



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 05:44 PM UTC

PDB ID : 7CWM / pdb_00007cwm
EMDB ID : EMD-30483
Title : Complex of SARS-CoV-2 spike protein and Fab P17 with one RBD in open state and two RBD in closed state
Authors : Wang, N.; Wang, X.
Deposited on : 2020-08-29
Resolution : 3.60 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

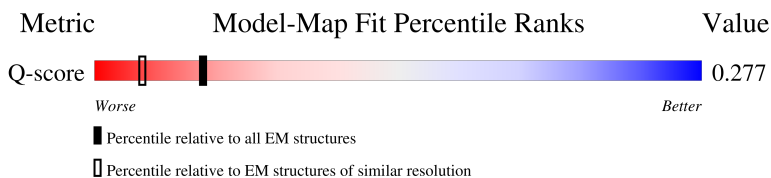
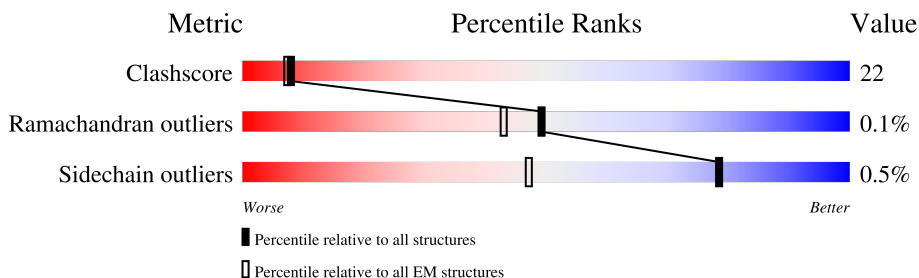
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



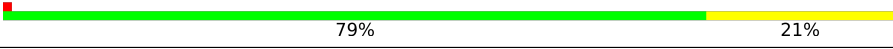
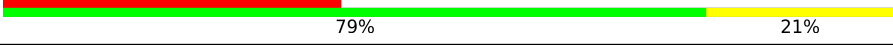
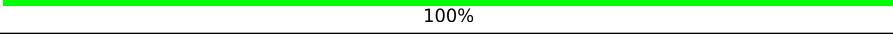
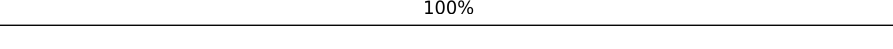
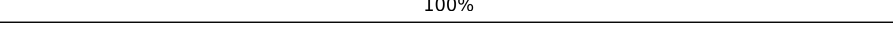
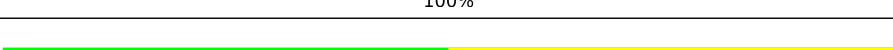
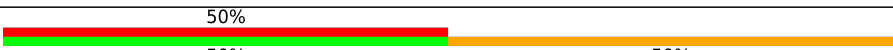
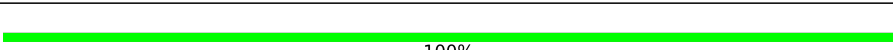
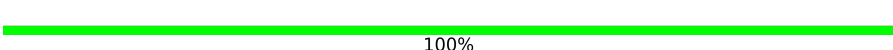
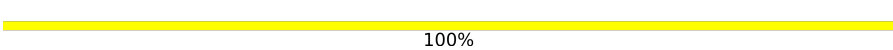
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12797 (3.10 - 4.10)

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 $\leq 5\%$. 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	
1	B	1273	
1	C	1273	
2	G	120	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	H	120	
2	I	120	
3	J	108	
3	K	108	
3	L	108	
4	D	2	
4	E	2	
4	F	2	
4	M	2	
4	N	2	
4	O	2	
4	P	2	
4	Q	2	
4	R	2	
4	S	2	
4	T	2	
4	U	2	
4	V	2	
4	W	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
4	NAG	S	1	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 30772 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	1056	Total	C	N	O	S	0	0
			8253	5267	1381	1568	37		
1	B	1071	Total	C	N	O	S	0	0
			8351	5330	1395	1587	39		
1	C	1072	Total	C	N	O	S	0	0
			8350	5329	1394	1588	39		

- Molecule 2 is a protein called P17 heavy chain.

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

- Molecule 3 is a protein called P17 light chain.

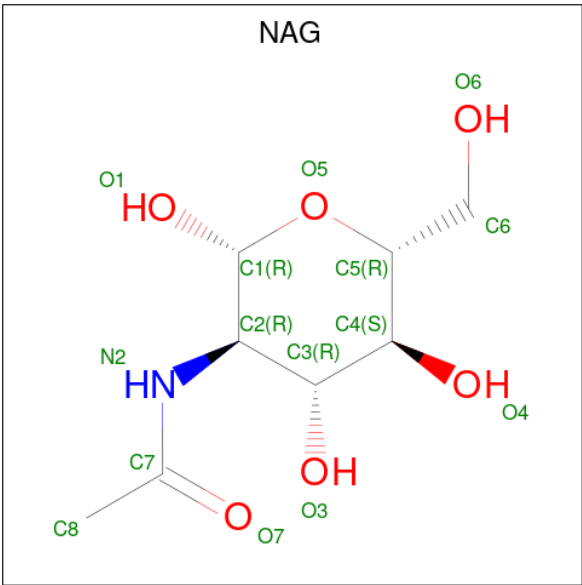
Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	108	Total	C	N	O	S	0	0
			814	510	137	165	2		
3	J	108	Total	C	N	O	S	0	0
			817	511	137	167	2		
3	K	108	Total	C	N	O	S	0	0
			817	511	137	167	2		

- Molecule 4 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
4	D	2	Total	C	N	O	0	0
			28	16	2	10		
4	E	2	Total	C	N	O	0	0
			28	16	2	10		
4	F	2	Total	C	N	O	0	0
			28	16	2	10		
4	M	2	Total	C	N	O	0	0
			28	16	2	10		
4	N	2	Total	C	N	O	0	0
			28	16	2	10		
4	O	2	Total	C	N	O	0	0
			28	16	2	10		
4	P	2	Total	C	N	O	0	0
			28	16	2	10		
4	Q	2	Total	C	N	O	0	0
			28	16	2	10		
4	R	2	Total	C	N	O	0	0
			28	16	2	10		
4	S	2	Total	C	N	O	0	0
			28	16	2	10		
4	T	2	Total	C	N	O	0	0
			28	16	2	10		
4	U	2	Total	C	N	O	0	0
			28	16	2	10		
4	V	2	Total	C	N	O	0	0
			28	16	2	10		
4	W	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

Continued on next page...

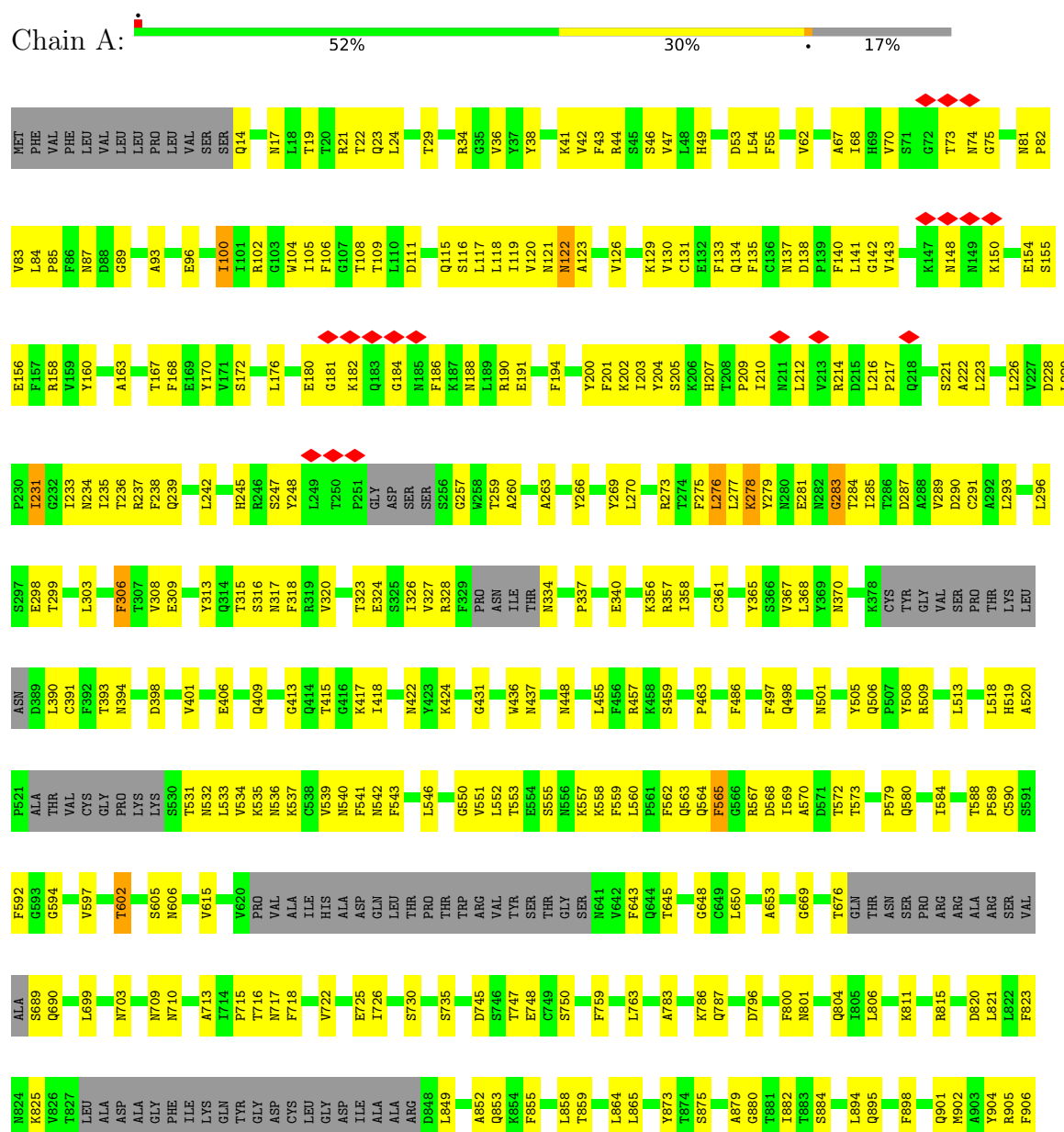
Continued from previous page...

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

3 Residue-property plots

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

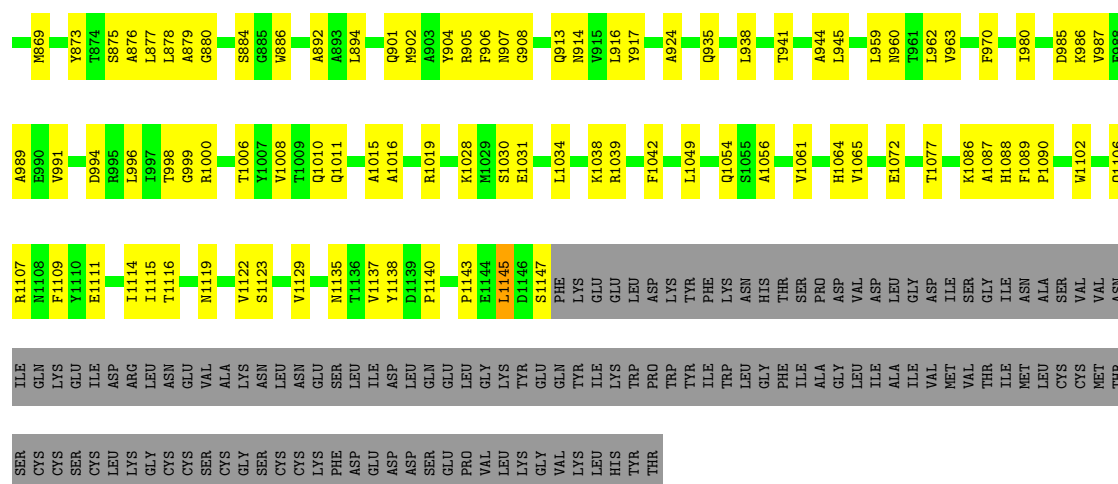


G857	Q965	A1087	SER
L888	F970	H1088	VAL
T859	F1089	P1090	VAL
	N978	R1091	ASN
L864		E1092	ILE
L865	S982	G1093	GLN
		R1107	LYS
M869	D994	Y1110	GLU
Y873		T998	ASP
T874	G999	Y1115	ARG
S875		T1116	LEU
	L1001	T1117	ASN
A879	T1006	D1118	VAL
G880	Y1007	V1122	GLY
T881	V1008	V1129	ASN
T883	T1009	I1132	GLY
S884	Q1010	I1137	LEU
	R1019	V1138	ASP
L894		D1139	LEU
Q895		P1140	GLN
F898	N1023	Q1142	GLU
	K1028		LEU
Q901	E1031		GLY
M902	C1032		GLY
R905			LYS
F906	K1038		TYR
N907	R1039		GLY
G908			GLY
	F1042		GLY
N914	V915		VAL
L916	H1048		LYS
	L1049		LEU
F927	H1050		TRP
	S1051		PRO
Q935	F1052		LYS
D936	P1053		TRP
S937	Q1054		ILE
L938			TRP
S939	H1058		LYS
			ASN
L945	Y1061		HIS
G946	F1062		THR
	L1063		PHE
	H1064		ILE
D950	V1065		ALA
			GLY
N953			LEU
	A1070		ILE
Q957	Q1071		ALA
A958	E1072		GLY
L959			ILE
N960	T1077		ILE
T961			GLY
L962	A1080		THR
V963	K1086		ILE
K964			ASN
			MET
			LEU
			ALA

