



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 02:33 AM UTC

PDB ID : 6CS1 / pdb_00006cs1
EMDB ID : EMD-7579
Title : SARS Spike Glycoprotein, Trypsin-cleaved, Stabilized variant, two S1 CTDs in an upwards conformation
Authors : Kirchdoerfer, R.N.; Wang, N.; Pallesen, J.; Turner, H.L.; Cottrell, C.A.; McLellan, J.S.; Ward, A.B.
Deposited on : 2018-03-19
Resolution : 4.60 Å (reported)
Based on initial models : 5X4S, 5I08, 2AJF

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:

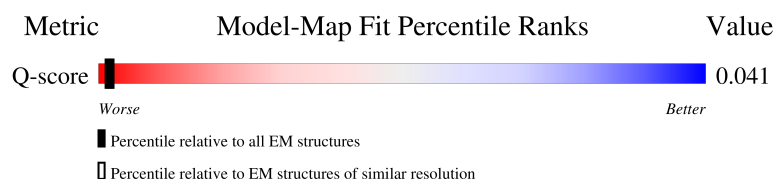
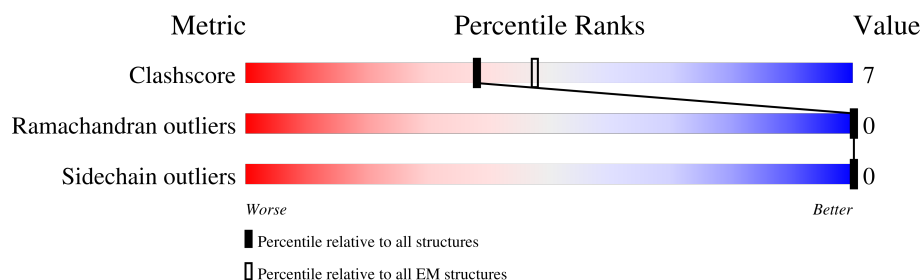
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13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

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2407 (4.10 - 5.10)

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	1215	52% 71% 17% 12%
1	B	1215	44% 71% 17% 12%
1	C	1215	45% 70% 18% 12%
2	D	2	100% 50% 50%

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Mol	Chain	Length	Quality of chain
2	F	2	100%
2	I	2	100%
2	J	2	100%
2	K	2	100%
2	M	2	100%
2	R	2	100%
2	T	2	100%
2	W	2	100%
3	E	3	100%
3	L	3	100%
3	Q	3	33%
3	U	3	100%
3	V	3	100%
3	X	3	100%
4	G	5	100%
4	H	5	60%
4	S	5	100%
5	N	4	100%
5	O	4	100%
5	P	4	50%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 25995 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

There are 42 discrepancies between the modelled and reference sequences:

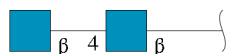
Chain	Residue	Modelled	Actual	Comment	Reference
B	577	ALA	SER	conflict	UNP P59594
B	968	PRO	LYS	engineered mutation	UNP P59594
B	969	PRO	VAL	engineered mutation	UNP P59594
B	1191	GLY	-	linker	UNP P59594
B	1192	SER	ALA	linker	UNP D9IEJ2
B	1220	GLY	-	expression tag	UNP D9IEJ2
B	1221	ARG	-	expression tag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

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

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



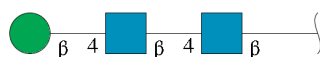
Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	2	Total	C	N	O	0	0
			28	16	2	10		
2	F	2	Total	C	N	O	0	0
			28	16	2	10		
2	I	2	Total	C	N	O	0	0
			28	16	2	10		
2	J	2	Total	C	N	O	0	0
			28	16	2	10		
2	K	2	Total	C	N	O	0	0
			28	16	2	10		
2	M	2	Total	C	N	O	0	0
			28	16	2	10		
2	R	2	Total	C	N	O	0	0
			28	16	2	10		

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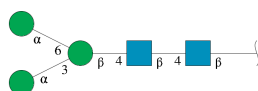
Mol	Chain	Residues	Atoms				AltConf	Trace
2	T	2	Total	C	N	O	0	0
			28	16	2	10		
2	W	2	Total	C	N	O	0	0
			28	16	2	10		

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



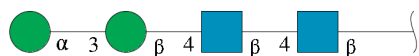
Mol	Chain	Residues	Atoms				AltConf	Trace
3	E	3	Total	C	N	O	0	0
			39	22	2	15		
3	L	3	Total	C	N	O	0	0
			39	22	2	15		
3	Q	3	Total	C	N	O	0	0
			39	22	2	15		
3	U	3	Total	C	N	O	0	0
			39	22	2	15		
3	V	3	Total	C	N	O	0	0
			39	22	2	15		
3	X	3	Total	C	N	O	0	0
			39	22	2	15		

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



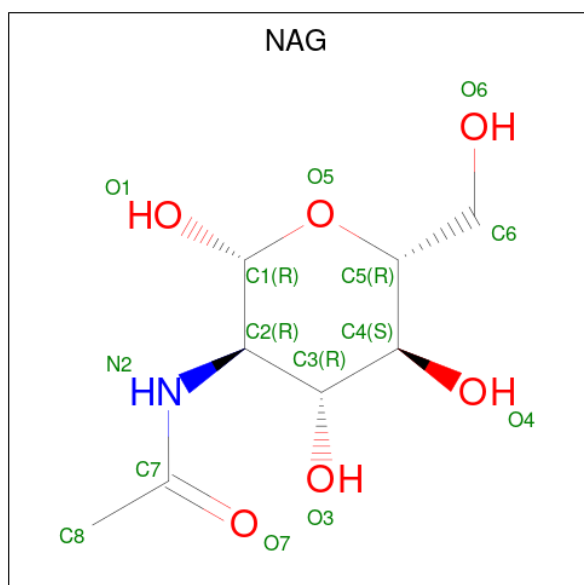
Mol	Chain	Residues	Atoms				AltConf	Trace
4	G	5	Total	C	N	O	0	0
			61	34	2	25		
4	H	5	Total	C	N	O	0	0
			61	34	2	25		
4	S	5	Total	C	N	O	0	0
			61	34	2	25		

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



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

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



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	B	1	Total	C	N	O	0
			14	8	1	5	

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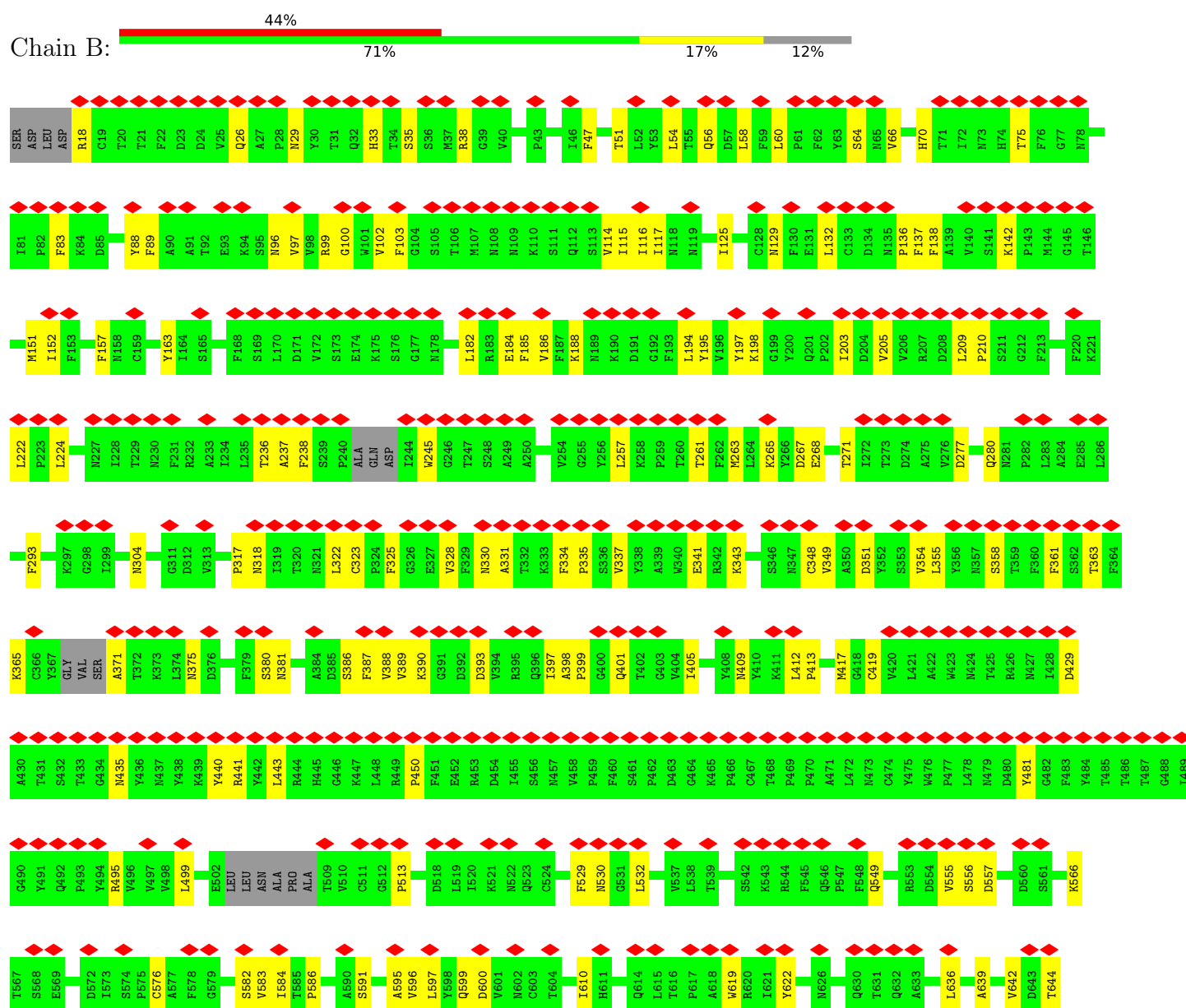
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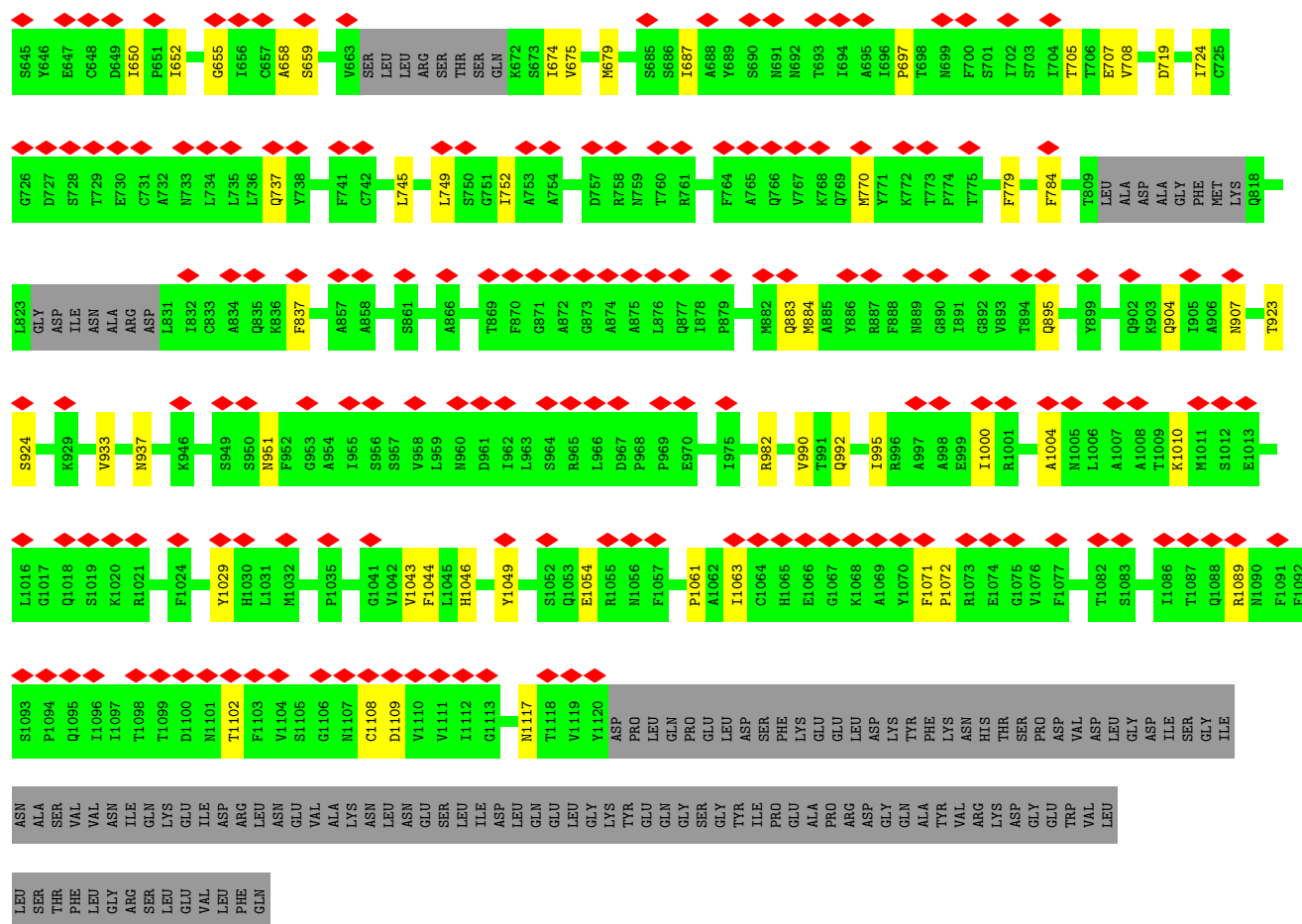
Mol	Chain	Residues	Atoms				AltConf
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	A	1	Total	C	N	O	0
			14	8	1	5	

3 Residue-property plots

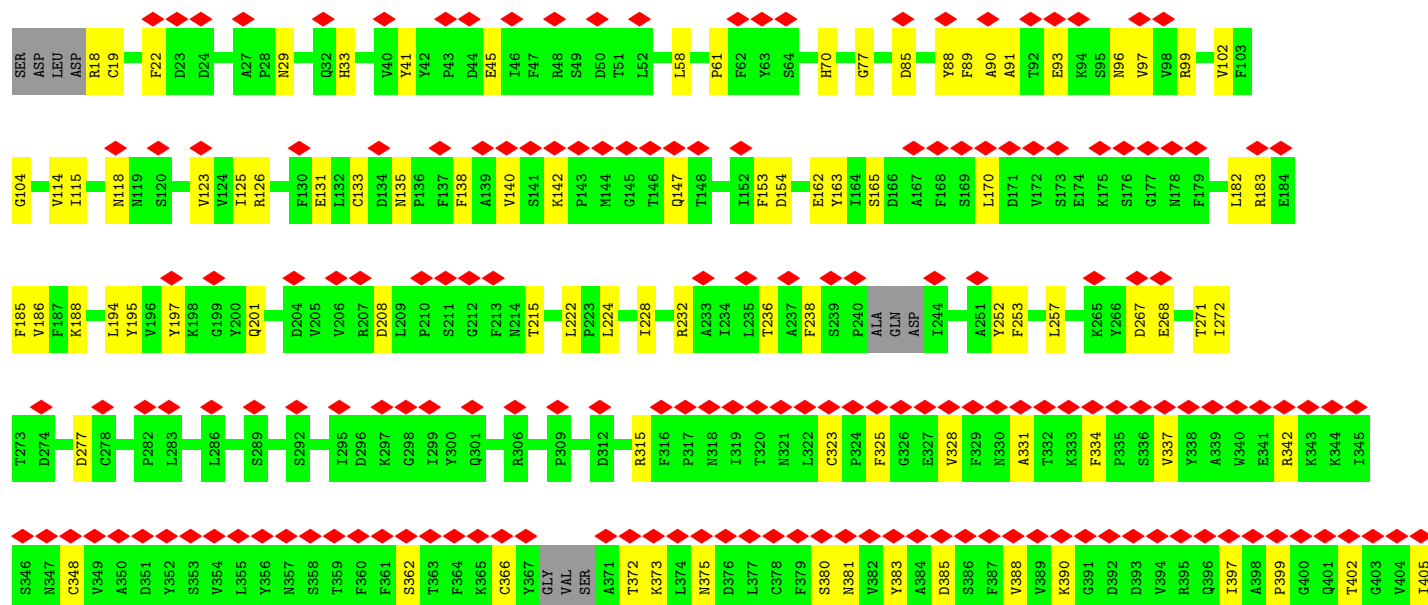
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

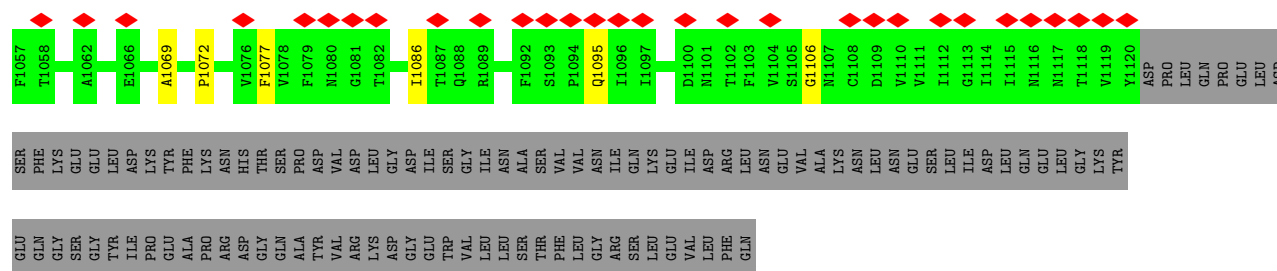




• Molecule 1: Spike glycoprotein,Fibrin



Q974	R882	V990	R996	E999	I1000	R1001	A1002	S1003	N1005	L1006	A1007	K1010	M1011	L1016	G1017	Q1018	S1019	K1020	N1021	V1022	D1023	G1026	K1027	G1028	H1029	N1030	L1031	M1032	S1033	F1034	P1035	Q1036	A1037	A1038	P1039	H1040	A954	G1041	V1042	N956	V1043	F1044	L1045	L1046	V1047	V1050	P1051	S1052	Q1053	E1054	R1055	N1056																																								
Q904	I905	A906	N907	Q908	F909	N910	K911	S914	Q915	I916	S917	D850	M851	A852	A853	A854	T855	T856	A857	A858	L859	V860	T863	A864	T865	A866	E801	E801	E802	E802	A874	A875	L876	Q877	T878	P879	F880	A881	N882	Q883	M884	A885	Y886	R887	F888	G892	V893	T894	Q895	N896	V897	E900	A971																																							
F837	L840	T841	V842	L843	P844	L847	T848	D849	D850	M851	L852	A853	A854	T855	T856	A857	A858	L859	V860	T863	A864	T865	A866	G867	W868	F870	G871	A872	N807	V808	T809	LEU	ALA	ASP	ALA	GLY	PHE	MET	LYS	Q818	E821	C822	L823	GLY	ASP	ILE	ASN	ALA	ARG	ASP	LEU	T832	C833	A834	Q835	R836																																				
M770	Y771	P774	T775	L776	G780	G781	F782	N783	D784	M785	T786	E787	D790	T791	T792	T793	T794	T795	T796	T797	T798	T799	T800	T801	T802	T803	T804	T805	T806	T807	T808	T809	T810	T811	T812	T813	T814	T815	T816	T817	T818	T819	T820	T821	T822	T823	T824	T825	T826	T827	T828	T829	T830	T831	T832	T833	T834	T835	T836	T837	T838	T839	T840	T841	T842	T843	T844	T845	T846	T847	T848	T849	T850	T851	T852	T853	T854	T855	T856	T857	T858	T859	T860	T861	T862	T863	T864	T865	T866	T867	T868	T869
N691	N692	A695	T698	N699	F700	S701	I702	S703	I704	T705	T706	E707	V708	S712	M713	A714	K715	T716	Y723	T724	G725	G726	D727	G731	L734	Q737	Y738	F741	G742	L745	A748	L749	I752	A753	D757	R758	N759	T760	F761	E762	V763	F764	A765	Q766	Y767	K768	Q769																																													
Y622	S623	T624	G625	N626	N627	V628	Q632	A633	G634	C635	L636	T637	G638	A639	E640	H641	V642	D643	Y646	E647	C648	D649	L650	P651	G653	A654	G655	L656	C657	A658	S659	T662	VAL	SER	LEU	LEU	ARG	SER	THR	SER	G1N	K672	S673	T674	V675	A676	Y677	T678	A683	D684	L688	T689	S690																																							
P469	P470	A471	L472	N473	C474	Y475	N476	P477	N479	D480	Y481	G482	F483	Y484	T485	T486	T487	G488	L489	G490	Y491	Q492	P493	Y494	R495	Y496	Y497	V498	L499	S500	F501	E502	LEU	LEU	ASN	ALA	PRO	ALA	T509	V510	C511	G512	P513	K514	L515	S516	L519	N528	F529	N530	G531	L532	R544	F545	Q546																																					
Q549	R553	D554	V555	S556	D557	D564	P565	K566	T567	S568	E569	D572	L573	A577	Y581	S582	V583	L584	T585	P586	G587	T588	S591	S592	E593	Y594	L597	Y598	Q599	D600	V601	N602	C603	T604	D605	V606	S607	T608	L609	L610	H611	M612	D613	Q614	L615	T616	P617	A618	Y619	R620	T621																																									
Y408	N409	Y410	K411	L412	P413	D414	D415	F416	M417	V420	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	D452	R453	D454	I455	S456	N457	V458	P459	F460	S461	P462	D463	G464	K465	P466	C467	T468																																		
C348	V349	A350	D351	Y352	S353	V354	L355	Y356	N357	S358	T359	F360	F361	S362	T363	F364	K365	C366	GLY	VAL	SER	A371	T372	K373	L374	N375	D376	L377	C378	F379	S380	N381	V382	Y383	A384	D385	S386	F387	V388	V389	K390	G391	D392	D393	V394	R395	Q396	I397	A398	P399	G400	Q401	T402	G403	V404	T405	A406	D407																																		
C278	S279	E285	L286	K287	C288	S289	V290	K291	I295	D296	K297	G298	Q301	T302	S303	N304	F305	R306	V307	V308	P309	S310	V314	P317	N318	I319	T320	N321	L322	C323	F324	F325	G326	G327	V328	F329	N330	A331	T332	K333	F334	P335	S336	V337	Y338	A339	W340	E341	R342	K343	K344	I345	S346	N347																																						
T215	L216	I219	F220	K221	L222	L224	G225	A226	N227	I228	T229	N230	F231	R232	A233	I234	L235	T236	A237	F238	S239	P240	A1A	G1N	ASP	I244	V245	G246	T247	S248	A249	A250	A251	Y252	F253	V254	G255	Y256	L257	K258	P259	T260	T261	L264	K265	Y266	N269	G270	T271	I272	T273	D274	A275	V276	D277																																					
T146	Q147	T148	H149	D154	N155	A156	F157	N158	C159	T160	F161	E162	Y163	I164	S165	D166	A167	F168	S169	L170	D171	V172	S173	E174	K175	S176	G177	N178	F179	K180	H181	L182	R183	E184	F185	V186	F187	K188	N189	K190	D191	G192	F193	L194	Y195	V196	Y197	K198	G199	I203	D204	L209	P210	S211	N214																																					
I81	P82	F83	K84	D85	G86	I87	Y88	F89	A90	T91	T92	E93	K94	S95	R99	G100	M101	V102	F103	G104	S105	T106	M107	N108	N109	K110	S111	Q112	S113	V114	I115	I116	I117	N118	N119	F185	V186	T121	N122	V123	V124	I125	C128	N129	F130	E131	L132	C133	D134	N135	A139	V140	S141	K142	P143	M144	G145																																			



