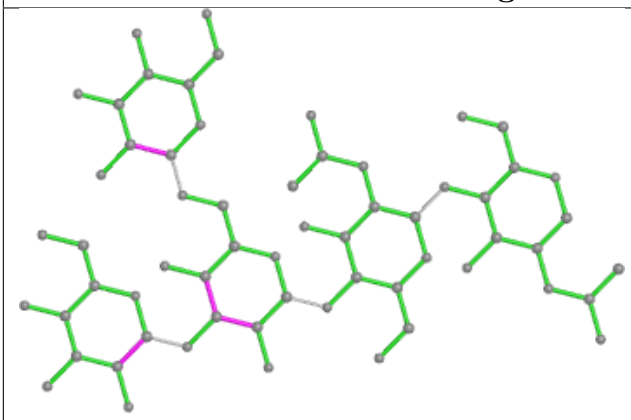


Torsions

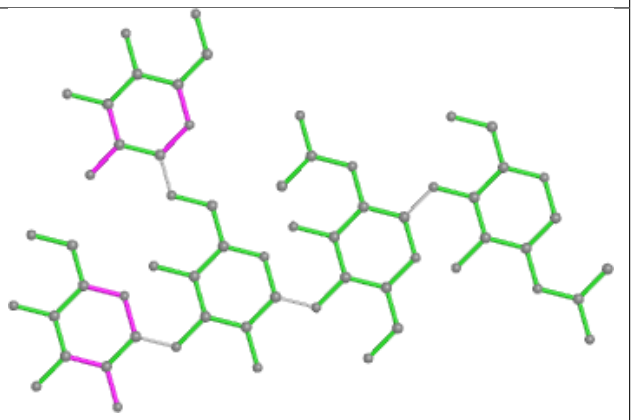


Rings

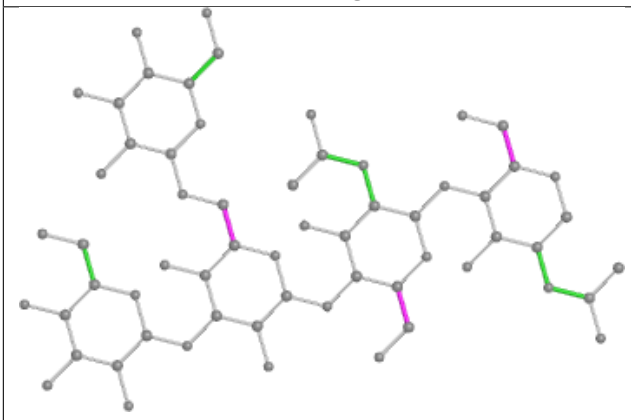
Oligosaccharide Chain S



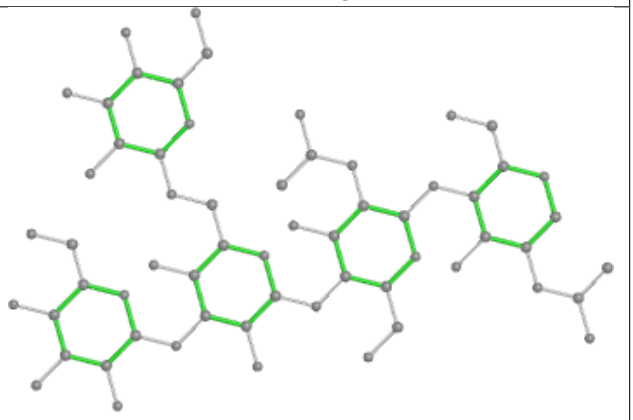
Bond lengths



Bond angles

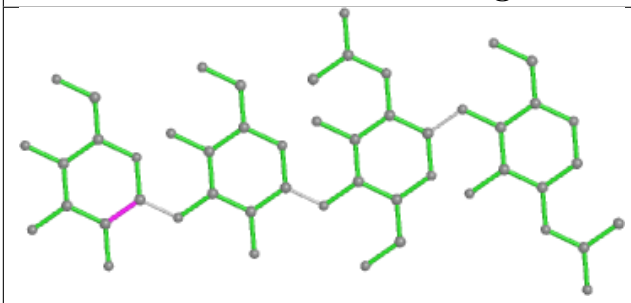


Torsions

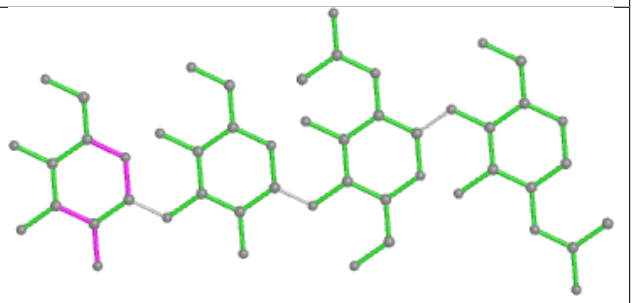


Rings

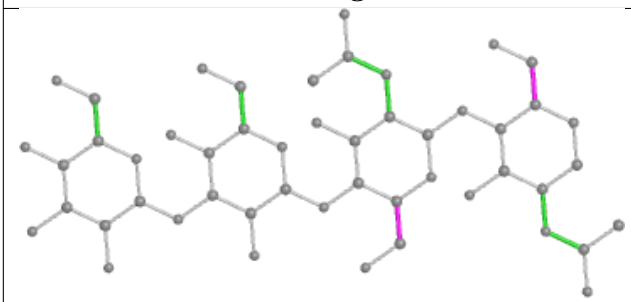
Oligosaccharide Chain N



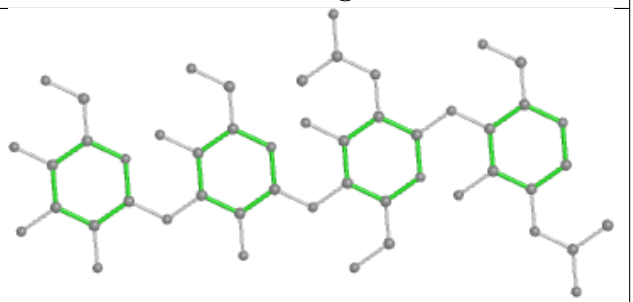
Bond lengths



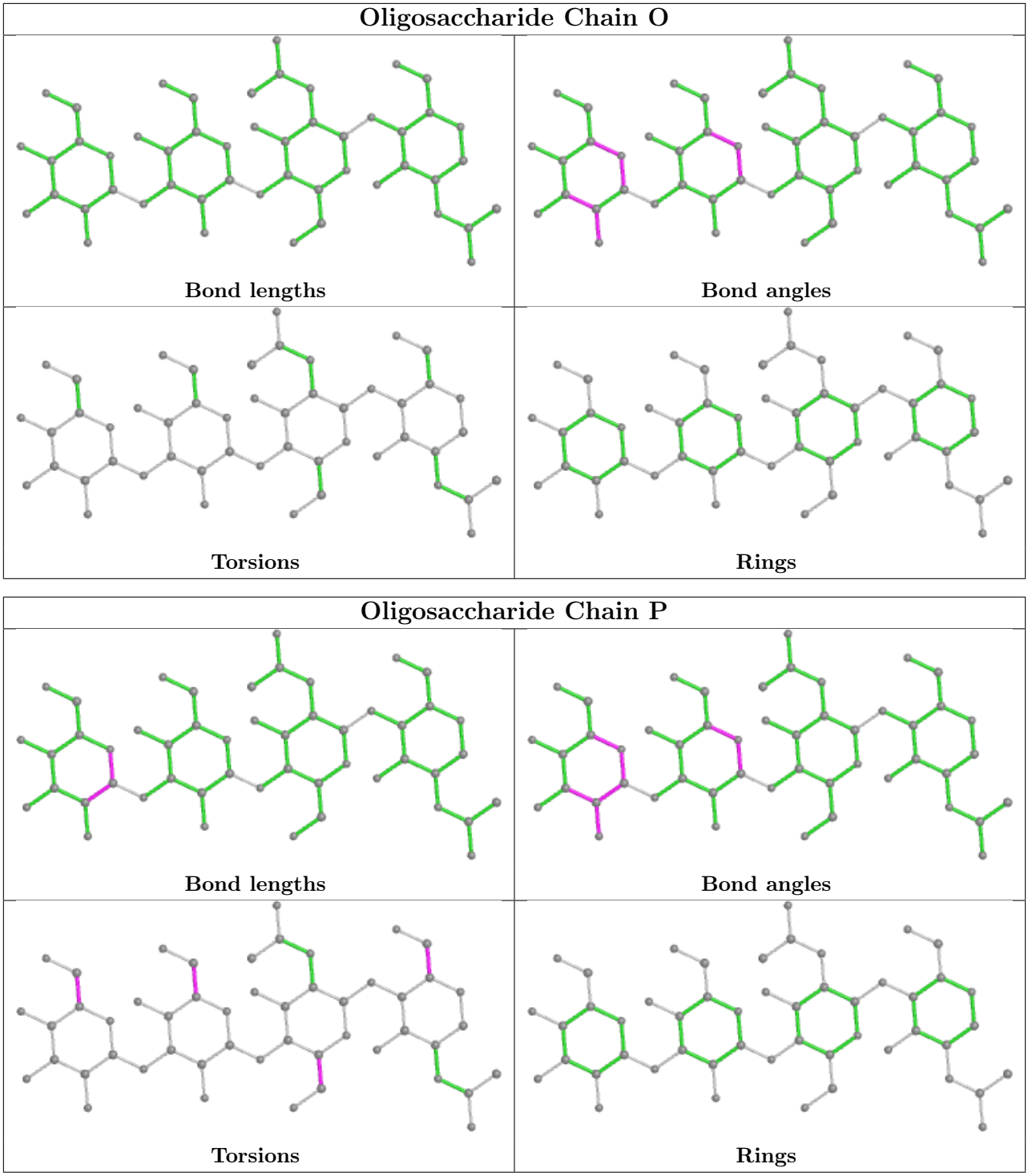
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

12 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	$\#\|Z\| > 2$
6	NAG	A	1317	1	14,14,15	0.41	0	17,19,21	0.41	0
6	NAG	A	1301	1	14,14,15	0.37	0	17,19,21	0.55	0
6	NAG	C	1321	1	14,14,15	0.43	0	17,19,21	0.46	0
6	NAG	A	1323	1	14,14,15	0.25	0	17,19,21	0.35	0
6	NAG	C	1308	1	14,14,15	0.27	0	17,19,21	0.40	0
6	NAG	B	1302	1	14,14,15	0.52	0	17,19,21	0.60	0
6	NAG	B	1322	1	14,14,15	0.24	0	17,19,21	0.60	0
6	NAG	A	1316	1	14,14,15	0.36	0	17,19,21	0.65	1 (5%)
6	NAG	B	1301	1	14,14,15	0.24	0	17,19,21	0.57	0
6	NAG	A	1307	1	14,14,15	0.20	0	17,19,21	0.43	0
6	NAG	C	1327	1	14,14,15	0.33	0	17,19,21	0.53	0
6	NAG	B	1323	1	14,14,15	0.19	0	17,19,21	0.36	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
