Full wwPDB EM Validation Report (i)

Nov 30, 2022 – 01:56 AM JST

PDB ID	:	7XNQ
EMDB ID	:	EMD-33323
Title	:	SARS-CoV-2 Omicron BA.4 variant spike
Authors	:	Wang, X.; Wang, L.
Deposited on	:	2022-04-29
Resolution	:	3.52 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

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

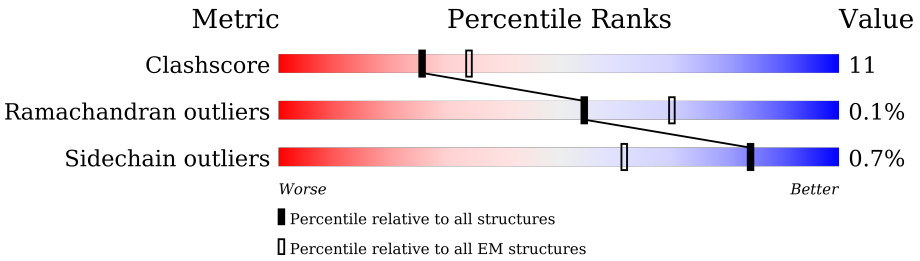
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.52 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	1268	20% 62% 23% 14%
1	B	1268	20% 63% 23% 14%
1	C	1268	20% 63% 22% • 14%
2	D	2	100% 50% 50%
2	E	2	50% 50% 50%
2	F	2	50% 50%
2	G	2	50% 100%
2	H	2	50% 100%

Continued on next page...

Continued from previous page...

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

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 26463 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1089	8499	5434	1412	1615	38	0	0
1	B	1089	8499	5434	1412	1615	38	0	0
1	C	1089	8499	5434	1412	1615	38	0	0

There are 129 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	ILE	THR	variant	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	27	SER	ALA	variant	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	140	ASP	GLY	variant	UNP P0DTC2
A	211	GLY	VAL	variant	UNP P0DTC2
A	337	ASP	GLY	variant	UNP P0DTC2
A	369	PHE	SER	variant	UNP P0DTC2
A	371	PRO	SER	variant	UNP P0DTC2
A	373	PHE	SER	variant	UNP P0DTC2
A	374	ALA	THR	variant	UNP P0DTC2
A	403	ASN	ASP	variant	UNP P0DTC2
A	406	SER	ARG	variant	UNP P0DTC2
A	415	ASN	LYS	variant	UNP P0DTC2
A	438	LYS	ASN	variant	UNP P0DTC2
A	450	ARG	LEU	variant	UNP P0DTC2
A	475	ASN	SER	variant	UNP P0DTC2
A	476	LYS	THR	variant	UNP P0DTC2
A	482	ALA	GLU	variant	UNP P0DTC2
A	484	VAL	PHE	variant	UNP P0DTC2
A	496	ARG	GLN	variant	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	499	TYR	ASN	variant	UNP P0DTC2
A	503	HIS	TYR	variant	UNP P0DTC2
A	612	GLY	ASP	variant	UNP P0DTC2
A	653	TYR	HIS	variant	UNP P0DTC2
A	656	SER	ASN	variant	UNP P0DTC2
A	677	LYS	ASN	variant	UNP P0DTC2
A	679	HIS	PRO	variant	UNP P0DTC2
A	681	ALA	ARG	variant	UNP P0DTC2
A	683	ALA	ARG	variant	UNP P0DTC2
A	762	LYS	ASN	variant	UNP P0DTC2
A	794	TYR	ASP	variant	UNP P0DTC2
A	815	PRO	PHE	variant	UNP P0DTC2
A	890	PRO	ALA	variant	UNP P0DTC2
A	897	PRO	ALA	variant	UNP P0DTC2
A	940	PRO	ALA	variant	UNP P0DTC2
A	952	HIS	GLN	variant	UNP P0DTC2
A	967	LYS	ASN	variant	UNP P0DTC2
A	984	PRO	LYS	engineered mutation	UNP P0DTC2
A	985	PRO	VAL	engineered mutation	UNP P0DTC2
B	22	ILE	THR	variant	UNP P0DTC2
B	?	-	LEU	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	27	SER	ALA	variant	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	140	ASP	GLY	variant	UNP P0DTC2
B	211	GLY	VAL	variant	UNP P0DTC2
B	337	ASP	GLY	variant	UNP P0DTC2
B	369	PHE	SER	variant	UNP P0DTC2
B	371	PRO	SER	variant	UNP P0DTC2
B	373	PHE	SER	variant	UNP P0DTC2
B	374	ALA	THR	variant	UNP P0DTC2
B	403	ASN	ASP	variant	UNP P0DTC2
B	406	SER	ARG	variant	UNP P0DTC2
B	415	ASN	LYS	variant	UNP P0DTC2
B	438	LYS	ASN	variant	UNP P0DTC2
B	450	ARG	LEU	variant	UNP P0DTC2
B	475	ASN	SER	variant	UNP P0DTC2
B	476	LYS	THR	variant	UNP P0DTC2
B	482	ALA	GLU	variant	UNP P0DTC2
B	484	VAL	PHE	variant	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	496	ARG	GLN	variant	UNP P0DTC2
B	499	TYR	ASN	variant	UNP P0DTC2
B	503	HIS	TYR	variant	UNP P0DTC2
B	612	GLY	ASP	variant	UNP P0DTC2
B	653	TYR	HIS	variant	UNP P0DTC2
B	656	SER	ASN	variant	UNP P0DTC2
B	677	LYS	ASN	variant	UNP P0DTC2
B	679	HIS	PRO	variant	UNP P0DTC2
B	681	ALA	ARG	variant	UNP P0DTC2
B	683	ALA	ARG	variant	UNP P0DTC2
B	762	LYS	ASN	variant	UNP P0DTC2
B	794	TYR	ASP	variant	UNP P0DTC2
B	815	PRO	PHE	variant	UNP P0DTC2
B	890	PRO	ALA	variant	UNP P0DTC2
B	897	PRO	ALA	variant	UNP P0DTC2
B	940	PRO	ALA	variant	UNP P0DTC2
B	952	HIS	GLN	variant	UNP P0DTC2
B	967	LYS	ASN	variant	UNP P0DTC2
B	984	PRO	LYS	engineered mutation	UNP P0DTC2
B	985	PRO	VAL	engineered mutation	UNP P0DTC2
C	22	ILE	THR	variant	UNP P0DTC2
C	?	-	LEU	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	27	SER	ALA	variant	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	140	ASP	GLY	variant	UNP P0DTC2
C	211	GLY	VAL	variant	UNP P0DTC2
C	337	ASP	GLY	variant	UNP P0DTC2
C	369	PHE	SER	variant	UNP P0DTC2
C	371	PRO	SER	variant	UNP P0DTC2
C	373	PHE	SER	variant	UNP P0DTC2
C	374	ALA	THR	variant	UNP P0DTC2
C	403	ASN	ASP	variant	UNP P0DTC2
C	406	SER	ARG	variant	UNP P0DTC2
C	415	ASN	LYS	variant	UNP P0DTC2
C	438	LYS	ASN	variant	UNP P0DTC2
C	450	ARG	LEU	variant	UNP P0DTC2
C	475	ASN	SER	variant	UNP P0DTC2
C	476	LYS	THR	variant	UNP P0DTC2
C	482	ALA	GLU	variant	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	484	VAL	PHE	variant	UNP P0DTC2
C	496	ARG	GLN	variant	UNP P0DTC2
C	499	TYR	ASN	variant	UNP P0DTC2
C	503	HIS	TYR	variant	UNP P0DTC2
C	612	GLY	ASP	variant	UNP P0DTC2
C	653	TYR	HIS	variant	UNP P0DTC2
C	656	SER	ASN	variant	UNP P0DTC2
C	677	LYS	ASN	variant	UNP P0DTC2
C	679	HIS	PRO	variant	UNP P0DTC2
C	681	ALA	ARG	variant	UNP P0DTC2
C	683	ALA	ARG	variant	UNP P0DTC2
C	762	LYS	ASN	variant	UNP P0DTC2
C	794	TYR	ASP	variant	UNP P0DTC2
C	815	PRO	PHE	variant	UNP P0DTC2
C	890	PRO	ALA	variant	UNP P0DTC2
C	897	PRO	ALA	variant	UNP P0DTC2
C	940	PRO	ALA	variant	UNP P0DTC2
C	952	HIS	GLN	variant	UNP P0DTC2
C	967	LYS	ASN	variant	UNP P0DTC2
C	984	PRO	LYS	engineered mutation	UNP P0DTC2
C	985	PRO	VAL	engineered mutation	UNP P0DTC2

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

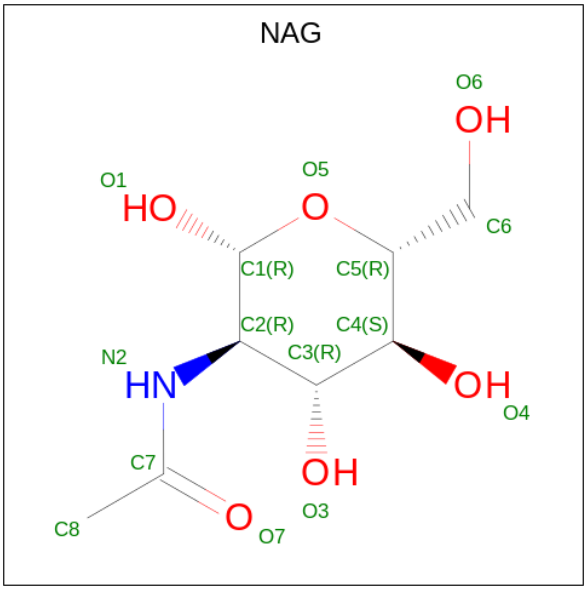
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	D	2	28	16	2	10	0	0
2	E	2	28	16	2	10	0	0
2	F	2	28	16	2	10	0	0
2	G	2	28	16	2	10	0	0
2	H	2	28	16	2	10	0	0
2	I	2	28	16	2	10	0	0

Continued on next page...

Continued from previous page...

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

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
3	A	1	154	88	11	55	0
3	A	1	154	88	11	55	0
3	A	1	154	88	11	55	0
3	A	1	154	88	11	55	0
3	A	1	154	88	11	55	0
3	A	1	154	88	11	55	0
3	A	1	154	88	11	55	0
3	A	1	154	88	11	55	0
3	A	1	154	88	11	55	0
3	A	1	154	88	11	55	0
3	A	1	154	88	11	55	0
3	B	1	154	88	11	55	0
3	B	1	154	88	11	55	0
3	B	1	154	88	11	55	0
3	B	1	154	88	11	55	0
3	B	1	154	88	11	55	0
3	B	1	154	88	11	55	0
3	B	1	154	88	11	55	0
3	B	1	154	88	11	55	0
3	B	1	154	88	11	55	0
3	B	1	154	88	11	55	0

Continued on next page...

Continued from previous page...

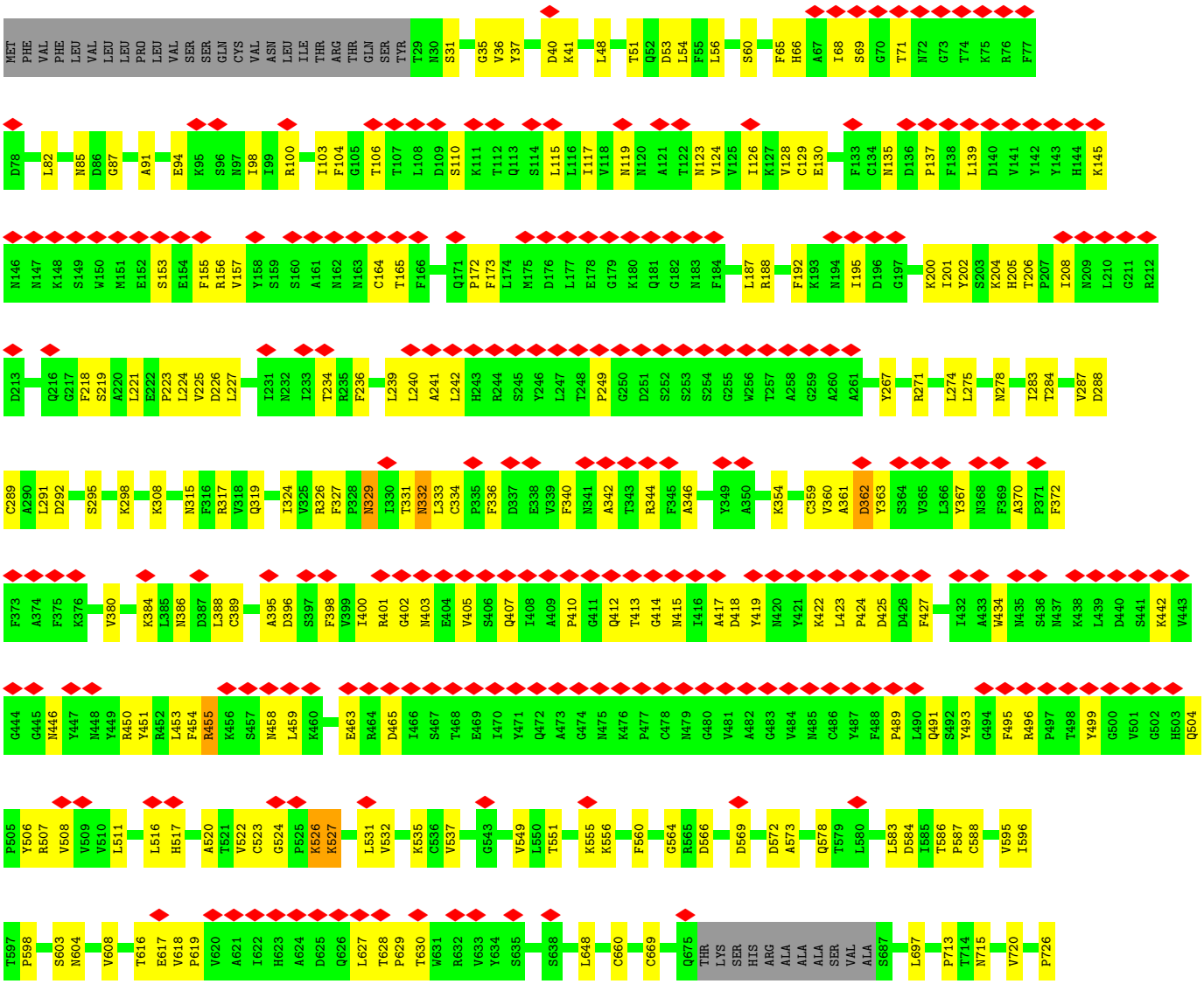
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
3	C	1	154	88	11	55	0
3	C	1	154	88	11	55	0
3	C	1	154	88	11	55	0
3	C	1	154	88	11	55	0
3	C	1	154	88	11	55	0
3	C	1	154	88	11	55	0
3	C	1	154	88	11	55	0
3	C	1	154	88	11	55	0
3	C	1	154	88	11	55	0
3	C	1	154	88	11	55	0
3	C	1	154	88	11	55	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Spike glycoprotein

Chain A:



T730 S733 V734 D735 C736 T737 M738 E746 L751 L752 Q753 S756 F757 L761 I768 N775 K784 Q785 P790 F795 F800 S801 Q802 I803 L804 K823 L826 ALA ASP ALA GLY PHE ILE LYS GLN TYR GLY ASP CYS LEU GLY ASP ILE ALA ALA ARG

ASP L847 F853 L856 T857 D865 E866 M867 I868 W884 L892 Q893 I894 P895 M898 Y902 R903 F904 V909 T910 Q911 L914 Q924 Q933 S937 S938 L946 V949 N953 T959 L960 Q963 K967 F968 G969 L979 D983 P984 P985

E988 I991 D992 R993 L994 I995 L1010 R1017 T1025 K1026 M1027 S1028 E1029 L1032 G1033 D1039 F1040 P1051 Q1052 G1057 V1063 Q1069 E1070 R1089 S1095 W1100 T1114 T1115 D1116 F1119 C1124 D1125 I1130 N1133 Y1136 D1137 P1138 L1139 Q1140 P1141 E1142

L1143 D1144 S1145 F1146 K1147 E1148 GLU LEU ASP LYS TYR PHE LYS ASN HIS THR SER PRO ASP VAL ASP LEU GLY ASP ILE SER GLY ILE ASN ALA SER VAL VAL ASN ILE GLN LYS GLU ILE ASP ARG LEU ASN GLU VAL ALA LYS ASN LEU ASN GLU SER LEU ILE ASP LEU GLN GLU LEU GLY

LYS TYR GLU GLN TYR ILE LYS TRP PRO TRP TYR ILE TRP LEU GLY PHE ILE ALA GLY LEU ILE ALA ILE VAL MET VAL THR ILE MET LEU CYS CYS MET THR SER CYS CYS SER CYS LEU LYS GLY CYS CYS SER CYS GLY SER CYS CYS LYS PHE ASP GLU ASP ASP SER GLU PRO VAL

LEU LYS GLY VAL LYS LEU HIS TYR THR

- Molecule 1: Spike glycoprotein

Chain B:

MET PHE VAL PHE LEU VAL LEU LEU PRO LEU VAL SER SER GLN CYS VAL ASN LEU ILE THR ARG THR GLN SER TYR T29 N30 S31 G35 V36 Y37 D40 K41 L48 T51 Q52 D53 L54 F55 L56 S60 W64 F65 H66 A67 I68 S69 G70 T71 N72 G73 T74 K75 R76

F77 D78 N79 P80 V81 L82 N85 D86 G87 A91 E94 K95 S96 N97 I98 I99 R100 G101 W102 I103 F104 G105 T106 T107 L108 D109 S110 K111 T112 Q113 S114 L115 L116 I117 V118 N119 N120 A121 T122 N123 V124 V125 I126 K127 V128 C129 E130 F133 C134 N135 D136 P137 F138 L139 D140 V141

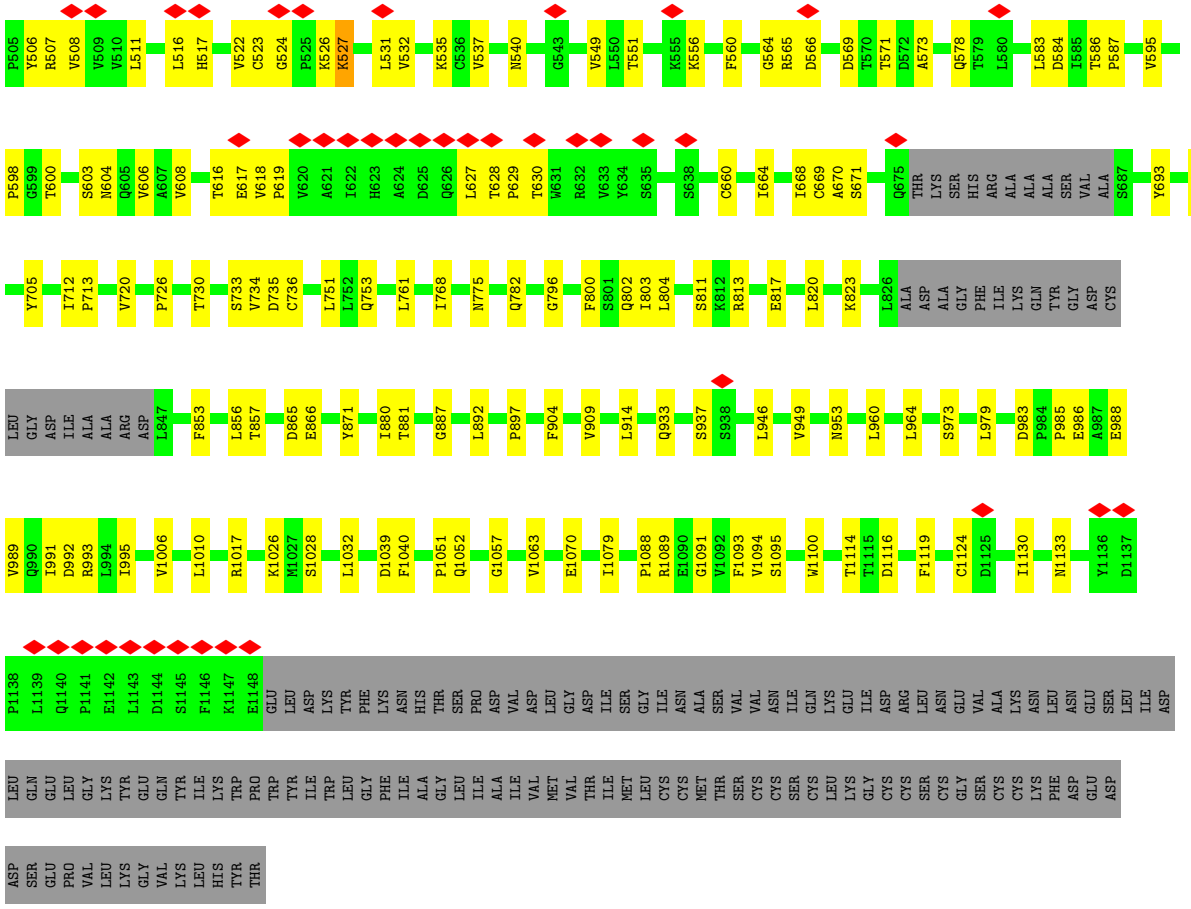
Y142 Y143 H144 K145 N146 N147 K148 S149 W150 M151 E152 S153 E154 F155 R156 V157 Y158 S159 S160 A161 N162 N163 C164 T165 F166 P172 F173 L174 M175 D176 L177 E178 G179 K180 Q181 G182 N183 F184 L187 R188 F192 K193 N194 I195 D196 G197 Y198 F199 K200 I201 Y202 S203 K204 H205 T206 P207 I208

N209 L210 G211 R212 D213 G216 G217 F218 S219 A220 L221 E222 P223 L224 V225 D226 L227 I231 N232 I233 T234 R235 F236 Q237 L240 A241 L242 H243 R244 S245 Y246 L247 T248 P249 G250 D251 S252 S253 S254 G255 W256 T257 A258 G259 A260 A261 A262 Y267 R271 L274 L275 N278

I283 T284 V287 D288 C289 A290 L291 D292 P293 L294 S295 K298 V306 E307 K308 N315 Q319 I324 V325 R326 F327 P328 N329 I330 T331 N332 L333 C334 P335 F336 D337 E338 V339 F340 N341 A342 T343 R344 F345 A346 Y349 A350 C359 V360 A361 D362 Y363 S364 V365 L366 Y367 N368

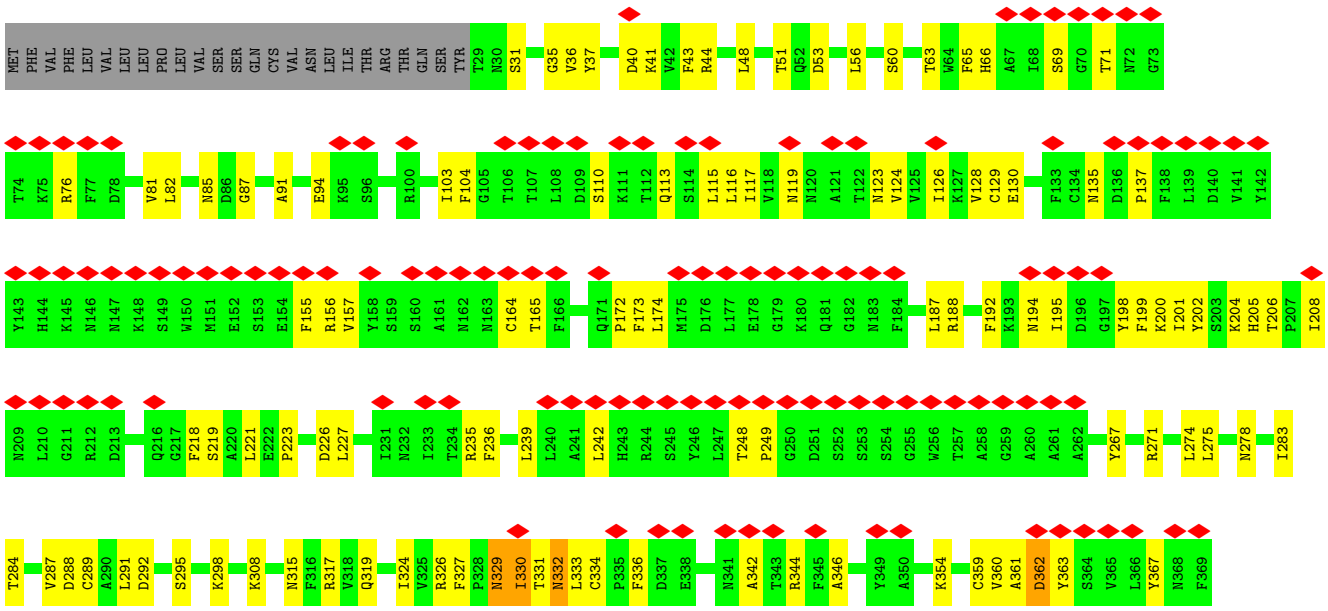
F369 A370 P371 F372 F373 A374 F375 K376 V380 K384 D387 L388 C389 F390 A395 D396 S397 F398 R401 G402 N403 E404 V405 S406 Q407 I408 A409 P410 G411 Q412 T413 G414 N415 I416 A417 D418 Y419 N420 Y421 K422 L423 P424 D425 D426 F427 I432 A433 W434 N435 S436 N437 K438 L439 D440

