



## wwPDB EM Validation Summary Report ⓘ

Jul 28, 2025 – 05:39 PM EDT

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.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev126  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0rc1  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.45.1

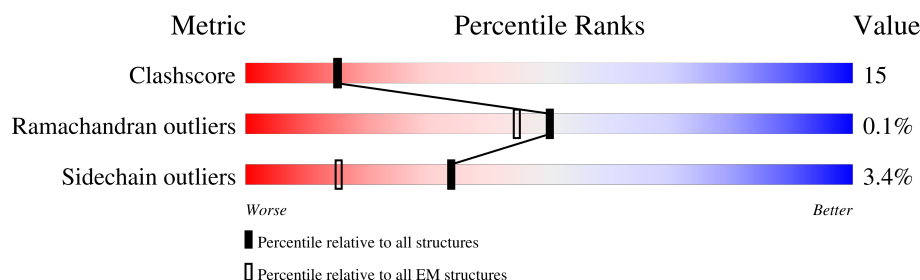
# 1 Overall quality at a glance

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.




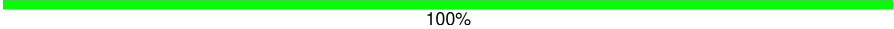
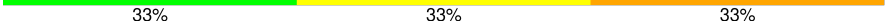
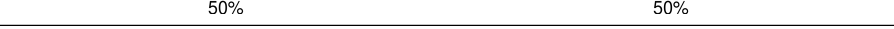

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 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	
2	E	3	
2	F	3	
2	I	3	
2	J	3	

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Mol	Chain	Length	Quality of chain
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.



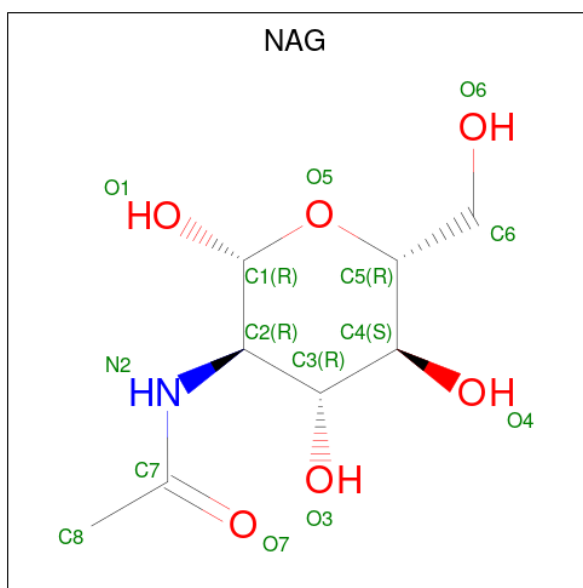
Mol	Chain	Residues	Atoms				AltConf	Trace
2	C	3	Total	C	N	O	0	0
			39	22	2	15		
2	D	3	Total	C	N	O	0	0
			39	22	2	15		
2	E	3	Total	C	N	O	0	0
			39	22	2	15		
2	F	3	Total	C	N	O	0	0
			39	22	2	15		
2	I	3	Total	C	N	O	0	0
			39	22	2	15		
2	J	3	Total	C	N	O	0	0
			39	22	2	15		
2	K	3	Total	C	N	O	0	0
			39	22	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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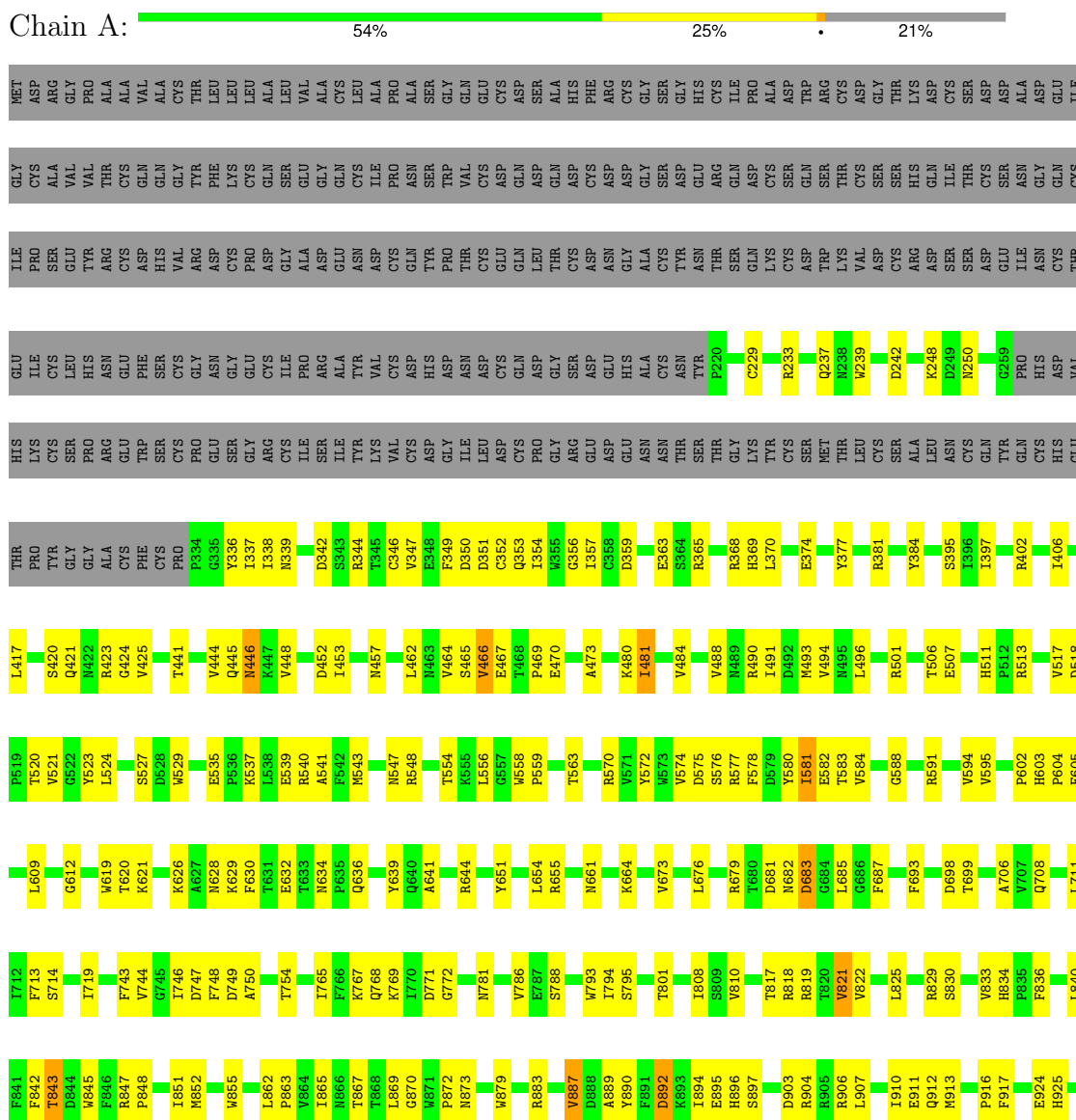
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Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	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











D2242	S2106	S1961	M1834	S1677	H1566	V1451	G1350	CYS	G1209	D1129	T1023	H896	Y799	V673
Y2247	D2113	P1963	L1835	W1685	L1567	T1452	N1351	ASP	D1212	T1130	E1024	S897	W800	S677
V2251	D2114	G1965	T1838	P1686	H1576	S1453	S1352	ARG	N1216	D1131	Q1025	D903	T801	H678
S2254	S2115	I1966	R1841	L1687	R1578	Q1454	S1354	ASN	D1217	N1132	C1026	R904	H804	L685
S2254	D2121	A1967	S1844	V1692	L1481	L1481	D1355	ASP	D1218	D1133	L1044	E910	I808	G686
I2257	T2124	L1973	I1845	K1696	V1462	V1462	N1357	GLY	E1219	C1134	G1045	E911	M811	F687
I2258	R2125	Y1974	E1846	L1712	G1485	G1485	G1359	MET	A1220	D1136	D1046	Q912	I808	G686
R2262	R2126	T1976	L1848	G1713	H1584	I1467	T1361	SER	T1224	K1141	C1051	A935	F693	F693
V2270	L2127	Q1979	D1853	L1714	M1588	I1468	E1362	ASP	R1225	N1142	H1052	I936	K816	G694
V2270	S2133	E1984	I1854	Q1718	R1589	V1469	E1363	LYS	P1227	C1149	D1056	V939	T817	F695
V2285	T2137	R1985	R1855	H1721	T1590	I1480	C1364	ASP	G1228	Q1150	E1057	R938	R818	C704
V2285	V2138	V1986	R1856	H1721	V1591	I1480	V1365	CYS	F1235	Q1153	Q1058	R940	R819	L711
I2290	T2139	R1987	R1857	F1722	V1592	S1483	Q1366	PRO	Q1236	F1154	L1059	R940	W821	I719
I2290	H2140	K1988	T1858	Y1723	V1593	D1484	E1367	GLN	C1237	N1155	C1060	G944	R829	R720
I2300	G2141	T1859	D1484	Y1723	I1597	D1484	F1368	PRO	C1238	C1156	T1062	R947	S830	
S2304	E2144	D1864	D1864	W1731	Q1487	Q1487	G1370	PHE	E1239	P1157	N1065	T948	W833	V732
K2305	N2145	L1868	L1868	C1740	W1491	W1491	K1372	ARG	I1242	N1158	S1068	V949	H834	M733
N2309	V2147	L1868	L1868	P1746	I1505	I1508	C1373	SER	I1244	R1160	A1071	I957	A837	F742
P2312	A2151	G1871	G1871	F1747	D1606	T1508	L1374	TRP	E1249	T1162	F1072	I960	F841	F743
P2313	N2163	F1872	F1872	V1751	L1612	L1510	G1378	GLN	C1250	F1166	E1078	I961	F842	G745
D2318	N2163	I1755	D1616	I1755	M1615	I1514	L1381	CYS	D1251	V1167	E1078	K961	T843	F746
N2319	A2164	I1756	D1616	I1756	M1615	I1514	L1381	GLN	G1252	V1167	E1078	K961	T843	D747
N2319	F2166	F1757	Y1618	F1757	Y1618	Y1618	K1386	GLY	P1254	D1170	C1079	T969	W845	F748
D2325	V2166	M1622	M1622	M1622	M1622	M1622	D1390	HIS	D1255	K1172	W1084	N972	F846	T754
V2326	E2168	L1636	L1636	L1636	L1636	L1636	D1390	ASN	C1256	C1173	D1087	N972	R847	I755
T2327	I2176	V1783	D1626	D1626	D1626	D1626	Q1402	CYS	L1257	V1175	D1087	C974	P848	K762
D2330	N2177	E1784	V1635	V1635	V1635	V1635	H1403	VAL	S1260	D1176	K1088	T978	M852	I765
K2331	R2181	M1905	V1635	V1635	V1635	V1635	C1404	ASN	D1261	G1177	H1090	H979	L862	F766
V2341	R2182	D1906	I1636	I1636	I1636	I1636	Y1405	LEU	E1262	G1178	D1091	P980	P863	K767
P2345	P2192	V1910	H1644	H1644	H1644	H1644	S1536	SER	H1263	D1179	C1092	N981	V864	Q768
P2366	H2194	D1927	P1645	P1645	P1645	P1645	K1537	VAL	P1268	E1180	G1095	C988	I865	K769
T2374	V2197	A1936	L1648	L1648	L1648	L1648	R1543	CYS	S1273	V1184	S1096	C988	T867	G772
Q2376	D2198	V1937	T1649	T1649	T1649	T1649	K1549	ASP	SER	L1185	D1097	V991	T868	T773
L2390	N2201	R1940	L1650	L1650	L1650	L1650	N1550	GLY	TYR	N1186	E1098	Q995	T868	G774
L2390	L2206	R1945	V1655	V1655	V1655	V1655	L1551	CYS	HIS	C1187	H1099	R996	N873	L777
A2393	Y2209	D1949	W1657	W1657	W1657	W1657	K1549	ASP	CYS	Q1191	C1109	R996	G874	L778
L2394	Y2209	T1951	T1658	T1658	T1658	T1658	N1550	ASP	HIS	F1192	C1109	R996	L875	A779
S2397	P2213	Q2093	R1660	R1660	R1660	R1660	E1422	CYS	ASP	K1193	T1112	P1001	M875	A780
L2398	R2233	M1954	V1665	V1665	V1665	V1665	S1423	PRO	ASN	D1198	Q1113	M1004	R883	N761
S2400	P2236	L1956	R1667	R1667	R1667	R1667	S1442	GLY	ASN	T1201	Y1114	M1004	L884	
L2401		L1960	M1563	M1563	M1563	M1563	Q1443	THR	ASN	G1202	M118	M1009	Y885	N785
								GLU	CYS	I1011	N118	M1009	Y885	N786
								SER	ILE	V1203	C1121	L1011	V887	
								ARG	HIS	T1204	I1122	G1015	D882	A790
								ALA	ALA	T1206	S1123	D1016	R893	W793
								TRP	ALA	R1206	K1124	D1016	I894	I794
								LEU	LEU		N1125	E1020	S795	S795

