



wwPDB EM Validation Summary Report ⓘ

Nov 7, 2023 – 10:16 AM JST

PDB ID : 6JPA
EMDB ID : EMD-9868
Title : Rabbit Cav1.1-Verapamil Complex
Authors : Zhao, Y.; Huang, G.; Wu, J.; Yan, N.
Deposited on : 2019-03-26
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev70
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

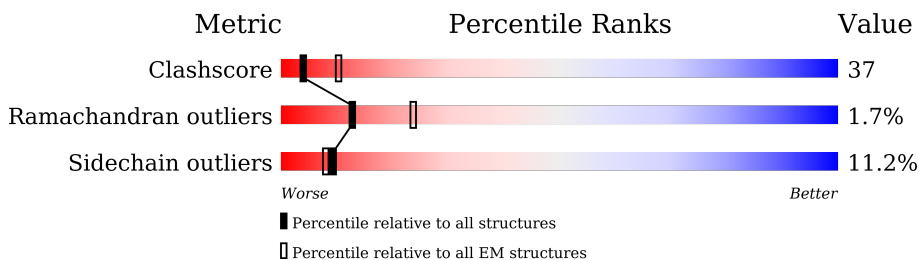
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.60 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.



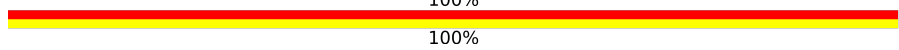
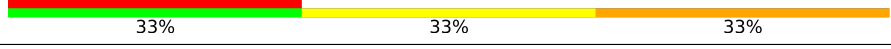
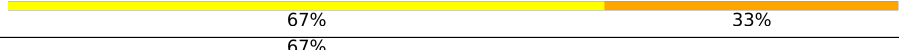

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	1506	
2	E	222	
3	B	450	
4	C	524	
5	F	1046	
6	D	2	
6	G	2	
6	J	2	

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Mol	Chain	Length	Quality of chain
6	K	2	100% 
7	H	3	33% 
7	I	3	67% 
8	L	3	67% 

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

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

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 22232 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 Voltage-dependent L-type calcium channel subunit alpha-1S.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1274	10219	6728	1668	1753	70	0	0

- Molecule 2 is a protein called Voltage-dependent calcium channel gamma-1 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	E	169	1326	872	216	220	18	0	0

- Molecule 3 is a protein called Voltage-dependent L-type calcium channel subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	B	100	710	455	125	129	1	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	75	GLN	-	expression tag	UNP P19517
B	76	GLY	-	expression tag	UNP P19517
B	77	PRO	-	expression tag	UNP P19517
B	78	HIS	-	expression tag	UNP P19517
B	79	MET	-	expression tag	UNP P19517

- Molecule 4 is a protein called Voltage-dependent L-type calcium channel subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	C	178	1367	876	232	254	5	0	0

- Molecule 5 is a protein called Voltage-dependent calcium channel subunit alpha-2/delta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	F	973	7804	4942	1320	1510	32	1	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	?	-	SER	See sequence details	UNP P13806

- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose.



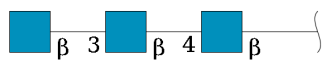
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	D	2	28	16	2	10	0	0
6	G	2	28	16	2	10	0	0
6	J	2	28	16	2	10	0	0
6	K	2	28	16	2	10	0	0

- Molecule 7 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.



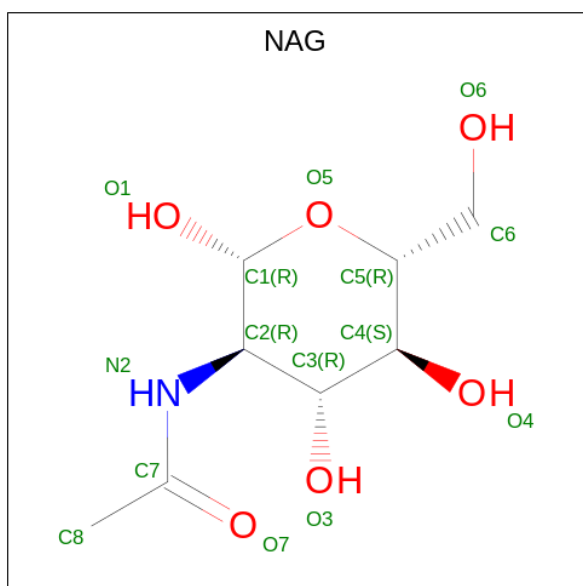
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
7	H	3	39	22	2	15	0	0
7	I	3	39	22	2	15	0	0

- Molecule 8 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms			AltConf	Trace	
			Total	C	N			O
8	L	3	42	24	3	15	0	0

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

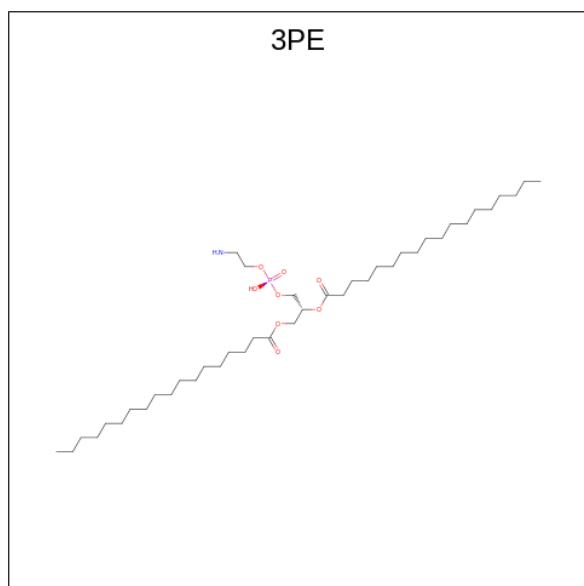


Mol	Chain	Residues	Atoms			AltConf	
			Total	C	N		O
9	A	1	14	8	1	5	0
9	F	1	14	8	1	5	0
9	F	1	14	8	1	5	0
9	F	1	14	8	1	5	0
9	F	1	14	8	1	5	0
9	F	1	14	8	1	5	0
9	F	1	14	8	1	5	0
9	F	1	14	8	1	5	0

- Molecule 10 is CALCIUM ION (three-letter code: CA) (formula: Ca).

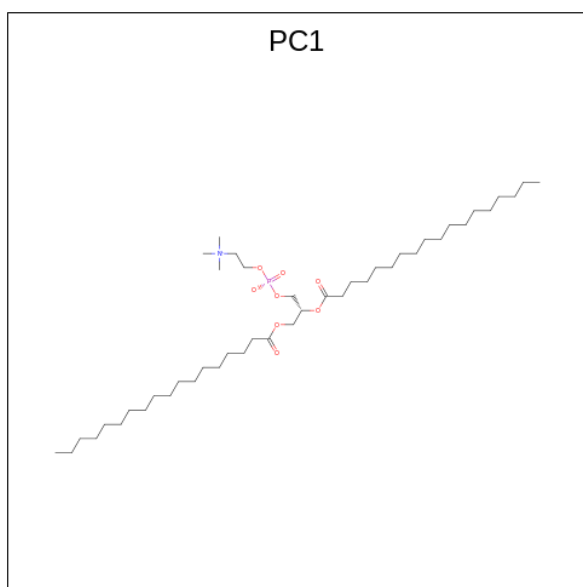
Mol	Chain	Residues	Atoms		AltConf
10	A	3	Total	Ca	0
			3	3	

- Molecule 11 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: C₄₁H₈₂NO₈P).



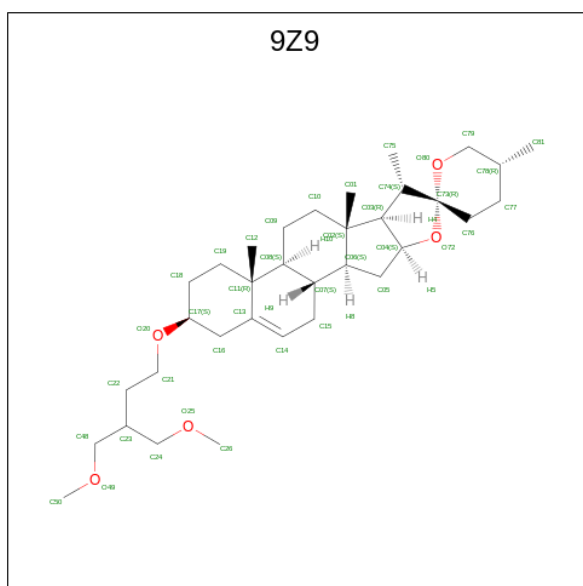
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
11	A	1	Total	C	N	O	P	0
			33	23	1	8	1	
11	A	1	Total	C	N	O	P	0
			19	10	1	7	1	
11	A	1	Total	C	N	O	P	0
			42	32	1	8	1	
11	A	1	Total	C	N	O	P	0
			36	26	1	8	1	
11	A	1	Total	C	N	O	P	0
			20	11	1	7	1	
11	A	1	Total	C	N	O	P	0
			35	25	1	8	1	
11	A	1	Total	C	N	O	P	0
			42	32	1	8	1	
11	A	1	Total	C	O	P		0
			39	30	8	1		

- Molecule 12 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: C₄₄H₈₈NO₈P).



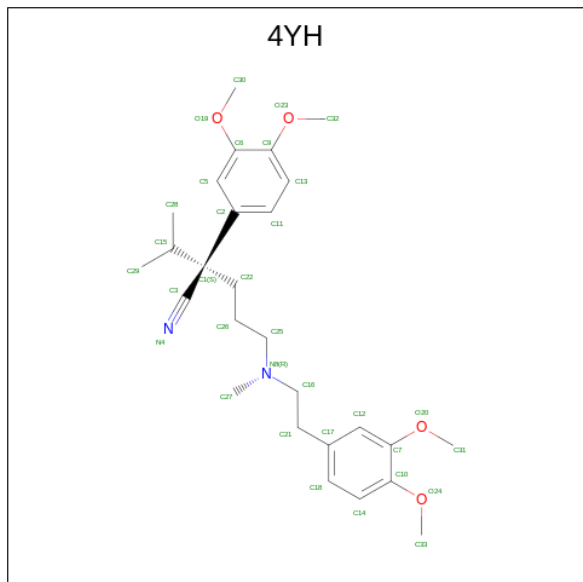
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
12	A	1	39	29	1	8	1	0
12	A	1	54	44	1	8	1	0

- Molecule 13 is (3beta,14beta,17beta,25R)-3-[4-methoxy-3-(methoxymethyl)butoxy]spirost-5-en (three-letter code: 9Z9) (formula: C₃₄H₅₆O₅).



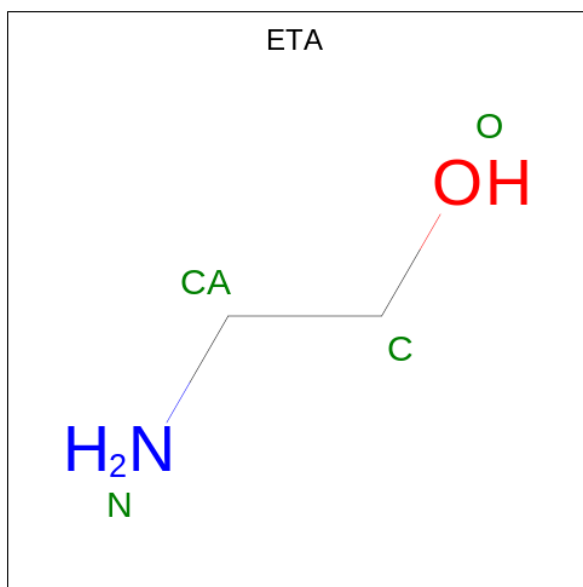
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
13	A	1	30	27	3	0

- Molecule 14 is (2S)-2-(3,4-dimethoxyphenyl)-5-{[2-(3,4-dimethoxyphenyl)ethyl](methyl)amino}-2-(propan-2-yl)pentanenitrile (three-letter code: 4YH) (formula: $C_{27}H_{38}N_2O_4$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
14	A	1	33	27	2	4	1
14	A	1	33	27	2	4	1

- Molecule 15 is ETHANOLAMINE (three-letter code: ETA) (formula: C_2H_7NO).

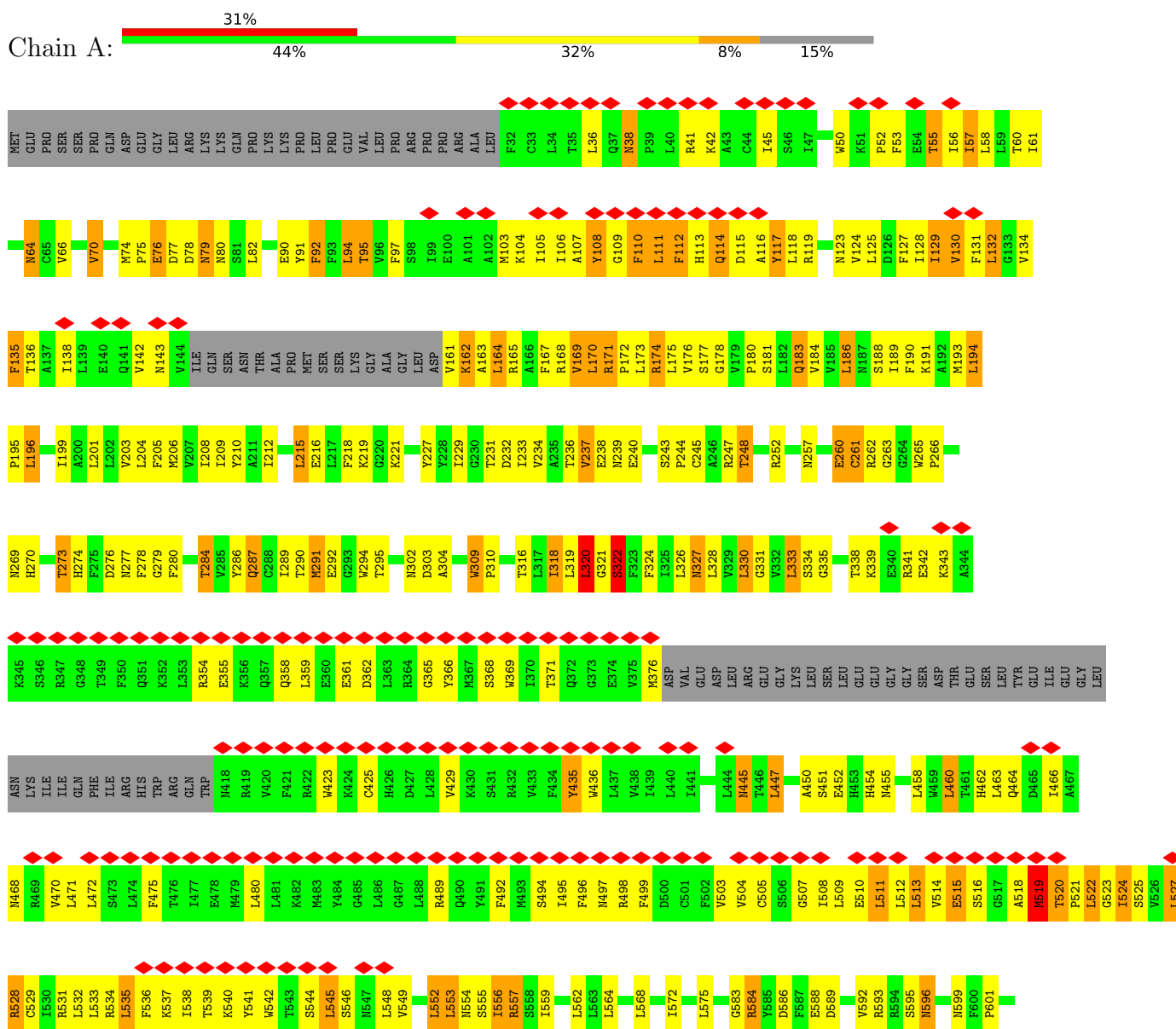


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
15	F	1	4	2	1	1	0

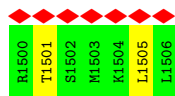
3 Residue-property plots i

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

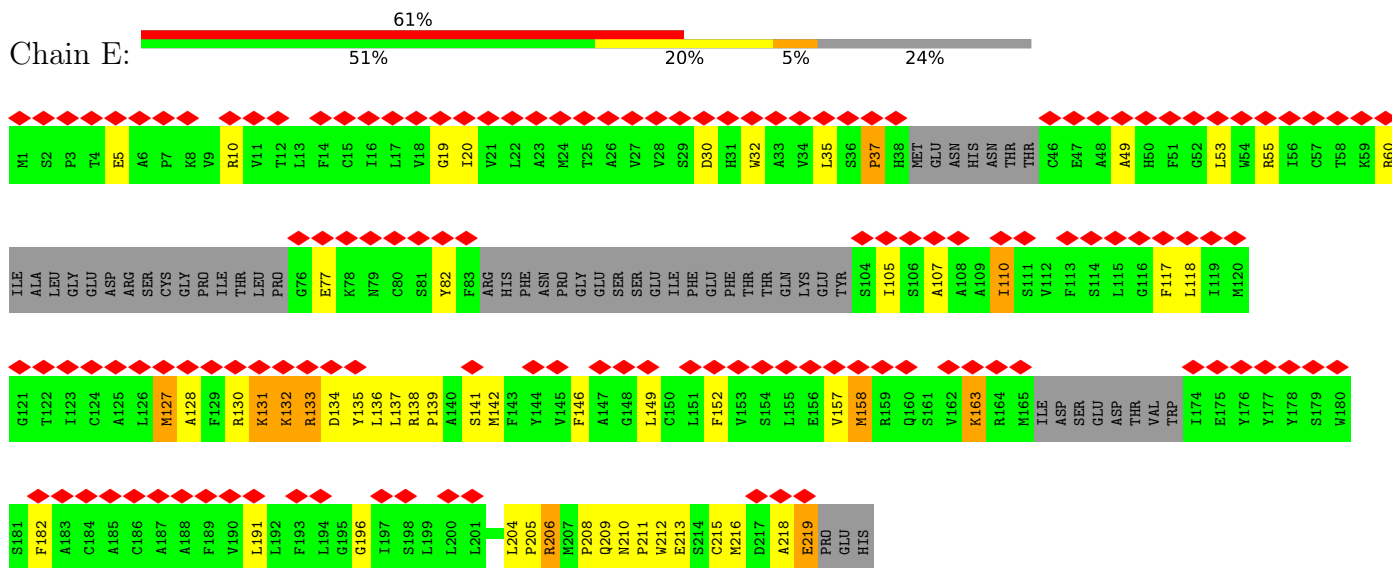
- Molecule 1: Voltage-dependent L-type calcium channel subunit alpha-1S



