



wwPDB EM Validation Summary Report ⓘ

Mar 6, 2026 – 06:05 PM UTC

PDB ID : 9CWM / pdb_00009cwm
EMDB ID : EMD-45967
Title : Cryo-EM structure of human Low-density lipoprotein receptor-related protein 2
Authors : Zhang, Z.; Lyu, M.
Deposited on : 2024-07-29
Resolution : 3.30 Å(reported)

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

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A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
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The types of validation reports are described at

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

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

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

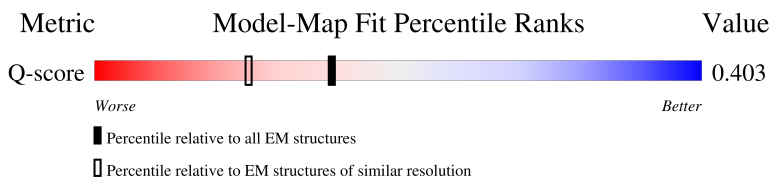
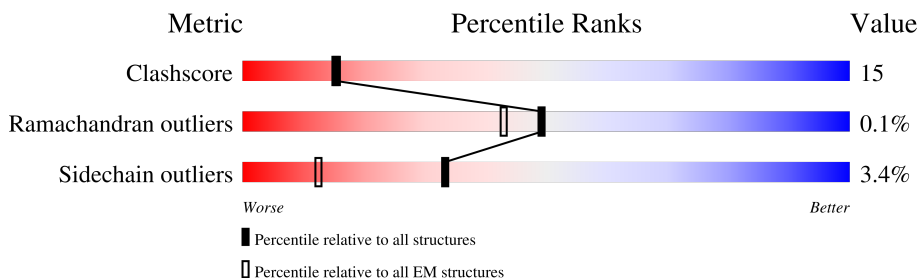
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 Å.

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




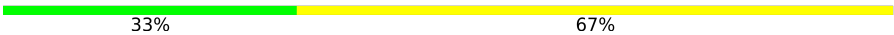


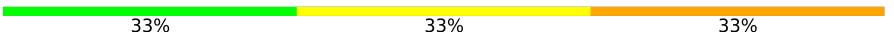



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 (2.80 - 3.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	4655	
1	B	4655	
2	C	3	
2	D	3	

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Mol	Chain	Length	Quality of chain
2	E	3	 67%33%
2	F	3	 100%
2	I	3	 33%67%
2	J	3	 33%67%
2	K	3	 67%33%
2	L	3	 100%
2	N	3	 33%33%33%
3	G	2	 50%50%
3	H	2	 50%50%
3	M	2	 50%50%

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	G	1	-	-	X	-

2 Entry composition [i](#)

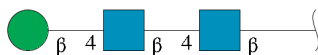
There are 4 unique types of molecules in this entry. The entry contains 58072 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Low-density lipoprotein receptor-related protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3695	Total	C	N	O	S	0	0
			28662	17831	4991	5563	277		
1	B	3692	Total	C	N	O	S	0	0
			28653	17828	4988	5560	277		

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



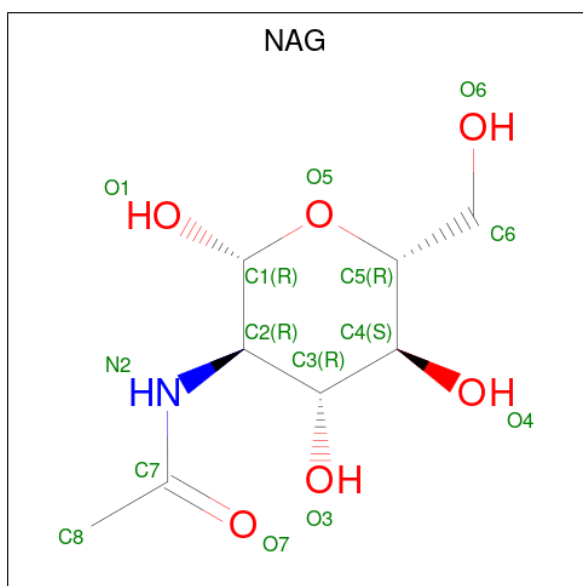
Mol	Chain	Residues	Atoms				AltConf	Trace
2	C	3	Total	C	N	O	0	0
			39	22	2	15		
2	D	3	Total	C	N	O	0	0
			39	22	2	15		
2	E	3	Total	C	N	O	0	0
			39	22	2	15		
2	F	3	Total	C	N	O	0	0
			39	22	2	15		
2	I	3	Total	C	N	O	0	0
			39	22	2	15		
2	J	3	Total	C	N	O	0	0
			39	22	2	15		
2	K	3	Total	C	N	O	0	0
			39	22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

- 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	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	M	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: $C_8H_{15}NO_6$).



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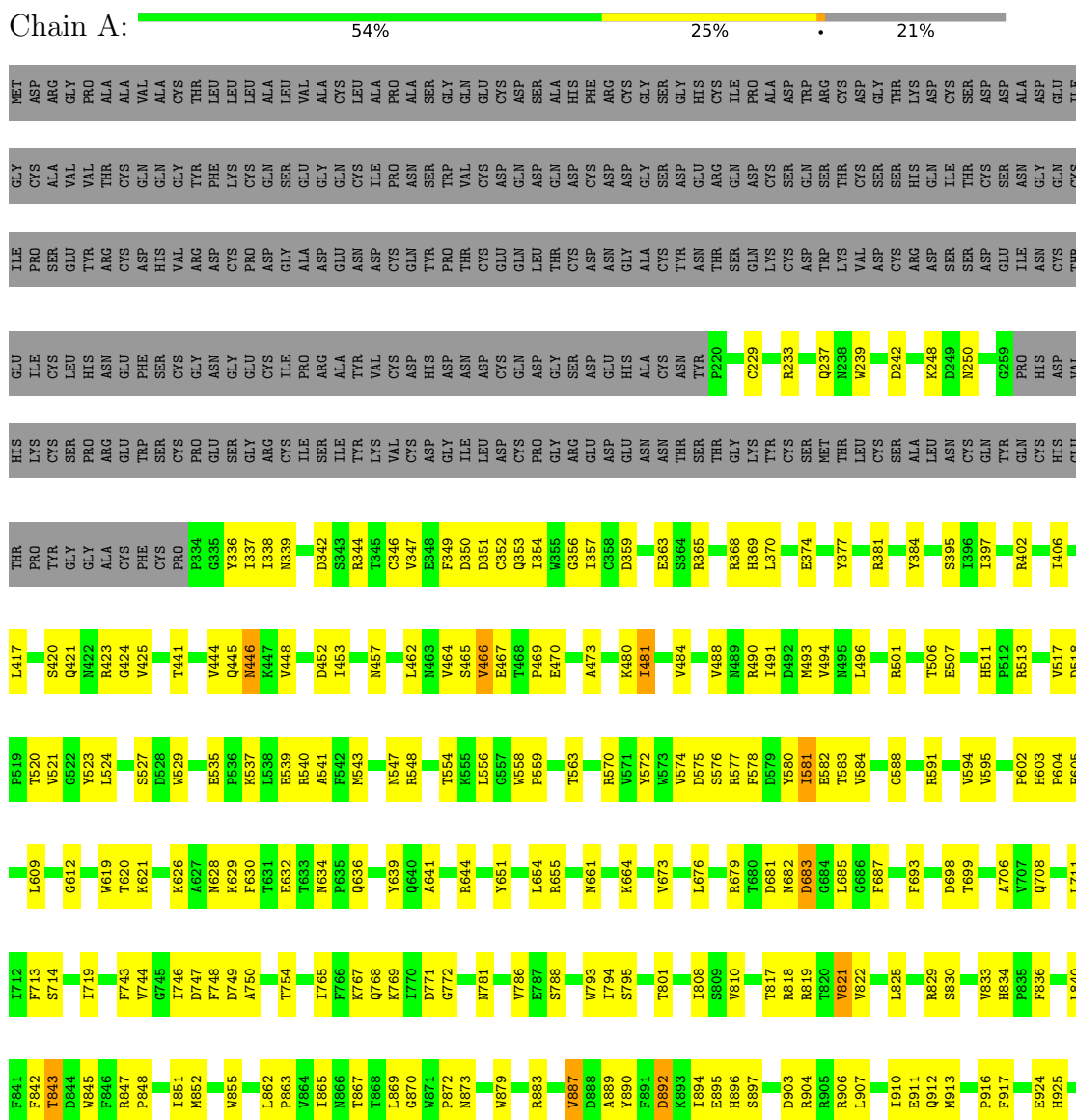
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Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C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

3 Residue-property plots

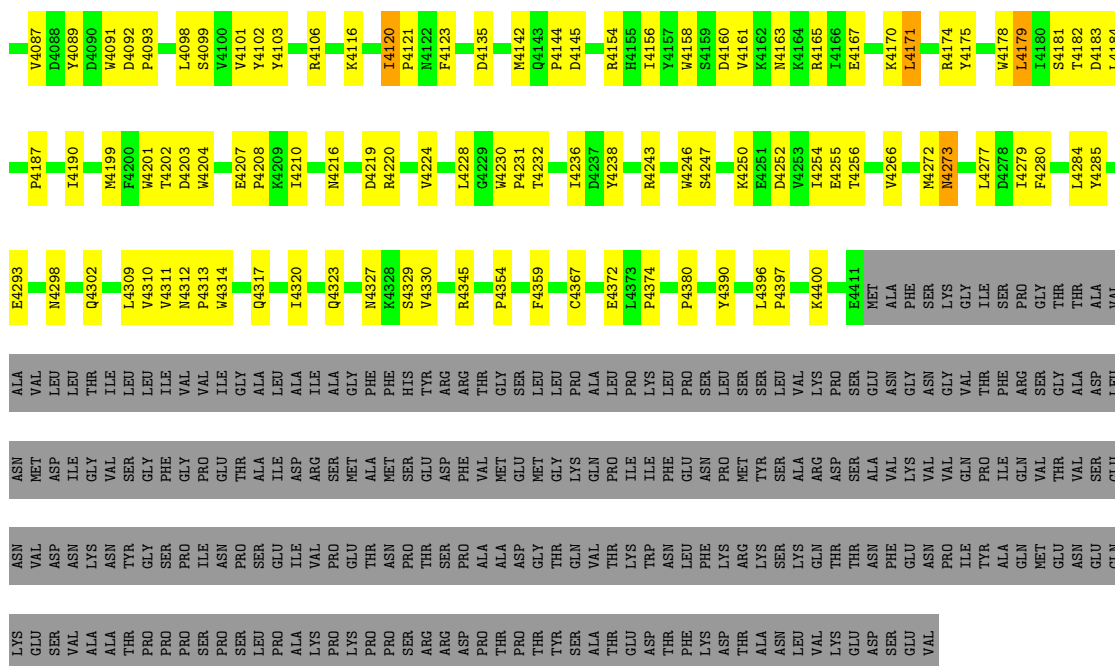
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Low-density lipoprotein receptor-related protein 2



