



Full wwPDB EM Validation Report ⓘ

Aug 3, 2026 – 11:13 am BST

PDB ID : 9G42 / pdb_00009g42
EMDB ID : EMD-51022
Title : Mouse Teneurin2 dimer variant A0B0
Authors : Berbeira-Santana, M.; Zhou, J.C.; el Omari, K.; Baker, L.; Seiradake, E.
Deposited on : 2024-07-12
Resolution : 2.82 Å(reported)
Based on initial model : .

This is a Full wwPDB EM Validation 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:

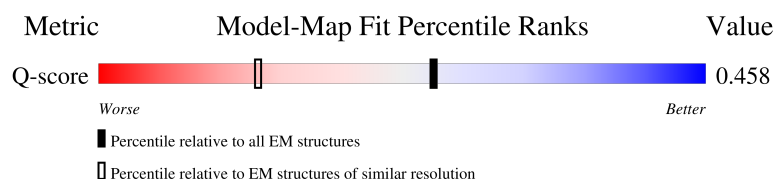
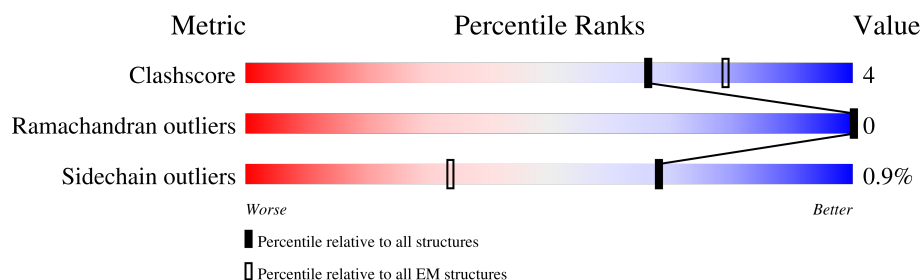
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal 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 2.82 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.



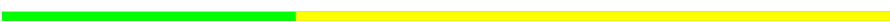
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11795 (2.32 - 3.32)

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	2394	
1	B	2394	
2	C	2	
2	E	2	

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Mol	Chain	Length	Quality of chain
2	F	2	 100%
2	H	2	 50%50%
3	D	3	 67%33%
3	G	3	 33%67%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 27562 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 Teneurin transmembrane protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1722	Total	C	N	O	S	0	0
			13616	8593	2355	2614	54		
1	B	1722	Total	C	N	O	S	0	0
			13616	8593	2355	2614	54		

There are 82 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	367	GLU	-	expression tag	UNP A0A0A0MQB7
A	368	THR	-	expression tag	UNP A0A0A0MQB7
A	369	GLY	-	expression tag	UNP A0A0A0MQB7
A	370	HIS	-	expression tag	UNP A0A0A0MQB7
A	371	HIS	-	expression tag	UNP A0A0A0MQB7
A	372	HIS	-	expression tag	UNP A0A0A0MQB7
A	373	HIS	-	expression tag	UNP A0A0A0MQB7
A	374	HIS	-	expression tag	UNP A0A0A0MQB7
A	375	HIS	-	expression tag	UNP A0A0A0MQB7
A	376	ARG	-	expression tag	UNP A0A0A0MQB7
A	377	GLY	-	expression tag	UNP A0A0A0MQB7
A	378	GLY	-	expression tag	UNP A0A0A0MQB7
A	379	LEU	-	expression tag	UNP A0A0A0MQB7
A	380	ASN	-	expression tag	UNP A0A0A0MQB7
A	381	ASP	-	expression tag	UNP A0A0A0MQB7
A	382	ILE	-	expression tag	UNP A0A0A0MQB7
A	383	PHE	-	expression tag	UNP A0A0A0MQB7
A	384	GLU	-	expression tag	UNP A0A0A0MQB7
A	385	ALA	-	expression tag	UNP A0A0A0MQB7
A	386	GLN	-	expression tag	UNP A0A0A0MQB7
A	387	LYS	-	expression tag	UNP A0A0A0MQB7
A	388	ILE	-	expression tag	UNP A0A0A0MQB7
A	389	GLU	-	expression tag	UNP A0A0A0MQB7
A	390	TRP	-	expression tag	UNP A0A0A0MQB7
A	391	HIS	-	expression tag	UNP A0A0A0MQB7
A	392	GLU	-	expression tag	UNP A0A0A0MQB7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	393	GLY	-	expression tag	UNP A0A0A0MQB7
A	394	GLY	-	expression tag	UNP A0A0A0MQB7
A	395	SER	-	expression tag	UNP A0A0A0MQB7
A	396	THR	-	expression tag	UNP A0A0A0MQB7
A	397	GLY	-	expression tag	UNP A0A0A0MQB7
A	737	GLU	-	insertion	UNP A0A0A0MQB7
A	?	-	LYS	deletion	UNP A0A0A0MQB7
A	?	-	GLU	deletion	UNP A0A0A0MQB7
A	?	-	PHE	deletion	UNP A0A0A0MQB7
A	?	-	LYS	deletion	UNP A0A0A0MQB7
A	?	-	HIS	deletion	UNP A0A0A0MQB7
A	?	-	SER	deletion	UNP A0A0A0MQB7
A	?	-	ASN	deletion	UNP A0A0A0MQB7
A	2759	GLY	-	expression tag	UNP A0A0A0MQB7
A	2760	THR	-	expression tag	UNP A0A0A0MQB7
B	367	GLU	-	expression tag	UNP A0A0A0MQB7
B	368	THR	-	expression tag	UNP A0A0A0MQB7
B	369	GLY	-	expression tag	UNP A0A0A0MQB7
B	370	HIS	-	expression tag	UNP A0A0A0MQB7
B	371	HIS	-	expression tag	UNP A0A0A0MQB7
B	372	HIS	-	expression tag	UNP A0A0A0MQB7
B	373	HIS	-	expression tag	UNP A0A0A0MQB7
B	374	HIS	-	expression tag	UNP A0A0A0MQB7
B	375	HIS	-	expression tag	UNP A0A0A0MQB7
B	376	ARG	-	expression tag	UNP A0A0A0MQB7
B	377	GLY	-	expression tag	UNP A0A0A0MQB7
B	378	GLY	-	expression tag	UNP A0A0A0MQB7
B	379	LEU	-	expression tag	UNP A0A0A0MQB7
B	380	ASN	-	expression tag	UNP A0A0A0MQB7
B	381	ASP	-	expression tag	UNP A0A0A0MQB7
B	382	ILE	-	expression tag	UNP A0A0A0MQB7
B	383	PHE	-	expression tag	UNP A0A0A0MQB7
B	384	GLU	-	expression tag	UNP A0A0A0MQB7
B	385	ALA	-	expression tag	UNP A0A0A0MQB7
B	386	GLN	-	expression tag	UNP A0A0A0MQB7
B	387	LYS	-	expression tag	UNP A0A0A0MQB7
B	388	ILE	-	expression tag	UNP A0A0A0MQB7
B	389	GLU	-	expression tag	UNP A0A0A0MQB7
B	390	TRP	-	expression tag	UNP A0A0A0MQB7
B	391	HIS	-	expression tag	UNP A0A0A0MQB7
B	392	GLU	-	expression tag	UNP A0A0A0MQB7
B	393	GLY	-	expression tag	UNP A0A0A0MQB7

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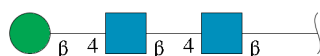
Chain	Residue	Modelled	Actual	Comment	Reference
B	394	GLY	-	expression tag	UNP A0A0A0MQB7
B	395	SER	-	expression tag	UNP A0A0A0MQB7
B	396	THR	-	expression tag	UNP A0A0A0MQB7
B	397	GLY	-	expression tag	UNP A0A0A0MQB7
B	737	GLU	-	insertion	UNP A0A0A0MQB7
B	?	-	LYS	deletion	UNP A0A0A0MQB7
B	?	-	GLU	deletion	UNP A0A0A0MQB7
B	?	-	PHE	deletion	UNP A0A0A0MQB7
B	?	-	LYS	deletion	UNP A0A0A0MQB7
B	?	-	HIS	deletion	UNP A0A0A0MQB7
B	?	-	SER	deletion	UNP A0A0A0MQB7
B	?	-	ASN	deletion	UNP A0A0A0MQB7
B	2759	GLY	-	expression tag	UNP A0A0A0MQB7
B	2760	THR	-	expression tag	UNP A0A0A0MQB7

- 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	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	H	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 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
3	D	3	Total	C	N	O	0	0
			39	22	2	15		

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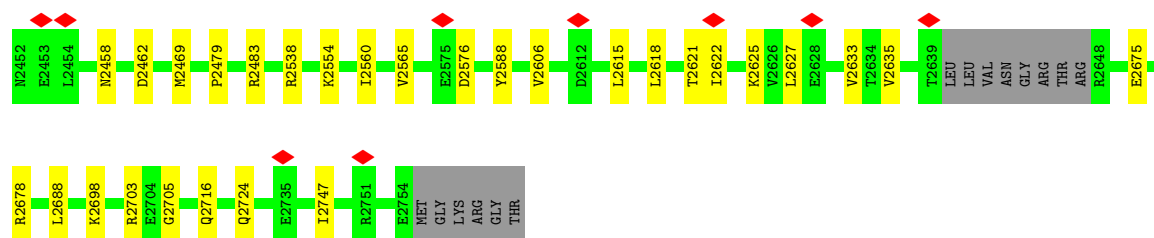
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	G	3	39	22	2	15	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

L2123	L1872	V1654	A1498	N1418	M1353	T1289	M1226	SER	HIS	GLY	CYS
I2127	Q1889	S1655	G1499	N1419	Y1354	M1290	K1227	ALA	ILE	ASP	GLU
Y2149	R1890	T1656	A1500	V1420	F1355	S1291	L1228	THR	ILE	LEU	VAL
M2156	R1896	E1679	A1501	I1421	D1356	R1292	L1229	LEU	GLY	TRP	CYS
Y2157	V1915	T1680	S1502	L1422	D1357	R1293	A1230	PHE	ASN	ASP	ASN
V2169	V1916	G1681	D1503	R1423	A1358	Y1294	F1231	ARG	GLY	CYS	LEU
L2176	W1922	D1687	C1504	I1424	T1359	R1295	A1232	GLU	PRO	ASP	ASP
H2217	M1925	D1726	C1506	E1426	M1360	V1297	L1234	ALA	ASN	THR	CYS
L2230	V1926	T1729	K1507	H1427	I1361	K1298	A1235	PHE	ILE	VAL	SER
R2235	L1927	S1736	N1511	Q1429	K1363	L1300	V1236	MET	CYS	ASP	CYS
D2236	S1931	V1744	D1512	V1430	D1365	S1301	G1237	SER	VAL	LEU	HIS
R2237	T1936	M1766	I1513	I1432	Q1366	G1302	D1238	GLN	SER	GLN	GLY
K2247	S1942	V1770	A1522	I1433	M1367	K1304	L1242	THR	ARG	ALA	VAL
I2248	S1943	H1773	L1527	A1434	G1368	D1305	F1243	VAL	GLY	CYS	VAL
D2249	R1944	H1777	N1528	G1435	S1371	A1307	G1245	TRP	GLN	ASN	GLY
D2250	T1949	VAL	S1529	R1436	T1372	G1308	D1246	ASN	ASP	ILE	CYS
Q2256	V1953	ALA	P1530	I1441	L1373	E1311	F1247	THR	GLY	THR	PRO
D2260	T1998	GLY	A1534	Q1441	L1374	V1312	N1248	PHE	THR	GLY	GLY
I2261	T1998	THR	V1535	Q1442	G1375	V1313	Y1249	TYR	LEU	ALA	GLY
N2275	L2012	ILE	D1538	P1443	M1377	A1314	R1251	ALA	CYS	ARG	TRP
R2285	L2015	THR	I1541	G1444	D1378	A1315	R1252	ASP	GLN	ASP	GLY
S2294	L2027	THR	Y1542	I1445	L1379	T1316	I1253	THR	GLY	LEU	LEU
Y2295	T2030	ILE	G1768	D1446	T1380	E1317	F1254	LEU	VAL	ASP	ASN
L2303	G2031	R1789	R1789	A1447	G1318	E1318	P1255	VAL	ASN	ILE	CYS
L2310	V2032	I1792	D1545	L1448	Q1319	C1320	P1256	THR	LYS	ILE	GLU
Y2331	K2051	E1804	L1546	L1449	L1321	L1322	I1257	GLY	ALA	VAL	GLU
E2342	D2057	R1808	G1547	S1456	F1323	D1324	R1257	GLU	GLN	ALA	ARG
L2360	M2068	R1809	I1549	A1457	E1325	E1326	G1207	ALA	THR	GLN	VAL
Q2374	I2069	E1810	R1550	L1458	A1326	A1326	M1206	GLY	CYS	GLY	CYS
Y2383	Y2075	I1818	S1571	E1459	R1327	C1328	G1207	VAL	LYS	THR	CYS
N2440	T2084	R1824	T1589	S1460	S1389	G1329	N1208	VAL	CYS	THR	ASP
M2443	S2092	V1925	Y1599	A1461	S1390	D1330	G1209	THR	ILE	ARG	PRO
N2448	H2112	H1826	D1606	A1463	M1391	D1331	R1266	ALA	TYR	ASP	GLY
S2451	F2113	G1827	N1616	I1464	D1392	D1330	N1267	GLN	MET	THR	THR
	G2114	L1831	K1621	S1467	Q1393	G1332	R1210	ILE	GLY	GLY	LEU
	V2118	L1831	T1622	Y1473	V1396	G1332	R1211	ASP	THR	GLY	THR
	D2122	D1834	R1623	E1476	R1397	K1333	R1212	LYS	THR	LYS	ASP
		R1862	I1641	T1477	L1398	A1334	S1213	ALA	THR	ALA	CYS
			T1642	D1478	E1399	V1335	I1214	LEU	PHE	ASP	LYS
			L1643	E1479	E1399	D1336	K1272	GLY	THR	ASP	GLY
			N1648	K1480	W1400	L1339	Y1273	ALA	ILE	LYS	ASN
				L1643	D1403	M1340	Y1274	LYS	ALA	ASP	LYS
					L1404	S1341	L1275	ASN	ALA	ASP	ASN
					M1405	P1342	A1276	GLY	GLY	GLY	GLU
					V1406	G1344	V1277	THR	THR	THR	THR
					M1409	I1345	G1284	GLY	GLY	GLY	GLY
					D1410	V1347	Y1285	LYS	LYS	LYS	LYS
					N1411	D1348	S1287	ASN	ASN	ASN	ASN
					L1416	E1417	D1288	GLY	GLY	GLY	GLY