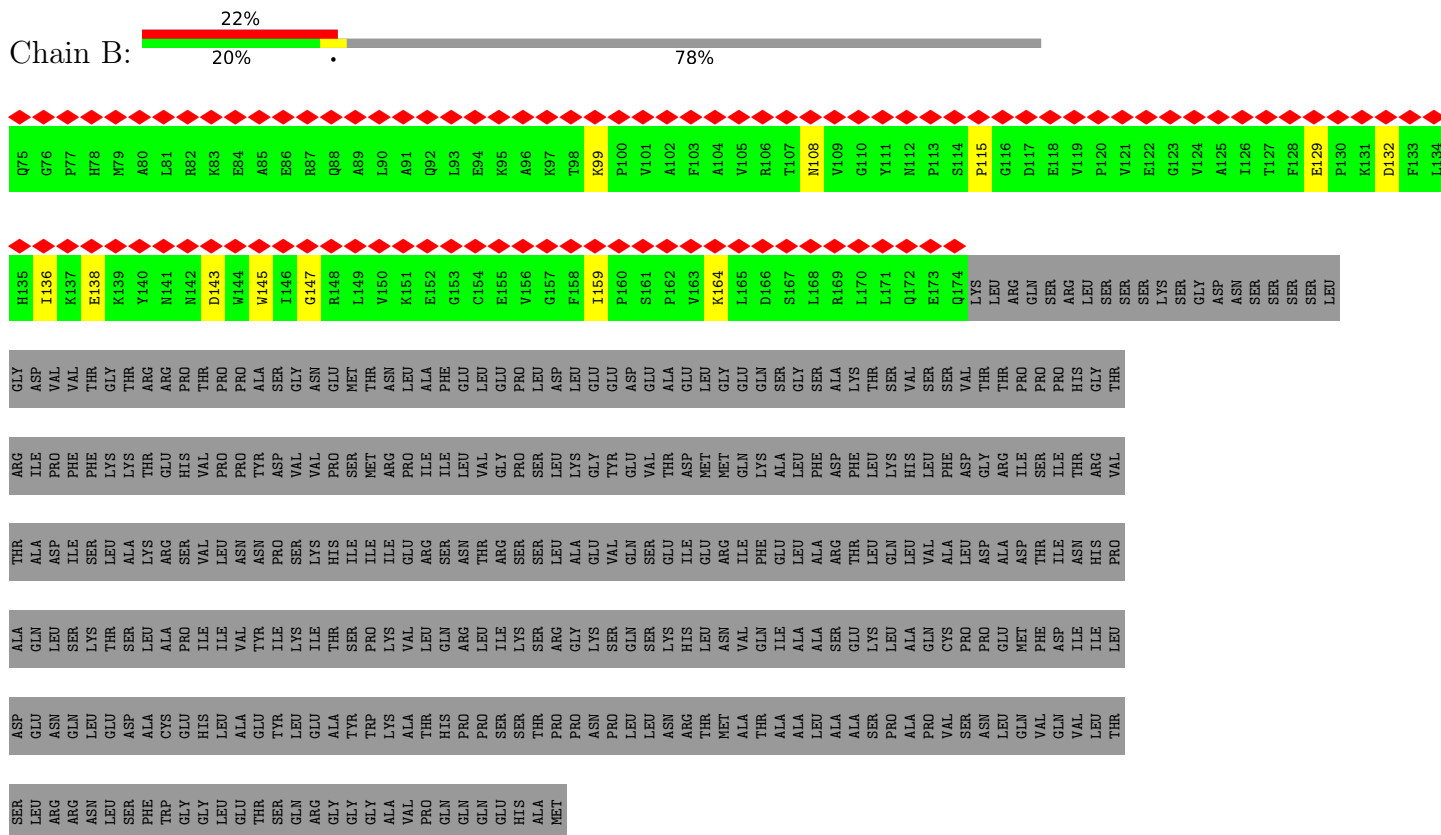
L604	L611	E614	P630	S631	Y632	P633	Y634	V635	L636	V637	C638	I639	L644	Y650	I651	L652	L653	N654	V655	F656	L657	A658	I659	A660	V661	D662	N663	L664	A665	E666	A667	E668	S669	L670	T671	S672	A673	Q674	K675	A676	K677	A678	E679	E680	R681	K682	R683	E684	K685	M686	S687	ARG	GLY	LEU								
PRO	ASP	LYS	THR	GLU	GLU	LYS	SER	VAL	MET	ALA	LYS	LEU	GLN	PRO	LYS	GLY	GLY	GLY	ILE	PRO	THR	THR	ALA	LYS	LEU	VAL	ASP	ASP	GLU	PHE	GLU	GLU	ASN	ASN	VAL	ASN	GLU	VAL	LYS	ASP	PRD	TYR	PRD	SER	ALA	ASP	PHE	PRO	GLY	ASP	ASP	GLU	GLU	ASP	GLU	GLU	PRD					
GLU	ILE	PRO	VAL	PRO	ARG	PRO	ARG	PRO	LEU	ALA	ALA	LEU	GLN	LYS	LYS	VAL	PRO	ILE	PRO	PRO	PHE	PHE	ILE	VAL	ASP	ASP	GLU	THR	THR	THR	THR	ASN	ASN	VAL	ASN	GLU	VAL	LYS	C792	H793	R794	I795	V796	N797	A798	T799	W800	F801	T802	N803	F804	I805	L806	L807	F808	L810						
L811	S812	S813	L816	F821	R822	R823	A824	E825	S826	Y827	R828	N829	Q830	I831	L832	G833	Y834	F835	D836	I837	A838	F839	T840	R900	S841	Y842	F843	T844	R845	R906	E846	I847	Y848	N909	R910	L849	K850	M851	T852	T853	Y854	G855	ALA	PHE	LEU	HIS	Q919	S920	V921	F922	V923	A924	I925	R926	T927	N869	I870	G929	I931	D872	L873	L874
V875	V876	A877	V878	S879	L880	I881	S882	M883	GLY	LEU	GLU	SER	THR	ILE	SER	V892	V893	K894	E895	L896	R897	A898	F899	R900	Y901	L902	R903	P904	L905	R906	A907	I908	N909	R910	L849	K850	M851	K912	G913	L914	K915	H916	V917	V918	Q919	S920	V921	F922	V923	A924	I925	R926	T927	N869	I870	G929	I931	D872	L873	L874		
L938	Q939	F940	M941	I945	G946	Q947	Q948	K951	F954	C957	N958	D959	I960	S961	M962	V893	M963	T964	E965	E966	E967	Y972	Y973	K976	D977	G978	D979	P980	T981	Q982	M983	E984	Q989	W990	I991	F997	D998	N999	V1000	A1003	M1004	L1007	V1010	Q919	E1014	G1015	P1017															
Q1018	R1022	D1025	E1028	E1029	D1030	P1033	M1037	R1038	V1039	I1046	I1052	F1055	M1056	I1059	G1062	F1063	V1064	I1065	V1066	T1067	F1068	Q1069	E1070	R980	T981	Q982	M983	E984	T1074	E1075	Y1076	K1077	M1078	C1079	E1080	L1081	D1082	K1083	M1084	Q1085	R1086	Q1087	G1088	V1089	Q1090	Y1091	A1092	L1093	K1094	A1095	R1096											
P1097	L1098	R1099	C1100	Y1101	I1102	P1103	K1104	M1105	P1106	Y1107	Y1109	Q1110	V1111	W1112	Y1113	V1114	V1115	T1116	S1117	Y1119	F1120	Y1122	L1123	M1124	F1125	I1128	M1131	T1132	L1135	G1136	M1137	Q1138	H1139	Y1140	H1141	Q1142	S1143	E1144	E1145	M1146	M1147	H1148	D1151	M1155	A1156	I1159	I1160	F1161	T1162													
L1163	M1165	I1166	K1168	L1169	L1170	A1171	F1172	K1173	A1174	R1175	D1180	P1181	M1182	M1183	L1188	I1189	V1190	I1194	I1195	D1196	V1197	I1198	L1199	E1201	I1202	D1203	T1204	F1205	L1206	ALA	SER	GLY	GLY	LEU	CYS	LEU	GLY	GLY	GLY	GLY	ASN	ASP	PRD	ASP	GLU	ALA	ARG	ILE														
SER	S1232	A1233	F1234	F1236	R1236	R1239	V1240	M1241	R1242	L1243	I1244	K1245	L1246	L1247	S1248	R1249	A1250	E1251	G1252	V1253	R1254	T1255	L1256	L1257	K1258	T1259	F1260	I1261	K1262	S1263	F1264	Q1265	A1266	L1267	A1271	L1272	L1277	F1278	F1279	I1280	Y1281	A1282	V1283	M1286	Q1287	F1288	F1289	G1290	K1291	L1292	A1293	L1294	V1295	T1298								
Q1299	I1300	M1301	R1302	Q1307	T1308	F1309	P1310	L1314	R1318	C1319	A1320	T1321	G1322	Q1326	L1329	L1330	A1331	C1332	S1333	Y1334	G1335	K1336	L1337	C1338	E1341	S1342	D1343	Y1344	A1345	P1346	G1347	E1348	E1349	C1352	G1353	T1354	M1355	F1356	A1357	Y1358	I1362	M1366	F1370	L1371	I1372	I1373	V1377															
I1380	M1381	D1382	N1383	F1384	D1385	Y1386	L1387	T1388	R1389	D1390	W1391	S1392	I1393	L1394	G1395	P1396	H1397	H1398	L1399	D1400	E1401	F1402	K1403	A1404	I1405	W1406	A1407	E1408	Y1409	D1410	P1411	E1412	A1413	K1414	G1415	R1416	I1417	K1418	H1419	L1420	D1421	V1422	V1423	T1424	L1425	L1426	R1427	F1428	I1429	Q1430	P1431	P1432	L1433	G1434	F1435	G1436	K1437	F1438	C1439			
P1440	H1441	R1442	V1443	A1444	C1445	K1446	R1447	L1448	V1449	G1450	M1451	N1452	M1453	P1454	L1455	N1456	S1457	D1458	G1459	T1460	V1461	T1462	F1463	N1464	A1465	T1466	L1467	F1468	A1469	L1470	V1471	R1472	T1473	A1474	L1475	K1476	I1477	K1478	T1479	E1480	G1481	N1482	F1483	E1484	Q1485	A1486	N1487	E1488	L1489	L1490	R1491	A1492	I1493	I1494	L1495	K1496	I1497	W1498	K1499			



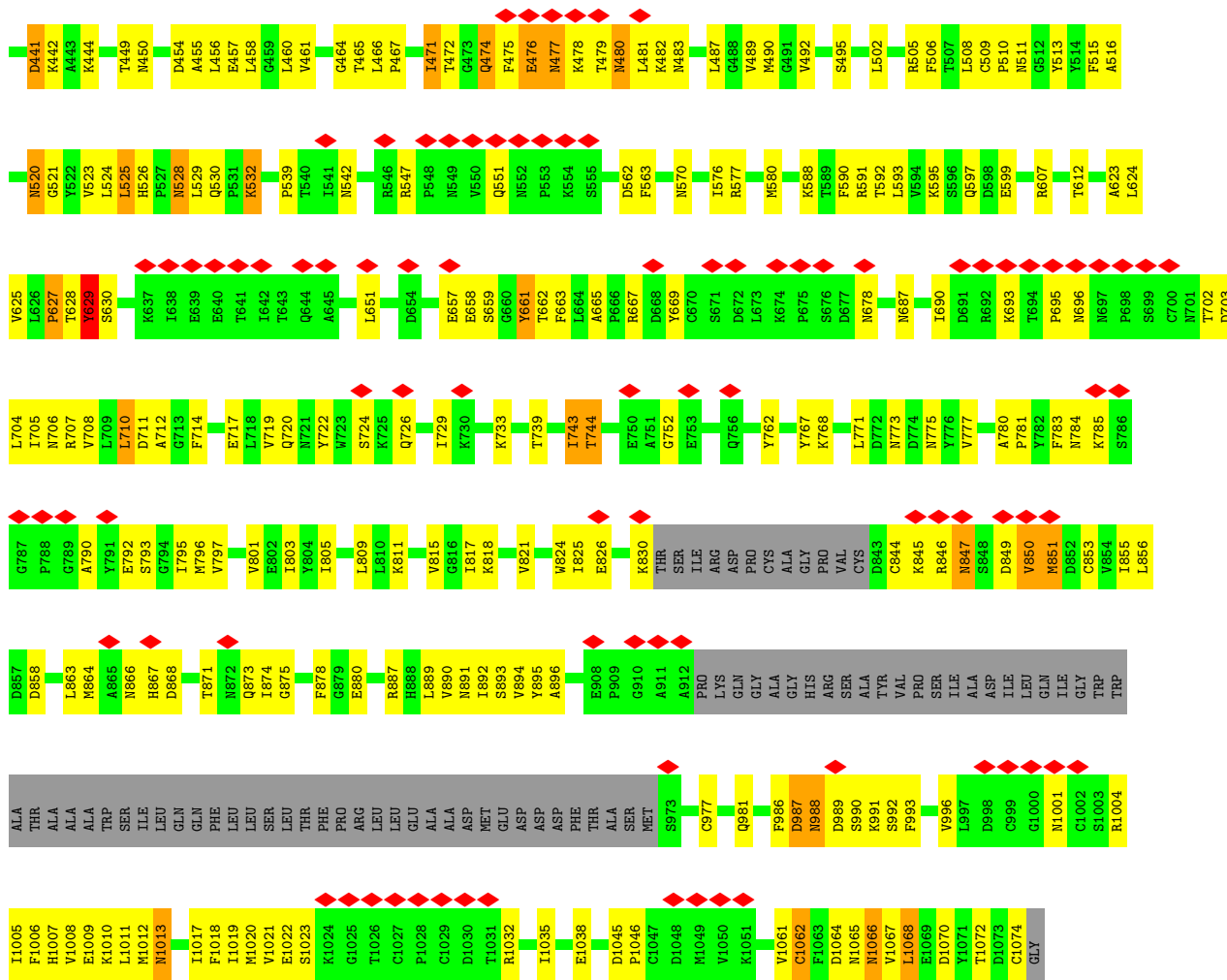
● Molecule 2: Voltage-dependent calcium channel gamma-1 subunit



● Molecule 3: Voltage-dependent L-type calcium channel subunit beta-1



● Molecule 4: Voltage-dependent L-type calcium channel subunit beta-1



• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose



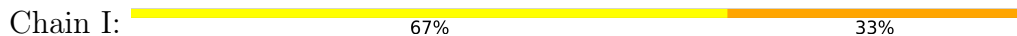
- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-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	433477	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	48	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.268	Depositor
Minimum map value	-0.142	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.025	Depositor
Map size (\AA)	349.12, 349.12, 349.12	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.091, 1.091, 1.091	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: 3PE, ETA, NAG, PC1, 9Z9, 4YH, CA, BMA

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	0.43	0/10463	0.62	0/14191
2	E	0.55	0/1358	0.69	0/1832
3	B	0.29	0/723	0.45	0/979
4	C	0.31	0/1394	0.49	0/1892
5	F	0.80	1/7974 (0.0%)	0.78	0/10816
All	All	0.59	1/21912 (0.0%)	0.67	0/29710

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	665	ALA	C-N	-6.89	1.21	1.34

There are no bond angle outliers.