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



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



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



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



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





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



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



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



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



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



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



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



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



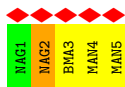
- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



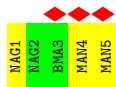
- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



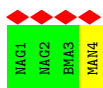
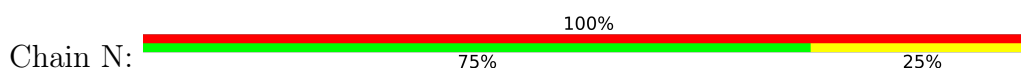
- Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



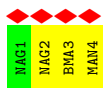
- Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	15314	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	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	0.131	Depositor
Minimum map value	-0.070	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.032	Depositor
Map size (Å)	329.59998, 329.59998, 329.59998	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.03, 1.03, 1.03	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, 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	0.23	0/8526	0.52	0/11601
1	B	0.23	0/8541	0.52	2/11622 (0.0%)
1	C	0.23	0/8538	0.51	0/11617
All	All	0.23	0/25605	0.51	2/34840 (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	1
All	All	0	3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	83	PHE	CA-C-N	5.05	131.19	121.54
1	B	83	PHE	C-N-CA	5.05	131.19	121.54

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	35	SER	Peptide
1	B	576	CYS	Peptide

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Mol	Chain	Res	Type	Group
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	8327	0	8068	137	0
1	B	8342	0	8088	128	0
1	C	8339	0	8082	146	0
2	D	28	0	25	1	0
2	F	28	0	25	0	0
2	I	28	0	25	0	0
2	J	28	0	25	1	0
2	K	28	0	25	0	0
2	M	28	0	25	0	0
2	R	28	0	25	0	0
2	T	28	0	25	0	0
2	W	28	0	25	0	0
3	E	39	0	34	0	0
3	L	39	0	34	1	0
3	Q	39	0	34	1	0
3	U	39	0	34	0	0
3	V	39	0	34	0	0
3	X	39	0	34	0	0
4	G	61	0	52	1	0
4	H	61	0	52	0	0
4	S	61	0	52	2	0
5	N	50	0	43	0	0
5	O	50	0	43	1	0
5	P	50	0	43	0	0
6	A	70	0	65	0	0
6	B	56	0	52	0	0
6	C	42	0	39	1	0
All	All	25995	0	25108	376	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 (376) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1089:ARG:HH21	1:C:876:LEU:HB2	1.57	0.68
1:A:188:LYS:HB2	1:A:195:TYR:HB2	1.76	0.67
1:A:390:LYS:HE3	1:A:392:ASP:HB2	1.75	0.66
1:C:93:GLU:HG3	1:C:183:ARG:HH21	1.59	0.66
1:C:131:GLU:HB2	1:C:154:ASP:HB2	1.77	0.65
1:B:341:GLU:HB3	1:B:386:SER:HB3	1.79	0.64
1:B:363:THR:HB	1:B:365:LYS:HG3	1.79	0.64
1:C:342:ARG:NH2	1:A:223:PRO:O	2.32	0.63
1:C:61:PRO:HB3	1:C:620:ARG:HH12	1.63	0.63
1:B:549:GLN:HA	1:C:45:GLU:HB2	1.81	0.63
1:C:901:ASN:HB3	1:C:904:GLN:HB3	1.81	0.62
1:C:366:CYS:HB2	1:C:373:LYS:HD2	1.81	0.62
1:B:582:SER:HB2	1:B:597:LEU:HB3	1.81	0.62
1:B:33:HIS:HB2	1:B:66:VAL:HB	1.80	0.61
1:C:449:ARG:NH2	1:A:189:ASN:O	2.34	0.61
1:B:390:LYS:HG3	1:B:481:TYR:HD1	1.64	0.61
1:B:1029:TYR:HB2	1:B:1049:TYR:HB3	1.83	0.61
1:A:636:LEU:HD21	1:A:639:ALA:HB3	1.83	0.61
1:A:745:LEU:HD22	1:A:990:VAL:HG21	1.81	0.61
1:C:91:ALA:HB3	1:C:183:ARG:HB2	1.83	0.60
1:C:529:PHE:HB2	1:C:532:LEU:HB2	1.83	0.60
1:C:547:PRO:HA	1:C:563:ARG:HH12	1.65	0.60
1:A:94:LYS:HB3	1:A:179:PHE:HA	1.82	0.60
1:B:555:VAL:HG11	1:C:818:GLN:HE22	1.67	0.60
1:C:421:LEU:HB3	1:C:497:VAL:HB	1.83	0.60
1:C:962:ILE:HG23	1:C:966:LEU:HD12	1.82	0.60
1:C:90:ALA:HB3	1:C:253:PHE:HB2	1.82	0.60
1:B:600:ASP:O	1:C:835:GLN:NE2	2.35	0.60
1:B:188:LYS:HB2	1:B:195:TYR:HB2	1.84	0.59
1:B:237:ALA:HB1	1:B:245:TRP:HB3	1.83	0.59
1:B:655:GLY:HA2	1:B:679:MET:HE2	1.84	0.59
1:B:322:LEU:HD22	1:B:351:ASP:HB3	1.84	0.59
1:B:419:CYS:HB2	1:B:499:LEU:HB2	1.84	0.59
1:B:659:SER:O	1:B:675:VAL:HG22	2.02	0.59
1:B:707:GLU:OE1	1:B:1046:HIS:NE2	2.35	0.59
1:C:18:ARG:N	1:C:153:PHE:O	2.35	0.59
1:C:277:ASP:OD2	1:C:620:ARG:NH2	2.35	0.59
1:B:337:VAL:HG22	1:B:387:PHE:HB2	1.85	0.59
1:A:659:SER:OG	1:A:675:VAL:CG2	2.51	0.59
1:B:331:ALA:HB3	1:B:334:PHE:HE1	1.68	0.59
1:C:562:VAL:HG13	1:C:573:ILE:HD11	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:133:CYS:O	1:C:232:ARG:NH2	2.37	0.58
1:A:582:SER:HB2	1:A:597:LEU:HB3	1.86	0.58
1:C:688:ALA:O	1:A:877:GLN:NE2	2.37	0.57
1:A:378:CYS:HA	1:A:511:CYS:HA	1.87	0.57
1:C:419:CYS:H	1:C:499:LEU:HB2	1.70	0.57
1:C:1105:SER:OG	1:A:896:ASN:ND2	2.37	0.57
1:A:102:VAL:HG22	1:A:115:ILE:HG12	1.85	0.57
1:A:100:GLY:HA3	1:A:117:ILE:HG22	1.86	0.57
1:C:456:SER:HB2	1:A:111:SER:HB3	1.87	0.57
1:A:690:SER:OG	1:A:692:ASN:OD1	2.23	0.57
1:C:96:ASN:O	1:C:99:ARG:NH1	2.37	0.57
1:B:18:ARG:HB2	1:B:151:MET:HE3	1.86	0.57
1:C:578:PHE:H	1:A:835:GLN:HE22	1.53	0.57
1:A:382:VAL:HG22	1:A:501:PHE:HA	1.87	0.57
1:B:895:GLN:NE2	1:A:1072:PRO:O	2.38	0.57
1:A:704:ILE:HG12	1:A:1047:VAL:HG22	1.86	0.57
1:B:138:PHE:HB2	1:B:236:THR:HA	1.86	0.56
1:B:375:ASN:ND2	1:B:513:PRO:O	2.36	0.56
1:C:445:HIS:HA	1:C:464:GLY:HA2	1.87	0.56
1:A:186:VAL:HB	1:A:197:TYR:HB2	1.86	0.56
1:C:337:VAL:HG11	1:C:405:ILE:HD12	1.86	0.56
1:B:737:GLN:OE1	1:A:951:ASN:ND2	2.39	0.56
1:C:439:LYS:NZ	1:C:480:ASP:OD1	2.37	0.56
1:A:328:VAL:HG11	1:A:345:ILE:HD11	1.87	0.56
1:A:715:LYS:HD2	1:A:753:ALA:HB1	1.87	0.56
1:B:705:THR:HB	1:B:1046:HIS:HB2	1.87	0.56
1:A:38:ARG:NH1	1:A:184:GLU:OE2	2.38	0.56
1:C:114:VAL:HG21	1:C:224:LEU:HD13	1.87	0.56
1:C:429:ASP:OD1	1:C:495:ARG:NH2	2.38	0.56
1:A:314:VAL:HG22	1:A:528:ASN:HB3	1.88	0.56
1:C:892:GLY:O	1:C:1090:ASN:ND2	2.39	0.56
1:A:102:VAL:HG11	1:A:132:LEU:HD11	1.88	0.56
1:A:871:GLY:HA3	1:A:1016:LEU:HB3	1.87	0.55
1:B:745:LEU:HD22	1:B:990:VAL:HG21	1.89	0.55
1:A:91:ALA:HB3	1:A:183:ARG:HB2	1.87	0.55
1:A:348:CYS:HB3	1:A:510:VAL:HG12	1.89	0.55
1:C:268:GLU:HB2	3:L:1:NAG:H82	1.88	0.55
1:B:186:VAL:HB	1:B:197:TYR:HB2	1.89	0.54
1:B:636:LEU:HD21	1:B:639:ALA:HB3	1.88	0.54
1:C:29:ASN:HD22	1:C:70:HIS:HB2	1.72	0.54
1:A:885:ALA:HB1	1:A:895:GLN:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1036:GLN:HB2	1:A:1043:VAL:HB	1.89	0.54
1:C:762:GLU:O	1:C:766:GLN:NE2	2.40	0.54
1:C:1072:PRO:O	1:A:895:GLN:NE2	2.41	0.54
1:A:342:ARG:NH2	1:A:502:GLU:OE1	2.41	0.54
1:A:348:CYS:SG	1:A:349:VAL:N	2.81	0.54
1:B:610:ILE:HG23	1:B:622:TYR:HE2	1.72	0.54
1:C:807:LYS:O	1:C:931:GLN:NE2	2.41	0.54
1:C:960:ASN:HA	1:C:963:LEU:HB2	1.90	0.54
1:A:619:TRP:HB2	1:A:622:TYR:HB2	1.90	0.54
1:A:41:TYR:HB3	1:A:216:LEU:HB2	1.90	0.54
1:B:389:VAL:HG11	1:B:397:ILE:HD11	1.90	0.53
1:C:99:ARG:HB3	1:C:118:ASN:HB3	1.90	0.53
1:C:429:ASP:O	1:C:435:ASN:ND2	2.41	0.53
1:C:557:ASP:OD2	1:A:949:SER:OG	2.25	0.53
1:B:265:LYS:HD2	1:B:293:PHE:HE2	1.72	0.53
1:C:186:VAL:HB	1:C:197:TYR:HB2	1.91	0.53
1:C:325:PHE:HB3	1:C:328:VAL:HB	1.90	0.53
1:C:323:CYS:N	1:C:348:CYS:SG	2.81	0.53
1:A:285:GLU:HB2	1:A:619:TRP:HH2	1.73	0.53
1:B:136:PRO:HB3	1:B:152:ILE:HA	1.91	0.53
1:B:334:PHE:HB2	1:B:388:VAL:HG23	1.91	0.53
1:B:687:ILE:HD11	1:C:875:ALA:HB1	1.89	0.53
1:C:188:LYS:HB2	1:C:195:TYR:HB2	1.90	0.53
1:B:412:LEU:HB3	1:B:417:MET:HE1	1.90	0.53
1:C:422:ALA:HB2	1:C:496:VAL:HG22	1.90	0.53
1:B:1072:PRO:O	1:C:895:GLN:NE2	2.42	0.53
1:C:832:ILE:HB	2:J:1:NAG:H83	1.91	0.53
1:B:26:GLN:HB2	1:B:75:THR:HA	1.91	0.53
1:B:719:ASP:OD1	1:A:304:ASN:ND2	2.41	0.53
1:C:804:LEU:HD13	1:C:1043:VAL:HG21	1.90	0.53
1:A:94:LYS:NZ	1:A:249:ALA:O	2.42	0.52
1:A:1018:GLN:HG3	1:A:1030:HIS:HD2	1.73	0.52
1:B:348:CYS:SG	1:B:349:VAL:N	2.82	0.52
1:C:1055:ARG:HA	6:C:1321:NAG:H82	1.91	0.52
1:A:409:ASN:HD21	1:A:440:TYR:HB2	1.73	0.52
1:C:449:ARG:N	1:C:452:GLU:OE1	2.42	0.52
1:B:413:PRO:HG3	1:B:450:PRO:HB3	1.92	0.52
1:B:724:ILE:O	1:B:982:ARG:NH1	2.40	0.52
1:A:1086:ILE:O	1:A:1095:GLN:N	2.42	0.52
1:B:58:LEU:HB3	1:B:257:LEU:HB3	1.90	0.52
1:B:114:VAL:HG21	1:B:224:LEU:HD13	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194:LEU:HB3	1:B:222:LEU:HB2	1.92	0.52
1:B:330:ASN:HB2	1:B:354:VAL:HG21	1.92	0.52
1:A:61:PRO:HG2	1:A:258:LYS:HD2	1.92	0.52
1:C:963:LEU:HD23	1:C:971:ALA:HB1	1.92	0.52
1:A:381:ASN:OD1	1:A:509:THR:N	2.42	0.52
1:A:896:ASN:O	1:A:900:GLU:N	2.41	0.52
1:B:619:TRP:HB2	1:B:622:TYR:HB2	1.90	0.52
1:A:444:ARG:NE	1:A:454:ASP:OD2	2.35	0.52
1:C:1073:ARG:NH1	1:C:1100:ASP:O	2.43	0.51
1:A:840:LEU:HD21	1:A:941:LEU:HD22	1.91	0.51
1:B:331:ALA:HB3	1:B:334:PHE:CE1	2.46	0.51
1:C:138:PHE:HB2	1:C:236:THR:HA	1.92	0.51
1:C:712:SER:HG	1:C:756:GLN:HE21	1.54	0.51
1:C:956:SER:H	1:C:962:ILE:HD11	1.75	0.51
1:C:954:ALA:HB2	1:C:977:ARG:HD3	1.91	0.51
1:A:116:ILE:HG12	1:A:125:ILE:HG23	1.92	0.51
1:B:96:ASN:O	1:B:99:ARG:NH1	2.44	0.51
1:B:129:ASN:HB2	1:B:157:PHE:HB2	1.91	0.51
1:A:131:GLU:HB3	1:A:155:ASN:H	1.76	0.51
1:A:35:SER:OG	1:A:64:SER:N	2.42	0.51
1:B:56:GLN:HB2	1:B:261:THR:HG22	1.93	0.51
1:C:409:ASN:HD21	1:C:440:TYR:HB2	1.75	0.51
1:C:267:ASP:OD1	1:C:271:THR:N	2.42	0.51
1:A:389:VAL:HG11	1:A:397:ILE:HD11	1.93	0.51
1:A:390:LYS:HB2	1:A:481:TYR:HD1	1.75	0.50
1:C:544:ARG:HH12	4:S:2:NAG:H82	1.76	0.50
1:C:315:ARG:NH1	1:C:517:THR:O	2.42	0.50
1:A:193:PHE:HA	1:A:223:PRO:HA	1.92	0.50
1:B:770:MET:N	1:A:683:ALA:O	2.44	0.50
1:C:824:GLY:HA3	1:C:831:LEU:HA	1.93	0.50
1:C:975:ILE:O	1:C:979:ILE:N	2.41	0.50
1:A:662:THR:HA	1:A:672:LYS:HA	1.92	0.50
1:A:702:ILE:HB	1:A:908:GLN:HB3	1.94	0.50
1:B:142:LYS:HD3	1:B:238:PHE:HB3	1.94	0.50
1:B:707:GLU:HB3	1:B:1044:PHE:HB2	1.94	0.50
1:C:521:LYS:NZ	1:C:569:GLU:OE2	2.41	0.50
1:A:35:SER:HB2	1:A:60:LEU:HD21	1.92	0.50
1:C:397:ILE:HG21	1:C:496:VAL:HG11	1.94	0.50
1:A:439:LYS:NZ	1:A:480:ASP:OD1	2.40	0.50
1:B:582:SER:OG	1:B:599:GLN:NE2	2.39	0.50
1:A:26:GLN:HB3	1:A:75:THR:HA	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:VAL:HB	1:A:220:PHE:HB2	1.94	0.49
1:B:380:SER:OG	1:B:381:ASN:N	2.44	0.49
1:B:393:ASP:HB3	1:B:405:ILE:HD11	1.94	0.49
1:B:429:ASP:O	1:B:435:ASN:ND2	2.45	0.49
1:A:184:GLU:O	1:A:199:GLY:N	2.43	0.49
1:A:360:PHE:HB3	1:A:423:TRP:HB2	1.94	0.49
1:C:99:ARG:HE	1:C:170:LEU:HD23	1.77	0.49
1:C:724:ILE:O	1:C:982:ARG:NH1	2.40	0.49
1:C:904:GLN:HG3	5:O:2:NAG:H82	1.93	0.49
1:A:388:VAL:HG22	1:A:495:ARG:HG2	1.94	0.49
1:C:97:VAL:HA	1:C:236:THR:HB	1.94	0.49
1:C:734:LEU:HD12	1:C:975:ILE:HD11	1.94	0.49
1:C:906:ALA:O	1:C:910:ASN:ND2	2.42	0.49
1:B:35:SER:HB2	1:B:60:LEU:HD21	1.95	0.49
1:B:185:PHE:HE1	1:B:198:LYS:HG3	1.78	0.49
1:B:268:GLU:HB2	2:D:1:NAG:H82	1.94	0.49
1:C:1094:PRO:HB2	3:Q:1:NAG:H61	1.95	0.49
1:A:607:SER:HA	1:A:610:ILE:HD12	1.94	0.49
1:B:116:ILE:HG12	1:B:125:ILE:HG12	1.95	0.49
1:C:1014:CYS:O	1:C:1033:SER:OG	2.31	0.48
1:C:459:PRO:HG2	1:C:469:PRO:HG3	1.94	0.48
1:A:758:ARG:NH1	1:A:762:GLU:OE2	2.46	0.48
1:A:887:ARG:NH1	1:A:1031:LEU:O	2.46	0.48
1:A:329:PHE:HE1	1:A:384:ALA:HB1	1.78	0.48
1:B:182:LEU:HB2	1:B:203:ILE:HD13	1.96	0.48
1:C:701:SER:HB3	1:C:1050:VAL:HB	1.96	0.48
1:A:323:CYS:N	1:A:348:CYS:SG	2.86	0.48
1:A:1086:ILE:HB	1:A:1095:GLN:HB2	1.95	0.48
1:A:380:SER:OG	1:A:381:ASN:N	2.47	0.48
1:C:123:VAL:N	1:C:165:SER:OG	2.46	0.48
1:C:717:SER:HB3	1:C:841:THR:HG23	1.95	0.48
1:A:420:VAL:HA	1:A:498:VAL:HG22	1.94	0.48
1:B:97:VAL:HG22	1:B:238:PHE:HE2	1.78	0.48
1:A:204:ASP:OD1	1:A:204:ASP:N	2.47	0.48
1:A:301:GLN:NE2	1:A:581:VAL:O	2.46	0.48
1:B:904:GLN:HA	1:B:907:ASN:HB2	1.96	0.48
1:A:885:ALA:HA	1:A:888:PHE:HD2	1.78	0.48
1:B:102:VAL:HG11	1:B:132:LEU:HD11	1.95	0.47
1:C:383:TYR:HB2	1:C:500:SER:HB3	1.95	0.47
1:A:39:GLY:HA3	1:A:60:LEU:HB3	1.96	0.47
1:A:88:TYR:HB2	1:A:257:LEU:HD21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:LYS:HB3	1:A:377:LEU:HB2	1.96	0.47
1:C:331:ALA:HB3	1:C:334:PHE:HE1	1.80	0.47
1:C:546:GLN:NE2	1:A:269:ASN:O	2.47	0.47
1:B:655:GLY:H	1:C:846:LEU:HD12	1.78	0.47
1:C:544:ARG:NH1	4:S:1:NAG:O6	2.46	0.47
1:B:51:THR:HB	1:A:555:VAL:HG12	1.95	0.47
1:B:584:ILE:HB	1:B:595:ALA:HB3	1.96	0.47
1:B:779:PHE:HB2	1:B:784:PHE:HE2	1.79	0.47
1:C:455:ILE:HD11	1:A:112:GLN:HE21	1.80	0.47
1:A:194:LEU:N	1:A:222:LEU:O	2.39	0.47
1:C:713:MET:O	1:C:756:GLN:NE2	2.48	0.47
1:C:917:GLN:HA	1:C:920:LEU:HB2	1.96	0.47
1:A:72:ILE:H	1:A:75:THR:HB	1.80	0.47
1:A:209:LEU:HD12	1:A:210:PRO:HD2	1.97	0.47
1:A:963:LEU:HD23	1:A:971:ALA:HB1	1.97	0.47
1:B:89:PHE:HB3	1:B:185:PHE:HB2	1.98	0.47
1:A:238:PHE:N	1:A:246:GLY:O	2.47	0.47
1:A:89:PHE:HB3	1:A:185:PHE:HB2	1.97	0.46
1:A:659:SER:OG	1:A:675:VAL:HG23	2.15	0.46
1:A:125:ILE:O	1:A:163:TYR:N	2.43	0.46
1:A:1032:MET:HG2	1:A:1047:VAL:HB	1.97	0.46
1:C:194:LEU:HD23	1:C:222:LEU:HD12	1.96	0.46
1:A:59:PHE:N	1:A:258:LYS:O	2.47	0.46
1:B:47:PHE:HD1	1:A:549:GLN:HE22	1.64	0.46
1:A:185:PHE:HE1	1:A:198:LYS:HG3	1.80	0.46
1:B:405:ILE:HA	1:B:409:ASN:HB2	1.98	0.46
1:C:372:THR:HA	1:C:375:ASN:HD22	1.80	0.46
1:C:390:LYS:HA	1:C:483:PHE:HE1	1.81	0.46
1:C:19:CYS:N	1:C:154:ASP:OD1	2.48	0.46
1:A:99:ARG:HH12	1:A:170:LEU:HD23	1.80	0.45
1:B:137:PHE:HB2	1:B:237:ALA:HB2	1.98	0.45
1:A:707:GLU:OE2	1:A:1010:LYS:NZ	2.49	0.45
1:B:103:PHE:HB2	1:B:114:VAL:HB	1.98	0.45
1:B:325:PHE:HA	1:B:328:VAL:HB	1.99	0.45
1:B:337:VAL:HG12	1:B:409:ASN:HB3	1.98	0.45
1:B:708:VAL:HG22	1:B:1043:VAL:HG22	1.99	0.45
1:A:83:PHE:O	1:A:86:GLY:N	2.42	0.45
1:A:790:ASP:OD2	1:A:793:LYS:N	2.46	0.45
1:B:337:VAL:HG21	1:B:389:VAL:HG12	1.98	0.45
1:B:583:VAL:HG22	1:B:596:VAL:HG12	1.98	0.45
1:C:182:LEU:HD23	1:C:201:GLN:HE21	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:586:PRO:HG2	1:B:591:SER:HB3	1.99	0.45
1:C:142:LYS:HG2	1:C:238:PHE:HB3	1.99	0.45
1:C:410:TYR:HE1	1:C:453:ARG:HD2	1.82	0.45
1:A:803:LEU:HA	1:A:806:ASN:HD22	1.82	0.45
1:B:318:ASN:HB2	1:B:566:LYS:HA	1.99	0.45
1:C:402:THR:HA	1:C:406:ALA:HB3	1.98	0.45
1:A:122:ASN:ND2	1:A:165:SER:O	2.49	0.45
1:B:652:ILE:HD11	1:B:658:ALA:HB2	1.98	0.45
1:B:1108:CYS:SG	1:B:1109:ASP:N	2.90	0.45
1:A:363:THR:OG1	1:A:420:VAL:O	2.34	0.45
1:B:440:TYR:HB3	1:B:481:TYR:CZ	2.51	0.45
1:B:267:ASP:OD1	1:B:271:THR:N	2.44	0.45
1:C:89:PHE:HB3	1:C:185:PHE:HB2	1.98	0.45
1:C:41:TYR:OH	1:C:58:LEU:O	2.32	0.44
1:B:328:VAL:HG22	1:B:343:LYS:HD3	2.00	0.44
1:B:697:PRO:HA	1:B:1054:GLU:HA	1.98	0.44
1:A:307:VAL:HB	1:A:577:ALA:HB3	1.99	0.44
1:A:869:THR:HG21	1:A:876:LEU:HD12	2.00	0.44
1:A:441:ARG:HG3	1:A:477:PRO:HB2	1.98	0.44
1:C:405:ILE:HD13	1:C:409:ASN:HD22	1.82	0.44
1:C:444:ARG:HH21	1:A:227:ASN:HD21	1.64	0.44
1:A:94:LYS:HZ2	1:A:179:PHE:HE1	1.66	0.44
1:C:22:PHE:H	1:C:135:ASN:HB2	1.81	0.44
1:C:956:SER:HB3	1:C:962:ILE:HG13	1.99	0.44
1:B:209:LEU:HD12	1:B:210:PRO:HD2	2.00	0.44
1:C:104:GLY:H	1:C:228:ILE:HG23	1.83	0.44
1:B:358:SER:HB3	1:B:361:PHE:HE2	1.83	0.44
1:A:286:LEU:HG	1:A:295:ILE:HD13	2.00	0.44
1:B:441:ARG:NH2	1:B:443:LEU:O	2.51	0.43
1:B:529:PHE:N	1:B:532:LEU:O	2.45	0.43
1:B:1072:PRO:HG2	1:C:895:GLN:HE21	1.82	0.43
1:C:385:ASP:HB2	1:C:498:VAL:HB	1.99	0.43
1:C:420:VAL:HG13	1:C:496:VAL:HG13	1.99	0.43
1:C:868:TRP:HZ3	1:C:883:GLN:HA	1.83	0.43
1:C:916:ILE:HD13	1:C:1045:LEU:HD22	2.00	0.43
1:A:63:TYR:O	1:A:620:ARG:NH2	2.51	0.43
1:C:61:PRO:HB3	1:C:620:ARG:NH1	2.29	0.43
1:C:652:ILE:HD11	1:C:658:ALA:HB2	1.99	0.43
1:C:1054:GLU:HG2	1:A:876:LEU:HD22	2.00	0.43
1:B:277:ASP:HB3	1:B:280:GLN:HG2	1.99	0.43
1:C:77:GLY:O	1:C:252:TYR:OH	2.28	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:ARG:NH1	1:B:184:GLU:OE2	2.50	0.43
1:C:362:SER:N	1:C:422:ALA:O	2.49	0.43
1:C:539:THR:HG23	1:C:572:ASP:HB2	2.01	0.43
1:A:125:ILE:HB	1:A:163:TYR:HB3	2.01	0.43
1:C:871:GLY:HA3	1:C:1016:LEU:HB3	2.00	0.43
1:A:307:VAL:HG22	1:A:615:LEU:HD23	2.01	0.43
1:B:388:VAL:HG22	1:B:495:ARG:HA	2.00	0.43
1:B:707:GLU:OE2	1:B:1010:LYS:NZ	2.38	0.43
1:B:992:GLN:HA	1:B:995:ILE:HD12	2.00	0.43
1:C:33:HIS:ND1	1:C:208:ASP:OD1	2.51	0.43
1:C:88:TYR:HB2	1:C:257:LEU:HD21	2.01	0.43
1:C:909:PHE:O	1:C:913:ILE:N	2.51	0.43
1:C:763:VAL:HG22	1:C:1008:ALA:HB2	2.01	0.43
1:A:89:PHE:HE2	1:A:91:ALA:HB2	1.83	0.43
1:A:652:ILE:HD11	1:A:658:ALA:HB2	2.01	0.43
1:B:586:PRO:HD3	1:B:674:ILE:HD11	2.00	0.43
1:C:126:ARG:HA	1:C:162:GLU:HG2	2.00	0.43
1:B:323:CYS:N	1:B:348:CYS:SG	2.92	0.43
1:C:443:LEU:HG	1:C:460:PHE:HB2	2.01	0.43
1:A:58:LEU:HD23	1:A:259:PRO:HB3	2.00	0.43
1:C:125:ILE:HD12	1:C:163:TYR:HB3	2.01	0.42
1:C:140:VAL:HG22	1:C:147:GLN:HA	2.01	0.42
1:A:310:SER:HB2	1:A:614:GLN:HE22	1.84	0.42
1:B:304:ASN:ND2	1:C:719:ASP:OD1	2.52	0.42
1:B:317:PRO:HD3	1:B:530:ASN:HB2	2.01	0.42
1:B:837:PHE:HZ	1:A:573:ILE:HG22	1.85	0.42
1:B:883:GLN:NE2	1:B:884:MET:SD	2.92	0.42
1:C:1036:GLN:HB2	1:C:1043:VAL:HB	2.02	0.42
1:A:88:TYR:N	1:A:255:GLY:O	2.40	0.42
1:B:650:ILE:HB	1:B:658:ALA:HB3	2.00	0.42
1:C:862:GLY:O	1:C:866:ALA:N	2.49	0.42
1:B:102:VAL:HG22	1:B:115:ILE:HG12	2.01	0.42
1:B:933:VAL:O	1:B:937:ASN:ND2	2.52	0.42
1:C:102:VAL:HG23	1:C:115:ILE:HG12	2.01	0.42
1:C:578:PHE:N	1:A:835:GLN:HE22	2.17	0.42
1:B:60:LEU:HB2	1:B:88:TYR:CE2	2.55	0.42
1:B:398:ALA:HB3	1:B:401:GLN:HG3	2.00	0.42
1:C:787:ILE:HG23	1:C:1036:GLN:HE22	1.83	0.42
1:C:1068:LYS:HG2	1:C:1107:ASN:HA	2.02	0.42
1:A:48:ARG:HB2	1:A:266:TYR:HD2	1.83	0.42
1:A:425:THR:HG21	1:A:495:ARG:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:399:PRO:HG3	1:B:417:MET:HG2	2.02	0.42
1:C:540:PRO:HA	1:C:571:LEU:HA	2.01	0.42
1:B:100:GLY:HA3	1:B:117:ILE:HG22	2.00	0.42
1:A:511:CYS:SG	1:A:512:GLY:N	2.90	0.42
1:B:355:LEU:HB3	1:B:371:ALA:HB1	2.02	0.41
1:A:430:ALA:HB2	1:A:493:PRO:HG3	2.02	0.41
1:C:999:GLU:OE2	1:A:1001:ARG:NH1	2.52	0.41
1:A:948:LEU:O	1:A:982:ARG:NH2	2.47	0.41
1:C:58:LEU:HD12	1:C:188:LYS:HE3	2.02	0.41
1:C:380:SER:OG	1:C:381:ASN:N	2.52	0.41
1:C:927:LEU:HD22	1:C:930:LEU:HD12	2.02	0.41
1:B:54:LEU:HD13	1:B:263:MET:HB2	2.01	0.41
1:B:904:GLN:HB2	4:G:2:NAG:H81	2.02	0.41
1:B:951:ASN:HD21	1:C:737:GLN:HB2	1.85	0.41
1:C:426:ARG:NH2	1:C:485:THR:O	2.47	0.41
1:A:390:LYS:HB2	1:A:481:TYR:CD1	2.55	0.41
1:B:35:SER:OG	1:B:64:SER:N	2.52	0.41
1:C:215:THR:HG23	1:C:272:ILE:HD12	2.03	0.41
1:B:1063:ILE:HG21	1:B:1117:ASN:HD22	1.86	0.41
1:C:334:PHE:HB2	1:C:388:VAL:HG23	2.02	0.41
1:A:1072:PRO:HD3	1:A:1077:PHE:CE2	2.56	0.41
1:C:445:HIS:CD2	1:C:461:SER:H	2.39	0.41
1:A:1069:ALA:N	1:A:1106:GLY:O	2.44	0.41
1:B:29:ASN:ND2	1:B:70:HIS:O	2.54	0.41
1:B:556:SER:OG	1:B:557:ASP:N	2.54	0.41
1:B:923:THR:OG1	1:B:924:SER:N	2.53	0.41
1:C:99:ARG:HB2	1:C:138:PHE:HE2	1.85	0.41
1:C:683:ALA:O	1:A:770:MET:N	2.54	0.41
1:A:373:LYS:HD3	1:A:376:ASP:HB2	2.03	0.41
1:A:441:ARG:HD3	1:A:444:ARG:HB2	2.03	0.41
1:A:564:ASP:HB3	1:A:569:GLU:H	1.86	0.41
1:B:1071:PHE:O	1:B:1102:THR:OG1	2.33	0.41
1:B:125:ILE:HB	1:B:163:TYR:HB3	2.02	0.40
1:B:1000:ILE:O	1:B:1004:ALA:N	2.54	0.40
1:C:689:TYR:HB3	1:A:776:LEU:HD22	2.03	0.40
1:B:115:ILE:HD11	1:B:132:LEU:HD21	2.03	0.40
1:C:457:ASN:H	1:A:110:LYS:HB3	1.86	0.40
1:C:546:GLN:HA	1:C:547:PRO:HD3	1.93	0.40
1:A:422:ALA:HA	1:A:496:VAL:HG22	2.03	0.40
1:A:723:TYR:OH	1:A:944:LEU:O	2.35	0.40
1:B:205:VAL:HG11	1:B:210:PRO:HG3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:335:PRO:HG2	1:B:341:GLU:HB2	2.03	0.40
1:B:642:VAL:HG12	1:B:644:THR:HG23	2.03	0.40
1:B:749:LEU:HD23	1:B:752:ILE:HD12	2.04	0.40
1:A:956:SER:HB3	1:A:962:ILE:HG23	2.03	0.40
1:B:1061:PRO:HB3	1:C:882:MET:HE1	2.02	0.40
1:C:399:PRO:HB2	1:C:414:ASP:HA	2.03	0.40
1:A:220:PHE:HB3	1:A:222:LEU:HG	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1052/1215 (87%)	979 (93%)	73 (7%)	0	100	100
1	B	1054/1215 (87%)	977 (93%)	77 (7%)	0	100	100
1	C	1054/1215 (87%)	977 (93%)	77 (7%)	0	100	100
All	All	3160/3645 (87%)	2933 (93%)	227 (7%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	925/1053 (88%)	925 (100%)	0	100	100
1	B	927/1053 (88%)	927 (100%)	0	100	100
1	C	926/1053 (88%)	926 (100%)	0	100	100
All	All	2778/3159 (88%)	2778 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	56	GLN
1	B	70	HIS
1	B	129	ASN
1	B	599	GLN
1	B	611	HIS
1	B	721	ASN
1	B	766	GLN
1	B	806	ASN
1	B	937	ASN
1	B	984	GLN
1	B	1036	GLN
1	C	29	ASN
1	C	78	ASN
1	C	129	ASN
1	C	201	GLN
1	C	375	ASN
1	C	599	GLN
1	C	611	HIS
1	C	721	ASN
1	C	759	ASN
1	C	818	GLN
1	C	835	GLN
1	C	917	GLN
1	C	931	GLN
1	C	984	GLN
1	C	993	GLN
1	C	1036	GLN
1	A	96	ASN
1	A	112	GLN
1	A	492	GLN
1	A	611	HIS
1	A	614	GLN

