



wwPDB EM Validation Summary Report ⓘ

Aug 25, 2026 – 12:50 am BST

PDB ID : 9IGS / pdb_00009igs
EMDB ID : EMD-52854
Title : Mouse teneurin-3 A1B1 isoform; microphthalmia-associated R2579W mutant;
compact dimer conformation
Authors : Gogou, C.; Meijer, D.H.
Deposited on : 2025-02-20
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

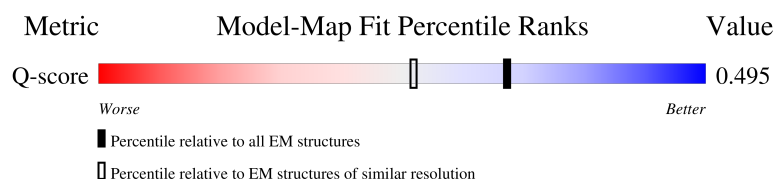
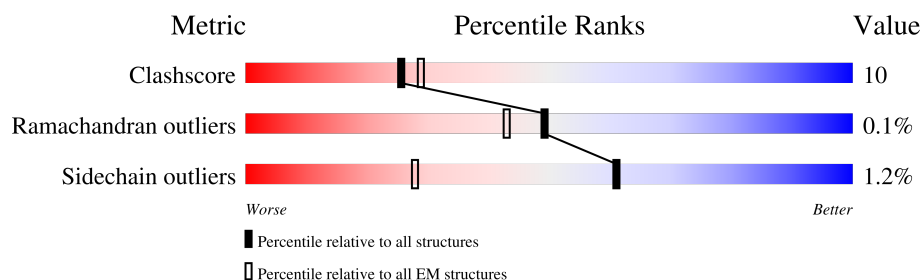
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

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 3.00 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	14081 (2.50 - 3.50)

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	2407	11% 61% 18% 22%
1	B	2407	11% 60% 18% 22%
2	C	2	50% 100%
2	D	2	50% 50%

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

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 29504 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 Isoform A1B1 of Teneurin-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1888	Total	C	N	O	S	0	0
			14527	9228	2504	2740	55		
1	B	1888	Total	C	N	O	S	0	0
			14527	9228	2504	2740	55		

There are 70 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	312	MET	-	initiating methionine	UNP Q9WTS6
A	313	ALA	-	expression tag	UNP Q9WTS6
A	314	ARG	-	expression tag	UNP Q9WTS6
A	315	PRO	-	expression tag	UNP Q9WTS6
A	316	LEU	-	expression tag	UNP Q9WTS6
A	317	CYS	-	expression tag	UNP Q9WTS6
A	318	THR	-	expression tag	UNP Q9WTS6
A	319	LEU	-	expression tag	UNP Q9WTS6
A	320	LEU	-	expression tag	UNP Q9WTS6
A	321	LEU	-	expression tag	UNP Q9WTS6
A	322	LEU	-	expression tag	UNP Q9WTS6
A	323	MET	-	expression tag	UNP Q9WTS6
A	324	ALA	-	expression tag	UNP Q9WTS6
A	325	THR	-	expression tag	UNP Q9WTS6
A	326	LEU	-	expression tag	UNP Q9WTS6
A	327	ALA	-	expression tag	UNP Q9WTS6
A	328	GLY	-	expression tag	UNP Q9WTS6
A	329	ALA	-	expression tag	UNP Q9WTS6
A	330	LEU	-	expression tag	UNP Q9WTS6
A	331	ALA	-	expression tag	UNP Q9WTS6
A	332	GLY	-	expression tag	UNP Q9WTS6
A	333	SER	-	expression tag	UNP Q9WTS6
A	334	HIS	-	expression tag	UNP Q9WTS6
A	335	HIS	-	expression tag	UNP Q9WTS6
A	336	HIS	-	expression tag	UNP Q9WTS6
A	337	HIS	-	expression tag	UNP Q9WTS6

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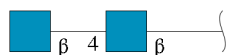
Chain	Residue	Modelled	Actual	Comment	Reference
A	338	HIS	-	expression tag	UNP Q9WTS6
A	339	HIS	-	expression tag	UNP Q9WTS6
A	340	GLY	-	expression tag	UNP Q9WTS6
A	341	SER	-	expression tag	UNP Q9WTS6
A	2332	ILE	THR	conflict	UNP Q9WTS6
A	2579	TRP	ARG	engineered mutation	UNP Q9WTS6
A	2716	ALA	-	expression tag	UNP Q9WTS6
A	2717	ALA	-	expression tag	UNP Q9WTS6
A	2718	ALA	-	expression tag	UNP Q9WTS6
B	312	MET	-	initiating methionine	UNP Q9WTS6
B	313	ALA	-	expression tag	UNP Q9WTS6
B	314	ARG	-	expression tag	UNP Q9WTS6
B	315	PRO	-	expression tag	UNP Q9WTS6
B	316	LEU	-	expression tag	UNP Q9WTS6
B	317	CYS	-	expression tag	UNP Q9WTS6
B	318	THR	-	expression tag	UNP Q9WTS6
B	319	LEU	-	expression tag	UNP Q9WTS6
B	320	LEU	-	expression tag	UNP Q9WTS6
B	321	LEU	-	expression tag	UNP Q9WTS6
B	322	LEU	-	expression tag	UNP Q9WTS6
B	323	MET	-	expression tag	UNP Q9WTS6
B	324	ALA	-	expression tag	UNP Q9WTS6
B	325	THR	-	expression tag	UNP Q9WTS6
B	326	LEU	-	expression tag	UNP Q9WTS6
B	327	ALA	-	expression tag	UNP Q9WTS6
B	328	GLY	-	expression tag	UNP Q9WTS6
B	329	ALA	-	expression tag	UNP Q9WTS6
B	330	LEU	-	expression tag	UNP Q9WTS6
B	331	ALA	-	expression tag	UNP Q9WTS6
B	332	GLY	-	expression tag	UNP Q9WTS6
B	333	SER	-	expression tag	UNP Q9WTS6
B	334	HIS	-	expression tag	UNP Q9WTS6
B	335	HIS	-	expression tag	UNP Q9WTS6
B	336	HIS	-	expression tag	UNP Q9WTS6
B	337	HIS	-	expression tag	UNP Q9WTS6
B	338	HIS	-	expression tag	UNP Q9WTS6
B	339	HIS	-	expression tag	UNP Q9WTS6
B	340	GLY	-	expression tag	UNP Q9WTS6
B	341	SER	-	expression tag	UNP Q9WTS6
B	2332	ILE	THR	conflict	UNP Q9WTS6
B	2579	TRP	ARG	engineered mutation	UNP Q9WTS6
B	2716	ALA	-	expression tag	UNP Q9WTS6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	2717	ALA	-	expression tag	UNP Q9WTS6
B	2718	ALA	-	expression tag	UNP Q9WTS6

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



Mol	Chain	Residues	Atoms				AltConf	Trace
2	C	2	Total	C	N	O	0	0
			28	16	2	10		
2	D	2	Total	C	N	O	0	0
			28	16	2	10		
2	E	2	Total	C	N	O	0	0
			28	16	2	10		
2	F	2	Total	C	N	O	0	0
			28	16	2	10		
2	G	2	Total	C	N	O	0	0
			28	16	2	10		
2	H	2	Total	C	N	O	0	0
			28	16	2	10		
2	I	2	Total	C	N	O	0	0
			28	16	2	10		
2	J	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



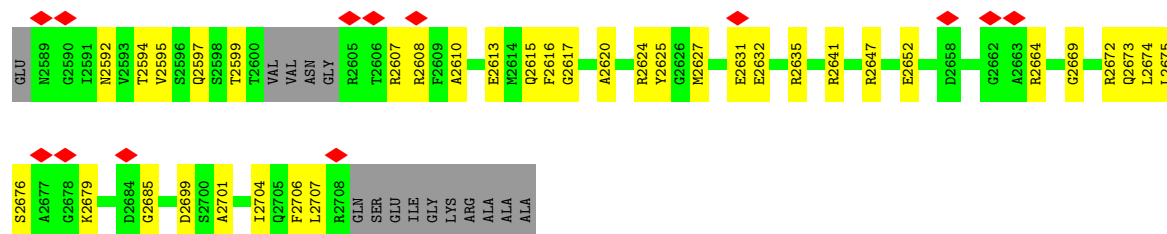
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
3	A	1	14	8	1	5	0
3	A	1	14	8	1	5	0
3	A	1	14	8	1	5	0
3	A	1	14	8	1	5	0
3	A	1	14	8	1	5	0
3	A	1	14	8	1	5	0
3	A	1	15	8	1	6	0
3	A	1	14	8	1	5	0
3	B	1	14	8	1	5	0
3	B	1	14	8	1	5	0
3	B	1	14	8	1	5	0
3	B	1	14	8	1	5	0
3	B	1	14	8	1	5	0
3	B	1	14	8	1	5	0

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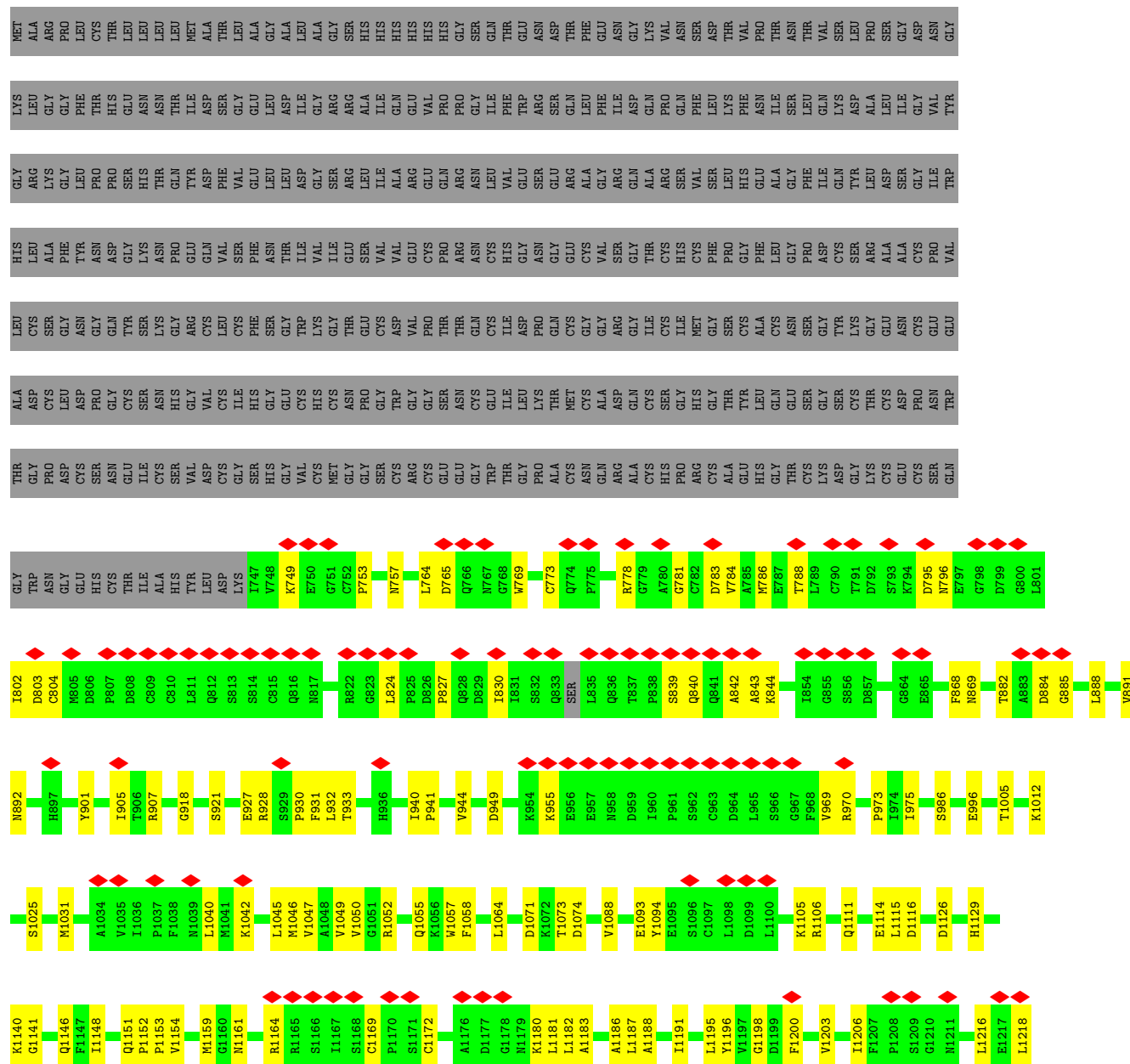
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Mol	Chain	Residues	Atoms				AltConf
3	B	1	Total	C	N	O	0
			15	8	1	6	
3	B	1	Total	C	N	O	0
			14	8	1	5	