D3747	Q3612	D3496	T3362	I3265	E3053	ASP	GLY	ASN	PRO	R2711	Y2607	V9513	S2409
D3750	C3613	L3502	A3363	R3288	D3054	VAL	GLY	PRO	ARG	C2712	T2608	L2614	S2414
S3773	D3614	Y3507	L3364	L3289	N3055	CYS	ARG	THR	GLU	I2713	R2614	D2615	T2414
S3774	C3619	C3508	P3367	P3270	D3056	THR	CYS	CYS	ILE	S2714	I2615	P2516	
R3775	N3622	M3509	T3371	A3271	E3063	ASP	PRO	THR	CYS	D2724	A2618	G2519	V2417
W3776	D3626	P3510	I3372	A3272	L3087	GLY	SER	THR	ASN	C2725	C2725	Y2520	V2421
I3777	D3626	C3512	N3376	E3273	P3073	THR	GLU	HIS	GLY	C2726	A2619	L2521	
H3780	H3629	C3512	N3376	V3277	T3074	ASP	ILE	THR	VAL	D2727	K2620	Y2522	L2424
Y3781	H3629	S3513	Y3380	D3278	C3075	ASN	CYS	SER	ASN	S2728	G2623	W2523	L2425
N3782	R3633	Q3516	Y3380	S3281	C3075	GLN	ASP	SER	CYS	E2733	H2629	K2531	Y2426
D3783	R3633	F3517	R3192	R3282	H3078	CYS	ASP	GLY	HIS	E2733	H2629	I2532	Y2427
C3784	F3640	L3518	Q3193	R3282	E3079	THR	ASN	GLU	ASP	A2737	L2633	E2532	S2428
D3789	R3641	E3390	N3194	K3283	E3079	ARG	ASN	PHE	ASN	L2738	L2634	R2534	S2428
E3790	N3644	N3522	S3195	L3284	C3081	ARG	CYS	CYS	THR	H2739	L2634	A2535	V2429
R3791	C3647	H3398	C3082	L3287	C3082	THR	GLY	ALA	SER	T2740	P2637	T2536	R2432
T3797	D3657	R3399	P3199	Y3200	R3086	CYS	ASP	SER	ASP	T2747	I2640	R2542	I2433
C3798	K3531	H3400	Y3200	Y3200	C3087	SER	MET	GLY	GLU	CYS	I2640	V2543	Y2434
H3799	C3532	I3413	F3203	F3203	C3087	GLU	THR	ARG	LYS	VAL	I2641	P2544	F2435
P3800	D3533	I3414	S3204	S3204	E3088	GLU	GLU	ILE	CYS	ALA	T2642	I2545	N2438
E3801	D3665	I3415	Y3208	S3297	E3088	THR	LYS	PRO	CYS	ASN	V2643	V2546	L2439
Y3802	E3666	I3415	C3091	D3298	M3090	ASP	ARG	GLN	ASP	GLY	V2644	S2547	A2440
Q3803	P3667	F3416	K3092	C3092	C3091	THR	ARG	GLN	ASP	ARG	S2548	S2548	S2441
Q3804	E3670	I3420	N3211	C3094	C3092	CYS	HIS	ARG	ARG	CYS	S2549	S2549	
G3808	T3682	T3423	L3221	D3099	C3094	GLY	TRP	THR	THR	GLN	I2648	L2550	Y2448
H3809	C3810	V3430	L3226	I3103	S3104	THR	HIS	TRP	THR	CYS	I2649	T2550	A2449
C3810	T3688	Y3436	V3229	D3106	D3106	GLY	GLN	TYR	CYS	GLN	Q2650	P2553	T2450
Y3811	F3318	N3446	F3318	I3106	C3107	LEU	CYS	ASP	ASP	SER	C2651	P2553	T2450
D3818	R3691	T3570	P3323	C3111	C3107	ILE	ASP	PHE	ASP	GLY	I2665	L2556	S2453
G3819	C3692	N3573	R3324	V3312	R3103	CYS	ASN	ASP	ASP	THR	I2665	L2556	S2453
S3820	I3693	A3574	G3325	G3325	S3104	PRO	ASN	SER	ALA	ASN	A2673	V2567	H2456
A3821	P3694	F3451	L3326	L3326	D3106	ILE	CYS	SER	ALA	THR	I2679	L2566	T2457
D3822	K3695	F3452	A3327	A3327	C3113	ASP	GLY	THR	THR	GLY	H2679	L2567	P2458
C3823	V3698	I3454	L3328	L3328	E3114	VAL	CYS	GLU	ILE	CYS	Q2673	Q2573	I2476
L3824	L3824	N3577	R3329	H3329	C3114	ASN	VAL	PRO	ILE	THR	Y2683	R2574	I2476
D3825	C3705	C3578	P3330	P3330	H3115	ASP	ASN	ALA	PRO	ARG	Y2684	I2575	L2486
E3829	R3706	S3582	Q3331	Q3331	H3124	ARG	ASP	SER	VAL	ASP	L2685	E2576	
C3832	D3707	D3583	Y3332	Y3332	H3124	THR	ARG	GLY	THR	CYS	R2685	R2585	M2489
P3833	N3708	E3584	C3332	C3332	T3129	PRO	PRO	GLY	TYR	ASN	R2689	E2586	I2490
T3834	S3709	D3585	L3335	L3335	N3035	ASP	HIS	LEU	LEU	ALA	S2491	S2491	V2502
R3835	D3710	R3461	Y3336	Y3336	L3130	THR	SER	CYS	CYS	ALA	V2587	V2587	S2492
F3836	E3711	N3467	W3337	W3337	C3135	ARG	GLU	GLU	ASP	THR	H2691	H2492	M2493
P3837	Q3712	F3468	Y3345	Y3345	S3136	CYS	THR	ARG	GLY	THR	C2692	L2494	G2494
R3838	H3720	C3469	I3346	I3346	Q3040	ILE	CYS	THR	ASP	GLU	V2694	E2495	
G3839	P3721	L3479	G3347	G3347	I3045	PRO	GLY	CYS	VAL	PHE	V2694	L2598	T2501
A3840	V3722	G3485	K3356	K3356	S3046	ALA	PRO	ALA	GLY	MET	S2704	L2600	CYS
Y3841	N3729	P3608	T3259	T3259	K3047	ASP	GLY	ASP	GLY	ASN	T2705	Y2601	L2502
C3842	Q3843	E3609	N3260	N3260	K3147	THR	PHE	GLU	ASP	ASN	T2706	G2603	L2503
D3744	D3744	S3610	K3261	K3261	R3148	VAL	THR	ASP	ASN	ARG	C2707	Q2603	R2505
M3846		W3611	I3360	I3360	R3148	CYS	LYS	SER	LYS	ARG	S2708	Y2604	
			S3361	S3361	V3151	ASP	GLY	ASP	GLU	ILE	I2710	Y2606	

F3847	LYS	LEU	E4072	L4179	E4293	VAL	GLU	GLN
E3848	PRO	ASN	E4072	L4180	Y4294	ALA	ASN	LYS
C3849	THR	GLY	D4080	S4181	W4295	VAL	VAL	GLU
K3850	PRO	GLY	D4080	Q4136	N4298	LEU	ASP	SER
N3851	LYS	PHE	Y4083	T4136	N4298	THR	ASN	VAL
V3853	CYS	ILE	T4084	T4130	Q4302	ILE	ASN	ALA
C3854	THR	CYS	Q4085	M4199	K4307	LEU	TYR	THR
I3855	GLU	SER	A4086	T4202	T4308	LEU	GLY	PRO
P3856	TYR	CYS	V4087	T4202	L4309	ILE	SER	PRO
P3857	GLU	THR	D4088	W4203	V4310	VAL	ILE	SER
Y3858	TYR	ALA	Y4089	W4204	V4311	ILE	ASN	PRO
Y3859	LYS	GLY	D4090	G4205	M4312	GLY	PRO	SER
D3862	CYS	F3995	W4091	P4208	W4313	ALA	SER	LEU
C3863	GLY	N3998	D4092	P4208	W4314	ALA	GLU	LEU
D3863	ASN	V3999	P4093	L4209	L4315	ILE	GLU	ALA
G3870	HIS	F4000	L4098	I4210	T4316	ILE	VAL	LYS
S3871	CYS	D4001	S4099	F4211	Q4317	ALA	PRO	PRO
D3872	ILE	S4004	V4100	S4212	I4320	GLY	GLU	LYS
E3873	PRO	C4005	V4101	D4219	F4321	ALA	THR	PRO
E3874	HIS	L4006	Y4102	D4219	H4322	PHE	ASN	PRO
L3875	ASP	D4007	Y4103	L4223	Q4323	HIS	THR	ARG
L3879	ASN	D4008	R4106	V4224	P4354	THR	GLU	ARG
D3880	CYS	C4017	K4116	L4228	F4359	ARG	PRO	ASP
F3889	ASP	C4021	I4120	G4229	C4367	THR	ALA	PRO
ARG	ALA	R4022	E4124	W4230	P4374	GLY	VAL	THR
CYS	ASP	R4025	D4135	P4231	P4380	LEU	GLN	ALA
ASN	CYS	G4026	D4242	D4243	C4381	ALA	VAL	THR
ASN	GLY	E4029	M4142	W4246	R4382	LEU	THR	GLU
ARG	TRP	C4030	P4144	S4247	Y4390	LEU	LYS	LEU
ILE	SER	Y4031	D4145	K4250	L4396	PRO	ASN	PHE
TVR	GLU	D4034	R4154	T4254	P4397	SER	PHE	LYS
HIS	LEU	G4035	H4155	E4255	C4397	LEU	LYS	ASP
GLU	GLY	F4036	T4156	T4256	K4400	LEU	ARG	THR
VAL	CYS	T4037	Y4157	I4257	Y4409	LEU	LYS	THR
ASN	LYS	S4038	W4158	G4261	E4411	VAL	THR	GLU
GLY	GLY	W4039	S4159	V4266	ALA	GLN	ASP	ASP
VAL	LYS	S4040	D4160	A4271	ALA	VAL	THR	GLU
ASP	GLU	D4041	N4163	M4272	PHE	GLY	ASN	GLU
ASP	ARG	R4042	R4165	I4166	SER	VAL	GLY	VAL
CYS	THR	C4045	E4167	L4277	ILE	VAL	ASN	PRO
GLY	GLU	C4046	K4170	D4278	THR	GLN	ILE	TYR
ASP	ASN	C4047	L4171	F4280	ILE	THR	ALA	ALA
ALA	THR	L4057	Y4059	L4284	ARG	GLN	GLN	GLN
GLY	GLN	Y4062	Y4067	W4286	PRO	VAL	VAL	VAL
THR	ASN	R4063	R4174	Y4175	GLY	THR	THR	THR
GLU	CYS	Y4067	W4178		THR	ALA	ASN	ALA
HIS	THR				ASP		SER	
CYS	GLN							

- 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, 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	0.26	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	76
1	B	3680/4655 (79%)	3478 (94%)	197 (5%)	5 (0%)	48	76
All	All	7363/9310 (79%)	6956 (94%)	400 (5%)	7 (0%)	50	76

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	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	3150/4105 (77%)	3038 (96%)	112 (4%)	30 57
All	All	6300/8210 (77%)	6085 (97%)	215 (3%)	34 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	1,2	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	1,2	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	1,2	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	1,2	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	1,3	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	1,2	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	1,2	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	1,2	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	1,2	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	1,3	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	1,2	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	1,2	-	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	1,2	-	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	1,2	-	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	1,2	-	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	1,3	-	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	1,2	-	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	1,2	-	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	1,2	-	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	1,2	-	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	1,3	-	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	1,2	-	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

