



Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 05:10 AM UTC

PDB ID : 9V6N / pdb_00009v6n
EMDB ID : EMD-64803
Title : Block based reconstruction of RVFV GnGc-Fab140 complex
Authors : Zhang, L.; Meng, K.; Xiang, Y.
Deposited on : 2025-05-27
Resolution : 3.40 Å(reported)

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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

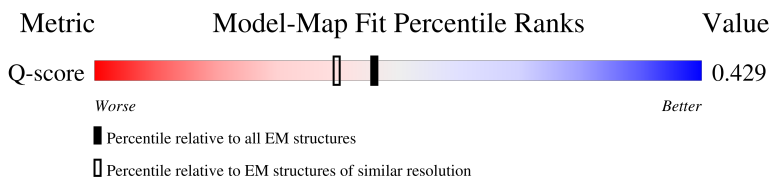
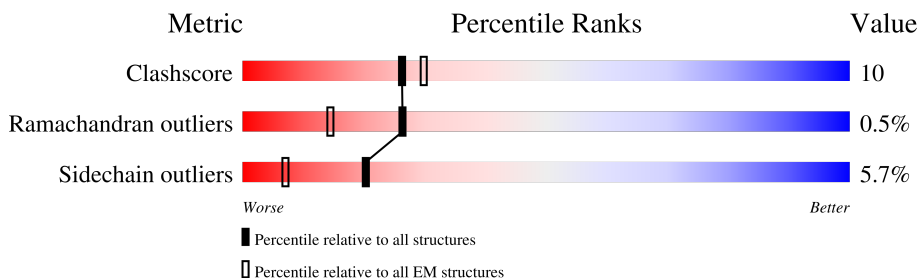
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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	14717 (2.90 - 3.90)

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	1064	
1	B	1064	
2	C	3	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6563 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 Envelopment polyprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	412	Total	C	N	O	S	0	0
			3119	1941	544	600	34		
1	B	444	Total	C	N	O	S	0	0
			3374	2093	582	671	28		

There are 44 discrepancies between the modelled and reference sequences:

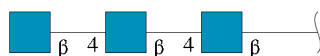
Chain	Residue	Modelled	Actual	Comment	Reference
A	1198	ASP	-	expression tag	UNP A2T069
A	1199	TYR	-	expression tag	UNP A2T069
A	1200	LYS	-	expression tag	UNP A2T069
A	1201	ASP	-	expression tag	UNP A2T069
A	1202	HIS	-	expression tag	UNP A2T069
A	1203	ASP	-	expression tag	UNP A2T069
A	1204	GLY	-	expression tag	UNP A2T069
A	1205	ASP	-	expression tag	UNP A2T069
A	1206	TYR	-	expression tag	UNP A2T069
A	1207	LYS	-	expression tag	UNP A2T069
A	1208	ASP	-	expression tag	UNP A2T069
A	1209	HIS	-	expression tag	UNP A2T069
A	1210	ASP	-	expression tag	UNP A2T069
A	1211	ILE	-	expression tag	UNP A2T069
A	1212	ASP	-	expression tag	UNP A2T069
A	1213	TYR	-	expression tag	UNP A2T069
A	1214	LYS	-	expression tag	UNP A2T069
A	1215	ASP	-	expression tag	UNP A2T069
A	1216	ASP	-	expression tag	UNP A2T069
A	1217	ASP	-	expression tag	UNP A2T069
A	1218	ASP	-	expression tag	UNP A2T069
A	1219	LYS	-	expression tag	UNP A2T069
B	1198	ASP	-	expression tag	UNP A2T069
B	1199	TYR	-	expression tag	UNP A2T069
B	1200	LYS	-	expression tag	UNP A2T069
B	1201	ASP	-	expression tag	UNP A2T069

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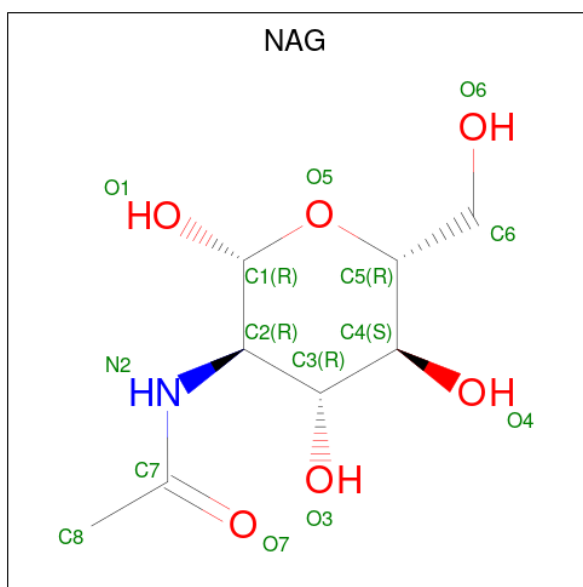
Chain	Residue	Modelled	Actual	Comment	Reference
B	1202	HIS	-	expression tag	UNP A2T069
B	1203	ASP	-	expression tag	UNP A2T069
B	1204	GLY	-	expression tag	UNP A2T069
B	1205	ASP	-	expression tag	UNP A2T069
B	1206	TYR	-	expression tag	UNP A2T069
B	1207	LYS	-	expression tag	UNP A2T069
B	1208	ASP	-	expression tag	UNP A2T069
B	1209	HIS	-	expression tag	UNP A2T069
B	1210	ASP	-	expression tag	UNP A2T069
B	1211	ILE	-	expression tag	UNP A2T069
B	1212	ASP	-	expression tag	UNP A2T069
B	1213	TYR	-	expression tag	UNP A2T069
B	1214	LYS	-	expression tag	UNP A2T069
B	1215	ASP	-	expression tag	UNP A2T069
B	1216	ASP	-	expression tag	UNP A2T069
B	1217	ASP	-	expression tag	UNP A2T069
B	1218	ASP	-	expression tag	UNP A2T069
B	1219	LYS	-	expression tag	UNP A2T069

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(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
			42	24	3	15		

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).



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

[illegible]

- Molecule 1: Envelopment polyprotein



PRO	HIS	LEU	ARG	ASN	ARG	PRO	GLY	GLY	LYS	HIS	ASN	TYR	ILE	ASP	GLY	THR	GLN	GLU	ASP	ALA	ALA	THR	THR	CYS	LYS	PRO	VAL	THR	THR	TYR	ALA	ALA	GLY	ALA	CYS	SER	SER	ASP	PHE	VAL	LEU	LEU	GLU	GLU	LYS	GLY	LYS	PHE	PRO	PRO	LEU	LEU	PHE	GLN	SER	TYR	ALA	HIS	HIS	ARG	THR	LEU	LEU	GLU	GLU	PRO
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VAL	HIS	ASP	THR	ILE	LEU	ALA	LYS	ASP	PRO	SER	CYS	ASP	LEU	GLN	SER	ALA	HIS	GLY	ASN	PRO	CYS	LYS	GLU	LYS	LEU	VAL	VAL	LYS	THR	HIS	CYS	PRO	ASN	ASP	TYR	GLN	SER	ALA	HIS	TYR	LEU	ASN	ASN	ASP	GLY	LYS	MET	ALA	ASP	VAL	LYS	PRO	PRO	LYS	TYR
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GLU	LEU	THR	GLU	ASP	CYS	ASN	PHE	CYS	CYS	ARG	GLN	MET	THR	GLY	ALA	ALA	SER	SER	TYR	PRO	LEU	GLN	GLN	CYS	CYS	SER	SER	GLU	ASP	ASP	GLY	GLY	SER	LYS	LYS	THR	LYS	MET	LYS	GLY	VAL	VAL	GLN	ALA	ALA	LEU	LYS	LYS	CYS	ASP	GLN	GLY
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LEU SER THR HIS GLU VAL VAL PHE LYS ASN SER LYS VAL TYR LEU ASP LYS LEU ASP LYS GLU GLU ASN LEU LEU THR GLU GLN HIS LYS GLY GLN TYR LYS GLY THR MET ASP SER GLY GLN THR LYS ARG GLU LEU

SER PHE ASP ILE SER GLN CYS PRO LYS LYS GLY HIS GLY SER LYS LYS CYS THR GLY ASP ALA ALA PHE CYS SER TYR TYR TYR TYR ASN VAL GLN GLN TYR TYR GLY GLY ILE VAL GLN GLN VAL SER GLY VAL TRP LYS LYS PRO LEU

CYS	VAL	GLY	TYR	GLU	ARG	VAL	VAL	VAL	LYS	ARG	GLU	LEU	SER	ALA	ALA	PRO	ILE	GLN	ARG	VAL	VAL	GLU	PRO	CYS	THR	THR	ILE	THR	LYS	CYS	GLU	PRO	HIS	GLY	LEU	VAL	VAL	VAL	ARG	SER	SER	SER	ILE	LYS	PHE	GLY	LYS	ILE	SER	SER	SER	ALA	VAL	VAL	CYS	VAL	VAL	THR	GLY	ASP
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GLN	SER	PRO	THR	GLU	ILE	THR	LEU	LYS	TYR	PRO	GLY	ILE	SER	SER	GLN	SER	SER	SER	ASP	ASP	GLN	SER	VAL	VAL	LYS	ILE	ALA	ALA	HIS	CYS	PRO	PRO	GLN	ASP	PRO	CYS	LEU	VAL	CYS	ALA	HIS	GLY	CYS	ILE	VAL	CYS	LEU	THR
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ASN	Tyr	GLN	CYS	HIS	THR	ALA	LEU	SER	ALA	PHE	VAL	VAL	VAL	PHE	PHE	PHE	SER	SER	ILE	ILE	ALA	ILE	ILE	ILE	CYS	LEU	CYS	ALA	ALA	VAL	VAL	LEU	LEU	Tyr	ARG	VAL	VAL	LEU	LEU	Lys	CYS	CYS	Lys	Val	Val	Leu	Asn	Pro	Pro	Thr	Met	Trp	Trp	Ile	Thr	Ala	Ala	Phe	Phe	Ile	Arg	Arg	Trp	Ile	Tyr	Tyr	Lys	Lys	Met
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Age Group	Percentage
18-24	15%
25-34	20%
35-44	25%
45-54	30%
55-64	35%
65-74	40%
75-84	45%
85+	50%

[illegible]