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Mol	Chain	Res	Type
1	A	733	ASN
1	A	759	ASN
1	A	806	ASN
1	A	877	GLN
1	A	896	ASN
1	A	907	ASN
1	A	910	ASN
1	A	917	GLN
1	A	951	ASN
1	A	984	GLN
1	A	1030	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

63 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	D	1	1,2	14,14,15	0.32	0	17,19,21	0.81	1 (5%)
2	NAG	D	2	2	14,14,15	0.26	0	17,19,21	0.58	0
3	NAG	E	1	1,3	14,14,15	0.56	0	17,19,21	0.64	0
3	NAG	E	2	3	14,14,15	0.20	0	17,19,21	0.60	0
3	BMA	E	3	3	11,11,12	0.70	0	15,15,17	0.87	1 (6%)
2	NAG	F	1	1,2	14,14,15	0.29	0	17,19,21	0.40	0
2	NAG	F	2	2	14,14,15	0.43	0	17,19,21	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	G	1	4,1	14,14,15	0.43	0	17,19,21	0.58	0
4	NAG	G	2	4	14,14,15	0.30	0	17,19,21	0.79	1 (5%)
4	BMA	G	3	4	11,11,12	1.52	2 (18%)	15,15,17	1.54	2 (13%)
4	MAN	G	4	4	11,11,12	0.77	0	15,15,17	1.12	2 (13%)
4	MAN	G	5	4	11,11,12	0.74	0	15,15,17	1.22	2 (13%)
4	NAG	H	1	4,1	14,14,15	0.20	0	17,19,21	0.76	1 (5%)
4	NAG	H	2	4	14,14,15	0.42	0	17,19,21	0.73	0
4	BMA	H	3	4	11,11,12	0.71	0	15,15,17	0.97	0
4	MAN	H	4	4	11,11,12	0.87	0	15,15,17	1.24	1 (6%)
4	MAN	H	5	4	11,11,12	0.76	0	15,15,17	1.23	2 (13%)
2	NAG	I	1	1,2	14,14,15	0.32	0	17,19,21	0.38	0
2	NAG	I	2	2	14,14,15	0.37	0	17,19,21	0.57	0
2	NAG	J	1	1,2	14,14,15	0.24	0	17,19,21	0.64	0
2	NAG	J	2	2	14,14,15	0.28	0	17,19,21	0.44	0
2	NAG	K	1	1,2	14,14,15	0.23	0	17,19,21	0.56	0
2	NAG	K	2	2	14,14,15	0.21	0	17,19,21	0.57	0
3	NAG	L	1	1,3	14,14,15	0.32	0	17,19,21	0.56	0
3	NAG	L	2	3	14,14,15	0.24	0	17,19,21	0.63	0
3	BMA	L	3	3	11,11,12	0.85	0	15,15,17	0.71	0
2	NAG	M	1	1,2	14,14,15	0.31	0	17,19,21	0.69	0
2	NAG	M	2	2	14,14,15	0.51	0	17,19,21	0.37	0
5	NAG	N	1	1,5	14,14,15	0.26	0	17,19,21	0.70	0
5	NAG	N	2	5	14,14,15	0.40	0	17,19,21	0.59	0
5	BMA	N	3	5	11,11,12	0.87	0	15,15,17	0.73	0
5	MAN	N	4	5	11,11,12	0.91	1 (9%)	15,15,17	1.31	2 (13%)
5	NAG	O	1	1,5	14,14,15	0.48	0	17,19,21	0.57	0
5	NAG	O	2	5	14,14,15	0.22	0	17,19,21	0.66	0
5	BMA	O	3	5	11,11,12	0.73	0	15,15,17	1.23	1 (6%)
5	MAN	O	4	5	11,11,12	0.93	0	15,15,17	0.96	2 (13%)
5	NAG	P	1	1,5	14,14,15	0.39	0	17,19,21	0.61	0
5	NAG	P	2	5	14,14,15	0.22	0	17,19,21	0.55	0
5	BMA	P	3	5	11,11,12	0.71	0	15,15,17	1.02	1 (6%)
5	MAN	P	4	5	11,11,12	1.33	2 (18%)	15,15,17	1.86	3 (20%)
3	NAG	Q	1	1,3	14,14,15	0.30	0	17,19,21	0.38	0
3	NAG	Q	2	3	14,14,15	0.19	0	17,19,21	0.58	0
3	BMA	Q	3	3	11,11,12	0.79	0	15,15,17	0.95	1 (6%)
2	NAG	R	1	1,2	14,14,15	0.47	0	17,19,21	0.62	0
2	NAG	R	2	2	14,14,15	0.25	0	17,19,21	0.55	0
4	NAG	S	1	4,1	14,14,15	0.36	0	17,19,21	0.63	0
4	NAG	S	2	4	14,14,15	0.48	0	17,19,21	0.72	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	BMA	S	3	4	11,11,12	1.13	2 (18%)	15,15,17	1.00	0
4	MAN	S	4	4	11,11,12	0.81	1 (9%)	15,15,17	1.16	2 (13%)
4	MAN	S	5	4	11,11,12	0.86	1 (9%)	15,15,17	1.25	2 (13%)
2	NAG	T	1	1,2	14,14,15	0.67	1 (7%)	17,19,21	0.83	0
2	NAG	T	2	2	14,14,15	0.45	0	17,19,21	0.44	0
3	NAG	U	1	1,3	14,14,15	0.61	1 (7%)	17,19,21	0.72	0
3	NAG	U	2	3	14,14,15	0.29	0	17,19,21	0.46	0
3	BMA	U	3	3	11,11,12	0.79	0	15,15,17	1.00	1 (6%)
3	NAG	V	1	1,3	14,14,15	0.40	0	17,19,21	1.09	1 (5%)
3	NAG	V	2	3	14,14,15	0.31	0	17,19,21	0.88	0
3	BMA	V	3	3	11,11,12	0.91	0	15,15,17	0.76	0
2	NAG	W	1	1,2	14,14,15	0.38	0	17,19,21	0.57	0
2	NAG	W	2	2	14,14,15	0.36	0	17,19,21	0.47	0
3	NAG	X	1	1,3	14,14,15	0.31	0	17,19,21	0.42	0
3	NAG	X	2	3	14,14,15	0.31	0	17,19,21	0.43	0
3	BMA	X	3	3	11,11,12	0.71	0	15,15,17	0.94	1 (6%)

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

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	U	2	3	-	2/6/23/26	0/1/1/1
3	BMA	U	3	3	-	1/2/19/22	0/1/1/1
3	NAG	V	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	V	2	3	-	0/6/23/26	0/1/1/1
3	BMA	V	3	3	-	1/2/19/22	0/1/1/1
2	NAG	W	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	W	2	2	-	2/6/23/26	0/1/1/1
3	NAG	X	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	X	2	3	-	2/6/23/26	0/1/1/1
3	BMA	X	3	3	-	2/2/19/22	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	3	BMA	C2-C3	3.50	1.57	1.52
5	P	4	MAN	O5-C1	2.96	1.48	1.43
5	P	4	MAN	C1-C2	2.83	1.59	1.52
4	G	3	BMA	C4-C3	2.54	1.58	1.52
5	N	4	MAN	C1-C2	2.33	1.57	1.52
4	S	3	BMA	C4-C3	2.29	1.58	1.52
4	S	3	BMA	C2-C3	2.26	1.55	1.52
4	S	5	MAN	C1-C2	2.20	1.57	1.52
2	T	1	NAG	O5-C1	-2.14	1.40	1.43
3	U	1	NAG	O5-C1	-2.09	1.40	1.43
4	S	4	MAN	C1-C2	2.01	1.57	1.52

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	P	4	MAN	C1-O5-C5	5.93	120.14	112.19
4	G	3	BMA	C2-C3-C4	3.94	117.78	110.86
4	H	5	MAN	C1-O5-C5	3.86	117.36	112.19
5	N	4	MAN	C1-O5-C5	3.84	117.33	112.19
4	H	4	MAN	C1-O5-C5	3.81	117.30	112.19
4	G	5	MAN	C1-O5-C5	3.67	117.11	112.19
4	S	5	MAN	C1-O5-C5	3.58	116.98	112.19
3	V	1	NAG	C1-O5-C5	3.57	116.97	112.19
5	O	3	BMA	C1-O5-C5	3.29	116.60	112.19
4	G	3	BMA	C1-C2-C3	3.20	114.30	109.64
4	G	4	MAN	C1-O5-C5	3.09	116.33	112.19
4	S	4	MAN	C1-O5-C5	3.05	116.27	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	U	3	BMA	C1-O5-C5	2.80	115.94	112.19
4	G	2	NAG	C1-O5-C5	2.67	115.76	112.19
2	D	1	NAG	C1-O5-C5	2.59	115.66	112.19
4	H	1	NAG	C1-O5-C5	2.57	115.63	112.19
3	X	3	BMA	C1-O5-C5	2.51	115.55	112.19
5	P	3	BMA	C1-O5-C5	2.46	115.48	112.19
5	O	4	MAN	C1-O5-C5	2.38	115.37	112.19
5	P	4	MAN	O2-C2-C3	-2.36	105.27	110.15
4	G	4	MAN	O2-C2-C3	-2.31	105.36	110.15
3	E	3	BMA	C1-O5-C5	2.30	115.27	112.19
4	G	5	MAN	O2-C2-C3	-2.29	105.41	110.15
5	N	4	MAN	O2-C2-C3	-2.29	105.42	110.15
4	S	4	MAN	O2-C2-C3	-2.17	105.66	110.15
4	S	5	MAN	O2-C2-C3	-2.16	105.67	110.15
5	P	4	MAN	C1-C2-C3	2.16	112.79	109.64
4	H	5	MAN	O2-C2-C3	-2.15	105.70	110.15
3	Q	3	BMA	C1-O5-C5	2.13	115.05	112.19
5	O	4	MAN	O2-C2-C3	-2.07	105.87	110.15

There are no chirality outliers.

