



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 05:37 AM UTC

PDB ID : 8EYH / pdb_00008eyh
EMDB ID : EMD-28688
Title : SARS-CoV-2 spike protein bound with a nanobody
Authors : Laughlin, Z.T.; Patel, A.; Ortlund, E.A.
Deposited on : 2022-10-27
Resolution : 3.75 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

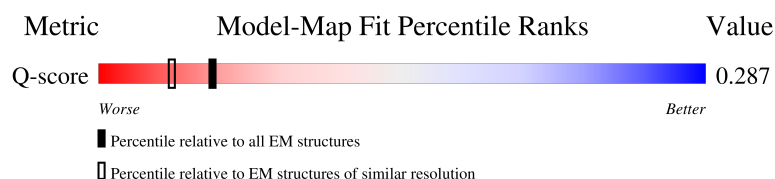
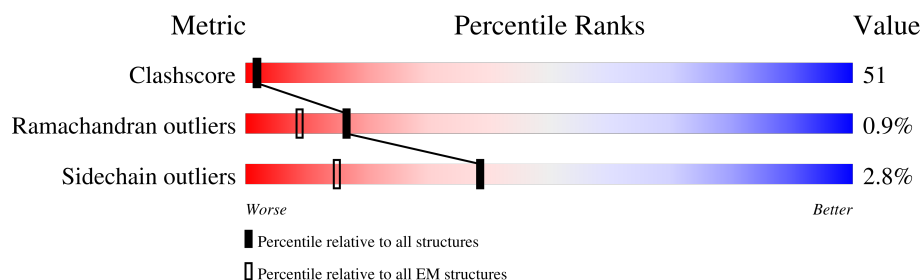
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 i

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

The reported resolution of this entry is 3.75 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	10301 (3.25 - 4.25)

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	D	118	59% 80% 20%
2	A	1136	37% 38% 55% 6%
2	B	1136	36% 35% 58% ..
2	C	1136	42% 36% 55% .. 6%

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Mol	Chain	Length	Quality of chain
3	E	2	50% 100%
3	F	2	100% 50% 50%
3	G	2	50% 50% 50%
3	H	2	50% 50% 50%
3	I	2	100% 100%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	I	1	-	-	X	-
4	NAG	C	1201	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 26575 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 Nanobody.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	118	Total	C	N	O	S	0	0
			868	543	147	174	4		

- Molecule 2 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1088	Total	C	N	O	S	0	0
			8515	5436	1421	1620	38		
2	C	1067	Total	C	N	O	S	0	0
			8350	5327	1395	1589	39		
2	A	1069	Total	C	N	O	S	0	0
			8366	5339	1397	1591	39		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	817	PRO	PHE	conflict	UNP P0DTC2
B	892	PRO	ALA	conflict	UNP P0DTC2
B	899	PRO	ALA	conflict	UNP P0DTC2
B	942	PRO	ALA	conflict	UNP P0DTC2
B	986	PRO	LYS	conflict	UNP P0DTC2
B	987	PRO	VAL	conflict	UNP P0DTC2
C	817	PRO	PHE	conflict	UNP P0DTC2
C	892	PRO	ALA	conflict	UNP P0DTC2
C	899	PRO	ALA	conflict	UNP P0DTC2
C	942	PRO	ALA	conflict	UNP P0DTC2
C	986	PRO	LYS	conflict	UNP P0DTC2
C	987	PRO	VAL	conflict	UNP P0DTC2
A	817	PRO	PHE	conflict	UNP P0DTC2
A	892	PRO	ALA	conflict	UNP P0DTC2
A	899	PRO	ALA	conflict	UNP P0DTC2
A	942	PRO	ALA	conflict	UNP P0DTC2
A	986	PRO	LYS	conflict	UNP P0DTC2

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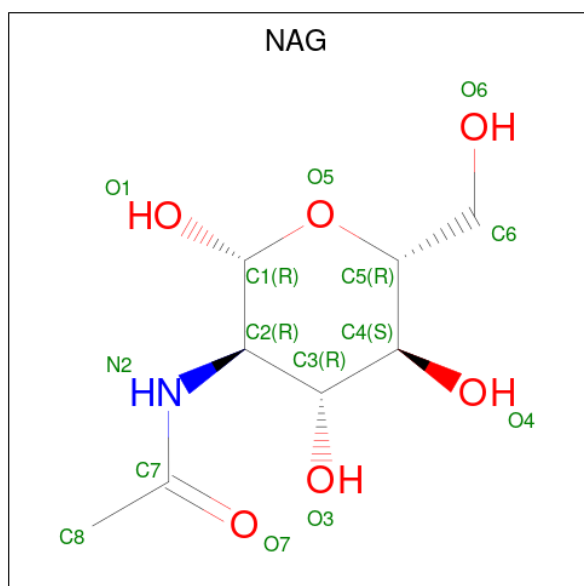
Chain	Residue	Modelled	Actual	Comment	Reference
A	987	PRO	VAL	conflict	UNP P0DTC2

- Molecule 3 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
3	E	2	Total	C	N	O	0	0
			28	16	2	10		
3	F	2	Total	C	N	O	0	0
			28	16	2	10		
3	G	2	Total	C	N	O	0	0
			28	16	2	10		
3	H	2	Total	C	N	O	0	0
			28	16	2	10		
3	I	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).



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

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

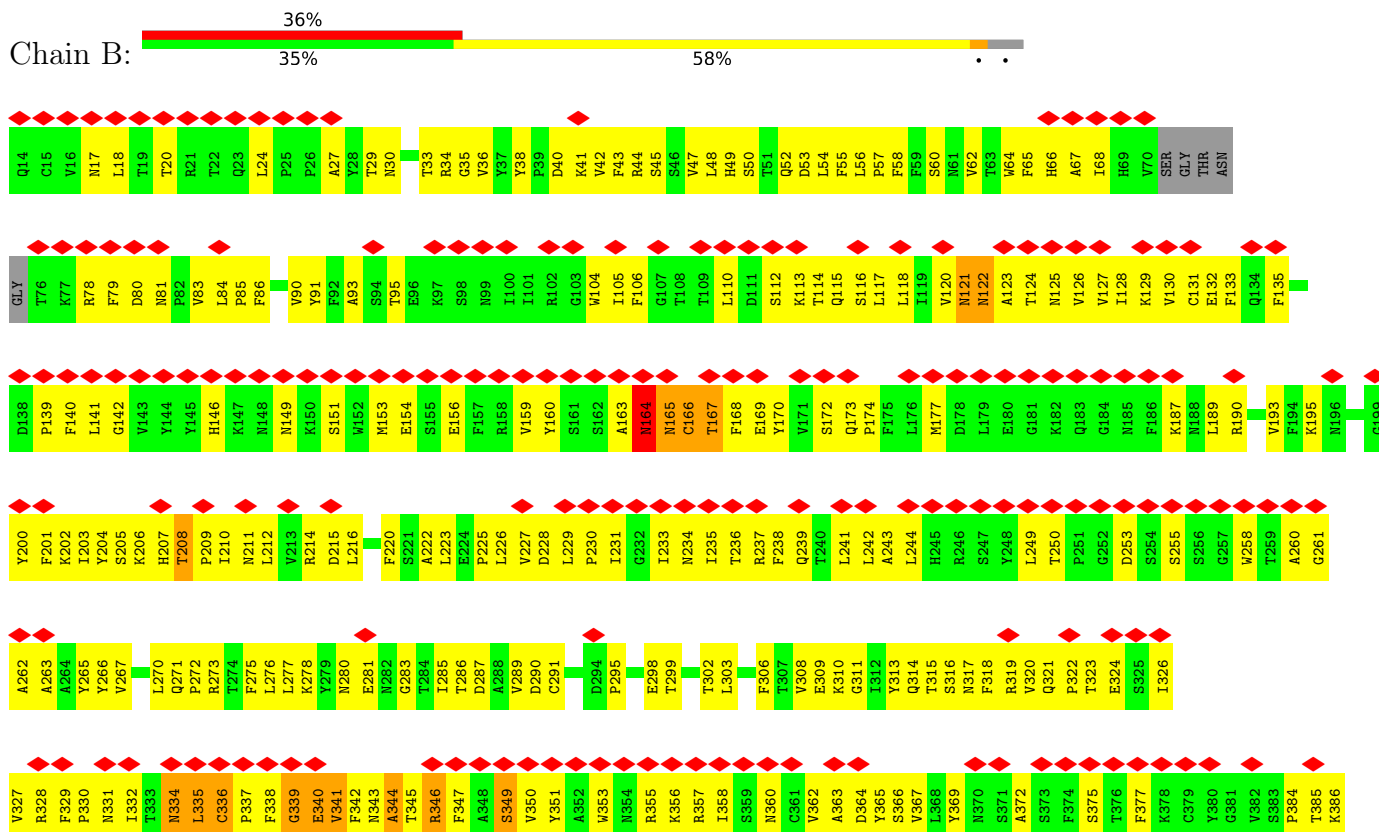
3 Residue-property plots [i](#)

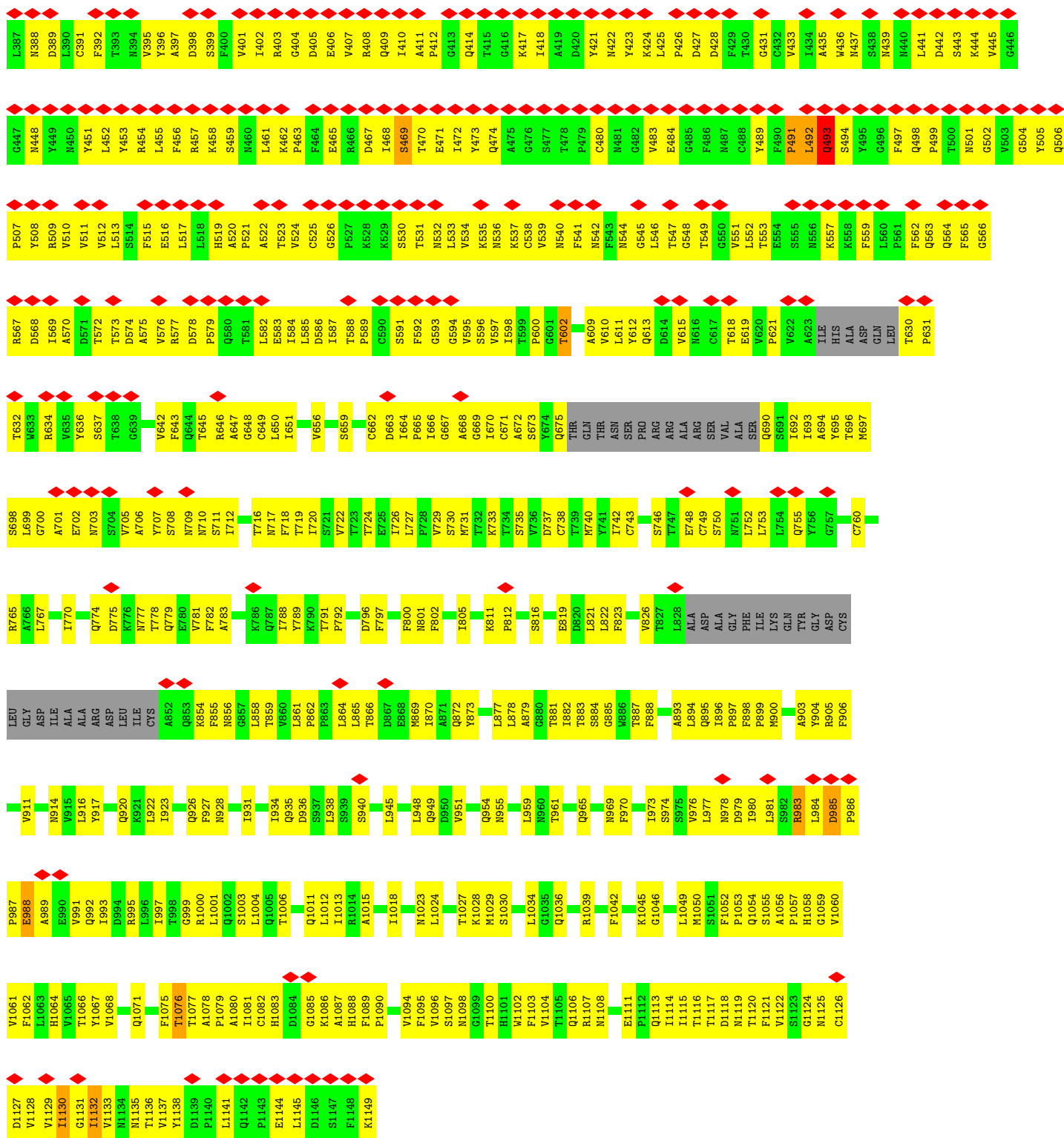
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Nanobody