S699	R700	I701	THR	THR	CYS	SER	T706	E707	G708	V709	N710	T711	K712	G713	R714	L715	F716	G717	L721	R722	A730	G731	L732	M733	L734	K735	G736	E739	D740	Q741	K746	L747	K748	C771	E782	V785	R792	D793	N794	G797	A798	E799	M809	R810
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[illegible]

L953
 Y956
 K957
 P958
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 Q962
 L963
 E964
 L969
 P972
 G979
 S980
 L981
 P982
 Q983
 T989
 F990
 A991
 V999
 A1009
 T1012
 N1017
 F1018
 E1019
 V1020
 D1021
 F1022
 T1023
 G1024
 A1025
 A1026
 C1029
 D1030
 A1031
 L1034
 N1035
 L1036
 T1037
 G1038
 C1039
 Y1040
 S1041

[illegible]

1121	1122	1123	1124	1125	1126	1133	1134	1135	1136	1137	1138	1139	1140	1141	1142	1143	1144	1145	1146	1147	1148	1149	1150	1151	1152	1153	1154	1155	1156	1157	1158	1159	1160	1161	1162	1163	1164	1165	1166	1167	1168	1169	1170	1171	1172	1173	1174	1175	1176	1177	1178	1179	1180	1181	1182	1183	1184	1185	1186	1187	1188	1189	1190	1191	1192	1193	1194	1195	1196	1197	1198	1199	1200	1201	1202	1203	1204	1205	1206	1207	1208	1209	1210	1211	1212	1213	1214	1215	1216	1217	1218	1219	1220	1221	1222	1223	1224	1225	1226	1227	1228	1229	1230	1231	1232	1233	1234	1235	1236	1237	1238	1239	1240	1241	1242	1243	1244	1245	1246	1247	1248	1249	1250	1251	1252	1253	1254	1255	1256	1257	1258	1259	1260	1261	1262	1263	1264	1265	1266	1267	1268	1269	1270	1271	1272	1273	1274	1275	1276	1277	1278	1279	1280	1281	1282	1283	1284	1285	1286	1287	1288	1289	1290	1291	1292	1293	1294	1295	1296	1297	1298	1299	1300	1301	1302	1303	1304	1305	1306	1307	1308	1309	1310	1311	1312	1313	1314	1315	1316	1317	1318	1319	1320	1321	1322	1323	1324	1325	1326	1327	1328	1329	1330	1331	1332	1333	1334	1335	1336	1337	1338	1339	1340	1341	1342	1343	1344	1345	1346	1347	1348	1349	1350	1351	1352	1353	1354	1355	1356	1357	1358	1359	1360	1361	1362	1363	1364	1365	1366	1367	1368	1369	1370	1371	1372	1373	1374	1375	1376	1377	1378	1379	1380	1381	1382	1383	1384	1385	1386	1387	1388	1389	1390	1391	1392	1393	1394	1395	1396	1397	1398	1399	1400	1401	1402	1403	1404	1405	1406	1407	1408	1409	1410	1411	1412	1413	1414	1415	1416	1417	1418	1419	1420	1421	1422	1423	1424	1425	1426	1427	1428	1429	1430	1431	1432	1433	1434	1435	1436	1437	1438	1439	1440	1441	1442	1443	1444	1445	1446	1447	1448	1449	1450	1451	1452	1453	1454	1455	1456	1457	1458	1459	1460	1461	1462	1463	1464	1465	1466	1467	1468	1469	1470	1471	1472	1473	1474	1475	1476	1477	1478	1479	1480	1481	1482	1483	1484	1485	1486	1487	1488	1489	1490	1491	1492	1493	1494	1495	1496	1497	1498	1499	1500	1501	1502	1503	1504	1505	1506	1507	1508	1509	1510	1511	1512	1513	1514	1515	1516	1517	1518	1519	1520	1521	1522	1523	1524	1525	1526	1527	1528	1529	1530	1531	1532	1533	1534	1535	1536	1537	1538	1539	1540	1541	1542	1543	1544	1545	1546	1547	1548	1549	1550	1551	1552	1553	1554	1555	1556	1557	1558	1559	1560	1561	1562	1563	1564	1565	1566	1567	1568	1569	1570	1571	1572	1573	1574	1575	1576	1577	1578	1579	1580
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- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



MAG1
MAG2
MAG3

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	811329	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.085	Depositor
Minimum map value	-0.036	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.014	Depositor
Map size (Å)	175.664, 175.664, 175.664	wwPDB
Map dimensions	160, 160, 160	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0979, 1.0979, 1.0979	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	0.16	0/3186	0.31	0/4300
1	B	0.27	0/3435	0.45	1/4640 (0.0%)
All	All	0.22	0/6621	0.39	1/8940 (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.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	1107	PRO	CA-N-CD	-6.78	102.51	112.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	180	LYS	Peptide
1	B	792	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	3119	0	3055	42	0
1	B	3374	0	3243	94	0
2	C	42	0	37	1	0
3	A	14	0	13	0	0
3	B	14	0	13	0	0
All	All	6563	0	6361	130	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.

