



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 01:40 AM UTC

PDB ID : 8E5B / pdb_00008e5b
EMDB ID : EMD-27909
Title : Human L-type voltage-gated calcium channel Cav1.3 in the presence of Amiodarone and Sofosbuvir at 3.3 Angstrom resolution
Authors : Gao, S.; Yao, X.; Yan, N.
Deposited on : 2022-08-20
Resolution : 3.30 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

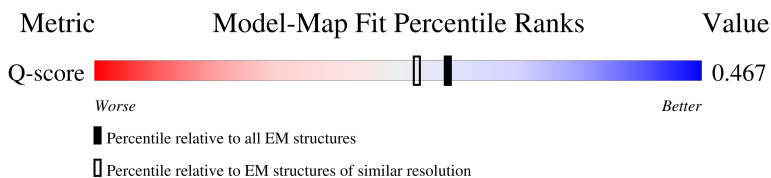
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	2161	
2	D	1103	
3	C	484	
4	B	3	

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Mol	Chain	Length	Quality of chain
5	E	2	100% 50% 50%
5	G	2	50% 100%
5	H	2	50% 100%
6	F	4	50% 25% 25% 50%

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 20310 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 Voltage-dependent L-type calcium channel subunit alpha-1D.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1230	Total	C	N	O	S	0	0
			9900	6517	1597	1715	71		

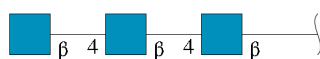
- Molecule 2 is a protein called Voltage-dependent calcium channel subunit alpha-2/delta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	948	Total	C	N	O	S	0	0
			7570	4803	1269	1467	31		

- Molecule 3 is a protein called Voltage-dependent L-type calcium channel subunit beta-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	324	Total	C	N	O	S	0	0
			2575	1619	467	479	10		

- Molecule 4 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
4	B	3	Total	C	N	O	0	0
			42	24	3	15		

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



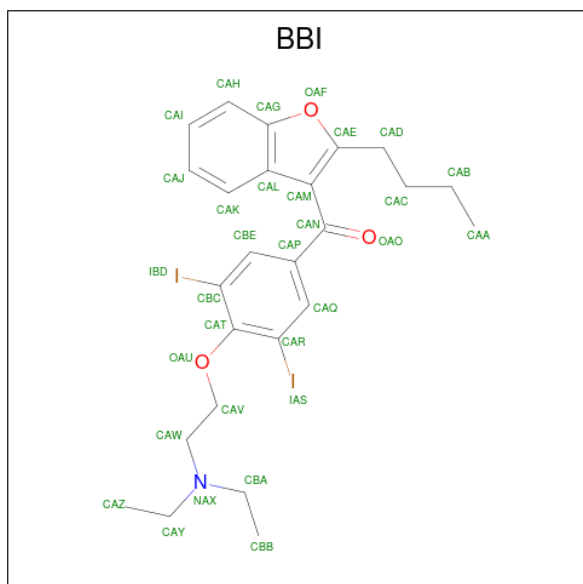
Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	2	Total	C	N	O	0	0
			28	16	2	10		
5	G	2	Total	C	N	O	0	0
			28	16	2	10		
5	H	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 6 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-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



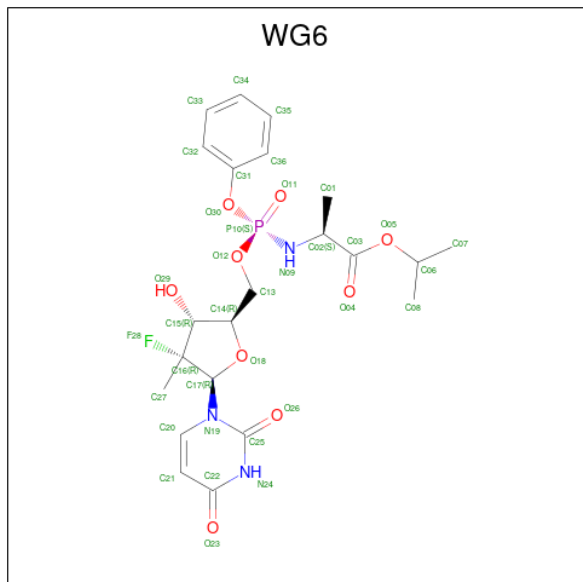
Mol	Chain	Residues	Atoms				AltConf	Trace
6	F	4	Total	C	N	O	0	0
			56	32	4	20		

- Molecule 7 is (2-butyl-1-benzofuran-3-yl){4-[2-(diethylamino)ethoxy]-3,5-diiodophenyl}methanone (CCD ID: BBI) (formula: C₂₅H₂₉I₂NO₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
7	A	1	Total	C	I	N	O	0
			31	25	2	1	3	

- Molecule 8 is Sofosbuvir (CCD ID: WG6) (formula: $C_{22}H_{29}FN_3O_9P$) (labeled as "Ligand of Interest" by depositor).

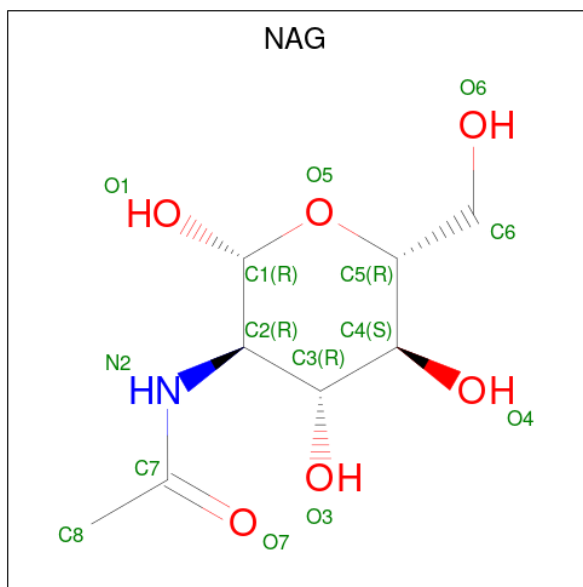


Mol	Chain	Residues	Atoms						AltConf
8	A	1	Total	C	F	N	O	P	0
			36	22	1	3	9	1	

- Molecule 9 is CALCIUM ION (CCD ID: CA) (formula: Ca).

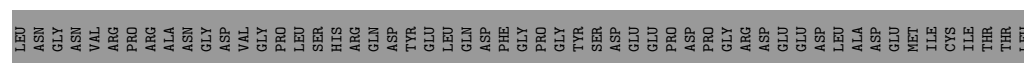
Mol	Chain	Residues	Atoms		AltConf
9	A	1	Total	Ca	0
			1	1	
9	D	1	Total	Ca	0
			1	1	

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

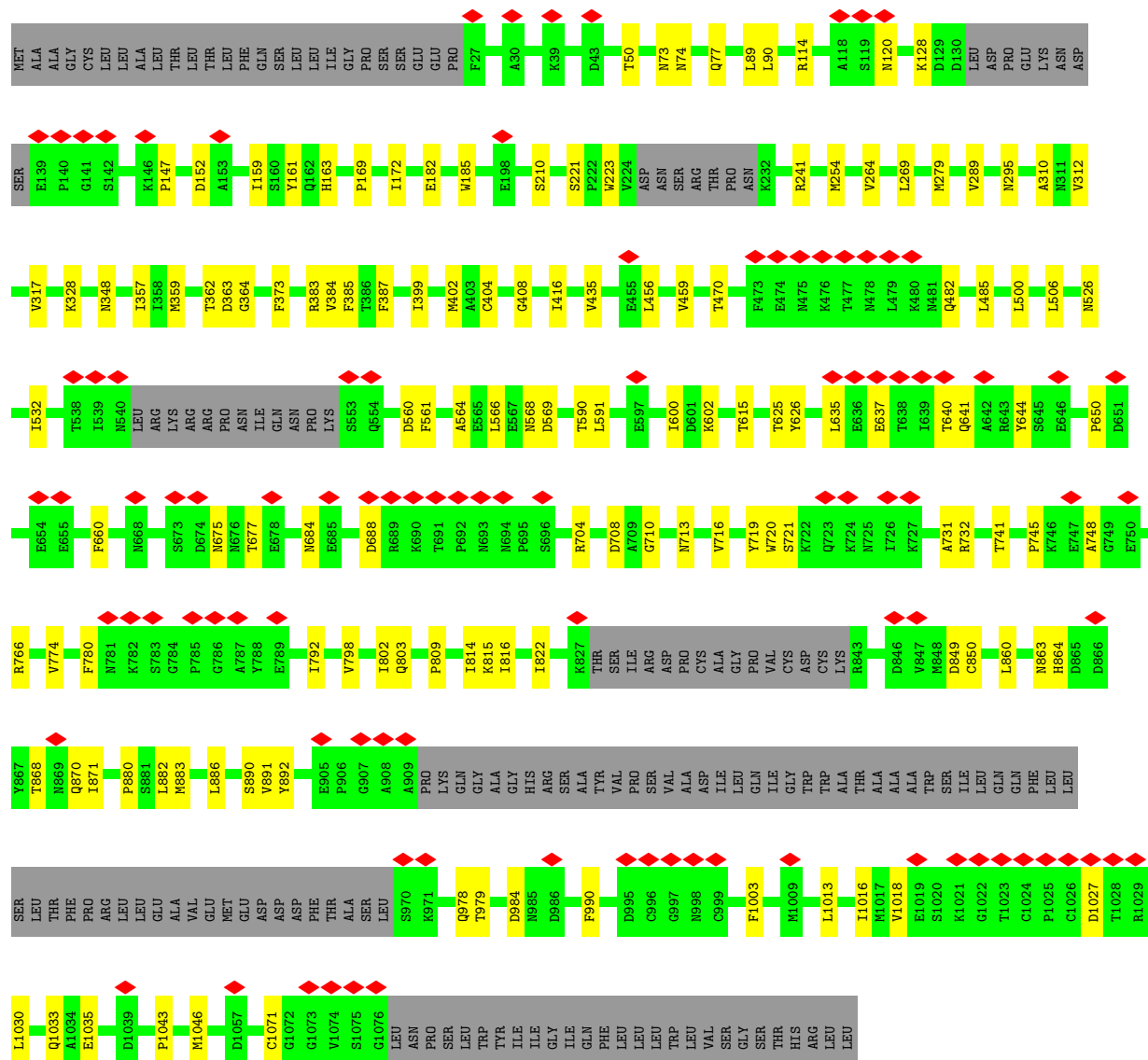
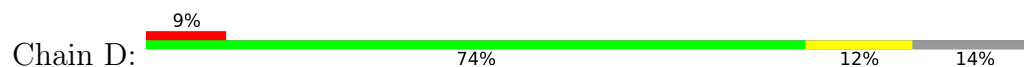