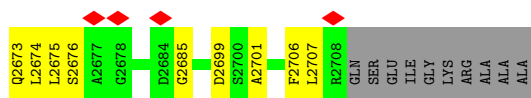




• Molecule 1: Isoform A1B1 of Tenascin-3



L1364	A1365	I1366	M1367	M1368	D1370	I1373	V1374	V1375	L1376	M1377	M1378	M1379	I1384	I1385	E1386	ASN	R1388	Q1389	A1393	A1394	G1395	R1396	P1397	MET	H1399	CYS	GLN	VAL	PRO	GLY	ASN	ASP	LEU	THR	ALA	LYS	D1265	L1266	T1267	K1268	M1269	A1270	V1273	M1274	G1275	T1276	G1277	S1354	Q1278	Q1279	CYS	LEU	PRO	PHE	ASP	GLU	ALA	ARG
T1450	ASP	G1452	G1459	E1463	C1464	D1465	C1466	K1467	M1468	D1469	M1378	A1470	ASN	C1472	D1473	C1474	S1477	G1478	D1479	A1494	A1495	S1496	P1497	D1498	A1504	I1509	L1520	A1530	S1531	P1532	Q1535	E1536	Y1538	I1539	A1412	A1413	F1540	D1541	T1545	Y1548	S1564	L1720	R1721	I1722	L1728	D1729	S1730	D1582	R1583	R1584	D1585							
P1586	M1587	R1588	M1589	V1593	V1594	S1595	M1598	Q1599	A1616	L1621	T1625	T1643	T1644	F1645	F1646	V1657	T1658	F1659	P1660	V1664	D1672	S1682	S1683	R1684	E1685	E1686	L1694	I1697	Q1707	Q1713	Y1716	L1720	R1721	I1722	L1728	D1729	S1730	D1582	R1583	R1584	D1585																	
H1731	T1734	H1737	A1740	M1744	P1745	M1751	M1752	G1756	E1757	M1761	L1762	V1763	E1764	V1765	R1766	Q1773	G1774	K1782	V1785	D1807	H1808	ARG	K1810	L1813	M1826	S1830	K1831	L1832	V1835	M1836	S1841	I1845	I1848	Q1849	R1850	G1851	T1852	T1853	S1854	Y1859																		
A1871	D1872	G1873	K1874	S1877	Y1878	T1879	K1883	V1886	L1887	L1888	R1893	I1896	F1897	E1898	M1901	N1902	D1903	R1904	L1905	T1908	T1909	M1910	P1911	T1917	R1922	S1923	I1924	M1932	P1933	P1934	E1935	S1936	M1937	A1938	S1939	I1940	D1943	Q1952	F1955	R1960	Q1969	E1974																
Y1977	D1978	S1979	T1980	R1981	V1982	S1983	D1987	G1991	M1997	L1998	Q1999	S2000	T2006	P2014	D2026	V2029	Y2035	D2038	M2046	T2050	N2051	E2052	T2053	D2064	K2074	V2077	D2081	N2082	Q2084	T2085	T2088	A2089	V2090	M2091	T2092	T2093	T2094	K2095	I2103																			
I2106	Q2107	Y2108	E2109	M2125	V2128	R2131	F2137	F2138	A2139	N2140	T2141	Y2144	A2145	Y2158	M2164	V2165	R2166	Y2167	N2168	L2171	N2174	L2177	L2178	N2179	P2180	S2181	S2182	S2183	A2184	R2185	L2186	L2189	R2196	L2200	L2207	D2208	E2209	D2210	G2211	F2212	Q2215	R2216	G2217															
Y2223	S2224	S2225	G2236	S2237	G2238	V2241	V2252	T2256	G2259	Q2263	F2264	F2265	Y2266	A2267	H2277	I2286	L2293	L2297	S2304	G2305	D2306	E2307	F2308	I2310	A2311	S2312	D2313	R2314	T2315	G2316	T2317	S2324	L2327	K2330	T2332	Q2333	F2342	M2345	Q2353	F2354																		
H2355	Y2359	L2366	R2371	D2372	Y2373	D2384	L2385	L2391	N2399	L2400	Y2401	N2402	F2403	R2404	N2405	I2412	H2413	D2414	V2415	Y2418	D2421	W2425	L2437	F2440	P2441	L2447	T2448	E2449	D2462	V2469	V2473	A2474	R2475	K2478	L2481	K2485	M2486	A2487	E2488	V2489																		
GLN	VAL	SER	ARG	ARG	LYS	ALA	GLY	ALA	E2499	L2511	L2518	L2530	ASN	ILE	ALA	N2534	E2535	D2536	C2537	I2538	K2539	V2540	V2543	L2544	F2548	Y2549	L2550	L2553	I2557	K2560	D2561	T2562	H2563	Y2564	F2565	L2566	P2571	E2572	S2573	D2574	L2575	G2576	T2577	L2578	W2579	LEU	THR	SER	GLY	ARG								
LYS	ALA	LEU	GLU	N2589	G2590	L2591	N2592	V2593	T2594	V2595	S2596	Q2597	T2599	T2600	VAL	ASN	ASN	GLY	R2605	T2606	R2607	R2608	F2609	A2610	E2613	T2614	Q2615	F2616	G2617	A2620	R2624	Y2625	G2626	M2627	E2631	E2632	R2635	R2641	R2647	E2652	D2658	G2662	A2663	R2664	G2669	R2672												



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



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



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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	59069	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.029	Depositor
Minimum map value	-0.011	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.00718	Depositor
Map size ($\text{\AA}$)	234.08, 234.08, 234.08	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.836, 0.836, 0.836	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

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	0.13	0/14846	0.32	3/20193 (0.0%)
1	B	0.13	0/14846	0.32	4/20193 (0.0%)
All	All	0.13	0/29692	0.32	7/40386 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1225	HIS	N-CA-C	6.98	122.16	112.45
1	B	1938	ALA	N-CA-C	-6.61	98.05	108.63
1	A	1938	ALA	N-CA-C	-6.61	98.06	108.63
1	A	1707	GLN	N-CA-CB	-5.70	103.01	110.88
1	B	1707	GLN	N-CA-CB	-5.68	103.04	110.88

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	907	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	B	907	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	14527	0	13814	293	0
1	B	14527	0	13814	294	0
2	C	28	0	25	0	0
2	D	28	0	25	0	0
2	E	28	0	25	2	0
2	F	28	0	25	0	0
2	G	28	0	25	0	0
2	H	28	0	25	0	0
2	I	28	0	25	2	0
2	J	28	0	25	0	0
3	A	113	0	106	3	0
3	B	113	0	106	4	0
All	All	29504	0	28040	593	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 10.

The worst 5 of 593 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:1697:ILE:HD12	1:A:1716:TYR:CE2	1.55	1.42
1:B:1697:ILE:HD12	1:B:1716:TYR:CE2	1.55	1.39
1:A:1697:ILE:CD1	1:A:1716:TYR:HE2	1.41	1.33
1:B:1697:ILE:CD1	1:B:1716:TYR:HE2	1.41	1.32
1:B:1625:THR:HB	1:B:1635:THR:CG2	1.84	1.07

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	1859/2407 (77%)	1720 (92%)	138 (7%)	1 (0%)	48	80
1	B	1859/2407 (77%)	1721 (93%)	137 (7%)	1 (0%)	48	80
All	All	3718/4814 (77%)	3441 (92%)	275 (7%)	2 (0%)	49	80

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	869	ASN
1	B	869	ASN

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1508/2075 (73%)	1490 (99%)	18 (1%)	63	82
1	B	1508/2075 (73%)	1490 (99%)	18 (1%)	63	82
All	All	3016/4150 (73%)	2980 (99%)	36 (1%)	61	82

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	2128	VAL
1	B	2595	VAL
1	B	2332	ILE
1	B	2518	LEU

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Mol	Chain	Res	Type
1	A	2332	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	2051	ASN
1	B	2534	ASN
1	B	2083	ASN
1	B	2263	GLN
1	B	2642	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

16 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	0.23	0	17,19,21	0.41	0
2	NAG	C	2	2	14,14,15	0.22	0	17,19,21	0.46	0
2	NAG	D	1	1,2	14,14,15	1.09	2 (14%)	17,19,21	1.12	1 (5%)
2	NAG	D	2	2	14,14,15	0.22	0	17,19,21	0.48	0
2	NAG	E	1	1,2	14,14,15	0.20	0	17,19,21	0.68	1 (5%)
2	NAG	E	2	2	14,14,15	0.57	0	17,19,21	1.26	1 (5%)
2	NAG	F	1	1,2	14,14,15	0.23	0	17,19,21	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	F	2	2	14,14,15	0.20	0	17,19,21	0.43	0
2	NAG	G	1	1,2	14,14,15	0.25	0	17,19,21	0.41	0
2	NAG	G	2	2	14,14,15	0.20	0	17,19,21	0.45	0
2	NAG	H	1	1,2	14,14,15	1.08	2 (14%)	17,19,21	1.12	1 (5%)
2	NAG	H	2	2	14,14,15	0.22	0	17,19,21	0.49	0
2	NAG	I	1	1,2	14,14,15	0.20	0	17,19,21	0.68	1 (5%)
2	NAG	I	2	2	14,14,15	0.56	0	17,19,21	1.26	1 (5%)
2	NAG	J	1	1,2	14,14,15	0.24	0	17,19,21	0.58	0
2	NAG	J	2	2	14,14,15	0.21	0	17,19,21	0.43	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	-	4/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	NAG	D	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	NAG	E	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	E	2	2	-	5/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	F	2	2	-	3/6/23/26	0/1/1/1
2	NAG	G	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	G	2	2	-	0/6/23/26	0/1/1/1
2	NAG	H	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	H	2	2	-	2/6/23/26	0/1/1/1
2	NAG	I	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	I	2	2	-	5/6/23/26	0/1/1/1
2	NAG	J	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	J	2	2	-	3/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1	NAG	O5-C1	2.89	1.48	1.43
2	H	1	NAG	O5-C1	2.88	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1	NAG	C1-C2	2.74	1.56	1.52
2	H	1	NAG	C1-C2	2.73	1.56	1.52

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	2	NAG	C2-N2-C7	4.31	129.04	122.90
2	I	2	NAG	C2-N2-C7	4.31	129.04	122.90
2	H	1	NAG	C1-O5-C5	4.11	117.77	112.19
2	D	1	NAG	C1-O5-C5	4.11	117.76	112.19
2	I	1	NAG	C1-O5-C5	2.28	115.28	112.19

There are no chirality outliers.