All (130) 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:B:1039:CYS:CB	1:B:1117:ILE:HD11	1.87	1.03
1:B:1039:CYS:HB2	1:B:1117:ILE:HD11	1.52	0.92
1:B:1039:CYS:HB2	1:B:1117:ILE:CD1	2.08	0.84
1:B:1039:CYS:SG	1:B:1117:ILE:HD11	2.20	0.80
1:A:511:CYS:HB2	1:B:1133:VAL:HG11	1.62	0.80
1:A:304:CYS:HA	1:A:456:CYS:HB3	1.65	0.79
1:B:1031:ALA:HB1	1:B:1050:LEU:HD11	1.66	0.76
1:B:885:TRP:HB2	1:B:1017:ASN:H	1.56	0.71
1:B:733:MET:HE3	1:B:733:MET:HA	1.76	0.68
1:A:304:CYS:HA	1:A:456:CYS:CB	2.25	0.67
1:B:913:TYR:HB2	1:B:981:LEU:HG	1.77	0.66
1:B:981:LEU:O	1:B:983:GLN:N	2.31	0.63
1:B:1039:CYS:CB	1:B:1117:ILE:CD1	2.68	0.63
1:B:746:LYS:HB2	1:B:864:THR:HB	1.80	0.61
1:B:699:SER:HB2	1:B:713:CYS:HB2	1.82	0.61
1:B:1038:GLY:HA3	1:B:1046:ALA:HA	1.82	0.61
1:B:1119:PRO:O	1:B:1120:PHE:C	2.43	0.61
1:B:701:ILE:HD13	1:B:734:LEU:HG	1.84	0.60
1:B:793:ASP:O	1:B:812:ASN:ND2	2.35	0.59
1:B:1034:LEU:HD13	2:C:1:NAG:H62	1.85	0.59
1:A:542:ALA:HB2	1:B:982:PRO:HB2	1.84	0.58
1:B:957:LYS:HB3	1:B:964:GLU:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1029:CYS:O	1:B:1106:ARG:NH1	2.28	0.58
1:B:890:LEU:HD11	1:B:1009:ALA:HB1	1.85	0.58
1:B:981:LEU:HD11	1:B:999:VAL:HG12	1.86	0.58
1:B:748:LYS:HB3	1:B:862:GLU:HB3	1.85	0.58
1:A:511:CYS:H	1:B:1133:VAL:HG22	1.67	0.58
1:A:511:CYS:HB2	1:B:1133:VAL:CG1	2.34	0.58
1:B:913:TYR:CB	1:B:981:LEU:HG	2.34	0.58
1:B:1042:CYS:HB3	1:B:1117:ILE:HD13	1.86	0.57
1:B:706:THR:HB	1:B:709:VAL:HG22	1.87	0.56
1:B:981:LEU:O	1:B:982:PRO:C	2.49	0.56
1:B:730:ALA:HB3	1:B:747:ILE:HB	1.88	0.56
1:A:367:LEU:HD13	1:A:422:ALA:HB2	1.87	0.56
1:B:1100:SER:HB2	1:B:1105:GLU:HA	1.87	0.56
1:A:376:GLU:OE2	1:A:384:THR:OG1	2.23	0.55
1:B:1120:PHE:O	1:B:1121:ASP:HB2	2.07	0.55
1:B:797:SER:OG	1:B:799:GLU:OE1	2.26	0.54
1:B:877:ALA:HB2	1:B:892:LEU:HD22	1.91	0.53
1:A:495:SER:O	1:A:520:THR:OG1	2.27	0.52
1:B:722:ARG:NH1	1:B:1009:ALA:H	2.08	0.52
1:A:511:CYS:O	1:B:1133:VAL:HG13	2.10	0.52
1:B:983:GLN:O	1:B:989:THR:HA	2.10	0.51
1:A:300:GLN:NE2	1:A:460:GLU:OE2	2.41	0.51
1:B:1037:THR:O	1:B:1047:ARG:N	2.44	0.51
1:B:847:LEU:HD12	1:B:972:PRO:HB2	1.92	0.51
1:A:263:ASP:N	1:A:263:ASP:OD1	2.41	0.50
1:A:360:ASP:OD1	1:A:446:GLN:HB3	2.11	0.50
1:A:512:VAL:HG22	1:A:527:PRO:HB3	1.93	0.50
1:B:1060:LEU:HD13	1:B:1062:ALA:H	1.76	0.50
1:B:1066:ASP:OD1	1:B:1066:ASP:N	2.33	0.50
1:A:225:ASP:O	1:A:227:PRO:HD3	2.12	0.49
1:B:1062:ALA:HB3	1:B:1071:ILE:HB	1.94	0.49
1:B:1122:ASP:N	1:B:1122:ASP:OD1	2.45	0.49
1:A:183:THR:HG22	1:A:184:TYR:H	1.77	0.49
1:B:712:LYS:HD2	1:B:1019:GLU:HB3	1.94	0.48
1:B:873:ILE:HD12	1:B:881:ARG:HG2	1.95	0.48
1:A:225:ASP:HB3	1:A:226:PRO:HD3	1.95	0.48
1:B:944:HIS:ND1	1:B:946:SER:OG	2.32	0.48
1:B:957:LYS:HG2	1:B:959:MET:HG2	1.95	0.48
1:B:1100:SER:HA	1:B:1106:ARG:HH21	1.78	0.47
1:A:541:MET:SD	1:A:541:MET:N	2.87	0.47
1:B:979:GLY:O	1:B:980:SER:C	2.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1029:CYS:HB3	1:B:1101:CYS:HB2	1.46	0.47
1:B:1076:GLU:HB2	1:B:1080:LYS:HD2	1.96	0.47
1:B:953:LEU:HD23	1:B:969:LEU:HD21	1.96	0.47
1:B:1052:ILE:HG21	1:B:1075:SER:HA	1.95	0.47
1:B:1060:LEU:HD22	1:B:1061:SER:H	1.78	0.47
1:A:276:GLU:OE2	1:A:285:ARG:NH1	2.47	0.47
1:A:378:LYS:HD3	1:A:393:GLU:HB2	1.97	0.47
1:A:303:PHE:O	1:A:456:CYS:HB2	2.15	0.47
1:A:319:LYS:HE2	1:A:319:LYS:HB3	1.67	0.47
1:B:1048:VAL:O	1:B:1084:GLN:N	2.31	0.47
1:A:504:VAL:HG12	1:A:540:HIS:HB2	1.96	0.46
1:B:1119:PRO:HB2	1:B:1121:ASP:O	2.15	0.46
1:B:730:ALA:O	1:B:746:LYS:HA	2.15	0.46
1:B:926:GLN:OE1	1:B:927:GLY:N	2.49	0.46
1:B:883:THR:OG1	1:B:884:ASN:N	2.48	0.46
1:B:898:SER:O	1:B:898:SER:OG	2.25	0.46
1:B:981:LEU:HD13	1:B:991:ALA:C	2.41	0.46
1:B:1045:GLY:HA3	1:B:1085:ILE:HD11	1.96	0.46
1:B:1073:LEU:HD13	1:B:1082:GLN:HB2	1.97	0.46
1:B:864:THR:HG23	1:B:869:SER:HB3	1.98	0.46
1:B:874:ASP:O	1:B:881:ARG:NH1	2.48	0.46
1:A:557:PRO:O	1:A:559:GLN:NE2	2.38	0.46
1:B:1036:LEU:HD13	1:B:1048:VAL:HG22	1.97	0.46
1:B:1062:ALA:HA	1:B:1099:TYR:HA	1.98	0.46
1:B:1049:CYS:HA	1:B:1083:CYS:HA	1.98	0.45
1:B:858:LYS:HE3	1:B:858:LYS:HB2	1.63	0.45
1:A:183:THR:HG22	1:A:184:TYR:N	2.31	0.45
1:A:232:GLN:HG3	1:A:272:PRO:HB3	1.97	0.45
1:B:865:ASP:OD1	1:B:866:PHE:N	2.50	0.45
1:B:721:ILE:O	1:B:721:ILE:HD12	2.17	0.44
1:B:696:GLN:HE21	1:B:717:GLY:HA3	1.82	0.44
1:A:199:LYS:O	1:A:204:GLN:NE2	2.51	0.44
1:B:710:ASN:HD21	1:B:1019:GLU:HB3	1.81	0.44
1:B:771:CYS:HB3	1:B:837:THR:HG22	1.98	0.44
1:A:324:VAL:HG23	1:A:464:VAL:HG12	1.99	0.44
1:A:562:CYS:HA	1:A:565:HIS:CE1	2.52	0.44
1:A:344:PRO:HB3	1:A:359:LEU:HD22	2.00	0.43
1:A:487:GLU:HG3	1:A:489:HIS:H	1.83	0.43
1:B:691:CYS:N	1:B:733:MET:HG2	2.32	0.43
1:A:366:ASN:ND2	1:A:368:LEU:HD23	2.32	0.43
1:B:959:MET:HE2	1:B:962:GLN:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:504:VAL:HG23	1:A:513:THR:HG22	2.00	0.43
1:B:1064:ASN:ND2	1:B:1066:ASP:OD1	2.52	0.43
1:A:260:LEU:HD21	1:A:347:VAL:HG21	1.99	0.43
1:B:1109:LEU:HD12	1:B:1110:VAL:N	2.33	0.43
1:A:471:LYS:HA	1:A:471:LYS:HD2	1.71	0.43
1:B:893:ASP:OD1	1:B:893:ASP:N	2.48	0.43
1:B:980:SER:O	1:B:983:GLN:HG2	2.19	0.43
1:B:1052:ILE:HD13	1:B:1082:GLN:HG2	2.01	0.43
1:B:701:ILE:HD12	1:B:741:GLN:HE21	1.84	0.42
1:A:331:LYS:HD2	1:A:331:LYS:HA	1.80	0.42
1:A:513:THR:HB	1:B:989:THR:HG21	2.02	0.42
1:B:712:LYS:HE2	1:B:712:LYS:HB2	1.78	0.42
1:B:870:VAL:HG23	1:B:870:VAL:O	2.19	0.42
1:A:197:LYS:HD3	1:A:197:LYS:HA	1.71	0.42
1:B:1117:ILE:N	1:B:1117:ILE:HD12	2.35	0.42
1:B:873:ILE:HD13	1:B:873:ILE:HA	1.94	0.41
1:B:811:GLU:OE2	1:B:956:TYR:OH	2.30	0.41
1:B:1097:PHE:C	1:B:1098:MET:HE3	2.45	0.41
1:B:809:MET:SD	1:B:949:ARG:HD3	2.61	0.41
1:A:445:ILE:HD12	1:A:445:ILE:HA	1.84	0.41
1:A:335:GLN:NE2	1:A:469:SER:H	2.19	0.41
1:B:837:THR:HG21	1:B:956:TYR:HE1	1.86	0.41
1:A:280:ASP:OD1	1:A:280:ASP:N	2.54	0.41
1:A:378:LYS:HG2	1:A:385:MET:SD	2.60	0.41
1:B:748:LYS:N	1:B:862:GLU:O	2.49	0.40
1:B:1064:ASN:OD1	1:B:1064:ASN:N	2.54	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	410/1064 (38%)	394 (96%)	15 (4%)	1 (0%)	43	71
1	B	440/1064 (41%)	406 (92%)	31 (7%)	3 (1%)	18	47
All	All	850/2128 (40%)	800 (94%)	46 (5%)	4 (0%)	26	54

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1121	ASP
1	B	982	PRO
1	A	228	SER
1	B	980	SER

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	352/912 (39%)	332 (94%)	20 (6%)	18	45
1	B	381/912 (42%)	359 (94%)	22 (6%)	18	45
All	All	733/1824 (40%)	691 (94%)	42 (6%)	20	45

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	190	SER
1	A	221	ILE
1	A	225	ASP
1	A	263	ASP
1	A	285	ARG
1	A	329	LEU
1	A	333	ASP
1	A	351	SER
1	A	390	THR
1	A	396	SER
1	A	413	CYS
1	A	457	VAL

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Mol	Chain	Res	Type
1	A	462	VAL
1	A	463	VAL
1	A	469	SER
1	A	477	GLU
1	A	493	VAL
1	A	510	VAL
1	A	513	THR
1	A	543	HIS
1	B	709	VAL
1	B	715	LEU
1	B	731	CYS
1	B	732	LEU
1	B	782	GLU
1	B	785	VAL
1	B	794	ASN
1	B	818	CYS
1	B	828	VAL
1	B	842	VAL
1	B	859	LEU
1	B	880	SER
1	B	893	ASP
1	B	915	ILE
1	B	931	GLU
1	B	960	ILE
1	B	980	SER
1	B	981	LEU
1	B	1012	THR
1	B	1023	VAL
1	B	1066	ASP
1	B	1085	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	166	HIS
1	A	380	GLN
1	A	389	GLN
1	A	401	GLN
1	A	408	HIS
1	B	817	GLN
1	B	986	ASN
1	B	1043	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 ⓘ

3 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	0.45	0	17,19,21	1.53	3 (17%)
2	NAG	C	2	2	14,14,15	0.39	0	17,19,21	1.35	2 (11%)
2	NAG	C	3	2	14,14,15	0.32	0	17,19,21	0.91	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	4/6/23/26	0/1/1/1
2	NAG	C	3	2	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	NAG	C1-O5-C5	-3.77	107.14	112.19
2	C	1	NAG	C4-C3-C2	3.26	115.79	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	NAG	C3-C4-C5	2.86	115.41	110.23
2	C	1	NAG	C1-O5-C5	-2.75	108.50	112.19
2	C	3	NAG	C2-N2-C7	-2.38	119.71	122.90
2	C	2	NAG	O5-C1-C2	-2.01	108.18	111.29

There are no chirality outliers.

All (10) torsion outliers are listed below:

