



## wwPDB EM Validation Summary Report ⓘ

Oct 27, 2024 – 03:03 PM JST

PDB ID : 7CWN  
EMDB ID : EMD-30484  
Title : P17-H014 Fab cocktail in complex with SARS-CoV-2 spike protein  
Authors : Wang, N.; Wang, X.  
Deposited on : 2020-08-29  
Resolution : 3.20 Å(reported)

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

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<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev113  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

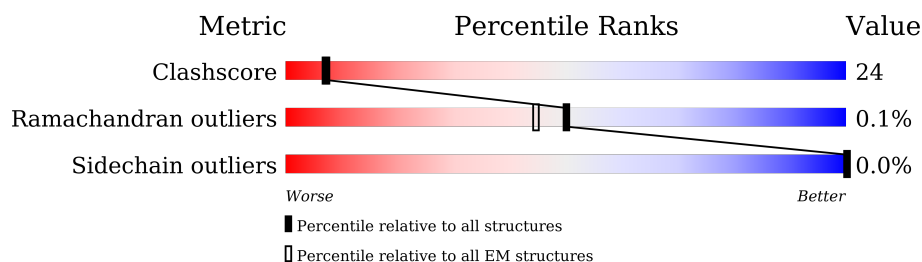
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.20 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 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  $\leq 5\%$ . 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	1273	 56%      28%      16%
1	B	1273	 56%      28%      16%
1	C	1273	 56%      29%      16%
2	G	213	 30%      36%      20%      14%
2	K	213	 30%      36%      20%      14%
2	L	213	 31%      36%      20%      13%
3	F	209	 19%      40%      11%      30%
3	I	209	 19%      41%      11%      29%

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Mol	Chain	Length	Quality of chain
3	J	209	
4	D	207	
4	M	207	
4	N	207	
5	E	214	
5	H	214	
5	O	214	
6	P	2	
6	Q	2	
6	R	2	
6	S	2	
6	T	2	
6	U	2	
6	V	2	
6	W	2	
6	X	2	
6	Y	2	
6	Z	2	
6	a	2	
6	b	2	
6	c	2	
6	d	2	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	NAG	Z	1	-	-	X	-

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 36191 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
1	A	1072	Total	C	N	O	S	0	0
			8348	5330	1392	1587	39		
1	B	1070	Total	C	N	O	S	0	0
			8339	5324	1392	1584	39		
1	C	1072	Total	C	N	O	S	0	0
			8351	5330	1395	1587	39		

- Molecule 2 is a protein called heavy chain of P17 Fab.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	K	120	Total	C	N	O	S	0	0
			918	574	165	175	4		
2	L	120	Total	C	N	O	S	0	0
			918	574	165	175	4		
2	G	120	Total	C	N	O	S	0	0
			918	574	165	175	4		

- Molecule 3 is a protein called light chain of P17 Fab.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	108	Total	C	N	O	S	0	0
			817	511	137	167	2		
3	J	107	Total	C	N	O	S	0	0
			813	509	136	166	2		
3	F	107	Total	C	N	O	S	0	0
			813	509	136	166	2		

- Molecule 4 is a protein called light chain of H014 Fab.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	107	Total	C	N	O	S	0	0
			844	540	140	162	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	N	107	Total	C	N	O	S	0	0
			844	540	140	162	2		
4	M	107	Total	C	N	O	S	0	0
			844	540	140	162	2		

- Molecule 5 is a protein called heavy chain of H014 Fab.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	122	Total	C	N	O	S	0	0
			929	589	147	189	4		
5	H	122	Total	C	N	O	S	0	0
			922	583	147	188	4		
5	O	122	Total	C	N	O	S	0	0
			929	589	147	189	4		

- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



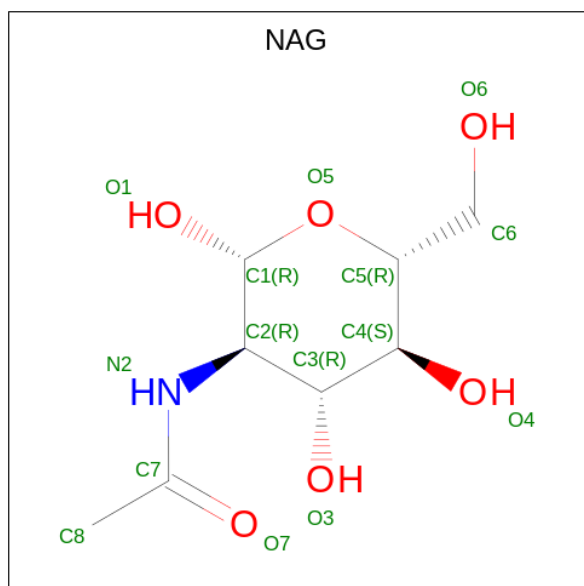
Mol	Chain	Residues	Atoms				AltConf	Trace
6	P	2	Total	C	N	O	0	0
			28	16	2	10		
6	Q	2	Total	C	N	O	0	0
			28	16	2	10		
6	R	2	Total	C	N	O	0	0
			28	16	2	10		
6	S	2	Total	C	N	O	0	0
			28	16	2	10		
6	T	2	Total	C	N	O	0	0
			28	16	2	10		
6	U	2	Total	C	N	O	0	0
			28	16	2	10		
6	V	2	Total	C	N	O	0	0
			28	16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

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Mol	Chain	Residues	Atoms				AltConf	Trace
6	Y	2	Total	C	N	O	0	0
			28	16	2	10		
6	Z	2	Total	C	N	O	0	0
			28	16	2	10		
6	a	2	Total	C	N	O	0	0
			28	16	2	10		
6	b	2	Total	C	N	O	0	0
			28	16	2	10		
6	c	2	Total	C	N	O	0	0
			28	16	2	10		
6	d	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

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



### 3 Residue-property plots [i](#)

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

#### • Molecule 1: Spike glycoprotein



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LEU	CYS	CYS	VAL	VAL	ASN	THR	SER	CYS	GLN	TYR1086	ASP	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP	CYS	LEU	GLY	ASP

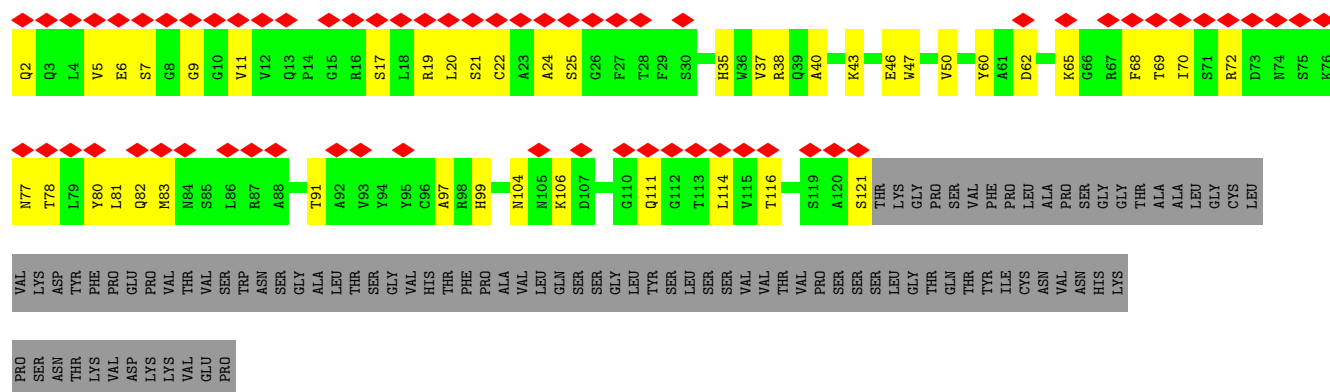
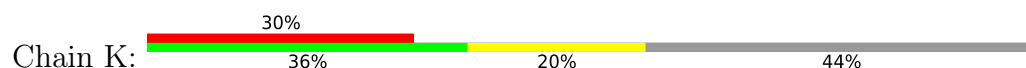
● Molecule 1: Spike glycoprotein



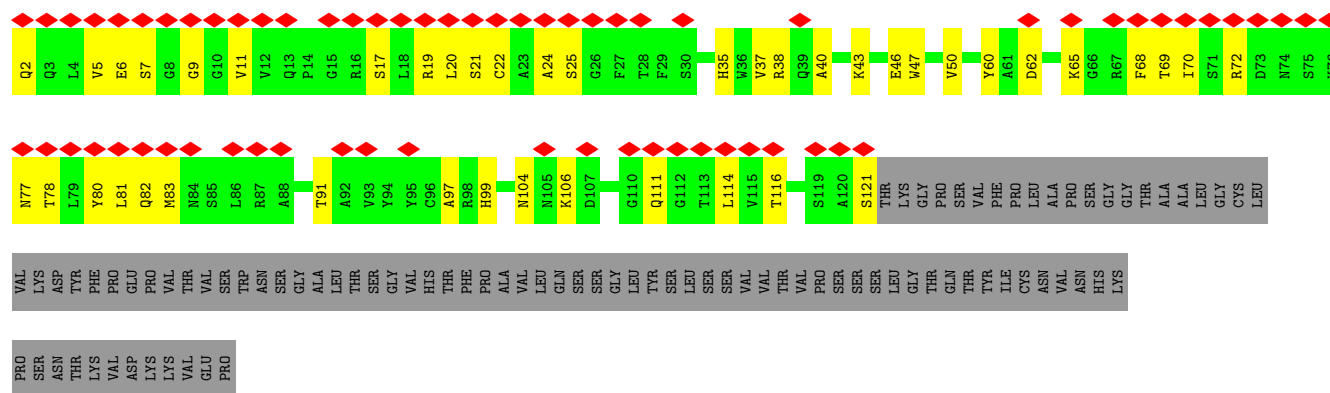
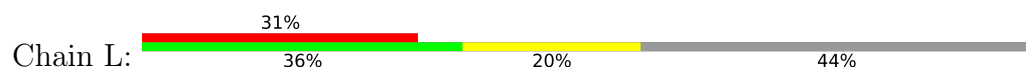
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P85	F86	N87	D88	G89	A93	E96	I100	I101	R102	G103	W104	I105	F106	G107	T108	T109	D111	Q115	S116	L117	L118	I119	V120	N121	N122	Y126	K129	V130	C131	E132	F133	Q134	F135	C136	N137	D138	P139	F140	L141	G142	V143	N148	N149	K150	E154	S155	E156	F157	R158	V159	
Y160	A163	T167	F168	E169	Y170	Y171	S172	L176	E180	G181	K182	Q183	ASP	G184	N185	F186	N188	L189	R190	E191	F194	Y200	F201	K202	T203	Y204	S205	K206	H207	T208	P209	I210	N211	L212	V213	R214	D215	L216	P217	S221	A222	L223	L226	V227	D228	L229	P230	L231	G232	F233	N234
T235	T236	R237	F238	Q239	L242	H245	R246	S247	Y248	L249	T250	P251	GLY	ASP	SER	S256	G257	W258	T259	A260	A263	Y266	Y269	L270	R273	L276	L277	L278	E281	G282	G283	T284	L285	V289	D290	C291	L296	S297	E298	T299	F306	T315	S316	N317	F318	R319					
V320	T323	E324	S325	L326	V327	R328	F329	P330	ASN	THR	ASN	L335	C336	P337	E340	T345	R346	A352	K356	R357	L358	S359	N360	Y365	S366	V367	L368	Y369	N370	S371	A372	S373	F377	Y380	S383	P384	L387	C391	F392	T393	N394	D398	V401	R417							
I418	N422	Y423	K424	G431	W436	N437	L441	D442	S443	K444	V445	G446	G447	N448	Y449	N450	R454	L455	F456	R457	K458	S459	P463	R466	D467	I468	S469	A475	G476	S477	F486	Q493	F497	Q498	P499	T500	N501	Y505	Q506	P507	Y508	R509	L513	L518	H519						
T523	G526	PRO	L533	V534	K535	N536	C537	V539	N540	F541	N542	F543	L546	G550	V551	L552	T553	K557	K558	F559	L560	P561	F562	Q563	Q564	F565	G566	R567	D568	I569	A570	D571	T572	T573	P579	Q580	I584	T588	P589	C590	S591	F592	G593	G594							
V597	N606	V615	V620	PRO	VAL	ALA	ILE	HIS	ALA	ASP	GLN	LEU	THR	PRO	THR	TRP	ARG	VAL	TYR	SER	THR	GLY	SER	N641	V642	F643	G644	T645	G648	C649	L650	A653	G669	T676	GLN	ASN	SER	PRO	ARG	ALA	ARG	ALA	VAL	ALA	VAL	S669	Q690	L699	N709		
N710	A713	I714	T715	T716	N717	F718	V722	E725	I726	S735	D745	S746	T747	S750	F759	L763	A783	K786	Q787	D796	F800	N801	Q804	K811	R815	D820	L821	L822	N824	K825	W826	T827	LEU	ALA	ASP	ALA	VAL	GLY	PHE	ILE	LYS	GLN	TYR								