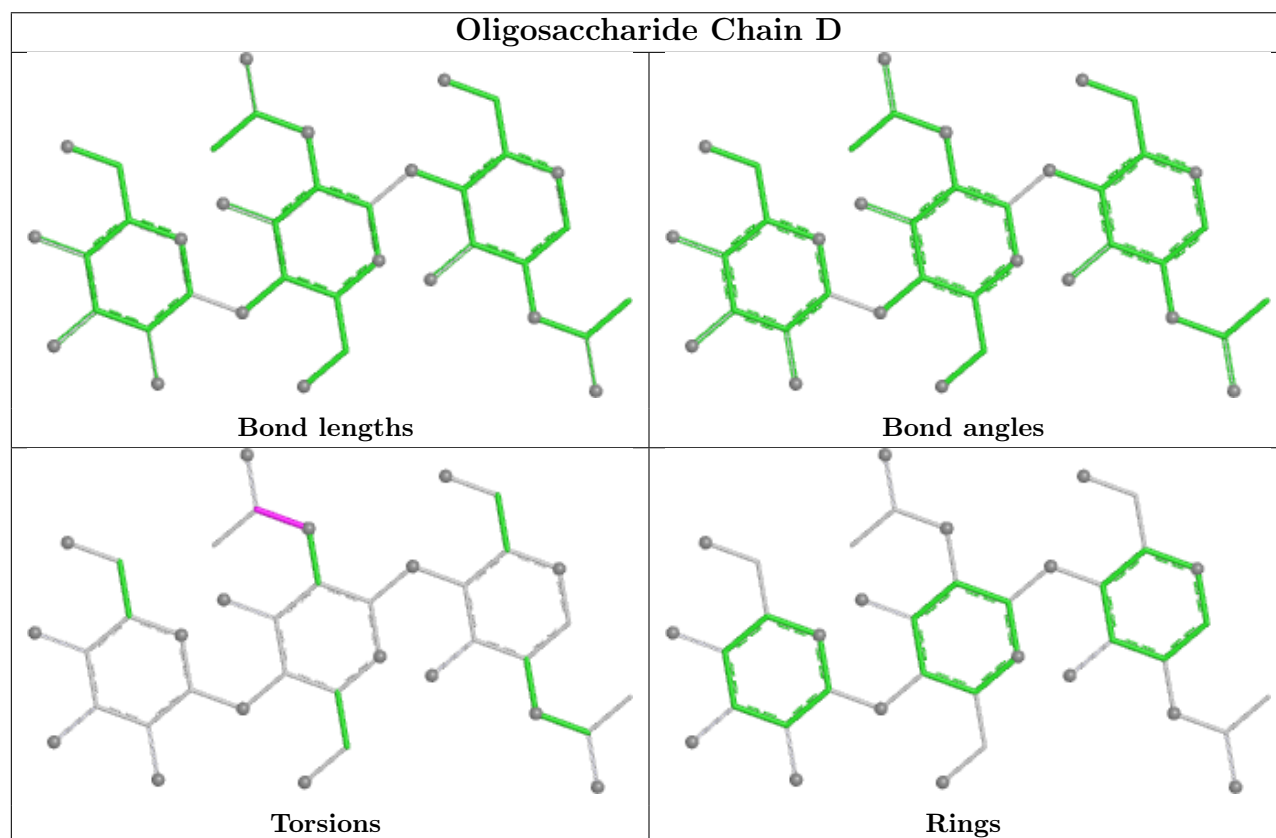
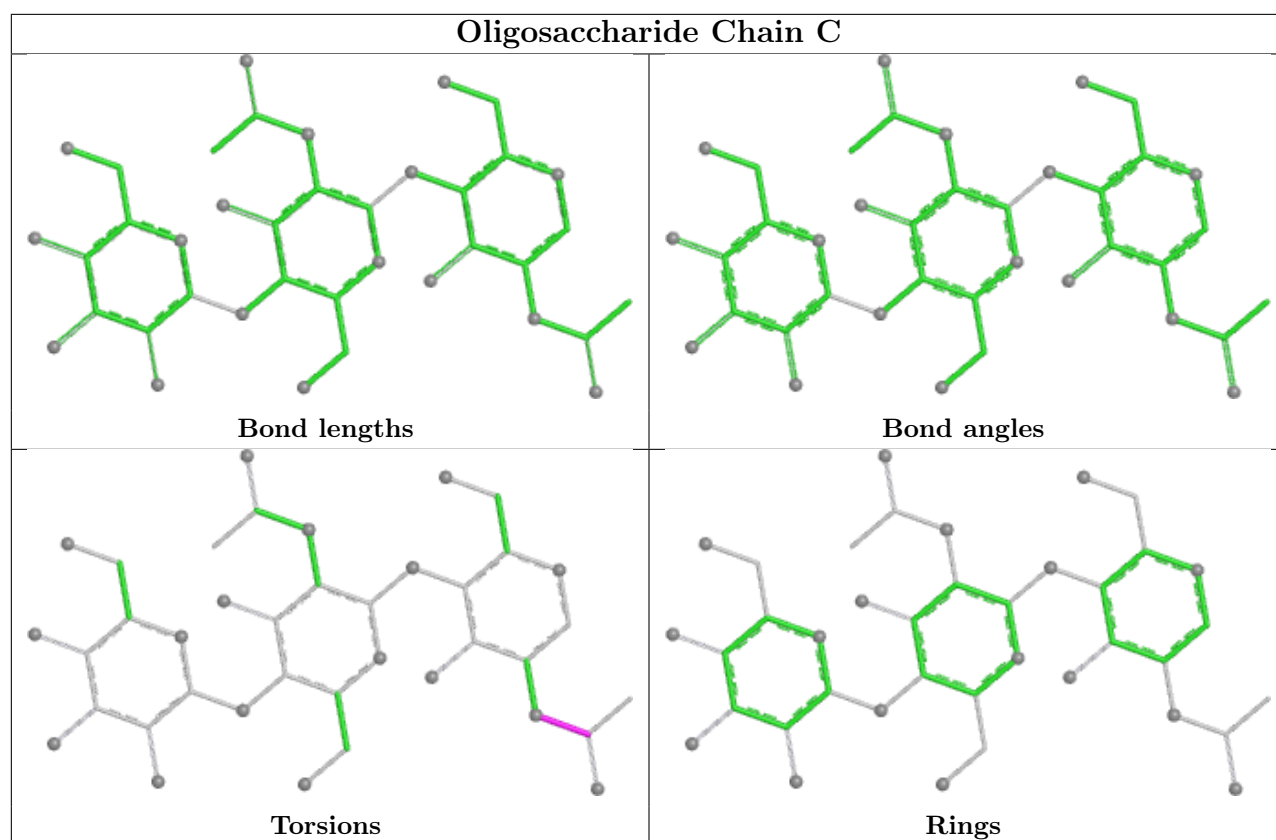
There are no ring outliers.

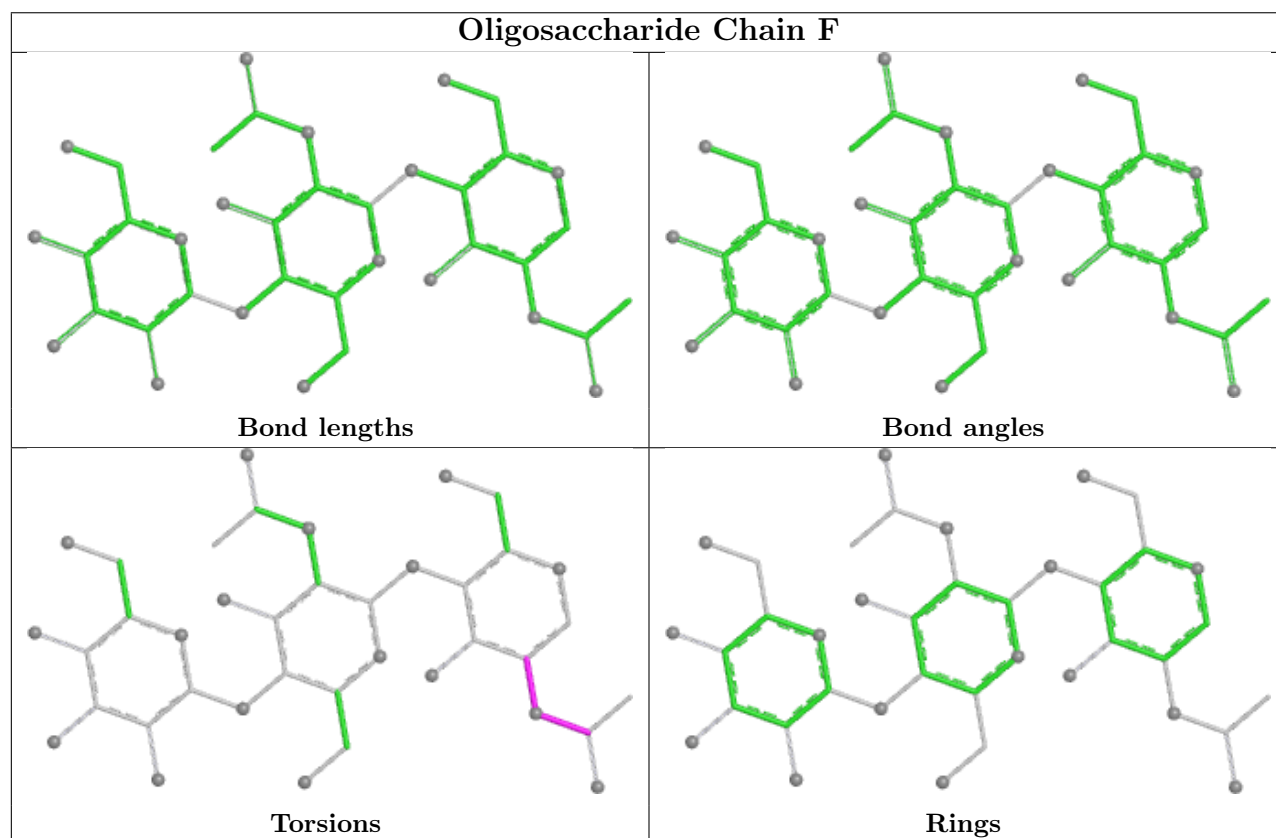
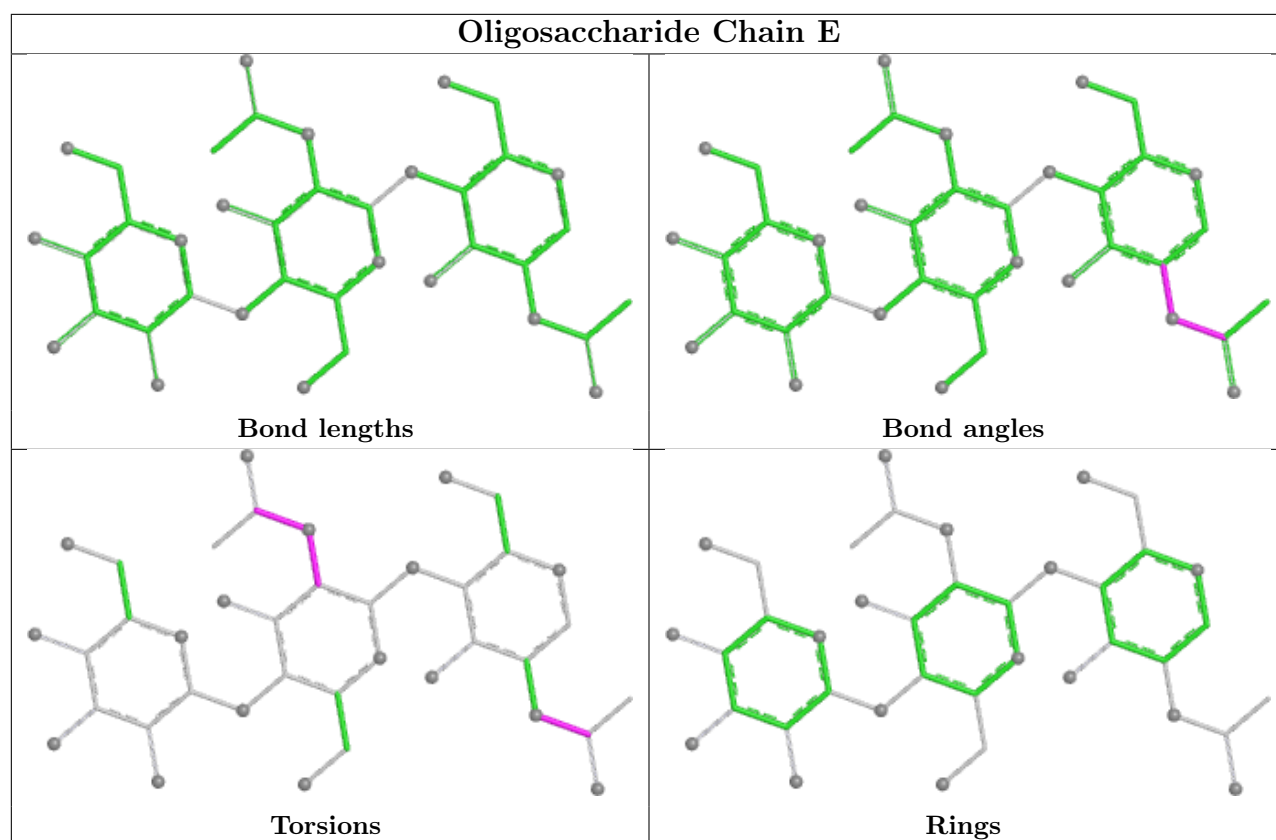
15 monomers are involved in 32 short contacts:

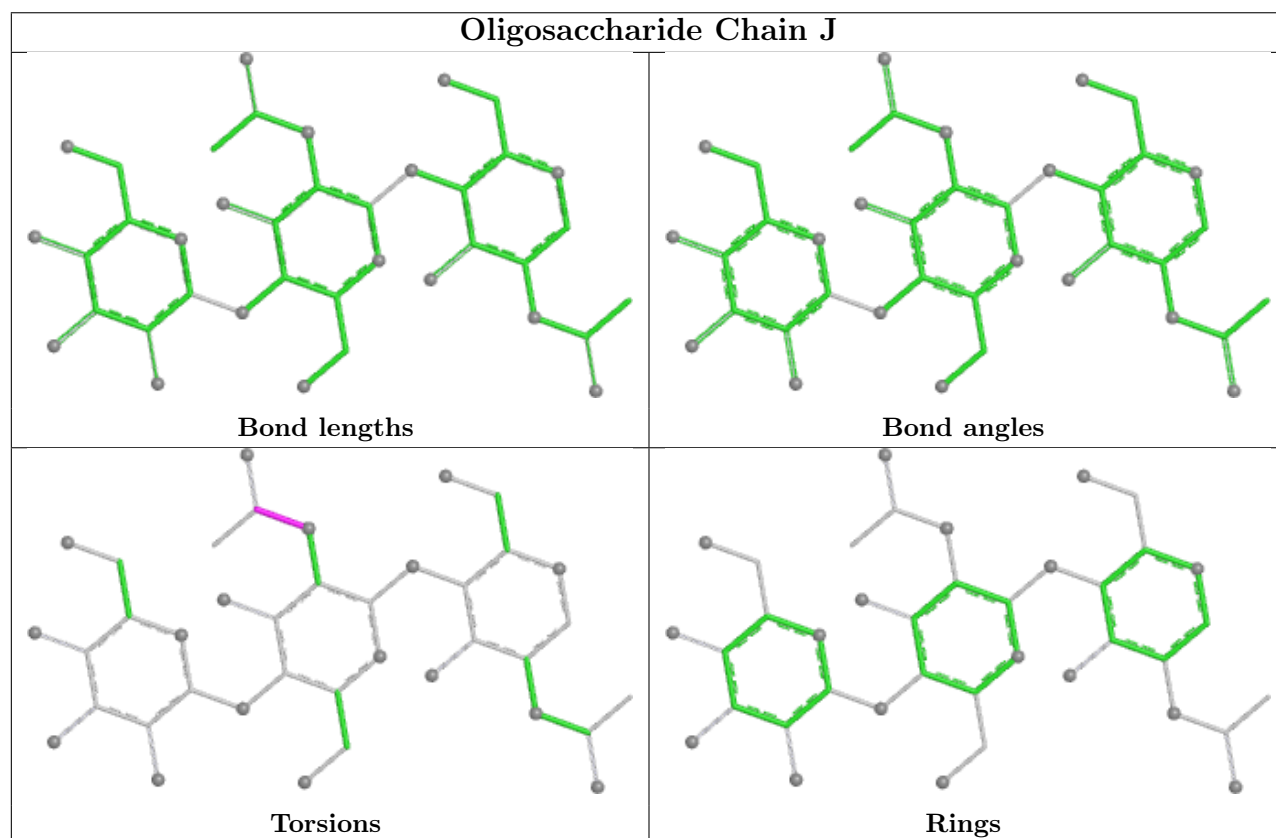
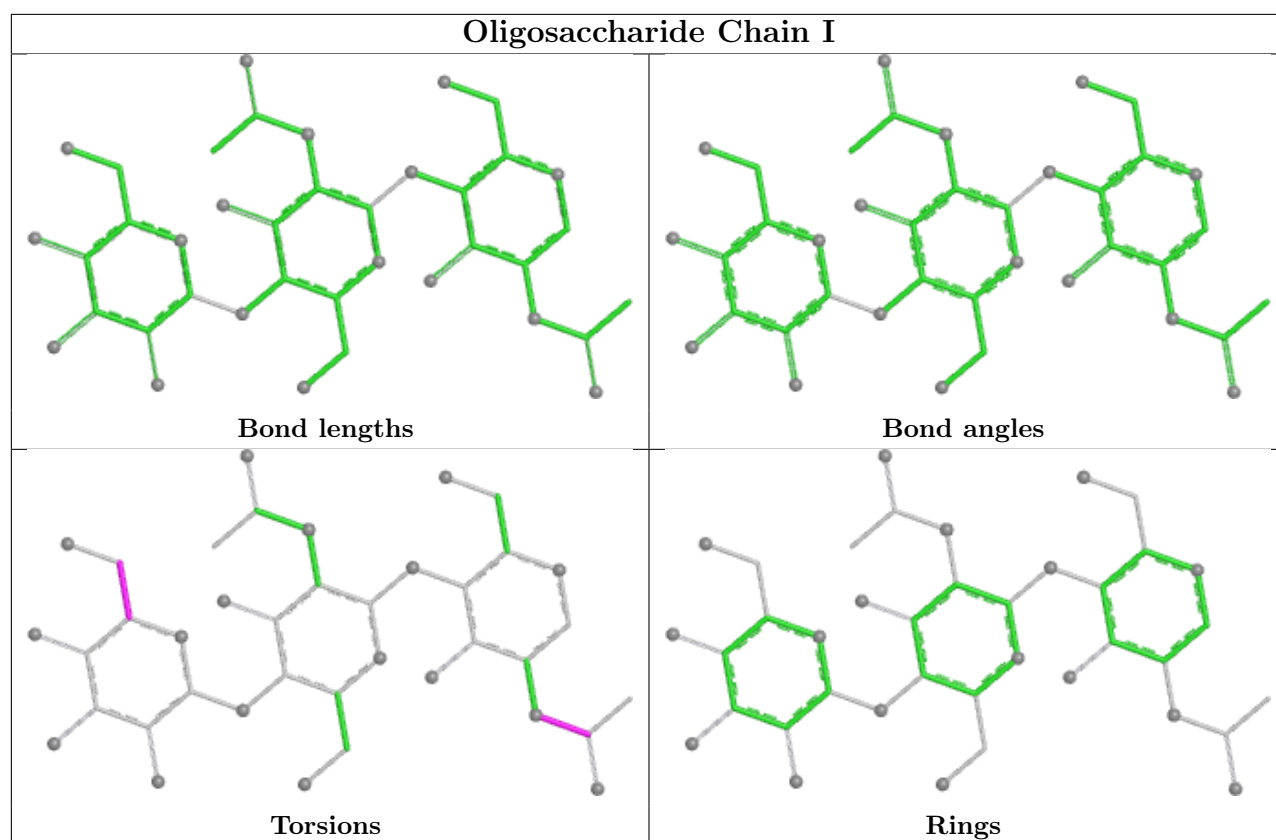
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	1	NAG	6	0
3	G	1	NAG	7	0
2	E	1	NAG	5	0
2	D	1	NAG	2	0
2	I	1	NAG	2	0
2	J	2	NAG	1	0
2	N	1	NAG	2	0
2	I	2	NAG	2	0
2	C	2	NAG	1	0
3	M	1	NAG	1	0
3	H	1	NAG	1	0
3	G	2	NAG	3	0
2	J	1	NAG	3	0
2	D	2	NAG	1	0
2	C	1	NAG	2	0

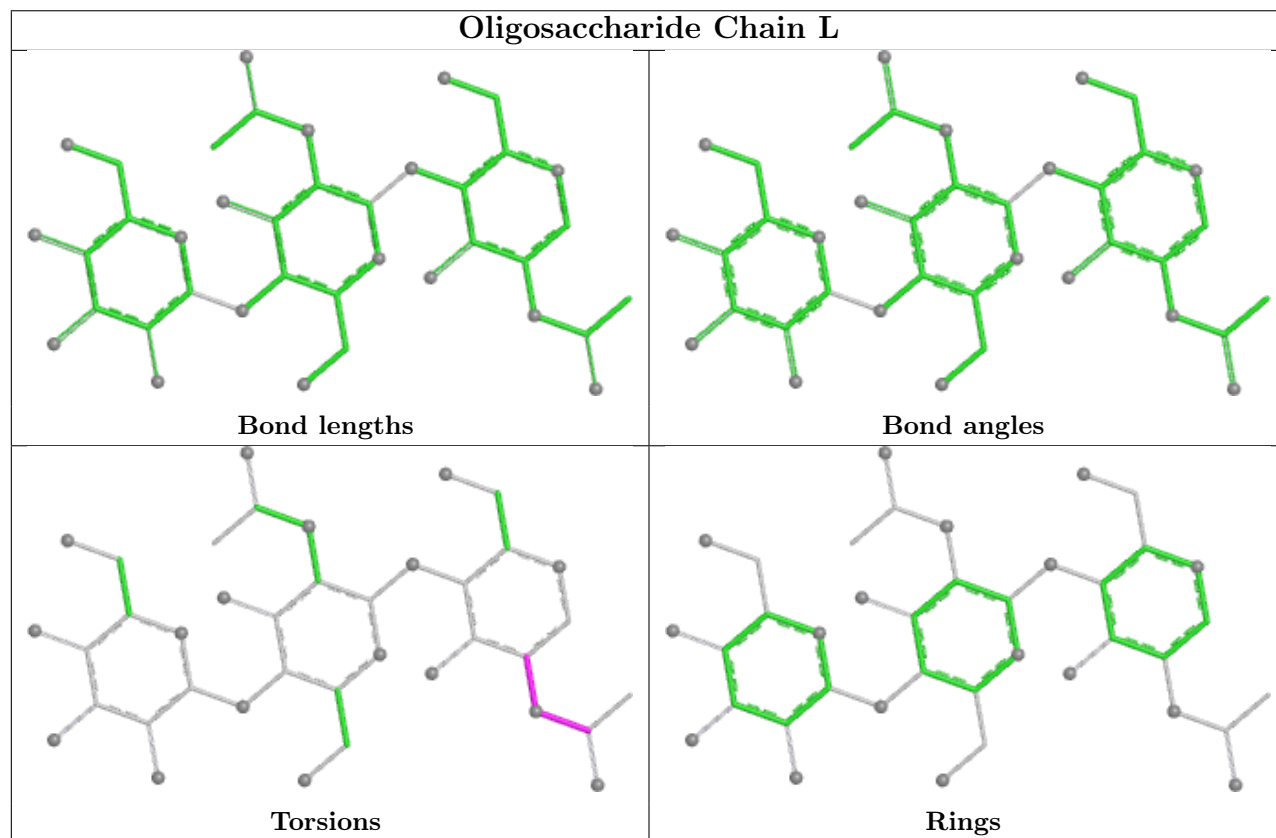
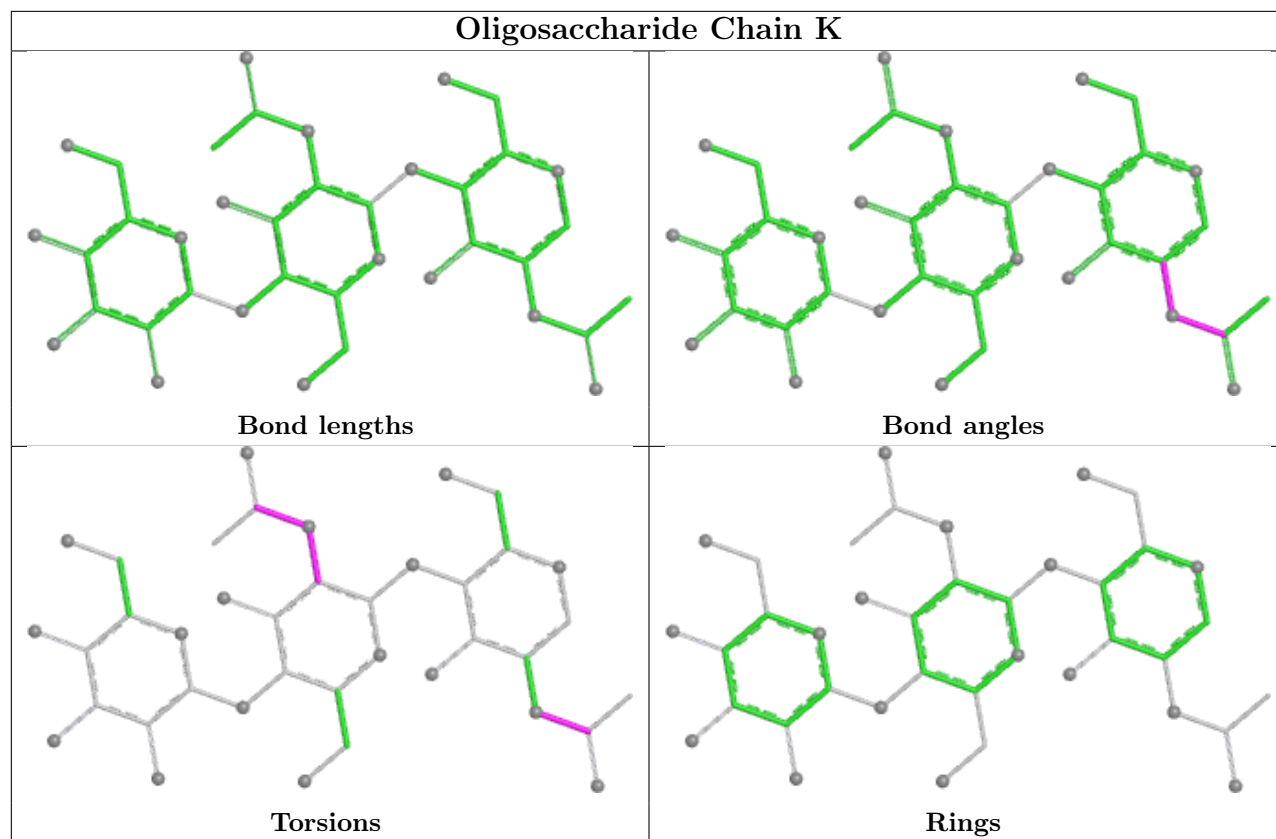
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