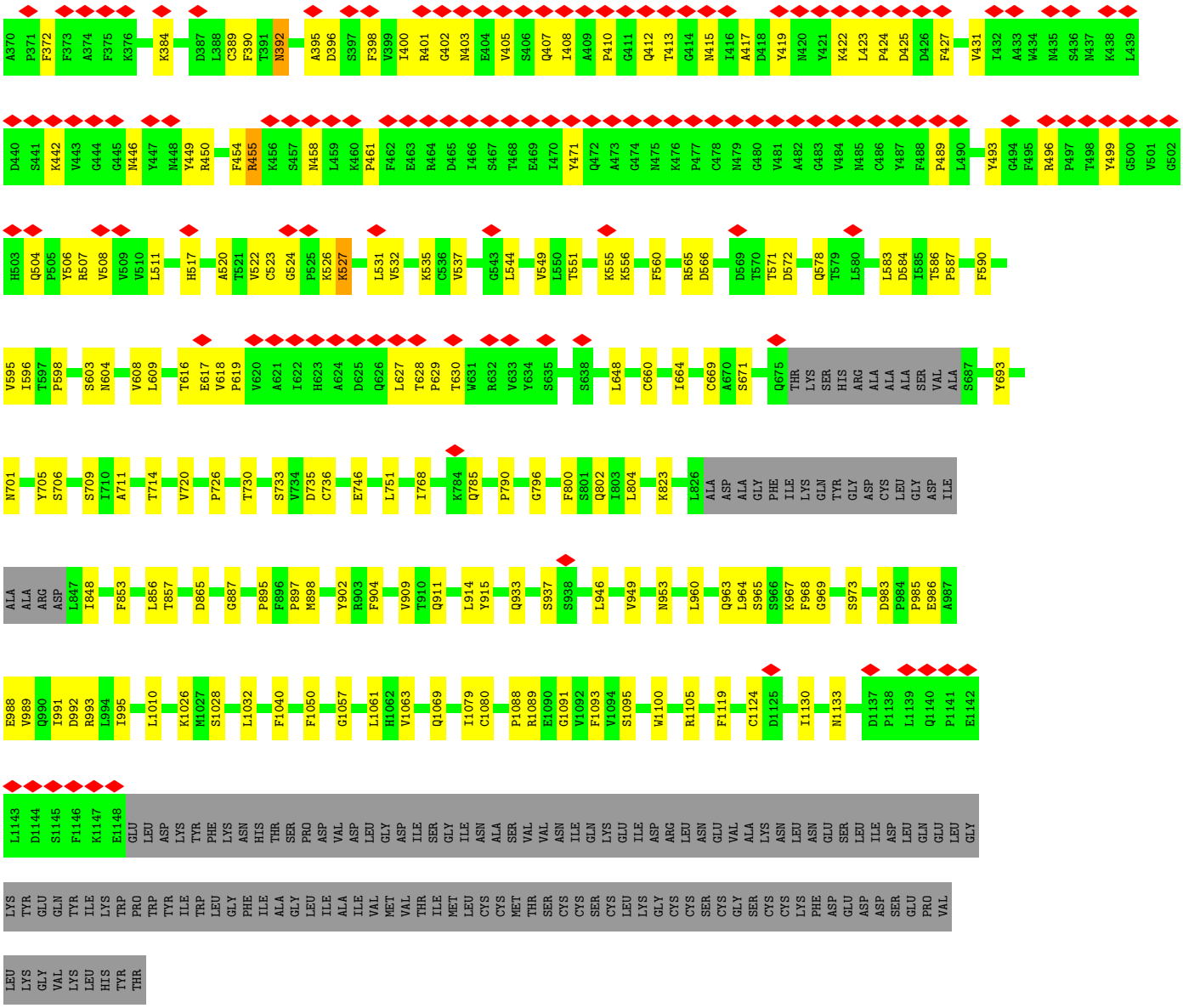
S441 K442 V443 G444 G445 N446 Y447 N448 Y449 R450 Y451 F454 R455 K456 S457 N458 L459 K460 E463 R464 D465 I466 S467 T468 E469 I470 Y471 Q472 A473 G474 N475 K476 P477 C478 N479 G480 V481 A482 G483 V484 N485 C486 Y487 F488 P489 L490 G494 F495 R496 P497 T498 Y499 G500 V501 G502 H503 Q504



- Molecule 1: Spike glycoprotein

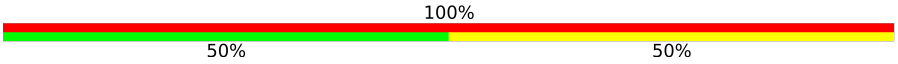
Chain C:





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

Chain D:



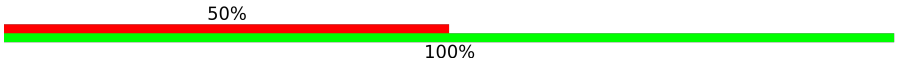
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:

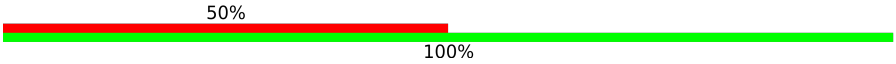
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:

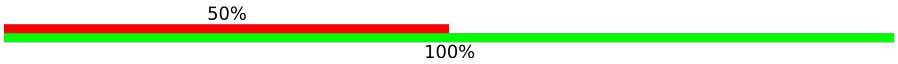
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G: 

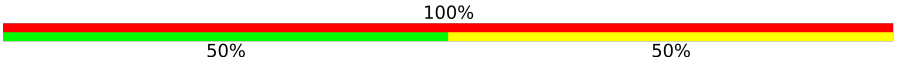
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H: 

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

Chain I: 

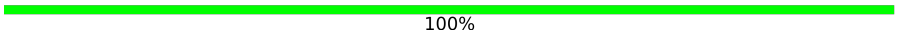
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J: 

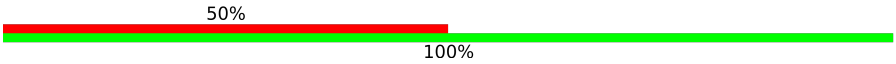
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:

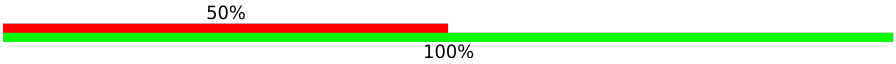
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L: 

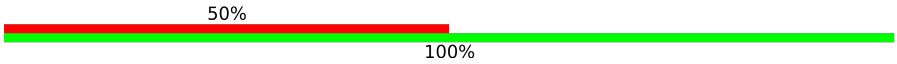
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M: 

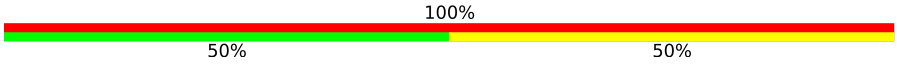
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N: 

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

Chain O: 

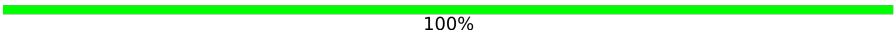
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P: 

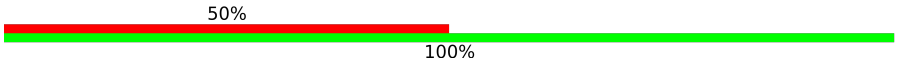
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:

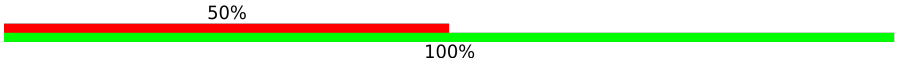
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R: 

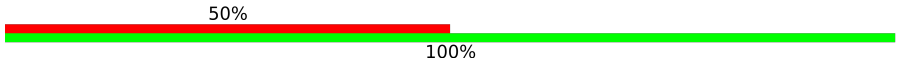
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S: 

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

Chain T: 

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

Chain U: 

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	129691	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K2 BASE (4k x 4k)	Depositor
Maximum map value	3.115	Depositor
Minimum map value	-1.963	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.067	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	332.8, 332.8, 332.8	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.26	0/8707	0.49	0/11860
1	B	0.26	0/8707	0.49	0/11860
1	C	0.26	0/8707	0.48	0/11860
All	All	0.26	0/26121	0.49	0/35580