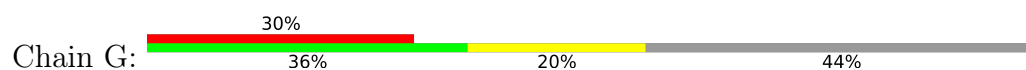
- Molecule 2: heavy chain of P17 Fab



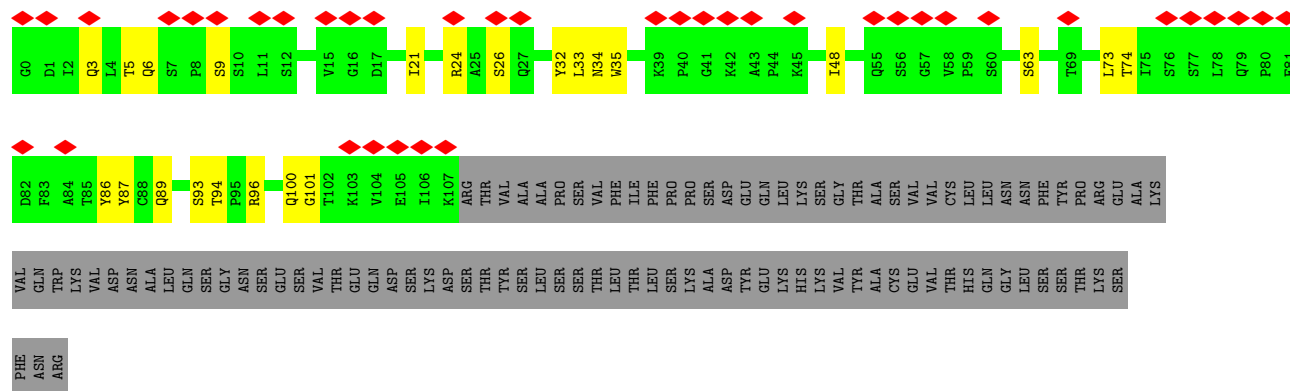
- Molecule 2: heavy chain of P17 Fab



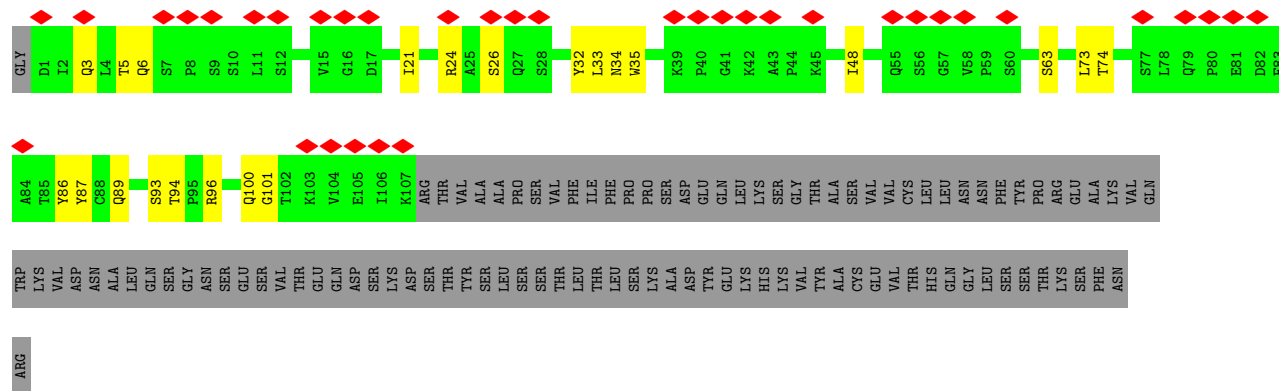
- Molecule 2: heavy chain of P17 Fab



- Molecule 3: light chain of P17 Fab

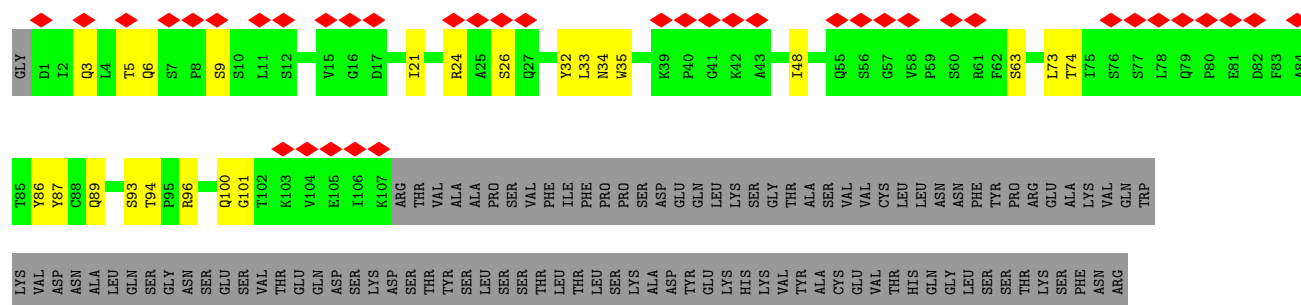


- Molecule 3: light chain of P17 Fab

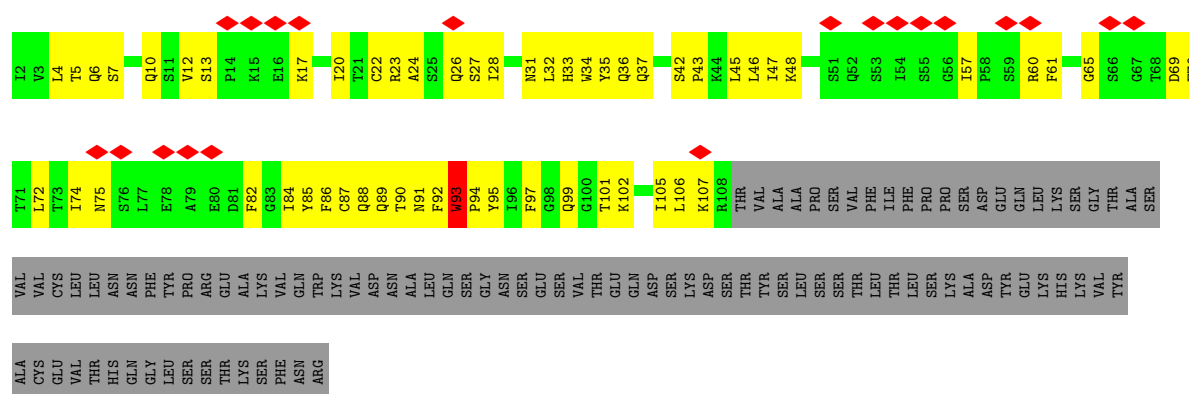
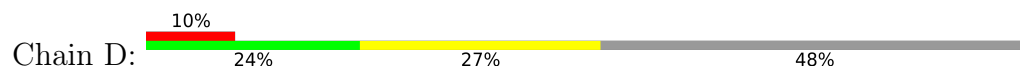


- Molecule 3: light chain of P17 Fab

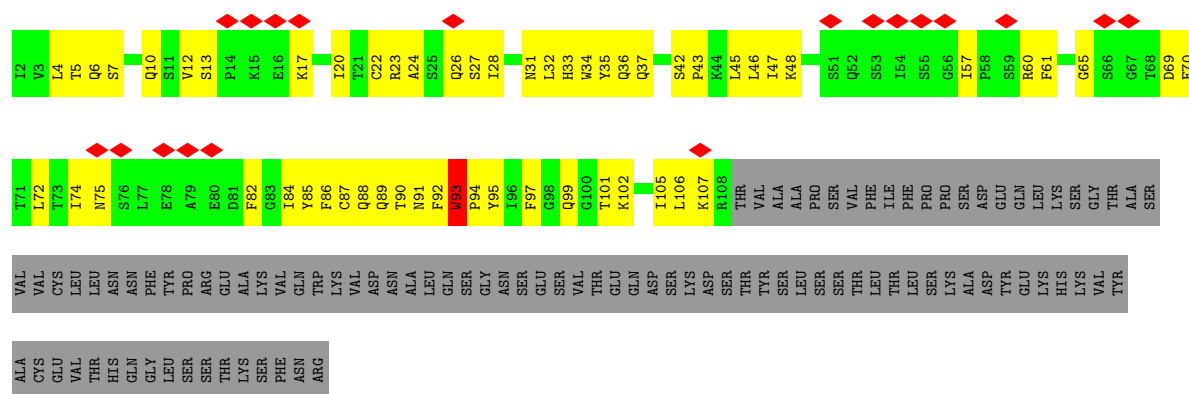
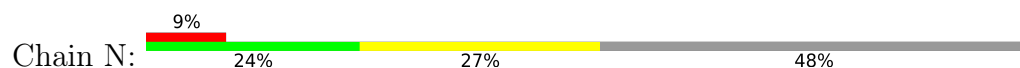




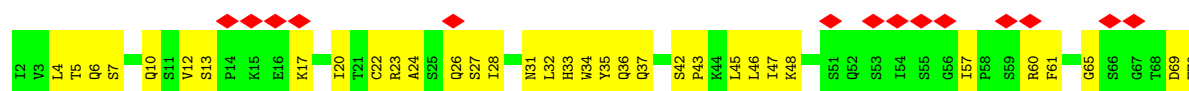
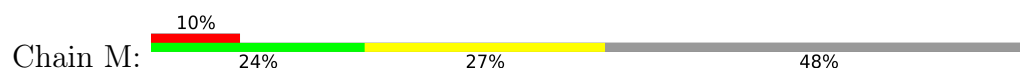
• Molecule 4: light chain of H014 Fab

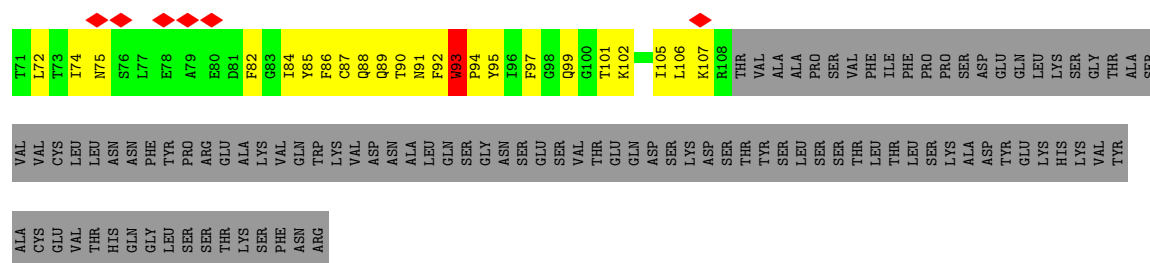


• Molecule 4: light chain of H014 Fab

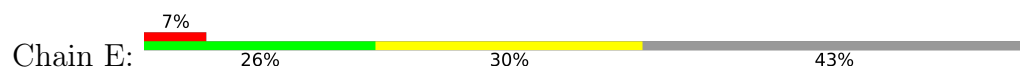


• Molecule 4: light chain of H014 Fab

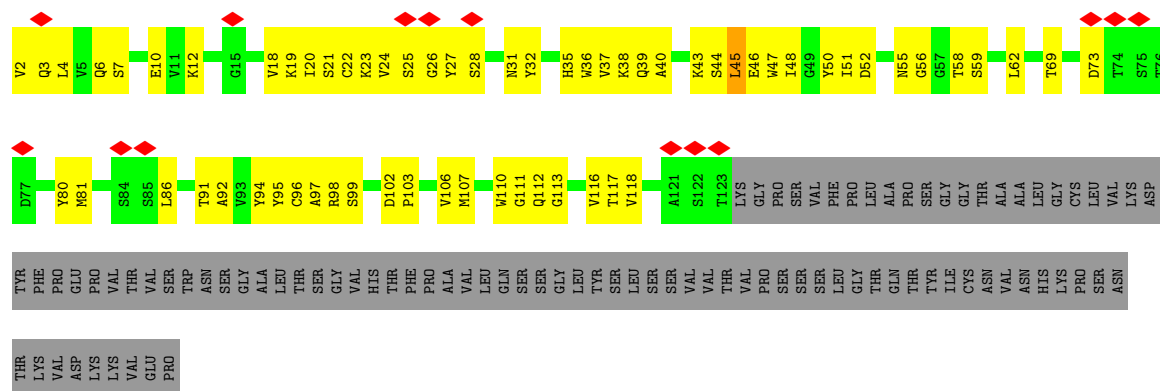
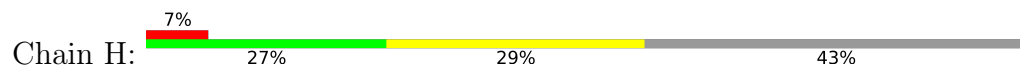




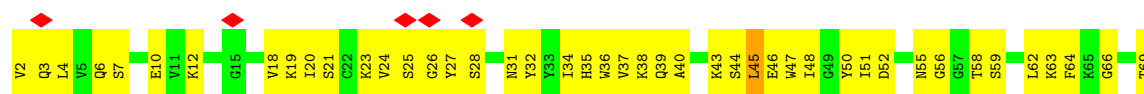
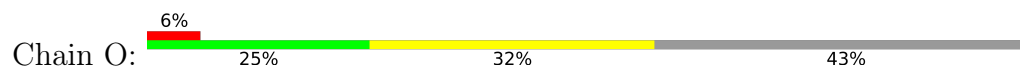
• Molecule 5: heavy chain of H014 Fab

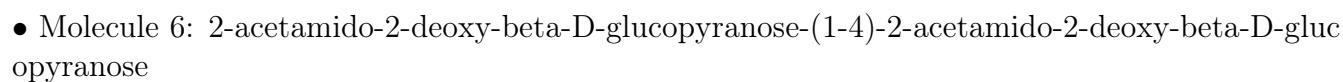


• Molecule 5: heavy chain of H014 Fab



• Molecule 5: heavy chain of H014 Fab





NAG1  
NAG2

- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

	NAG1	NAG2
1	0.00	0.00
2	0.00	0.00
3	0.00	0.00
4	0.00	0.00
5	0.00	0.00
6	0.00	0.00
7	0.00	0.00
8	0.00	0.00
9	0.00	0.00
10	0.00	0.00
11	0.00	0.00
12	0.00	0.00
13	0.00	0.00
14	0.00	0.00
15	0.00	0.00
16	0.00	0.00
17	0.00	0.00
18	0.00	0.00
19	0.00	0.00
20	0.00	0.00
21	0.00	0.00
22	0.00	0.00
23	0.00	0.00
24	0.00	0.00
25	0.00	0.00
26	0.00	0.00
27	0.00	0.00
28	0.00	0.00
29	0.00	0.00
30	0.00	0.00
31	0.00	0.00
32	0.00	0.00
33	0.00	0.00
34	0.00	0.00
35	0.00	0.00
36	0.00	0.00
37	0.00	0.00
38	0.00	0.00
39	0.00	0.00
40	0.00	0.00
41	0.00	0.00
42	0.00	0.00
43	0.00	0.00
44	0.00	0.00
45	0.00	0.00
46	0.00	0.00
47	0.00	0.00
48	0.00	0.00
49	0.00	0.00
50	0.00	0.00
51	0.00	0.00
52	0.00	0.00
53	0.00	0.00
54	0.00	0.00
55	0.00	0.00
56	0.00	0.00
57	0.00	0.00
58	0.00	0.00
59	0.00	0.00
60	0.00	0.00
61	0.00	0.00
62	0.00	0.00
63	0.00	0.00
64	0.00	0.00
65	0.00	0.00
66	0.00	0.00
67	0.00	0.00
68	0.00	0.00
69	0.00	0.00
70	0.00	0.00
71	0.00	0.00
72	0.00	0.00
73	0.00	0.00
74	0.00	0.00
75	0.00	0.00
76	0.00	0.00
77	0.00	0.00
78	0.00	0.00
79	0.00	0.00
80	0.00	0.00
81	0.00	0.00
82	0.00	0.00
83	0.00	0.00
84	0.00	0.00
85	0.00	0.00
86	0.00	0.00
87	0.00	0.00
88	0.00	0.00
89	0.00	0.00
90	0.00	0.00
91	0.00	0.00
92	0.00	0.00
93	0.00	0.00
94	0.00	0.00
95	0.00	0.00
96	0.00	0.00
97	0.00	0.00
98	0.00	0.00
99	0.00	0.00
100	0.00	0.00

- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

NAG1  
NAG2

- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

NAG1  
NAG2

- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

NAG1  
NAG2

- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:  100%



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:  100%



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d:  50%  100%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	175063	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.058	Depositor
Minimum map value	-0.018	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.00538	Depositor
Map size (Å)	416.0, 416.0, 416.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

## 5 Model quality

### 5.1 Standard geometry

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	0.44	0/8539	0.57	2/11622 (0.0%)
1	B	0.45	0/8529	0.58	2/11606 (0.0%)
1	C	0.46	0/8542	0.58	1/11625 (0.0%)
2	G	0.37	0/937	0.60	0/1269
2	K	0.37	0/937	0.60	0/1269
2	L	0.37	0/937	0.60	0/1269
3	F	0.38	0/830	0.59	0/1126
3	I	0.38	0/834	0.59	0/1131
3	J	0.38	0/830	0.59	0/1126
4	D	0.45	0/865	0.72	2/1171 (0.2%)
4	M	0.45	0/865	0.72	2/1171 (0.2%)
4	N	0.45	0/865	0.72	2/1171 (0.2%)
5	E	0.45	0/952	0.69	1/1298 (0.1%)
5	H	0.46	0/944	0.69	1/1287 (0.1%)
5	O	0.45	0/952	0.69	1/1298 (0.1%)
All	All	0.44	0/36358	0.60	14/49439 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	5
1	C	0	3
2	G	0	1
2	K	0	1
2	L	0	1
All	All	0	15

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	93	TRP	CB-CA-C	6.77	123.93	110.40
4	N	93	TRP	CB-CA-C	6.76	123.93	110.40
4	D	93	TRP	CB-CA-C	6.75	123.91	110.40
4	D	93	TRP	CA-CB-CG	6.17	125.42	113.70
4	M	93	TRP	CA-CB-CG	6.15	125.38	113.70

There are no chirality outliers.

5 of 15 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1145	LEU	Peptide
1	A	248	TYR	Peptide
1	A	391	CYS	Peptide
1	A	565	PHE	Peptide
1	B	248	TYR	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8348	0	8120	433	0
1	B	8339	0	8119	393	0
1	C	8351	0	8123	421	0
2	G	918	0	885	26	0
2	K	918	0	885	26	0
2	L	918	0	885	27	0
3	F	813	0	797	17	0
3	I	817	0	800	17	0
3	J	813	0	797	15	0
4	D	844	0	827	114	0
4	M	844	0	827	114	0
4	N	844	0	827	115	0
5	E	929	0	873	78	0
5	H	922	0	866	77	0
5	O	929	0	873	81	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	P	28	0	25	1	0
6	Q	28	0	25	0	0
6	R	28	0	25	1	0
6	S	28	0	25	0	0
6	T	28	0	25	0	0
6	U	28	0	25	1	0
6	V	28	0	25	0	0
6	W	28	0	25	1	0
6	X	28	0	25	0	0
6	Y	28	0	25	2	0
6	Z	28	0	25	7	0
6	a	28	0	25	0	0
6	b	28	0	25	0	0
6	c	28	0	25	0	0
6	d	28	0	25	0	0
7	A	84	0	78	1	0
7	B	70	0	65	1	0
7	C	70	0	65	0	0
All	All	36191	0	35087	1669	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 24.