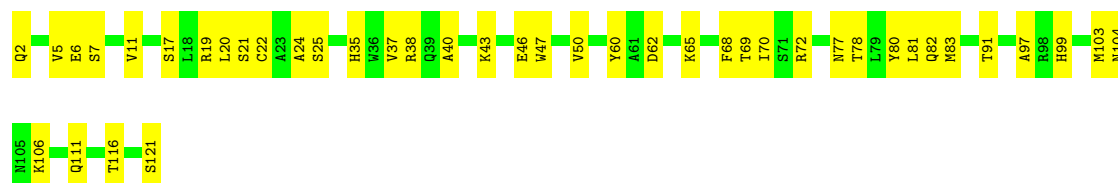
● Molecule 1: Spike glycoprotein



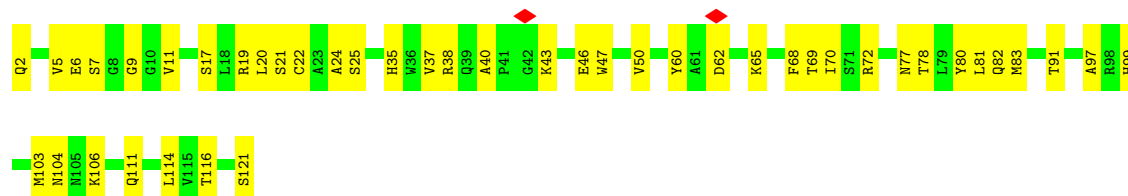
MET	P85	A163	F238	P330	M448	A570	I670	I770
PHE	F86	T167	Q239	ASN		D571	G671	Q774
VAL	N87	F168	L242	ILE	L455	T572	A672	K786
THR	G89	E169	H245	N334	F456	D578	S673	Y789
LEU	A93	Y170	Y248	P337	K458	P579	G675	
GLN	E96	S172	L249	E340	S459	E583	T676	D796
LEU	I100	G181	T250	K356	P463	I584	THR	F800
PRO	R101	K182	P251	K357	E465	T587	ASN	N801
VAL	G183	ASP	GLY	R358	F466	T588	SER	
SER	W104	K184	SER	C361	F497	P589	ARG	Q804
GLY	I105	F186	S256			C590	ALA	I805
ASN	G107	K187	A263	S365	N501	S591	ARG	L806
LYS	T108	N185	A264	S366	Y505	G594	ARG	D808
GLY	T109	L188	L285	S367	Q506	T599	VAL	K811
ASN	D111	L189	Y266	L368	P507	P600	ALA	
LYS	Q115	E191	Y269	Y369	Y508	V608	S689	R815
GLY	S116	F194	L270	C379	R509	V615	Q690	S816
ASP	Y36			G381	L513	V620	Y695	E819
ASP	Y37	Y200	F275	V382	L518	PRO	S704	L822
LEU	Y38	F201	L276	S383	L518	VAL		F823
GLN		K202	L277	P384	A522	ALA	N709	N824
GLY	K41	V120	K278	T385	T523	ILE	N710	K825
VAL	V42	N121	Y279	K386	V524	HIS	S711	N826
LYS	F43	N122		L387		ALA	I712	T827
TYR	R44	A123		N388	P527	ASP	L714	LEU
GLY	S45	V126	G283	N389	LYS	GLN	F715	ASP
VAL	S46		T284	L390	THR	LEU	T716	ALA
LYS	D53	V130	T285	C391	SER	THR	N717	GLY
LEU	L54	C131	T286	F392	T531	PRO	F718	PHE
HIS	F55	E132	A288	N394	H532	THR		ILE
TYR		Q134	V289		V534	TRP	V722	LYS
	V62	F140	L296	V401		VAL	E725	GLN
	T63	L141	C301	E406	N542	TYR	I726	TYR
	W64	G142	T302	Q409	F543	SER	I742	GLY
	F65	V143	L303	P412	N544	GLY	C743	ASP
	H66	Y144	A304	P412	G545	SER	S746	GLY
	A67	Y145	S305	K417	L546	GLY	T747	ASP
	H69	H146	F306	T418	S555	ILE	E748	ALA
	V70	K147	T307			ALA	T749	ALA
	T73	N148	V308	N422	L560	ALA	C750	ALA
	N74	K150	S316	Y423	P561	THR	S750	ARG
	G75	E164	N317	F562	F562	GLY		
		S155	F318	Q563	L650	THR	L753	D848
	R78	F79	R319	Q564	T651	GLY		L849
	D80	N81	V320	F565	G652	THR	Y763	I850
	F157	E156	I233	G566	A653	GLY	C760	T781
	R158	F159	N234	R567	E661	ILE		Q853
	V83	Y160	T236	D568	L763	ALA		K854
	L84		F329			ALA		L858



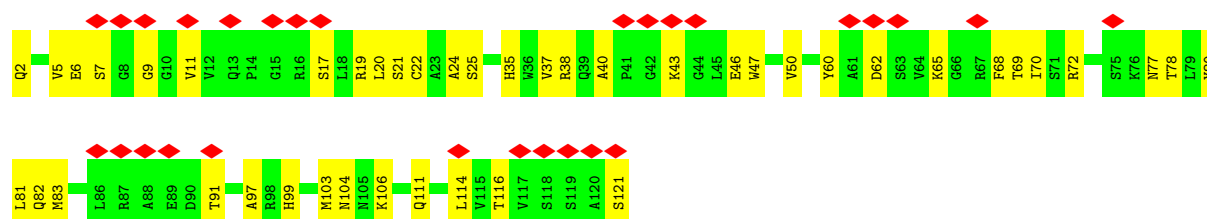
- Molecule 2: P17 heavy chain



- Molecule 2: P17 heavy chain

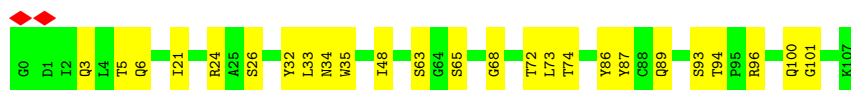


- Molecule 2: P17 heavy chain

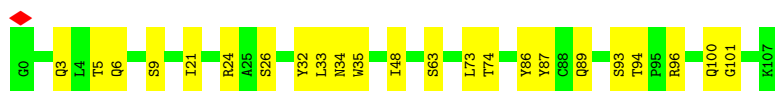
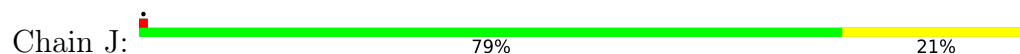


- Molecule 3: P17 light chain

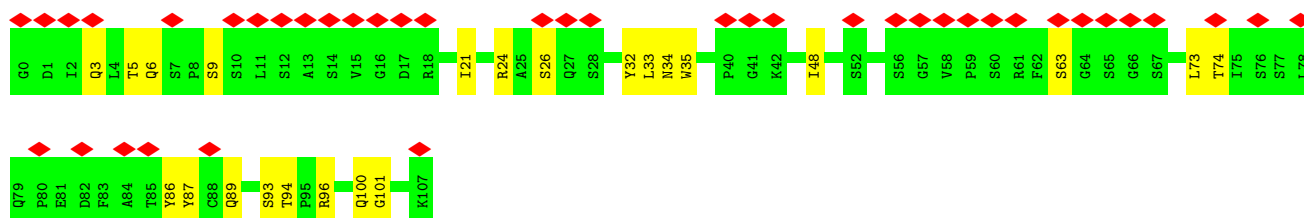
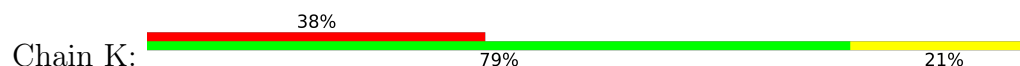




- Molecule 3: P17 light chain



- Molecule 3: P17 light chain



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



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



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



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





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

Chain N:  100%



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

Chain O:  100%



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

Chain P:  50% 50%



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

Chain Q:  100%



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

Chain R:  100%



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

Chain S:  50% 50%



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

Chain T:  100%

MAG1
MAG2

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

Chain U:  50% 50%

MAG1
MAG2

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

Chain V:  100%

MAG1
MAG2

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

Chain W:  100%

MAG1
MAG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	150376	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	0.039	Depositor
Minimum map value	-0.006	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.00503	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	0.47	0/8439	0.71	5/11478 (0.0%)
1	B	0.44	0/8541	0.66	4/11622 (0.0%)
1	C	0.50	0/8540	0.73	3/11622 (0.0%)
2	G	0.32	0/937	0.63	0/1269
2	H	0.32	0/937	0.64	0/1269
2	I	0.32	0/937	0.64	0/1269
3	J	0.33	0/834	0.63	0/1131
3	K	0.33	0/834	0.63	0/1131
3	L	0.33	0/831	0.63	0/1127
All	All	0.45	0/30830	0.69	12/41918 (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	4
1	C	0	2
2	G	0	1
2	H	0	1
2	I	0	1
All	All	0	13

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	100	ILE	N-CA-C	-10.78	102.85	113.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	100	ILE	N-CA-C	-10.78	102.85	113.20
1	B	301	CYS	N-CA-C	-8.75	102.38	113.23
1	A	283	GLY	CA-C-O	-6.08	116.30	122.56
1	A	849	LEU	N-CA-C	-5.69	106.11	113.16

There are no chirality outliers.

5 of 13 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	8253	0	8039	510	0
1	B	8351	0	8128	461	0
1	C	8350	0	8124	441	0
2	G	918	0	885	26	0
2	H	918	0	885	27	0
2	I	918	0	885	27	0
3	J	817	0	800	17	0
3	K	817	0	800	17	0
3	L	814	0	797	36	0
4	D	28	0	25	3	0
4	E	28	0	25	0	0
4	F	28	0	25	1	0
4	M	28	0	25	0	0
4	N	28	0	25	2	0
4	O	28	0	25	0	0
4	P	28	0	25	1	0
4	Q	28	0	25	0	0
4	R	28	0	25	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	S	28	0	25	7	0
4	T	28	0	25	0	0
4	U	28	0	25	1	0
4	V	28	0	25	0	0
4	W	28	0	25	4	0
5	A	70	0	65	1	0
5	B	84	0	78	1	0
5	C	70	0	65	0	0
All	All	30772	0	29901	1349	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 22.

The worst 5 of 1349 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:22:THR:CG2	1:C:78:ARG:HD2	1.28	1.61
1:B:276:LEU:HD11	1:B:306:PHE:CE1	1.32	1.59
1:C:234:ASN:HD22	4:S:1:NAG:C1	1.10	1.59
1:C:63:THR:CG2	1:C:65:PHE:CZ	1.85	1.57
1:C:63:THR:HG21	1:C:65:PHE:CZ	1.36	1.53

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	961/1273 (76%)	884 (92%)	76 (8%)	1 (0%)	48	79
1	B	1057/1273 (83%)	984 (93%)	72 (7%)	1 (0%)	48	79
1	C	1058/1273 (83%)	978 (92%)	80 (8%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	G	118/120 (98%)	106 (90%)	12 (10%)	0	100	100
2	H	118/120 (98%)	106 (90%)	12 (10%)	0	100	100
2	I	118/120 (98%)	106 (90%)	12 (10%)	0	100	100
3	J	106/108 (98%)	97 (92%)	9 (8%)	0	100	100
3	K	106/108 (98%)	97 (92%)	9 (8%)	0	100	100
3	L	106/108 (98%)	97 (92%)	9 (8%)	0	100	100
All	All	3748/4503 (83%)	3455 (92%)	291 (8%)	2 (0%)	49	79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	986	LYS
1	B	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	918/1112 (83%)	909 (99%)	9 (1%)	68	75
1	B	929/1112 (84%)	927 (100%)	2 (0%)	87	85
1	C	928/1112 (84%)	921 (99%)	7 (1%)	73	77
2	G	96/98 (98%)	96 (100%)	0	100	100
2	H	96/98 (98%)	96 (100%)	0	100	100
2	I	96/98 (98%)	96 (100%)	0	100	100
3	J	93/93 (100%)	93 (100%)	0	100	100
3	K	93/93 (100%)	93 (100%)	0	100	100
3	L	92/93 (99%)	92 (100%)	0	100	100
All	All	3341/3909 (86%)	3323 (100%)	18 (0%)	78	80

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	385	THR
1	C	524	VAL
1	C	391	CYS
1	A	985	ASP
1	C	382	VAL

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

Mol	Chain	Res	Type
3	L	90	GLN
3	J	79	GLN
1	B	239	GLN
1	B	165	ASN
3	J	90	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

28 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	$\# Z > 2$
4	NAG	D	1	4,1	14,14,15	1.58	1 (7%)	17,19,21	1.40	2 (11%)
4	NAG	D	2	4	14,14,15	0.22	0	17,19,21	0.52	0
4	NAG	E	1	4,1	14,14,15	0.35	0	17,19,21	0.48	0
4	NAG	E	2	4	14,14,15	0.30	0	17,19,21	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	F	1	4,1	14,14,15	0.48	0	17,19,21	0.47	0
4	NAG	F	2	4	14,14,15	0.21	0	17,19,21	0.48	0
4	NAG	M	1	4,1	14,14,15	0.44	0	17,19,21	0.42	0
4	NAG	M	2	4	14,14,15	0.29	0	17,19,21	0.45	0
4	NAG	N	1	4,1	14,14,15	0.31	0	17,19,21	0.99	1 (5%)
4	NAG	N	2	4	14,14,15	0.49	0	17,19,21	1.23	2 (11%)
4	NAG	O	1	4,1	14,14,15	0.33	0	17,19,21	0.51	0
4	NAG	O	2	4	14,14,15	0.31	0	17,19,21	0.41	0
4	NAG	P	1	4,1	14,14,15	0.47	0	17,19,21	0.46	0
4	NAG	P	2	4	14,14,15	0.17	0	17,19,21	0.47	0
4	NAG	Q	1	4,1	14,14,15	0.49	0	17,19,21	0.53	0
4	NAG	Q	2	4	14,14,15	0.25	0	17,19,21	0.39	0
4	NAG	R	1	4,1	14,14,15	0.47	0	17,19,21	0.41	0
4	NAG	R	2	4	14,14,15	0.23	0	17,19,21	0.46	0
4	NAG	S	1	4,1	14,14,15	1.19	2 (14%)	17,19,21	1.10	2 (11%)
4	NAG	S	2	4	14,14,15	0.35	0	17,19,21	0.45	0
4	NAG	T	1	4,1	14,14,15	0.51	0	17,19,21	0.48	0
4	NAG	T	2	4	14,14,15	0.32	0	17,19,21	0.41	0
4	NAG	U	1	4,1	14,14,15	0.44	0	17,19,21	0.46	0
4	NAG	U	2	4	14,14,15	0.27	0	17,19,21	0.37	0
4	NAG	V	1	4,1	14,14,15	0.42	0	17,19,21	0.47	0
4	NAG	V	2	4	14,14,15	0.27	0	17,19,21	0.38	0
4	NAG	W	1	4,1	14,14,15	0.27	0	17,19,21	0.65	0
4	NAG	W	2	4	14,14,15	0.26	0	17,19,21	0.65	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
4	NAG	D	1	4,1	-	3/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
4	NAG	E	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	E	2	4	-	2/6/23/26	0/1/1/1
4	NAG	F	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	F	2	4	-	2/6/23/26	0/1/1/1
4	NAG	M	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	M	2	4	-	2/6/23/26	0/1/1/1
4	NAG	N	1	4,1	-	3/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	N	2	4	-	0/6/23/26	0/1/1/1
4	NAG	O	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	O	2	4	-	2/6/23/26	0/1/1/1
4	NAG	P	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	P	2	4	-	2/6/23/26	0/1/1/1
4	NAG	Q	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	Q	2	4	-	1/6/23/26	0/1/1/1
4	NAG	R	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	R	2	4	-	2/6/23/26	0/1/1/1
4	NAG	S	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	S	2	4	-	2/6/23/26	0/1/1/1
4	NAG	T	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	T	2	4	-	2/6/23/26	0/1/1/1
4	NAG	U	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	U	2	4	-	2/6/23/26	0/1/1/1
4	NAG	V	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	V	2	4	-	2/6/23/26	0/1/1/1
4	NAG	W	1	4,1	-	3/6/23/26	0/1/1/1
4	NAG	W	2	4	-	1/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1	NAG	O5-C1	-5.67	1.34	1.43
4	S	1	NAG	O5-C1	-3.69	1.37	1.43
4	S	1	NAG	C1-C2	-2.14	1.49	1.52

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	N	2	NAG	C1-O5-C5	3.78	117.25	112.19
4	D	1	NAG	C3-C4-C5	3.61	116.78	110.23
4	S	1	NAG	C3-C4-C5	3.17	115.98	110.23
4	N	2	NAG	C1-C2-N2	2.67	114.64	110.43
4	N	1	NAG	C4-C3-C2	-2.62	107.18	111.02

There are no chirality outliers.