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8499	0	8260	222	0
1	B	8499	0	8259	212	0
1	C	8499	0	8259	213	0
2	D	28	0	25	1	0
2	E	28	0	25	0	0
2	F	28	0	25	1	0
2	G	28	0	25	0	0
2	H	28	0	25	0	0
2	I	28	0	25	0	0
2	J	28	0	25	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	K	28	0	25	0	0
2	L	28	0	25	0	0
2	M	28	0	25	0	0
2	N	28	0	25	0	0
2	O	28	0	25	0	0
2	P	28	0	25	1	0
2	Q	28	0	24	0	0
2	R	28	0	25	0	0
2	S	28	0	25	0	0
2	T	28	0	25	0	0
2	U	28	0	25	0	0
3	A	154	0	141	0	0
3	B	154	0	141	1	0
3	C	154	0	141	1	0
All	All	26463	0	25650	594	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (594) 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:524:GLY:HA3	1:B:526:LYS:HZ3	1.04	1.18
1:C:524:GLY:HA3	1:C:526:LYS:HZ3	1.06	1.10
1:A:524:GLY:HA3	1:A:526:LYS:HZ3	1.18	1.08
1:A:527:LYS:HE3	1:A:527:LYS:HA	1.49	0.94
1:C:527:LYS:HE3	1:C:527:LYS:HA	1.51	0.92
1:B:527:LYS:HE3	1:B:527:LYS:HA	1.51	0.92
1:B:524:GLY:HA3	1:B:526:LYS:NZ	1.90	0.84
1:C:389:CYS:HA	1:C:523:CYS:HB3	1.56	0.84
1:A:360:VAL:HG13	1:A:524:GLY:HA2	1.59	0.84
1:A:389:CYS:HA	1:A:523:CYS:HB3	1.57	0.84
1:B:389:CYS:HA	1:B:523:CYS:HB3	1.56	0.84
1:C:524:GLY:HA3	1:C:526:LYS:NZ	1.91	0.84
1:A:407:GLN:HG2	1:A:412:GLN:HG2	1.57	0.83
1:A:753:GLN:HE22	1:C:969:GLY:H	1.26	0.81
1:A:524:GLY:HA3	1:A:526:LYS:NZ	1.98	0.78
1:B:360:VAL:HG13	1:B:524:GLY:HA2	1.67	0.76
1:B:345:PHE:HB3	1:B:397:SER:HB3	1.67	0.76
1:B:332:ASN:OD1	1:B:359:CYS:HA	1.88	0.73
1:B:454:PHE:HB3	1:B:489:PRO:HB3	1.69	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:360:VAL:HG13	1:C:524:GLY:HA2	1.69	0.72
1:A:560:PHE:HD2	1:B:41:LYS:HZ2	1.36	0.71
1:B:324:ILE:HD12	1:B:537:VAL:HG21	1.72	0.71
1:C:454:PHE:HB3	1:C:489:PRO:HB3	1.73	0.70
1:C:344:ARG:HH21	1:C:346:ALA:H	1.38	0.69
1:A:336:PHE:CE1	1:A:361:ALA:HB1	2.27	0.69
1:A:911:GLN:NE2	1:C:1088:PRO:O	2.26	0.69
1:B:344:ARG:HH21	1:B:346:ALA:H	1.41	0.69
1:B:242:LEU:HD21	1:B:248:THR:HG21	1.72	0.69
1:C:336:PHE:CE1	1:C:361:ALA:HB1	2.28	0.69
1:A:344:ARG:HH21	1:A:346:ALA:H	1.39	0.69
1:A:895:PRO:HA	1:C:705:TYR:HE2	1.58	0.68
1:B:336:PHE:CE1	1:B:361:ALA:HB1	2.29	0.68
1:B:1088:PRO:O	1:C:911:GLN:NE2	2.27	0.68
1:C:117:ILE:HG12	1:C:126:ILE:HG23	1.76	0.68
1:C:69:SER:HB2	1:C:242:LEU:HD23	1.75	0.68
1:C:173:PHE:O	1:C:205:HIS:NE2	2.26	0.68
1:C:407:GLN:HG2	1:C:412:GLN:HG2	1.74	0.68
1:A:753:GLN:HE21	1:C:967:LYS:HB2	1.59	0.68
1:C:401:ARG:HG2	1:C:403:ASN:H	1.57	0.68
1:C:119:ASN:HD21	1:C:174:LEU:HB2	1.58	0.67
1:A:173:PHE:O	1:A:205:HIS:NE2	2.27	0.67
1:B:595:VAL:HG22	1:B:608:VAL:HG12	1.77	0.67
1:B:173:PHE:O	1:B:205:HIS:NE2	2.27	0.67
1:A:454:PHE:HB3	1:A:489:PRO:HB3	1.76	0.66
1:C:392:ASN:HD22	1:C:392:ASN:N	1.95	0.65
1:A:595:VAL:HG22	1:A:608:VAL:HG12	1.78	0.65
1:C:802:GLN:NE2	1:C:933:GLN:OE1	2.30	0.65
1:B:87:GLY:HA2	1:B:192:PHE:O	1.96	0.65
1:B:128:VAL:HB	1:B:165:THR:HB	1.78	0.65
1:A:360:VAL:HG13	1:A:524:GLY:CA	2.25	0.65
1:B:117:ILE:HG12	1:B:126:ILE:HG23	1.79	0.65
1:A:332:ASN:OD1	1:A:332:ASN:N	2.27	0.64
1:A:117:ILE:HG12	1:A:126:ILE:HG23	1.79	0.64
1:A:802:GLN:NE2	1:A:933:GLN:OE1	2.30	0.64
1:C:333:LEU:HD23	1:C:334:CYS:N	2.13	0.64
1:C:271:ARG:NH1	1:C:288:ASP:OD2	2.30	0.64
1:A:104:PHE:HB2	1:A:115:LEU:HB2	1.79	0.64
1:A:756:SER:OG	1:C:963:GLN:OE1	2.12	0.64
1:A:823:LYS:HE3	1:A:937:SER:HA	1.80	0.64
1:B:69:SER:HB2	1:B:242:LEU:HD23	1.78	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:128:VAL:HB	1:C:165:THR:HB	1.80	0.64
1:C:595:VAL:HG22	1:C:608:VAL:HG12	1.80	0.64
1:A:331:THR:HA	1:A:360:VAL:CG2	2.28	0.64
1:A:526:LYS:HE2	1:A:526:LYS:H	1.60	0.64
1:A:735:ASP:OD2	1:C:315:ASN:ND2	2.30	0.63
1:B:802:GLN:NE2	1:B:933:GLN:OE1	2.31	0.63
1:B:395:ALA:HB2	1:B:511:LEU:HD13	1.80	0.63
1:B:319:GLN:NE2	1:B:628:THR:OG1	2.24	0.63
1:B:524:GLY:CA	1:B:526:LYS:HZ3	1.97	0.63
1:C:395:ALA:HB2	1:C:511:LEU:HD13	1.80	0.63
1:A:94:GLU:OE2	1:A:188:ARG:NH1	2.30	0.62
1:B:271:ARG:NH1	1:B:288:ASP:OD2	2.32	0.62
1:B:705:TYR:HE1	1:C:895:PRO:HA	1.64	0.62
1:A:195:ILE:HB	1:A:200:LYS:HZ3	1.65	0.62
1:B:344:ARG:NH2	1:B:346:ALA:O	2.32	0.62
1:C:401:ARG:HB2	1:C:493:TYR:CE1	2.35	0.62
1:A:271:ARG:NH1	1:A:288:ASP:OD2	2.33	0.62
1:A:395:ALA:HB2	1:A:511:LEU:HD13	1.81	0.62
1:B:333:LEU:HD23	1:B:334:CYS:N	2.14	0.62
1:B:94:GLU:OE2	1:B:188:ARG:NH1	2.32	0.62
1:C:94:GLU:OE2	1:C:188:ARG:NH1	2.32	0.61
1:C:499:TYR:O	1:C:504:GLN:NE2	2.32	0.61
1:B:124:VAL:HG13	1:B:172:PRO:HA	1.82	0.61
1:A:627:LEU:HG	1:A:630:THR:H	1.65	0.61
1:B:627:LEU:HG	1:B:630:THR:H	1.65	0.61
1:C:556:LYS:NZ	2:D:1:NAG:O6	2.32	0.61
1:A:442:LYS:HD3	1:A:446:ASN:HA	1.83	0.61
1:A:924:GLN:HE21	2:F:1:NAG:H62	1.65	0.61
1:C:51:THR:HG22	1:C:53:ASP:H	1.66	0.61
1:C:330:ILE:HD12	1:C:332:ASN:H	1.65	0.61
1:B:499:TYR:O	1:B:504:GLN:NE2	2.34	0.60
1:C:823:LYS:HE3	1:C:937:SER:HA	1.82	0.60
1:C:319:GLN:NE2	1:C:628:THR:OG1	2.24	0.60
1:A:1028:SER:HA	1:A:1032:LEU:HD12	1.81	0.60
1:A:361:ALA:O	1:A:363:TYR:CD1	2.55	0.60
1:A:124:VAL:HG13	1:A:172:PRO:HA	1.83	0.60
1:B:315:ASN:ND2	1:C:735:ASP:OD2	2.34	0.60
1:B:823:LYS:HE3	1:B:937:SER:HA	1.84	0.60
1:B:98:ILE:HG22	1:B:240:LEU:HD11	1.83	0.59
1:A:333:LEU:HD23	1:A:334:CYS:N	2.17	0.59
1:A:775:ASN:OD1	1:A:1017:ARG:NH1	2.35	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:51:THR:HG22	1:B:53:ASP:H	1.66	0.59
1:C:361:ALA:O	1:C:363:TYR:CD1	2.55	0.59
1:A:555:LYS:NZ	1:A:572:ASP:OD2	2.35	0.59
1:B:361:ALA:O	1:B:363:TYR:CD1	2.55	0.59
1:A:317:ARG:NH1	1:A:588:CYS:SG	2.75	0.59
1:A:736:CYS:HB3	1:A:751:LEU:HD21	1.84	0.59
1:A:153:SER:HA	1:A:156:ARG:HH22	1.68	0.59
1:C:627:LEU:HG	1:C:630:THR:H	1.67	0.59
1:A:556:LYS:NZ	2:J:1:NAG:O6	2.32	0.59
1:B:326:ARG:HH21	1:B:578:GLN:HB2	1.68	0.58
1:C:442:LYS:HD3	1:C:446:ASN:HA	1.84	0.58
1:B:104:PHE:HB2	1:B:115:LEU:HB2	1.85	0.58
1:B:733:SER:HG	1:B:857:THR:HG1	1.51	0.58
1:B:155:PHE:HD2	1:B:157:VAL:HG13	1.67	0.58
1:B:361:ALA:O	1:B:363:TYR:N	2.36	0.58
1:A:332:ASN:O	1:A:359:CYS:HB2	2.03	0.58
1:B:442:LYS:HD3	1:B:446:ASN:HA	1.85	0.58
1:C:326:ARG:HH21	1:C:578:GLN:HB2	1.69	0.58
1:C:410:PRO:HB3	1:C:423:LEU:HB2	1.86	0.58
1:C:124:VAL:HG13	1:C:172:PRO:HA	1.84	0.58
1:C:275:LEU:HD23	1:C:283:ILE:HD13	1.86	0.58
1:A:517:HIS:HB2	1:B:41:LYS:HB3	1.86	0.57
1:A:800:PHE:HD1	1:A:803:ILE:HD11	1.67	0.57
1:A:453:LEU:HB2	1:A:491:GLN:HB2	1.85	0.57
1:A:979:LEU:O	1:C:384:LYS:NZ	2.35	0.57
1:A:319:GLN:NE2	1:A:628:THR:OG1	2.26	0.57
1:C:736:CYS:HB3	1:C:751:LEU:HD21	1.86	0.57
1:B:992:ASP:HA	1:B:995:ILE:HG22	1.86	0.57
1:C:40:ASP:OD2	1:C:44:ARG:NH2	2.38	0.57
1:C:192:PHE:CD1	1:C:201:ILE:HD12	2.39	0.57
1:A:326:ARG:HH21	1:A:578:GLN:HB2	1.70	0.57
1:A:424:PRO:HG2	1:A:427:PHE:HB2	1.87	0.57
1:A:98:ILE:HG23	1:A:242:LEU:HD13	1.87	0.57
1:C:361:ALA:O	1:C:363:TYR:N	2.37	0.57
1:A:324:ILE:HD12	1:A:537:VAL:HG21	1.87	0.56
1:A:344:ARG:NH2	1:A:346:ALA:O	2.38	0.56
1:A:422:LYS:HZ1	1:A:458:ASN:HB2	1.68	0.56
1:B:664:ILE:HD12	1:B:668:ILE:HG22	1.87	0.56
1:C:199:PHE:CE1	1:C:201:ILE:HD11	2.39	0.56
1:A:51:THR:HG22	1:A:53:ASP:H	1.70	0.56
1:A:784:LYS:HG3	1:A:785:GLN:HG3	1.85	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:104:PHE:HB2	1:C:115:LEU:HB2	1.86	0.56
1:C:344:ARG:NH2	1:C:346:ALA:O	2.38	0.56
1:C:526:LYS:HE2	1:C:526:LYS:H	1.70	0.56
1:B:195:ILE:HB	1:B:200:LYS:HZ3	1.68	0.56
1:C:417:ALA:HB1	1:C:422:LYS:HD3	1.86	0.56
1:C:137:PRO:HD3	1:C:155:PHE:HB3	1.87	0.56
1:C:1026:LYS:NZ	1:C:1040:PHE:O	2.37	0.56
1:A:1051:PRO:O	1:A:1052:GLN:NE2	2.38	0.56
1:A:128:VAL:HB	1:A:165:THR:HB	1.86	0.56
1:C:135:ASN:ND2	1:C:156:ARG:O	2.37	0.56
1:A:499:TYR:O	1:A:504:GLN:NE2	2.39	0.56
1:B:153:SER:HA	1:B:156:ARG:HH22	1.71	0.56
1:C:334:CYS:SG	1:C:360:VAL:C	2.84	0.56
1:C:392:ASN:N	1:C:392:ASN:ND2	2.52	0.56
1:C:398:PHE:HD2	1:C:508:VAL:HB	1.70	0.56
1:A:361:ALA:O	1:A:363:TYR:N	2.39	0.55
1:A:988:GLU:HA	1:A:991:ILE:HB	1.86	0.55
1:B:556:LYS:NZ	2:P:1:NAG:O6	2.34	0.55
1:A:1089:ARG:HG2	1:A:1119:PHE:HD1	1.70	0.55
1:C:344:ARG:HH12	1:C:449:TYR:HE1	1.54	0.55
1:A:401:ARG:HG2	1:A:403:ASN:H	1.70	0.55
1:B:564:GLY:HA3	1:B:573:ALA:HB3	1.88	0.55
1:B:964:LEU:O	1:B:973:SER:OG	2.23	0.55
1:B:64:TRP:NE1	1:B:66:HIS:HB2	2.21	0.55
1:C:334:CYS:SG	1:C:360:VAL:N	2.79	0.55
1:A:342:ALA:O	1:A:507:ARG:NH1	2.39	0.55
1:A:627:LEU:HD12	1:A:629:PRO:HG2	1.88	0.55
1:B:334:CYS:SG	1:B:360:VAL:C	2.85	0.55
1:B:345:PHE:CE2	1:B:507:ARG:HD2	2.42	0.55
1:A:308:LYS:HG3	1:A:598:PRO:HA	1.87	0.55
1:A:422:LYS:NZ	1:A:458:ASN:HB2	2.22	0.55
1:B:603:SER:OG	1:B:604:ASN:N	2.39	0.55
1:C:308:LYS:HG3	1:C:598:PRO:HA	1.89	0.55
1:C:531:LEU:HD11	1:C:583:LEU:HD21	1.89	0.55
1:C:992:ASP:HA	1:C:995:ILE:HG22	1.89	0.55
1:B:308:LYS:HG3	1:B:598:PRO:HA	1.89	0.54
1:C:856:LEU:HD11	1:C:960:LEU:HD23	1.88	0.54
1:C:324:ILE:HD12	1:C:537:VAL:HG21	1.89	0.54
1:A:226:ASP:OD1	1:A:227:LEU:N	2.41	0.54
1:B:1026:LYS:NZ	1:B:1040:PHE:O	2.40	0.54
1:B:37:TYR:HA	1:B:221:LEU:H	1.71	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:361:ALA:O	1:B:363:TYR:HD1	1.90	0.54
1:C:291:LEU:HD23	1:C:292:ASP:HB2	1.89	0.54
1:A:331:THR:HA	1:A:360:VAL:HG21	1.89	0.54
1:A:768:ILE:HD11	1:A:1010:LEU:HD23	1.90	0.54
1:B:288:ASP:OD1	1:B:289:CYS:N	2.41	0.54
1:B:410:PRO:HB3	1:B:423:LEU:HB2	1.90	0.54
1:C:720:VAL:HG22	1:C:1063:VAL:HG22	1.89	0.54
1:C:1050:PHE:HB2	1:C:1061:LEU:HB2	1.90	0.54
1:A:361:ALA:O	1:A:363:TYR:HD1	1.91	0.54
1:C:544:LEU:HD11	1:C:571:THR:HG21	1.90	0.53
1:A:65:PHE:HE2	1:A:82:LEU:HD11	1.72	0.53
1:A:425:ASP:HB3	1:C:985:PRO:HB3	1.89	0.53
1:B:135:ASN:ND2	1:B:156:ARG:O	2.40	0.53
1:B:291:LEU:HD23	1:B:292:ASP:HB2	1.90	0.53
1:B:713:PRO:HA	1:B:1070:GLU:HA	1.89	0.53
1:A:564:GLY:HA3	1:A:573:ALA:HB3	1.90	0.53
1:C:1095:SER:HB3	1:C:1100:TRP:CD2	2.43	0.53
1:B:627:LEU:HD12	1:B:629:PRO:HG2	1.90	0.53
1:C:887:GLY:HA3	1:C:1032:LEU:HD12	1.90	0.53
1:A:135:ASN:ND2	1:A:156:ARG:O	2.41	0.53
1:A:288:ASP:OD1	1:A:289:CYS:N	2.42	0.53
1:A:895:PRO:HB2	1:A:898:MET:HG3	1.91	0.53
1:B:517:HIS:HB2	1:C:41:LYS:HB3	1.91	0.53
1:C:195:ILE:HB	1:C:200:LYS:HZ3	1.74	0.53
1:C:1089:ARG:HG2	1:C:1119:PHE:HD1	1.73	0.53
1:B:417:ALA:HB1	1:B:422:LYS:HD3	1.90	0.53
1:C:532:VAL:HG21	1:C:535:LYS:HB2	1.90	0.53
1:A:1095:SER:HB3	1:A:1100:TRP:CD2	2.44	0.53
1:B:817:GLU:HA	1:B:820:LEU:HD12	1.91	0.53
1:C:327:PHE:O	1:C:578:GLN:NE2	2.41	0.53
1:B:1095:SER:HB3	1:B:1100:TRP:CD2	2.44	0.52
1:C:603:SER:OG	1:C:604:ASN:N	2.42	0.52
1:A:291:LEU:HD23	1:A:292:ASP:HB2	1.91	0.52
1:A:398:PHE:HD2	1:A:508:VAL:HB	1.73	0.52
1:B:401:ARG:HG2	1:B:403:ASN:H	1.74	0.52
1:B:880:ILE:HG13	1:B:881:THR:HG23	1.91	0.52
1:C:865:ASP:N	1:C:865:ASP:OD1	2.41	0.52
1:A:532:VAL:HG21	1:A:535:LYS:HB2	1.91	0.52
1:C:71:THR:H	1:C:76:ARG:HB2	1.74	0.52
1:B:334:CYS:SG	1:B:360:VAL:N	2.82	0.52
1:B:768:ILE:HD11	1:B:1010:LEU:HD23	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:361:ALA:O	1:C:363:TYR:HD1	1.92	0.52
1:C:627:LEU:HD12	1:C:629:PRO:HG2	1.92	0.52
1:A:603:SER:OG	1:A:604:ASN:N	2.42	0.52
1:B:64:TRP:HE1	1:B:66:HIS:HB2	1.74	0.52
1:B:332:ASN:O	1:B:359:CYS:HB2	2.10	0.52
1:B:701:ASN:ND2	1:C:785:GLN:OE1	2.43	0.52
1:B:331:THR:HA	1:B:360:VAL:HG23	1.92	0.52
1:B:367:TYR:HA	1:B:372:PHE:HE1	1.75	0.52
1:A:726:PRO:HB3	1:A:949:VAL:HG21	1.92	0.51
1:B:560:PHE:HD2	1:C:41:LYS:HE3	1.74	0.51
1:A:87:GLY:HA2	1:A:192:PHE:O	2.10	0.51
1:B:415:ASN:HA	1:B:419:TYR:HD2	1.75	0.51
1:B:1051:PRO:O	1:B:1052:GLN:NE2	2.41	0.51
1:A:100:ARG:HG3	1:A:241:ALA:HB3	1.91	0.51
1:A:697:LEU:HD22	1:B:871:TYR:CE1	2.45	0.51
1:B:664:ILE:HD11	1:B:670:ALA:HB2	1.92	0.51
1:B:887:GLY:HA3	1:B:1032:LEU:HD12	1.93	0.51
1:C:206:THR:HG22	1:C:208:ILE:HG12	1.93	0.51
1:A:730:THR:HB	1:A:953:ASN:ND2	2.25	0.51
1:B:1114:THR:OG1	1:B:1116:ASP:OD1	2.20	0.51
1:C:768:ILE:HD11	1:C:1010:LEU:HD23	1.93	0.51
1:A:569:ASP:OD2	1:B:973:SER:OG	2.25	0.51
1:B:81:VAL:HG21	1:B:235:ARG:HD3	1.93	0.51
1:A:992:ASP:HA	1:A:995:ILE:HG22	1.91	0.51
1:B:31:SER:OG	1:B:60:SER:O	2.24	0.51
1:B:110:SER:HA	1:B:130:GLU:HB3	1.93	0.51
1:A:331:THR:HG22	1:A:360:VAL:HG21	1.93	0.51
1:B:736:CYS:HB3	1:B:751:LEU:HD21	1.92	0.51
1:C:367:TYR:HA	1:C:372:PHE:HE1	1.76	0.51
1:A:334:CYS:SG	1:A:360:VAL:N	2.84	0.50
1:B:532:VAL:HG21	1:B:535:LYS:HB2	1.92	0.50
1:C:288:ASP:OD1	1:C:289:CYS:N	2.44	0.50
1:A:327:PHE:O	1:A:578:GLN:NE2	2.43	0.50
1:A:800:PHE:HB3	1:A:804:LEU:HD23	1.92	0.50
1:B:224:LEU:HG	1:B:225:VAL:HG23	1.94	0.50
1:B:811:SER:OG	1:B:813:ARG:NH1	2.43	0.50
1:A:31:SER:OG	1:A:60:SER:O	2.26	0.50
1:A:524:GLY:CA	1:A:526:LYS:HZ3	2.08	0.50
1:A:753:GLN:NE2	1:C:969:GLY:H	2.01	0.50
1:C:389:CYS:HA	1:C:523:CYS:CB	2.37	0.50
1:C:204:LYS:HE2	1:C:219:SER:HB3	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1114:THR:OG1	1:A:1116:ASP:OD1	2.19	0.50
1:C:332:ASN:O	1:C:359:CYS:HB2	2.11	0.50
1:C:63:THR:HG22	3:C:1301:NAG:H82	1.93	0.50
1:A:618:VAL:HB	1:A:619:PRO:HD3	1.94	0.50
1:B:327:PHE:O	1:B:578:GLN:NE2	2.45	0.50
1:B:398:PHE:HD2	1:B:508:VAL:HB	1.77	0.49
1:A:137:PRO:HD3	1:A:155:PHE:HB3	1.94	0.49
1:C:103:ILE:HG13	1:C:239:LEU:HD11	1.94	0.49
1:C:331:THR:HA	1:C:360:VAL:CG2	2.41	0.49
1:C:549:VAL:N	1:C:586:THR:O	2.45	0.49
1:C:946:LEU:HD21	1:C:1057:GLY:HA3	1.93	0.49
1:B:36:VAL:HG11	1:B:218:PHE:CE1	2.47	0.49
1:B:204:LYS:HE2	1:B:219:SER:HB3	1.94	0.49
1:B:531:LEU:HD11	1:B:583:LEU:HD21	1.93	0.49
1:C:113:GLN:HB3	1:C:128:VAL:HG12	1.93	0.49
1:A:415:ASN:HA	1:A:419:TYR:HD2	1.78	0.49
1:C:317:ARG:HD2	1:C:590:PHE:HB2	1.94	0.49
1:C:333:LEU:HD23	1:C:334:CYS:H	1.77	0.49
1:A:334:CYS:SG	1:A:360:VAL:C	2.90	0.49
1:A:895:PRO:HA	1:C:705:TYR:CE2	2.43	0.49
1:A:967:LYS:HB2	1:B:753:GLN:NE2	2.27	0.49
1:B:35:GLY:HA3	1:B:56:LEU:HD23	1.94	0.49
1:C:329:ASN:OD1	1:C:329:ASN:N	2.43	0.49
1:A:204:LYS:HE2	1:A:219:SER:HB3	1.95	0.49
1:B:123:ASN:OD1	1:B:124:VAL:N	2.41	0.49
1:A:720:VAL:HG22	1:A:1063:VAL:HG22	1.95	0.49
1:B:856:LEU:HD11	1:B:960:LEU:HD23	1.95	0.49
1:C:331:THR:HA	1:C:360:VAL:HG23	1.95	0.49
1:A:418:ASP:HA	1:A:422:LYS:HE3	1.95	0.49
1:B:992:ASP:OD1	1:B:993:ARG:N	2.46	0.49
1:C:618:VAL:HB	1:C:619:PRO:HD3	1.95	0.49
1:B:174:LEU:HA	1:B:205:HIS:HE2	1.77	0.49
1:C:800:PHE:HB3	1:C:804:LEU:HD23	1.95	0.49
1:A:367:TYR:HA	1:A:372:PHE:HE1	1.77	0.48
1:B:206:THR:HG22	1:B:208:ILE:HG12	1.95	0.48
1:B:360:VAL:HG13	1:B:524:GLY:CA	2.41	0.48
1:C:986:GLU:O	1:C:989:VAL:HG12	2.13	0.48
1:B:275:LEU:HD23	1:B:283:ILE:HD13	1.95	0.48
1:B:415:ASN:ND2	1:B:451:TYR:OH	2.46	0.48
1:A:85:ASN:HB2	1:A:267:TYR:HB3	1.95	0.48
1:A:123:ASN:OD1	1:A:124:VAL:N	2.43	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:455:ARG:HD3	1:A:459:LEU:HB2	1.95	0.48
1:B:407:GLN:HG2	1:B:412:GLN:HG2	1.96	0.48
1:C:116:LEU:HD23	1:C:117:ILE:N	2.29	0.48
1:C:988:GLU:HA	1:C:991:ILE:HB	1.96	0.48
1:A:103:ILE:HG13	1:A:239:LEU:HD11	1.95	0.48
1:A:384:LYS:NZ	1:B:979:LEU:O	2.41	0.48
1:B:424:PRO:HG2	1:B:427:PHE:HB2	1.96	0.48
1:B:113:GLN:HB3	1:B:128:VAL:HG12	1.96	0.48
1:B:1089:ARG:HG2	1:B:1119:PHE:HD1	1.77	0.48
1:C:726:PRO:HB3	1:C:949:VAL:HG21	1.94	0.48
1:C:796:GLY:HA3	1:C:897:PRO:HG3	1.96	0.48
1:A:36:VAL:HG11	1:A:218:PHE:CE1	2.48	0.48
1:A:853:PHE:HB3	1:C:587:PRO:HG2	1.95	0.48
1:B:155:PHE:CD2	1:B:157:VAL:HG13	2.48	0.48
1:C:226:ASP:OD1	1:C:227:LEU:N	2.46	0.48
1:B:726:PRO:HB3	1:B:949:VAL:HG21	1.96	0.48
1:C:660:CYS:HB2	1:C:669:CYS:HB3	1.59	0.48
1:C:714:THR:OG1	1:C:1069:GLN:O	2.28	0.48
1:A:41:LYS:HB3	1:C:517:HIS:CG	2.49	0.48
1:A:419:TYR:HD1	1:A:455:ARG:HG2	1.79	0.48
1:B:85:ASN:HB2	1:B:267:TYR:HB3	1.96	0.48
1:A:959:THR:O	1:A:963:GLN:HB2	2.13	0.48
1:B:618:VAL:HB	1:B:619:PRO:HD3	1.95	0.48
1:C:123:ASN:OD1	1:C:124:VAL:N	2.42	0.48
1:A:206:THR:HG22	1:A:208:ILE:HG12	1.96	0.47
1:B:569:ASP:OD2	1:C:965:SER:N	2.46	0.47
1:B:730:THR:HB	1:B:953:ASN:ND2	2.29	0.47
1:C:1124:CYS:HB2	1:C:1130:ILE:HD13	1.95	0.47
1:B:1091:GLY:O	1:C:902:TYR:OH	2.28	0.47
1:B:587:PRO:HG2	1:C:853:PHE:HB3	1.96	0.47
1:A:336:PHE:HE1	1:A:361:ALA:HB1	1.77	0.47
1:A:493:TYR:HB3	1:A:495:PHE:CE2	2.49	0.47
1:A:713:PRO:HA	1:A:1070:GLU:HA	1.96	0.47
1:A:992:ASP:OD1	1:A:993:ARG:N	2.48	0.47
1:B:329:ASN:OD1	1:B:329:ASN:N	2.43	0.47
1:C:37:TYR:HA	1:C:221:LEU:H	1.80	0.47
1:C:400:ILE:HG12	1:C:401:ARG:H	1.80	0.47
1:C:555:LYS:NZ	1:C:572:ASP:OD2	2.47	0.47
1:C:730:THR:HB	1:C:953:ASN:ND2	2.30	0.47
1:A:110:SER:HA	1:A:130:GLU:HB3	1.95	0.47
1:A:413:THR:HA	1:A:417:ALA:HB3	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:516:LEU:HG	1:A:517:HIS:ND1	2.29	0.47
1:B:516:LEU:HG	1:B:517:HIS:ND1	2.28	0.47
1:B:983:ASP:HB2	1:B:985:PRO:HD2	1.96	0.47
1:B:733:SER:OG	1:B:857:THR:OG1	2.25	0.47
1:A:275:LEU:HD23	1:A:283:ILE:HD13	1.96	0.47
1:B:401:ARG:HA	1:B:495:PHE:HZ	1.79	0.47
1:B:419:TYR:HD1	1:B:455:ARG:HG2	1.79	0.47
1:B:720:VAL:HG22	1:B:1063:VAL:HG22	1.97	0.47
1:B:1124:CYS:HB2	1:B:1130:ILE:HD13	1.96	0.47
1:C:81:VAL:HG21	1:C:235:ARG:HD3	1.97	0.47
1:C:392:ASN:HD22	1:C:392:ASN:H	1.63	0.47
1:C:424:PRO:HG2	1:C:427:PHE:HB2	1.96	0.47
1:C:565:ARG:HE	1:C:571:THR:HG22	1.80	0.47
1:A:271:ARG:HD3	1:A:271:ARG:HA	1.80	0.47
1:B:64:TRP:CH2	1:B:261:ALA:HB2	2.50	0.47
1:B:342:ALA:HB3	1:B:345:PHE:HE1	1.80	0.47
1:B:796:GLY:HA3	1:B:897:PRO:HG3	1.97	0.47
1:C:36:VAL:HG11	1:C:218:PHE:CZ	2.49	0.47
1:C:964:LEU:O	1:C:973:SER:OG	2.23	0.47
1:A:549:VAL:N	1:A:586:THR:O	2.47	0.47
1:A:946:LEU:HD21	1:A:1057:GLY:HA3	1.97	0.47
1:A:329:ASN:OD1	1:A:329:ASN:N	2.46	0.46
1:A:331:THR:HA	1:A:360:VAL:HG23	1.96	0.46
1:B:361:ALA:O	1:B:362:ASP:C	2.54	0.46
1:C:342:ALA:O	1:C:507:ARG:NH1	2.47	0.46
1:C:898:MET:HG2	1:C:915:TYR:OH	2.14	0.46
1:A:98:ILE:HG22	1:A:240:LEU:HD11	1.96	0.46
1:B:389:CYS:HA	1:B:523:CYS:CB	2.37	0.46
1:B:1039:ASP:HB3	1:C:1028:SER:HB3	1.97	0.46
1:C:110:SER:HA	1:C:130:GLU:HB3	1.97	0.46
1:C:419:TYR:HD1	1:C:455:ARG:HG2	1.81	0.46
1:A:35:GLY:HA3	1:A:56:LEU:HD23	1.97	0.46
1:A:37:TYR:OH	1:A:54:LEU:O	2.21	0.46
1:A:757:PHE:O	1:A:761:LEU:HG	2.14	0.46
1:A:1124:CYS:HB2	1:A:1130:ILE:HD13	1.96	0.46
1:B:66:HIS:NE2	1:B:249:PRO:O	2.47	0.46
1:A:155:PHE:CD2	1:A:157:VAL:HG13	2.50	0.46
1:A:790:PRO:HG2	1:C:705:TYR:HB3	1.98	0.46
1:B:565:ARG:HE	1:B:571:THR:HG22	1.81	0.46
1:A:82:LEU:N	1:A:236:PHE:O	2.36	0.46
1:C:904:PHE:CD2	1:C:914:LEU:HB2	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:549:VAL:N	1:B:586:THR:O	2.47	0.46
1:C:566:ASP:OD1	1:C:566:ASP:N	2.46	0.46
1:A:201:ILE:HB	1:A:225:VAL:HB	1.98	0.46
1:C:194:ASN:ND2	1:C:199:PHE:HB2	2.31	0.46
1:C:361:ALA:O	1:C:362:ASP:C	2.53	0.46
1:A:66:HIS:NE2	1:A:249:PRO:O	2.47	0.45
1:A:753:GLN:NE2	1:C:967:LYS:HB2	2.29	0.45
1:C:87:GLY:HA2	1:C:192:PHE:O	2.16	0.45
1:A:531:LEU:HD11	1:A:583:LEU:HD21	1.98	0.45
1:A:983:ASP:OD1	1:A:983:ASP:N	2.49	0.45
1:B:325:VAL:HG22	1:B:540:ASN:HB3	1.98	0.45
1:C:551:THR:HG23	1:C:584:ASP:HB3	1.98	0.45
1:C:904:PHE:HB3	1:C:909:VAL:HG23	1.99	0.45
1:C:360:VAL:HG13	1:C:524:GLY:CA	2.43	0.45
1:A:1025:THR:O	1:A:1029:GLU:HG3	2.16	0.45
1:B:199:PHE:HE1	1:B:201:ILE:HD11	1.81	0.45
1:B:401:ARG:HA	1:B:495:PHE:CZ	2.51	0.45
1:A:389:CYS:HA	1:A:523:CYS:CB	2.38	0.45
1:A:1039:ASP:HB3	1:B:1028:SER:HB3	1.98	0.45
1:B:564:GLY:HA2	1:C:43:PHE:HB3	1.98	0.45
1:B:566:ASP:OD1	1:B:566:ASP:N	2.42	0.45
1:A:738:MET:HE3	1:C:317:ARG:HD3	1.99	0.45
1:A:616:THR:HG23	1:A:617:GLU:HG3	1.99	0.45
1:C:192:PHE:HD1	1:C:201:ILE:HD12	1.82	0.45
1:A:733:SER:OG	1:A:857:THR:OG1	2.27	0.45
1:A:892:LEU:HB3	1:C:711:ALA:HB3	1.97	0.45
1:B:800:PHE:HB3	1:B:804:LEU:HD23	1.99	0.45
1:B:904:PHE:CD2	1:B:914:LEU:HB2	2.51	0.45
1:C:415:ASN:HA	1:C:419:TYR:HD2	1.81	0.45
1:A:295:SER:HA	1:A:298:LYS:HG2	1.99	0.45
1:B:37:TYR:OH	1:B:54:LEU:O	2.21	0.45
1:B:201:ILE:HB	1:B:225:VAL:HB	1.98	0.45
1:C:85:ASN:HB2	1:C:267:TYR:HB3	1.97	0.45
1:C:992:ASP:OD1	1:C:993:ARG:N	2.50	0.45
1:A:414:GLY:O	1:A:418:ASP:N	2.46	0.45
1:A:560:PHE:HB2	1:B:41:LYS:NZ	2.32	0.45
1:A:660:CYS:HB2	1:A:669:CYS:HB3	1.66	0.45
1:A:145:LYS:HA	1:A:145:LYS:HD3	1.83	0.44
1:A:785:GLN:OE1	1:C:701:ASN:ND2	2.44	0.44
1:A:856:LEU:HD11	1:A:960:LEU:HD23	1.98	0.44
1:B:331:THR:HA	1:B:360:VAL:CG2	2.47	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:342:ALA:O	1:B:507:ARG:NH1	2.50	0.44
1:A:106:THR:HG22	1:A:234:THR:H	1.82	0.44
1:A:596:ILE:HD12	1:A:648:LEU:HD11	1.97	0.44
1:A:902:TYR:OH	1:C:1091:GLY:O	2.26	0.44
1:B:202:TYR:CD1	1:B:223:PRO:HA	2.53	0.44
1:B:396:ASP:OD1	1:B:396:ASP:N	2.49	0.44
1:C:471:TYR:HB2	1:C:489:PRO:HG3	1.98	0.44
1:C:596:ILE:HD12	1:C:648:LEU:HD11	1.98	0.44
1:A:37:TYR:HA	1:A:221:LEU:H	1.82	0.44
1:A:522:VAL:O	1:A:522:VAL:HG23	2.17	0.44
1:B:195:ILE:HB	1:B:200:LYS:NZ	2.31	0.44
1:C:1080:CYS:HB2	1:C:1124:CYS:HB2	1.88	0.44
1:A:396:ASP:OD1	1:A:396:ASP:N	2.50	0.44
1:A:738:MET:HE1	1:C:317:ARG:HH11	1.82	0.44
1:B:333:LEU:HD23	1:B:334:CYS:H	1.81	0.44
1:B:705:TYR:HB3	1:C:790:PRO:HG2	2.00	0.44
1:A:40:ASP:OD1	1:A:40:ASP:N	2.50	0.44
1:B:761:LEU:HB3	1:B:1006:VAL:HG21	1.98	0.44
1:C:287:VAL:HG21	1:C:298:LYS:HD2	2.00	0.44
1:C:524:GLY:CA	1:C:526:LYS:HZ3	1.99	0.44
1:B:48:LEU:HD12	1:B:274:LEU:HD21	1.99	0.44
1:C:295:SER:HA	1:C:298:LYS:HG2	2.00	0.44
1:B:782:GLN:OE1	1:B:1028:SER:OG	2.36	0.44
1:C:198:TYR:HB3	1:C:200:LYS:HE3	1.99	0.44
1:C:413:THR:HA	1:C:417:ALA:HB3	1.99	0.44
1:A:713:PRO:HD3	1:B:892:LEU:HD13	1.99	0.44
1:B:413:THR:HA	1:B:417:ALA:HB3	2.00	0.44
1:C:35:GLY:HA3	1:C:56:LEU:HD23	1.99	0.44
1:C:616:THR:HG23	1:C:617:GLU:HG3	2.00	0.44
1:A:278:ASN:HB2	1:A:284:THR:HG23	2.00	0.43
1:B:82:LEU:HB2	1:B:236:PHE:HB3	2.00	0.43
1:C:390:PHE:HB2	1:C:522:VAL:HG23	2.00	0.43
1:A:315:ASN:ND2	1:B:735:ASP:OD2	2.51	0.43
1:A:402:GLY:O	1:A:405:VAL:HG12	2.19	0.43
1:A:202:TYR:CD1	1:A:223:PRO:HA	2.53	0.43
1:A:551:THR:HG23	1:A:584:ASP:HB3	1.99	0.43
1:B:775:ASN:OD1	1:B:1017:ARG:NH1	2.51	0.43
1:C:389:CYS:HB3	1:C:520:ALA:HB1	1.99	0.43
1:A:129:CYS:HB2	1:A:164:CYS:HB3	1.98	0.43
1:A:195:ILE:HB	1:A:200:LYS:NZ	2.30	0.43
1:A:389:CYS:HB3	1:A:520:ALA:HB1	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:616:THR:HG23	1:B:617:GLU:HG3	2.00	0.43
1:B:336:PHE:HE1	1:B:361:ALA:HB1	1.80	0.43
1:C:396:ASP:OD1	1:C:396:ASP:N	2.50	0.43
1:B:295:SER:HA	1:B:298:LYS:HG2	2.01	0.43
1:B:946:LEU:HD21	1:B:1057:GLY:HA3	2.01	0.43
1:C:202:TYR:CD1	1:C:223:PRO:HA	2.54	0.43
1:C:242:LEU:HD21	1:C:248:THR:HG21	2.01	0.43
1:A:517:HIS:HD2	1:B:41:LYS:HG2	1.84	0.43
1:A:734:VAL:HG12	1:A:856:LEU:HD13	2.00	0.43
1:A:746:GLU:OE2	1:A:746:GLU:N	2.45	0.43
1:C:330:ILE:CD1	1:C:332:ASN:H	2.31	0.43
1:A:967:LYS:NZ	1:B:753:GLN:HE21	2.16	0.43
1:B:226:ASP:OD1	1:B:227:LEU:N	2.52	0.43
1:A:354:LYS:HA	1:A:354:LYS:HD2	1.92	0.43
1:B:278:ASN:HB2	1:B:284:THR:HG23	2.00	0.43
1:C:82:LEU:HB2	1:C:236:PHE:HB3	2.00	0.43
1:A:380:VAL:HG21	1:A:388:LEU:HD11	2.01	0.42
1:A:904:PHE:HB3	1:A:909:VAL:HG23	2.01	0.42
1:B:390:PHE:HB2	1:B:522:VAL:HG23	2.01	0.42
1:C:1100:TRP:HB2	1:C:1133:ASN:ND2	2.34	0.42
1:B:517:HIS:CB	1:C:41:LYS:HB3	2.49	0.42
1:C:195:ILE:HB	1:C:200:LYS:NZ	2.34	0.42
1:C:336:PHE:HE1	1:C:361:ALA:HB1	1.79	0.42
1:C:983:ASP:OD1	1:C:983:ASP:N	2.51	0.42
1:A:82:LEU:O	1:A:236:PHE:N	2.53	0.42
1:A:405:VAL:HG11	1:A:506:TYR:HD2	1.84	0.42
1:B:904:PHE:HB3	1:B:909:VAL:HG23	2.01	0.42
1:C:48:LEU:HD12	1:C:274:LEU:HD21	2.00	0.42
1:A:336:PHE:CE1	1:A:361:ALA:CB	3.02	0.42
1:A:398:PHE:HZ	1:A:400:ILE:HD12	1.84	0.42
1:A:587:PRO:HG2	1:B:853:PHE:HB3	2.01	0.42
1:B:712:ILE:HD12	1:B:1094:VAL:HG21	2.01	0.42
1:C:402:GLY:O	1:C:405:VAL:HG12	2.19	0.42
1:A:68:ILE:HG13	1:A:69:SER:N	2.34	0.42
1:A:865:ASP:OD1	1:A:866:GLU:N	2.52	0.42
1:B:660:CYS:HB2	1:B:669:CYS:HB3	1.66	0.42
1:B:865:ASP:OD1	1:B:866:GLU:N	2.51	0.42
1:B:1100:TRP:HB2	1:B:1133:ASN:ND2	2.33	0.42
1:B:64:TRP:CD1	1:B:66:HIS:HB2	2.54	0.42
1:C:671:SER:HB3	1:C:693:TYR:HE2	1.85	0.42
1:A:224:LEU:HG	1:A:225:VAL:HG23	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:894:ILE:CD1	1:C:1105:ARG:HH22	2.32	0.42
1:A:1100:TRP:HB2	1:A:1133:ASN:ND2	2.34	0.42
1:B:409:ALA:HA	1:B:410:PRO:HD3	1.92	0.42
1:B:455:ARG:HD3	1:B:459:LEU:HB2	2.02	0.42
1:A:41:LYS:HE3	1:C:560:PHE:HB2	2.02	0.42
1:A:904:PHE:CD2	1:A:914:LEU:HB2	2.54	0.42
1:A:969:GLY:H	1:B:753:GLN:HE22	1.68	0.42
1:A:969:GLY:H	1:B:753:GLN:NE2	2.18	0.42
1:B:306:VAL:HG22	1:B:600:THR:HG23	2.01	0.42
1:B:983:ASP:N	1:B:983:ASP:OD1	2.53	0.42
1:B:1079:ILE:HG12	1:B:1093:PHE:CE2	2.55	0.42
1:A:386:ASN:CG	1:A:526:LYS:HD2	2.40	0.42
1:C:278:ASN:HB2	1:C:284:THR:HG23	2.01	0.42
1:A:1026:LYS:NZ	1:A:1040:PHE:O	2.52	0.41
1:B:294:LEU:HB2	1:B:606:VAL:HG11	2.01	0.41
1:C:336:PHE:CE1	1:C:361:ALA:CB	3.02	0.41
1:A:985:PRO:HB3	1:B:425:ASP:HB3	2.01	0.41
1:B:137:PRO:HD3	1:B:155:PHE:HB3	2.01	0.41
1:A:48:LEU:HD12	1:A:274:LEU:HD21	2.01	0.41
1:A:332:ASN:O	1:A:360:VAL:N	2.53	0.41
1:A:795:PHE:HD1	1:C:705:TYR:HE1	1.68	0.41
1:C:91:ALA:HB1	1:C:187:LEU:HD11	2.01	0.41
1:C:135:ASN:H	1:C:157:VAL:HA	1.84	0.41
1:C:425:ASP:N	1:C:425:ASP:OD1	2.52	0.41
1:A:91:ALA:HB1	1:A:187:LEU:HD11	2.02	0.41
1:A:715:ASN:HD22	1:A:1069:GLN:HG3	1.86	0.41
1:A:400:ILE:HG12	1:A:401:ARG:H	1.86	0.41
1:A:884:TRP:HB3	1:A:1033:GLY:HA2	2.02	0.41
1:B:102:TRP:HD1	1:B:236:PHE:HZ	1.69	0.41
1:B:287:VAL:HG21	1:B:298:LYS:HD2	2.02	0.41
1:B:560:PHE:CD2	1:C:41:LYS:HE3	2.53	0.41
1:B:671:SER:HB3	1:B:693:TYR:HE2	1.85	0.41
1:B:800:PHE:CD1	1:B:803:ILE:HD11	2.55	0.41
1:B:986:GLU:O	1:B:989:VAL:HG12	2.20	0.41
1:B:71:THR:H	1:B:76:ARG:HB2	1.85	0.41
1:B:91:ALA:HB1	1:B:187:LEU:HD11	2.02	0.41
1:B:405:VAL:HG11	1:B:506:TYR:HD2	1.85	0.41
1:C:82:LEU:N	1:C:236:PHE:O	2.41	0.41
1:C:354:LYS:HA	1:C:354:LYS:HD2	1.91	0.41
1:A:361:ALA:O	1:A:362:ASP:C	2.58	0.41
1:A:434:TRP:HE1	1:A:507:ARG:NH2	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:ASN:O	1:B:237:GLN:NE2	2.53	0.41
1:C:31:SER:OG	1:C:60:SER:O	2.21	0.41
1:C:66:HIS:NE2	1:C:249:PRO:O	2.54	0.41
1:C:733:SER:O	1:C:857:THR:OG1	2.38	0.41
1:B:526:LYS:HE2	1:B:526:LYS:H	1.85	0.41
1:C:65:PHE:HE2	1:C:82:LEU:HD11	1.85	0.41
1:C:129:CYS:HB2	1:C:164:CYS:HB3	1.96	0.41
1:C:609:LEU:HD22	1:C:664:ILE:HG23	2.02	0.41
1:C:1079:ILE:HG12	1:C:1093:PHE:CE2	2.56	0.41
1:A:41:LYS:HE3	1:C:560:PHE:HD2	1.84	0.41
1:A:415:ASN:ND2	1:A:451:TYR:OH	2.52	0.41
1:B:437:ASN:HB3	1:B:504:GLN:HB3	2.03	0.41
1:B:734:VAL:HG12	1:B:856:LEU:HD13	2.03	0.41
1:C:405:VAL:HG11	1:C:506:TYR:CD2	2.56	0.41
1:C:458:ASN:OD1	1:C:458:ASN:N	2.54	0.41
1:C:968:PHE:O	1:C:993:ARG:HG2	2.21	0.41
1:A:340:PHE:HZ	1:A:370:ALA:HB3	1.86	0.41
1:A:410:PRO:HB3	1:A:423:LEU:HB2	2.02	0.41
1:A:425:ASP:N	1:A:425:ASP:OD1	2.54	0.41
1:B:271:ARG:HD3	1:B:271:ARG:HA	1.78	0.41
1:B:405:VAL:HG11	1:B:506:TYR:CD2	2.56	0.41
1:C:271:ARG:HA	1:C:271:ARG:HD3	1.80	0.41
1:C:408:ILE:HG12	1:C:431:VAL:HG11	2.03	0.41
1:C:422:LYS:HG3	1:C:461:PRO:HG3	2.02	0.41
1:C:746:GLU:OE2	1:C:746:GLU:N	2.45	0.40
1:C:1095:SER:HB3	1:C:1100:TRP:CE3	2.56	0.40
1:A:287:VAL:HG21	1:A:298:LYS:HD2	2.04	0.40
1:A:332:ASN:CG	1:A:359:CYS:HA	2.41	0.40
1:B:380:VAL:HG21	1:B:388:LEU:HD11	2.02	0.40
1:C:706:SER:HB3	1:C:709:SER:HB3	2.02	0.40
1:A:648:LEU:HD12	1:A:648:LEU:HA	1.84	0.40
1:A:868:ILE:HD13	1:A:868:ILE:HA	1.87	0.40
1:B:425:ASP:OD1	1:B:425:ASP:N	2.54	0.40
1:B:551:THR:HG23	1:B:584:ASP:HB3	2.03	0.40
1:B:988:GLU:HA	1:B:991:ILE:HB	2.04	0.40
1:A:71:THR:HG23	1:A:139:LEU:HD22	2.01	0.40
1:A:463:GLU:OE2	3:B:1306:NAG:N2	2.49	0.40
1:A:465:ASP:N	1:A:465:ASP:OD1	2.53	0.40
1:A:566:ASP:OD1	1:A:566:ASP:N	2.52	0.40
1:B:1095:SER:HB3	1:B:1100:TRP:CE3	2.57	0.40
1:C:848:ILE:HD12	1:C:848:ILE:H	1.86	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:340:PHE:HZ	1:B:370:ALA:HB3	1.87	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	1083/1268 (85%)	1017 (94%)	65 (6%)	1 (0%)	51 84
1	B	1083/1268 (85%)	1016 (94%)	66 (6%)	1 (0%)	51 84
1	C	1083/1268 (85%)	1017 (94%)	65 (6%)	1 (0%)	51 84
All	All	3249/3804 (85%)	3050 (94%)	196 (6%)	3 (0%)	54 84