The worst 5 of 1669 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:C:234:ASN:HD22	6:Z:1:NAG:C1	1.10	1.63
1:A:276:LEU:HD11	1:A:306:PHE:CE1	1.32	1.59
1:C:22:THR:CG2	1:C:78:ARG:HD2	1.28	1.58
1:C:63:THR:HG21	1:C:65:PHE:CZ	1.36	1.57
1:A:234:ASN:HD22	6:P:1:NAG:C1	1.03	1.56

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	1058/1273 (83%)	985 (93%)	72 (7%)	1 (0%)	48	80
1	B	1056/1273 (83%)	976 (92%)	80 (8%)	0	100	100
1	C	1058/1273 (83%)	977 (92%)	81 (8%)	0	100	100
2	G	118/213 (55%)	106 (90%)	12 (10%)	0	100	100
2	K	118/213 (55%)	106 (90%)	12 (10%)	0	100	100
2	L	118/213 (55%)	106 (90%)	12 (10%)	0	100	100
3	F	105/209 (50%)	96 (91%)	9 (9%)	0	100	100
3	I	106/209 (51%)	97 (92%)	9 (8%)	0	100	100
3	J	105/209 (50%)	96 (91%)	9 (9%)	0	100	100
4	D	105/207 (51%)	99 (94%)	5 (5%)	1 (1%)	13	47
4	M	105/207 (51%)	99 (94%)	5 (5%)	1 (1%)	13	47
4	N	105/207 (51%)	99 (94%)	5 (5%)	1 (1%)	13	47
5	E	120/214 (56%)	114 (95%)	6 (5%)	0	100	100
5	H	120/214 (56%)	114 (95%)	6 (5%)	0	100	100
5	O	120/214 (56%)	114 (95%)	6 (5%)	0	100	100
All	All	4517/6348 (71%)	4184 (93%)	329 (7%)	4 (0%)	50	80

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	93	TRP
4	N	93	TRP
4	M	93	TRP
1	A	24	LEU

### 5.3.2 Protein sidechains ⓘ

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	928/1112 (84%)	928 (100%)	0	100	100
1	B	927/1112 (83%)	926 (100%)	1 (0%)	92	98
1	C	928/1112 (84%)	928 (100%)	0	100	100
2	G	96/178 (54%)	96 (100%)	0	100	100
2	K	96/178 (54%)	96 (100%)	0	100	100
2	L	96/178 (54%)	96 (100%)	0	100	100
3	F	93/184 (50%)	93 (100%)	0	100	100
3	I	93/184 (50%)	93 (100%)	0	100	100
3	J	93/184 (50%)	93 (100%)	0	100	100
4	D	96/187 (51%)	96 (100%)	0	100	100
4	M	96/187 (51%)	96 (100%)	0	100	100
4	N	96/187 (51%)	96 (100%)	0	100	100
5	E	99/181 (55%)	99 (100%)	0	100	100
5	H	98/181 (54%)	98 (100%)	0	100	100
5	O	99/181 (55%)	99 (100%)	0	100	100
All	All	3934/5526 (71%)	3933 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	533	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 64 such sidechains are listed below:

Mol	Chain	Res	Type
2	G	104	ASN
3	F	90	GLN
1	C	66	HIS
1	C	61	ASN
4	M	6	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.



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

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

## 5.5 Carbohydrates ⓘ

30 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	$\# Z  > 2$
6	NAG	P	1	1,6	14,14,15	1.65	1 (7%)	17,19,21	1.39	2 (11%)
6	NAG	P	2	6	14,14,15	0.20	0	17,19,21	0.52	0
6	NAG	Q	1	1,6	14,14,15	0.34	0	17,19,21	0.50	0
6	NAG	Q	2	6	14,14,15	0.33	0	17,19,21	0.40	0
6	NAG	R	1	1,6	14,14,15	0.50	0	17,19,21	0.45	0
6	NAG	R	2	6	14,14,15	0.18	0	17,19,21	0.45	0
6	NAG	S	1	1,6	14,14,15	0.52	0	17,19,21	0.51	0
6	NAG	S	2	6	14,14,15	0.26	0	17,19,21	0.38	0
6	NAG	T	1	1,6	14,14,15	0.48	0	17,19,21	0.39	0
6	NAG	T	2	6	14,14,15	0.24	0	17,19,21	0.45	0
6	NAG	U	1	1,6	14,14,15	1.66	1 (7%)	17,19,21	1.39	2 (11%)
6	NAG	U	2	6	14,14,15	0.22	0	17,19,21	0.50	0
6	NAG	V	1	1,6	14,14,15	0.36	0	17,19,21	0.46	0
6	NAG	V	2	6	14,14,15	0.31	0	17,19,21	0.39	0
6	NAG	W	1	1,6	14,14,15	0.51	0	17,19,21	0.45	0
6	NAG	W	2	6	14,14,15	0.21	0	17,19,21	0.46	0
6	NAG	X	1	1,6	14,14,15	0.46	0	17,19,21	0.40	0
6	NAG	X	2	6	14,14,15	0.29	0	17,19,21	0.43	0
6	NAG	Y	1	1,6	14,14,15	0.32	0	17,19,21	0.98	1 (5%)
6	NAG	Y	2	6	14,14,15	0.47	0	17,19,21	1.22	2 (11%)
6	NAG	Z	1	1,6	14,14,15	1.20	1 (7%)	17,19,21	1.11	2 (11%)
6	NAG	Z	2	6	14,14,15	0.34	0	17,19,21	0.44	0
6	NAG	a	1	1,6	14,14,15	0.53	0	17,19,21	0.46	0
6	NAG	a	2	6	14,14,15	0.34	0	17,19,21	0.39	0
6	NAG	b	1	1,6	14,14,15	0.47	0	17,19,21	0.45	0
6	NAG	b	2	6	14,14,15	0.25	0	17,19,21	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	NAG	c	1	1,6	14,14,15	0.44	0	17,19,21	0.46	0
6	NAG	c	2	6	14,14,15	0.28	0	17,19,21	0.37	0
6	NAG	d	1	1,6	14,14,15	0.27	0	17,19,21	0.70	0
6	NAG	d	2	6	14,14,15	0.25	0	17,19,21	0.71	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	P	1	1,6	-	4/6/23/26	0/1/1/1
6	NAG	P	2	6	-	0/6/23/26	0/1/1/1
6	NAG	Q	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	Q	2	6	-	2/6/23/26	0/1/1/1
6	NAG	R	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	R	2	6	-	2/6/23/26	0/1/1/1
6	NAG	S	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	S	2	6	-	1/6/23/26	0/1/1/1
6	NAG	T	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	T	2	6	-	2/6/23/26	0/1/1/1
6	NAG	U	1	1,6	-	4/6/23/26	0/1/1/1
6	NAG	U	2	6	-	0/6/23/26	0/1/1/1
6	NAG	V	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	V	2	6	-	2/6/23/26	0/1/1/1
6	NAG	W	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	W	2	6	-	2/6/23/26	0/1/1/1
6	NAG	X	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	X	2	6	-	2/6/23/26	0/1/1/1
6	NAG	Y	1	1,6	-	3/6/23/26	0/1/1/1
6	NAG	Y	2	6	-	0/6/23/26	0/1/1/1
6	NAG	Z	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	Z	2	6	-	2/6/23/26	0/1/1/1
6	NAG	a	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	a	2	6	-	2/6/23/26	0/1/1/1
6	NAG	b	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	b	2	6	-	2/6/23/26	0/1/1/1
6	NAG	c	1	1,6	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	c	2	6	-	2/6/23/26	0/1/1/1
6	NAG	d	1	1,6	-	3/6/23/26	0/1/1/1
6	NAG	d	2	6	-	2/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	P	1	NAG	O5-C1	-5.99	1.34	1.43
6	U	1	NAG	O5-C1	-5.99	1.34	1.43
6	Z	1	NAG	O5-C1	-3.89	1.37	1.43

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Y	2	NAG	C1-O5-C5	3.72	117.24	112.19
6	P	1	NAG	C3-C4-C5	3.66	116.76	110.24
6	U	1	NAG	C3-C4-C5	3.66	116.76	110.24
6	Z	1	NAG	C3-C4-C5	3.23	116.00	110.24
6	Y	1	NAG	C4-C3-C2	-2.59	107.22	111.02

There are no chirality outliers.

5 of 51 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	Y	1	NAG	C8-C7-N2-C2
6	Y	1	NAG	O7-C7-N2-C2
6	d	1	NAG	C8-C7-N2-C2
6	d	1	NAG	O7-C7-N2-C2
6	Q	2	NAG	O5-C5-C6-O6

There are no ring outliers.

7 monomers are involved in 13 short contacts:

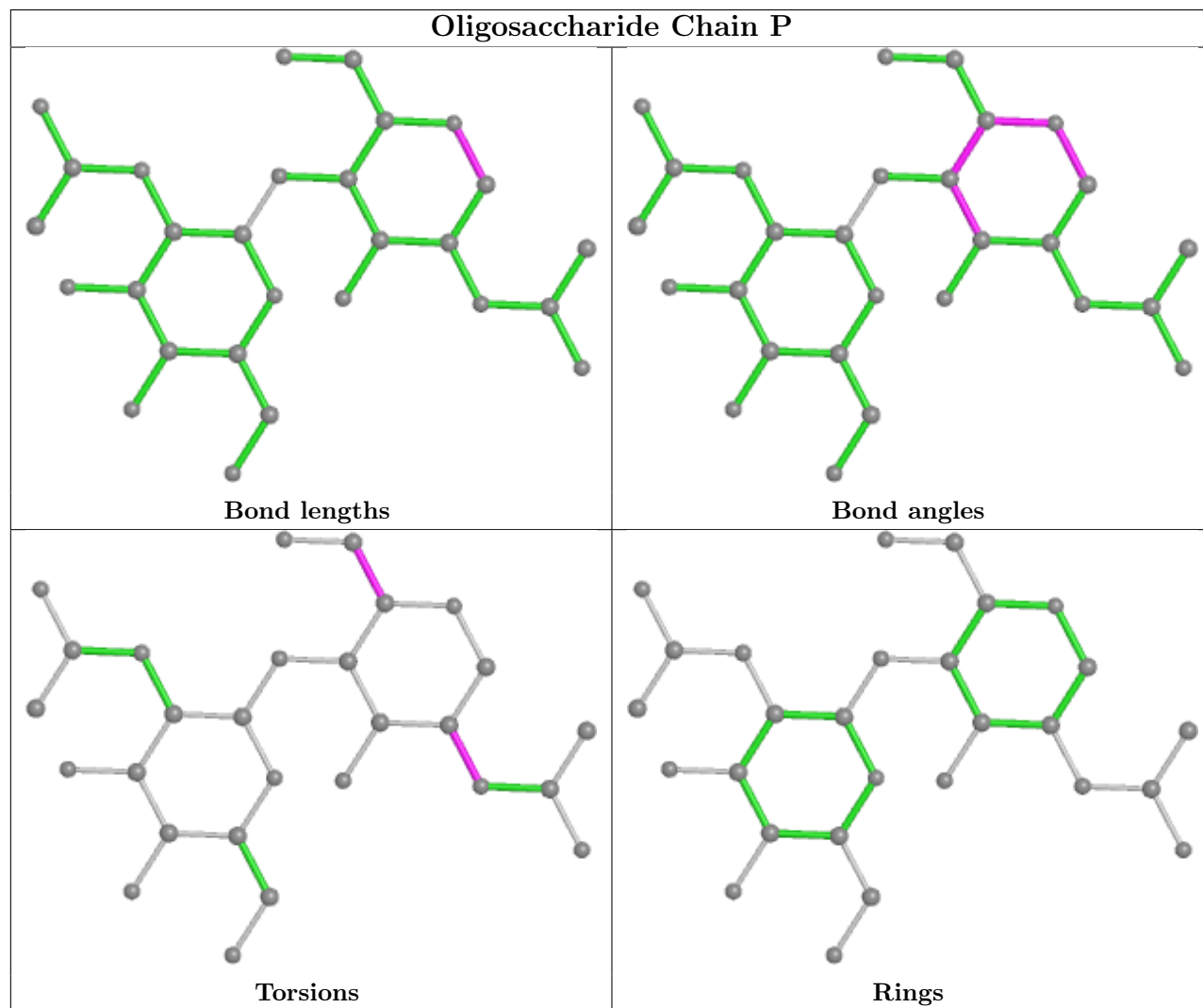
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	W	1	NAG	1	0
6	P	1	NAG	1	0
6	Y	2	NAG	2	0
6	U	1	NAG	1	0
6	Y	1	NAG	2	0
6	Z	1	NAG	7	0