6	NAG	A	1317	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1301	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1321	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1323	1	-	0/6/23/26	0/1/1/1
6	NAG	C	1308	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1302	1	-	1/6/23/26	0/1/1/1
6	NAG	B	1322	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1316	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1301	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1307	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1327	1	-	1/6/23/26	0/1/1/1
6	NAG	B	1323	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	1316	NAG	C1-O5-C5	2.25	115.24	112.19

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1316	NAG	O5-C5-C6-O6
6	B	1322	NAG	O5-C5-C6-O6
6	C	1321	NAG	O5-C5-C6-O6
6	A	1301	NAG	O5-C5-C6-O6
6	A	1307	NAG	O5-C5-C6-O6
6	C	1308	NAG	O5-C5-C6-O6
6	B	1301	NAG	O5-C5-C6-O6
6	A	1316	NAG	C4-C5-C6-O6
6	A	1307	NAG	C4-C5-C6-O6
6	B	1323	NAG	C4-C5-C6-O6
6	A	1301	NAG	C4-C5-C6-O6
6	C	1308	NAG	C4-C5-C6-O6
6	B	1301	NAG	C4-C5-C6-O6
6	B	1322	NAG	C4-C5-C6-O6
6	B	1323	NAG	O5-C5-C6-O6
6	C	1321	NAG	C4-C5-C6-O6
6	A	1317	NAG	O5-C5-C6-O6
6	B	1302	NAG	C4-C5-C6-O6
6	A	1317	NAG	C4-C5-C6-O6
6	C	1327	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	1321	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.