All (85) torsion outliers are listed below:

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

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

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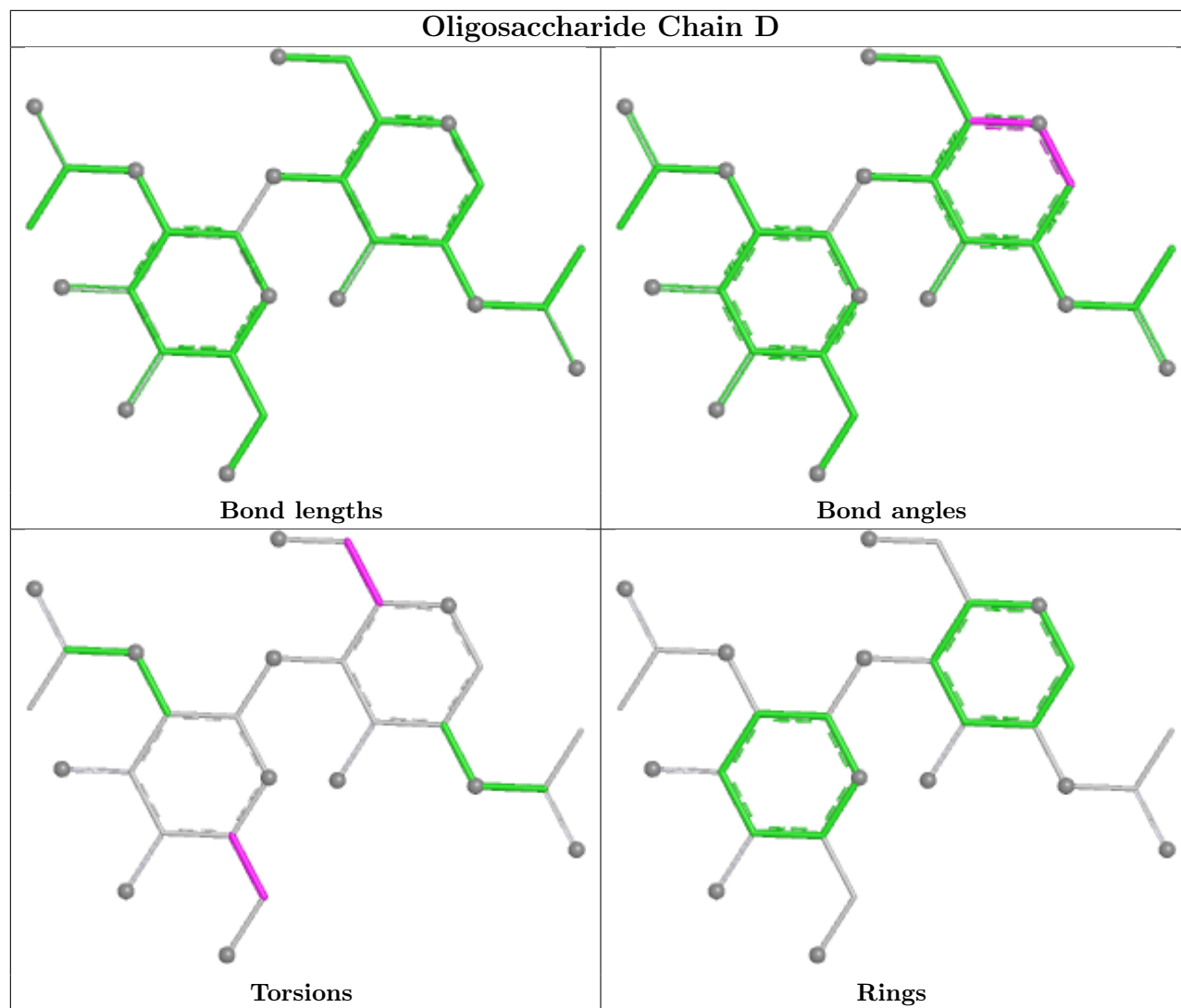
Mol	Chain	Res	Type	Atoms
5	P	3	BMA	C4-C5-C6-O6
5	N	2	NAG	O5-C5-C6-O6
4	S	1	NAG	C4-C5-C6-O6
2	R	1	NAG	C4-C5-C6-O6
2	I	2	NAG	O5-C5-C6-O6
2	T	2	NAG	O5-C5-C6-O6
3	U	2	NAG	C4-C5-C6-O6
3	V	3	BMA	O5-C5-C6-O6
4	H	3	BMA	C4-C5-C6-O6
2	R	1	NAG	O5-C5-C6-O6
2	F	2	NAG	C4-C5-C6-O6
4	G	1	NAG	C4-C5-C6-O6
2	T	1	NAG	O5-C5-C6-O6
4	S	2	NAG	C4-C5-C6-O6
3	U	3	BMA	C4-C5-C6-O6
4	G	2	NAG	C4-C5-C6-O6
3	Q	3	BMA	C4-C5-C6-O6
5	N	1	NAG	C4-C5-C6-O6
4	H	3	BMA	O5-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6
2	R	2	NAG	C1-C2-N2-C7
3	Q	2	NAG	C1-C2-N2-C7
3	X	1	NAG	O5-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6

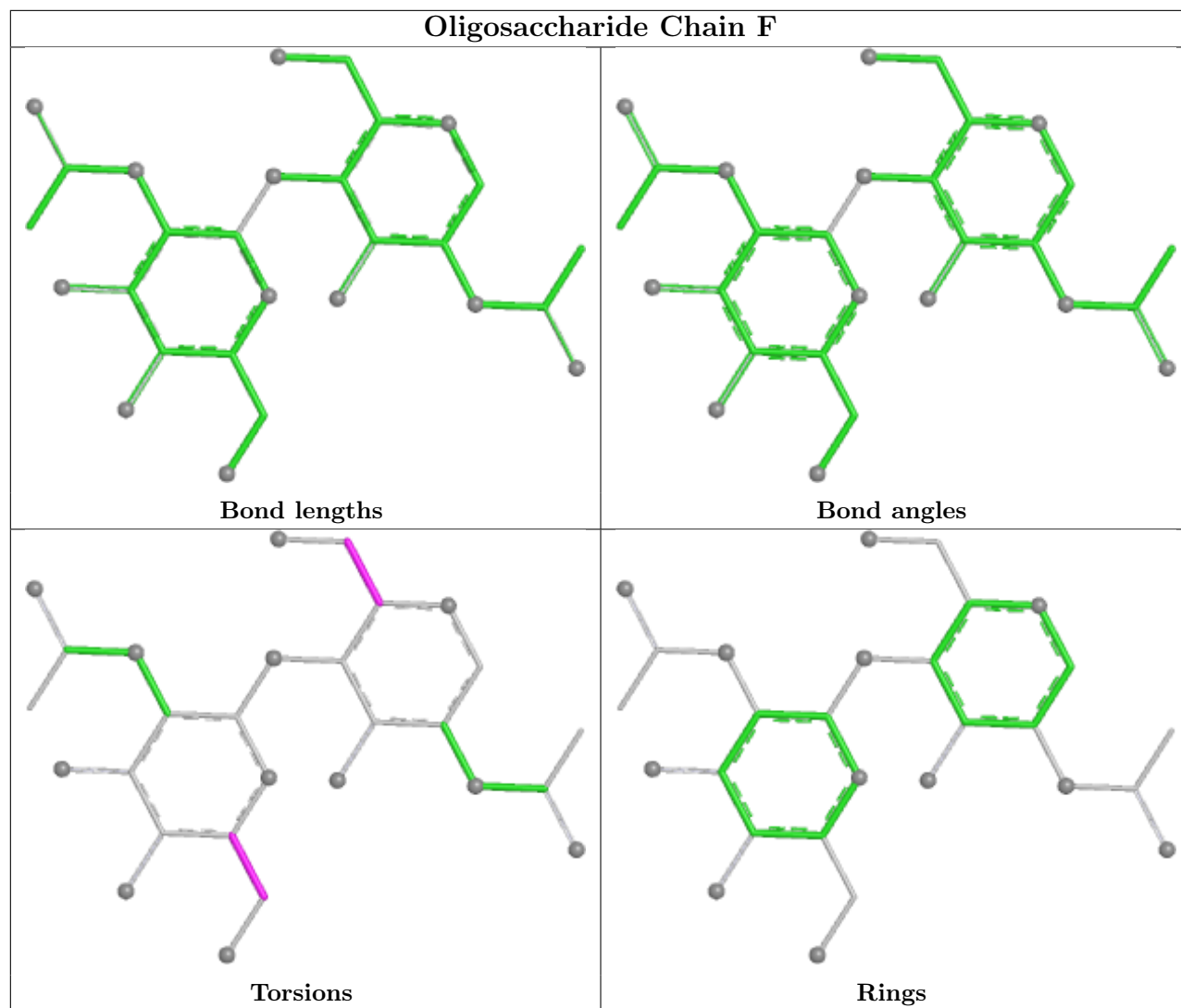
There are no ring outliers.

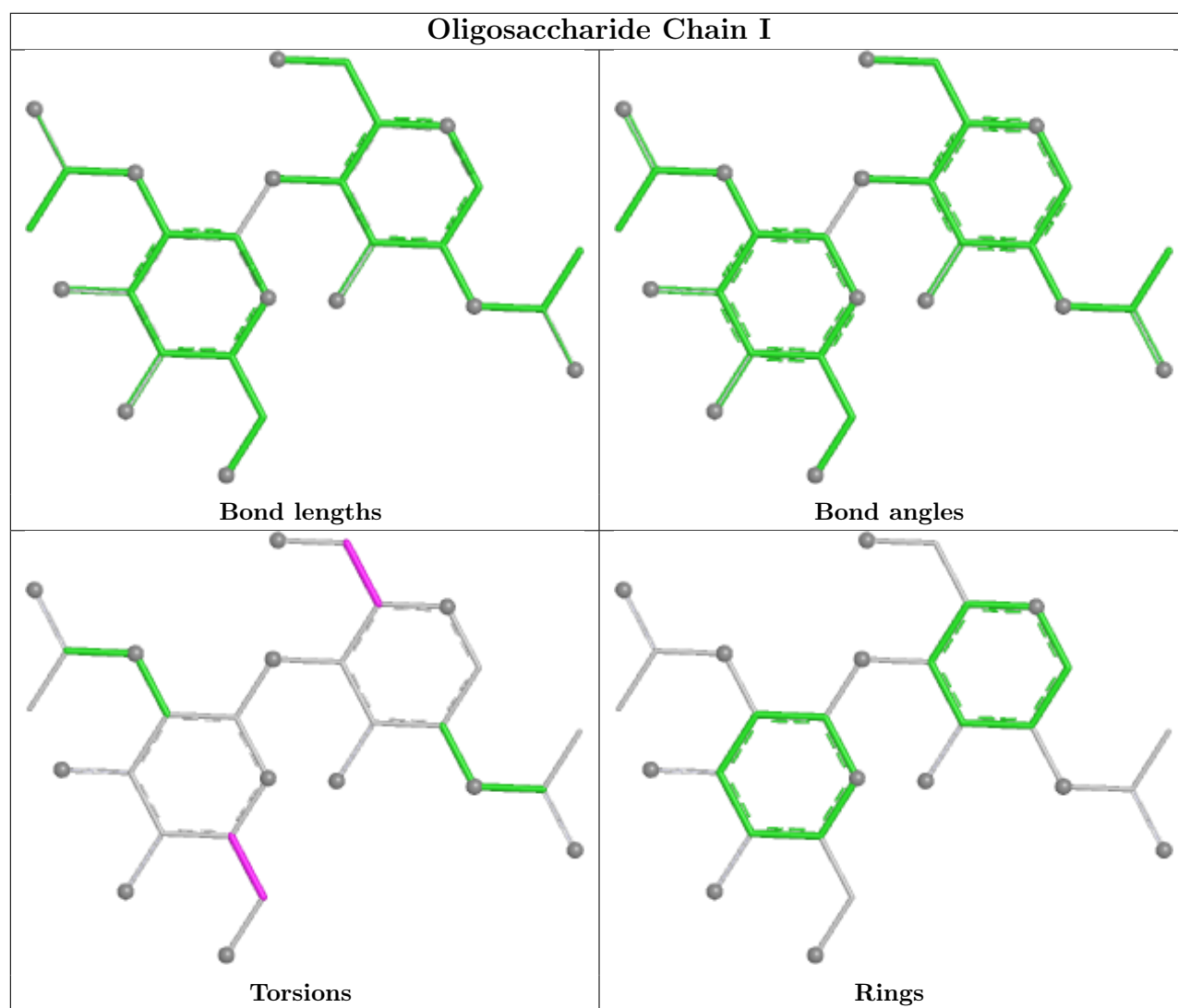
8 monomers are involved in 8 short contacts:

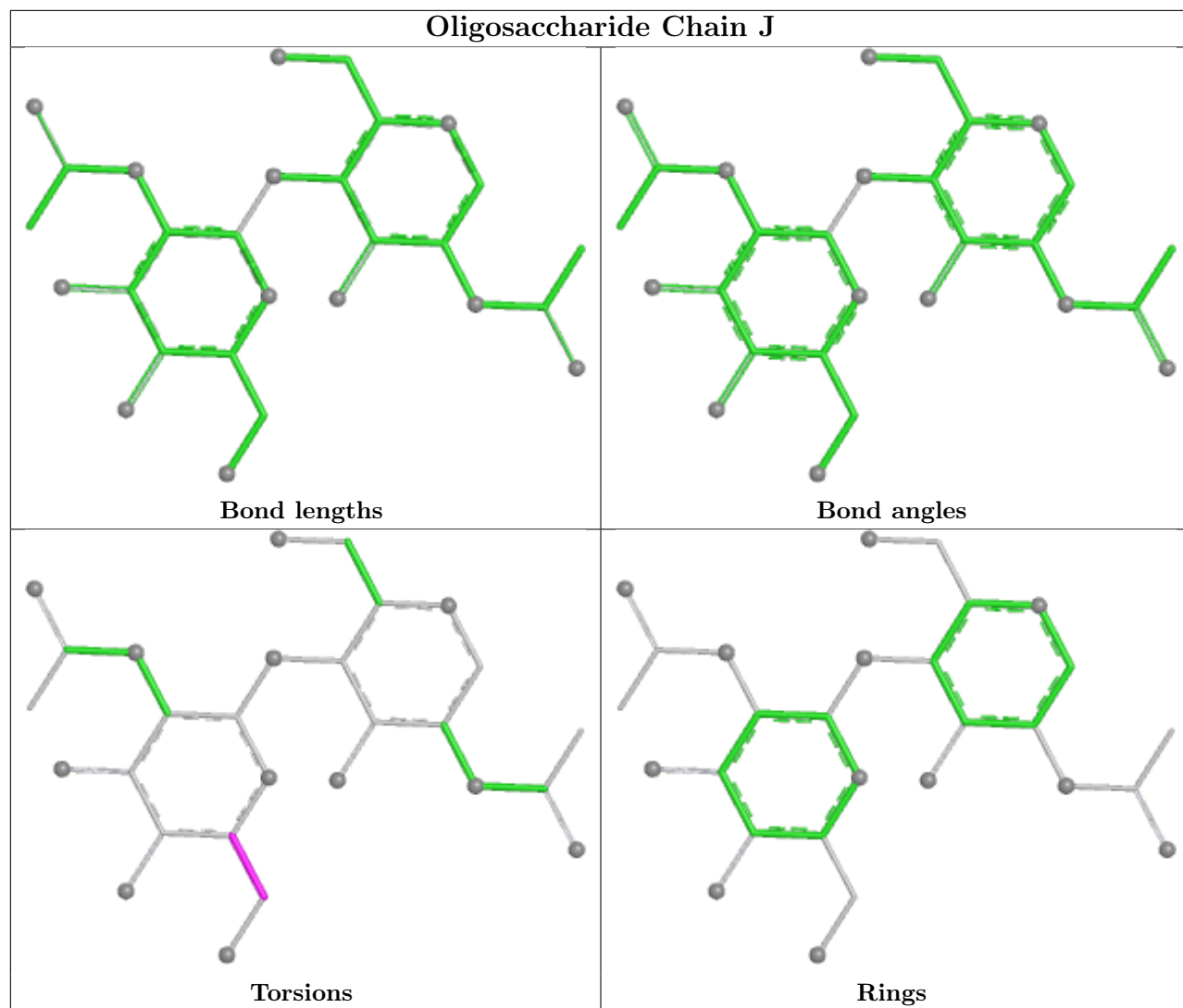
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1	NAG	1	0
3	Q	1	NAG	1	0
4	G	2	NAG	1	0
2	J	1	NAG	1	0
4	S	1	NAG	1	0
3	L	1	NAG	1	0
4	S	2	NAG	1	0
5	O	2	NAG	1	0

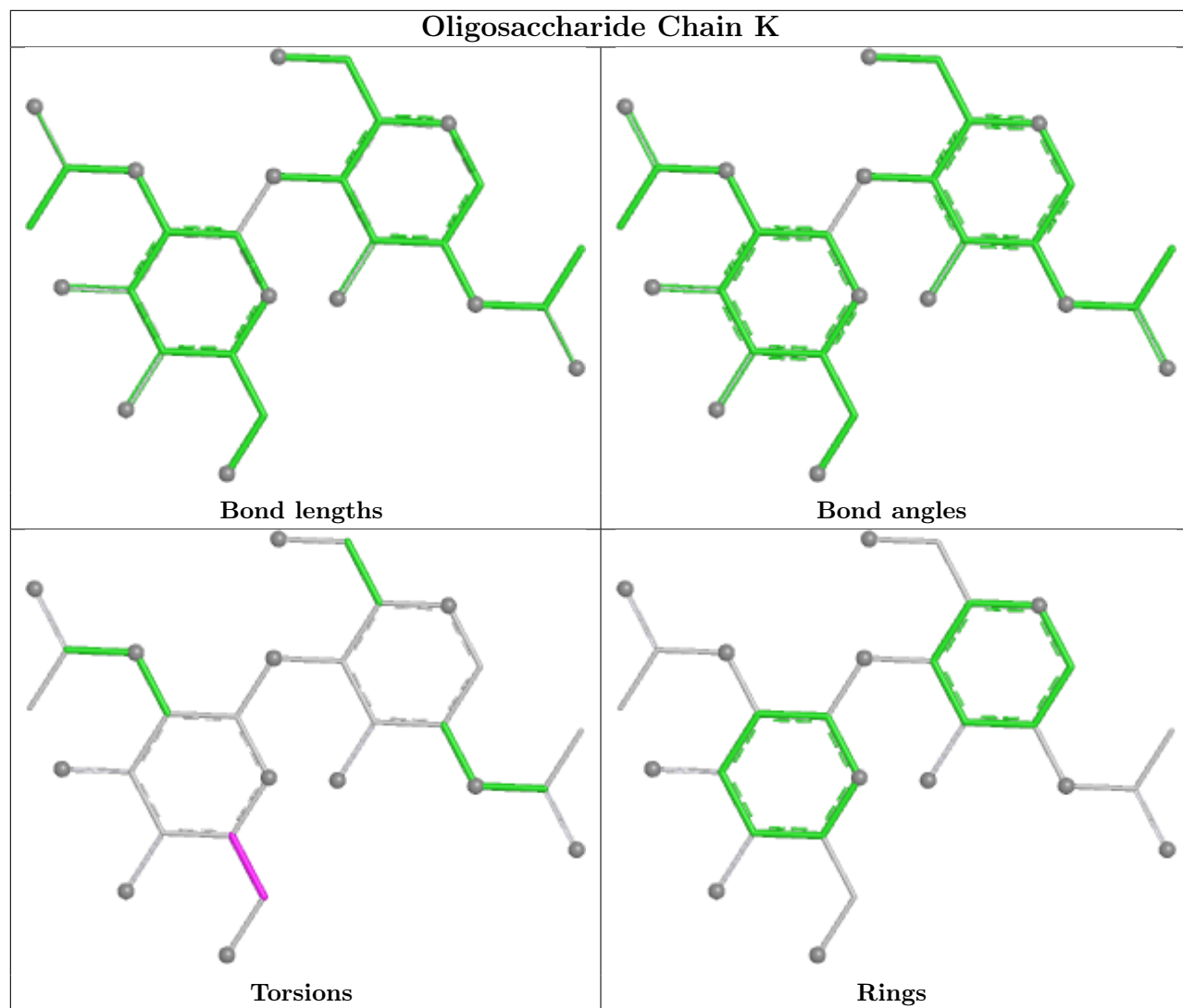
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