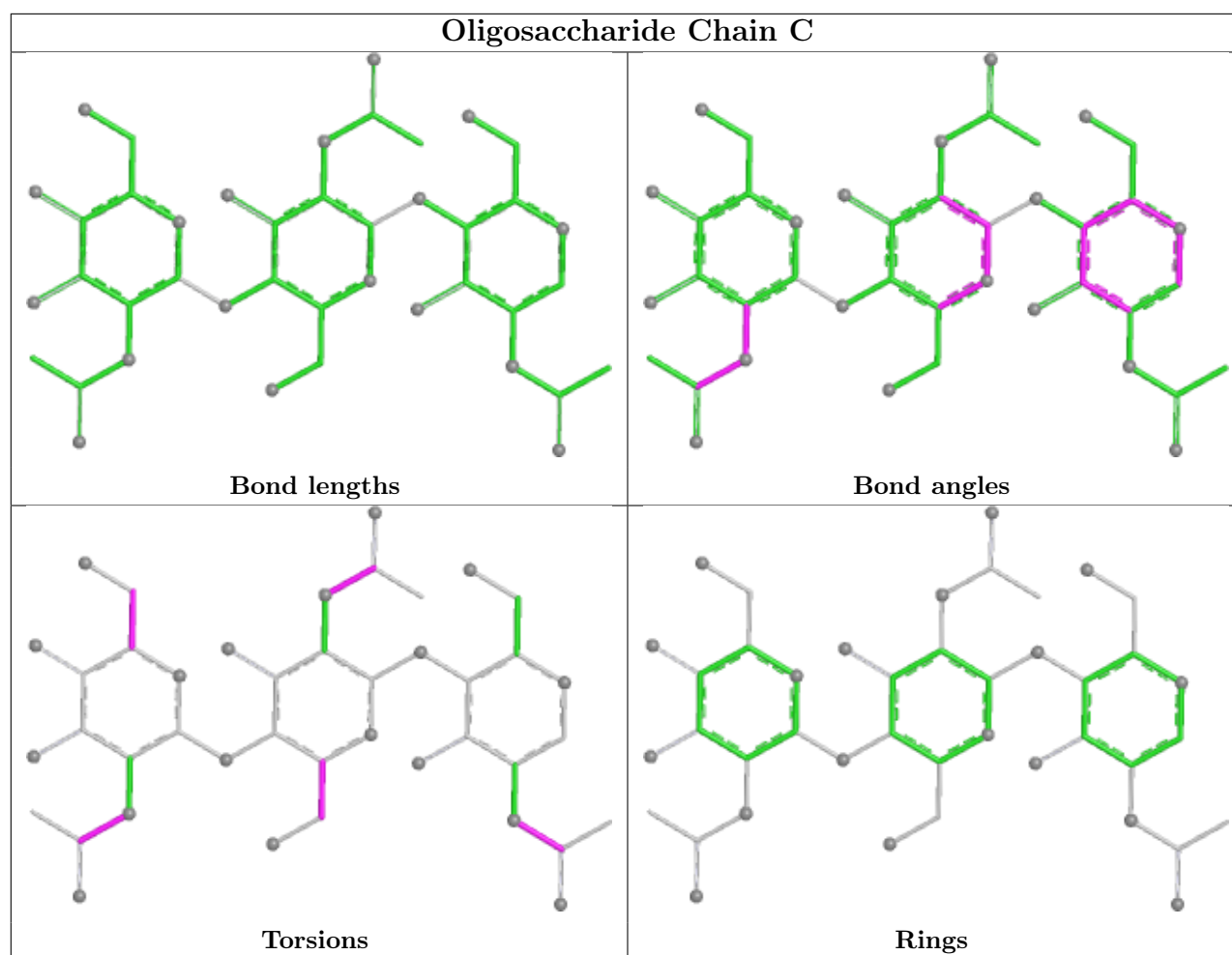
Mol	Chain	Res	Type	Atoms
2	C	2	NAG	C8-C7-N2-C2
2	C	2	NAG	O7-C7-N2-C2
2	C	3	NAG	O5-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
2	C	3	NAG	C4-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
2	C	3	NAG	C8-C7-N2-C2
2	C	3	NAG	O7-C7-N2-C2
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	NAG	1	0

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



5.6 Ligand geometry [i](#)

2 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	B	1301	1	14,14,15	0.20	0	17,19,21	0.45	0
3	NAG	A	1301	1	14,14,15	0.24	0	17,19,21	0.41	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	B	1301	1	-	4/6/23/26	0/1/1/1
3	NAG	A	1301	1	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

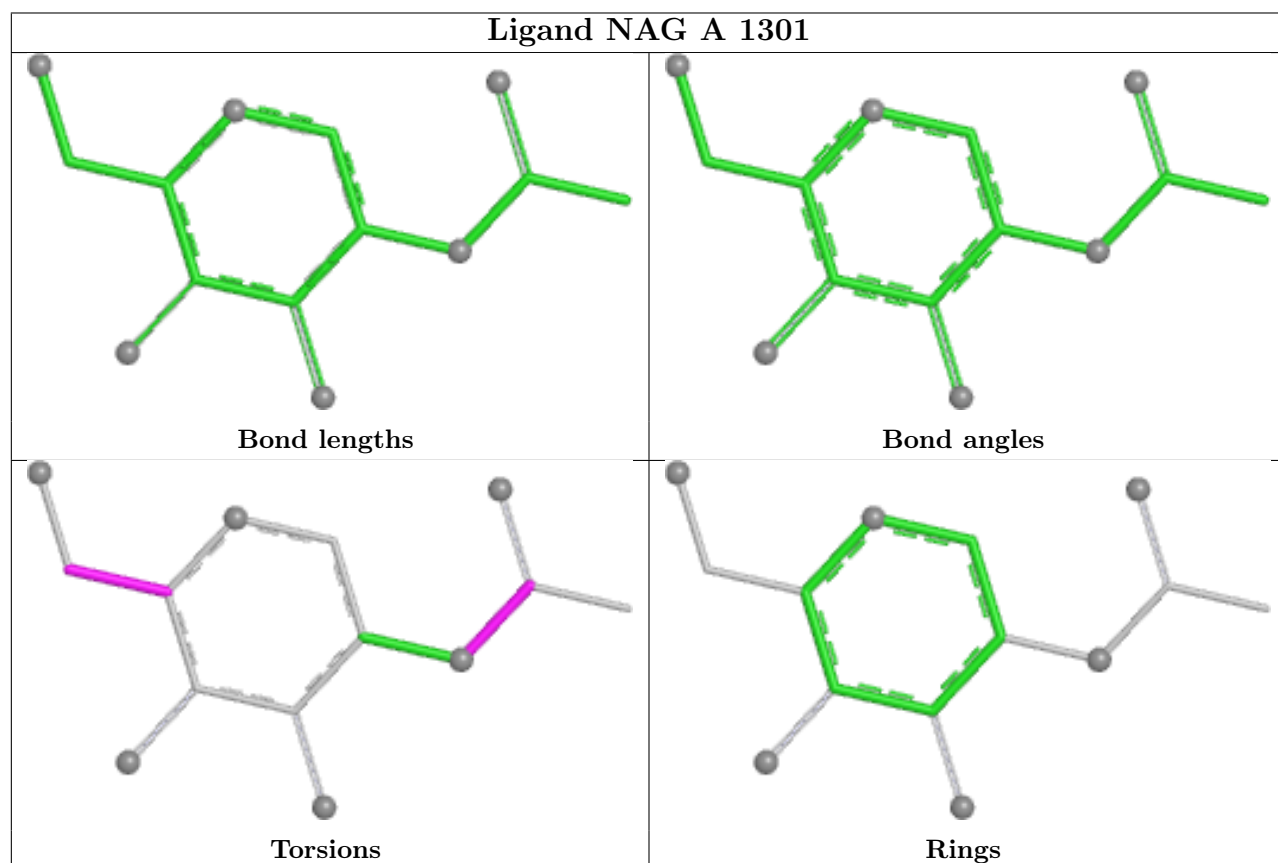
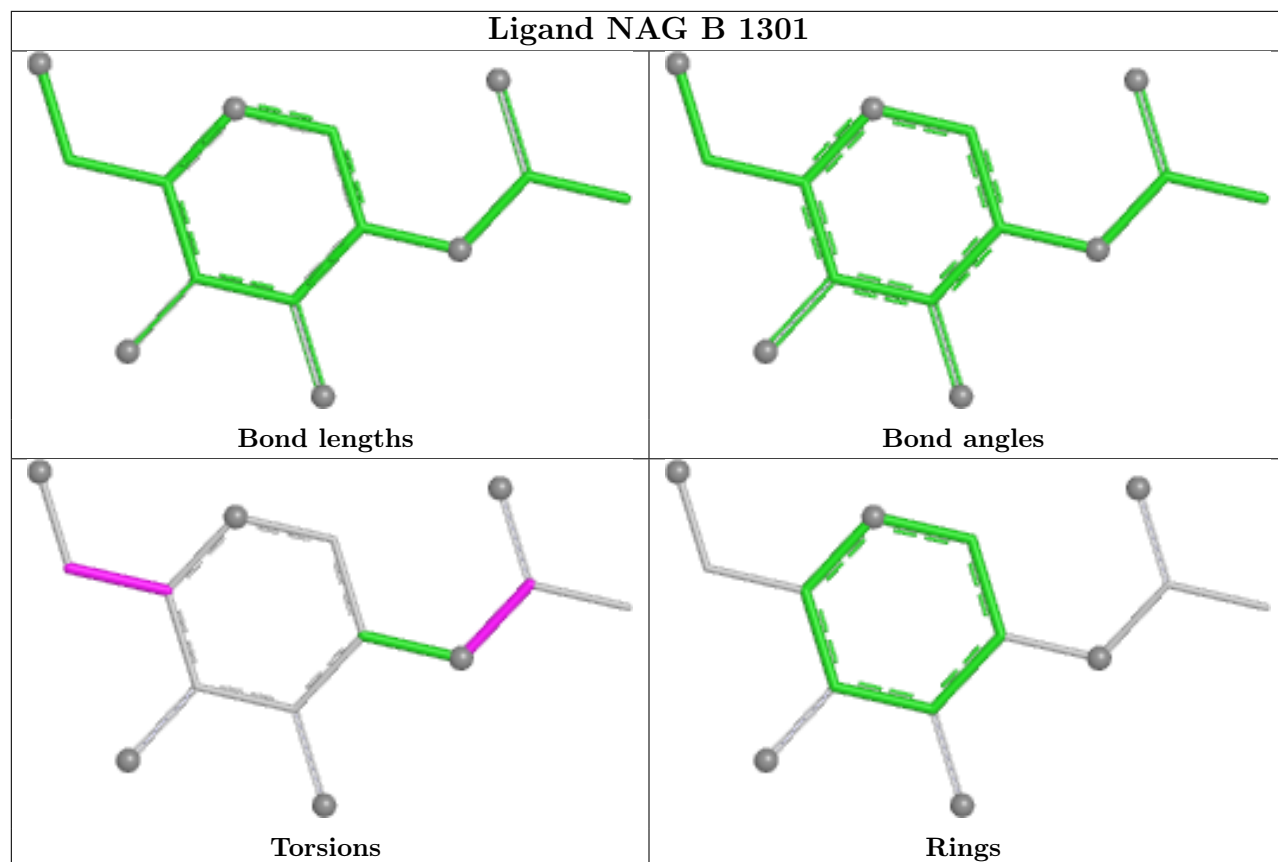
All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1301	NAG	O5-C5-C6-O6
3	B	1301	NAG	C4-C5-C6-O6
3	A	1301	NAG	C8-C7-N2-C2
3	A	1301	NAG	O7-C7-N2-C2
3	B	1301	NAG	C8-C7-N2-C2
3	B	1301	NAG	O7-C7-N2-C2
3	A	1301	NAG	O5-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 all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

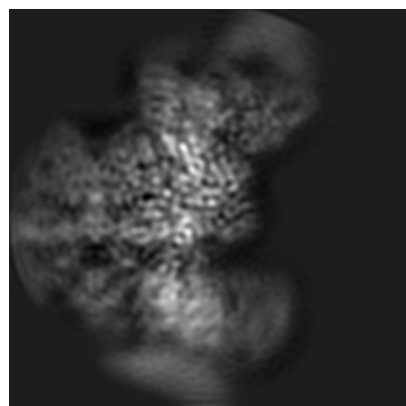
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-64803. These allow visual inspection of the internal detail of the map and identification of artifacts.