5 of 48 torsion outliers are listed below:

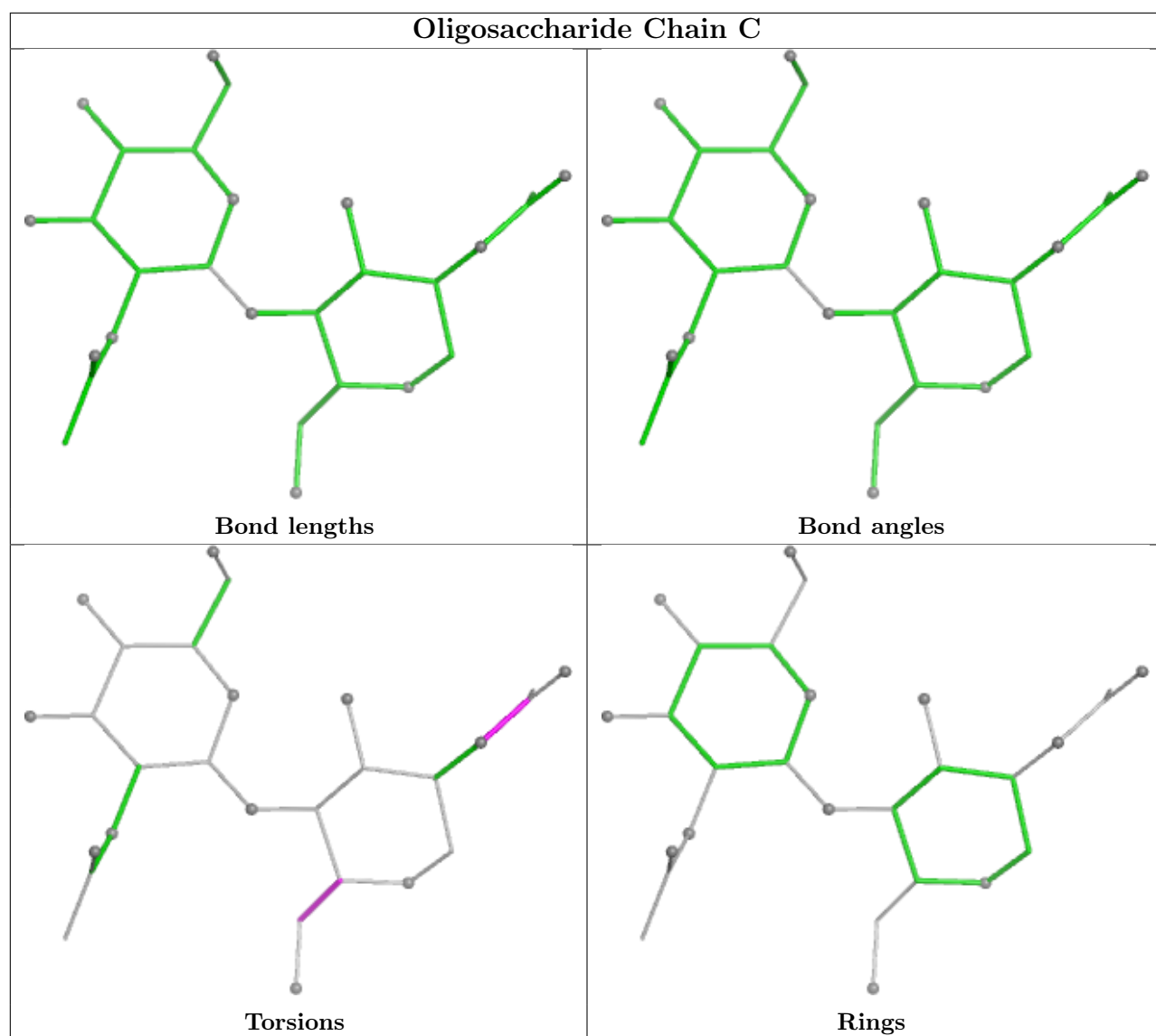
Mol	Chain	Res	Type	Atoms
2	D	2	NAG	O5-C5-C6-O6
2	H	2	NAG	O5-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
2	H	1	NAG	C4-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6

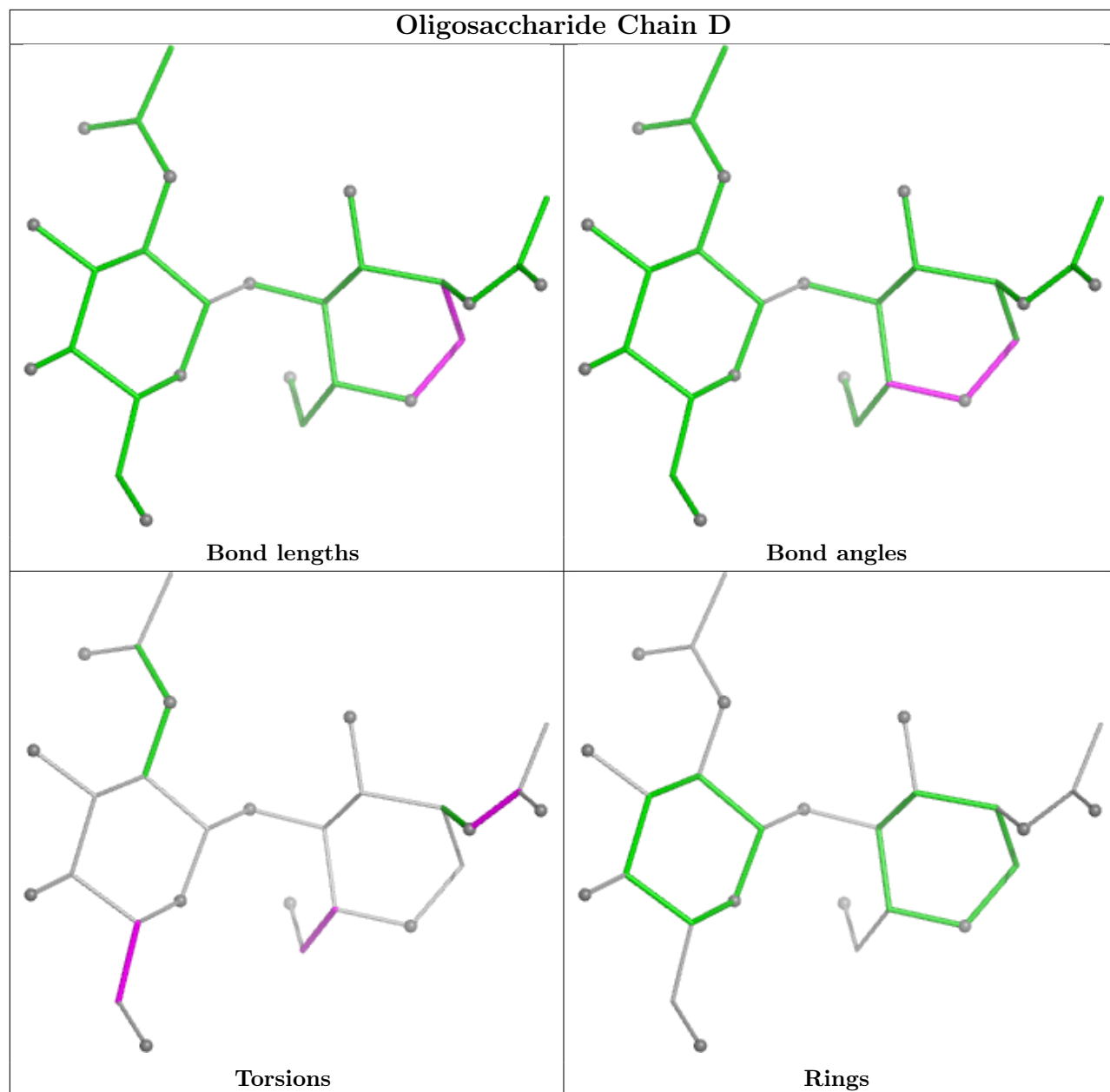
There are no ring outliers.

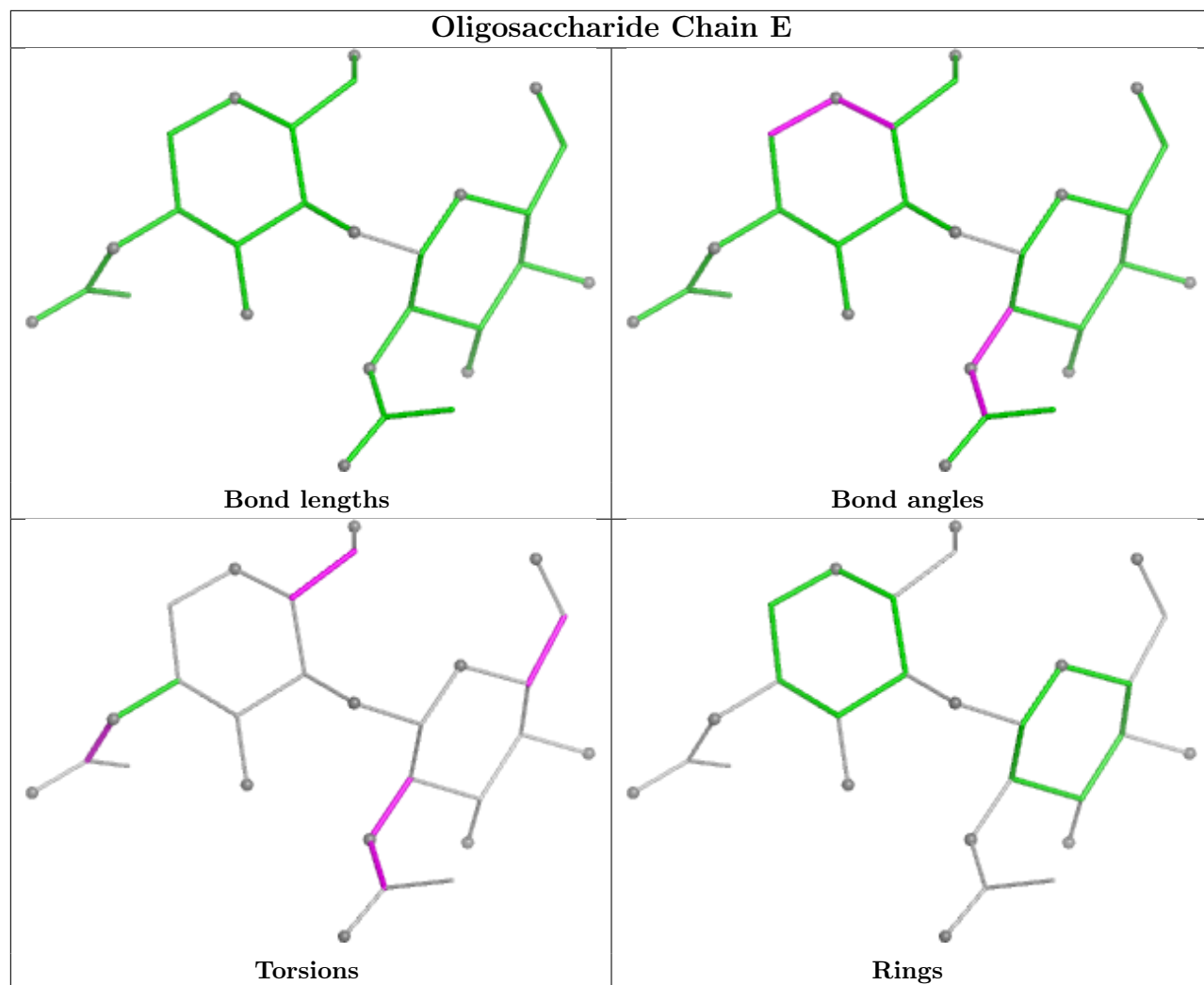
4 monomers are involved in 4 short contacts:

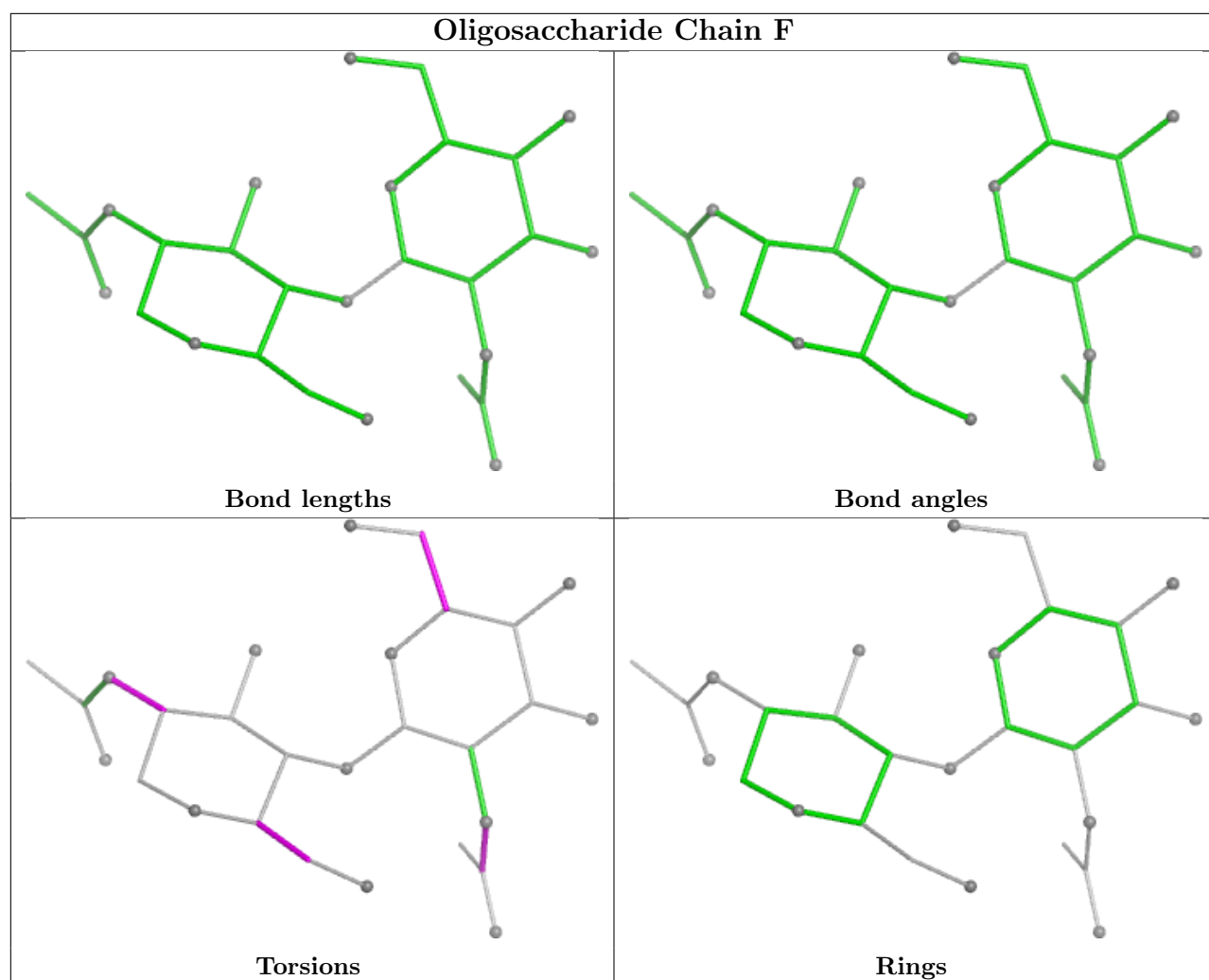
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	2	NAG	2	0
2	E	1	NAG	1	0
2	I	1	NAG	1	0
2	I	2	NAG	2	0