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

Chain C:  100%



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

Chain E:  50%



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

Chain F:  100%



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

Chain H:  50%

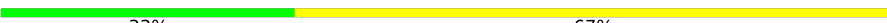


- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:  67%



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

Chain G:  33%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	38045	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 ($e^-/\text{\AA}^2$)	41.503	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.776	Depositor
Minimum map value	-0.016	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.036	Depositor
Recommended contour level	0.134	Depositor
Map size (Å)	290.5, 290.5, 290.5	wwPDB
Map dimensions	350, 350, 350	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

5 Model quality

5.1 Standard geometry

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	0.16	0/13907	0.42	0/18861
1	B	0.16	0/13907	0.42	0/18861
All	All	0.16	0/27814	0.42	0/37722

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	3
1	B	0	3
All	All	0	6

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1017	ARG	Sidechain
1	A	1761	ARG	Sidechain
1	A	1789	ARG	Sidechain
1	B	1017	ARG	Sidechain
1	B	1789	ARG	Sidechain
1	B	2483	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	13616	0	13350	101	0
1	B	13616	0	13351	113	0
2	C	28	0	25	0	0
2	E	28	0	25	0	0
2	F	28	0	25	0	0
2	H	28	0	25	0	0
3	D	39	0	34	0	0
3	G	39	0	34	0	0
4	A	70	0	65	1	0
4	B	70	0	65	2	0
All	All	27562	0	26999	214	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 4.

All (214) 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:1017:ARG:HH12	1:A:1425:THR:HG21	1.48	0.77
1:B:1346:ALA:HB1	1:B:1406:VAL:HG23	1.77	0.67
1:A:1346:ALA:HB1	1:A:1406:VAL:HG23	1.77	0.66
1:A:1504:CYS:SG	1:A:1505:ASP:N	2.69	0.66
1:B:1504:CYS:SG	1:B:1505:ASP:N	2.69	0.65
1:A:1206:MET:HB2	1:A:1551:ILE:HB	1.80	0.64
1:B:1089:ARG:HB2	1:B:1140:GLU:HB3	1.80	0.64
1:B:1237:GLY:HA2	1:B:1277:VAL:HG11	1.80	0.64
1:B:1206:MET:HB2	1:B:1551:ILE:HB	1.81	0.63
1:B:1830:LEU:HD12	1:B:1831:LEU:HB2	1.81	0.63
1:A:1237:GLY:HA2	1:A:1277:VAL:HG11	1.81	0.63
1:A:1072:SER:HB3	1:A:1157:LEU:HD22	1.82	0.62
1:A:1830:LEU:HD12	1:A:1831:LEU:HB2	1.80	0.62
1:B:2118:VAL:HG22	1:B:2127:ILE:HG12	1.81	0.62
1:A:1810:GLU:HB2	1:A:1818:ILE:HB	1.82	0.61
1:B:2027:ASP:HB3	1:B:2031:GLY:H	1.64	0.61
1:B:1773:HIS:HB2	4:B:2805:NAG:H81	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1766:ASN:HA	1:A:2030:THR:HG23	1.84	0.60
1:B:2057:ASP:HA	1:B:2075:TYR:HB2	1.84	0.60
1:A:2027:ASP:HB3	1:A:2031:GLY:H	1.67	0.59
1:B:1319:GLN:HG3	1:B:1340:MET:HA	1.84	0.59
1:B:1249:TYR:OH	1:B:1261:SER:OG	2.20	0.59
1:A:1319:GLN:HG3	1:A:1340:MET:HA	1.84	0.59
1:A:1829:ASN:ND2	1:A:1847:ASP:OD2	2.34	0.59
1:B:1421:ILE:HB	1:B:1434:ALA:HB3	1.85	0.58
1:B:1766:ASN:HA	1:B:2030:THR:HG23	1.86	0.58
1:B:1810:GLU:HB2	1:B:1818:ILE:HB	1.85	0.58
1:B:1467:SER:HA	1:B:1535:VAL:HG11	1.86	0.57
1:A:1467:SER:HA	1:A:1535:VAL:HG11	1.86	0.57
1:A:1421:ILE:HB	1:A:1434:ALA:HB3	1.87	0.57
1:B:2112:HIS:NE2	1:B:2114:GLY:O	2.37	0.57
1:A:1473:TYR:HB3	1:A:1485:LEU:HD11	1.85	0.57
1:B:1473:TYR:HB3	1:B:1485:LEU:HD11	1.86	0.57
1:A:1089:ARG:HB2	1:A:1140:GLU:HB3	1.87	0.56
1:A:1136:SER:HB3	1:A:1152:LYS:HD3	1.87	0.56
1:B:2217:HIS:HA	1:B:2230:LEU:HB2	1.85	0.56
1:A:2076:THR:HG23	1:A:2085:ALA:HB3	1.87	0.56
1:A:2149:TYR:HB3	1:A:2157:TYR:HB3	1.87	0.56
1:A:2440:ASN:HB3	1:A:2443:MET:HB3	1.88	0.56
1:A:2588:TYR:HB2	1:A:2606:VAL:HG23	1.88	0.56
1:A:1803:ILE:HG12	1:A:1825:VAL:HG22	1.87	0.56
1:A:2057:ASP:HA	1:A:2075:TYR:HB2	1.88	0.56
1:B:2688:LEU:HD23	1:B:2747:ILE:HD13	1.88	0.55
1:B:1480:LYS:HE2	1:B:1508:ASN:HD21	1.72	0.55
1:A:1249:TYR:OH	1:A:1261:SER:OG	2.21	0.55
1:A:1480:LYS:HE2	1:A:1508:ASN:HD21	1.71	0.55
1:A:2058:LYS:HE3	1:A:2060:ILE:HD11	1.88	0.55
1:A:2560:ILE:HG12	1:A:2565:VAL:HG22	1.88	0.55
1:B:2560:ILE:HG12	1:B:2565:VAL:HG22	1.89	0.54
1:A:2032:VAL:HB	1:A:2051:LYS:HD2	1.88	0.54
1:A:2217:HIS:HA	1:A:2230:LEU:HB2	1.88	0.54
1:B:1089:ARG:HH21	1:B:1104:SER:HB3	1.72	0.54
1:B:1234:LEU:HB3	1:B:1534:ALA:HB2	1.90	0.54
1:B:1679:GLU:OE2	1:B:2538:ARG:NH1	2.41	0.54
1:A:2169:VAL:HG23	1:A:2451:SER:HB3	1.90	0.54
1:B:1242:LEU:HD23	1:B:1253:ILE:HD12	1.89	0.54
1:B:1808:ARG:NH2	1:B:1834:ASP:OD1	2.41	0.54
1:B:2176:LEU:HD21	1:B:2360:LEU:HB3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2295:TYR:HD2	1:A:2303:LEU:HB2	1.73	0.53
1:B:2032:VAL:HB	1:B:2051:LYS:HD2	1.90	0.53
1:A:1242:LEU:HD23	1:A:1253:ILE:HD12	1.90	0.53
1:A:1534:ALA:HB3	1:A:1542:TYR:HB2	1.90	0.53
1:B:1616:ASN:OD1	1:B:1862:ARG:NH1	2.41	0.53
1:B:2069:ILE:HD13	1:B:2092:SER:HB2	1.91	0.53
1:A:1017:ARG:HH21	1:A:1429:GLN:HB2	1.74	0.53
1:A:2285:ARG:HB3	1:A:2294:SER:HB3	1.90	0.53
1:B:1363:LYS:HE3	1:B:1373:LEU:HB2	1.91	0.53
1:B:1534:ALA:HB3	1:B:1542:TYR:HB2	1.90	0.52
1:B:2440:ASN:HB3	1:B:2443:MET:HB3	1.90	0.52
1:A:1363:LYS:HE3	1:A:1373:LEU:HB2	1.91	0.52
1:A:1234:LEU:HB3	1:A:1534:ALA:HB2	1.90	0.52
1:B:2295:TYR:HD2	1:B:2303:LEU:HB2	1.75	0.52
1:A:1616:ASN:OD1	1:A:1862:ARG:NH1	2.42	0.52
1:B:1890:ARG:NH1	1:B:2458:ASN:O	2.43	0.52
1:B:2615:LEU:HD21	1:B:2635:VAL:HG11	1.91	0.52
1:A:2374:GLN:HB2	1:A:2383:TYR:HB3	1.92	0.51
1:A:2576:ASP:HB3	1:A:2627:LEU:HD13	1.93	0.51
1:B:2169:VAL:HG23	1:B:2451:SER:HB3	1.92	0.51
1:A:1387:CYS:HA	1:A:1432:ILE:HD12	1.92	0.51
1:B:1017:ARG:HH12	1:B:1425:THR:HG21	1.76	0.51
1:B:2149:TYR:HB3	1:B:2157:TYR:HB3	1.92	0.51
1:B:2675:GLU:OE1	1:B:2678:ARG:NH1	2.43	0.51
1:B:1017:ARG:NH2	1:B:1425:THR:OG1	2.41	0.51
1:B:1942:SER:OG	1:B:1944:ARG:NH1	2.44	0.51
1:A:1679:GLU:OE2	1:A:2538:ARG:NH1	2.44	0.51
1:A:1681:GLY:HA2	1:A:2554:LYS:HD3	1.93	0.51
1:A:1931:SER:O	1:A:1931:SER:OG	2.29	0.50
1:A:2068:MET:HE1	1:A:2294:SER:HB2	1.93	0.50
1:B:2588:TYR:HB2	1:B:2606:VAL:HG23	1.93	0.50
1:A:2069:ILE:HD13	1:A:2092:SER:HB2	1.94	0.49
1:B:1289:THR:O	1:B:1292:ARG:NE	2.45	0.49
1:B:2084:ILE:HD11	1:B:2310:LEU:HD12	1.94	0.49
1:A:1890:ARG:NH1	1:A:2458:ASN:O	2.44	0.49
1:A:2176:LEU:HD21	1:A:2360:LEU:HB3	1.93	0.49
1:B:1889:GLN:OE1	1:B:1896:ARG:NH2	2.46	0.49
1:B:1824:ARG:NH2	1:B:1827:GLY:O	2.46	0.48
1:B:1230:ALA:HB3	1:B:1247:PHE:HB2	1.95	0.48
1:B:1387:CYS:HA	1:B:1432:ILE:HD12	1.95	0.48
1:B:2618:LEU:O	1:B:2625:LYS:NZ	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1090:VAL:HB	1:A:1105:PHE:HB2	1.95	0.48
1:B:1509:ASP:HB3	1:B:1512:CYS:HB2	1.96	0.48
1:A:1916:TRP:HB3	1:A:1927:LEU:HD11	1.95	0.48
1:A:1230:ALA:HB3	1:A:1247:PHE:HB2	1.95	0.48
1:A:1289:THR:O	1:A:1292:ARG:NE	2.46	0.48
1:B:1792:ILE:HD13	1:B:2479:PRO:HG2	1.96	0.47
1:B:1017:ARG:HH21	1:B:1429:GLN:HB2	1.79	0.47
1:B:1621:LYS:HD2	1:B:1623:ARG:HH12	1.78	0.47
1:B:2374:GLN:HB2	1:B:2383:TYR:HB3	1.96	0.47
1:B:1164:PRO:HB3	1:B:1177:THR:HB	1.96	0.47
1:B:2716:GLN:NE2	1:B:2724:GLN:OE1	2.46	0.47
1:B:1275:LEU:HD22	1:B:1284:LEU:HD21	1.97	0.46
1:A:1509:ASP:HB3	1:A:1512:CYS:HB2	1.96	0.46
1:B:1770:VAL:HG22	1:B:1792:ILE:HG23	1.97	0.46
1:B:2260:ASP:OD1	1:B:2275:ASN:ND2	2.49	0.46
1:A:1275:LEU:HD22	1:A:1284:LEU:HD21	1.97	0.46
1:B:2285:ARG:HB2	1:B:2294:SER:HB3	1.97	0.46
1:B:2462:ASP:N	1:B:2462:ASP:OD1	2.48	0.46
1:A:2050:ARG:HD3	1:A:2058:LYS:HE2	1.98	0.46
1:B:1264:GLU:N	1:B:1306:LEU:O	2.46	0.46
1:B:1641:ILE:HG12	1:B:1656:THR:HG22	1.96	0.46
1:B:2576:ASP:HB3	1:B:2627:LEU:HD13	1.98	0.46
1:A:1264:GLU:N	1:A:1306:LEU:O	2.46	0.45
1:A:2726:TYR:OH	1:A:2751:ARG:NH2	2.48	0.45
1:B:1916:TRP:HB3	1:B:1927:LEU:HD11	1.99	0.45
1:A:1347:VAL:HG22	1:A:1353:MET:HG2	1.99	0.45
1:A:2194:GLN:OE1	1:A:2447:ASN:ND2	2.43	0.45
1:B:1687:ASP:HB3	4:B:2803:NAG:H83	1.98	0.45
1:B:1789:ARG:HG2	1:B:1804:GLU:HG3	1.98	0.45
1:B:2122:ASP:OD1	1:B:2123:ILE:N	2.50	0.45
1:A:1877:VAL:HG12	1:A:1888:LEU:HD23	1.99	0.45
1:A:1275:LEU:HB3	1:A:1284:LEU:HD11	1.99	0.44
1:A:1374:LEU:HD22	1:A:1398:LEU:HD22	1.99	0.44
1:B:1571:SER:O	1:B:1571:SER:OG	2.34	0.44
1:B:1936:ILE:HB	1:B:1949:THR:HB	1.98	0.44
1:B:2235:ARG:HE	1:B:2235:ARG:HB3	1.58	0.44
1:A:1950:MET:HE2	1:A:1950:MET:HB3	1.83	0.44
1:B:1931:SER:O	1:B:1931:SER:OG	2.30	0.44
1:B:2698:LYS:HD2	1:B:2705:GLY:HA2	1.99	0.44
1:A:1477:THR:HB	1:A:1530:PRO:HD2	2.00	0.44
1:A:1925:MET:HE1	1:A:2436:PRO:HG2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2084:ILE:HD11	1:A:2310:LEU:HD12	2.00	0.44
1:A:1236:VAL:HG23	1:A:1534:ALA:HB1	2.00	0.44
1:A:1687:ASP:HB3	4:A:2803:NAG:H83	1.99	0.43
1:A:1696:ASN:OD1	1:A:1696:ASN:N	2.50	0.43
1:B:1020:PRO:HG2	1:B:1153:ARG:HG3	1.99	0.43
1:B:2012:LEU:HD21	1:B:2015:ILE:HD11	1.99	0.43
1:A:2012:LEU:HD21	1:A:2015:ILE:HD11	1.99	0.43
1:A:2122:ASP:OD1	1:A:2123:ILE:N	2.50	0.43
1:B:1477:THR:HB	1:B:1530:PRO:HD2	1.99	0.43
1:A:2150:GLU:HG2	1:A:2155:LEU:HA	2.00	0.43
1:B:2247:LYS:HB2	1:B:2256:GLN:HB3	1.99	0.43
1:A:1981:ILE:HB	1:A:1994:SER:HB2	2.01	0.43
1:B:2618:LEU:HD13	1:B:2633:VAL:HG11	2.01	0.43
1:A:1789:ARG:HG2	1:A:1804:GLU:HG3	2.01	0.43
1:B:1236:VAL:HG23	1:B:1534:ALA:HB1	2.00	0.43
1:B:2068:MET:HE1	1:B:2294:SER:HB2	1.99	0.43
1:B:2331:TYR:HE2	1:B:2342:GLU:HB2	1.81	0.43
1:A:2056:VAL:O	1:A:2077:TYR:OH	2.35	0.43
1:B:1998:THR:OG1	1:B:2251:ASP:OD2	2.31	0.43
1:A:1945:LEU:HD12	1:A:1945:LEU:HA	1.91	0.43
1:B:1681:GLY:HA2	1:B:2554:LYS:HD3	2.00	0.43
1:A:2235:ARG:HE	1:A:2235:ARG:HB3	1.59	0.43
1:B:1118:ASP:OD1	1:B:1118:ASP:N	2.45	0.43
1:B:1729:THR:HB	1:B:1744:VAL:HB	2.01	0.43
1:A:1989:ARG:NH2	1:A:2010:SER:O	2.52	0.42
1:B:1589:THR:HG22	1:B:1599:TYR:HB2	2.01	0.42
1:B:1275:LEU:HB3	1:B:1284:LEU:HD11	2.00	0.42
1:A:1396:VAL:HG21	1:A:1430:VAL:HG21	2.01	0.42
1:B:1374:LEU:HD22	1:B:1398:LEU:HD22	2.01	0.42
1:B:1648:ASN:OD1	1:B:1648:ASN:N	2.52	0.42
1:A:1872:LEU:HD13	1:A:2469:MET:HE2	2.01	0.42
1:B:2261:ILE:HG12	1:B:2703:ARG:HG2	2.00	0.42
1:A:1086:ASN:HB2	1:A:1141:TYR:HD2	1.85	0.42
1:B:1347:VAL:HG22	1:B:1353:MET:HG2	2.00	0.42
1:B:1396:VAL:HG21	1:B:1430:VAL:HG21	2.00	0.42
1:A:1416:LEU:HD22	1:A:1464:ILE:HG23	2.01	0.42
1:A:1998:THR:OG1	1:A:2251:ASP:OD2	2.31	0.42
1:A:2164:ASP:OD1	1:A:2168:ARG:N	2.52	0.42
1:A:2540:LYS:HB3	1:A:2543:HIS:HB2	2.01	0.42
1:B:1942:SER:OG	1:B:1942:SER:O	2.35	0.42
1:A:1498:ALA:HB2	1:A:1522:ALA:HB1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1161:GLU:OE2	1:B:1192:ASN:ND2	2.53	0.41
1:B:1872:LEU:HD13	1:B:2469:MET:HE2	2.02	0.41
1:B:2448:ASN:OD1	1:B:2451:SER:OG	2.38	0.41
1:B:2622:ILE:HD13	1:B:2622:ILE:HA	1.91	0.41
1:A:1648:ASN:OD1	1:A:1648:ASN:N	2.53	0.41
1:B:1289:THR:HA	1:B:1342:PRO:HG2	2.03	0.41
1:A:1063:LEU:HB3	1:A:1066:ARG:HG3	2.02	0.41
1:A:1236:VAL:HG11	1:A:1537:PRO:HD3	2.03	0.41
1:A:1821:ARG:NH2	1:A:2524:LEU:O	2.54	0.41
1:A:2622:ILE:HD13	1:A:2622:ILE:HA	1.91	0.41
1:B:1498:ALA:HB2	1:B:1522:ALA:HB1	2.01	0.41
1:B:1726:ASP:OD1	1:B:1726:ASP:N	2.52	0.41
1:B:2068:MET:HE3	1:B:2068:MET:HB3	1.88	0.41
1:A:1199:PRO:HB2	1:A:1521:TYR:CE1	2.56	0.41
1:A:1760:LEU:HD23	1:A:1772:PHE:HZ	1.86	0.41
1:B:1063:LEU:HB3	1:B:1066:ARG:HG3	2.02	0.41
1:A:2068:MET:HE3	1:A:2068:MET:HB3	1.90	0.40
1:A:2698:LYS:HD2	1:A:2705:GLY:HA2	2.02	0.40
1:A:1235:ALA:HB3	1:A:1243:PHE:HB2	2.03	0.40
1:A:1476:GLU:OE1	1:A:1484:ARG:NE	2.48	0.40
1:A:2262:PHE:HE2	1:A:2404:THR:HB	1.84	0.40
1:B:1235:ALA:HB3	1:B:1243:PHE:HB2	2.03	0.40
1:B:1416:LEU:HD22	1:B:1464:ILE:HG23	2.02	0.40
1:A:2732:LEU:HD23	1:A:2732:LEU:HA	1.92	0.40
1:B:1268:SER:HA	1:B:1269:PRO:HD3	1.91	0.40
1:B:1643:LEU:HD22	1:B:1654:VAL:HG22	2.03	0.40
1:B:2615:LEU:HD23	1:B:2621:THR:HA	2.03	0.40
1:A:1409:MET:HE3	1:A:1409:MET:HB2	1.88	0.40
1:B:1165:SER:HB2	1:B:1171:SER:HA	2.04	0.40
1:B:1409:MET:HE3	1:B:1409:MET:HB2	1.99	0.40
1:B:2237:ARG:NH1	1:B:2249:ASP:O	2.54	0.40
1:A:1792:ILE:HD13	1:A:2479:PRO:HG2	2.04	0.40
1:B:1348:ASP:HB2	1:B:1354:TYR:HE1	1.87	0.40