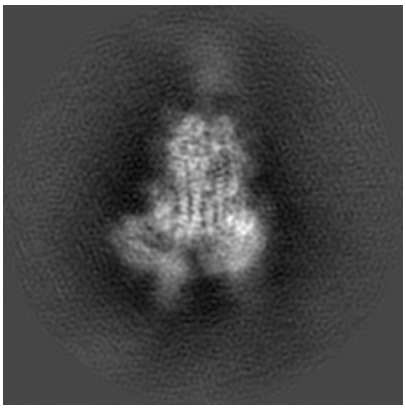
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-7579. These allow visual inspection of the internal detail of the map and identification of artifacts.

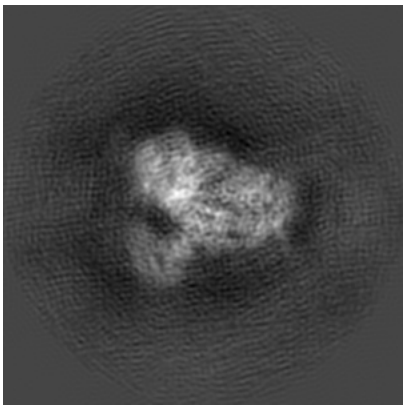
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

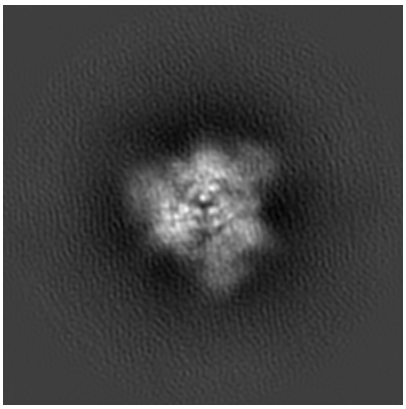
6.1.1 Primary map



X

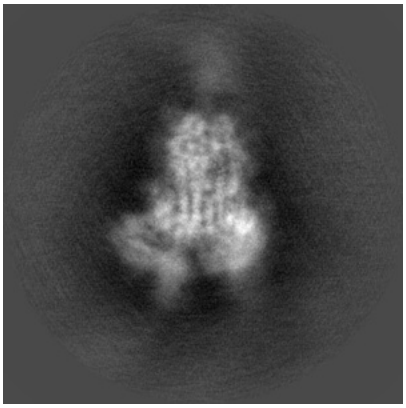


Y

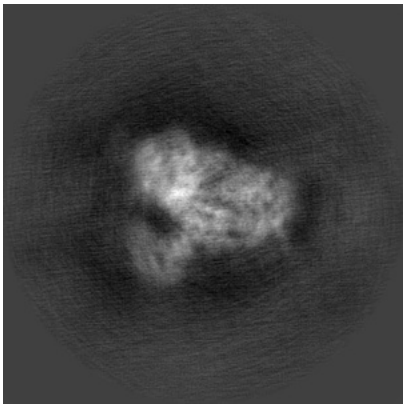


Z

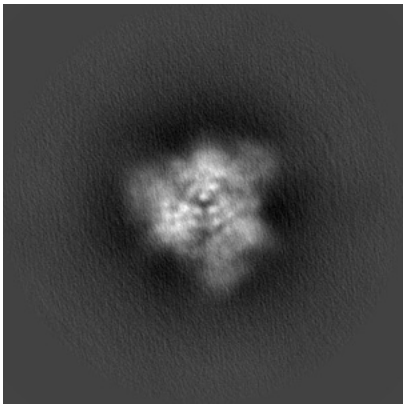
6.1.2 Raw map



X



Y

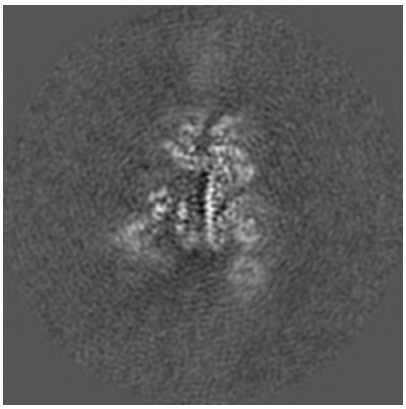


Z

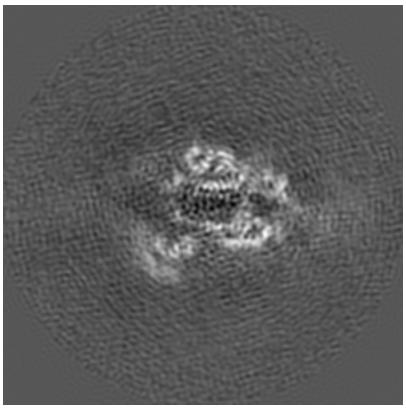
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

