



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 03:19 AM UTC

PDB ID : 6CRZ / pdb_00006crz
EMDB ID : EMD-7577
Title : SARS Spike Glycoprotein, Trypsin-cleaved, Stabilized variant, C3 symmetry
Authors : Kirchdoerfer, R.N.; Wang, N.; Pallesen, J.; Turner, H.L.; Cottrell, C.A.;
McLellan, J.S.; Ward, A.B.
Deposited on : 2018-03-19
Resolution : 3.30 Å (reported)
Based on initial models : 2AJF, 5X4S, 5I08

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

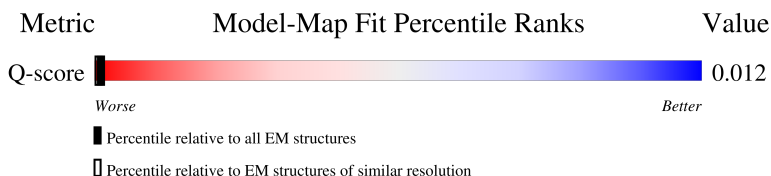
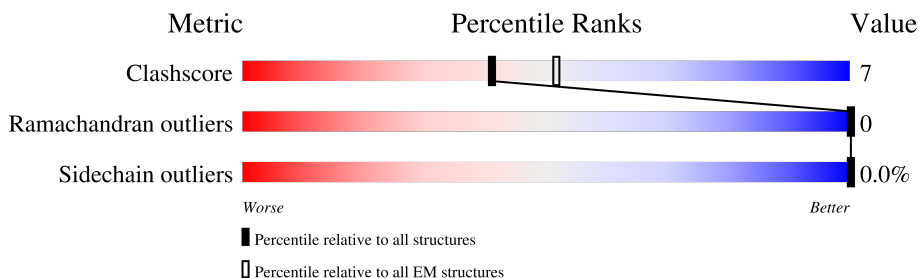
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 3.30 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	15087 (2.80 - 3.80)

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	1215	79% 71% 17% 12%
1	B	1215	74% 73% 15% 12%
1	C	1215	75% 71% 17% 12%
2	D	3	100% 67% 33%

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Mol	Chain	Length	Quality of chain
2	F	3	100% 67%33%
2	J	3	100% 100%
2	K	3	100% 67%33%
2	M	3	100% 100%
2	N	3	67% 67%33%
2	R	3	100% 33%67%
2	T	3	100% 67%33%
2	U	3	100% 67%33%
3	E	4	100% 75%25%
4	G	2	100% 50%50%
4	H	2	100% 100%
4	I	2	100% 100%
4	L	2	100% 50%50%
4	O	2	100% 50%50%
4	P	2	100% 100%
4	Q	2	100% 100%
4	V	2	100% 100%
5	S	4	100% 50%50%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 25909 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Spike glycoprotein,Fibritin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1068	Total	C	N	O	S	0	0
			8339	5328	1379	1586	46		
1	B	1068	Total	C	N	O	S	0	0
			8342	5331	1379	1586	46		
1	C	1069	Total	C	N	O	S	0	0
			8343	5329	1380	1588	46		

There are 42 discrepancies between the modelled and reference sequences:

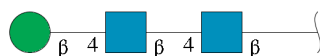
Chain	Residue	Modelled	Actual	Comment	Reference
A	577	ALA	SER	conflict	UNP P59594
A	968	PRO	LYS	engineered mutation	UNP P59594
A	969	PRO	VAL	engineered mutation	UNP P59594
A	1191	GLY	-	linker	UNP P59594
A	1192	SER	ALA	linker	UNP D9IEJ2
A	1220	GLY	-	expression tag	UNP D9IEJ2
A	1221	ARG	-	expression tag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

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

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



Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	3	Total	C	N	O	0	0
			39	22	2	15		
2	F	3	Total	C	N	O	0	0
			39	22	2	15		
2	J	3	Total	C	N	O	0	0
			39	22	2	15		
2	K	3	Total	C	N	O	0	0
			39	22	2	15		
2	M	3	Total	C	N	O	0	0
			39	22	2	15		
2	N	3	Total	C	N	O	0	0
			39	22	2	15		
2	R	3	Total	C	N	O	0	0
			39	22	2	15		

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Mol	Chain	Residues	Atoms				AltConf	Trace
2	T	3	Total	C	N	O	0	0
			39	22	2	15		
2	U	3	Total	C	N	O	0	0
			39	22	2	15		

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



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

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



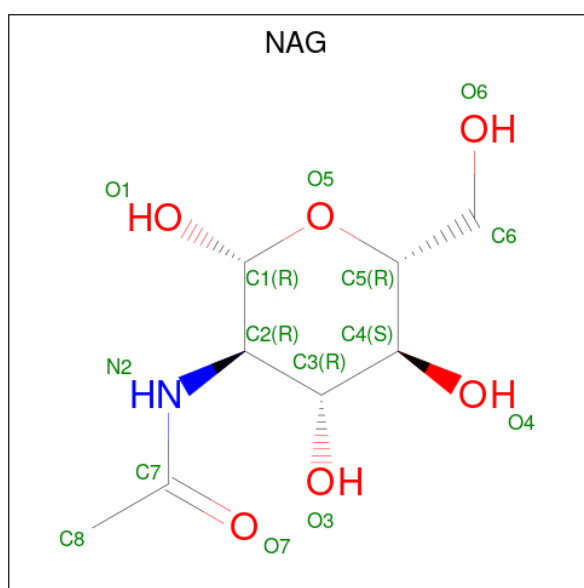
Mol	Chain	Residues	Atoms				AltConf	Trace
4	G	2	Total	C	N	O	0	0
			28	16	2	10		
4	H	2	Total	C	N	O	0	0
			28	16	2	10		
4	I	2	Total	C	N	O	0	0
			28	16	2	10		
4	L	2	Total	C	N	O	0	0
			28	16	2	10		
4	O	2	Total	C	N	O	0	0
			28	16	2	10		
4	P	2	Total	C	N	O	0	0
			28	16	2	10		
4	Q	2	Total	C	N	O	0	0
			28	16	2	10		
4	V	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

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



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

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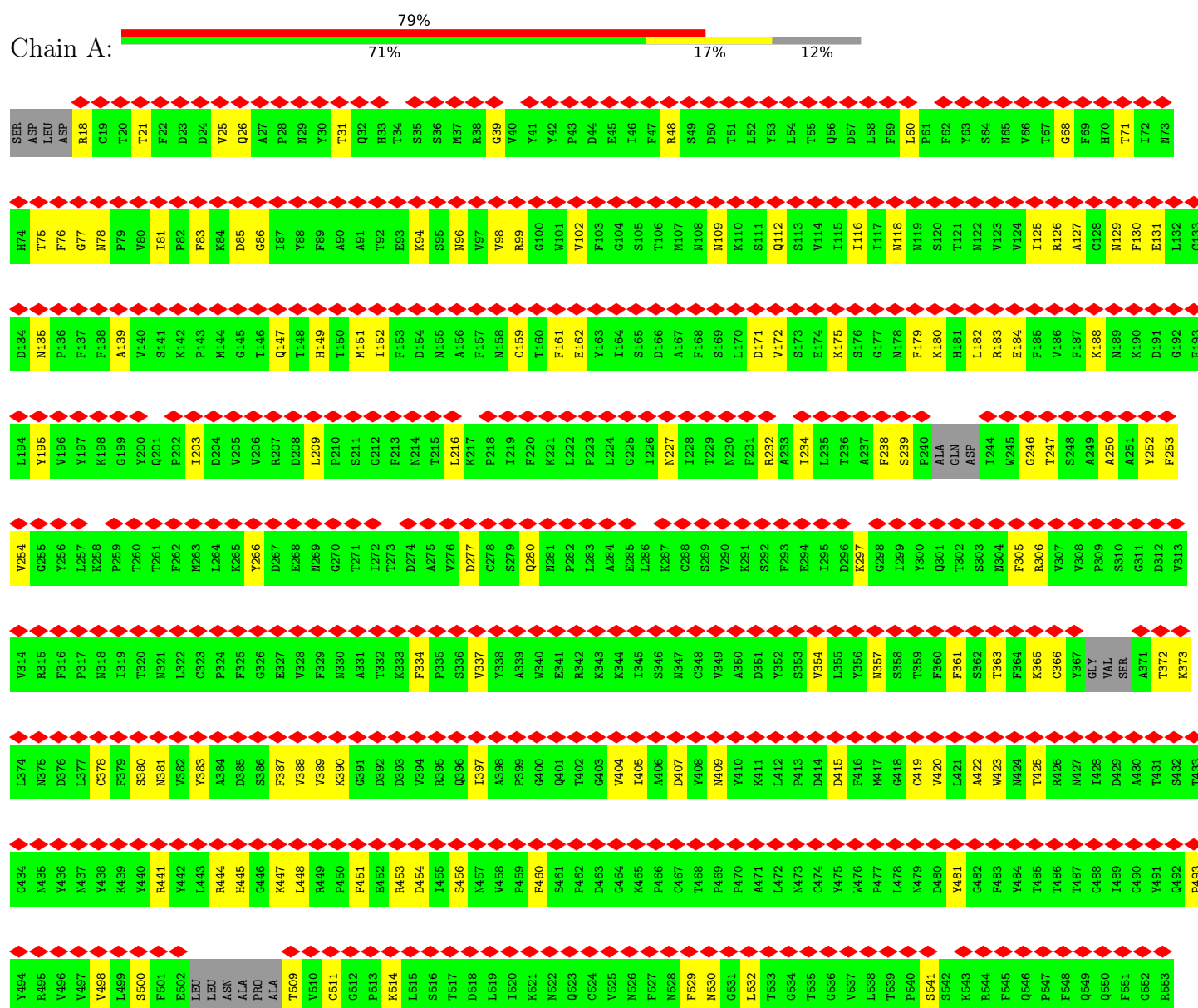
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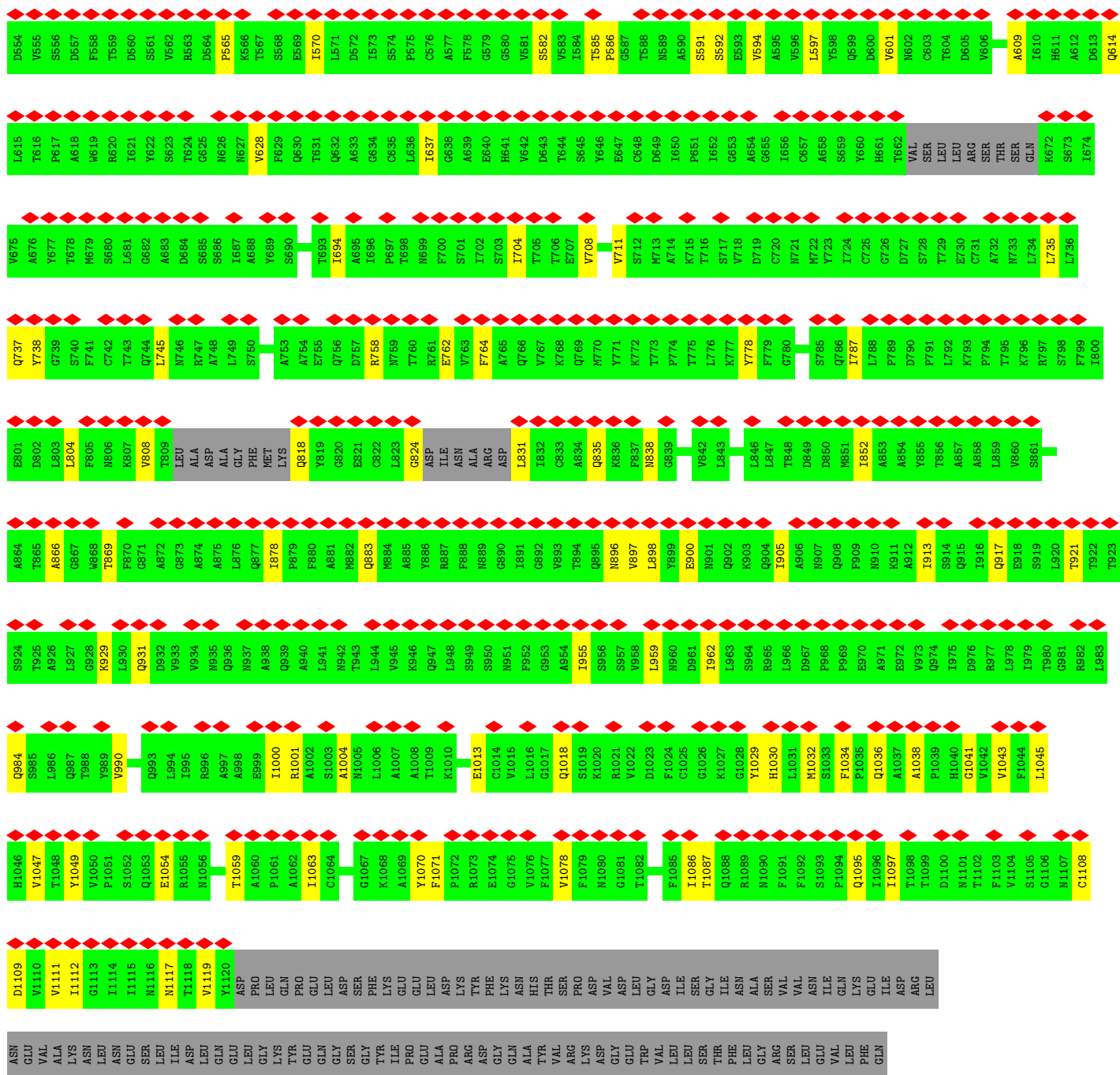
Mol	Chain	Residues	Atoms				AltConf
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	

3 Residue-property plots

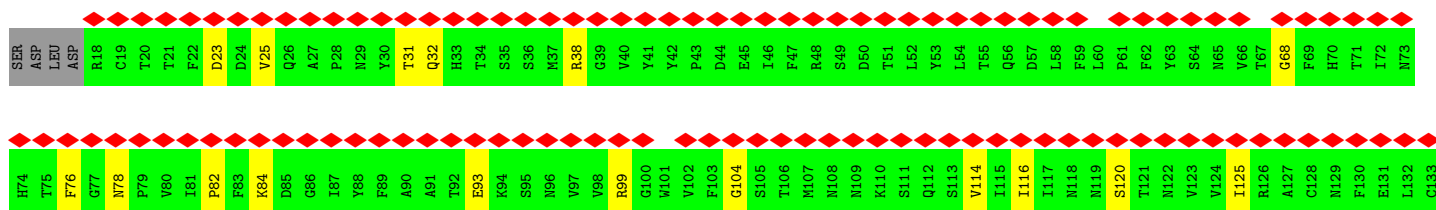
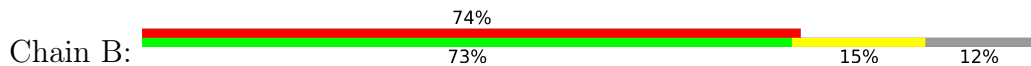
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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,Fibrin



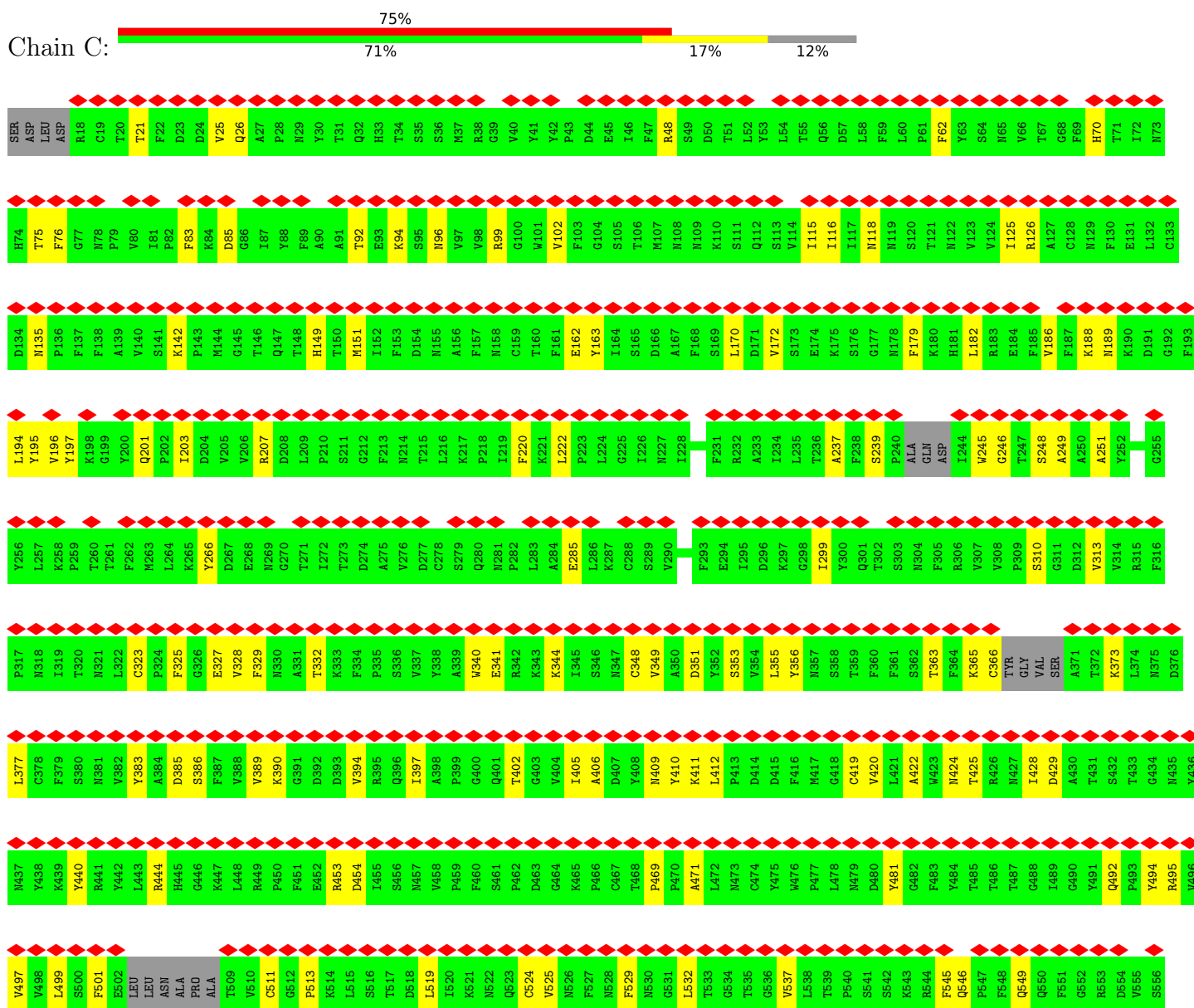


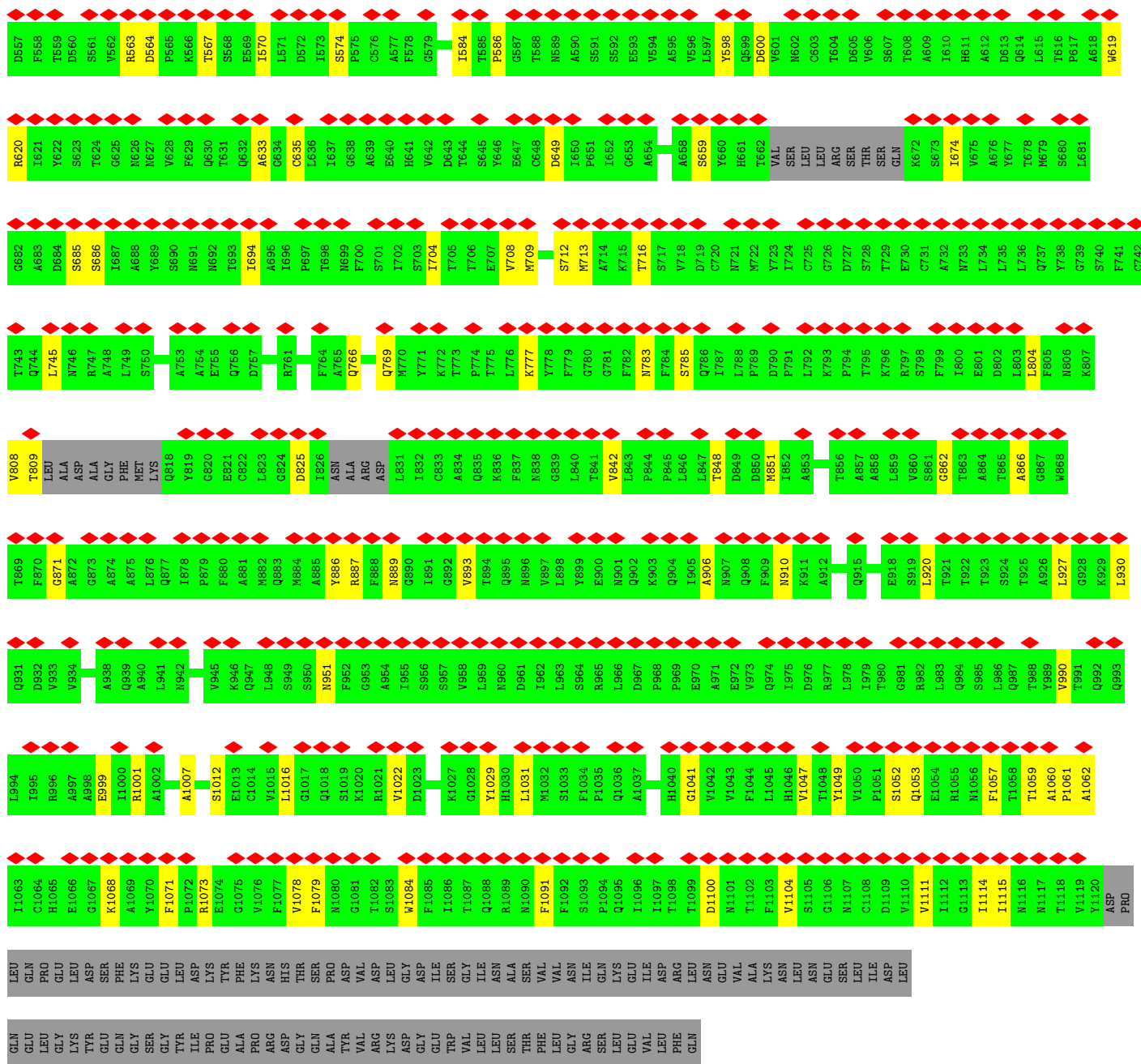
● Molecule 1: Spike glycoprotein, Fibritin