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	A	10219	0	10305	935	0
2	E	1326	0	1345	124	0
3	B	710	0	633	6	0
4	C	1367	0	1343	96	0
5	F	7804	0	7608	539	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	28	0	25	8	0
6	G	28	0	25	1	0
6	J	28	0	25	0	0
6	K	28	0	25	8	0
7	H	39	0	34	4	0
7	I	39	0	34	1	0
8	L	42	0	37	11	0
9	A	14	0	13	3	0
9	F	98	0	91	15	0
10	A	3	0	0	0	0
11	A	266	0	341	49	0
12	A	93	0	140	13	0
13	A	30	0	0	6	0
14	A	66	0	76	12	0
15	F	4	0	0	2	0
All	All	22232	0	22100	1640	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 37.

The worst 5 of 1640 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:A:462:HIS:CE1	1:A:466:ILE:HD11	1.40	1.56
5:F:784:ASN:ND2	9:F:1120:NAG:C1	1.69	1.52
5:F:678:ASN:HD21	6:K:1:NAG:C1	1.19	1.52
5:F:326:ASN:ND2	9:F:1104:NAG:C1	1.72	1.51
1:A:136:THR:HG22	1:A:164:LEU:CD2	1.42	1.49

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	1260/1506 (84%)	1106 (88%)	117 (9%)	37 (3%)	4	7
2	E	159/222 (72%)	146 (92%)	11 (7%)	2 (1%)	12	24
3	B	98/450 (22%)	89 (91%)	9 (9%)	0	100	100
4	C	174/524 (33%)	164 (94%)	10 (6%)	0	100	100
5	F	968/1046 (92%)	876 (90%)	86 (9%)	6 (1%)	25	47
All	All	2659/3748 (71%)	2381 (90%)	233 (9%)	45 (2%)	13	18

5 of 45 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	36	LEU
1	A	76	GLU
1	A	110	PHE
1	A	129	ILE
1	A	237	VAL

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	1097/1327 (83%)	923 (84%)	174 (16%)	2	4
2	E	143/192 (74%)	133 (93%)	10 (7%)	15	30
3	B	58/391 (15%)	57 (98%)	1 (2%)	60	81
4	C	143/460 (31%)	141 (99%)	2 (1%)	67	85
5	F	868/924 (94%)	796 (92%)	72 (8%)	11	22
All	All	2309/3294 (70%)	2050 (89%)	259 (11%)	9	10

5 of 259 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	F	542	ASN
5	F	707	ARG
1	A	906	ARG

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Mol	Chain	Res	Type
1	A	899	LEU
5	F	793	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 50 such sidechains are listed below:

Mol	Chain	Res	Type
5	F	228	ASN
5	F	477	ASN
5	F	1066	ASN
5	F	299	ASN
5	F	372	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

17 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	NAG	D	1	6	14,14,15	0.28	0	17,19,21	1.02	1 (5%)
6	NAG	D	2	6	14,14,15	0.32	0	17,19,21	0.56	0
6	NAG	G	1	6,5	14,14,15	0.28	0	17,19,21	0.63	0
6	NAG	G	2	6	14,14,15	0.28	0	17,19,21	0.58	0
7	NAG	H	1	5,7	14,14,15	0.73	1 (7%)	17,19,21	0.70	0
7	NAG	H	2	7	14,14,15	0.37	0	17,19,21	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	BMA	H	3	7	11,11,12	0.74	0	15,15,17	0.97	1 (6%)
7	NAG	I	1	5,7	14,14,15	0.84	1 (7%)	17,19,21	0.82	0
7	NAG	I	2	7	14,14,15	1.63	1 (7%)	17,19,21	0.91	1 (5%)
7	BMA	I	3	7	11,11,12	0.92	0	15,15,17	1.04	1 (6%)
6	NAG	J	1	6,5	14,14,15	0.56	0	17,19,21	0.62	0
6	NAG	J	2	6	14,14,15	0.33	0	17,19,21	0.39	0
6	NAG	K	1	6	14,14,15	0.28	0	17,19,21	0.65	0
6	NAG	K	2	6	14,14,15	0.29	0	17,19,21	0.57	0
8	NAG	L	1	5,8	14,14,15	0.29	0	17,19,21	0.65	0
8	NAG	L	2	8	14,14,15	0.31	0	17,19,21	0.69	0
8	NAG	L	3	8	14,14,15	0.29	0	17,19,21	1.34	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
6	NAG	D	1	6	-	5/6/23/26	0/1/1/1
6	NAG	D	2	6	-	2/6/23/26	0/1/1/1
6	NAG	G	1	6,5	-	0/6/23/26	0/1/1/1
6	NAG	G	2	6	-	3/6/23/26	0/1/1/1
7	NAG	H	1	5,7	-	0/6/23/26	0/1/1/1
7	NAG	H	2	7	-	2/6/23/26	0/1/1/1
7	BMA	H	3	7	-	0/2/19/22	0/1/1/1
7	NAG	I	1	5,7	-	2/6/23/26	0/1/1/1
7	NAG	I	2	7	-	2/6/23/26	0/1/1/1
7	BMA	I	3	7	-	2/2/19/22	0/1/1/1
6	NAG	J	1	6,5	-	2/6/23/26	0/1/1/1
6	NAG	J	2	6	-	0/6/23/26	0/1/1/1
6	NAG	K	1	6	-	4/6/23/26	0/1/1/1
6	NAG	K	2	6	-	6/6/23/26	0/1/1/1
8	NAG	L	1	5,8	-	2/6/23/26	0/1/1/1
8	NAG	L	2	8	-	5/6/23/26	0/1/1/1
8	NAG	L	3	8	-	4/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	2	NAG	O5-C1	-5.91	1.34	1.43
7	I	1	NAG	O5-C1	-2.67	1.39	1.43
7	H	1	NAG	O5-C1	-2.36	1.39	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	L	3	NAG	C1-O5-C5	4.38	118.13	112.19
6	D	1	NAG	C3-C4-C5	2.52	114.73	110.24
7	H	3	BMA	C1-O5-C5	2.41	115.46	112.19
7	I	2	NAG	C4-C3-C2	2.24	114.30	111.02
7	I	3	BMA	O5-C1-C2	-2.02	107.66	110.77

There are no chirality outliers.

5 of 41 torsion outliers are listed below:

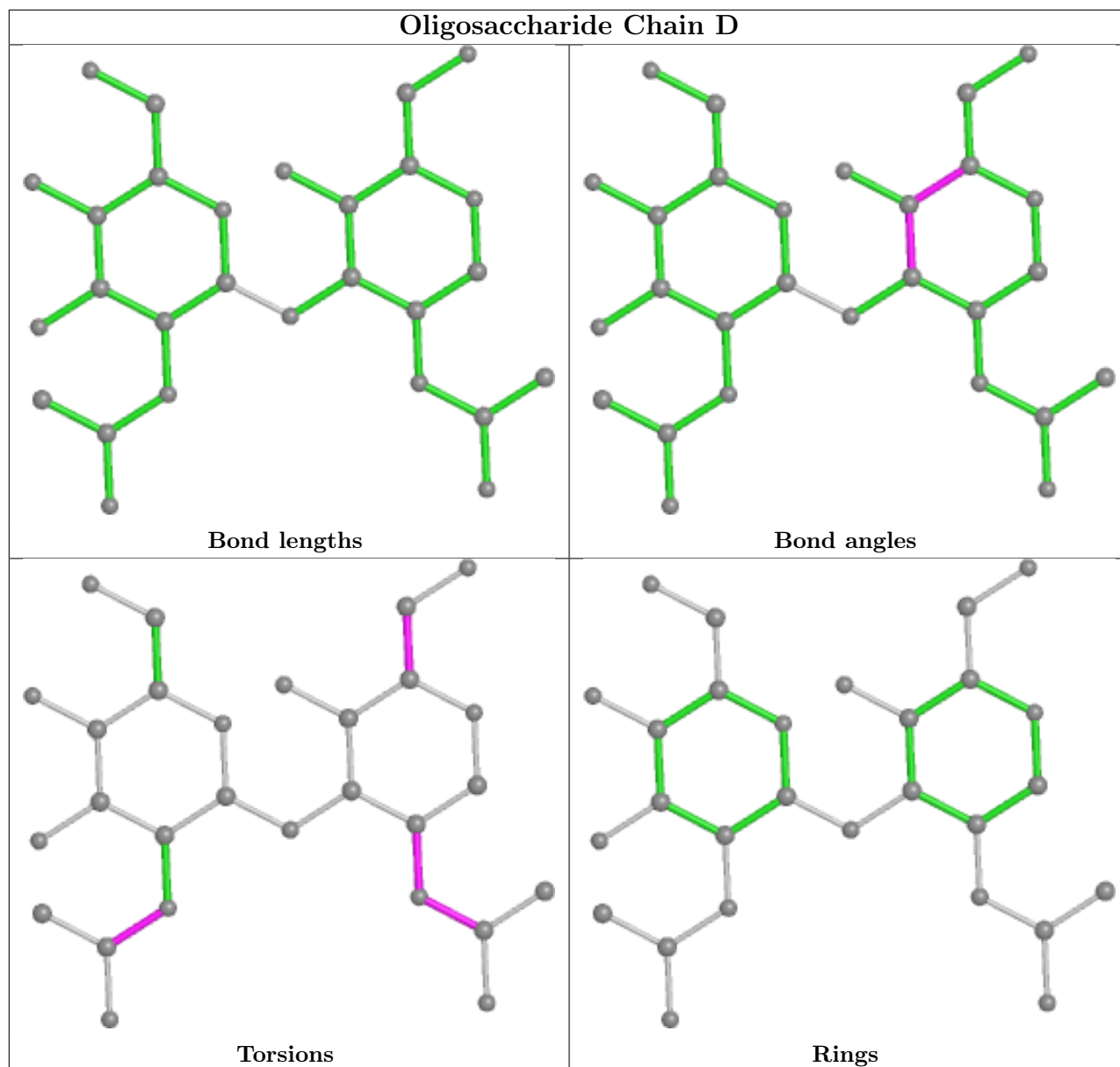
Mol	Chain	Res	Type	Atoms
6	D	1	NAG	C8-C7-N2-C2
6	D	1	NAG	O7-C7-N2-C2
6	K	1	NAG	C8-C7-N2-C2
6	K	1	NAG	O7-C7-N2-C2
8	L	1	NAG	C8-C7-N2-C2

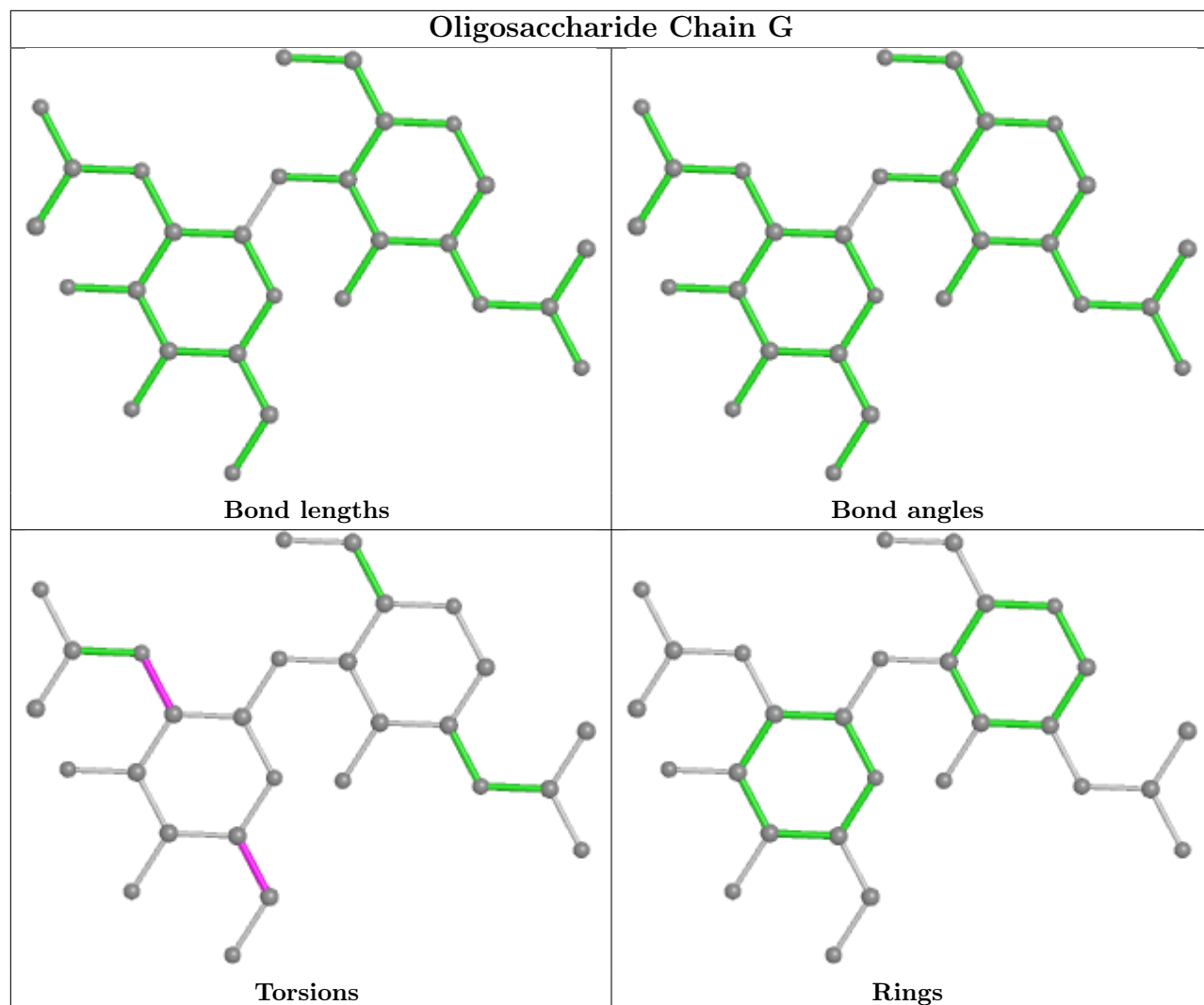
There are no ring outliers.