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	1716/2394 (72%)	1660 (97%)	56 (3%)	0	100	100
1	B	1716/2394 (72%)	1665 (97%)	51 (3%)	0	100	100
All	All	3432/4788 (72%)	3325 (97%)	107 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	1495/2056 (73%)	1479 (99%)	16 (1%)	65	86
1	B	1495/2056 (73%)	1484 (99%)	11 (1%)	76	91
All	All	2990/4112 (73%)	2963 (99%)	27 (1%)	68	89

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1071	LYS
1	A	1130	LEU
1	A	1135	VAL
1	A	1137	VAL
1	A	1195	LEU
1	A	1216	CYS
1	A	1477	THR
1	A	1510	VAL

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Mol	Chain	Res	Type
1	A	1588	TYR
1	A	1696	ASN
1	A	1925	MET
1	A	1953	VAL
1	A	2106	ILE
1	A	2543	HIS
1	A	2567	THR
1	A	2606	VAL
1	B	1060	LEU
1	B	1114	THR
1	B	1195	LEU
1	B	1216	CYS
1	B	1477	THR
1	B	1510	VAL
1	B	1915	VAL
1	B	1925	MET
1	B	1953	VAL
1	B	2112	HIS
1	B	2156	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1395	GLN
1	A	1429	GLN
1	A	1508	ASN
1	A	1575	GLN
1	A	1657	GLN
1	A	1745	GLN
1	A	1750	ASN
1	A	1773	HIS
1	A	1777	HIS
1	A	1961	HIS
1	A	1969	ASN
1	A	2311	HIS
1	A	2337	HIS
1	A	2411	GLN
1	A	2505	GLN
1	A	2697	GLN
1	B	1395	GLN
1	B	1508	ASN
1	B	1657	GLN

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Mol	Chain	Res	Type
1	B	1745	GLN
1	B	1773	HIS
1	B	1961	HIS
1	B	2337	HIS
1	B	2374	GLN
1	B	2448	ASN
1	B	2505	GLN
1	B	2651	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

14 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	0.22	0	17,19,21	0.50	0
2	NAG	C	2	2	14,14,15	0.24	0	17,19,21	0.54	0
3	NAG	D	1	3,1	14,14,15	0.30	0	17,19,21	0.72	1 (5%)
3	NAG	D	2	3	14,14,15	0.47	0	17,19,21	0.45	0
3	BMA	D	3	3	11,11,12	0.66	0	15,15,17	0.84	0
2	NAG	E	1	2,1	14,14,15	0.23	0	17,19,21	0.79	1 (5%)
2	NAG	E	2	2	14,14,15	0.48	0	17,19,21	0.55	0
2	NAG	F	1	2,1	14,14,15	0.23	0	17,19,21	0.49	0
2	NAG	F	2	2	14,14,15	0.26	0	17,19,21	0.51	0
3	NAG	G	1	3,1	14,14,15	0.23	0	17,19,21	0.80	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	G	2	3	14,14,15	0.44	0	17,19,21	0.49	0
3	BMA	G	3	3	11,11,12	0.66	0	15,15,17	0.82	1 (6%)
2	NAG	H	1	2,1	14,14,15	0.25	0	17,19,21	0.76	1 (5%)
2	NAG	H	2	2	14,14,15	0.43	0	17,19,21	0.50	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	-	3/6/23/26	0/1/1/1
3	NAG	D	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
3	BMA	D	3	3	-	0/2/19/22	0/1/1/1
2	NAG	E	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	E	2	2	-	3/6/23/26	0/1/1/1
2	NAG	F	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	F	2	2	-	3/6/23/26	0/1/1/1
3	NAG	G	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	3/6/23/26	0/1/1/1
3	BMA	G	3	3	-	0/2/19/22	0/1/1/1
2	NAG	H	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	H	2	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1	NAG	C1-O5-C5	2.64	115.77	112.19
2	H	1	NAG	C1-O5-C5	2.54	115.64	112.19
3	G	1	NAG	C1-O5-C5	2.43	115.49	112.19
3	G	3	BMA	C1-O5-C5	2.06	114.98	112.19
3	D	1	NAG	C1-O5-C5	2.01	114.91	112.19

There are no chirality outliers.