T943	L944	V945	K946	Q947	L948	S949	S950	N951	F952	G953	A954	Y955	S956	S957	V958	L959	N960	D961	L962	L963	S964	R965	L966	D967	P968	P969	E970	A971	E972	V973	Q974	I975	D976	R977	L978	T979	T980	G981	N982	Q984	S985	L986	Q987	T988	Q989	Q990	L991	A992	E993	I994	R995	A996	E997	S998	E999	I1000	R1001	A1008	T1009			
F870	G871	G872	G873	A874	A875	L876	Q877	L878	P879	F880	A881	M882	Q883	N884	A885	Y886	R887	F888	N889	G890	I891	G892	V893	T894	V897	L898	Y899	E900	N901	Q902	I905	A906	N910	K911	L912	T913	S914	Q915	T922	T923	S924	T925	A926	K929	L930	Q931	D932	Q936	N937	A938	Q939	A940										
C742	T743	A744	L745	N746	R747	A748	L749	S750	G751	A754	E755	Q756	D757	R758	R761	E762	V763	F764	A765	Q766	V767	K768	Q769	Y770	Y771	K772	T773	P774	T775	L776	K777	F778	F779	F782	N783	F784	I787	L788	P789	D790	F791	L792	K793	F794	T795	K796	R797	S798	F799	I800	E801	L804	F805	N806								
K807	T808	LEU	T809	ALA	ASP	ALA	GLY	PHE	MET	LYS	Q818	Y819	G820	E821	C822	L823	GLY	ASP	ILE	ASN	ALA	ARG	ASP	L831	I832	C833	K836	F837	N838	G839	N840	T841	V842	L843	R844	P845	L846	L847	T848	D849	D850	M851	A854	Y855	A858	L859	V860	S861	T862	T863	A864	T865	A866	G867	T868							
V870	G871	G872	G873	A874	A875	L876	Q877	L878	P879	F880	A881	M882	Q883	N884	A885	Y886	R887	F888	N889	G890	I891	G892	V893	T894	V897	L898	Y899	E900	N901	Q902	I905	A906	N910	K911	L912	T913	S914	Q915	T922	T923	S924	T925	A926	K929	L930	Q931	D932	Q936	N937	A938	Q939	A940										
L194	Y195	V196	Y197	K198	G199	Y200	Q201	P202	I203	D204	V205	V206	R207	D208	L209	P210	S211	G212	F213	N214	T215	L216	A217	P218	I219	F220	K221	L222	P223	L224	G225	I226	N227	I228	S229	N230	F231	R232	V233	I234	L235	T236	A237	F238	I239	S239	P240	ALA	GLM	ASP	I244	W245	G246	R306	V307	S248	GLY	A249	A250	G311	Y252	F253
V254	Q255	Y256	L257	K258	P259	T260	T261	F262	M263	L264	K265	Y266	D267	E268	N269	G270	T271	T272	T273	D274	A275	V276	D277	C278	S279	Q280	N281	P282	L283	A284	E285	L286	K287	C288	S289	V290	K291	S292	F293	E294	I295	D296	K297	G298	I299	S299	Y300	Q301	T302	S303	N304	F305	K306	V308	P309	S310	G311	D312	V313			
V314	R315	F316	P317	N318	I319	T320	N321	L322	C323	P324	G325	G326	E327	V328	F329	N330	T332	D333	F334	P335	S336	V337	Y338	A339	U340	E341	R342	K343	K344	I345	S346	N347	C348	V349	A350	D351	Y352	S353	V354	L355	Y356	N357	S358	T359	F360	G361	S362	T363	F364	K365	C366	Y367	GLY	VAL	SER	A371	T372	K373				
L374	N375	D376	L377	C378	F379	S380	N381	Y382	Y383	A384	D385	S386	F387	V388	V389	K390	G391	D392	D393	V394	R395	Q396	I397	Y398	S399	G400	Q401	T402	G403	Y404	I405	A406	D407	Y408	N409	Y410	K411	L412	P413	D414	D415	F416	N417	G418	C419	Y420	L421	A422	N423	N424	T425	R426	N427	I428	D429	A430	T431	S432	T433			
G434	N435	Y436	N437	Y438	K439	Y440	R441	Y442	L443	R444	H445	G446	K447	L448	R449	P450	F451	E452	R453	D454	L455	S456	N457	Y458	P459	F460	S461	P462	D463	G464	K465	P466	C467	T468	P469	A470	L471	L472	N473	C474	Y475	N476	P477	L478	N479	D480	Y481	G482	F483	Y484	T485	T486	T487	G488	T489	G490	Q491	P492				
Y494	R495	Y496	V497	V498	L499	S500	F501	E502	LEU	LEU	ASN	ALA	PRO	T509	V510	C511	G512	P513	K514	L515	S516	T517	D518	L519	I520	K521	N522	Q523	C524	V525	N526	F527	N528	P529	N530	G531	L532	T533	G534	G535	V537	L538	T539	P540	S541	S542	K543	R544	F545	Q546	P547	Q548	Q550	F551	G552	R553						
D554	V555	S556	D557	F558	T559	D560	S561	V562	R563	D564	P565	K566	T567	S568	E569	I570	L571	D572	L573	S574	P575	C576	A577	F578	G579	G580	V581	S582	V583	L584	T585	P586	N589	A590	S591	S592	E593	V594	A595	V596	L597	Y598	Q599	D600	V601	N602	C603	T604	D605	V606	S607	T608	A609	T610	H611	A612	D613	Q614				
L615	T616	P617	A618	N619	R620	L621	Y622	S623	T624	G625	N626	N627	V628	F629	D630	T631	Q632	A633	G634	L635	L636	L637	H641	V642	D643	T644	S645	Y646	E647	C648	D649	I650	P651	L652	G653	A654	G655	L656	C657	A658	S659	V660	H661	T662	V663	SER	LEU	LEU	ARG	THR	SER	GLN	K672	S673	L674	V675	A676					
Y677	T678	N679	S680	L681	G682	A683	D684	S685	S686	L687	A688	Y689	S690	N691	N692	T693	T694	A695	T696	P697	T698	N699	F700	S701	I702	E707	P710	V711	S712	N713	A714	K715	T716	S717	V718	G719	C720	N721	I724	C725	G726	D727	S728	T729	E730	C731	A732	N733	L734	L735	L736	Q737	Y738	G739	S740	F741						

- Molecule 1: Spike glycoprotein, Fibrin







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



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



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



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



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



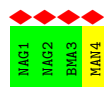
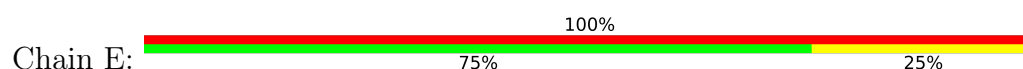
- Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



- 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



- 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 5: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	162177	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 ($e^-/\text{\AA}^2$)	65	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	29000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.374	Depositor
Minimum map value	-0.191	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.069	Depositor
Map size (Å)	329.59998, 329.59998, 329.59998	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.03, 1.03, 1.03	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.30	0/8538	0.58	0/11617
1	B	0.29	0/8541	0.59	2/11622 (0.0%)
1	C	0.30	1/8541 (0.0%)	0.57	0/11621
All	All	0.30	1/25620 (0.0%)	0.58	2/34860 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	3
All	All	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	142	LYS	C-N	5.26	1.39	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1070	TYR	CA-C-N	10.44	136.12	121.61
1	B	1070	TYR	C-N-CA	10.44	136.12	121.61

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	85	ASP	Peptide
1	B	1080	ASN	Peptide
1	C	207	ARG	Peptide
1	C	525	VAL	Peptide
1	C	85	ASP	Peptide

5.2 Too-close contacts

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	8339	0	8083	135	0
1	B	8342	0	8088	113	0
1	C	8343	0	8086	122	0
2	D	39	0	34	0	0
2	F	39	0	34	0	0
2	J	39	0	34	0	0
2	K	39	0	34	0	0
2	M	39	0	34	0	0
2	N	39	0	34	0	0
2	R	39	0	34	0	0
2	T	39	0	34	0	0
2	U	39	0	34	0	0
3	E	50	0	43	0	0
4	G	28	0	25	1	0
4	H	28	0	25	0	0
4	I	28	0	25	0	0
4	L	28	0	25	0	0
4	O	28	0	25	0	0
4	P	28	0	25	0	0
4	Q	28	0	25	0	0
4	V	28	0	25	0	0
5	S	50	0	43	0	0
6	A	56	0	52	1	0
6	B	70	0	65	1	0
6	C	84	0	78	0	0
All	All	25909	0	25044	350	0