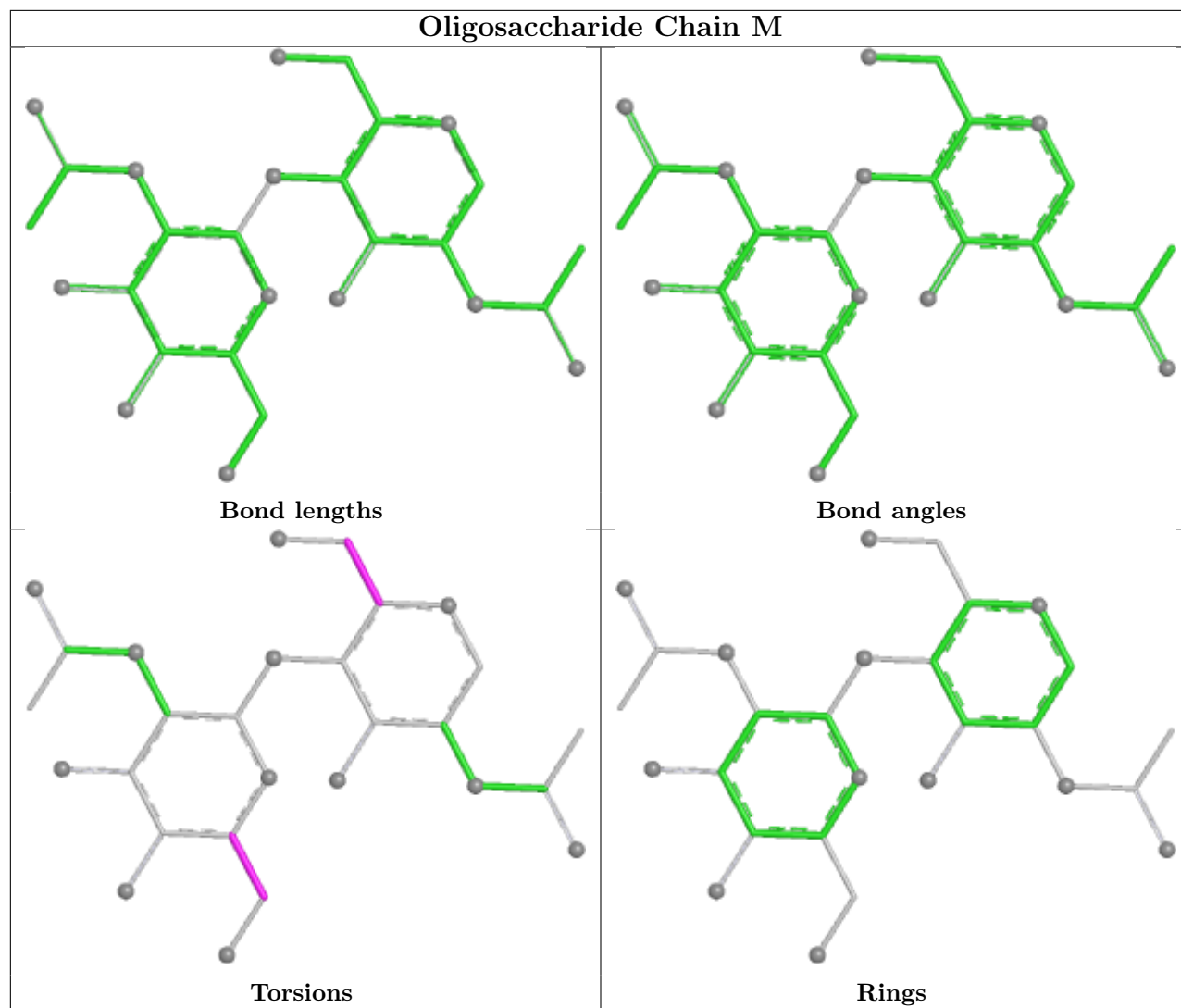


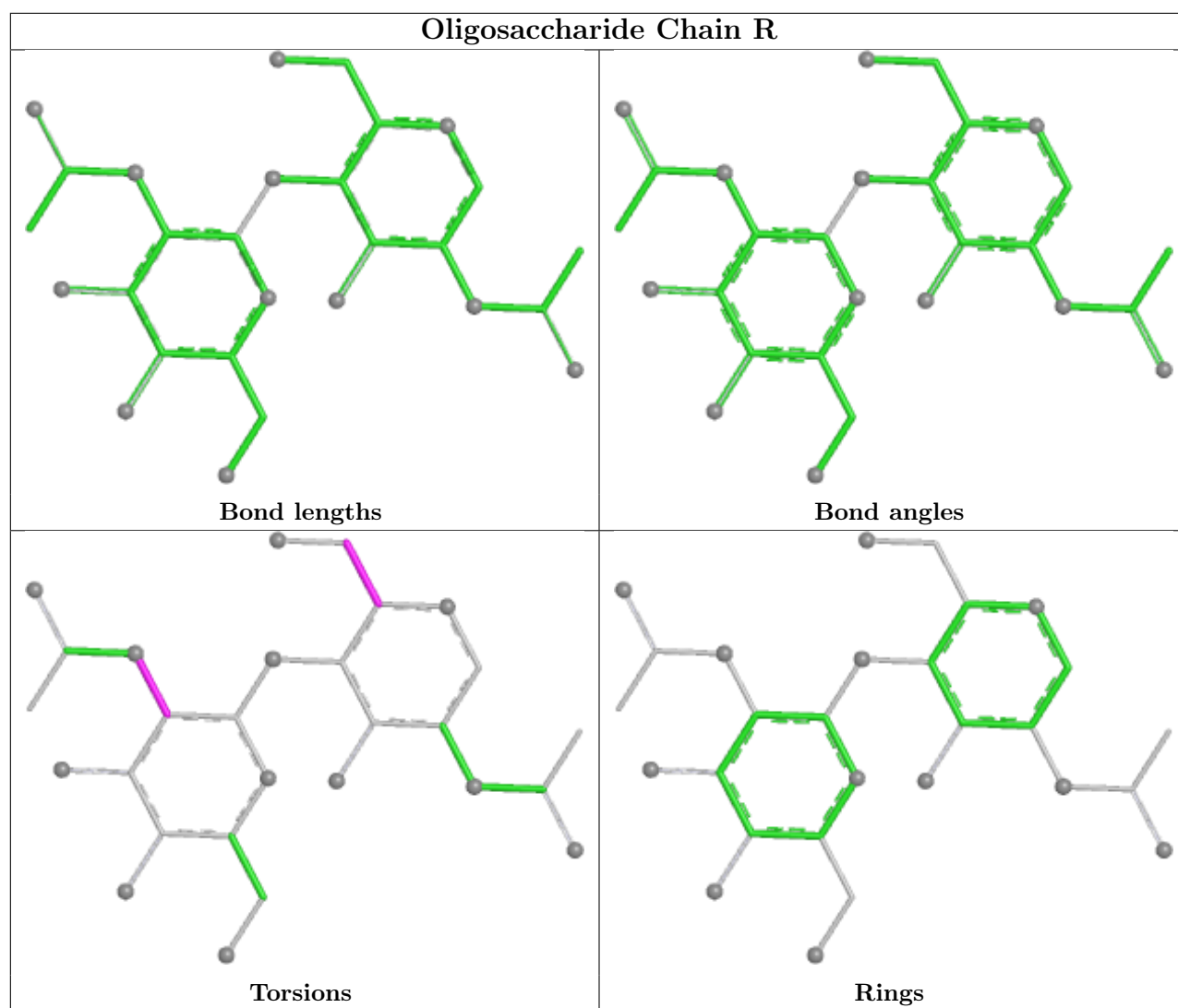


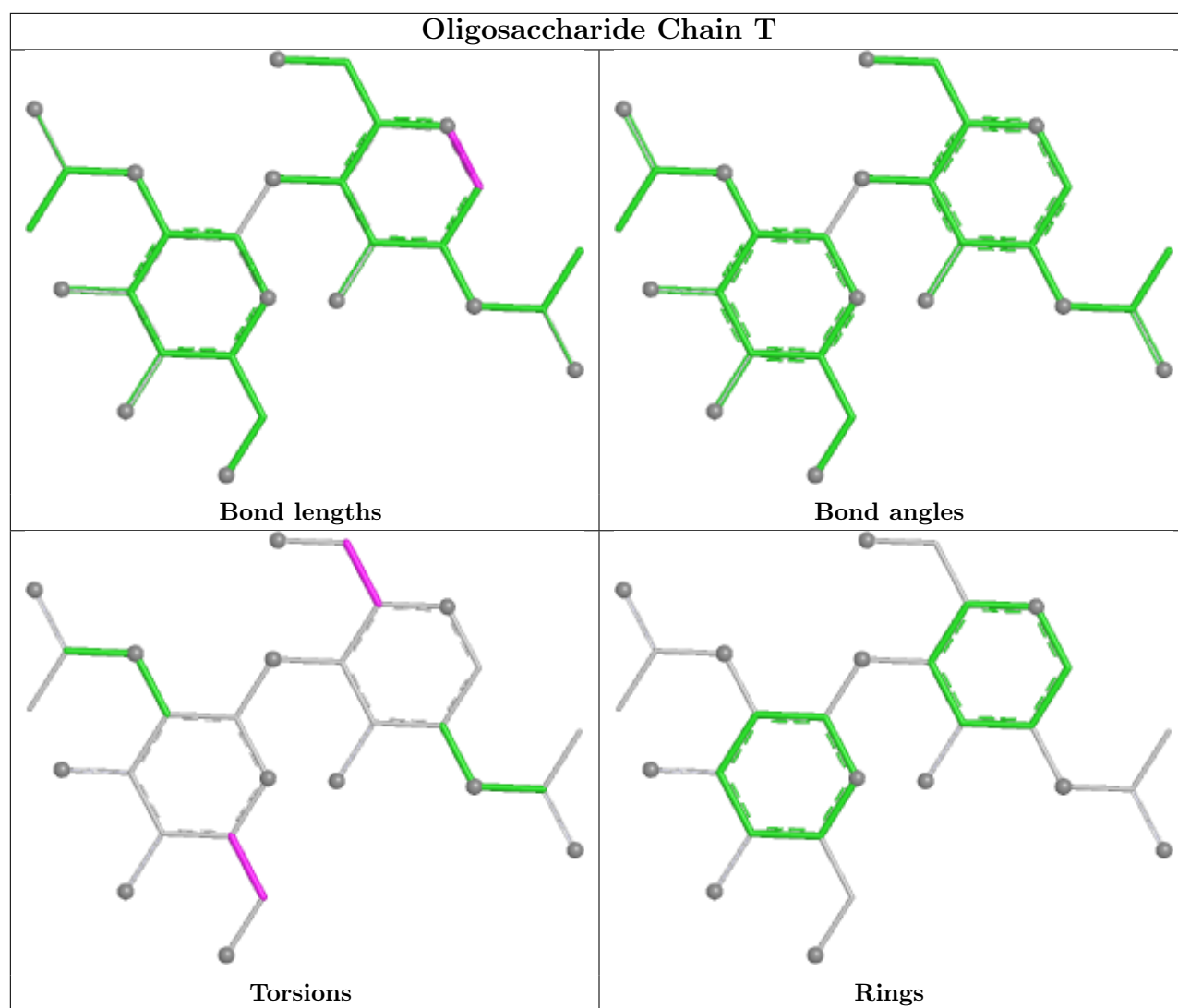


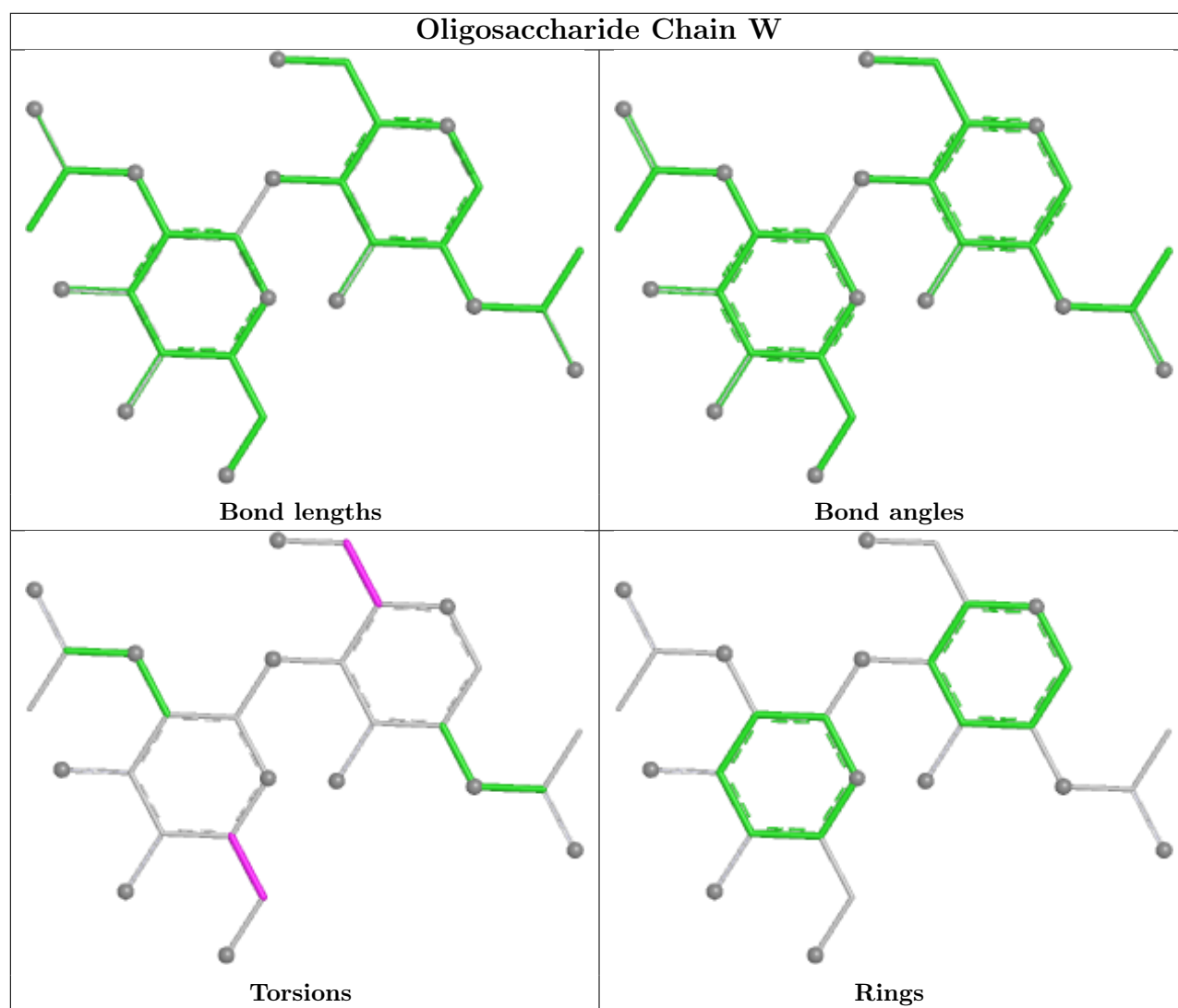


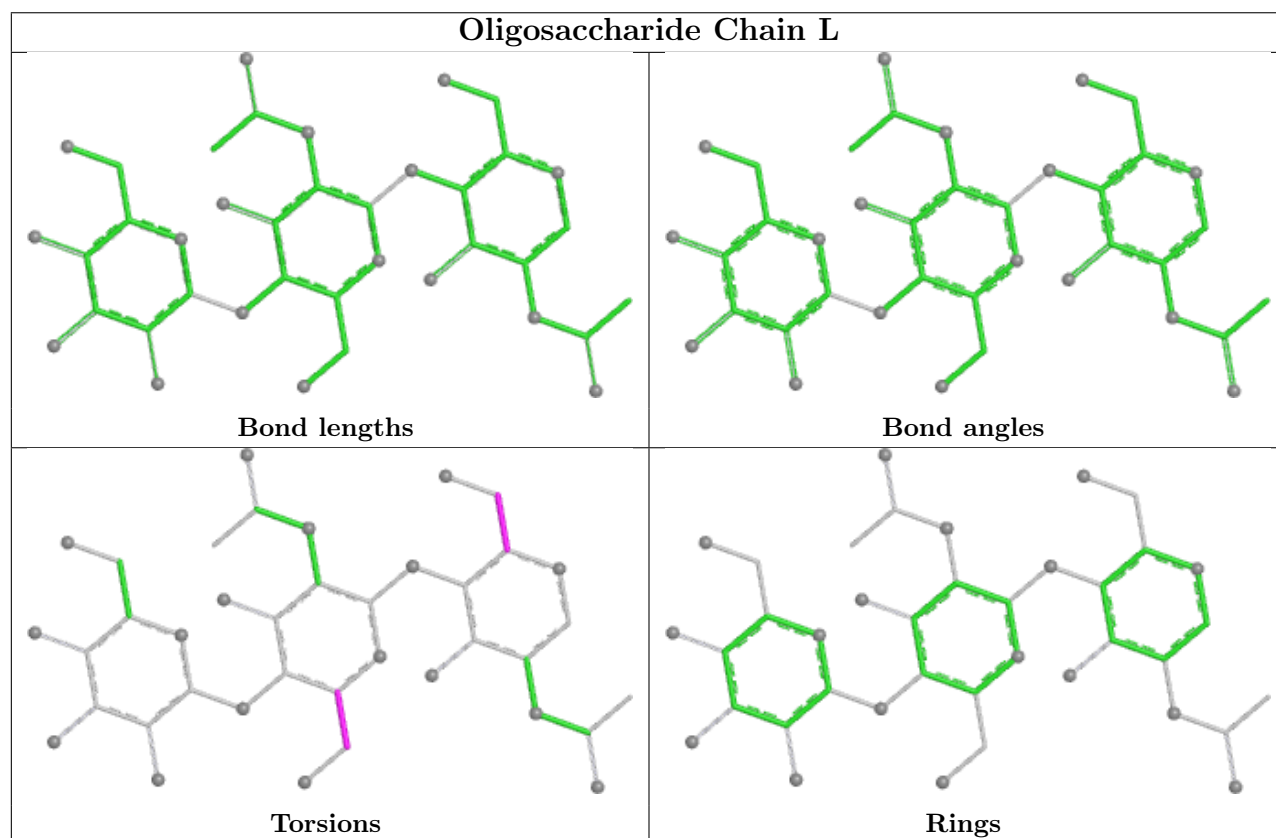
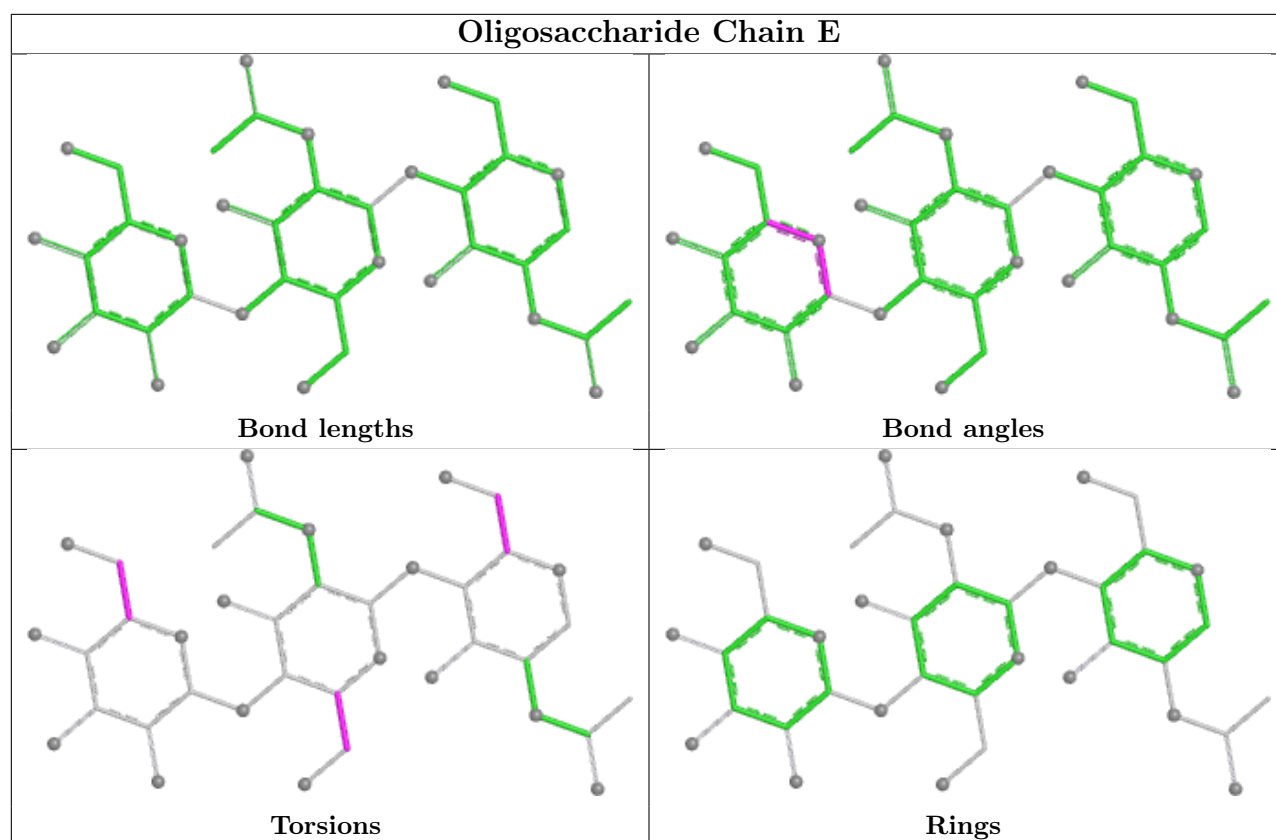


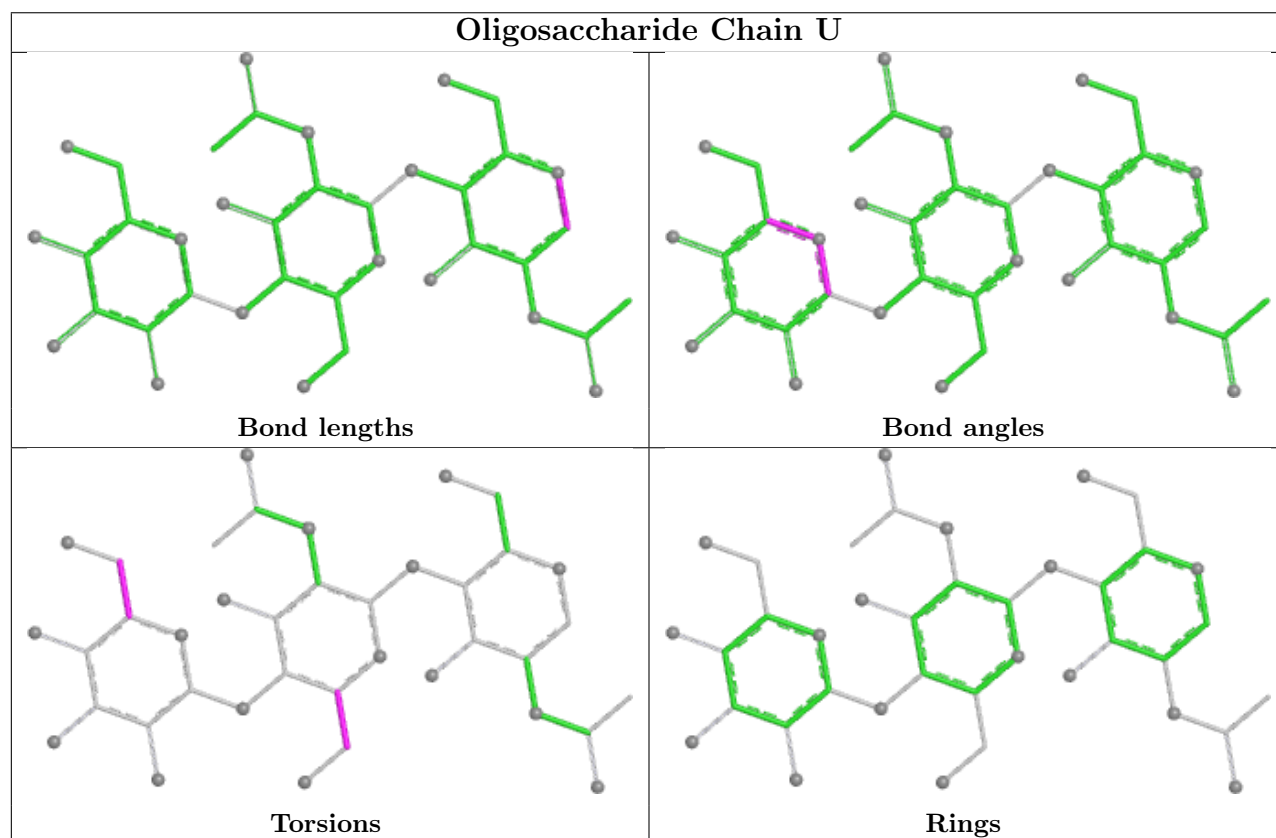
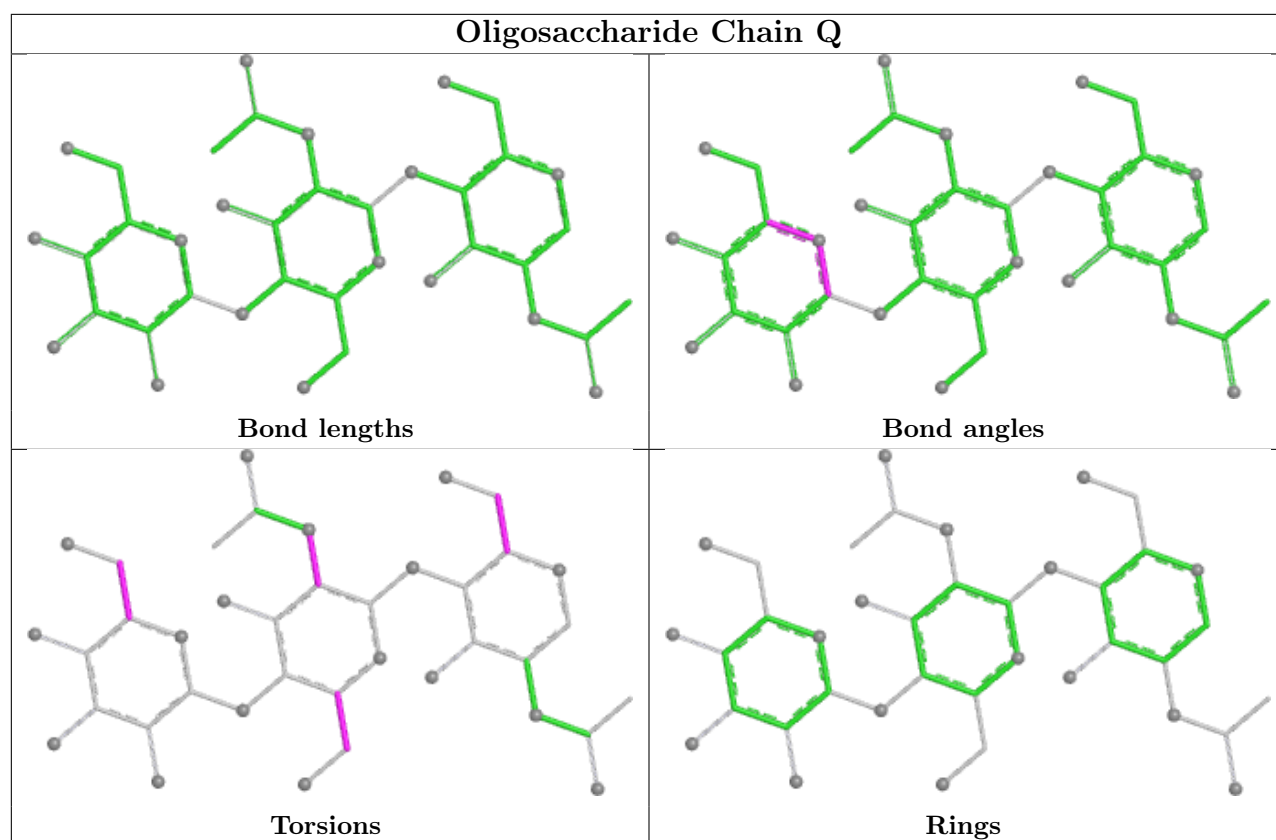