5 of 45 torsion outliers are listed below:

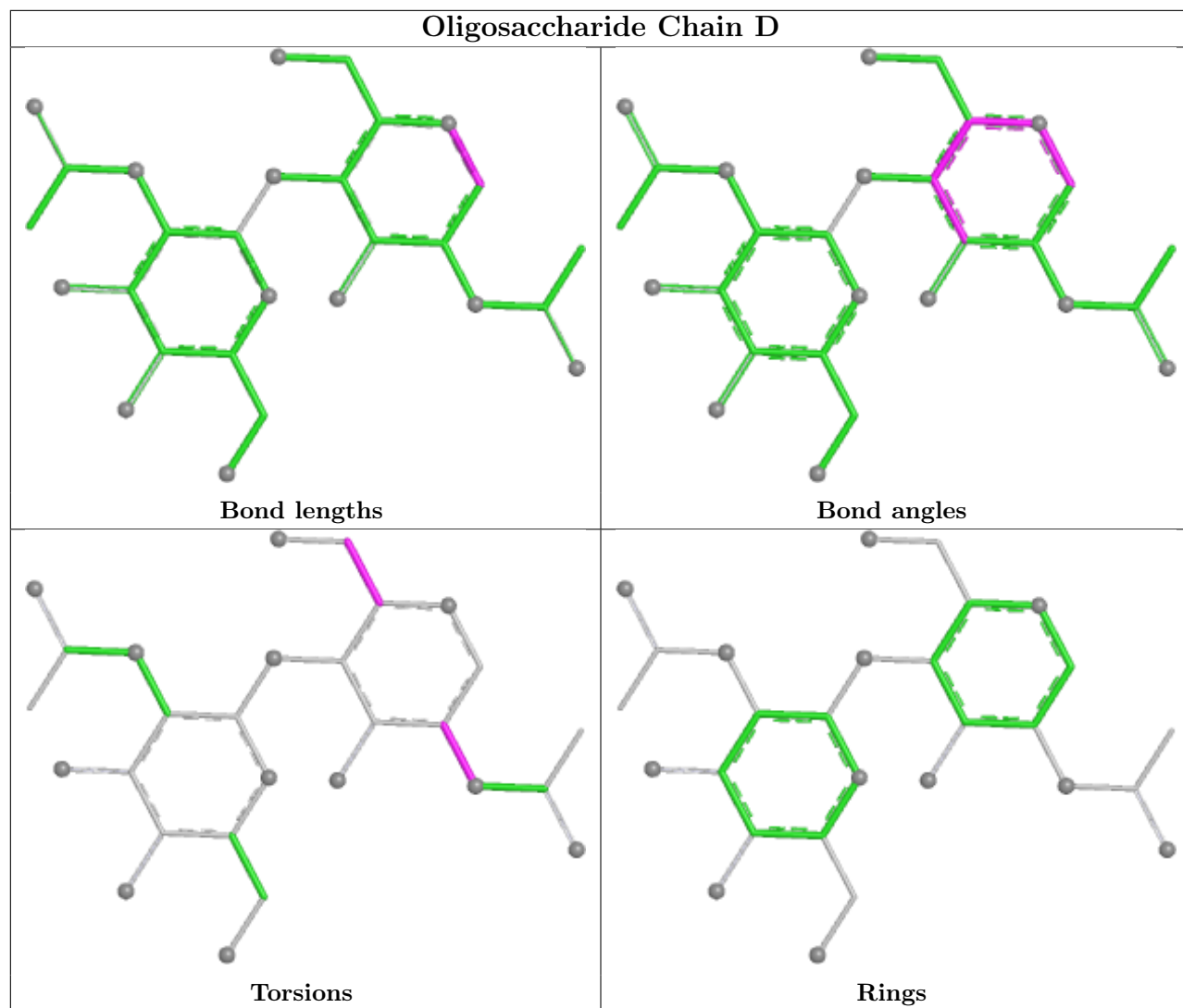
Mol	Chain	Res	Type	Atoms
4	N	1	NAG	C8-C7-N2-C2
4	N	1	NAG	O7-C7-N2-C2
4	W	1	NAG	C1-C2-N2-C7
4	W	1	NAG	C8-C7-N2-C2
4	W	1	NAG	O7-C7-N2-C2

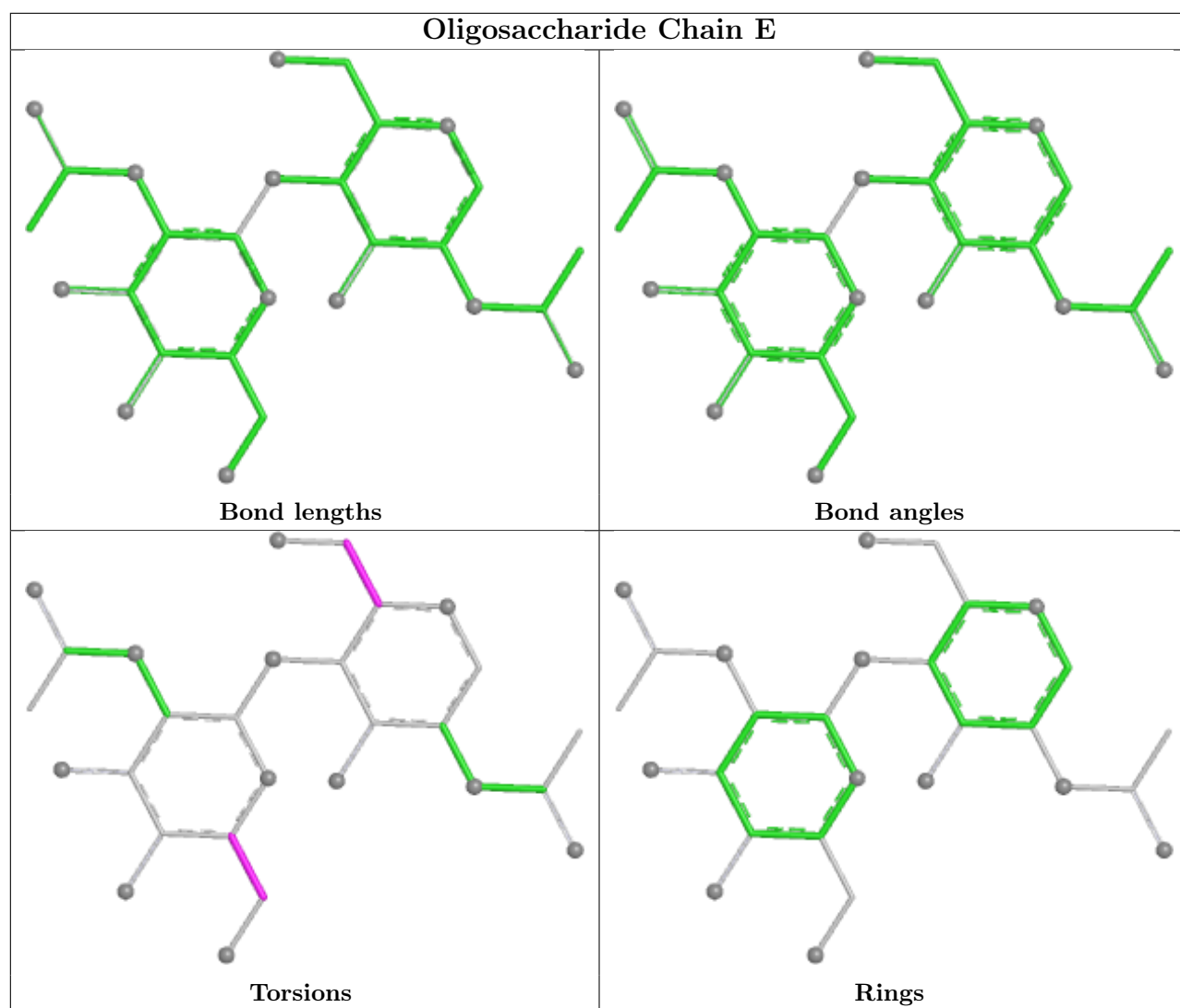
There are no ring outliers.

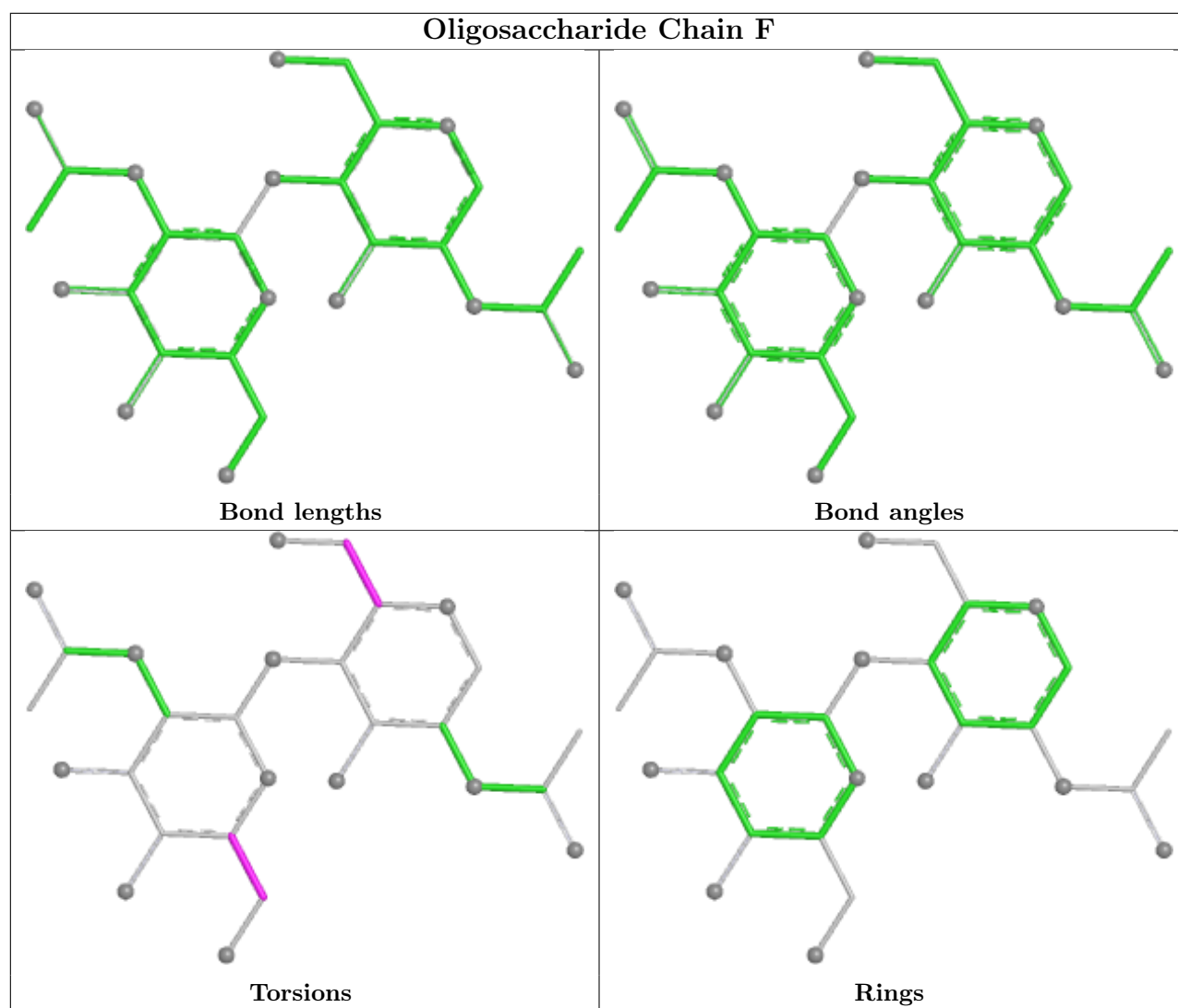
9 monomers are involved in 19 short contacts:

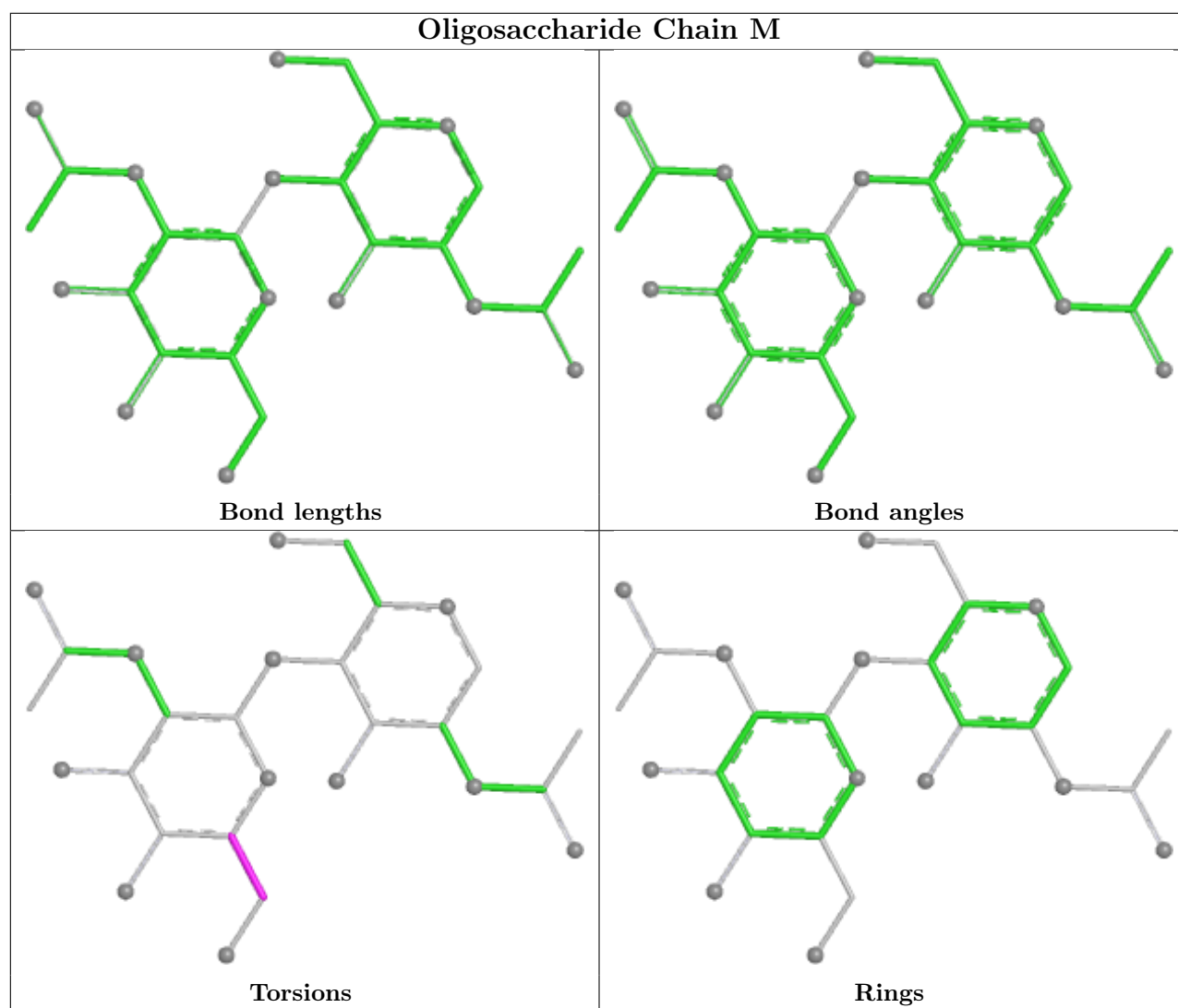
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	P	1	NAG	1	0
4	U	1	NAG	1	0
4	N	2	NAG	2	0
4	F	1	NAG	1	0
4	W	1	NAG	3	0
4	S	1	NAG	7	0
4	W	2	NAG	1	0
4	D	1	NAG	3	0
4	N	1	NAG	2	0

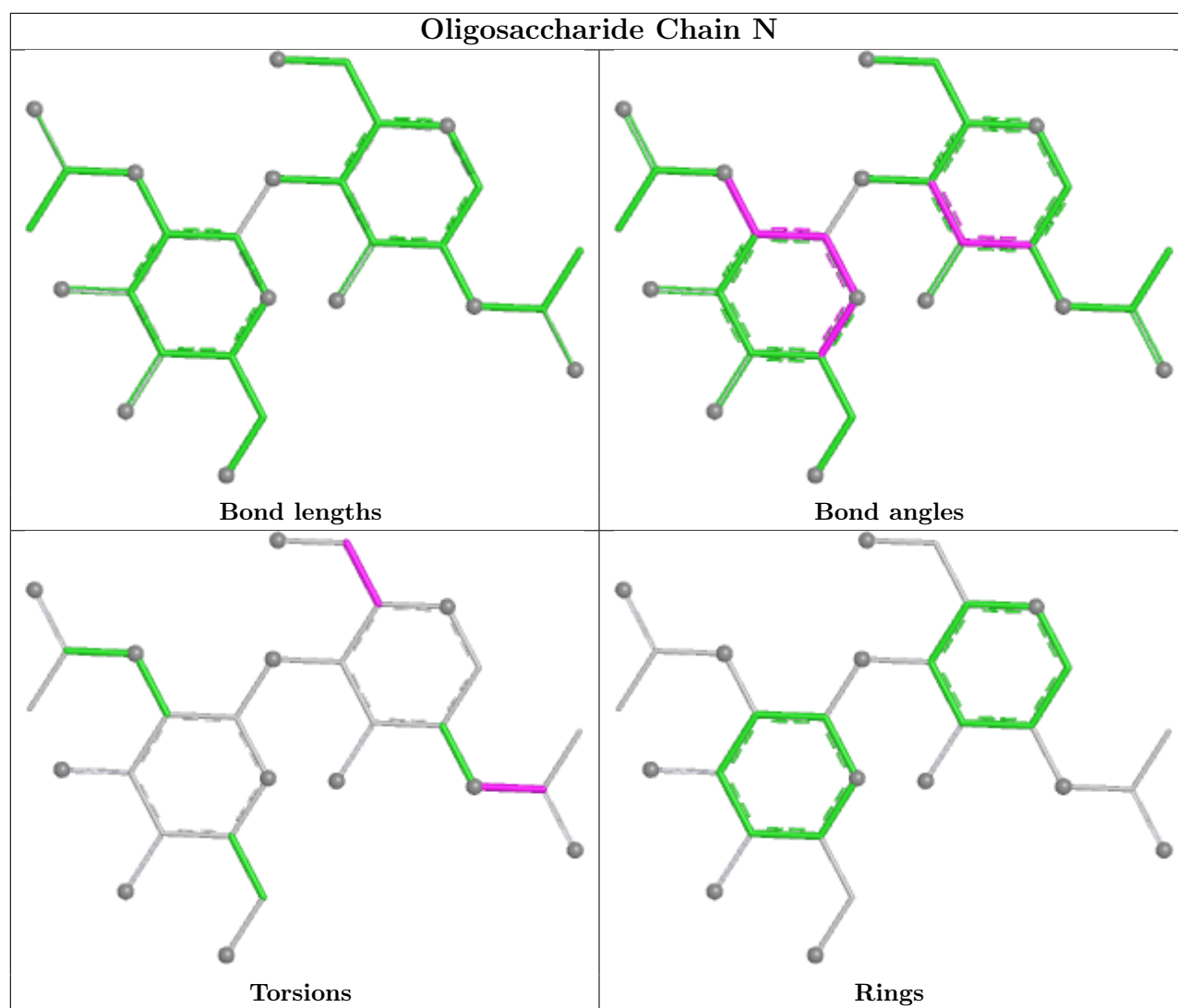
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