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
10	D	1	14	8	1	5	0

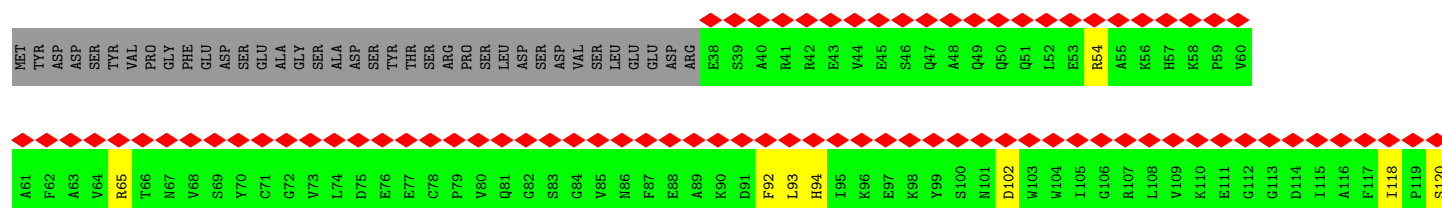
PHE	ARG	THR	CYS	TYR	TYR	GLY	GLY	LEU	E1567	T1507	L1416	ASN	M1232	G1159	P955	LYS
ASN	ARG	THR	LEU	THR	THR	GLN	ASN	VAL	Q1568	L1508	L1419	SER	D1235	E1160	S969	ILE
ASN	ARG	THR	GLN	TYR	TYR	VAL	ASN	GLY	A1569	L1509	K1419	GLU	A1236	E1161	F970	ALA
SER	SER	THR	SER	ARG	ILE	THR	VAL	ALA	N1570	R1510	D1426	SER	M1237	K1161	ILE	PRO
GLN	SER	ASP	GLN	SER	ASN	LYS	ASN	LYS	E1571	R1511	N1428	ARG	D1238	Y1162	GLY	GLU
ASN	GLN	ASP	ASN	THR	ASN	ASN	ASN	ASN	E1572	I1512	M1428	ILE	I1239	Y1163	ILE	GLY
ASN	ASN	THR	ASN	THR	THR	THR	THR	THR	L1573	Q1513	E1431	S1314	M1242	K1164	SER	SER
ASN	THR	THR	ASN	THR	THR	THR	THR	THR	R1574	P1514	L1450	I1315	M1242	C1166	ALA	PHE
ASN	THR	THR	ASN	THR	THR	THR	THR	THR	A1575	P1515	L1450	T1316	M1242	C1166	ALA	PHE
ASN	THR	THR	ASN	THR	THR	THR	THR	THR	V1576	L1516	L1450	F1317	M1252	E1167	ILE	ILE
ASN	THR	THR	ASN	THR	THR	THR	THR	THR	I1577	G1517	L1450	F1318	V1253	SER	SER	LEU
ASN	THR	THR	ASN	THR	THR	THR	THR	THR	F1518	F1518	F1453	R1319	V1256	I1169	1982	SER
ASN	THR	THR	ASN	THR	THR	THR	THR	THR	L1578	G1519	L1454	L1320	I1257	L983	1983	LYS
ASN	THR	THR	ASN	THR	THR	THR	THR	THR	K1579	K1520	V1460	F1321	I1257	R984	1984	THR
ASN	THR	THR	ASN	THR	THR	THR	THR	THR	I1580	K1520	V1460	F1322	I1257	R984	1984	ASN
ASN	THR	THR	ASN	THR	THR	THR	THR	THR	V1581	L1521	M1464	V1323	I1257	R987	1987	PRO
ASN	THR	THR	ASN	THR	THR	THR	THR	THR	K1582	C1522	D1465	M1324	A1258	K1172	1987	PRO
ASN	THR	THR	ASN	THR	THR	THR	THR	THR	K1583	P1523	N1466	R1325	F1259	Q1174	K999	G878
ASN	THR	THR	ASN	THR	THR	THR	THR	THR	T1584	H1524	F1467	L1326	K1260	Q1175	G1800	C379
ASN	THR	THR	ASN	THR	THR	THR	THR	THR	S1585	R1525	D1468	V1327	K1262	C1176	L1001	H880
ASN	THR	THR	ASN	THR	THR	THR	THR	THR	M1586	V1526	Y1469	K1328	K1263	Y1176	K1002	K981
ASN	THR	THR	ASN	THR	THR	THR	THR	THR	K1587	L1470	T1471	L1329	K1263	Y1176	H1003	L882
ASN	THR	THR	ASN	THR	THR	THR	THR	THR	L1588	L1472	R1472	L1330	F1265	A1179	I1018	L882
ASN	THR	THR	ASN	THR	THR	THR	THR	THR	L1589	D1473	W1474	S1331	S1266	L1190	I1018	I883
ASN	THR	THR	ASN	THR	THR	THR	THR	THR	ASP	K1530	H1474	R1332	D1267	K1181	T1022	H886
ASN	THR	THR	ASN	THR	THR	THR	THR	THR	GLN	R1531	S1475	R1333	F1272	A1182	T1022	H886
ASN	THR	THR	ASN	THR	THR	THR	THR	THR	VAL	V1532	I1476	E1334	D1273	P1184	V1034	H890
ASN	THR	THR	ASN	THR	THR	THR	THR	THR	VAL	A1533	L1477	G1335	D1274	P1184	V1034	H890
ASN	THR	THR	ASN	THR	THR	THR	THR	THR	PRO	M1534	G1478	E1335	S1275	L1185	K1038	V894
ASN	THR	THR	ASN	THR	THR	THR	THR	THR	PRO	M1534	G1478	E1335	L1275	L1185	K1038	V894
ASN	THR	THR	ASN	THR	THR	THR	THR	THR	ALA	M1535	H1480	F1343	I1276	R1186	D1046	M897
ASN	THR	THR	ASN	THR	THR	THR	THR	THR	GLY	M1536	H1480	F1343	I1277	R1187	E1047	M897
ASN	THR	THR	ASN	THR	THR	THR	THR	THR	ASP	M1537	D1483	L1385	I1278	Y1188	F1059	S911
ASN	THR	THR	ASN	THR	THR	THR	THR	THR	ASP	P1537	E1484	L1385	I1279	I1189	F1059	S911
ASN	THR	THR	ASN	THR	THR	THR	THR	THR	GLU	L1538	E1484	L1385	K1279	I1189	F1059	S911
ASN	THR	THR	ASN	THR	THR	THR	THR	THR	VAL	M1539	F1485	L1385	K1191	K1191	D1064	H912
ASN	THR	THR	ASN	THR	THR	THR	THR	THR	VAL	S1540	K1486	L1385	N1192	N1192	G1065	D923
ASN	THR	THR	ASN	THR	THR	THR	THR	THR	VAL	D1541	K1486	M1377	P1193	P1193	D1066	D923
ASN	THR	THR	ASN	THR	THR	THR	THR	THR	GLY	G1542	I1488	R1378	Y1194	Y1194	V1067	E933
ASN	THR	THR	ASN	THR	THR	THR	THR	THR	THR	T1543	I1488	D1379	Y1194	Y1194	D1068	E933
ASN	THR	THR	ASN	THR	THR	THR	THR	THR	ALA	V1544	W1489	Q1382	A1285	Q1195	W1103	K937
ASN	THR	THR	ASN	THR	THR	THR	THR	THR	ALA	M1545	S1490	Q1382	L1286	Q1195	W1103	K937
ASN	THR	THR	ASN	THR	THR	THR	THR	THR	THR	M1545	S1490	Q1382	L1286	Q1195	W1103	K937
ASN	THR	THR	ASN	THR	THR	THR	THR	THR	THR	F1546	E1491	R1385	S1287	K1197	P1104	H938
ASN	THR	THR	ASN	THR	THR	THR	THR	THR	THR	M1546	E1491	R1385	S1287	K1197	P1104	H938
ASN	THR	THR	ASN	THR	THR	THR	THR	THR	THR	M1547	Y1492	N1388	A1288	F1198	G942	G942
ASN	THR	THR	ASN	THR	THR	THR	THR	THR	THR	M1548	D1493	N1388	ALA	W1199	S1113	G942
ASN	THR	THR	ASN	THR	THR	THR	THR	THR	THR	A1548	P1494	N1388	ASP	W1199	S1113	G942
ASN	THR	THR	ASN	THR	THR	THR	THR	THR	THR	T1549	E1495	T1391	PRO	G1115	G1115	ALA
ASN	THR	THR	ASN	THR	THR	THR	THR	THR	THR	L1550	E1495	F1392	THR	E1116	E1116	ALA
ASN	THR	THR	ASN	THR	THR	THR	THR	THR	THR	F1551	A1496	F1392	GLU	I1121	I1121	ALA
ASN	THR	THR	ASN	THR	THR	THR	THR	THR	THR	A1552	K1497	P1393	SER	F1206	F1206	ALA
ASN	THR	THR	ASN	THR	THR	THR	THR	THR	THR	L1553	K1498	P1393	GLU	F1207	F1207	ALA
ASN	THR	THR	ASN	THR	THR	THR	THR	THR	THR	L1554	R1499	R1401	ASN	E1208	E1208	ALA
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ASN	THR	THR	ASN	THR	THR	THR	THR	THR	THR	R1555	I1500	T1404	VAL	M1210	M1210	ALA
ASN	THR	THR	ASN	THR	THR	THR	THR	THR	THR	T1556	I1501	A1407	VAL	M1211	M1211	ALA
ASN	THR	THR	ASN	THR	THR	THR	THR	THR	THR	A1557	H1502	A1407	THR	F1212	F1212	ALA
ASN	THR	THR	ASN	THR	THR	THR	THR	THR	THR	L1558	H1503	E1410	ALA	L1222	L1222	ALA
ASN	THR	THR	ASN	THR	THR	THR	THR	THR	THR	K1559	L1503	E1410	ALA	A1223	A1223	ALA
ASN	THR	THR	ASN	THR	THR	THR	THR	THR	THR	T1560	V1505	E1410	ALA	M1224	M1224	ALA
ASN	THR	THR	ASN	THR	THR	THR	THR	THR	THR	K1561	V1506	E1410	ALA	Y1227	Y1227	ALA
ASN	THR	THR	ASN	THR	THR	THR	THR	THR	THR	L1562	V1506	E1410	ALA	K1231	K1231	ALA
ASN	THR	THR	ASN	THR	THR	THR	THR	THR	THR	E1563	V1506	E1410	ALA	K1231	K1231	ALA
ASN	THR	THR	ASN	THR	THR	THR	THR	THR	THR	Q1564	V1506	E1410	ALA	K1231	K1231	ALA
ASN	THR	THR	ASN	THR	THR	THR	THR	THR	THR	N1565	V1506	E1410	ALA	K1231	K1231	ALA
ASN	THR	THR	ASN	THR	THR	THR	THR	THR	THR	L1566	V1506	E1410	ALA	K1231	K1231	ALA

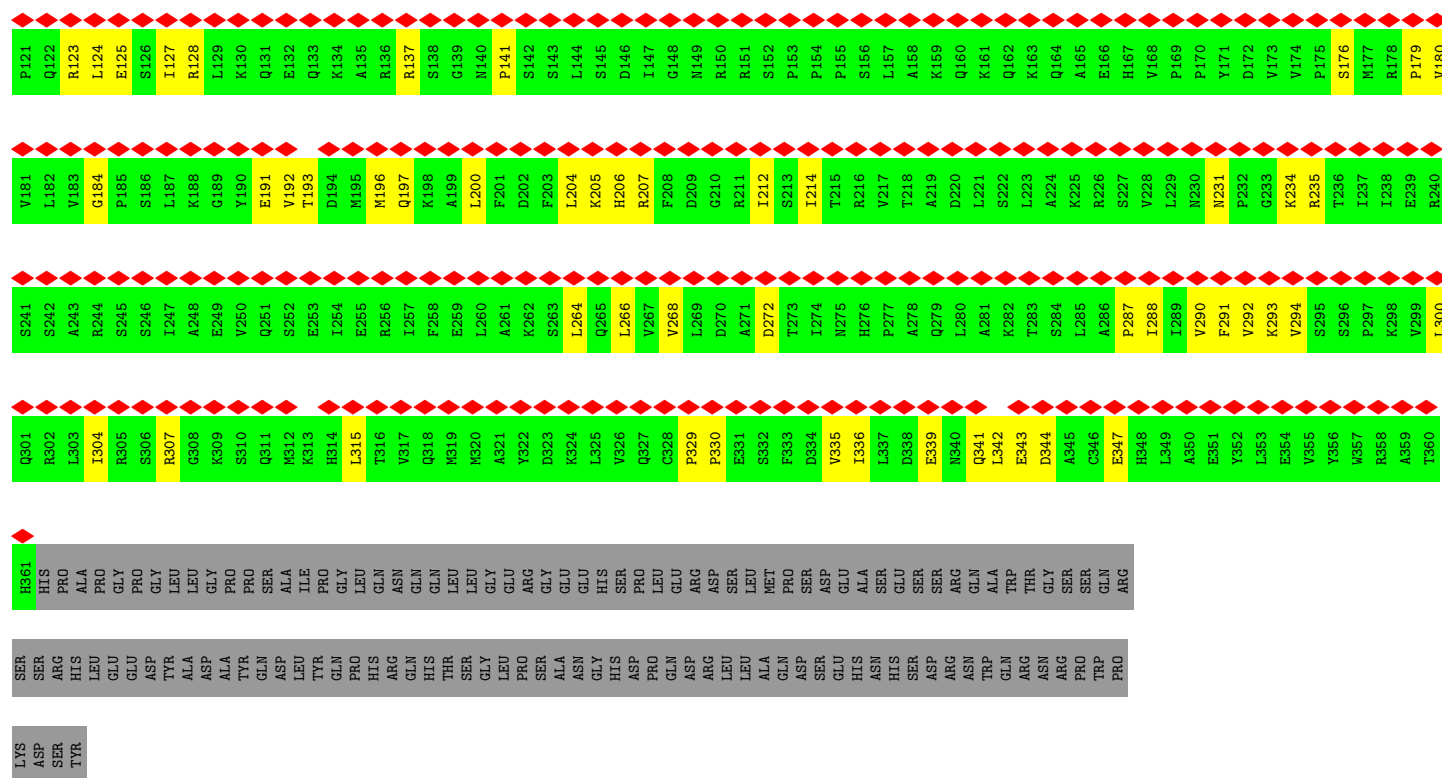


• Molecule 2: Voltage-dependent calcium channel subunit alpha-2/delta-1



• Molecule 3: Voltage-dependent L-type calcium channel subunit beta-3





- Molecule 4: 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



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



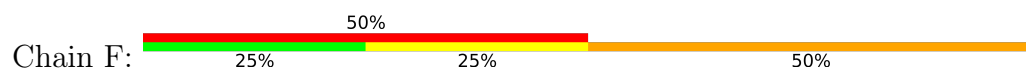
- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: 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-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	69718	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1900	Depositor
Maximum defocus (nm)	2100	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.152	Depositor
Minimum map value	-0.088	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	311.91998, 311.91998, 311.91998	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.114, 1.114, 1.114	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, NAG, WG6, BBI

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	0/10127	0.30	0/13716
2	D	0.14	0/7728	0.28	0/10477
3	C	0.10	0/2624	0.25	0/3544
All	All	0.13	0/20479	0.28	0/27737

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	9900	0	10071	139	0
2	D	7570	0	7370	88	0
3	C	2575	0	2619	41	0
4	B	42	0	37	2	0
5	E	28	0	25	1	0
5	G	28	0	25	0	0
5	H	28	0	25	1	0
6	F	56	0	49	4	0
7	A	31	0	29	10	0
8	A	36	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	A	1	0	0	0	0
9	D	1	0	0	0	0
10	D	14	0	13	0	0
All	All	20310	0	20263	277	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 7.