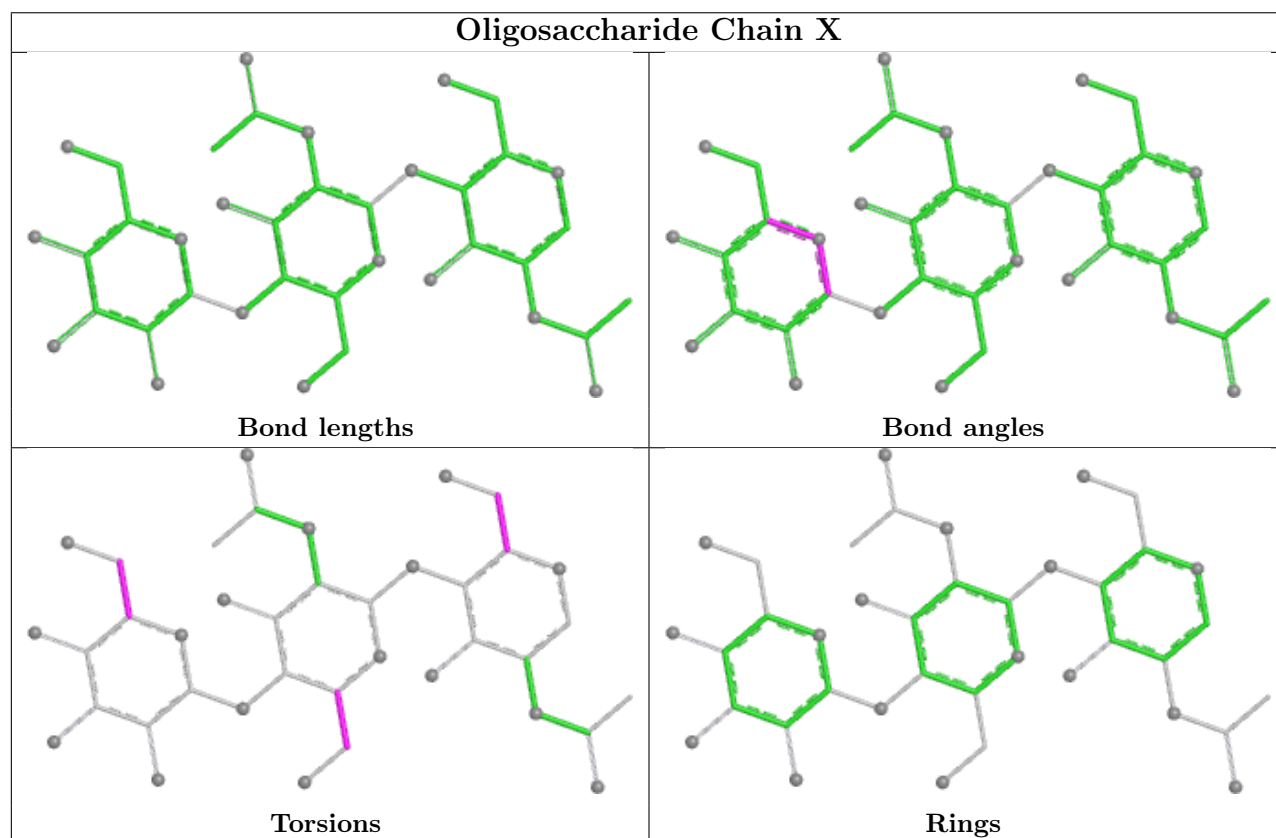
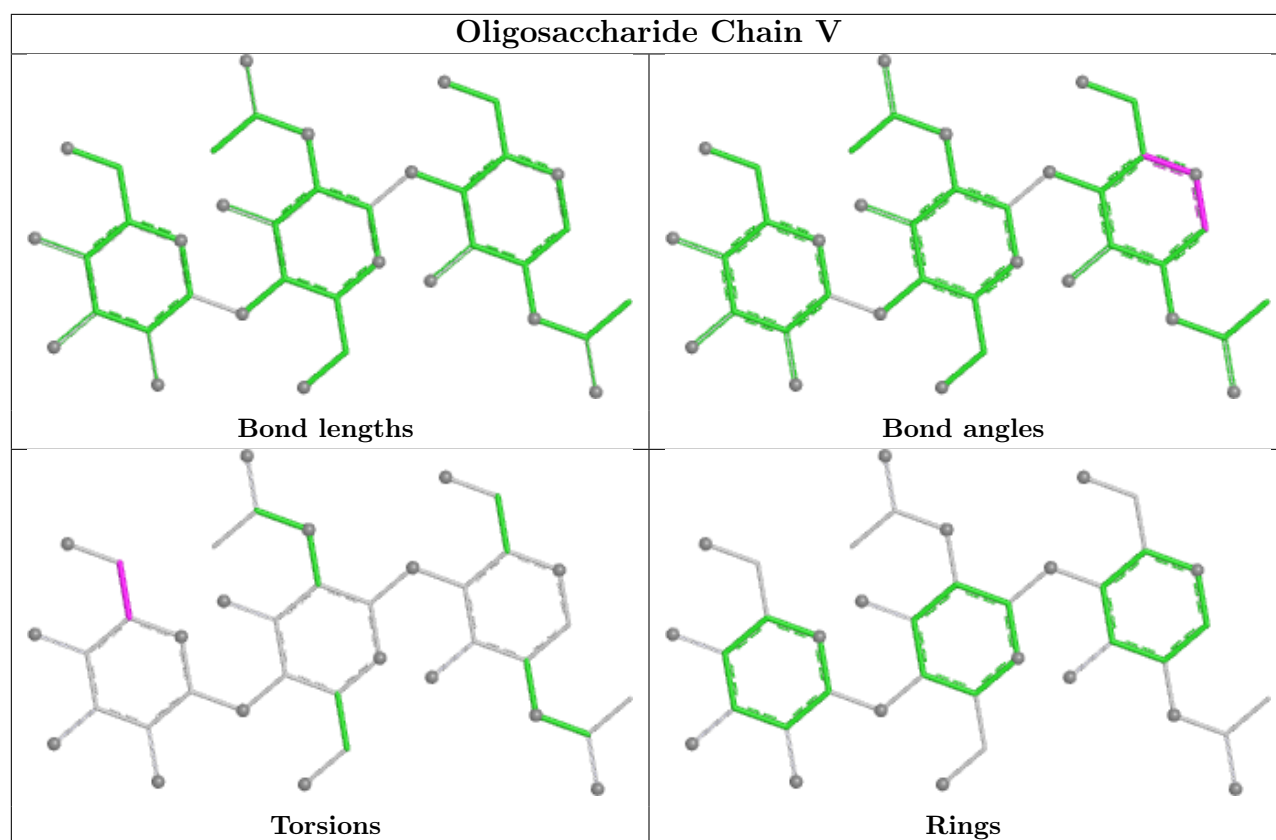


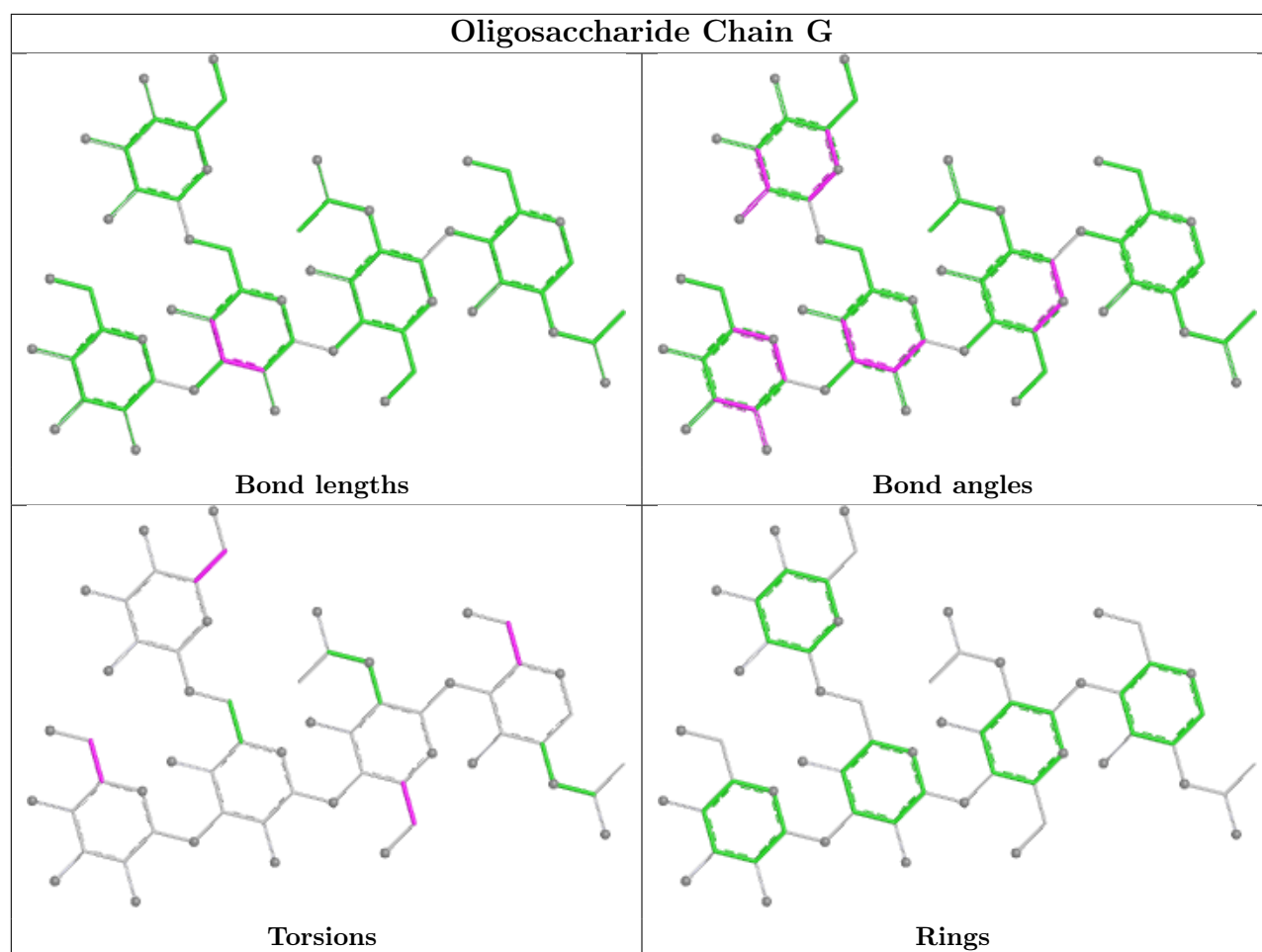


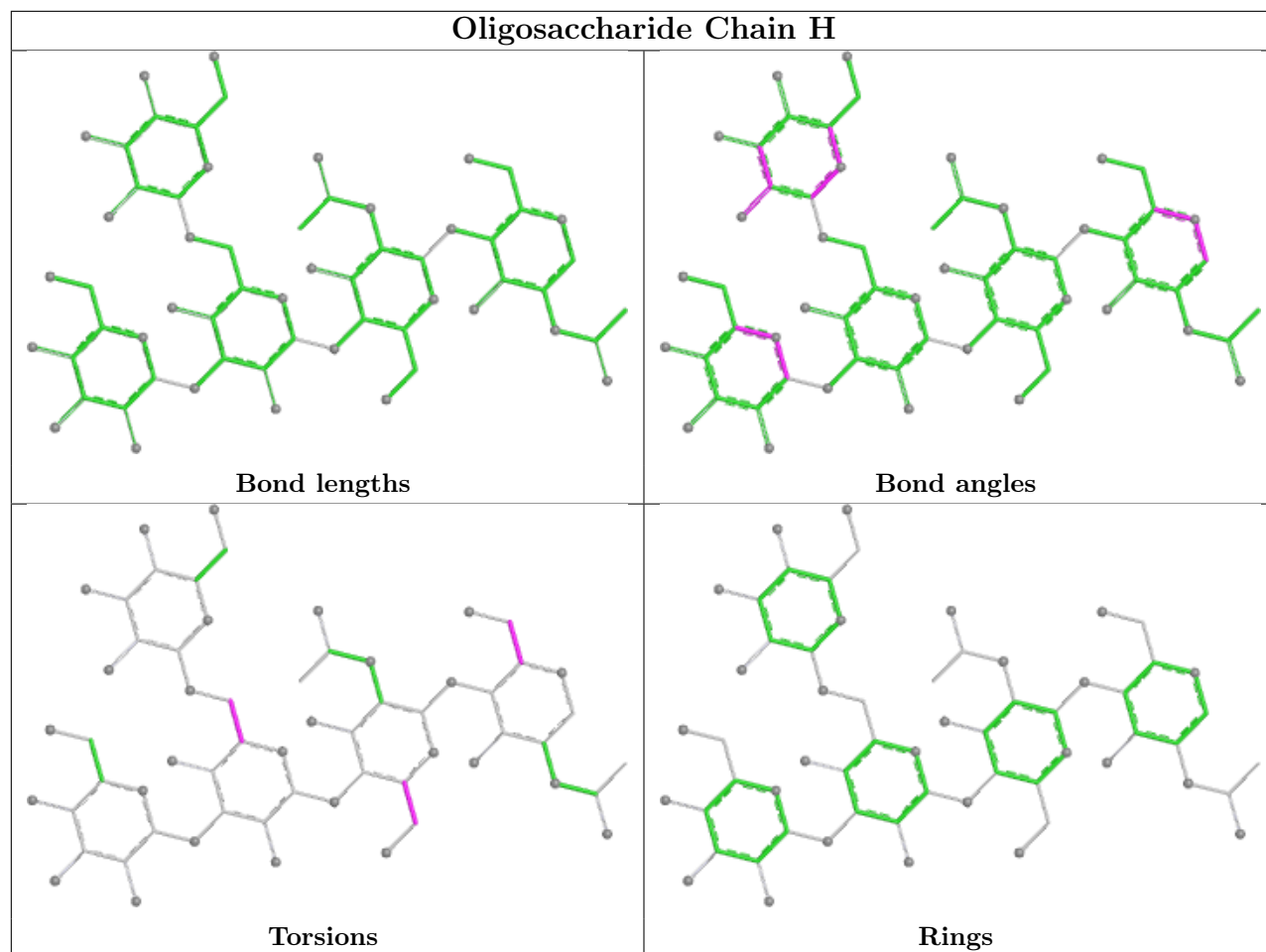


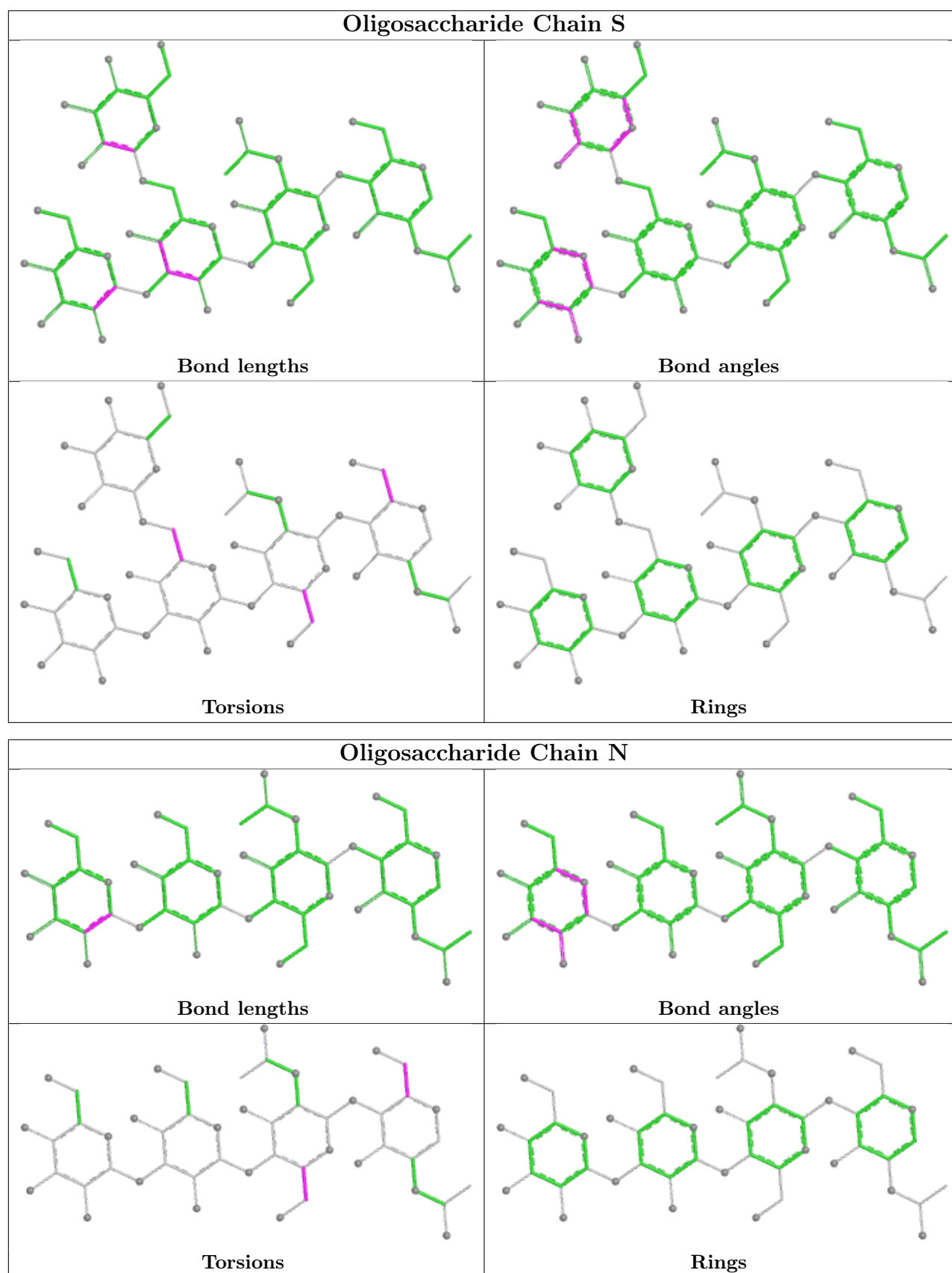


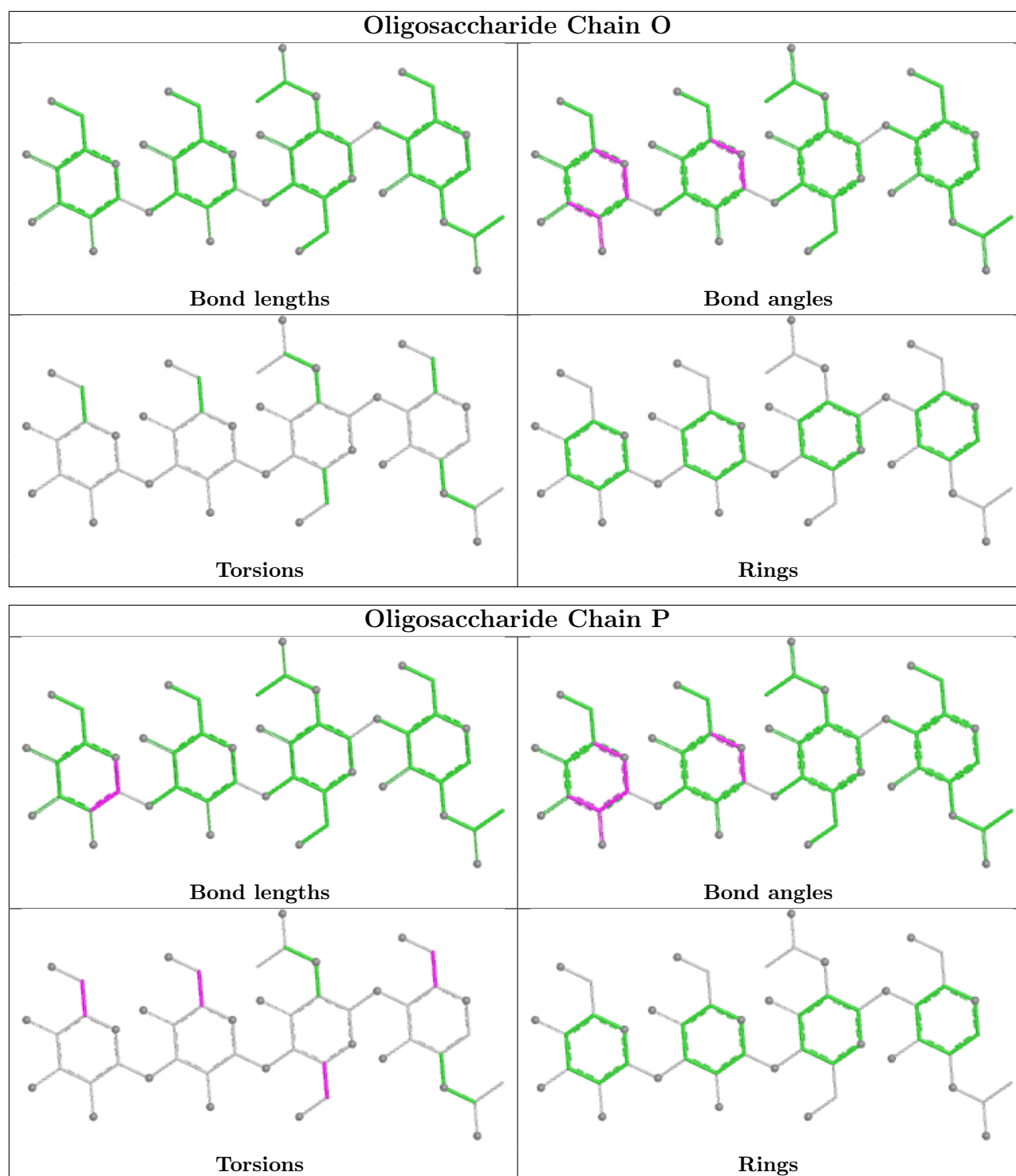












5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	NAG	A	1323	1	14,14,15	0.26	0	17,19,21	0.37	0
6	NAG	B	1322	1	14,14,15	0.24	0	17,19,21	0.62	0
6	NAG	C	1327	1	14,14,15	0.33	0	17,19,21	0.55	0
6	NAG	A	1301	1	14,14,15	0.39	0	17,19,21	0.57	0
6	NAG	A	1316	1	14,14,15	0.38	0	17,19,21	0.67	1 (5%)
6	NAG	A	1317	1	14,14,15	0.42	0	17,19,21	0.43	0
6	NAG	C	1308	1	14,14,15	0.28	0	17,19,21	0.42	0
6	NAG	B	1302	1	14,14,15	0.56	0	17,19,21	0.62	0
6	NAG	B	1323	1	14,14,15	0.19	0	17,19,21	0.38	0
6	NAG	C	1321	1	14,14,15	0.46	0	17,19,21	0.48	0
6	NAG	A	1307	1	14,14,15	0.20	0	17,19,21	0.45	0
6	NAG	B	1301	1	14,14,15	0.25	0	17,19,21	0.59	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	A	1323	1	-	0/6/23/26	0/1/1/1
6	NAG	B	1322	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1327	1	-	1/6/23/26	0/1/1/1
6	NAG	A	1301	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1316	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1317	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1308	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1302	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1323	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1321	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1307	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1301	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1316	NAG	C1-O5-C5	2.28	115.24	112.19

There are no chirality outliers.