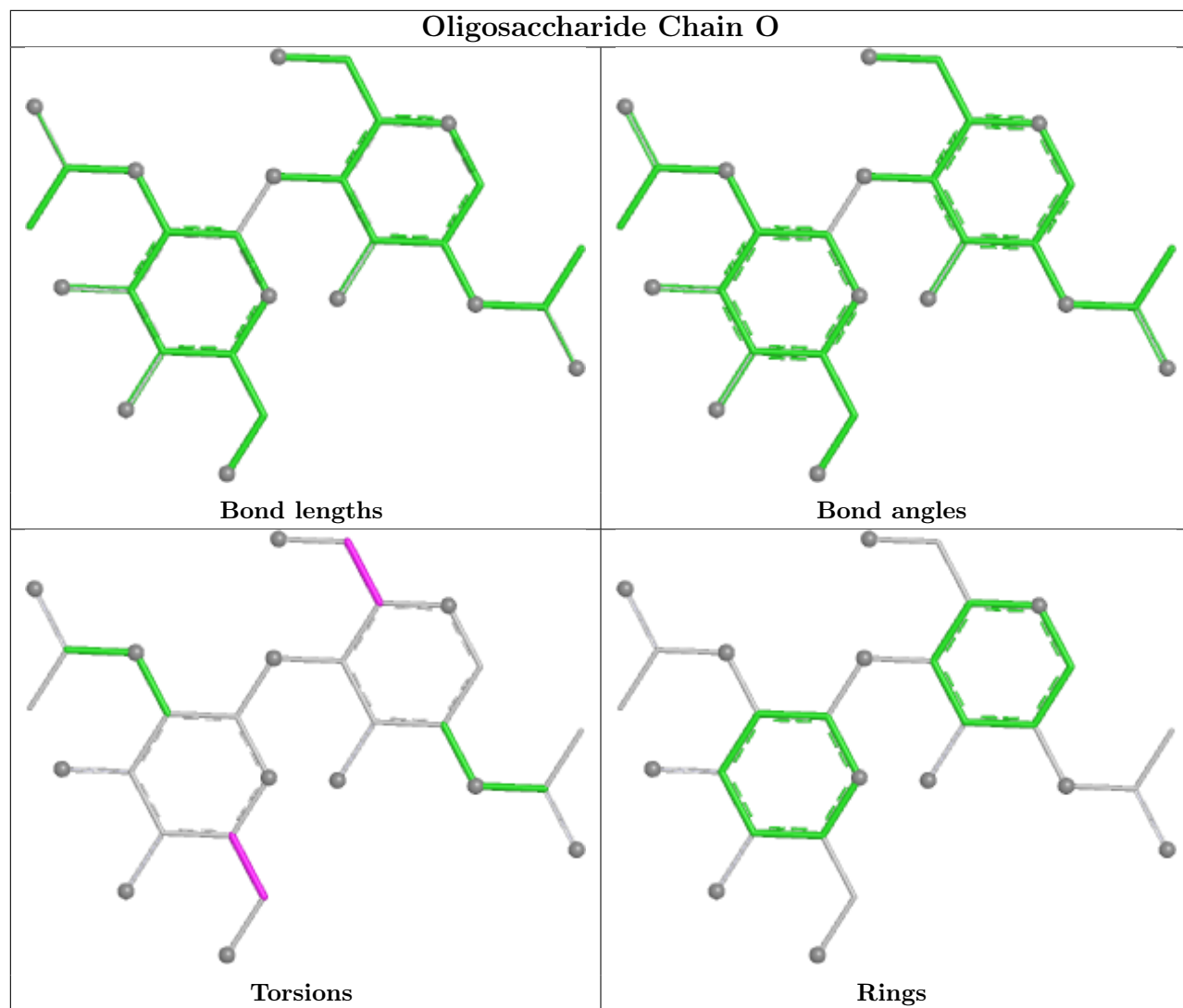


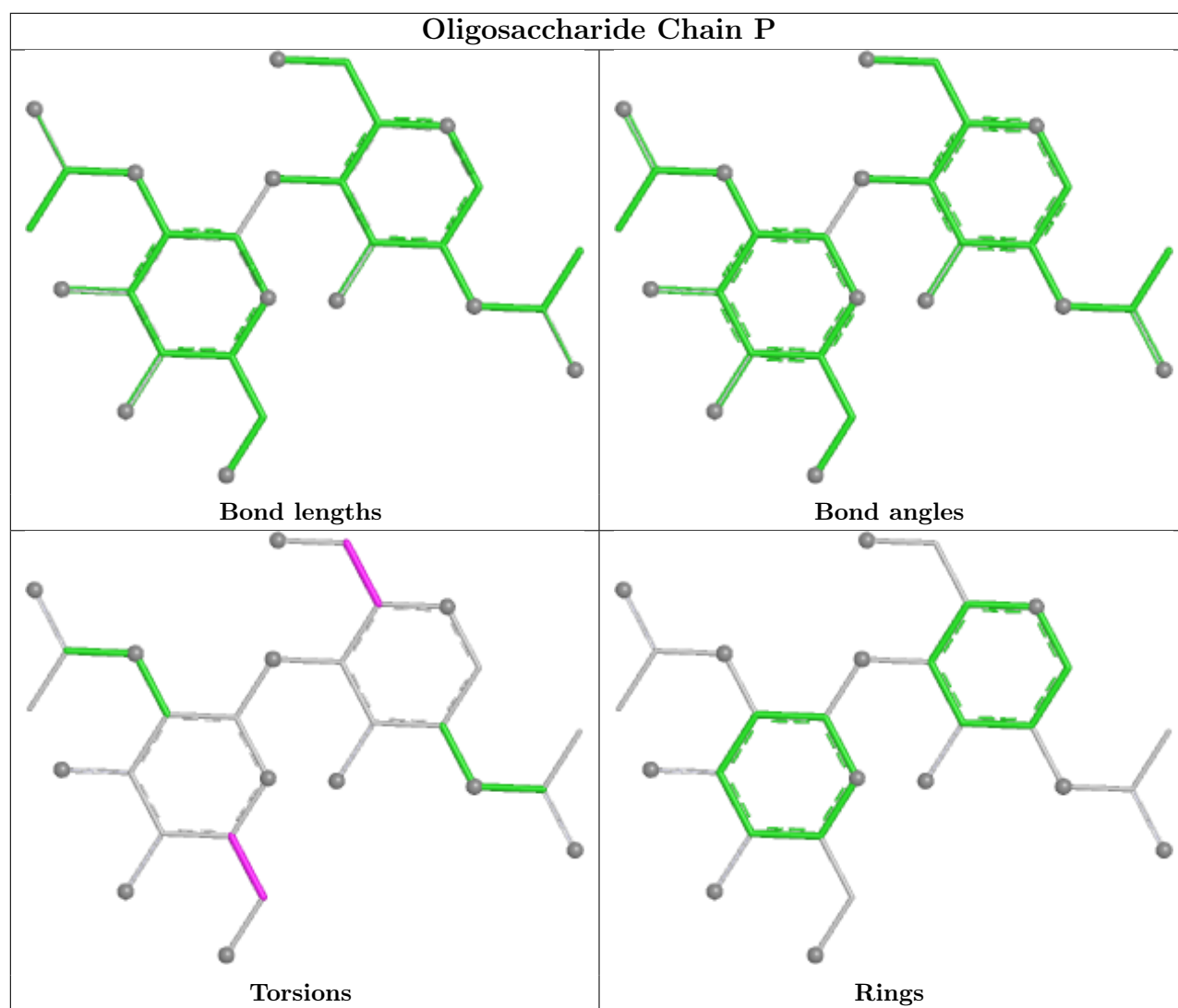


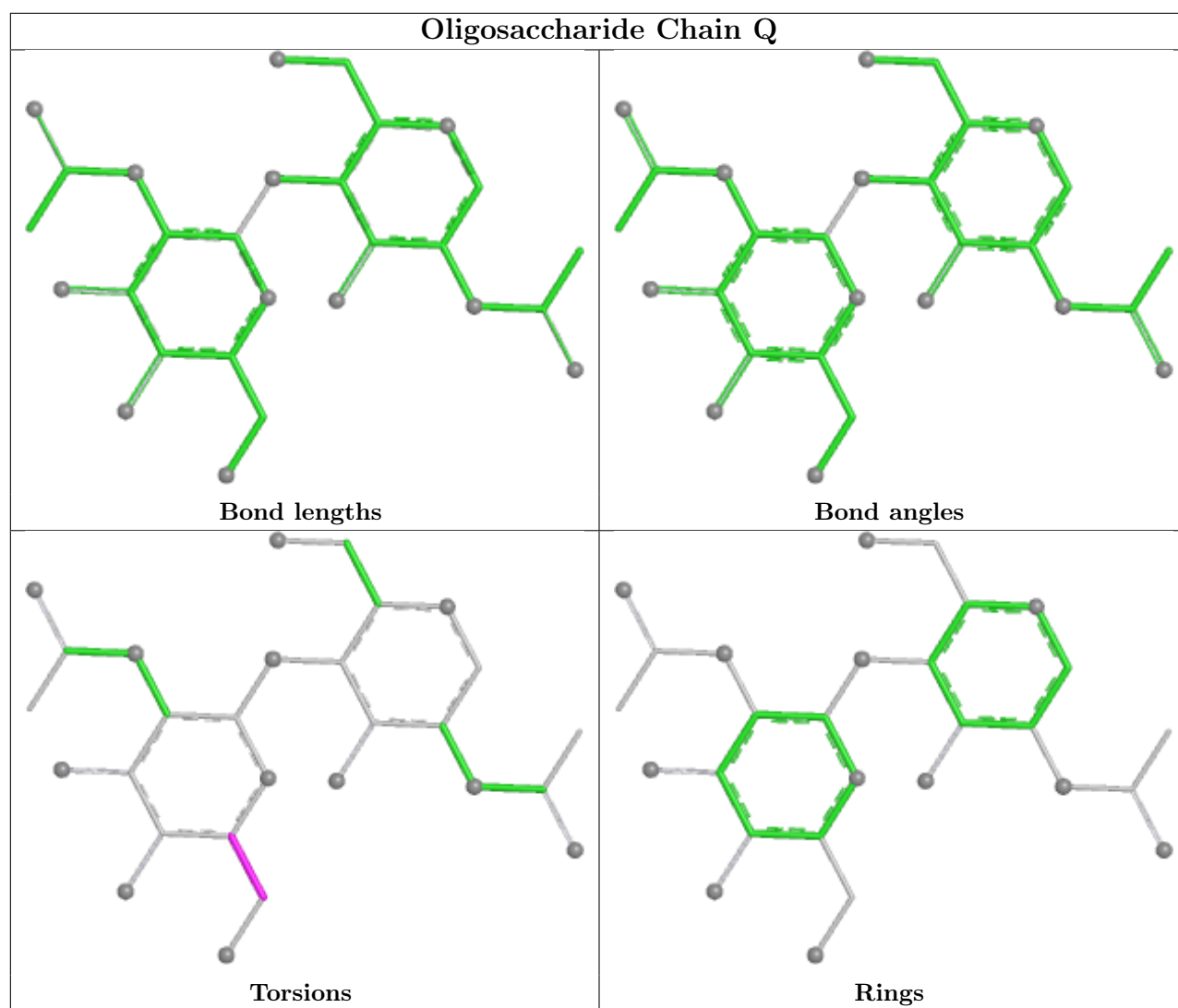


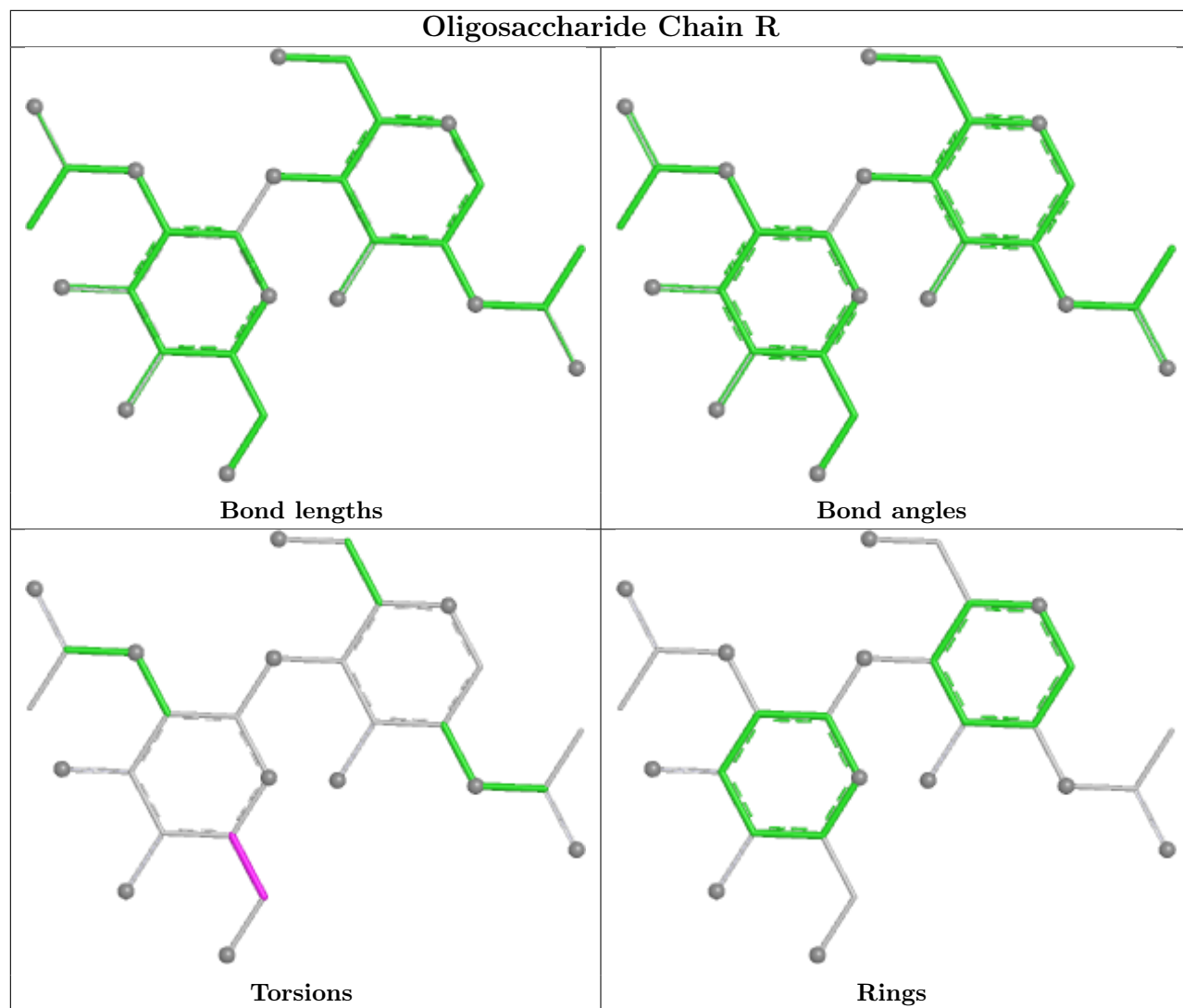


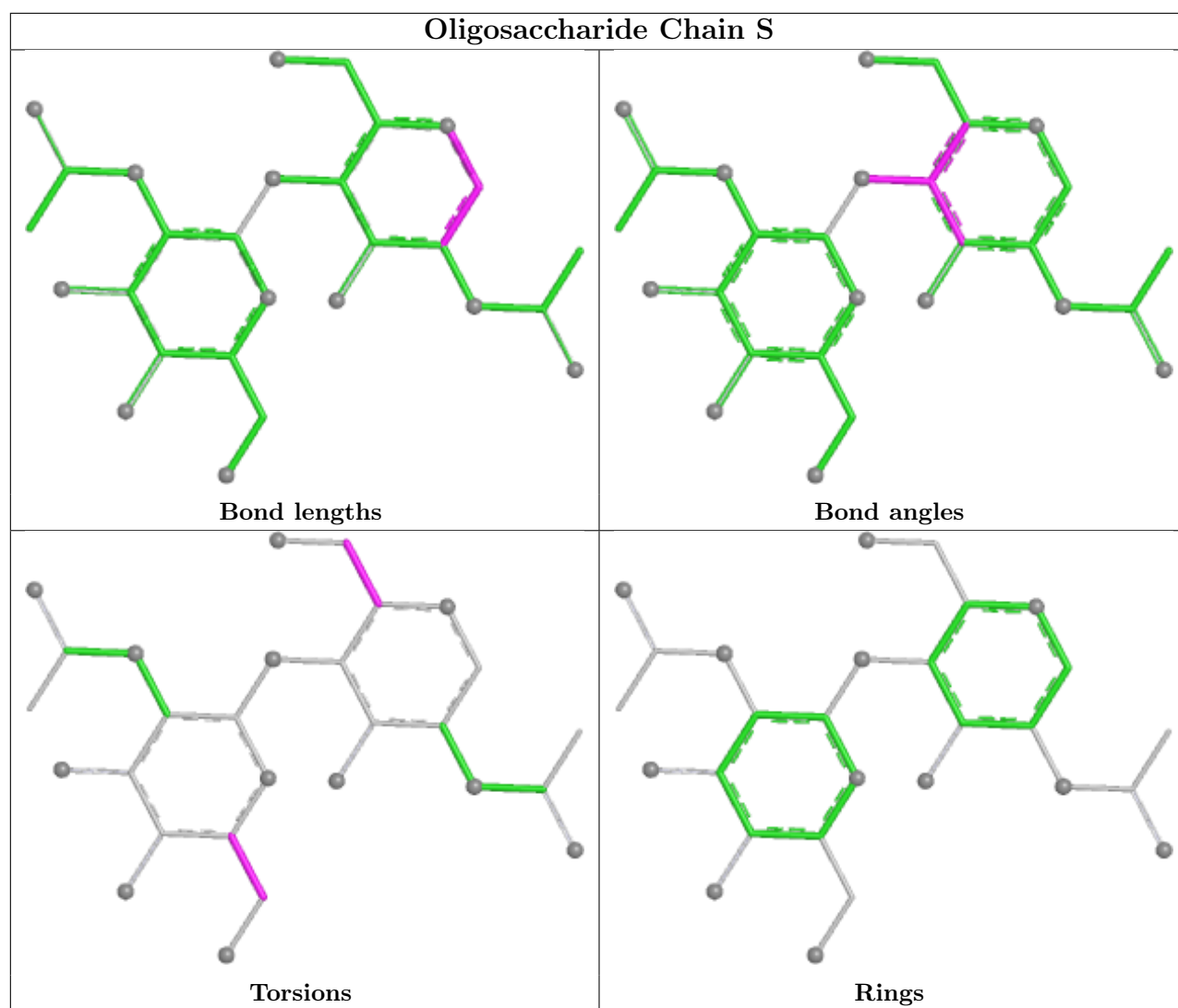


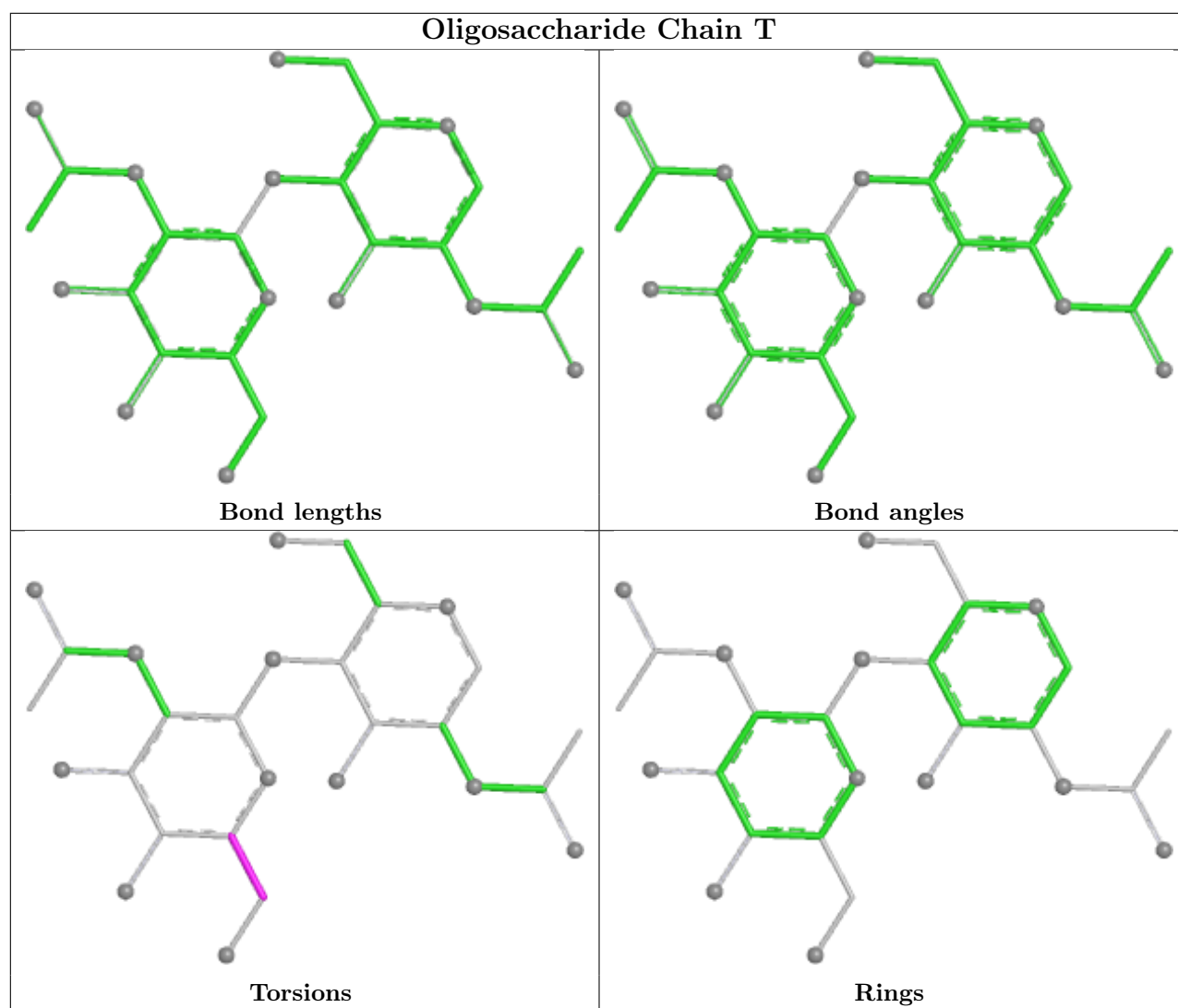


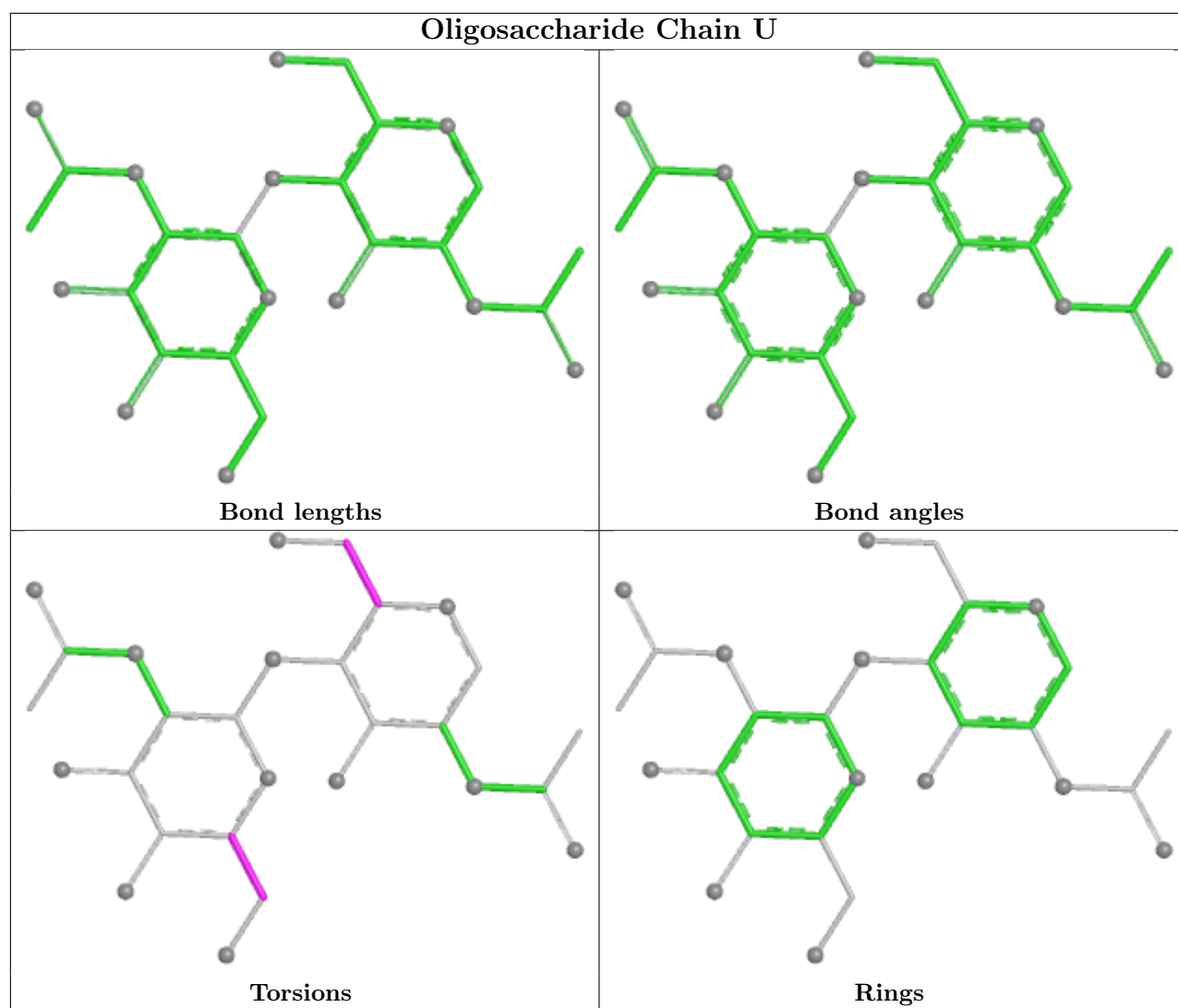


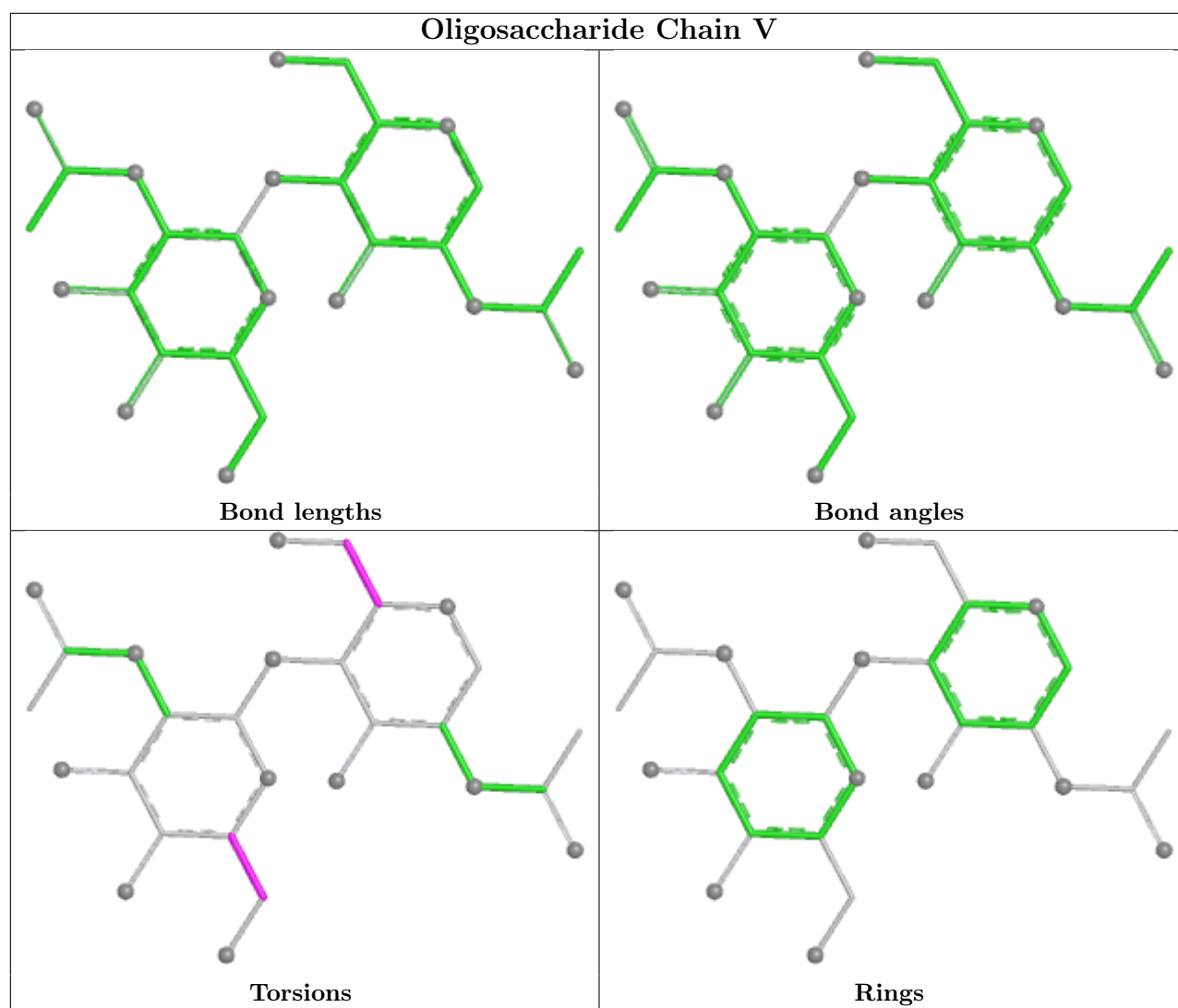


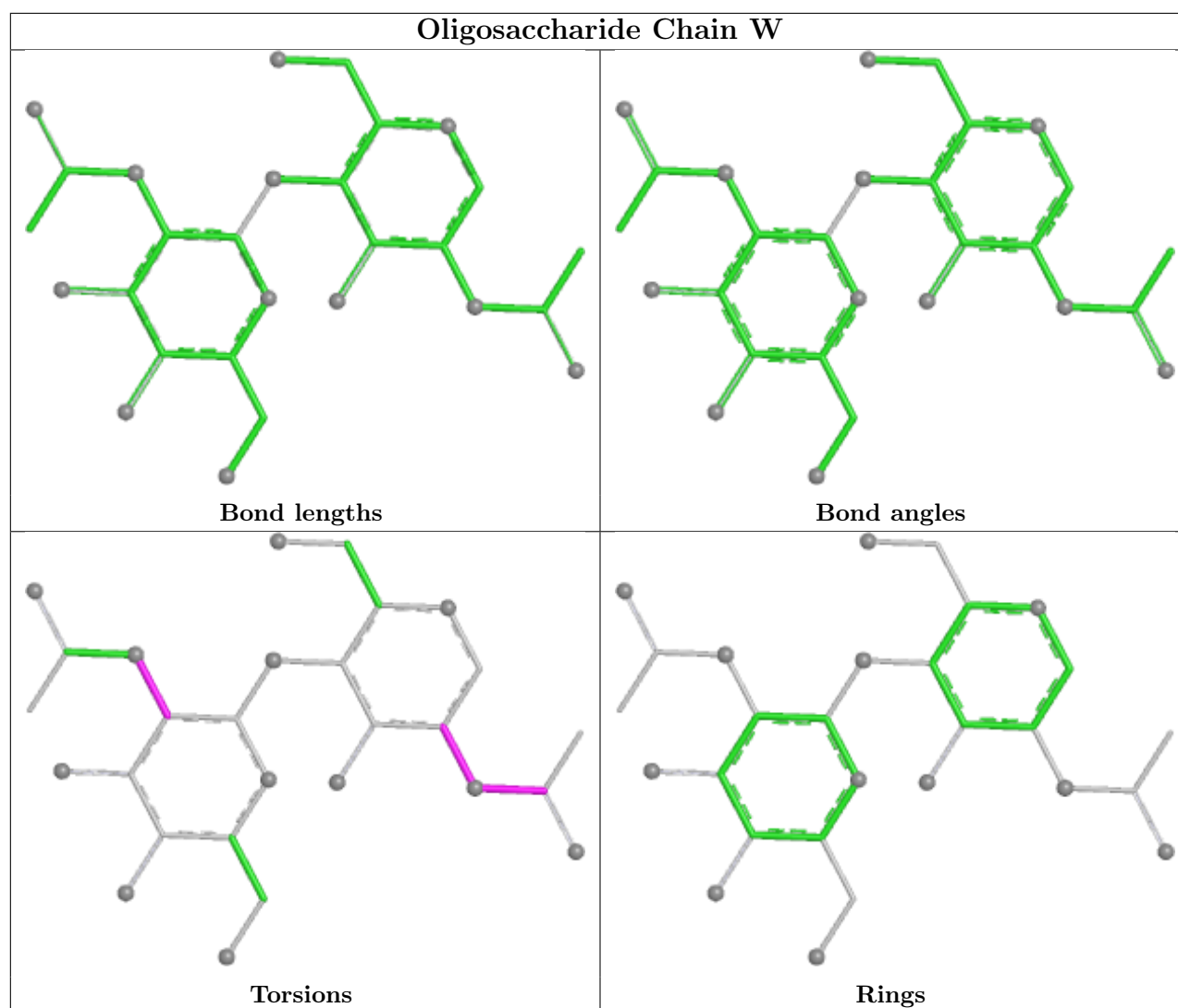












5.6 Ligand geometry [i](#)

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	$\# Z > 2$
5	NAG	A	1302	1	14,14,15	0.47	0	17,19,21	0.51	0
5	NAG	C	1301	1	14,14,15	0.41	0	17,19,21	0.43	0
5	NAG	A	1301	1	14,14,15	0.21	0	17,19,21	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	A	1304	1	14,14,15	0.57	0	17,19,21	0.37	0
5	NAG	C	1304	1	14,14,15	0.46	0	17,19,21	0.52	0
5	NAG	C	1305	1	14,14,15	0.25	0	17,19,21	0.53	0
5	NAG	B	1306	1	14,14,15	0.21	0	17,19,21	0.62	0
5	NAG	B	1305	1	14,14,15	0.53	0	17,19,21	0.37	0
5	NAG	C	1302	1	14,14,15	0.67	0	17,19,21	0.46	0
5	NAG	B	1304	1	14,14,15	0.22	0	17,19,21	0.45	0
5	NAG	C	1303	1	14,14,15	0.33	0	17,19,21	0.38	0
5	NAG	A	1303	1	14,14,15	0.19	0	17,19,21	0.45	0
5	NAG	B	1302	1	14,14,15	0.22	0	17,19,21	0.36	0
5	NAG	A	1305	1	14,14,15	0.23	0	17,19,21	0.64	0
5	NAG	B	1303	1	14,14,15	0.46	0	17,19,21	0.49	0
5	NAG	B	1301	1	14,14,15	0.37	0	17,19,21	0.41	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
5	NAG	A	1302	1	-	1/6/23/26	0/1/1/1
5	NAG	C	1301	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1301	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1304	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1304	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1305	1	-	1/6/23/26	0/1/1/1
5	NAG	B	1306	1	-	1/6/23/26	0/1/1/1
5	NAG	B	1305	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1302	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1304	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1303	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1303	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1302	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1305	1	-	1/6/23/26	0/1/1/1
5	NAG	B	1303	1	-	1/6/23/26	0/1/1/1
5	NAG	B	1301	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	1302	NAG	O5-C5-C6-O6
5	A	1304	NAG	C4-C5-C6-O6
5	B	1305	NAG	C4-C5-C6-O6
5	A	1304	NAG	O5-C5-C6-O6
5	B	1305	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
5	A	1304	NAG	1	0
5	B	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.