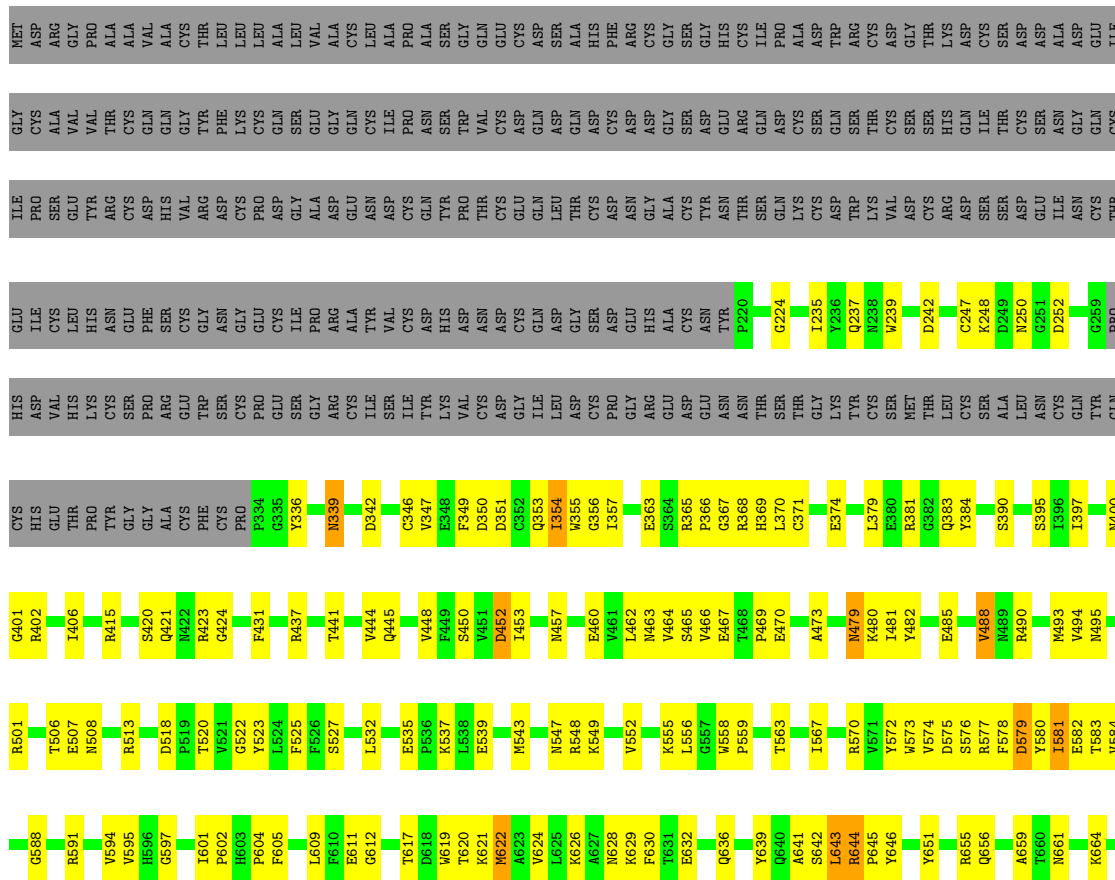






• Molecule 1: Low-density lipoprotein receptor-related protein 2

Chain B: 53% 25% 21%



D2242	S2106	S1961	M1834	S1677	H1566	V1451	G1350	CYS	G1209	D1129	T1023	H896	V673
Y2247	D2113	P1963	L1835	V1685	L1567	T1452	N1351	ASP	D1212	T1130	E1024	S897	S677
V2251	D2114	G1965	T1838	P1686	H1576	S1453	S1352	ARG	N1216	D1131	Q1025	D903	H678
S2254	S2115	I1966	R1841	L1687	R1578	Q1454	S1354	ASN	S1217	N1132	C1026	R904	L685
S2254	D2121	A1967	S1844	V1692	L1481	L1481	D1355	ASP	D1218	D1133	L1044	E910	G686
I2257	T2124	L1973	I1845	K1696	V1462	V1462	N1357	GLY	E1219	C1134	Q1045	E911	F687
I2258	R2125	Y1974	V1847	L1712	G1465	G1465	G1359	MET	A1220	D1136	D1046	Q912	G686
R2262	R2126	T1976	L1848	G1713	M1584	I1467	T1361	SER	T1224	K1141	C1051	A935	F693
V2270	T2127	Q1979	D1853	L1714	M1588	I1468	E1362	ASP	R1225	N1142	H1052	I936	G694
V2270	S2133	I1984	R1854	Q1718	A1589	V1469	E1363	LYS	P1227	C1149	D1056	V939	F695
V2285	T2137	R1855	T1590	H1721	T1590	I1480	C1364	ASP	G1228	Q1150	E1057	R938	C704
V2285	V2138	V1856	V1591	H1721	V1591	I1480	V1365	PRO	F1235	Q1153	Q1058	R940	L711
I2290	T2139	R1857	V1592	F1722	V1592	S1483	Q1366	THR	Q1236	F1154	L1059	R940	I719
I2290	H2140	T1858	V1593	Y1723	V1593	D1484	E1367	GLN	C1237	N1155	C1060	R829	R720
I2300	G2141	T1859	I1597	Y1723	V1593	D1484	F1368	PRO	C1238	C1156	G1061	R830	
S2304	E2144	D1864	Q1487	Y1731	I1597	Q1487	G1370	PHE	E1239	P1157	T1062	T948	V732
K2305	N2145	I1905	C1601	C1740	C1601	W1491	A1371	ARG	I1242	N1158	N1065	V949	M733
N2309	G2146	L1868	I1508	P1746	I1606	I1508	C1373	CYS	I1243	R1160	S1068	I957	F742
P2312	A2151	G1871	T1509	F1747	D1612	T1509	L1374	SER	I1244	C1161	A1071	I958	F743
P2313	A2151	F1872	L1510	V1751	L1612	L1510	G1378	TRP	E1249	T1162	F1072	H959	V744
D2318	N2163	I1874	I1514	I1755	M1615	I1514	L1381	GLN	C1250	F1166	E1078	K961	G745
N2319	A2164	G1875	D1616	I1756	D1616	W1518	S1385	CYS	D1251	V1167	E1078	I960	I746
N2319	T2165	I1756	S1617	F1757	Y1618	V1519	K1386	LEU	G1252	G1170	C1079	Q968	D747
D2325	V2166	F1757	Y1618	F1757	Y1618	V1519	K1386	GLY	P1254	D1171	I1080	T969	F748
V2326	E2167	M1622	M1622	F1757	Y1618	V1519	K1386	HIS	D1255	K1172	W1084	N972	T754
T2327	E2168	M1622	M1622	F1757	Y1618	V1519	K1386	ASN	C1256	K1172	D1087	N972	I755
D2330	T2176	D1626	D1626	F1757	Y1618	V1519	K1386	ILE	L1257	C1174	A973	C974	K762
K2331	N2177	V1783	V1783	E1784	V1635	Y1528	H1403	CYS	S1260	D1176	K1088	T978	I765
V2341	R2181	M1904	M1904	F1785	V1635	Y1528	H1403	VAL	D1261	G1177	H1089	H979	F766
P2345	R2182	D1906	D1906	D1786	I1636	I1536	G1404	ASN	E1262	G1178	H1090	H979	F766
P2345	R2182	V1910	V1910	Y1791	I1636	I1536	Y1405	LEU	H1263	S1178	D1091	N981	K767
P2366	P2192	D1927	D1927	Y1791	I1636	I1536	Y1405	SER	P1268	D1179	C1092	C988	K769
T2374	V2197	A1936	A1936	Y1801	V1655	R1543	R1412	CYS	P1268	V1184	G1095	C988	G772
Q2375	D2198	V1937	V1937	T1804	V1655	R1543	R1412	ASP	S1273	L1185	S1096	V991	T773
Q2376	N2201	V2066	V2066	V1804	V1655	R1543	R1412	GLY	SER	N1186	D1097	V991	G774
L2390	W2206	V2067	V2067	L1820	V1655	R1543	R1412	ASP	TYR	C1187	E1098	Q995	I777
A2393	Y2209	M2068	M2068	G1821	V1655	R1543	R1412	CYS	PHE	Q1191	H1099	R996	L778
L2394	Y2209	M2069	M2069	P1822	V1655	R1543	R1412	ASP	HIS	F1192	C1109	R996	A779
S2397	P2213	A2072	A2072	P1822	V1655	R1543	R1412	PRO	CYS	K1193	T1112	P1001	A780
L2398	P2213	H2083	H2083	P1822	V1655	R1543	R1412	ASN	ASP	D1198	Q1113	M1004	N761
S2400	T2233	Q2083	Q2083	P1822	V1655	R1543	R1412	GLY	ASN	C1193	Y1114	M1004	N761
S2400	P2236	T1951	T1951	P1822	V1655	R1543	R1412	THR	ASN	T1201	M1118	M1009	N785
L2401	P2236	Q2084	Q2084	P1822	V1655	R1543	R1412	GLU	CYS	G1202	N1118	M1010	V786
		M1954	M1954	P1822	V1655	R1543	R1412	SER	ILE	L1011	C1121	L1011	V887
		T1855	T1855	P1822	V1655	R1543	R1412	ARG	HIS	V1203	C1121	L1011	A790
		L1956	L1956	P1822	V1655	R1543	R1412	ALA	ARG	T1294	I1122	G1015	D882
		L1960	L1960	P1822	V1655	R1543	R1412	ALA	ALA	T1294	S1123	D1016	R893
				P1822	V1655	R1543	R1412	TRP	TRP	N1206	K1124	I894	I794
				P1822	V1655	R1543	R1412	LEU	LEU		N1125	E1020	S795

D3747	Q3612	D3496	T3362	I3265	E3053	ASP	GLY	ASN	PRO	R2711	V2607	V9513	S2409
D3750	C3613	L3502	A3363	R3288	D3054	VAL	GLY	PRO	ARG	C2712	T2608	L2614	S2414
S3773	D3614	Y3607	L3364	L3289	N3055	CYS	ARG	THR	GLU	I2713	R2614	D2615	T2414
S3774	C3619	C3508	P3367	A3271	E3063	THR	ILE	CYS	ILE	S2714	I2615	P2516	
R3775	N3622	M3509	T3371	A3272	L3087	ASP	PRO	THR	CYS	D2724	A2618	G2519	V2417
W3776	D3626	P3510	I3372	E3273	P3073	THR	GLY	THR	ASN	C2725	C2725	Y2520	V2421
I3777	D3626	C3512	N3376	V3277	L3074	ASP	THR	VAL	GLY	D2726	A2619	L2521	
H3780	H3629	C3513	D3278	D3277	T3074	GLU	ILE	CYS	VAL	G2728	R2620	W2523	L2424
Y3781	R3633	Y3380	Y3378	V3277	C3075	ASN	ASP	ASN	ASN	S2729	G2623	Y2426	L2425
N3782	F3517	Q3516	R3192	S3281	H3078	GLN	GLY	SER	HIS	E2733	W2629	I2532	Y2427
D3783	L3518	Y3388	R3193	R3282	E3079	CYS	ASP	GLU	ASP	A2737	L2633	E2532	S2428
C3784	F3640	E3389	Q3193	K3283	L3088	THR	ASN	PHE	ASN	L2738	L2634	R2534	V2429
D3789	R3641	E3390	N3194	L3284	A3081	ARG	GLN	GLN	ASN	H2739	L2634	A2535	
E3790	N3644	N3522	S3195	S3195	C3082	THR	CYS	CYS	THR	T2740	P2637	T2536	R2432
R3791	I3526	H3398	P3199	P3199	R3086	CYS	ASP	SER	ASP	T2747	I2640	R2542	I2433
R3796	P3527	H3400	Y3200	Y3200	C3087	SER	MET	GLY	GLU	CYS	I2641	V2543	Y2434
T3797	L3528	T3401	F3203	L3294	C3088	GLU	THR	ARG	LYS	VAL	R2642	P2544	F2435
C3798	K3531	I3413	S3204	S3204	E3089	GLU	GLU	CYS	ASN	ALA	T2642	I2545	N2438
H3799	C3532	T3414	S3204	S3204	A3089	ILE	GLU	ILE	CYS	ASN	V2643	V2546	L2439
P3800	D3533	I3415	Y3208	S3297	M3090	PHE	LYS	PRO	PRO	GLY	V2644	G2547	A2440
E3801	D3665	F3416	Y3208	D3298	K3091	THR	THR	ASP	ASP	ARG		S2548	S2441
Y3802	E3666	I3420	N3211	G3302	K3092	CYS	ARG	ARG	ARG	CYS	K2648	S2549	
Q3804	P3667	I3420	N3211	H3303	L3093	GLY	HIS	THR	THR	VAL	Q2649	L2550	Y2448
E3808	F3670	T3423	L3221	R3304	C3094	TYR	GLN	CYS	CYS	GLN	Q2650	P2553	A2449
H3809	C3560	V3430	L3226	F3318	D3099	LEU	GLN	ASP	SER	S2756	C2651	T2450	
C3810	S3567	Y3436	V3229	C3319	N3103	ILE	ASN	ASP	ASN	S2757	N2652	L2556	S2453
Y3811	T3570	N3446	V3229	F3318	S3104	PHE	GLN	ASP	HIS	R2764	N2653	V2567	H2456
G3818	T3570	N3446	L3226	C3311	D3106	ASP	ASP	ASP	THR	S2765	E2656	L2566	T2457
G3819	N3573	R3450	R3236	P3323	K3107	ARG	SER	ALA	SER	C2766	I2665	V2567	P2458
S3820	A3574	F3451	R3236	R3324	G3110	CYS	GLU	ALA	THR		A2673	D2568	G2466
A3821	H3575	F3452	R3236	G3325	I3111	ASP	PHE	SER	ILE	G2774	H2679	L2572	D2474
D3822	Q3576	D3453	K3239	L3326	N3112	THR	LEU	ASP	ASP	C2775	Q2573	Q2573	W2475
C3823	N3577	I3454	R3240	A3327	E3113	ASN	CYS	GLU	ILE	L2776	R2574	I2575	I2476
L3824	C3578	H3455	R3240	L3328	H3115	ASP	VAL	PRO	PRO	F2777	Y2684	I2575	
D3825	C3705	H3458	W3243	P3330	R3129	ASP	ASN	ALA	ARG	ARG	L2685	E2576	L2486
E3829	R3706	P3458	I3244	Q3331	H3124	ARG	ASP	SER	VAL	ASP	A2686	R2489	M2489
C3832	D3707	F3459	D3245	Y3332	T3129	PRO	ARG	GLY	TYR	CYS	R2689	E2586	I2490
P3833	N3708	Y3460	D3245	L3335	N3035	THR	THR	HIS	LEU	ASN	ALA	W2491	S2491
T3834	S3709	R3461	Q3249	Y3336	L3130	ASP	ARG	SER	CYS	ALA	K2690	V2587	S2492
R3835	D3710	N3467	I3251	Y3337	C3135	ARG	ARG	GLU	ASP	THR	H2691	C2692	W2493
F3836	E3711	F3468	E3252	W3337	S3136	CYS	CYS	ARG	GLY	THR	C2692	L2494	G2494
P3837	Q3712	C3469	R3253	Y3345	Q3040	ILE	ILE	THR	ASP	GLU	I2694	E2495	
H3838	H3720	L3479	F3255	I3346	I3045	PRO	PRO	CYS	VAL	PHE	V2694	L2598	T2501
G3839	P3721	W3599	F3255	Q3347	S3046	GLY	GLN	ALA	GLY	MET	S2704	T2599	V2502
A3840	V3722	G3485	T3259	K3356	K3047	ASP	THR	ASP	GLY	ASN	T2705	G2601	L2503
Y3841	N3729	P3608	N3260	K3147	R3148	GLU	THR	GLU	ASP	ASN	T2706	G2603	A2504
C3842	Q3843	E3609	K3261	R3147	R3148	PHE	VAL	ASP	ASP	ARG	C2707	Q2603	R2505
D3744		S3610	I3360	I3360	V3151	LYS	CYS	SER	SER	ARG	S2708	Y2604	
M3846		W3611	S3361	S3361	D3052	ASP	GLY	ASP	GLU	ILE	I2710	Y2606	