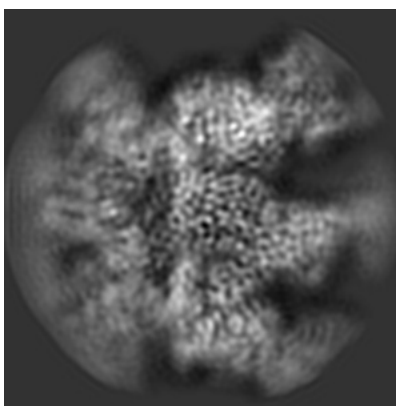
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

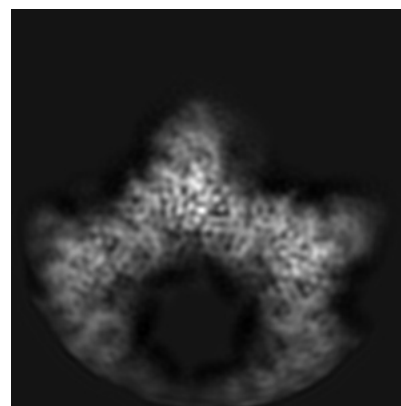
6.1.1 Primary map



X

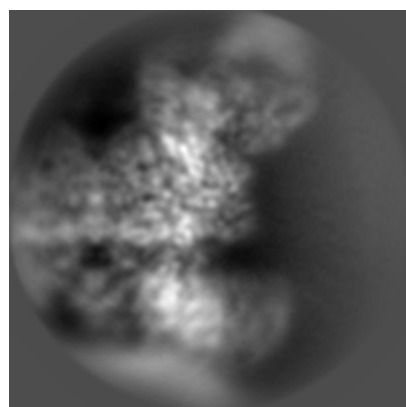


Y

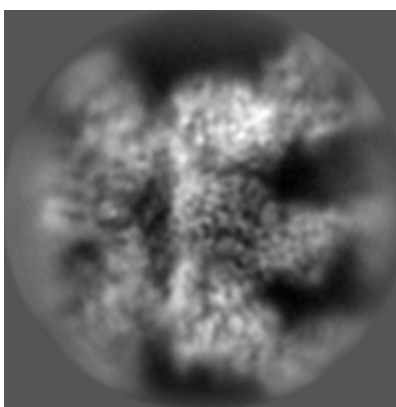


Z

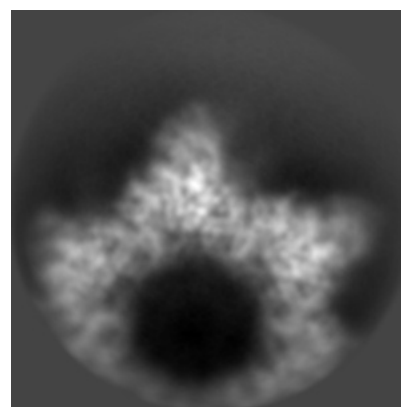
6.1.2 Raw map



X



Y

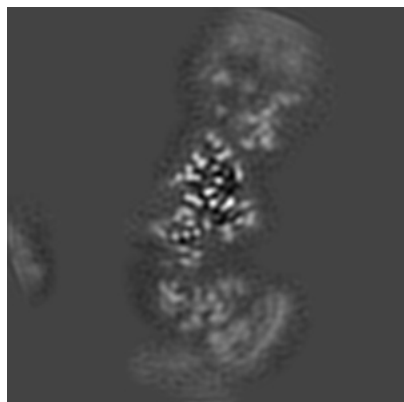


Z

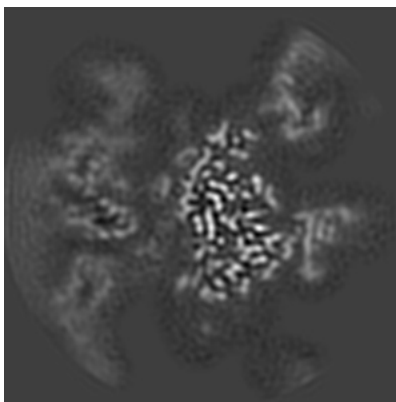
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

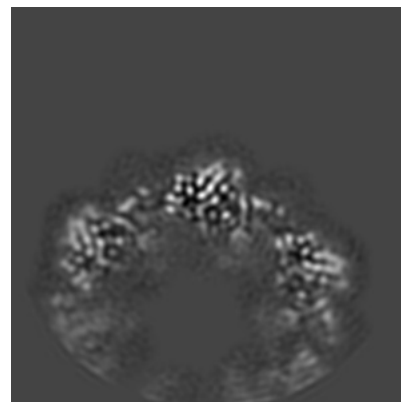
6.2.1 Primary map



X Index: 80

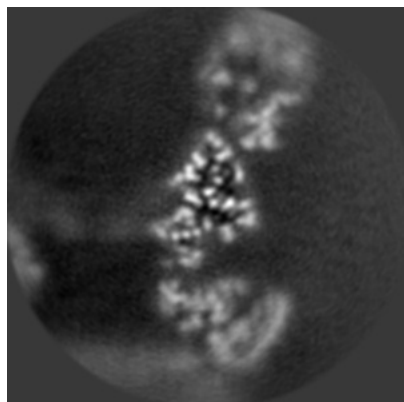


Y Index: 80

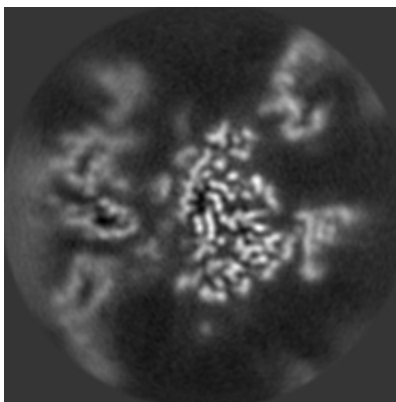


Z Index: 80

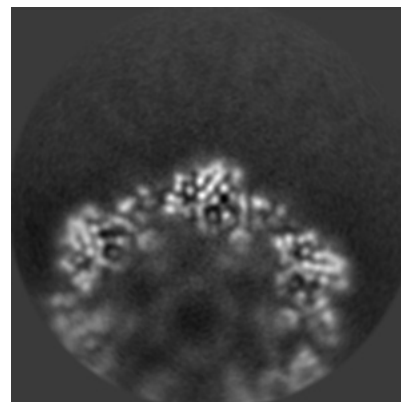
6.2.2 Raw map



X Index: 80



Y Index: 80

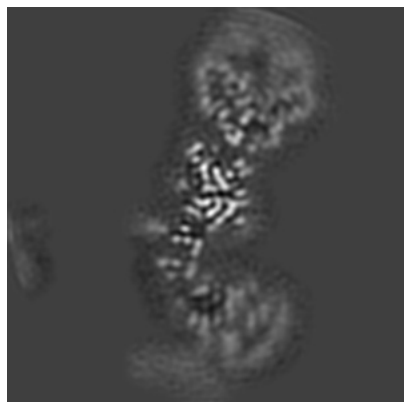


Z Index: 80

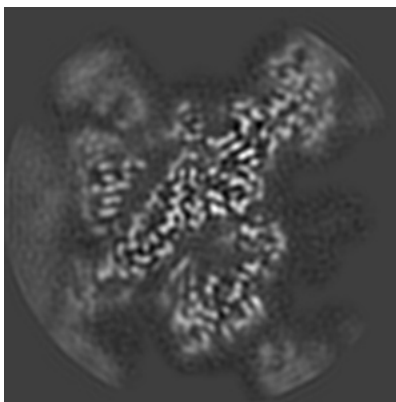
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

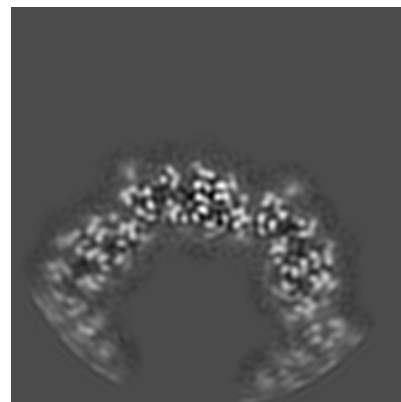
6.3.1 Primary map



X Index: 75

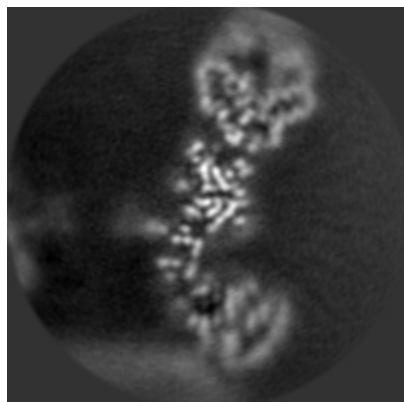


Y Index: 72

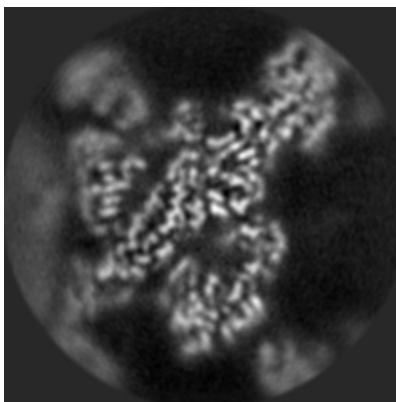


Z Index: 93

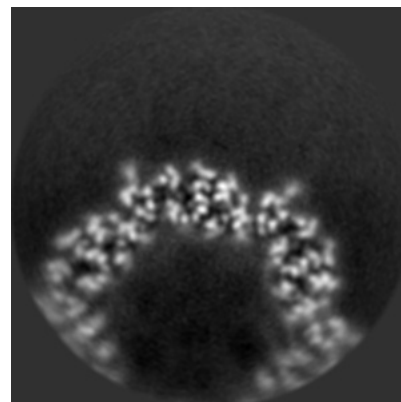
6.3.2 Raw map



X Index: 75



Y Index: 72

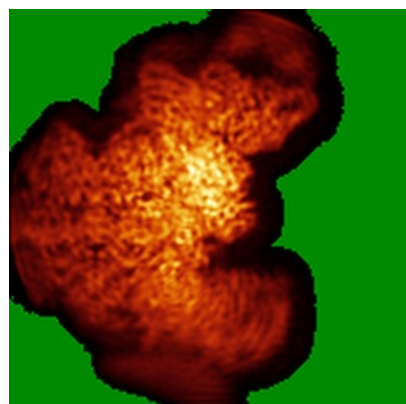


Z Index: 93

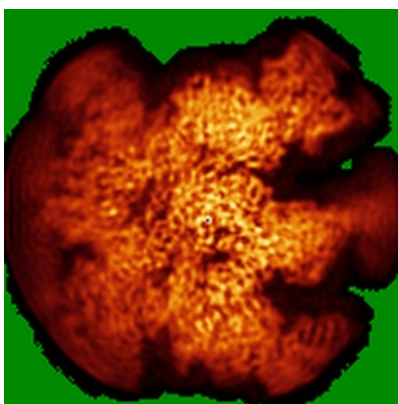
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X