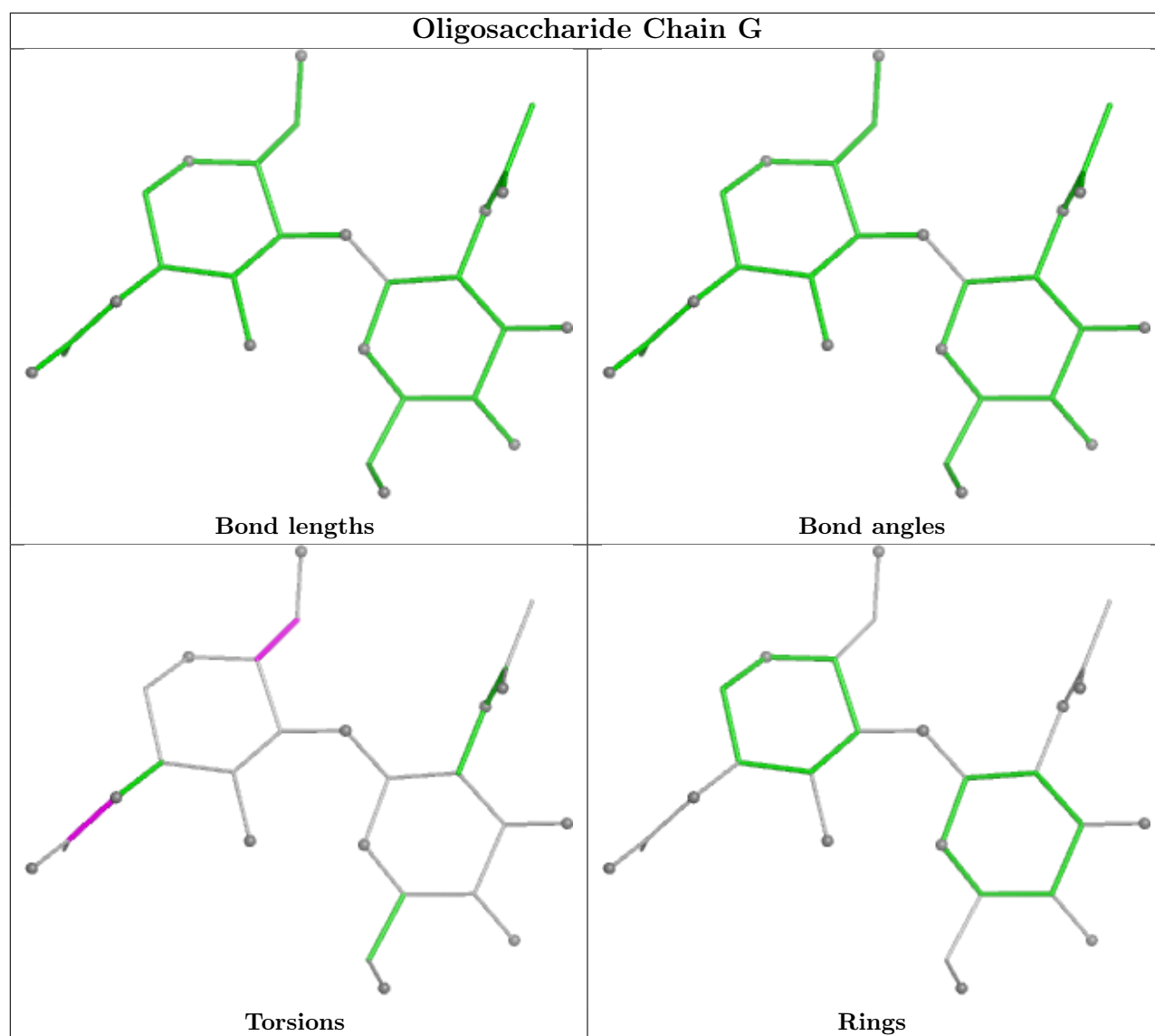
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