All (277) 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:1391:THR:HG22	1:A:1393:PRO:HD2	1.59	0.84
1:A:377:MET:HG2	1:A:378:GLY:H	1.45	0.80
2:D:822:ILE:HD11	2:D:868:THR:HG21	1.66	0.76
1:A:1187:ARG:HH21	1:A:1494:PRO:HB3	1.52	0.75
1:A:377:MET:HE1	1:A:381:LEU:HD23	1.69	0.75
3:C:231:ASN:HB3	3:C:234:LYS:HE2	1.72	0.72
1:A:294:ILE:HG13	1:A:348:ASP:HA	1.70	0.71
7:A:2201:BBI:IAS	7:A:2201:BBI:CAV	3.09	0.71
1:A:1193:PRO:HA	1:A:1196:TYR:HB3	1.74	0.69
1:A:1509:LEU:HD13	1:A:1512:ILE:HD12	1.74	0.68
1:A:1534:MET:SD	1:A:1556:THR:OG1	2.51	0.68
3:C:179:PRO:HG2	3:C:287:PRO:HB3	1.76	0.68
3:C:339:GLU:HG3	3:C:341:GLN:H	1.59	0.67
2:D:404:CYS:HB3	2:D:1071:CYS:HA	1.77	0.67
1:A:348:ASP:HB2	1:A:1227:TYR:HB2	1.77	0.66
1:A:367:THR:HG21	1:A:1401:ARG:HG3	1.77	0.66
2:D:704:ARG:NH1	2:D:708:ASP:OD2	2.28	0.65
3:C:94:HIS:NE2	3:C:176:SER:O	2.30	0.64
1:A:1382:GLN:HG3	1:A:1410:GLU:HB3	1.79	0.63
1:A:1360:LEU:HD22	1:A:1454:LEU:HD12	1.81	0.62
1:A:1222:LEU:HD21	1:A:1322:ARG:HD2	1.80	0.62
2:D:435:VAL:HG21	2:D:482:GLN:HA	1.80	0.62
2:D:716:VAL:HA	2:D:720:TRP:HB2	1.82	0.62
1:A:740:ASN:OD1	8:A:2202:WG6:C27	2.48	0.62
2:D:802:ILE:HG22	2:D:803:GLN:HG2	1.80	0.62
1:A:587:PHE:O	1:A:631:ARG:NH2	2.32	0.62
2:D:359:MET:HG2	2:D:385:PHE:HB2	1.82	0.62
1:A:1534:MET:HE1	1:A:1552:ALA:HB1	1.83	0.61
1:A:1162:GLU:OE1	1:A:1164:LYS:NZ	2.31	0.61
1:A:126:LYS:HG3	1:A:127:PRO:HD3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:542:SER:OG	1:A:555:GLN:NE2	2.33	0.60
1:A:165:GLU:OE2	1:A:246:ARG:NH1	2.28	0.60
7:A:2201:BBI:H21	7:A:2201:BBI:OAU	2.01	0.60
3:C:207:ARG:NH2	3:C:347:GLU:OE1	2.35	0.59
2:D:416:ILE:HD12	2:D:416:ILE:H	1.68	0.59
2:D:182:GLU:OE2	2:D:210:SER:OG	2.18	0.58
3:C:294:VAL:HG21	3:C:300:LEU:HD13	1.85	0.58
2:D:357:ILE:HD12	2:D:359:MET:HE3	1.84	0.58
1:A:199:LEU:HA	1:A:202:PHE:CE1	2.38	0.58
3:C:205:LYS:NZ	3:C:206:HIS:CE1	2.71	0.58
1:A:563:LEU:HD21	1:A:599:ILE:HA	1.86	0.58
2:D:90:LEU:HD12	2:D:615:THR:HG21	1.86	0.58
1:A:166:TYR:O	1:A:170:ILE:HD12	2.04	0.58
3:C:192:VAL:HG13	3:C:193:THR:HG23	1.85	0.58
2:D:732:ARG:HG2	2:D:814:ILE:HG22	1.86	0.57
2:D:295:ASN:ND2	2:D:328:LYS:O	2.32	0.57
2:D:289:VAL:HG12	2:D:310:ALA:HB2	1.86	0.57
1:A:536:ASN:HB2	1:A:562:LEU:HD21	1.87	0.57
2:D:185:TRP:HA	4:B:1:NAG:H82	1.86	0.57
1:A:911:SER:OG	1:A:1426:ASP:OD2	2.23	0.56
2:D:357:ILE:HG22	2:D:383:ARG:HB2	1.86	0.56
6:F:3:NAG:H83	6:F:3:NAG:H3	1.86	0.56
1:A:1169:ASP:OD1	1:A:1172:GLN:NE2	2.39	0.56
6:F:4:NAG:H3	6:F:4:NAG:H83	1.87	0.56
7:A:2201:BBI:H24	7:A:2201:BBI:H30	1.87	0.56
2:D:675:ASN:ND2	2:D:677:THR:OG1	2.39	0.56
1:A:370:LEU:HD12	1:A:386:PHE:HB2	1.86	0.55
4:B:2:NAG:H83	4:B:2:NAG:H3	1.86	0.55
1:A:1198:PHE:HB3	1:A:1258:ALA:HB2	1.89	0.55
1:A:1570:ASN:HB3	1:A:1574:ARG:HH21	1.72	0.55
3:C:212:ILE:HG22	3:C:266:LEU:HB2	1.87	0.55
1:A:1489:TRP:HA	1:A:1508:LEU:HD11	1.88	0.55
1:A:1155:PHE:HB3	1:A:1464:MET:HG3	1.88	0.55
2:D:254:MET:HE3	2:D:359:MET:SD	2.47	0.55
3:C:304:ILE:HG21	3:C:315:LEU:HB2	1.89	0.55
1:A:143:LEU:HD11	1:A:243:ARG:HG2	1.89	0.55
1:A:274:ILE:HD11	1:A:404:VAL:HG21	1.89	0.54
1:A:1499:ARG:HB3	1:A:1543:THR:HA	1.90	0.54
2:D:169:PRO:HG2	2:D:172:ILE:HD12	1.89	0.54
2:D:254:MET:HE1	2:D:279:MET:HG2	1.89	0.54
1:A:1187:ARG:HB2	1:A:1189:ILE:HG12	1.88	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:214:ILE:HA	3:C:268:VAL:HB	1.90	0.53
1:A:1103:TRP:CD1	1:A:1104:PRO:HD3	2.44	0.53
1:A:1314:SER:OG	1:A:1315:ILE:N	2.38	0.53
2:D:880:PRO:HB3	2:D:1030:LEU:HA	1.90	0.53
1:A:1450:LEU:HD23	7:A:2201:BBI:H3	1.91	0.53
1:A:285:TYR:O	1:A:385:TYR:OH	2.25	0.53
1:A:1343:PHE:HD1	1:A:1466:ASN:HD21	1.56	0.53
2:D:568:ASN:OD1	2:D:569:ASP:N	2.42	0.53
2:D:716:VAL:O	2:D:721:SER:N	2.41	0.53
1:A:519:ALA:O	1:A:522:SER:OG	2.22	0.52
1:A:1379:ASP:OD2	1:A:1385:ARG:NH1	2.42	0.52
1:A:1450:LEU:HD23	7:A:2201:BBI:CAA	2.40	0.52
2:D:348:ASN:OD1	5:E:1:NAG:N2	2.43	0.52
3:C:234:LYS:HG3	3:C:235:ARG:HG2	1.90	0.52
1:A:1501:LYS:HG3	1:A:1503:LEU:H	1.75	0.51
1:A:1272:PHE:HZ	1:A:1324:MET:HB3	1.75	0.51
2:D:849:ASP:OD1	2:D:864:HIS:NE2	2.43	0.51
2:D:147:PRO:HB3	2:D:163:HIS:CE1	2.46	0.51
3:C:291:PHE:HB3	3:C:336:ILE:HD12	1.93	0.51
1:A:143:LEU:HD21	1:A:243:ARG:HD2	1.93	0.51
1:A:1235:ASP:O	1:A:1239:ILE:HG12	2.11	0.51
2:D:363:ASP:OD1	2:D:364:GLY:N	2.44	0.51
3:C:205:LYS:HZ1	3:C:206:HIS:CE1	2.29	0.51
7:A:2201:BBI:IAS	7:A:2201:BBI:H17	2.81	0.50
1:A:543:GLU:HG2	1:A:555:GLN:HE22	1.76	0.50
2:D:128:LYS:HB3	2:D:223:TRP:HB3	1.93	0.50
2:D:883:MET:HE1	2:D:892:TYR:HD2	1.76	0.50
1:A:276:LEU:HG	1:A:280:PHE:HE2	1.77	0.50
1:A:1001:LEU:HD13	1:A:1355:LEU:HD23	1.94	0.50
1:A:577:LEU:HD23	1:A:582:TYR:HE1	1.77	0.50
1:A:244:VAL:O	1:A:247:PRO:HD2	2.13	0.49
1:A:366:TRP:HE1	1:A:1404:THR:HG21	1.77	0.49
2:D:849:ASP:HA	2:D:864:HIS:CE1	2.47	0.49
3:C:339:GLU:HG2	3:C:344:ASP:HB2	1.93	0.49
2:D:591:LEU:HA	2:D:602:LYS:HA	1.94	0.49
2:D:860:LEU:HD12	2:D:1013:LEU:HD21	1.93	0.49
1:A:1224:MET:HE3	1:A:1237:MET:HE1	1.95	0.49
1:A:441:TRP:CD1	3:C:342:LEU:HD13	2.48	0.49
1:A:1187:ARG:HD3	1:A:1491:GLU:HA	1.95	0.49
1:A:1211:MET:HA	1:A:1211:MET:HE2	1.94	0.49
2:D:373:PHE:CE2	2:D:402:MET:HG2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:373:PHE:HE2	2:D:402:MET:HG2	1.77	0.49
1:A:1495:GLU:HG2	1:A:1497:LYS:HD3	1.94	0.48
2:D:660:PHE:HB2	2:D:741:THR:HG22	1.94	0.48
7:A:2201:BBI:IAS	7:A:2201:BBI:H16	2.82	0.48
1:A:377:MET:HG2	1:A:378:GLY:N	2.21	0.48
2:D:637:GLU:HB3	2:D:640:THR:HG22	1.95	0.48
1:A:999:LYS:HE3	1:A:1003:HIS:HB2	1.96	0.48
5:H:1:NAG:H61	5:H:2:NAG:HN2	1.77	0.48
1:A:1377:MET:SD	1:A:1388:ASN:ND2	2.86	0.48
2:D:456:LEU:HD23	2:D:459:VAL:HG11	1.96	0.48
3:C:205:LYS:NZ	3:C:206:HIS:HE1	2.11	0.48
2:D:1043:PRO:HA	2:D:1046:MET:HG3	1.95	0.48
1:A:131:PHE:HZ	1:A:171:ILE:HD11	1.78	0.47
2:D:74:ASN:HD22	2:D:77:GLN:HG2	1.79	0.47
2:D:745:PRO:HG2	2:D:748:ALA:HB3	1.94	0.47
1:A:620:CYS:O	1:A:624:LEU:HG	2.14	0.47
1:A:744:LEU:HD13	8:A:2202:WG6:O26	2.14	0.47
1:A:1510:ARG:NH1	1:A:1519:GLY:O	2.45	0.47
2:D:860:LEU:O	2:D:871:ILE:HD11	2.13	0.47
1:A:1401:ARG:HH12	1:A:1407:ALA:HB3	1.79	0.47
2:D:591:LEU:HD13	2:D:600:ILE:HG21	1.97	0.47
3:C:205:LYS:HZ1	3:C:206:HIS:HE1	1.61	0.47
1:A:1573:LEU:HD23	1:A:1584:THR:HG21	1.96	0.47
1:A:1335:GLY:HA2	1:A:1338:THR:HG22	1.96	0.47
2:D:566:LEU:HD13	2:D:591:LEU:HD12	1.96	0.47
3:C:125:GLU:HA	3:C:128:ARG:HG2	1.96	0.47
1:A:149:PHE:HB3	1:A:153:ASP:HB3	1.95	0.47
2:D:485:LEU:HD22	6:F:1:NAG:H82	1.96	0.47
1:A:442:ILE:HG13	3:C:196:MET:HB2	1.95	0.47
1:A:1114:ASN:ND2	1:A:1121:ILE:HD11	2.30	0.47
7:A:2201:BBI:H29	8:A:2202:WG6:C13	2.44	0.47
8:A:2202:WG6:C07	8:A:2202:WG6:C01	2.92	0.47
1:A:1508:LEU:O	1:A:1512:ILE:HG13	2.15	0.47
1:A:139:ASN:ND2	1:A:246:ARG:HD3	2.30	0.46
2:D:73:ASN:HD21	2:D:506:LEU:HD23	1.80	0.46
2:D:1003:PHE:HB3	2:D:1018:VAL:HG23	1.97	0.46
3:C:196:MET:HE1	3:C:292:VAL:HG21	1.97	0.46
1:A:638:ASN:HD21	1:A:761:LEU:HD22	1.80	0.46
1:A:363:MET:HE3	1:A:394:SER:OG	2.15	0.46
1:A:1034:VAL:O	1:A:1038:LYS:HB2	2.16	0.46
1:A:1499:ARG:HA	1:A:1544:VAL:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1113:SER:OG	1:A:1125:ARG:NH2	2.40	0.46
1:A:1177:GLU:O	1:A:1181:LYS:HG2	2.16	0.46
2:D:1027:ASP:OD1	2:D:1027:ASP:N	2.47	0.46
1:A:153:ASP:OD1	1:A:154:SER:N	2.47	0.46
2:D:114:ARG:CZ	2:D:120:ASN:HD21	2.29	0.46
1:A:542:SER:HG	1:A:555:GLN:HE21	1.62	0.45
1:A:1151:VAL:HG12	1:A:1460:VAL:HG11	1.99	0.45
1:A:955:PHE:HE2	1:A:1002:LYS:HE3	1.81	0.45
2:D:891:VAL:HG23	2:D:990:PHE:HE1	1.80	0.45
1:A:287:ILE:HG12	1:A:1223:ALA:HB2	1.98	0.45
1:A:725:GLY:O	1:A:728:VAL:HG12	2.16	0.45
2:D:780:PHE:CE1	2:D:870:GLN:HA	2.51	0.45
3:C:124:LEU:HA	3:C:127:ILE:HG22	1.96	0.45
2:D:399:ILE:HA	2:D:402:MET:HE3	1.99	0.45
1:A:240:ARG:HD3	1:A:243:ARG:HH12	1.81	0.45
1:A:257:LEU:HD21	1:A:656:LEU:HD13	1.98	0.45
2:D:568:ASN:HD22	2:D:590:THR:HG22	1.81	0.45
2:D:362:THR:HG21	2:D:399:ILE:HD12	1.99	0.45
1:A:349:ASN:OD1	1:A:350:PHE:N	2.50	0.45
1:A:1512:ILE:HB	1:A:1517:GLY:HA3	1.99	0.45
2:D:254:MET:HE1	2:D:279:MET:CG	2.46	0.45
2:D:731:ALA:HB3	2:D:815:LYS:HG3	1.98	0.45
1:A:132:ILE:O	1:A:136:ILE:HG12	2.17	0.45
2:D:635:LEU:HD13	2:D:641:GLN:HB2	1.97	0.44
1:A:894:VAL:HA	1:A:897:MET:HG2	1.99	0.44
1:A:1477:LEU:HG	1:A:1478:GLY:H	1.82	0.44
1:A:1453:PHE:HB2	7:A:2201:BBi:OAO	2.18	0.44
1:A:1547:ASN:HA	1:A:1550:LEU:HG	1.98	0.44
2:D:312:VAL:HG21	2:D:532:ILE:HD11	1.99	0.44
2:D:625:THR:HG22	2:D:626:TYR:N	2.32	0.44
3:C:290:VAL:HA	3:C:335:VAL:HB	1.99	0.44
2:D:470:THR:HG21	6:F:1:NAG:H5	1.99	0.44
1:A:154:SER:OG	1:A:155:ASN:N	2.51	0.44
1:A:687:THR:OG1	1:A:689:ASP:OD1	2.26	0.44
1:A:1555:ARG:HD2	1:A:1555:ARG:HA	1.74	0.44
1:A:344:ILE:HG12	1:A:721:PRO:HG3	1.98	0.44
2:D:279:MET:HE1	2:D:387:PHE:CZ	2.52	0.44
2:D:883:MET:HE1	2:D:892:TYR:CD2	2.51	0.44
3:C:137:ARG:HD2	3:C:141:PRO:HG2	1.99	0.44
3:C:180:VAL:HG12	3:C:288:ILE:HB	2.00	0.44
1:A:335:SER:OG	1:A:336:GLY:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1392:PHE:HB3	1:A:1393:PRO:HD3	2.00	0.44
1:A:1222:LEU:HD11	1:A:1322:ARG:HG3	1.99	0.43
1:A:1510:ARG:NH2	1:A:1520:LYS:HD3	2.33	0.43
2:D:886:LEU:HD22	2:D:891:VAL:HG11	2.00	0.43
1:A:168:PHE:HA	1:A:171:ILE:HG22	1.99	0.43
1:A:1256:VAL:O	1:A:1261:PRO:HD3	2.17	0.43
2:D:979:THR:HG23	2:D:1033:GLN:HG2	2.01	0.43
1:A:577:LEU:HD23	1:A:582:TYR:CE1	2.53	0.43
2:D:317:VAL:HG21	2:D:1043:PRO:HG2	2.00	0.43
2:D:780:PHE:HE1	2:D:870:GLN:HA	1.83	0.43
2:D:560:ASP:OD1	2:D:561:PHE:N	2.52	0.43
1:A:1319:ARG:O	1:A:1322:ARG:HG2	2.19	0.43
1:A:1242:MET:HG2	1:A:1284:VAL:HG23	1.99	0.43
1:A:1252:MET:HE1	1:A:1277:VAL:HB	2.00	0.43
3:C:264:LEU:HD23	3:C:264:LEU:O	2.19	0.43
1:A:1472:ARG:HG2	1:A:1474:TRP:CZ3	2.54	0.43
2:D:384:VAL:O	2:D:408:GLY:HA3	2.19	0.43
2:D:644:TYR:CE1	2:D:710:GLY:HA3	2.54	0.43
2:D:159:ILE:HG22	2:D:221:SER:HB2	2.00	0.43
2:D:849:ASP:HA	2:D:864:HIS:HE1	1.83	0.42
1:A:1197:LYS:O	1:A:1201:VAL:HG23	2.19	0.42
2:D:766:ARG:HH21	2:D:774:VAL:HG13	1.84	0.42
2:D:625:THR:HG22	2:D:626:TYR:H	1.83	0.42
3:C:120:SER:O	3:C:124:LEU:N	2.34	0.42
3:C:205:LYS:HZ2	3:C:206:HIS:CE1	2.36	0.42
1:A:426:ARG:HA	1:A:426:ARG:HD2	1.79	0.42
2:D:526:ASN:ND2	2:D:564:ALA:O	2.45	0.42
3:C:200:LEU:O	3:C:204:LEU:HG	2.19	0.42
1:A:626:ILE:O	1:A:629:VAL:HG22	2.20	0.42
2:D:650:PRO:HD3	2:D:684:ASN:HD21	1.84	0.42
3:C:54:ARG:HE	3:C:54:ARG:HB2	1.61	0.42
3:C:65:ARG:HD3	3:C:92:PHE:CZ	2.55	0.42
1:A:171:ILE:O	1:A:175:GLU:HG2	2.19	0.42
1:A:425:LEU:HD12	1:A:645:ASN:OD1	2.20	0.42
1:A:984:ARG:NE	1:A:987:ARG:HH12	2.18	0.42
1:A:1550:LEU:HD12	1:A:1551:PHE:N	2.34	0.42
1:A:203:VAL:HA	1:A:206:ILE:HG12	2.02	0.42
1:A:1252:MET:SD	1:A:1274:SER:HA	2.60	0.42
1:A:1450:LEU:CD2	7:A:2201:BB1:H1	2.49	0.42
3:C:93:LEU:HG	3:C:118:ILE:HG12	2.01	0.42
1:A:381:LEU:N	1:A:382:PRO:HD2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1276:ILE:HD13	1:A:1321:PHE:HD1	1.85	0.42
1:A:206:ILE:HG13	1:A:207:VAL:N	2.34	0.41
2:D:688:ASP:OD1	2:D:688:ASP:N	2.50	0.41
2:D:798:VAL:HG23	2:D:809:PRO:HD2	2.02	0.41
2:D:89:LEU:HD22	2:D:500:LEU:HD11	2.02	0.41
3:C:184:GLY:O	3:C:197:GLN:NE2	2.51	0.41
1:A:301:CYS:HA	1:A:333:CYS:HB3	2.01	0.41
1:A:1046:ASP:HB3	1:A:1059:PHE:CE2	2.54	0.41
2:D:850:CYS:HB2	2:D:863:ASN:ND2	2.35	0.41
1:A:540:ILE:HG21	1:A:623:LEU:HD13	2.02	0.41
1:A:301:CYS:HB3	1:A:333:CYS:HB3	2.02	0.41
1:A:358:PHE:O	1:A:361:ILE:HG22	2.20	0.41
2:D:359:MET:HA	2:D:385:PHE:O	2.21	0.41
3:C:102:ASP:HB3	3:C:123:ARG:HD3	2.02	0.41
3:C:343:GLU:O	3:C:347:GLU:HG2	2.21	0.41
2:D:890:SER:OG	2:D:984:ASP:OD1	2.36	0.41
1:A:204:ILE:HG21	1:A:246:ARG:HG3	2.03	0.41
1:A:235:ASP:N	1:A:235:ASP:OD1	2.53	0.41
1:A:1416:LEU:O	1:A:1419:LYS:HG2	2.20	0.41
1:A:1489:TRP:HH2	1:A:1546:PHE:HB2	1.84	0.41
3:C:179:PRO:O	3:C:288:ILE:N	2.53	0.41
3:C:291:PHE:CE2	3:C:293:LYS:HB3	2.55	0.41
1:A:1343:PHE:CZ	1:A:1470:LEU:HD11	2.56	0.41
2:D:241:ARG:HA	2:D:241:ARG:HD2	1.89	0.41
2:D:264:VAL:O	2:D:269:LEU:HB2	2.20	0.41
2:D:792:ILE:O	2:D:816:ILE:N	2.49	0.41
3:C:272:ASP:OD1	3:C:272:ASP:N	2.43	0.41
1:A:169:LEU:O	1:A:173:THR:HG23	2.22	0.40
1:A:1187:ARG:NH1	1:A:1491:GLU:O	2.54	0.40
2:D:50:THR:O	2:D:719:TYR:OH	2.27	0.40
2:D:152:ASP:OD2	2:D:161:TYR:OH	2.36	0.40
2:D:978:GLN:NE2	2:D:1035:GLU:OE2	2.53	0.40
3:C:336:ILE:HD12	3:C:336:ILE:HA	1.91	0.40
1:A:292:LEU:HD23	1:A:292:LEU:HA	1.94	0.40
1:A:1468:ASP:N	1:A:1468:ASP:OD1	2.54	0.40
2:D:713:ASN:C	2:D:713:ASN:HD22	2.29	0.40
3:C:191:GLU:HG3	3:C:307:ARG:NH1	2.36	0.40
3:C:329:PRO:HA	3:C:330:PRO:HD3	1.99	0.40
1:A:162:GLU:HG3	1:A:163:LYS:N	2.37	0.40
1:A:1018:ILE:O	1:A:1022:THR:HG22	2.22	0.40
1:A:1253:VAL:HA	1:A:1256:VAL:HG12	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:882:LEU:HD21	2:D:1016:ILE:HD12	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1214/2161 (56%)	1154 (95%)	60 (5%)	0	100	100
2	D	936/1103 (85%)	891 (95%)	45 (5%)	0	100	100
3	C	322/484 (66%)	312 (97%)	10 (3%)	0	100	100
All	All	2472/3748 (66%)	2357 (95%)	115 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1086/1902 (57%)	1086 (100%)	0	100	100
2	D	837/971 (86%)	837 (100%)	0	100	100
3	C	287/426 (67%)	287 (100%)	0	100	100
All	All	2210/3299 (67%)	2210 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	341	ASN
1	A	536	ASN
1	A	555	GLN
1	A	638	ASN
1	A	884	ASN
1	A	1086	ASN
1	A	1171	ASN
1	A	1381	ASN
2	D	472	GLN
2	D	824	ASN
3	C	149	ASN
3	C	206	HIS
3	C	275	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](#)