• Molecule 2: Spike glycoprotein

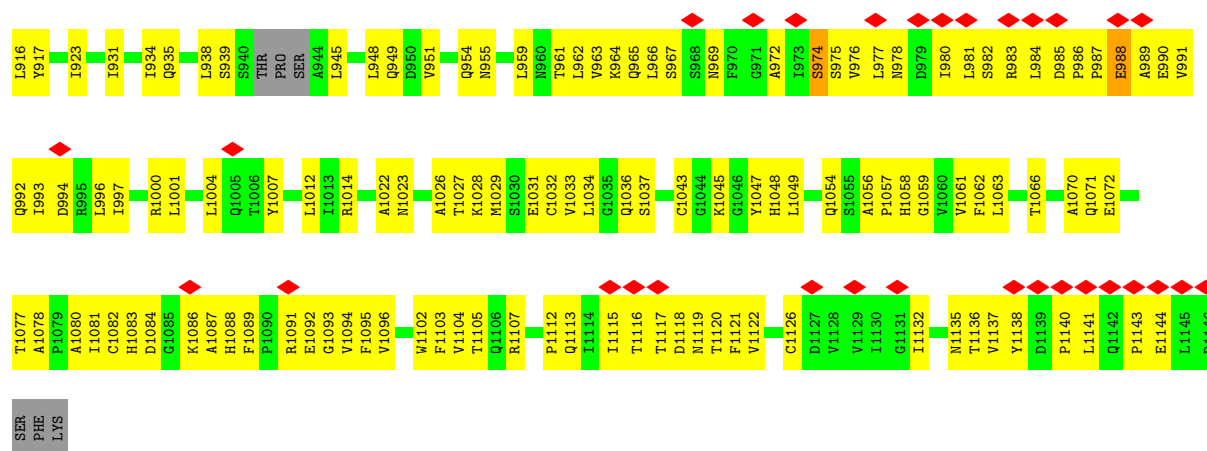




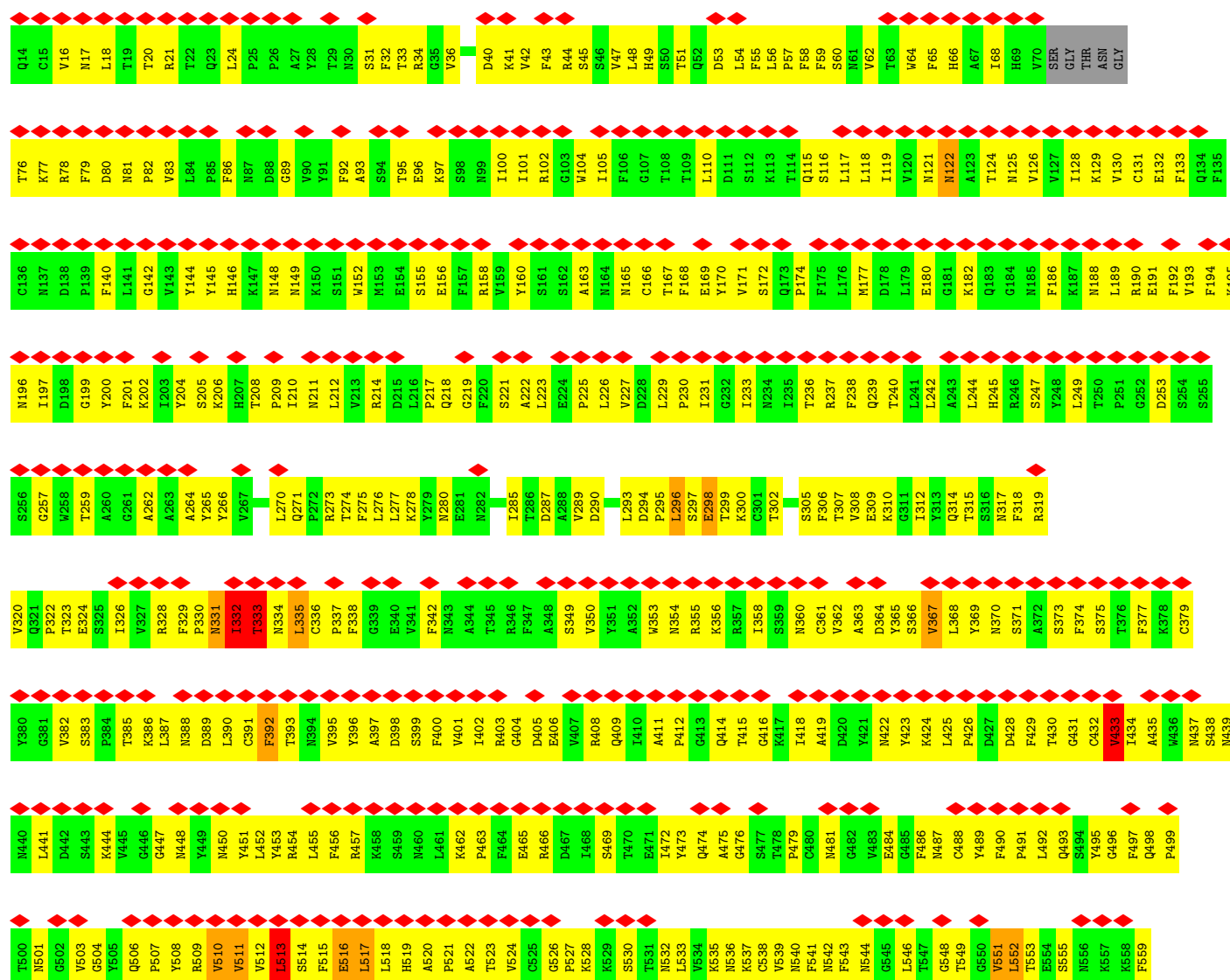
• Molecule 2: Spike glycoprotein

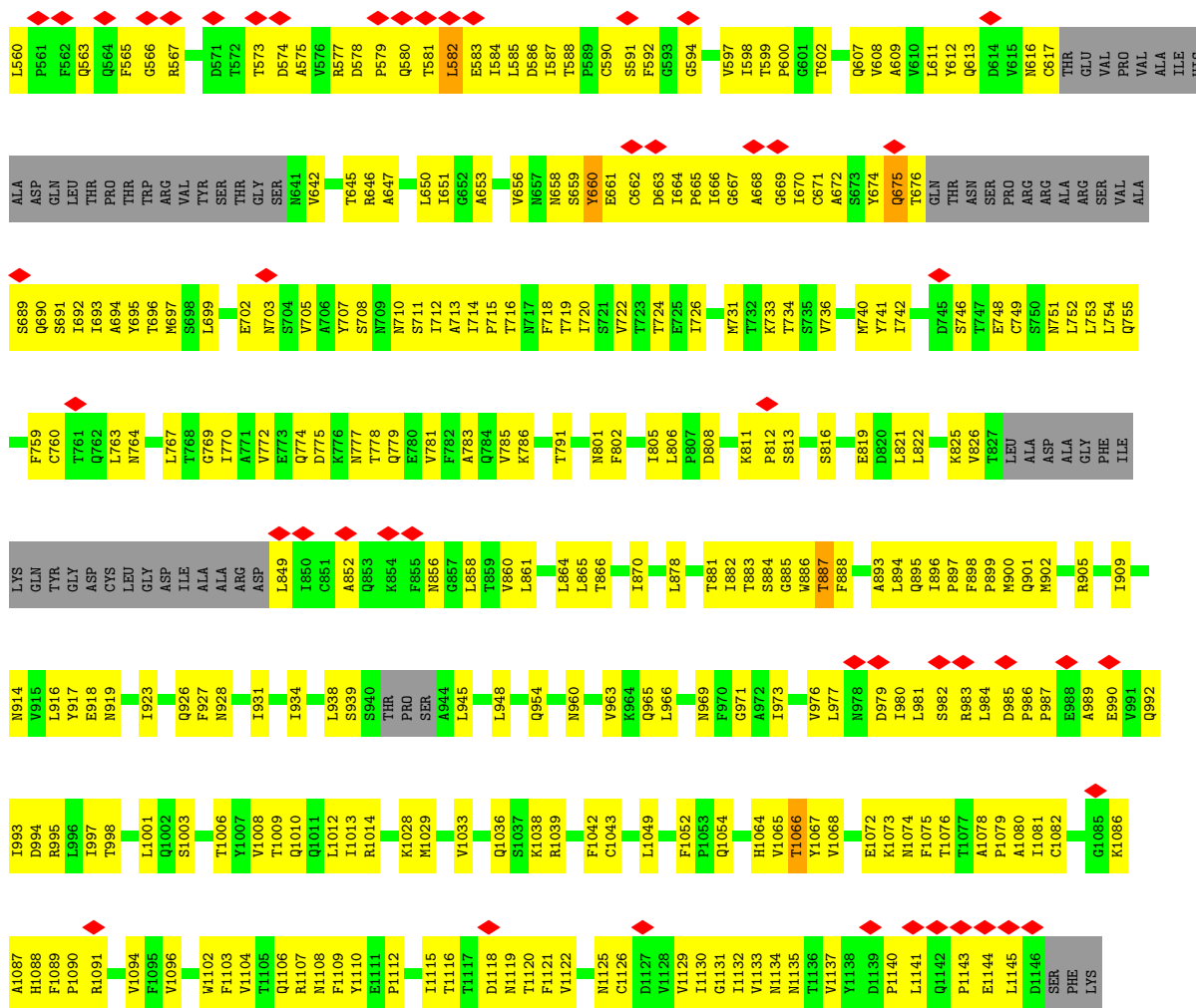


LEU I1E	C851	A852	T778	Q779	Q853	Q854	Q855	Q856	Q857	L888	V860	L889	V861	L861	P862	P863	L864	L865	L866	T866	N869	L877	L878	L879	G880	P889	S810	L882	T883	S884	S885	W886	L887	F888	G889	A890	W890	P892	A893	L894	Q895	L896	P897	F898	P899	N900	Q901	M902	A903	Q904	R905	L906	N907	G908	I909	G910	V911	T912	Q913	N914	V915																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
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S711	I712	A713	T714	Q715	Q716	Q717	Q718	Q719	Q720	T721	T722	T723	T724	T725	T726	T727	T728	T729	T730	T731	T732	T733	T734	T735	T736	T737	T738	T739	T740	T741	T742	T743	T744	T745	T746	T747	T748	T749	T750	T751	T752	T753	T754	T755	T756	T757	T758	T759	T760	T761	T762	T763	T764	T765	T766	T767	T768	T769	T770	T771	T772	T773	T774																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
T775	T776	T777	T778	T779	T780	T781	T782	T783	T784	T785	T786	T787	T788	T789	T790	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	T870	T871	T872	T873	T874	T875	T876	T877	T878	T879	T880	T881	T882	T883	T884	T885	T886	T887	T888	T889	T890	T891	T892	T893	T894	T895	T896	T897	T898	T899	T900	T901	T902	T903	T904	T905	T906	T907	T908	T909	T910	T911	T912	T913	T914	T915	T916	T917	T918	T919	T920	T921	T922	T923	T924	T925	T926	T927	T928	T929	T930	T931	T932	T933	T934	T935	T936	T937	T938	T939	T940	T941	T942	T943	T944	T945	T946	T947	T948	T949	T950	T951	T952	T953	T954	T955	T956	T957	T958	T959	T960	T961	T962	T963	T964	T965	T966	T967	T968	T969	T970	T971	T972	T973	T974	T975	T976	T977	T978	T979	T980	T981	T982	T983	T984	T985	T986	T987	T988	T989	T990	T991	T992	T993	T994	T995	T996	T997	T998	T999	T1000	T1001	T1002	T1003	T1004	T1005	T1006	T1007	T1008	T1009	T1010	T1011	T1012	T1013	T1014	T1015	T1016	T1017	T1018	T1019	T1020	T1021	T1022	T1023	T1024	T1025	T1026	T1027	T1028	T1029	T1030	T1031	T1032	T1033	T1034	T1035	T1036	T1037	T1038	T1039	T1040	T1041	T1042	T1043	T1044	T1045	T1046	T1047	T1048	T1049	T1050	T1051	T1052	T1053	T1054	T1055	T1056	T1057	T1058	T1059	T1060	T1061	T1062	T1063	T1064	T1065	T1066	T1067	T1068	T1069	T1070	T1071	T1072	T1073	T1074	T1075	T1076	T1077	T1078	T1079	T1080	T1081	T1082	T1083	T1084	T1085	T1086	T1087	T1088	T1089	T1090	T1091	T1092	T1093	T1094	T1095	T1096	T1097	T1098	T1099	T1100	T1101	T1102	T1103	T1104	T1105	T1106	T1107	T1108	T1109	T1110	T1111	T1112	T1113	T1114	T1115	T1116	T1117	T1118	T1119	T1120	T1121	T1122	T1123	T1124	T1125	T1126	T1127	T1128	T1129	T1130	T1131	T1132	T1133	T1134	T1135	T1136	T1137	T1138	T1139	T1140	T1141	T1142	T1143	T1144	T1145	T1146	T1147	T1148	T1149	T1150	T1151	T1152	T1153	T1154	T1155	T1156	T1157	T1158	T1159	T1160	T1161	T1162	T1163	T1164	T1165	T1166	T1167	T1168	T1169	T1170	T1171	T1172	T1173	T1174	T1175	T1176	T1177	T1178	T1179	T1180	T1181	T1182	T1183	T1184	T1185	T1186	T1187	T1188	T1189	T1190	T1191	T1192	T1193	T1194	T1195	T1196	T1197	T1198	T1199	T1200	T1201	T1202	T1203	T1204	T1205	T1206	T1207	T1208	T1209	T1210	T1211	T1212	T1213	T1214	T1215	T1216	T1217	T1218	T1219	T1220	T1221	T1222	T1223	T1224	T1225	T1226	T1227	T1228	T1229	T1230	T1231	T1232	T1233	T1234	T1235	T1236	T1237	T1238	T1239	T1240	T1241	T1242	T1243	T1244	T1245	T1246	T1247	T1248	T1249	T1250	T1251	T1252	T1253	T1254	T1255	T1256	T1257	T1258	T1259	T1260	T1261	T1262	T1263	T1264	T1265	T1266	T1267	T1268	T1269	T1270	T1271	T1272	T1273	T1274	T1275	T1276	T1277	T1278	T1279	T1280	T1281	T1282	T1283	T1284	T1285	T1286	T1287	T1288	T1289	T1290	T1291	T1292	T1293	T1294	T1295	T1296	T1297	T1298	T1299	T1300	T1301	T1302	T1303	T1304	T1305	T1306	T1307	T1308	T1309	T1310	T1311	T1312	T1313	T1314	T1315	T1316	T1317	T1318	T1319	T1320	T1321	T1322	T1323	T1324	T1325	T1326	T1327	T1328	T1329	T1330	T1331	T1332	T1333	T1334	T1335	T1336	T1337	T1338	T1339	T1340	T1341	T1342	T1343	T1344	T1345	T1346	T1347	T1348	T1349	T1350	T1351	T1352	T1353	T1354	T1355	T1356	T1357	T1358	T1359	T1360	T1361	T1362	T1363	T1364	T1365	T1366	T1367	T1368	T1369	T1370	T1371	T1372	T1373	T1374	T1375	T1376	T1377	T1378	T1379	T1380	T1381	T1382	T1383	T1384	T1385	T1386	T1387	T1388	T1389	T1390	T1391	T1392	T1393	T1394	T1395	T1396	T1397	T1398	T1399	T1400	T1401	T1402	T1403	T1404	T1405	T1406	T1407	T1408	T1409	T1410	T1411	T1412	T1413	T1414	T1415	T1416	T1417	T1418	T1419	T1420	T1421	T1422	T1423	T1424	T1425	T1426	T1427	T1428	T1429	T1430	T1431	T1432	T1433	T1434	T1435	T1436	T1437	T1438	T1439	T1440	T1441	T1442	T1443	T1444	T1445	T1446	T1447	T1448	T1449	T1450	T1451	T1452	T1453	T1454	T1455	T1456	T1457	T1458	T1459	T1460	T1461	T1462	T1463	T1464	T1465	T1466	T1467	T1468	T1469	T1470	T1471	T1472	T1473	T1474	T1475	T1476	T1477	T1478	T1479	T1480	T1481	T1482	T1483	T1484	T1485	T1486	T1487	T1488	T1489	T1490	T1491	T1492	T1493	T1494	T1495	T1496	T1497	T1498	T1499	T1500	T1501	T1502	T1503	T1504	T1505	T1506	T1507	T1508	T1509
A570	D571	T572	T573	D574	A575	A576	A577	A578	A579	A580	A581	A582	A583	A584	A585	A586	A587	A588	A589	A590	A591	A592	A593	A594	A595	A596	A597	A598	A599	A600	A601	A602	A603	A604	A605	A606	A607	A608	A609	A610	A611	A612	A613	A614	A615	A616	A617	A618	A619	A620	A621	A622	A623	A624	A625	A626	A627	A628	A629	A630	A631	A632	A633	A634	A635	A636	A637	A638	A639	A640	A641	A642	A643	A644	A645	A646	A647	A648	A649	A650	A651	A652	A653	A654	A655	A656	A657	A658	A659	A660	A661	A662	A663	A664	A665	A666	A667	A668	A669	A670	A671	A672	A673	A674	A675	A676	A677	A678	A679	A680	A681	A682	A683	A684	A685	A686	A687	A688	A689	A690	A691	A692	A693	A694	A695	A696	A697	A698	A699	A700	A701	A702	A703	A704	A705	A706	A707	A708	A709	A710	A711	A712	A713	A714	A715	A716	A717	A718	A719	A720	A721	A722	A723	A724	A725	A726	A727	A728	A729	A730	A731	A732	A733	A734	A735	A736	A737	A738	A739	A740	A741	A742	A743	A744	A745	A746	A747	A748	A749	A750	A751	A752	A753	A754	A755	A756	A757	A758	A759	A760	A761	A762	A763	A764	A765	A766	A767	A768	A769	A770	A771	A772	A773	A774	A775	A776	A777	A778	A779	A780	A781	A782	A783	A784	A785	A786	A787	A788	A789	A790	A791	A792	A793	A794	A795	A796	A797	A798	A799	A800	A801	A802	A803	A804	A805	A806	A807	A808	A809	A810	A811	A812	A813	A814	A815	A816	A817	A818	A819	A820	A821	A822	A823	A824	A825	A826	A827	A828	A829	A830	A831	A832	A833	A834	A835	A836	A837	A838	A839	A840	A841	A842	A843	A844	A845	A846	A847	A848	A849	A850	A851	A852	A853	A854	A855	A856	A857	A858	A859	A860	A861	A862	A863	A864	A865	A866	A867	A868	A869	A870	A871	A872	A873	A874	A875	A876	A877	A878	A879	A880	A881	A882	A883	A884	A885	A886	A887	A888	A889	A890	A891	A892	A893	A894	A895	A896	A897	A898	A899	A900	A901	A902	A903	A904	A905	A906	A907	A908	A909	A910	A911	A912	A913	A914	A915																																																																																																																																																																																																																																																																																																																																																																																																					
Q14	C15	V16	M17	L18	T19	T20	R21	T22	Q23	L24	P25	P26	A27	Y28	T29	N30	S31	V36	Y37	Y38	P39	D40	K41	V42	F43	R44	S45	S46	V47	L48	H49	S50	T51	Q52	D53	L54	F55	L56	S80	N61	V62	T63	A64	F65	H66	A67	I68	H69	SER	GLY	THR	ASN	GLY	T76	K77	R78																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
F79	D80	N81	P82	V83	L84	P85	F86	N87	D88	G89	V90	Y91	E96	K97	S98	N99	I100	I101	G103	S161	S162	A163	N164	N165	C166	T167	F168	D111	S112	K113	T114	Q115	S116	P174	F175	L176	M177	D178	L179	E180	G181	K182	Q183	G184	N185	K187	N188	C131	GLY	THR	ASN	E191	Q134	F135	C136	D138	P139	F140	L141																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
G142	V143	Y144	Y145	H146	K147	N148	N149	K150	S151	V152	M153	E154	S155	E156	F157	R158	V159	Y160	S161	A163	N164	N165	C166	T167	F168	E169	V170	V171	S172	Q173	P174	F175	L176	M177	D178	L179	E180	G181	K182	Q183	G184	N185	F186	K187	N188	C131	GLY	THR	ASN	E191	Q134	F135	C136	D138	P139	F140	L141																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
K202	I203	Y204	S205	K206	H207	T210	N211	P212	L212	V213	R214	D215	L216	P217	Q218	G219	F220	S221	A222	L223	E224	P225	L																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							



• Molecule 2: Spike glycoprotein





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



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



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



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



- Molecule 3: 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, Not provided	
Number of particles used	615492	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	63.81	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	66.367	Depositor
Minimum map value	-45.933	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.755	Depositor
Recommended contour level	5	Depositor
Map size (Å)	444.7456, 444.7456, 444.7456	wwPDB
Map dimensions	416, 416, 416	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0691, 1.0691, 1.0691	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	D	0.10	0/886	0.24	0/1198
2	A	0.26	0/8562	0.38	1/11654 (0.0%)
2	B	0.26	1/8719 (0.0%)	0.37	0/11874
2	C	0.30	0/8546	0.40	0/11632
All	All	0.27	1/26713 (0.0%)	0.38	1/36358 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	164	ASN	N-CA	5.01	1.49	1.46

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	337	PRO	N-CA-C	-6.11	107.65	114.92

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	868	0	831	18	0
2	A	8366	0	8167	894	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	8515	0	8324	1113	0
2	C	8350	0	8147	982	0
3	E	28	0	25	0	0
3	F	28	0	25	6	0
3	G	28	0	25	4	0
3	H	28	0	25	4	0
3	I	28	0	25	11	0
4	A	126	0	116	9	0
4	B	98	0	91	6	0
4	C	112	0	104	18	0
All	All	26575	0	25905	2677	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 51.

The worst 5 of 2677 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)
2:B:343:ASN:HD21	3:I:1:NAG:C1	1.07	1.63
2:C:331:ASN:ND2	4:C:1201:NAG:C1	1.77	1.47
2:C:331:ASN:HD21	4:C:1201:NAG:C1	1.31	1.41
2:B:343:ASN:ND2	3:I:1:NAG:C1	1.93	1.30
2:A:334:ASN:HA	2:A:362:VAL:HG13	1.18	1.16

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	D	116/118 (98%)	110 (95%)	6 (5%)	0	100	100
2	A	1057/1136 (93%)	957 (90%)	90 (8%)	10 (1%)	14	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	1078/1136 (95%)	963 (89%)	110 (10%)	5 (0%)	24	56
2	C	1055/1136 (93%)	933 (88%)	107 (10%)	15 (1%)	9	36
All	All	3306/3526 (94%)	2963 (90%)	313 (10%)	30 (1%)	16	43

5 of 30 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	329	PHE
2	C	330	PRO
2	C	450	ASN
2	A	332	ILE
2	A	367	VAL

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	D	89/89 (100%)	89 (100%)	0	100	100
2	A	937/990 (95%)	912 (97%)	25 (3%)	39	58
2	B	954/990 (96%)	925 (97%)	29 (3%)	36	56
2	C	935/990 (94%)	906 (97%)	29 (3%)	35	56
All	All	2915/3059 (95%)	2832 (97%)	83 (3%)	38	57

5 of 83 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	988	GLU
2	A	517	LEU
2	A	271	GLN
2	A	433	VAL
2	A	582	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 44 such sidechains are listed below:

Mol	Chain	Res	Type
2	A	137	ASN
2	A	544	ASN
2	A	239	GLN
2	A	487	ASN
2	A	926	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 ⓘ

10 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	$\# Z > 2$
3	NAG	E	1	3,2	14,14,15	0.25	0	17,19,21	0.45	0
3	NAG	E	2	3	14,14,15	0.25	0	17,19,21	0.44	0
3	NAG	F	1	3,2	14,14,15	0.67	1 (7%)	17,19,21	0.98	1 (5%)
3	NAG	F	2	3	14,14,15	0.24	0	17,19,21	0.45	0
3	NAG	G	1	3,2	14,14,15	0.39	0	17,19,21	0.49	0
3	NAG	G	2	3	14,14,15	0.26	0	17,19,21	0.41	0
3	NAG	H	1	3,2	14,14,15	0.64	1 (7%)	17,19,21	0.64	0
3	NAG	H	2	3	14,14,15	0.27	0	17,19,21	0.44	0
3	NAG	I	1	3	14,14,15	0.48	0	17,19,21	0.37	0
3	NAG	I	2	3	14,14,15	0.36	0	17,19,21	0.41	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	E	1	3,2	-	1/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	NAG	F	1	3,2	-	3/6/23/26	0/1/1/1
3	NAG	F	2	3	-	3/6/23/26	0/1/1/1
3	NAG	G	1	3,2	-	3/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
3	NAG	H	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	H	2	3	-	3/6/23/26	0/1/1/1
3	NAG	I	1	3	-	4/6/23/26	0/1/1/1
3	NAG	I	2	3	-	3/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	1	NAG	O5-C1	-2.22	1.40	1.43
3	F	1	NAG	O5-C1	2.14	1.47	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	1	NAG	C1-O5-C5	3.73	117.18	112.19

There are no chirality outliers.

5 of 26 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	1	NAG	C1-C2-N2-C7
3	F	2	NAG	C4-C5-C6-O6
3	I	1	NAG	O5-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6

There are no ring outliers.

6 monomers are involved in 25 short contacts:

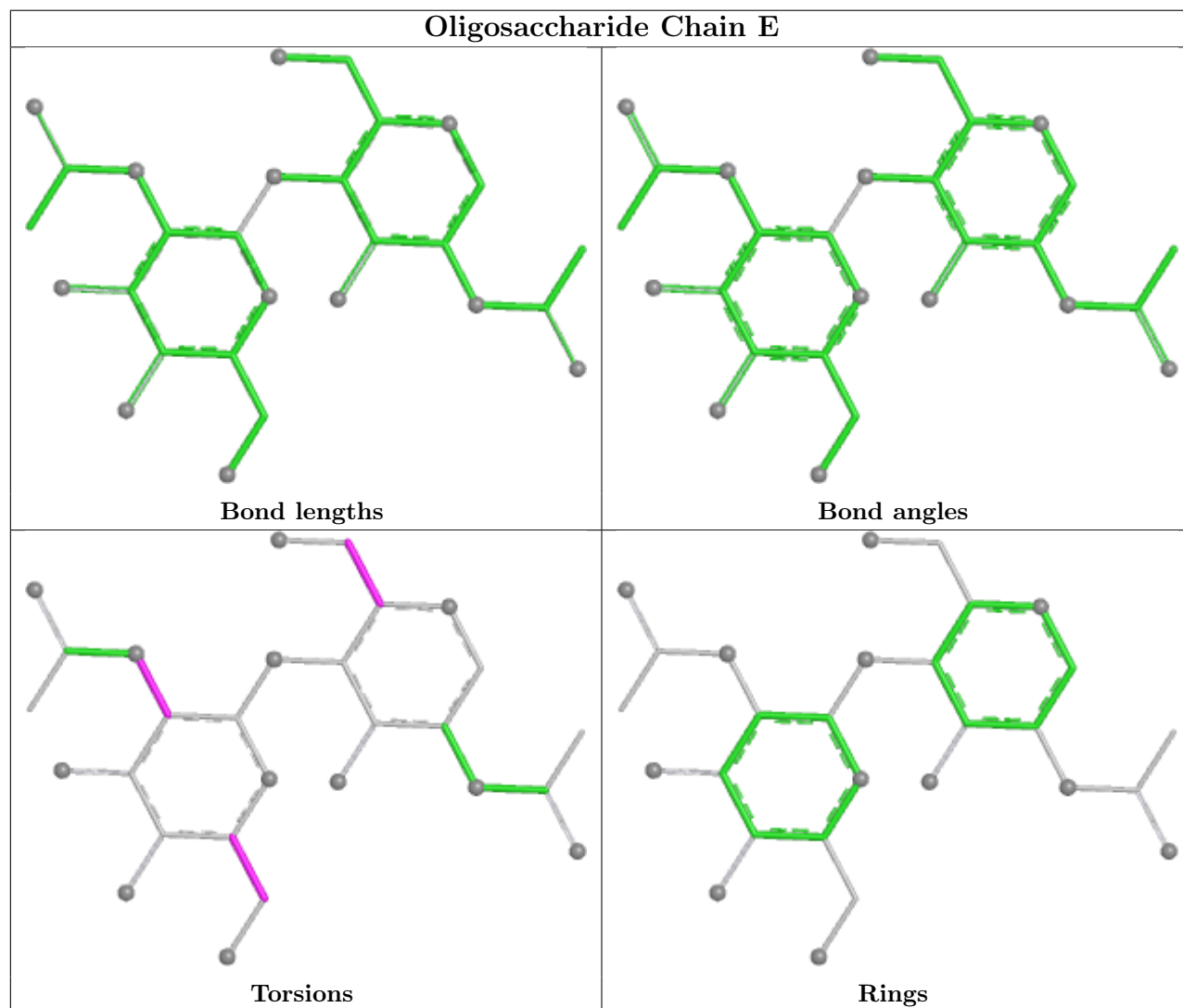
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	1	NAG	3	0
3	I	1	NAG	11	0