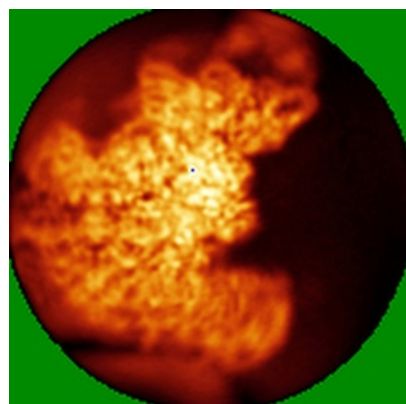


Y

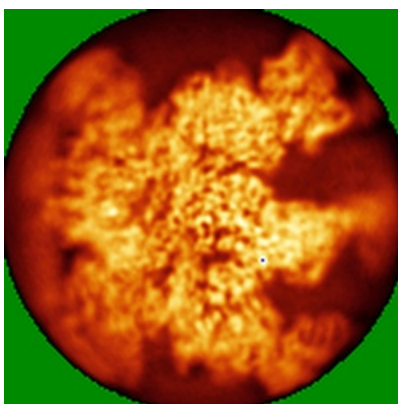


Z

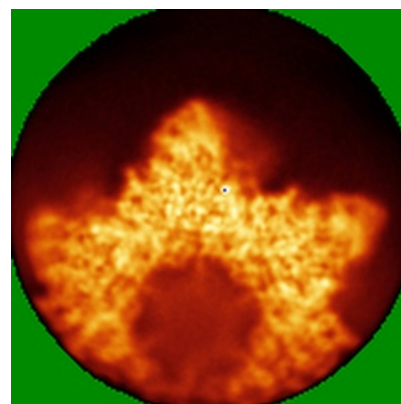
6.4.2 Raw map



X



Y

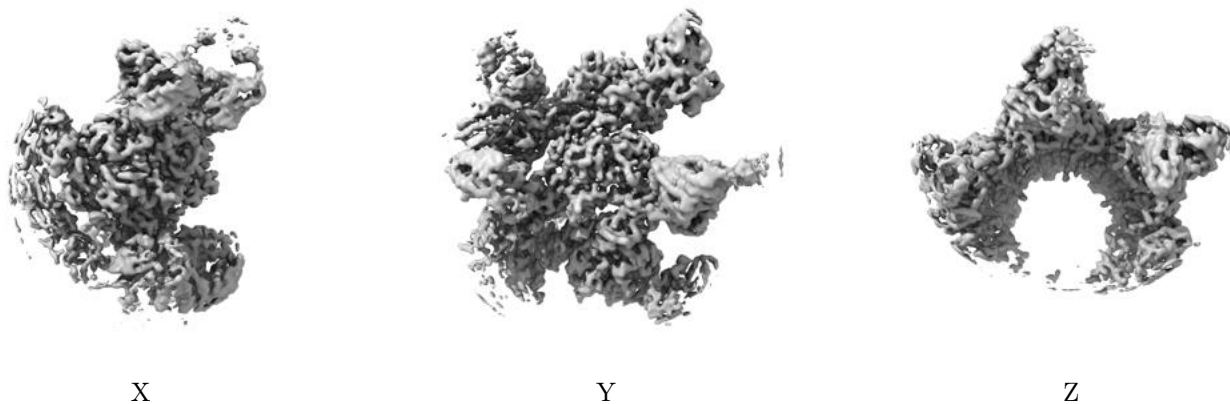


Z

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.

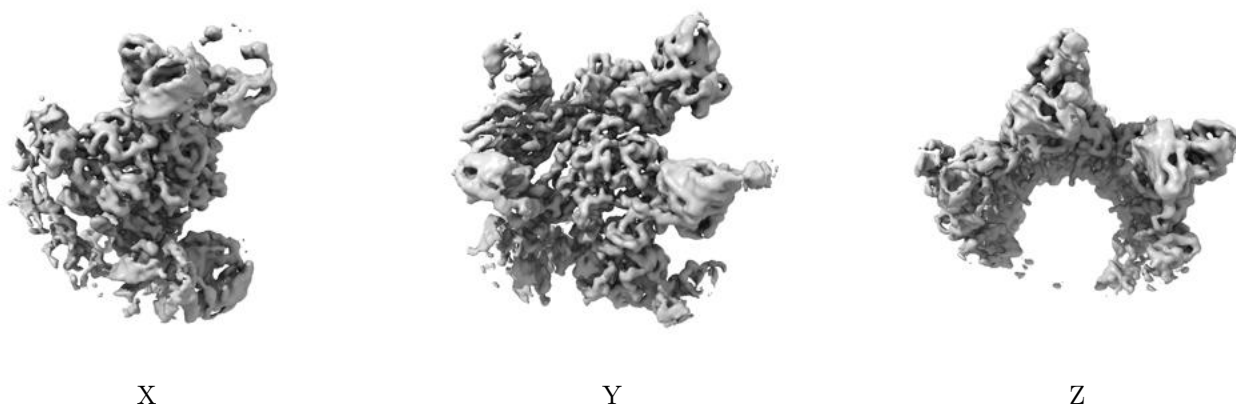
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.014. 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.

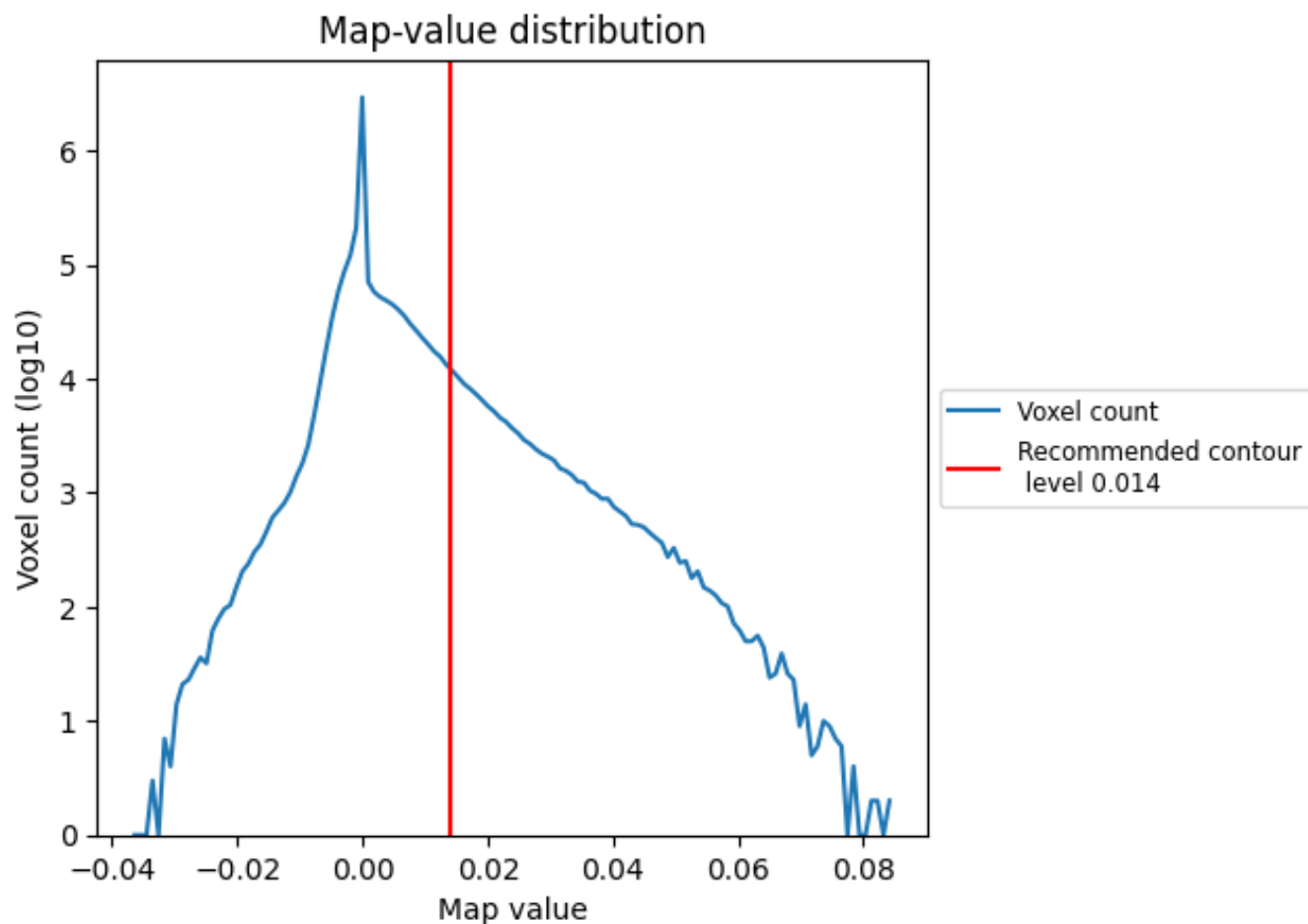
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