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

All (350) 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:405:ILE:HA	1:C:409:ASN:HB2	1.74	0.70
1:A:1034:PHE:HB2	1:A:1045:LEU:HB2	1.77	0.67
1:C:444:ARG:HE	1:C:454:ASP:HB2	1.60	0.67
1:A:188:LYS:HB3	1:A:195:TYR:HB2	1.76	0.66
1:A:227:ASN:HB2	1:C:444:ARG:HH22	1.61	0.66
1:A:99:ARG:HH22	1:A:172:VAL:HA	1.60	0.66
1:B:337:VAL:HG22	1:B:387:PHE:HB2	1.78	0.65
1:A:334:PHE:HB2	1:A:388:VAL:HG23	1.78	0.65
1:B:1018:GLN:NE2	1:B:1030:HIS:O	2.29	0.65
1:C:285:GLU:OE1	1:C:619:TRP:NE1	2.30	0.65
1:C:341:GLU:HB3	1:C:386:SER:HB3	1.79	0.65
1:B:563:ARG:HA	1:B:570:ILE:HA	1.80	0.63
1:A:704:ILE:HG12	1:A:1047:VAL:HG22	1.79	0.63
1:B:93:GLU:HG3	1:B:183:ARG:HH21	1.64	0.63
1:C:366:CYS:SG	1:C:373:LYS:NZ	2.72	0.63
1:A:441:ARG:NH2	1:A:456:SER:O	2.32	0.62
1:A:99:ARG:HB3	1:A:118:ASN:HB3	1.80	0.62
1:A:99:ARG:HH12	1:A:172:VAL:HG12	1.65	0.62
1:A:126:ARG:NH2	1:A:159:CYS:SG	2.73	0.62
1:C:1068:LYS:HB3	1:C:1104:VAL:HG21	1.82	0.61
1:C:349:VAL:HG12	1:C:511:CYS:H	1.65	0.61
1:B:1034:PHE:HB2	1:B:1045:LEU:HB2	1.83	0.61
1:B:707:GLU:OE2	1:B:1010:LYS:NZ	2.33	0.61
1:C:355:LEU:HD22	1:C:419:CYS:HB2	1.82	0.61
1:C:188:LYS:HB2	1:C:195:TYR:HB2	1.81	0.61
1:C:325:PHE:HB3	1:C:328:VAL:HB	1.83	0.60
1:B:993:GLN:OE1	1:B:996:ARG:NH1	2.35	0.60
1:C:323:CYS:N	1:C:348:CYS:SG	2.74	0.60
1:A:26:GLN:HB2	1:A:75:THR:HA	1.84	0.60
1:A:18:ARG:HB2	1:A:151:MET:HG2	1.82	0.60
1:A:1036:GLN:HB2	1:A:1043:VAL:HB	1.83	0.60
1:B:142:LYS:HE2	1:B:240:PRO:HD3	1.83	0.60
1:A:541:SER:HB3	1:A:570:ILE:HG22	1.84	0.59
1:A:898:LEU:HD23	1:A:905:ILE:HD13	1.84	0.59
1:C:355:LEU:HD11	1:C:499:LEU:HD22	1.84	0.59
1:A:99:ARG:NH2	1:A:171:ASP:O	2.35	0.59
1:B:377:LEU:O	1:B:512:GLY:N	2.35	0.59
1:A:415:ASP:O	1:B:965:ARG:NH2	2.36	0.59
1:A:1001:ARG:NH2	1:C:999:GLU:OE2	2.36	0.59
1:B:716:THR:HG22	1:B:842:VAL:HG22	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:511:CYS:HB3	1:A:514:LYS:HD2	1.83	0.58
1:A:708:VAL:HG12	1:A:1043:VAL:HG22	1.86	0.58
1:C:716:THR:HG22	1:C:842:VAL:HG22	1.85	0.58
1:B:138:PHE:HB2	1:B:236:THR:HA	1.86	0.58
1:B:323:CYS:N	1:B:348:CYS:SG	2.77	0.58
1:C:70:HIS:HA	1:C:251:ALA:HA	1.85	0.58
1:B:152:ILE:HD13	1:B:234:ILE:HD13	1.85	0.58
1:C:186:VAL:HB	1:C:197:TYR:HB2	1.86	0.57
1:C:425:THR:HG21	1:C:495:ARG:HE	1.67	0.57
1:A:1086:ILE:HB	1:A:1095:GLN:HB2	1.86	0.57
1:B:550:GLN:OE1	1:B:563:ARG:NH2	2.37	0.57
1:A:1078:VAL:HG21	1:A:1087:THR:HG22	1.86	0.57
1:B:38:ARG:NH1	1:B:184:GLU:OE2	2.38	0.57
1:B:388:VAL:HG22	1:B:495:ARG:HG2	1.86	0.56
1:A:126:ARG:HB2	1:A:130:PHE:HZ	1.69	0.56
1:A:529:PHE:HB2	1:A:532:LEU:HB3	1.87	0.56
1:C:402:THR:HA	1:C:406:ALA:HB3	1.87	0.56
1:C:862:GLY:O	1:C:866:ALA:N	2.38	0.56
1:A:628:VAL:HG22	1:A:637:ILE:HG12	1.88	0.56
1:A:1038:ALA:HB2	1:A:1043:VAL:HG23	1.88	0.56
1:C:389:VAL:HG11	1:C:397:ILE:HD11	1.87	0.56
1:A:78:ASN:O	1:A:232:ARG:NH1	2.38	0.56
1:B:416:PHE:HB3	1:B:502:GLU:HB2	1.87	0.56
1:A:239:SER:HB3	1:A:246:GLY:H	1.70	0.56
1:A:354:VAL:HA	1:A:357:ASN:HB2	1.87	0.56
1:A:984:GLN:OE1	1:B:984:GLN:NE2	2.34	0.56
1:B:277:ASP:OD2	1:B:280:GLN:NE2	2.35	0.56
1:C:529:PHE:HB2	1:C:532:LEU:HB2	1.87	0.56
1:C:563:ARG:HA	1:C:570:ILE:HA	1.87	0.55
1:B:99:ARG:HH22	1:B:120:SER:HA	1.71	0.55
1:B:206:VAL:HG12	1:B:207:ARG:HG3	1.88	0.55
1:C:194:LEU:HD23	1:C:222:LEU:HD12	1.88	0.55
1:C:777:LYS:HD3	1:C:785:SER:HA	1.88	0.55
1:A:277:ASP:HB3	1:A:280:GLN:HG2	1.88	0.55
1:A:453:ARG:NH2	1:B:158:ASN:O	2.39	0.55
1:B:409:ASN:HD21	1:B:440:TYR:HB2	1.72	0.55
1:C:92:THR:HB	1:C:251:ALA:HB3	1.88	0.55
1:C:125:ILE:HB	1:C:163:TYR:HB3	1.89	0.55
1:A:824:GLY:HA3	1:A:831:LEU:HA	1.89	0.55
1:C:239:SER:HB3	1:C:246:GLY:H	1.71	0.55
1:B:383:TYR:HB2	1:B:500:SER:HB3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:351:ASP:HB3	1:C:513:PRO:HD3	1.88	0.54
1:C:96:ASN:O	1:C:99:ARG:NH1	2.41	0.54
1:A:404:VAL:O	1:A:409:ASN:ND2	2.41	0.54
1:A:1029:TYR:HB2	1:A:1049:TYR:HB3	1.90	0.54
1:C:409:ASN:HD21	1:C:440:TYR:HB2	1.72	0.54
1:A:381:ASN:OD1	1:A:509:THR:N	2.41	0.54
1:B:999:GLU:OE2	1:C:1001:ARG:NH2	2.40	0.54
1:A:109:ASN:O	1:A:129:ASN:ND2	2.41	0.54
1:B:953:GLY:O	1:B:977:ARG:NH1	2.41	0.54
1:C:745:LEU:HD22	1:C:990:VAL:HG21	1.89	0.54
1:A:116:ILE:HA	1:A:125:ILE:HG12	1.90	0.53
1:A:149:HIS:HB3	1:A:151:MET:HG3	1.90	0.53
1:C:99:ARG:HB3	1:C:118:ASN:HB3	1.90	0.53
1:C:340:TRP:HE1	1:C:453:ARG:HB3	1.73	0.53
1:A:383:TYR:HB2	1:A:500:SER:HB3	1.89	0.53
1:B:78:ASN:ND2	1:B:136:PRO:O	2.42	0.53
1:A:25:VAL:HG23	1:A:76:PHE:HB2	1.89	0.53
1:C:906:ALA:O	1:C:910:ASN:ND2	2.42	0.53
1:A:758:ARG:NH1	1:A:762:GLU:OE2	2.42	0.53
1:C:1029:TYR:HB2	1:C:1049:TYR:HB3	1.91	0.53
1:B:419:CYS:H	1:B:499:LEU:HB2	1.74	0.53
1:C:353:SER:HA	1:C:356:TYR:HB3	1.90	0.53
1:A:737:GLN:OE1	1:C:951:ASN:ND2	2.39	0.53
1:A:955:ILE:HG23	1:A:962:ILE:HG12	1.91	0.53
1:A:182:LEU:HB2	1:A:203:ILE:HD13	1.91	0.53
1:C:327:GLU:HG2	1:C:328:VAL:HG23	1.90	0.53
1:A:126:ARG:HG2	1:A:162:GLU:HG3	1.91	0.53
1:B:1068:LYS:HA	1:B:1107:ASN:HA	1.89	0.53
1:C:783:ASN:N	1:C:910:ASN:OD1	2.42	0.52
1:A:139:ALA:HB3	1:A:149:HIS:HB2	1.91	0.52
1:B:1063:ILE:HD11	1:B:1097:ILE:HD13	1.91	0.52
1:A:896:ASN:O	1:A:900:GLU:N	2.38	0.52
1:A:71:THR:HB	1:A:250:ALA:HB3	1.92	0.52
1:A:425:THR:OG1	1:A:493:PRO:O	2.27	0.52
1:A:778:TYR:HB3	4:G:1:NAG:H81	1.90	0.52
1:A:337:VAL:HG11	1:A:405:ILE:HD12	1.92	0.52
1:B:887:ARG:NH1	1:B:1031:LEU:O	2.43	0.52
1:C:299:ILE:HG12	1:C:584:ILE:HG12	1.90	0.52
1:A:407:ASP:OD2	1:A:447:LYS:NZ	2.39	0.52
1:C:373:LYS:NZ	1:C:419:CYS:SG	2.79	0.52
1:A:378:CYS:HA	1:A:511:CYS:HA	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:642:VAL:HB	1:B:677:TYR:HB3	1.91	0.52
1:B:690:SER:OG	1:B:692:ASN:OD1	2.27	0.52
1:B:398:ALA:HB3	1:B:401:GLN:HG3	1.91	0.51
1:A:1030:HIS:NE2	1:A:1032:MET:O	2.44	0.51
1:B:883:GLN:HE21	1:B:887:ARG:HE	1.58	0.51
1:B:1080:ASN:HB2	1:B:1085:PHE:HE1	1.75	0.51
1:A:175:LYS:HZ2	1:A:180:LYS:HD2	1.75	0.51
1:A:390:LYS:HD3	1:A:481:TYR:HB3	1.92	0.51
1:B:32:GLN:HG3	6:B:1301:NAG:H3	1.92	0.51
1:B:429:ASP:OD1	1:B:495:ARG:NH2	2.42	0.51
1:A:1112:ILE:HG23	6:A:1310:NAG:H62	1.93	0.51
1:B:99:ARG:HB2	1:B:138:PHE:HE2	1.76	0.51
1:A:380:SER:OG	1:A:381:ASN:N	2.44	0.51
1:A:297:LYS:HG3	1:A:586:PRO:HA	1.93	0.50
1:C:149:HIS:HB3	1:C:151:MET:HE2	1.91	0.50
1:A:1086:ILE:HG12	1:A:1097:ILE:HG12	1.94	0.50
1:A:94:LYS:HB3	1:A:179:PHE:HA	1.92	0.50
1:B:282:PRO:HB2	1:B:594:VAL:HG21	1.92	0.50
1:C:930:LEU:HD21	1:C:1041:GLY:HA3	1.93	0.50
1:B:822:CYS:HA	1:B:833:CYS:HA	1.92	0.50
1:C:340:TRP:NE1	1:C:453:ARG:HB3	2.27	0.50
1:A:405:ILE:HA	1:A:409:ASN:HB2	1.94	0.50
1:B:459:PRO:HD2	1:B:469:PRO:HB2	1.94	0.50
1:B:762:GLU:O	1:B:766:GLN:NE2	2.39	0.50
1:C:62:PHE:O	1:C:620:ARG:NH2	2.45	0.50
1:A:184:GLU:HG2	1:A:216:LEU:HD21	1.94	0.50
1:A:366:CYS:HA	1:A:419:CYS:HA	1.93	0.50
1:A:818:GLN:O	1:A:838:ASN:ND2	2.44	0.50
1:A:337:VAL:HG22	1:A:387:PHE:HB2	1.92	0.49
1:A:711:VAL:HG12	1:A:1004:ALA:HA	1.93	0.49
1:A:764:PHE:HE2	1:A:852:ILE:HG23	1.78	0.49
1:B:405:ILE:HA	1:B:409:ASN:HB2	1.93	0.49
1:C:1057:PHE:HB3	1:C:1078:VAL:HB	1.94	0.49
1:A:112:GLN:HE22	1:C:453:ARG:HH21	1.60	0.49
1:B:316:PHE:HB3	1:B:513:PRO:HB2	1.94	0.49
1:A:99:ARG:NH1	1:A:147:GLN:OE1	2.46	0.49
1:B:422:ALA:HB1	1:B:494:TYR:HB3	1.94	0.49
1:C:804:LEU:HD22	1:C:927:LEU:HD11	1.94	0.49
1:A:609:ALA:HB1	1:A:614:GLN:HB2	1.93	0.49
1:B:334:PHE:HB2	1:B:388:VAL:HG23	1.94	0.49
1:B:389:VAL:HG11	1:B:397:ILE:HD11	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1013:GLU:OE1	1:C:1022:VAL:N	2.46	0.49
1:C:886:TYR:HA	1:C:889:ASN:HD22	1.78	0.49
1:A:878:ILE:HG13	1:C:694:ILE:HG12	1.95	0.48
1:B:807:LYS:HD2	1:B:924:SER:HB2	1.95	0.48
1:B:591:SER:OG	1:B:592:SER:N	2.46	0.48
1:B:958:VAL:HG12	1:B:961:ASP:H	1.77	0.48
1:C:99:ARG:HE	1:C:170:LEU:HD23	1.77	0.48
1:C:1073:ARG:NH1	1:C:1100:ASP:O	2.46	0.48
1:B:871:GLY:HA3	1:B:1016:LEU:HB3	1.94	0.48
1:C:237:ALA:HB1	1:C:245:TRP:HB3	1.95	0.48
1:C:94:LYS:HB3	1:C:179:PHE:HA	1.95	0.48
1:B:25:VAL:HG13	1:B:76:PHE:HB3	1.96	0.48
1:C:25:VAL:HG22	1:C:76:PHE:HD2	1.79	0.48
1:A:445:HIS:H	1:A:460:PHE:HZ	1.61	0.48
1:A:808:VAL:HA	1:A:931:GLN:HE21	1.79	0.48
1:B:194:LEU:HB3	1:B:222:LEU:HB2	1.95	0.48
1:B:322:LEU:HA	1:B:349:VAL:H	1.78	0.48
1:B:582:SER:HB2	1:B:597:LEU:HB3	1.94	0.48
1:C:424:ASN:ND2	1:C:492:GLN:OE1	2.46	0.48
1:C:332:THR:O	1:C:495:ARG:NH1	2.47	0.48
1:C:394:VAL:HG21	1:C:494:TYR:HD2	1.78	0.48
1:A:1029:TYR:O	1:A:1049:TYR:N	2.44	0.48
1:C:586:PRO:HD3	1:C:674:ILE:HD11	1.96	0.48
1:A:48:ARG:HB2	1:A:266:TYR:CD2	2.49	0.47
1:C:422:ALA:HB1	1:C:494:TYR:HB3	1.95	0.47
1:C:429:ASP:OD2	1:C:495:ARG:NH2	2.47	0.47
1:A:804:LEU:HD13	1:A:1043:VAL:HG21	1.96	0.47
1:A:441:ARG:HH22	1:A:456:SER:HB3	1.80	0.47
1:A:1070:TYR:HD2	1:A:1119:VAL:HG21	1.78	0.47
1:B:116:ILE:HG12	1:B:125:ILE:HG12	1.95	0.47
1:C:182:LEU:HD22	1:C:203:ILE:HD12	1.96	0.47
1:C:196:VAL:HB	1:C:220:PHE:H	1.80	0.47
1:C:344:LYS:HA	1:C:383:TYR:HA	1.97	0.47
1:C:804:LEU:HD21	1:C:920:LEU:HD13	1.95	0.47
1:C:1062:ALA:HB3	1:C:1114:ILE:HG12	1.97	0.47
1:C:1111:VAL:HB	1:C:1114:ILE:HD11	1.97	0.47
1:B:331:ALA:HB3	1:B:334:PHE:HE1	1.79	0.47
1:C:126:ARG:HG2	1:C:162:GLU:HG3	1.97	0.47
1:A:708:VAL:HG23	1:A:929:LYS:HD2	1.97	0.46
1:A:1000:ILE:O	1:A:1004:ALA:N	2.47	0.46
1:C:102:VAL:HG23	1:C:115:ILE:HG12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:ARG:NH2	1:B:210:PRO:O	2.47	0.46
1:A:361:PHE:HA	1:A:423:TRP:HB2	1.97	0.46
1:A:711:VAL:HG22	1:A:1041:GLY:HA2	1.97	0.46
1:B:429:ASP:O	1:B:435:ASN:ND2	2.38	0.46
1:C:1062:ALA:O	1:C:1115:ILE:N	2.38	0.46
1:B:348:CYS:SG	1:B:349:VAL:N	2.89	0.46
1:C:712:SER:OG	1:C:713:MET:N	2.49	0.46
1:A:878:ILE:HG23	1:A:883:GLN:HE21	1.80	0.46
1:B:23:ASP:HB3	1:B:244:ILE:HG23	1.97	0.46
1:A:389:VAL:HG11	1:A:397:ILE:HD11	1.99	0.45
1:A:405:ILE:HD13	1:A:409:ASN:HD22	1.81	0.45
1:C:99:ARG:CZ	1:C:172:VAL:HG12	2.45	0.45
1:B:328:VAL:HG13	1:B:343:LYS:HD2	1.98	0.45
1:A:835:GLN:NE2	1:C:600:ASP:O	2.48	0.45
1:B:326:GLY:HA2	1:B:330:ASN:HB3	1.99	0.45
1:A:48:ARG:HB2	1:A:266:TYR:HD2	1.80	0.45
1:A:1018:GLN:NE2	1:A:1030:HIS:O	2.44	0.45
1:C:537:VAL:HB	1:C:574:SER:HB3	1.97	0.45
1:B:405:ILE:HG12	1:B:409:ASN:HD22	1.82	0.45
1:C:598:TYR:HB2	1:C:635:CYS:HB2	1.98	0.45
1:A:102:VAL:HB	1:A:232:ARG:HB3	1.99	0.45
1:B:188:LYS:HE3	1:B:195:TYR:HD2	1.82	0.45
1:A:363:THR:HG21	1:A:422:ALA:HB3	1.99	0.44
1:B:337:VAL:HG12	1:B:409:ASN:HB3	2.00	0.44
1:A:897:VAL:HA	1:A:900:GLU:HB2	1.99	0.44
1:A:109:ASN:HD22	1:A:131:GLU:HG2	1.82	0.44
1:A:585:THR:HB	1:A:594:VAL:HG12	1.98	0.44
1:C:425:THR:HB	1:C:428:ILE:HB	1.98	0.44
1:A:917:GLN:O	1:A:921:THR:OG1	2.27	0.44
1:C:871:GLY:HA2	1:C:1016:LEU:HD22	1.98	0.44
1:A:31:THR:O	1:A:68:GLY:N	2.42	0.44
1:B:114:VAL:HG11	1:B:224:LEU:HD13	1.98	0.44
1:A:582:SER:HB2	1:A:597:LEU:HB3	2.00	0.44
1:B:1057:PHE:HB3	1:B:1078:VAL:HG13	2.00	0.44
1:C:310:SER:N	1:C:524:CYS:O	2.50	0.44
1:A:591:SER:OG	1:A:592:SER:N	2.50	0.44
1:B:521:LYS:HD3	1:B:540:PRO:HD3	1.99	0.44
1:A:959:LEU:HD23	1:A:962:ILE:HD12	2.00	0.44
1:B:1063:ILE:HG23	1:B:1117:ASN:HB3	2.00	0.44
1:C:808:VAL:HG12	1:C:809:THR:HG23	2.00	0.44
1:B:352:TYR:HB3	1:B:355:LEU:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:92:THR:N	1:C:251:ALA:O	2.47	0.43
1:C:766:GLN:NE2	1:C:1012:SER:OG	2.45	0.43
1:A:81:ILE:HG21	1:A:254:VAL:HG21	1.98	0.43
1:A:98:VAL:O	1:A:183:ARG:NH2	2.46	0.43
1:A:745:LEU:HD22	1:A:990:VAL:HG21	2.00	0.43
1:C:564:ASP:OD2	1:C:567:THR:OG1	2.25	0.43
1:C:1071:PHE:HZ	1:C:1111:VAL:HG21	1.83	0.43
1:A:451:PHE:HD2	1:B:192:GLY:HA3	1.82	0.43
1:A:866:ALA:O	1:A:869:THR:OG1	2.33	0.43
1:A:1108:CYS:SG	1:A:1109:ASP:N	2.91	0.43
1:C:685:SER:OG	1:C:686:SER:N	2.51	0.43
1:B:584:ILE:HB	1:B:595:ALA:HB3	1.99	0.43
1:C:390:LYS:HE2	1:C:481:TYR:HD1	1.83	0.43
1:C:1012:SER:HA	1:C:1016:LEU:HD12	2.01	0.43
1:A:444:ARG:NH1	1:A:454:ASP:OD2	2.52	0.43
1:A:238:PHE:H	1:A:247:THR:HA	1.83	0.43
1:B:324:PRO:HD2	1:B:345:ILE:HG23	2.01	0.43
1:A:1063:ILE:HG12	1:A:1117:ASN:HD22	1.83	0.43
1:B:31:THR:O	1:B:68:GLY:N	2.50	0.43
1:B:82:PRO:HB3	1:B:84:LYS:HE3	2.00	0.43
1:B:822:CYS:HB3	1:B:833:CYS:HB2	1.91	0.43
1:C:709:MET:HE2	1:C:1007:ALA:HB2	2.00	0.43
1:B:182:LEU:HB2	1:B:203:ILE:HD13	1.99	0.43
1:A:420:VAL:HG22	1:A:498:VAL:HG22	2.00	0.43
1:A:694:ILE:HG22	1:A:1059:THR:HB	2.01	0.43
1:B:179:PHE:HB2	1:B:205:VAL:HB	2.00	0.42
1:B:277:ASP:HB3	1:B:280:GLN:HG2	2.01	0.42
1:A:365:LYS:NZ	1:A:366:CYS:O	2.49	0.42
1:B:186:VAL:HG13	1:B:257:LEU:HD11	2.02	0.42
1:A:21:THR:HG22	1:A:135:ASN:H	1.84	0.42
1:A:96:ASN:O	1:A:99:ARG:NE	2.51	0.42
1:A:152:ILE:HD13	1:A:234:ILE:HD13	2.02	0.42
1:B:955:ILE:HB	1:B:974:GLN:HE22	1.83	0.42
1:C:704:ILE:HG12	1:C:1047:VAL:HG22	2.02	0.42
1:A:127:ALA:HB3	1:A:161:PHE:H	1.84	0.42
1:C:385:ASP:OD2	1:C:410:TYR:OH	2.37	0.42
1:A:787:ILE:HD11	1:A:913:ILE:HD12	2.01	0.42
1:B:104:GLY:HA2	1:B:226:ILE:HD12	2.01	0.42
1:B:203:ILE:HB	1:B:205:VAL:HG23	2.01	0.42
1:B:282:PRO:HG3	1:B:619:TRP:CE2	2.55	0.42
1:B:758:ARG:O	1:B:762:GLU:N	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1052:SER:OG	1:C:1053:GLN:N	2.52	0.42
1:B:248:SER:OG	1:B:249:ALA:N	2.52	0.42
1:A:209:LEU:HB2	1:A:253:PHE:CZ	2.55	0.42
1:B:286:LEU:HD11	1:B:300:TYR:HB2	2.01	0.42
1:B:429:ASP:OD2	1:B:495:ARG:NE	2.49	0.42
1:B:1029:TYR:HB2	1:B:1049:TYR:HB3	2.00	0.42
1:C:26:GLN:HB2	1:C:75:THR:HA	2.02	0.42
1:C:83:PHE:HE2	1:C:189:ASN:HB2	1.84	0.42
1:C:848:THR:H	1:C:851:MET:HE3	1.84	0.42
1:B:285:GLU:OE1	1:B:619:TRP:NE1	2.52	0.42
1:C:248:SER:OG	1:C:249:ALA:N	2.51	0.42
1:B:697:PRO:O	1:B:1092:PHE:N	2.53	0.42
1:C:329:PHE:HA	1:C:497:VAL:HG21	2.01	0.42
1:C:365:LYS:HB2	1:C:420:VAL:HB	2.02	0.42
1:A:77:GLY:O	1:A:252:TYR:OH	2.33	0.42
1:B:923:THR:OG1	1:B:924:SER:N	2.51	0.42
1:B:1079:PHE:HB2	1:B:1084:TRP:CH2	2.54	0.42
1:B:197:TYR:CD1	1:B:218:PRO:HA	2.55	0.41
1:A:1054:GLU:HG2	1:B:876:LEU:HD21	2.01	0.41
1:B:710:PRO:HA	1:B:1041:GLY:HA3	2.03	0.41
1:C:377:LEU:HB3	1:C:501:PHE:HZ	1.85	0.41
1:C:887:ARG:NH1	1:C:1031:LEU:O	2.51	0.41
1:A:444:ARG:HH22	1:A:448:LEU:HG	1.84	0.41
1:B:631:THR:OG1	1:B:634:GLY:N	2.49	0.41
1:C:116:ILE:HG12	1:C:125:ILE:HG12	2.02	0.41
1:C:600:ASP:N	1:C:633:ALA:O	2.44	0.41
1:B:1080:ASN:HB3	1:B:1083:SER:H	1.86	0.41
1:C:1079:PHE:HB2	1:C:1084:TRP:CD2	2.55	0.41
1:A:83:PHE:CZ	1:A:86:GLY:HA2	2.56	0.41
1:A:96:ASN:HB2	1:A:99:ARG:HH21	1.86	0.41
1:A:305:PHE:HZ	1:A:601:VAL:HG11	1.85	0.41
1:C:545:PHE:HB2	1:C:563:ARG:HH21	1.86	0.41
1:B:663:VAL:H	1:B:672:LYS:N	2.19	0.41
1:C:182:LEU:HD23	1:C:201:GLN:HE21	1.86	0.41
1:C:546:GLN:H	1:C:549:GLN:HB2	1.86	0.41
1:A:39:GLY:HA3	1:A:60:LEU:HB3	2.02	0.41
1:A:372:THR:HG21	1:B:968:PRO:HD3	2.02	0.41
1:A:1071:PHE:HZ	1:A:1111:VAL:HG21	1.85	0.41
1:B:683:ALA:HB3	1:C:769:GLN:HG2	2.03	0.41
1:B:888:PHE:HE2	1:B:898:LEU:HD13	1.86	0.41
1:B:1080:ASN:HB3	1:B:1082:THR:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99:ARG:HH21	1:C:170:LEU:HG	1.85	0.41
1:A:112:GLN:NE2	1:C:453:ARG:HH21	2.19	0.41
1:A:735:LEU:HA	1:A:738:TYR:HD2	1.86	0.41
1:A:1111:VAL:HG13	1:B:899:TYR:HB3	2.02	0.41
1:C:893:VAL:HA	1:C:1091:PHE:HE1	1.86	0.41
1:A:102:VAL:N	1:A:232:ARG:O	2.42	0.40
1:B:788:LEU:HA	1:B:788:LEU:HD23	1.82	0.40
1:C:363:THR:HG21	1:C:394:VAL:HG11	2.03	0.40
1:C:649:ASP:HB3	1:C:659:SER:HB2	2.03	0.40
1:C:313:VAL:HG11	1:C:519:LEU:HD12	2.03	0.40
1:A:306:ARG:NH2	1:B:727:ASP:OD1	2.43	0.40
1:B:76:PHE:CZ	1:B:235:LEU:HB2	2.56	0.40
1:C:411:LYS:NZ	1:C:412:LEU:O	2.38	0.40
1:A:373:LYS:HE2	1:B:965:ARG:HG2	2.04	0.40
1:B:632:GLN:HE21	1:C:825:ASP:HA	1.86	0.40
1:C:21:THR:HB	1:C:135:ASN:HB2	2.04	0.40
1:C:25:VAL:HA	1:C:76:PHE:HB3	2.02	0.40
1:C:48:ARG:HB2	1:C:266:TYR:CD2	2.57	0.40
1:C:469:PRO:HA	1:C:471:ALA:H	1.87	0.40
1:C:1059:THR:HG22	1:C:1078:VAL:HG12	2.02	0.40
1:A:530:ASN:H	1:A:565:PRO:HG2	1.87	0.40
1:B:405:ILE:O	1:B:410:TYR:N	2.40	0.40
1:C:1060:ALA:HA	1:C:1061:PRO:HD3	1.93	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1054/1215 (87%)	962 (91%)	92 (9%)	0	100	100
1	B	1054/1215 (87%)	973 (92%)	81 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	1055/1215 (87%)	982 (93%)	73 (7%)	0	100	100
All	All	3163/3645 (87%)	2917 (92%)	246 (8%)	0	100	100

There are no Ramachandran outliers to report.

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	926/1053 (88%)	926 (100%)	0	100	100
1	B	927/1053 (88%)	927 (100%)	0	100	100
1	C	927/1053 (88%)	926 (100%)	1 (0%)	88	90
All	All	2780/3159 (88%)	2779 (100%)	1 (0%)	100	100

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

Mol	Chain	Res	Type
1	C	708	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	GLN
1	A	230	ASN
1	A	396	GLN
1	A	424	ASN
1	A	630	GLN
1	A	786	GLN
1	A	883	GLN
1	A	908	GLN
1	A	931	GLN
1	A	974	GLN
1	A	1040	HIS

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Mol	Chain	Res	Type
1	B	32	GLN
1	B	74	HIS
1	B	109	ASN
1	B	147	GLN
1	B	733	ASN
1	B	806	ASN
1	B	877	GLN
1	B	883	GLN
1	B	951	ASN
1	B	1018	GLN
1	B	1053	GLN
1	C	74	HIS
1	C	112	GLN
1	C	201	GLN
1	C	375	ASN
1	C	550	GLN
1	C	759	ASN
1	C	889	ASN
1	C	908	GLN
1	C	1018	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 ⓘ

51 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	D	1	1,2	14,14,15	0.41	0	17,19,21	0.61	0
2	NAG	D	2	2	14,14,15	0.31	0	17,19,21	1.09	1 (5%)
2	BMA	D	3	2	11,11,12	0.92	0	15,15,17	0.76	0
3	NAG	E	1	1,3	14,14,15	0.38	0	17,19,21	0.64	0
3	NAG	E	2	3	14,14,15	0.29	0	17,19,21	0.51	0
3	BMA	E	3	3	11,11,12	0.63	0	15,15,17	0.84	0
3	MAN	E	4	3	11,11,12	0.79	0	15,15,17	1.04	2 (13%)
2	NAG	F	1	1,2	14,14,15	0.53	0	17,19,21	0.66	0
2	NAG	F	2	2	14,14,15	0.36	0	17,19,21	0.47	0
2	BMA	F	3	2	11,11,12	0.64	0	15,15,17	0.98	1 (6%)
4	NAG	G	1	1,4	14,14,15	0.45	0	17,19,21	0.57	0
4	NAG	G	2	4	14,14,15	0.23	0	17,19,21	0.53	0
4	NAG	H	1	1,4	14,14,15	0.39	0	17,19,21	0.66	0
4	NAG	H	2	4	14,14,15	0.27	0	17,19,21	0.58	0
4	NAG	I	1	1,4	14,14,15	0.72	0	17,19,21	0.64	0
4	NAG	I	2	4	14,14,15	0.49	0	17,19,21	0.50	0
2	NAG	J	1	1,2	14,14,15	0.29	0	17,19,21	0.47	0
2	NAG	J	2	2	14,14,15	0.30	0	17,19,21	0.51	0
2	BMA	J	3	2	11,11,12	0.86	0	15,15,17	0.78	0
2	NAG	K	1	1,2	14,14,15	0.36	0	17,19,21	0.64	1 (5%)
2	NAG	K	2	2	14,14,15	0.33	0	17,19,21	0.52	0
2	BMA	K	3	2	11,11,12	0.80	0	15,15,17	0.77	0
4	NAG	L	1	1,4	14,14,15	0.29	0	17,19,21	0.39	0
4	NAG	L	2	4	14,14,15	0.22	0	17,19,21	0.66	1 (5%)
2	NAG	M	1	1,2	14,14,15	0.31	0	17,19,21	0.58	0
2	NAG	M	2	2	14,14,15	0.46	0	17,19,21	0.64	0
2	BMA	M	3	2	11,11,12	0.76	0	15,15,17	0.81	0
2	NAG	N	1	1,2	14,14,15	0.37	0	17,19,21	0.55	0
2	NAG	N	2	2	14,14,15	0.23	0	17,19,21	0.71	1 (5%)
2	BMA	N	3	2	11,11,12	0.84	0	15,15,17	0.74	0
4	NAG	O	1	1,4	14,14,15	0.43	0	17,19,21	0.79	1 (5%)
4	NAG	O	2	4	14,14,15	0.60	0	17,19,21	0.40	0
4	NAG	P	1	1,4	14,14,15	0.27	0	17,19,21	0.51	0
4	NAG	P	2	4	14,14,15	0.30	0	17,19,21	0.44	0
4	NAG	Q	1	1,4	14,14,15	0.31	0	17,19,21	0.52	0
4	NAG	Q	2	4	14,14,15	0.34	0	17,19,21	0.44	0
2	NAG	R	1	1,2	14,14,15	0.22	0	17,19,21	1.01	1 (5%)
2	NAG	R	2	2	14,14,15	0.20	0	17,19,21	0.60	0
2	BMA	R	3	2	11,11,12	0.72	0	15,15,17	0.93	1 (6%)
5	NAG	S	1	1,5	14,14,15	0.39	0	17,19,21	0.43	0
5	NAG	S	2	5	14,14,15	0.26	0	17,19,21	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	BMA	S	3	5	11,11,12	0.82	0	15,15,17	1.35	1 (6%)
5	MAN	S	4	5	11,11,12	0.97	1 (9%)	15,15,17	1.23	2 (13%)
2	NAG	T	1	1,2	14,14,15	0.61	0	17,19,21	0.60	0
2	NAG	T	2	2	14,14,15	0.31	0	17,19,21	0.72	0
2	BMA	T	3	2	11,11,12	0.64	0	15,15,17	1.00	1 (6%)
2	NAG	U	1	1,2	14,14,15	0.44	0	17,19,21	0.48	0
2	NAG	U	2	2	14,14,15	0.36	0	17,19,21	0.63	1 (5%)
2	BMA	U	3	2	11,11,12	0.75	0	15,15,17	0.83	0
4	NAG	V	1	1,4	14,14,15	0.27	0	17,19,21	0.41	0
4	NAG	V	2	4	14,14,15	0.26	0	17,19,21	0.52	0

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

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	S	4	MAN	C1-C2	2.51	1.58	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	S	3	BMA	C1-O5-C5	3.84	117.33	112.19
2	D	2	NAG	C1-O5-C5	3.54	116.94	112.19
2	R	1	NAG	C1-O5-C5	3.26	116.55	112.19
5	S	4	MAN	C1-O5-C5	2.97	116.17	112.19
2	F	3	BMA	C1-O5-C5	2.89	116.06	112.19
3	E	4	MAN	C1-O5-C5	2.57	115.62	112.19
4	O	1	NAG	C1-O5-C5	2.54	115.59	112.19
2	T	3	BMA	C1-O5-C5	2.51	115.54	112.19
2	R	3	BMA	C1-O5-C5	2.48	115.51	112.19
2	N	2	NAG	C1-O5-C5	2.42	115.43	112.19
4	L	2	NAG	C1-O5-C5	2.34	115.33	112.19
2	U	2	NAG	C1-O5-C5	2.11	115.02	112.19
5	S	4	MAN	O2-C2-C3	-2.11	105.78	110.15
3	E	4	MAN	O2-C2-C3	-2.10	105.81	110.15
2	K	1	NAG	C1-O5-C5	2.04	114.92	112.19

There are no chirality outliers.