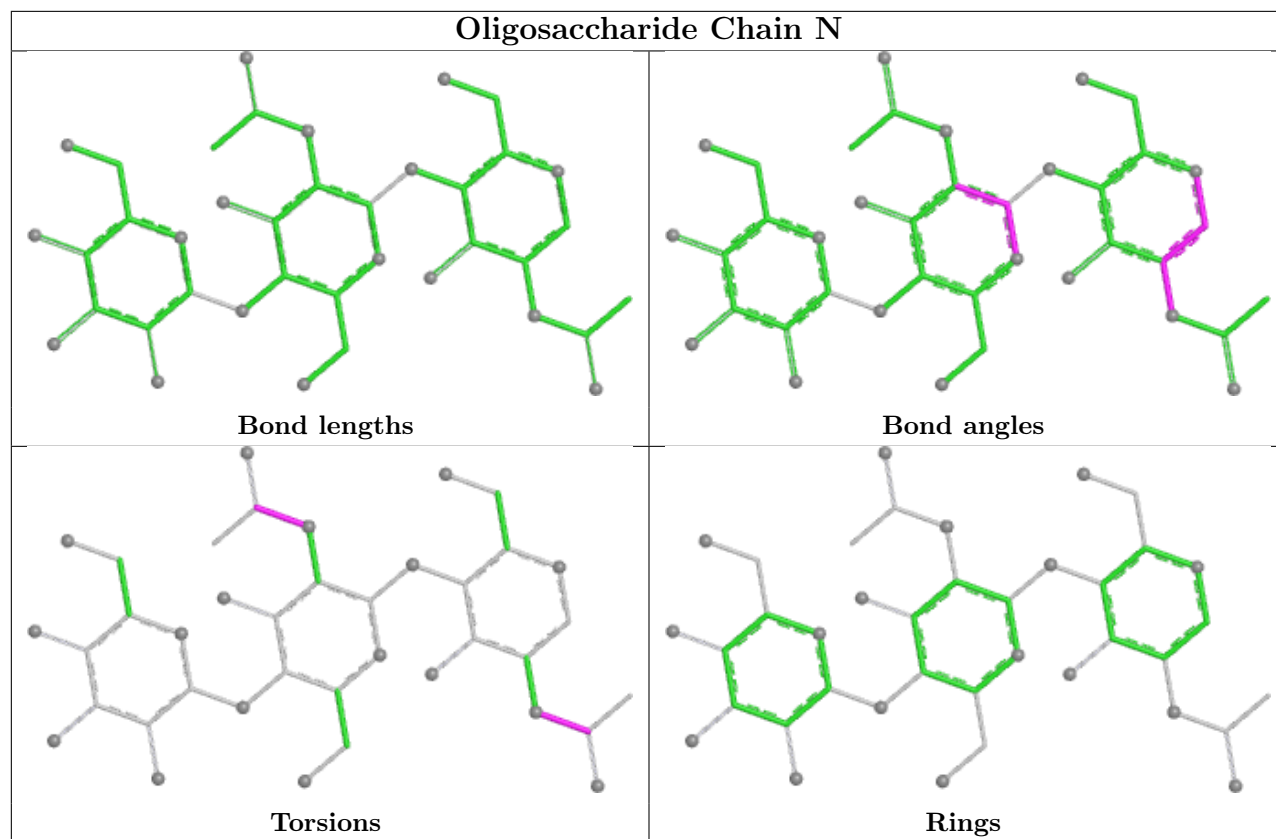


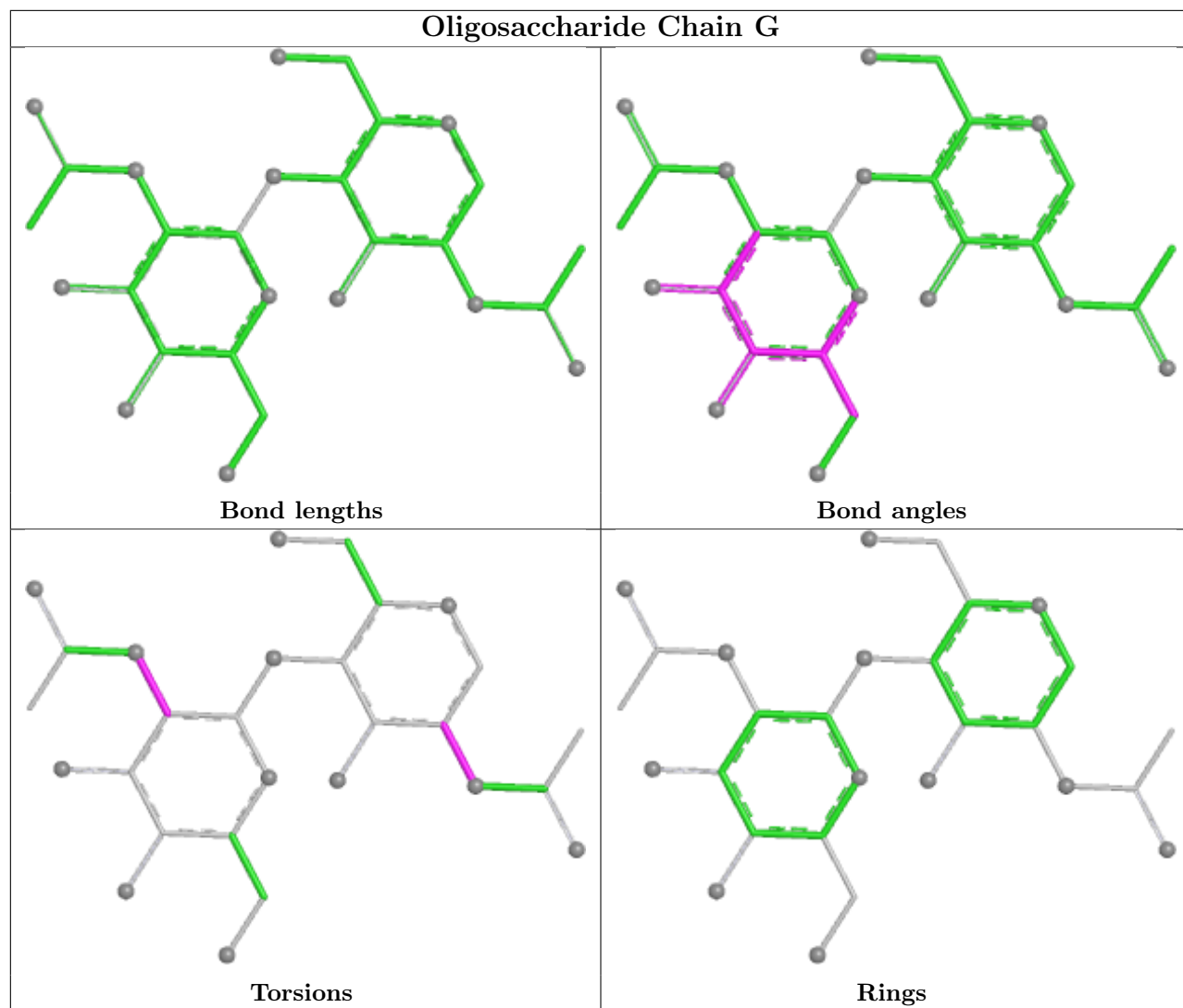


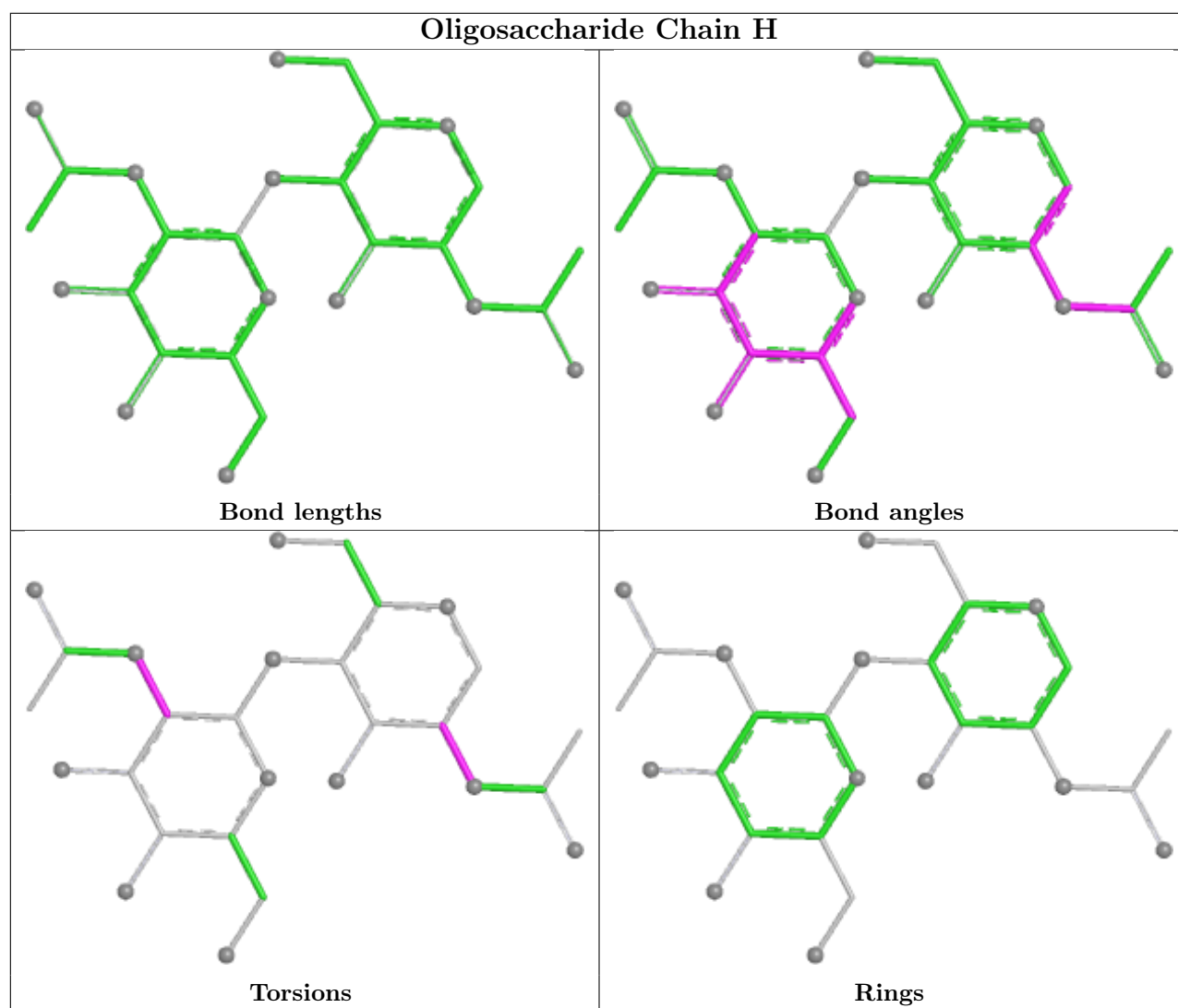


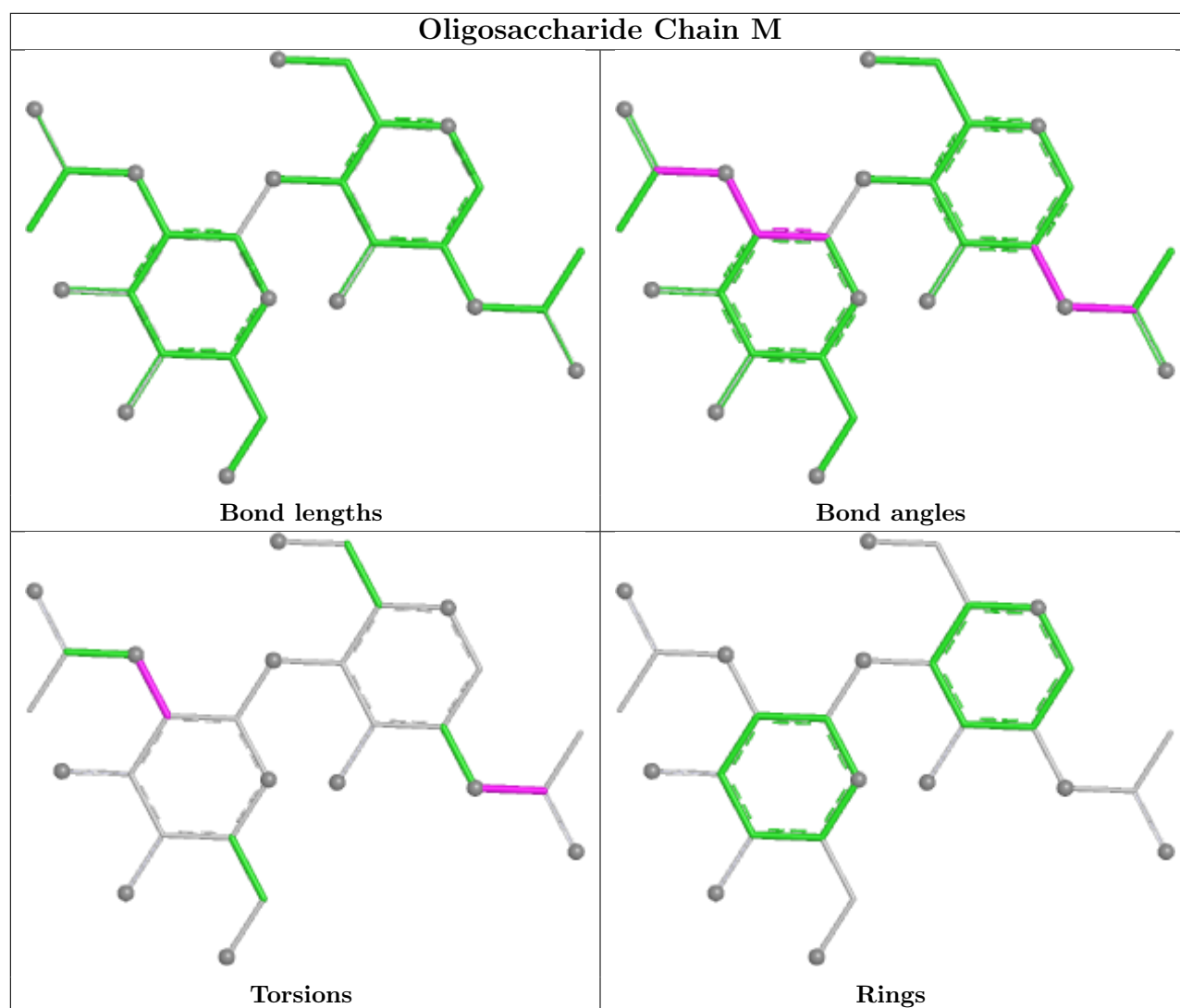












## 5.6 Ligand geometry [i](#)

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	B	4709	1	14,14,15	0.28	0	17,19,21	0.64	0
4	NAG	A	4703	1	14,14,15	0.28	0	17,19,21	0.66	0
4	NAG	B	4705	1	14,14,15	0.28	0	17,19,21	0.61	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	A	4707	1	14,14,15	0.26	0	17,19,21	0.67	0
4	NAG	B	4708	1	14,14,15	0.36	0	17,19,21	0.99	1 (5%)
4	NAG	A	4706	1	14,14,15	0.28	0	17,19,21	0.64	0
4	NAG	A	4712	1	14,14,15	0.39	0	17,19,21	0.79	1 (5%)
4	NAG	B	4703	1	14,14,15	0.30	0	17,19,21	0.68	0
4	NAG	B	4702	1	14,14,15	0.27	0	17,19,21	0.71	0
4	NAG	B	4704	1	14,14,15	0.27	0	17,19,21	0.74	0
4	NAG	A	4701	1	14,14,15	0.28	0	17,19,21	0.61	0
4	NAG	A	4708	1	14,14,15	0.37	0	17,19,21	0.76	1 (5%)
4	NAG	B	4710	1	14,14,15	0.28	0	17,19,21	0.64	0
4	NAG	B	4711	1	14,14,15	0.38	0	17,19,21	0.48	0
4	NAG	A	4702	1	14,14,15	0.29	0	17,19,21	0.75	0
4	NAG	A	4709	1	14,14,15	0.27	0	17,19,21	0.69	0
4	NAG	B	4706	1	14,14,15	0.27	0	17,19,21	0.67	0
4	NAG	A	4705	1	14,14,15	0.27	0	17,19,21	0.66	0
4	NAG	A	4711	1	14,14,15	0.38	0	17,19,21	0.50	0
4	NAG	A	4710	1	14,14,15	0.26	0	17,19,21	0.52	0
4	NAG	B	4701	1	14,14,15	0.26	0	17,19,21	0.67	0
4	NAG	B	4707	1	14,14,15	0.26	0	17,19,21	0.67	0
4	NAG	A	4704	1	14,14,15	0.28	0	17,19,21	0.60	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