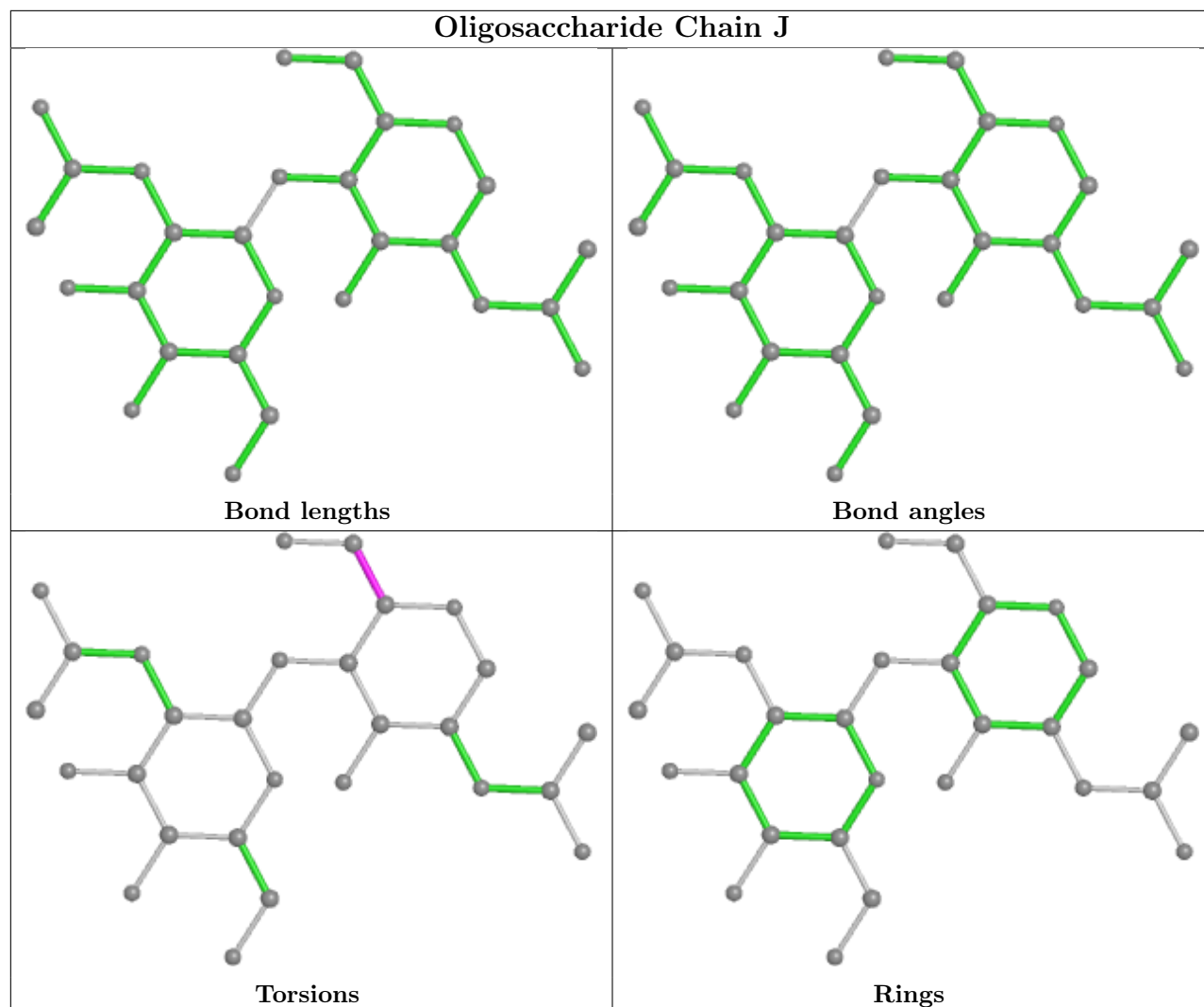
11 monomers are involved in 33 short contacts:

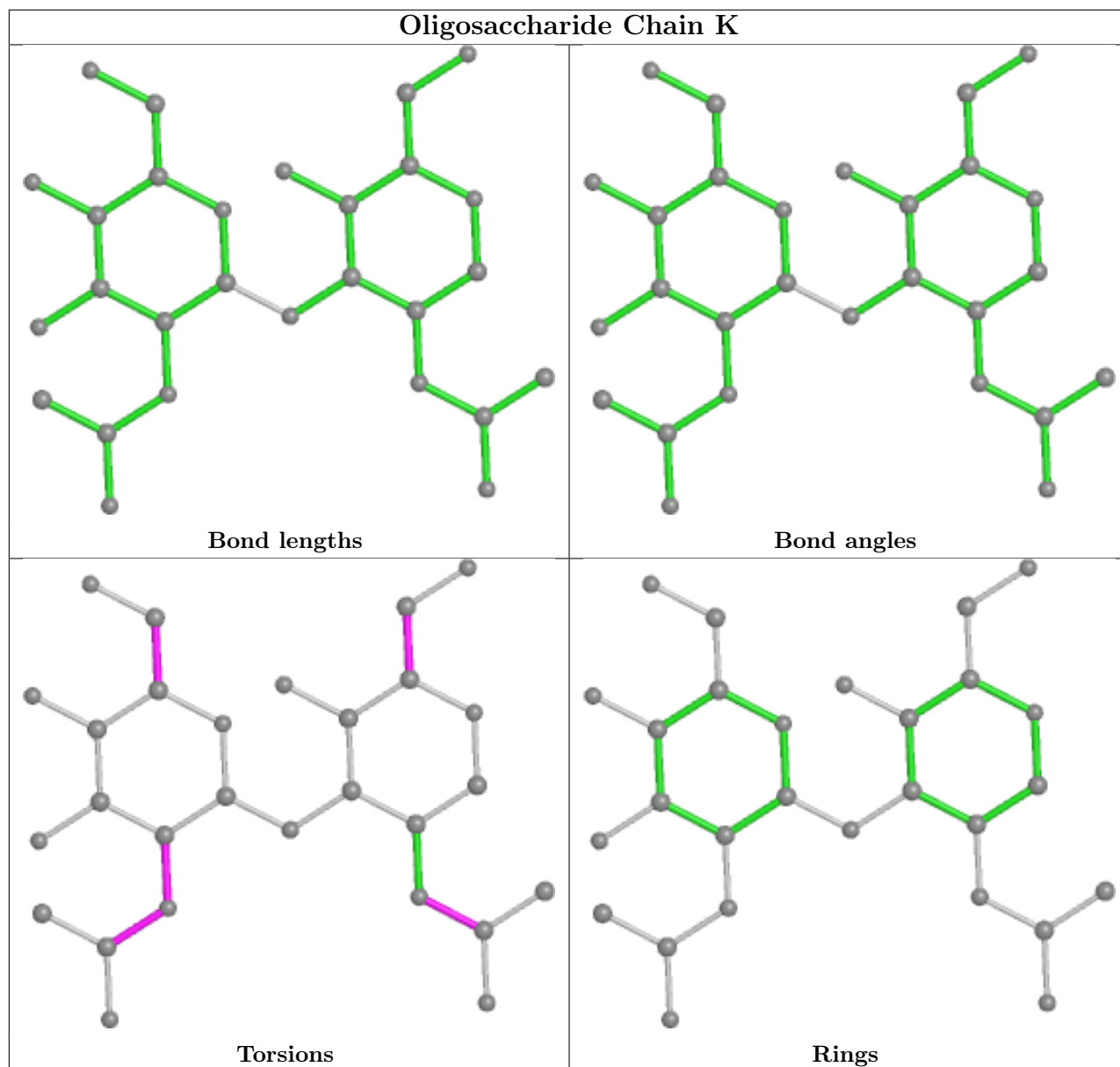
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	K	2	NAG	5	0
7	H	1	NAG	4	0
7	I	1	NAG	1	0
6	K	1	NAG	5	0
6	D	1	NAG	8	0
8	L	2	NAG	2	0
6	D	2	NAG	4	0
8	L	3	NAG	4	0
6	G	1	NAG	1	0
6	G	2	NAG	1	0
8	L	1	NAG	6	0

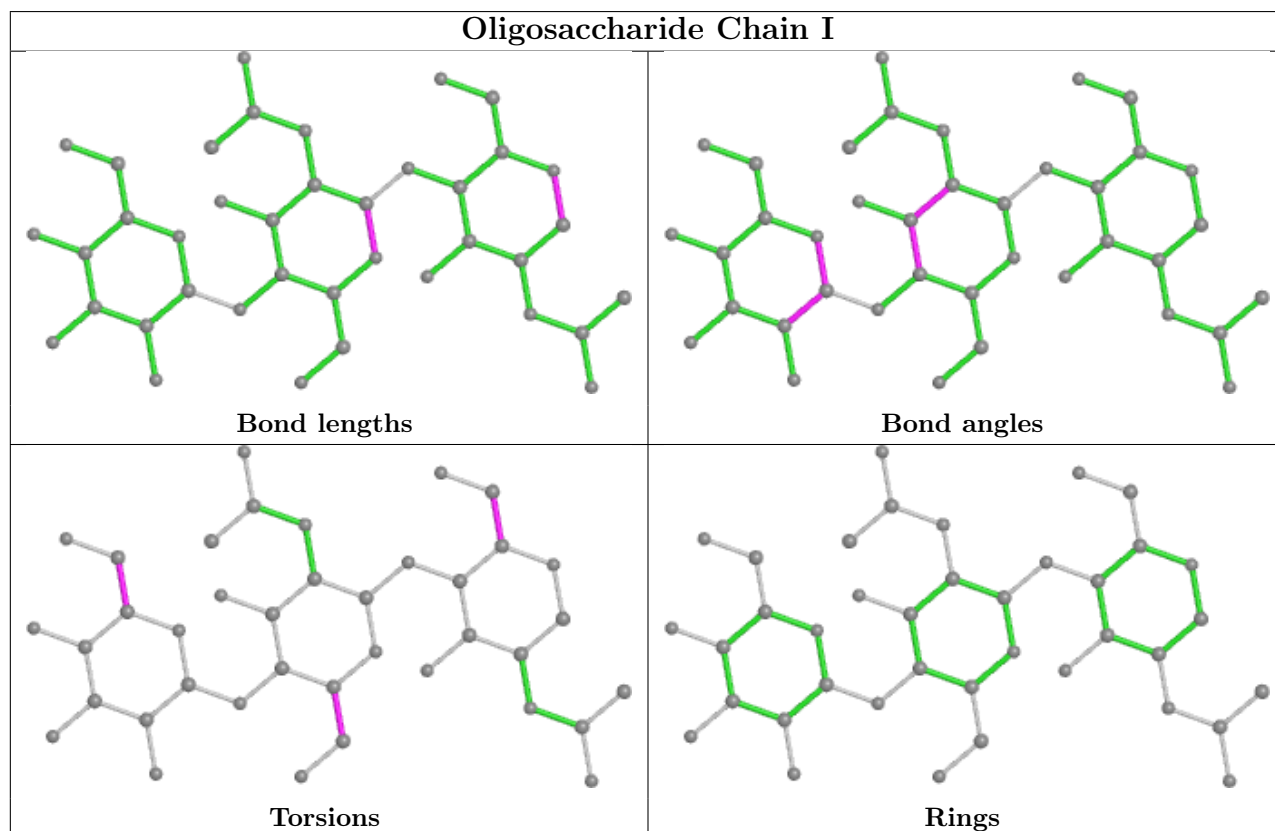
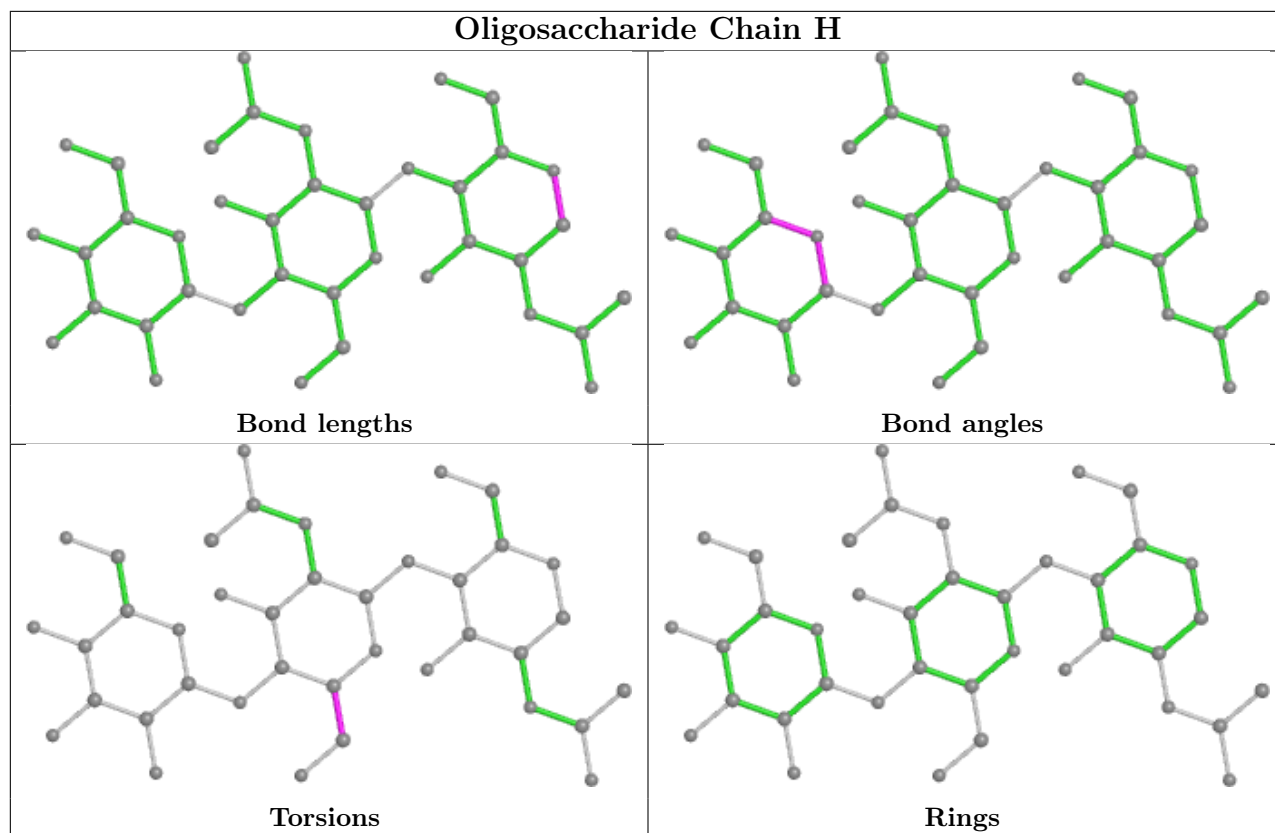
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

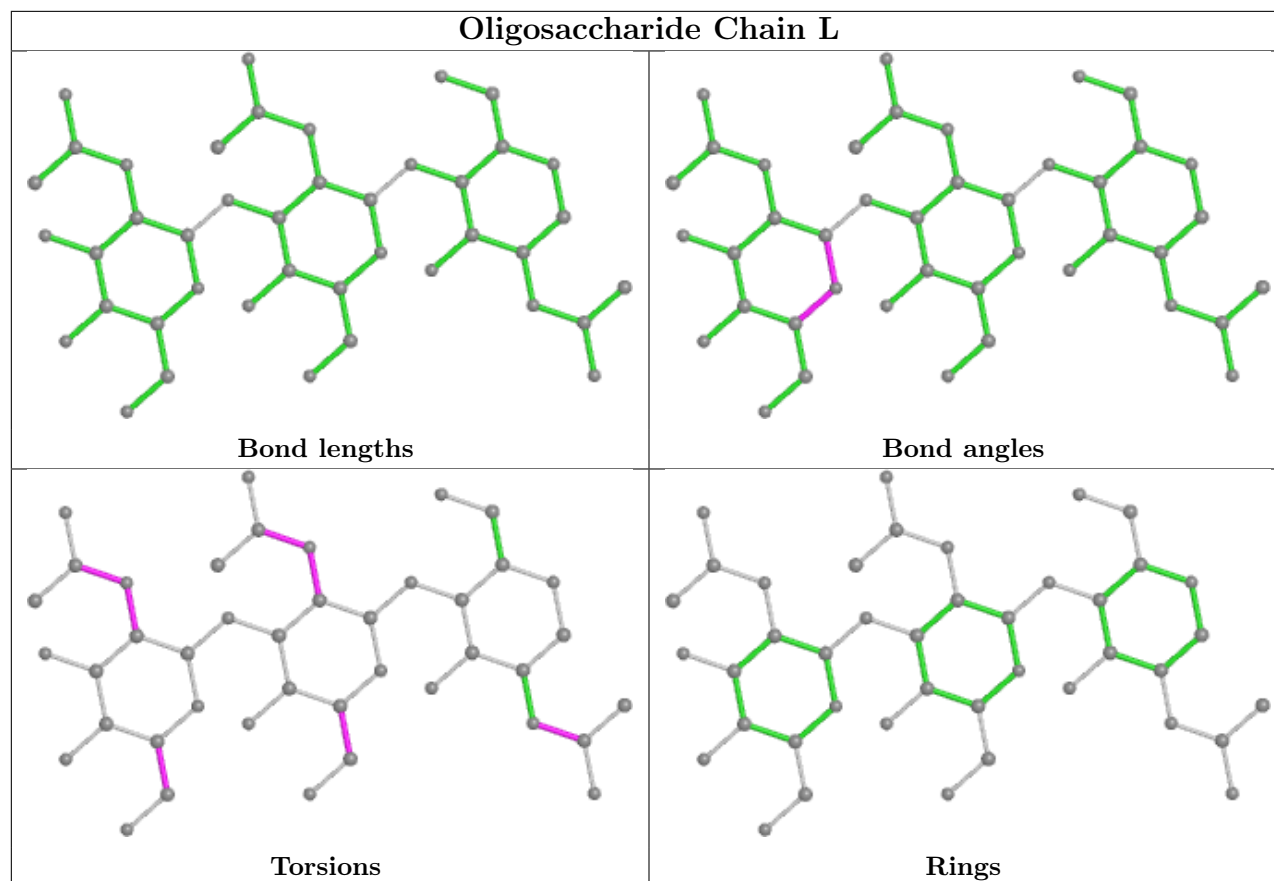












5.6 Ligand geometry [i](#)

Of 25 ligands modelled in this entry, 3 are monoatomic - leaving 22 for Mogul analysis.