F3847	LYS	L4179	E4293	VAL	LEU	GLU	GLN
E3848	PRO	T4180	Y4294	ALA	ASN	ASN	LYS
C3849	THR	S4181	W4295	VAL	ASP	VAL	GLU
K3850	PRO	D4080	N4298	LEU	ILE	ASP	SER
N3851	LYS	Q4136	N4298	THR	GLY	ASN	VAL
V3853	CYS	T4190	Q4302	ILE	VAL	ASN	ALA
C3854	THR	M4199	K4307	LEU	SER	THR	THR
L3855	GLU	T4202	T4308	LEU	GLY	GLY	PRO
P3856	TYR	D4088	L4309	VAL	PHE	PRO	PRO
P3857	GLU	Y4089	V4310	VAL	PRO	ILE	SER
Y3858	TYR	W4204	V4311	ILE	ASN	ASN	PRO
Y3859	LYS	G4205	M4312	GLY	PRO	PRO	SER
D3862	CYS	P4208	W4313	ALA	SER	LEU	LEU
C3863	GLY	D4092	W4314	ALA	ILE	PRO	ALA
G3870	GLY	P4093	L4316	ILE	ASP	GLU	ALA
S3871	HIS	L4098	T4316	ILE	ARG	VAL	LYS
S3871	CYS	S4099	Q4317	ALA	SER	PRO	PRO
D3872	ILE	V4100	I4320	GLY	GLU	GLU	LYS
E3873	PRO	V4101	F4321	PHE	THR	THR	PRO
E3874	HIS	Y4102	H4322	ALA	ASN	ASN	PRO
L3875	ASP	Y4103	Q4323	HIS	SER	PRO	SER
D3879	ASN	R4106	P4354	TYR	GLU	ARG	ARG
D3880	CYS	K4116	F4359	ARG	ASP	SER	ASP
F3889	ASP	L4223	C4367	THR	PRO	PRO	PRO
ARG	ALA	V4224	P4374	THR	GLN	ALA	THR
CYS	ASP	L4228	P4380	GLY	LYS	VAL	ALA
ASN	ASP	G4229	C4381	VAL	PRO	THR	THR
ASN	GLY	T4120	R4382	THR	ILE	GLU	GLU
ASN	ASP	R4022	D4145	LEU	LYS	ASN	ASP
CYS	ASP	R4025	D4242	LEU	PHE	LEU	ASN
GLY	ASP	G4026	R4243	ALA	ASN	GLU	LYS
TRP	TRP	E4029	W4246	LEU	PRO	PHE	LYS
SER	SER	C4030	S4247	LEU	ILE	ARG	THR
GLU	ASP	V4031	P4144	LEU	PHE	LYS	ALA
LEU	GLU	D4034	D4145	PRO	GLU	LYS	LEU
GLY	LEU	G4035	R4154	SER	ASN	GLU	VAL
CYS	CYS	F4036	H4155	LEU	PRO	LYS	ASP
ASN	ASN	T4037	T4156	SER	MET	ASN	THR
LYS	LYS	S4038	Y4157	LEU	TYR	LYS	ALA
GLY	GLY	W4039	W4158	LEU	SER	SER	ASN
LYS	LYS	S4040	S4159	VAL	ALA	LYS	LEU
GLU	GLU	D4041	D4160	VAL	ARG	GLN	VAL
ARG	ARG	R4042	N4163	THR	THR	THR	THR
CYS	CYS	K4045	K4164	ASN	ALA	ASN	VAL
GLY	GLY	R4046	R4165	GLY	VAL	LYS	GLY
ASP	ASP	C4047	I4166	ASN	VAL	GLU	VAL
THR	THR	L4057	E4167	GLY	VAL	ASN	PRO
ASN	ASN	L4057	K4170	VAL	ILE	PRO	ILE
CYS	CYS	P4059	L4171	THR	THR	ALA	THR
GLN	GLN	V4062	R4174	ARG	PRO	GLN	GLN
ASN	ASN	R4063	Y4175	SER	VAL	MET	VAL
CYS	CYS	Y4067	W4178	GLY	THR	GLU	GLU
THR	THR			THR	VAL	ASN	ALA
GLN	GLN			ASP	SER	GLU	ASP

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

Chain C:  33% 67%

NAG1
NAG2
BNA3

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

Chain D:  33% 67%

NAG1
NAG2
BNA3

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

Chain E:  67% 33%



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

Chain F:



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

Chain I:



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

Chain J:



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

Chain K:



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

Chain L:



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

Chain N:



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

Chain G:  50% 50%

MAG1
MAG2

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

Chain H:  50% 50%

MAG1
MAG2

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

Chain M:  50% 50%

MAG1
MAG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	111811	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.033	Depositor
Minimum map value	-0.060	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	547.84, 547.84, 547.84	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	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: BMA, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.26	5/29362 (0.0%)	0.43	4/39957 (0.0%)
1	B	0.25	6/29354 (0.0%)	0.43	7/39946 (0.0%)
All	All	0.26	11/58716 (0.0%)	0.43	11/79903 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	480	LYS	C-N	9.10	1.44	1.33
1	B	842	PHE	C-N	8.55	1.44	1.33
1	B	995	GLN	C-N	8.00	1.45	1.33
1	A	995	GLN	C-N	7.15	1.44	1.33
1	A	843	THR	C-N	6.31	1.41	1.33

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2726	GLY	N-CA-C	-9.85	102.41	115.32
1	A	2726	GLY	N-CA-C	-9.74	102.56	115.32
1	B	3819	GLY	N-CA-C	-6.17	107.74	115.08
1	B	842	PHE	O-C-N	5.58	129.92	123.17
1	A	480	LYS	O-C-N	5.54	130.43	123.23

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	819	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	28662	0	26485	823	0
1	B	28653	0	26477	829	0
2	C	39	0	34	2	0
2	D	39	0	34	2	0
2	E	39	0	34	5	0
2	F	39	0	34	0	0
2	I	39	0	34	3	0
2	J	39	0	34	3	0
2	K	39	0	34	6	0
2	L	39	0	34	0	0
2	N	39	0	34	2	0
3	G	28	0	25	7	0
3	H	28	0	25	1	0
3	M	28	0	25	1	0
4	A	168	0	156	1	0
4	B	154	0	143	2	0
All	All	58072	0	53642	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 15.

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:4329:SER:HB2	3:G:1:NAG:C1	1.75	1.16
1:A:4007:ASP:HA	1:A:4025:LYS:HA	1.10	1.09
1:B:1228:GLY:HA3	1:B:3195:SER:HA	1.51	0.91
1:A:4007:ASP:HA	1:A:4025:LYS:CA	2.00	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3611:TRP:HA	1:B:3614:ASP:HB3	1.55	0.88

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	3683/4655 (79%)	3478 (94%)	203 (6%)	2 (0%)	48	75
1	B	3680/4655 (79%)	3478 (94%)	197 (5%)	5 (0%)	48	75
All	All	7363/9310 (79%)	6956 (94%)	400 (5%)	7 (0%)	49	75

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1160	ARG
1	A	821	VAL
1	A	960	LEU
1	B	821	VAL
1	B	646	TYR

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	3150/4105 (77%)	3047 (97%)	103 (3%)	33	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	3150/4105 (77%)	3038 (96%)	112 (4%)	31 58
All	All	6300/8210 (77%)	6085 (97%)	215 (3%)	33 59

5 of 215 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	643	LEU
1	B	1649	THR
1	B	3858	TYR
1	B	821	VAL
1	B	1184	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 132 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	3300	ASN
1	B	3385	HIS
1	B	4163	ASN
1	A	3400	HIS
1	A	3376	ASN

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 ⓘ

33 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	C	1	2,1	14,14,15	0.29	0	17,19,21	0.70	0
2	NAG	C	2	2	14,14,15	0.31	0	17,19,21	0.73	0
2	BMA	C	3	2	11,11,12	0.23	0	15,15,17	0.53	0
2	NAG	D	1	2,1	14,14,15	0.32	0	17,19,21	0.61	0
2	NAG	D	2	2	14,14,15	0.27	0	17,19,21	0.75	0
2	BMA	D	3	2	11,11,12	0.21	0	15,15,17	0.50	0
2	NAG	E	1	2,1	14,14,15	0.30	0	17,19,21	0.82	1 (5%)
2	NAG	E	2	2	14,14,15	0.26	0	17,19,21	0.68	0
2	BMA	E	3	2	11,11,12	0.21	0	15,15,17	0.55	0
2	NAG	F	1	2,1	14,14,15	0.25	0	17,19,21	0.50	0
2	NAG	F	2	2	14,14,15	0.29	0	17,19,21	0.61	0
2	BMA	F	3	2	11,11,12	0.21	0	15,15,17	0.56	0
3	NAG	G	1	3	14,14,15	0.40	0	17,19,21	0.76	0
3	NAG	G	2	3	14,14,15	0.40	0	17,19,21	2.00	4 (23%)
3	NAG	H	1	3,1	14,14,15	0.36	0	17,19,21	1.33	2 (11%)
3	NAG	H	2	3	14,14,15	0.39	0	17,19,21	2.00	4 (23%)
2	NAG	I	1	2,1	14,14,15	0.31	0	17,19,21	0.66	0
2	NAG	I	2	2	14,14,15	0.31	0	17,19,21	0.80	0
2	BMA	I	3	2	11,11,12	0.22	0	15,15,17	0.51	0
2	NAG	J	1	2,1	14,14,15	0.33	0	17,19,21	0.58	0
2	NAG	J	2	2	14,14,15	0.26	0	17,19,21	0.66	0
2	BMA	J	3	2	11,11,12	0.21	0	15,15,17	0.52	0
2	NAG	K	1	2,1	14,14,15	0.31	0	17,19,21	0.80	1 (5%)
2	NAG	K	2	2	14,14,15	0.25	0	17,19,21	0.68	0
2	BMA	K	3	2	11,11,12	0.22	0	15,15,17	0.56	0
2	NAG	L	1	2,1	14,14,15	0.25	0	17,19,21	0.49	0
2	NAG	L	2	2	14,14,15	0.27	0	17,19,21	0.63	0
2	BMA	L	3	2	11,11,12	0.21	0	15,15,17	0.55	0
3	NAG	M	1	3,1	14,14,15	0.42	0	17,19,21	1.05	1 (5%)
3	NAG	M	2	3	14,14,15	0.40	0	17,19,21	1.02	2 (11%)
2	NAG	N	1	2,1	14,14,15	0.39	0	17,19,21	1.21	2 (11%)
2	NAG	N	2	2	14,14,15	0.41	0	17,19,21	1.10	1 (5%)
2	BMA	N	3	2	11,11,12	0.21	0	15,15,17	0.51	0

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

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

There are no bond length outliers.

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	2	NAG	O5-C5-C6	6.53	120.37	107.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	2	NAG	O5-C5-C6	6.52	120.35	107.66
2	N	2	NAG	O5-C1-C2	3.81	117.18	111.29
3	H	1	NAG	C1-C2-N2	3.69	116.25	110.43
3	H	1	NAG	C2-N2-C7	3.45	127.53	122.90

There are no chirality outliers.

5 of 38 torsion outliers are listed below:

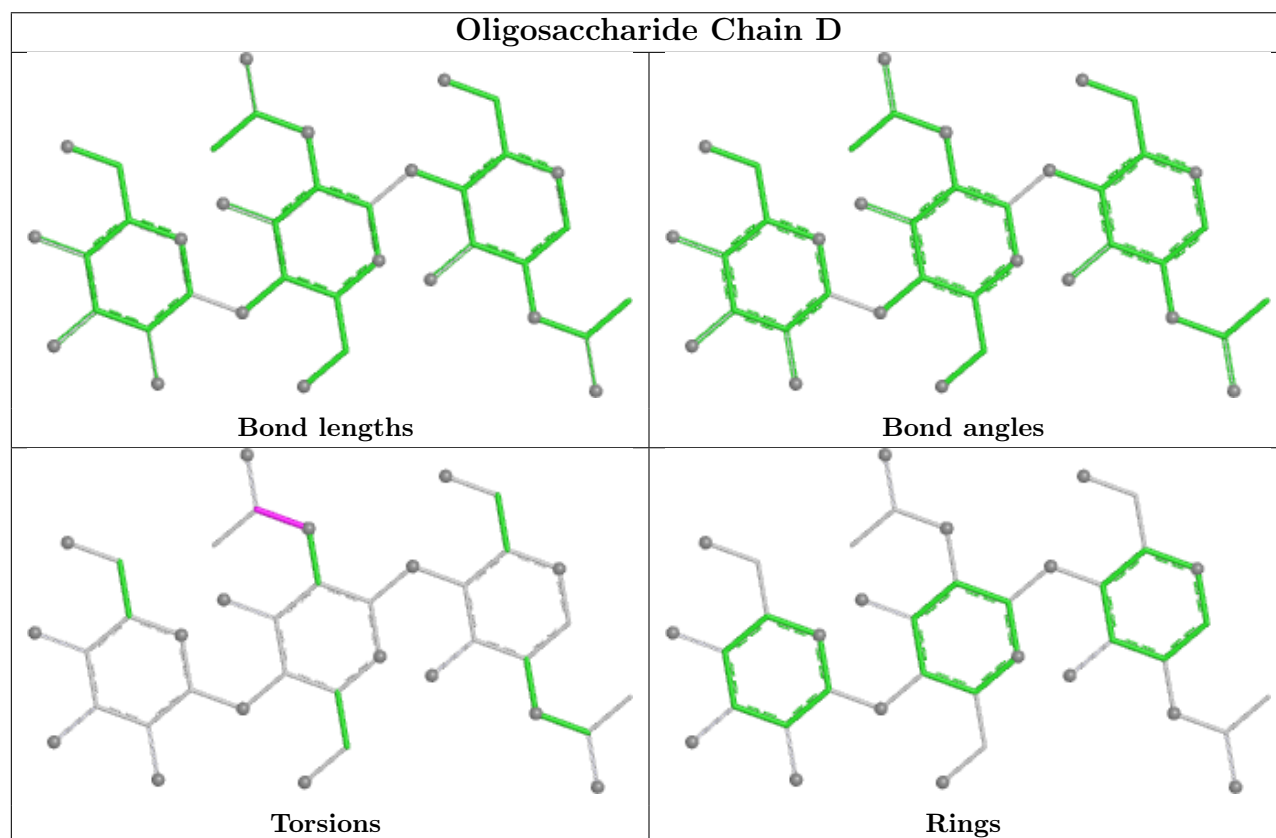
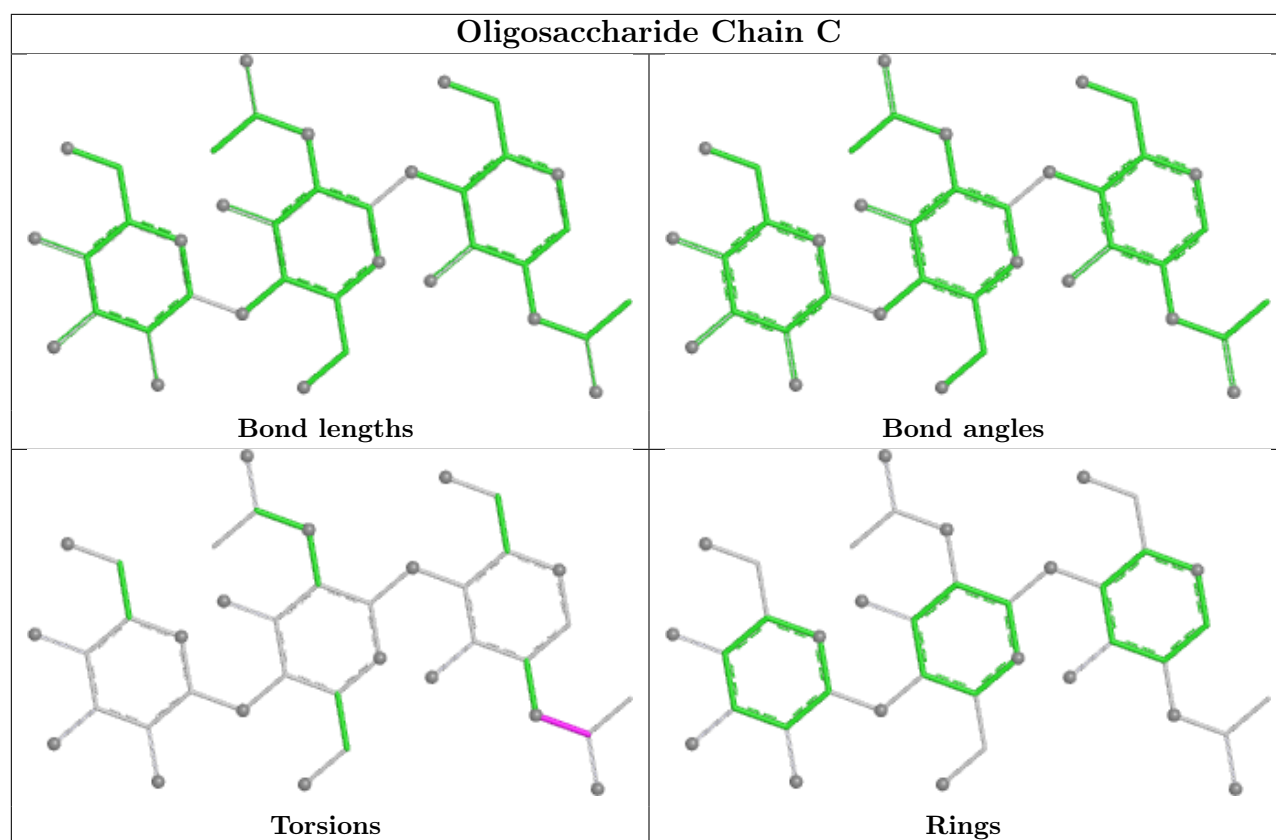
Mol	Chain	Res	Type	Atoms
2	E	1	NAG	C8-C7-N2-C2
2	E	1	NAG	O7-C7-N2-C2
2	E	2	NAG	C3-C2-N2-C7
2	E	2	NAG	C8-C7-N2-C2
2	E	2	NAG	O7-C7-N2-C2