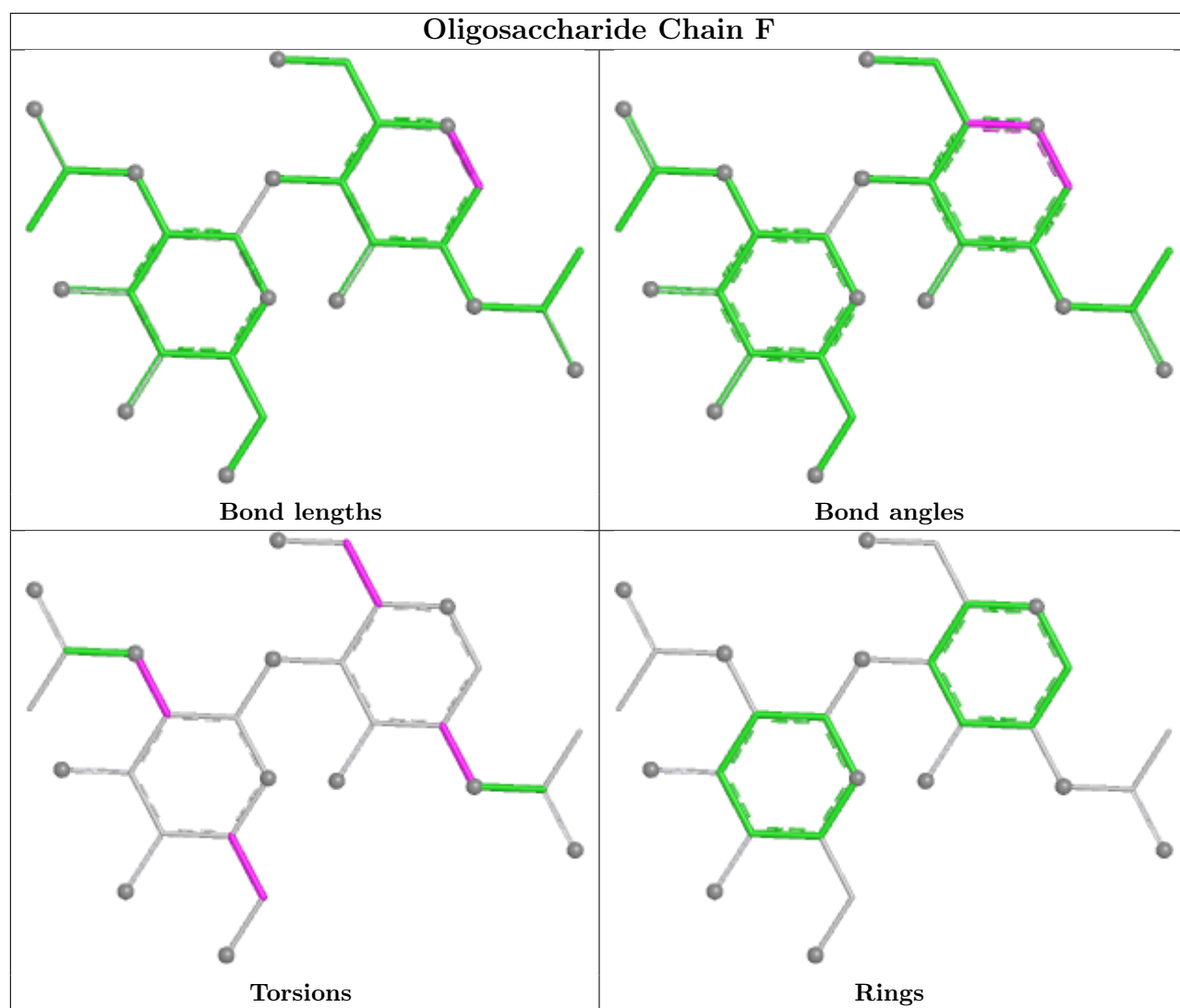
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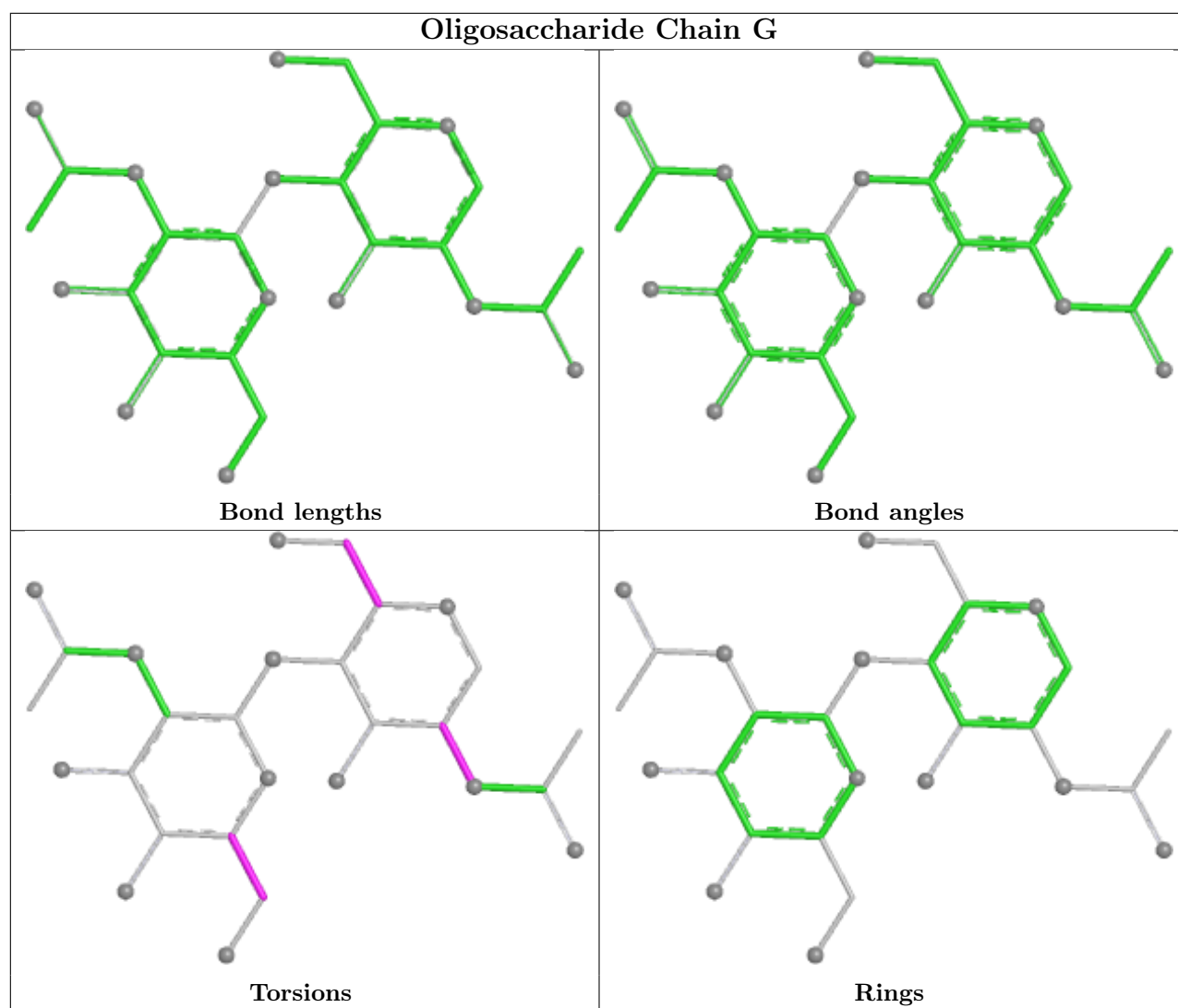
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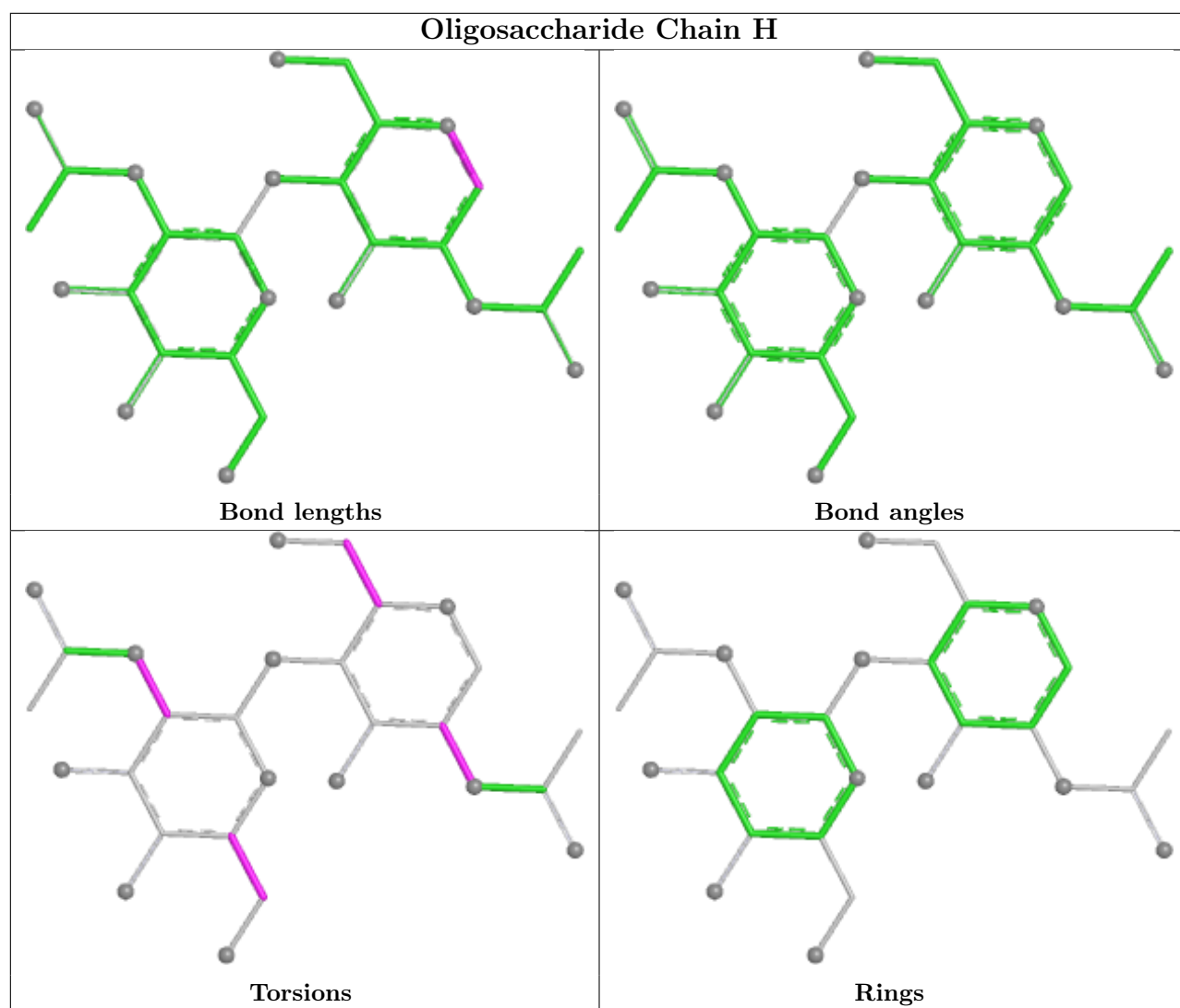
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	1	NAG	6	0
3	H	2	NAG	1	0
3	G	1	NAG	4	0
3	I	2	NAG	1	0

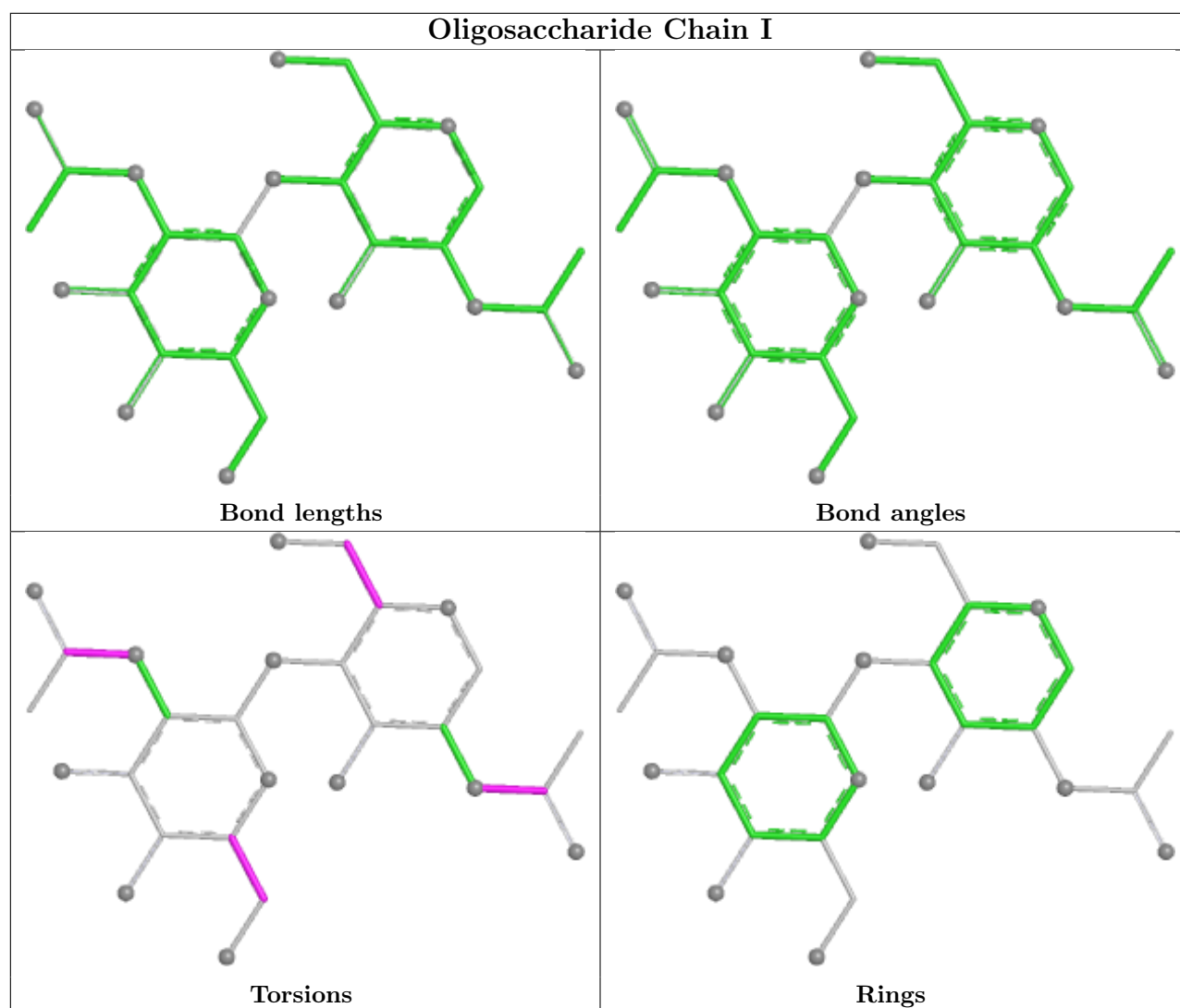
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

24 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	$\# Z > 2$
4	NAG	C	1205	2	14,14,15	0.21	0	17,19,21	0.40	0
4	NAG	A	1207	2	14,14,15	0.27	0	17,19,21	0.42	0
4	NAG	B	1301	2	14,14,15	0.58	0	17,19,21	0.82	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	C	1207	2	14,14,15	0.24	0	17,19,21	0.50	0
4	NAG	A	1209	2	14,14,15	0.43	0	17,19,21	0.35	0
4	NAG	B	1305	-	14,14,15	1.65	2 (14%)	17,19,21	1.23	3 (17%)
4	NAG	A	1206	2	14,14,15	0.22	0	17,19,21	0.44	0
4	NAG	B	1307	2	14,14,15	0.26	0	17,19,21	0.45	0
4	NAG	C	1202	2	14,14,15	0.53	0	17,19,21	0.79	1 (5%)
4	NAG	A	1203	2	14,14,15	0.23	0	17,19,21	0.44	0
4	NAG	C	1203	2	14,14,15	0.24	0	17,19,21	0.43	0
4	NAG	A	1201	2	14,14,15	0.50	0	17,19,21	0.76	1 (5%)
4	NAG	B	1302	2	14,14,15	0.22	0	17,19,21	0.44	0
4	NAG	C	1206	2	14,14,15	0.31	0	17,19,21	0.34	0
4	NAG	A	1205	2	14,14,15	0.25	0	17,19,21	0.43	0
4	NAG	C	1201	-	14,14,15	0.61	0	17,19,21	0.58	0
4	NAG	B	1306	2	14,14,15	0.23	0	17,19,21	0.42	0
4	NAG	B	1303	2	14,14,15	0.28	0	17,19,21	0.43	0
4	NAG	B	1304	2	14,14,15	0.28	0	17,19,21	0.40	0
4	NAG	A	1202	-	14,14,15	2.70	7 (50%)	17,19,21	1.23	2 (11%)
4	NAG	A	1204	2	14,14,15	0.23	0	17,19,21	0.44	0
4	NAG	C	1204	2	14,14,15	0.25	0	17,19,21	0.42	0
4	NAG	A	1208	2	14,14,15	0.23	0	17,19,21	0.46	0
4	NAG	C	1208	-	14,14,15	0.99	0	17,19,21	0.94	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	1205	2	-	1/6/23/26	0/1/1/1
4	NAG	A	1207	2	-	3/6/23/26	0/1/1/1
4	NAG	B	1301	2	-	4/6/23/26	0/1/1/1
4	NAG	C	1207	2	-	2/6/23/26	0/1/1/1
4	NAG	A	1209	2	-	3/6/23/26	0/1/1/1
4	NAG	B	1305	-	-	2/6/23/26	0/1/1/1
4	NAG	A	1206	2	-	1/6/23/26	0/1/1/1
4	NAG	B	1307	2	-	2/6/23/26	0/1/1/1
4	NAG	C	1202	2	-	1/6/23/26	0/1/1/1
4	NAG	A	1203	2	-	4/6/23/26	0/1/1/1
4	NAG	C	1203	2	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1201	2	-	4/6/23/26	0/1/1/1
4	NAG	B	1302	2	-	4/6/23/26	0/1/1/1
4	NAG	C	1206	2	-	2/6/23/26	0/1/1/1
4	NAG	A	1205	2	-	2/6/23/26	0/1/1/1
4	NAG	C	1201	-	-	4/6/23/26	0/1/1/1
4	NAG	B	1306	2	-	2/6/23/26	0/1/1/1
4	NAG	B	1303	2	-	4/6/23/26	0/1/1/1
4	NAG	B	1304	2	-	4/6/23/26	0/1/1/1
4	NAG	A	1202	-	-	0/6/23/26	0/1/1/1
4	NAG	A	1204	2	-	2/6/23/26	0/1/1/1
4	NAG	C	1204	2	-	2/6/23/26	0/1/1/1
4	NAG	A	1208	2	-	2/6/23/26	0/1/1/1
4	NAG	C	1208	-	-	4/6/23/26	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1305	NAG	C1-C2	5.23	1.59	1.52
4	A	1202	NAG	O5-C5	4.45	1.52	1.43
4	A	1202	NAG	C3-C2	4.25	1.61	1.52
4	A	1202	NAG	C8-C7	-3.49	1.43	1.50
4	A	1202	NAG	C2-N2	-3.48	1.40	1.46

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1301	NAG	C1-O5-C5	3.04	116.27	112.19
4	A	1202	NAG	O7-C7-C8	-2.95	116.80	122.05
4	C	1202	NAG	C1-O5-C5	2.88	116.05	112.19
4	A	1201	NAG	C1-O5-C5	2.75	115.87	112.19
4	B	1305	NAG	O5-C5-C4	-2.72	104.20	110.83

There are no chirality outliers.

5 of 62 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	1204	NAG	C4-C5-C6-O6
4	A	1209	NAG	C4-C5-C6-O6
4	B	1301	NAG	C4-C5-C6-O6

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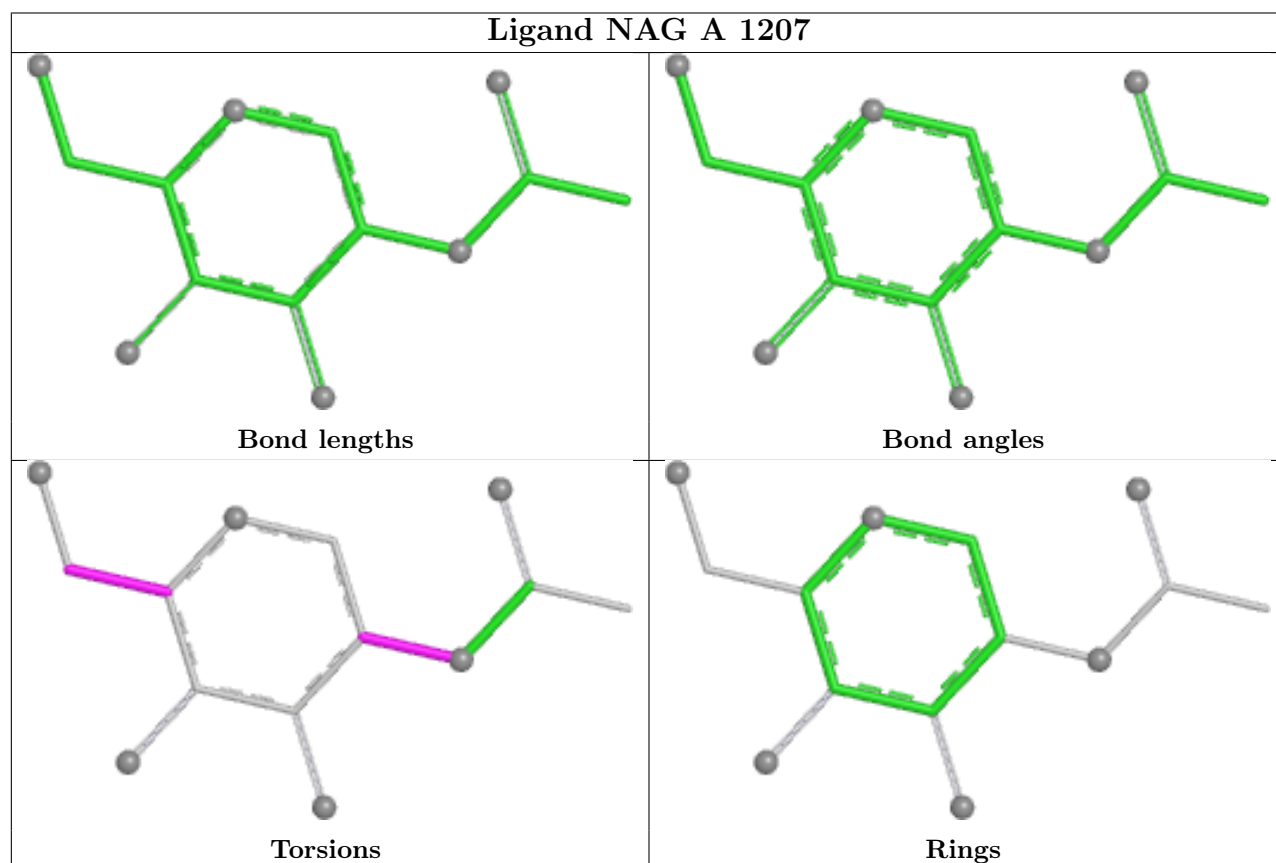
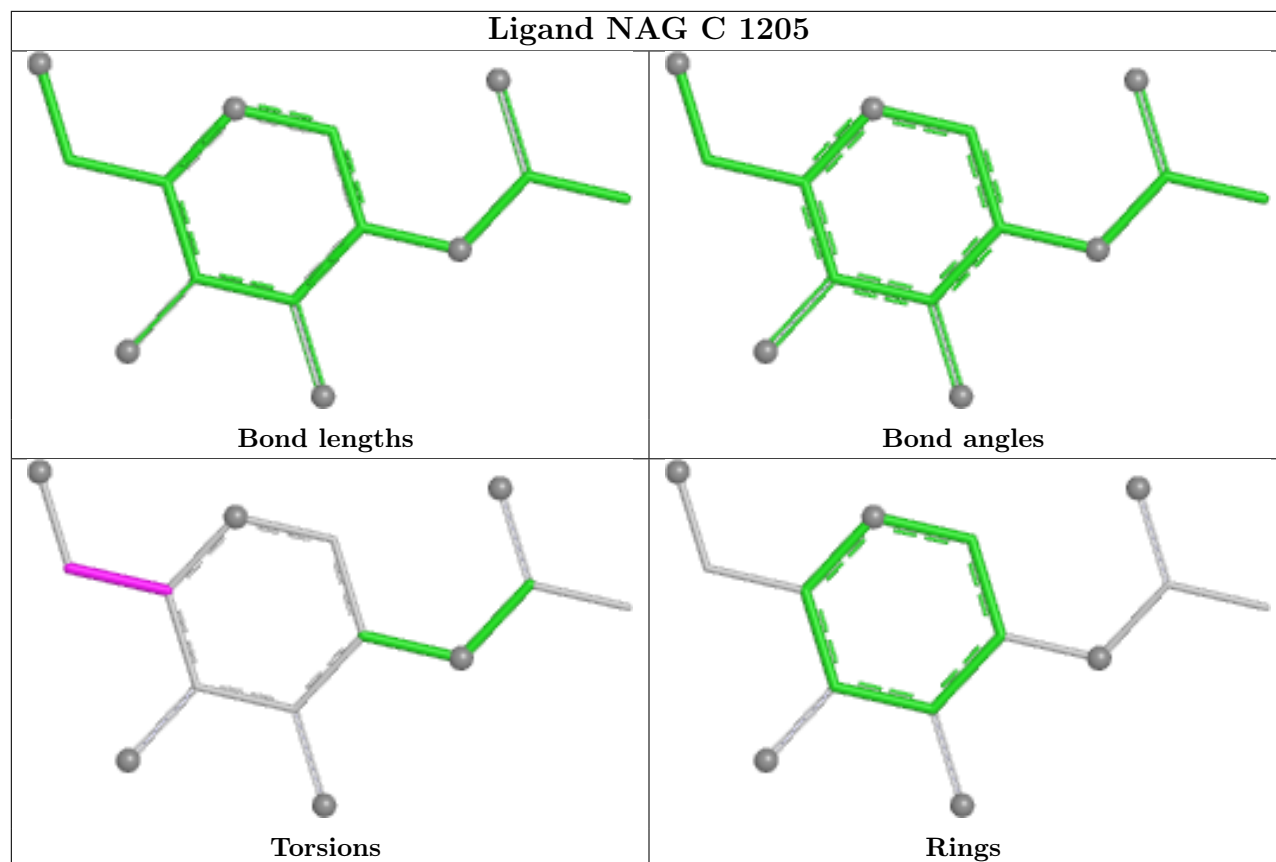
Mol	Chain	Res	Type	Atoms
4	A	1203	NAG	C4-C5-C6-O6
4	A	1205	NAG	O5-C5-C6-O6