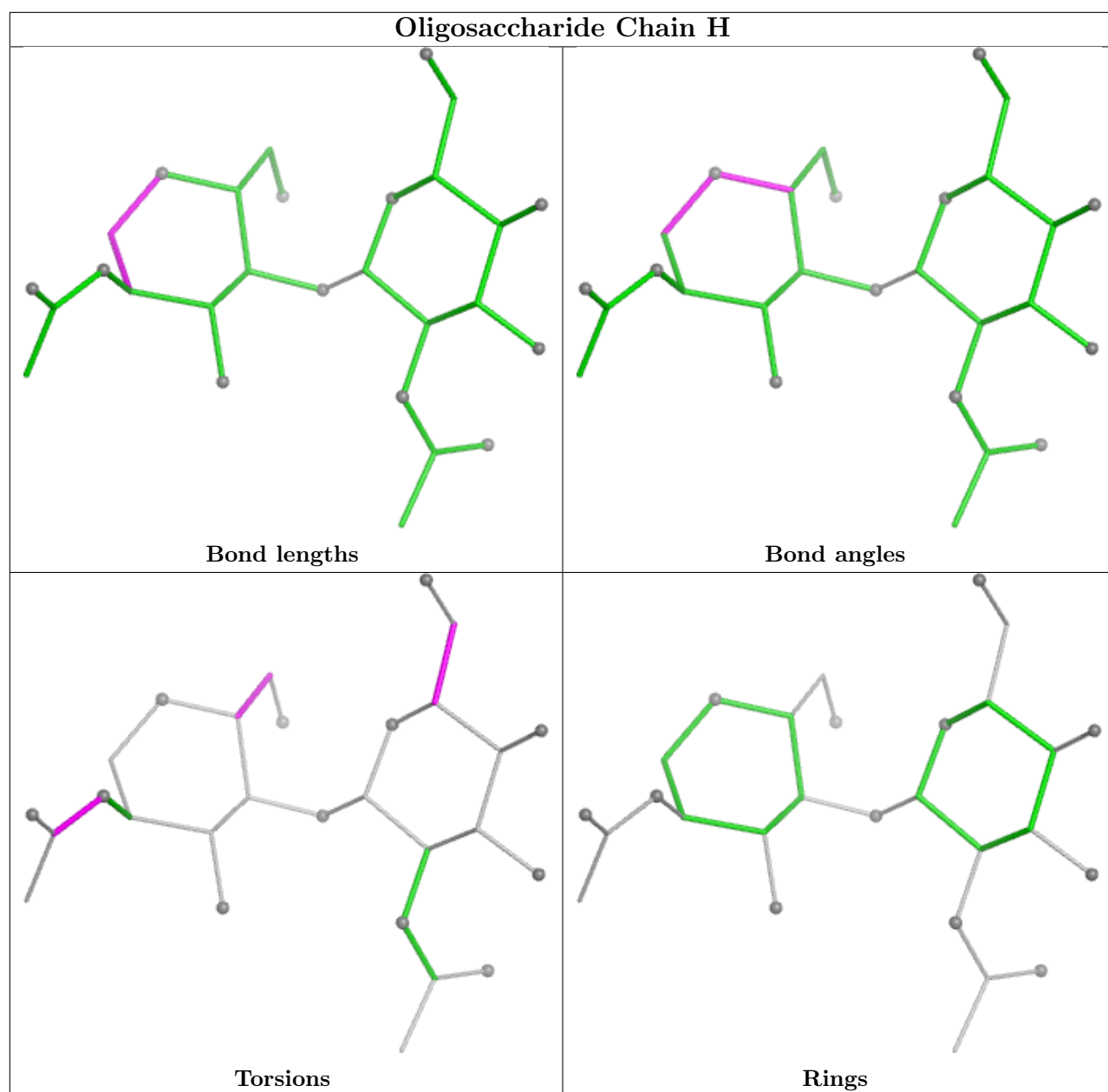


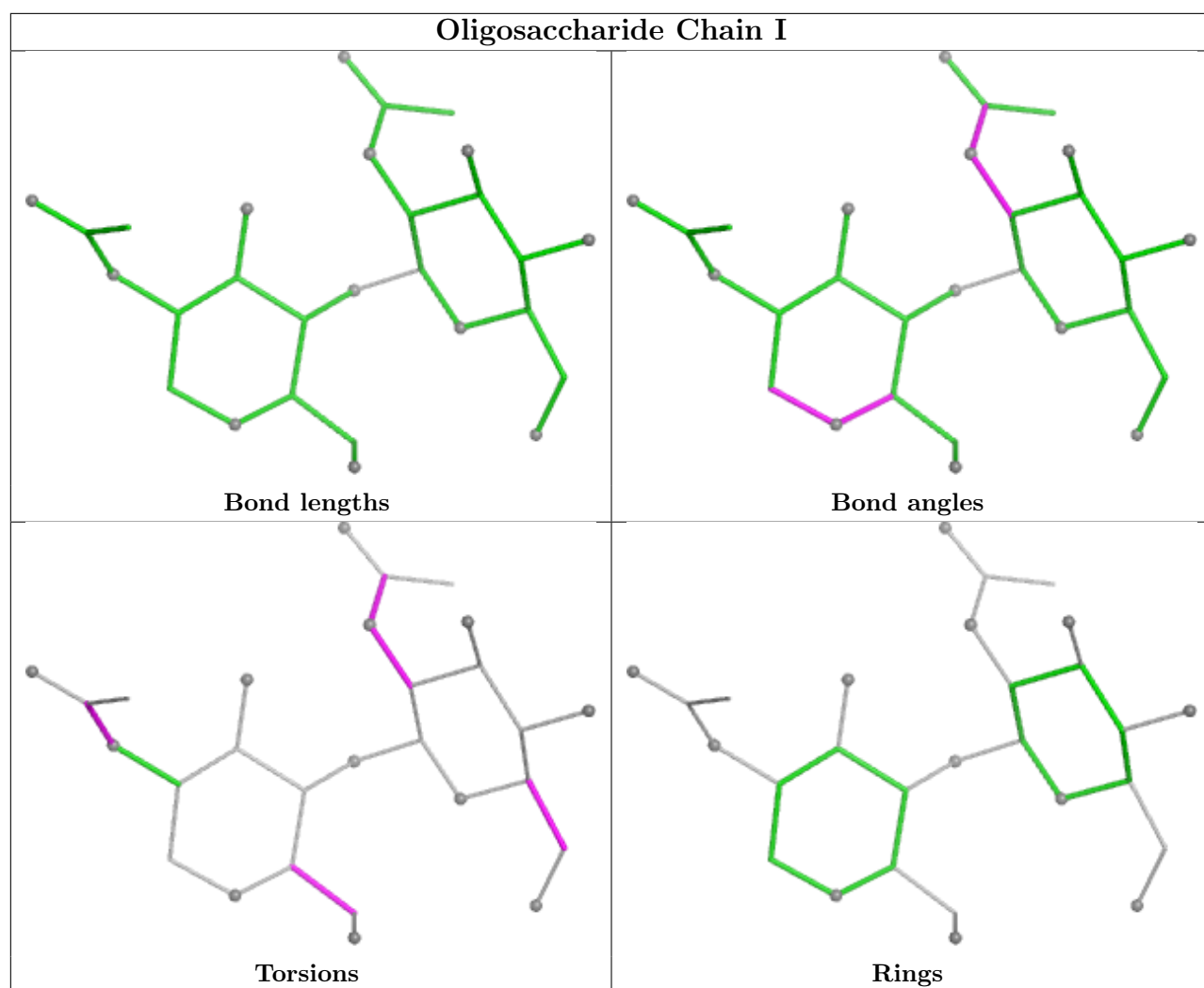


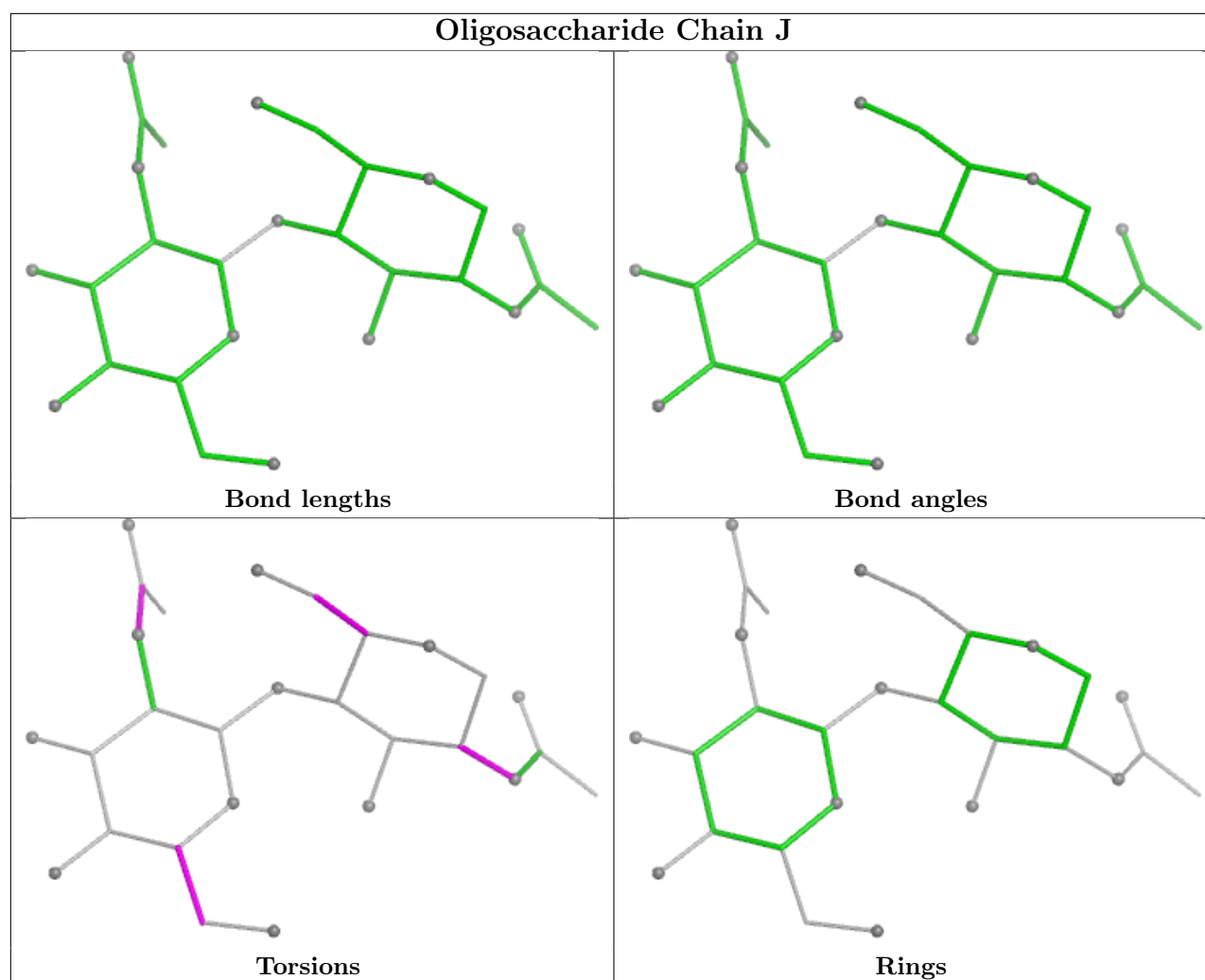












5.6 Ligand geometry [i](#)

16 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	$\# Z > 2$
3	NAG	A	2807	-	15,15,15	0.23	0	21,21,21	0.30	0
3	NAG	A	2802	1	14,14,15	0.17	0	17,19,21	0.35	0
3	NAG	B	2803	1	14,14,15	0.34	0	17,19,21	0.55	0
3	NAG	B	2804	1	14,14,15	0.55	0	17,19,21	0.43	0
3	NAG	B	2807	-	15,15,15	0.22	0	21,21,21	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	B	2808	1	14,14,15	0.40	0	17,19,21	0.72	1 (5%)
3	NAG	B	2806	1	14,14,15	0.30	0	17,19,21	0.45	0
3	NAG	A	2806	1	14,14,15	0.32	0	17,19,21	0.45	0
3	NAG	A	2801	1	14,14,15	0.31	0	17,19,21	0.90	1 (5%)
3	NAG	B	2805	1	14,14,15	1.09	2 (14%)	17,19,21	1.63	3 (17%)
3	NAG	A	2804	1	14,14,15	0.53	0	17,19,21	0.43	0
3	NAG	B	2801	1	14,14,15	0.32	0	17,19,21	0.90	1 (5%)
3	NAG	A	2803	1	14,14,15	0.32	0	17,19,21	0.55	0
3	NAG	A	2808	1	14,14,15	0.40	0	17,19,21	0.73	1 (5%)
3	NAG	A	2805	1	14,14,15	1.10	2 (14%)	17,19,21	1.63	3 (17%)
3	NAG	B	2802	1	14,14,15	0.16	0	17,19,21	0.34	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	2807	-	-	4/6/26/26	0/1/1/1
3	NAG	A	2802	1	-	4/6/23/26	0/1/1/1
3	NAG	B	2803	1	-	4/6/23/26	0/1/1/1
3	NAG	B	2804	1	-	2/6/23/26	0/1/1/1
3	NAG	B	2807	-	-	4/6/26/26	0/1/1/1
3	NAG	B	2808	1	-	2/6/23/26	0/1/1/1
3	NAG	B	2806	1	-	2/6/23/26	0/1/1/1
3	NAG	A	2806	1	-	2/6/23/26	0/1/1/1
3	NAG	A	2801	1	-	0/6/23/26	0/1/1/1
3	NAG	B	2805	1	-	5/6/23/26	0/1/1/1
3	NAG	A	2804	1	-	2/6/23/26	0/1/1/1
3	NAG	B	2801	1	-	0/6/23/26	0/1/1/1
3	NAG	A	2803	1	-	4/6/23/26	0/1/1/1
3	NAG	A	2808	1	-	2/6/23/26	0/1/1/1
3	NAG	A	2805	1	-	5/6/23/26	0/1/1/1
3	NAG	B	2802	1	-	4/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2805	NAG	O5-C1	3.35	1.49	1.43
3	A	2805	NAG	O5-C1	3.29	1.49	1.43
3	A	2805	NAG	C1-C2	2.34	1.55	1.52
3	B	2805	NAG	C1-C2	2.21	1.55	1.52

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2805	NAG	C1-O5-C5	4.36	118.09	112.19
3	B	2805	NAG	C1-O5-C5	4.35	118.08	112.19
3	B	2805	NAG	C2-N2-C7	4.27	128.99	122.90
3	A	2805	NAG	C2-N2-C7	4.27	128.98	122.90
3	B	2801	NAG	C1-O5-C5	3.30	116.67	112.19

There are no chirality outliers.

5 of 46 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2805	NAG	C4-C5-C6-O6
3	B	2805	NAG	C4-C5-C6-O6
3	A	2803	NAG	O5-C5-C6-O6
3	B	2803	NAG	O5-C5-C6-O6
3	A	2807	NAG	O5-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2803	NAG	1	0
3	B	2805	NAG	3	0
3	A	2803	NAG	1	0
3	A	2805	NAG	2	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.

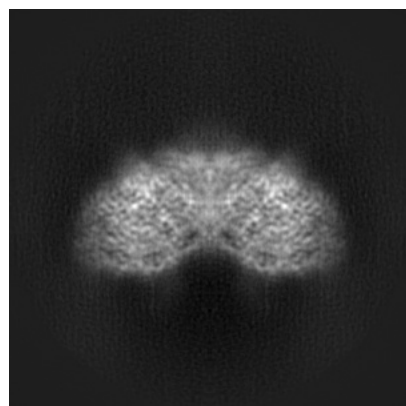
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52854. These allow visual inspection of the internal detail of the map and identification of artifacts.

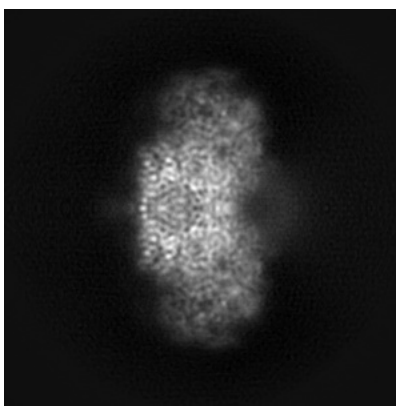
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

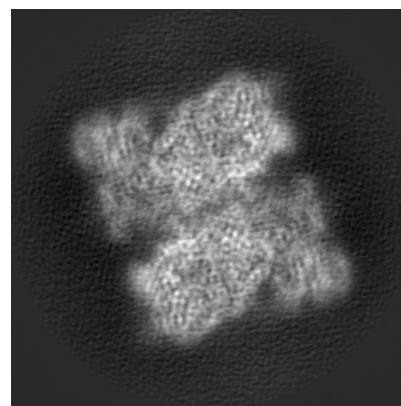
6.1.1 Primary map



X

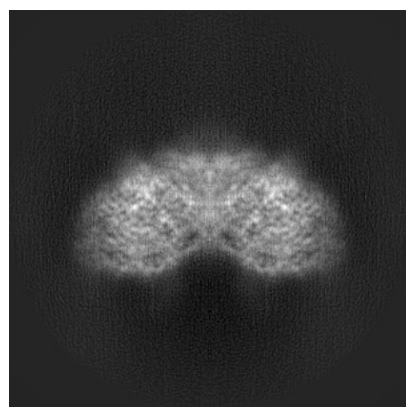


Y

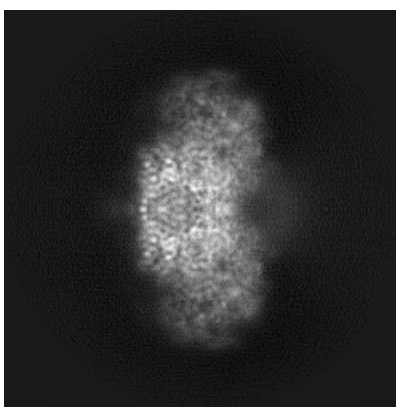


Z

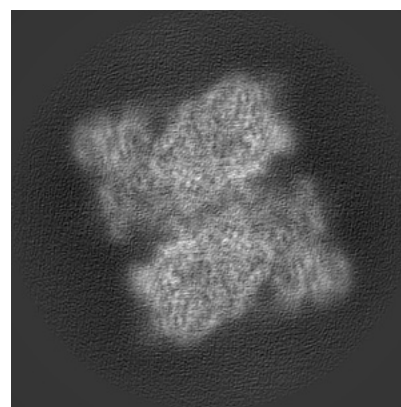
6.1.2 Raw map



X



Y

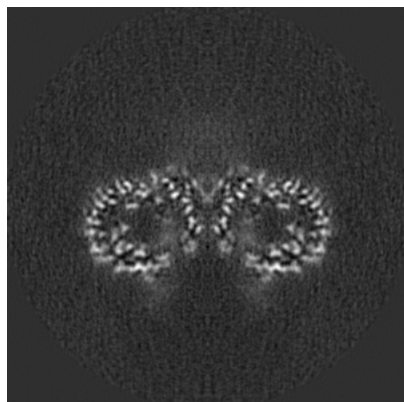


Z

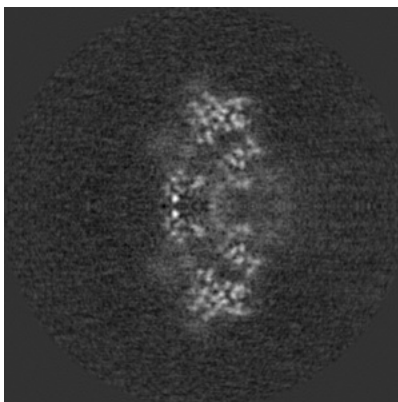
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