13 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	$\# Z > 2$
4	NAG	B	1	4,2	14,14,15	0.47	0	17,19,21	0.51	0
4	NAG	B	2	4	14,14,15	0.44	0	17,19,21	1.32	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	B	3	4	14,14,15	0.35	0	17,19,21	0.45	0
5	NAG	E	1	5,2	14,14,15	0.47	0	17,19,21	0.51	0
5	NAG	E	2	5	14,14,15	0.50	0	17,19,21	0.80	0
6	NAG	F	1	6,2	14,14,15	0.31	0	17,19,21	0.53	0
6	NAG	F	2	6	14,14,15	0.18	0	17,19,21	0.46	0
6	NAG	F	3	6	14,14,15	1.01	1 (7%)	17,19,21	1.73	3 (17%)
6	NAG	F	4	6	14,14,15	0.51	0	17,19,21	1.35	2 (11%)
5	NAG	G	1	5,2	14,14,15	0.26	0	17,19,21	0.42	0
5	NAG	G	2	5	14,14,15	0.25	0	17,19,21	0.52	0
5	NAG	H	1	5,2	14,14,15	0.55	0	17,19,21	0.41	0
5	NAG	H	2	5	14,14,15	0.23	0	17,19,21	0.42	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	1	4,2	-	0/6/23/26	0/1/1/1
4	NAG	B	2	4	-	5/6/23/26	0/1/1/1
4	NAG	B	3	4	-	4/6/23/26	0/1/1/1
5	NAG	E	1	5,2	-	4/6/23/26	0/1/1/1
5	NAG	E	2	5	-	4/6/23/26	0/1/1/1
6	NAG	F	1	6,2	-	2/6/23/26	0/1/1/1
6	NAG	F	2	6	-	0/6/23/26	0/1/1/1
6	NAG	F	3	6	-	4/6/23/26	0/1/1/1
6	NAG	F	4	6	-	5/6/23/26	0/1/1/1
5	NAG	G	1	5,2	-	2/6/23/26	0/1/1/1
5	NAG	G	2	5	-	2/6/23/26	0/1/1/1
5	NAG	H	1	5,2	-	2/6/23/26	0/1/1/1
5	NAG	H	2	5	-	4/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	3	NAG	O5-C1	3.19	1.49	1.43