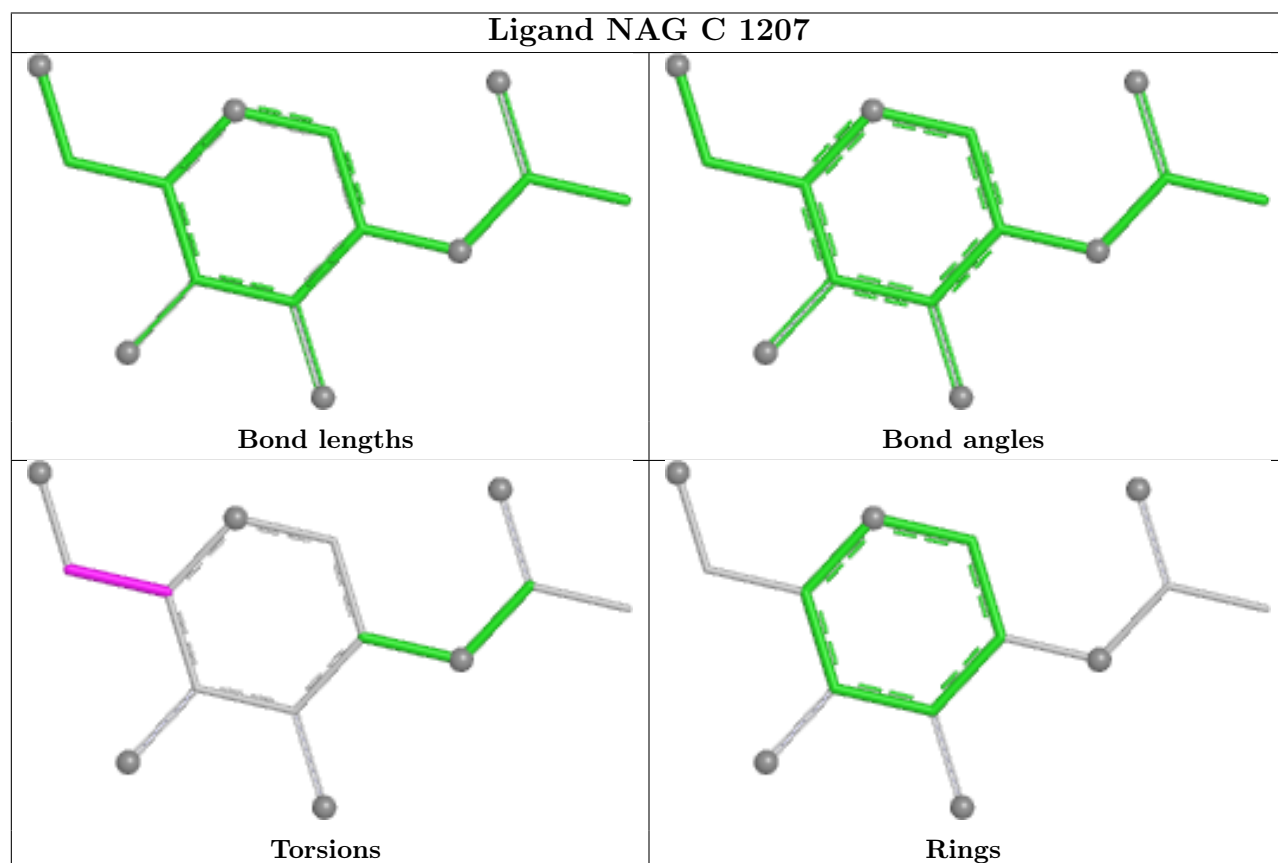
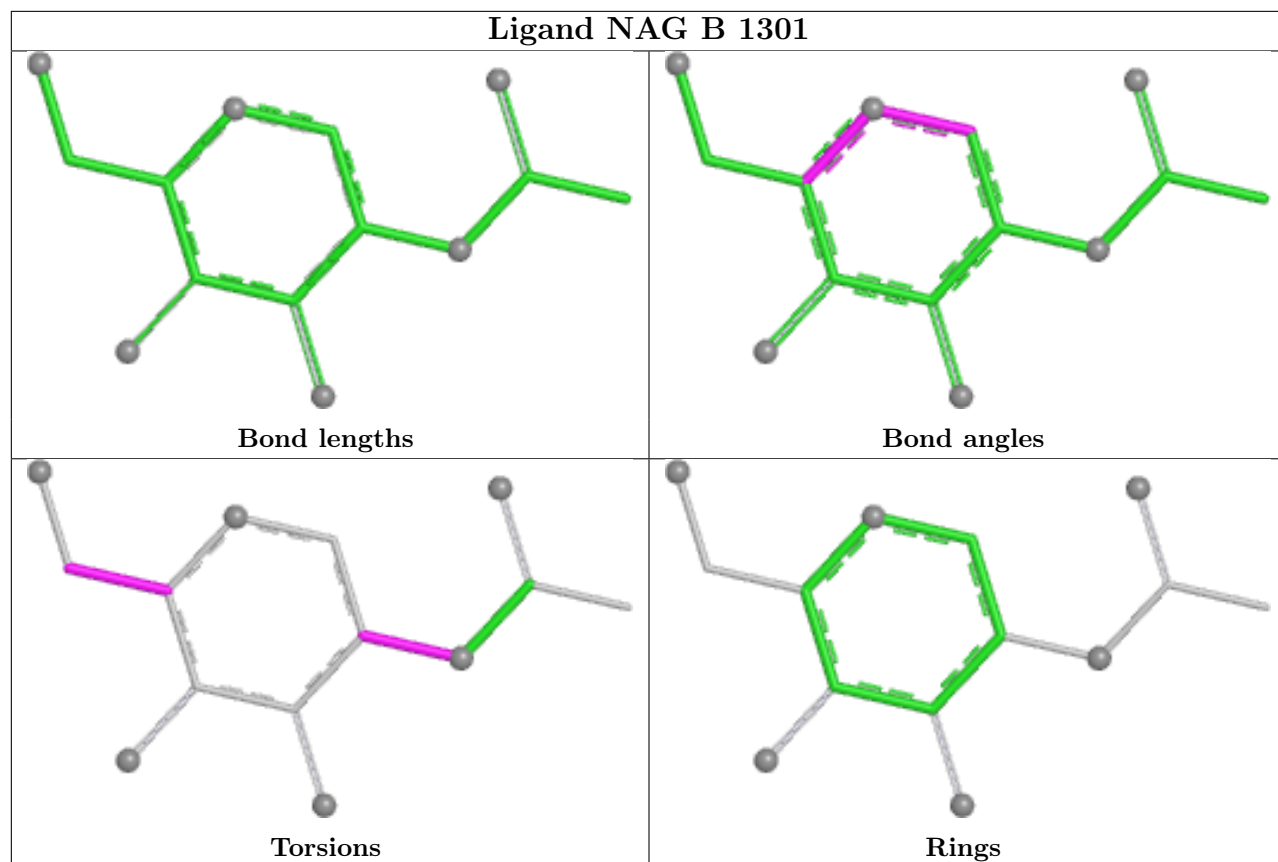
There are no ring outliers.

11 monomers are involved in 33 short contacts:

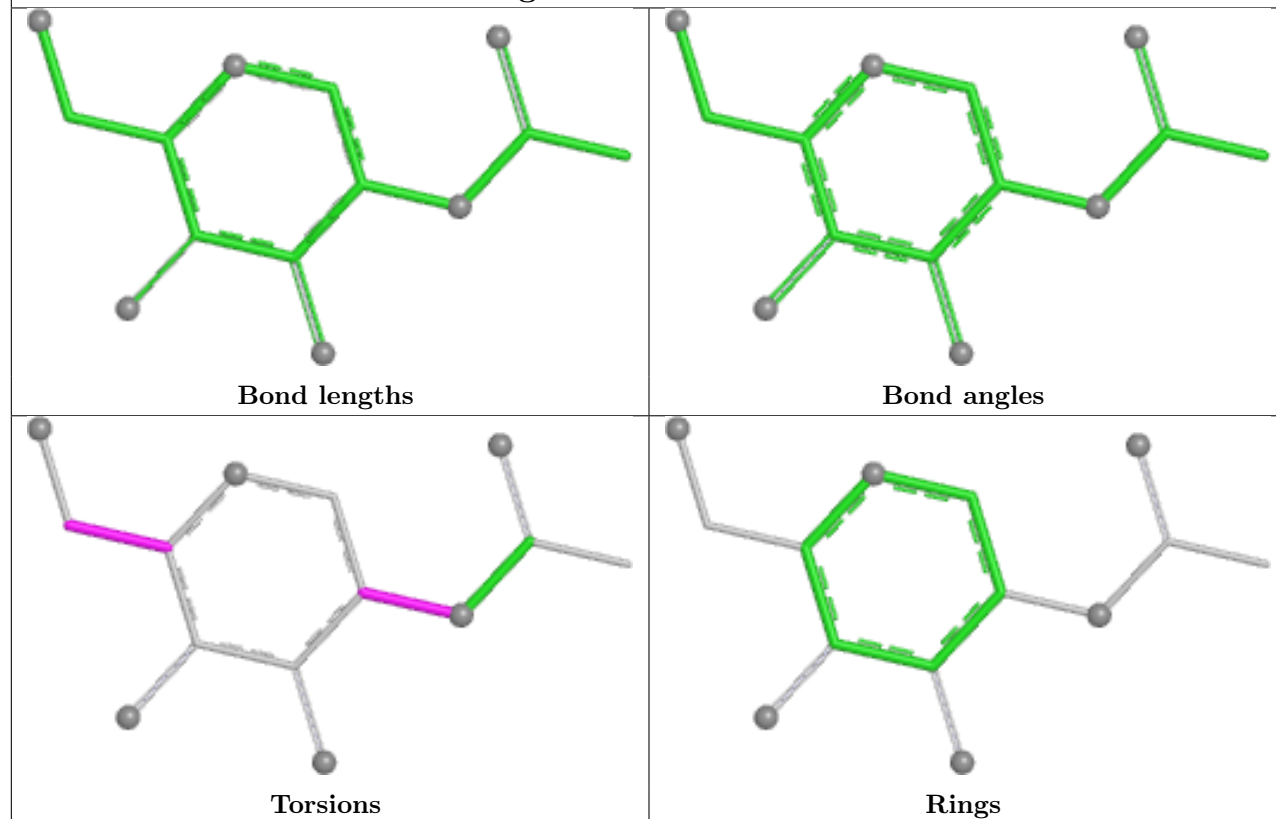
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1205	NAG	1	0
4	A	1207	NAG	1	0
4	B	1301	NAG	1	0
4	B	1307	NAG	3	0
4	C	1206	NAG	5	0
4	C	1201	NAG	9	0
4	B	1303	NAG	1	0
4	B	1304	NAG	1	0
4	A	1202	NAG	5	0
4	A	1204	NAG	3	0
4	C	1208	NAG	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

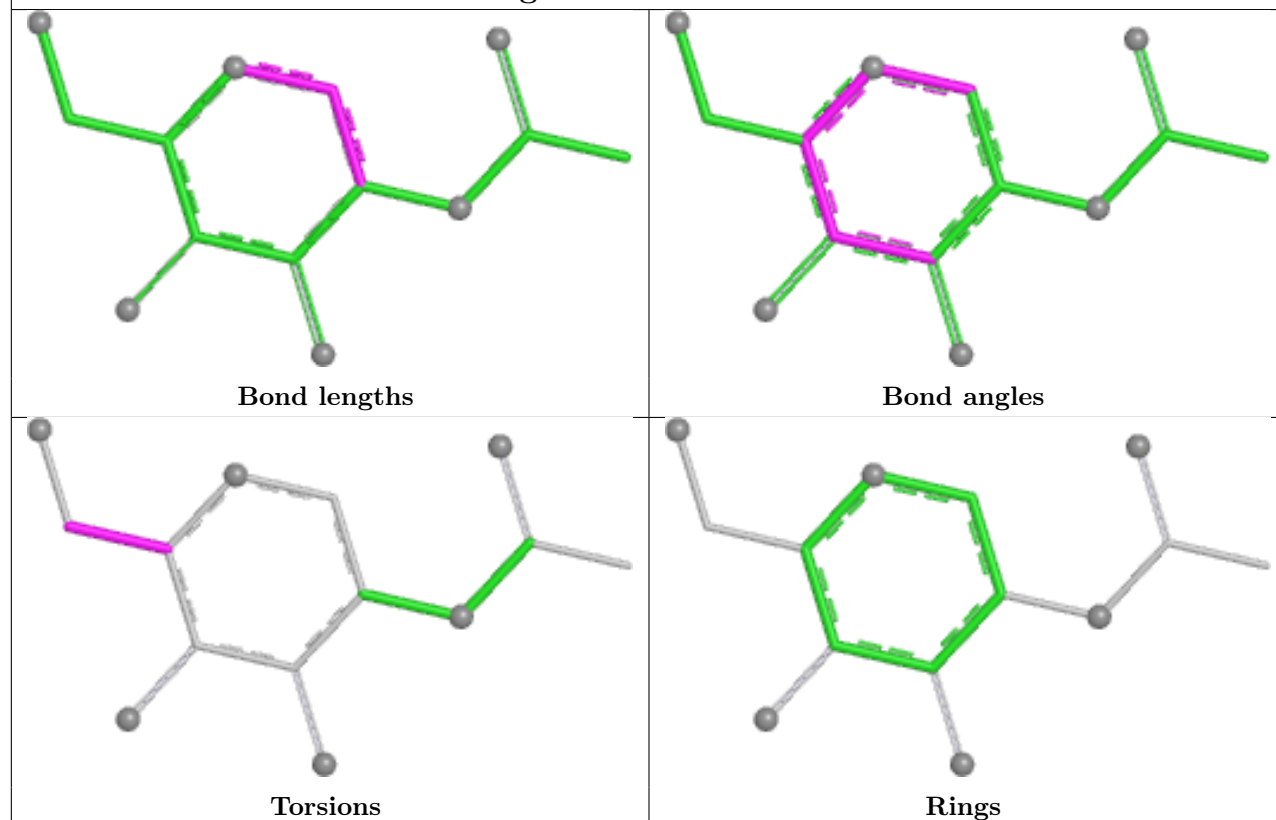


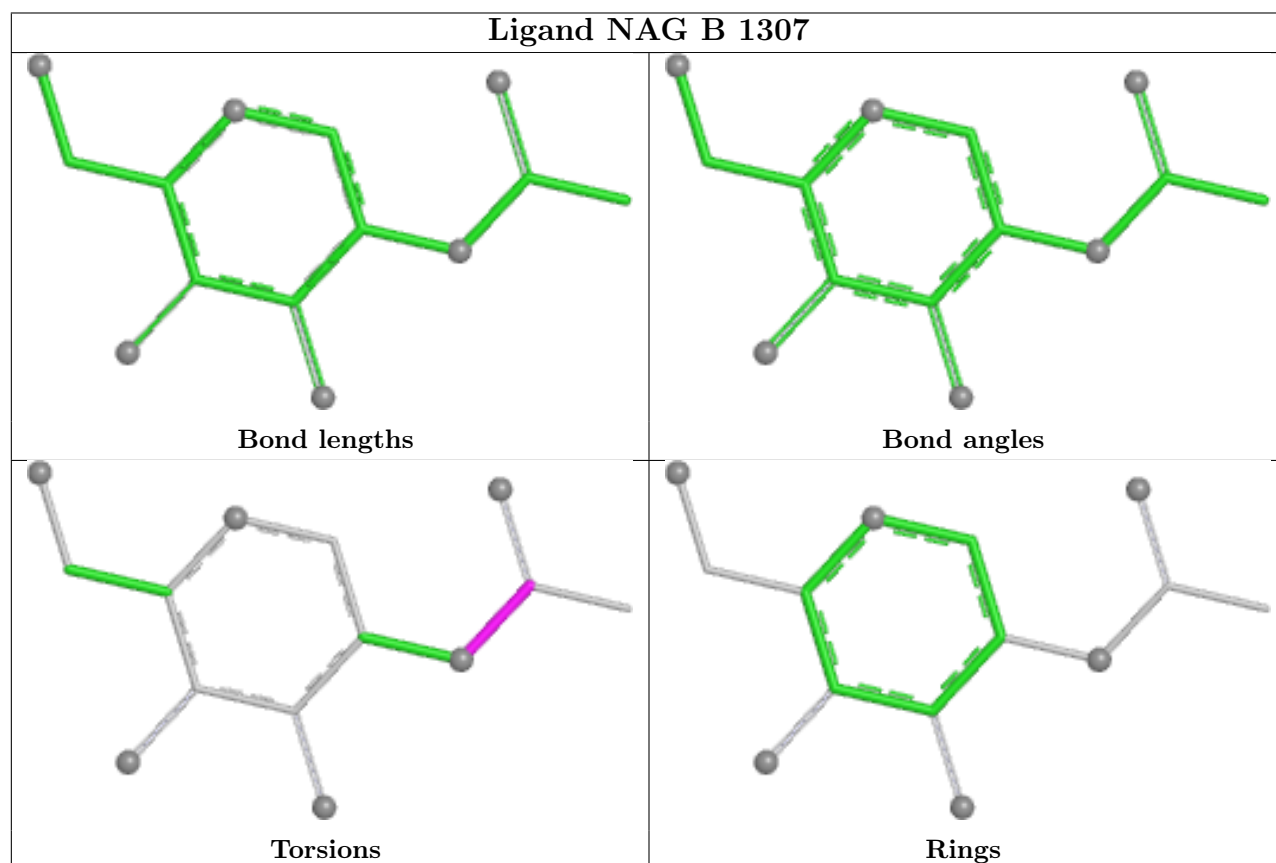
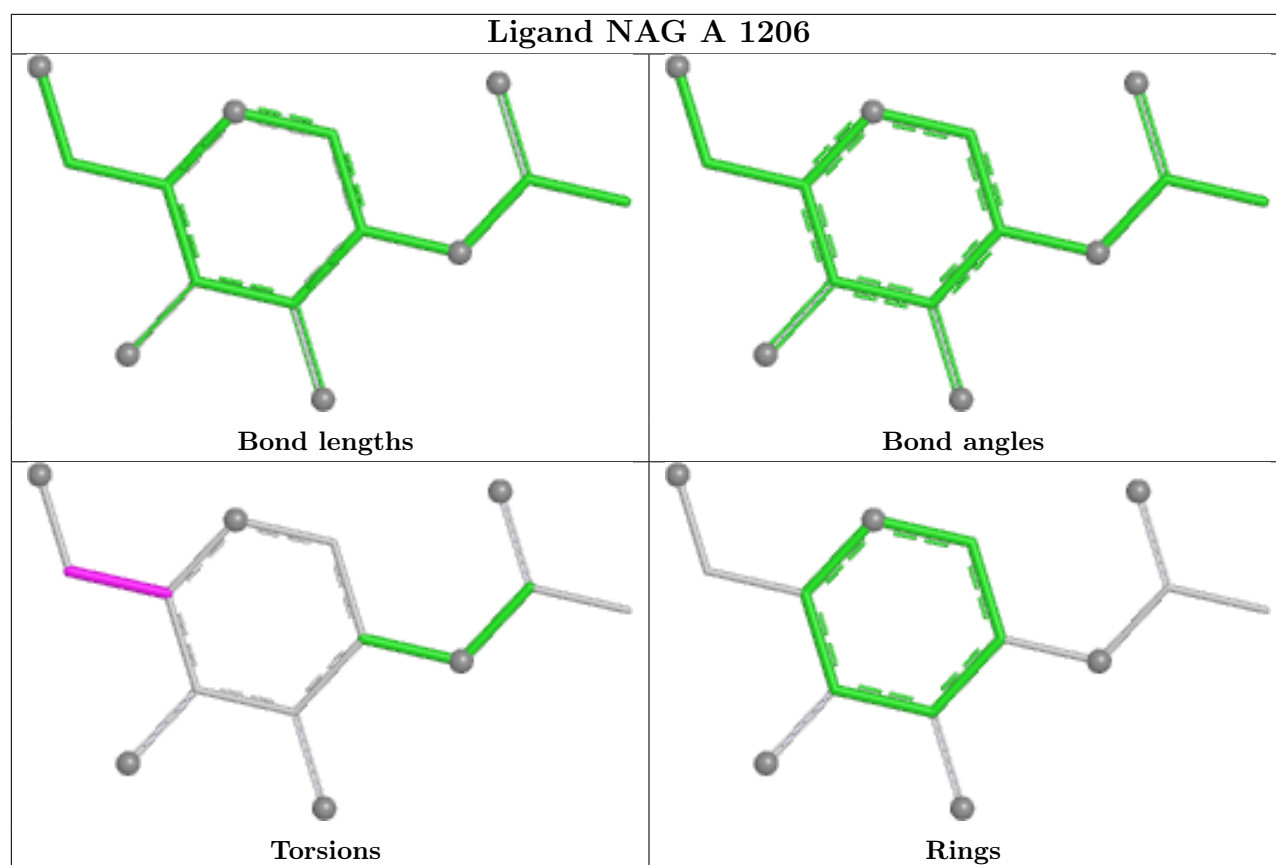