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	362	ASP
1	B	362	ASP
1	C	362	ASP

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	946/1107 (86%)	938 (99%)	8 (1%)	81 91

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	946/1107 (86%)	941 (100%)	5 (0%)	88 95
1	C	946/1107 (86%)	938 (99%)	8 (1%)	81 91
All	All	2838/3321 (86%)	2817 (99%)	21 (1%)	84 93

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	119	ASN
1	A	329	ASN
1	A	332	ASN
1	A	450	ARG
1	A	455	ARG
1	A	496	ARG
1	A	526	LYS
1	A	527	LYS
1	B	119	ASN
1	B	329	ASN
1	B	450	ARG
1	B	496	ARG
1	B	527	LYS
1	C	329	ASN
1	C	330	ILE
1	C	332	ASN
1	C	392	ASN
1	C	450	ARG
1	C	455	ARG
1	C	496	ARG
1	C	527	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	753	GLN
1	A	953	ASN
1	A	1133	ASN
1	C	119	ASN
1	C	194	ASN
1	C	392	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

36 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	D	1	1,2	14,14,15	0.20	0	17,19,21	0.39	0
2	NAG	D	2	2	14,14,15	0.24	0	17,19,21	0.42	0
2	NAG	E	1	1,2	14,14,15	0.98	1 (7%)	17,19,21	1.28	1 (5%)
2	NAG	E	2	2	14,14,15	0.21	0	17,19,21	0.46	0
2	NAG	F	1	1,2	14,14,15	0.20	0	17,19,21	0.48	0
2	NAG	F	2	2	14,14,15	0.22	0	17,19,21	0.44	0
2	NAG	G	1	1,2	14,14,15	0.30	0	17,19,21	0.52	0
2	NAG	G	2	2	14,14,15	0.24	0	17,19,21	0.41	0
2	NAG	H	1	1,2	14,14,15	0.31	0	17,19,21	0.53	0
2	NAG	H	2	2	14,14,15	0.28	0	17,19,21	0.41	0
2	NAG	I	1	1,2	14,14,15	0.24	0	17,19,21	0.48	0
2	NAG	I	2	2	14,14,15	0.23	0	17,19,21	0.43	0
2	NAG	J	1	1,2	14,14,15	0.20	0	17,19,21	0.40	0
2	NAG	J	2	2	14,14,15	0.24	0	17,19,21	0.43	0
2	NAG	K	1	1,2	14,14,15	0.47	0	17,19,21	0.76	1 (5%)
2	NAG	K	2	2	14,14,15	0.21	0	17,19,21	0.50	0
2	NAG	L	1	1,2	14,14,15	0.20	0	17,19,21	0.44	0
2	NAG	L	2	2	14,14,15	0.22	0	17,19,21	0.42	0
2	NAG	M	1	1,2	14,14,15	0.26	0	17,19,21	0.49	0
2	NAG	M	2	2	14,14,15	0.23	0	17,19,21	0.41	0
2	NAG	N	1	1,2	14,14,15	0.32	0	17,19,21	0.53	0
2	NAG	N	2	2	14,14,15	0.26	0	17,19,21	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	O	1	1,2	14,14,15	0.25	0	17,19,21	0.49	0
2	NAG	O	2	2	14,14,15	0.23	0	17,19,21	0.42	0
2	NAG	P	1	1,2	14,14,15	0.20	0	17,19,21	0.38	0
2	NAG	P	2	2	14,14,15	0.23	0	17,19,21	0.42	0
2	NAG	Q	1	1,2	14,14,15	0.42	0	17,19,21	0.76	1 (5%)
2	NAG	Q	2	2	14,14,15	0.22	0	17,19,21	0.52	0
2	NAG	R	1	1,2	14,14,15	0.34	0	17,19,21	0.44	0
2	NAG	R	2	2	14,14,15	0.25	0	17,19,21	0.48	0
2	NAG	S	1	1,2	14,14,15	0.29	0	17,19,21	0.53	0
2	NAG	S	2	2	14,14,15	0.24	0	17,19,21	0.42	0
2	NAG	T	1	1,2	14,14,15	0.29	0	17,19,21	0.52	0
2	NAG	T	2	2	14,14,15	0.31	0	17,19,21	0.41	0
2	NAG	U	1	1,2	14,14,15	0.23	0	17,19,21	0.49	0
2	NAG	U	2	2	14,14,15	0.24	0	17,19,21	0.42	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	D	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	NAG	E	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1
2	NAG	G	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	G	2	2	-	2/6/23/26	0/1/1/1
2	NAG	H	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	H	2	2	-	1/6/23/26	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	-	2/6/23/26	0/1/1/1
2	NAG	J	2	2	-	2/6/23/26	0/1/1/1
2	NAG	K	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	K	2	2	-	2/6/23/26	0/1/1/1
2	NAG	L	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	L	2	2	-	2/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	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
2	NAG	N	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	N	2	2	-	1/6/23/26	0/1/1/1
2	NAG	O	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	O	2	2	-	2/6/23/26	0/1/1/1
2	NAG	P	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	P	2	2	-	2/6/23/26	0/1/1/1
2	NAG	Q	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	Q	2	2	-	2/6/23/26	0/1/1/1
2	NAG	R	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	R	2	2	-	2/6/23/26	0/1/1/1
2	NAG	S	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	S	2	2	-	2/6/23/26	0/1/1/1
2	NAG	T	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	T	2	2	-	2/6/23/26	0/1/1/1
2	NAG	U	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	U	2	2	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1	NAG	O5-C1	3.52	1.49	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	1	NAG	C1-O5-C5	4.98	118.93	112.19
2	K	1	NAG	C1-O5-C5	2.37	115.40	112.19
2	Q	1	NAG	C1-O5-C5	2.31	115.32	112.19

There are no chirality outliers.

All (64) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	L	1	NAG	O5-C5-C6-O6
2	K	1	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

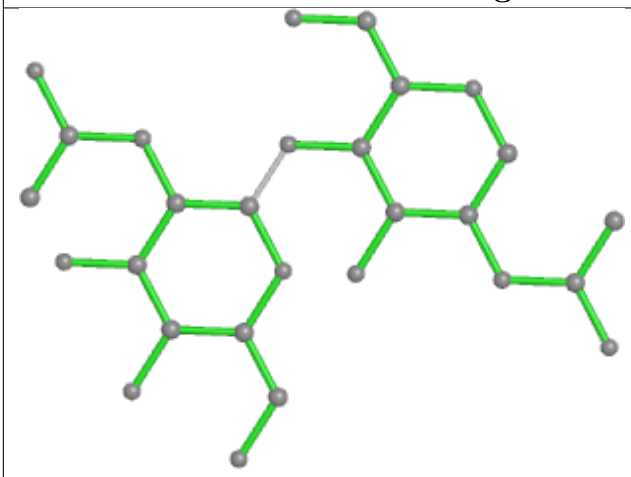
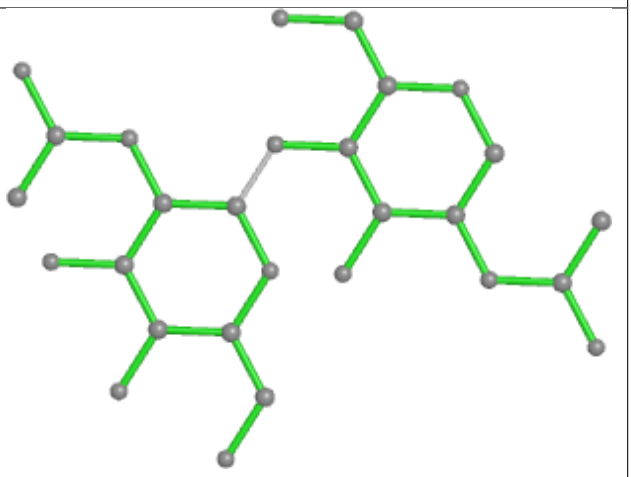
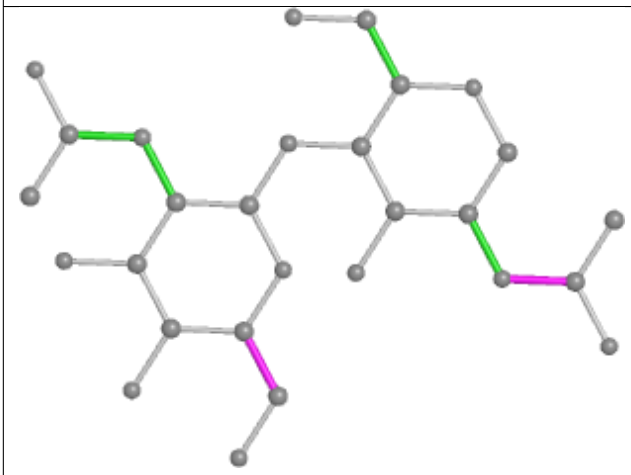
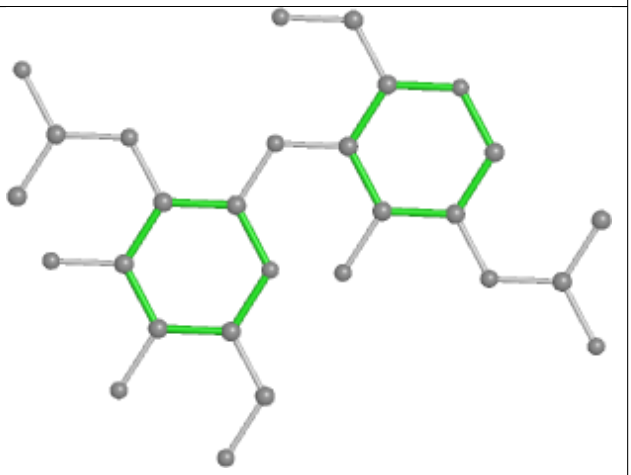
Mol	Chain	Res	Type	Atoms
2	U	1	NAG	C4-C5-C6-O6
2	O	1	NAG	O5-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6
2	O	1	NAG	C4-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
2	I	1	NAG	C4-C5-C6-O6
2	I	1	NAG	O5-C5-C6-O6
2	N	2	NAG	O5-C5-C6-O6
2	H	2	NAG	O5-C5-C6-O6
2	T	2	NAG	C4-C5-C6-O6
2	I	2	NAG	C4-C5-C6-O6
2	O	2	NAG	C4-C5-C6-O6
2	U	2	NAG	C4-C5-C6-O6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

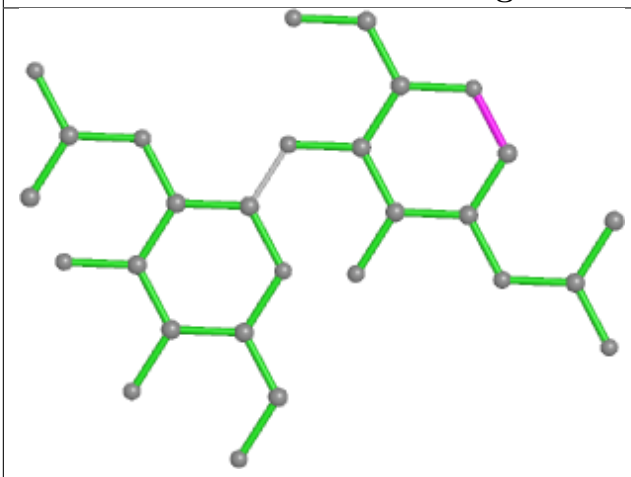
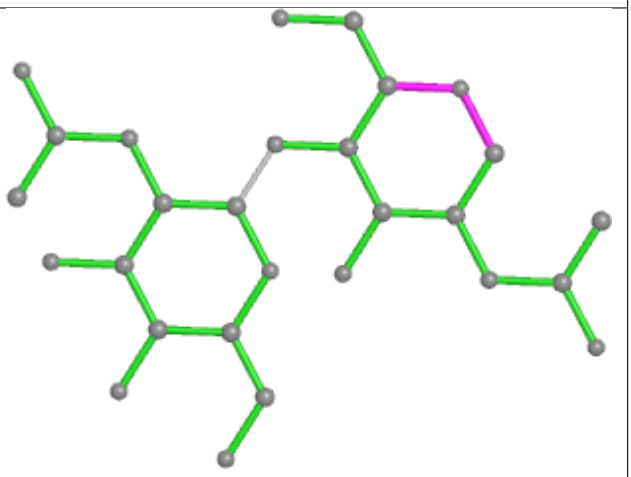
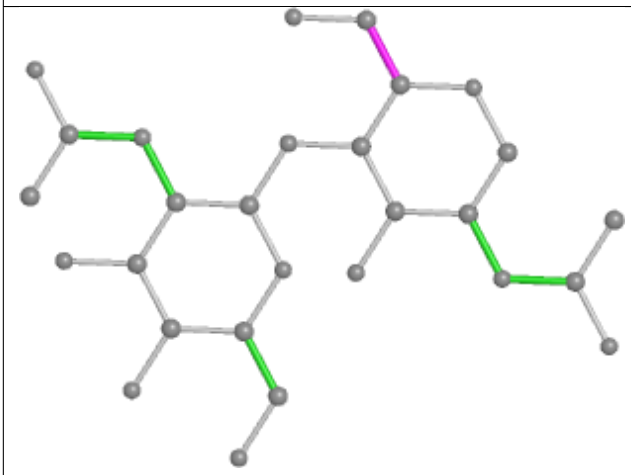
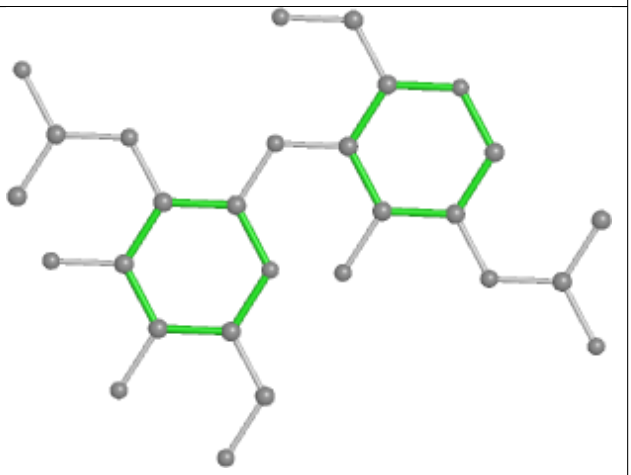
There are no ring outliers.

4 monomers are involved in 4 short contacts:

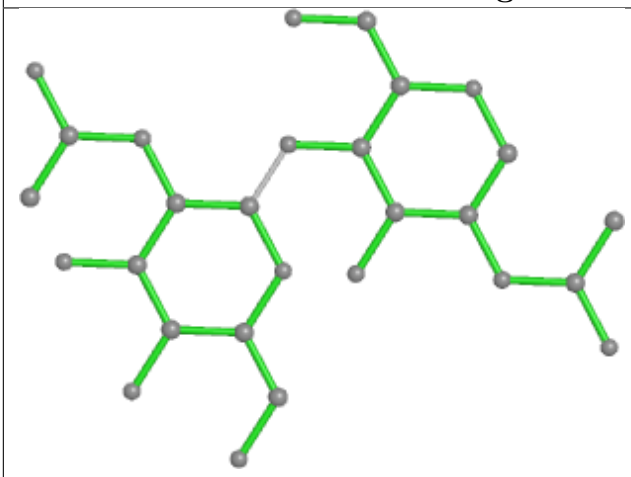
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	1	NAG	1	0
2	D	1	NAG	1	0
2	P	1	NAG	1	0
2	J	1	NAG	1	0

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

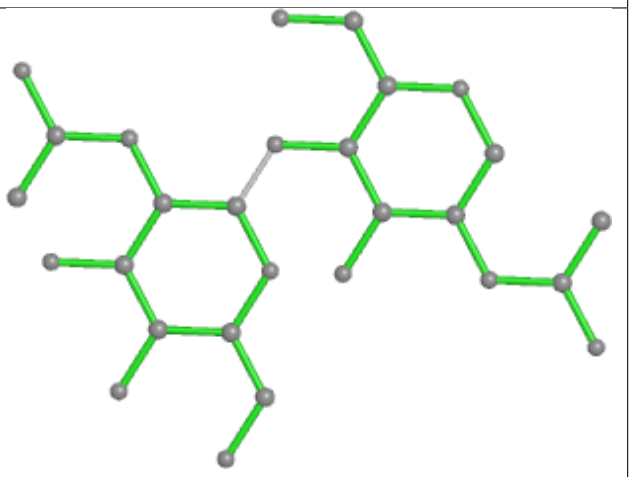
Oligosaccharide Chain D	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain E	
 Bond lengths	 Bond angles
 Torsions	 Rings