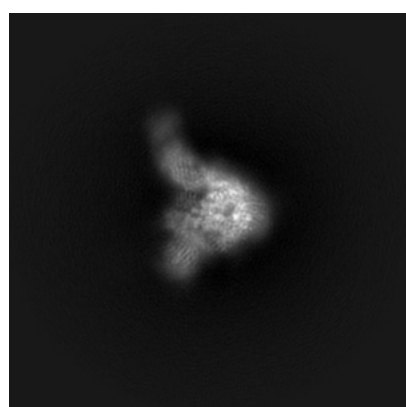
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30483. These allow visual inspection of the internal detail of the map and identification of artifacts.

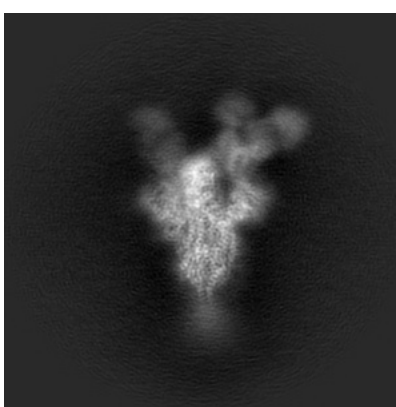
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

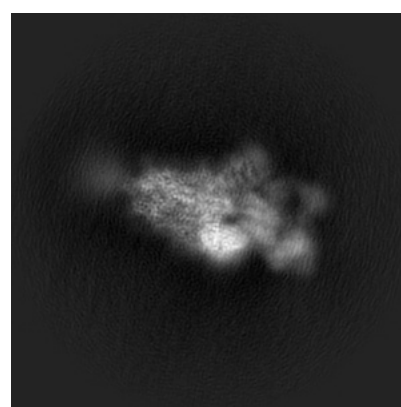
6.1.1 Primary map



X



Y

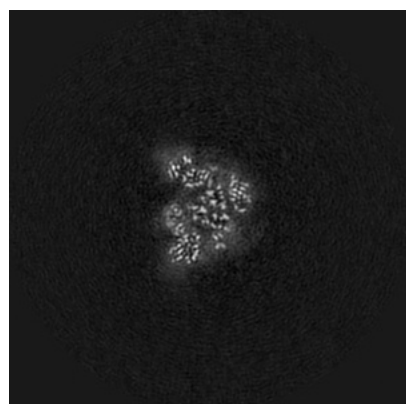


Z

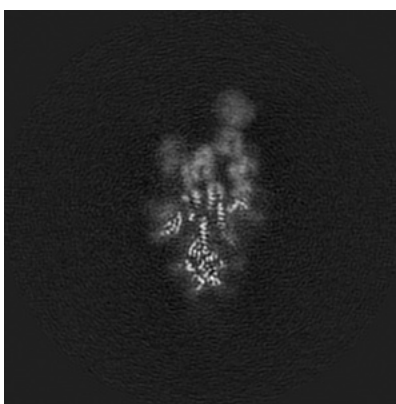
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

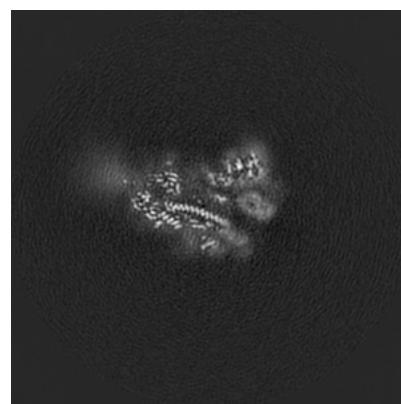
6.2.1 Primary map



X Index: 200



Y Index: 200

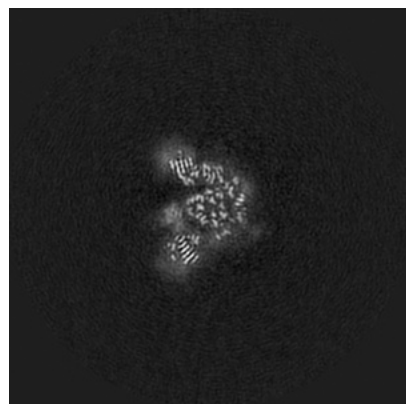


Z Index: 200

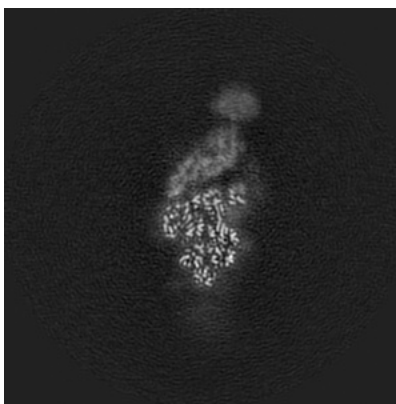
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

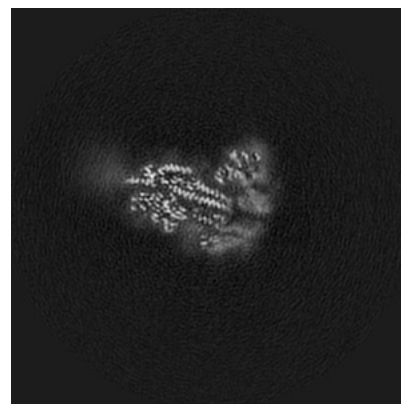
6.3.1 Primary map



X Index: 205



Y Index: 212

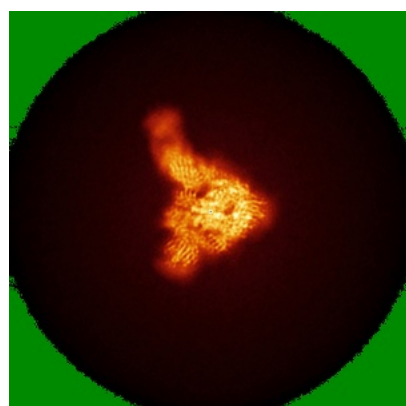


Z Index: 194

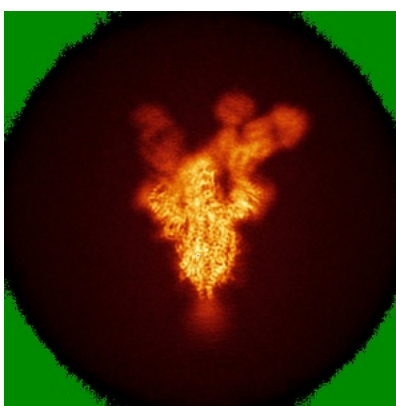
The images above show the largest variance slices of the map in three orthogonal directions.

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

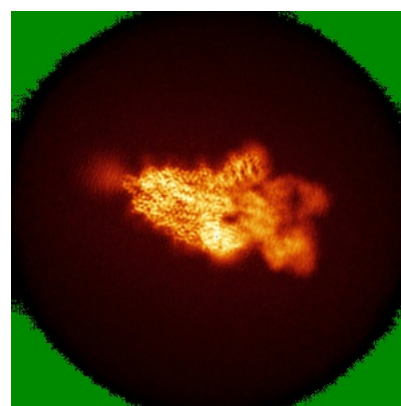
6.4.1 Primary map



X



Y



Z

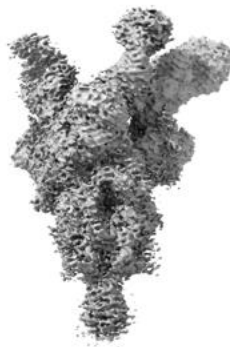
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

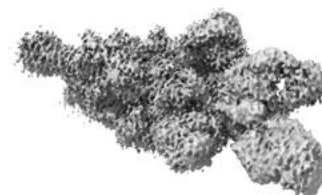
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.00503. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

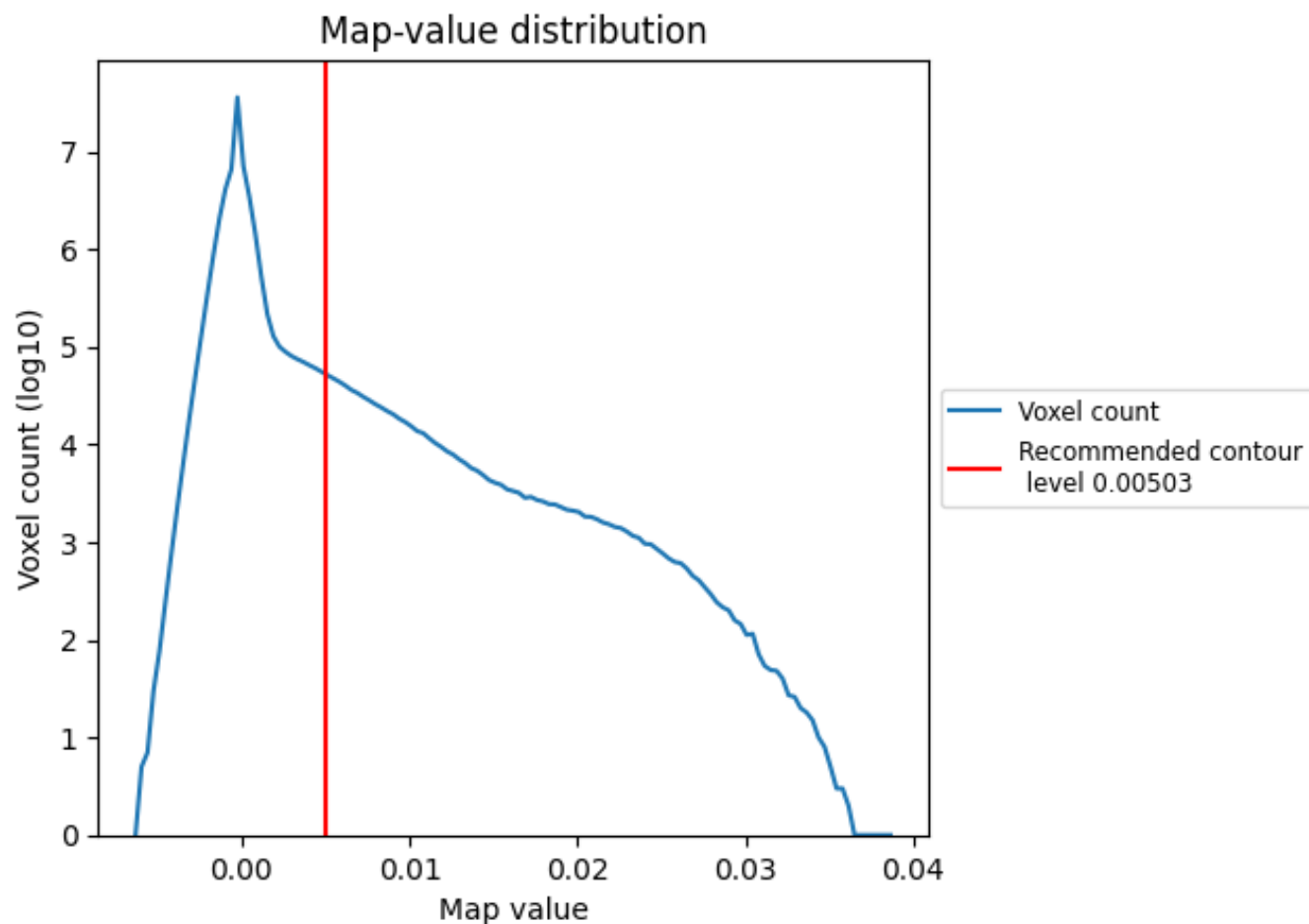
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

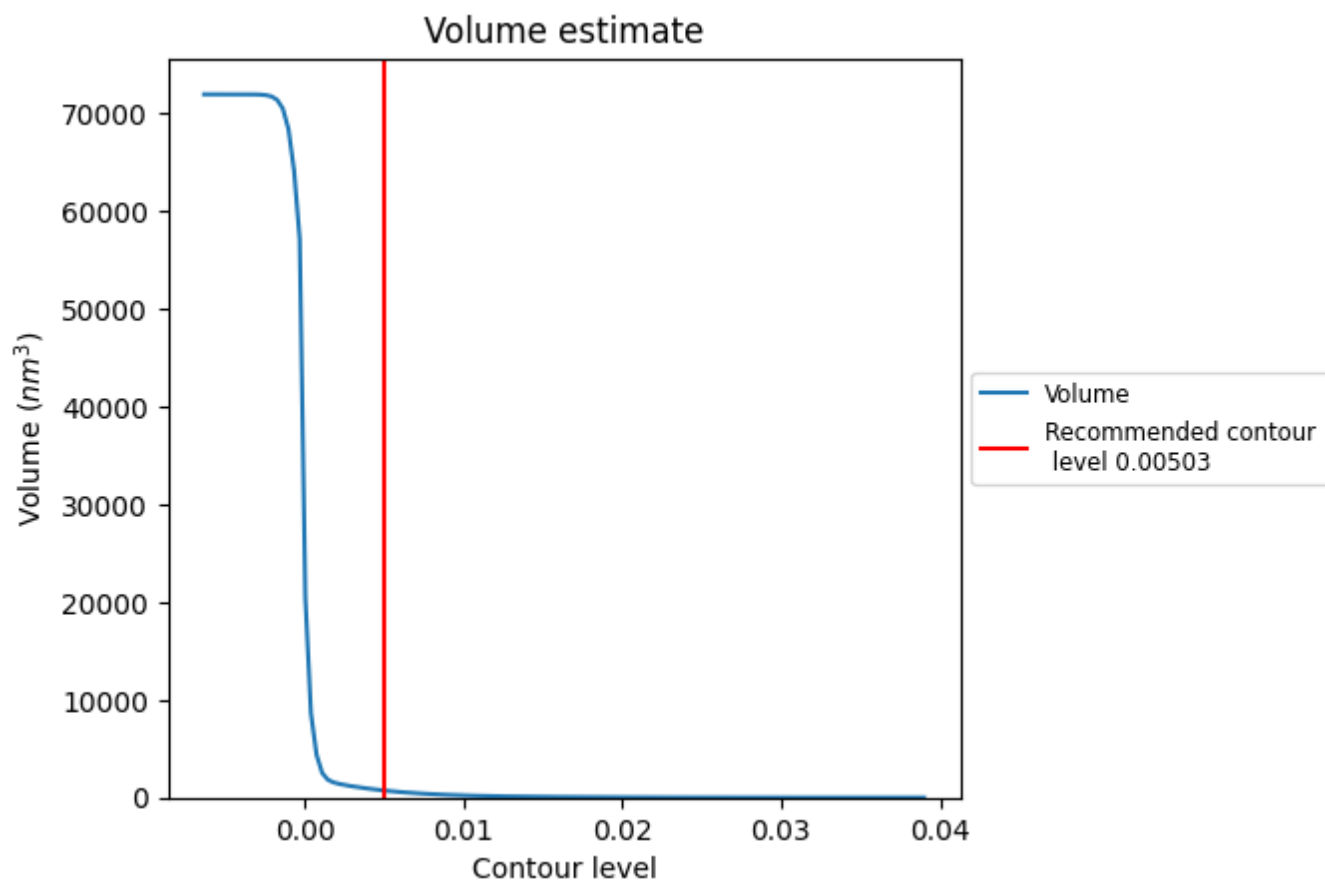
This section contains the results of statistical analysis of the map.