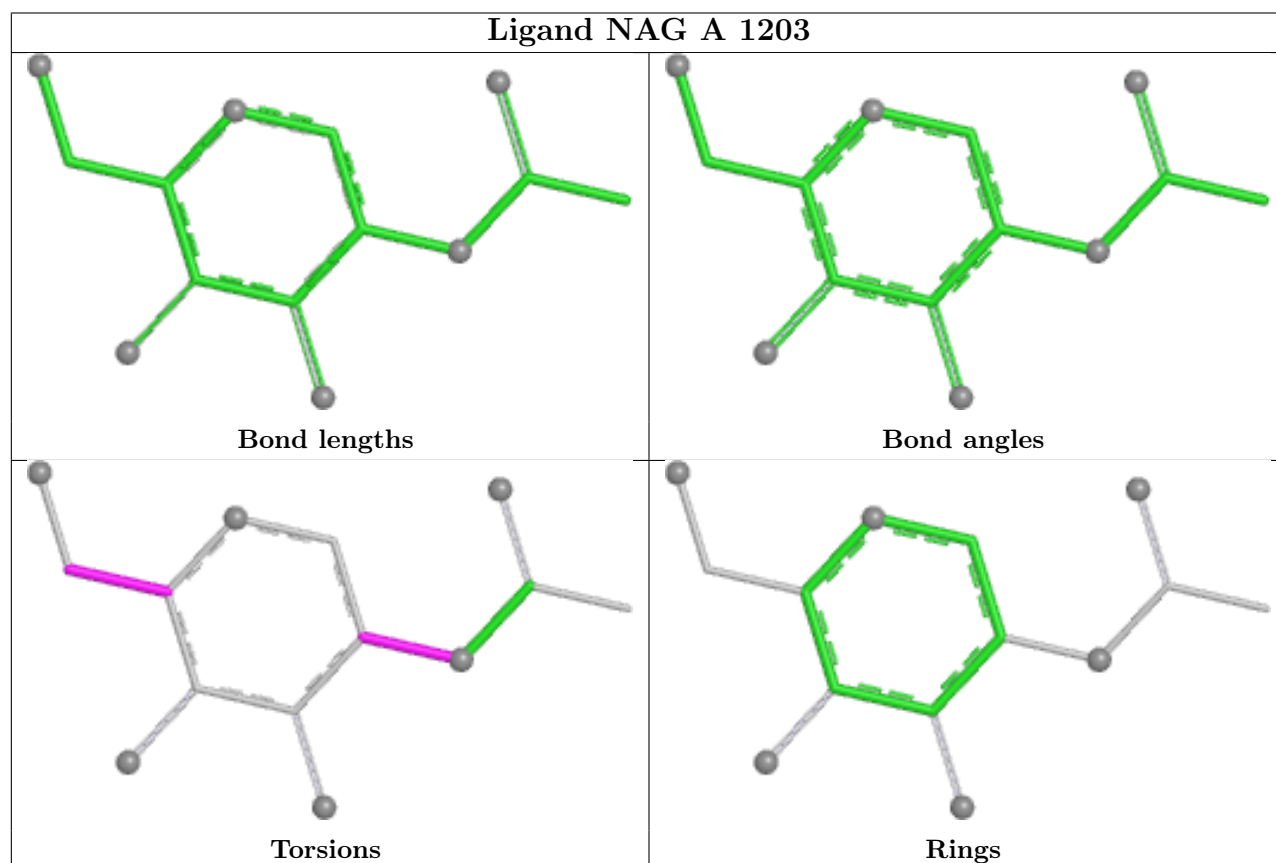
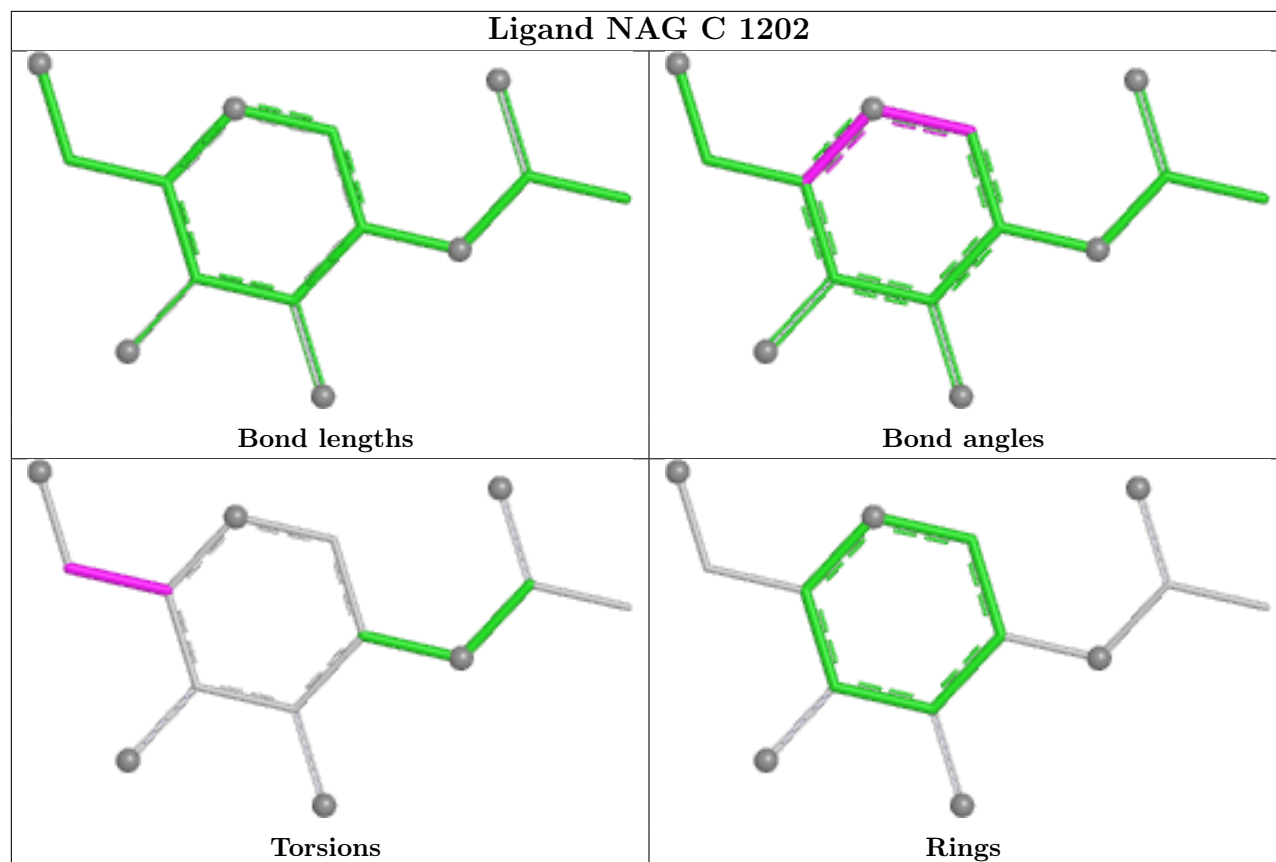
Ligand NAG A 1209