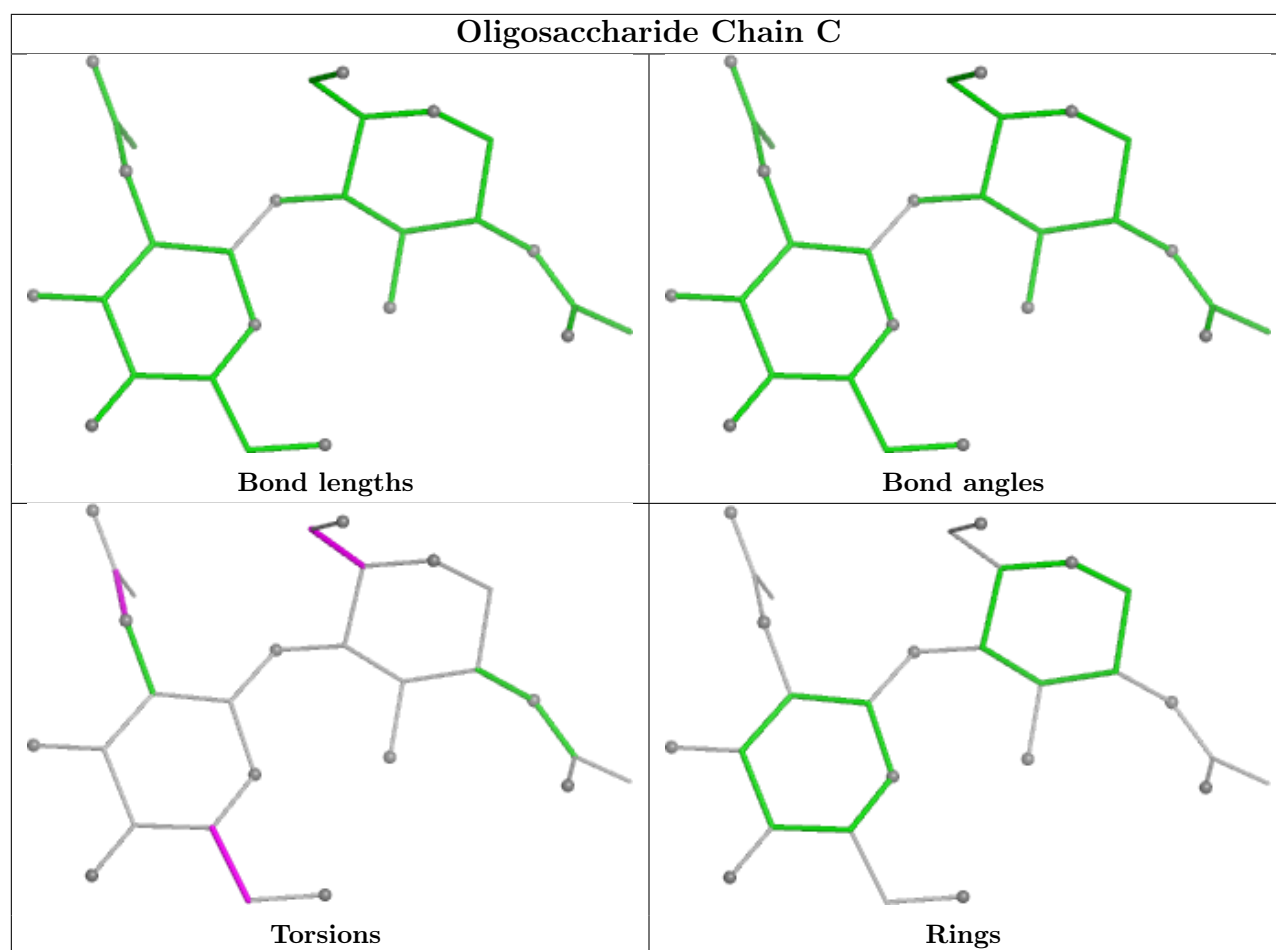
All (32) torsion outliers are listed below:

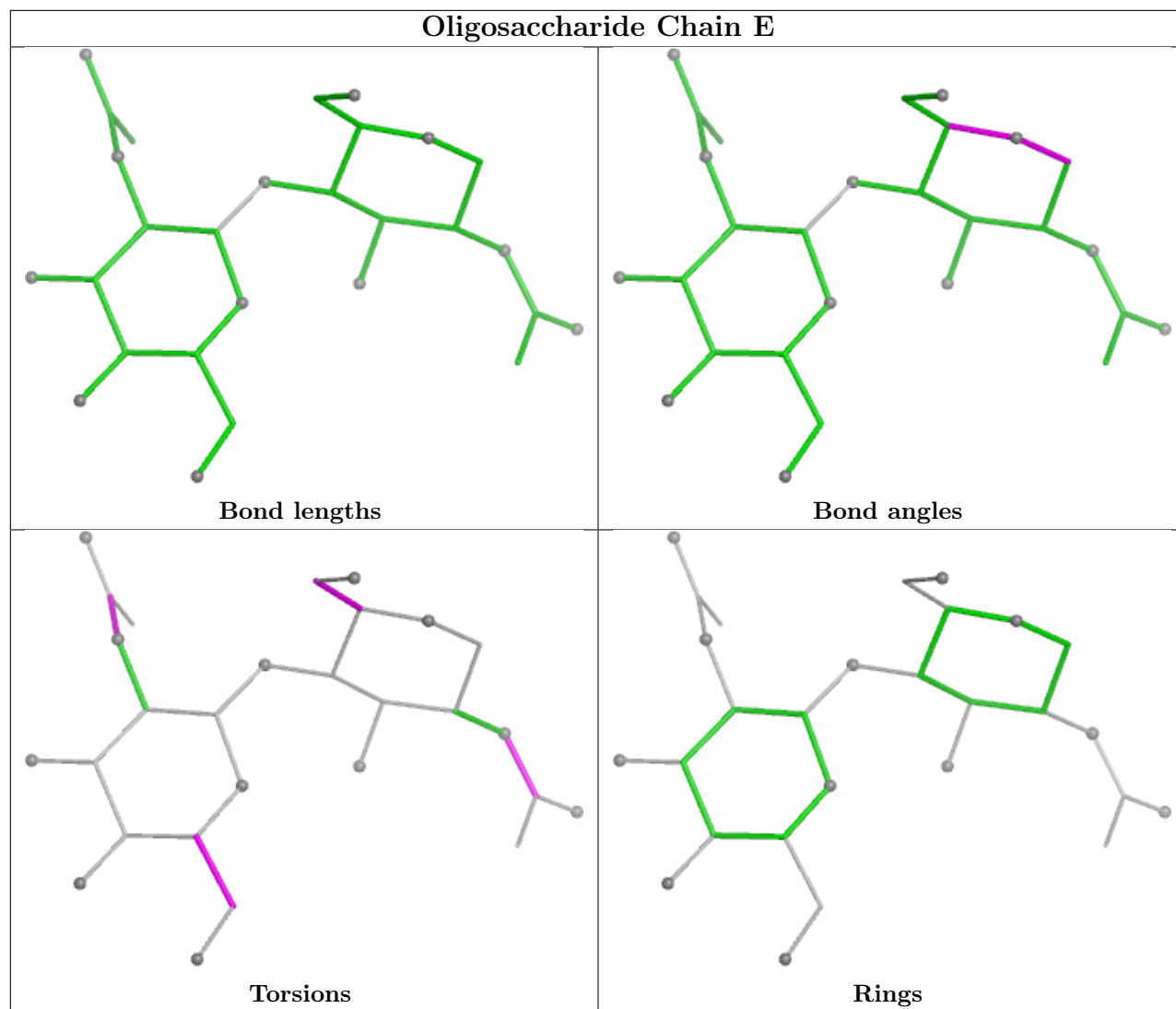
Mol	Chain	Res	Type	Atoms
2	E	1	NAG	O5-C5-C6-O6
2	H	1	NAG	O5-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6
3	D	1	NAG	O5-C5-C6-O6
2	F	1	NAG	O5-C5-C6-O6
2	H	1	NAG	C4-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6
2	F	1	NAG	C4-C5-C6-O6
3	D	1	NAG	C4-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
2	C	2	NAG	C8-C7-N2-C2
2	C	2	NAG	O7-C7-N2-C2
2	E	1	NAG	C8-C7-N2-C2
2	E	1	NAG	O7-C7-N2-C2
2	E	2	NAG	C8-C7-N2-C2
2	E	2	NAG	O7-C7-N2-C2
2	F	2	NAG	C8-C7-N2-C2
2	F	2	NAG	O7-C7-N2-C2
2	H	1	NAG	C8-C7-N2-C2
2	H	1	NAG	O7-C7-N2-C2
3	D	1	NAG	C8-C7-N2-C2
3	D	1	NAG	O7-C7-N2-C2
3	G	1	NAG	C8-C7-N2-C2
3	G	1	NAG	O7-C7-N2-C2
3	G	2	NAG	C8-C7-N2-C2
3	G	2	NAG	O7-C7-N2-C2
2	H	2	NAG	C4-C5-C6-O6
2	H	2	NAG	O5-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6

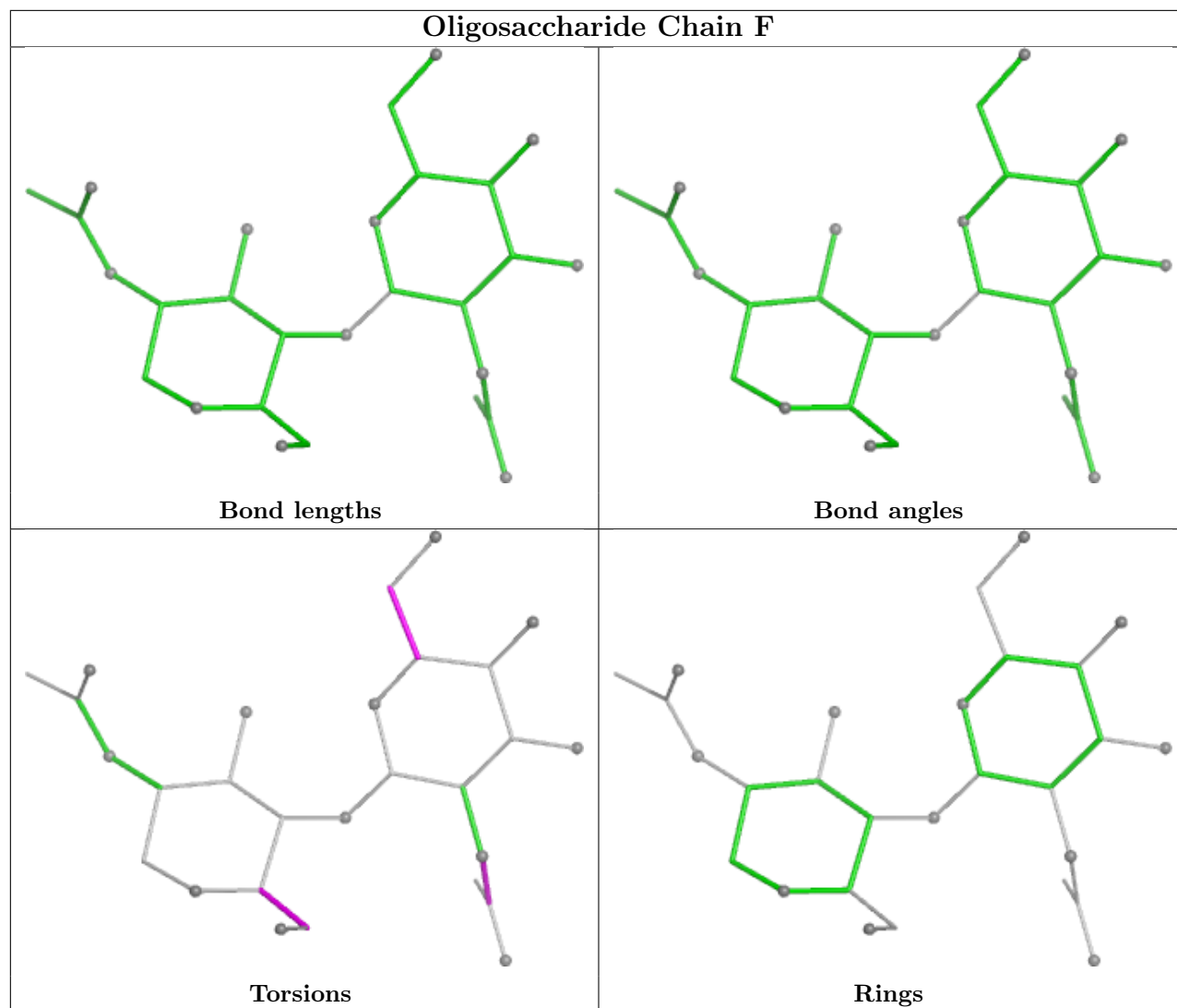
There are no ring outliers.