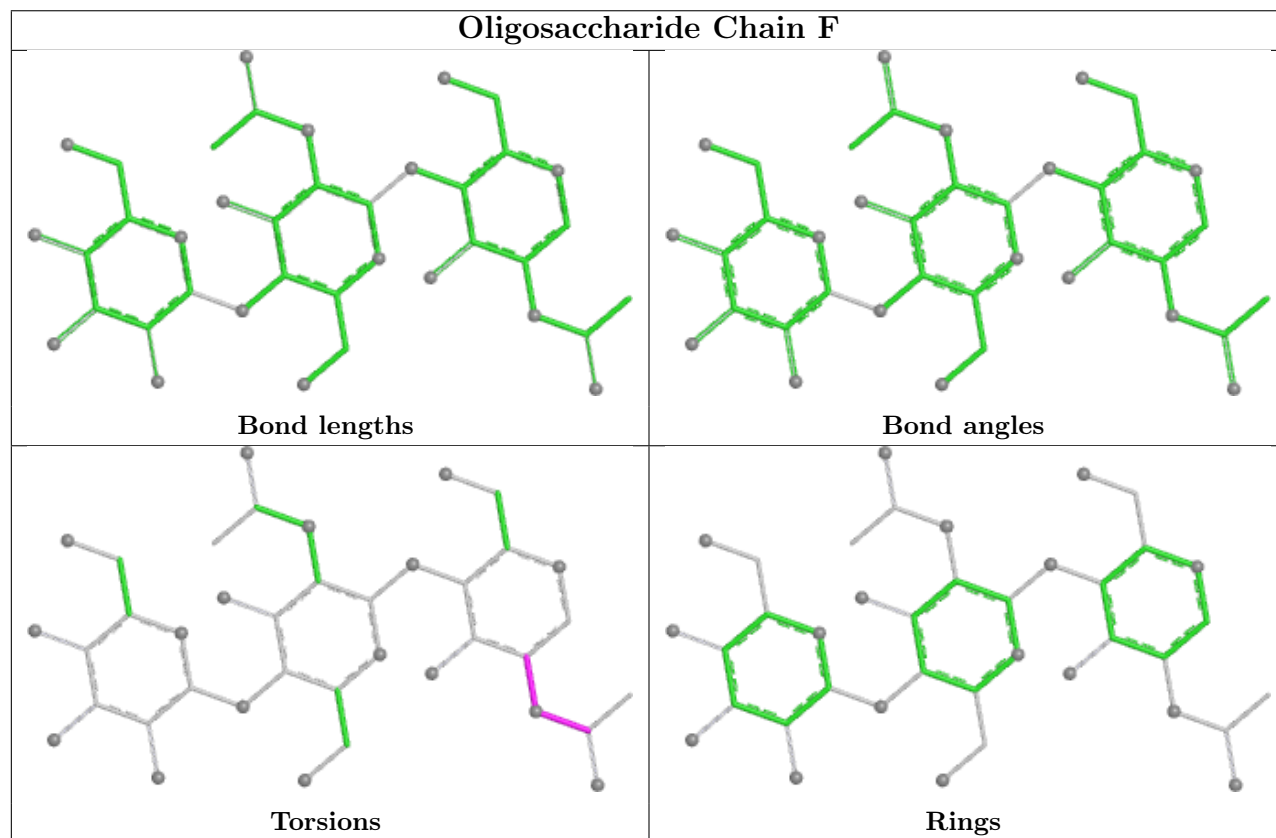
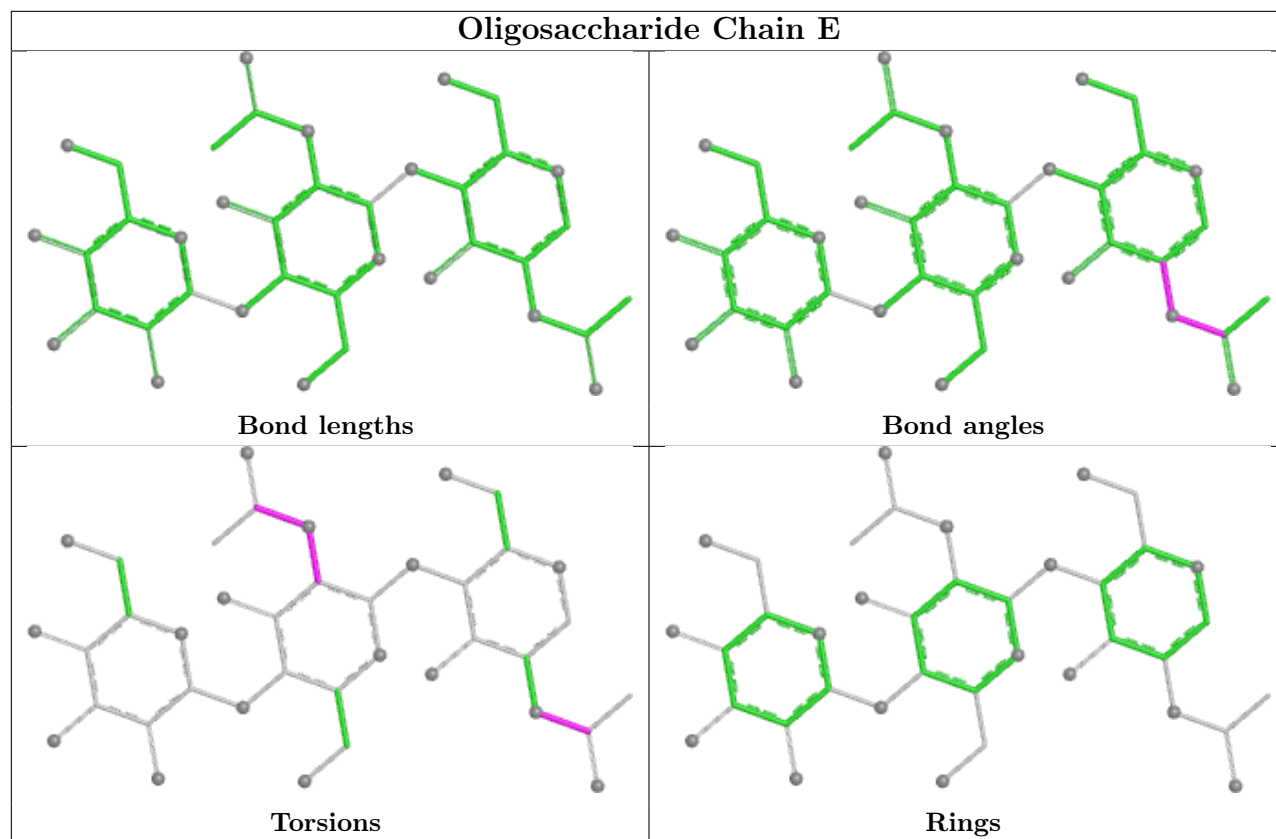
There are no ring outliers.

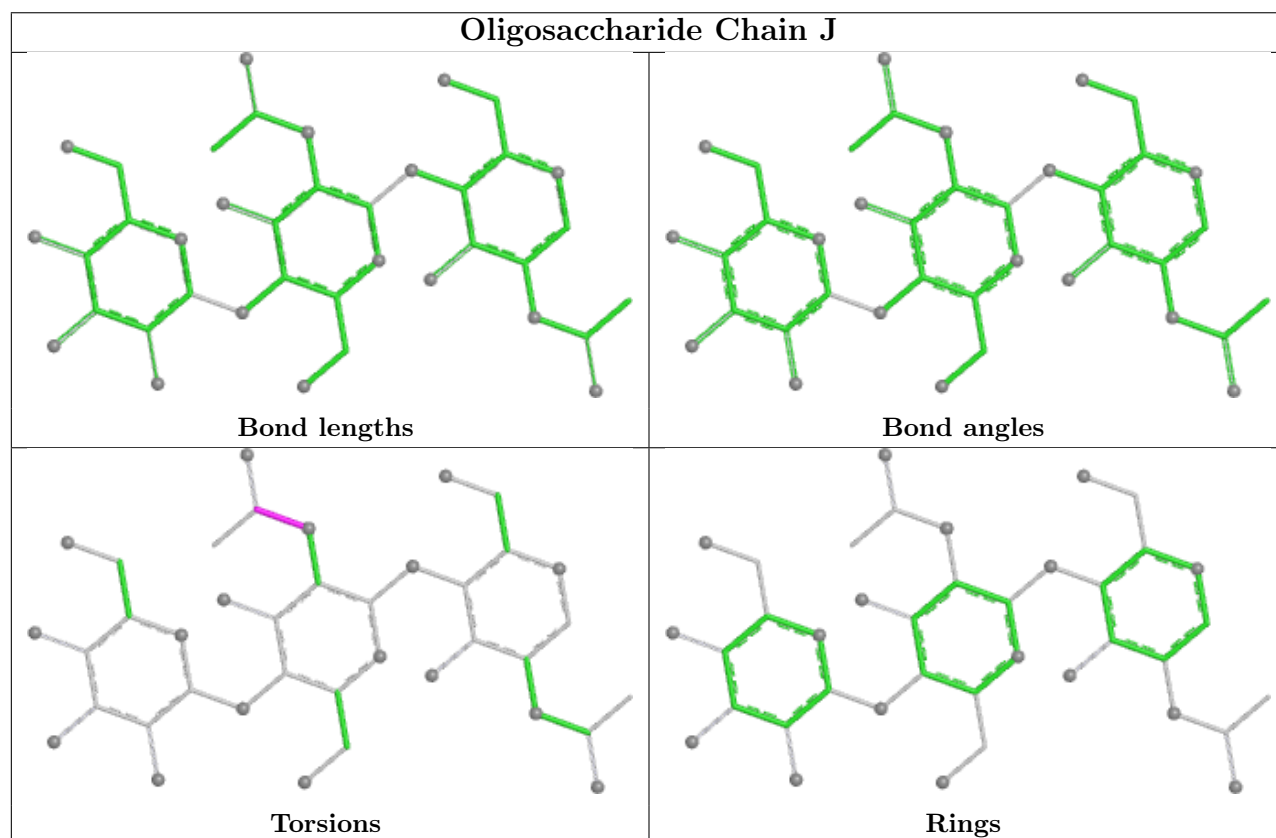
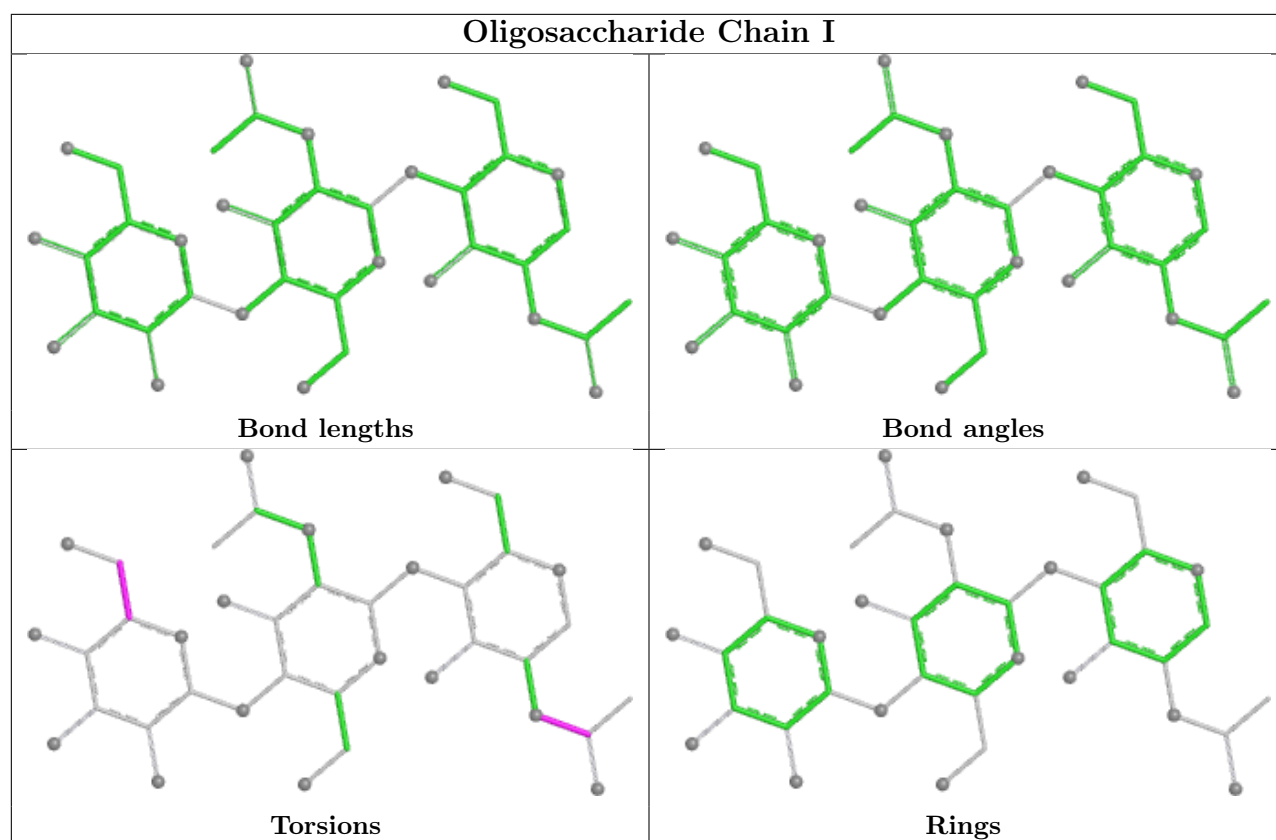
15 monomers are involved in 32 short contacts:

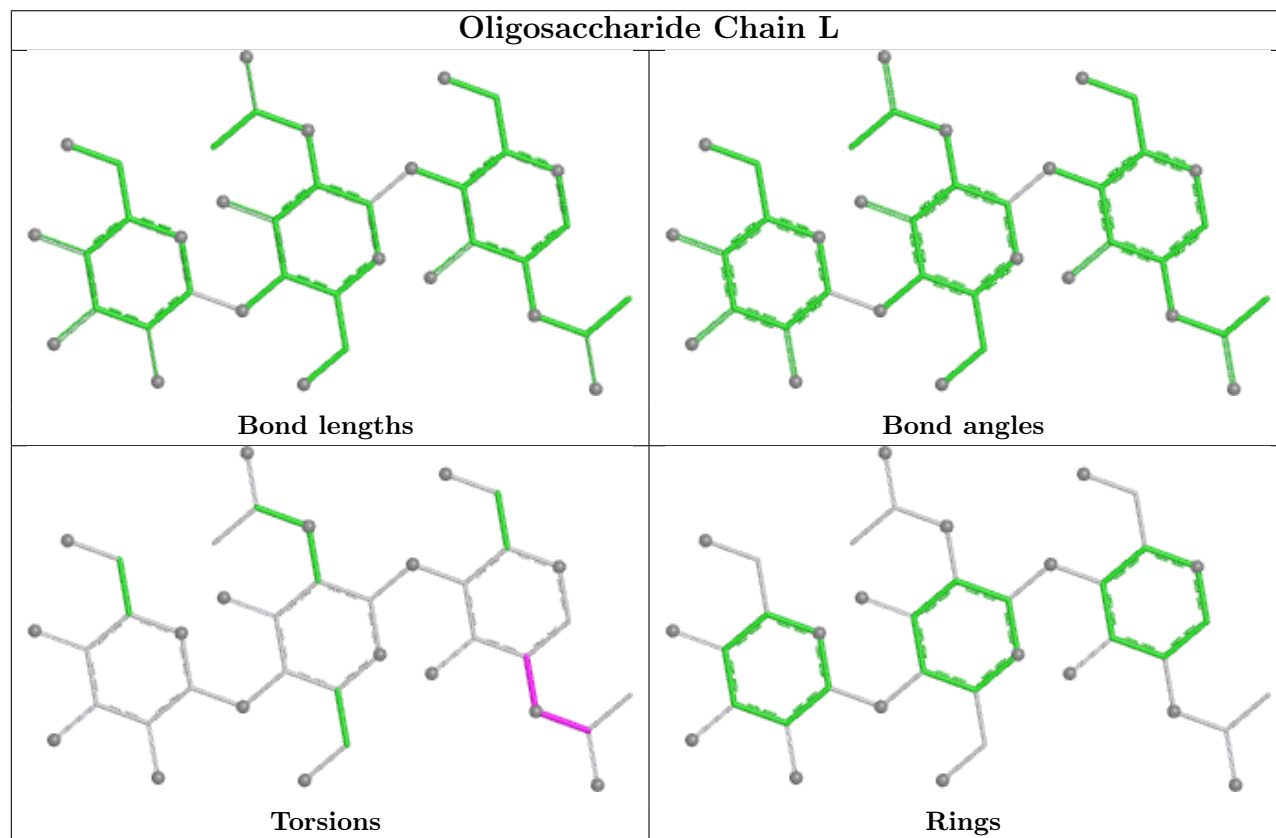
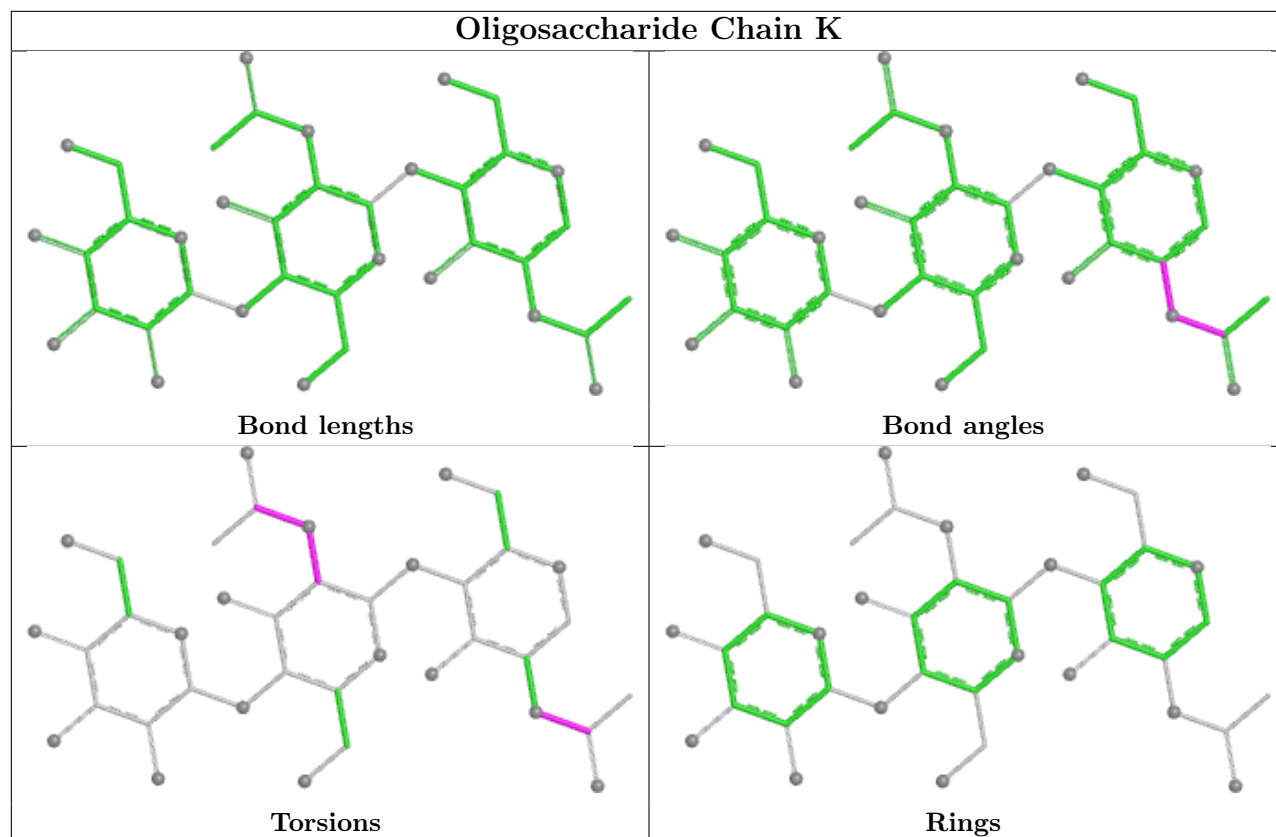
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	M	1	NAG	1	0
2	C	1	NAG	2	0
3	G	1	NAG	7	0
2	I	2	NAG	2	0
2	E	1	NAG	5	0
2	D	2	NAG	1	0
2	I	1	NAG	2	0
2	D	1	NAG	2	0
2	J	1	NAG	3	0
3	H	1	NAG	1	0
2	K	1	NAG	6	0
3	G	2	NAG	3	0
2	N	1	NAG	2	0
2	J	2	NAG	1	0
2	C	2	NAG	1	0

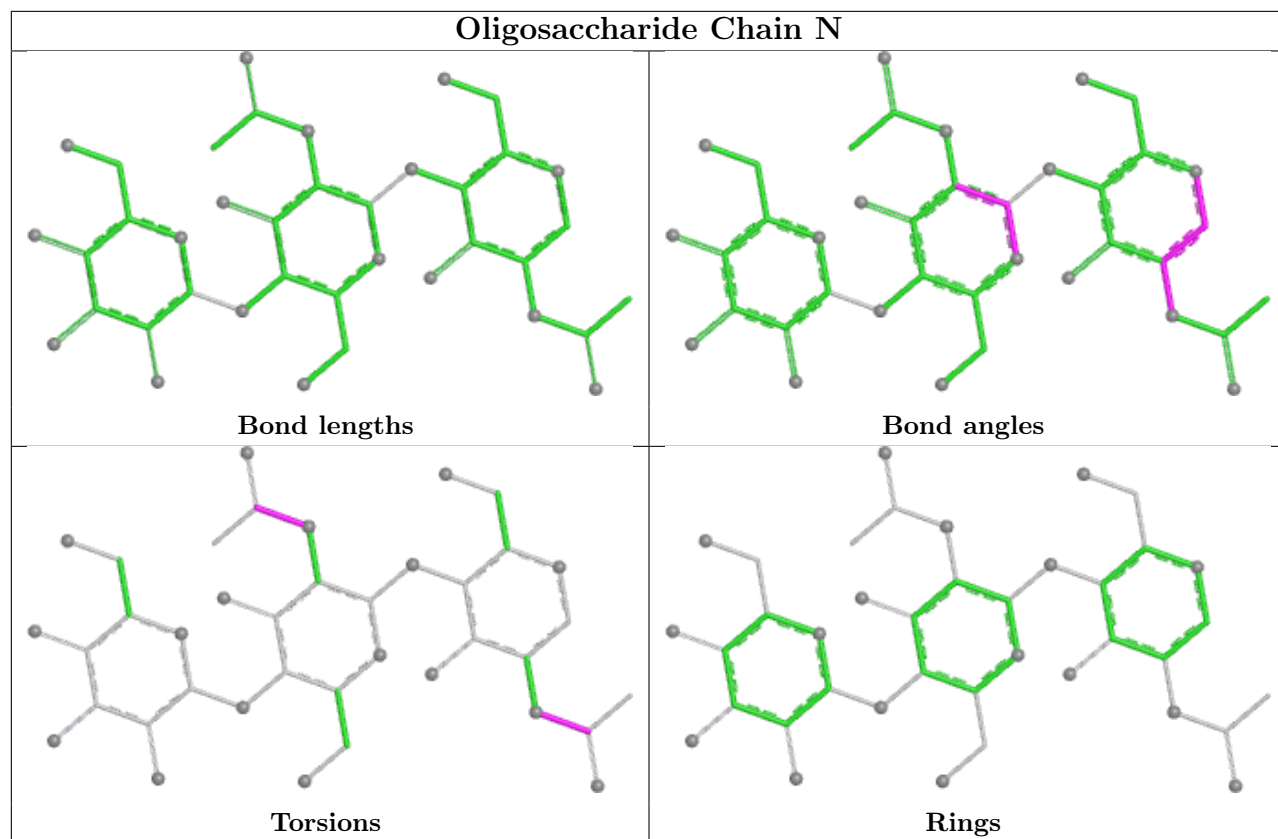
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