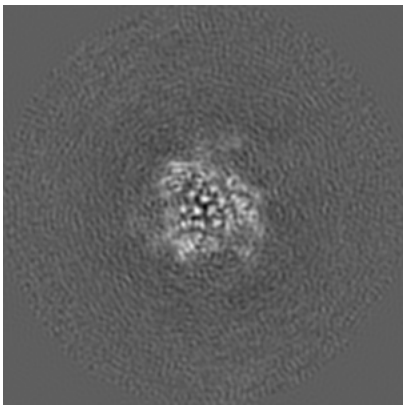
6.2.1 Primary map



X Index: 160

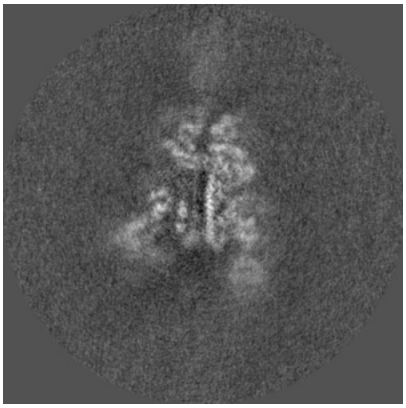


Y Index: 160

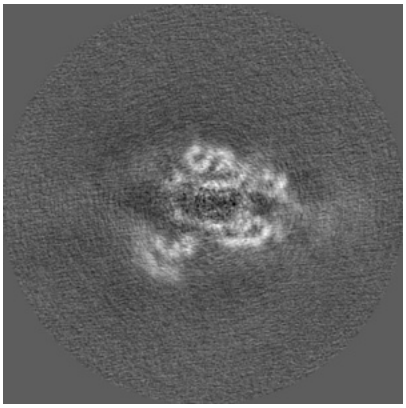


Z Index: 160

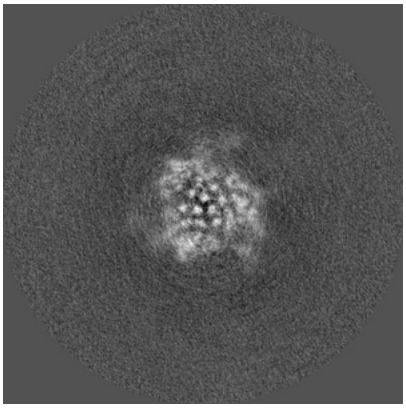
6.2.2 Raw map



X Index: 160



Y Index: 160

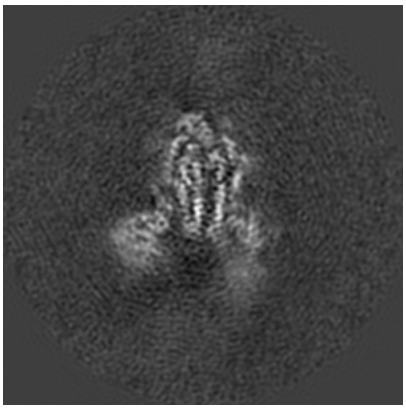


Z Index: 160

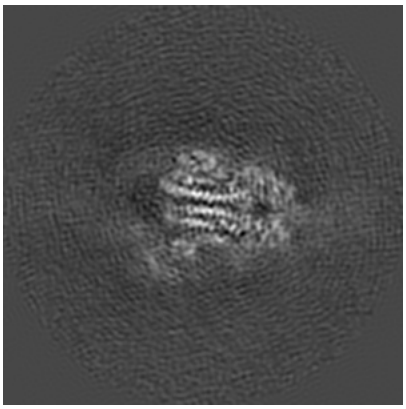
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

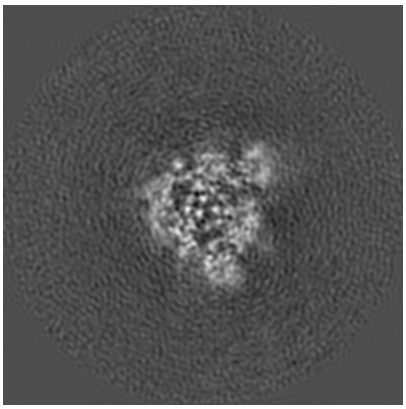
6.3.1 Primary map



X Index: 168

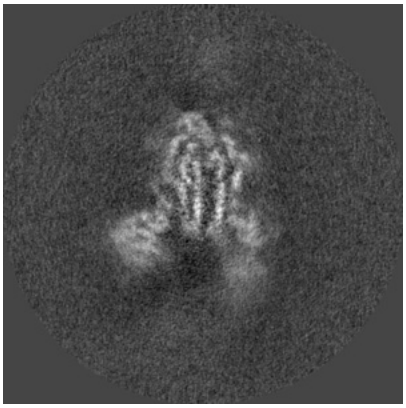


Y Index: 155

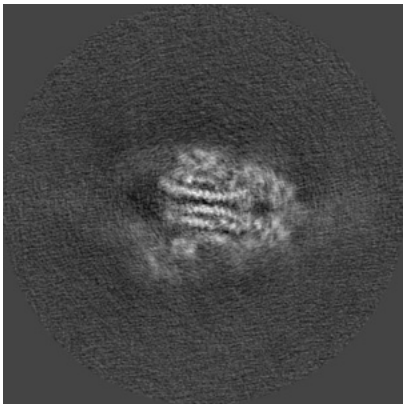


Z Index: 147

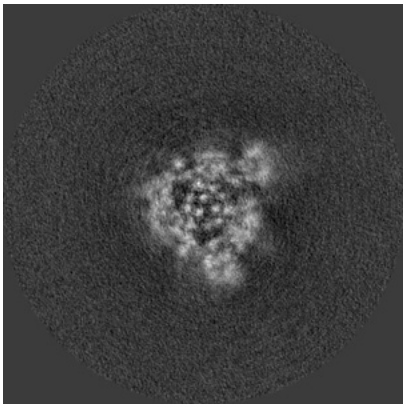
6.3.2 Raw map



X Index: 168



Y Index: 155



Z Index: 147

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 0.032. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

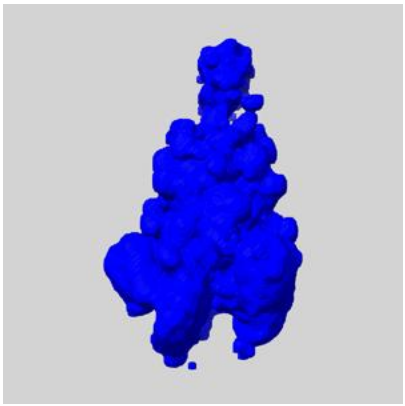
6.5 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

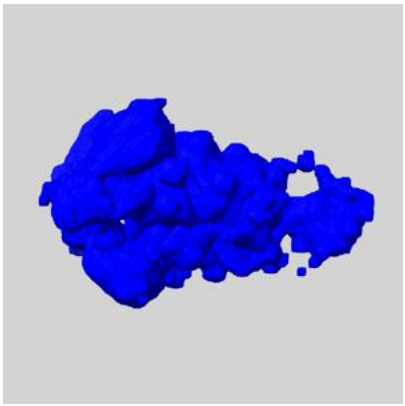
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

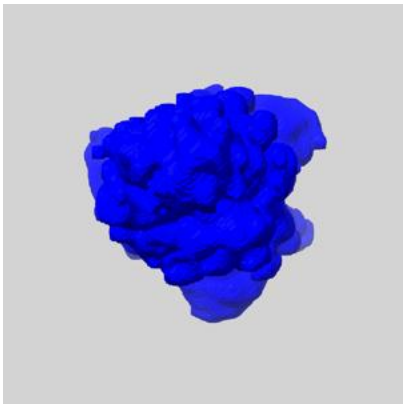
6.5.1 emd_7579_msk_1.map (i)