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	3	NAG	C1-O5-C5	4.64	118.40	112.19
6	F	3	NAG	C2-N2-C7	4.58	129.04	122.90
6	F	4	NAG	C2-N2-C7	4.58	129.04	122.90
4	B	2	NAG	C2-N2-C7	4.54	128.99	122.90
6	F	4	NAG	C1-C2-N2	2.22	113.93	110.43
6	F	3	NAG	C1-C2-N2	2.09	113.73	110.43
4	B	2	NAG	C1-C2-N2	2.09	113.73	110.43

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	G	1	NAG	O5-C5-C6-O6
4	B	3	NAG	C4-C5-C6-O6
5	E	2	NAG	C4-C5-C6-O6
5	G	2	NAG	O5-C5-C6-O6
5	G	1	NAG	C4-C5-C6-O6
5	E	1	NAG	O5-C5-C6-O6
6	F	1	NAG	O5-C5-C6-O6
4	B	2	NAG	C8-C7-N2-C2
4	B	2	NAG	O7-C7-N2-C2
4	B	3	NAG	C8-C7-N2-C2
4	B	3	NAG	O7-C7-N2-C2
5	H	1	NAG	C8-C7-N2-C2
5	H	1	NAG	O7-C7-N2-C2
5	H	2	NAG	C8-C7-N2-C2
5	H	2	NAG	O7-C7-N2-C2
6	F	3	NAG	C8-C7-N2-C2
6	F	3	NAG	O7-C7-N2-C2
6	F	4	NAG	C8-C7-N2-C2
6	F	4	NAG	O7-C7-N2-C2
5	E	2	NAG	O5-C5-C6-O6
4	B	3	NAG	O5-C5-C6-O6
5	H	2	NAG	O5-C5-C6-O6
5	G	2	NAG	C4-C5-C6-O6
5	E	1	NAG	C4-C5-C6-O6
6	F	4	NAG	O5-C5-C6-O6
6	F	1	NAG	C4-C5-C6-O6
5	E	2	NAG	C1-C2-N2-C7
5	H	2	NAG	C4-C5-C6-O6
5	E	1	NAG	C3-C2-N2-C7
4	B	2	NAG	C4-C5-C6-O6
4	B	2	NAG	C1-C2-N2-C7

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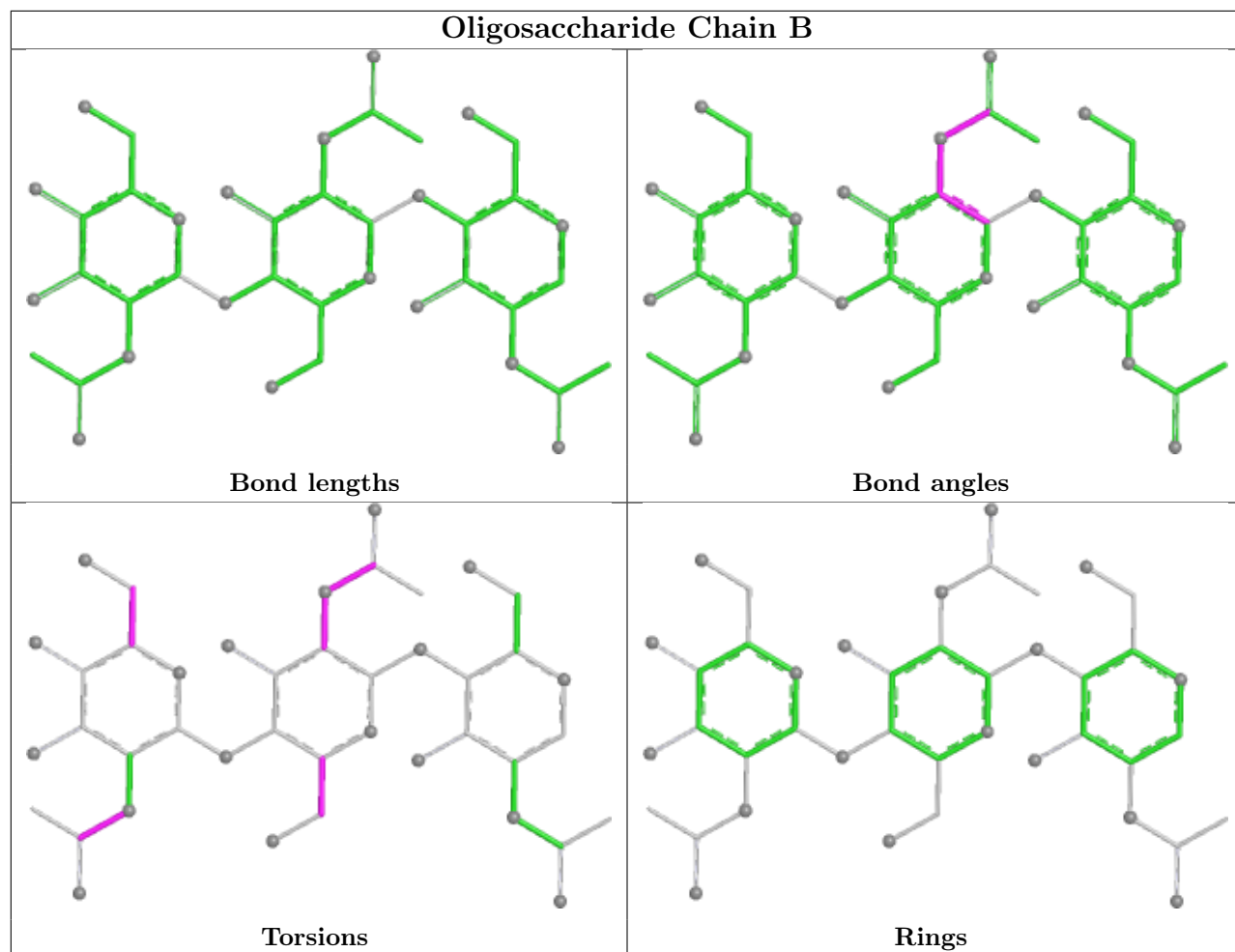
Mol	Chain	Res	Type	Atoms
5	E	1	NAG	C1-C2-N2-C7
6	F	3	NAG	C1-C2-N2-C7
6	F	4	NAG	C1-C2-N2-C7
4	B	2	NAG	C3-C2-N2-C7
5	E	2	NAG	C3-C2-N2-C7
6	F	3	NAG	C3-C2-N2-C7
6	F	4	NAG	C3-C2-N2-C7

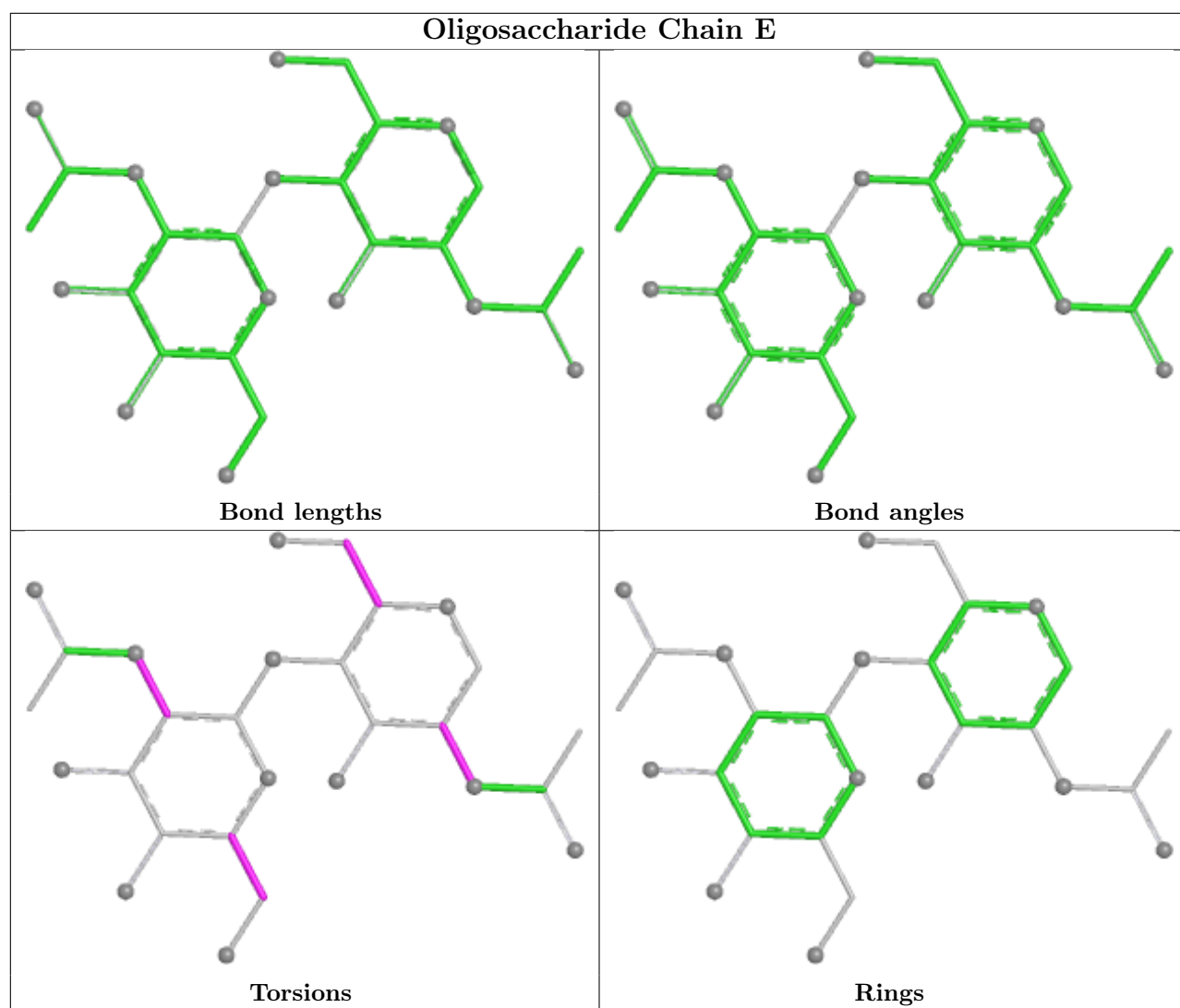
There are no ring outliers.