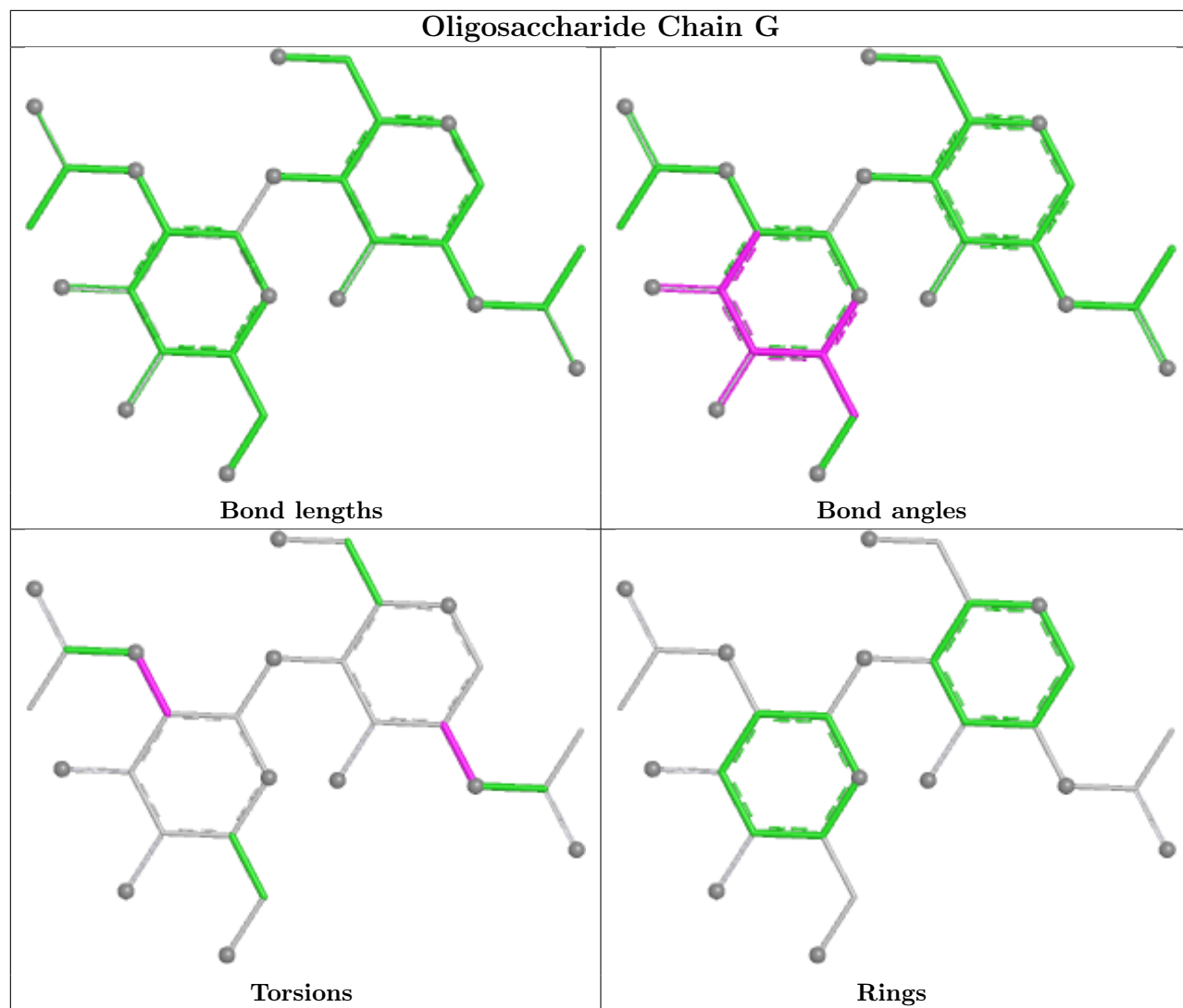


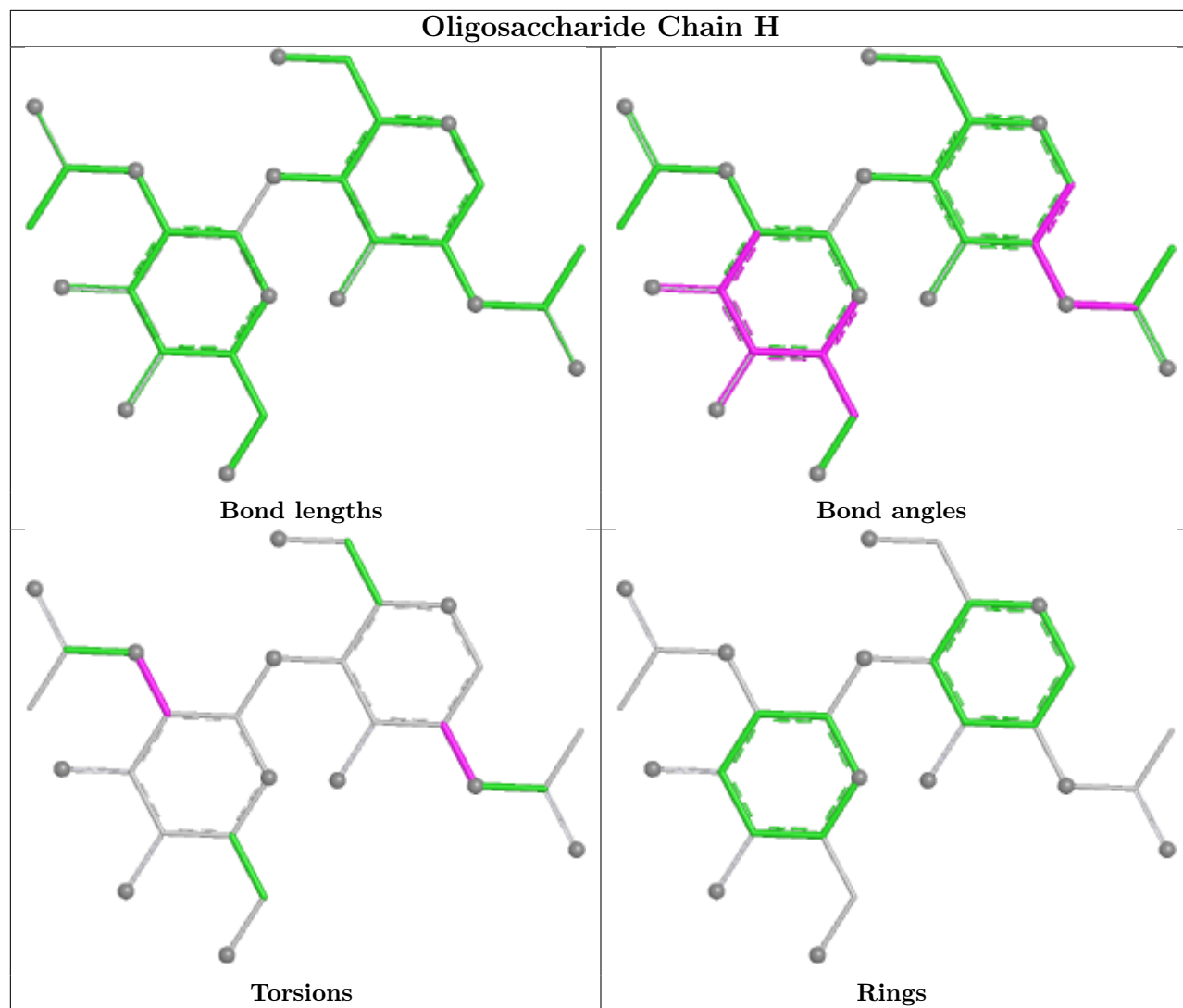


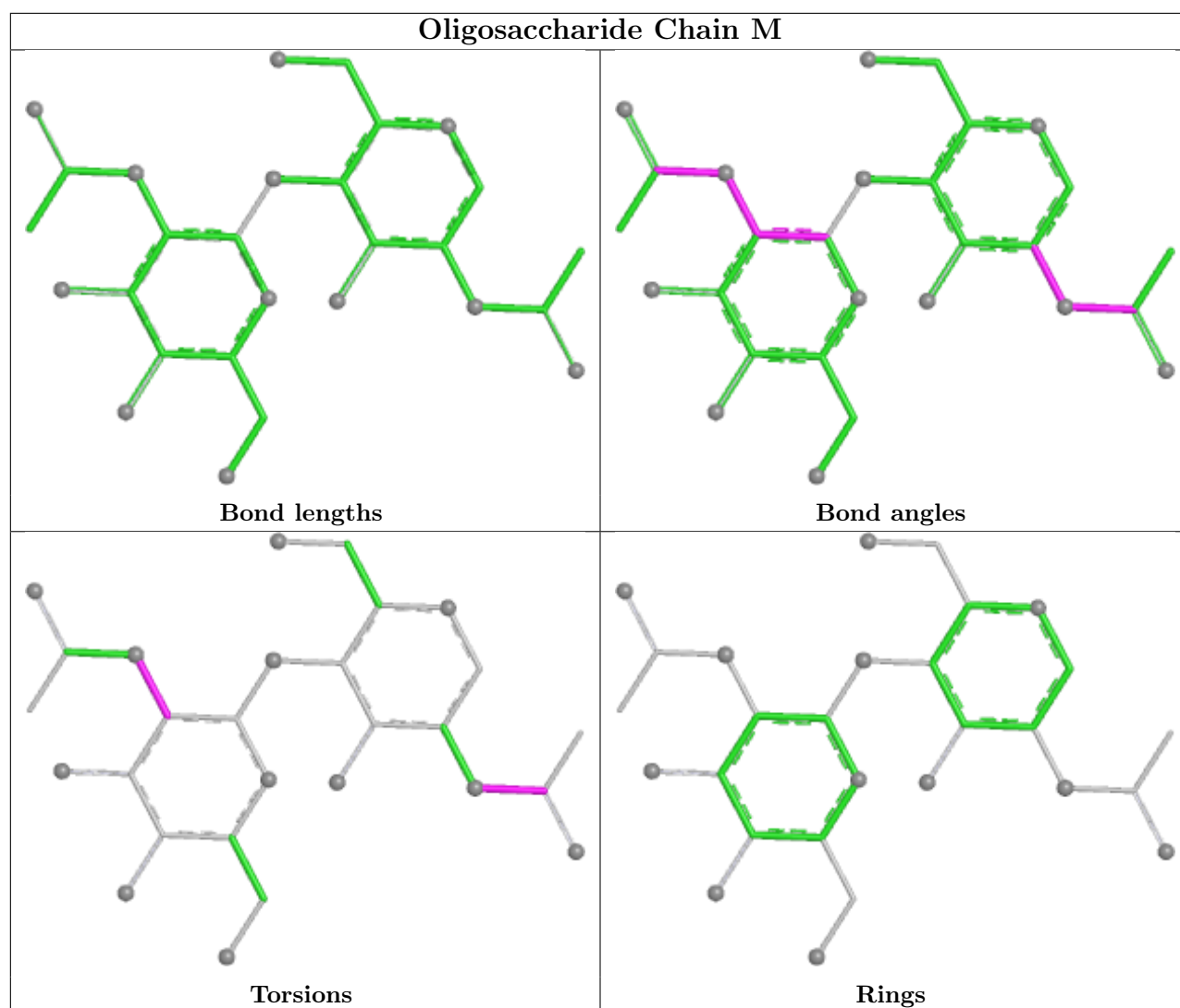












5.6 Ligand geometry [i](#)

23 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	A	4705	1	14,14,15	0.27	0	17,19,21	0.66	0
4	NAG	A	4709	1	14,14,15	0.27	0	17,19,21	0.69	0
4	NAG	B	4704	1	14,14,15	0.27	0	17,19,21	0.74	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	A	4703	1	14,14,15	0.28	0	17,19,21	0.66	0
4	NAG	A	4702	1	14,14,15	0.29	0	17,19,21	0.75	0
4	NAG	B	4709	1	14,14,15	0.28	0	17,19,21	0.64	0
4	NAG	A	4701	1	14,14,15	0.28	0	17,19,21	0.61	0
4	NAG	A	4711	1	14,14,15	0.38	0	17,19,21	0.50	0
4	NAG	B	4708	1	14,14,15	0.36	0	17,19,21	0.99	1 (5%)
4	NAG	B	4702	1	14,14,15	0.27	0	17,19,21	0.71	0
4	NAG	A	4704	1	14,14,15	0.28	0	17,19,21	0.60	0
4	NAG	B	4703	1	14,14,15	0.30	0	17,19,21	0.68	0
4	NAG	B	4705	1	14,14,15	0.28	0	17,19,21	0.61	0
4	NAG	B	4701	1	14,14,15	0.26	0	17,19,21	0.67	0
4	NAG	B	4710	1	14,14,15	0.28	0	17,19,21	0.64	0
4	NAG	A	4707	1	14,14,15	0.26	0	17,19,21	0.67	0
4	NAG	B	4711	1	14,14,15	0.38	0	17,19,21	0.48	0
4	NAG	A	4708	1	14,14,15	0.37	0	17,19,21	0.76	1 (5%)
4	NAG	B	4707	1	14,14,15	0.26	0	17,19,21	0.67	0
4	NAG	A	4710	1	14,14,15	0.26	0	17,19,21	0.52	0
4	NAG	A	4706	1	14,14,15	0.28	0	17,19,21	0.64	0
4	NAG	B	4706	1	14,14,15	0.27	0	17,19,21	0.67	0
4	NAG	A	4712	1	14,14,15	0.39	0	17,19,21	0.79	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	A	4705	1	-	0/6/23/26	0/1/1/1
4	NAG	A	4709	1	-	2/6/23/26	0/1/1/1
4	NAG	B	4704	1	-	2/6/23/26	0/1/1/1
4	NAG	A	4703	1	-	3/6/23/26	0/1/1/1
4	NAG	A	4702	1	-	2/6/23/26	0/1/1/1
4	NAG	B	4709	1	-	0/6/23/26	0/1/1/1
4	NAG	A	4701	1	-	0/6/23/26	0/1/1/1
4	NAG	A	4711	1	-	0/6/23/26	0/1/1/1
4	NAG	B	4708	1	-	3/6/23/26	0/1/1/1
4	NAG	B	4702	1	-	2/6/23/26	0/1/1/1
4	NAG	A	4704	1	-	0/6/23/26	0/1/1/1
4	NAG	B	4703	1	-	2/6/23/26	0/1/1/1
4	NAG	B	4705	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	4701	1	-	0/6/23/26	0/1/1/1
4	NAG	B	4710	1	-	0/6/23/26	0/1/1/1
4	NAG	A	4707	1	-	3/6/23/26	0/1/1/1
4	NAG	B	4711	1	-	0/6/23/26	0/1/1/1
4	NAG	A	4708	1	-	1/6/23/26	0/1/1/1
4	NAG	B	4707	1	-	3/6/23/26	0/1/1/1
4	NAG	A	4710	1	-	3/6/23/26	0/1/1/1
4	NAG	A	4706	1	-	2/6/23/26	0/1/1/1
4	NAG	B	4706	1	-	0/6/23/26	0/1/1/1
4	NAG	A	4712	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	4708	NAG	C2-N2-C7	3.44	127.50	122.90
4	A	4712	NAG	C2-N2-C7	2.43	126.15	122.90
4	A	4708	NAG	C2-N2-C7	2.26	125.92	122.90

There are no chirality outliers.