All (21) 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	1322	NAG	O5-C5-C6-O6
6	C	1321	NAG	O5-C5-C6-O6
6	A	1307	NAG	O5-C5-C6-O6
6	B	1301	NAG	O5-C5-C6-O6
6	C	1308	NAG	O5-C5-C6-O6
6	A	1316	NAG	C4-C5-C6-O6
6	A	1307	NAG	C4-C5-C6-O6
6	C	1308	NAG	C4-C5-C6-O6
6	B	1301	NAG	C4-C5-C6-O6
6	B	1323	NAG	C4-C5-C6-O6
6	B	1322	NAG	C4-C5-C6-O6
6	A	1301	NAG	C4-C5-C6-O6
6	B	1323	NAG	O5-C5-C6-O6
6	C	1321	NAG	C4-C5-C6-O6
6	A	1317	NAG	O5-C5-C6-O6
6	B	1302	NAG	C4-C5-C6-O6
6	A	1317	NAG	C4-C5-C6-O6
6	C	1327	NAG	C4-C5-C6-O6
6	B	1302	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	1321	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

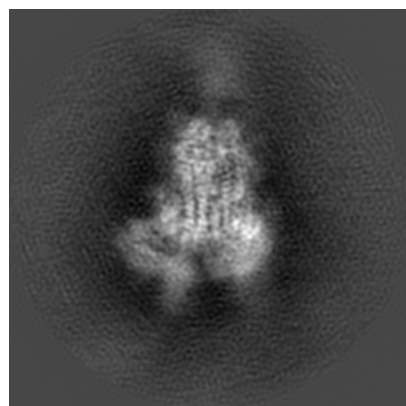
6 Map visualisation [i](#)

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

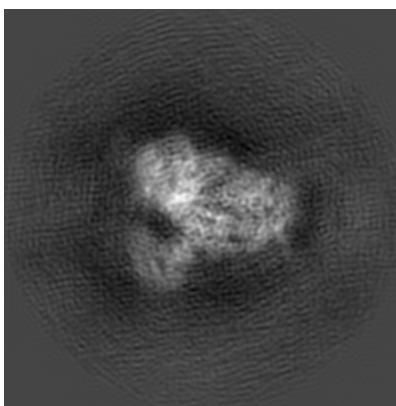
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

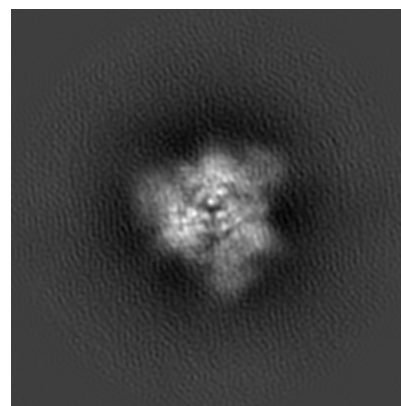
6.1.1 Primary map



X

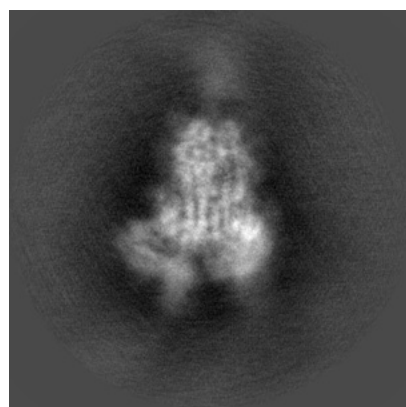


Y

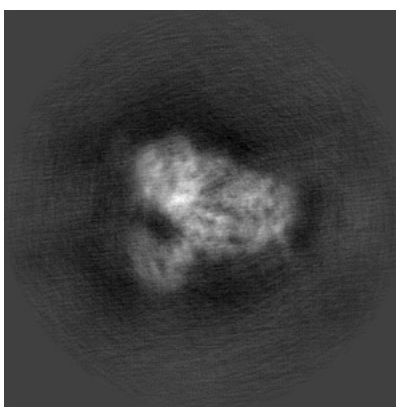


Z

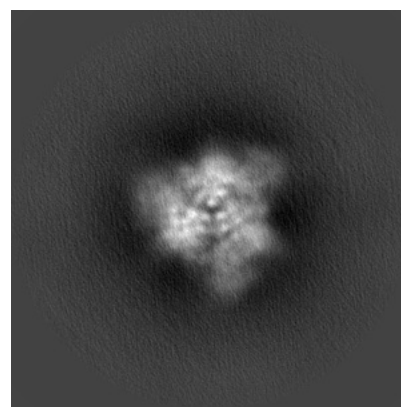
6.1.2 Raw map



X



Y

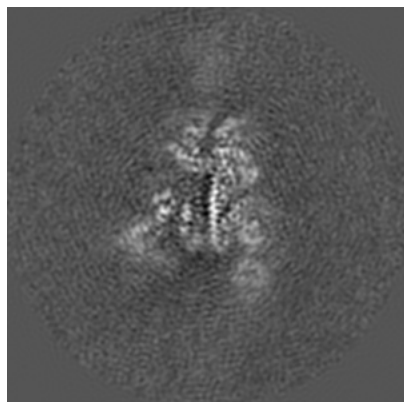


Z

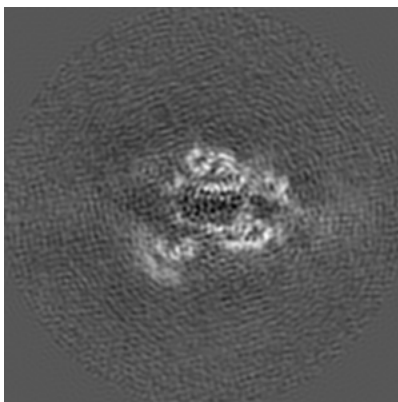
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

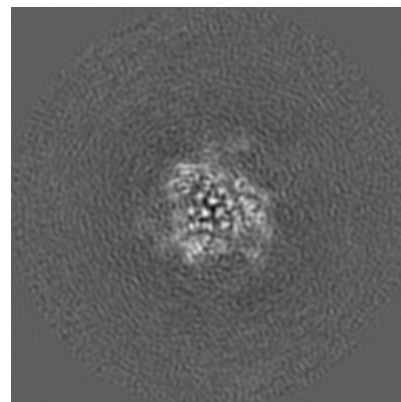
6.2.1 Primary map



X Index: 160

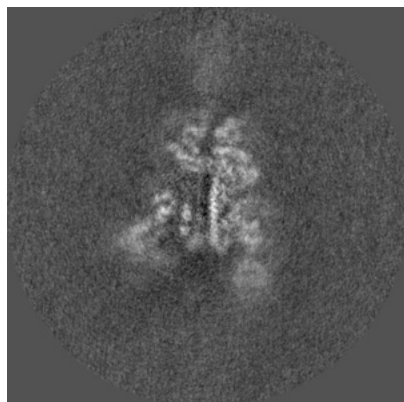


Y Index: 160

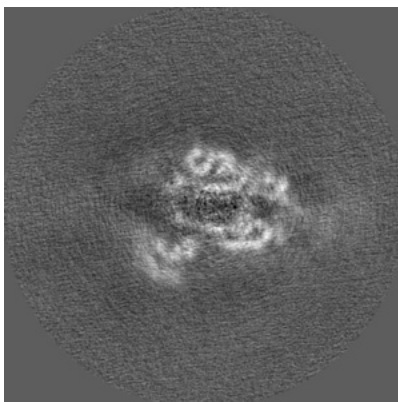


Z Index: 160

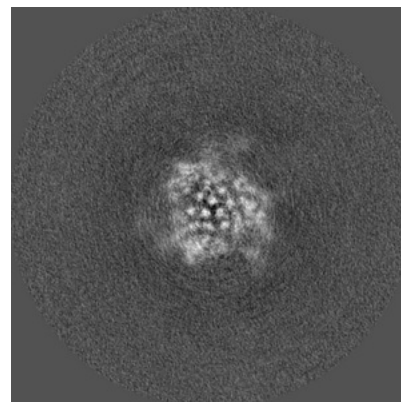
6.2.2 Raw map



X Index: 160



Y Index: 160

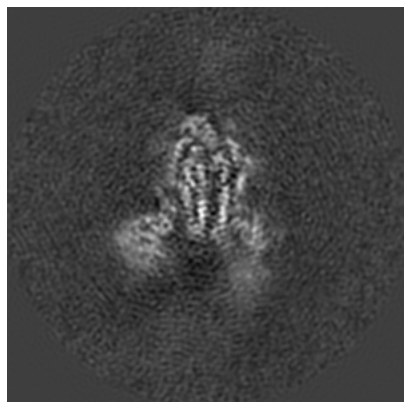


Z Index: 160

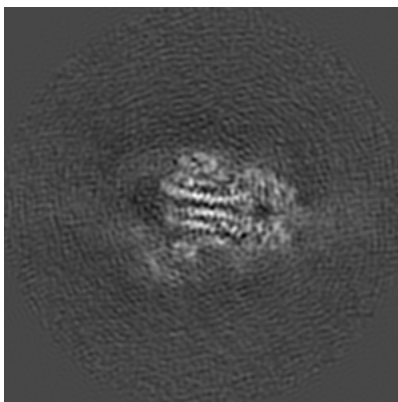
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

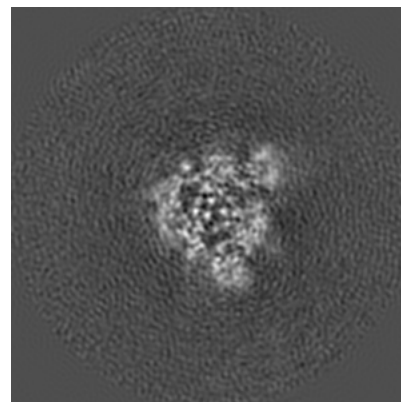
6.3.1 Primary map



X Index: 168

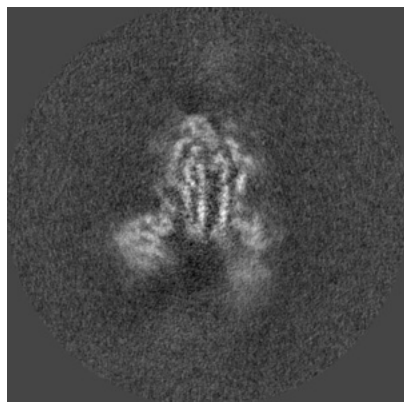


Y Index: 155

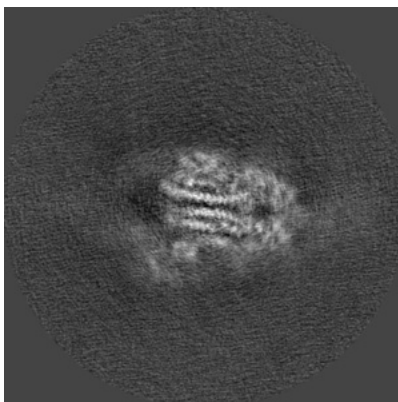


Z Index: 147

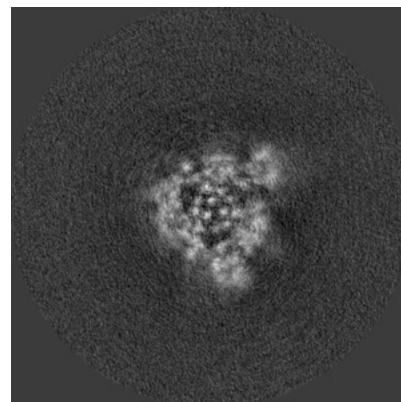
6.3.2 Raw map



X Index: 168



Y Index: 155

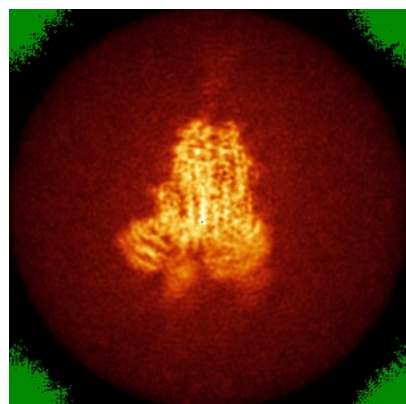


Z Index: 147

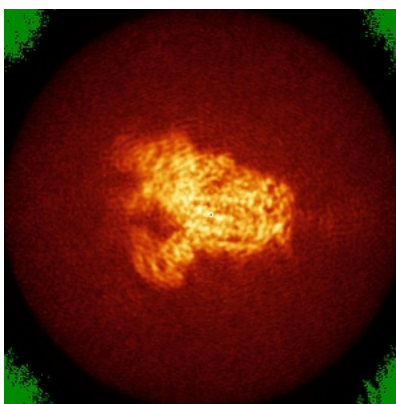
The images above show the largest variance slices of the map in three orthogonal directions.

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

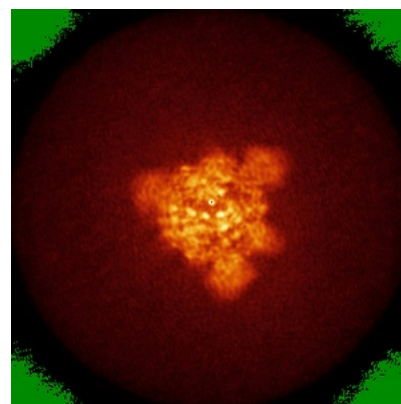
6.4.1 Primary map



X

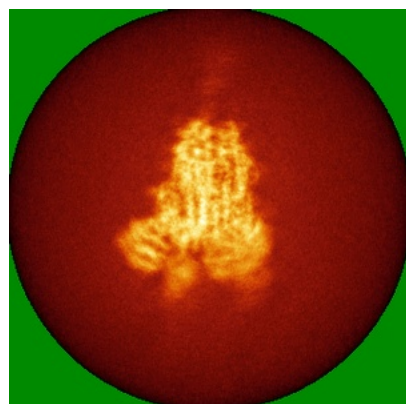


Y

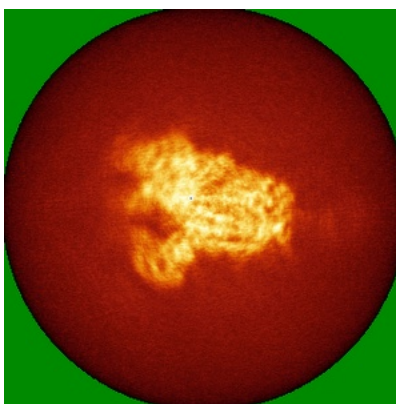


Z

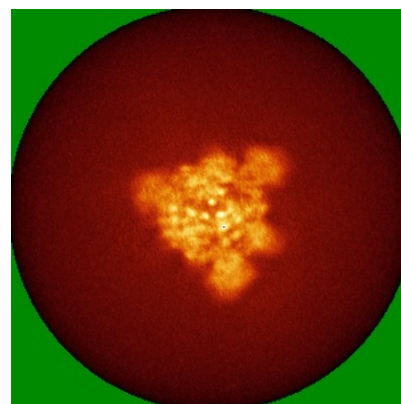
6.4.2 Raw map



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 0.032. 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.

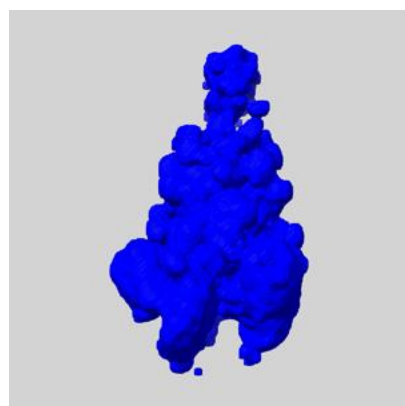
6.6 Mask visualisation [i](#)

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

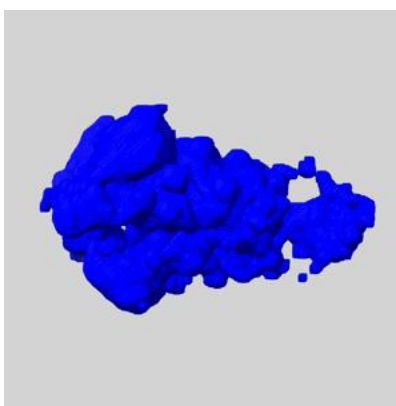
A mask typically either:

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

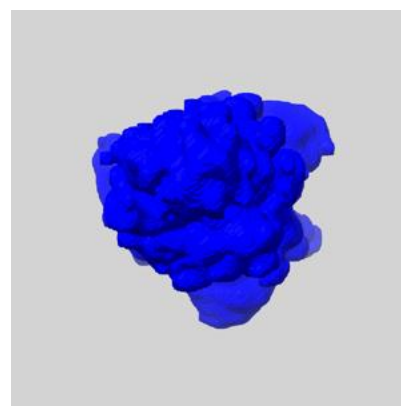
6.6.1 emd_7579_msk_1.map [i](#)