X



Y

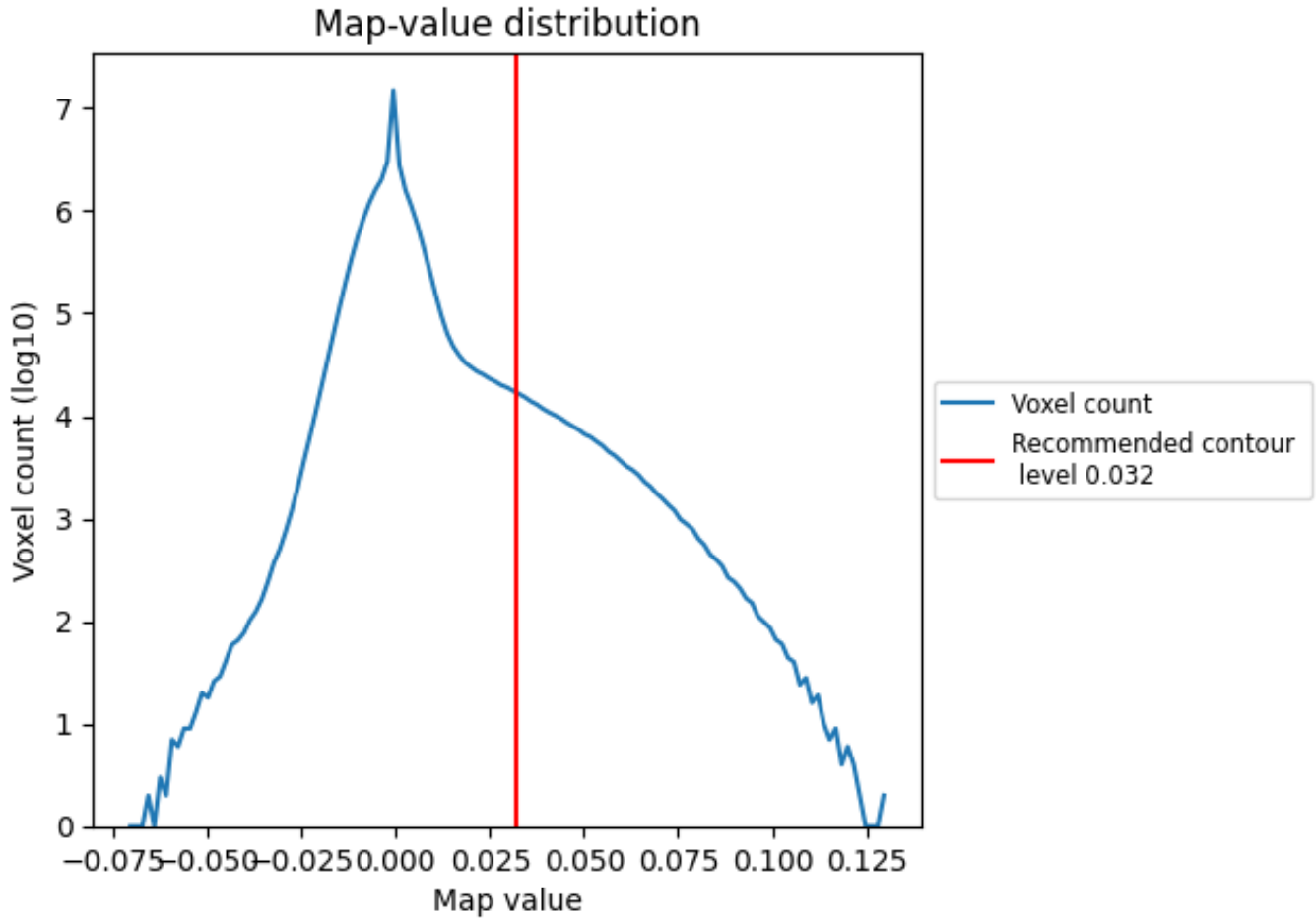


Z

7 Map analysis

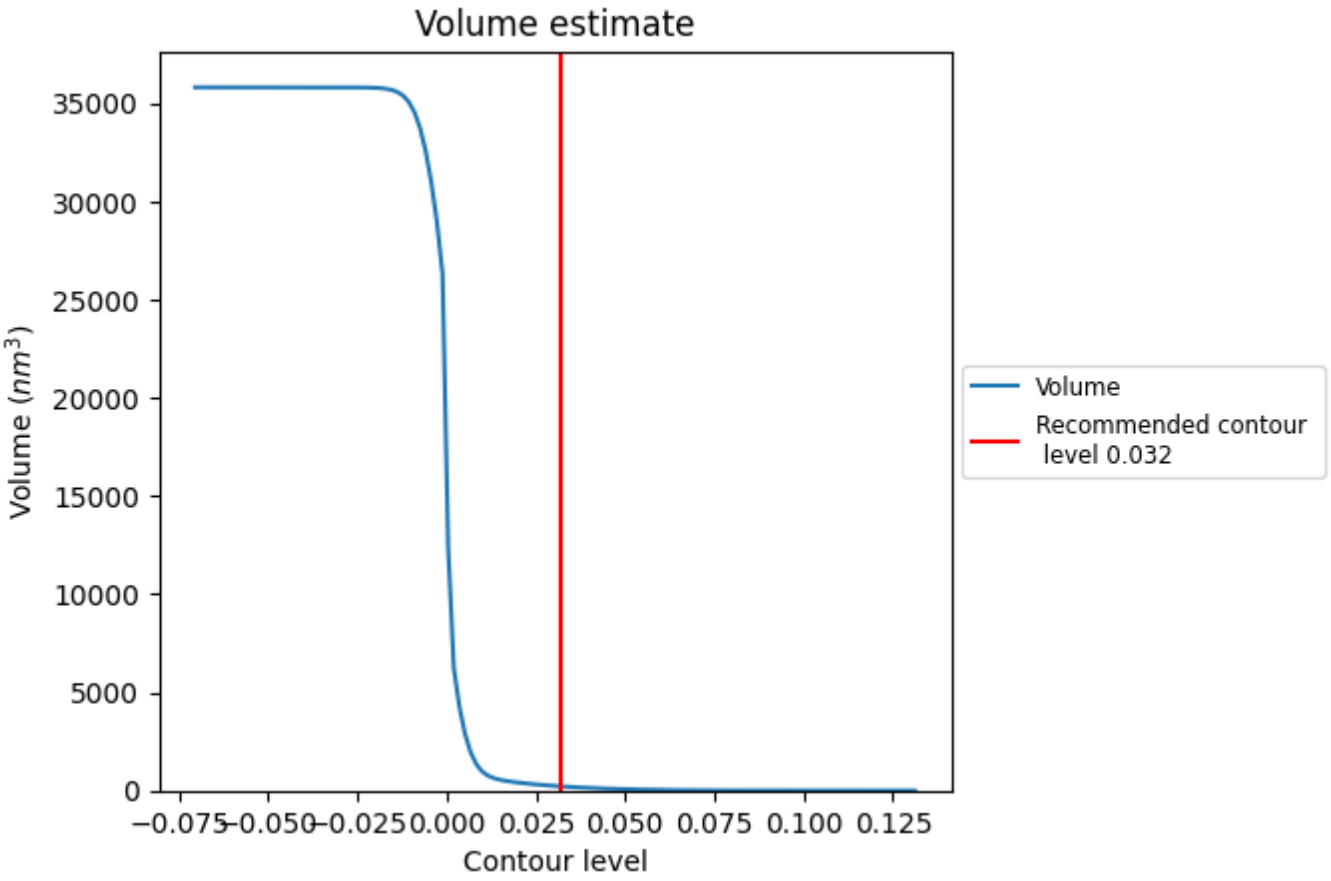
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