5 of 29 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	4707	NAG	C8-C7-N2-C2
4	A	4707	NAG	O7-C7-N2-C2
4	A	4710	NAG	C1-C2-N2-C7
4	A	4710	NAG	C8-C7-N2-C2
4	A	4710	NAG	O7-C7-N2-C2

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	4702	NAG	1	0
4	B	4703	NAG	1	0
4	B	4701	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

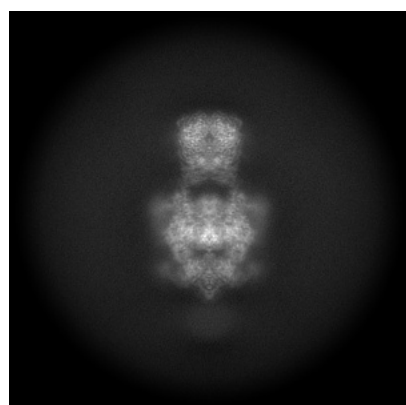
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45967. These allow visual inspection of the internal detail of the map and identification of artifacts.

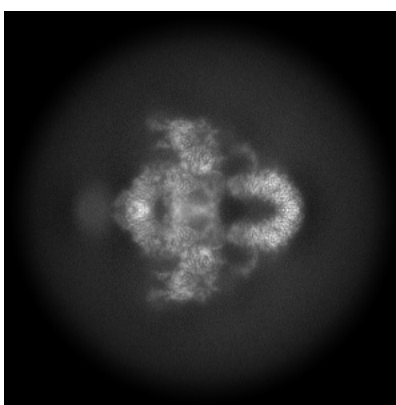
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

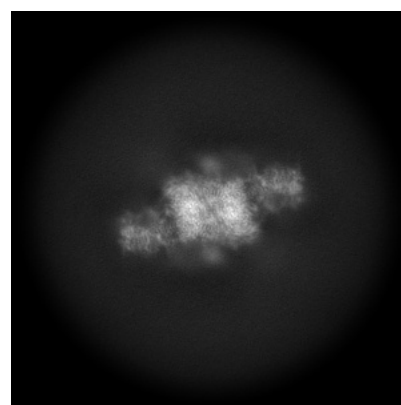
6.1.1 Primary map



X



Y

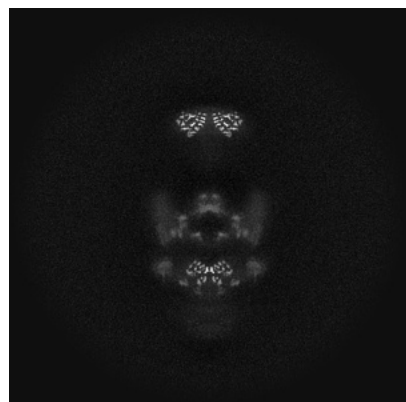


Z

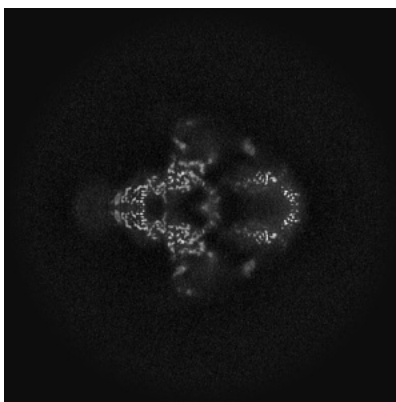
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

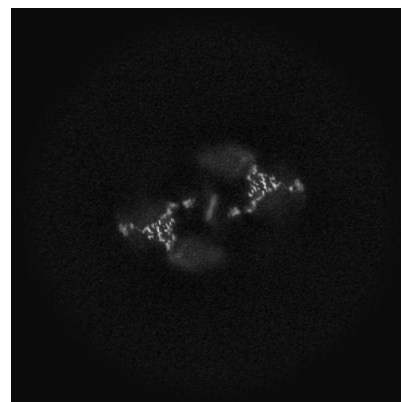
6.2.1 Primary map



X Index: 256



Y Index: 256

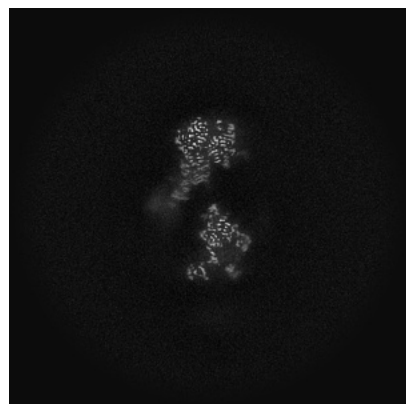


Z Index: 256

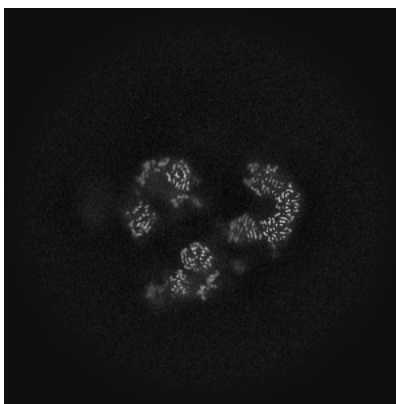
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

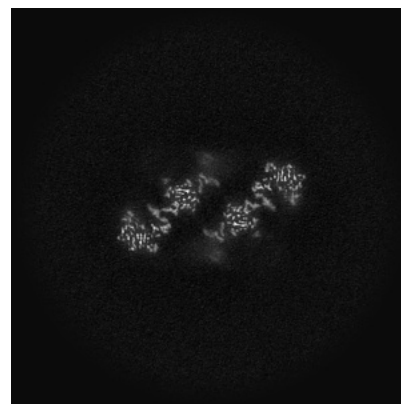
6.3.1 Primary map



X Index: 224



Y Index: 233

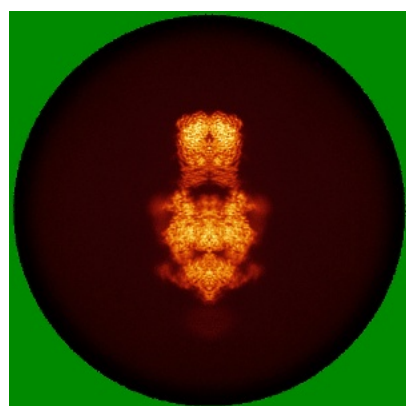


Z Index: 231

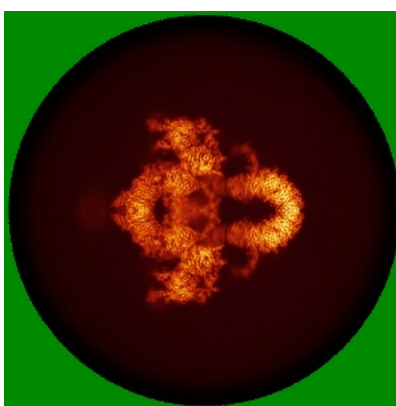
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X



Y

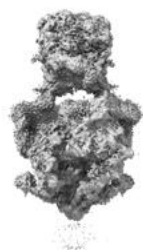


Z

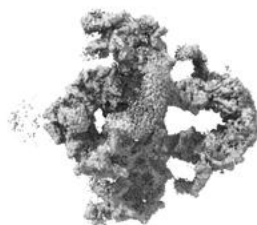
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

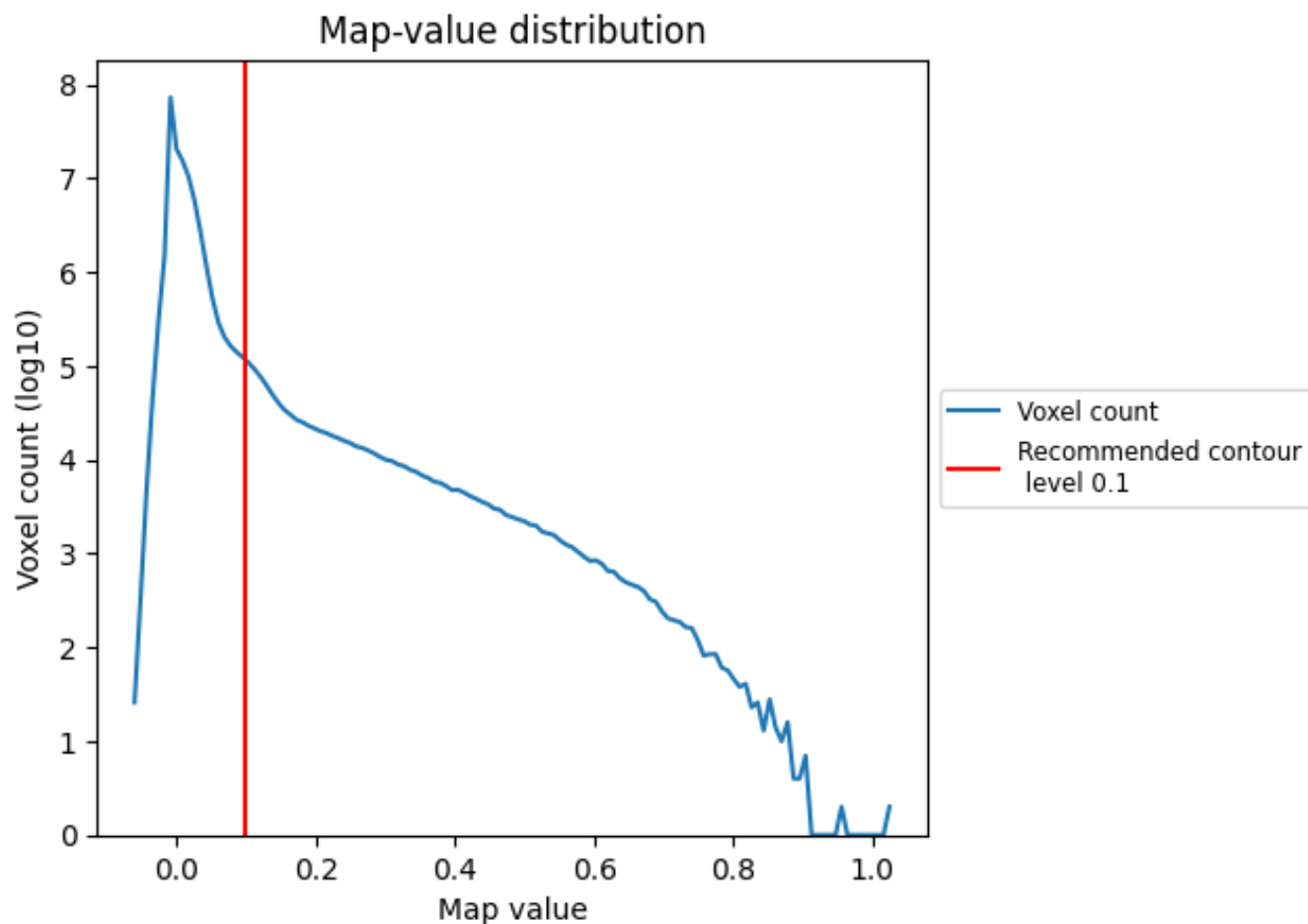
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

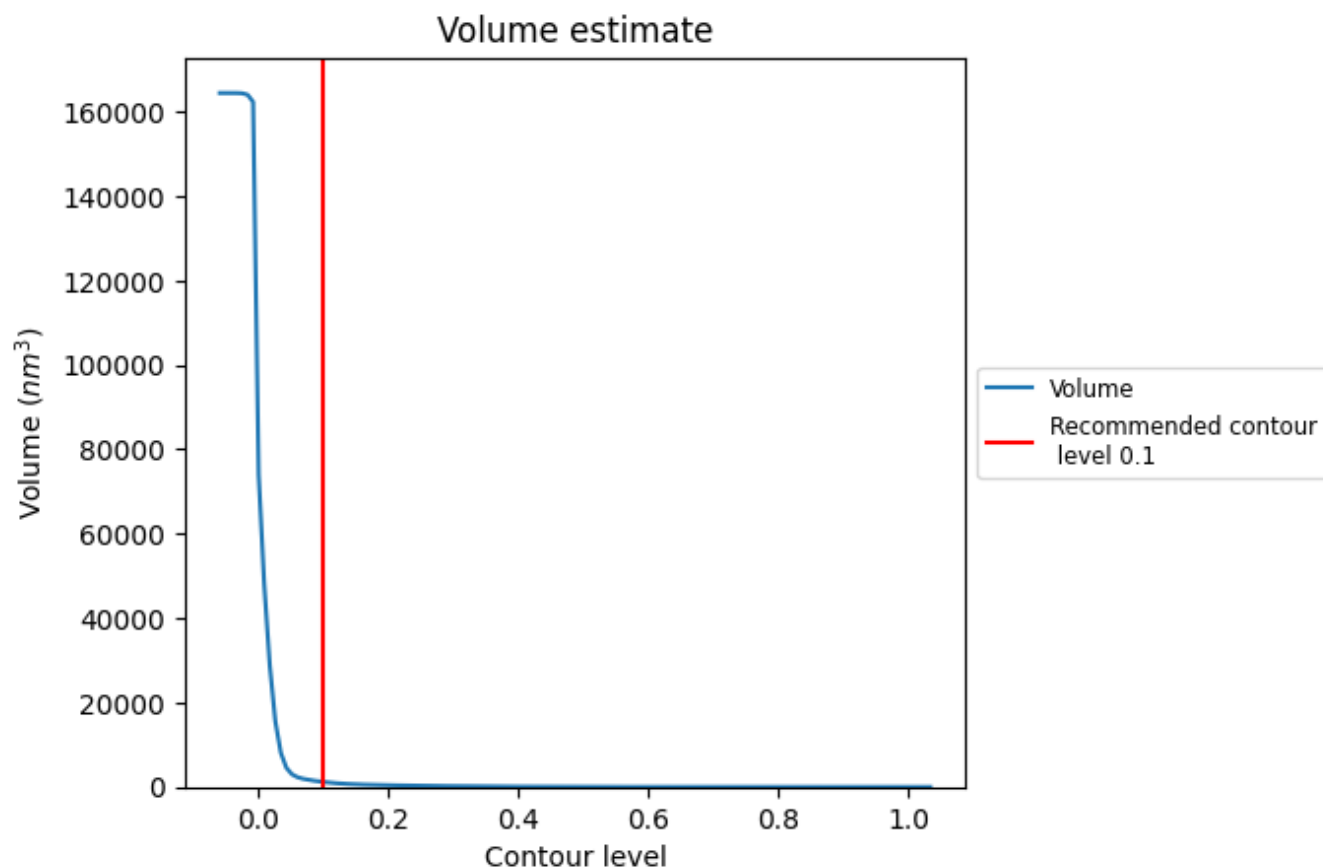
This section contains the results of statistical analysis of the map.