All (71) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	K	2	NAG	O5-C5-C6-O6
2	N	3	BMA	C4-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	K	3	BMA	O5-C5-C6-O6
4	O	1	NAG	O5-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
4	P	2	NAG	O5-C5-C6-O6
4	O	1	NAG	C4-C5-C6-O6
2	R	3	BMA	O5-C5-C6-O6
4	L	2	NAG	O5-C5-C6-O6
2	M	1	NAG	O5-C5-C6-O6
2	N	3	BMA	O5-C5-C6-O6
2	T	2	NAG	O5-C5-C6-O6
2	K	2	NAG	C4-C5-C6-O6
4	G	1	NAG	O5-C5-C6-O6
2	N	1	NAG	C4-C5-C6-O6
2	N	1	NAG	O5-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
2	F	1	NAG	O5-C5-C6-O6
5	S	1	NAG	O5-C5-C6-O6
2	K	3	BMA	C4-C5-C6-O6
2	T	3	BMA	O5-C5-C6-O6
2	T	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	F	1	NAG	C4-C5-C6-O6
2	F	2	NAG	C4-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
5	S	1	NAG	C4-C5-C6-O6
2	R	2	NAG	O5-C5-C6-O6
5	S	2	NAG	O5-C5-C6-O6
2	M	1	NAG	C4-C5-C6-O6
4	I	2	NAG	O5-C5-C6-O6
2	R	3	BMA	C4-C5-C6-O6
4	L	2	NAG	C4-C5-C6-O6
4	P	2	NAG	C4-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	R	2	NAG	C4-C5-C6-O6
3	E	4	MAN	O5-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6
2	J	3	BMA	C4-C5-C6-O6
2	M	3	BMA	O5-C5-C6-O6
4	P	1	NAG	O5-C5-C6-O6
4	G	2	NAG	C4-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
3	E	4	MAN	C4-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6
4	Q	1	NAG	C4-C5-C6-O6
4	G	1	NAG	C4-C5-C6-O6
3	E	3	BMA	O5-C5-C6-O6
2	J	3	BMA	O5-C5-C6-O6
4	I	1	NAG	O5-C5-C6-O6
5	S	2	NAG	C4-C5-C6-O6
3	E	3	BMA	C4-C5-C6-O6
4	I	2	NAG	C4-C5-C6-O6
4	V	1	NAG	C4-C5-C6-O6
2	R	1	NAG	O5-C5-C6-O6
2	U	2	NAG	O5-C5-C6-O6
2	M	2	NAG	C4-C5-C6-O6
4	Q	1	NAG	O5-C5-C6-O6
2	M	3	BMA	C4-C5-C6-O6
2	M	2	NAG	O5-C5-C6-O6
4	L	1	NAG	O5-C5-C6-O6
4	V	1	NAG	O5-C5-C6-O6
4	Q	2	NAG	C4-C5-C6-O6
4	Q	2	NAG	O5-C5-C6-O6
2	J	1	NAG	C4-C5-C6-O6

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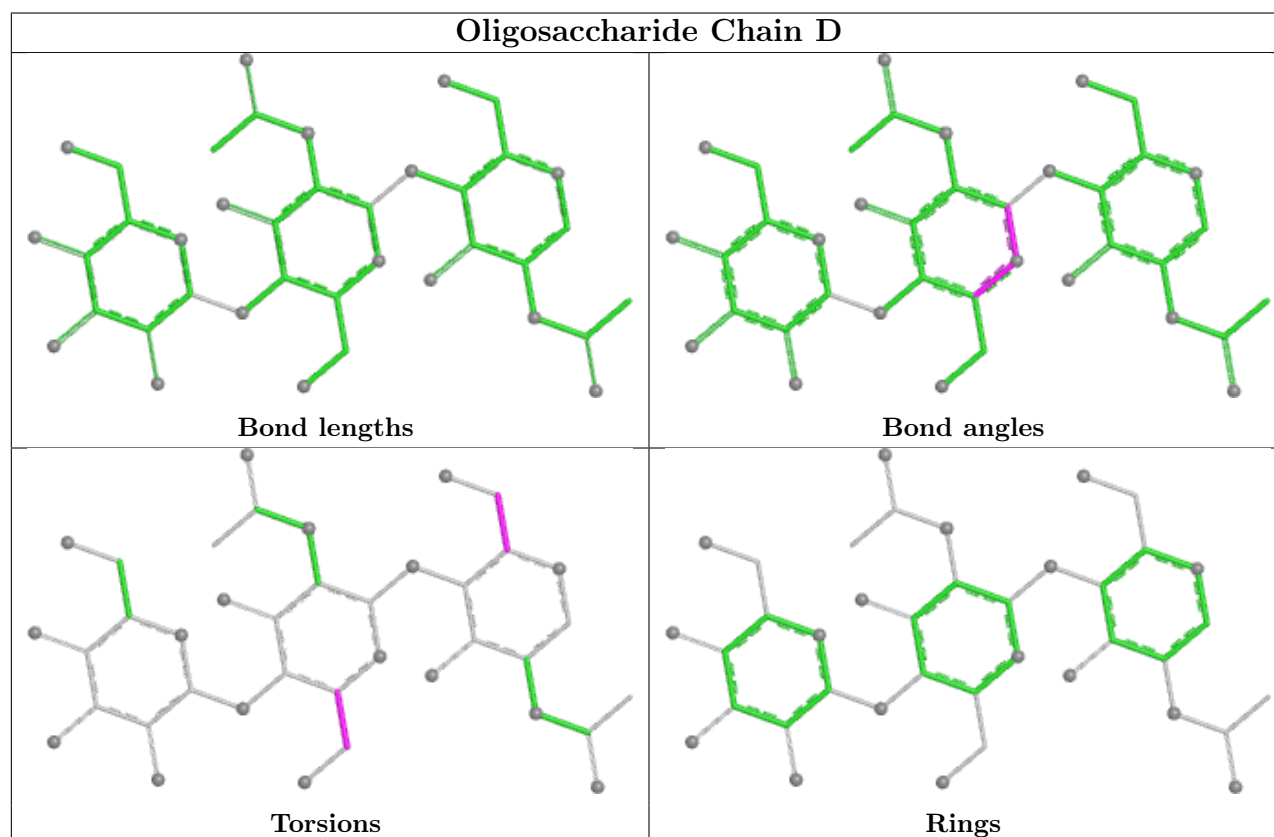
Mol	Chain	Res	Type	Atoms
5	S	3	BMA	O5-C5-C6-O6
2	U	1	NAG	C1-C2-N2-C7
4	Q	2	NAG	C1-C2-N2-C7
2	T	3	BMA	C4-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
4	P	1	NAG	C4-C5-C6-O6

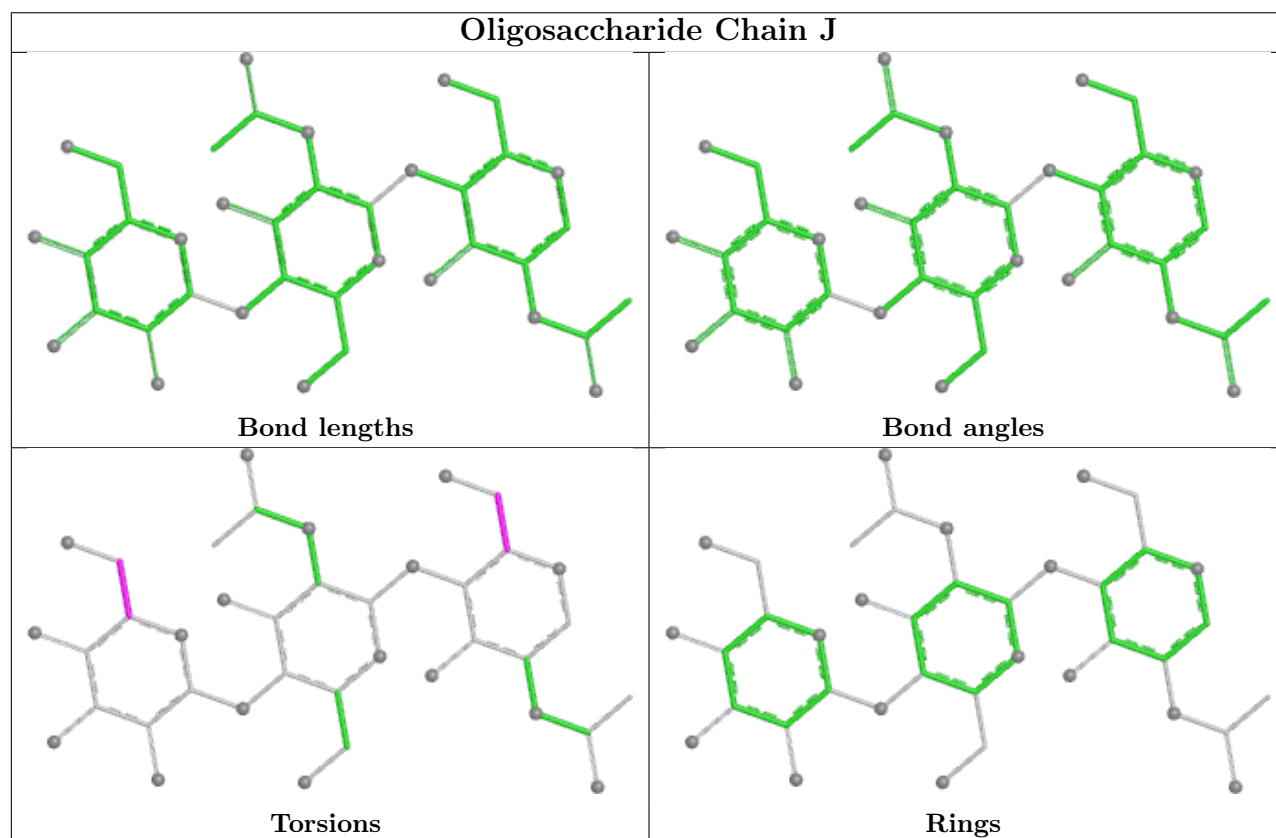
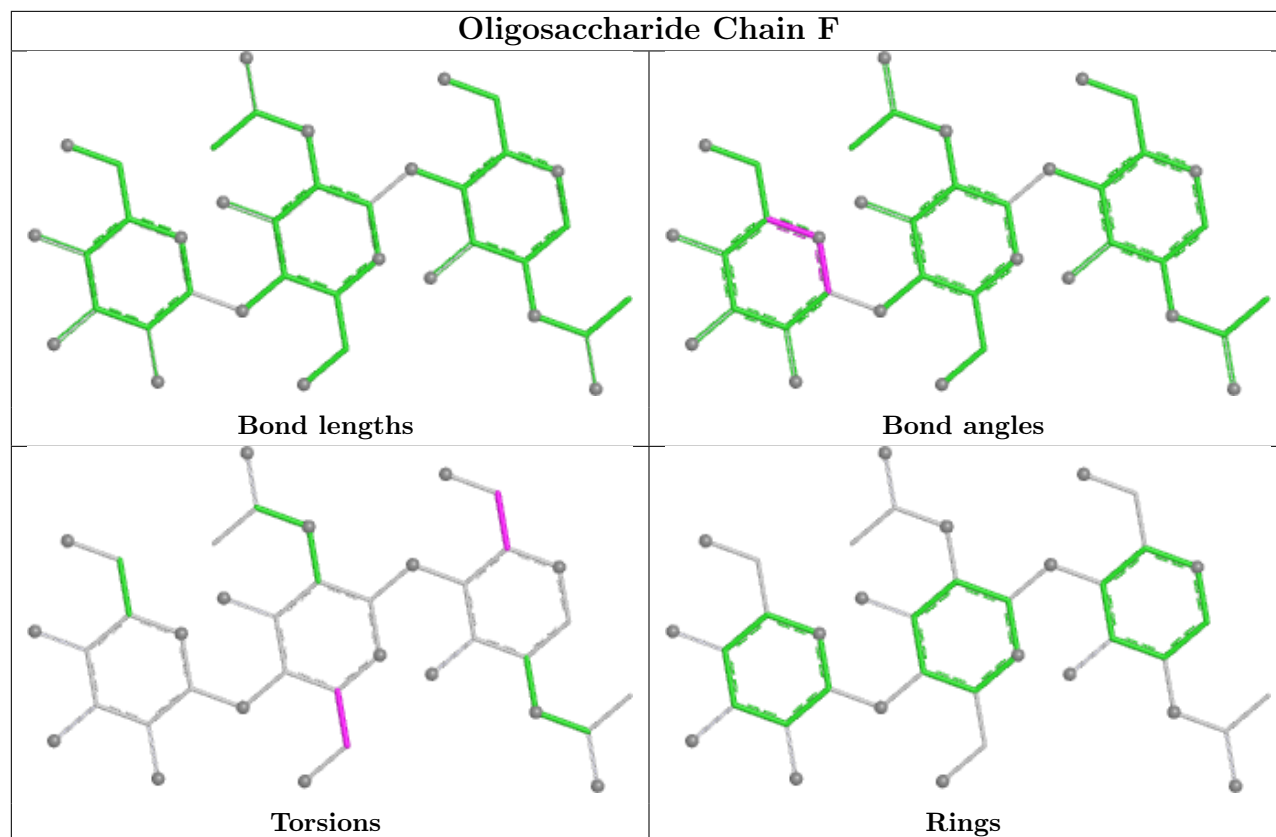
There are no ring outliers.

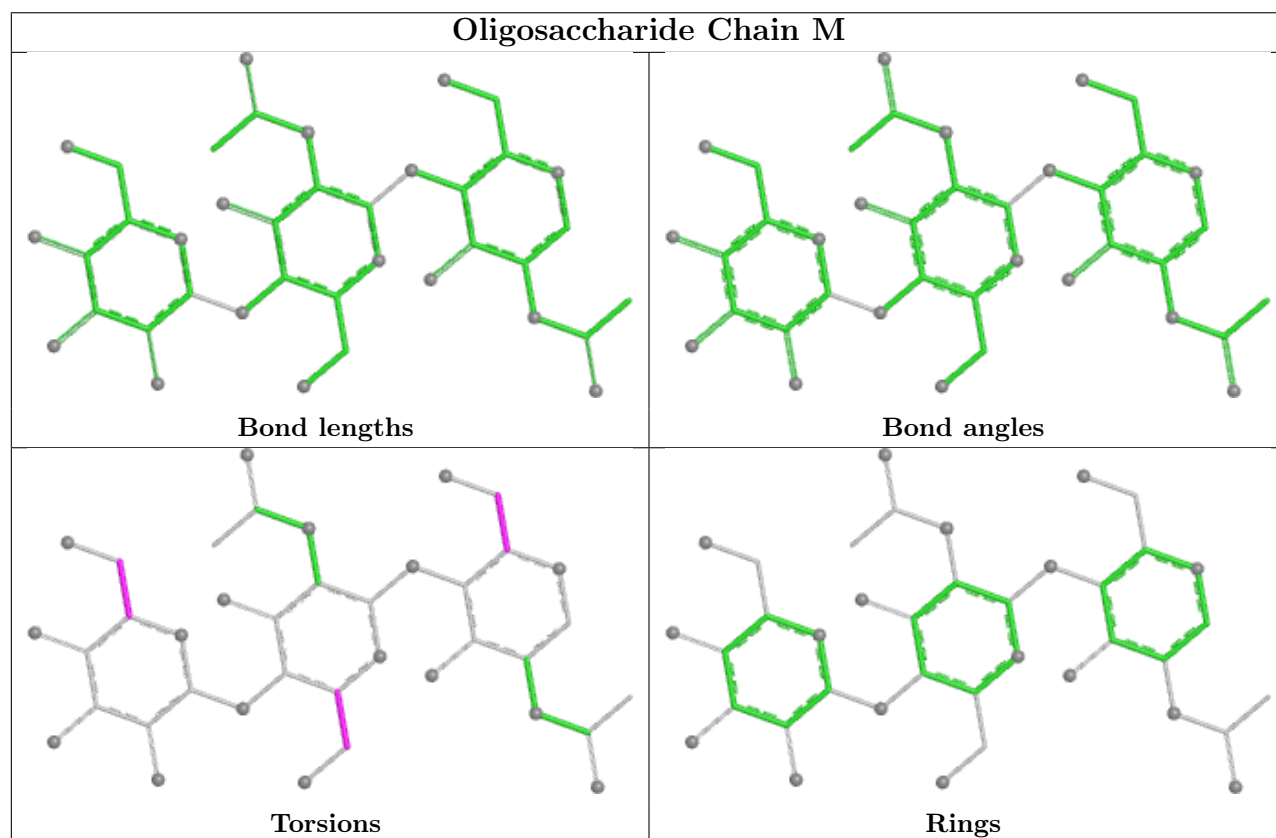
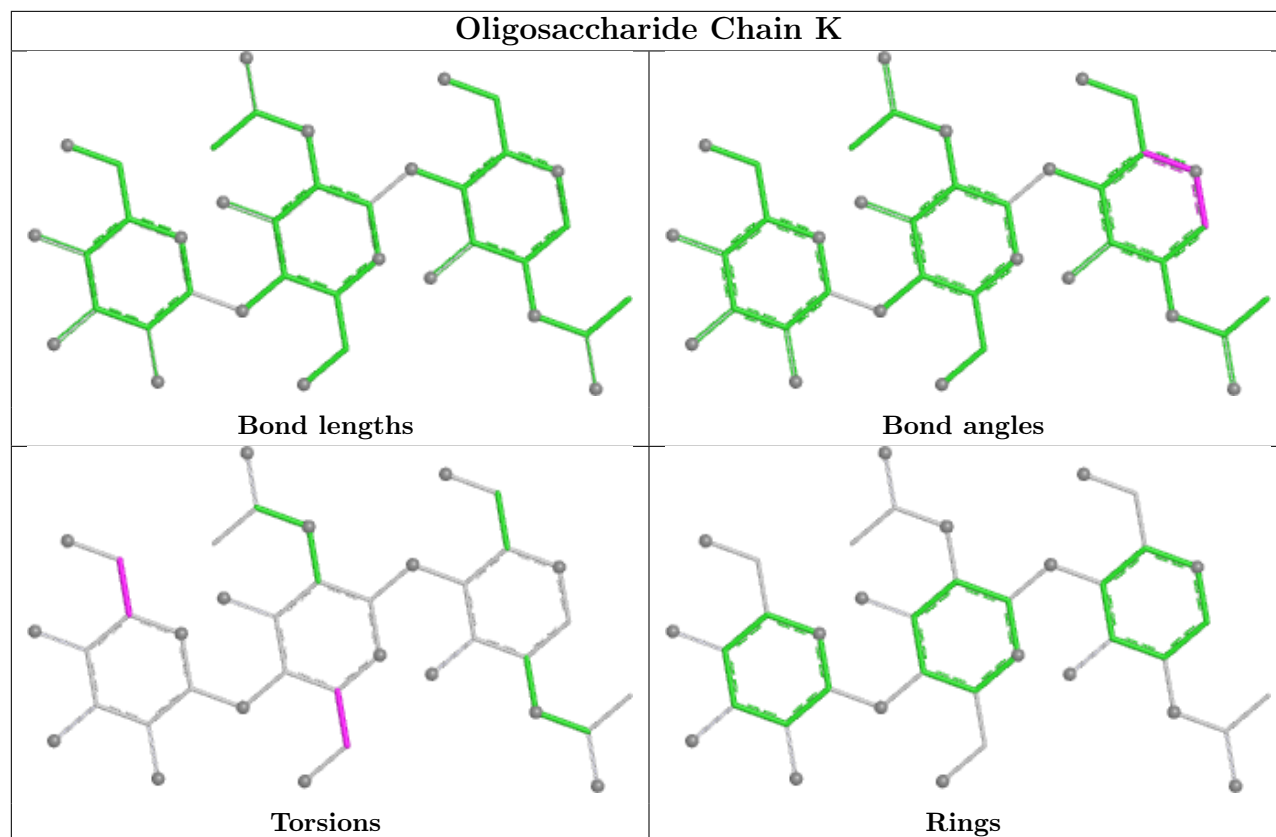
1 monomer is involved in 1 short contact:

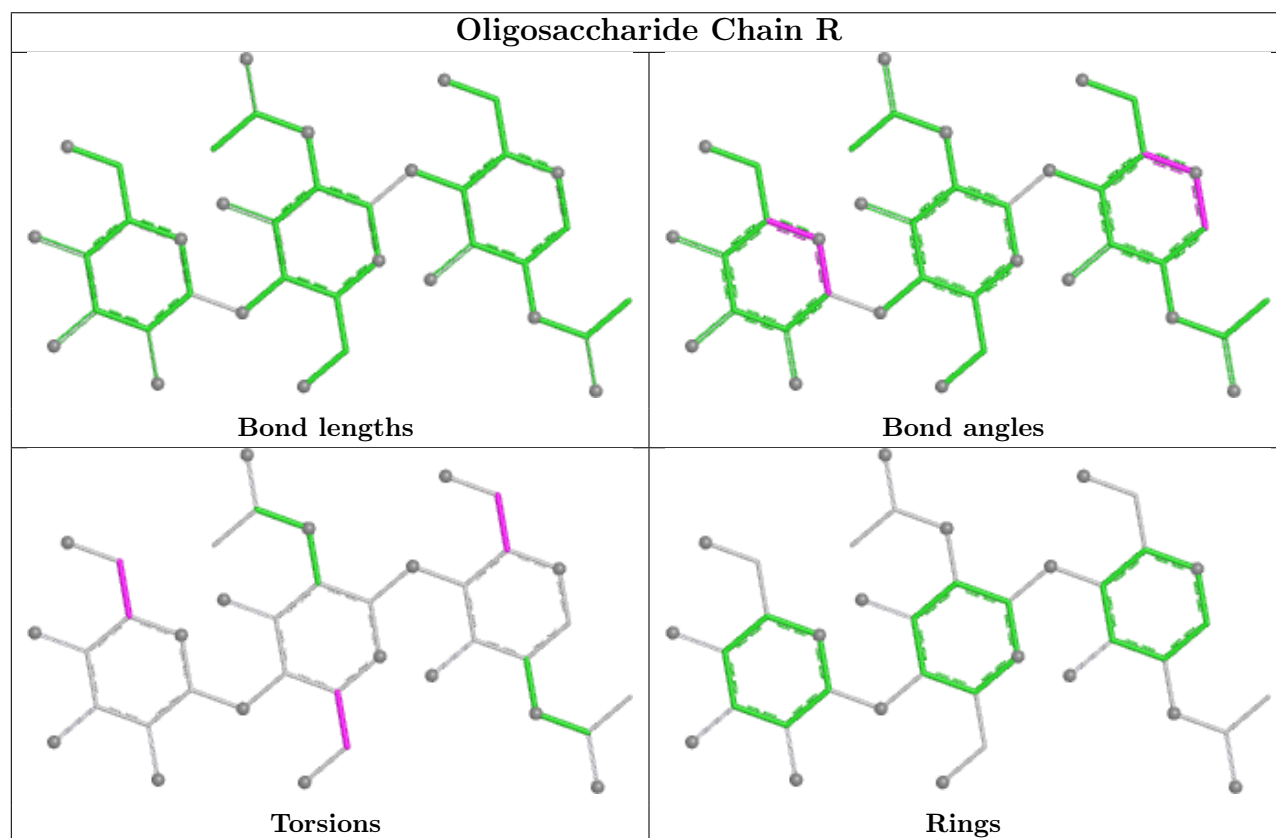
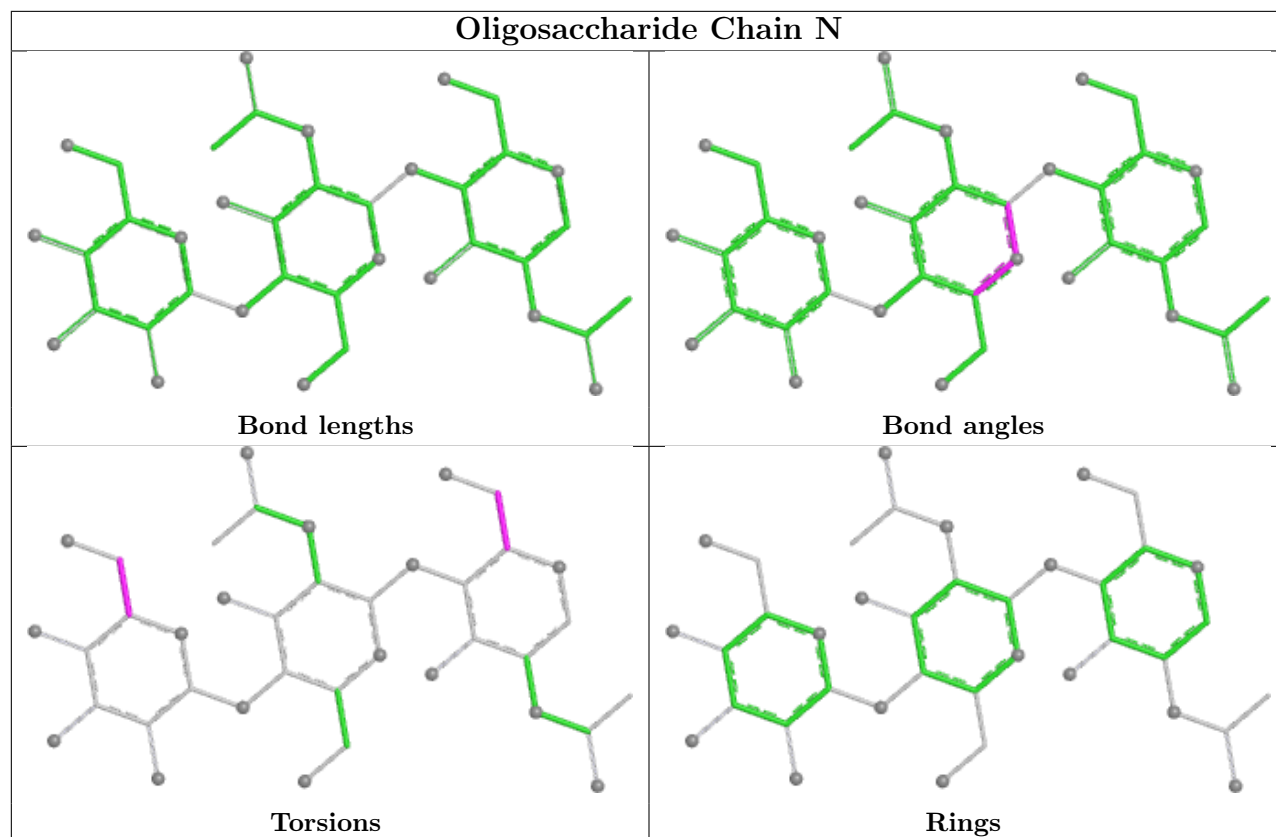
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	1	NAG	1	0

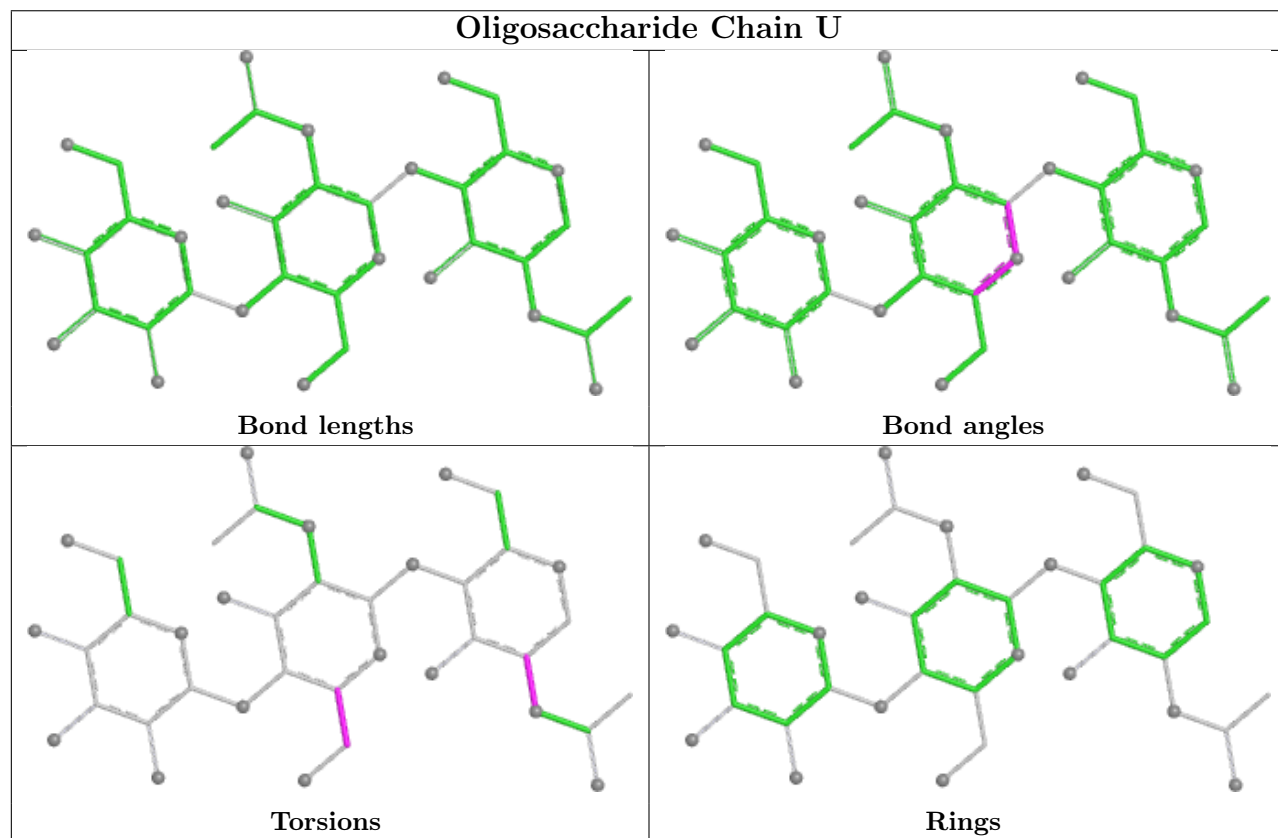
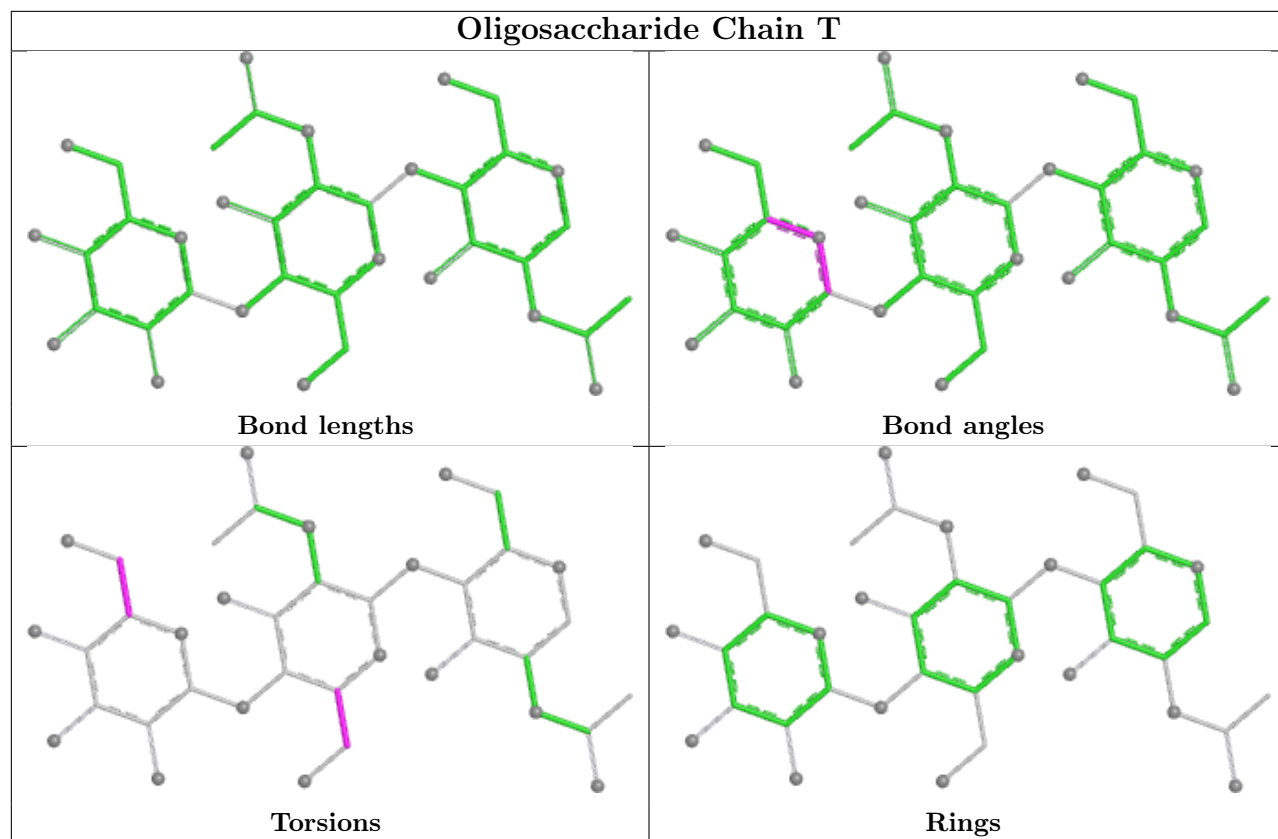
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