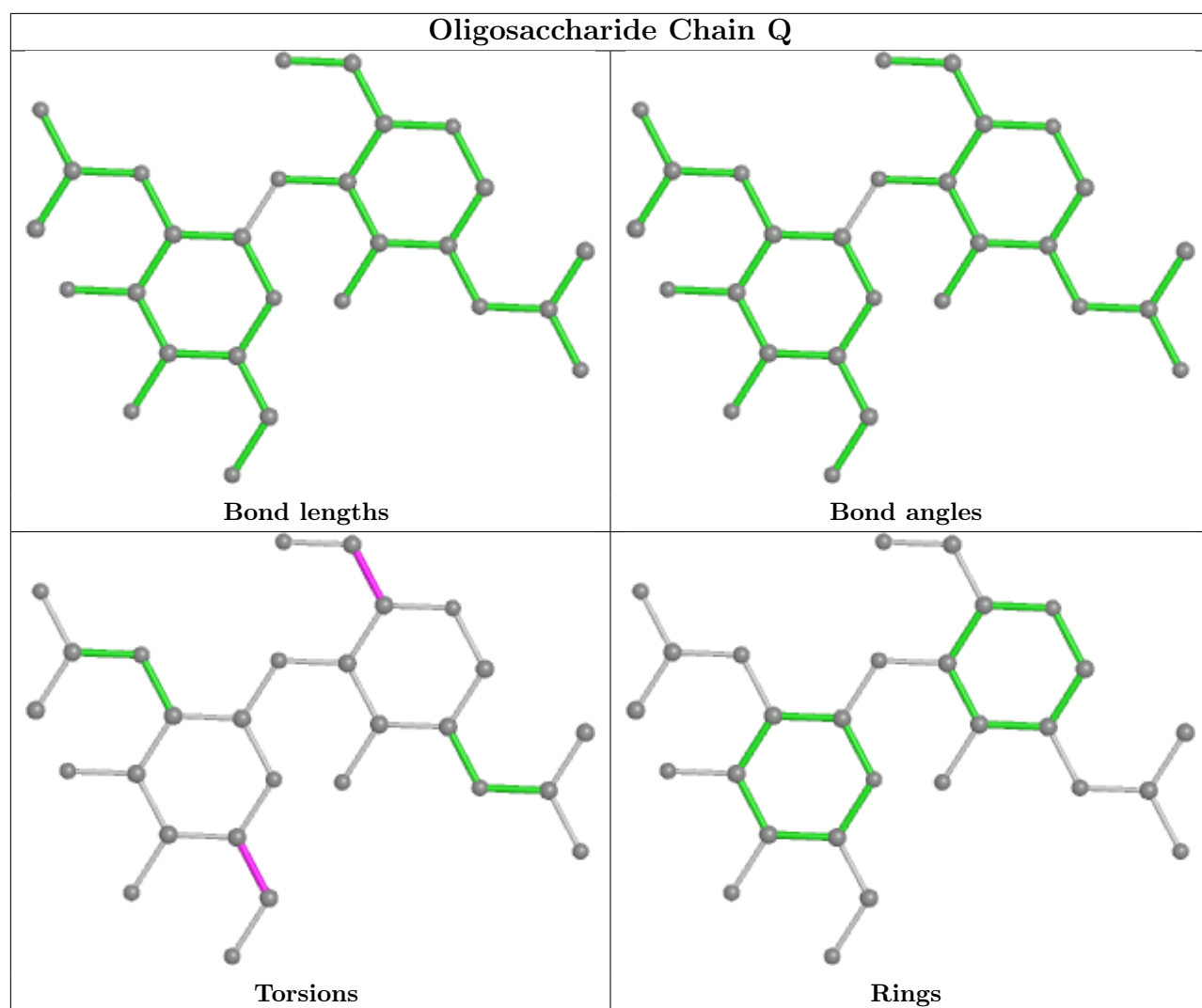
*Continued on next page...*

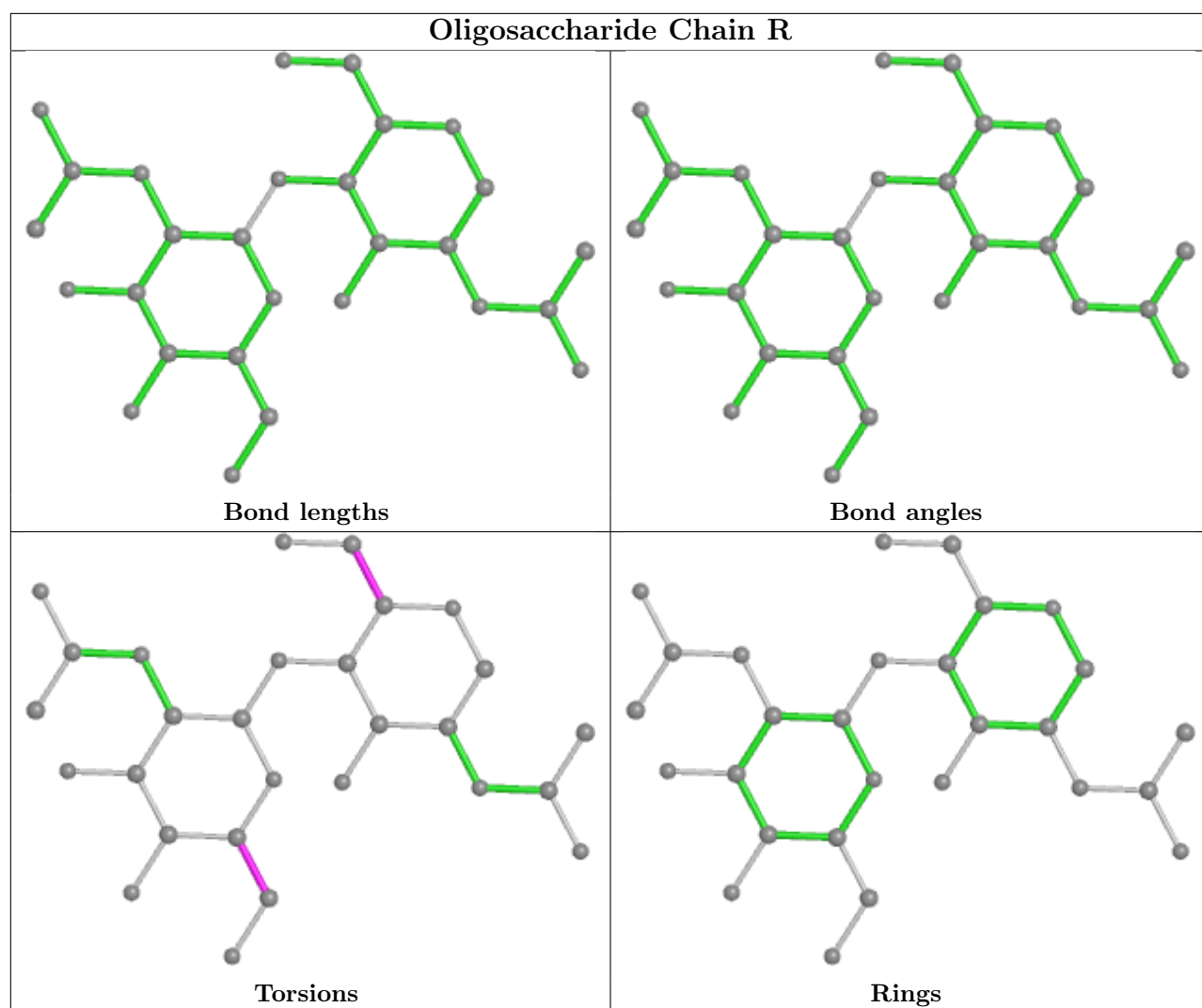
*Continued from previous page...*

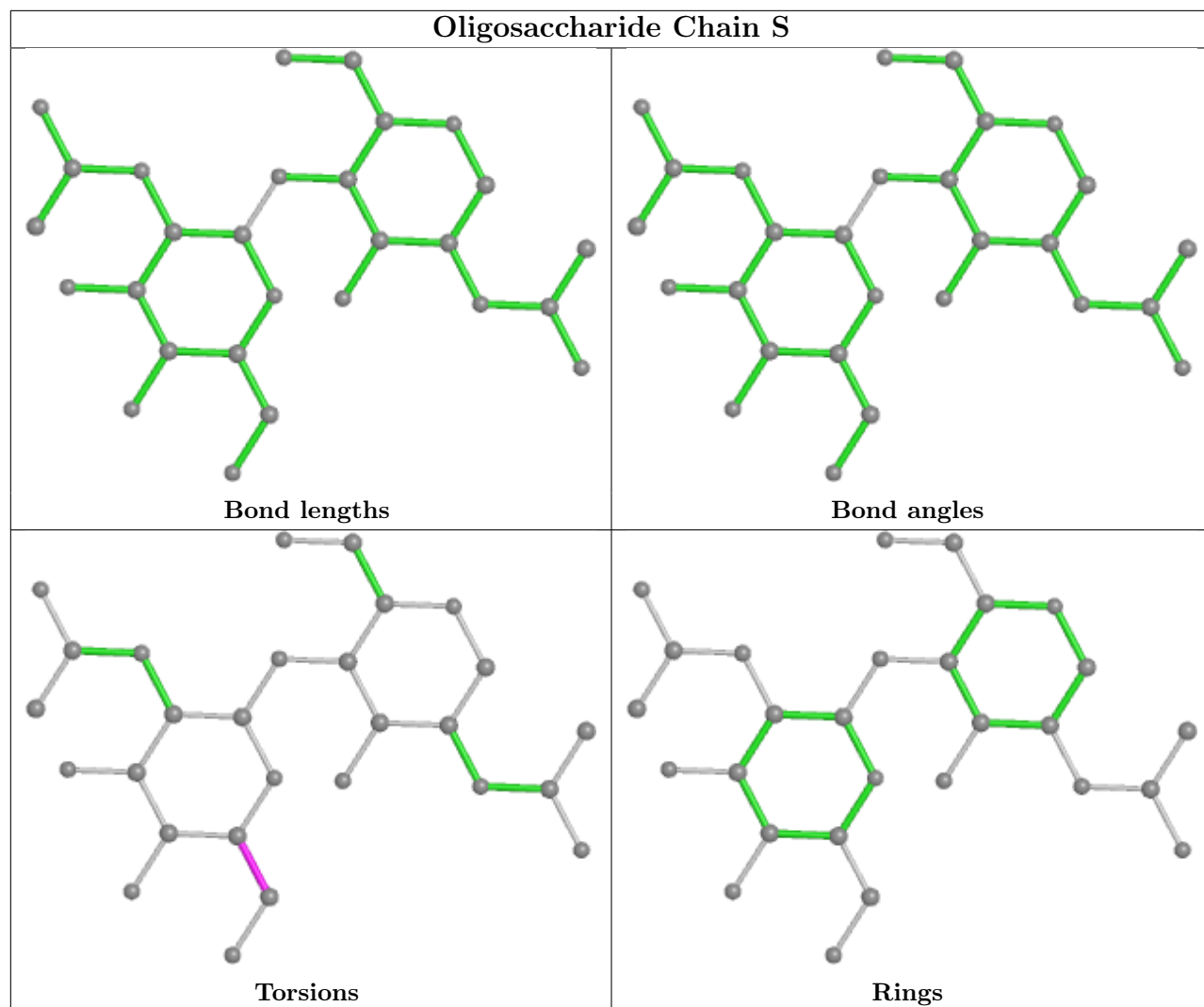
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	R	1	NAG	1	0

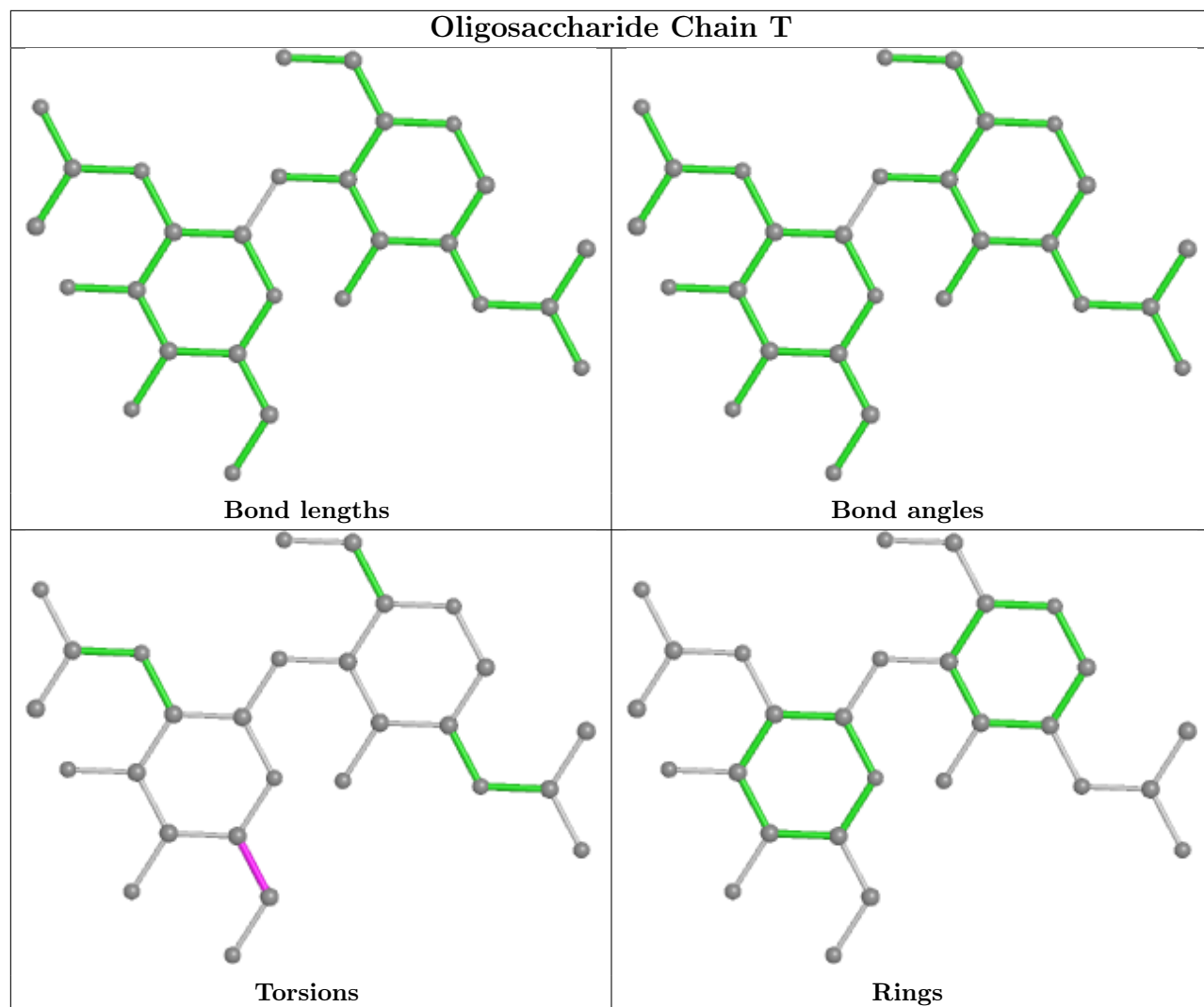
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