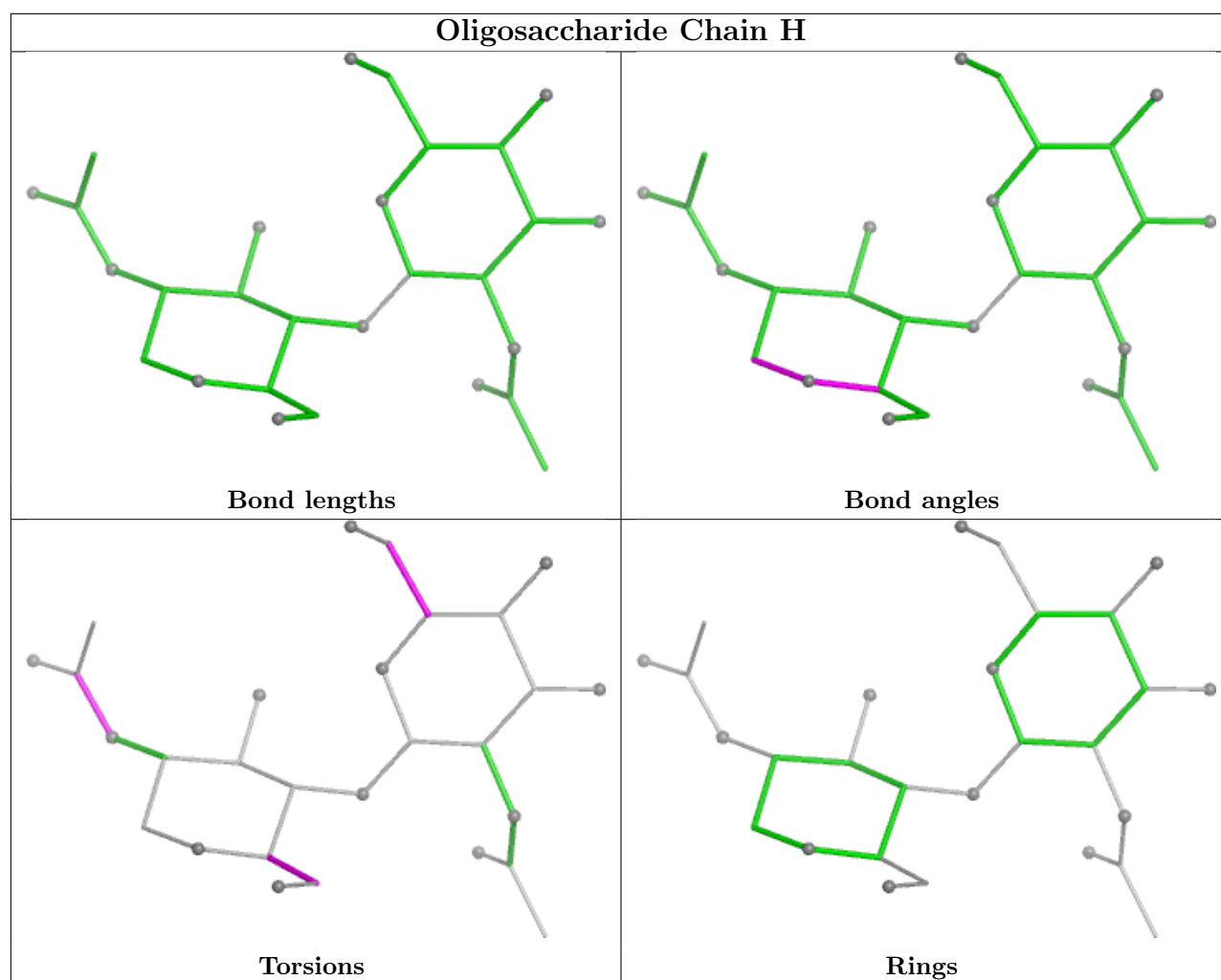
No monomer is involved in short contacts.

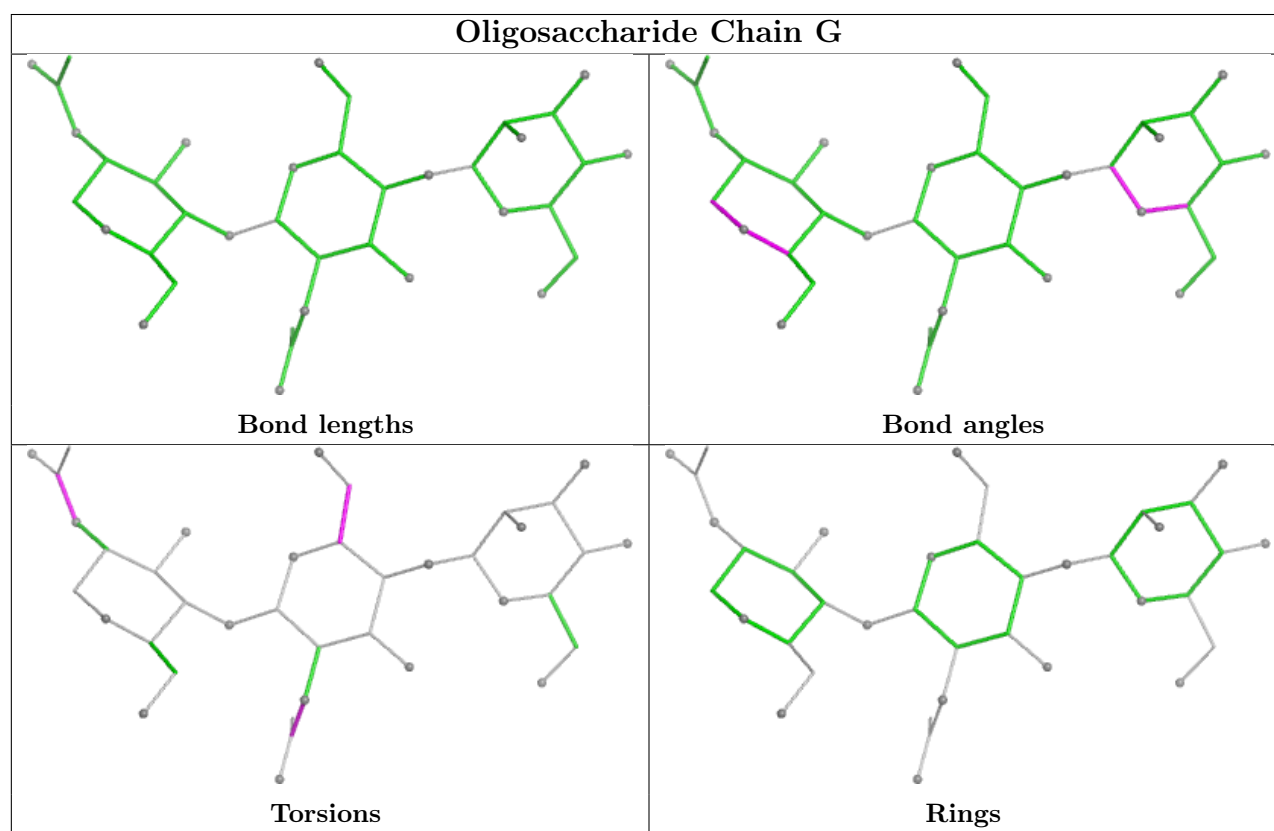
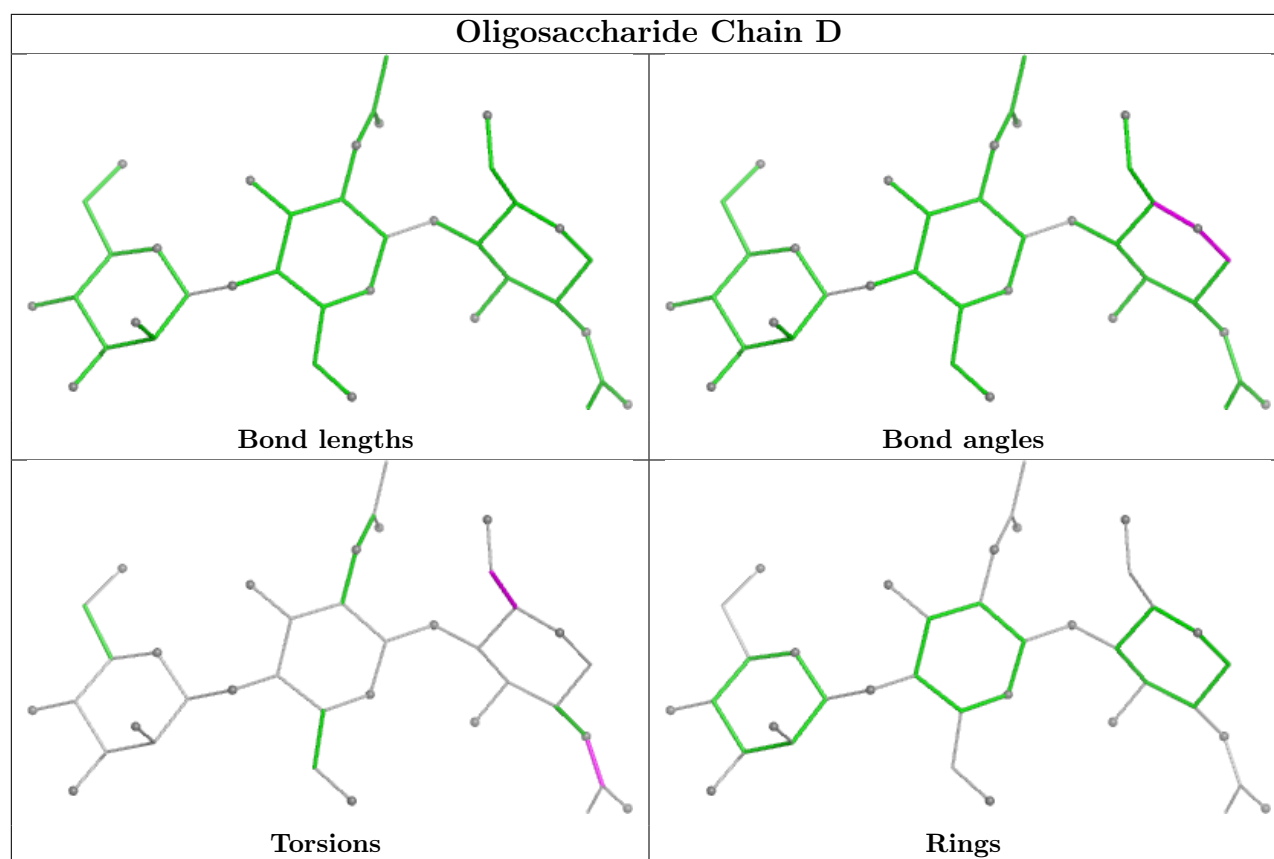
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry

10 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	2804	1	14,14,15	0.36	0	17,19,21	0.54	0
4	NAG	B	2803	1	14,14,15	0.54	0	17,19,21	0.58	0
4	NAG	B	2802	1	14,14,15	0.36	0	17,19,21	0.53	0
4	NAG	A	2804	1	14,14,15	0.30	0	17,19,21	0.56	0
4	NAG	B	2801	1	14,14,15	0.39	0	17,19,21	0.60	1 (5%)
4	NAG	B	2805	1	14,14,15	0.39	0	17,19,21	0.98	1 (5%)
4	NAG	A	2803	1	14,14,15	0.56	0	17,19,21	0.73	0
4	NAG	A	2805	1	14,14,15	0.31	0	17,19,21	0.97	1 (5%)
4	NAG	A	2801	1	14,14,15	0.43	0	17,19,21	0.94	1 (5%)
4	NAG	A	2802	1	14,14,15	0.36	0	17,19,21	0.55	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	2804	1	-	0/6/23/26	0/1/1/1
4	NAG	B	2803	1	-	4/6/23/26	0/1/1/1
4	NAG	B	2802	1	-	2/6/23/26	0/1/1/1
4	NAG	A	2804	1	-	2/6/23/26	0/1/1/1
4	NAG	B	2801	1	-	0/6/23/26	0/1/1/1
4	NAG	B	2805	1	-	3/6/23/26	0/1/1/1
4	NAG	A	2803	1	-	4/6/23/26	0/1/1/1
4	NAG	A	2805	1	-	3/6/23/26	0/1/1/1
4	NAG	A	2801	1	-	2/6/23/26	0/1/1/1
4	NAG	A	2802	1	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2805	NAG	C2-N2-C7	2.98	127.15	122.90
4	B	2805	NAG	C2-N2-C7	2.88	127.01	122.90
4	A	2801	NAG	C2-N2-C7	2.86	126.97	122.90
4	B	2801	NAG	C1-O5-C5	2.17	115.13	112.19

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2805	NAG	O5-C5-C6-O6
4	B	2803	NAG	O5-C5-C6-O6
4	A	2804	NAG	C4-C5-C6-O6
4	A	2803	NAG	O5-C5-C6-O6
4	A	2805	NAG	C4-C5-C6-O6
4	A	2803	NAG	C4-C5-C6-O6
4	B	2803	NAG	C4-C5-C6-O6
4	A	2802	NAG	C8-C7-N2-C2
4	A	2802	NAG	O7-C7-N2-C2
4	A	2803	NAG	C8-C7-N2-C2
4	A	2803	NAG	O7-C7-N2-C2
4	B	2802	NAG	C8-C7-N2-C2
4	B	2802	NAG	O7-C7-N2-C2
4	B	2803	NAG	C8-C7-N2-C2
4	B	2803	NAG	O7-C7-N2-C2
4	A	2804	NAG	O5-C5-C6-O6
4	B	2805	NAG	O5-C5-C6-O6
4	B	2805	NAG	C4-C5-C6-O6
4	A	2801	NAG	O5-C5-C6-O6
4	A	2802	NAG	C4-C5-C6-O6
4	A	2801	NAG	C3-C2-N2-C7
4	A	2805	NAG	C3-C2-N2-C7
4	B	2805	NAG	C3-C2-N2-C7

There are no ring outliers.

3 monomers are involved in 3 short contacts:

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

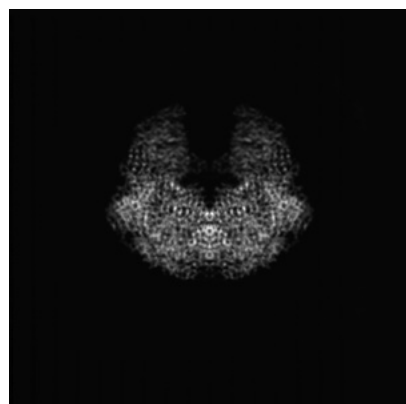
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51022. These allow visual inspection of the internal detail of the map and identification of artifacts.