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.

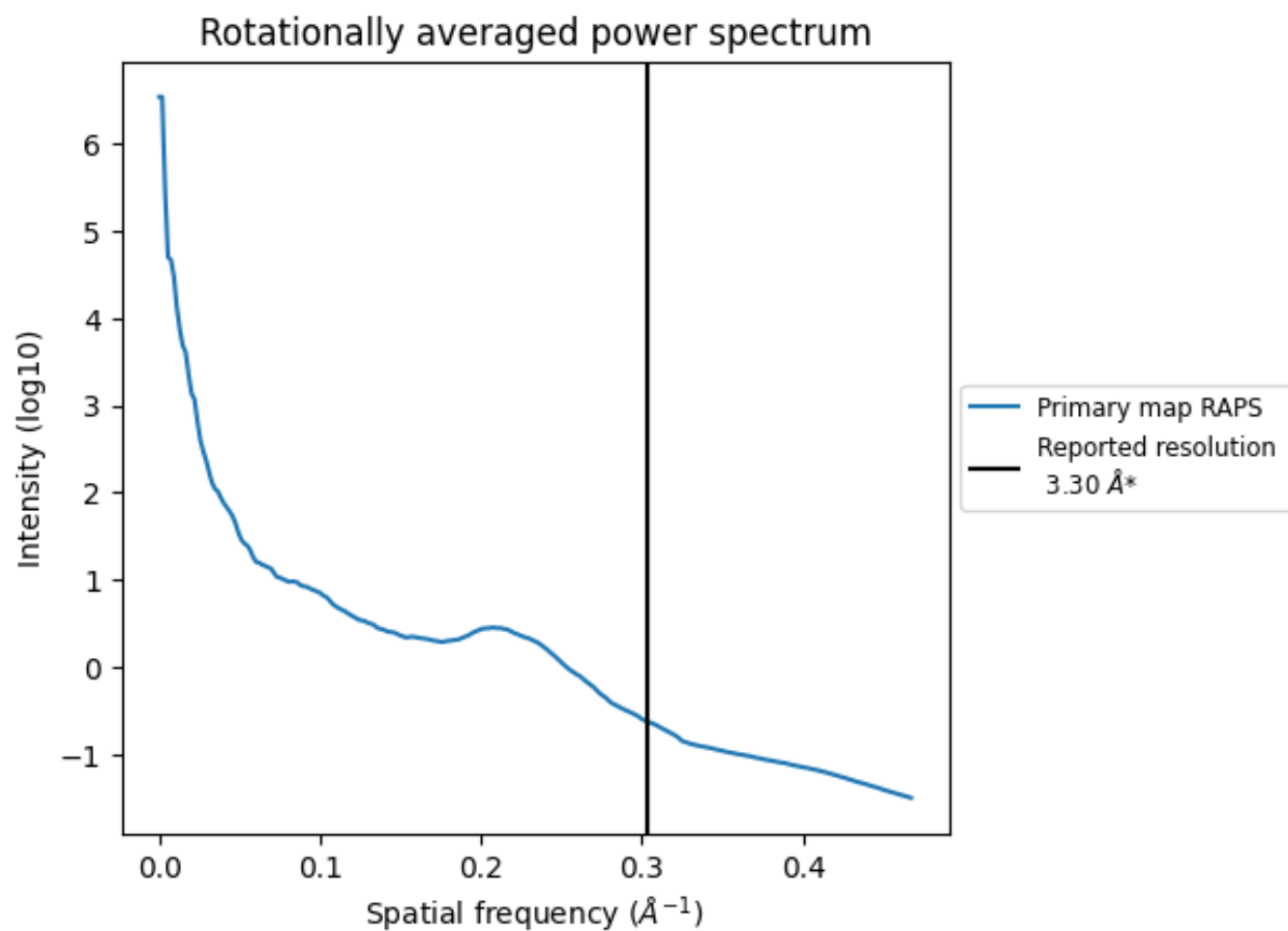
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1187 nm^3 ; this corresponds to an approximate mass of 1072 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



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

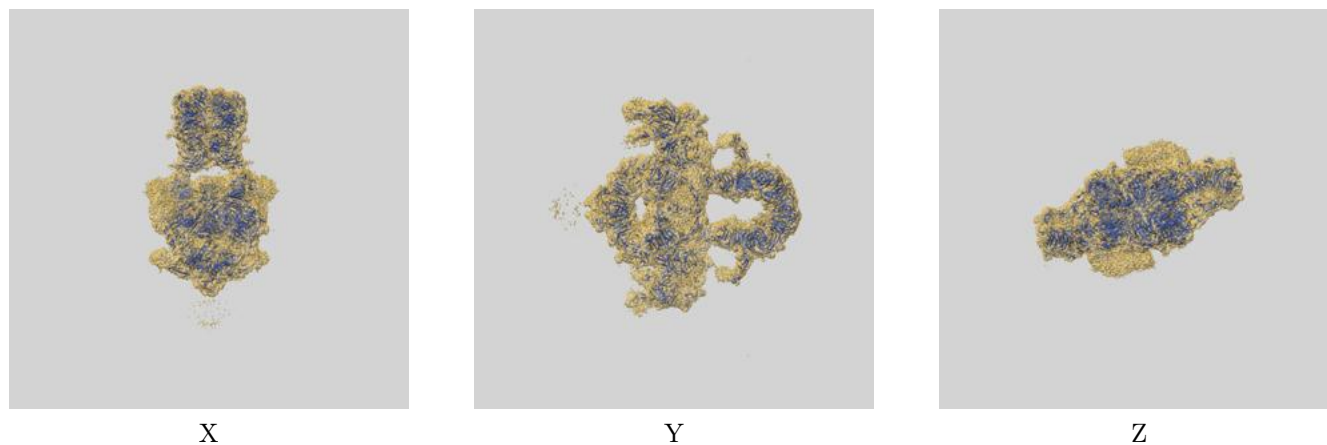
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

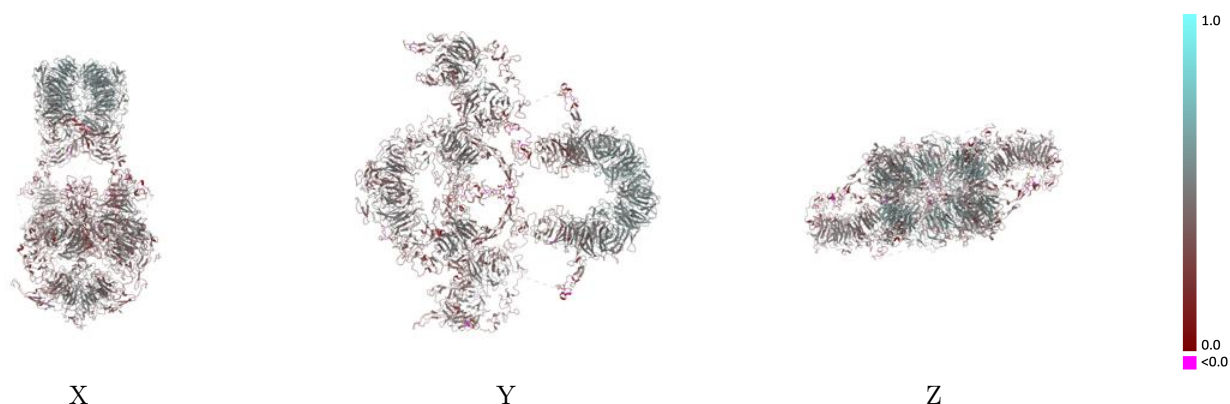
This section contains information regarding the fit between EMDB map EMD-45967 and PDB model 9CWM. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



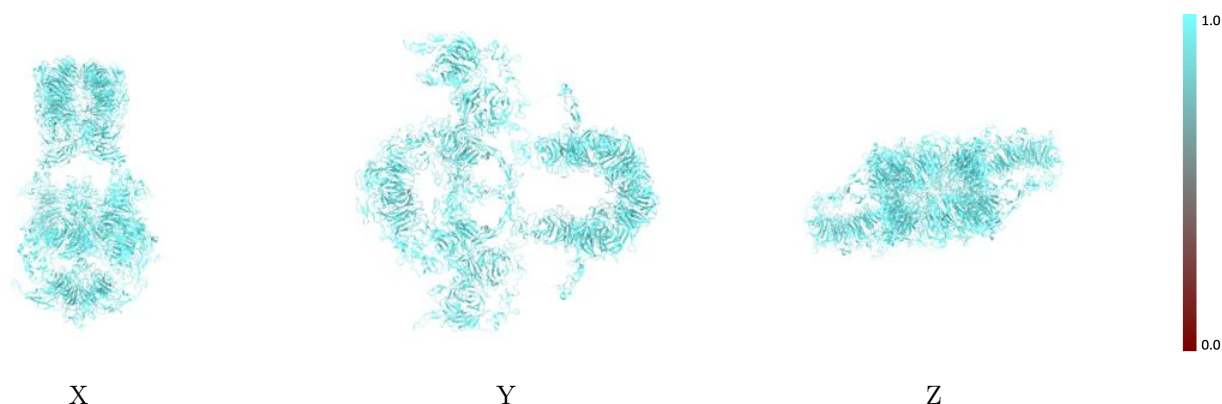
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



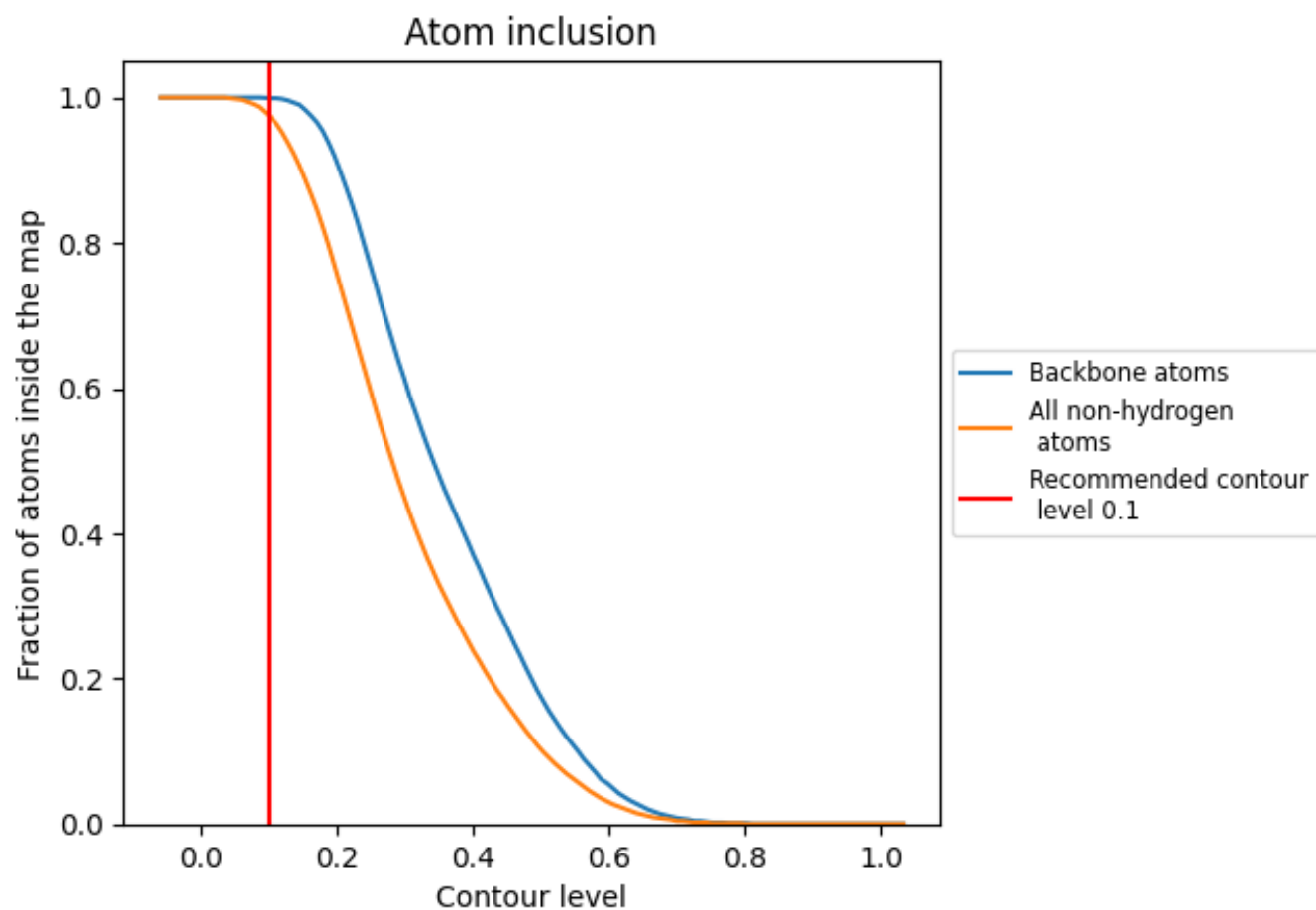
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).































9.4 Atom inclusion ⓘ



At the recommended contour level, 100% of all backbone atoms, 98% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9750	 0.4030
A	 0.9760	 0.4050
B	 0.9750	 0.4010
C	 0.9490	 0.4310
D	 0.9490	 0.3520
E	 1.0000	 0.4100
F	 0.8970	 0.1850
G	 0.8930	 0.3650
H	 1.0000	 0.4200
I	 0.9740	 0.4470
J	 0.9490	 0.3580
K	 1.0000	 0.4160
L	 0.8970	 0.2190
M	 0.9640	 0.3420
N	 0.8210	 0.1740