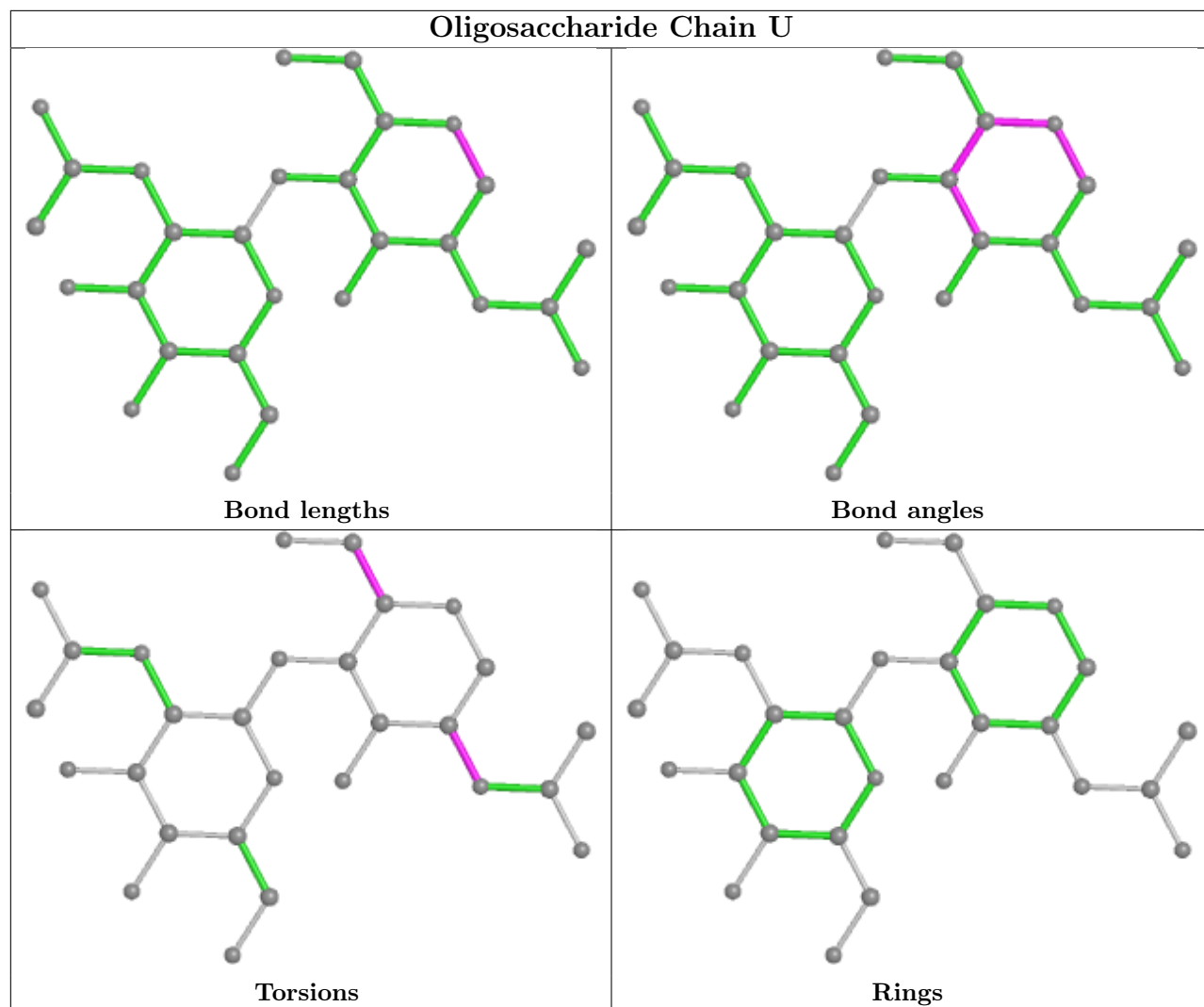


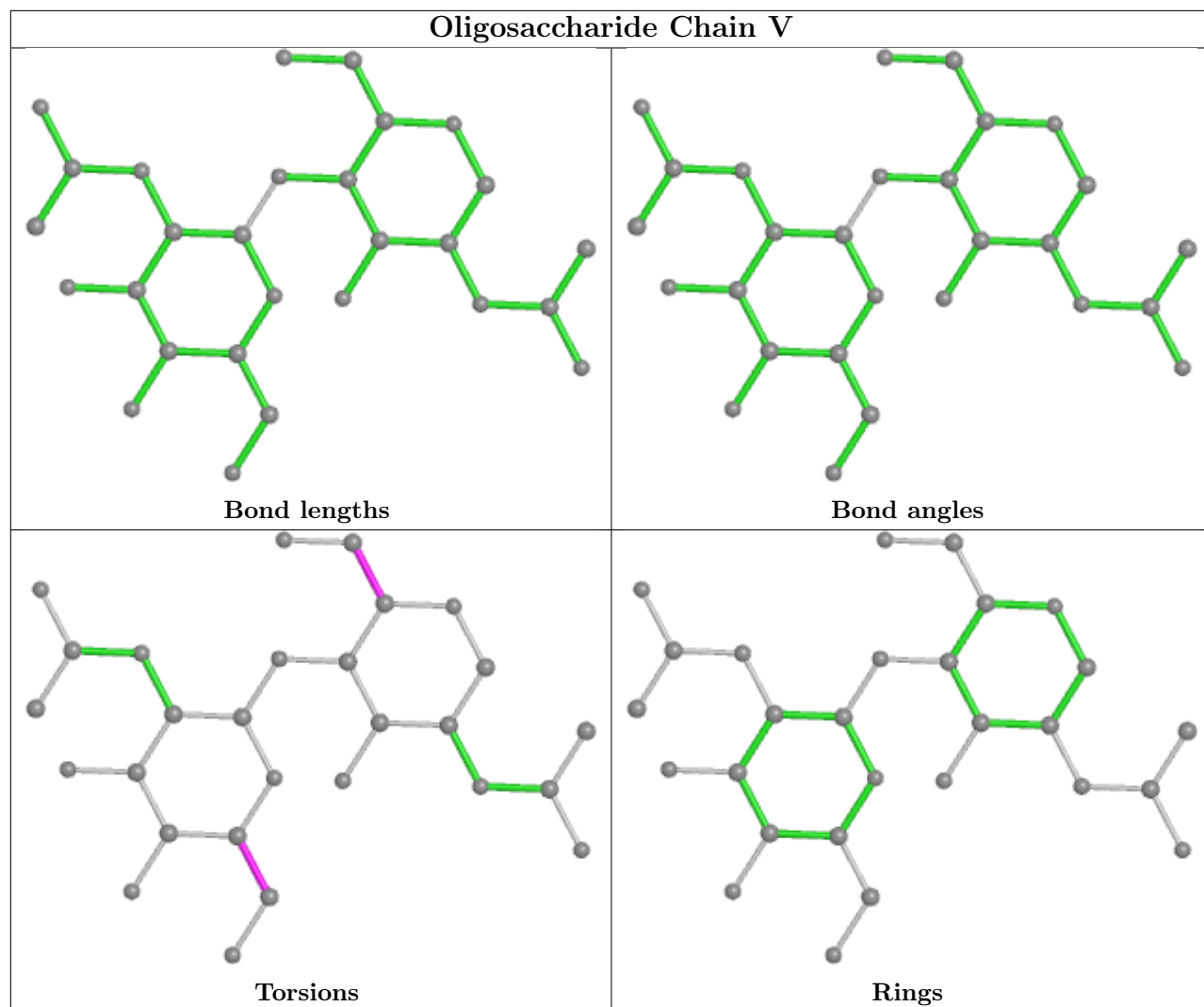


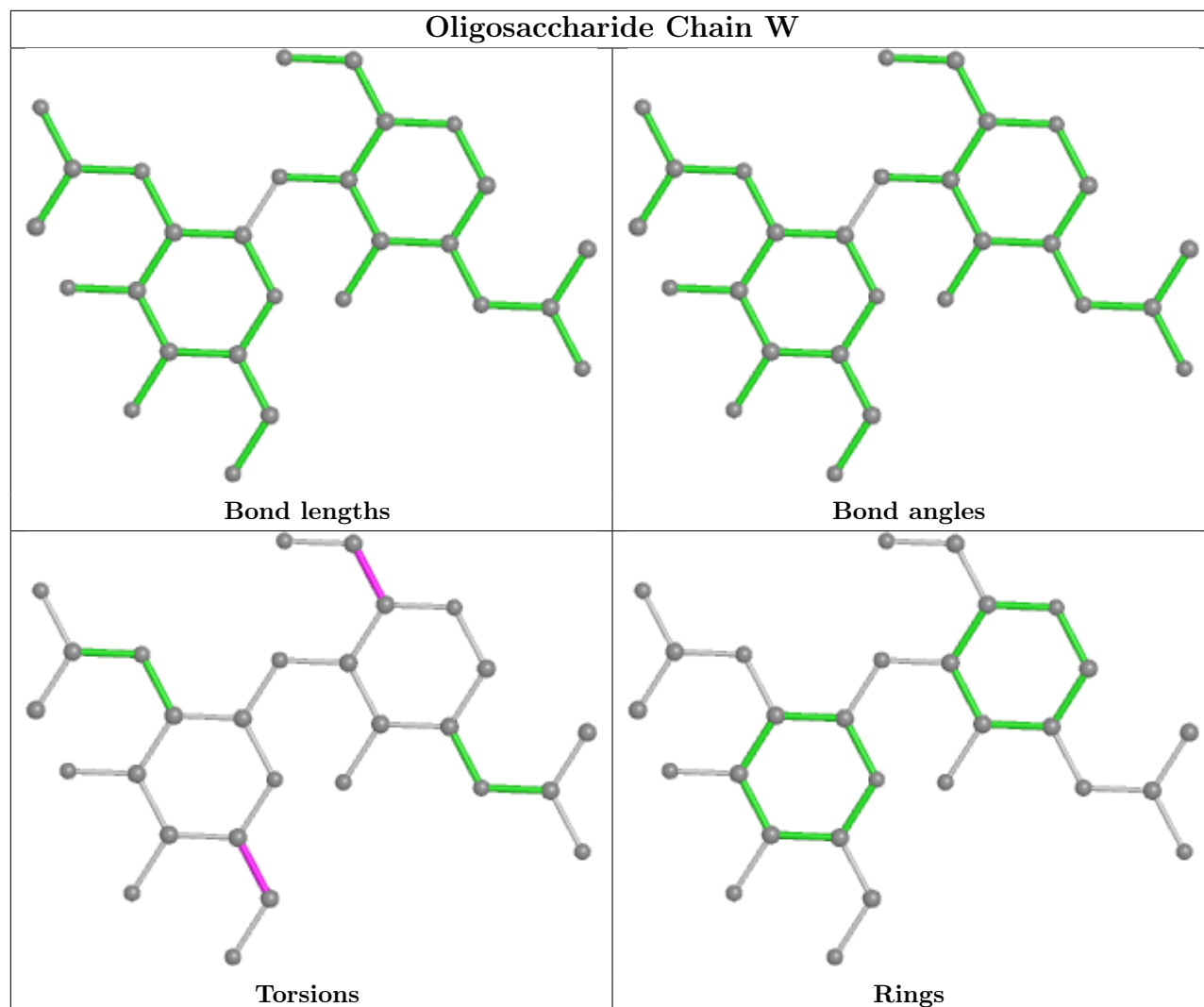


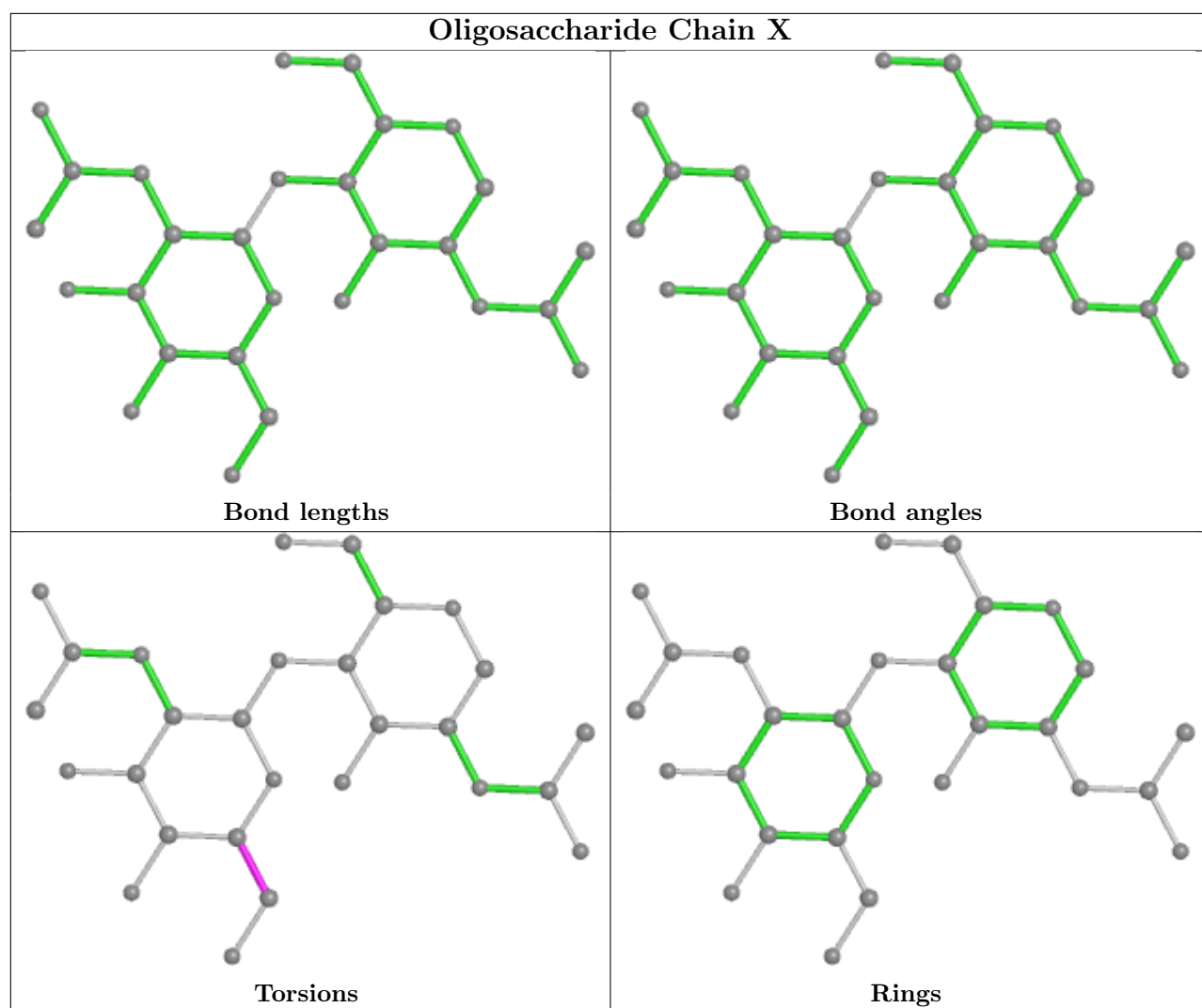


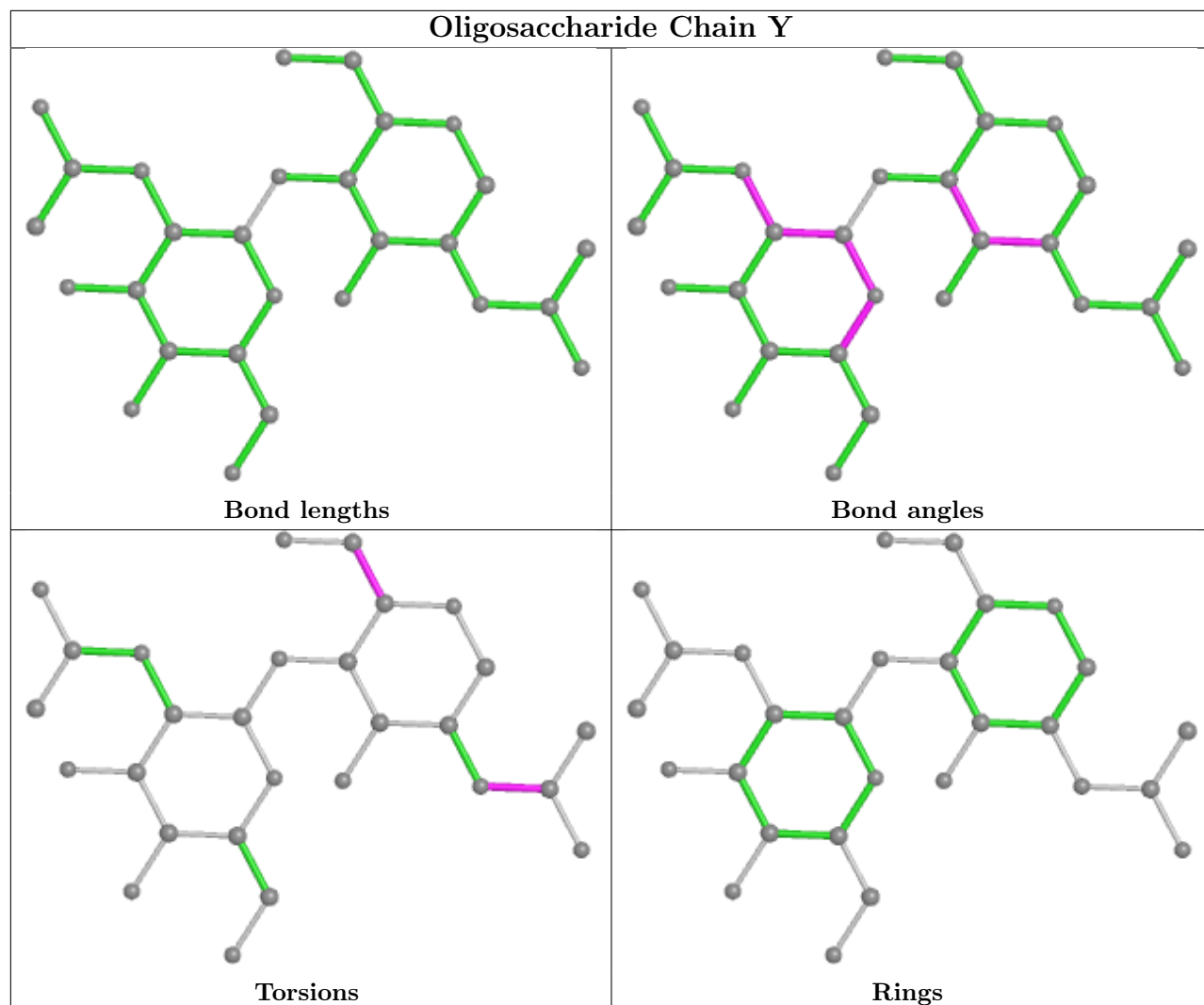


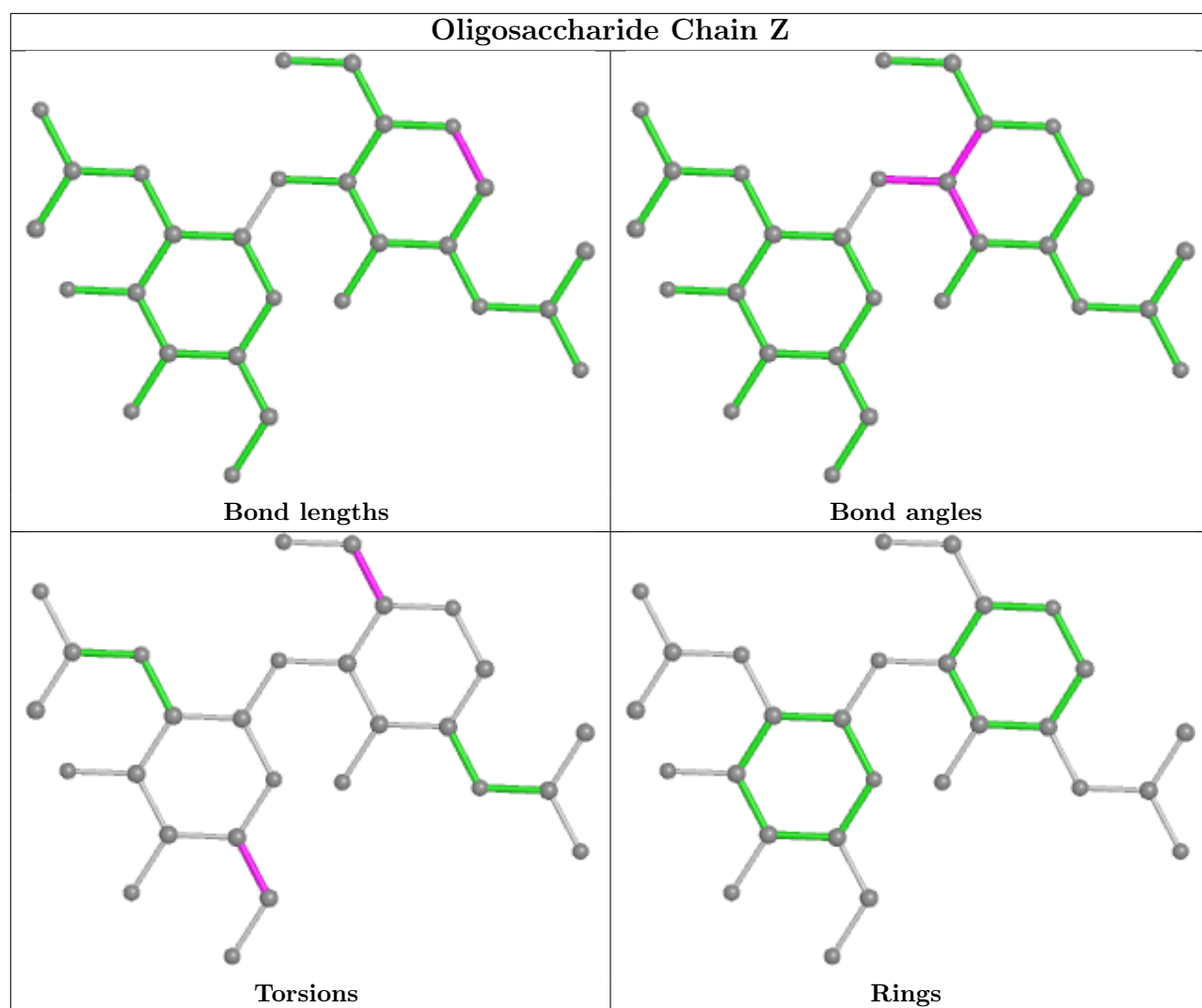


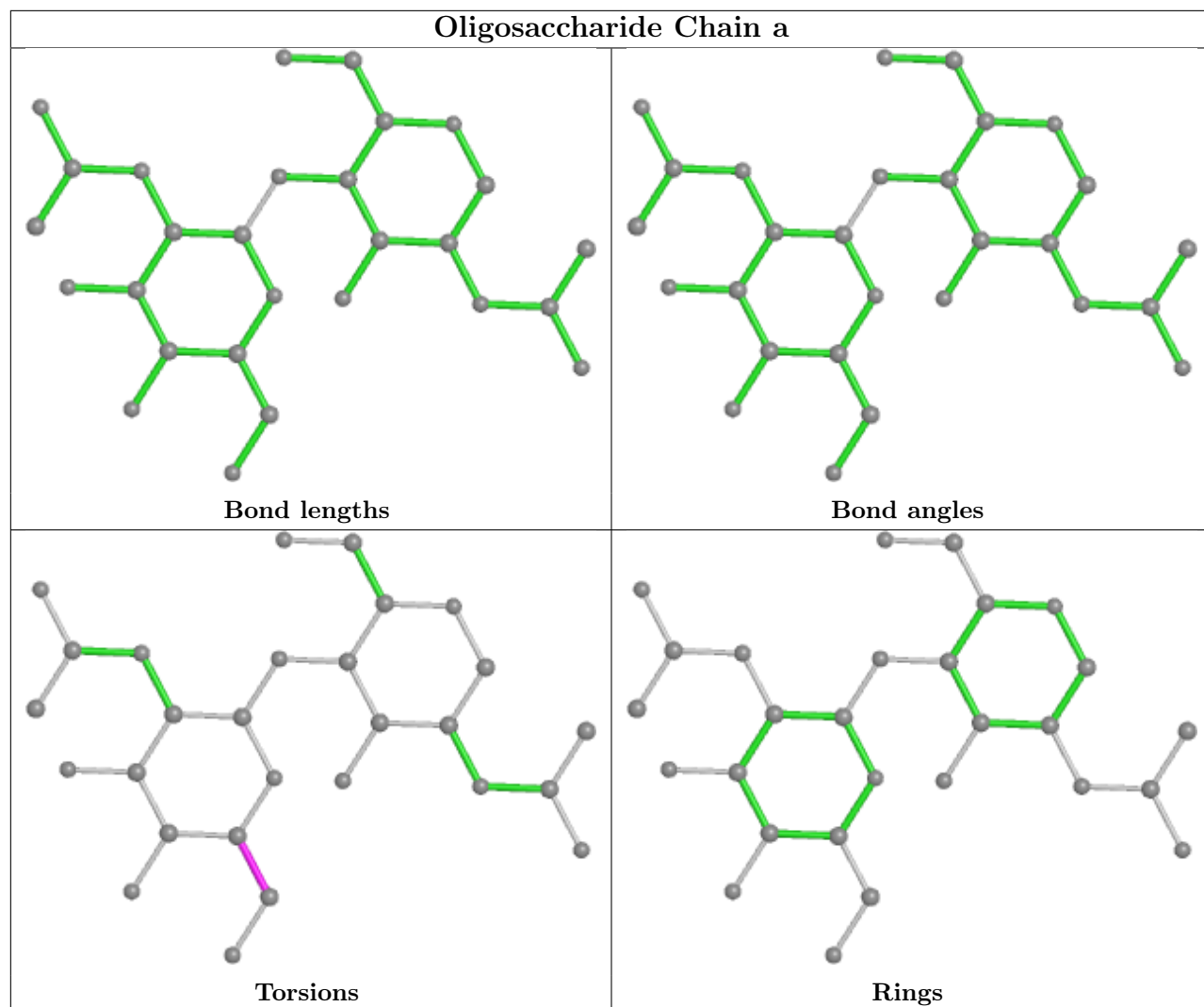


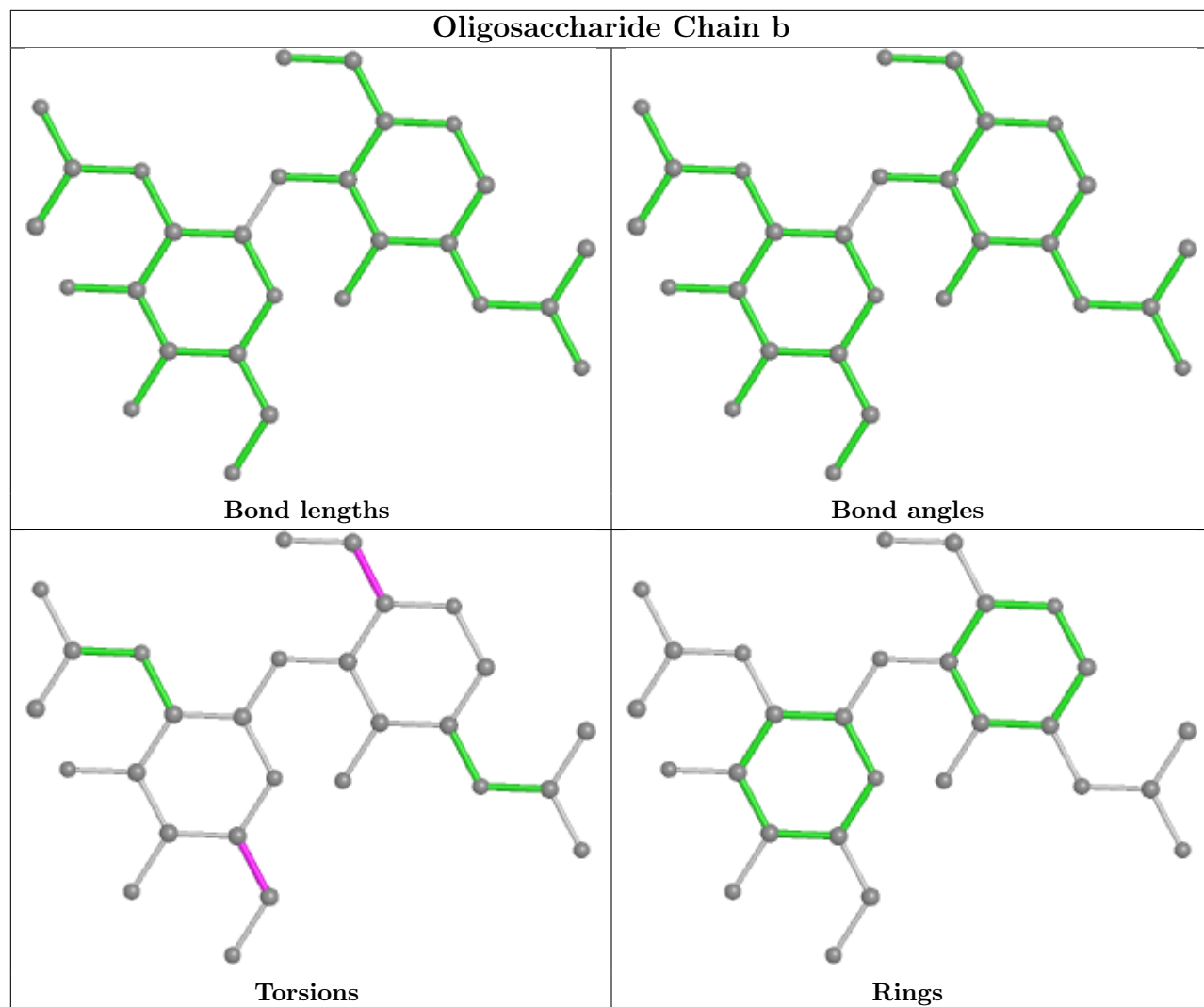




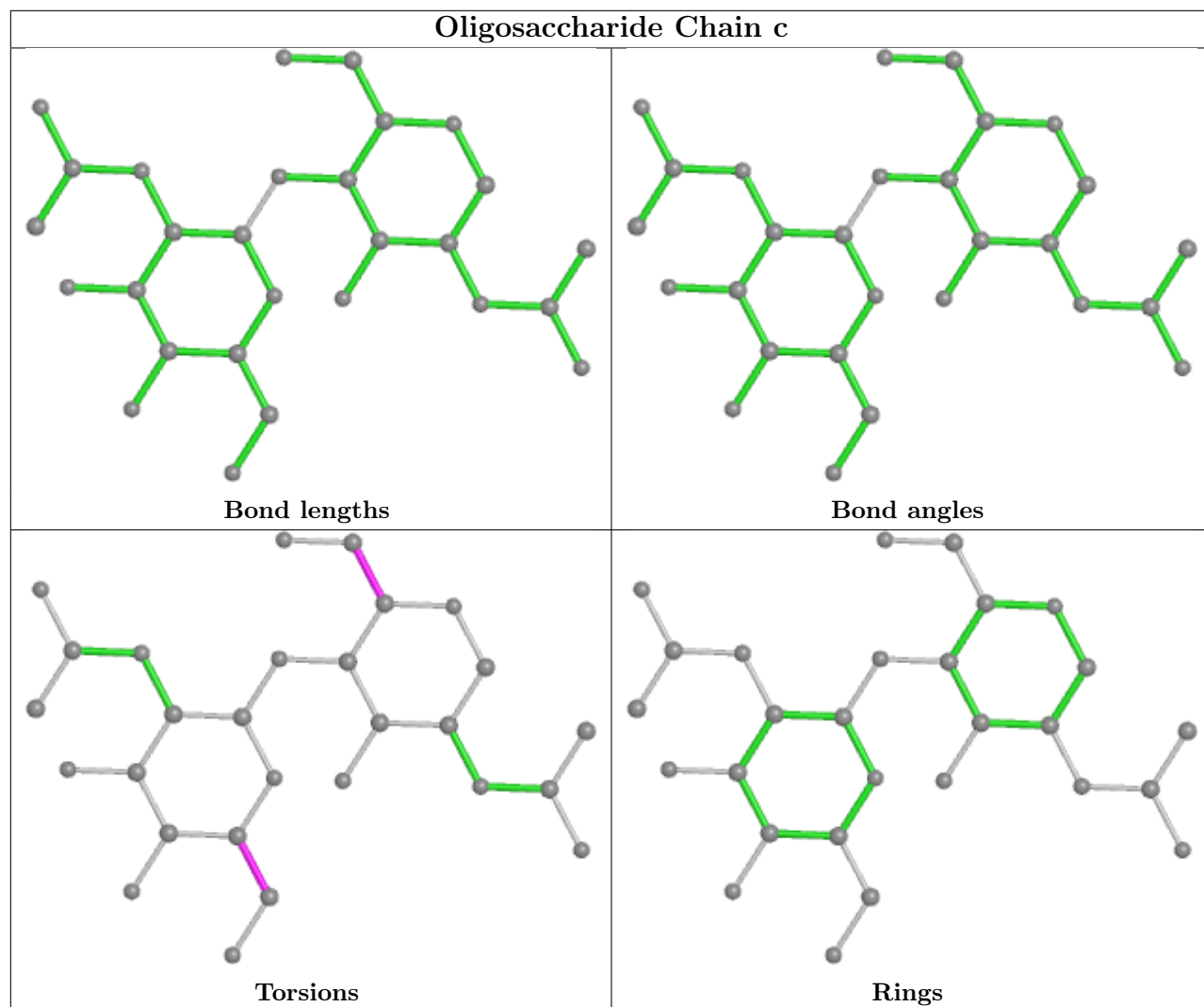


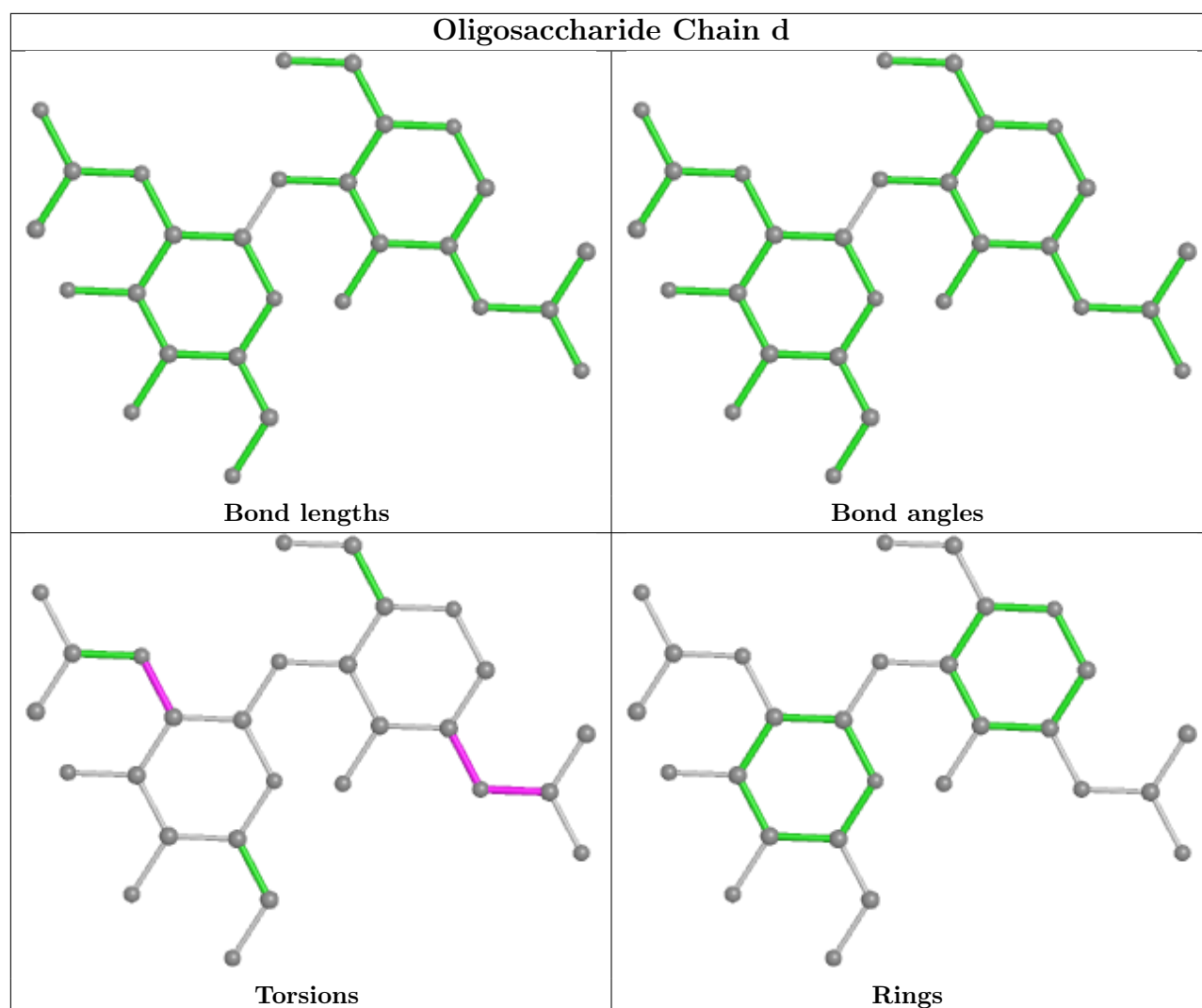












## 5.6 Ligand geometry [i](#)

16 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	$\# Z  > 2$
7	NAG	A	1301	1	14,14,15	0.34	0	17,19,21	0.38	0
7	NAG	A	1302	1	14,14,15	0.22	0	17,19,21	0.35	0
7	NAG	C	1304	1	14,14,15	0.48	0	17,19,21	0.51	0
7	NAG	A	1304	1	14,14,15	0.22	0	17,19,21	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	NAG	B	1303	1	14,14,15	0.19	0	17,19,21	0.43	0
7	NAG	C	1301	1	14,14,15	0.39	0	17,19,21	0.41	0
7	NAG	B	1301	1	14,14,15	0.22	0	17,19,21	0.34	0
7	NAG	B	1302	1	14,14,15	0.49	0	17,19,21	0.49	0
7	NAG	B	1304	1	14,14,15	0.59	1 (7%)	17,19,21	0.37	0