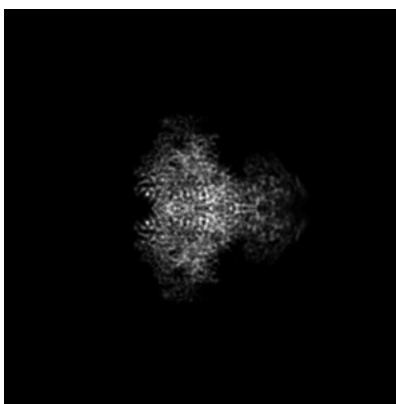
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

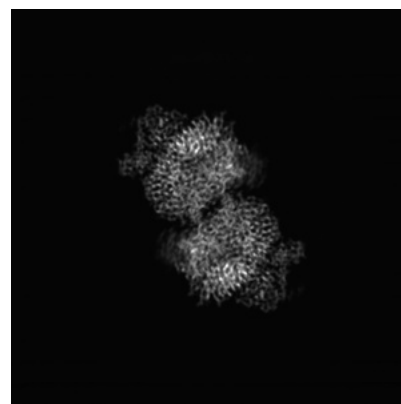
6.1.1 Primary map



X

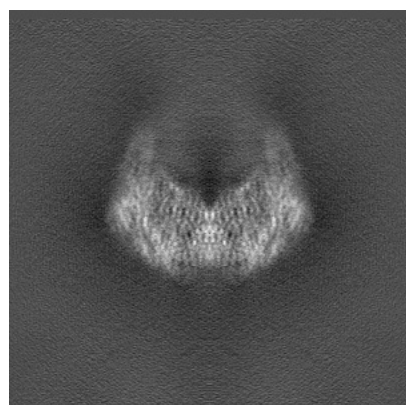


Y

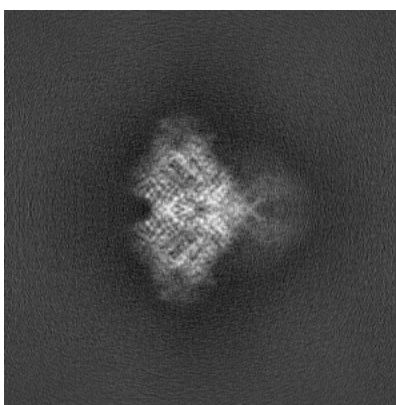


Z

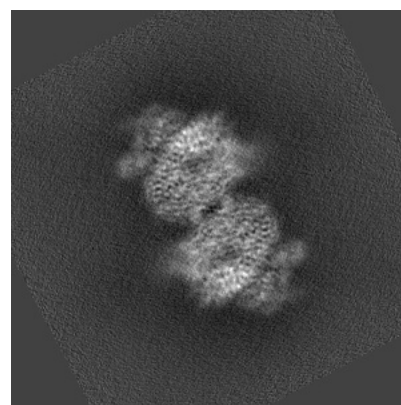
6.1.2 Raw map



X



Y



Z

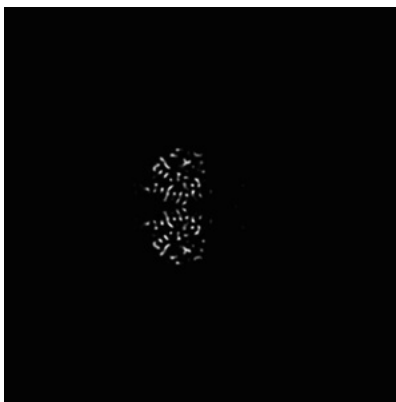
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

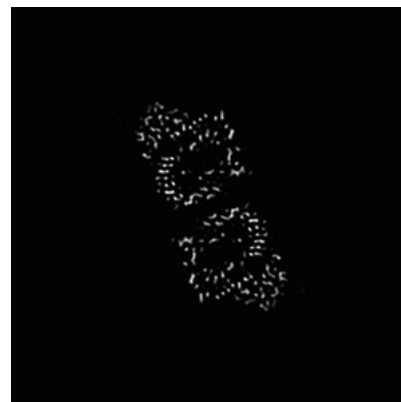
6.2.1 Primary map



X Index: 175

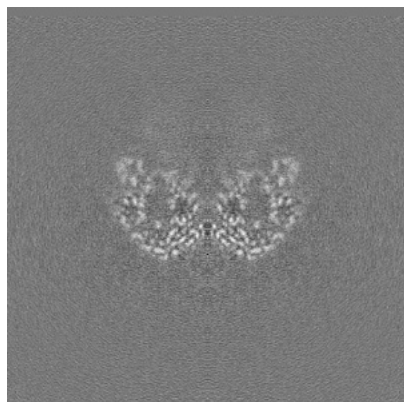


Y Index: 175

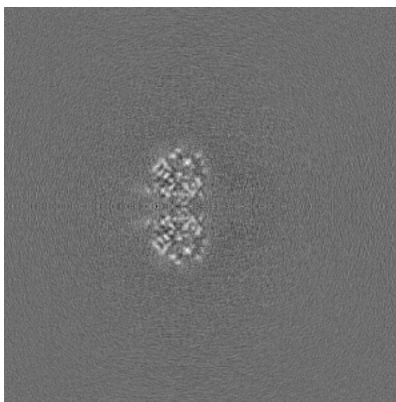


Z Index: 175

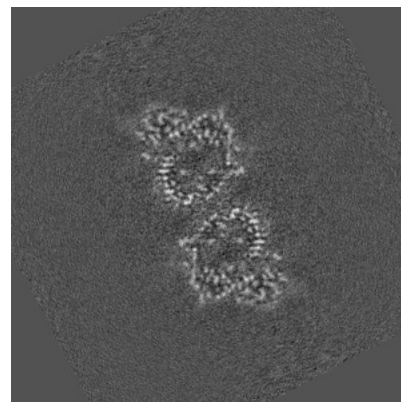
6.2.2 Raw map



X Index: 175



Y Index: 175



Z Index: 175

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: 185

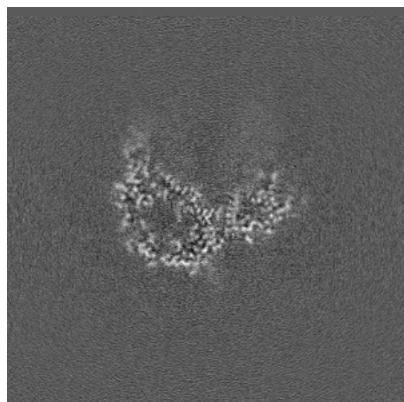


Y Index: 119

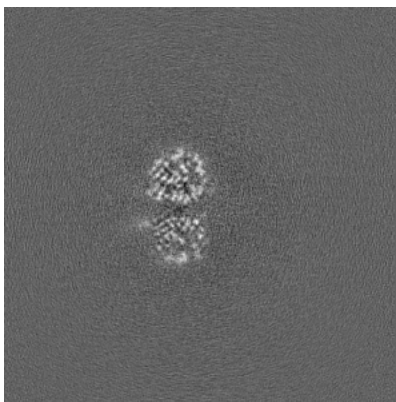


Z Index: 171

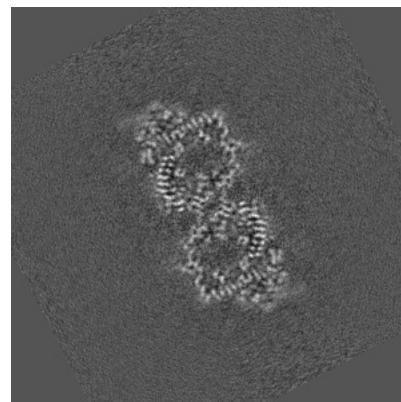
6.3.2 Raw map



X Index: 187



Y Index: 173

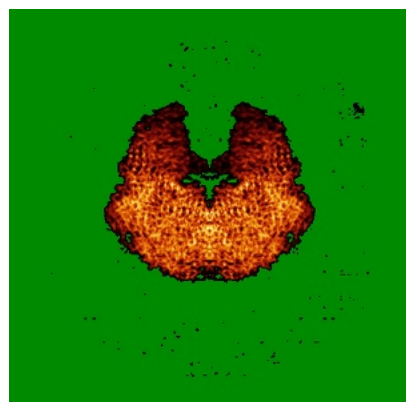


Z Index: 172

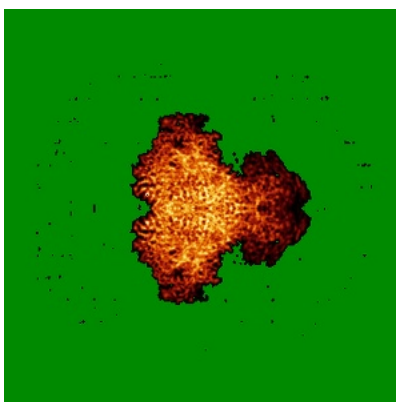
The images above show the largest variance slices of the map in three orthogonal directions.

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

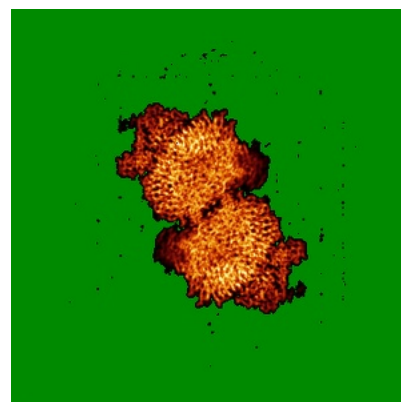
6.4.1 Primary map



X

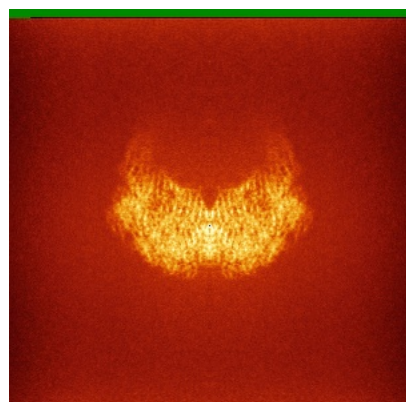


Y

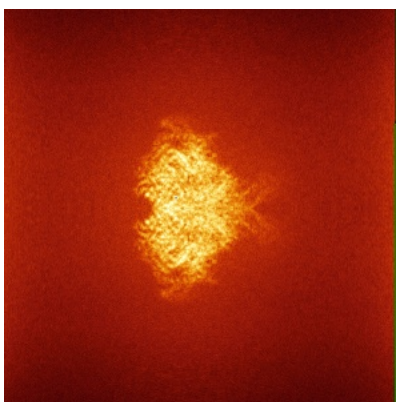


Z

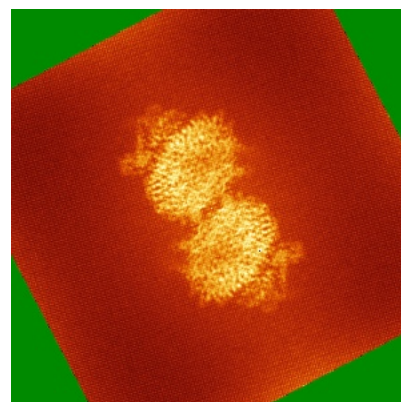
6.4.2 Raw map



X



Y

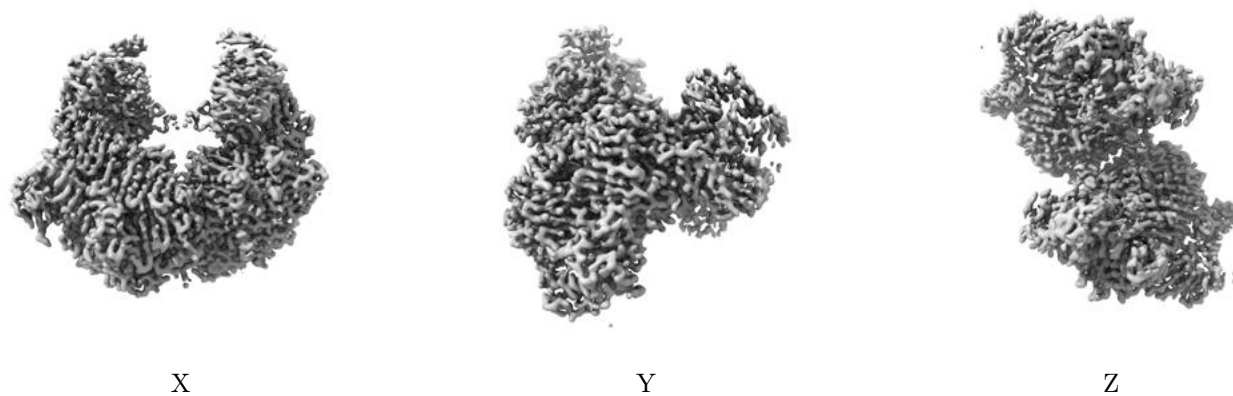


Z

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.