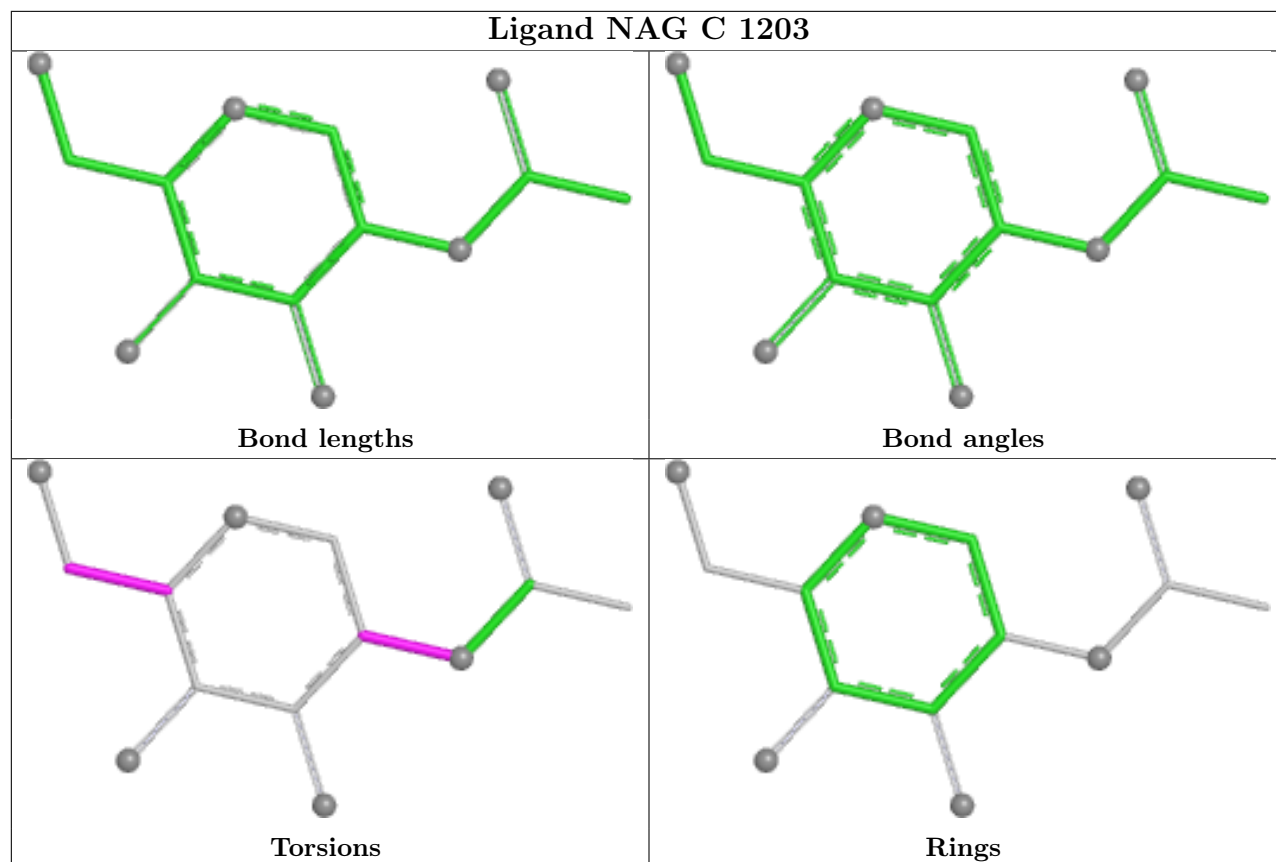
Ligand NAG B 1305



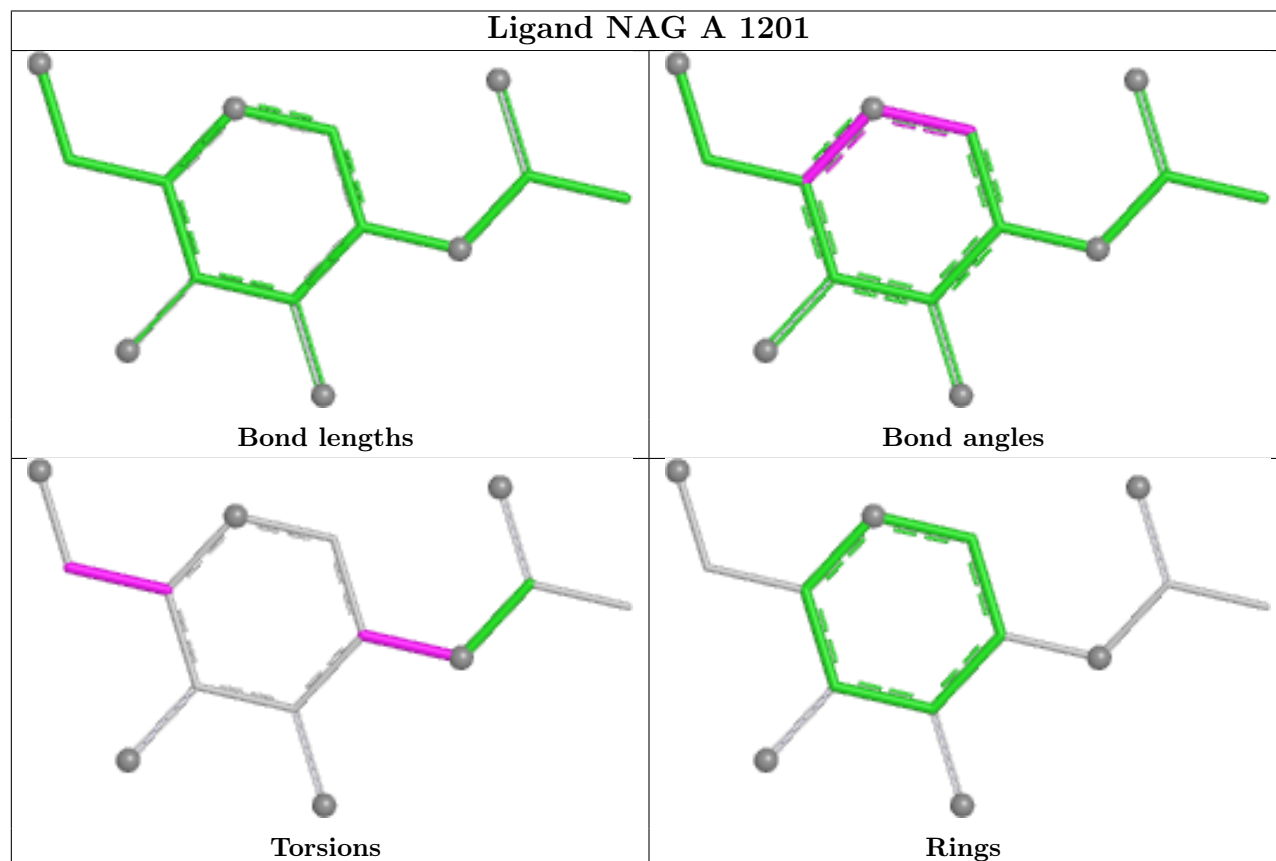




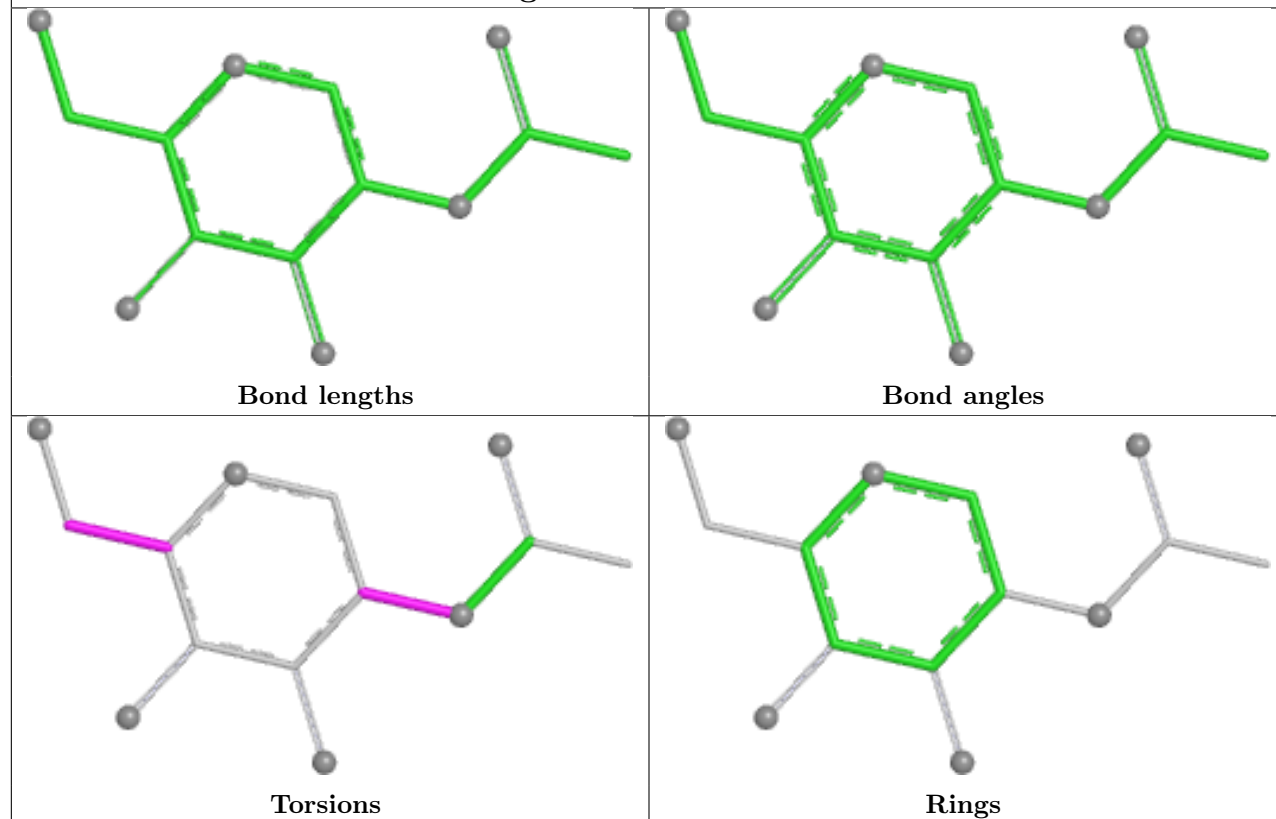
Ligand NAG C 1203



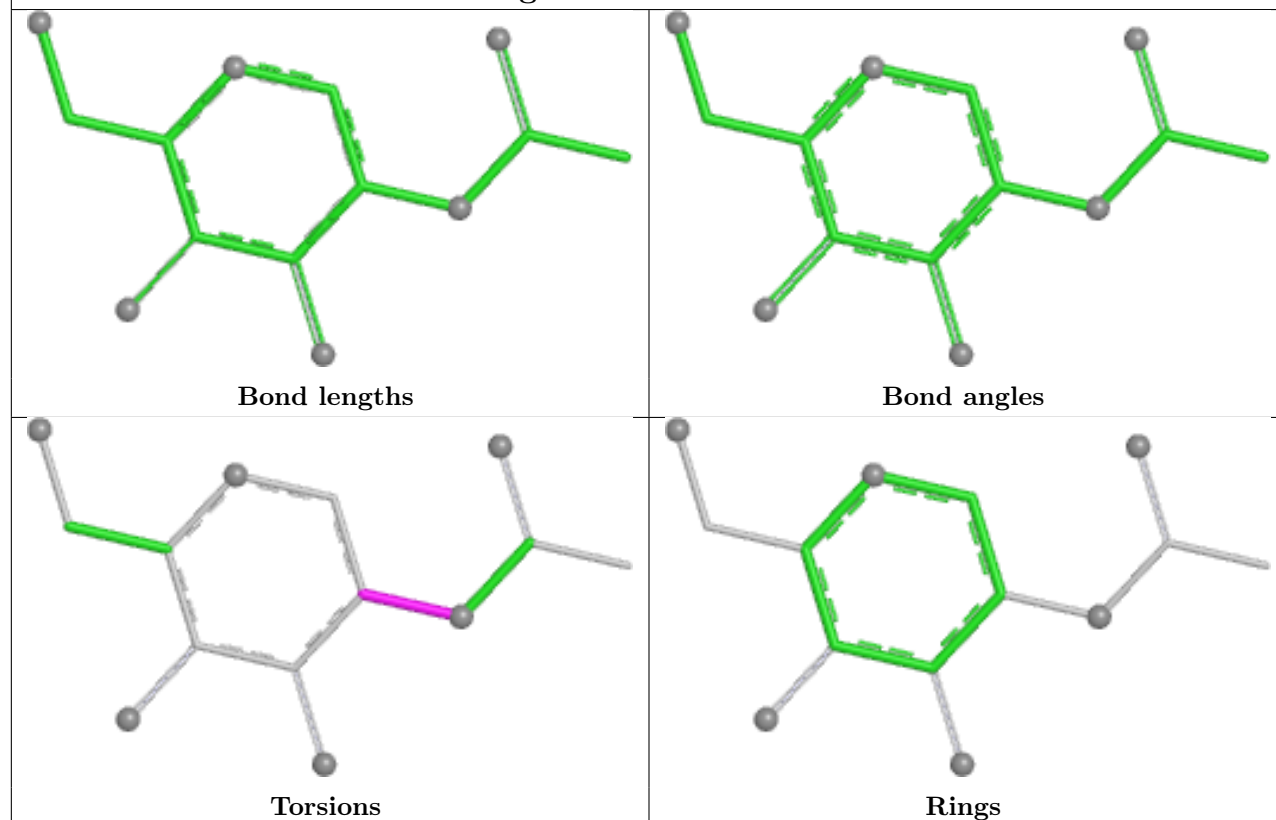
Ligand NAG A 1201



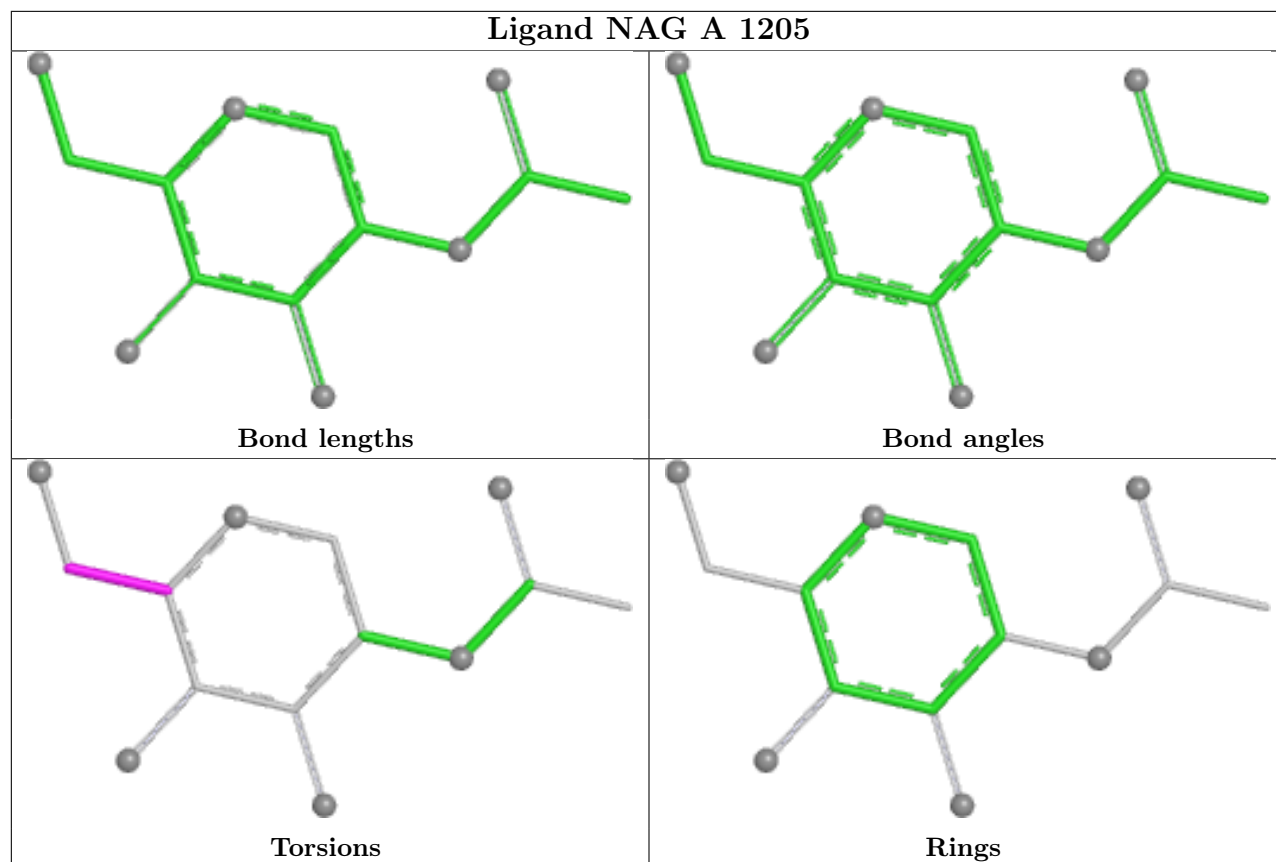
Ligand NAG B 1302



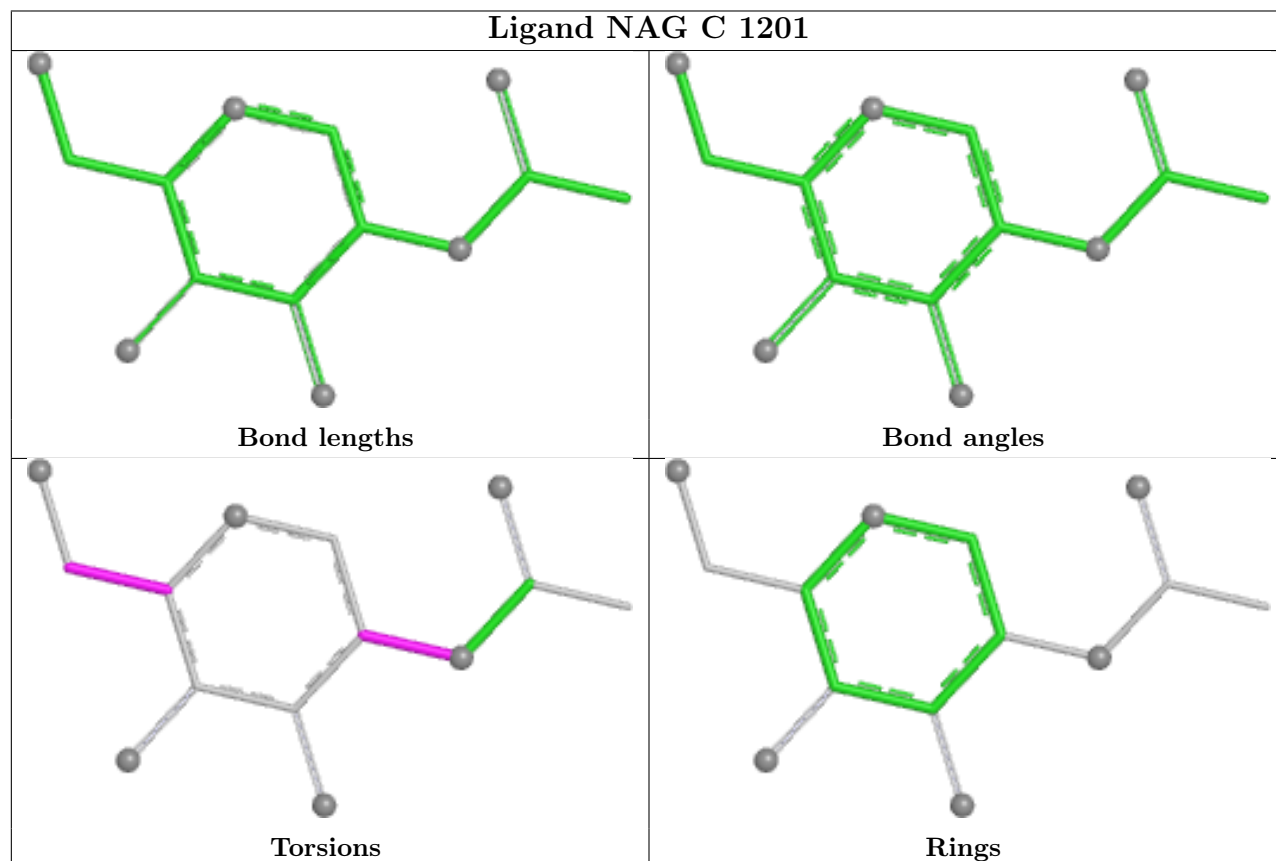
Ligand NAG C 1206

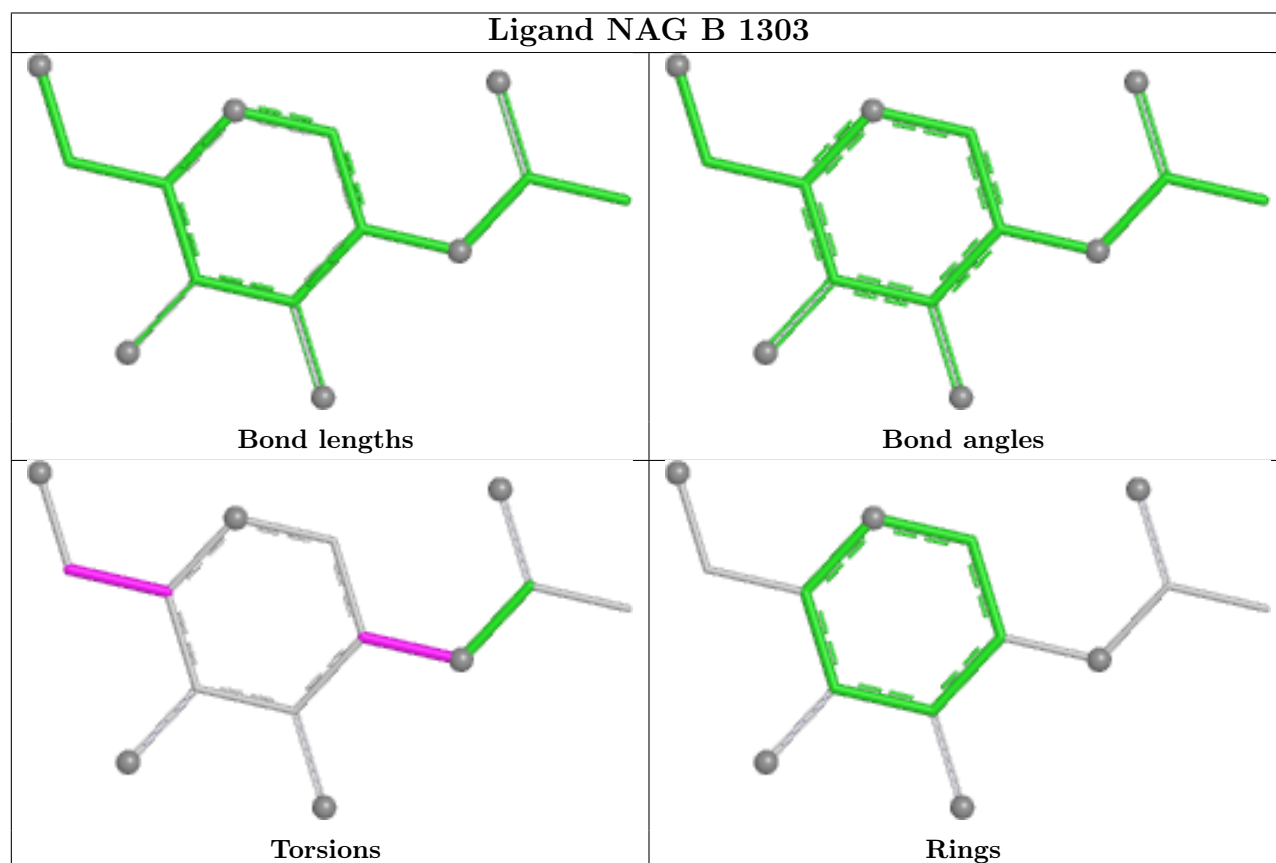
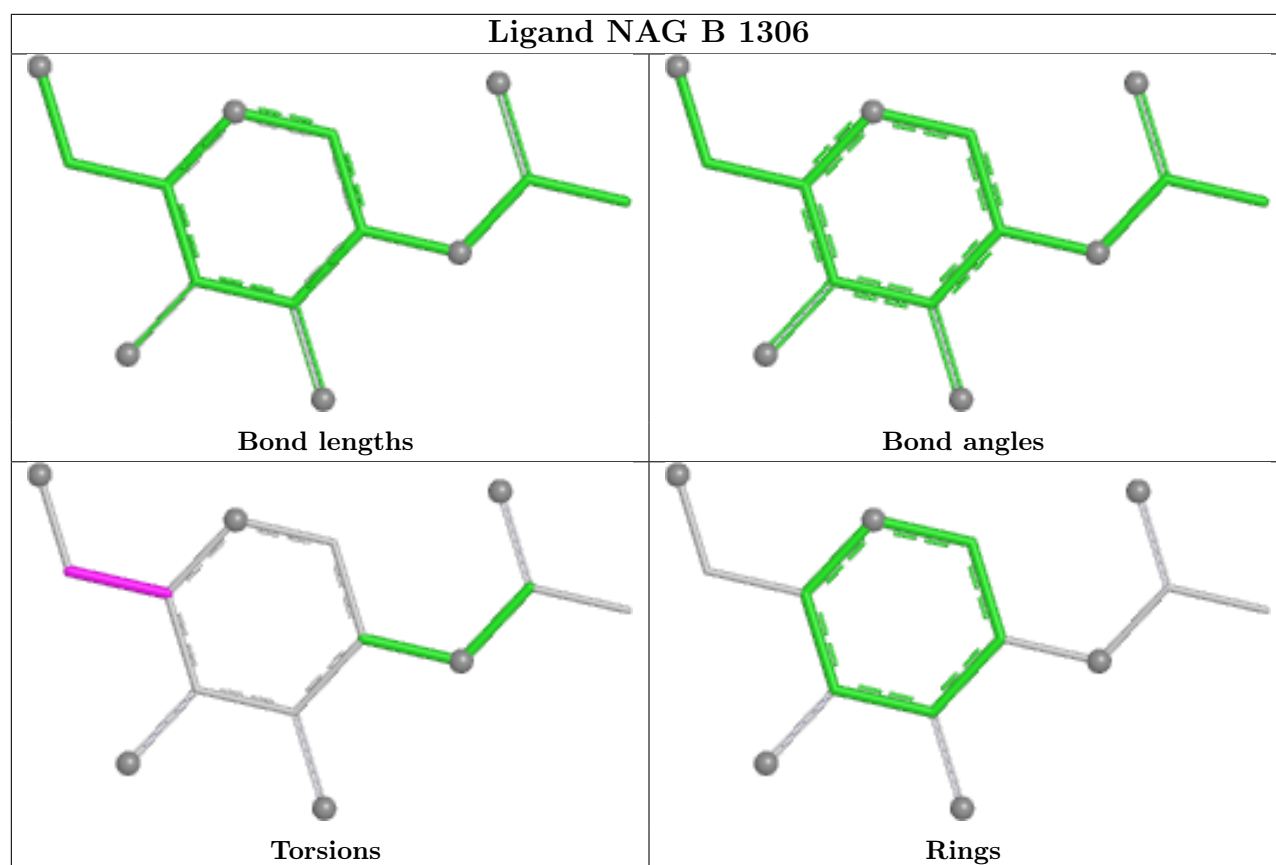


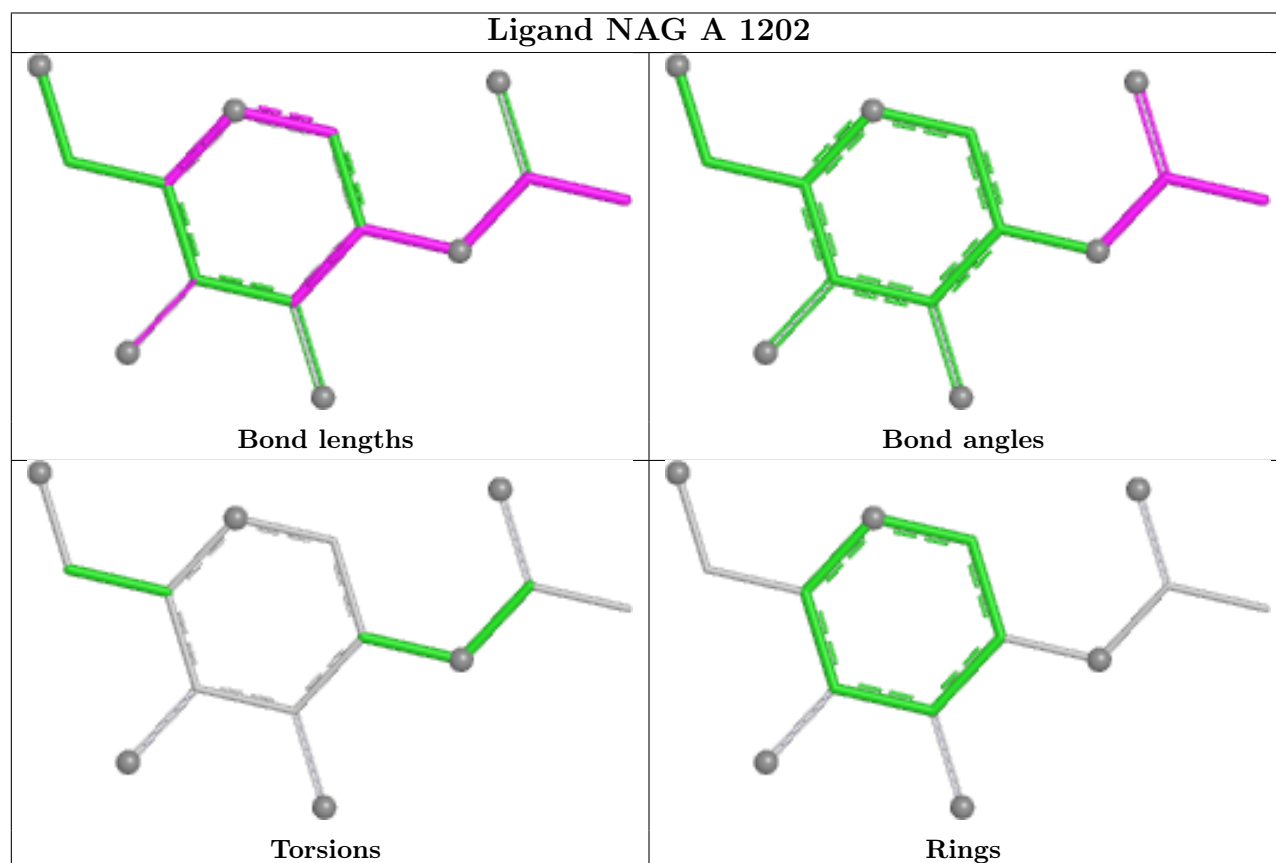
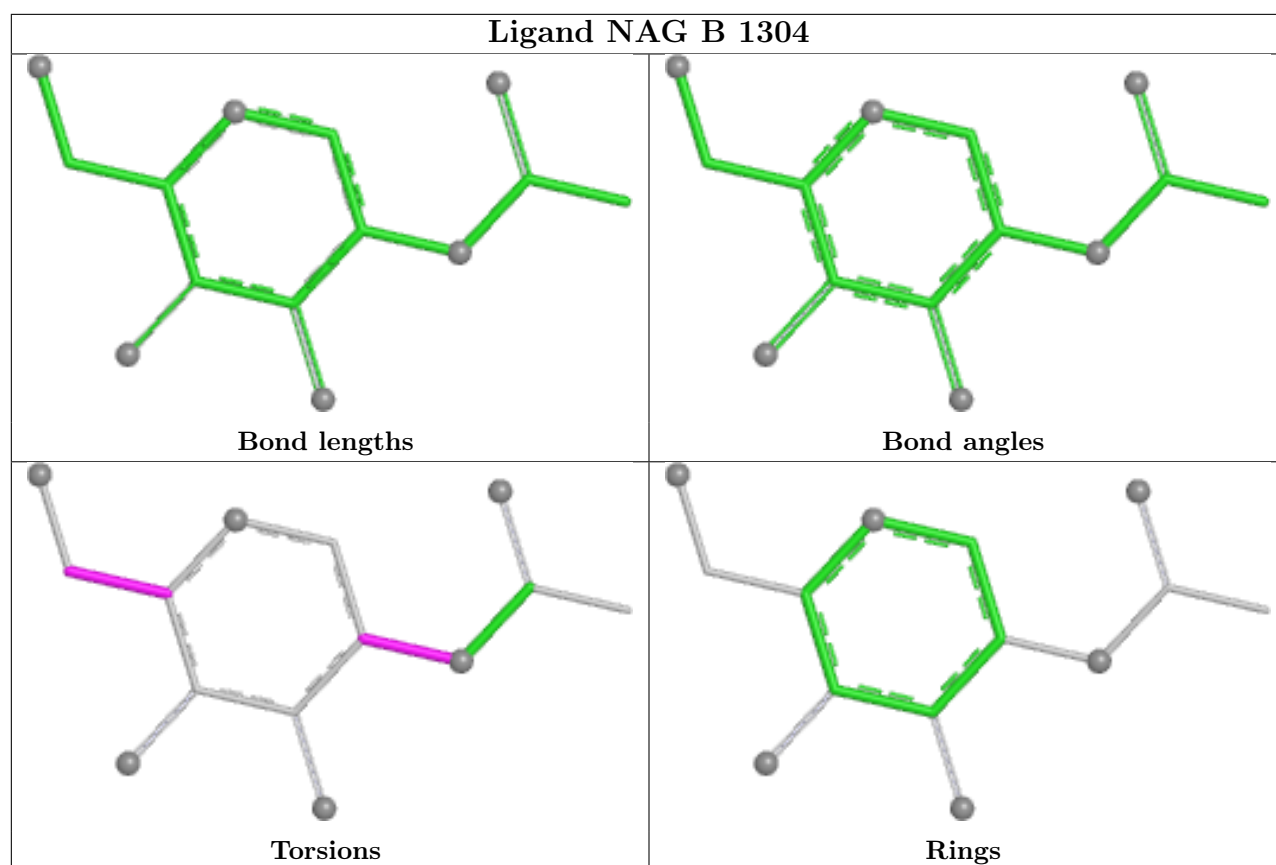
Ligand NAG A 1205