7	NAG	C	1302	1	14,14,15	0.67	0	17,19,21	0.44	0
7	NAG	C	1303	1	14,14,15	0.32	0	17,19,21	0.37	0
7	NAG	A	1306	1	14,14,15	0.21	0	17,19,21	0.60	0
7	NAG	A	1305	1	14,14,15	0.57	0	17,19,21	0.36	0
7	NAG	B	1305	1	14,14,15	0.23	0	17,19,21	0.62	0
7	NAG	A	1303	1	14,14,15	0.48	0	17,19,21	0.48	0
7	NAG	C	1305	1	14,14,15	0.24	0	17,19,21	0.51	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	A	1301	1	-	0/6/23/26	0/1/1/1
7	NAG	A	1302	1	-	0/6/23/26	0/1/1/1
7	NAG	C	1304	1	-	2/6/23/26	0/1/1/1
7	NAG	A	1304	1	-	0/6/23/26	0/1/1/1
7	NAG	B	1303	1	-	0/6/23/26	0/1/1/1
7	NAG	C	1301	1	-	0/6/23/26	0/1/1/1
7	NAG	B	1301	1	-	0/6/23/26	0/1/1/1
7	NAG	B	1302	1	-	1/6/23/26	0/1/1/1
7	NAG	B	1304	1	-	2/6/23/26	0/1/1/1
7	NAG	C	1302	1	-	2/6/23/26	0/1/1/1
7	NAG	C	1303	1	-	0/6/23/26	0/1/1/1
7	NAG	A	1306	1	-	1/6/23/26	0/1/1/1
7	NAG	A	1305	1	-	2/6/23/26	0/1/1/1
7	NAG	B	1305	1	-	1/6/23/26	0/1/1/1
7	NAG	A	1303	1	-	1/6/23/26	0/1/1/1
7	NAG	C	1305	1	-	1/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	1304	NAG	O5-C1	-2.02	1.40	1.43

There are no bond angle outliers.