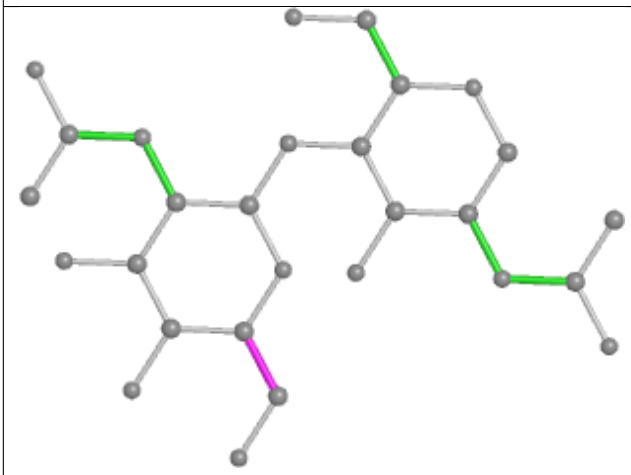
Oligosaccharide Chain F



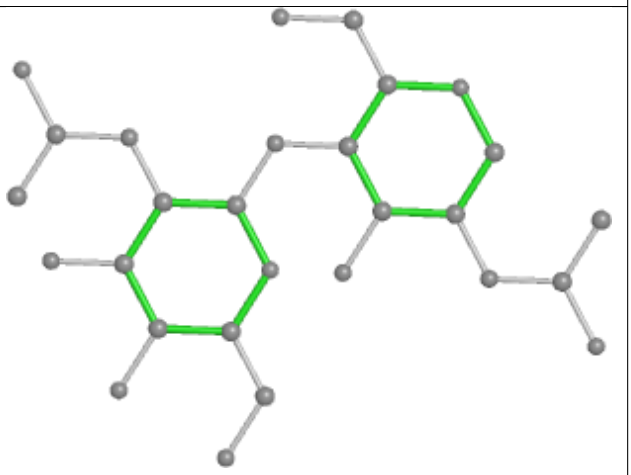
Bond lengths



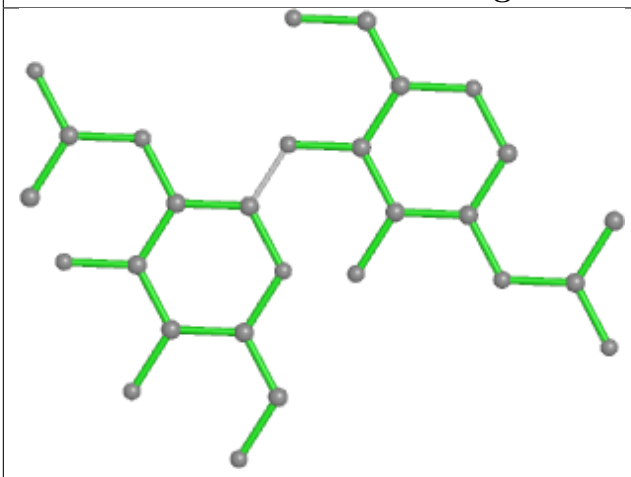
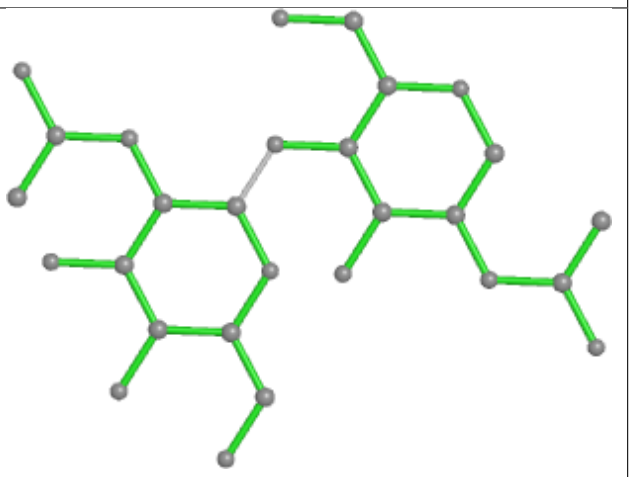
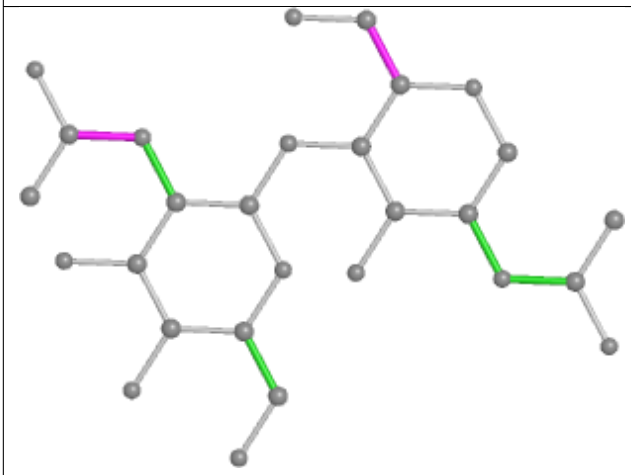
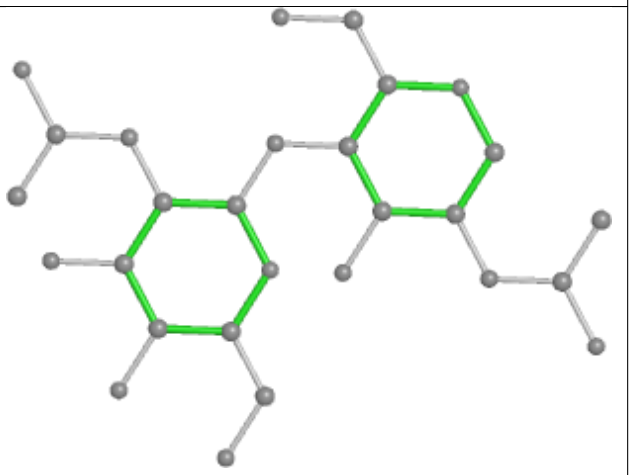
Bond angles

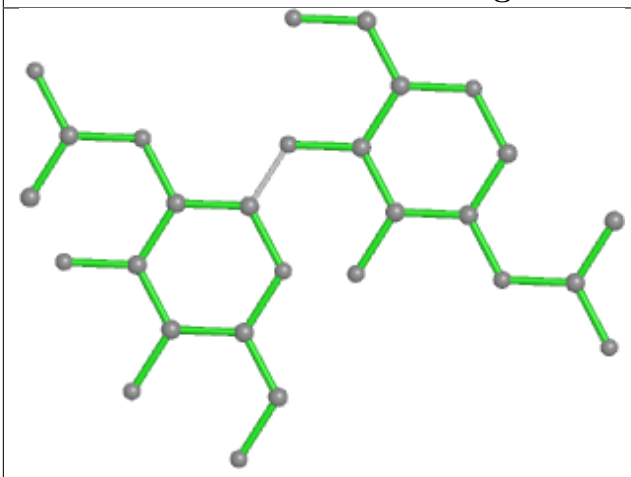
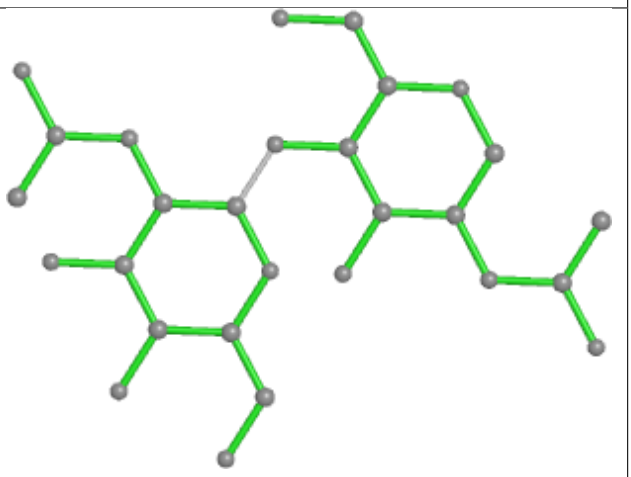
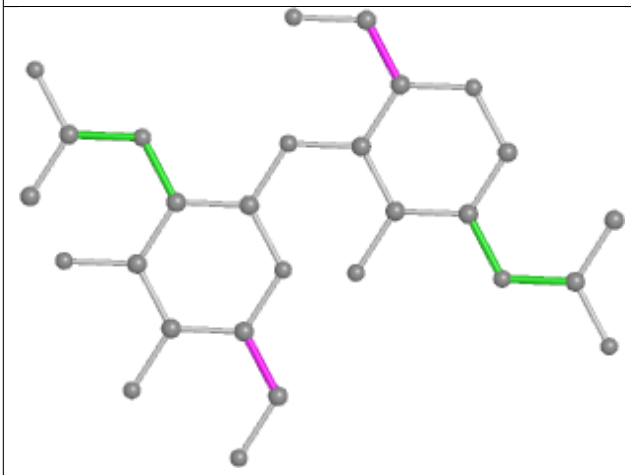
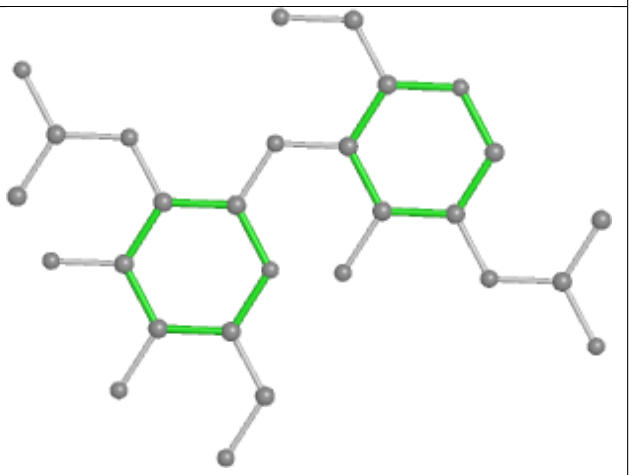


Torsions

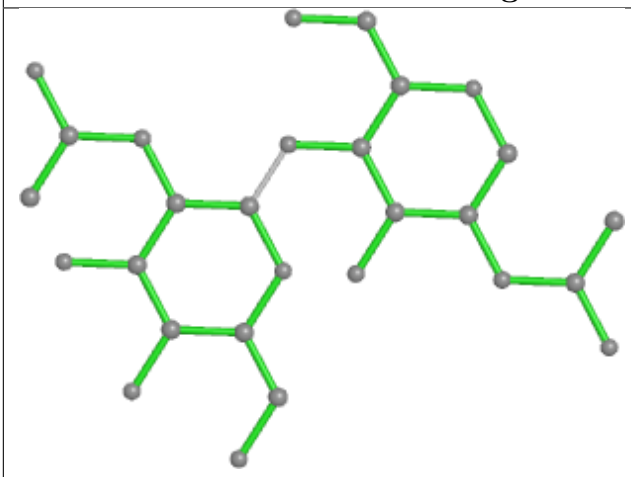


Rings

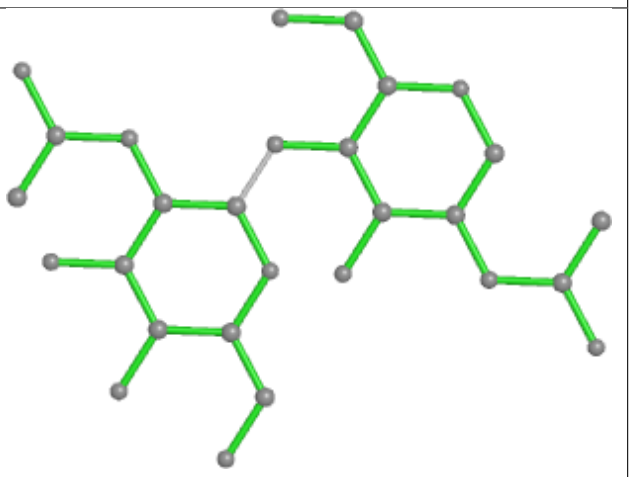
Oligosaccharide Chain G	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain H	
 Bond lengths	 Bond angles
 Torsions	 Rings

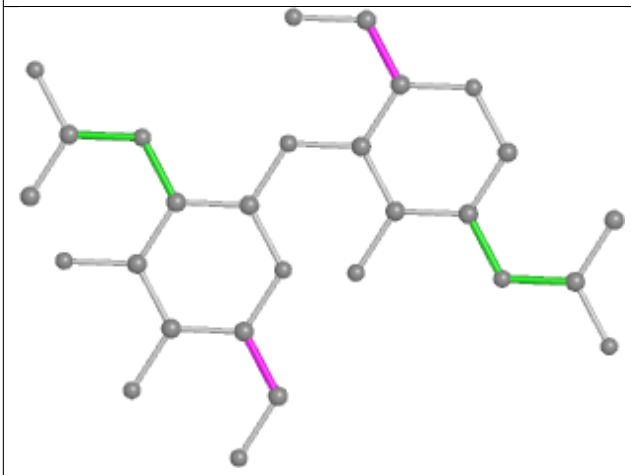
Oligosaccharide Chain I



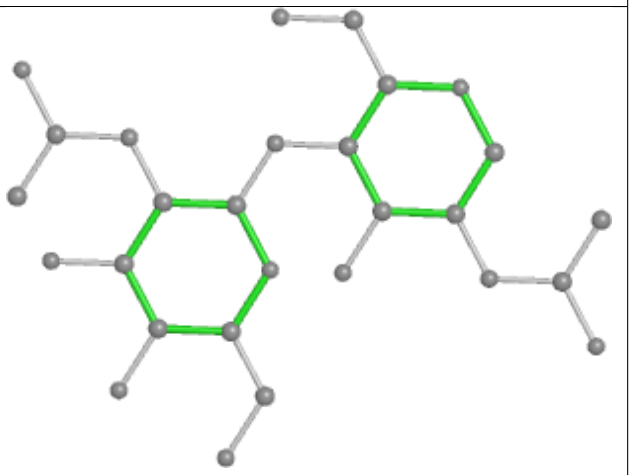
Bond lengths



Bond angles

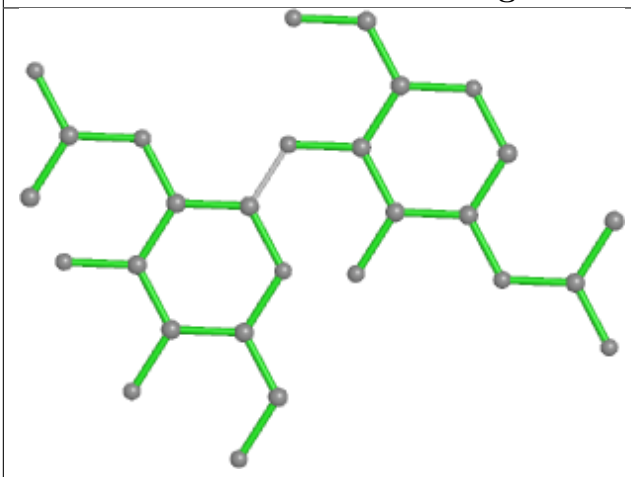


Torsions

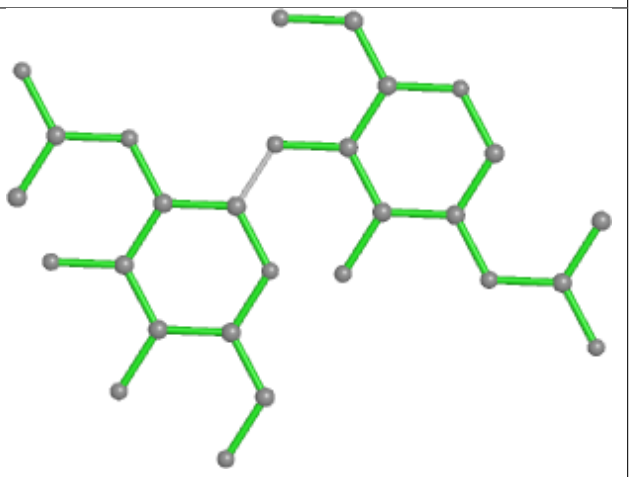


Rings

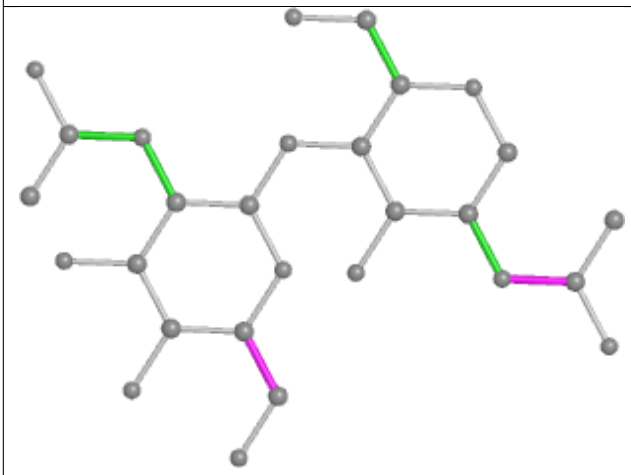
Oligosaccharide Chain J



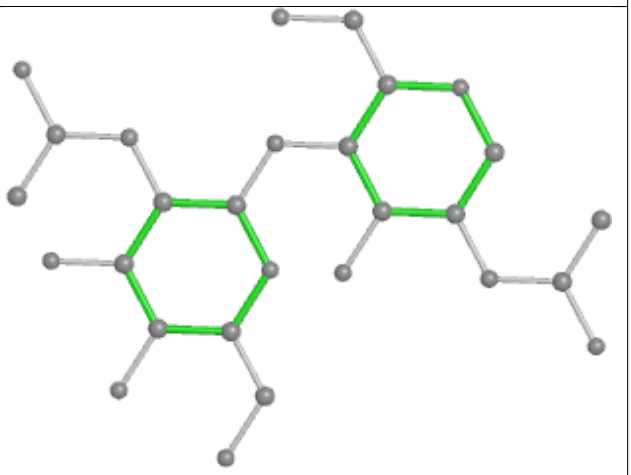
Bond lengths



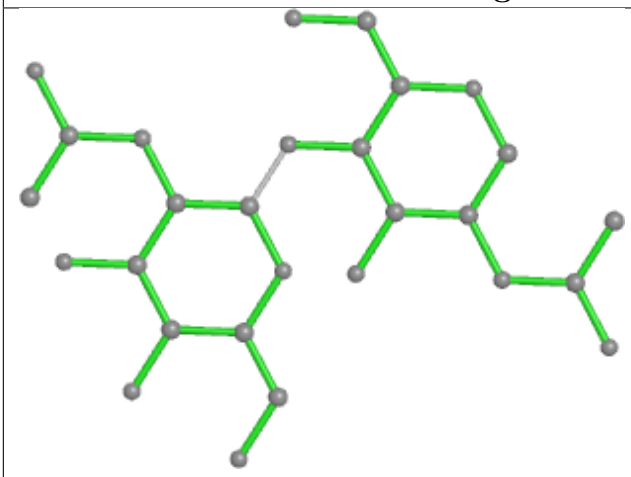
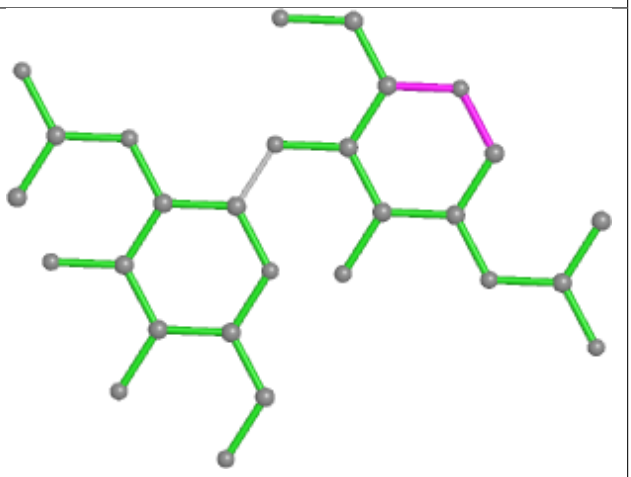
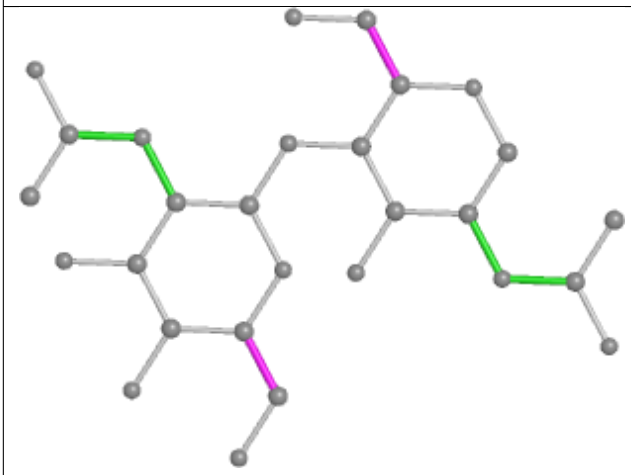
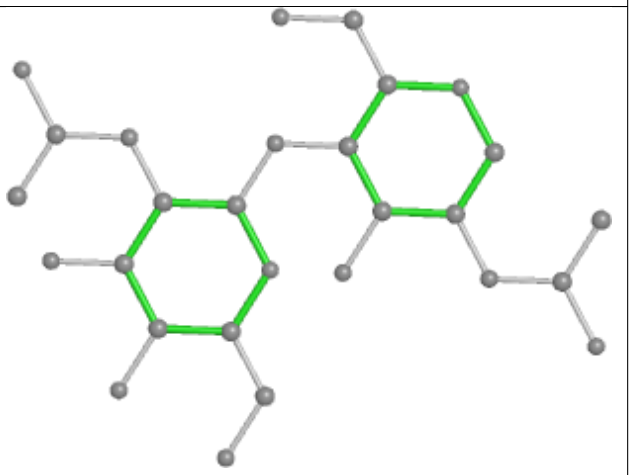
Bond angles

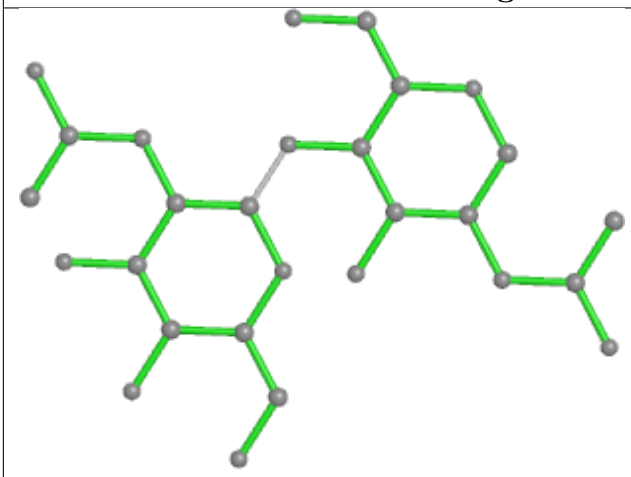
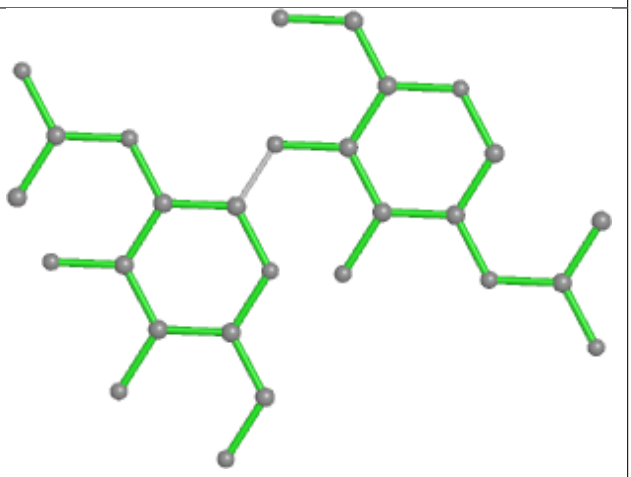
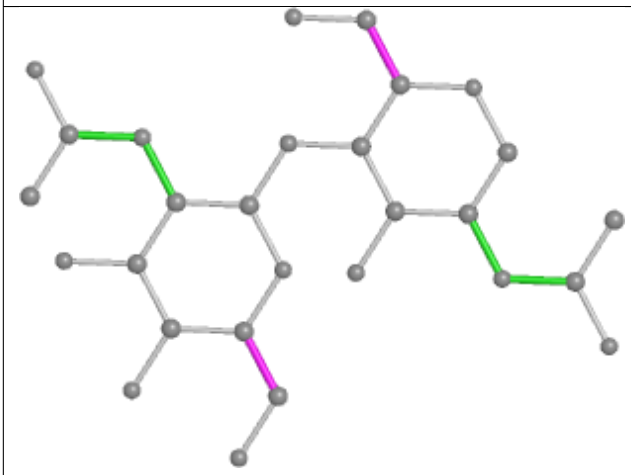
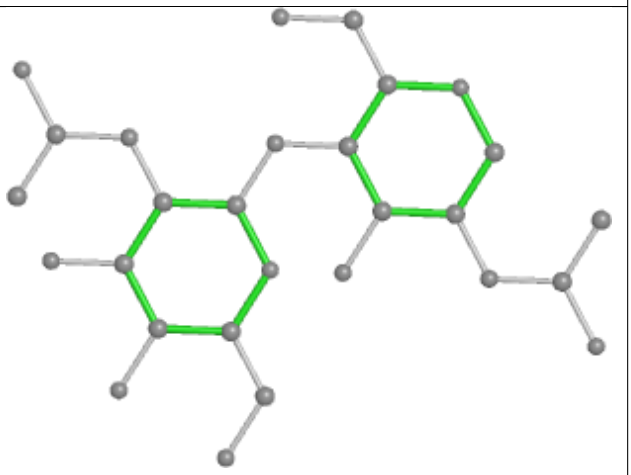