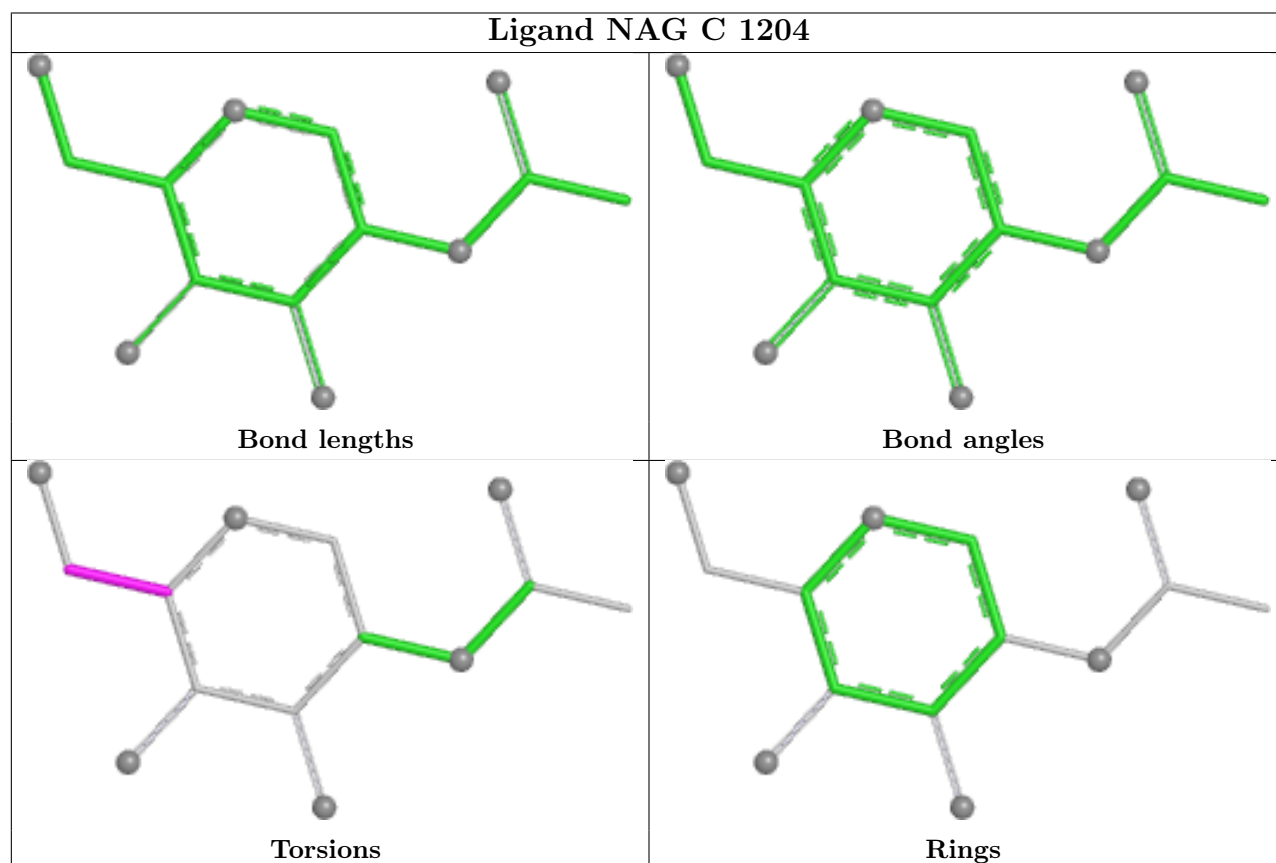
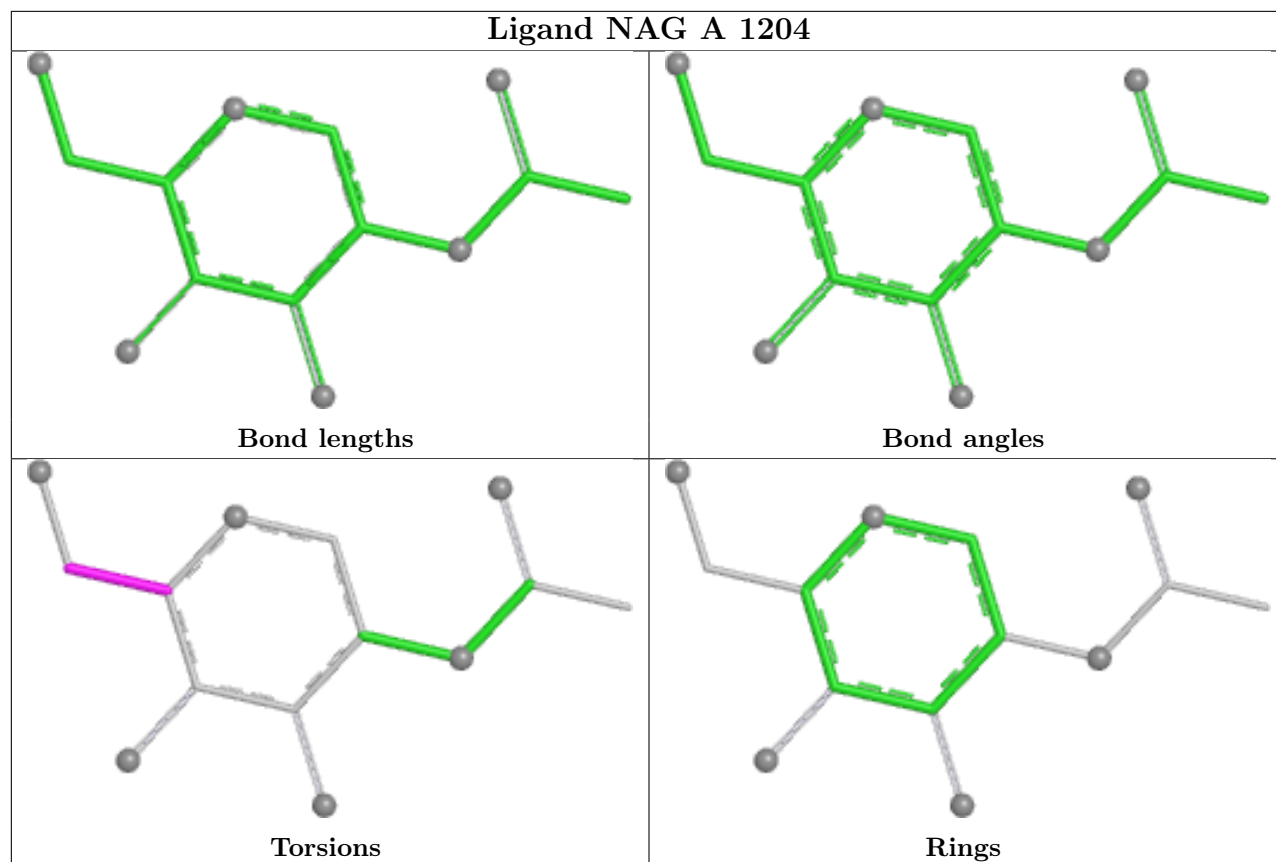


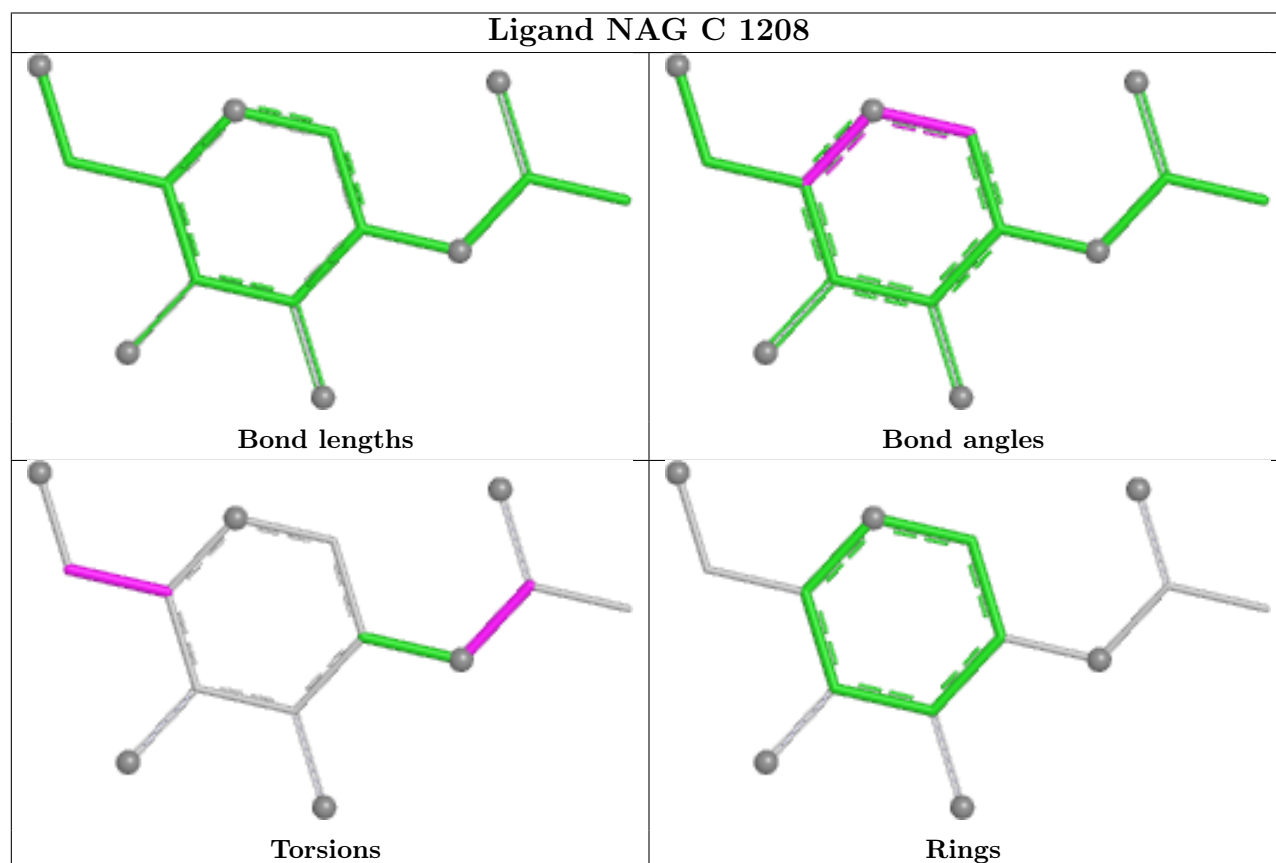
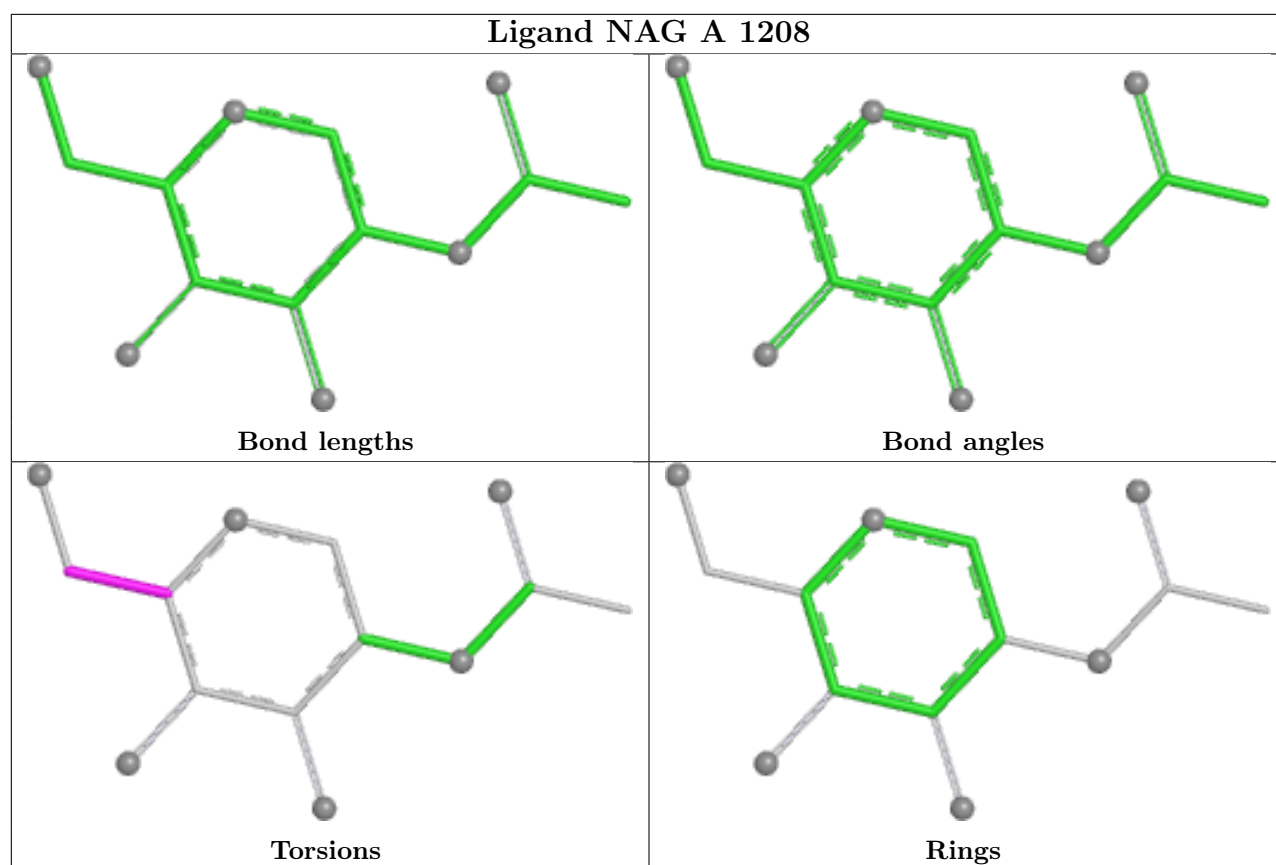
Ligand NAG C 1201











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.

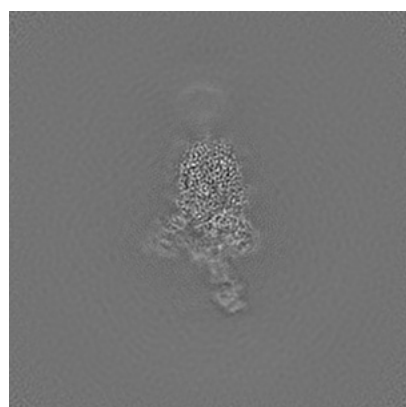
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-28688. These allow visual inspection of the internal detail of the map and identification of artifacts.

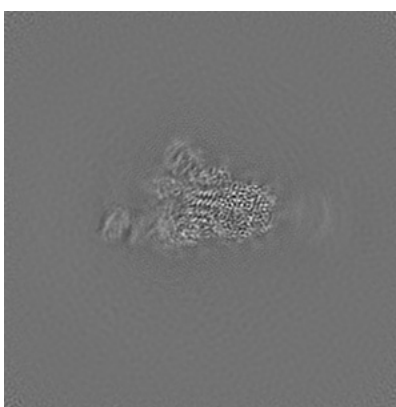
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

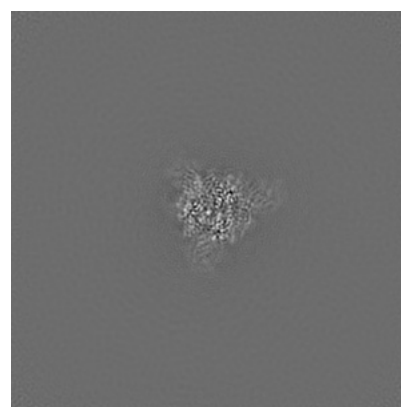
6.1.1 Primary map



X



Y

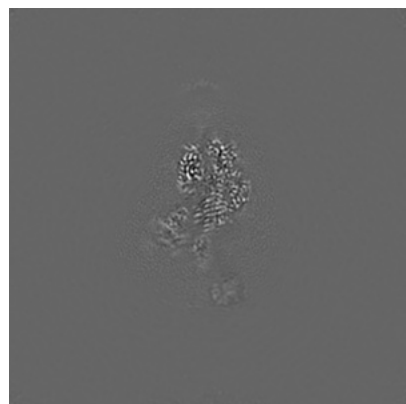


Z

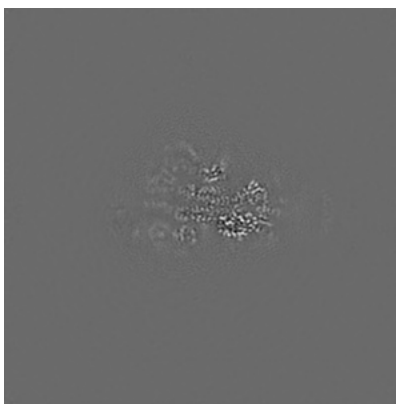
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

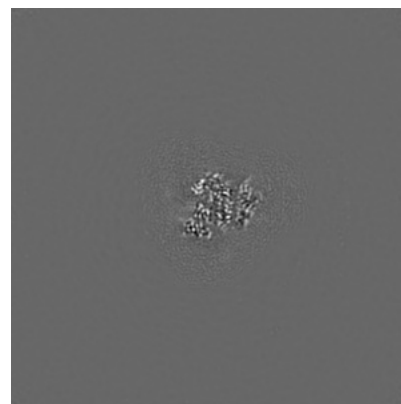
6.2.1 Primary map



X Index: 208



Y Index: 208



Z Index: 208

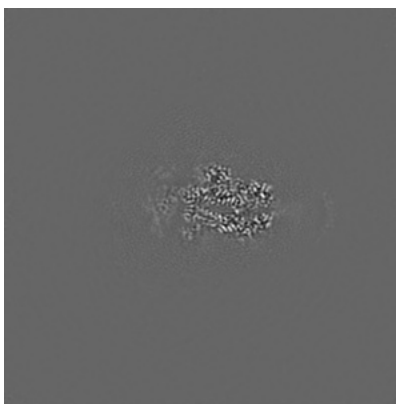
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

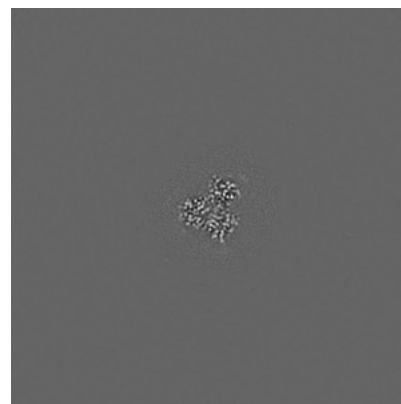
6.3.1 Primary map



X Index: 219



Y Index: 198

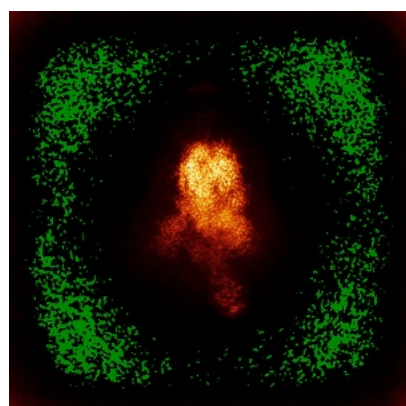


Z Index: 246

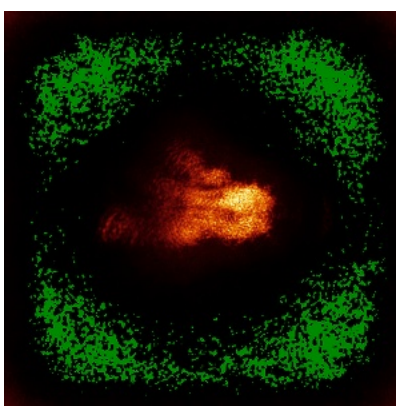
The images above show the largest variance slices of the map in three orthogonal directions.

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

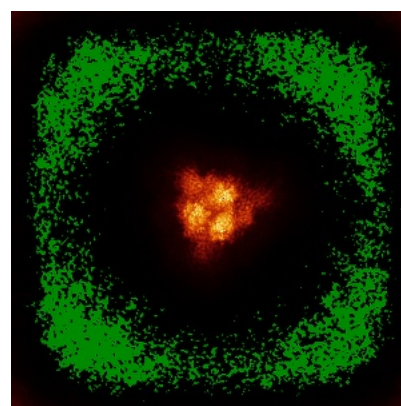
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 5.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

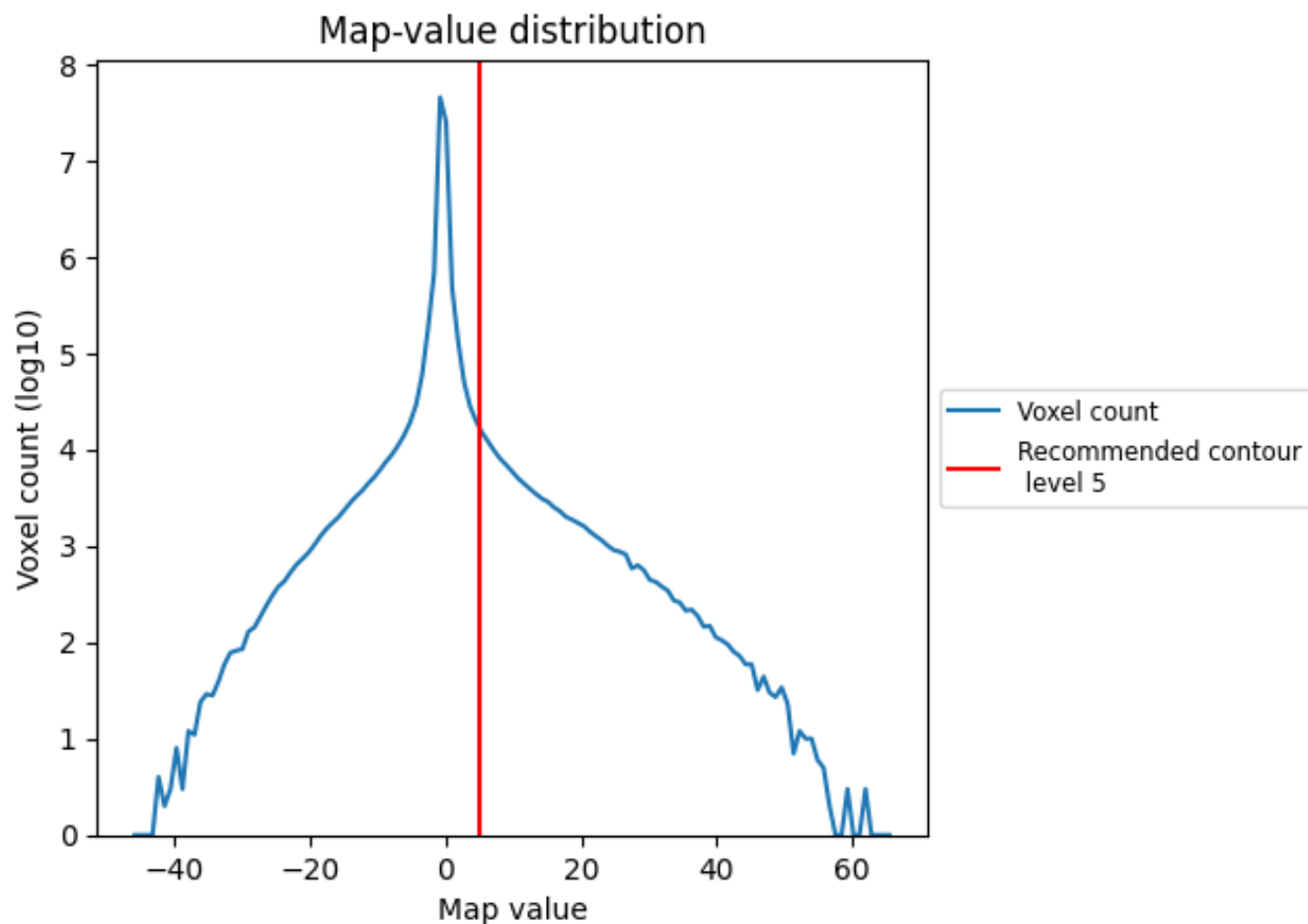
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