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	1302	NAG	O5-C5-C6-O6
7	A	1305	NAG	C4-C5-C6-O6
7	B	1304	NAG	C4-C5-C6-O6
7	A	1305	NAG	O5-C5-C6-O6
7	B	1304	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	1304	NAG	1	0
7	A	1305	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.

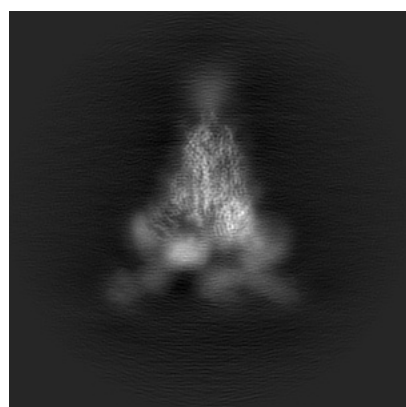
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30484. These allow visual inspection of the internal detail of the map and identification of artifacts.

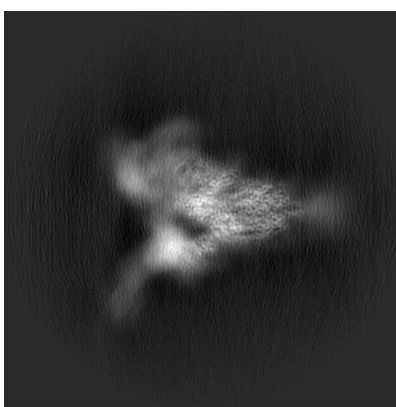
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

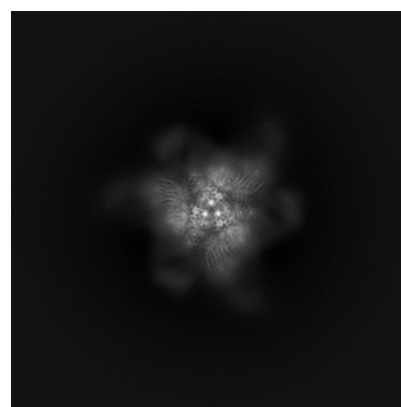
#### 6.1.1 Primary map



X



Y

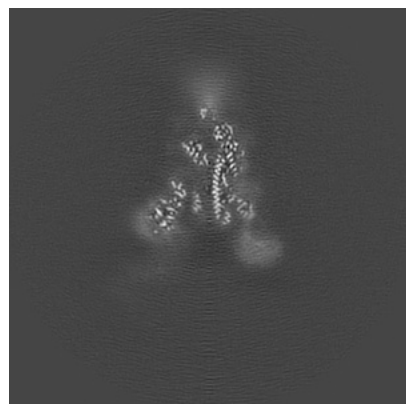


Z

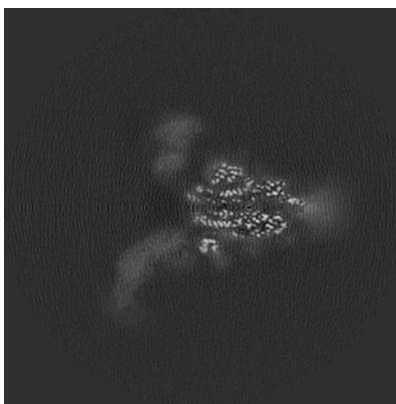
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

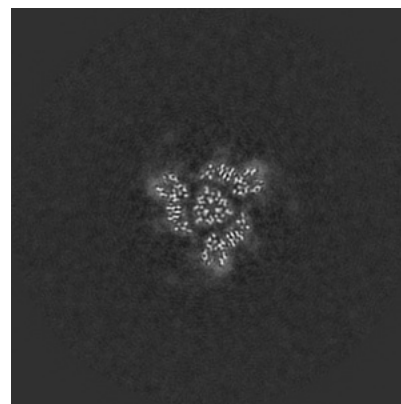
#### 6.2.1 Primary map



X Index: 200



Y Index: 200

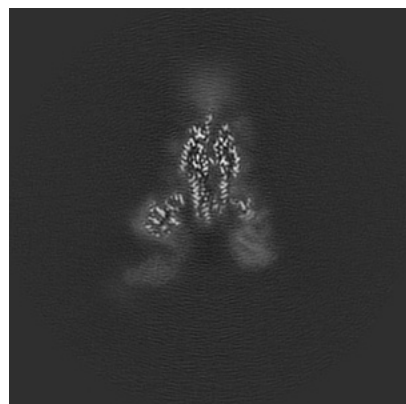


Z Index: 200

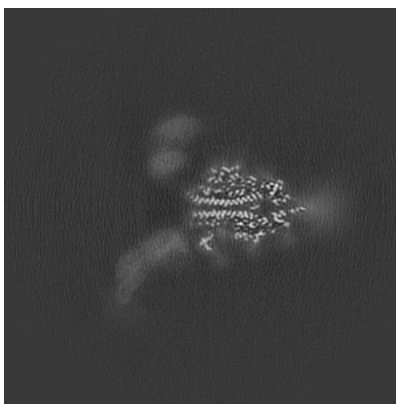
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

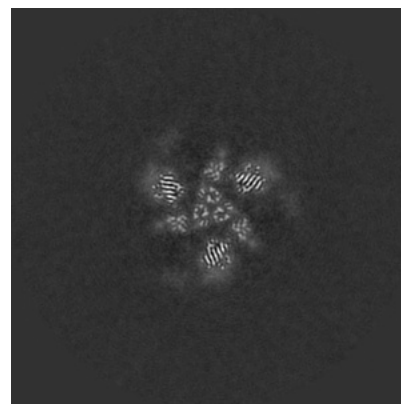
### 6.3.1 Primary map



X Index: 209



Y Index: 196

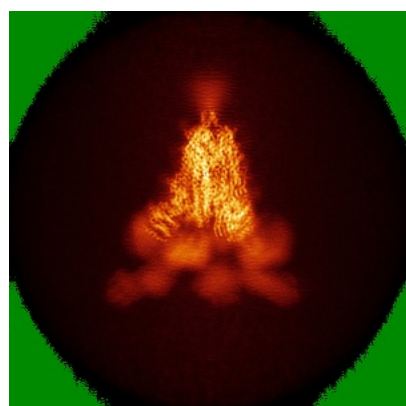


Z Index: 194

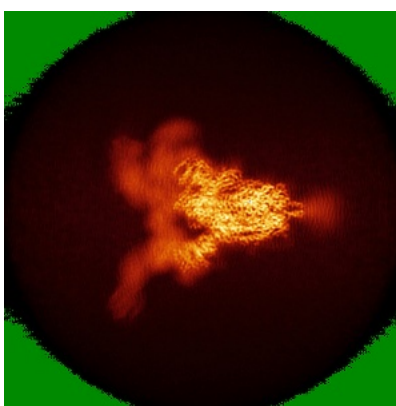
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

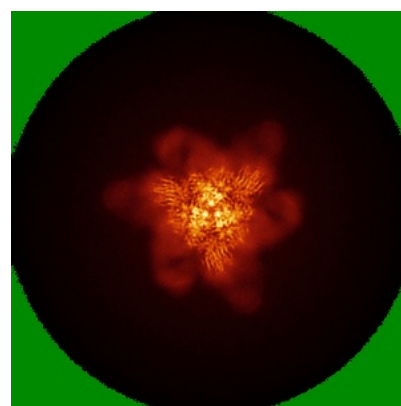
### 6.4.1 Primary map



X



Y

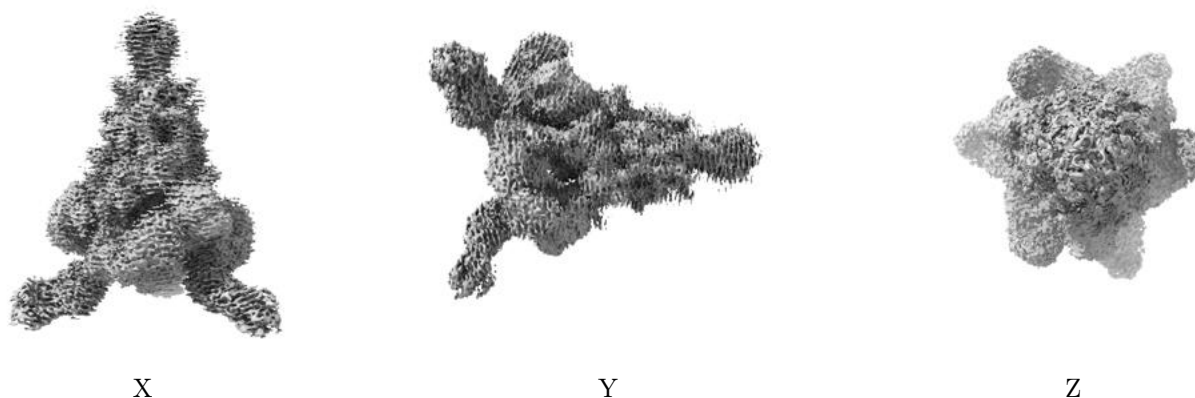


Z

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

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00538. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

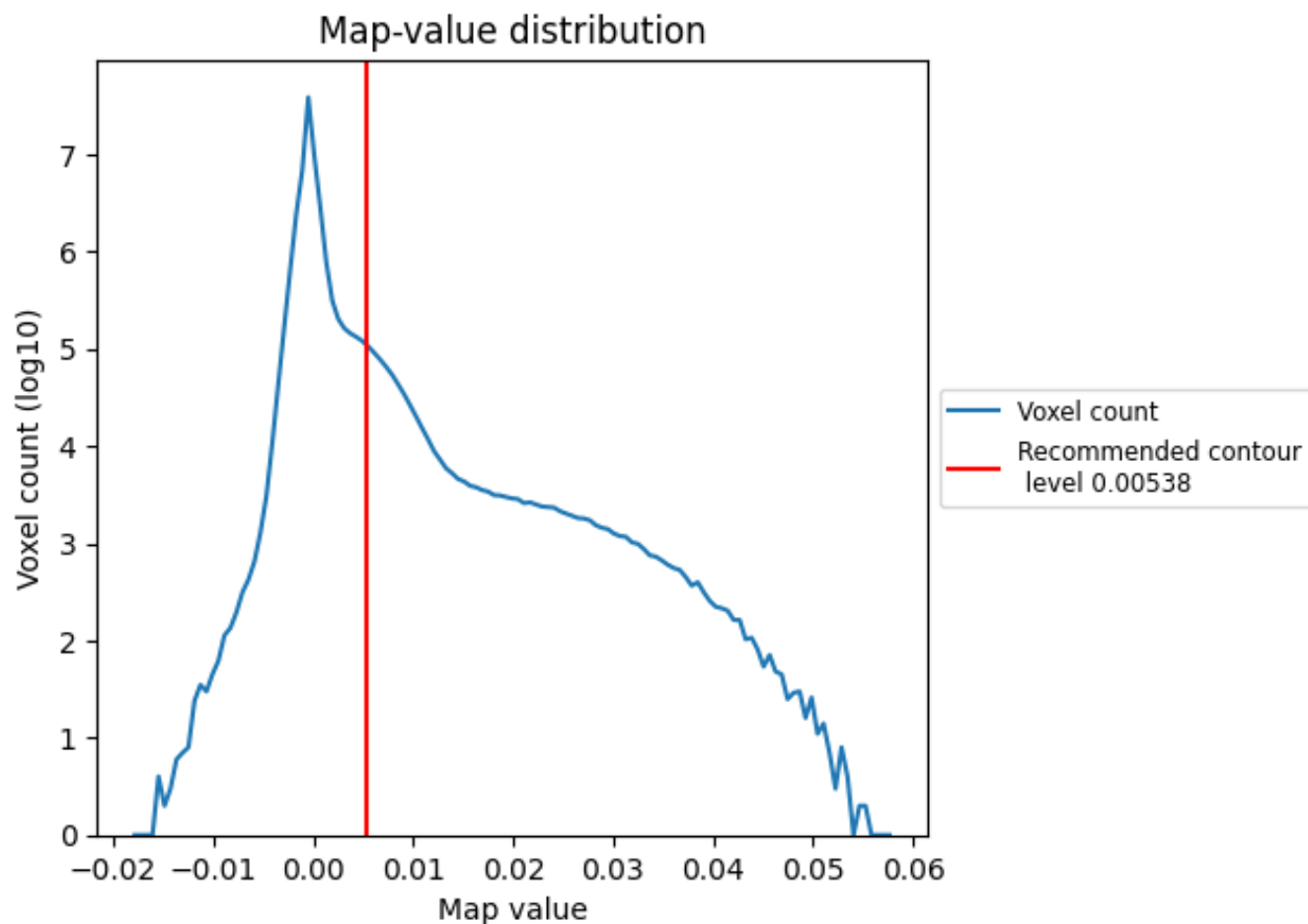
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