X



Y

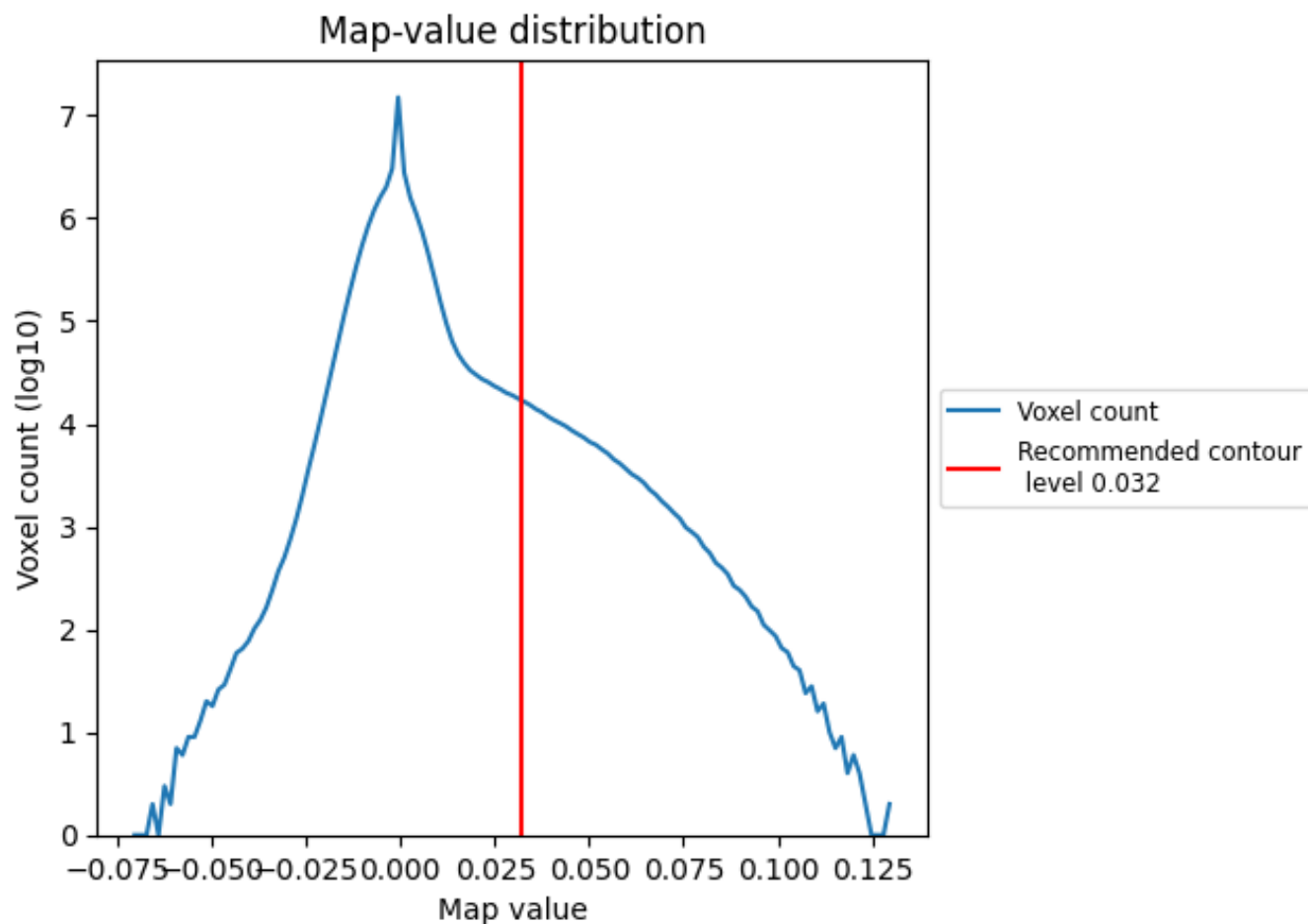


Z

7 Map analysis [i](#)

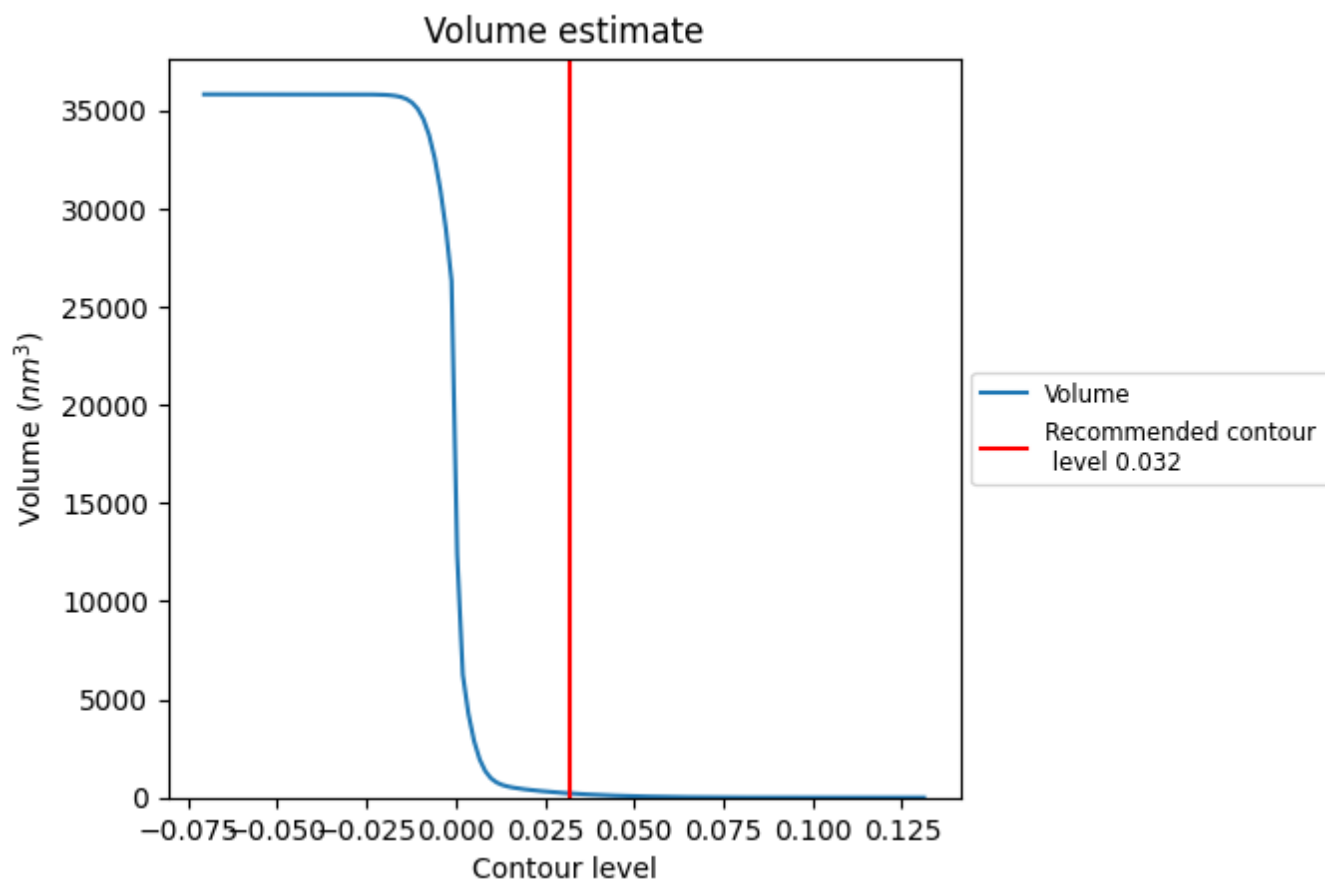
This section contains the results of statistical analysis of the map.

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.

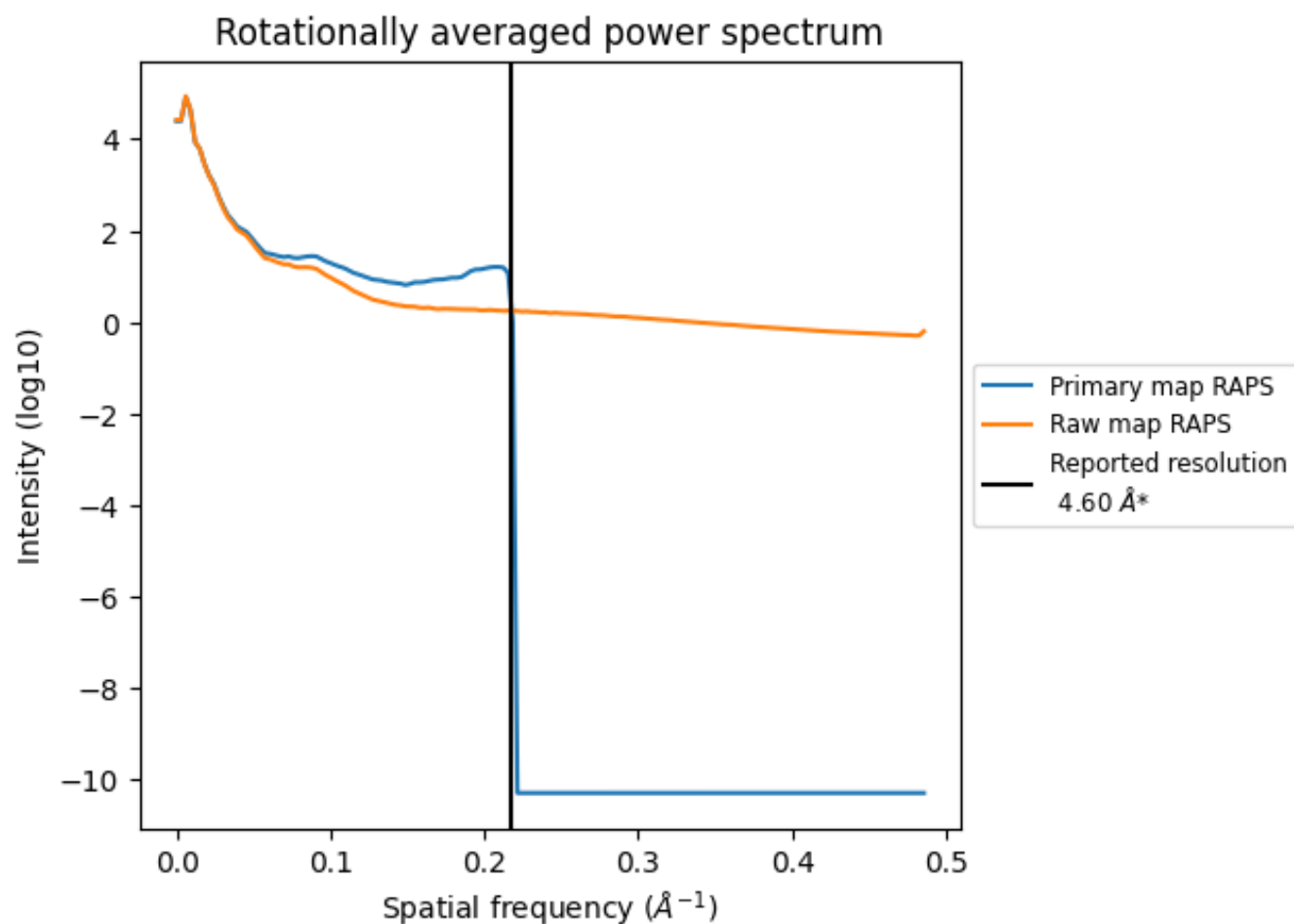
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 213 nm³; this corresponds to an approximate mass of 192 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

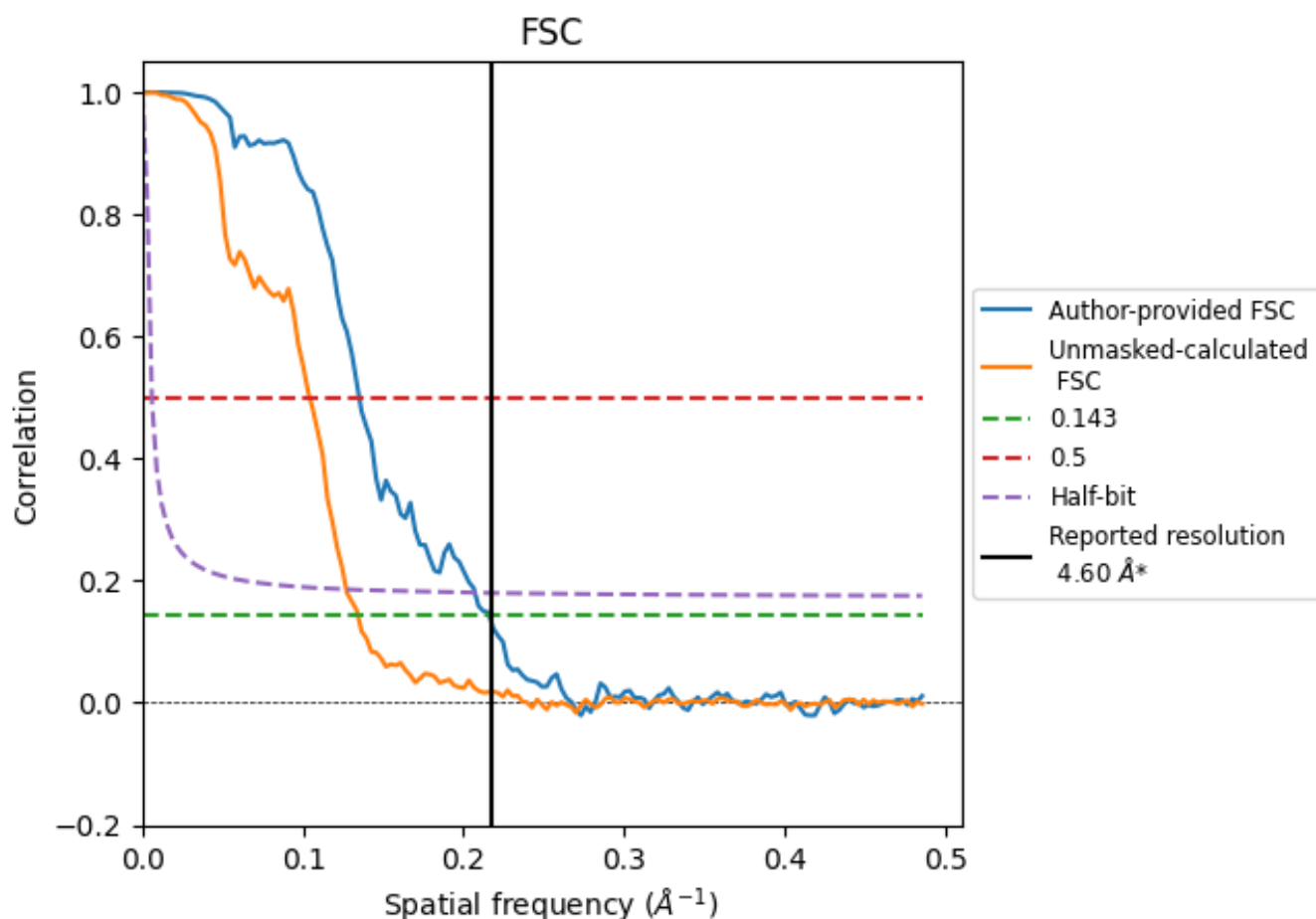


*Reported resolution corresponds to spatial frequency of 0.217 Å⁻¹

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 0.217 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

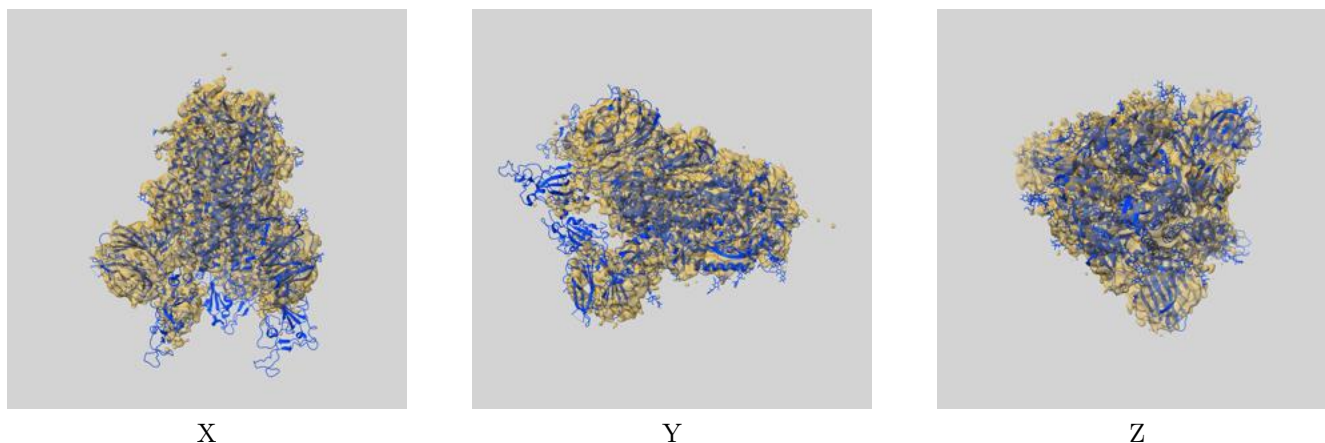
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.60	-	-
Author-provided FSC curve	4.63	7.41	4.83
Unmasked-calculated*	7.45	9.60	7.87

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.45 differs from the reported value 4.6 by more than 10 %

9 Map-model fit [i](#)

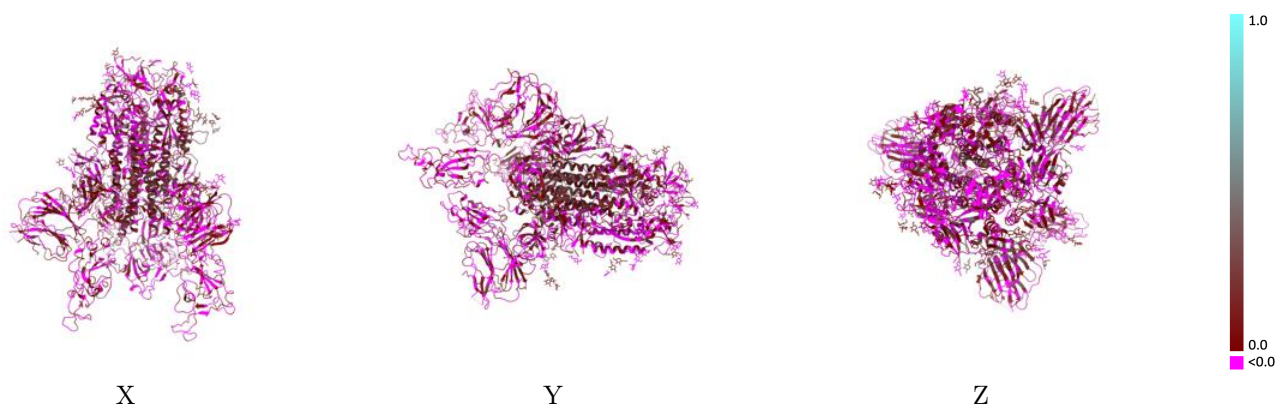
This section contains information regarding the fit between EMDB map EMD-7579 and PDB model 6CS1. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



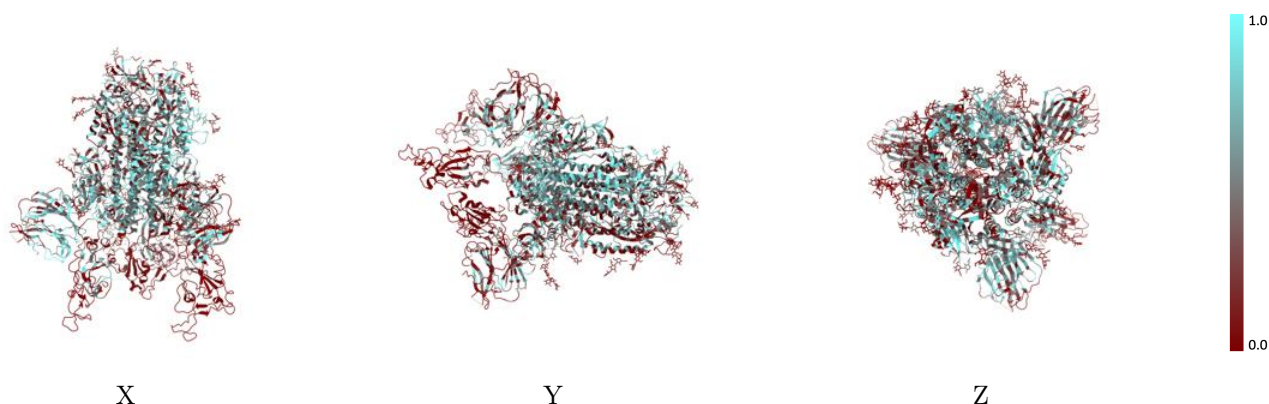
The images above show the 3D surface view of the map at the recommended contour level 0.032 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



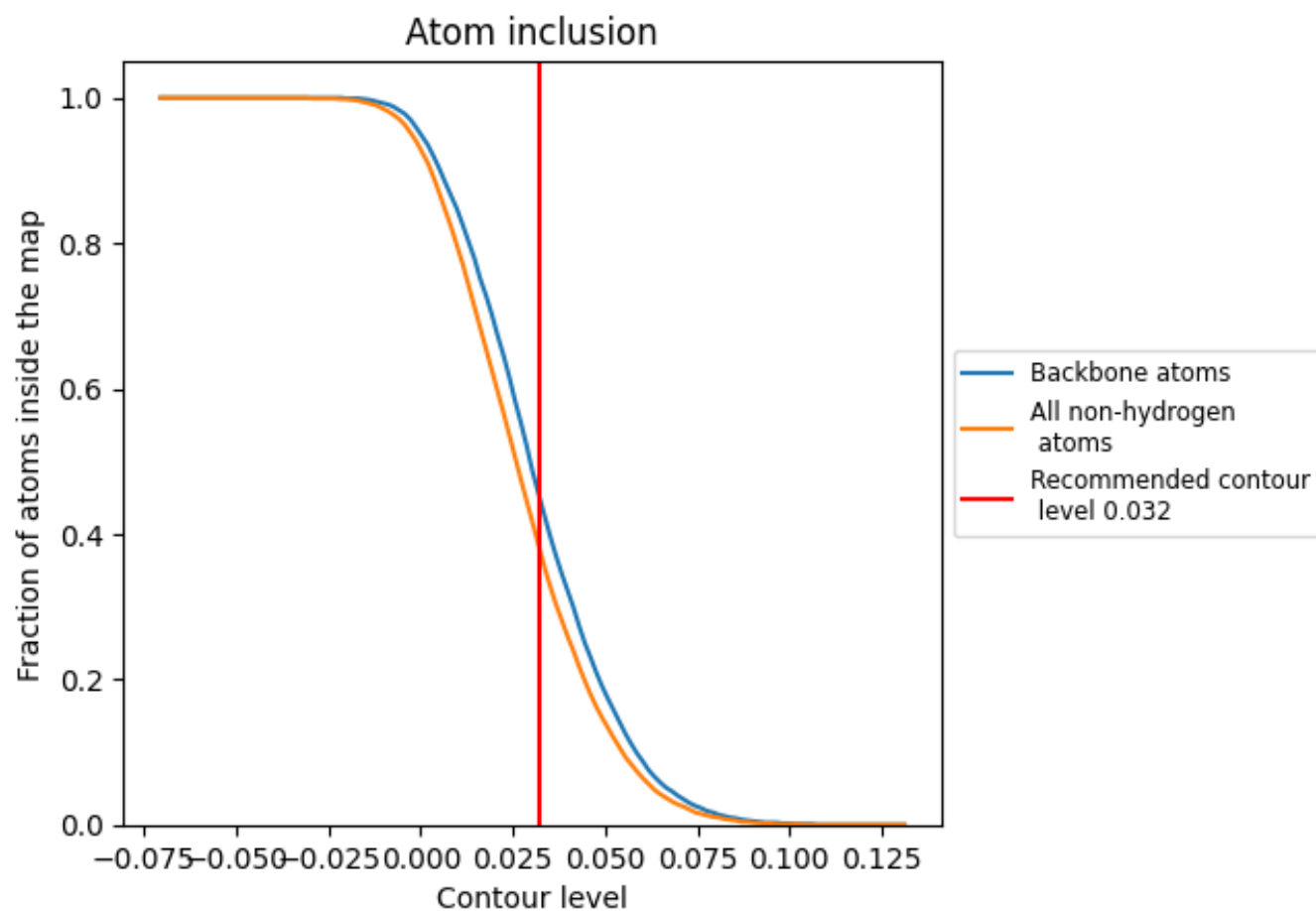
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.032).

9.4 Atom inclusion [i](#)



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

9.5 Map-model fit summary

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

Chain	Atom inclusion	Q-score
All	 0.3840	 0.0410
A	 0.3430	 0.0250
B	 0.4190	 0.0580
C	 0.4130	 0.0380
D	 0.0000	 -0.1130
E	 0.0260	 -0.0080
F	 0.0360	 0.0870
G	 0.1640	 0.0420
H	 0.4100	 0.2230
I	 0.1430	 0.0230
J	 0.1430	 -0.0700
K	 0.1790	 0.1480
L	 0.0510	 -0.0060
M	 0.1790	 0.0430
N	 0.1000	 0.0850
O	 0.2000	 0.1490
P	 0.2600	 0.0770
Q	 0.5130	 0.1790
R	 0.0000	 -0.0930
S	 0.0000	 0.0890
T	 0.1790	 0.0940
U	 0.0000	 -0.1300
V	 0.0260	 -0.0160
W	 0.0000	 -0.0130
X	 0.0260	 -0.0640