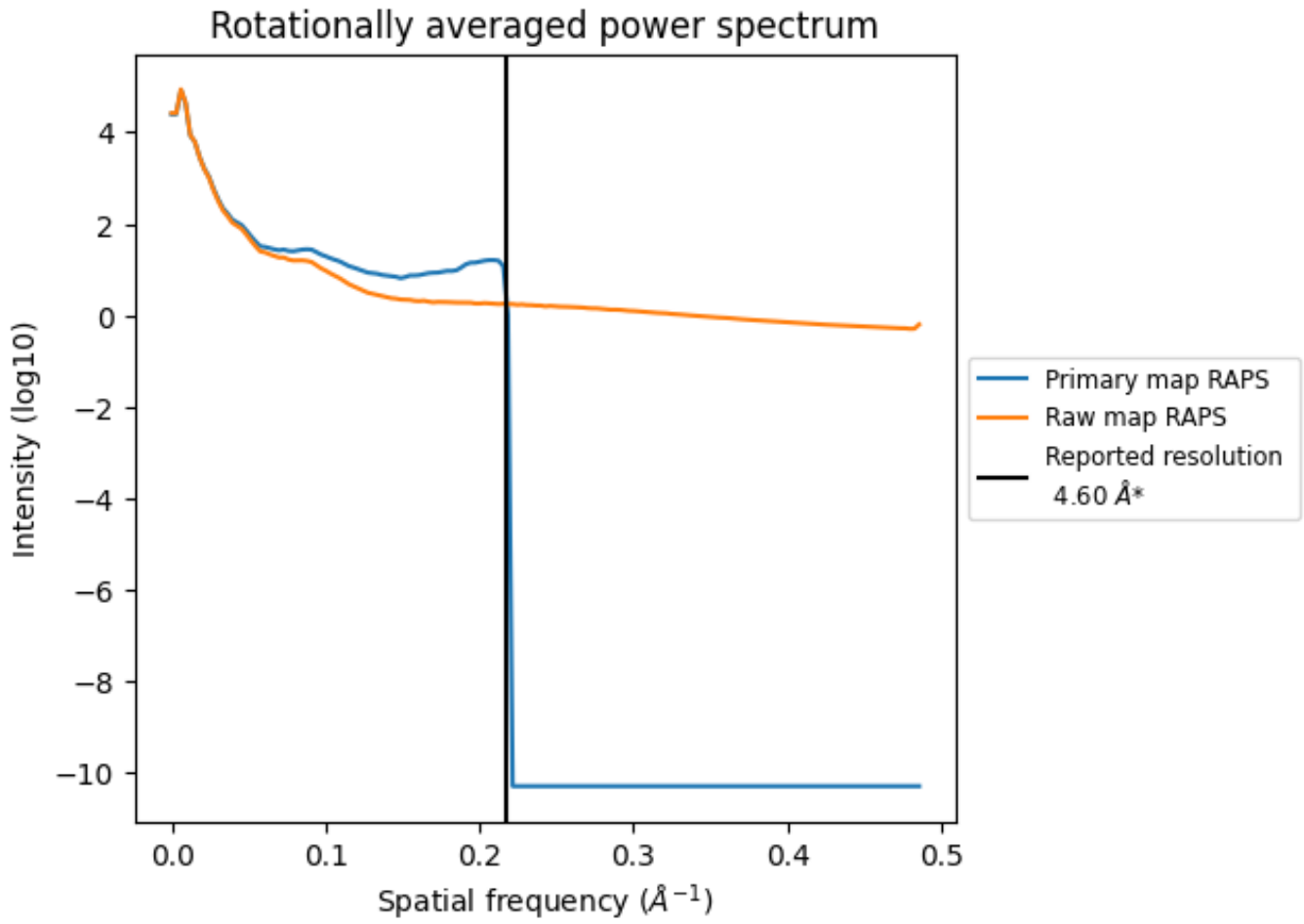
7.2 Volume estimate



The volume at the recommended contour level is 213 nm^3; this corresponds to an approximate mass of 192 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)