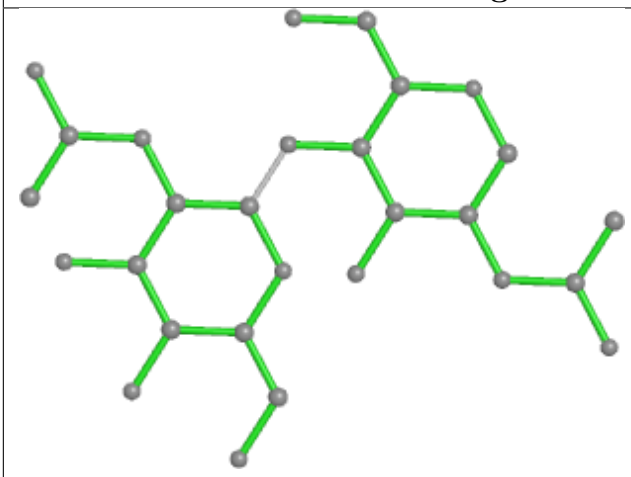
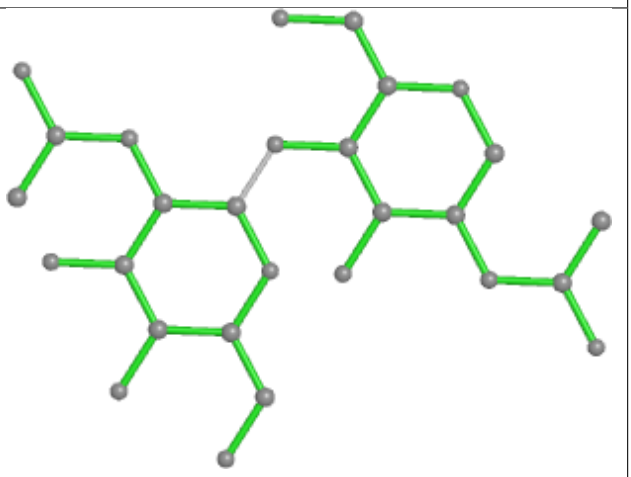
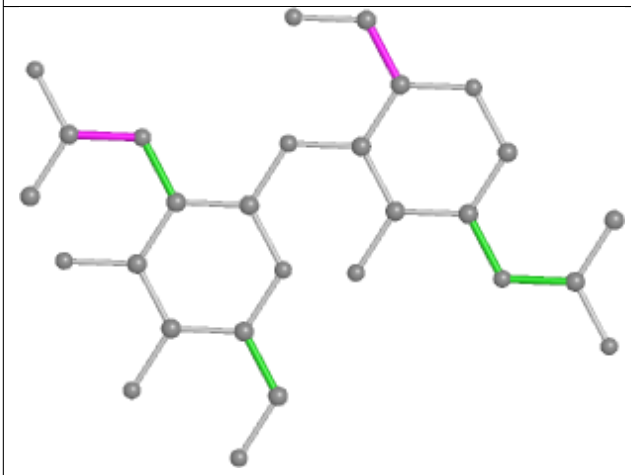
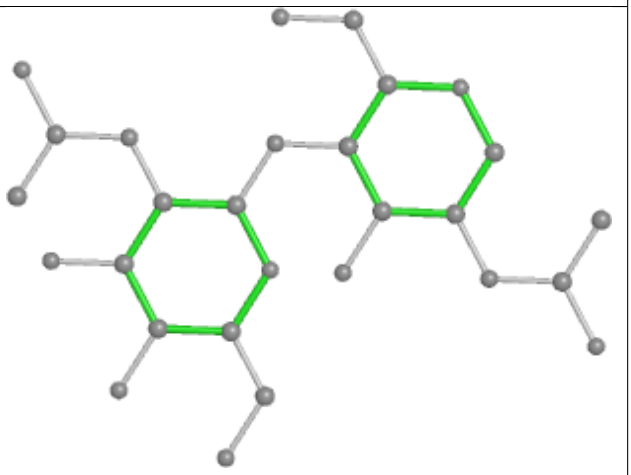
Torsions

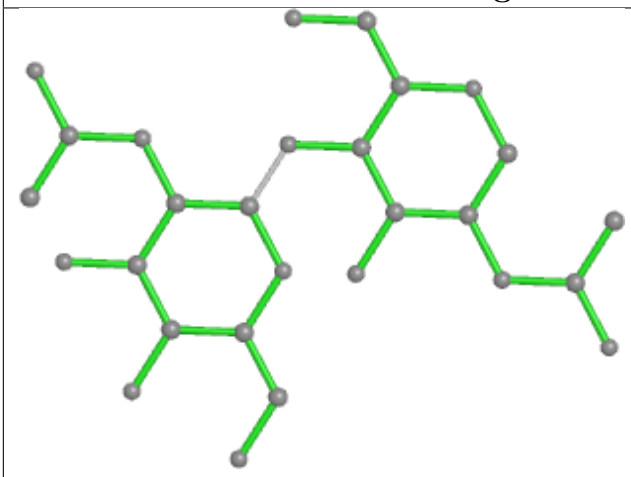
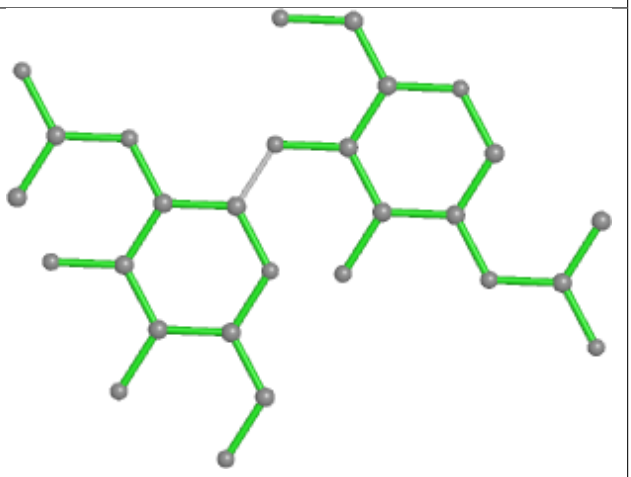
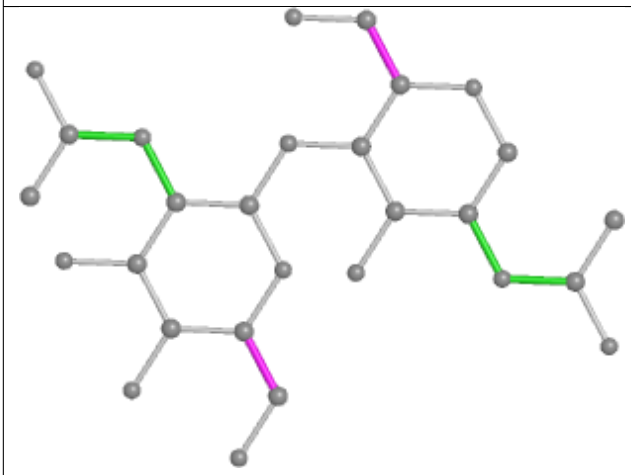
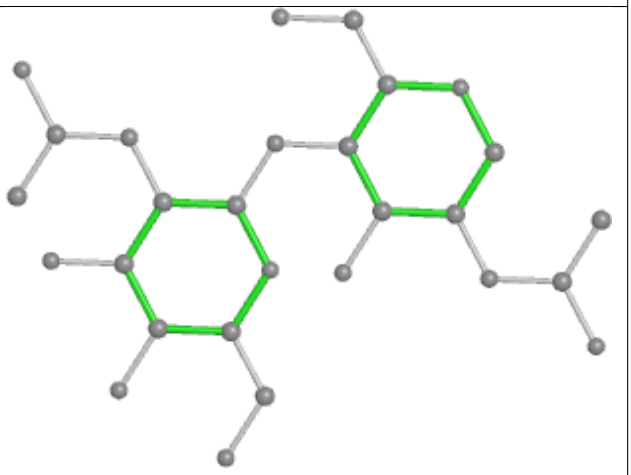


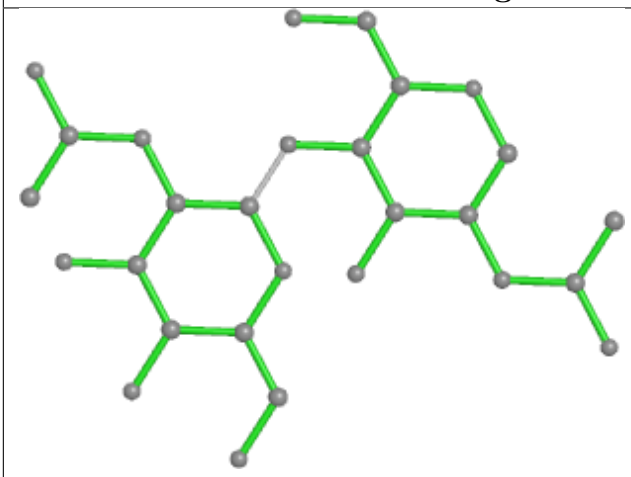
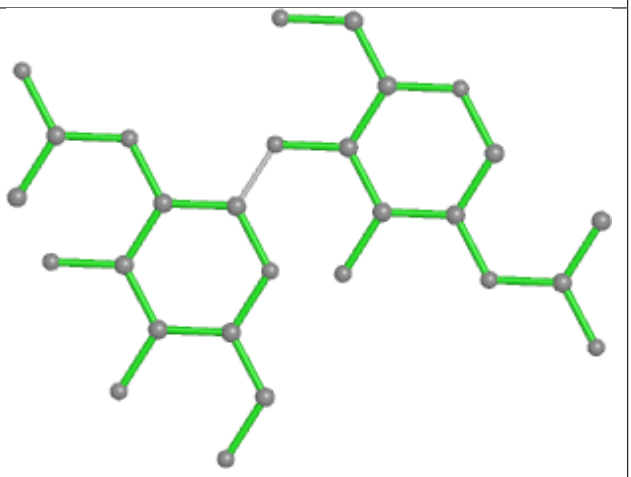
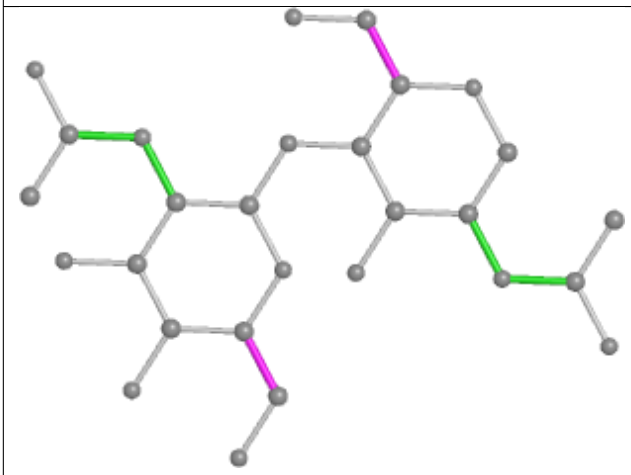
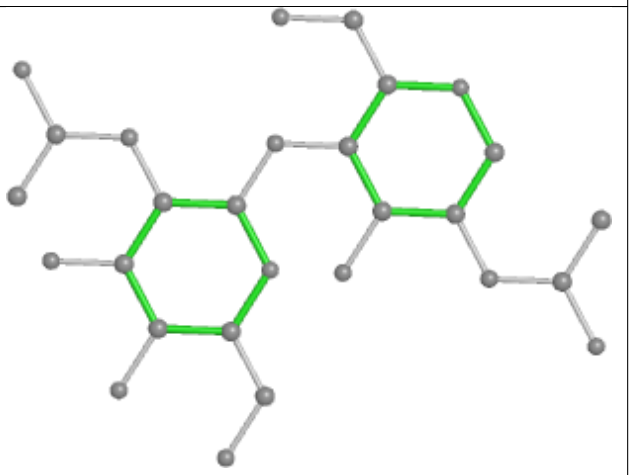
Rings

Oligosaccharide Chain K	
 Bond lengths	 Bond angles
 Torsions	 Rings

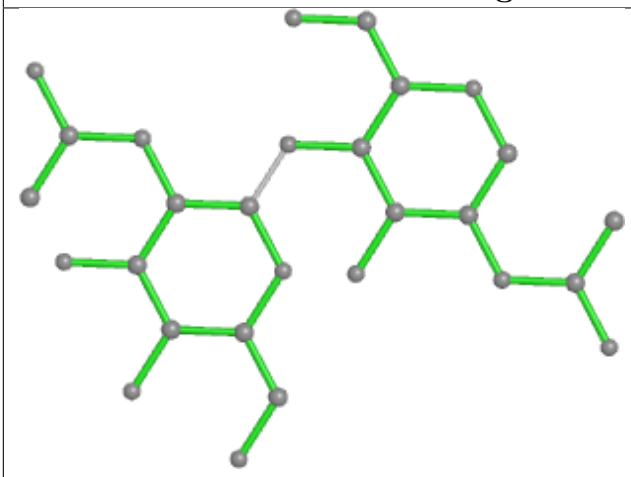
Oligosaccharide Chain L	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain M	
 Bond lengths	 Bond angles
 Torsions	 Rings

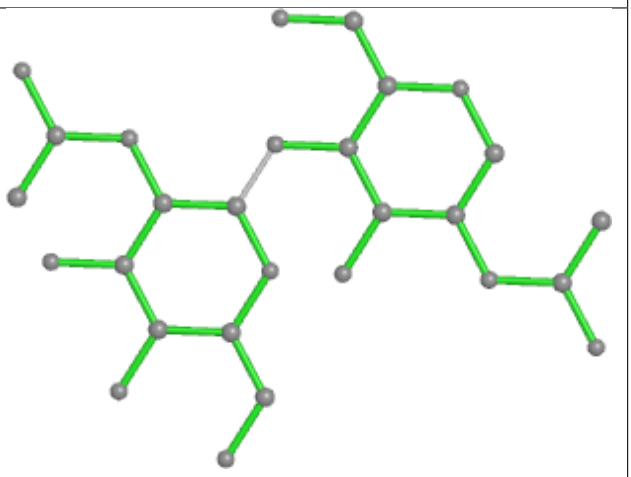
Oligosaccharide Chain N	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain O	
 Bond lengths	 Bond angles
 Torsions	 Rings

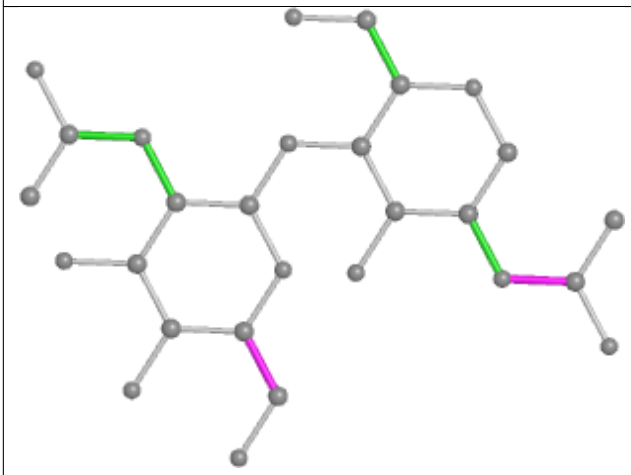
Oligosaccharide Chain P



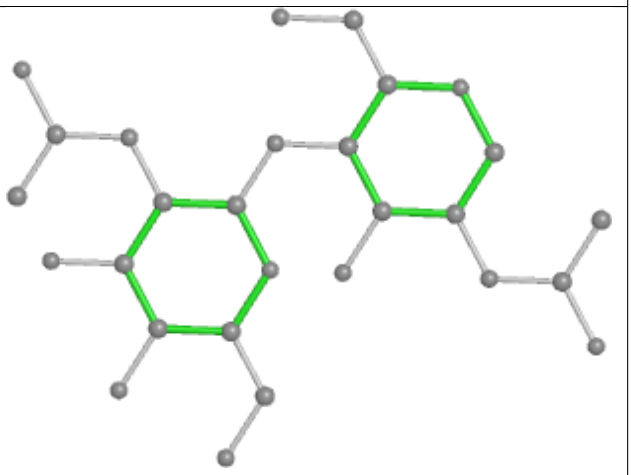
Bond lengths



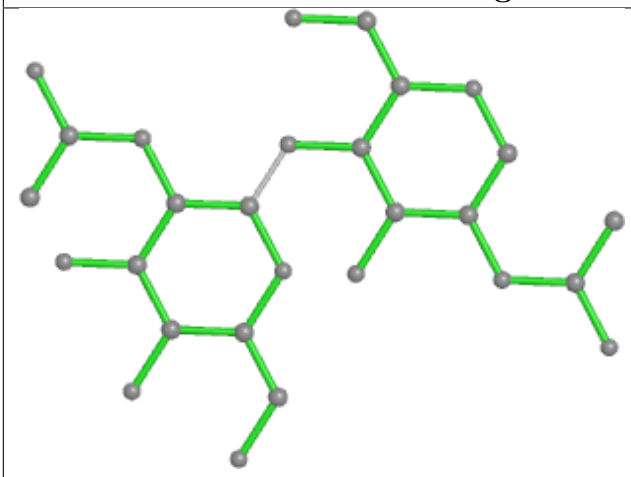
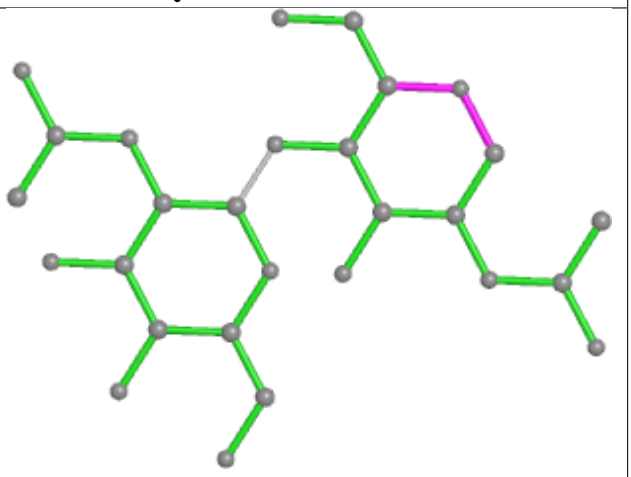
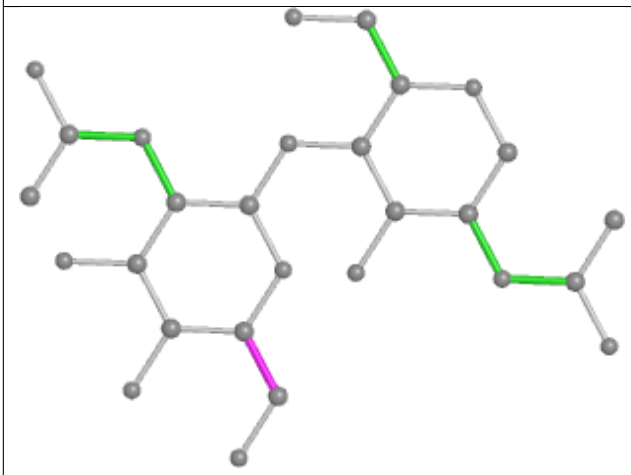
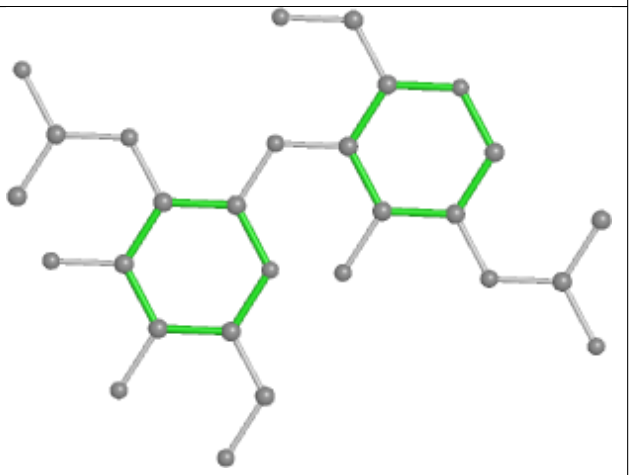
Bond angles

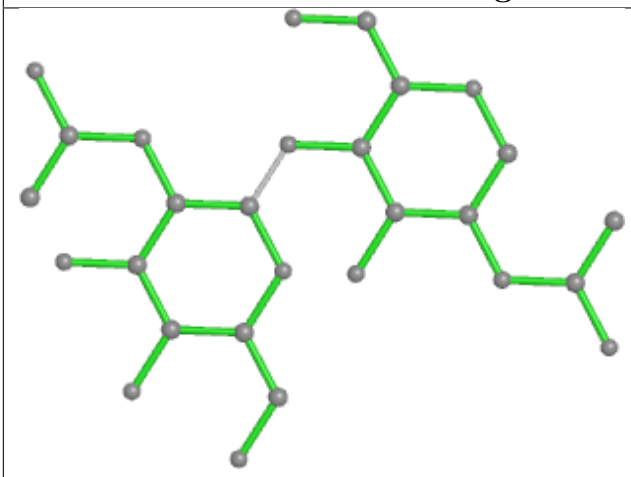
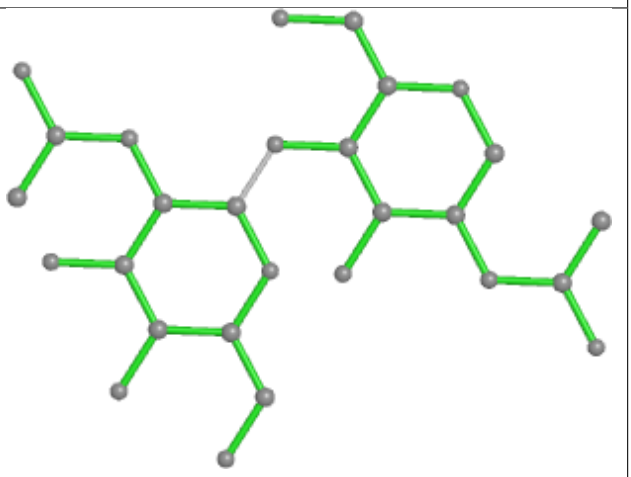
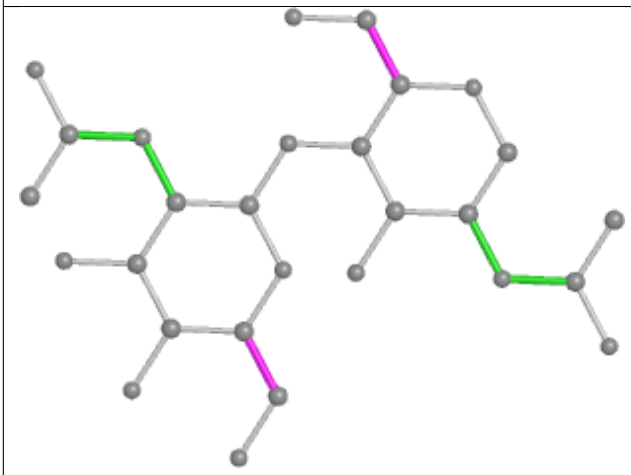
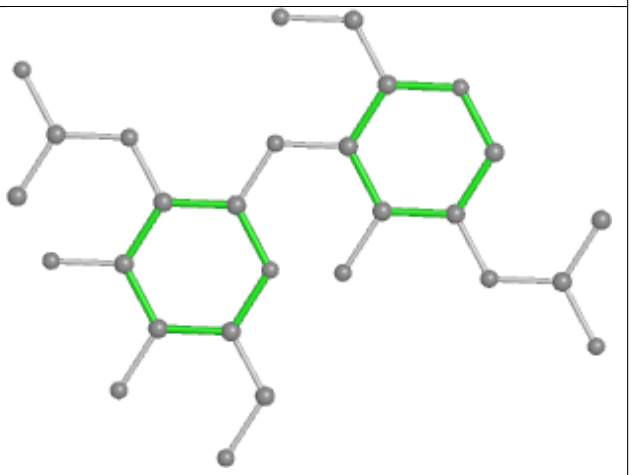


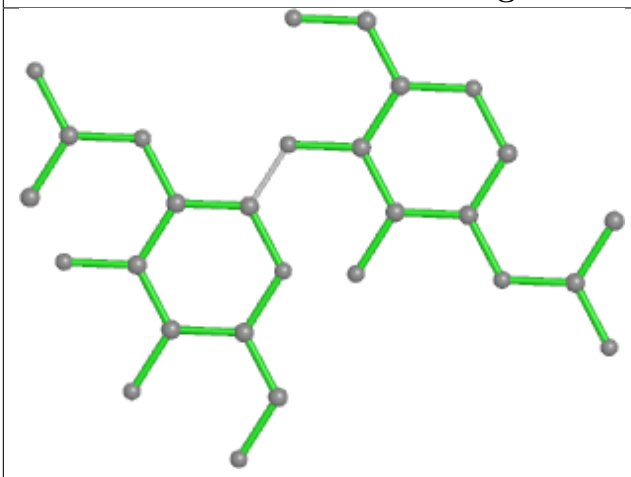
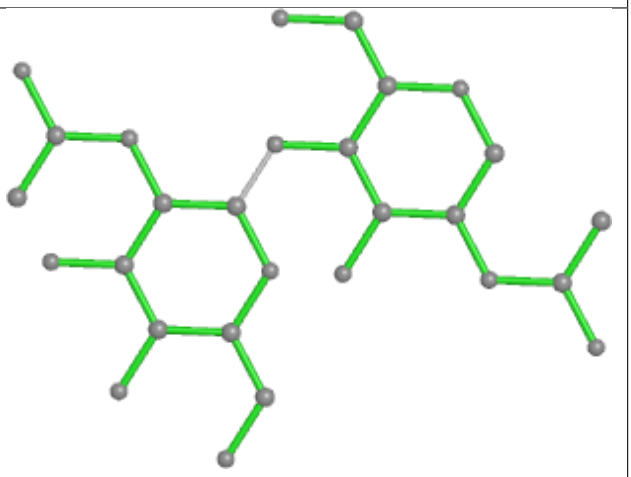
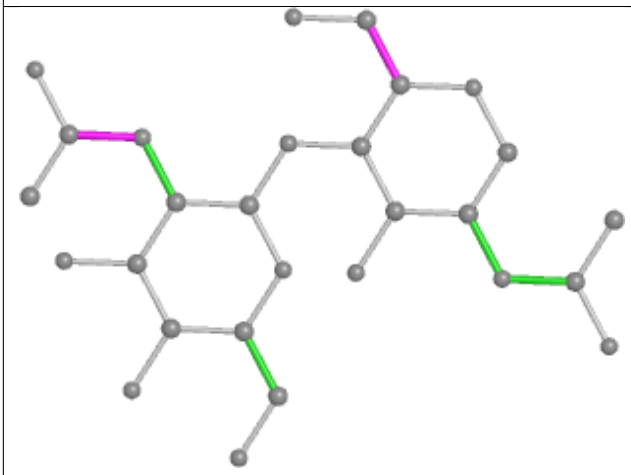
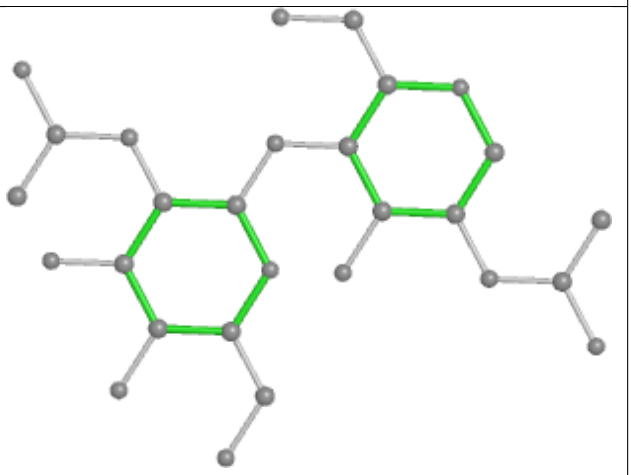
Torsions