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

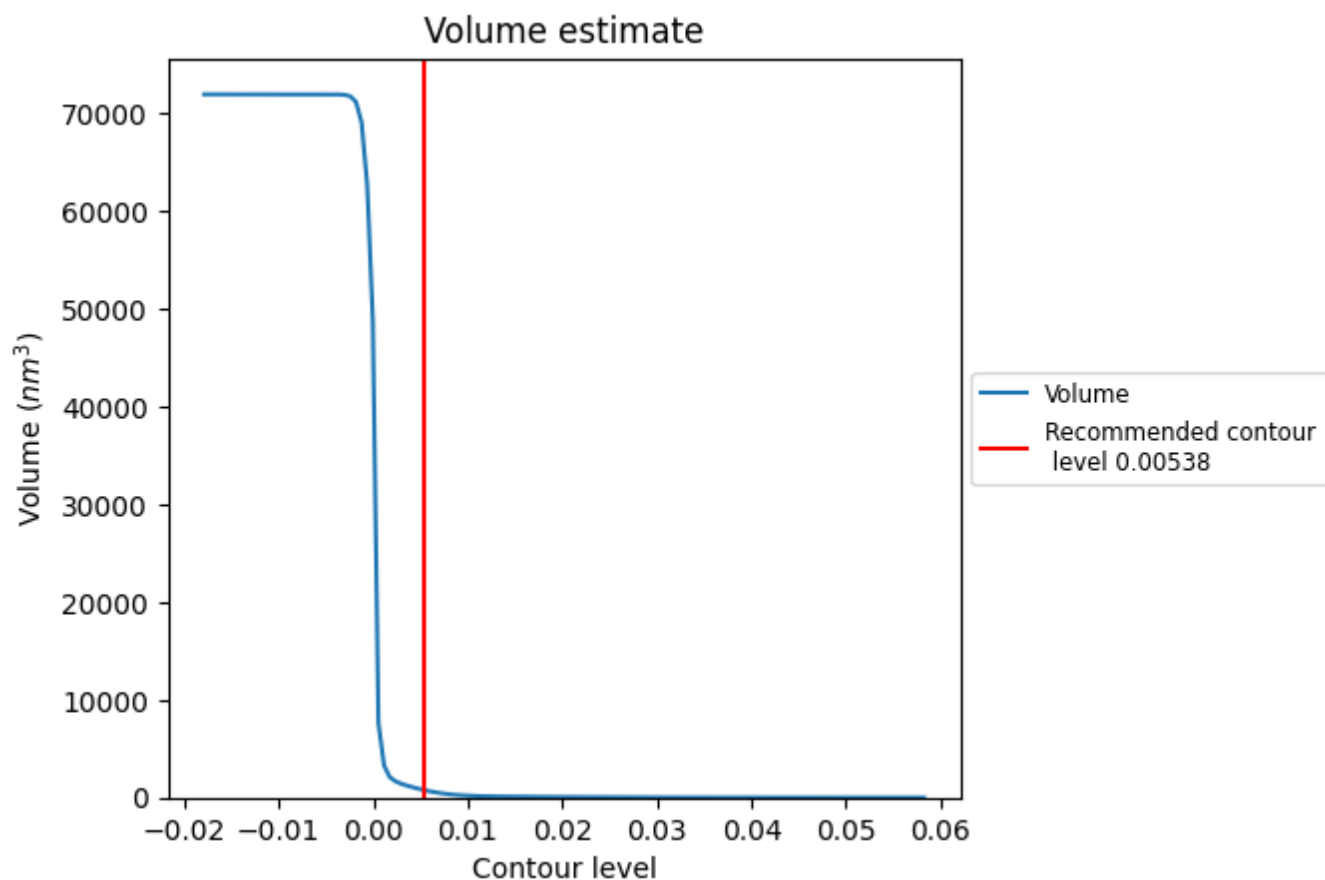
### 7.1 Map-value distribution [i](#)



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



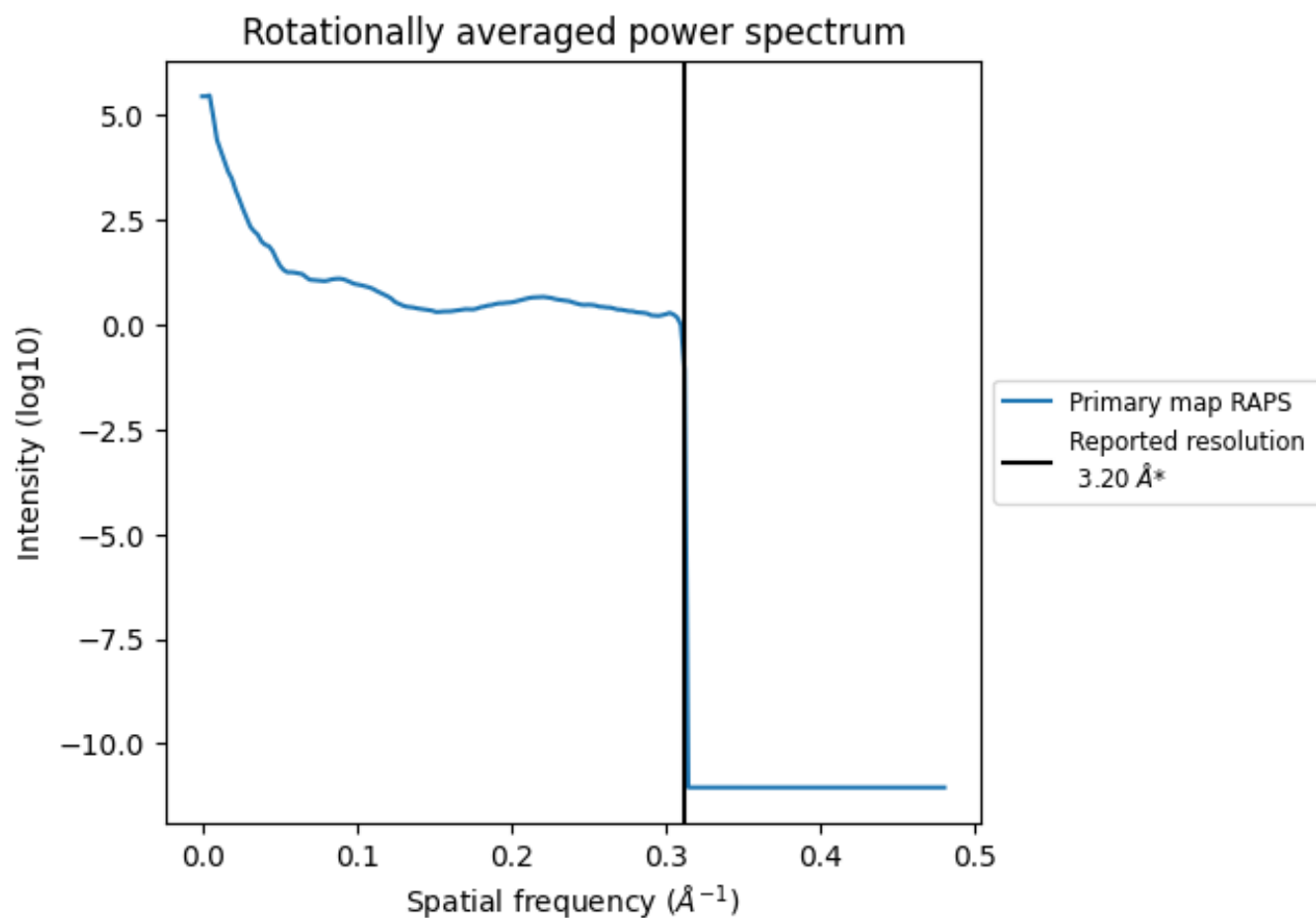
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 763 nm<sup>3</sup>; this corresponds to an approximate mass of 689 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 ⓘ



\*Reported resolution corresponds to spatial frequency of 0.312  $\text{\AA}^{-1}$

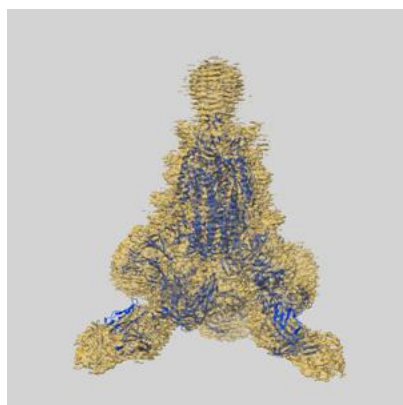
## 8 Fourier-Shell correlation

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

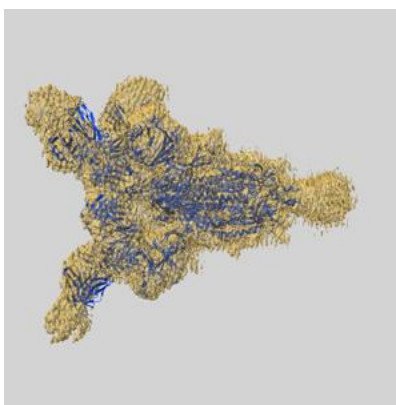
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-30484 and PDB model 7CWN. Per-residue inclusion information can be found in section [3](#) on page [9](#).

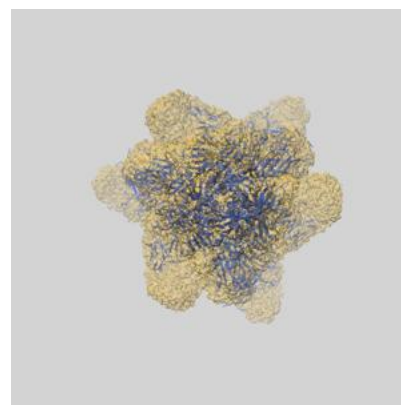
### 9.1 Map-model overlay [i](#)



X



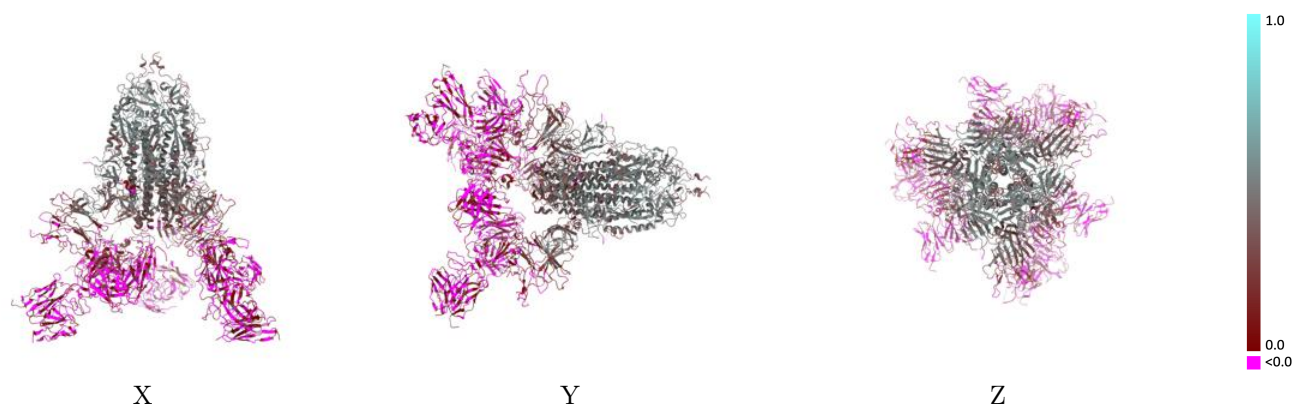
Y



Z

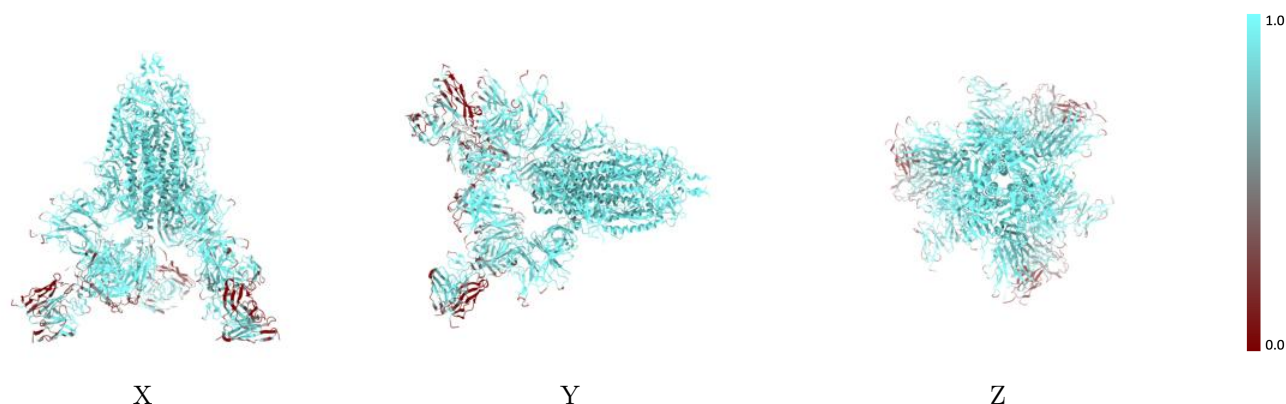
The images above show the 3D surface view of the map at the recommended contour level 0.00538 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



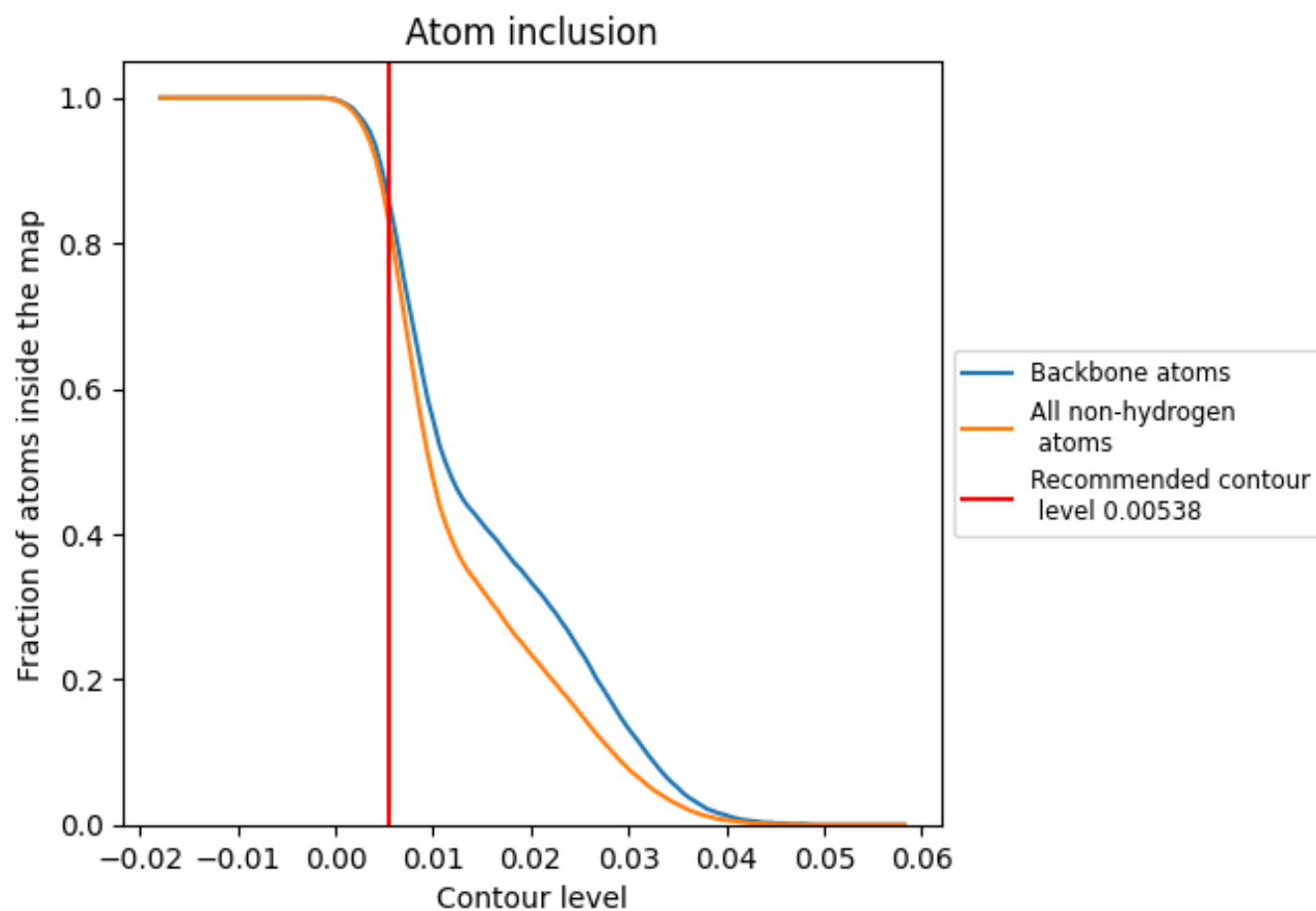
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.00538).































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.00538) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8370	 0.2240
A	 0.9070	 0.3080
B	 0.9090	 0.3100
C	 0.9100	 0.3100
D	 0.7790	 0.0090
E	 0.8550	 0.0200
F	 0.6080	 -0.0030
G	 0.4180	 0.0440
H	 0.8550	 0.0110
I	 0.6010	 -0.0000
J	 0.6330	 0.0040
K	 0.4280	 0.0490
L	 0.4320	 0.0470
M	 0.7730	 0.0070
N	 0.7840	 0.0120
O	 0.8540	 0.0150
P	 0.2860	 0.0240
Q	 0.7860	 0.3560
R	 0.9290	 0.3420
S	 0.8210	 0.3320
T	 0.8210	 0.3530
U	 0.2860	 0.0060
V	 0.7860	 0.3830
W	 0.9290	 0.3460
X	 0.8210	 0.3750
Y	 0.7860	 0.2490
Z	 0.3210	 0.0990
a	 0.7860	 0.3580
b	 0.8930	 0.3670
c	 0.7860	 0.2380
d	 0.5710	 0.1250