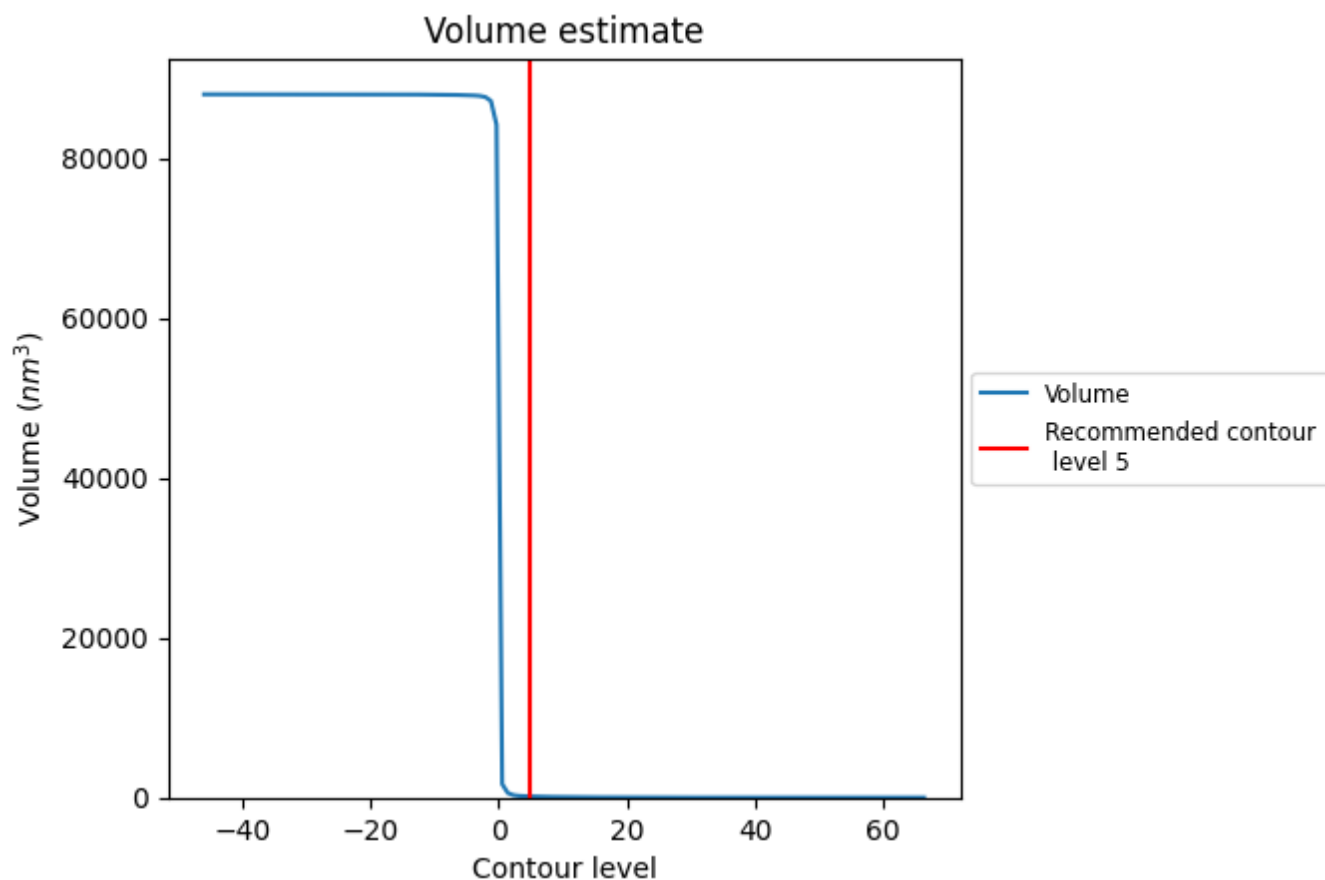
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

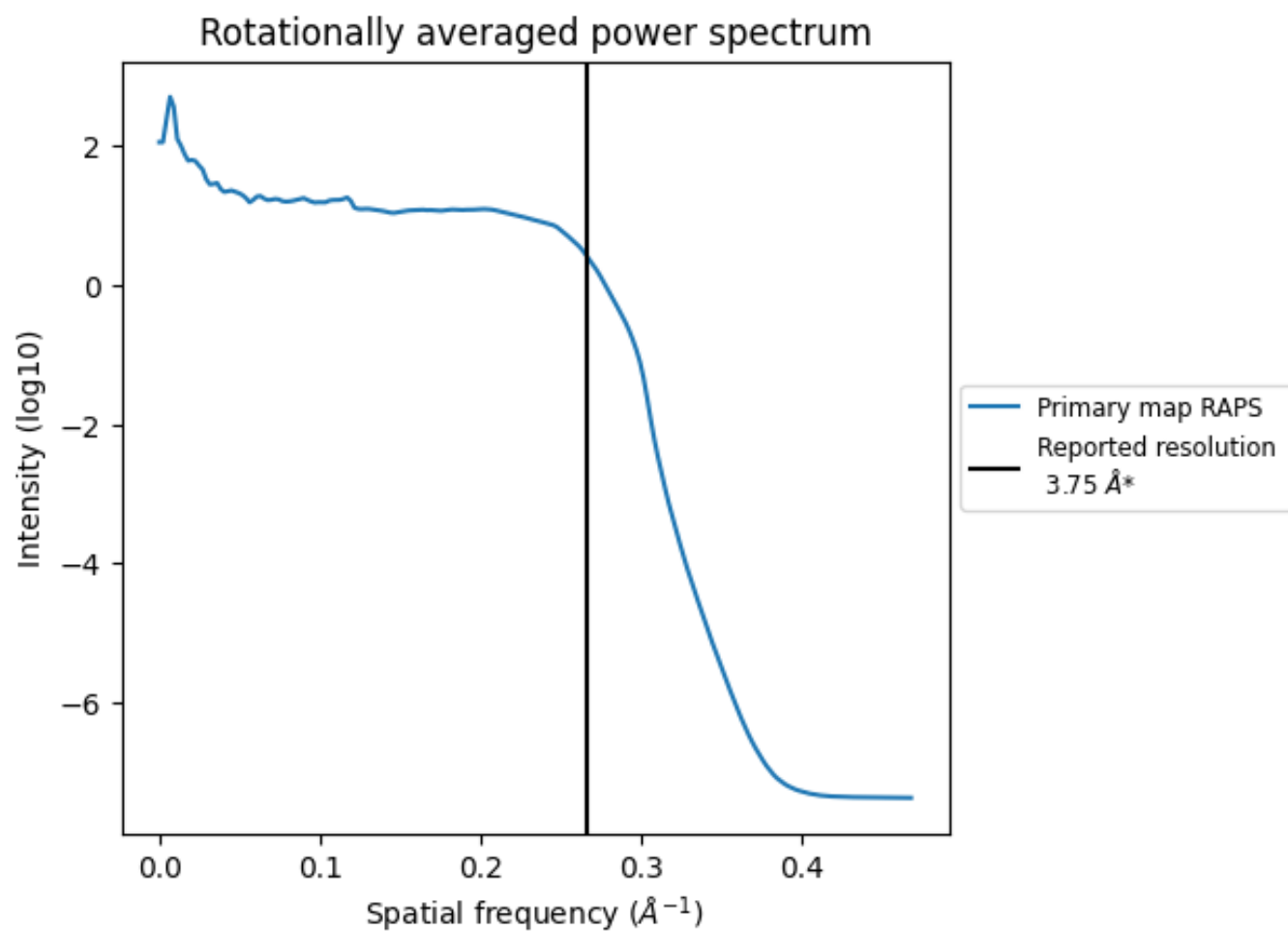
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 138 nm³; this corresponds to an approximate mass of 125 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 ⓘ

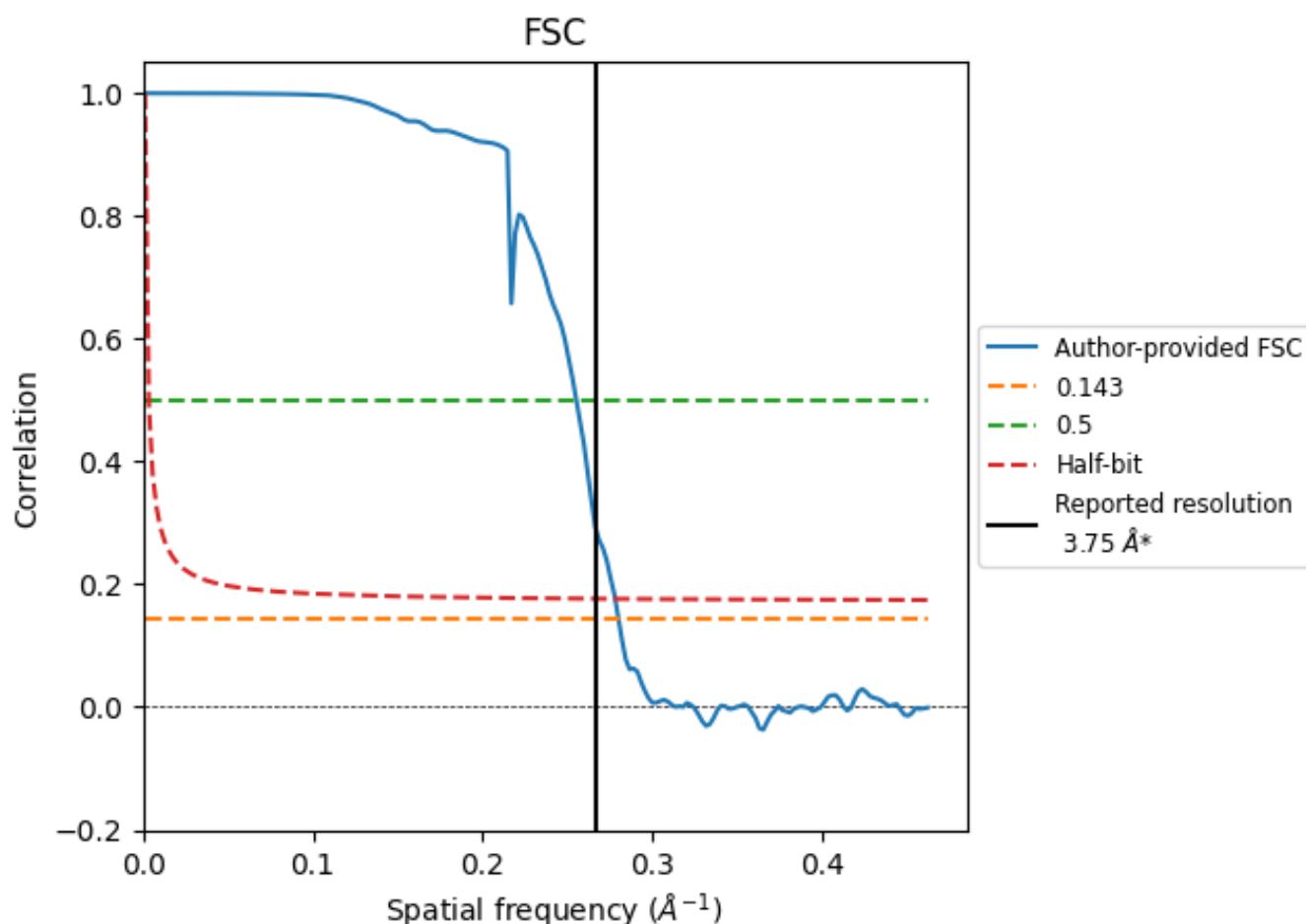


*Reported resolution corresponds to spatial frequency of 0.267 Å⁻¹

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 0.267 Å⁻¹

8.2 Resolution estimates [i](#)

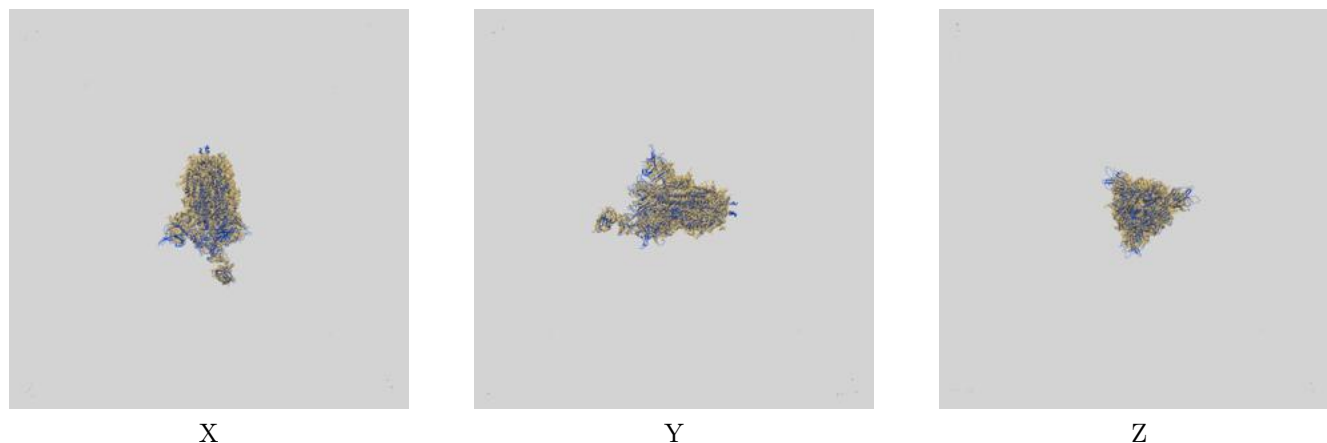
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	3.75	-
Author-provided FSC curve	3.57	3.92	3.60
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

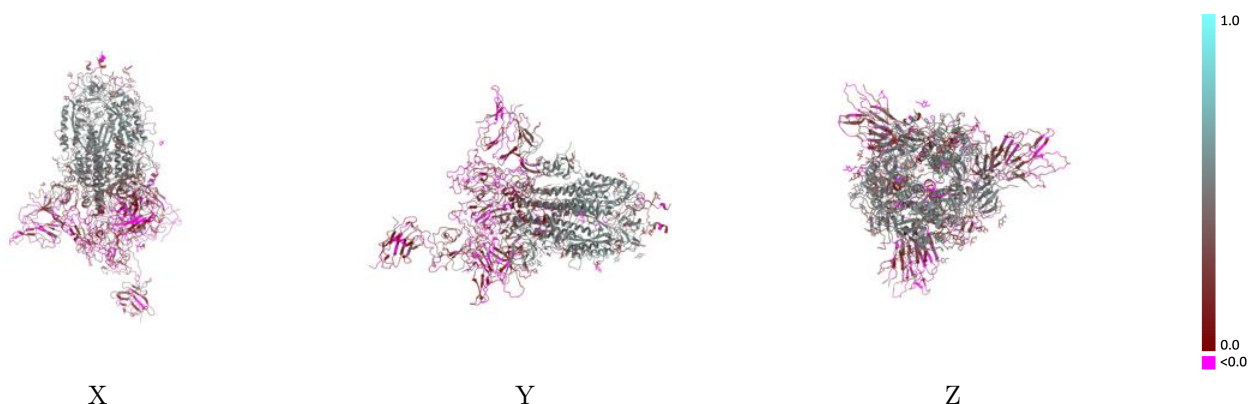
This section contains information regarding the fit between EMDB map EMD-28688 and PDB model 8EYH. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

9.1 Map-model overlay [i](#)



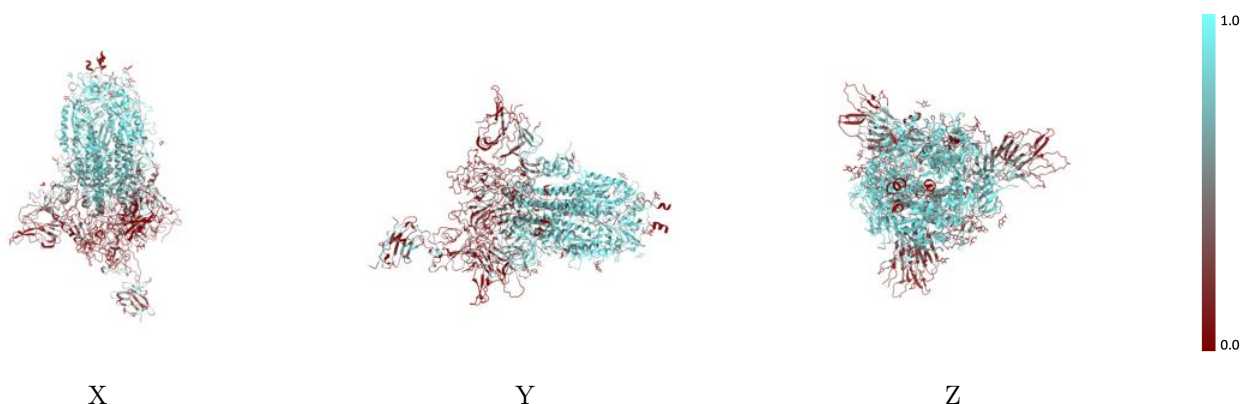
The images above show the 3D surface view of the map at the recommended contour level 5.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



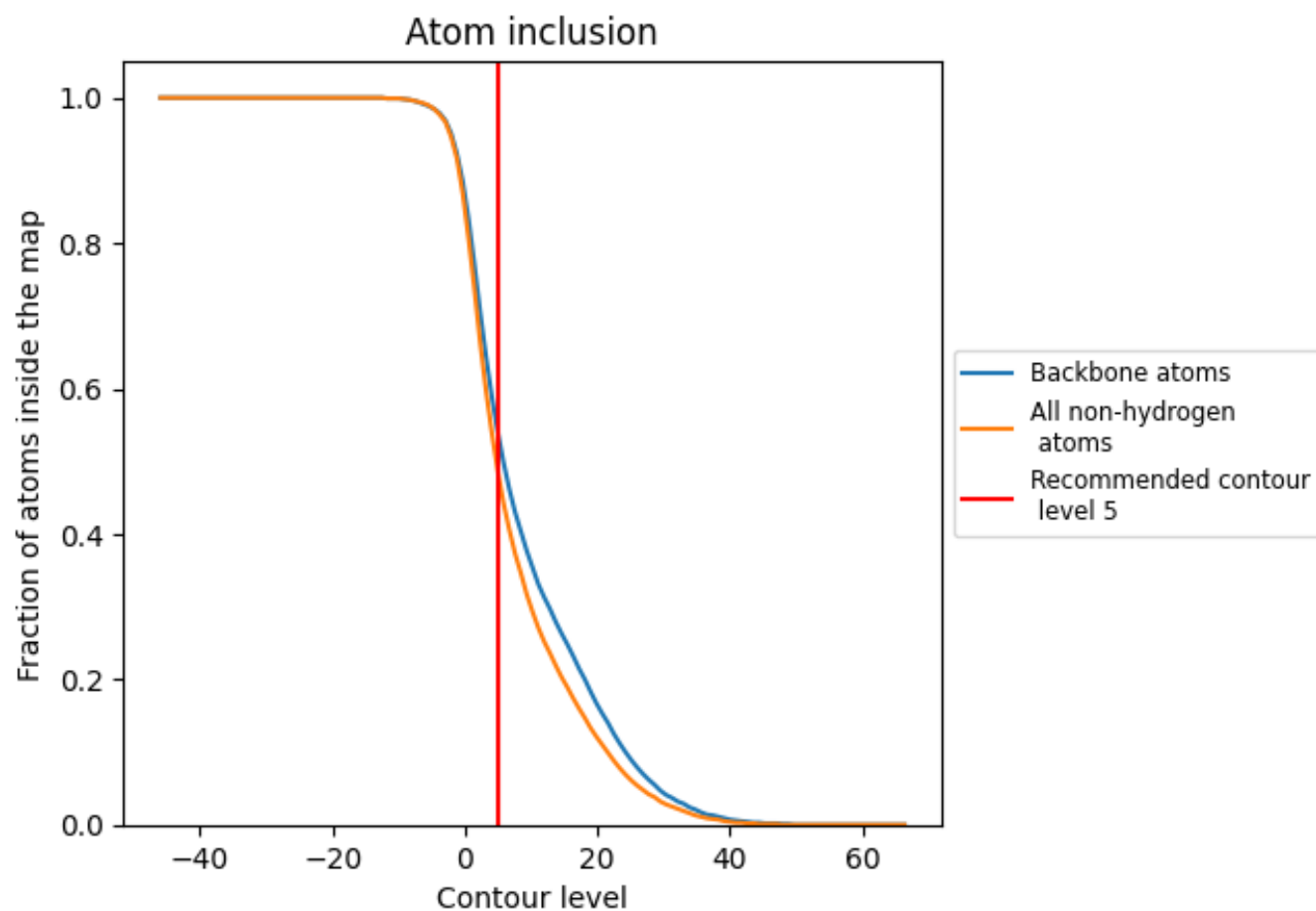
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 54% of all backbone atoms, 48% 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 (5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4850	0.2870
A	0.4980	0.3080
B	0.5100	0.3000
C	0.4630	0.2720
D	0.3500	0.1460
E	0.3210	0.1470
F	0.1790	0.0860
G	0.3570	0.1290
H	0.2140	0.0730
I	0.0710	-0.0470

1.0

0.0

<0.0