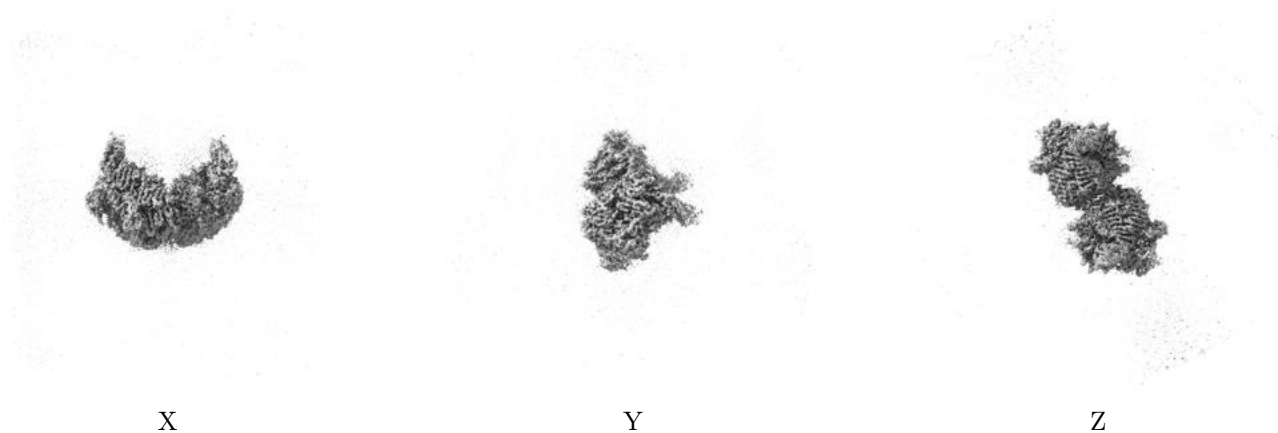
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.134. 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.

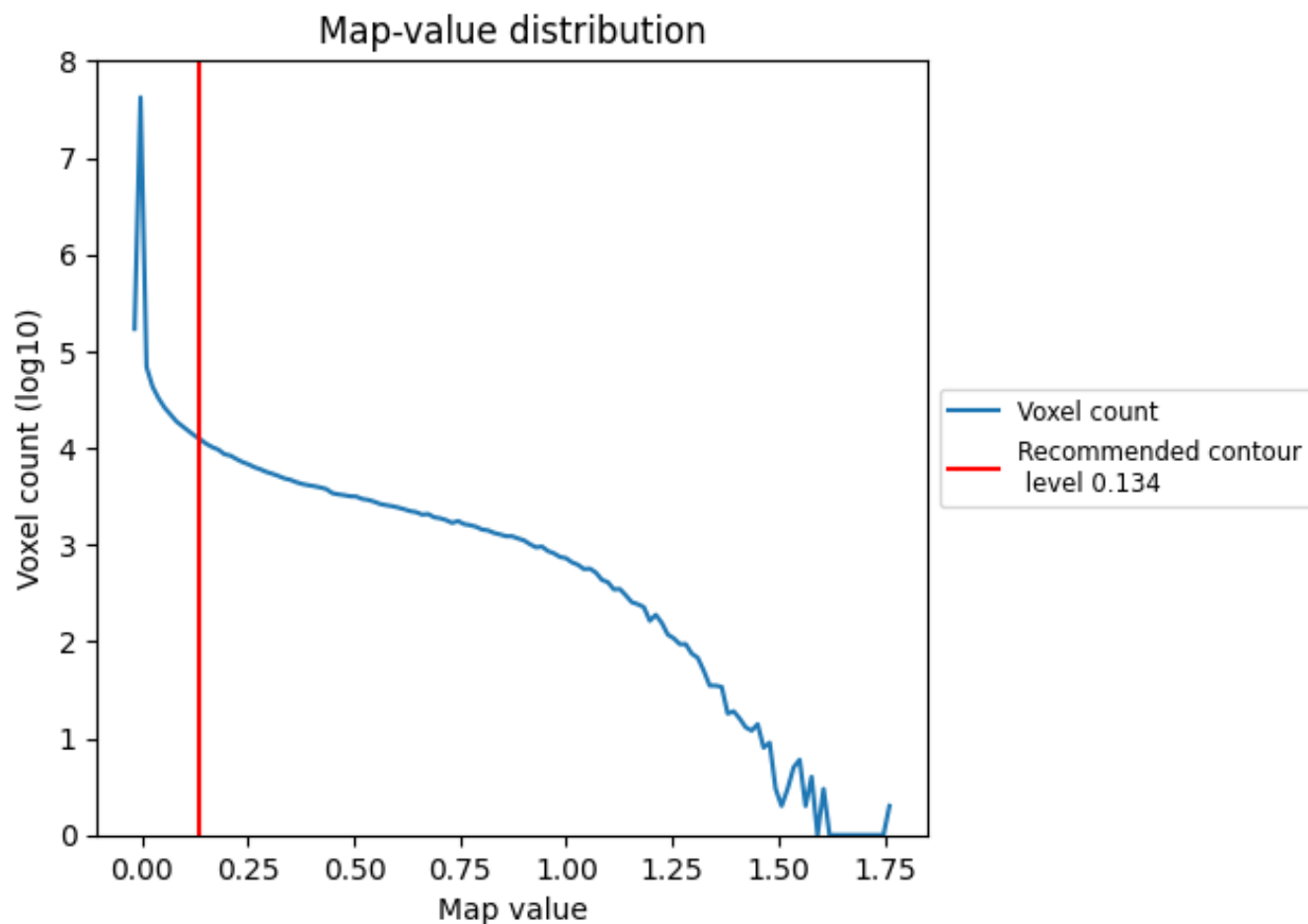
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

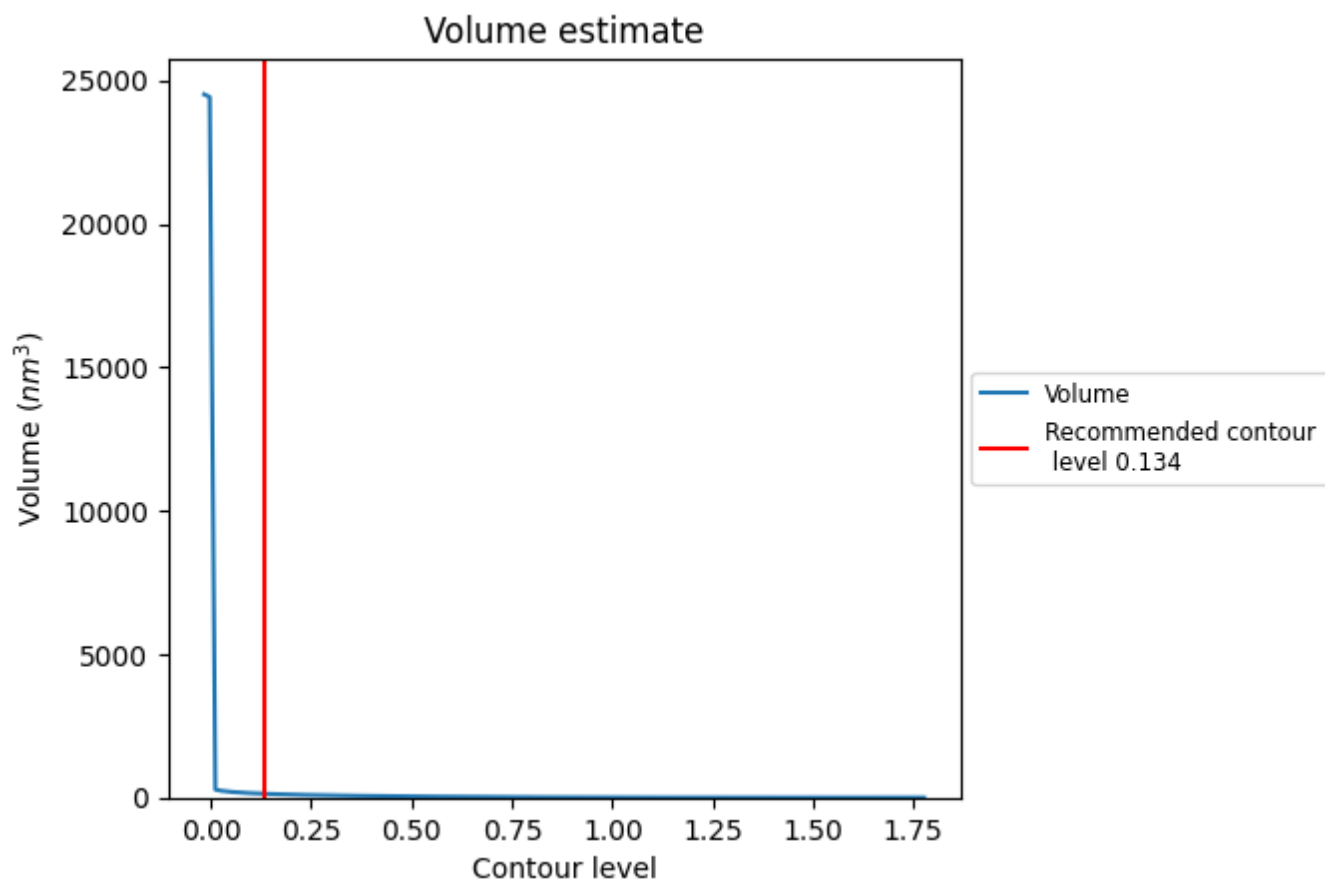
This section contains the results of statistical analysis of the map.

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.

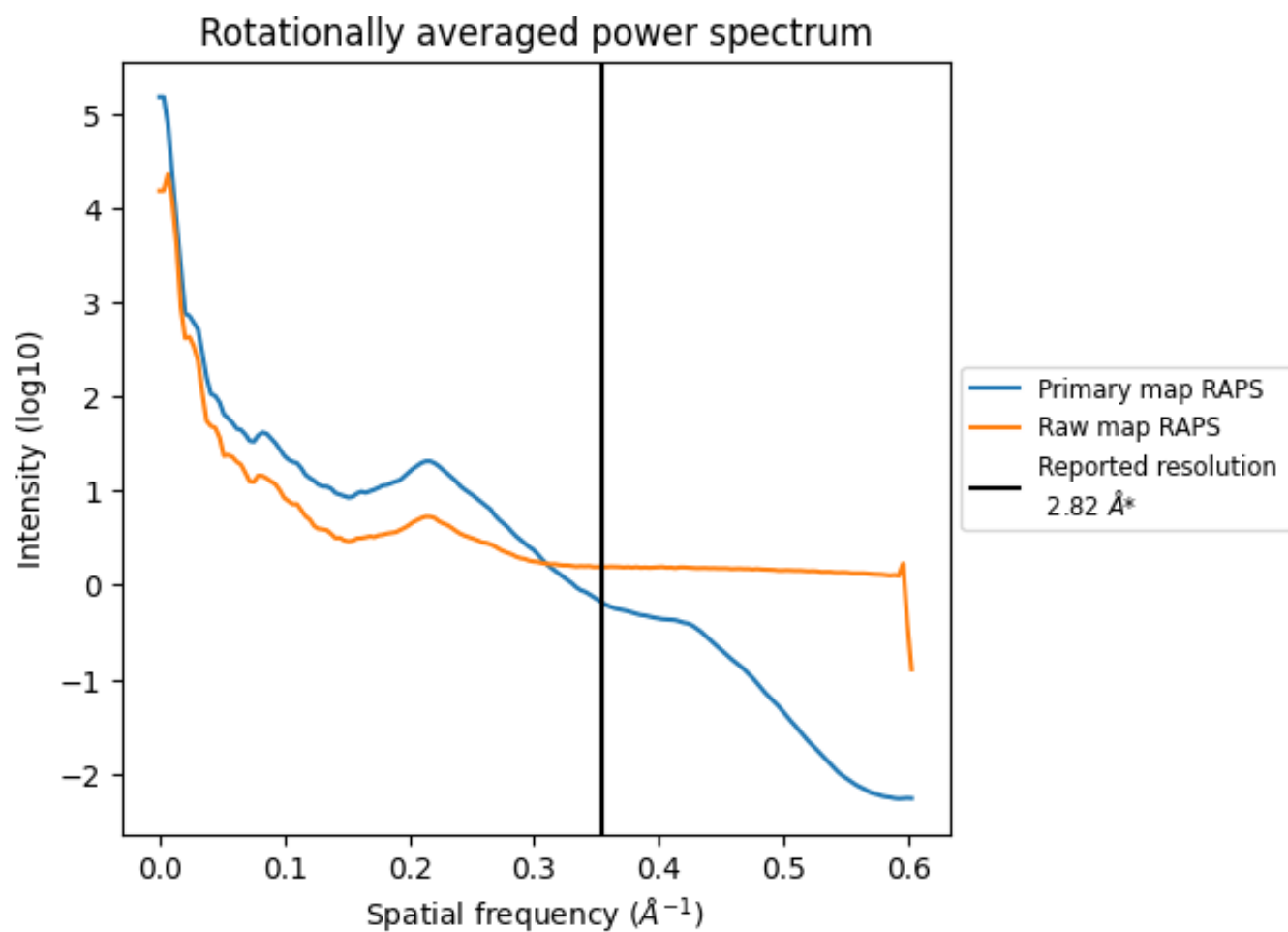
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 133 nm³; this corresponds to an approximate mass of 120 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 ⓘ