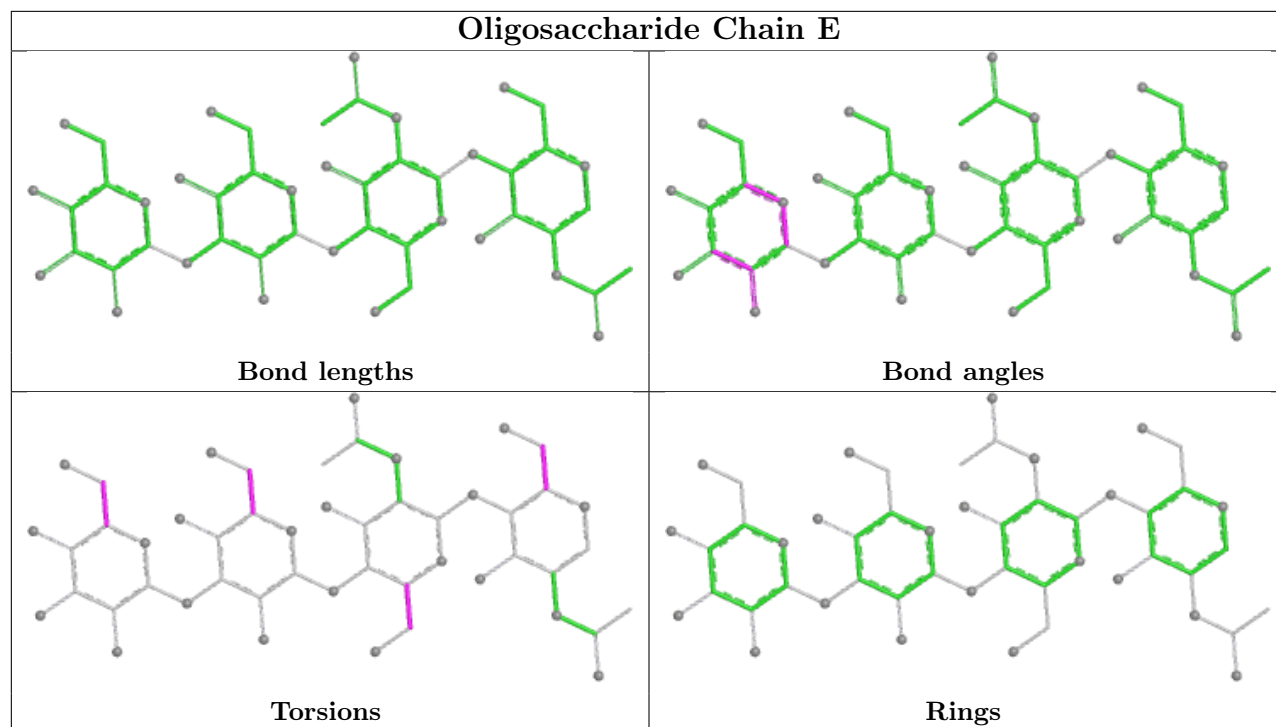


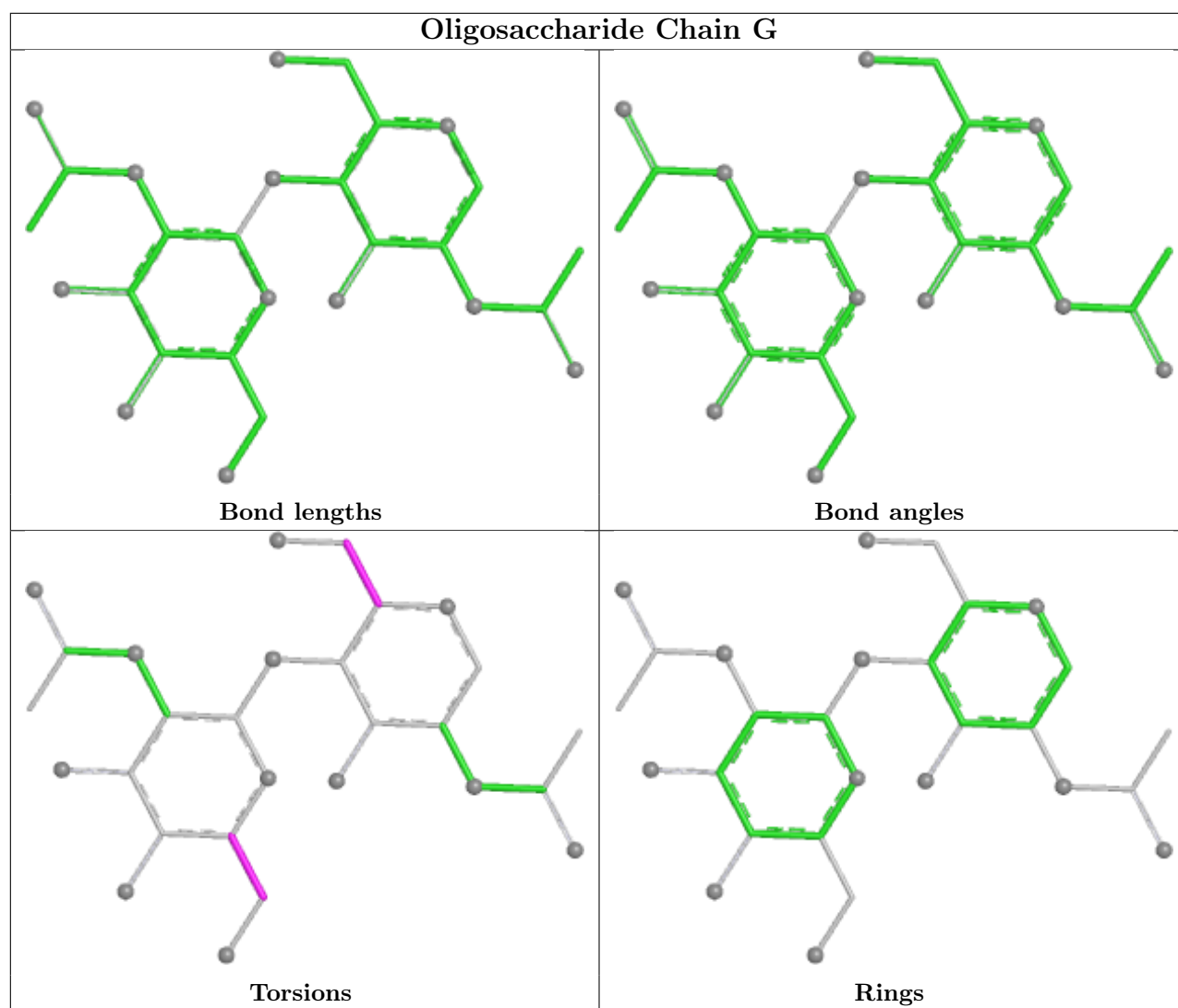


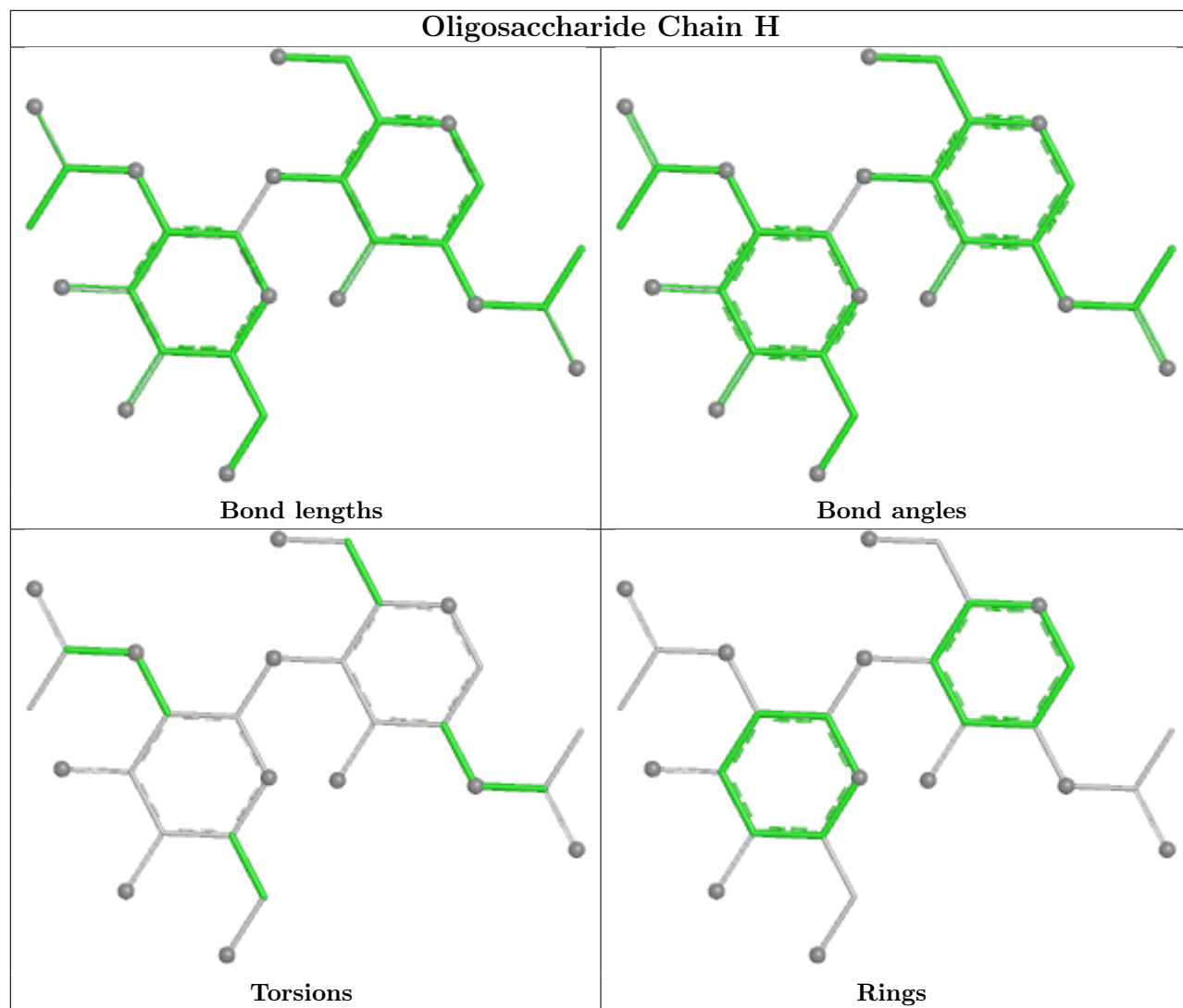


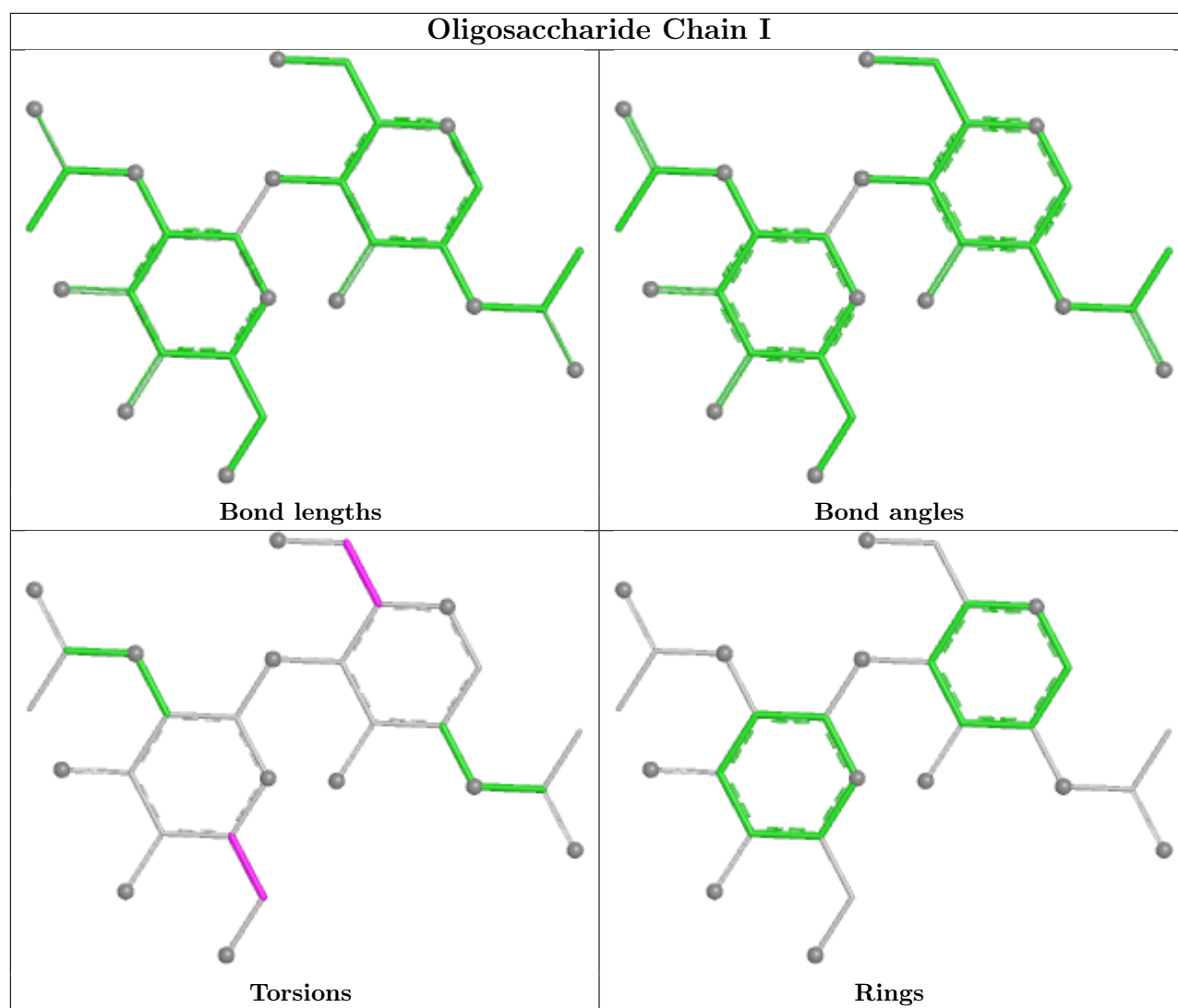


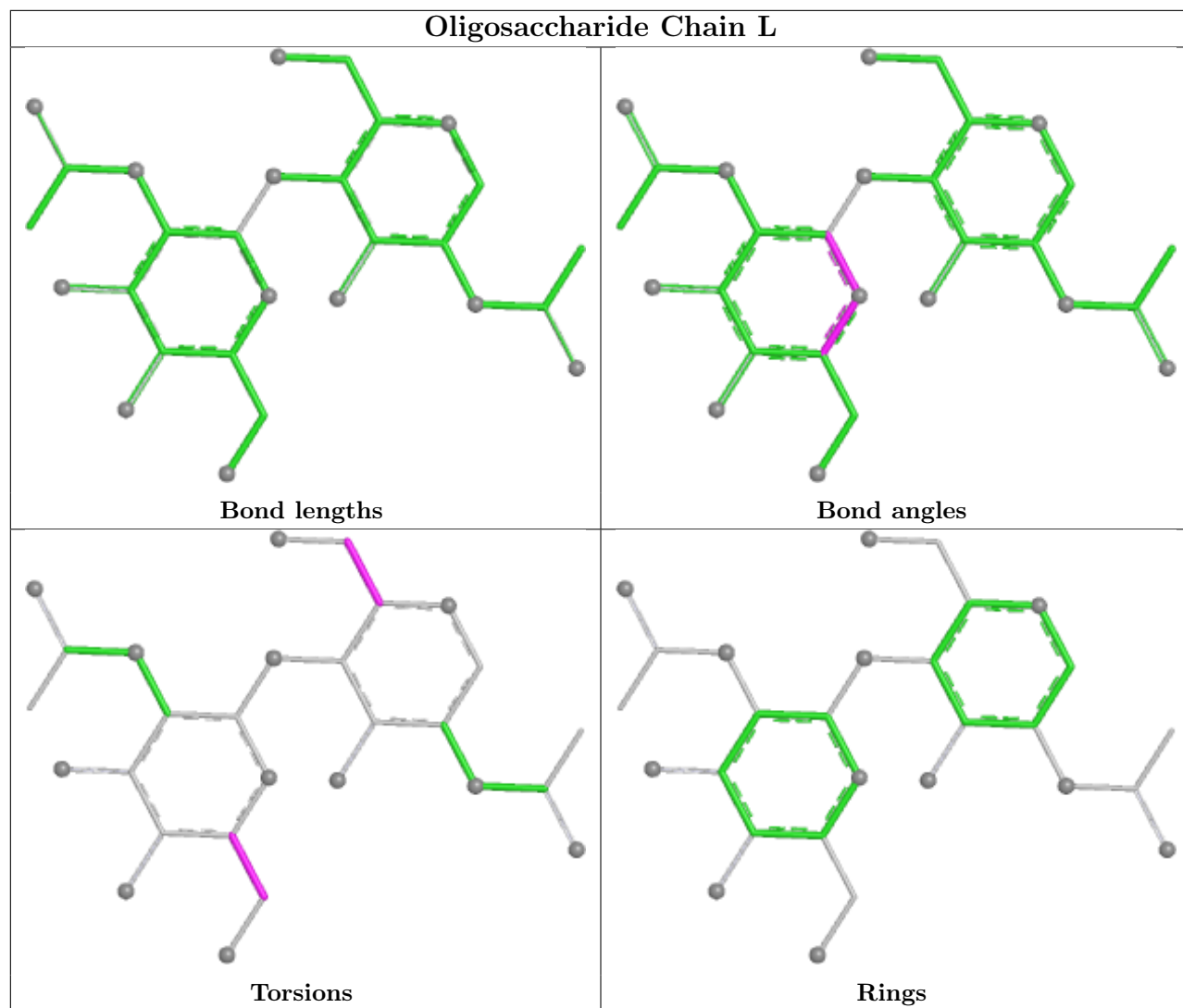


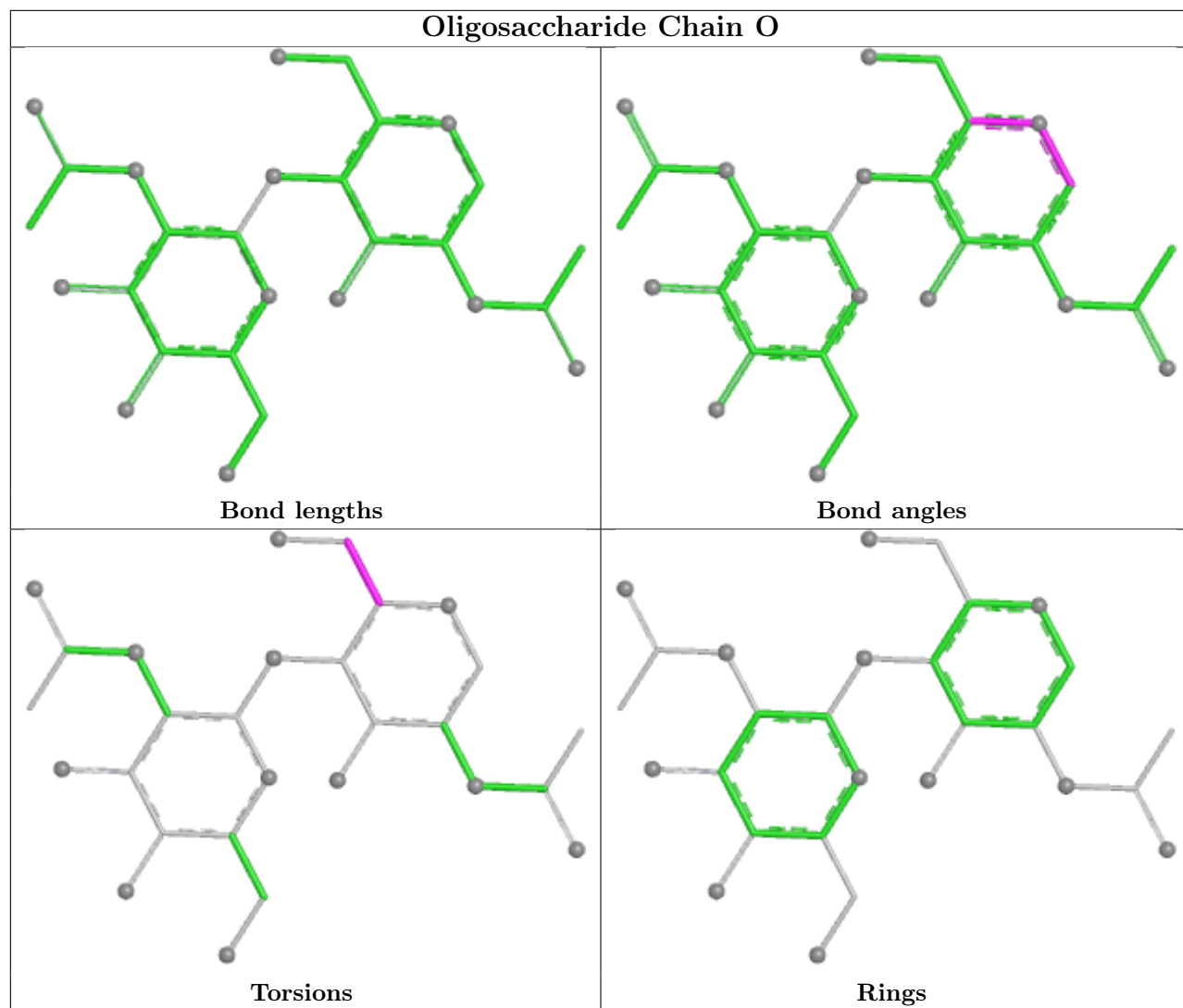


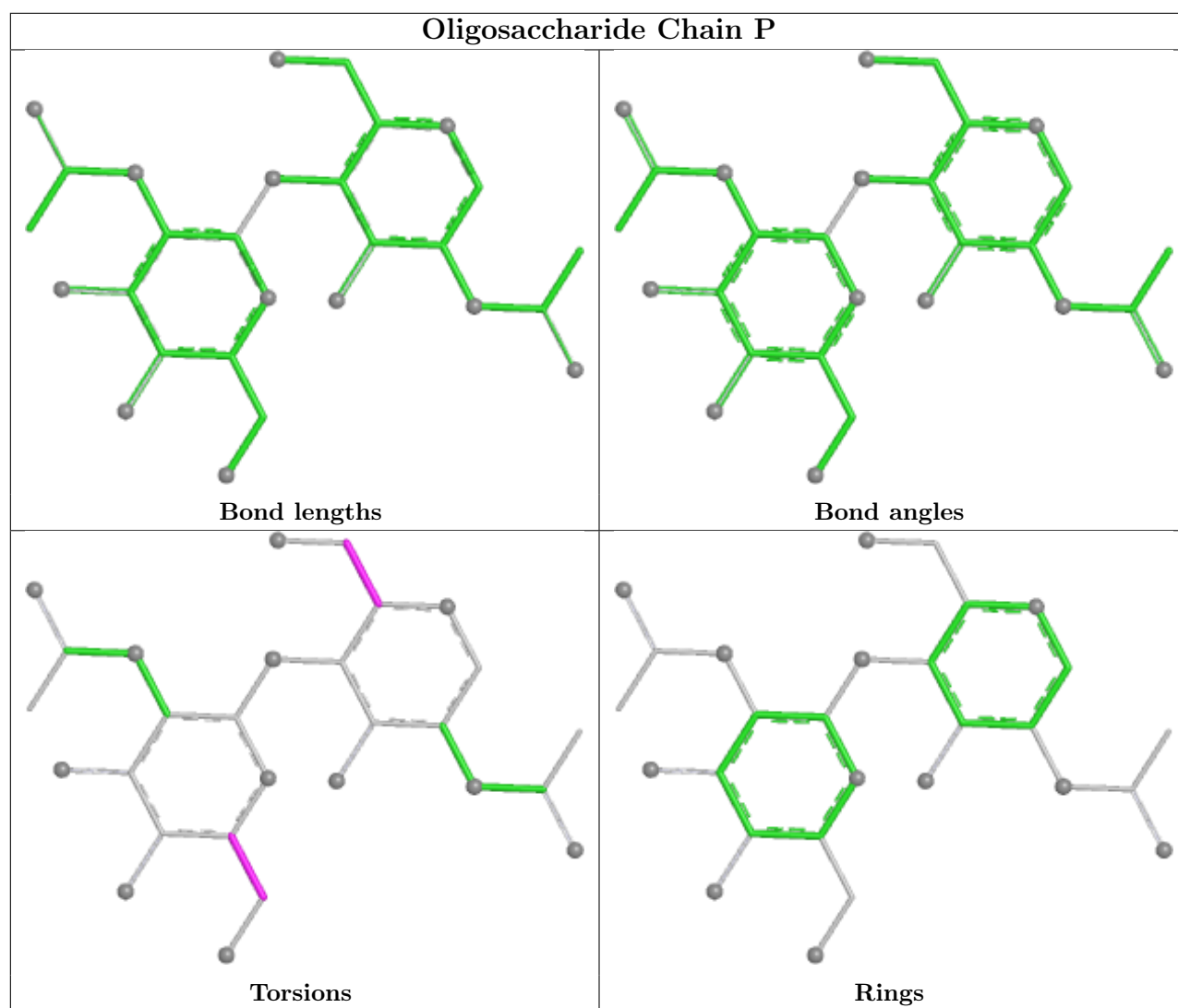


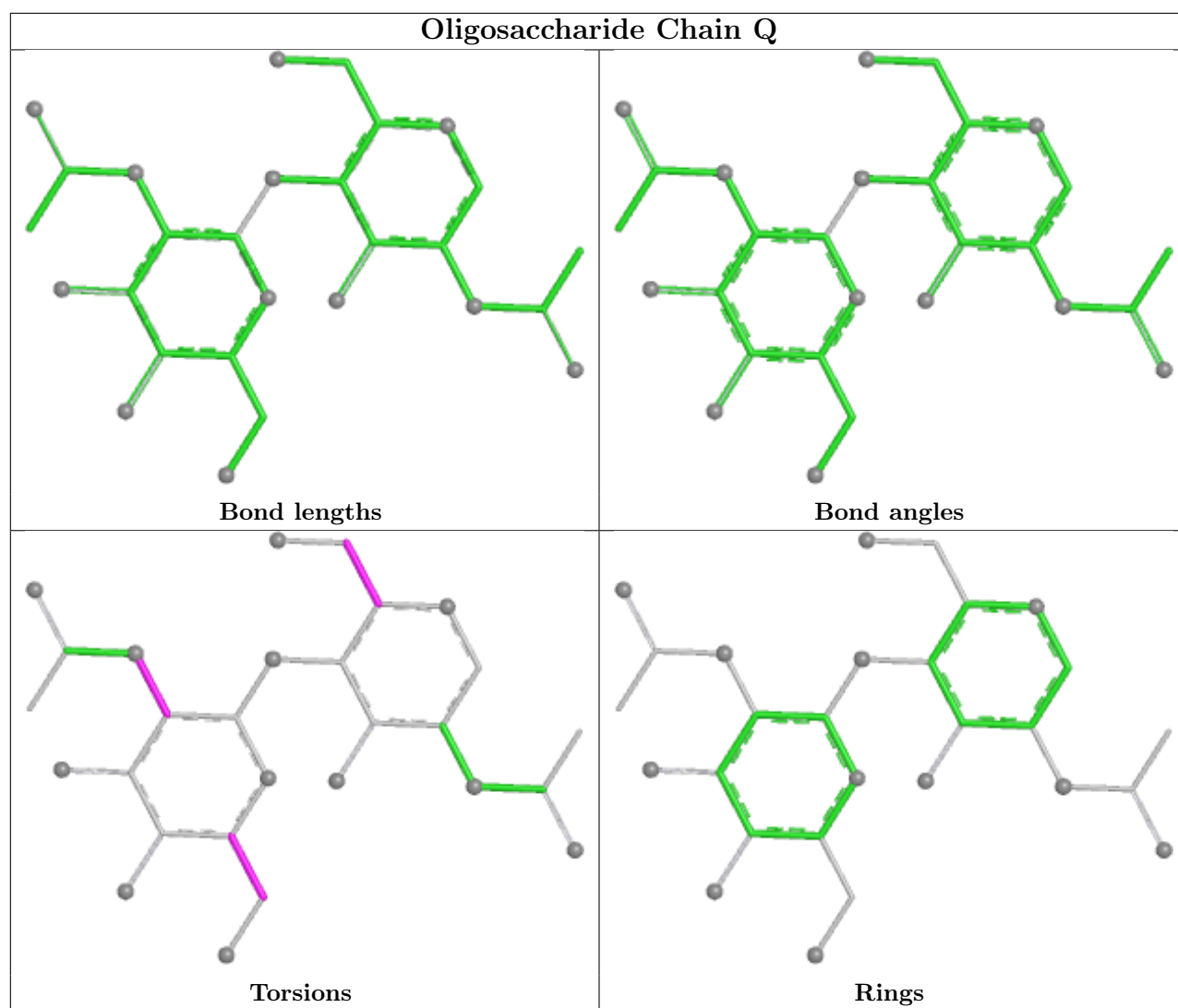


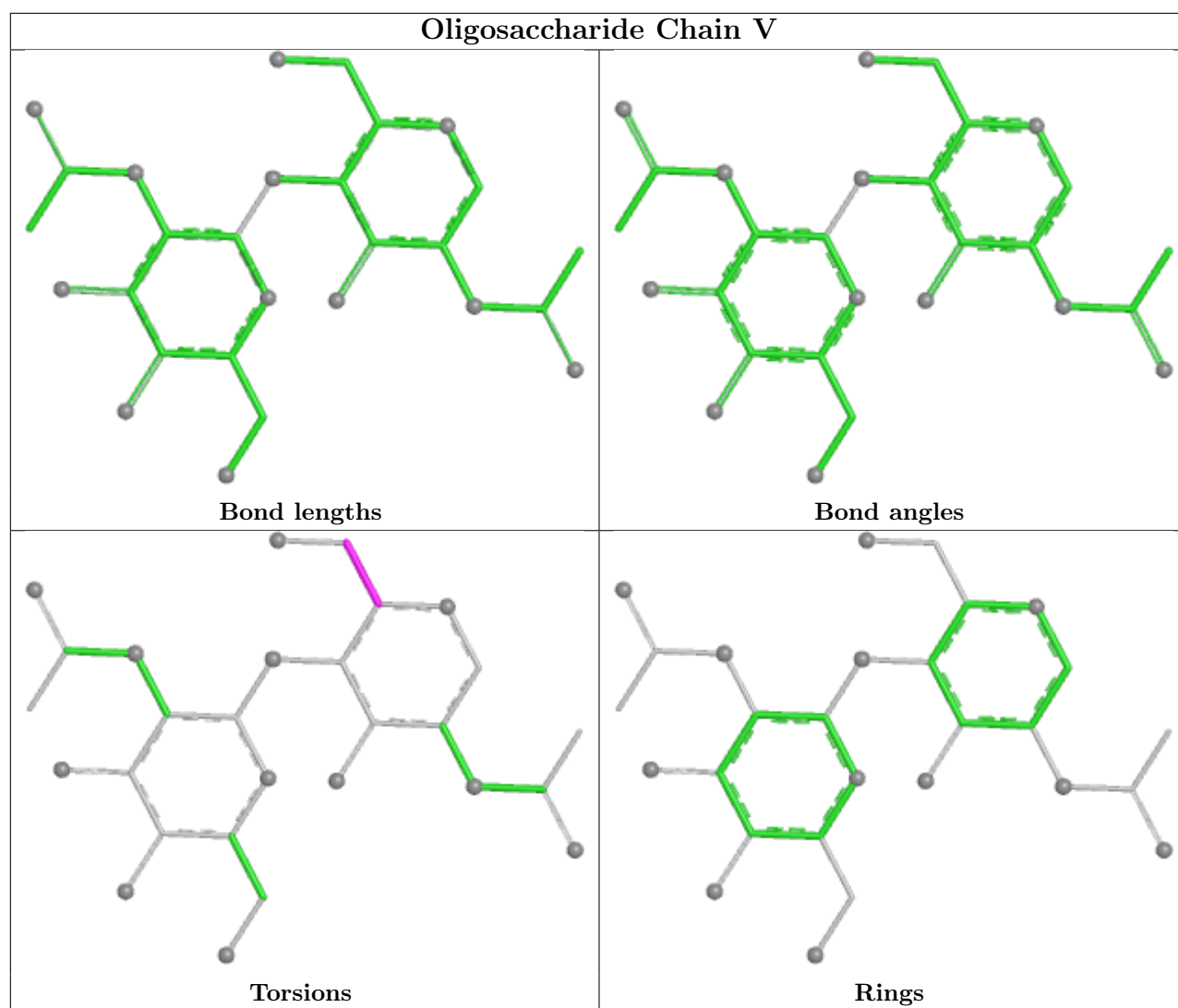


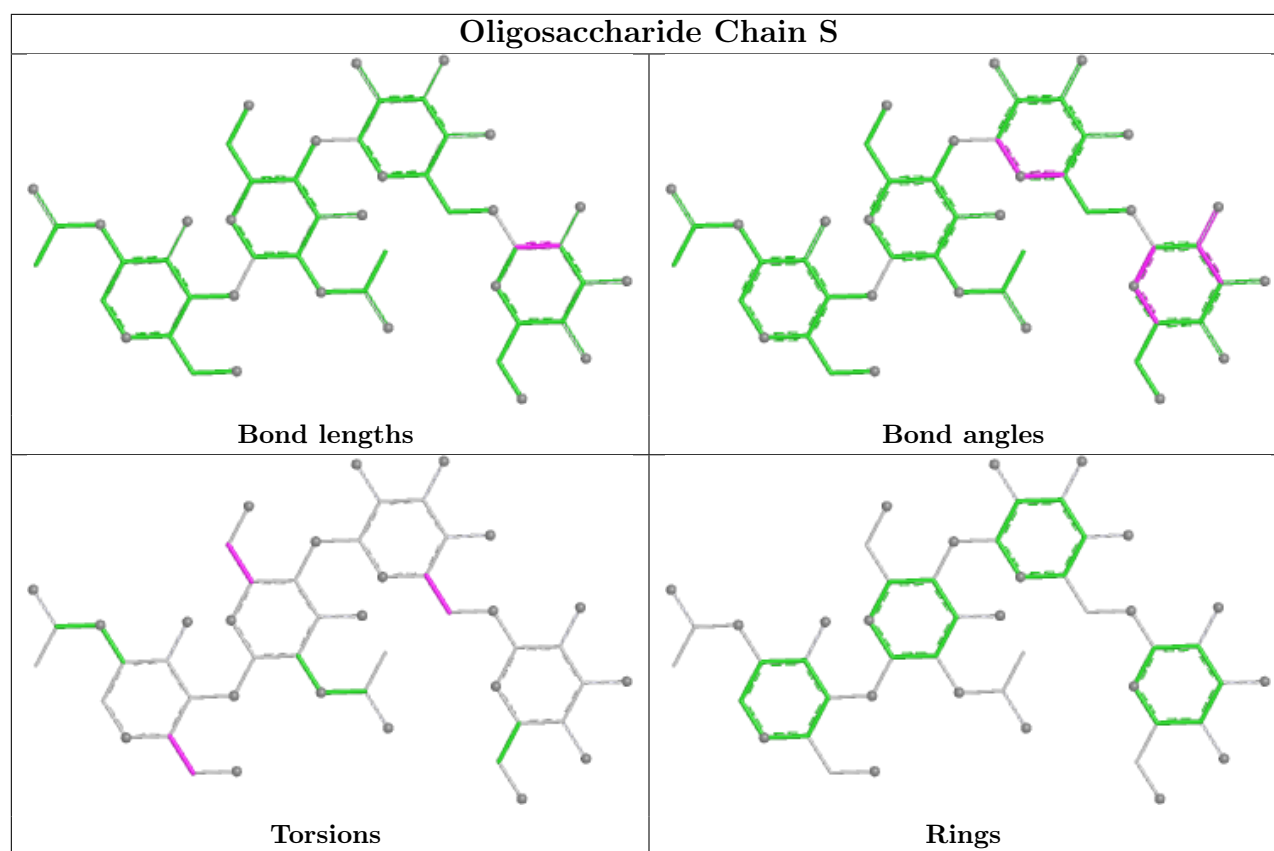












5.6 Ligand geometry [i](#)

15 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	NAG	B	1301	1	14,14,15	0.28	0	17,19,21	0.41	0
6	NAG	C	1304	1	14,14,15	0.47	0	17,19,21	0.72	1 (5%)
6	NAG	A	1301	1	14,14,15	0.42	0	17,19,21	0.75	1 (5%)
6	NAG	A	1305	1	14,14,15	0.44	0	17,19,21	0.54	0
6	NAG	B	1320	1	14,14,15	0.27	0	17,19,21	0.66	1 (5%)
6	NAG	C	1320	1	14,14,15	0.47	0	17,19,21	0.63	1 (5%)
6	NAG	A	1310	1	14,14,15	0.23	0	17,19,21	0.65	1 (5%)
6	NAG	C	1312	1	14,14,15	0.35	0	17,19,21	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	B	1308	1	14,14,15	0.33	0	17,19,21	0.49	0
6	NAG	C	1307	1	14,14,15	0.32	0	17,19,21	0.34	0
6	NAG	A	1316	1	14,14,15	0.46	0	17,19,21	0.67	1 (5%)
6	NAG	C	1308	1	14,14,15	0.27	0	17,19,21	0.67	1 (5%)
6	NAG	C	1301	1	14,14,15	0.36	0	17,19,21	0.64	1 (5%)
6	NAG	B	1321	1	14,14,15	0.27	0	17,19,21	0.46	0
6	NAG	B	1311	1	14,14,15	0.41	0	17,19,21	0.43	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	B	1301	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1304	1	-	0/6/23/26	0/1/1/1
6	NAG	A	1301	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1305	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1320	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1320	1	-	0/6/23/26	0/1/1/1
6	NAG	A	1310	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1312	1	-	0/6/23/26	0/1/1/1
6	NAG	B	1308	1	-	1/6/23/26	0/1/1/1
6	NAG	C	1307	1	-	1/6/23/26	0/1/1/1
6	NAG	A	1316	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1308	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1301	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1321	1	-	0/6/23/26	0/1/1/1
6	NAG	B	1311	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1301	NAG	C1-O5-C5	2.58	115.65	112.19
6	C	1304	NAG	C1-O5-C5	2.58	115.65	112.19
6	B	1320	NAG	C1-O5-C5	2.38	115.37	112.19
6	A	1316	NAG	C1-O5-C5	2.35	115.34	112.19
6	C	1308	NAG	C1-O5-C5	2.32	115.30	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1310	NAG	C1-O5-C5	2.18	115.11	112.19
6	C	1301	NAG	C1-O5-C5	2.15	115.06	112.19
6	C	1320	NAG	C1-O5-C5	2.12	115.03	112.19

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1316	NAG	O5-C5-C6-O6
6	A	1301	NAG	O5-C5-C6-O6
6	B	1320	NAG	O5-C5-C6-O6
6	A	1316	NAG	C4-C5-C6-O6
6	A	1301	NAG	C4-C5-C6-O6
6	A	1305	NAG	O5-C5-C6-O6
6	B	1311	NAG	C4-C5-C6-O6