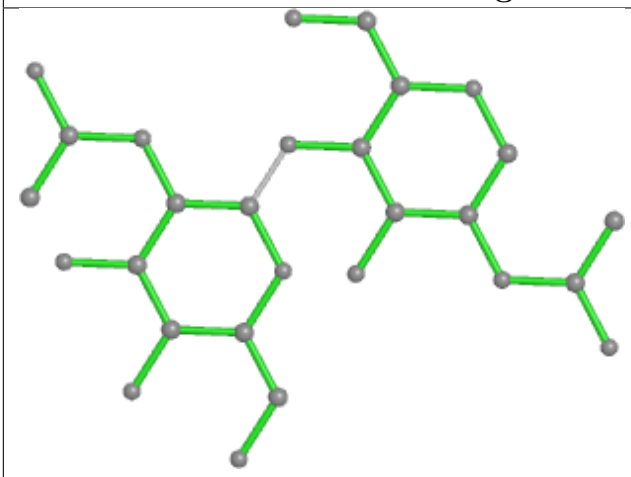
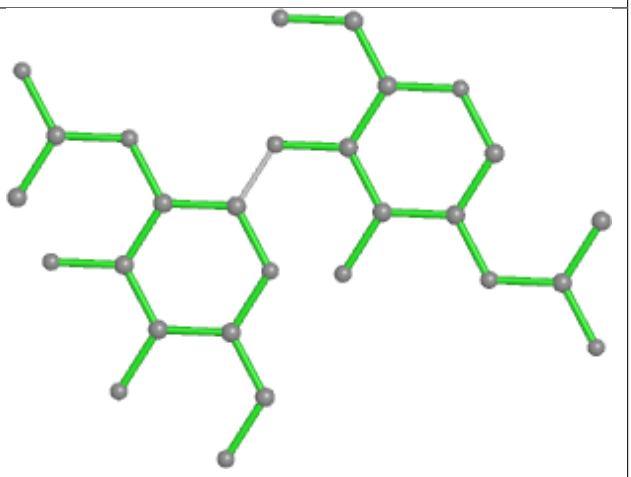
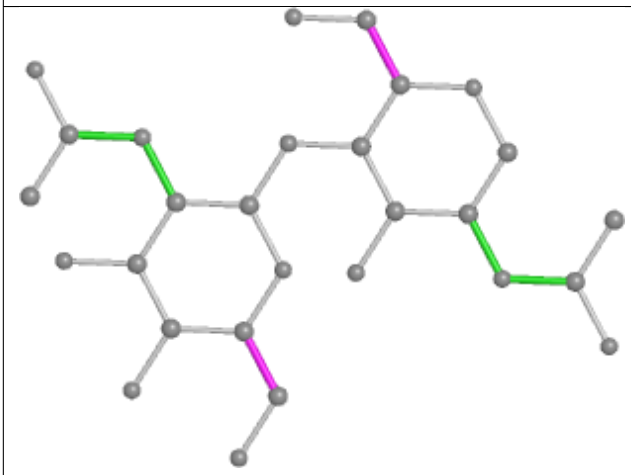
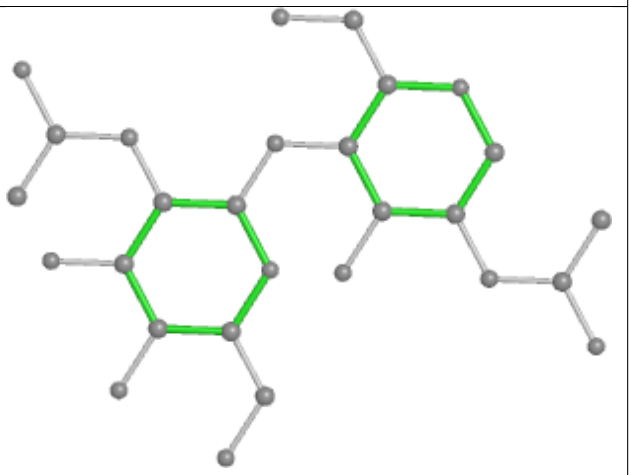


Rings

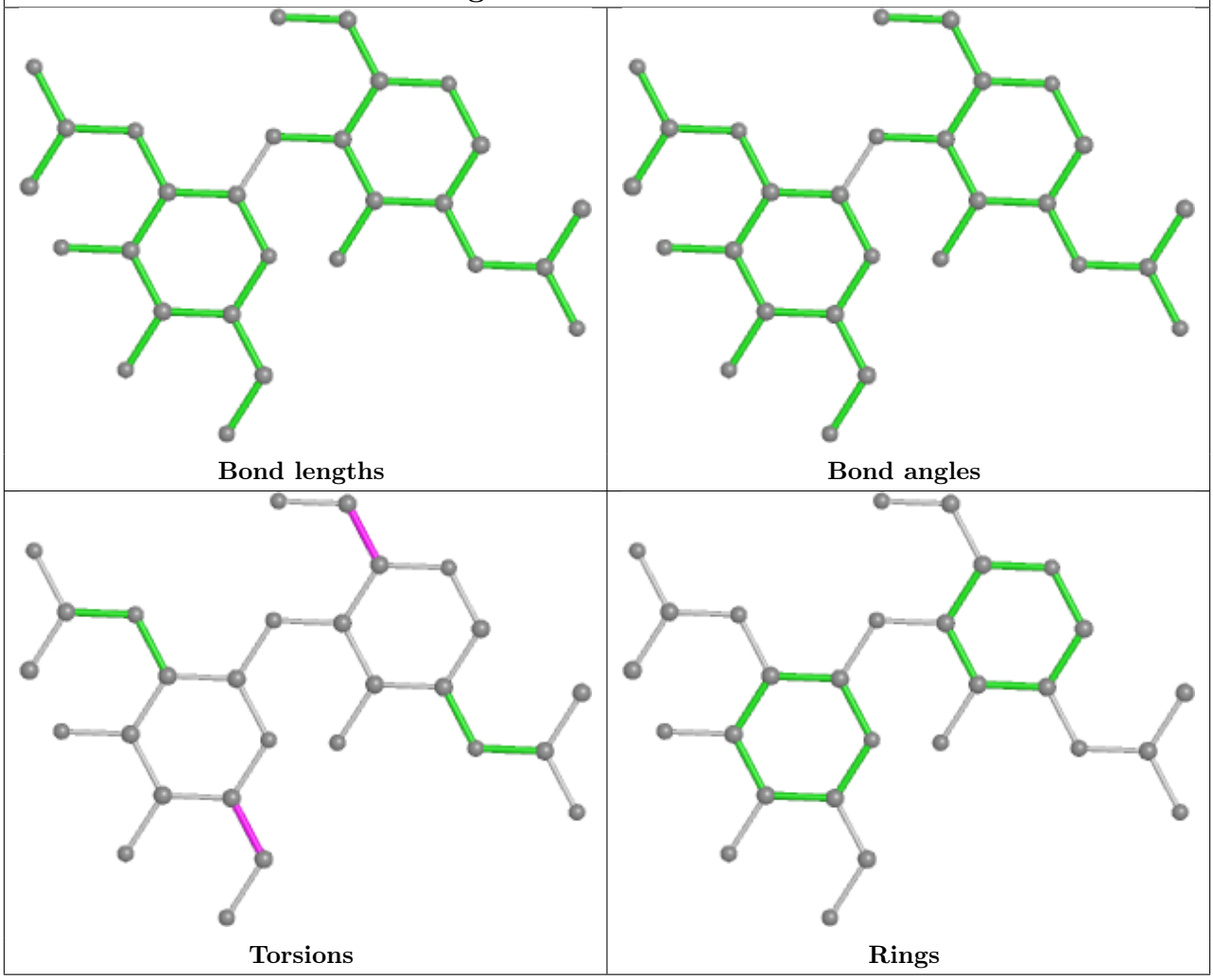
Oligosaccharide Chain Q	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain R	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain S	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain T	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain U



5.6 Ligand geometry (i)

33 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	B	1302	1	14,14,15	0.23	0	17,19,21	0.41	0
3	NAG	A	1311	1	14,14,15	0.22	0	17,19,21	0.41	0
3	NAG	B	1305	1	14,14,15	0.51	0	17,19,21	0.90	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	C	1304	1	14,14,15	0.32	0	17,19,21	0.35	0
3	NAG	B	1301	1	14,14,15	0.25	0	17,19,21	0.50	0
3	NAG	A	1302	1	14,14,15	0.29	0	17,19,21	0.49	0
3	NAG	C	1308	1	14,14,15	0.28	0	17,19,21	0.48	0
3	NAG	A	1310	1	14,14,15	0.22	0	17,19,21	0.41	0
3	NAG	B	1304	1	14,14,15	0.36	0	17,19,21	0.35	0
3	NAG	B	1309	1	14,14,15	0.27	0	17,19,21	0.43	0
3	NAG	C	1302	1	14,14,15	0.22	0	17,19,21	0.42	0
3	NAG	C	1310	1	14,14,15	0.23	0	17,19,21	0.42	0
3	NAG	B	1307	1	14,14,15	0.22	0	17,19,21	0.42	0
3	NAG	A	1308	1	14,14,15	0.30	0	17,19,21	0.48	0
3	NAG	B	1306	1	14,14,15	0.21	0	17,19,21	0.44	0
3	NAG	C	1311	1	14,14,15	0.20	0	17,19,21	0.41	0
3	NAG	A	1304	1	14,14,15	0.34	0	17,19,21	0.35	0
3	NAG	A	1307	1	14,14,15	0.21	0	17,19,21	0.42	0
3	NAG	A	1305	1	14,14,15	0.52	0	17,19,21	0.91	2 (11%)
3	NAG	A	1309	1	14,14,15	0.27	0	17,19,21	0.43	0
3	NAG	B	1308	1	14,14,15	0.28	0	17,19,21	0.48	0
3	NAG	C	1307	1	14,14,15	0.23	0	17,19,21	0.43	0
3	NAG	B	1303	1	14,14,15	0.21	0	17,19,21	0.44	0
3	NAG	C	1303	1	14,14,15	0.20	0	17,19,21	0.45	0
3	NAG	C	1305	1	14,14,15	0.52	0	17,19,21	0.91	2 (11%)
3	NAG	C	1309	1	14,14,15	0.27	0	17,19,21	0.42	0
3	NAG	A	1301	1	14,14,15	0.24	0	17,19,21	0.48	0
3	NAG	A	1306	1	14,14,15	0.21	0	17,19,21	0.44	0
3	NAG	A	1303	1	14,14,15	0.20	0	17,19,21	0.44	0
3	NAG	B	1311	1	14,14,15	0.21	0	17,19,21	0.40	0
3	NAG	C	1301	1	14,14,15	0.26	0	17,19,21	0.45	0
3	NAG	B	1310	1	14,14,15	0.23	0	17,19,21	0.43	0
3	NAG	C	1306	1	14,14,15	0.21	0	17,19,21	0.43	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
3	NAG	B	1302	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1311	1	-	1/6/23/26	0/1/1/1
3	NAG	B	1305	1	-	4/6/23/26	0/1/1/1
3	NAG	C	1304	1	-	1/6/23/26	0/1/1/1
3	NAG	B	1301	1	-	2/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	1302	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1308	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1310	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1304	1	-	1/6/23/26	0/1/1/1
3	NAG	B	1309	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1302	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1310	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1307	1	-	1/6/23/26	0/1/1/1
3	NAG	A	1308	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1306	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1311	1	-	1/6/23/26	0/1/1/1
3	NAG	A	1304	1	-	1/6/23/26	0/1/1/1
3	NAG	A	1307	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1305	1	-	4/6/23/26	0/1/1/1
3	NAG	A	1309	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1308	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1307	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1303	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1303	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1305	1	-	4/6/23/26	0/1/1/1
3	NAG	C	1309	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1301	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1306	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1303	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1311	1	-	1/6/23/26	0/1/1/1
3	NAG	C	1301	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1310	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1306	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1305	NAG	C3-C4-C5	2.44	114.59	110.24
3	B	1305	NAG	C3-C4-C5	2.43	114.58	110.24
3	C	1305	NAG	C3-C4-C5	2.42	114.55	110.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1305	NAG	C1-O5-C5	2.12	115.06	112.19
3	C	1305	NAG	C1-O5-C5	2.07	115.00	112.19

There are no chirality outliers.

All (65) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1306	NAG	O5-C5-C6-O6
3	A	1302	NAG	O5-C5-C6-O6
3	A	1306	NAG	O5-C5-C6-O6
3	B	1306	NAG	O5-C5-C6-O6
3	A	1301	NAG	O5-C5-C6-O6
3	A	1303	NAG	O5-C5-C6-O6
3	B	1308	NAG	O5-C5-C6-O6
3	C	1308	NAG	O5-C5-C6-O6
3	A	1308	NAG	O5-C5-C6-O6
3	B	1301	NAG	O5-C5-C6-O6
3	B	1302	NAG	O5-C5-C6-O6
3	B	1303	NAG	O5-C5-C6-O6
3	C	1301	NAG	O5-C5-C6-O6
3	C	1303	NAG	O5-C5-C6-O6
3	B	1306	NAG	C4-C5-C6-O6
3	B	1309	NAG	C4-C5-C6-O6
3	C	1308	NAG	C4-C5-C6-O6
3	C	1309	NAG	C4-C5-C6-O6
3	C	1302	NAG	O5-C5-C6-O6
3	A	1309	NAG	O5-C5-C6-O6
3	A	1306	NAG	C4-C5-C6-O6
3	A	1309	NAG	C4-C5-C6-O6
3	C	1306	NAG	C4-C5-C6-O6
3	B	1309	NAG	O5-C5-C6-O6
3	C	1309	NAG	O5-C5-C6-O6
3	A	1303	NAG	C4-C5-C6-O6
3	A	1308	NAG	C4-C5-C6-O6
3	B	1303	NAG	C4-C5-C6-O6
3	B	1308	NAG	C4-C5-C6-O6
3	C	1303	NAG	C4-C5-C6-O6
3	A	1302	NAG	C4-C5-C6-O6
3	B	1302	NAG	C4-C5-C6-O6
3	C	1302	NAG	C4-C5-C6-O6
3	A	1301	NAG	C4-C5-C6-O6
3	C	1307	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	1305	NAG	C8-C7-N2-C2
3	A	1305	NAG	O7-C7-N2-C2
3	B	1305	NAG	C8-C7-N2-C2
3	B	1305	NAG	O7-C7-N2-C2
3	C	1305	NAG	C8-C7-N2-C2
3	C	1305	NAG	O7-C7-N2-C2
3	C	1310	NAG	O5-C5-C6-O6
3	A	1310	NAG	O5-C5-C6-O6
3	B	1310	NAG	O5-C5-C6-O6
3	A	1305	NAG	O5-C5-C6-O6
3	A	1307	NAG	O5-C5-C6-O6
3	B	1301	NAG	C4-C5-C6-O6
3	C	1301	NAG	C4-C5-C6-O6
3	C	1305	NAG	O5-C5-C6-O6
3	C	1310	NAG	C4-C5-C6-O6
3	B	1305	NAG	O5-C5-C6-O6
3	B	1307	NAG	O5-C5-C6-O6
3	B	1310	NAG	C4-C5-C6-O6
3	A	1310	NAG	C4-C5-C6-O6
3	B	1304	NAG	O5-C5-C6-O6
3	A	1304	NAG	O5-C5-C6-O6
3	C	1304	NAG	O5-C5-C6-O6
3	A	1311	NAG	O5-C5-C6-O6
3	B	1311	NAG	O5-C5-C6-O6
3	C	1311	NAG	O5-C5-C6-O6
3	A	1305	NAG	C4-C5-C6-O6
3	C	1305	NAG	C4-C5-C6-O6
3	B	1305	NAG	C4-C5-C6-O6
3	C	1307	NAG	C4-C5-C6-O6
3	A	1307	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1306	NAG	1	0
3	C	1301	NAG	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

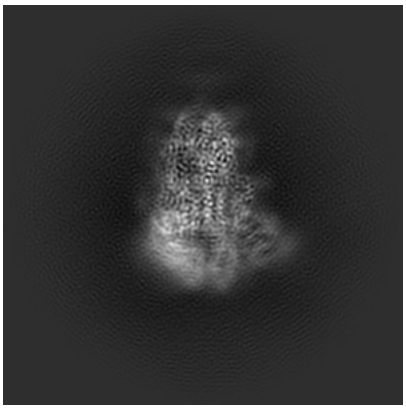
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-33323. These allow visual inspection of the internal detail of the map and identification of artifacts.

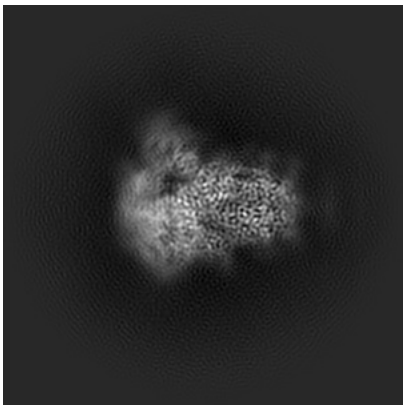
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

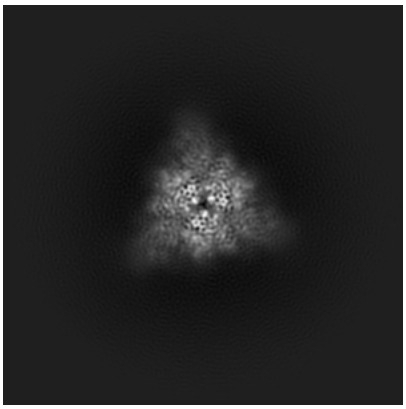
6.1.1 Primary map



X

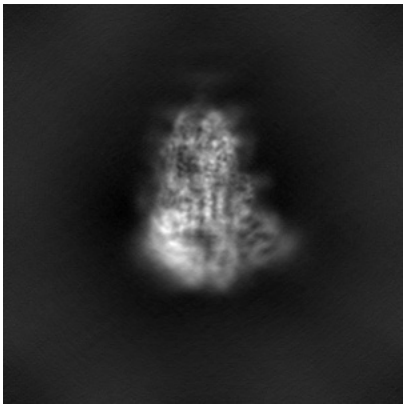


Y

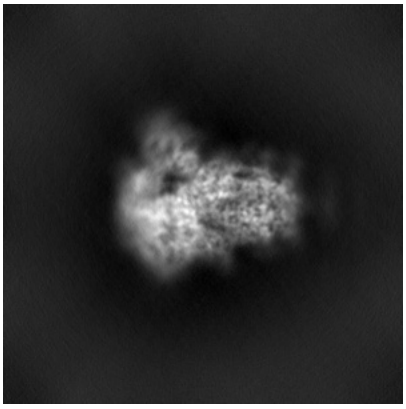


Z

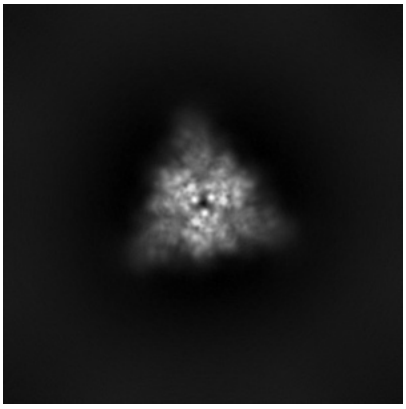
6.1.2 Raw map



X



Y

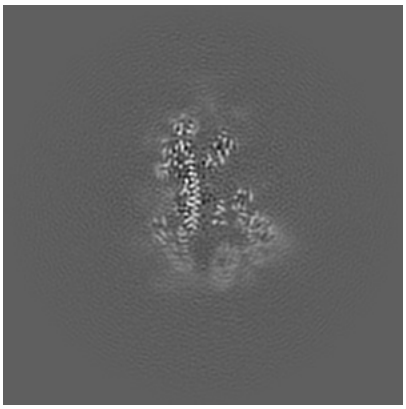


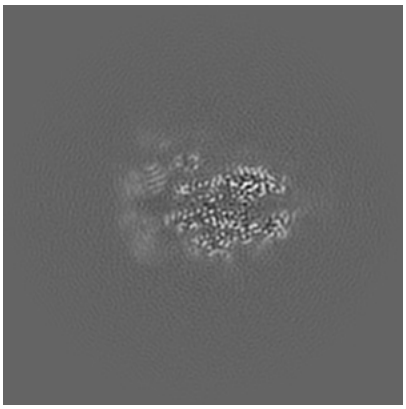
Z

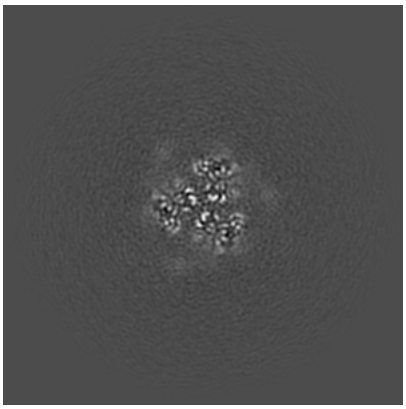
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

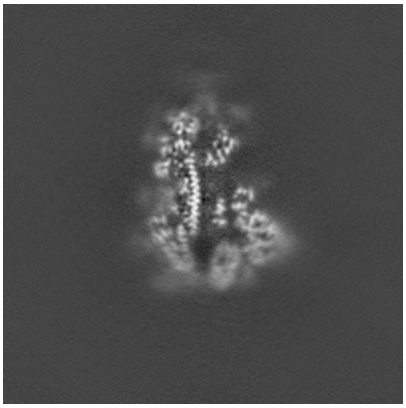
6.2.1 Primary map

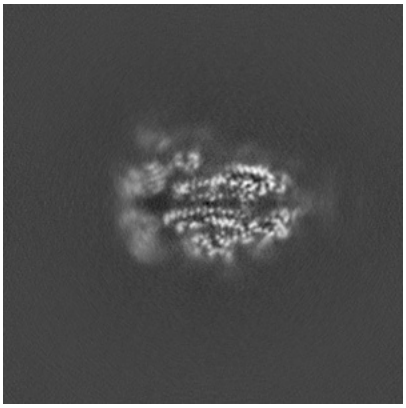

X Index: 160

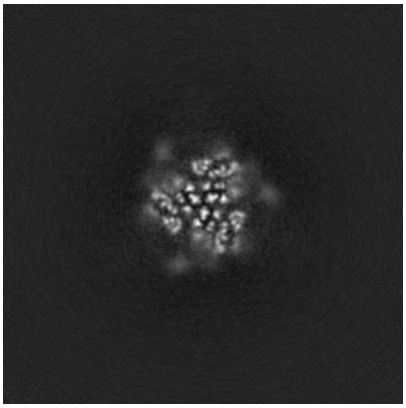

Y Index: 160


Z Index: 160

6.2.2 Raw map


X Index: 160

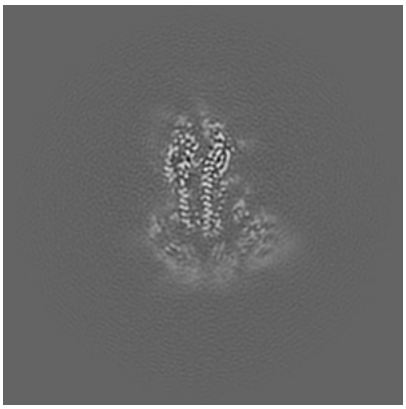

Y Index: 160


Z Index: 160

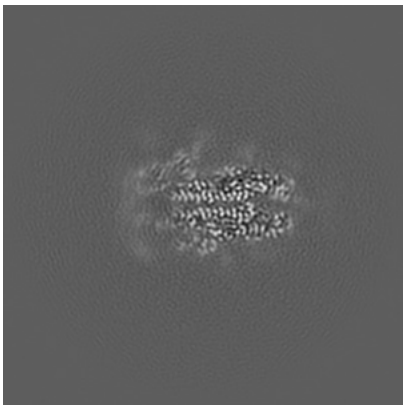
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

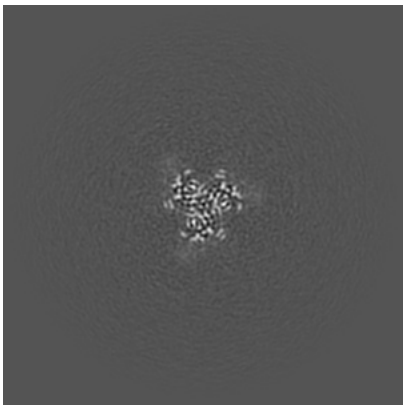
6.3.1 Primary map



X Index: 153

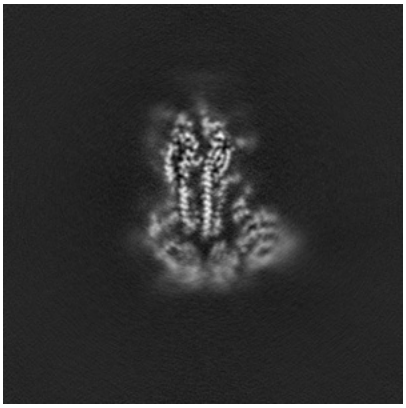


Y Index: 165

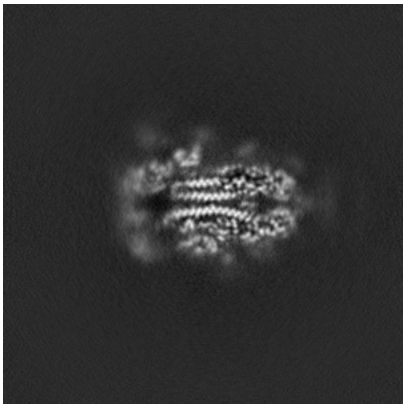


Z Index: 193

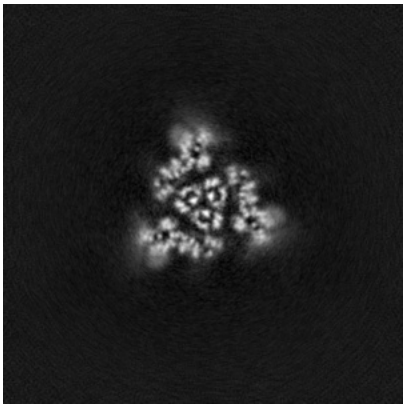
6.3.2 Raw map



X Index: 153



Y Index: 163



Z Index: 141

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 0.4. 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.