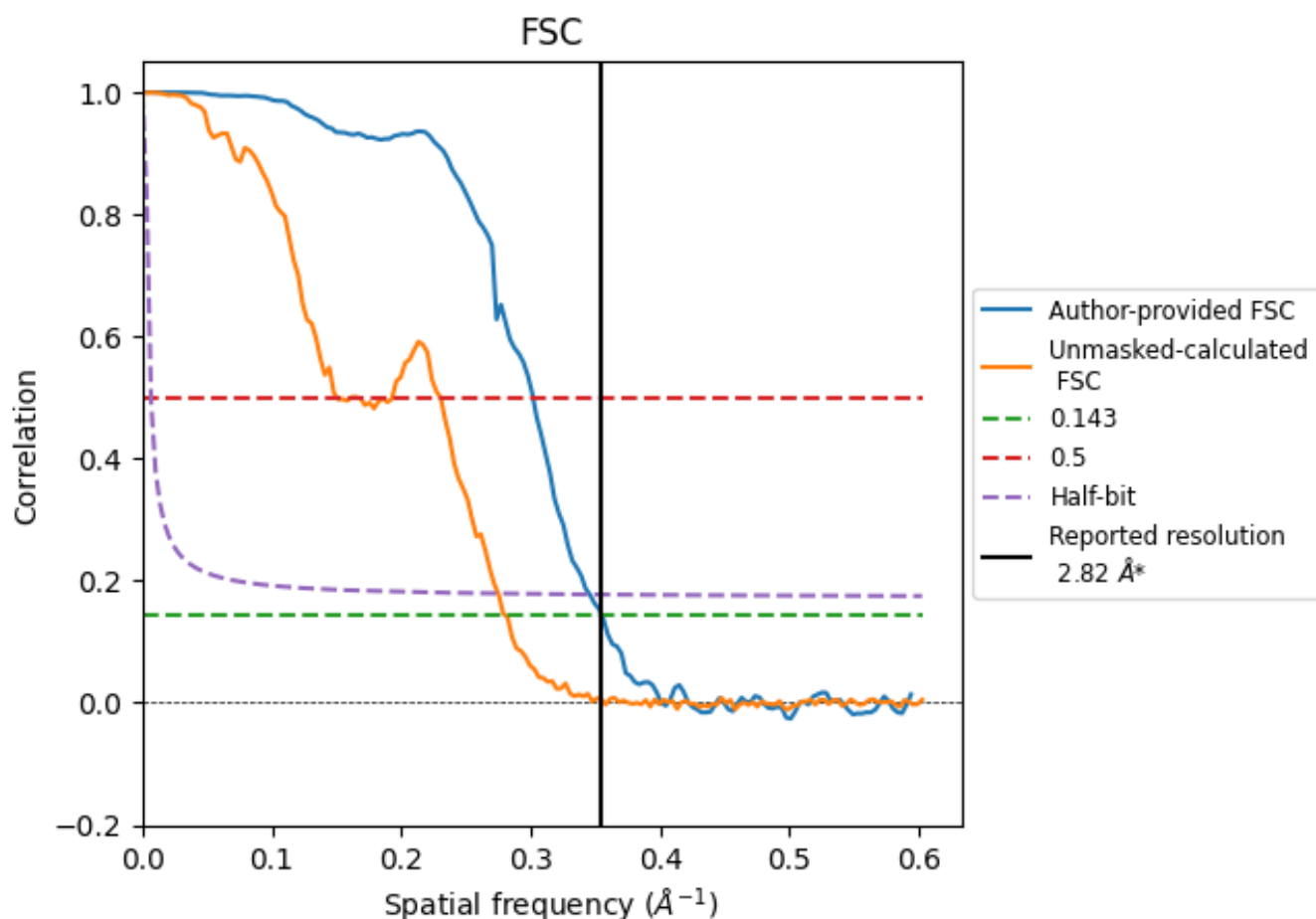


*Reported resolution corresponds to spatial frequency of $0.355 \text{ \AA}^{-1}$

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 0.355 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

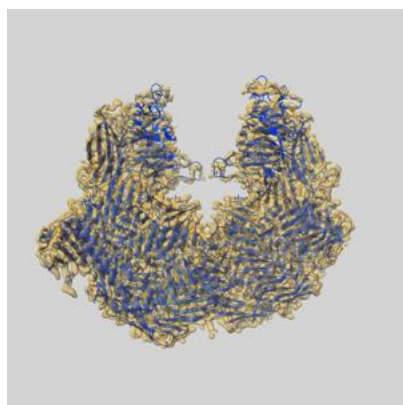
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.82	-	-
Author-provided FSC curve	2.82	3.31	2.89
Unmasked-calculated*	3.57	6.64	3.64

*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 3.57 differs from the reported value 2.82 by more than 10 %

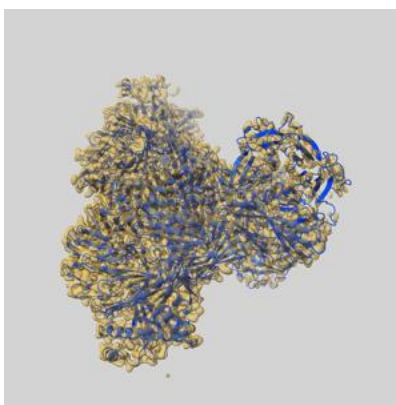
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-51022 and PDB model 9G42. Per-residue inclusion information can be found in section [3](#) on page [8](#).

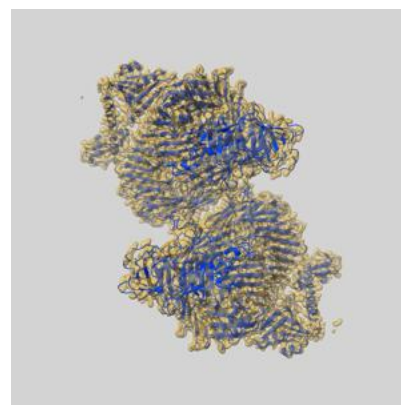
9.1 Map-model overlay [i](#)



X



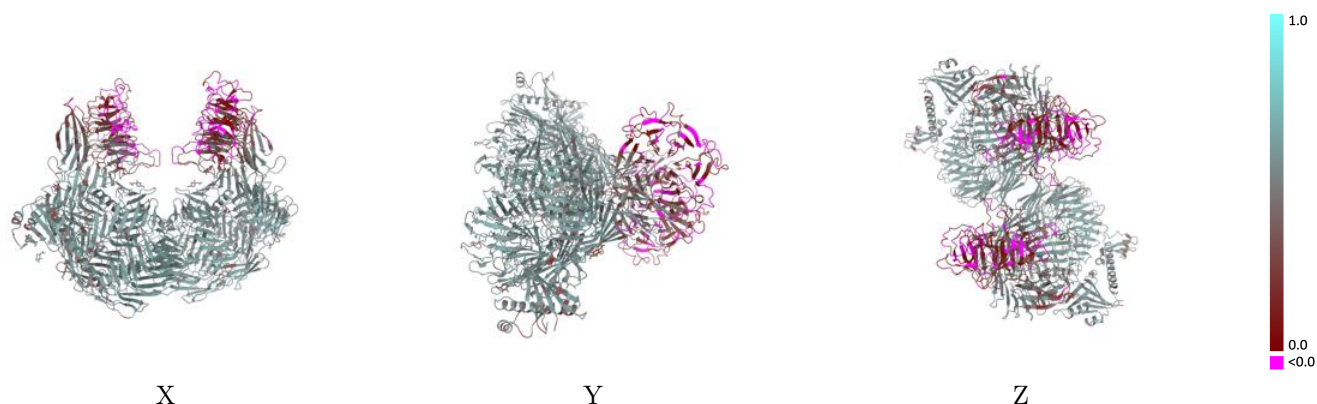
Y



Z

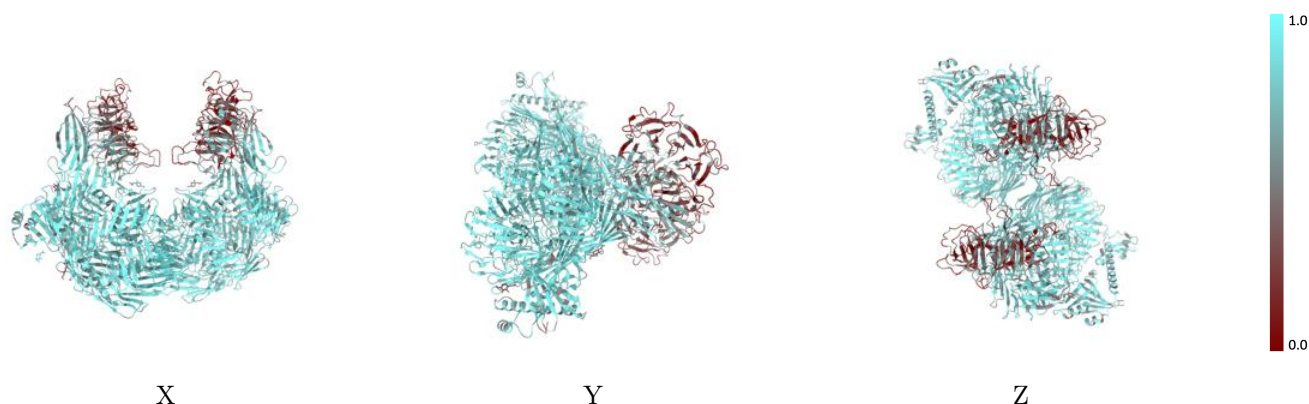
The images above show the 3D surface view of the map at the recommended contour level 0.134 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



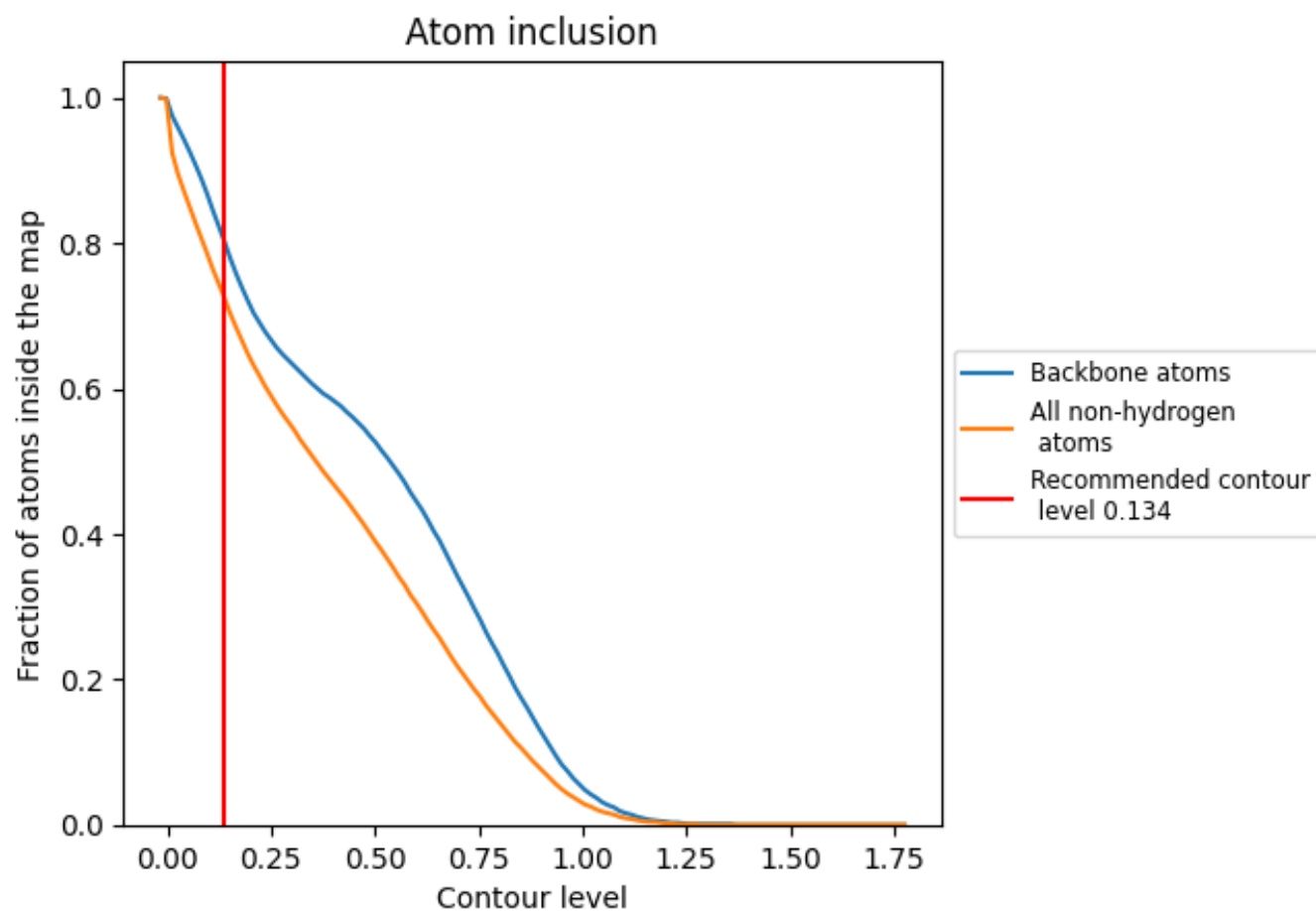
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.134).

9.4 Atom inclusion ⓘ



At the recommended contour level, 81% of all backbone atoms, 73% 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 (0.134) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7300	0.4580
A	0.7300	0.4580
B	0.7290	0.4590
C	0.7500	0.4570
D	0.7440	0.4890
E	0.6790	0.4460
F	0.7500	0.4500
G	0.7690	0.4940
H	0.7860	0.4340

1.0

0.0

<0.0