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
11	3PE	A	1907	-	35,35,50	1.10	2 (5%)	38,40,55	1.18	4 (10%)
11	3PE	A	1913	-	38,38,50	1.11	2 (5%)	42,43,55	1.08	3 (7%)
9	NAG	F	1120	-	14,14,15	0.30	0	17,19,21	0.62	0
9	NAG	F	1121	-	14,14,15	0.45	0	17,19,21	0.52	0
11	3PE	A	1905	-	18,18,50	1.07	1 (5%)	20,22,55	1.07	2 (10%)
14	4YH	A	1915[A]	-	32,34,34	3.66	14 (43%)	36,46,46	1.88	11 (30%)
9	NAG	F	1114	5	14,14,15	0.23	0	17,19,21	0.65	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	NAG	F	1122	-	14,14,15	0.29	0	17,19,21	0.62	0
9	NAG	A	1901	-	14,14,15	0.70	1 (7%)	17,19,21	0.81	0
11	3PE	A	1906	-	41,41,50	1.04	2 (4%)	44,46,55	1.12	4 (9%)
9	NAG	F	1107	5	14,14,15	0.29	0	17,19,21	0.64	0
9	NAG	F	1104	-	14,14,15	0.30	0	17,19,21	0.71	0
15	ETA	F	1101	-	3,3,3	0.41	0	2,2,2	0.52	0
12	PC1	A	1910	-	53,53,53	0.89	2 (3%)	59,61,61	1.03	5 (8%)
14	4YH	A	1916[B]	-	32,34,34	0.97	3 (9%)	36,46,46	1.66	11 (30%)
11	3PE	A	1912	-	41,41,50	1.00	2 (4%)	44,46,55	1.18	3 (6%)
13	9Z9	A	1914	-	35,35,44	0.64	1 (2%)	58,58,68	1.09	4 (6%)
11	3PE	A	1911	-	34,34,50	1.11	2 (5%)	37,39,55	1.21	4 (10%)
9	NAG	F	1115	5	14,14,15	0.81	1 (7%)	17,19,21	1.00	1 (5%)
12	PC1	A	1909	-	38,38,53	1.06	2 (5%)	44,46,61	1.06	2 (4%)
11	3PE	A	1904	-	32,32,50	1.14	2 (6%)	35,37,55	1.25	2 (5%)
11	3PE	A	1908	-	19,19,50	1.03	1 (5%)	21,23,55	1.19	2 (9%)

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
11	3PE	A	1907	-	-	10/39/39/54	-
11	3PE	A	1913	-	-	15/40/40/54	-
9	NAG	F	1120	-	-	2/6/23/26	0/1/1/1
9	NAG	F	1121	-	-	0/6/23/26	0/1/1/1
11	3PE	A	1905	-	-	7/20/20/54	-
14	4YH	A	1915[A]	-	-	14/32/35/35	0/2/2/2
9	NAG	F	1114	5	-	0/6/23/26	0/1/1/1
9	NAG	F	1122	-	-	2/6/23/26	0/1/1/1
9	NAG	A	1901	-	-	2/6/23/26	0/1/1/1
11	3PE	A	1906	-	-	23/45/45/54	-
9	NAG	F	1107	5	-	2/6/23/26	0/1/1/1
9	NAG	F	1104	-	-	3/6/23/26	0/1/1/1
15	ETA	F	1101	-	-	1/1/1/1	-
12	PC1	A	1910	-	-	31/57/57/57	-
14	4YH	A	1916[B]	-	-	14/32/35/35	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	3PE	A	1912	-	-	20/45/45/54	-
13	9Z9	A	1914	-	-	-	0/6/6/6
11	3PE	A	1911	-	-	19/38/38/54	-
9	NAG	F	1115	5	-	0/6/23/26	0/1/1/1
12	PC1	A	1909	-	-	11/42/42/57	-
11	3PE	A	1904	-	-	20/36/36/54	-
11	3PE	A	1908	-	-	7/22/22/54	-

The worst 5 of 38 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	1915[A]	4YH	C5-C2	8.32	1.53	1.39
14	A	1915[A]	4YH	C11-C13	7.81	1.53	1.38
14	A	1915[A]	4YH	C14-C18	7.74	1.52	1.38
14	A	1915[A]	4YH	C12-C17	7.60	1.52	1.39
14	A	1915[A]	4YH	C9-C6	5.66	1.52	1.40

The worst 5 of 59 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	1912	3PE	O21-C21-C22	4.95	122.18	111.50
14	A	1915[A]	4YH	C21-C16-N8	-4.83	104.86	112.56
11	A	1904	3PE	O21-C21-C22	4.63	121.49	111.50
13	A	1914	9Z9	O80-C73-C76	4.63	115.07	110.77
11	A	1906	3PE	O21-C21-C22	4.21	120.58	111.50

There are no chirality outliers.

5 of 203 torsion outliers are listed below:

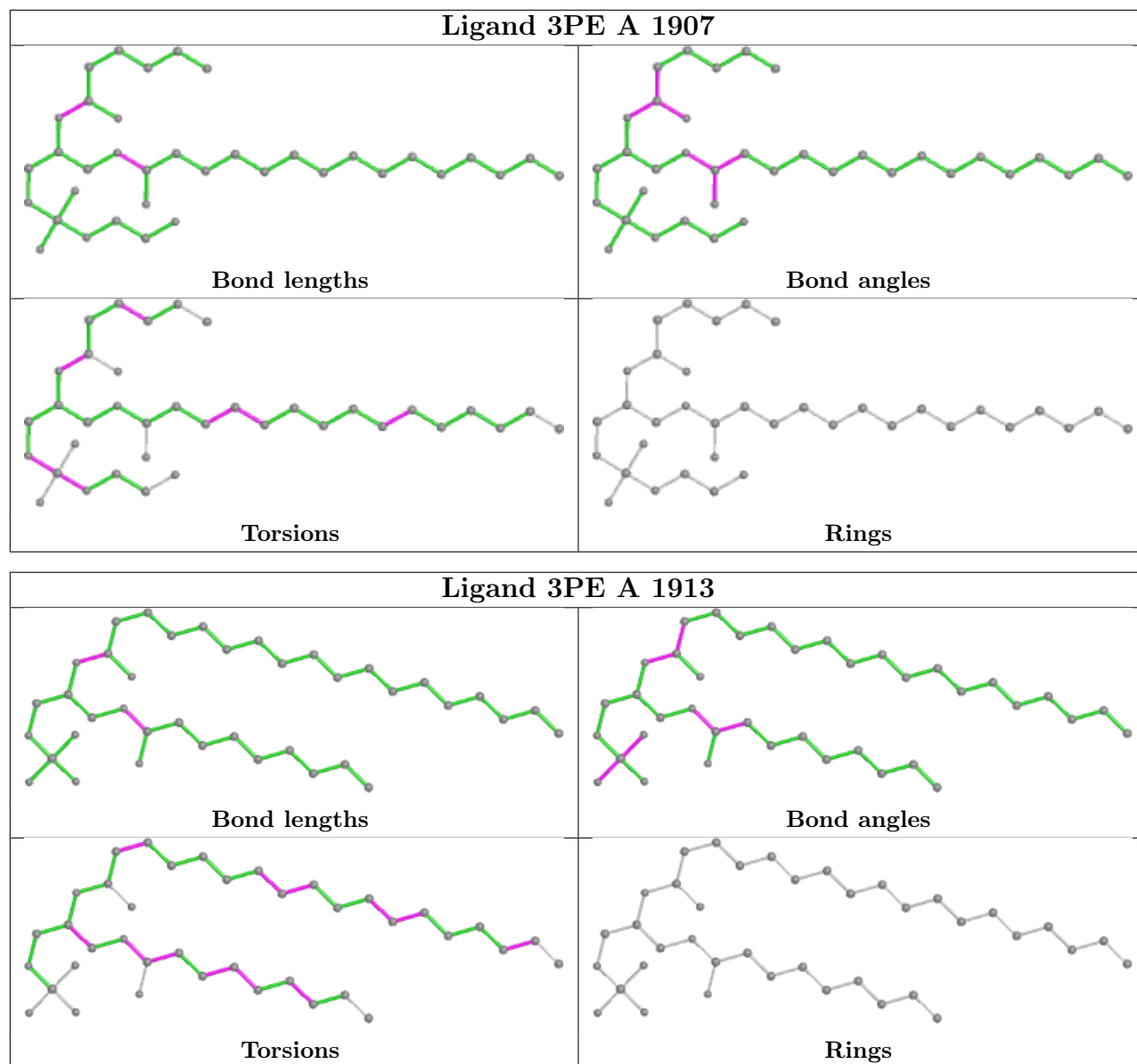
Mol	Chain	Res	Type	Atoms
9	F	1104	NAG	C8-C7-N2-C2
9	F	1104	NAG	O7-C7-N2-C2
11	A	1904	3PE	C1-O11-P-O12
11	A	1904	3PE	C1-O11-P-O13
11	A	1904	3PE	C1-O11-P-O14

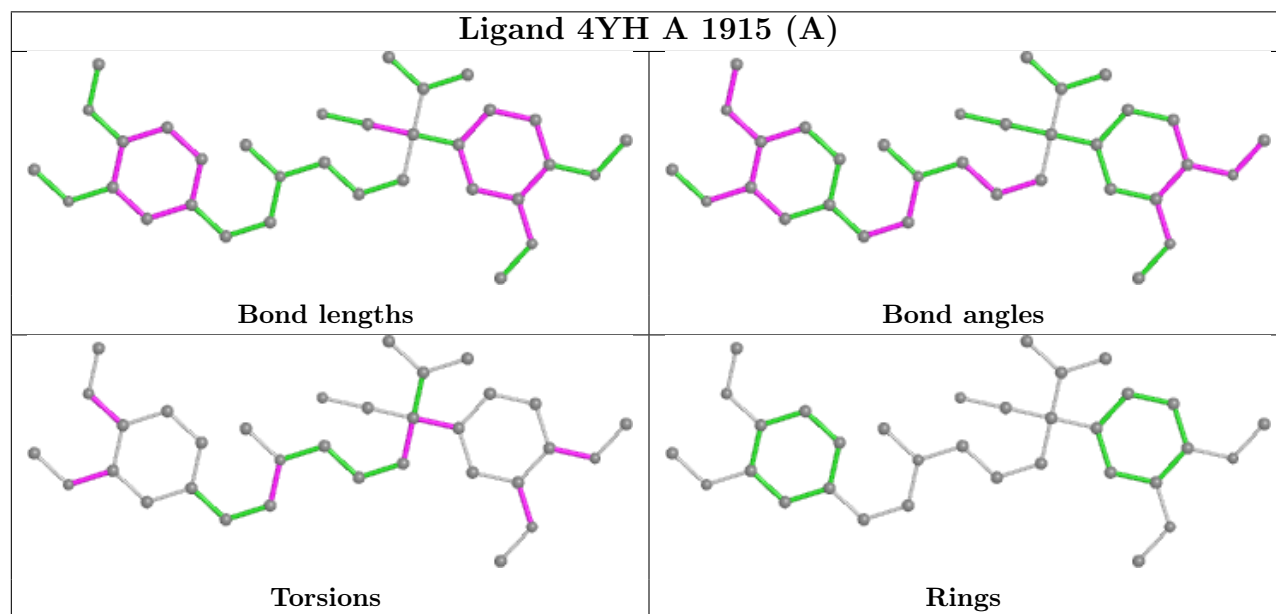
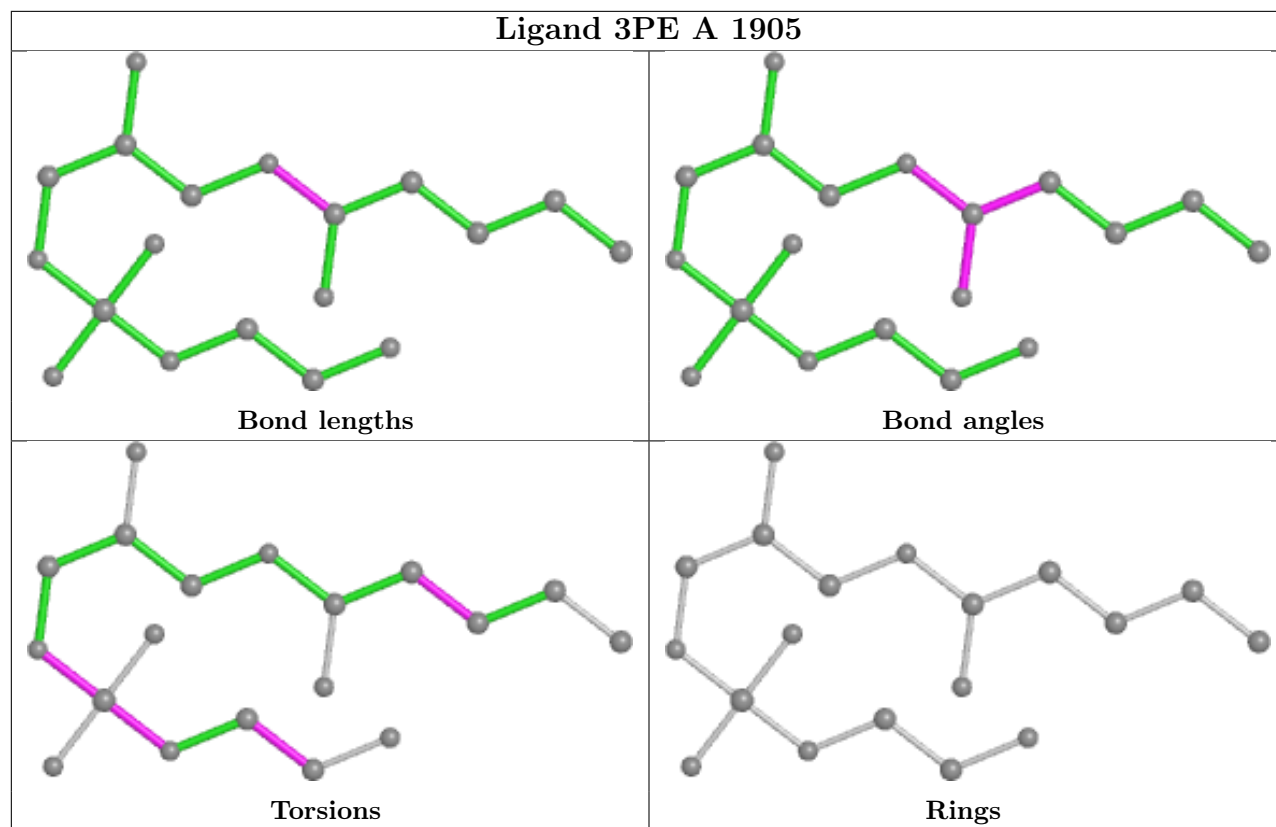
There are no ring outliers.