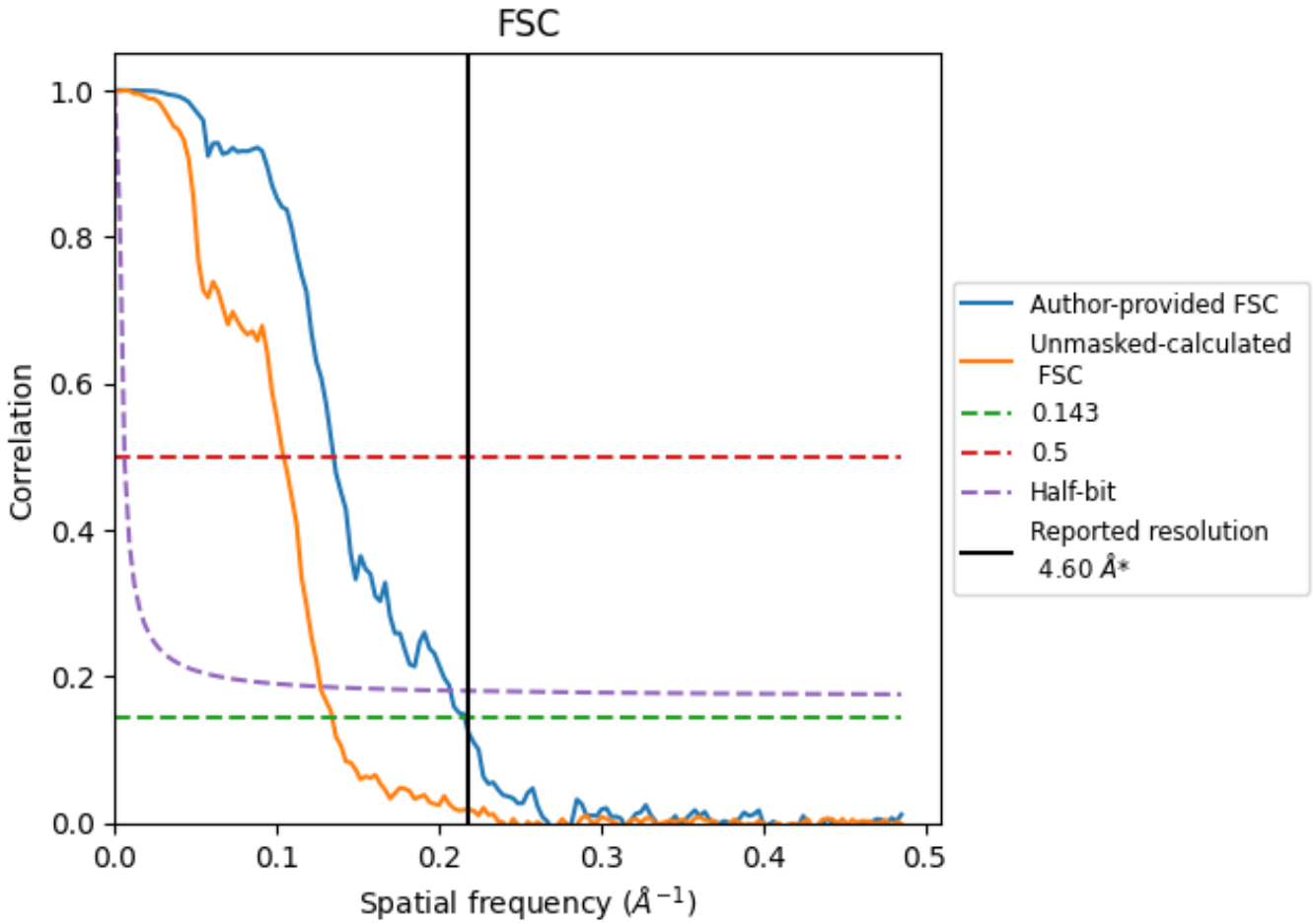


*Reported resolution corresponds to spatial frequency of 0.217 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.217 Å^{-1}

8.2 Resolution estimates (i)

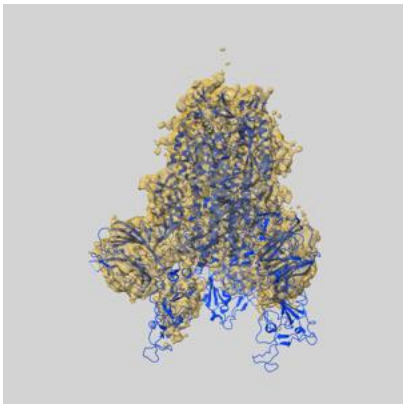
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.60	-	-
Author-provided FSC curve	4.63	7.41	4.83
Unmasked-calculated*	7.45	9.60	7.87

*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 7.45 differs from the reported value 4.6 by more than 10 %

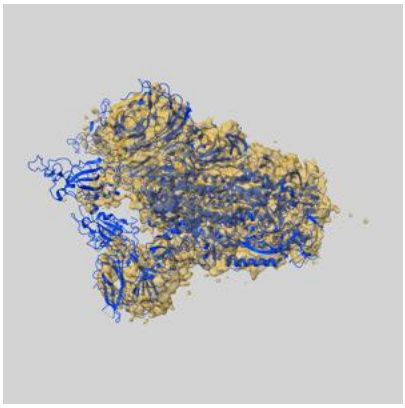
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-7579 and PDB model 6CS1. Per-residue inclusion information can be found in section 3 on page 9.

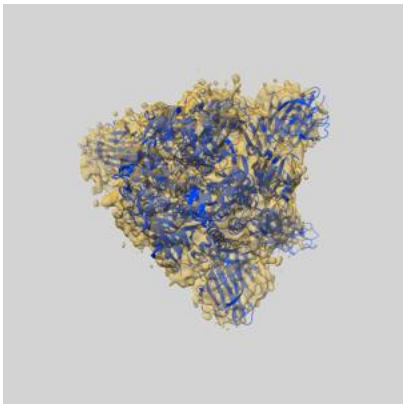
9.1 Map-model overlay



X



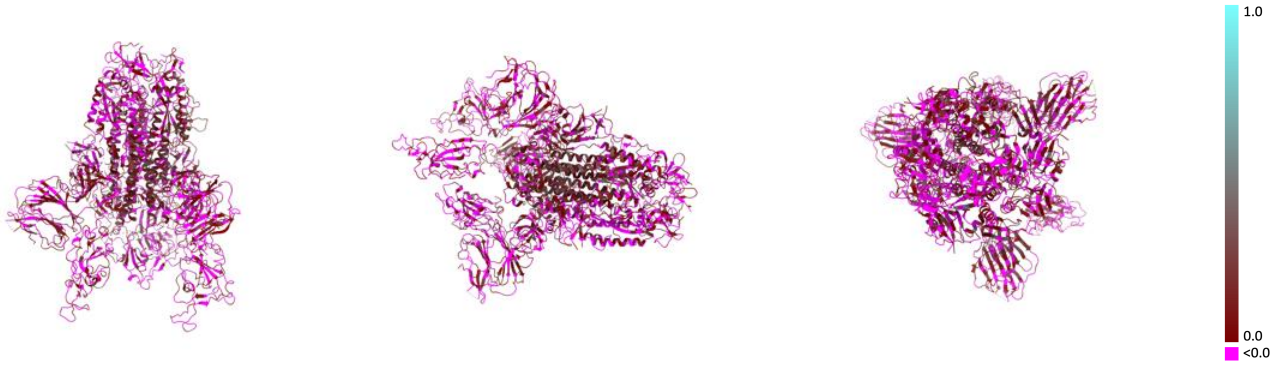
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.032 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.