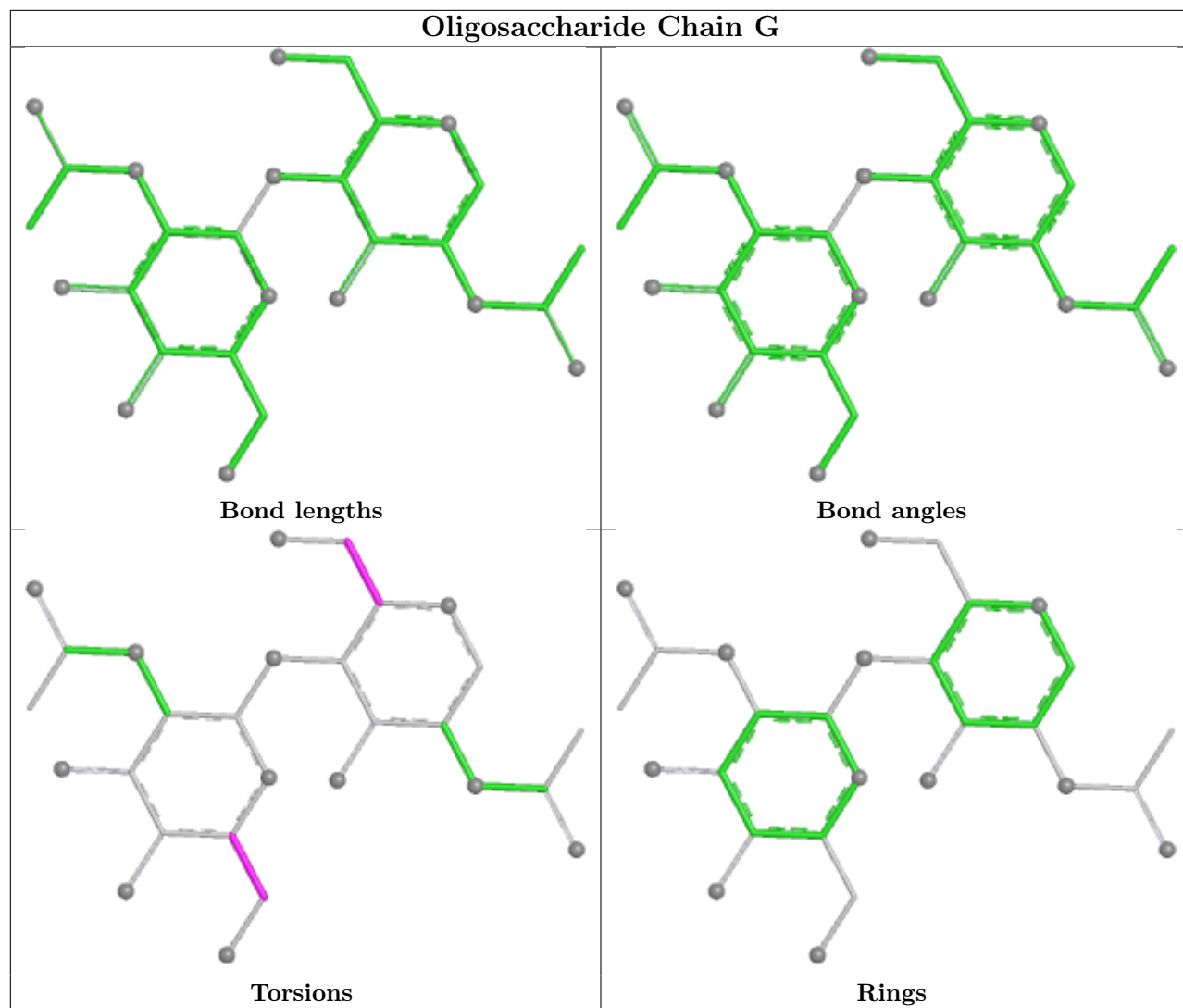
8 monomers are involved in 8 short contacts:

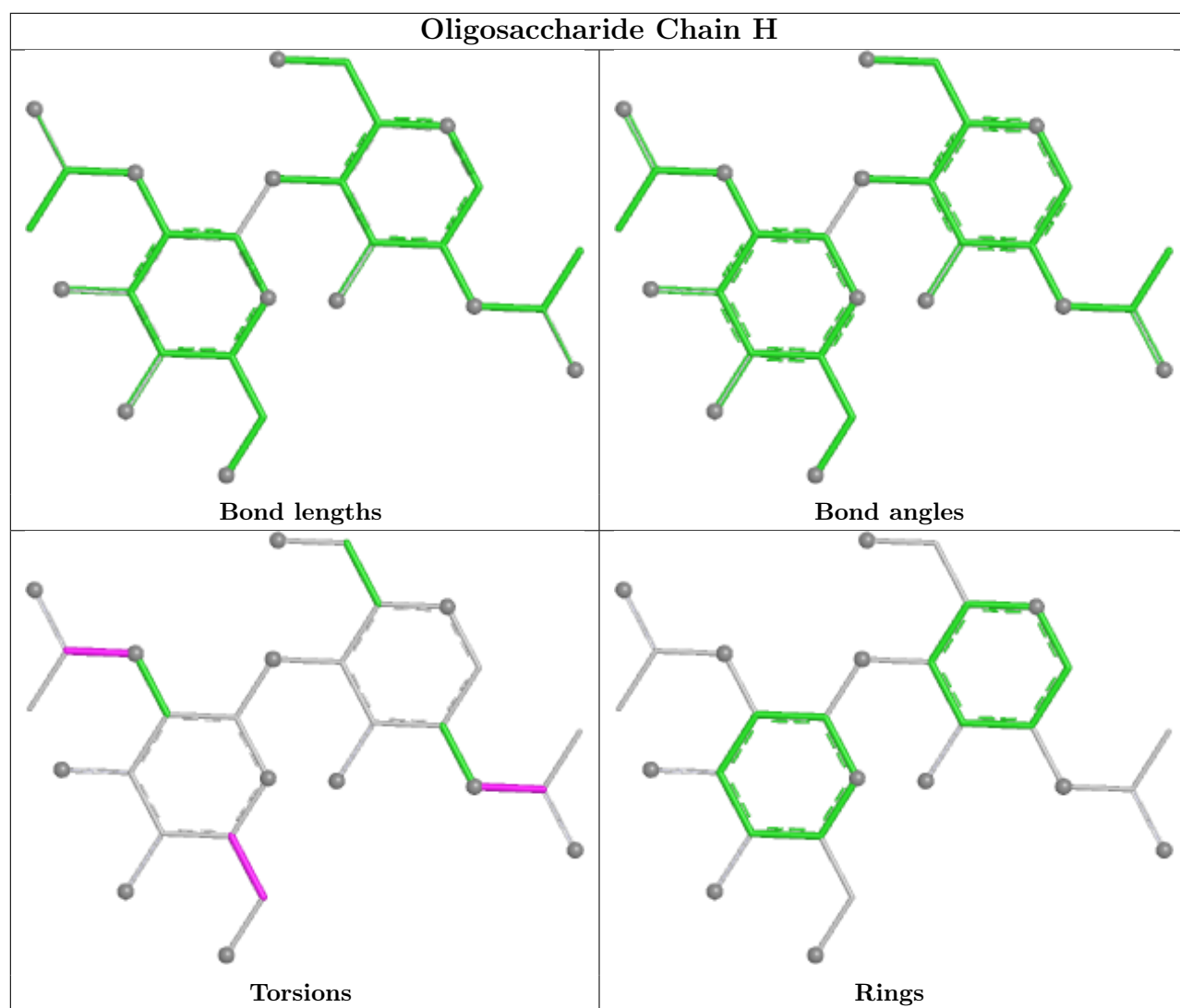
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	1	NAG	2	0
6	F	4	NAG	1	0
5	E	1	NAG	1	0
4	B	1	NAG	1	0
5	H	2	NAG	1	0
5	H	1	NAG	1	0
6	F	3	NAG	1	0
4	B	2	NAG	1	0

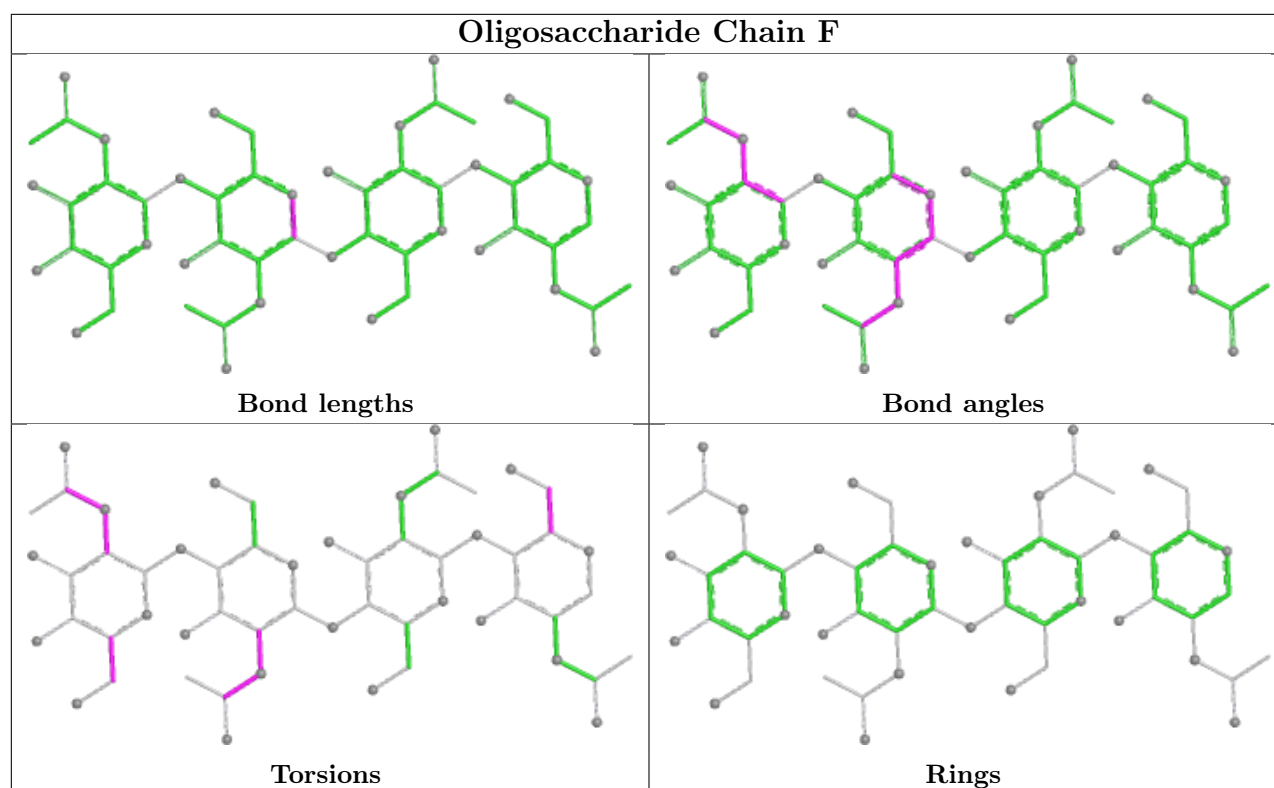
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 for Mogul analysis.