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.

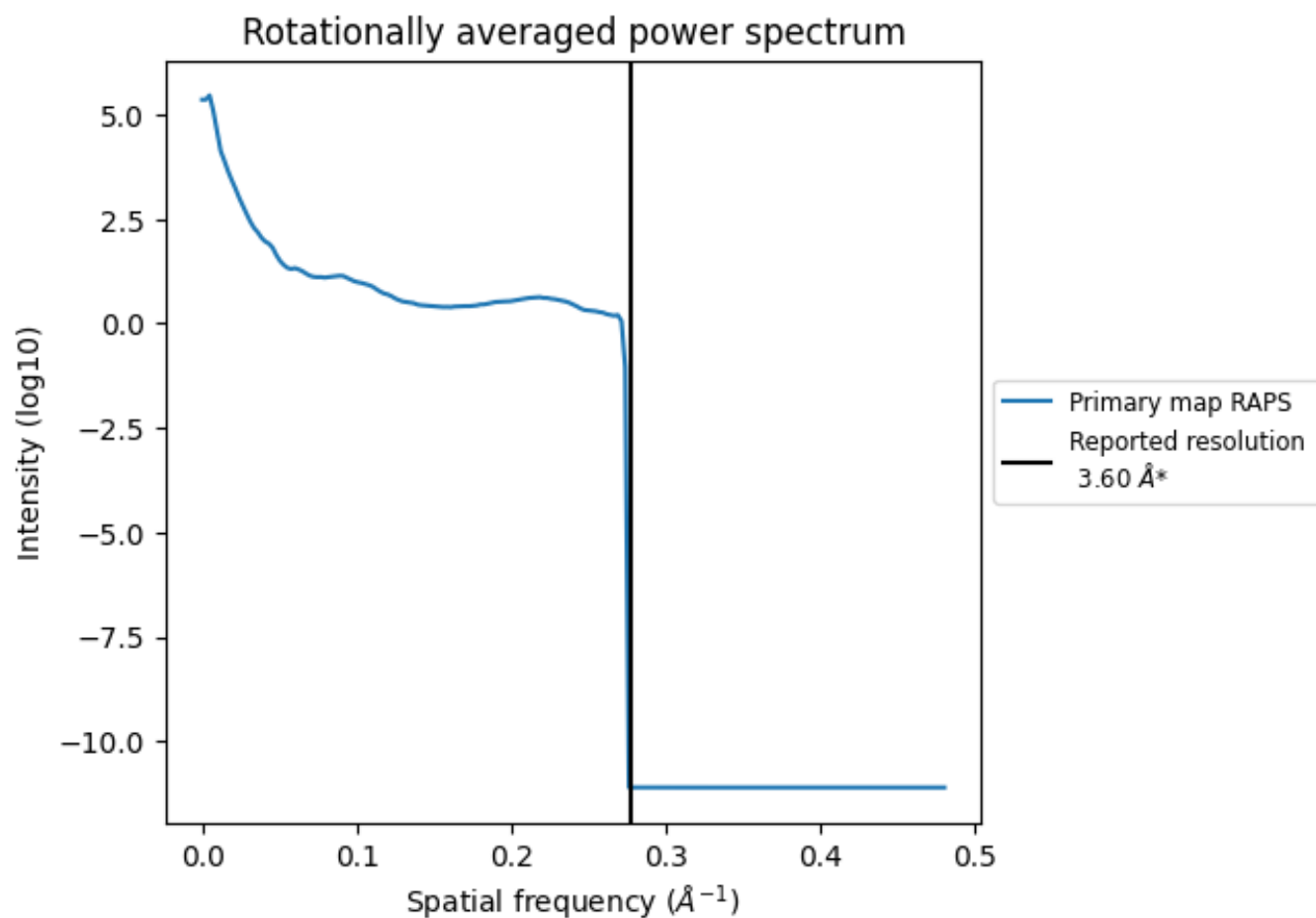
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 720 nm^3 ; this corresponds to an approximate mass of 650 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 0.278 $\text{\AA}^{-1}$

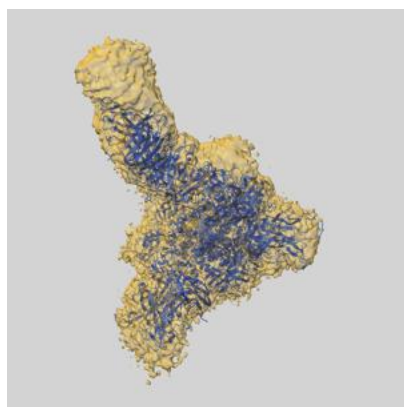
8 Fourier-Shell correlation ⓘ

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

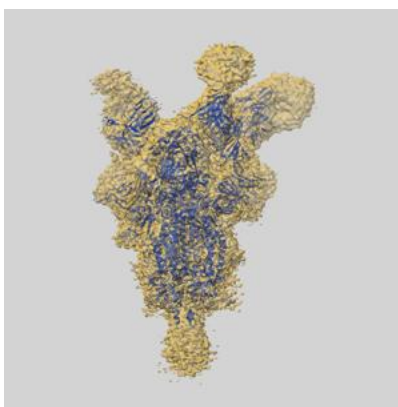
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-30483 and PDB model 7CWM. Per-residue inclusion information can be found in section [3](#) on page [8](#).

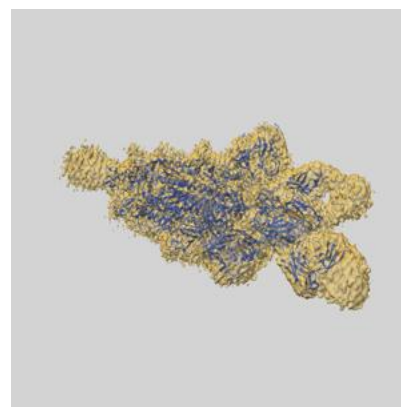
9.1 Map-model overlay [i](#)



X



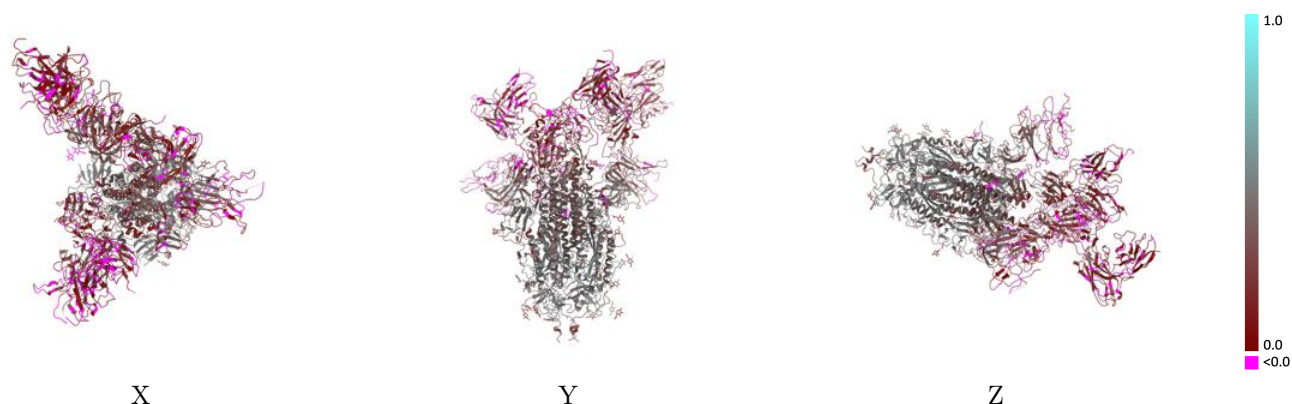
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.00503 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](#)

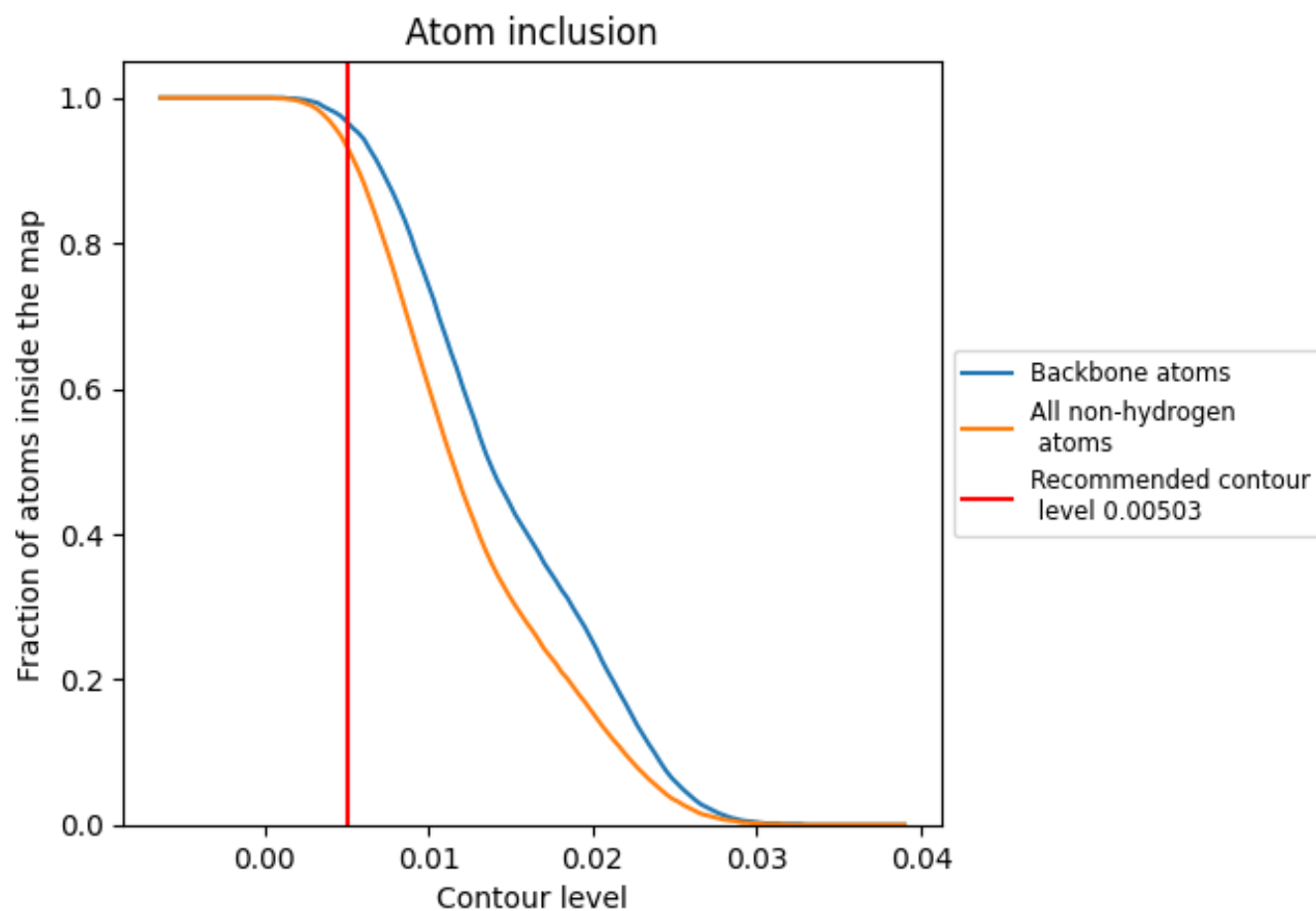


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 93% 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 (0.00503) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9330	 0.2770
A	 0.9470	 0.3140
B	 0.9530	 0.3060
C	 0.9580	 0.3140
D	 0.8570	 0.2490
E	 0.9640	 0.4540
F	 0.8930	 0.2920
G	 0.9680	 0.1480
H	 0.9520	 0.1490
I	 0.7110	 0.0700
J	 0.9590	 0.1110
K	 0.5690	 0.0460
L	 0.9120	 0.1390
M	 0.8930	 0.2800
N	 0.8570	 0.2210
O	 0.9290	 0.4120
P	 0.8930	 0.2350
Q	 0.9290	 0.4380
R	 0.8210	 0.2920
S	 0.3210	 -0.0890
T	 0.8570	 0.4200
U	 0.8570	 0.2920
V	 0.8570	 0.3130
W	 0.6790	 0.2690