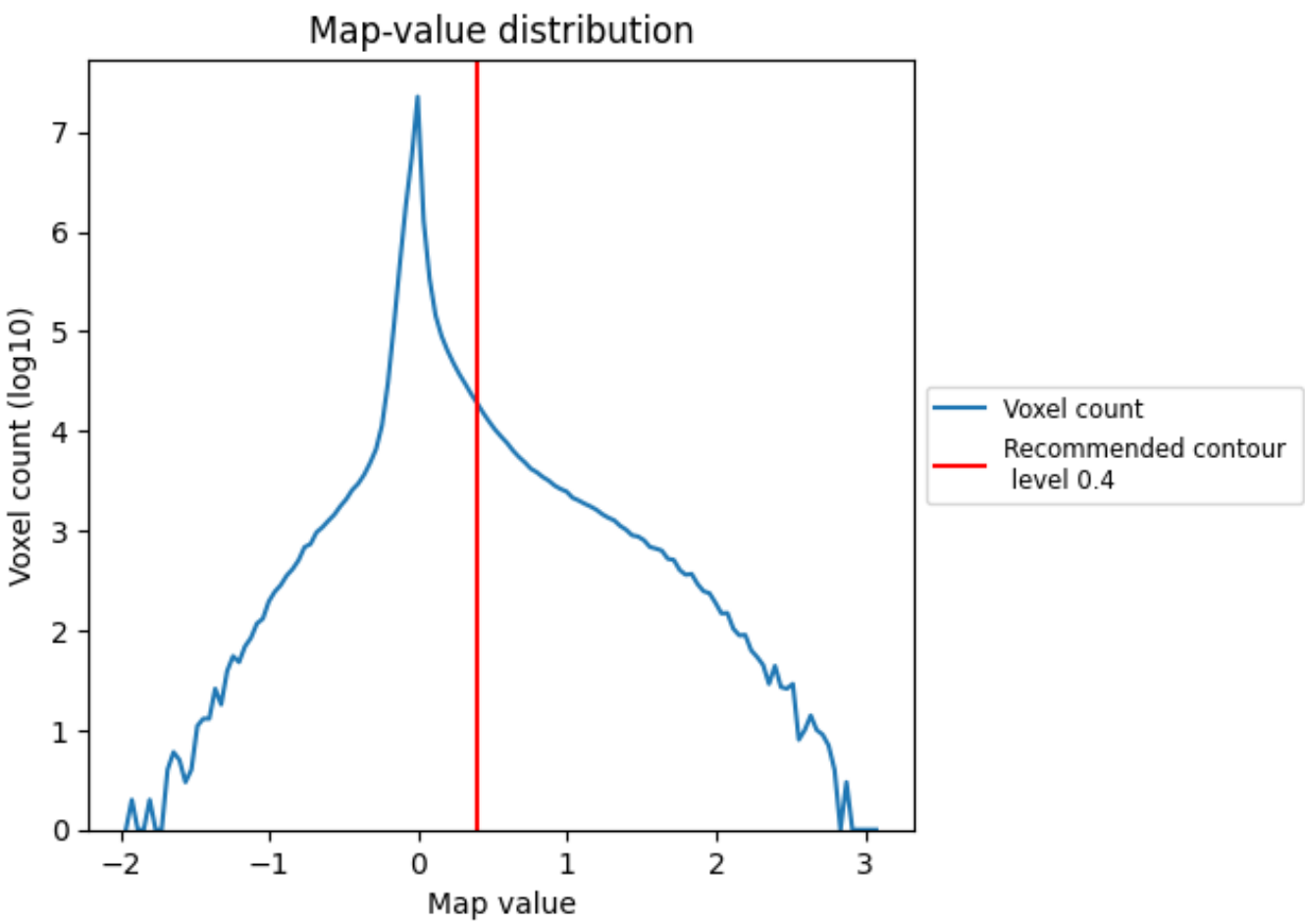
6.5 Mask visualisation (i)

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

7 Map analysis (i)

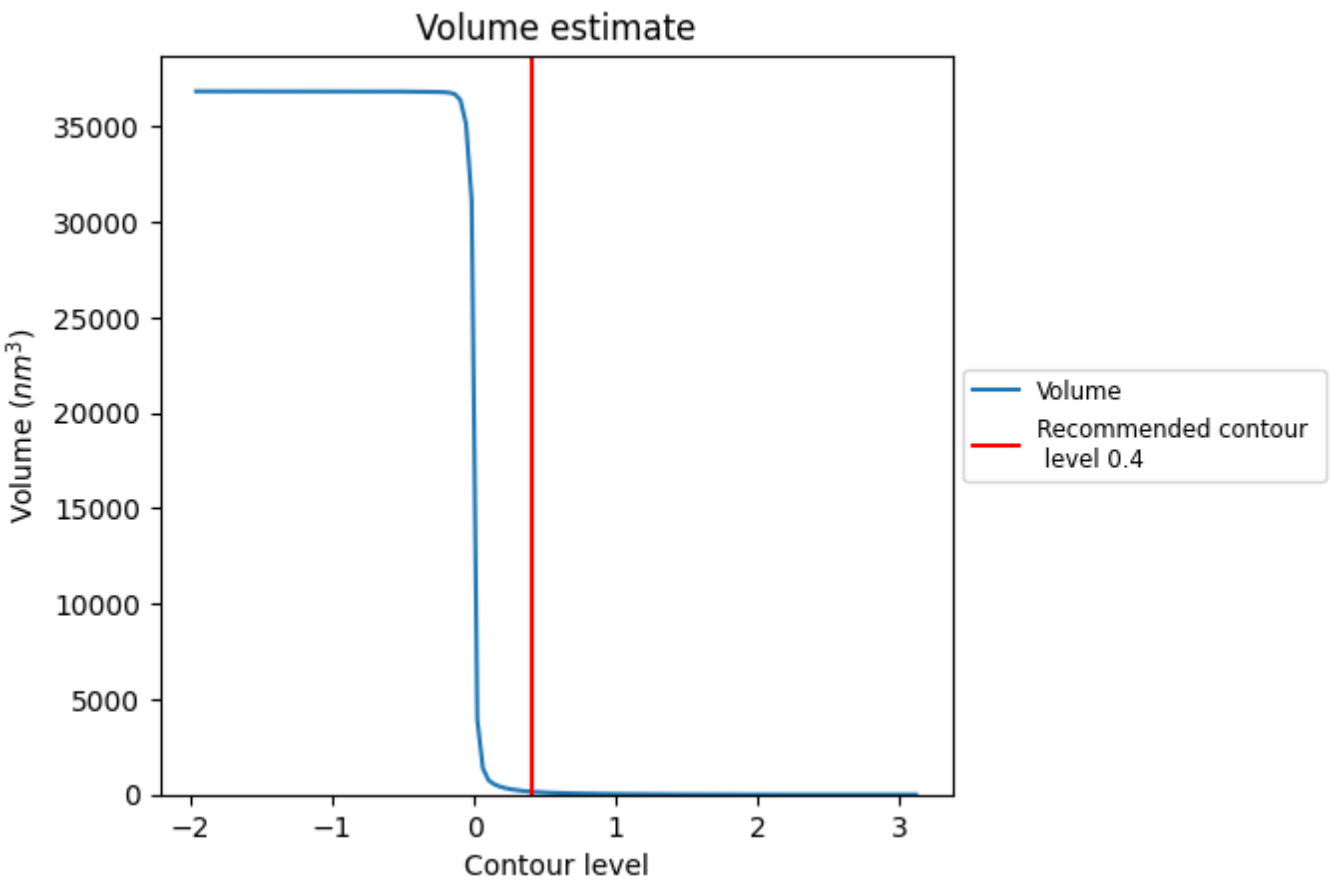
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

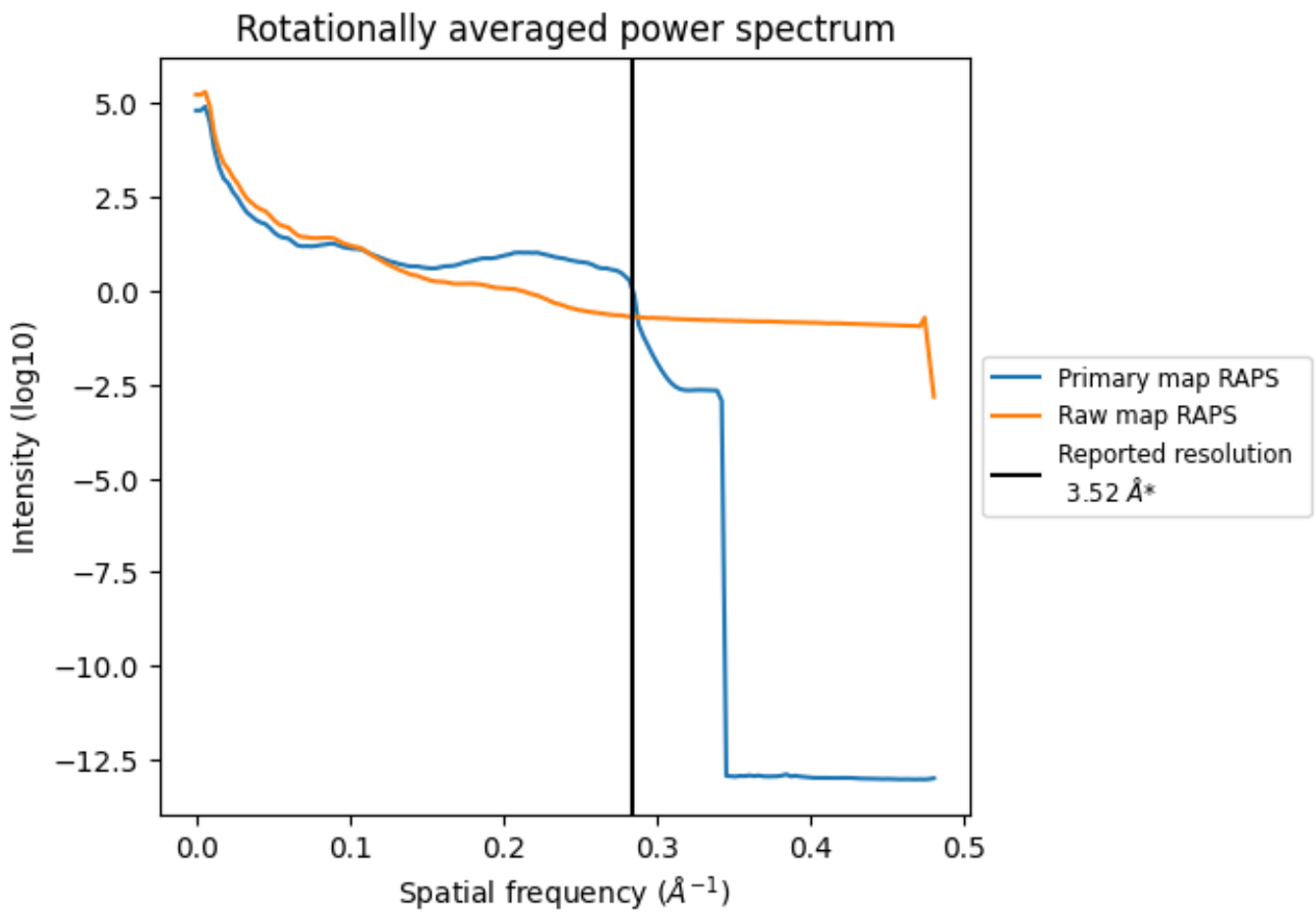
7.2 Volume estimate (i)



The volume at the recommended contour level is 152 nm^3; this corresponds to an approximate mass of 138 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)

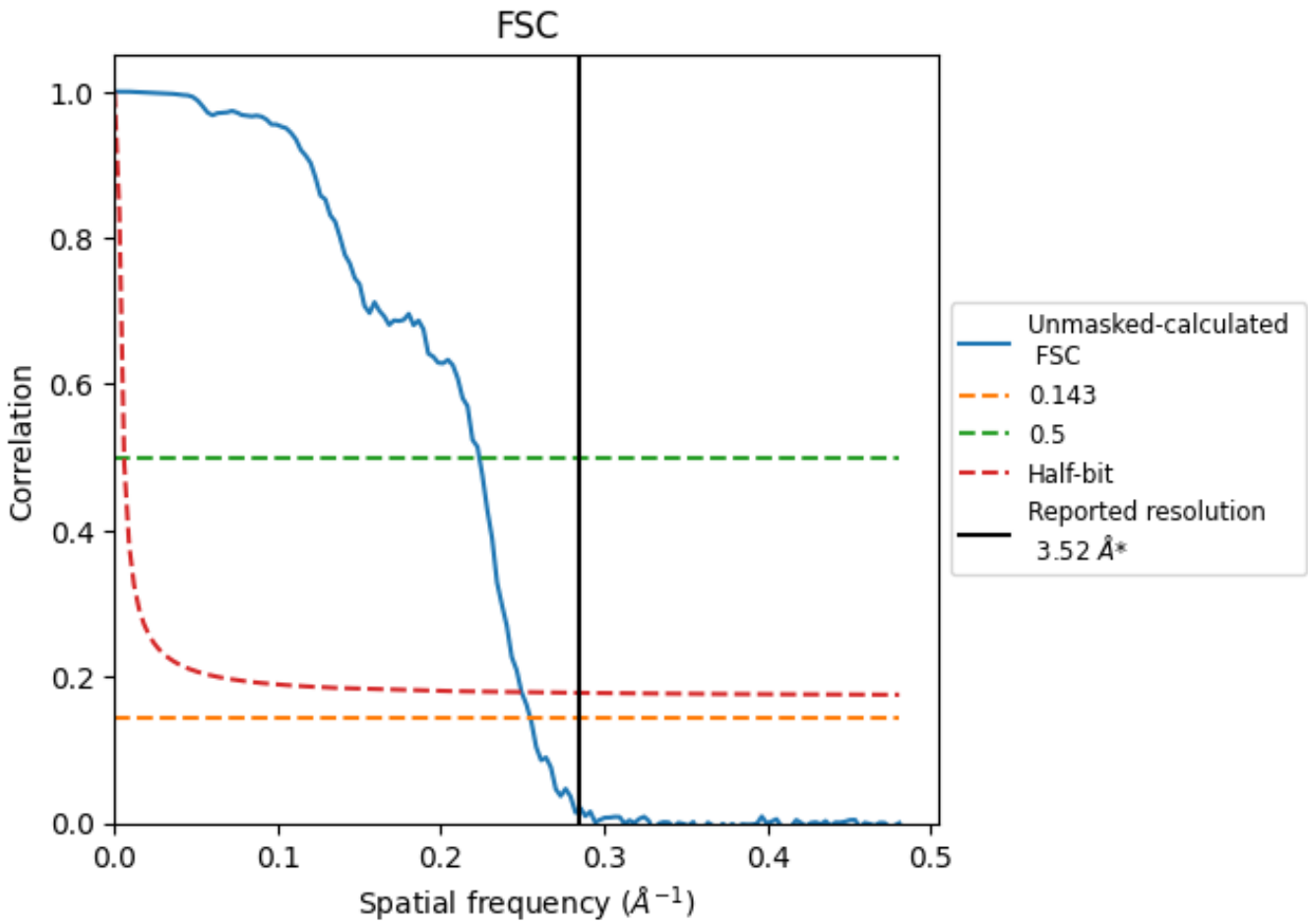


*Reported resolution corresponds to spatial frequency of 0.284 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.284 Å^{-1}

8.2 Resolution estimates (i)

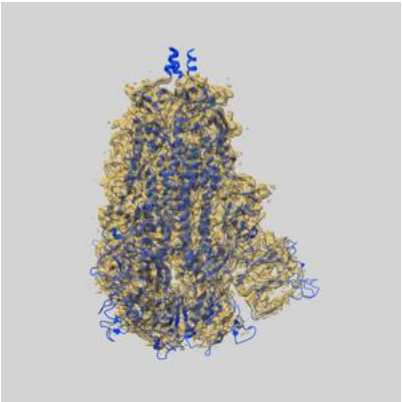
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.52	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.92	4.47	4.01

*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 3.92 differs from the reported value 3.52 by more than 10 %

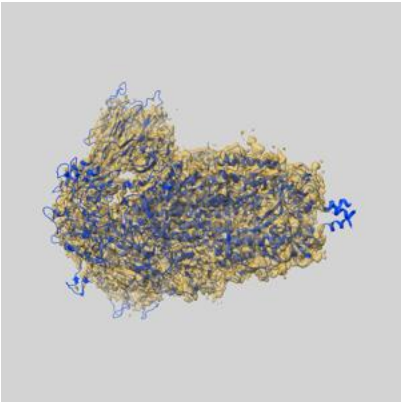
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-33323 and PDB model 7XNQ. Per-residue inclusion information can be found in section 3 on page 11.

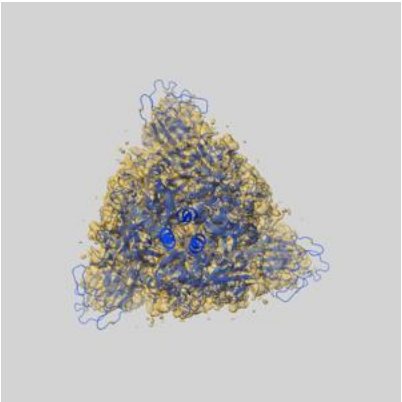
9.1 Map-model overlay (i)



X



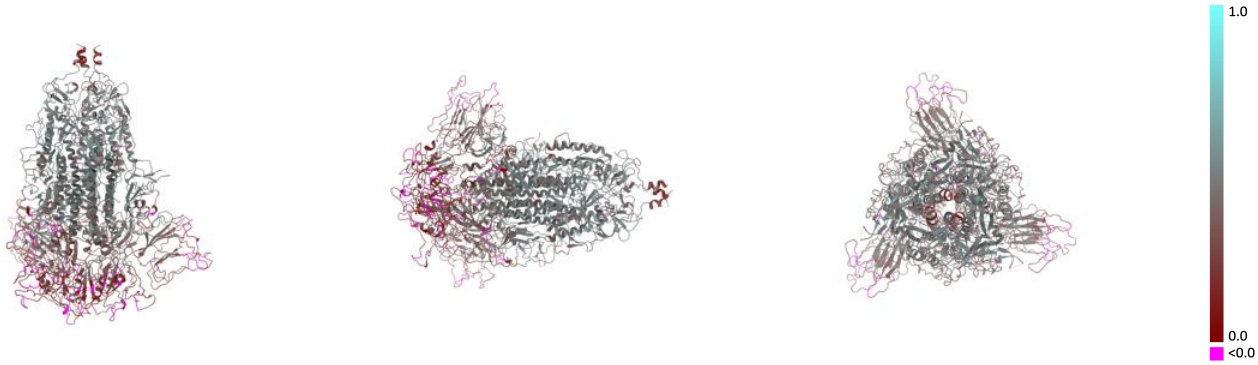
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

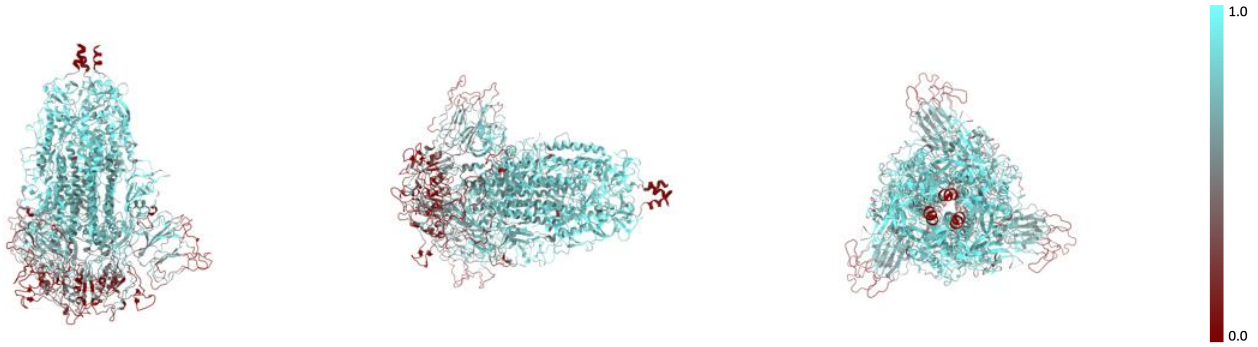
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

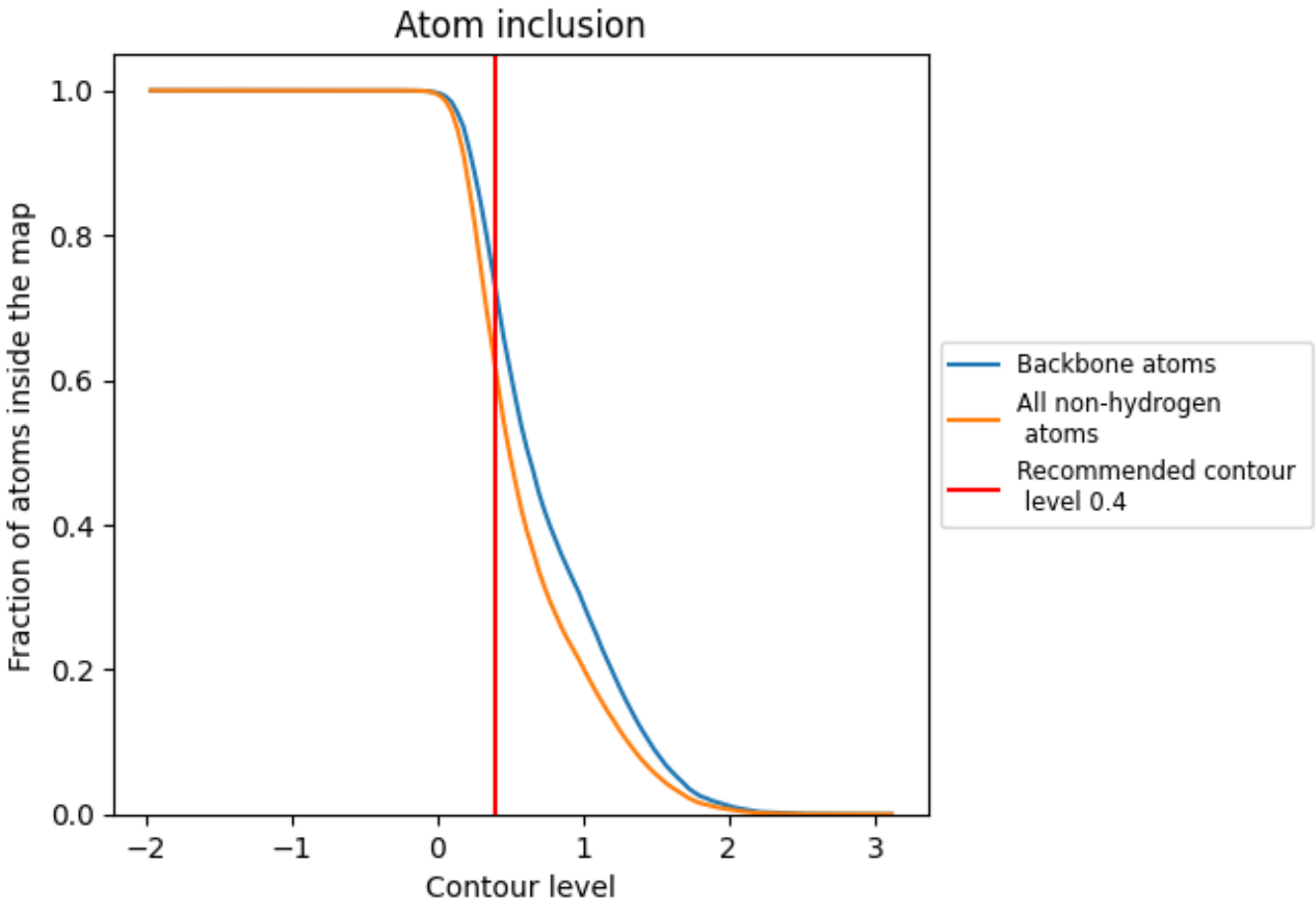
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.4).

9.4 Atom inclusion (i)



At the recommended contour level, 73% of all backbone atoms, 61% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6144	0.3690
A	0.6173	0.3700
B	0.6210	0.3690
C	0.6184	0.3680
D	0.1786	0.2820
E	0.3929	0.3550
F	0.5714	0.3510
G	0.6071	0.3860
H	0.2857	0.3290
I	0.2500	0.3770
J	0.1786	0.2630
K	0.3571	0.3570
L	0.5714	0.3960
M	0.6071	0.3740
N	0.3214	0.3280
O	0.2500	0.3770
P	0.1786	0.2910
Q	0.3571	0.3300
R	0.6786	0.4070
S	0.6071	0.3760
T	0.2857	0.3300
U	0.2500	0.3820