4	NAG	B	4709	1	-	0/6/23/26	0/1/1/1
4	NAG	A	4703	1	-	3/6/23/26	0/1/1/1
4	NAG	B	4705	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	4708	1	-	3/6/23/26	0/1/1/1
4	NAG	A	4706	1	-	2/6/23/26	0/1/1/1
4	NAG	A	4712	1	-	1/6/23/26	0/1/1/1
4	NAG	B	4703	1	-	2/6/23/26	0/1/1/1
4	NAG	B	4702	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	4701	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	4710	1	-	0/6/23/26	0/1/1/1

Continued on next page...

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	4711	1	-	0/6/23/26	0/1/1/1
4	NAG	A	4702	1	-	2/6/23/26	0/1/1/1
4	NAG	A	4709	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	4705	1	-	0/6/23/26	0/1/1/1
4	NAG	A	4711	1	-	0/6/23/26	0/1/1/1
4	NAG	A	4710	1	-	3/6/23/26	0/1/1/1
4	NAG	B	4701	1	-	0/6/23/26	0/1/1/1
4	NAG	B	4707	1	-	3/6/23/26	0/1/1/1
4	NAG	A	4704	1	-	0/6/23/26	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	B	4703	NAG	1	0
4	A	4702	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.

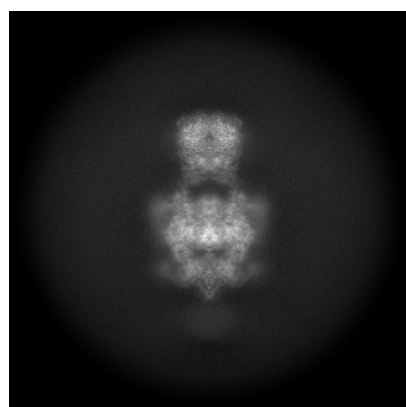
## 6 Map visualisation [i](#)

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.

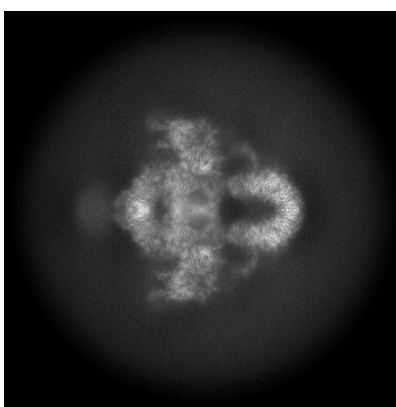
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

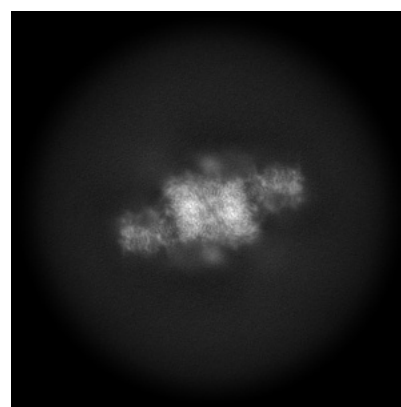
#### 6.1.1 Primary map



X



Y

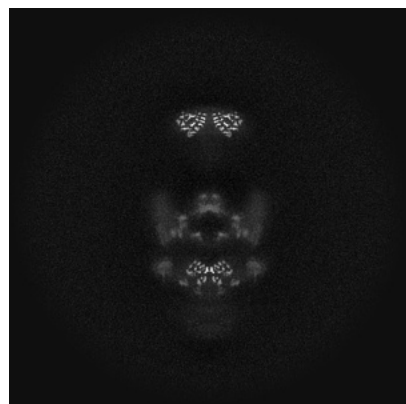


Z

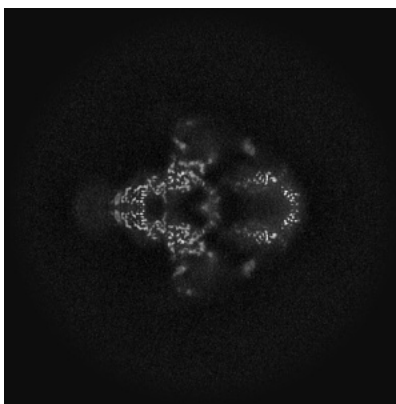
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