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	$\# Z > 2$
10	NAG	D	1201	2	14,14,15	0.38	0	17,19,21	0.50	0
8	WG6	A	2202	-	34,38,38	3.39	15 (44%)	46,56,56	2.58	15 (32%)
7	BB1	A	2201	-	33,33,33	1.52	5 (15%)	44,45,45	1.98	5 (11%)

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
10	NAG	D	1201	2	-	2/6/23/26	0/1/1/1
8	WG6	A	2202	-	-	15/28/48/48	0/3/3/3
7	BBI	A	2201	-	-	9/22/22/22	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	2202	WG6	P10-O30	11.41	1.71	1.58
8	A	2202	WG6	P10-N09	8.62	1.72	1.61
8	A	2202	WG6	C17-N19	5.94	1.61	1.46
7	A	2201	BBI	OAF-CAE	-5.65	1.30	1.38
8	A	2202	WG6	P10-O12	5.19	1.71	1.57
8	A	2202	WG6	C13-C14	4.96	1.66	1.51
8	A	2202	WG6	C25-N19	3.86	1.44	1.38
7	A	2201	BBI	CAM-CAE	3.84	1.40	1.36
8	A	2202	WG6	C25-N24	3.42	1.43	1.38
8	A	2202	WG6	O05-C03	3.11	1.41	1.34
8	A	2202	WG6	C02-C03	2.89	1.62	1.51
8	A	2202	WG6	C21-C22	2.84	1.49	1.43
7	A	2201	BBI	OAF-CAG	-2.52	1.34	1.38
8	A	2202	WG6	C20-N19	2.50	1.44	1.38
8	A	2202	WG6	C22-N24	2.45	1.42	1.38
7	A	2201	BBI	OAO-CAN	-2.30	1.18	1.23
8	A	2202	WG6	O29-C15	-2.19	1.38	1.42
7	A	2201	BBI	CAP-CAN	2.07	1.53	1.49
8	A	2202	WG6	C14-C15	2.03	1.56	1.53
8	A	2202	WG6	C20-C21	2.02	1.39	1.35

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	2202	WG6	O18-C17-N19	10.67	117.80	108.23
7	A	2201	BBI	CAD-CAE-CAM	-8.40	125.67	133.84
7	A	2201	BBI	OAF-CAE-CAD	6.38	124.89	115.22
8	A	2202	WG6	O05-C03-C02	5.84	120.61	110.83
7	A	2201	BBI	CAG-OAF-CAE	5.48	111.45	106.04
8	A	2202	WG6	C17-N19-C20	4.40	125.61	121.26
8	A	2202	WG6	P10-O30-C31	3.79	132.54	122.35
8	A	2202	WG6	O05-C03-O04	-3.71	117.26	123.95
8	A	2202	WG6	C03-C02-N09	3.40	117.66	111.47
8	A	2202	WG6	O12-P10-N09	3.23	114.82	108.00
8	A	2202	WG6	C17-N19-C25	-3.16	113.55	117.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	2201	BBI	CAH-CAG-CAL	-3.01	120.12	123.58
8	A	2202	WG6	O18-C14-C15	-2.99	100.55	104.46
8	A	2202	WG6	O26-C25-N19	-2.86	119.08	122.80
8	A	2202	WG6	O12-P10-O11	-2.55	106.70	114.27
8	A	2202	WG6	P10-O12-C13	2.41	128.24	119.24
8	A	2202	WG6	C22-N24-C25	-2.32	123.73	126.61
8	A	2202	WG6	C06-O05-C03	2.28	120.96	117.71
8	A	2202	WG6	O30-P10-O11	-2.26	112.63	115.68
7	A	2201	BBI	CAL-CAM-CAE	-2.02	104.90	106.75

There are no chirality outliers.

All (26) torsion outliers are listed below:

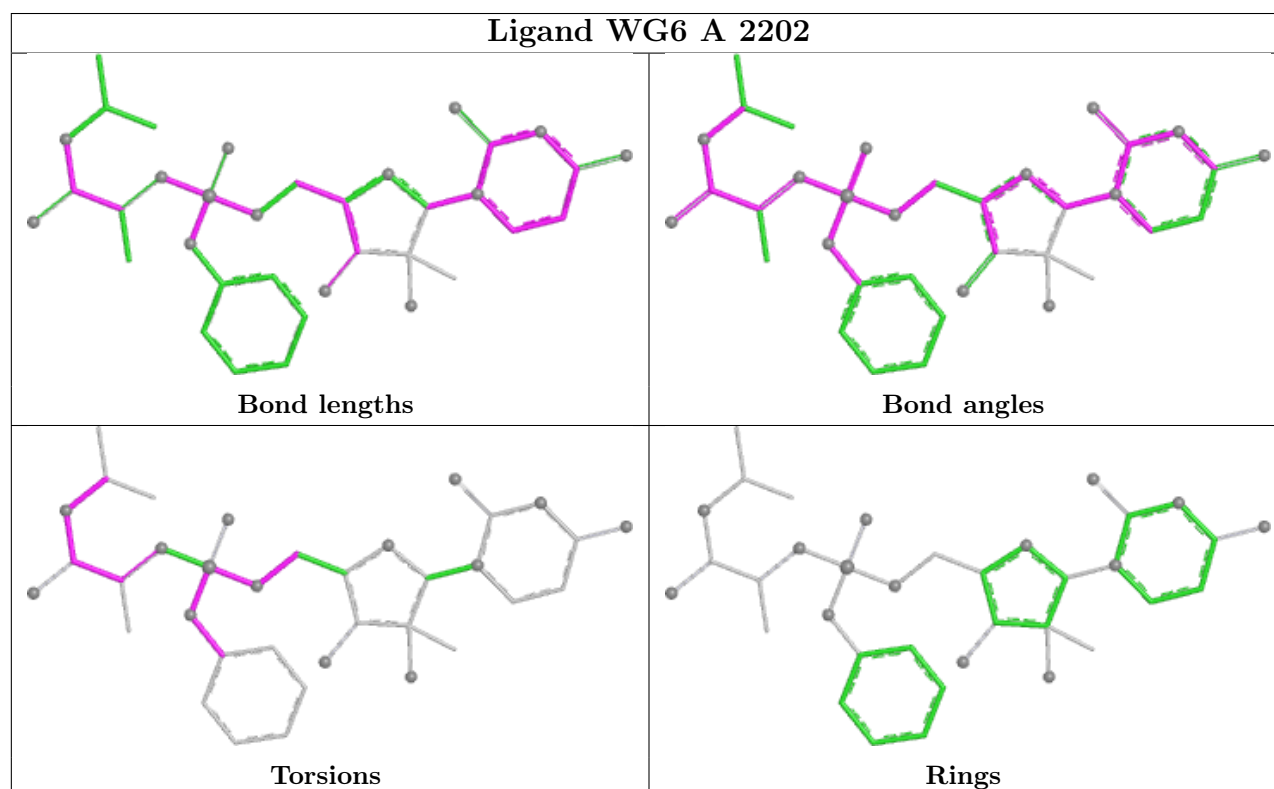
Mol	Chain	Res	Type	Atoms
7	A	2201	BBI	CAR-CAT-OAU-CAV
7	A	2201	BBI	CAV-CAW-NAX-CBA
8	A	2202	WG6	N09-C02-C03-O04
8	A	2202	WG6	N09-C02-C03-O05
8	A	2202	WG6	C03-C02-N09-P10
8	A	2202	WG6	C02-C03-O05-C06
8	A	2202	WG6	O04-C03-O05-C06
8	A	2202	WG6	C08-C06-O05-C03
7	A	2201	BBI	CAW-CAV-OAU-CAT
7	A	2201	BBI	CAB-CAC-CAD-CAE
7	A	2201	BBI	CAZ-CAY-NAX-CAW
7	A	2201	BBI	CAZ-CAY-NAX-CBA
8	A	2202	WG6	C31-O30-P10-O12
8	A	2202	WG6	C01-C02-C03-O05
8	A	2202	WG6	C01-C02-C03-O04
8	A	2202	WG6	C31-O30-P10-O11
8	A	2202	WG6	C14-C13-O12-P10
10	D	1201	NAG	C3-C2-N2-C7
7	A	2201	BBI	CAA-CAB-CAC-CAD
8	A	2202	WG6	C36-C31-O30-P10
8	A	2202	WG6	C31-O30-P10-N09
8	A	2202	WG6	C13-O12-P10-N09
10	D	1201	NAG	C1-C2-N2-C7
8	A	2202	WG6	C32-C31-O30-P10
7	A	2201	BBI	CBC-CAT-OAU-CAV
7	A	2201	BBI	CAV-CAW-NAX-CAY

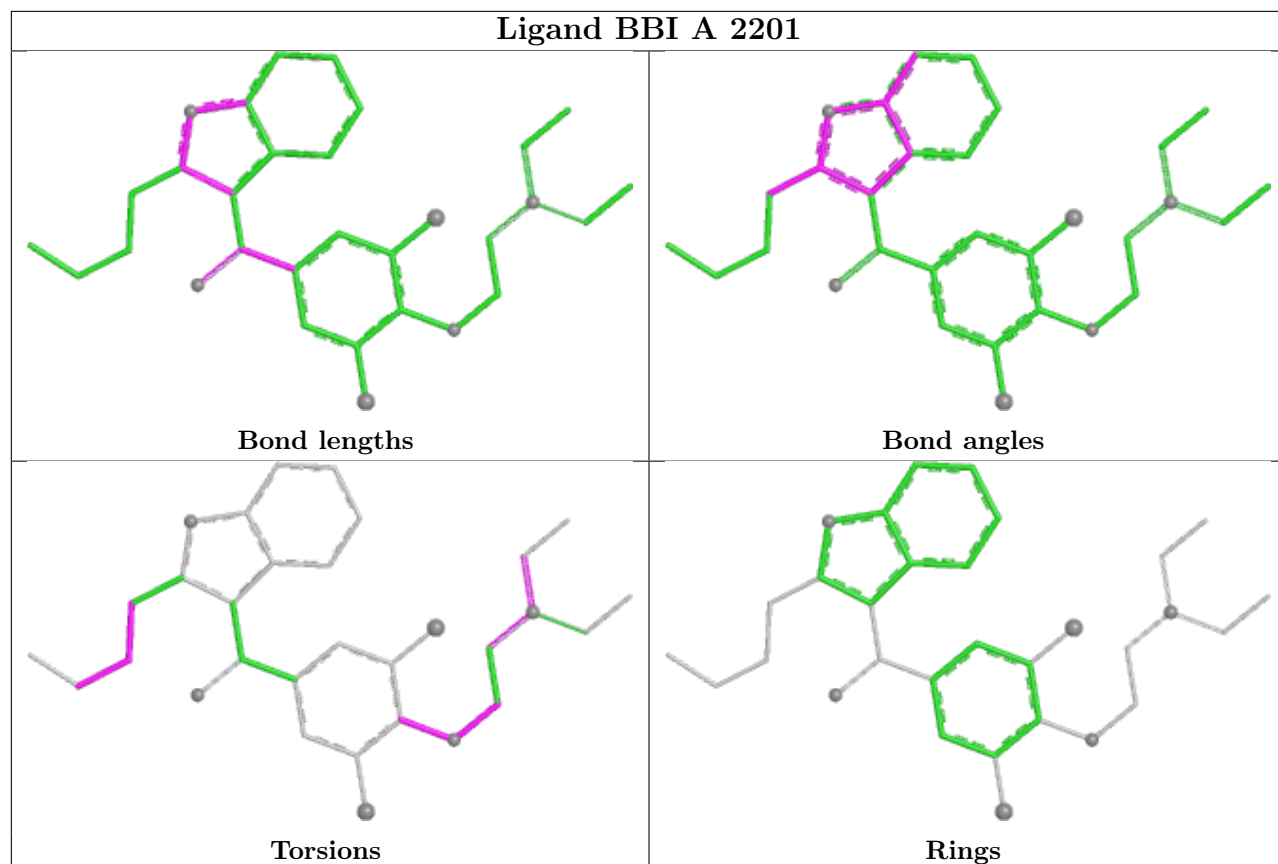
There are no ring outliers.

2 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	2202	WG6	4	0
7	A	2201	BB1	10	0

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.

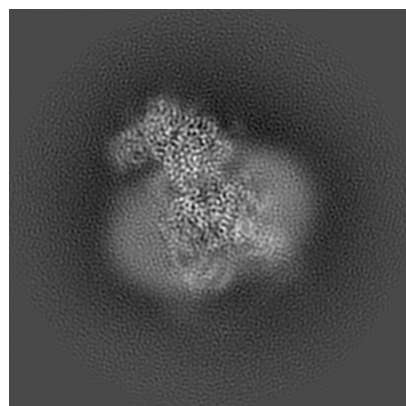
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27909. These allow visual inspection of the internal detail of the map and identification of artifacts.