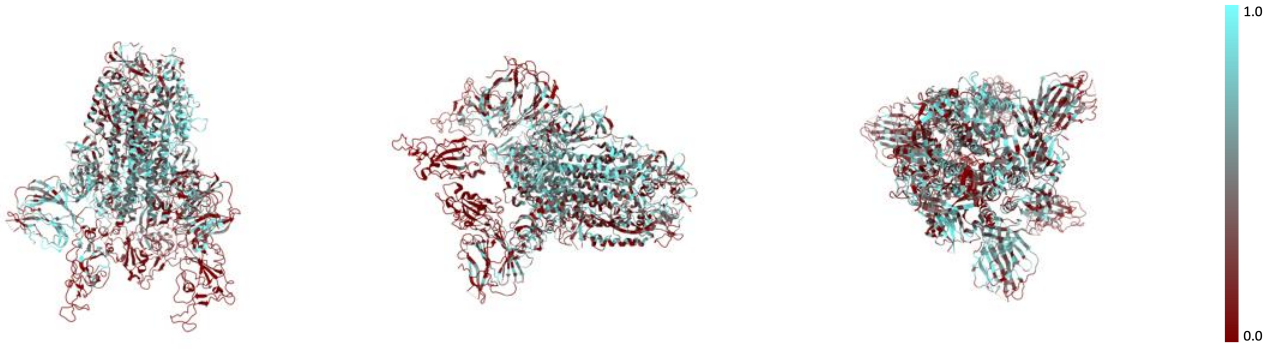
9.2 Q-score mapped to coordinate model (i)



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.

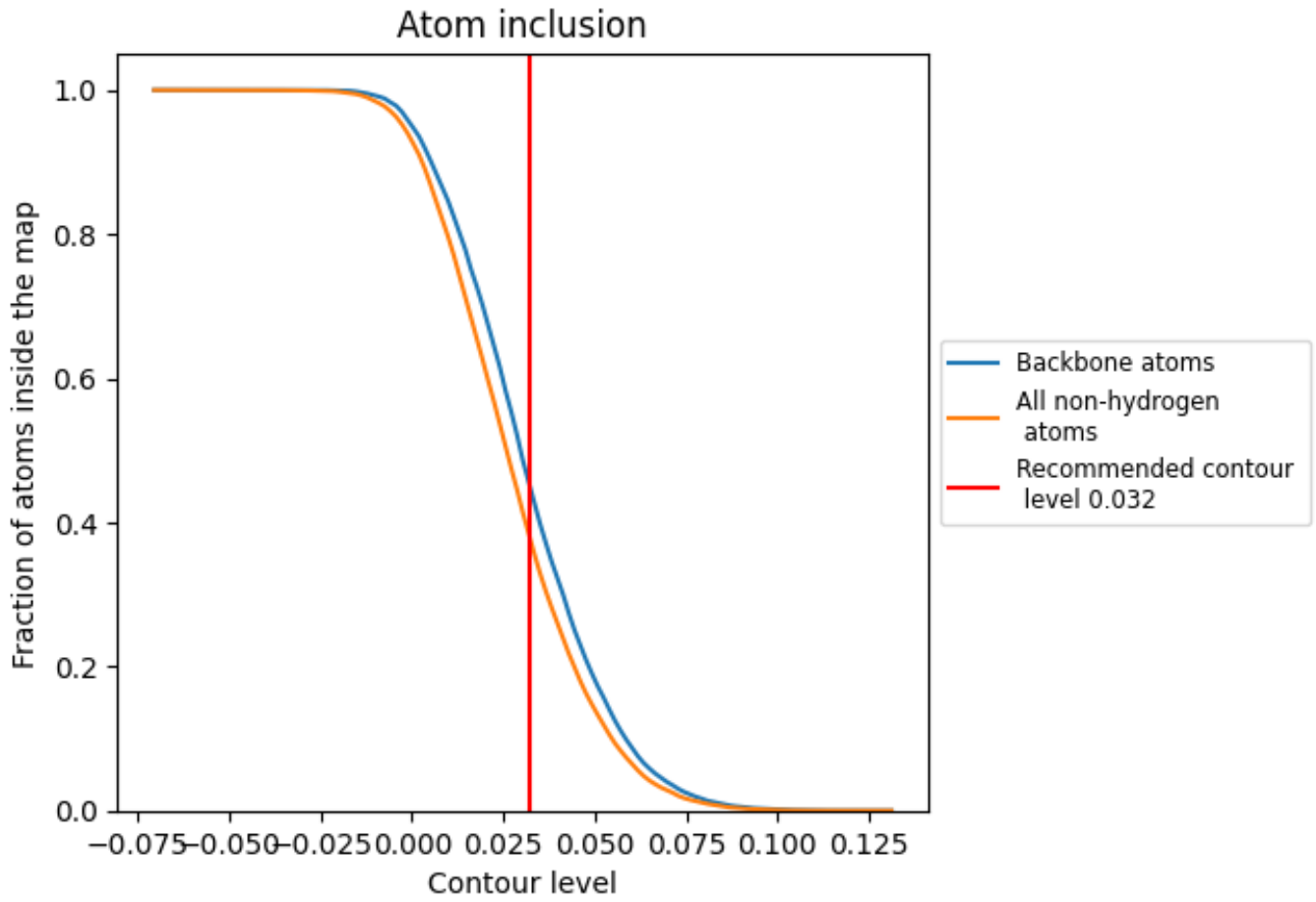
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.032).

9.4 Atom inclusion (i)



At the recommended contour level, 46% of all backbone atoms, 38% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.032) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.3839	0.0410
A	0.3434	0.0250
B	0.4195	0.0580
C	0.4132	0.0380
D	0.0000	-0.1130
E	0.0256	-0.0080
F	0.0357	0.0870
G	0.1639	0.0420
H	0.4098	0.2230
I	0.1429	0.0230
J	0.1429	-0.0700
K	0.1786	0.1480
L	0.0513	-0.0060
M	0.1786	0.0430
N	0.1000	0.0850
O	0.2000	0.1490
P	0.2600	0.0770
Q	0.5128	0.1790
R	0.0000	-0.0930
S	0.0000	0.0890
T	0.1786	0.0940
U	0.0000	-0.1300
V	0.0256	-0.0160
W	0.0000	-0.0130
X	0.0256	-0.0640