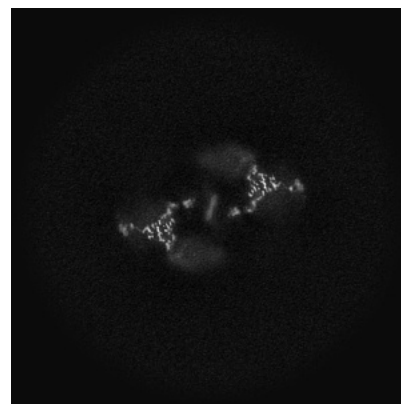
#### 6.2.1 Primary map



X Index: 256



Y Index: 256

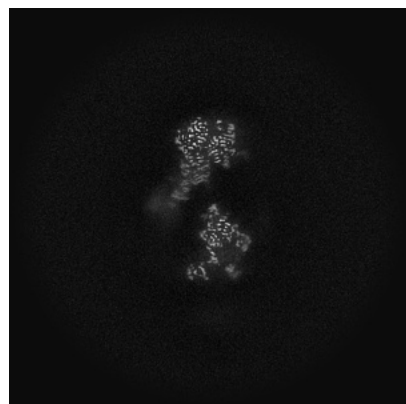


Z Index: 256

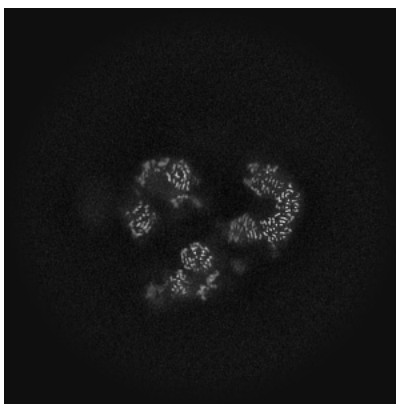
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

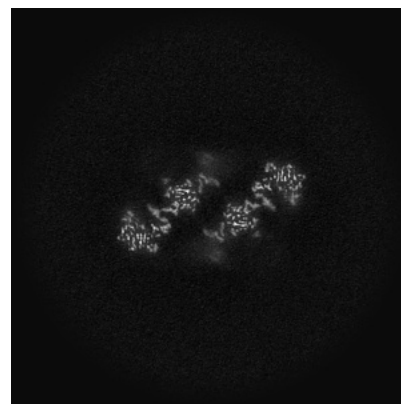
### 6.3.1 Primary map



X Index: 224



Y Index: 233

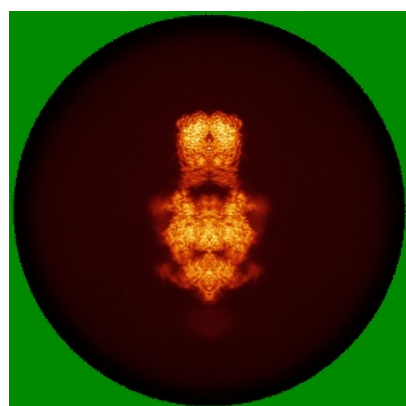


Z Index: 231

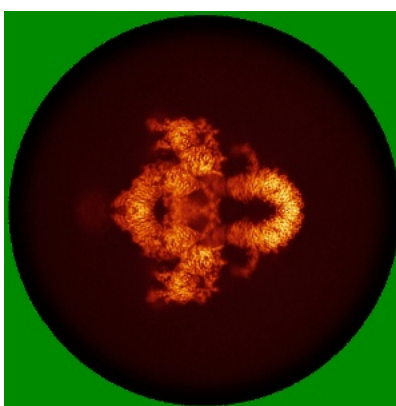
The images above show the largest variance slices of the map in three orthogonal directions.

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

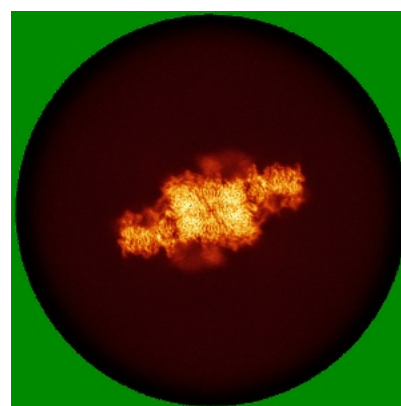
### 6.4.1 Primary map



X



Y

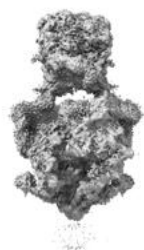


Z

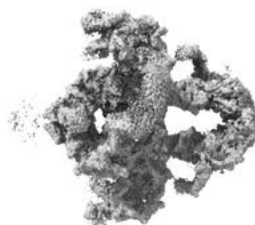
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 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.

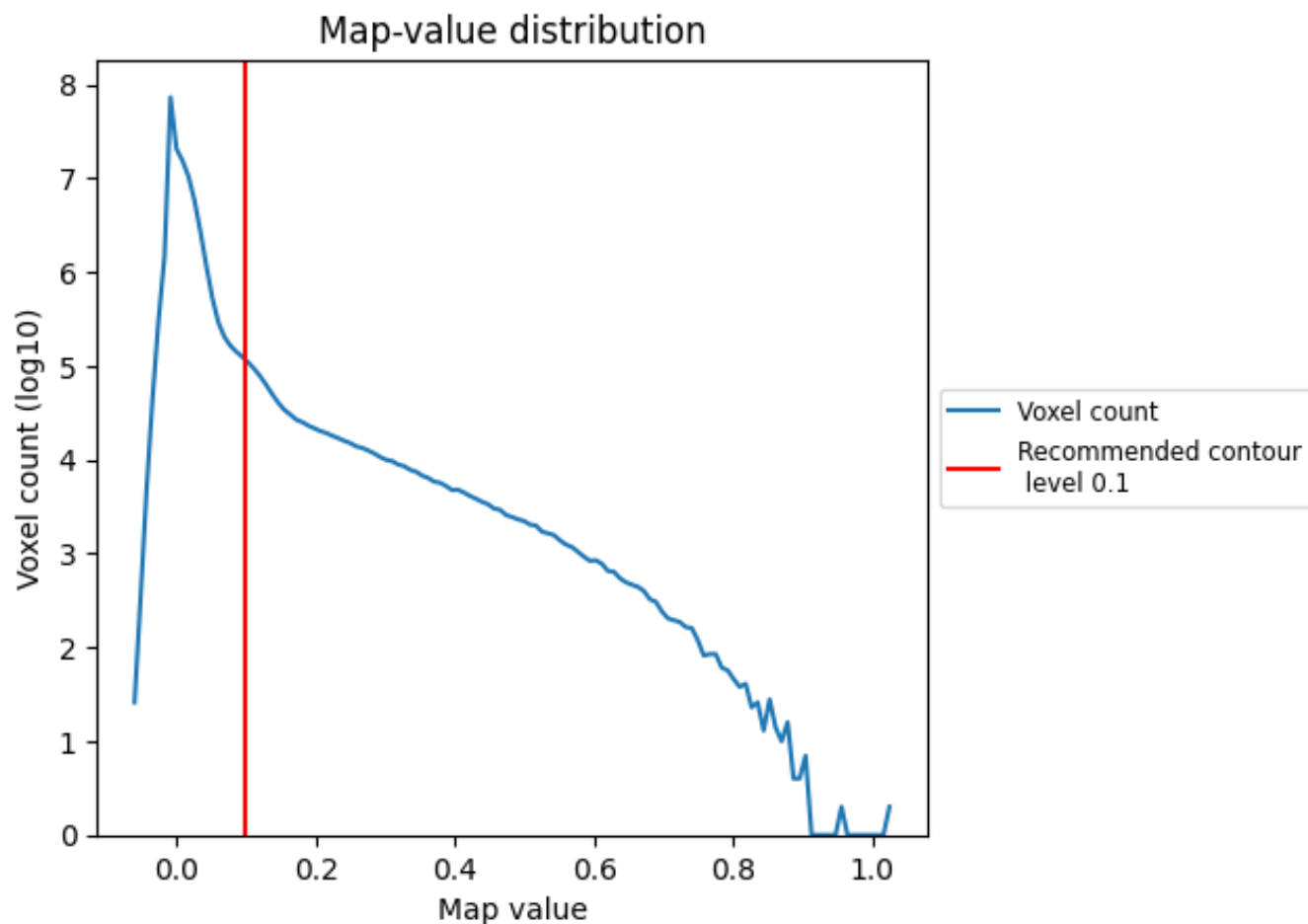
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

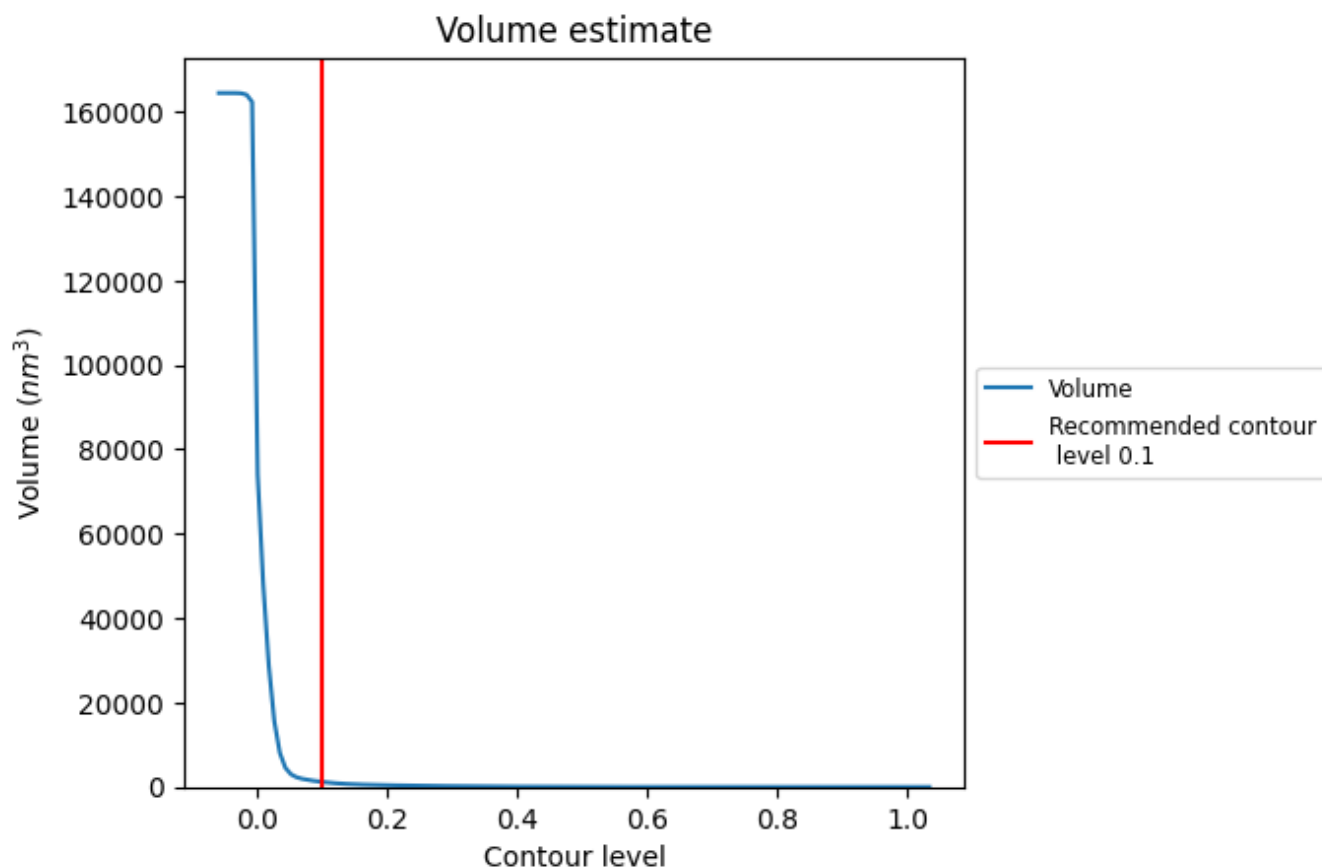
This section contains the results of statistical analysis of the map.