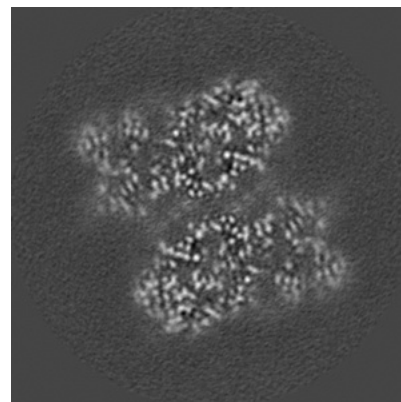
6.2.1 Primary map



X Index: 140

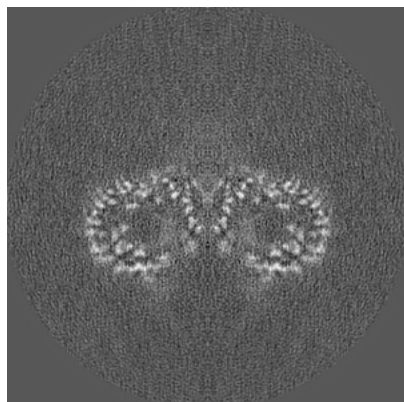


Y Index: 140

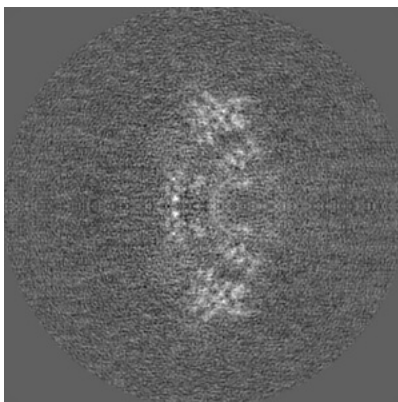


Z Index: 140

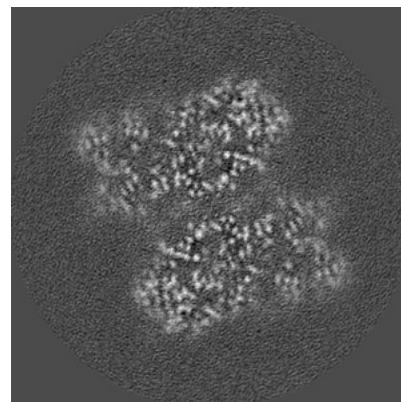
6.2.2 Raw map



X Index: 140



Y Index: 140

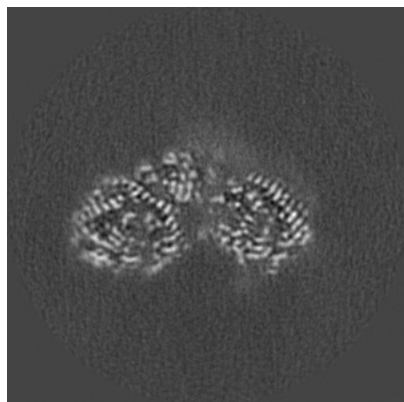


Z Index: 140

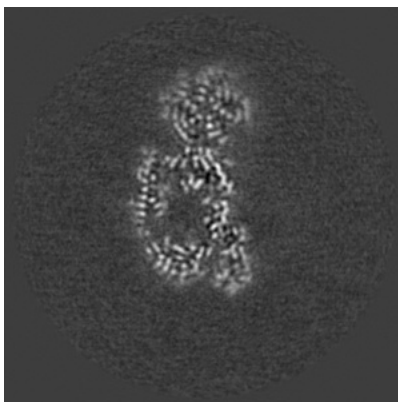
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

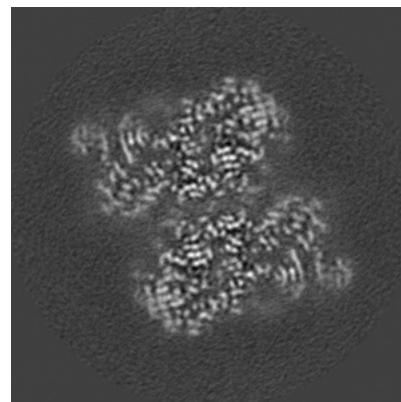
6.3.1 Primary map



X Index: 118

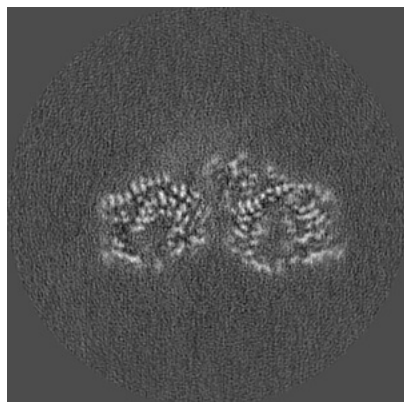


Y Index: 95

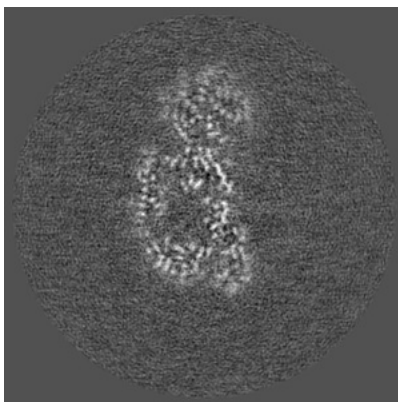


Z Index: 144

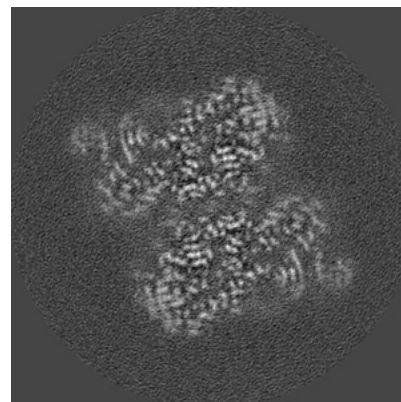
6.3.2 Raw map



X Index: 156



Y Index: 95

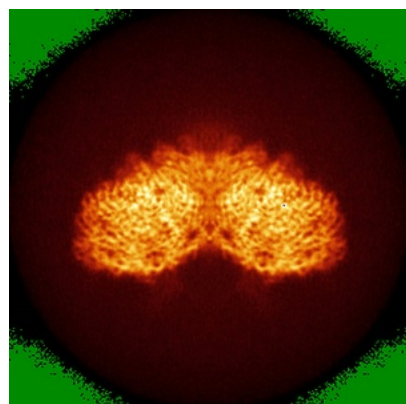


Z Index: 144

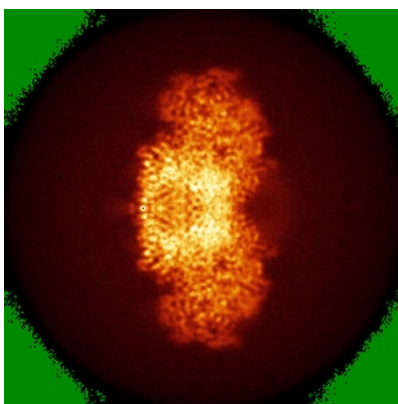
The images above show the largest variance slices of the map in three orthogonal directions.

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

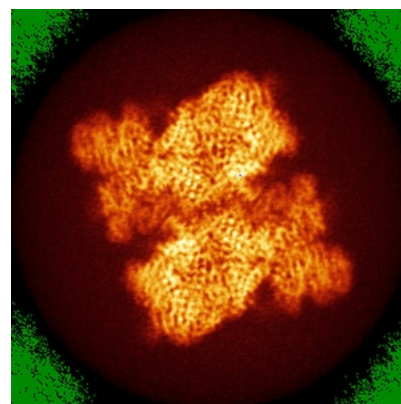
6.4.1 Primary map



X

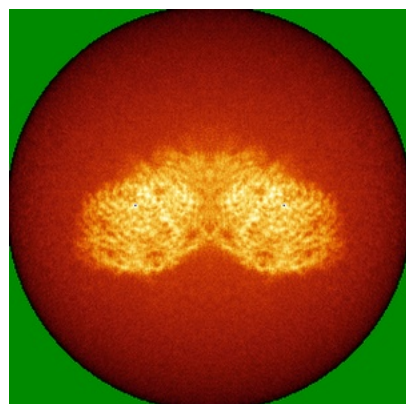


Y

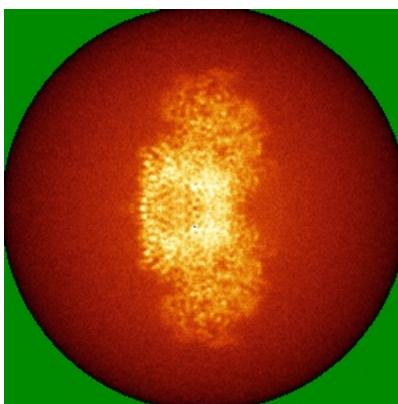


Z

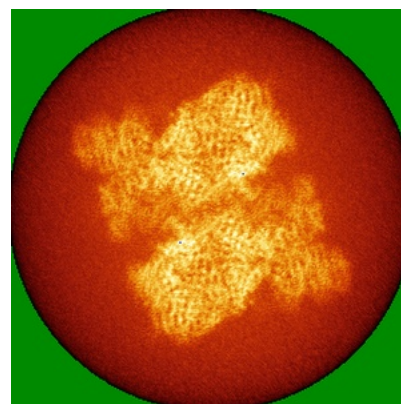
6.4.2 Raw map



X



Y

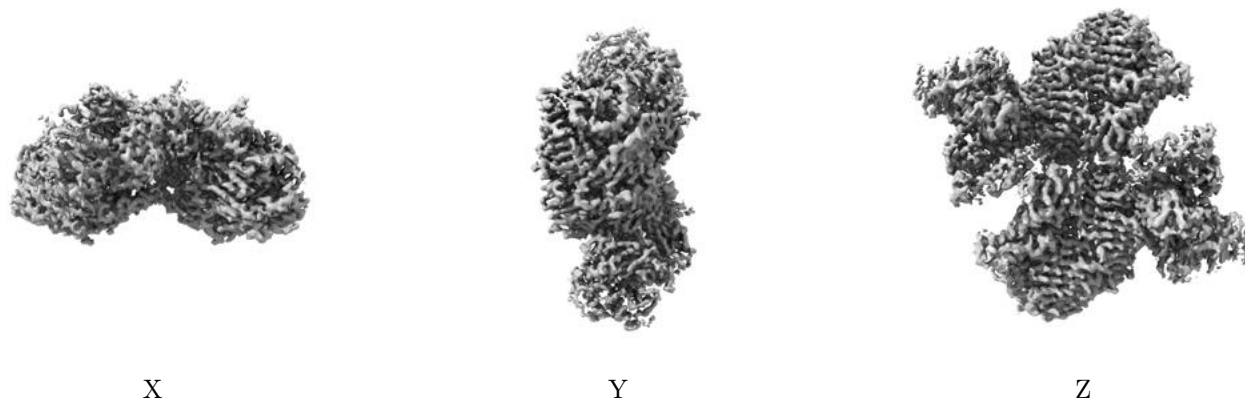


Z

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

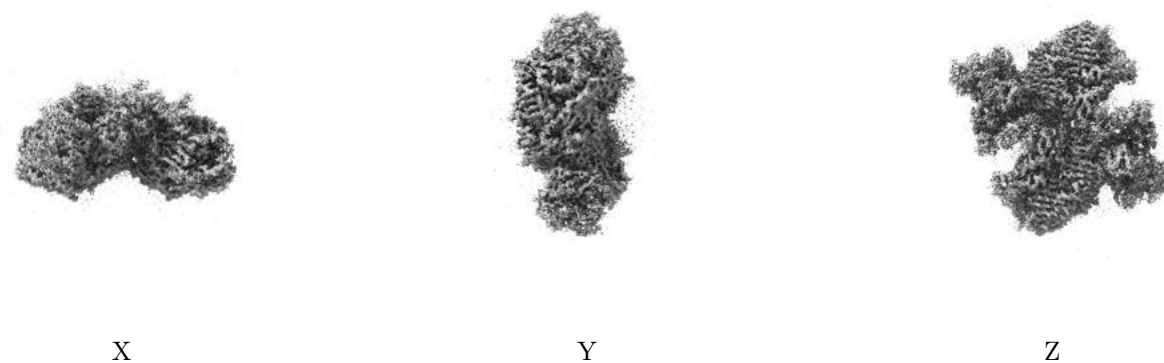
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00718. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