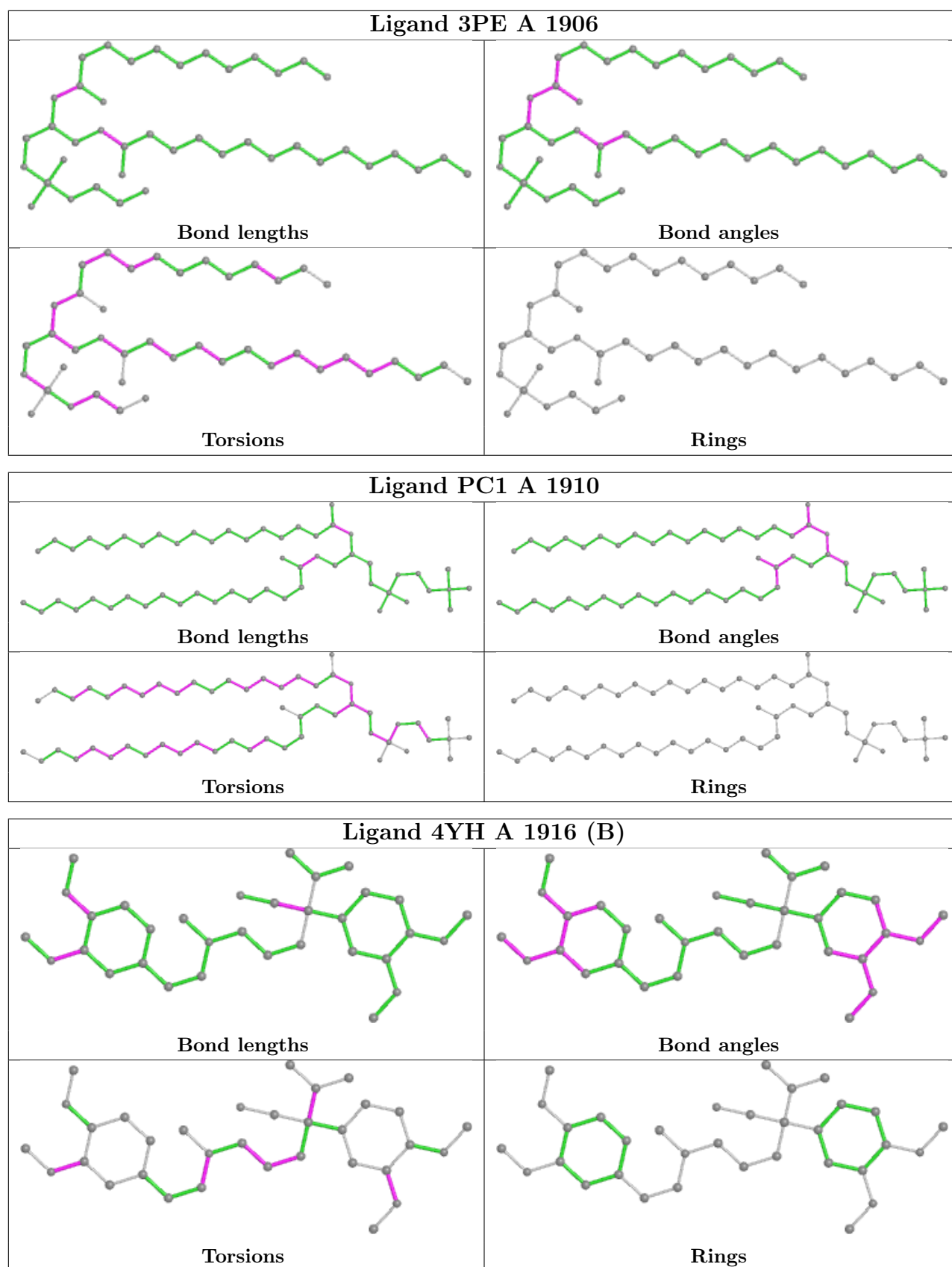
21 monomers are involved in 100 short contacts:

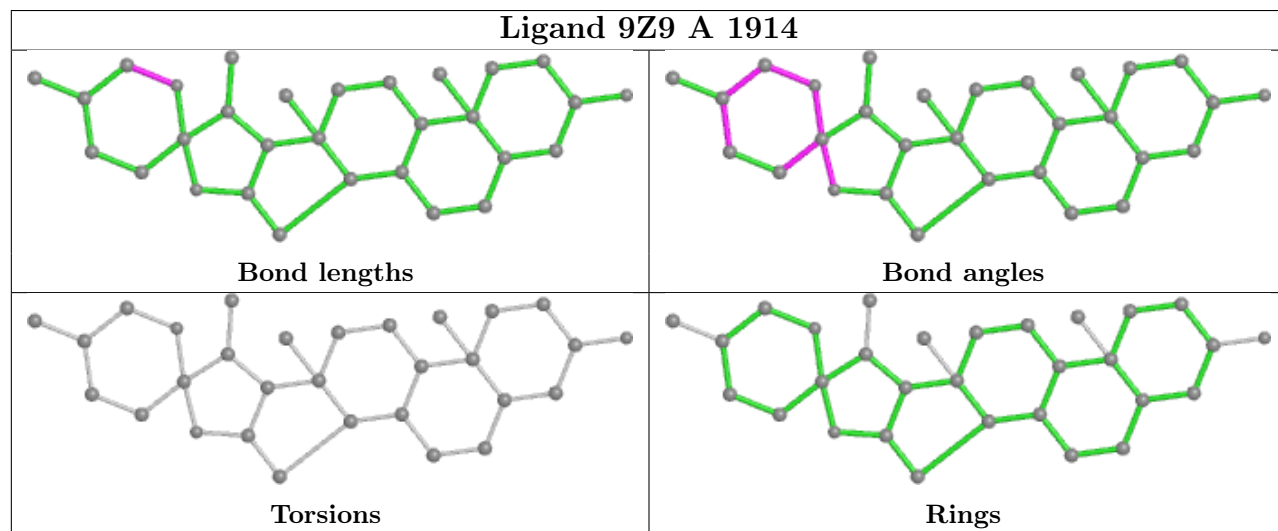
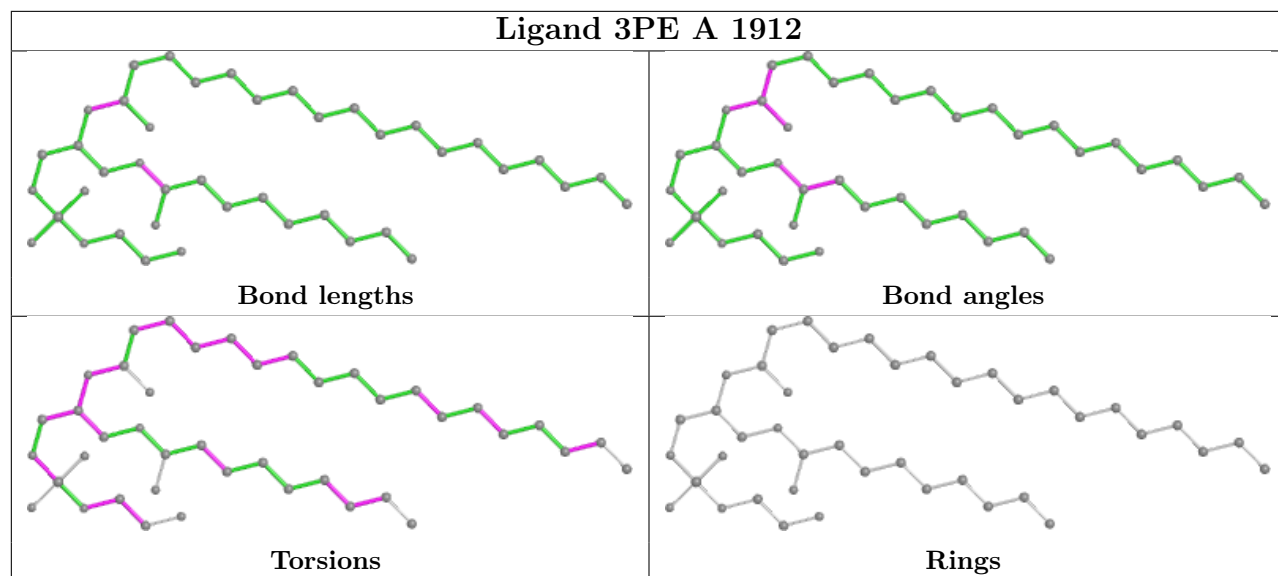
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	1907	3PE	7	0
11	A	1913	3PE	8	0
9	F	1120	NAG	2	0
9	F	1121	NAG	3	0
11	A	1905	3PE	2	0
14	A	1915[A]	4YH	5	0
9	F	1122	NAG	4	0
9	A	1901	NAG	3	0
11	A	1906	3PE	4	0
9	F	1107	NAG	1	0
9	F	1104	NAG	3	0
15	F	1101	ETA	2	0
12	A	1910	PC1	5	0
14	A	1916[B]	4YH	7	0
11	A	1912	3PE	14	0
13	A	1914	9Z9	6	0
11	A	1911	3PE	5	0
9	F	1115	NAG	2	0
12	A	1909	PC1	8	0
11	A	1904	3PE	3	0
11	A	1908	3PE	9	0

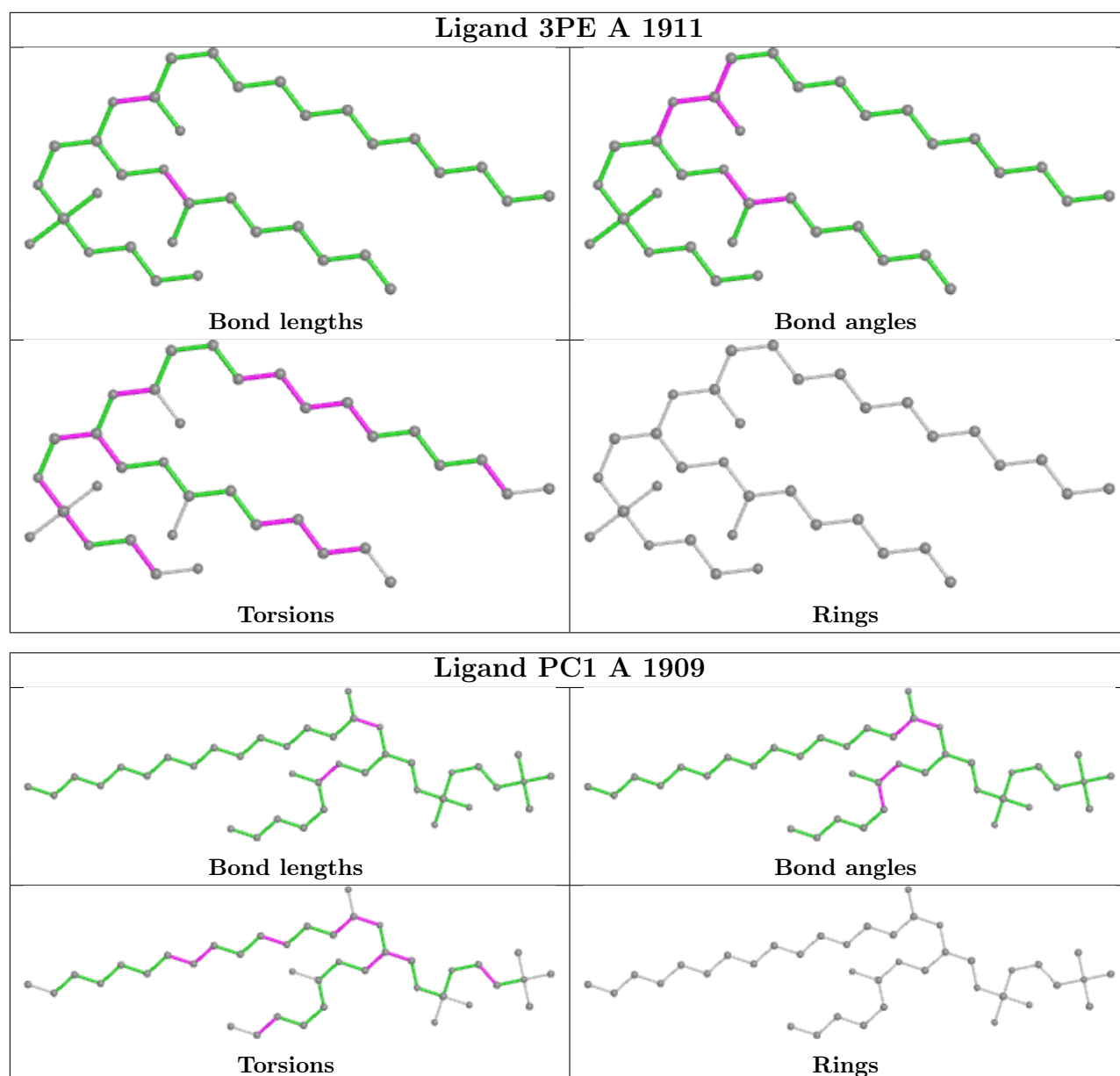
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