### 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](#)

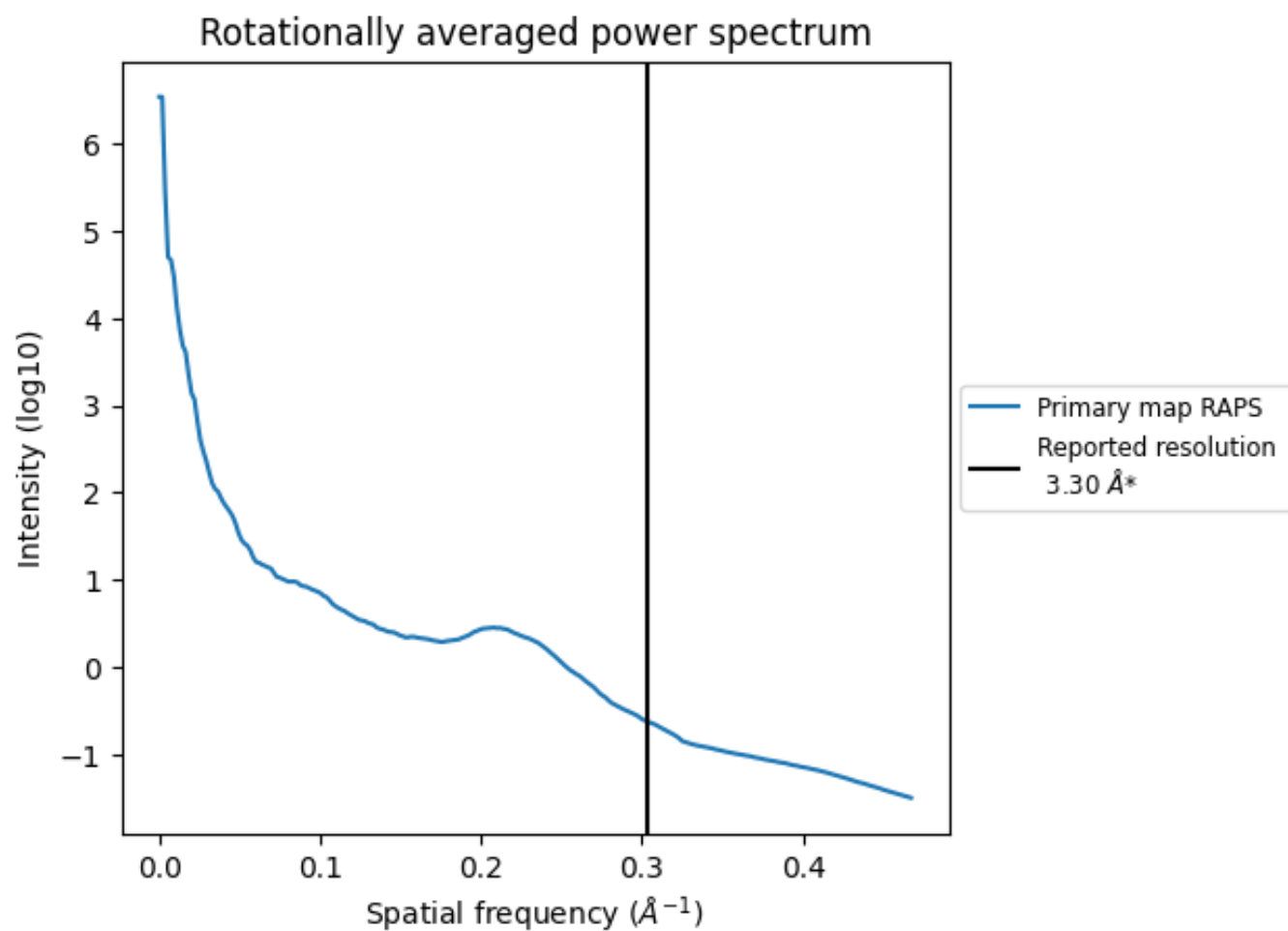


The volume at the recommended contour level is 1187 nm<sup>3</sup>; this corresponds to an approximate mass of 1072 kDa.

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<sup>-1</sup>

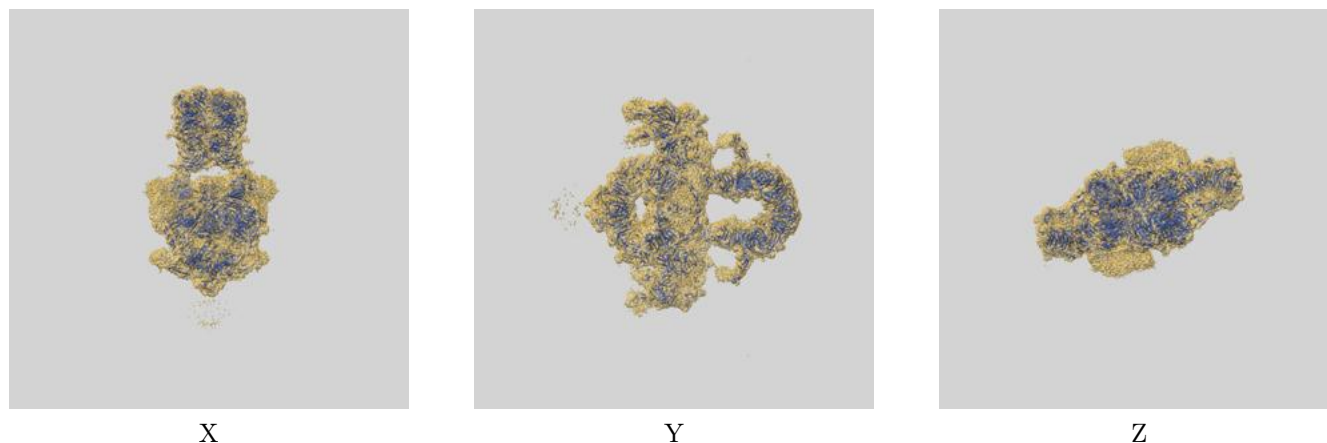
## 8 Fourier-Shell correlation

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

## 9 Map-model fit [i](#)

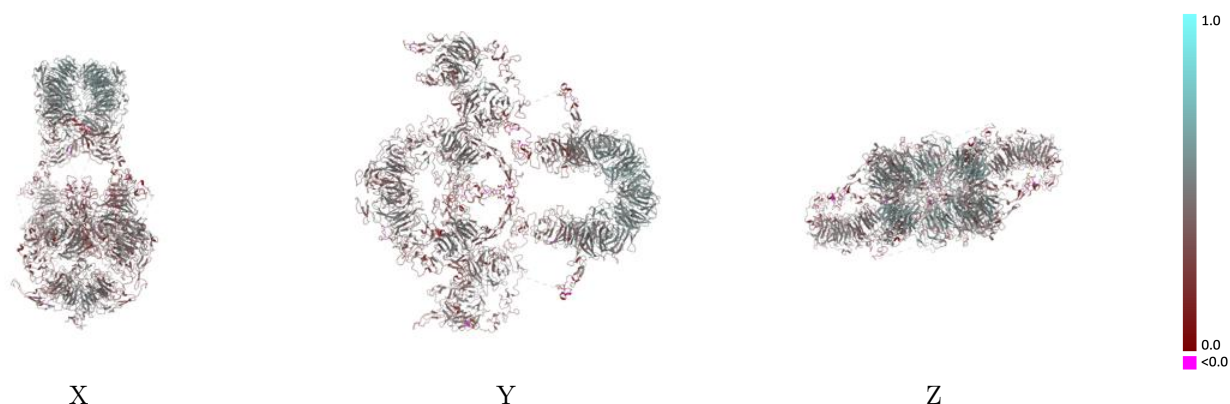
This section contains information regarding the fit between EMDB map EMD-45967 and PDB model 9CWM. Per-residue inclusion information can be found in section [3](#) on page [7](#).

### 9.1 Map-model overlay [i](#)



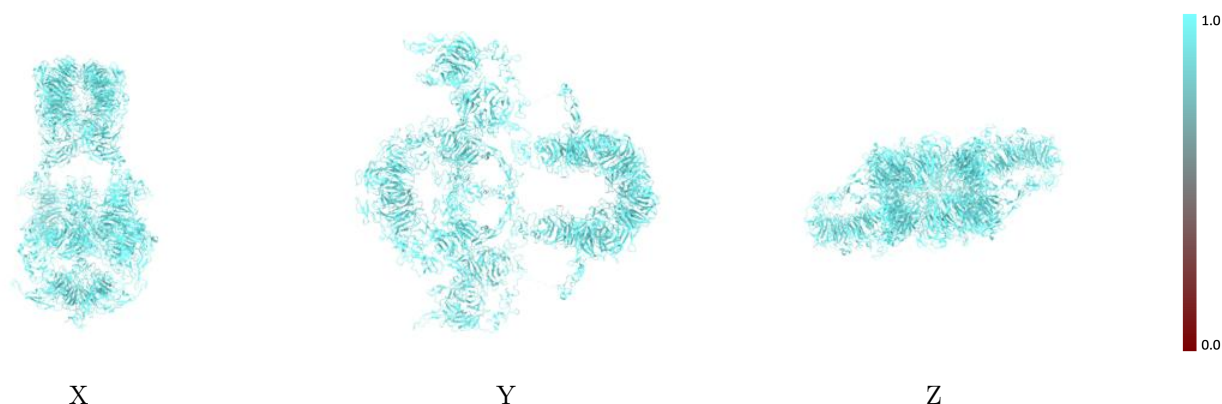
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



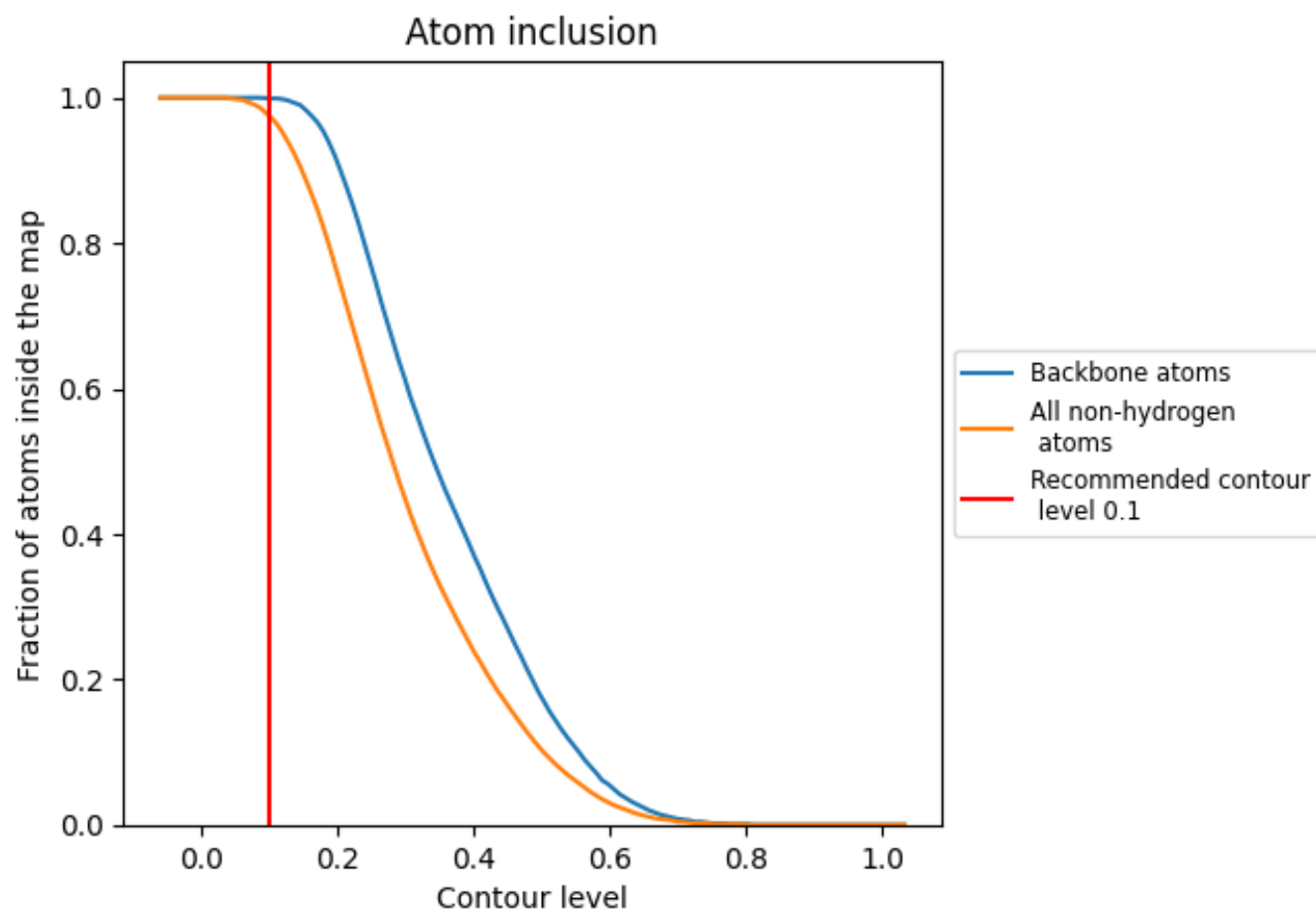
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