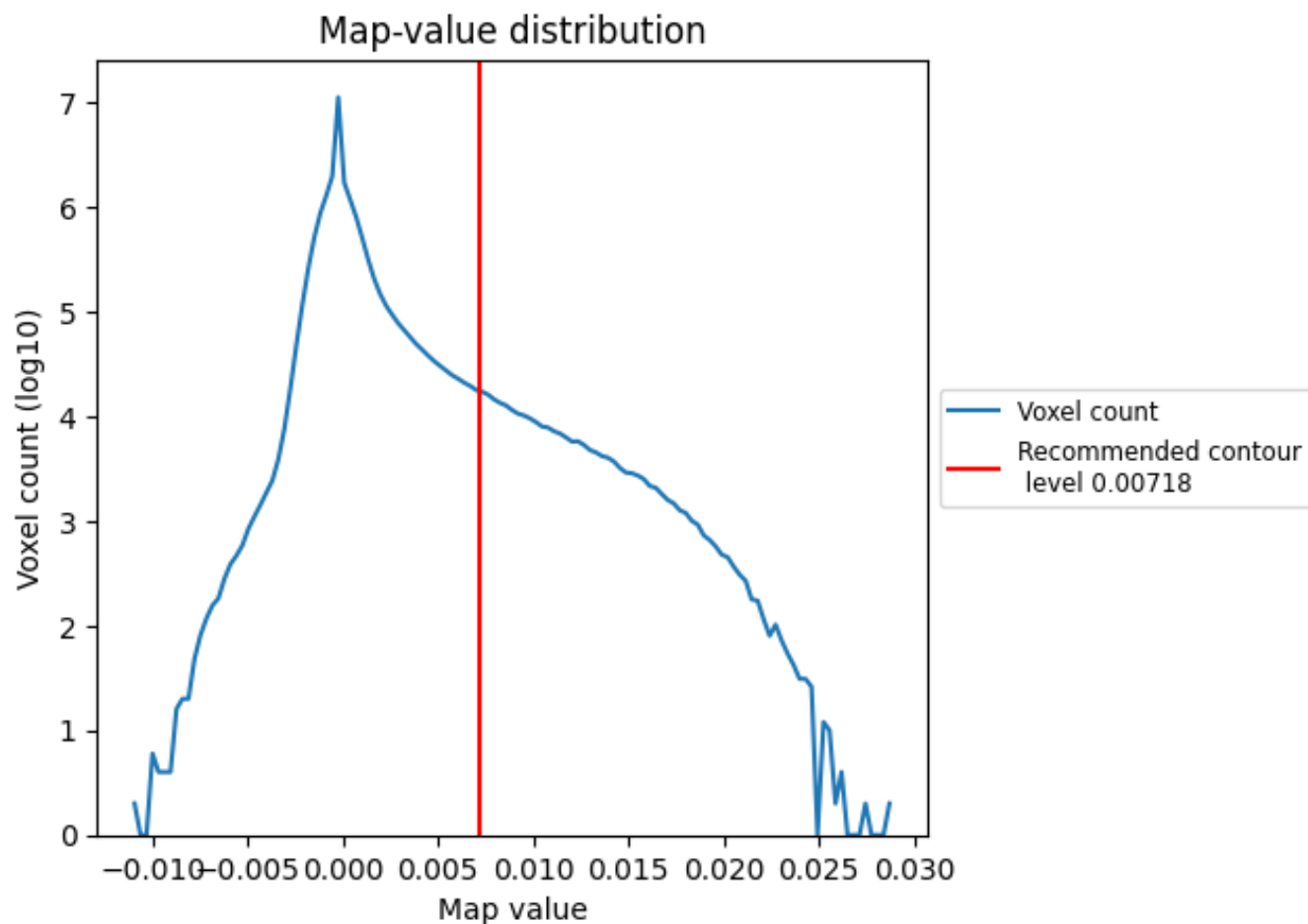
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

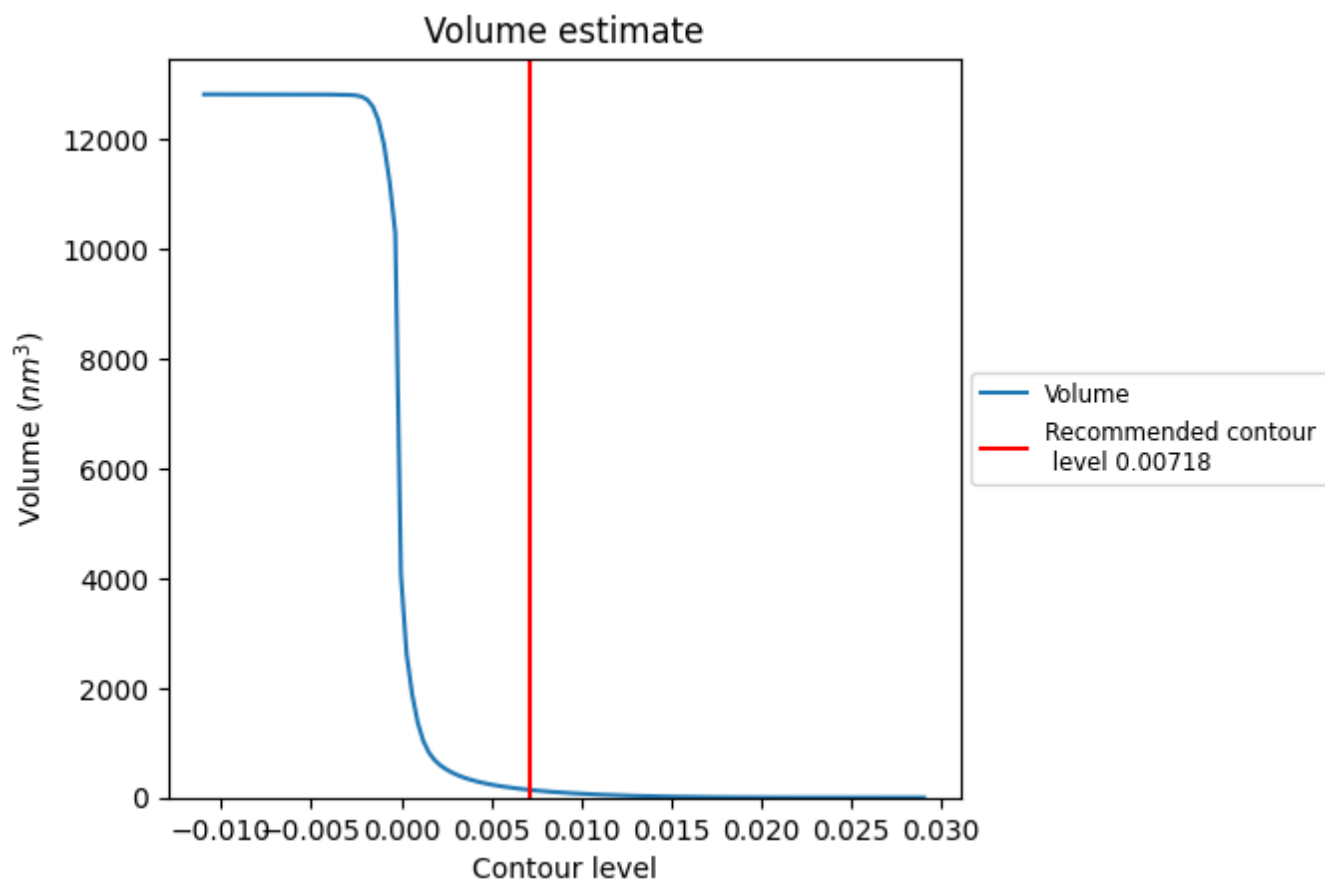
This section contains the results of statistical analysis of the map.

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.

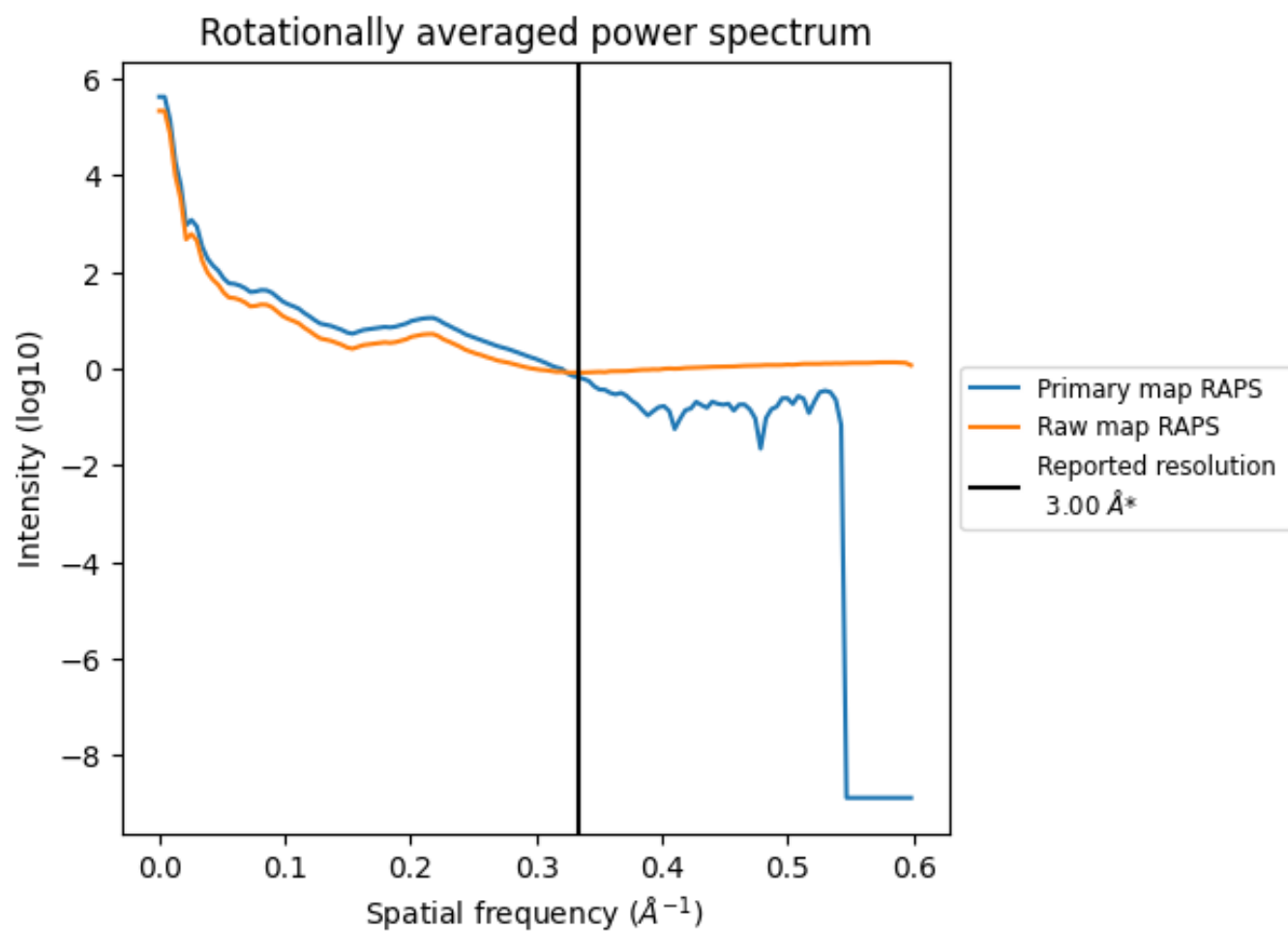
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 139 nm³; this corresponds to an approximate mass of 126 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 ⓘ