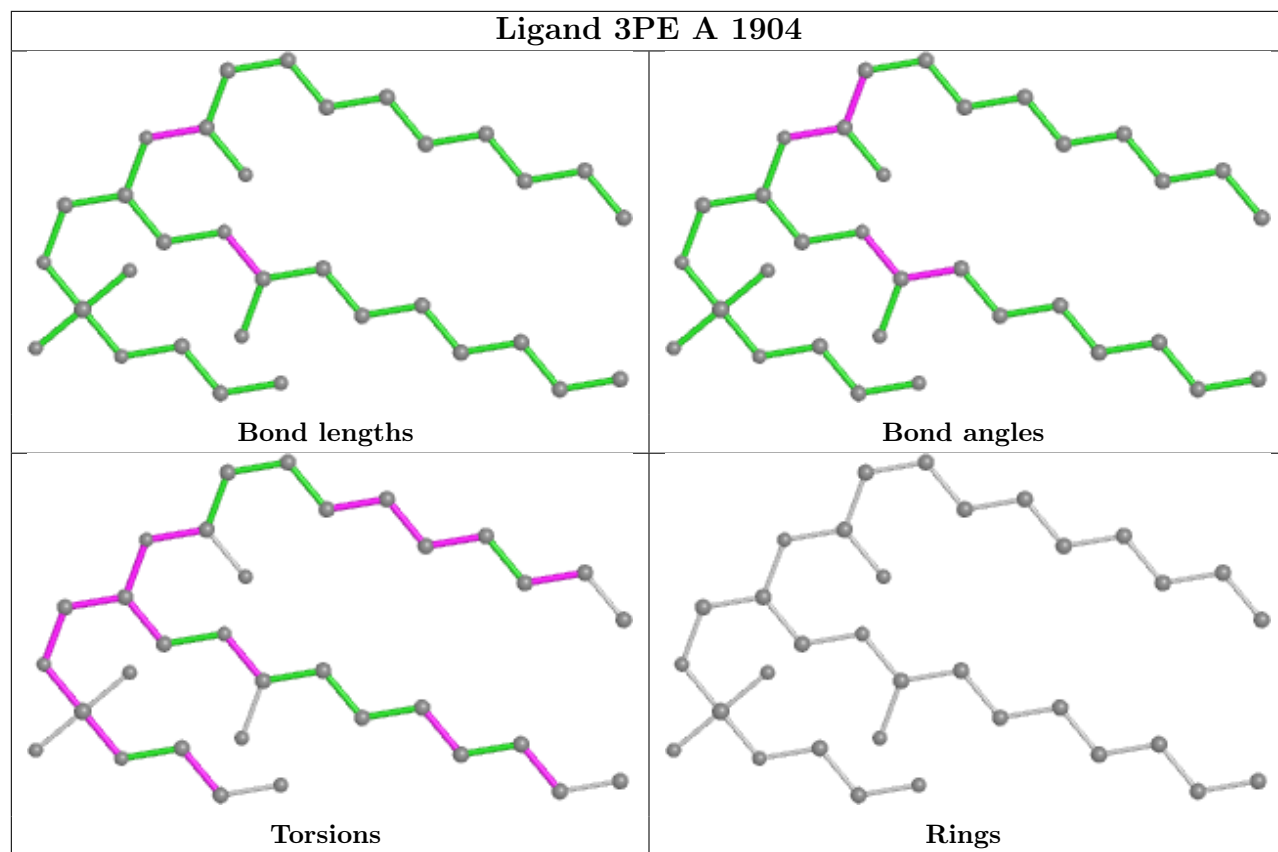


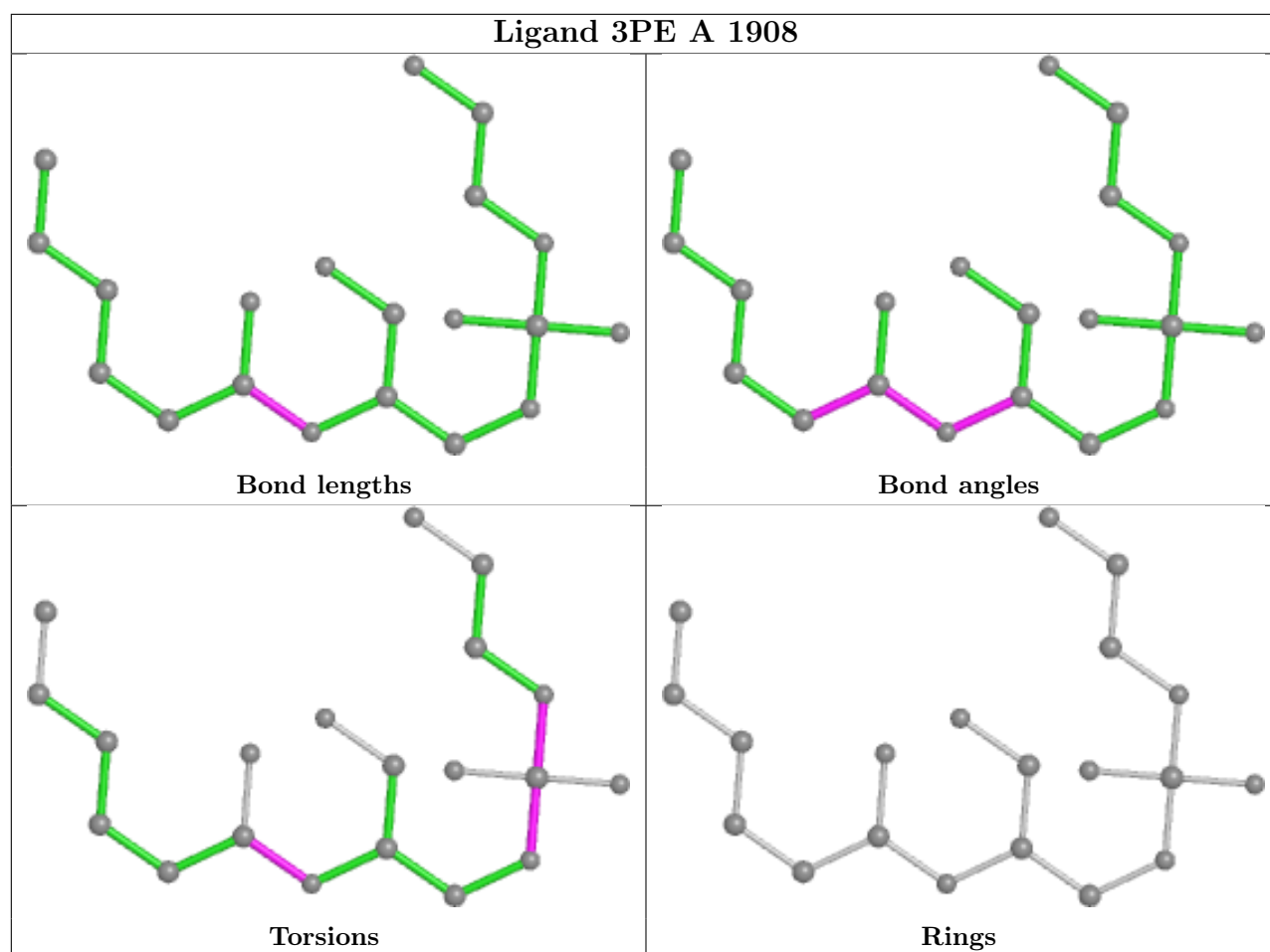












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

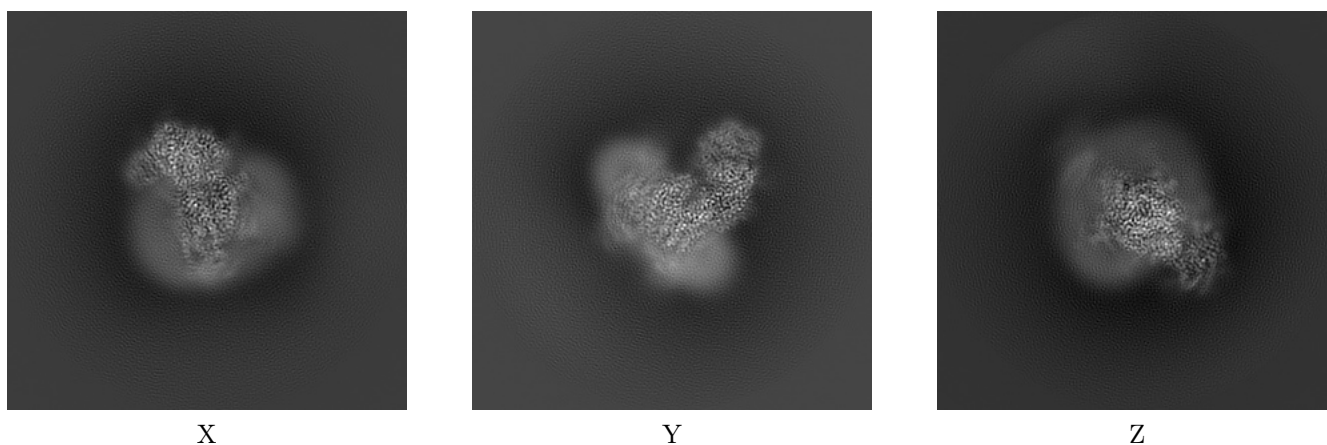
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9868. 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](#)

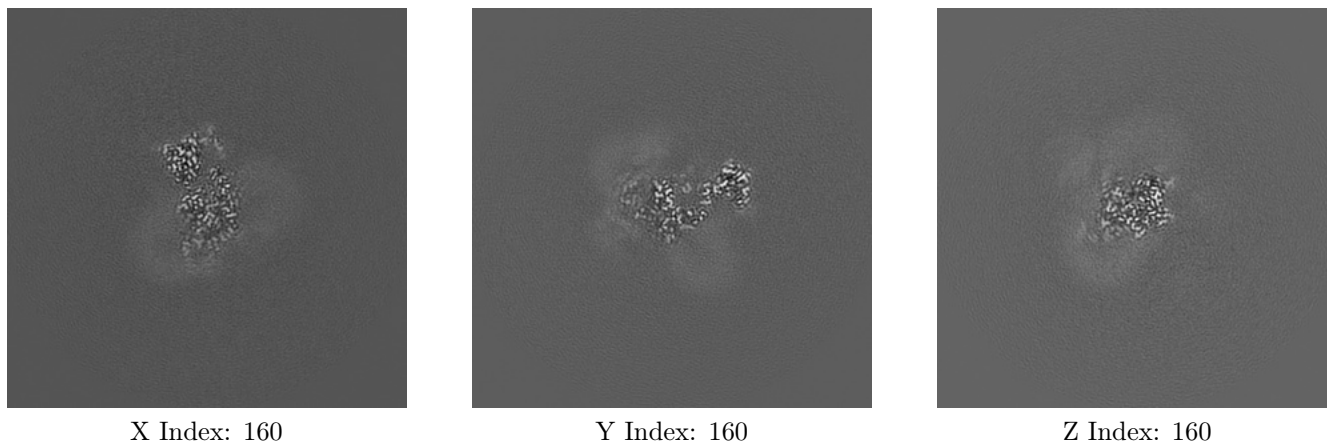
6.1.1 Primary map



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

6.2 Central slices [i](#)

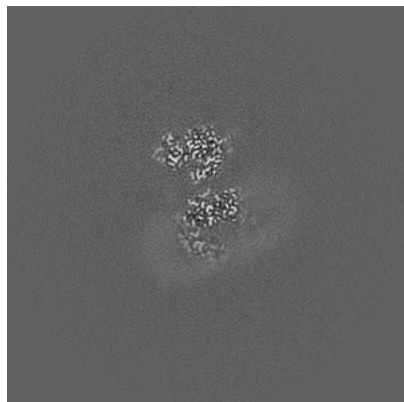
6.2.1 Primary map



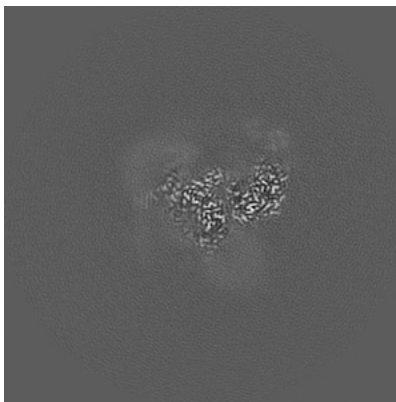
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

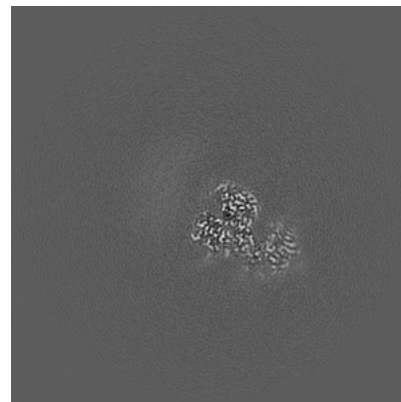
6.3.1 Primary map



X Index: 173



Y Index: 150

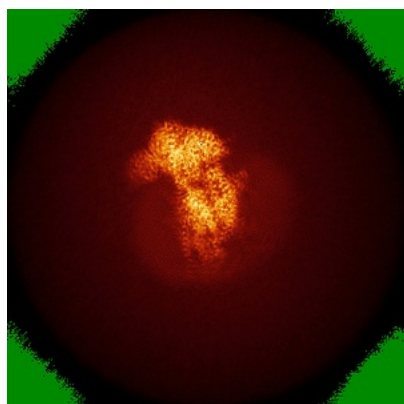


Z Index: 205

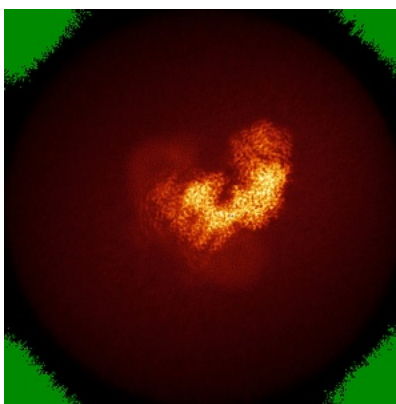
The images above show the largest variance slices of the map in three orthogonal directions.

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

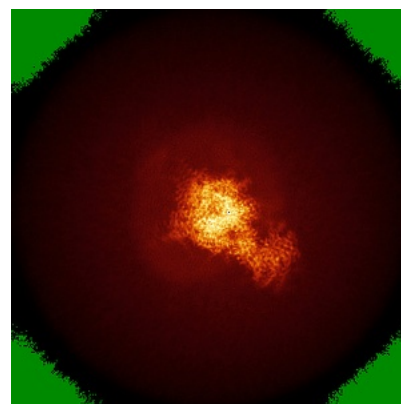
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

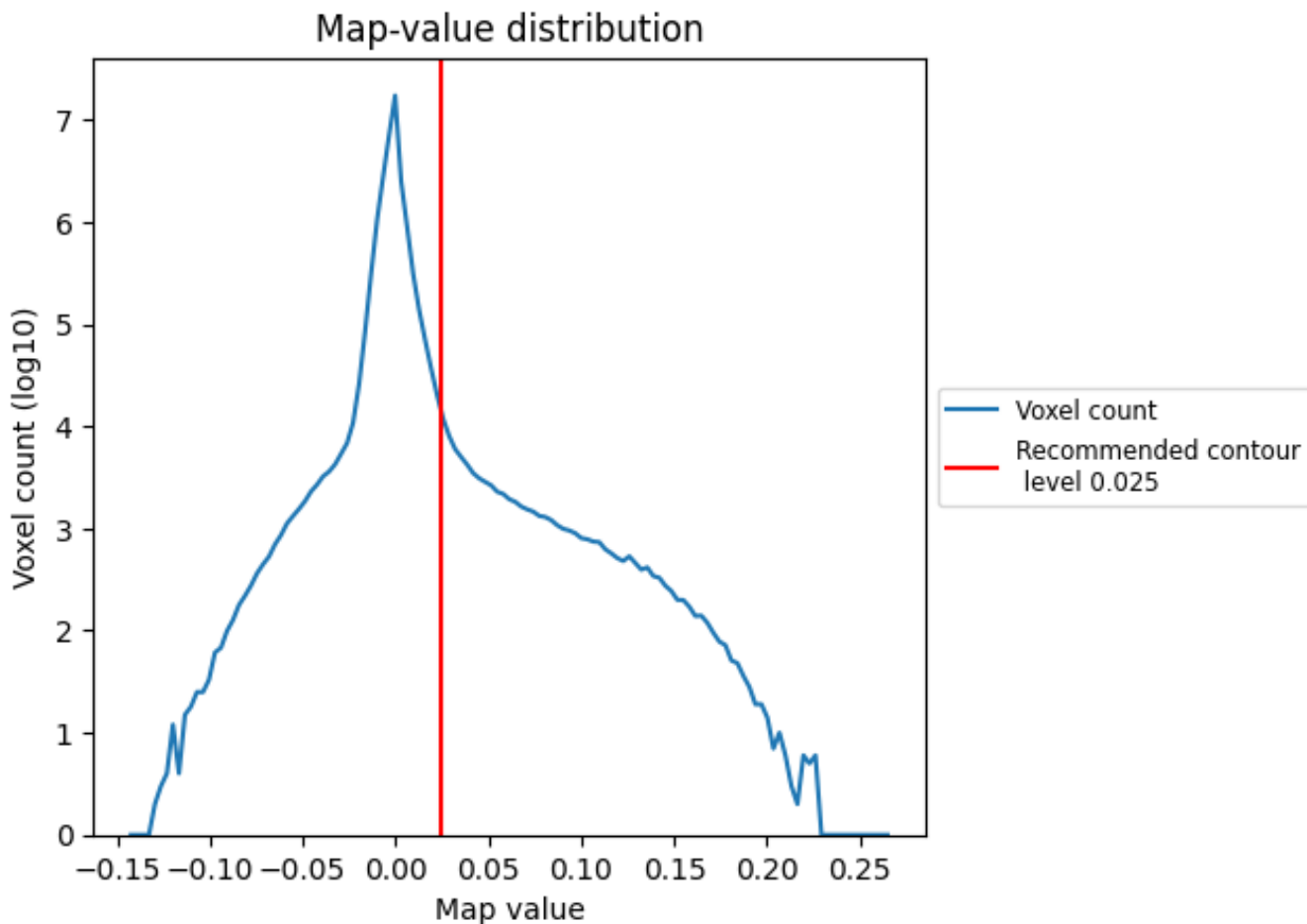
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