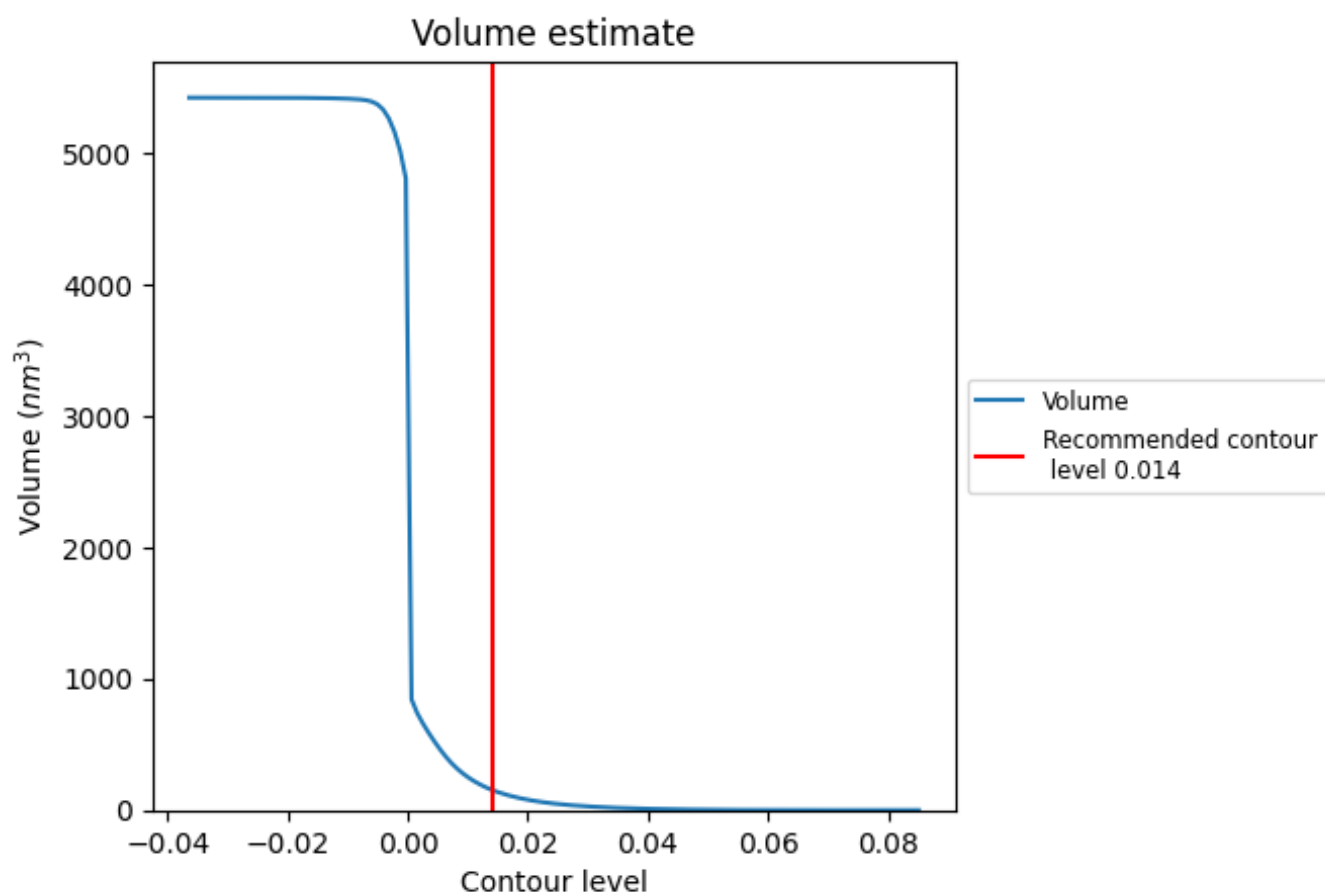
This section contains the results of statistical analysis of the map.

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.

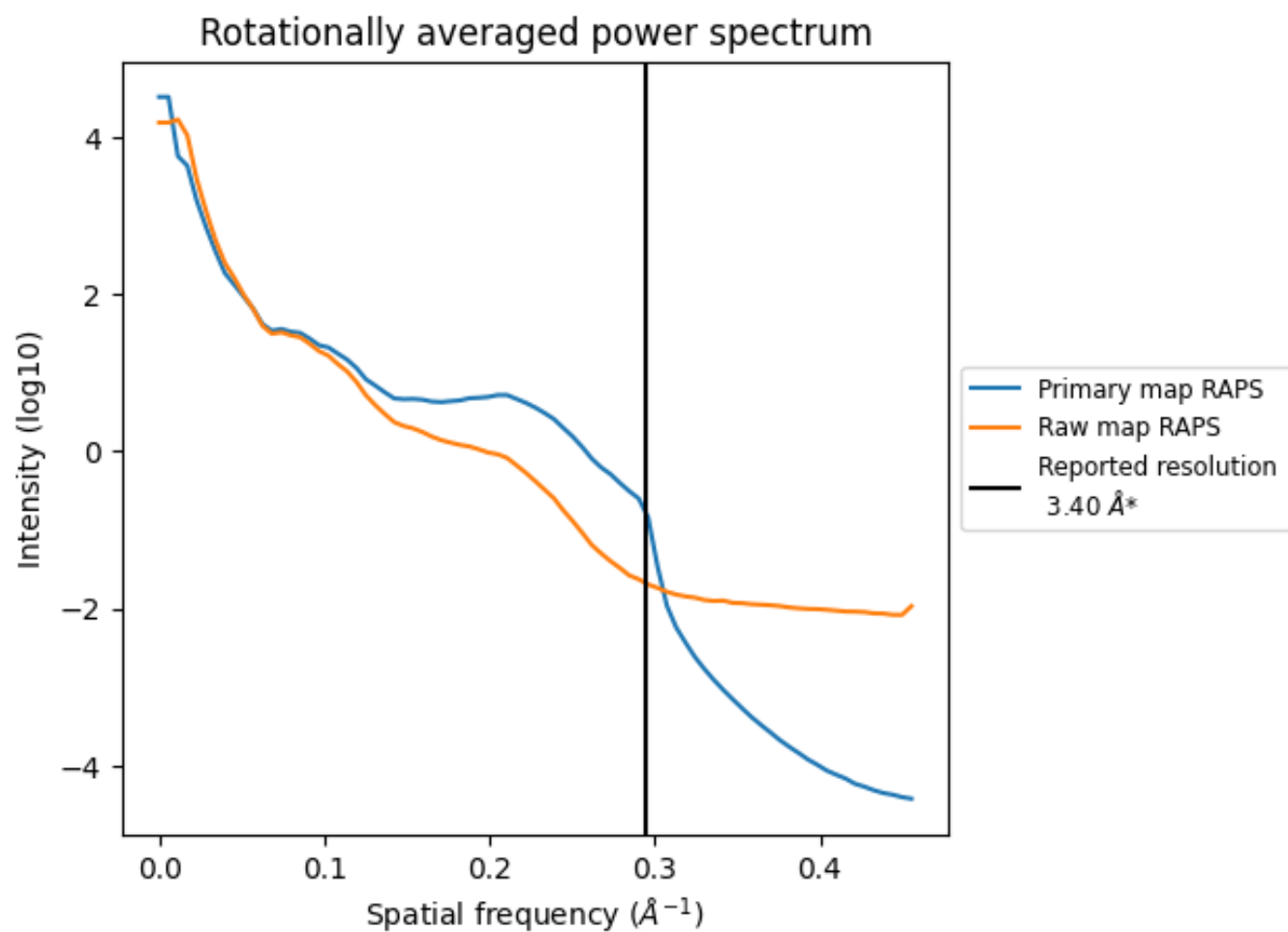
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 154 nm³; this corresponds to an approximate mass of 139 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 ⓘ

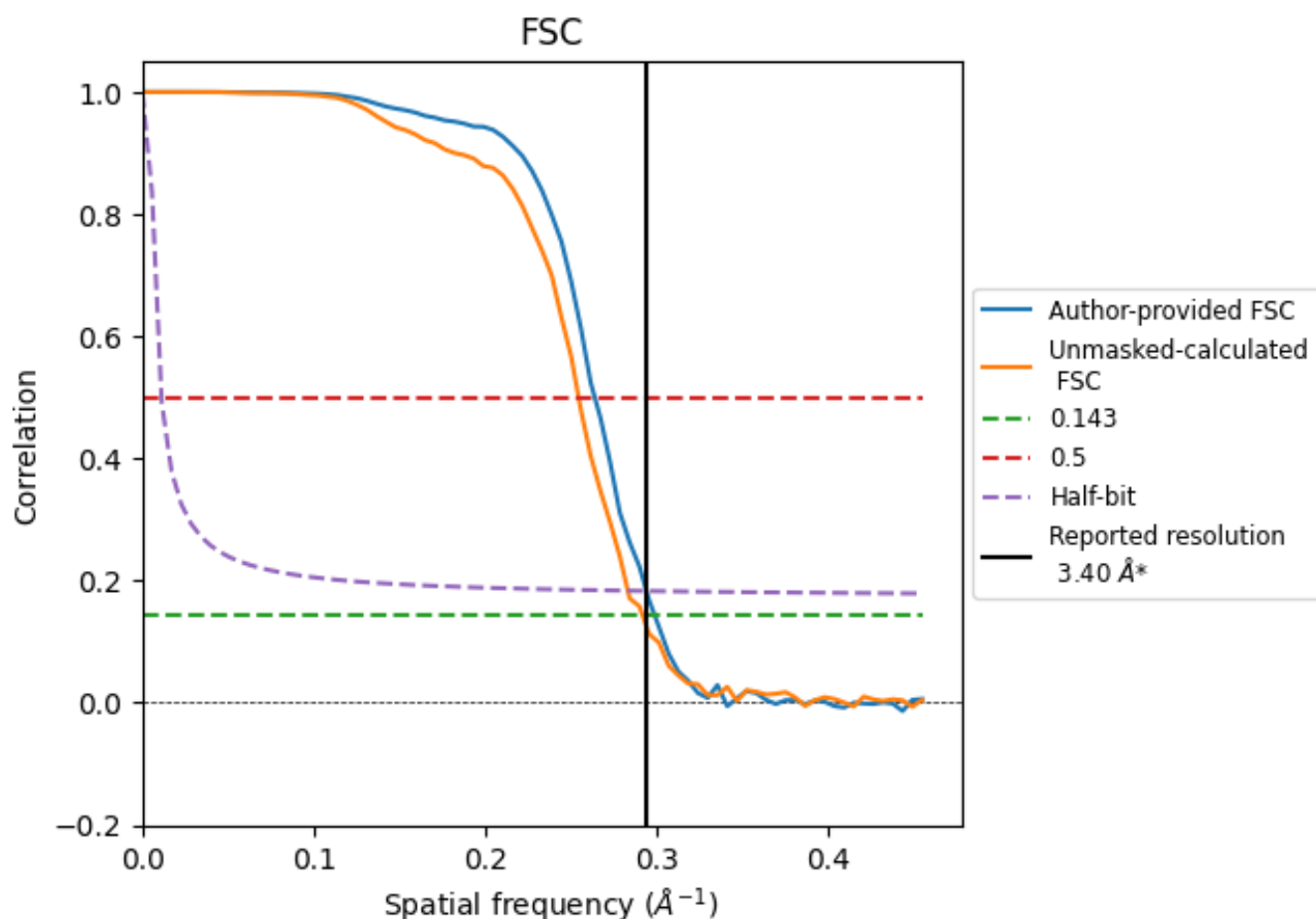


*Reported resolution corresponds to spatial frequency of $0.294 \text{ \AA}^{-1}$