6	A	1310	NAG	O5-C5-C6-O6
6	B	1311	NAG	O5-C5-C6-O6
6	B	1301	NAG	O5-C5-C6-O6
6	B	1301	NAG	C4-C5-C6-O6
6	B	1320	NAG	C4-C5-C6-O6
6	A	1310	NAG	C4-C5-C6-O6
6	C	1308	NAG	O5-C5-C6-O6
6	C	1301	NAG	O5-C5-C6-O6
6	C	1308	NAG	C4-C5-C6-O6
6	C	1301	NAG	C4-C5-C6-O6
6	B	1308	NAG	O5-C5-C6-O6
6	A	1305	NAG	C4-C5-C6-O6
6	C	1307	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
6	B	1301	NAG	1	0
6	A	1310	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

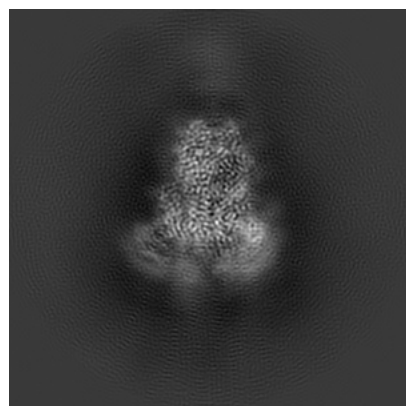
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7577. These allow visual inspection of the internal detail of the map and identification of artifacts.

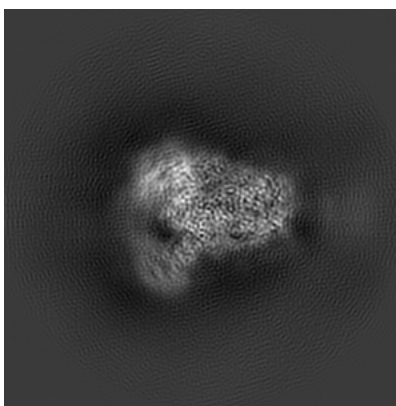
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

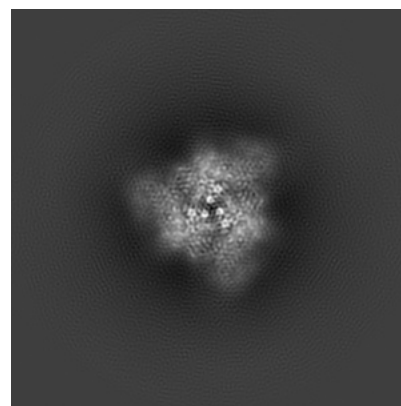
6.1.1 Primary map



X

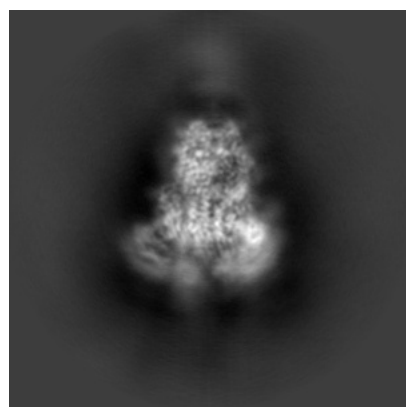


Y

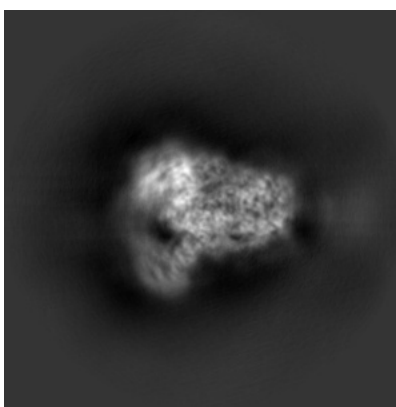


Z

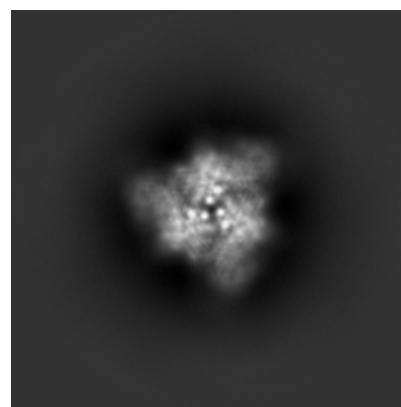
6.1.2 Raw map



X



Y

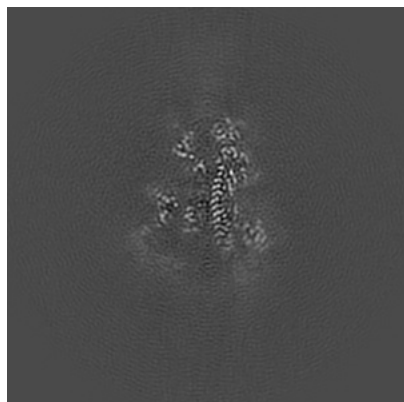


Z

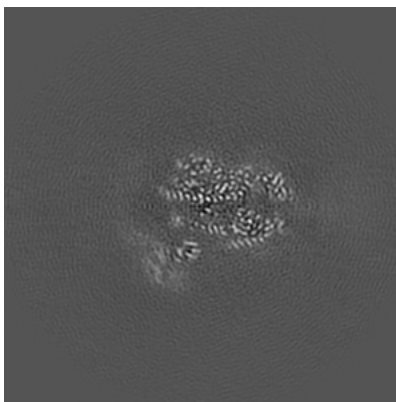
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

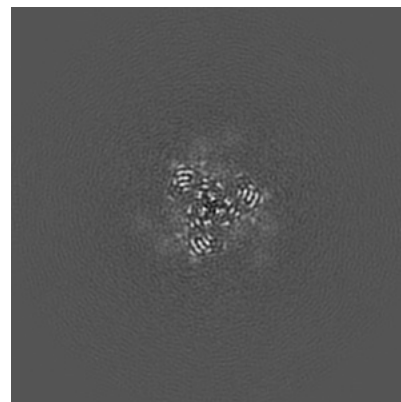
6.2.1 Primary map



X Index: 160

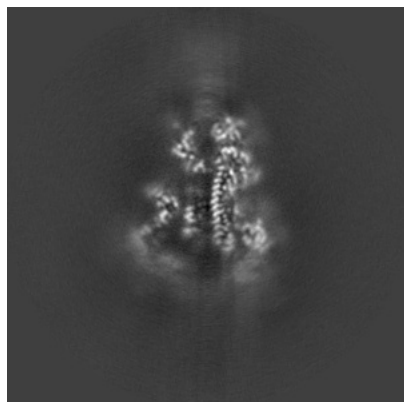


Y Index: 160

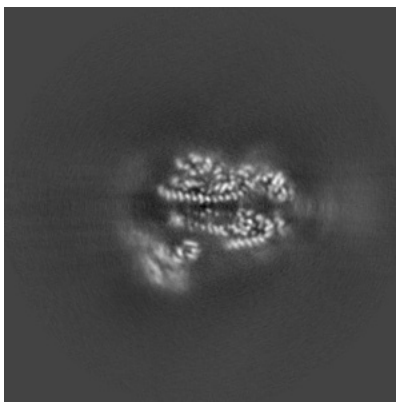


Z Index: 160

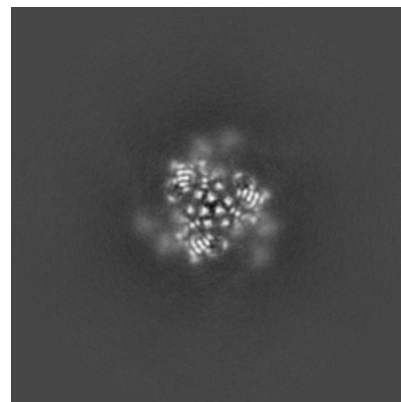
6.2.2 Raw map



X Index: 160



Y Index: 160

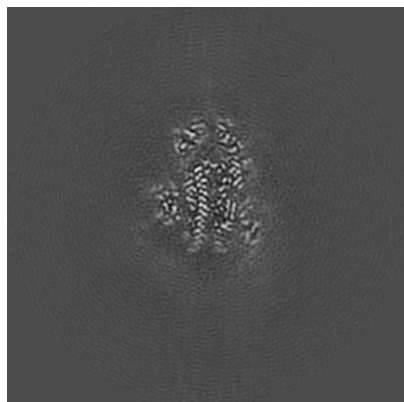


Z Index: 160

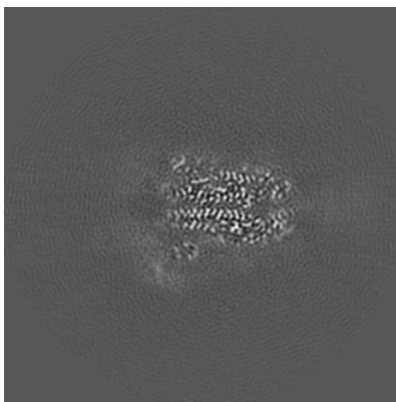
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

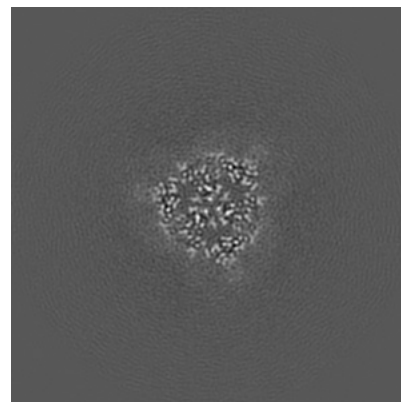
6.3.1 Primary map



X Index: 154

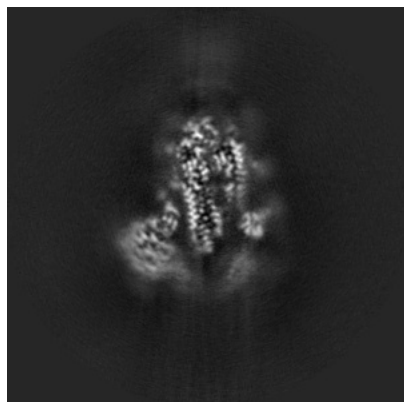


Y Index: 155

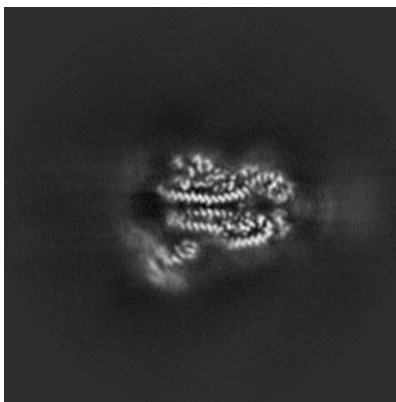


Z Index: 148

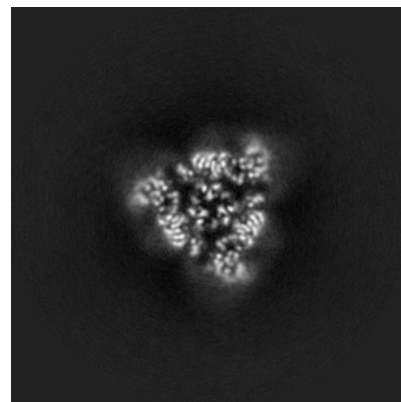
6.3.2 Raw map



X Index: 171



Y Index: 158

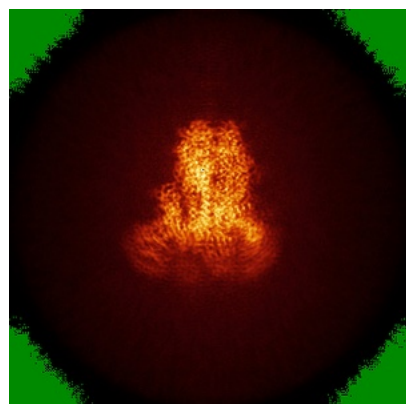


Z Index: 144

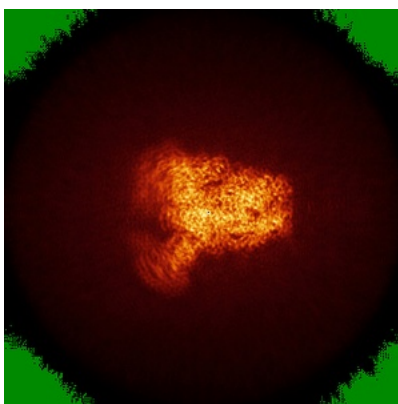
The images above show the largest variance slices of the map in three orthogonal directions.

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

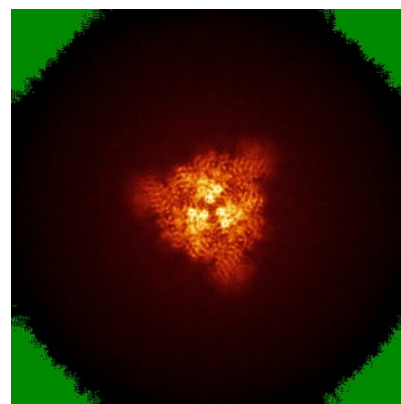
6.4.1 Primary map



X

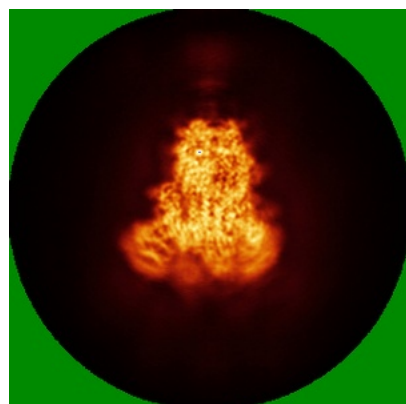


Y

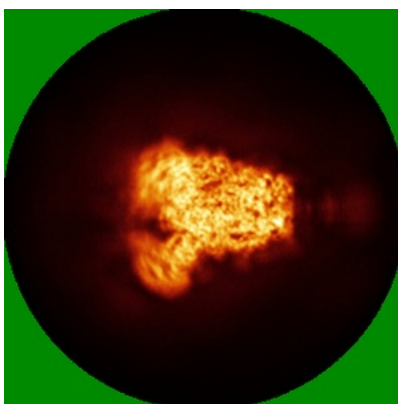


Z

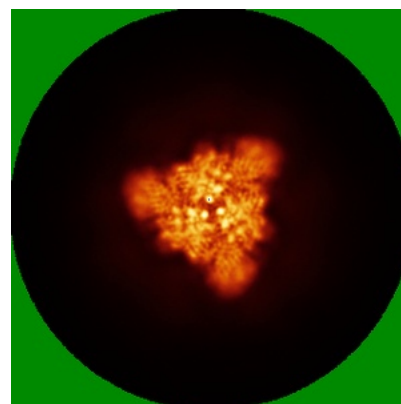
6.4.2 Raw map



X



Y



Z

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

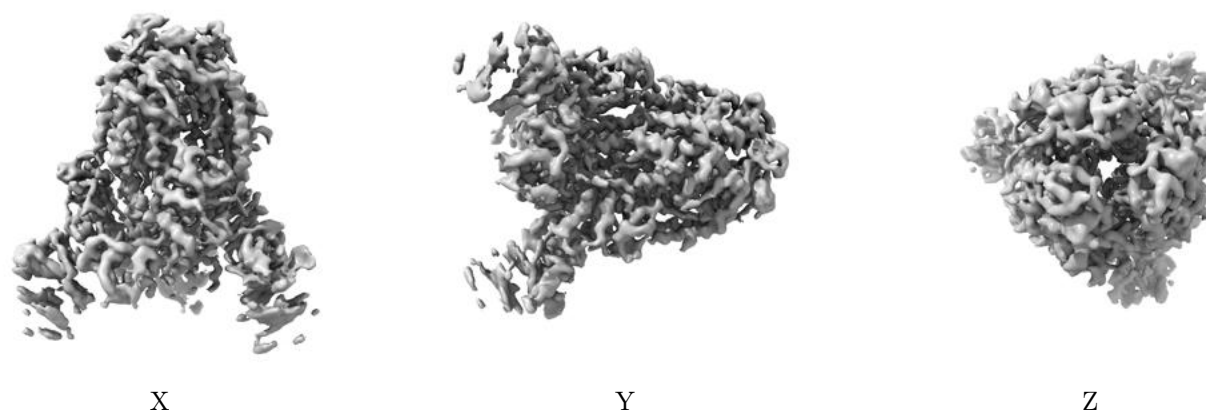
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.069. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

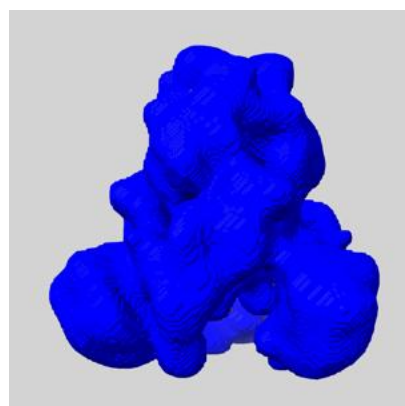
6.6 Mask visualisation [i](#)

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

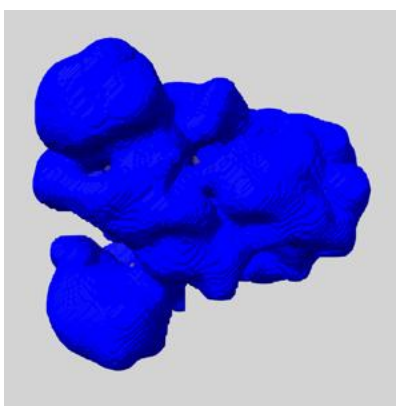
A mask typically either:

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

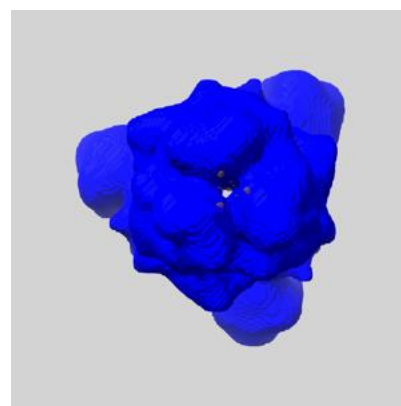
6.6.1 emd_7577_msk_1.map [i](#)



X



Y

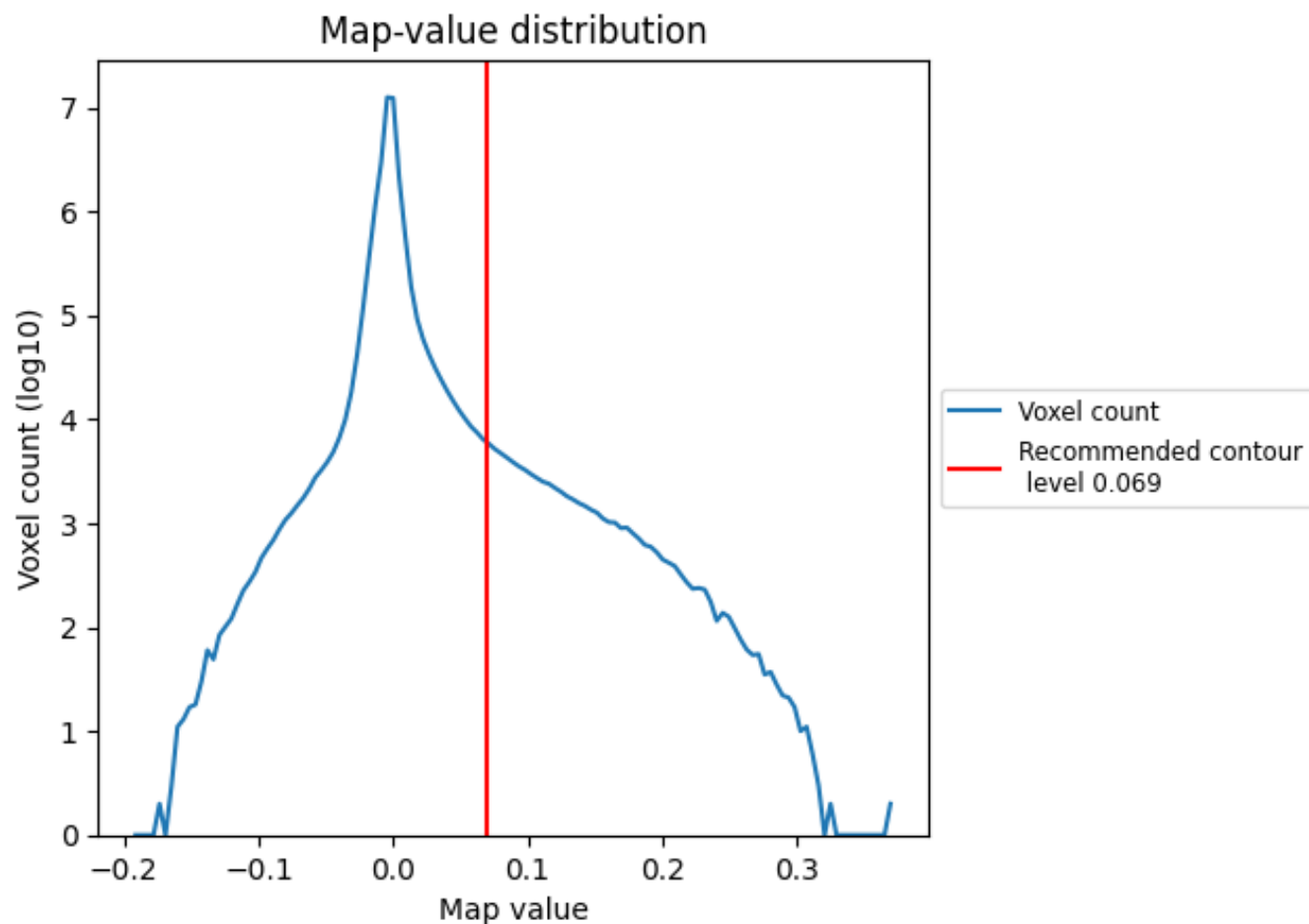


Z

7 Map analysis [i](#)

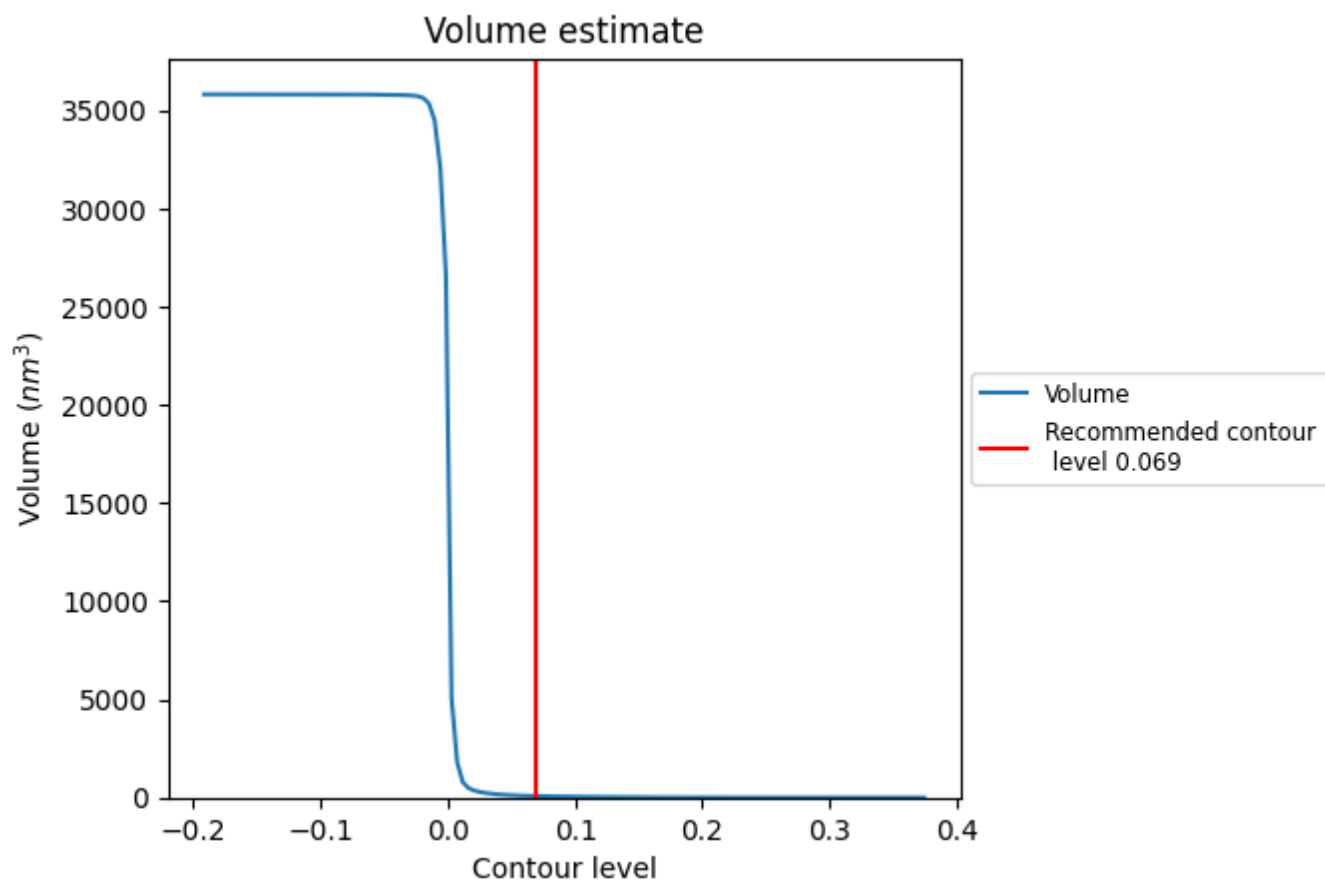
This section contains the results of statistical analysis of the map.

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.

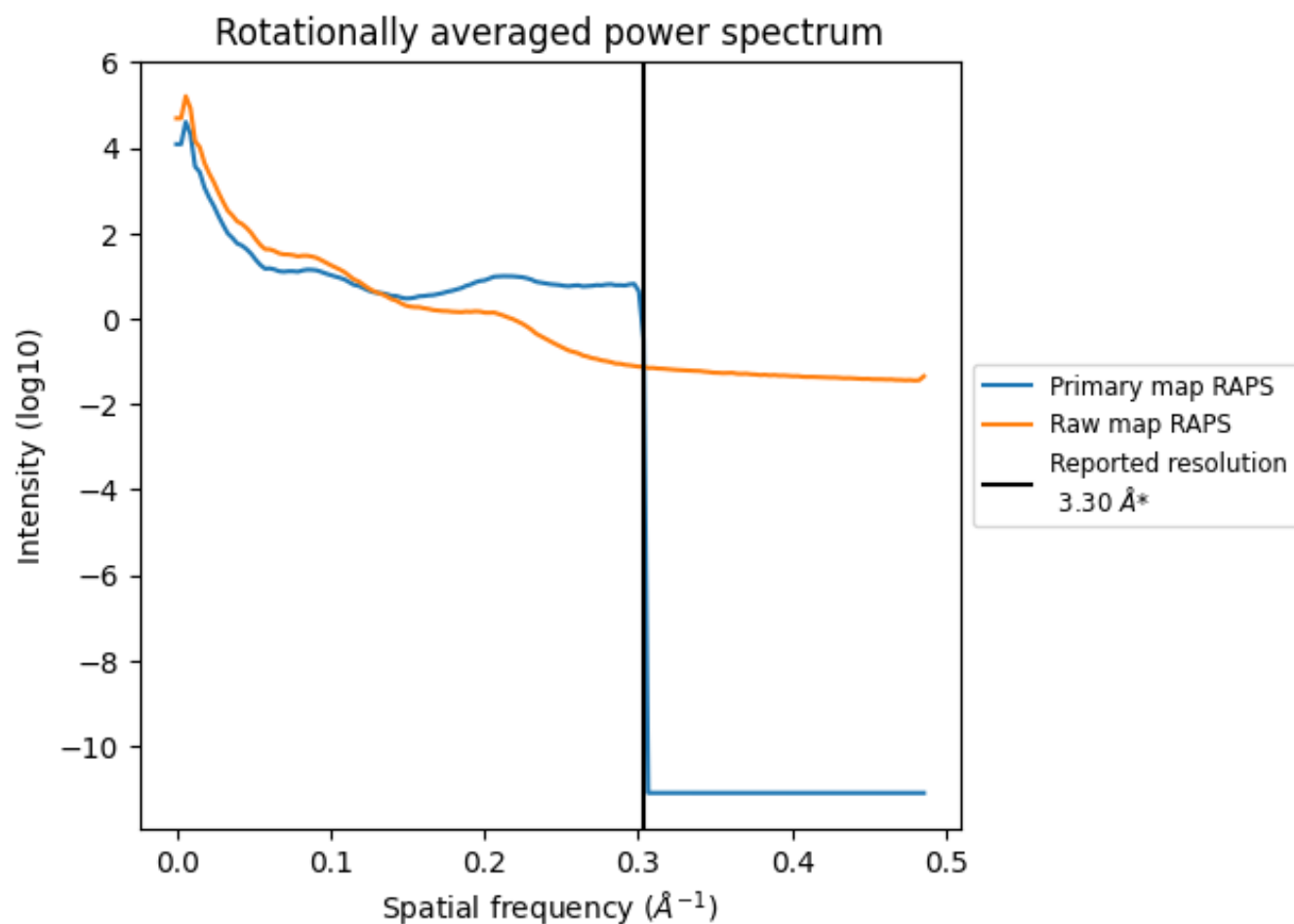
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 76 nm³; this corresponds to an approximate mass of 69 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 ⓘ

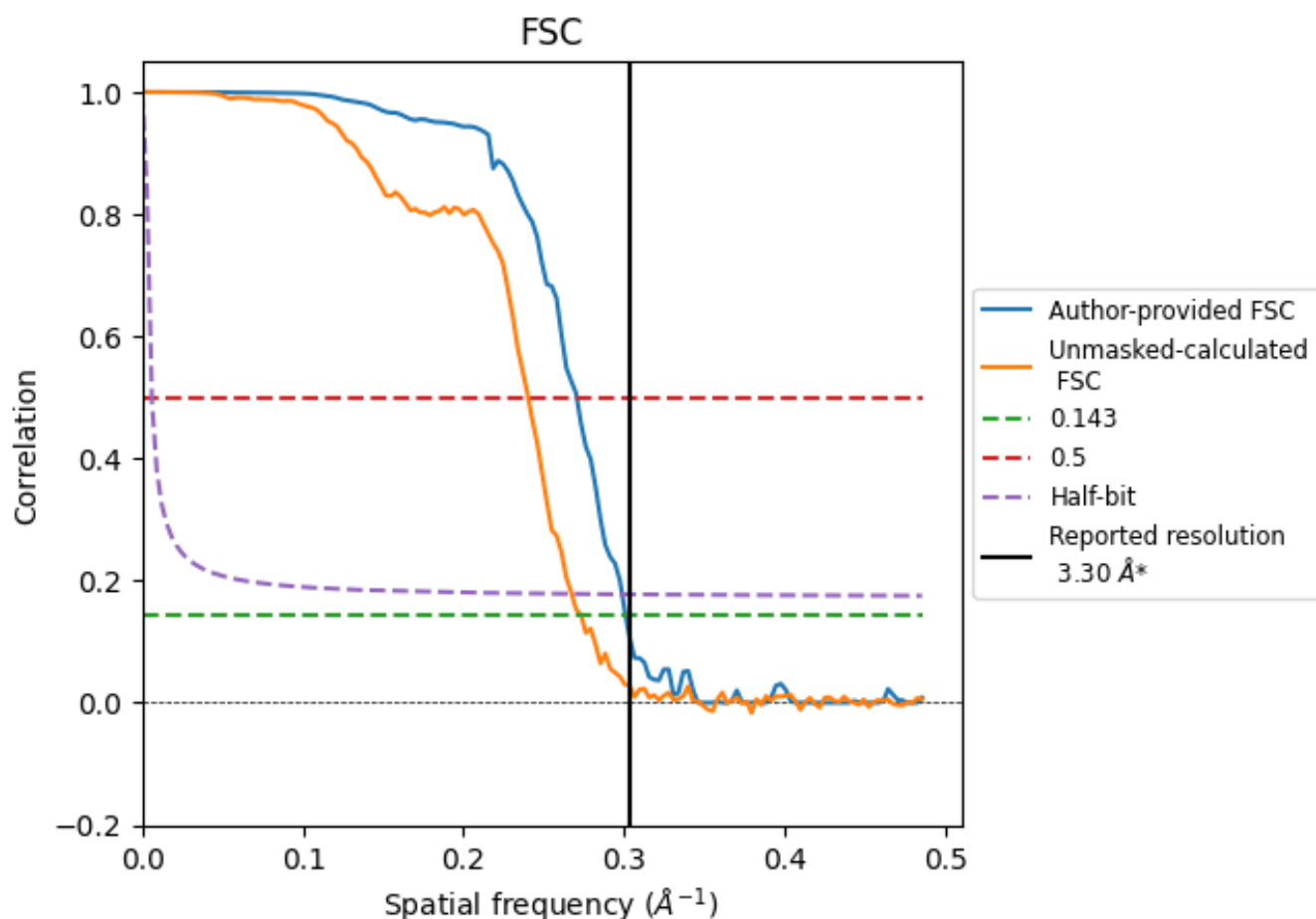


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.303 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.32	3.70	3.35
Unmasked-calculated*	3.66	4.16	3.74

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.66 differs from the reported value 3.3 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-7577 and PDB model 6CRZ. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)

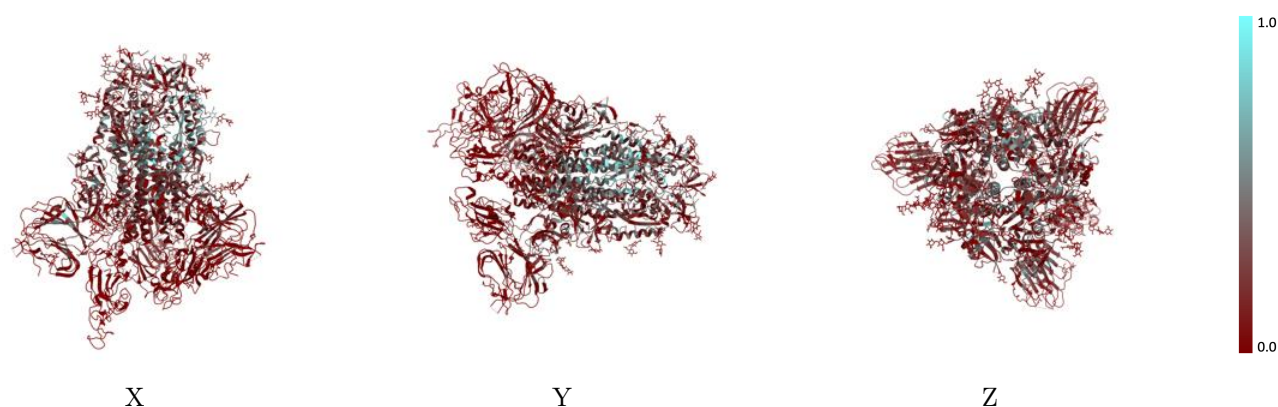
This section was not generated.

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



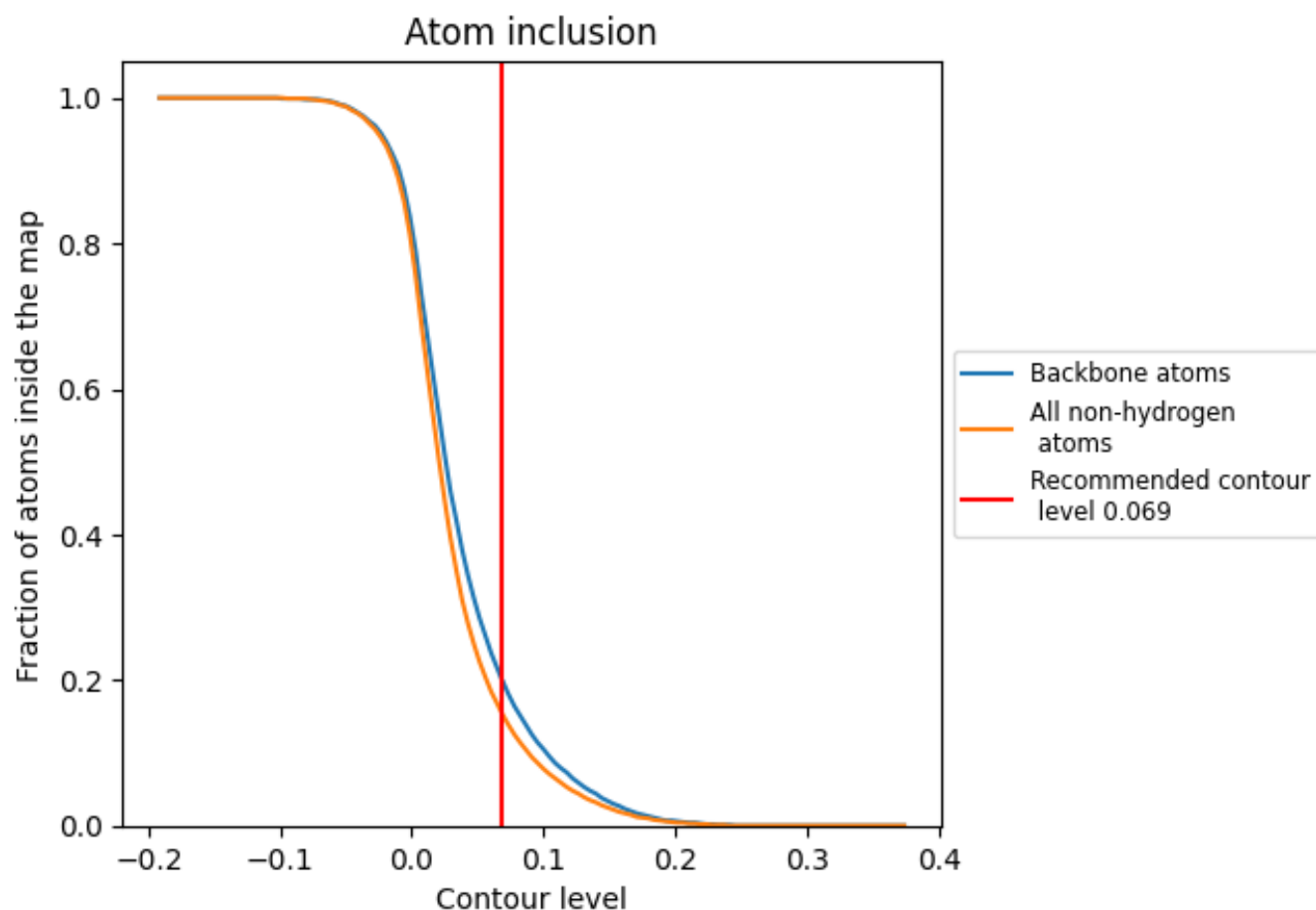
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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 (0.069).

9.4 Atom inclusion [i](#)



At the recommended contour level, 20% of all backbone atoms, 15% 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 (0.069) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.1530	 0.0120
A	 0.1340	 -0.0150
B	 0.1700	 0.0210
C	 0.1640	 0.0260
D	 0.0000	 0.0350
E	 0.0000	 0.0250
F	 0.0260	 0.0960
G	 0.0000	 0.0900
H	 0.0000	 -0.1420
I	 0.0360	 0.1790
J	 0.0000	 0.0160
K	 0.0000	 0.1370
L	 0.0000	 -0.0100
M	 0.1030	 0.1100
N	 0.2310	 0.1470
O	 0.0710	 0.0270
P	 0.0000	 0.0610
Q	 0.0000	 0.0040
R	 0.0260	 0.0140
S	 0.0000	 0.0070
T	 0.0000	 -0.0360
U	 0.1790	 0.1640
V	 0.0000	 -0.0670