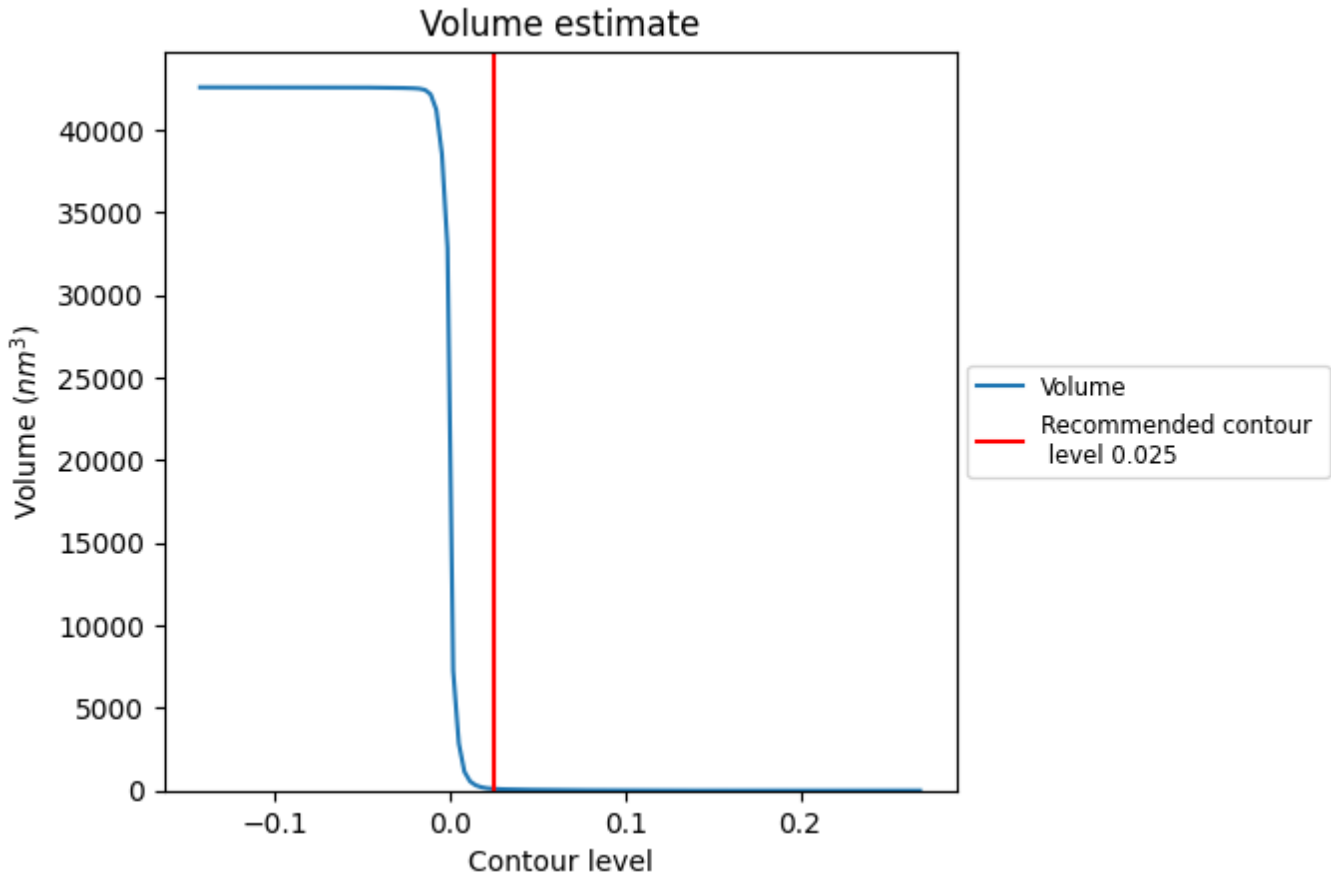
This section contains the results of statistical analysis of the map.

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.

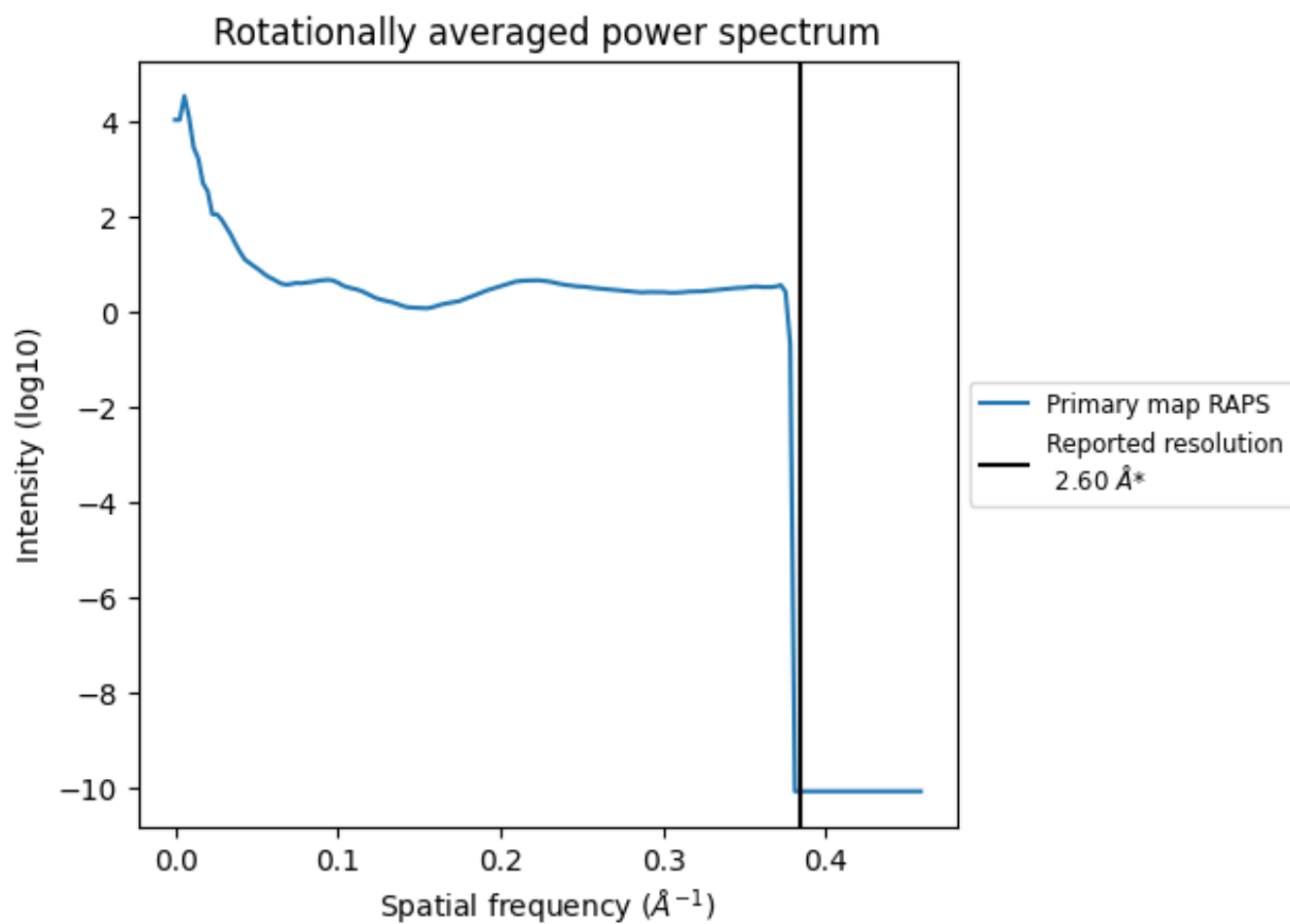
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 106 nm^3 ; this corresponds to an approximate mass of 96 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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.385 Å⁻¹

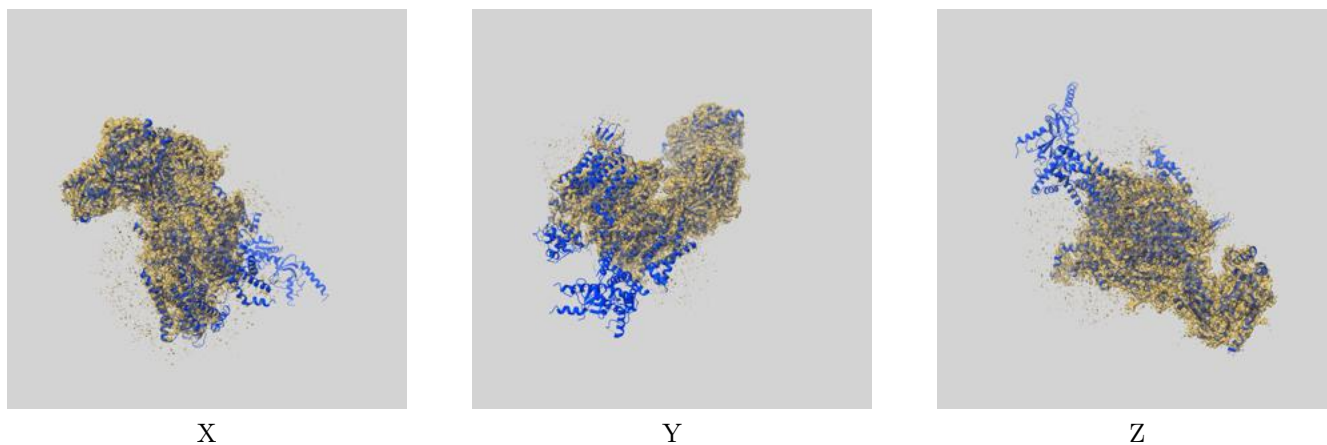
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

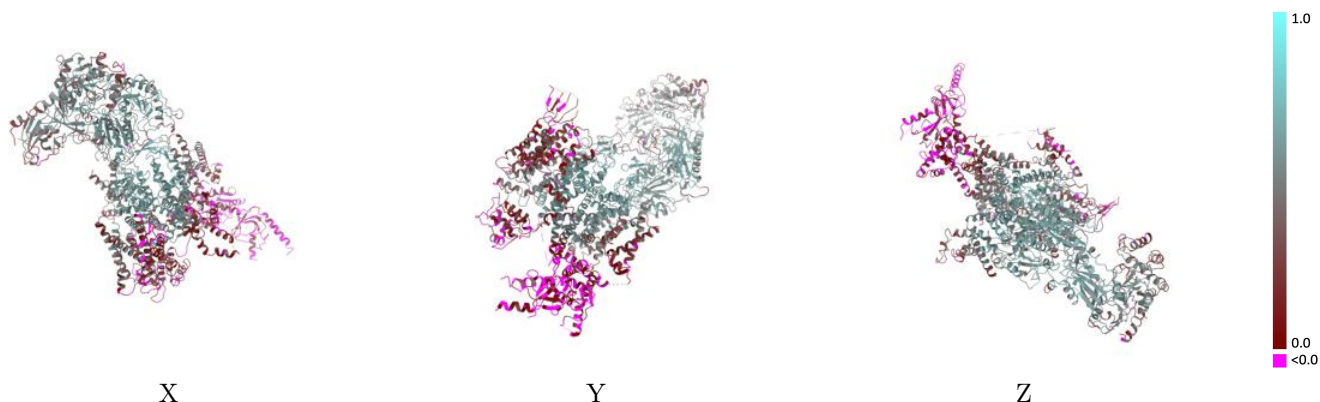
This section contains information regarding the fit between EMDB map EMD-9868 and PDB model 6JPA. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



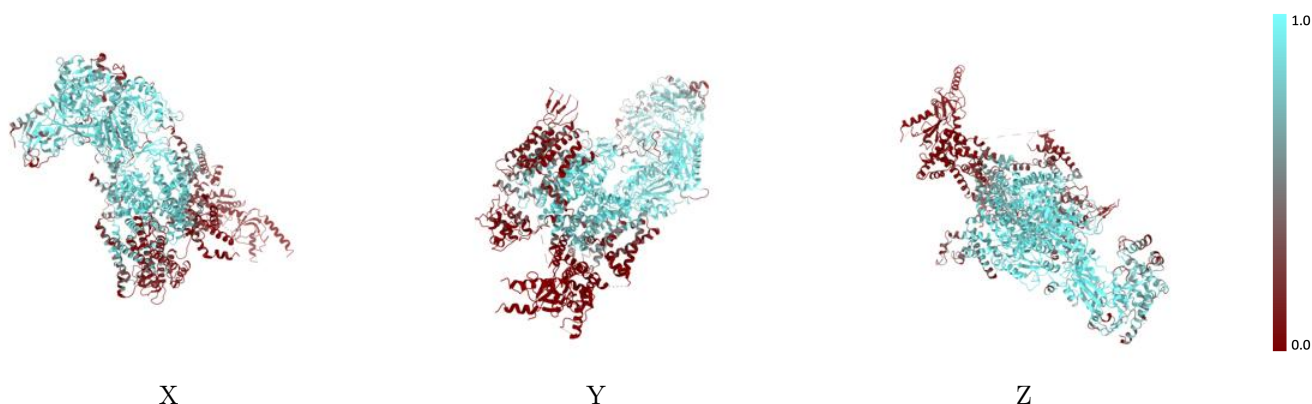
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



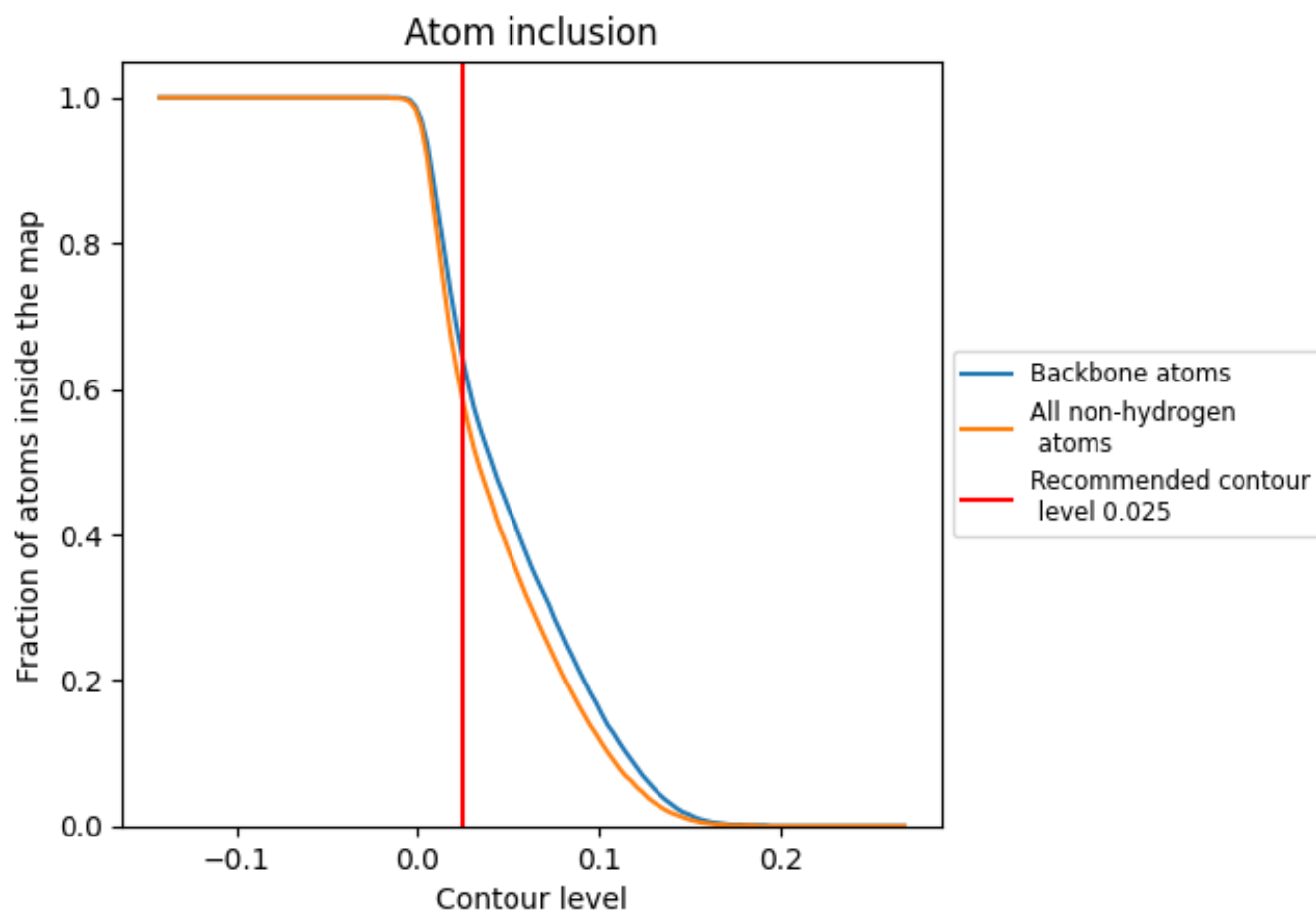
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.025).



























9.4 Atom inclusion [i](#)



At the recommended contour level, 64% of all backbone atoms, 58% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5800	 0.4000
A	 0.5910	 0.4260
B	 0.0000	 -0.0070
C	 0.0000	 0.0090
D	 0.3930	 0.3430
E	 0.2140	 0.1960
F	 0.7830	 0.5060
G	 0.4290	 0.3500
H	 0.4870	 0.2720
I	 0.8720	 0.5240
J	 0.6070	 0.4340
K	 0.1070	 0.2320
L	 0.1910	 0.1980