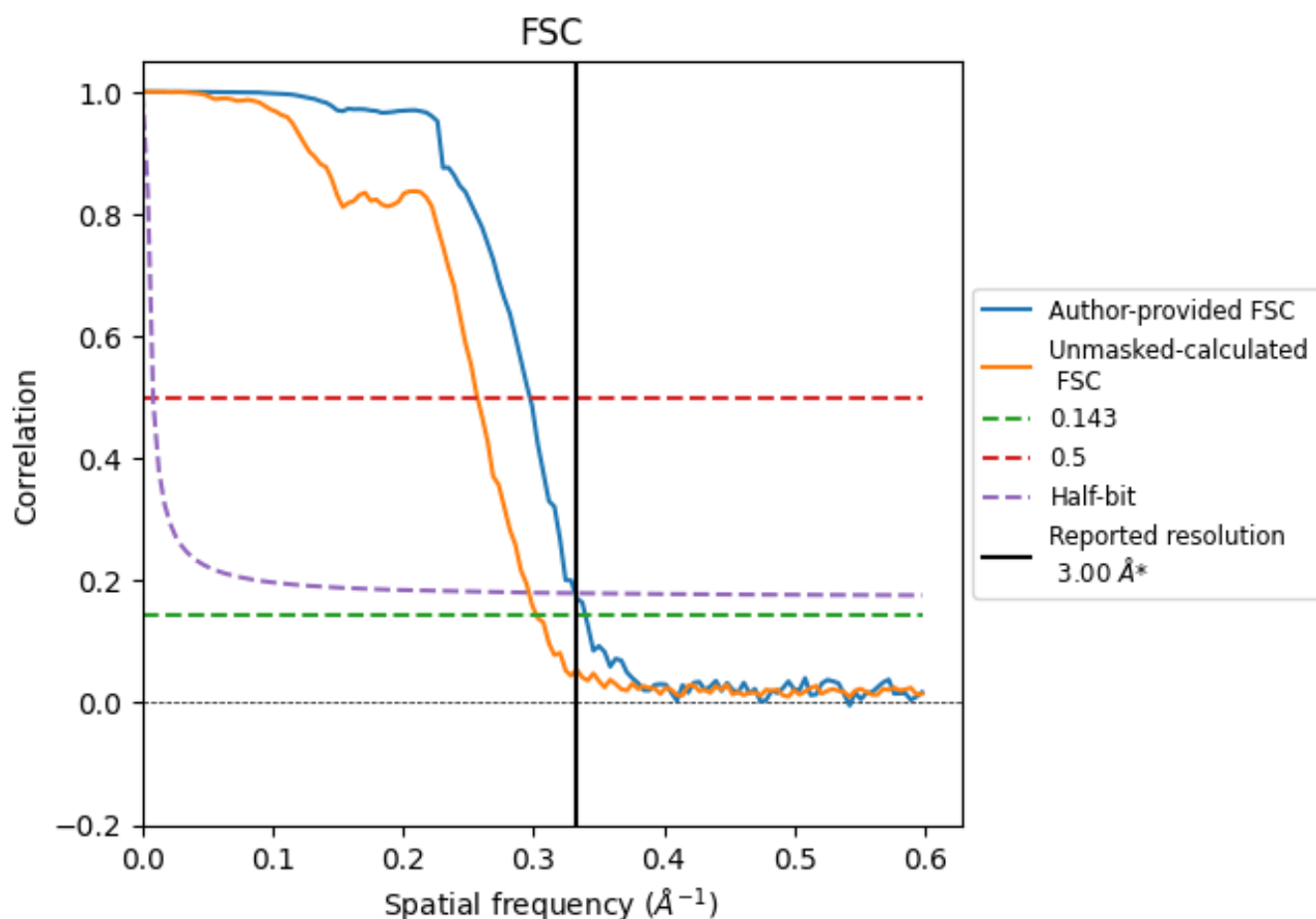


*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

8.2 Resolution estimates [i](#)

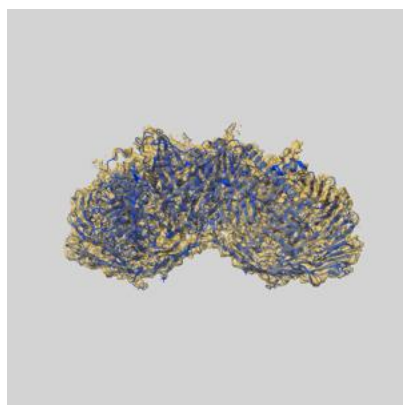
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	2.94	3.36	3.01
Unmasked-calculated*	3.31	3.89	3.37

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.31 differs from the reported value 3.0 by more than 10 %

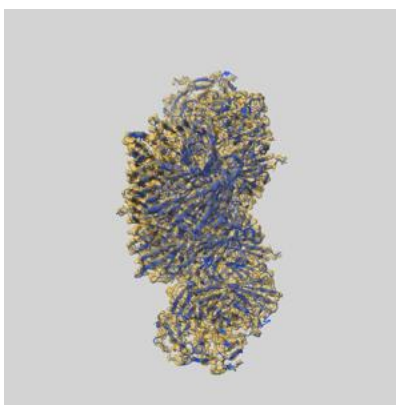
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-52854 and PDB model 9IGS. Per-residue inclusion information can be found in section [3](#) on page [9](#).

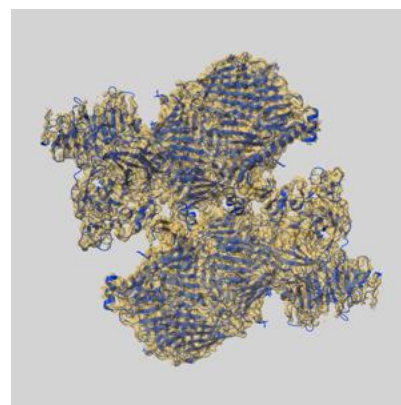
9.1 Map-model overlay [i](#)



X



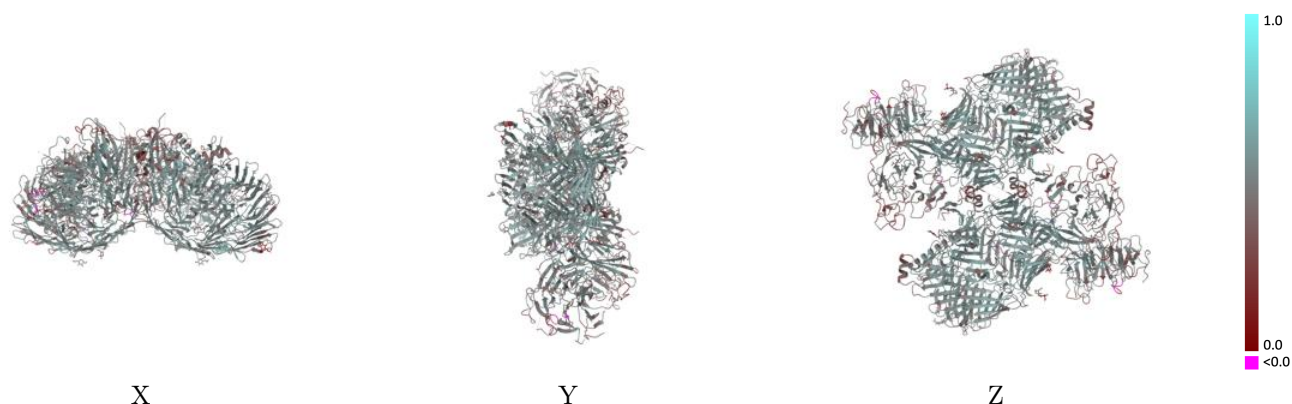
Y



Z

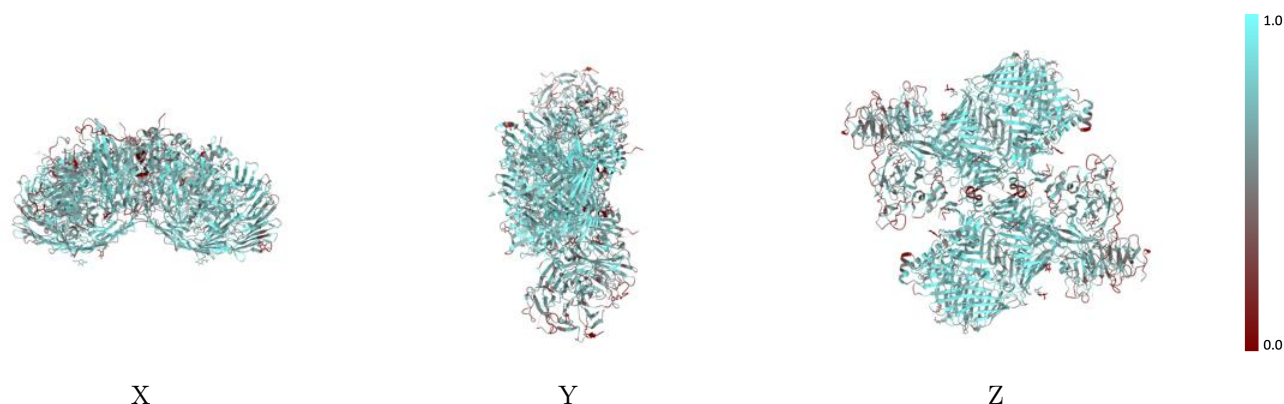
The images above show the 3D surface view of the map at the recommended contour level 0.00718 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



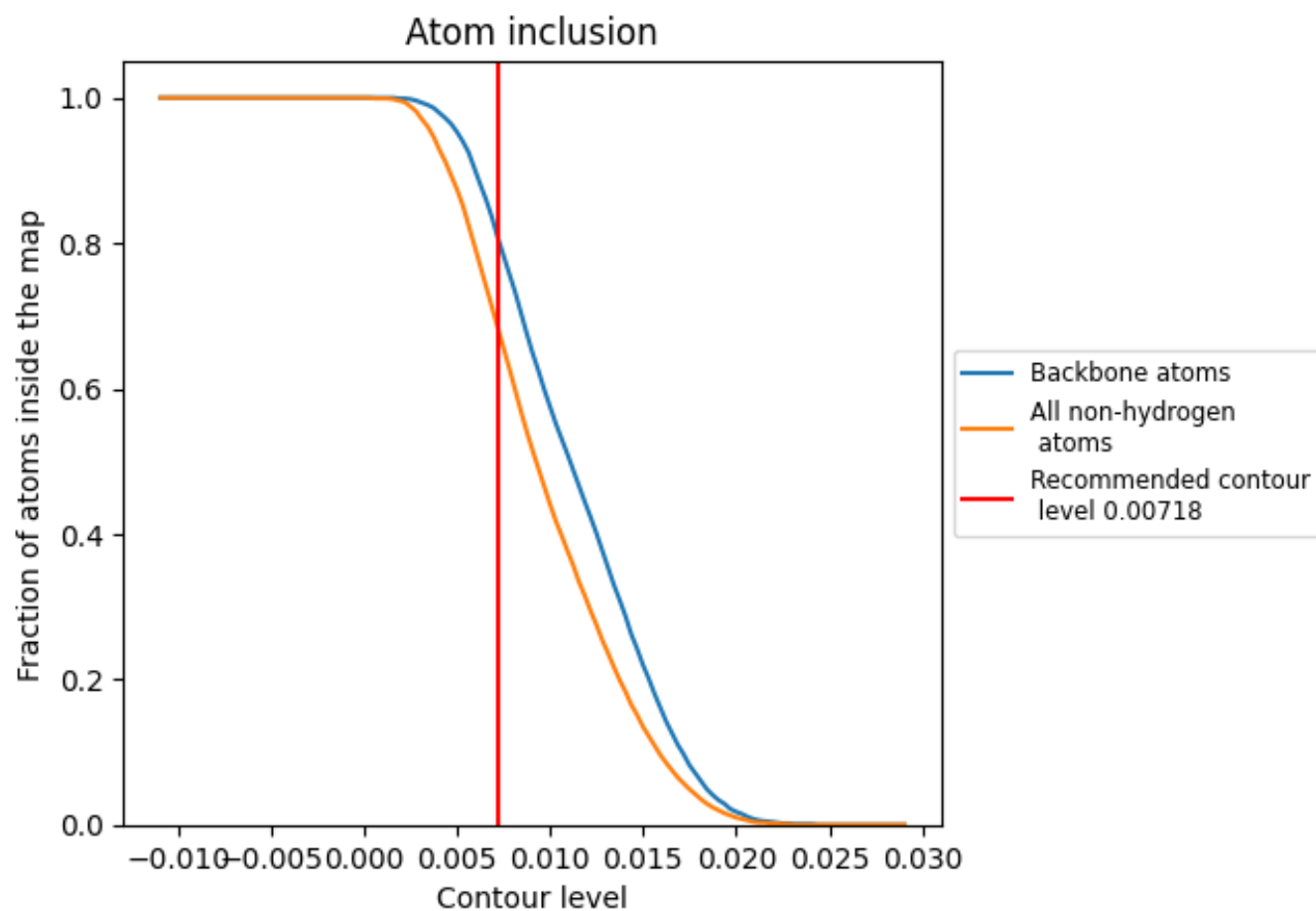
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00718).

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 68% 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 (0.00718) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6840	0.4950
A	0.6860	0.4960
B	0.6860	0.4960
C	0.3930	0.4370
D	0.2860	0.3210
E	0.3210	0.2920
F	0.5360	0.4760
G	0.3930	0.4180
H	0.2860	0.3430
I	0.3210	0.2790
J	0.5710	0.4750

1.0

0.0

<0.0