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 0.294 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

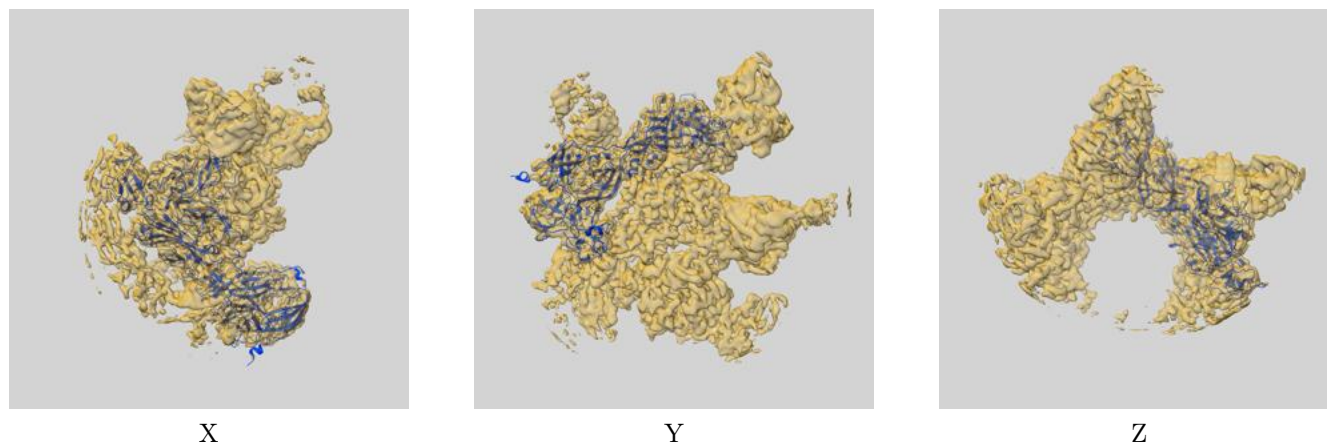
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.34	3.79	3.40
Unmasked-calculated*	3.42	3.92	3.53

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

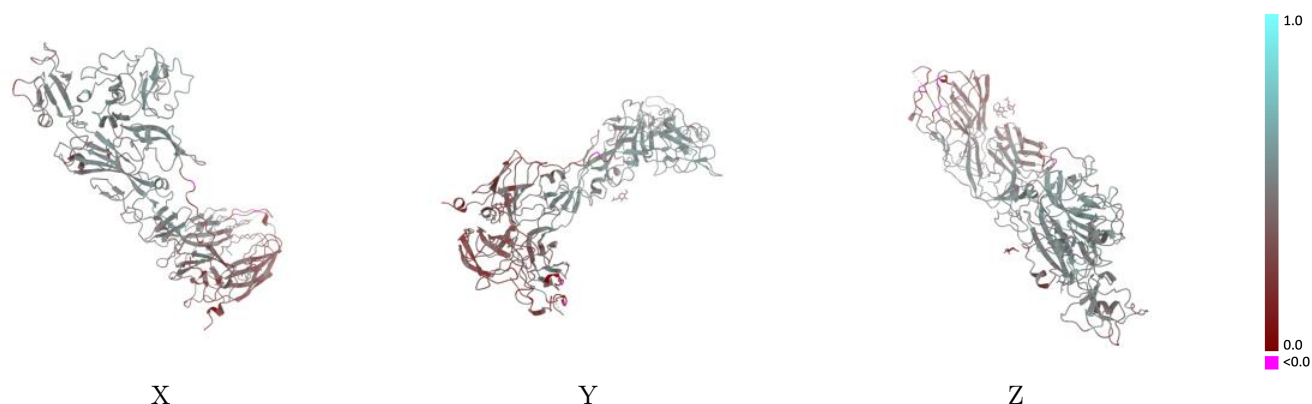
This section contains information regarding the fit between EMDB map EMD-64803 and PDB model 9V6N. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



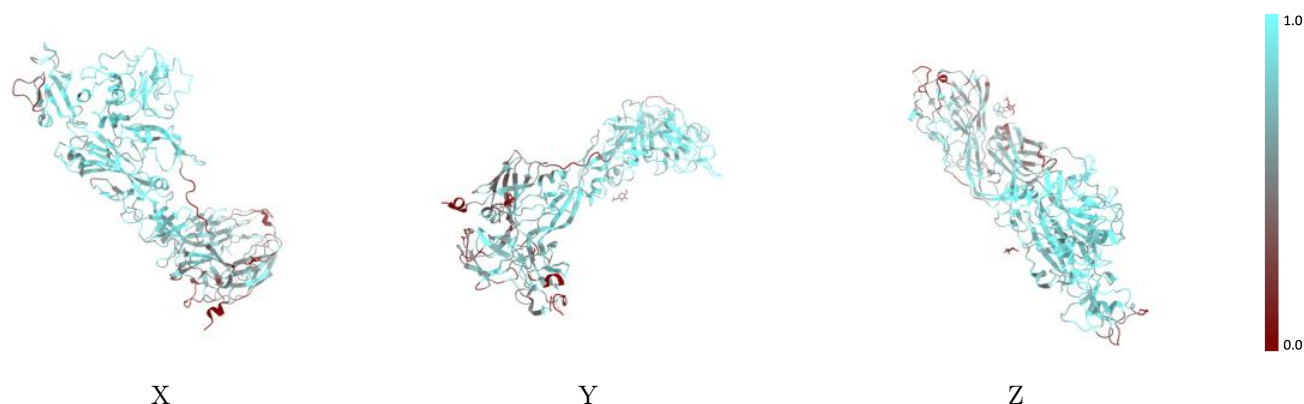
The images above show the 3D surface view of the map at the recommended contour level 0.014 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



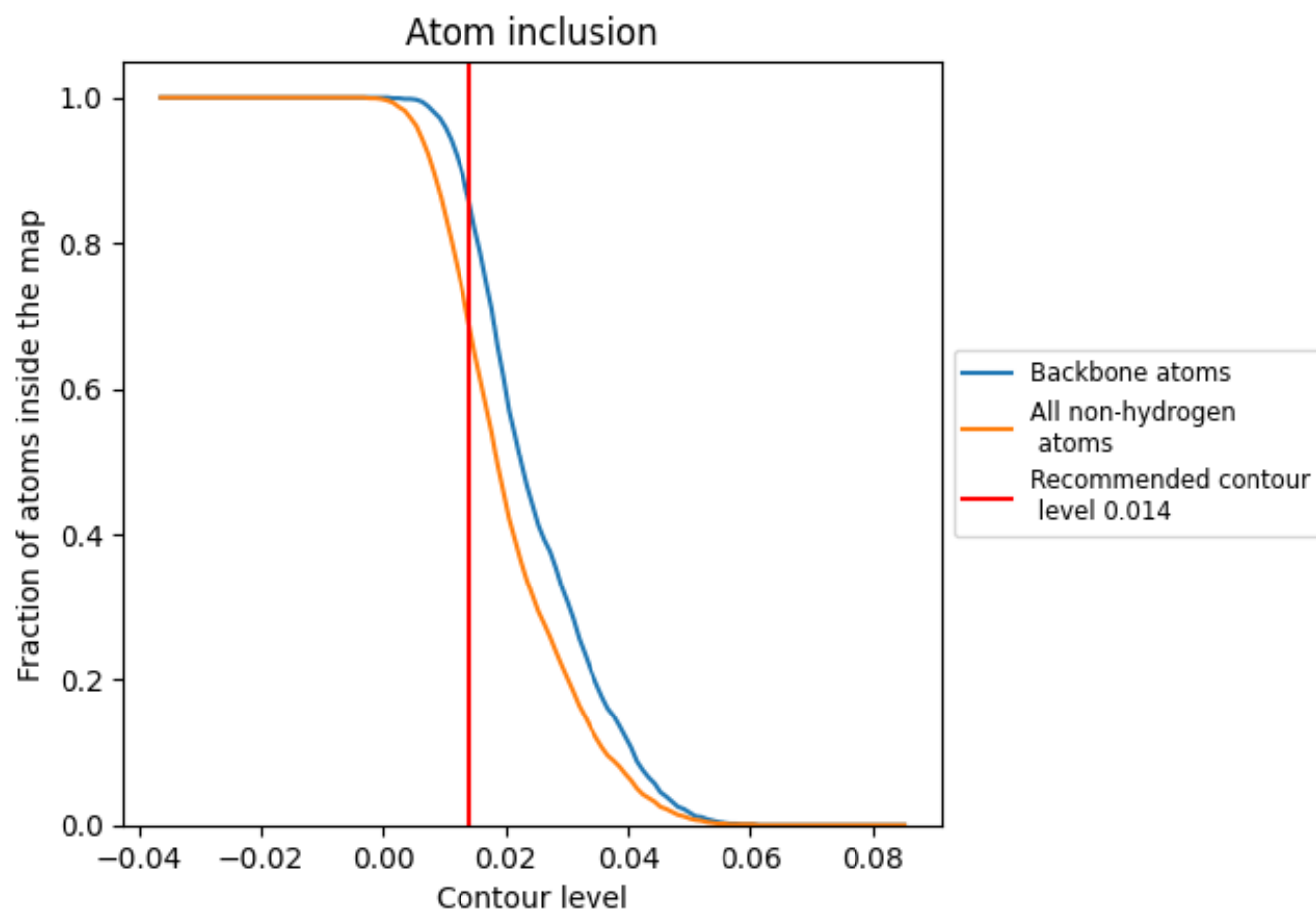
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.014).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 69% 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 (0.014) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6890	0.4290
A	0.7270	0.4590
B	0.6580	0.4030
C	0.4290	0.3370