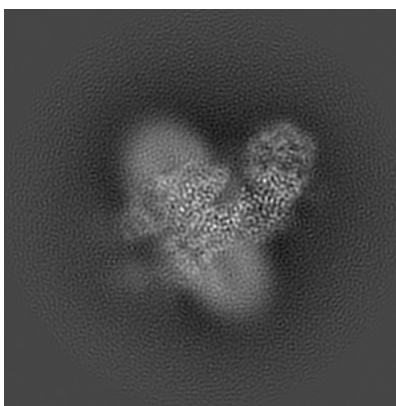
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

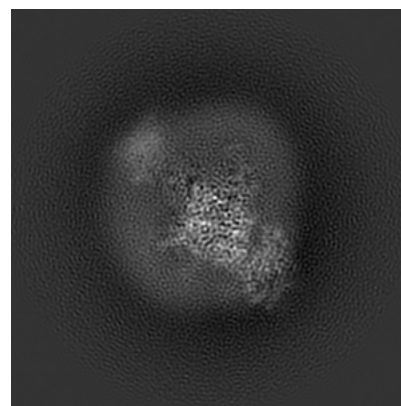
6.1.1 Primary map



X

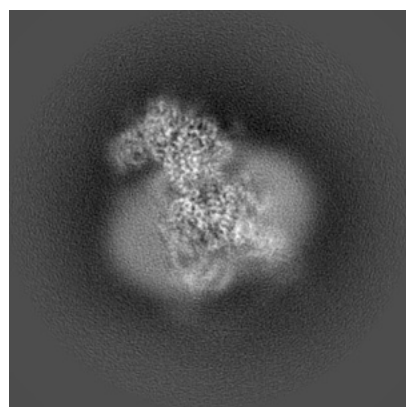


Y

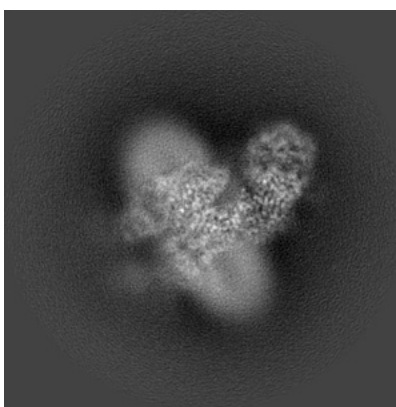


Z

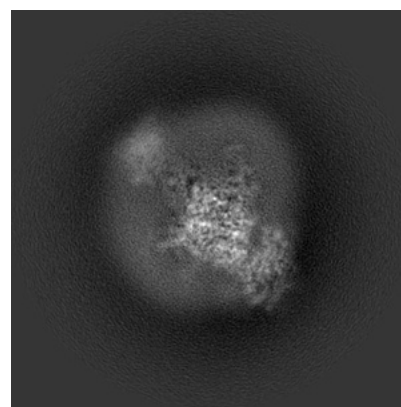
6.1.2 Raw map



X



Y

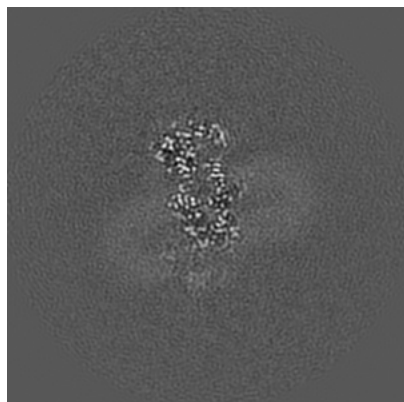


Z

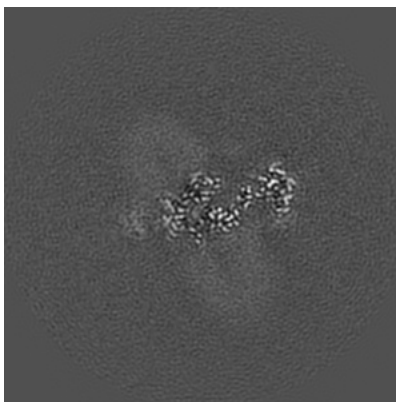
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

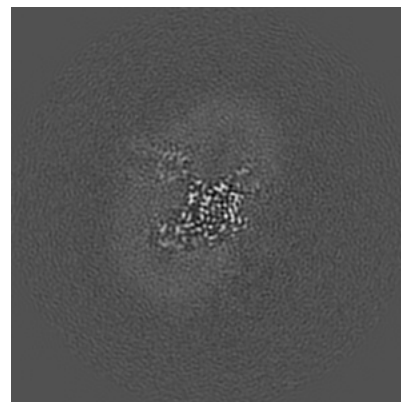
6.2.1 Primary map



X Index: 140

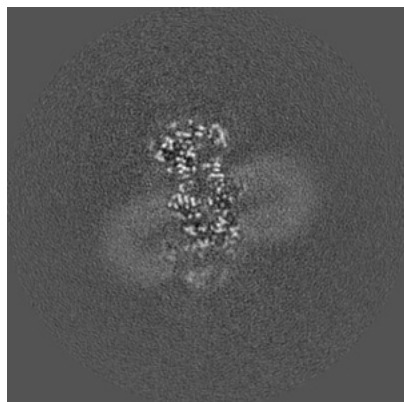


Y Index: 140

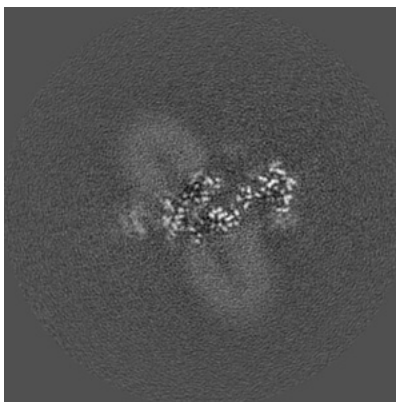


Z Index: 140

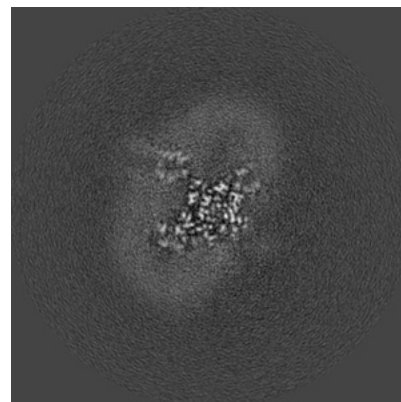
6.2.2 Raw map



X Index: 140



Y Index: 140

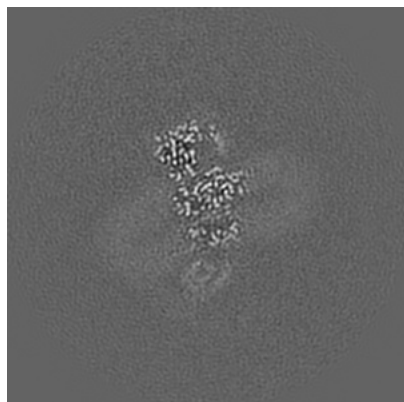


Z Index: 140

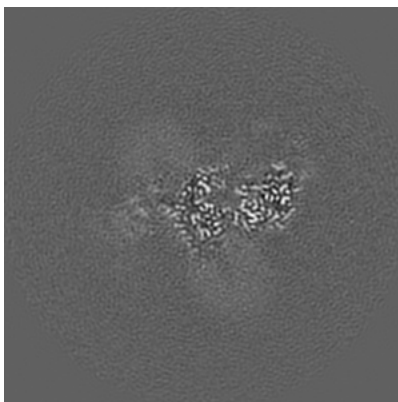
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

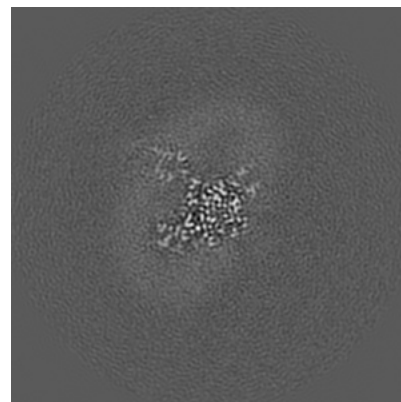
6.3.1 Primary map



X Index: 135

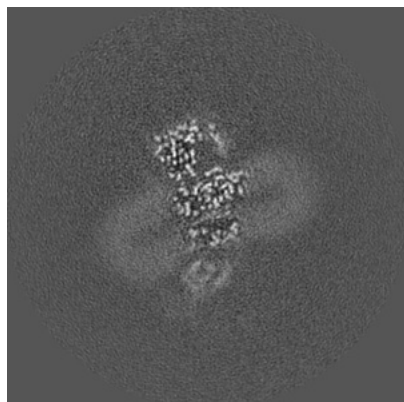


Y Index: 130

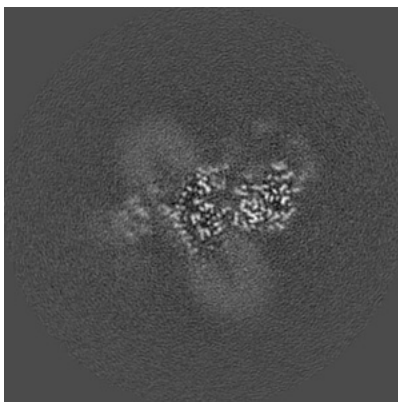


Z Index: 141

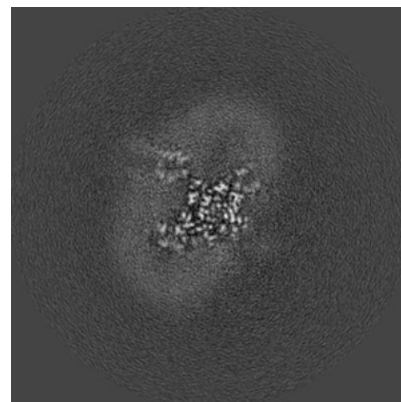
6.3.2 Raw map



X Index: 135



Y Index: 130

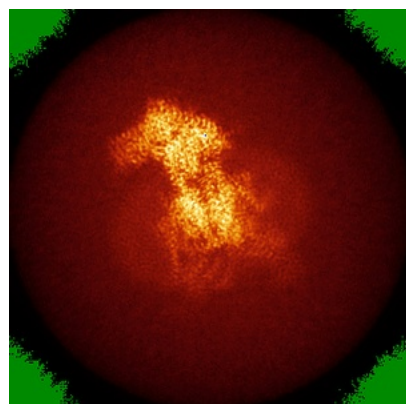


Z Index: 140

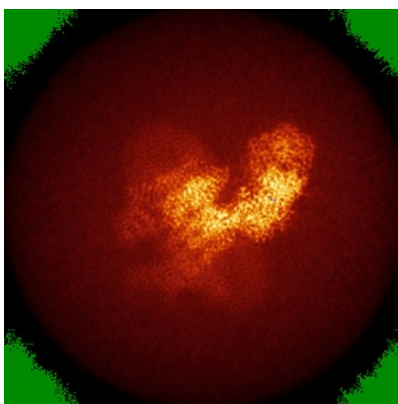
The images above show the largest variance slices of the map in three orthogonal directions.

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

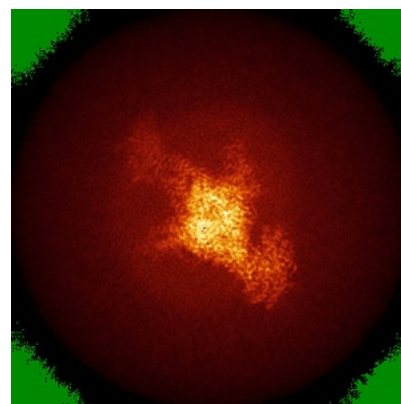
6.4.1 Primary map



X

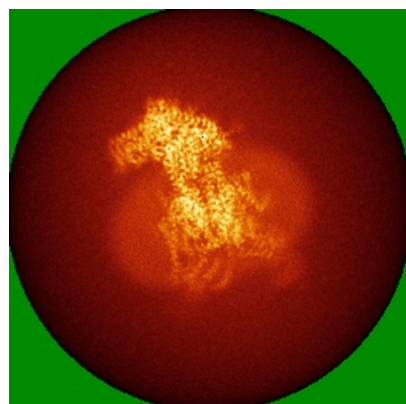


Y

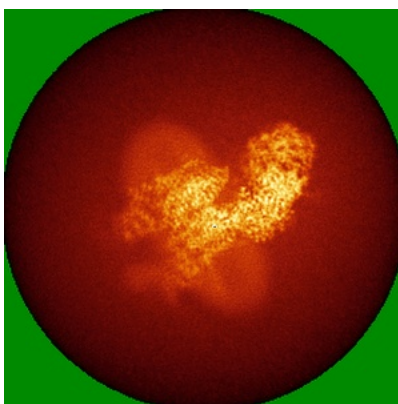


Z

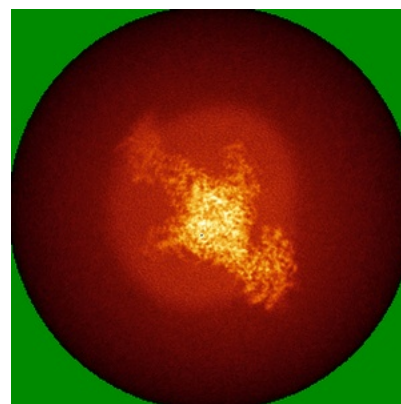
6.4.2 Raw map



X



Y



Z

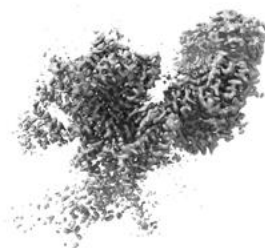
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

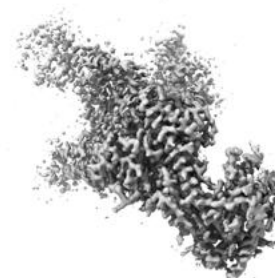
6.5.1 Primary map



X



Y



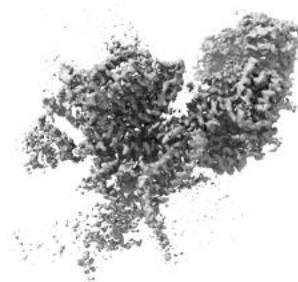
Z

The images above show the 3D surface view of the map at the recommended contour level 0.025. 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



X



Y



Z

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.

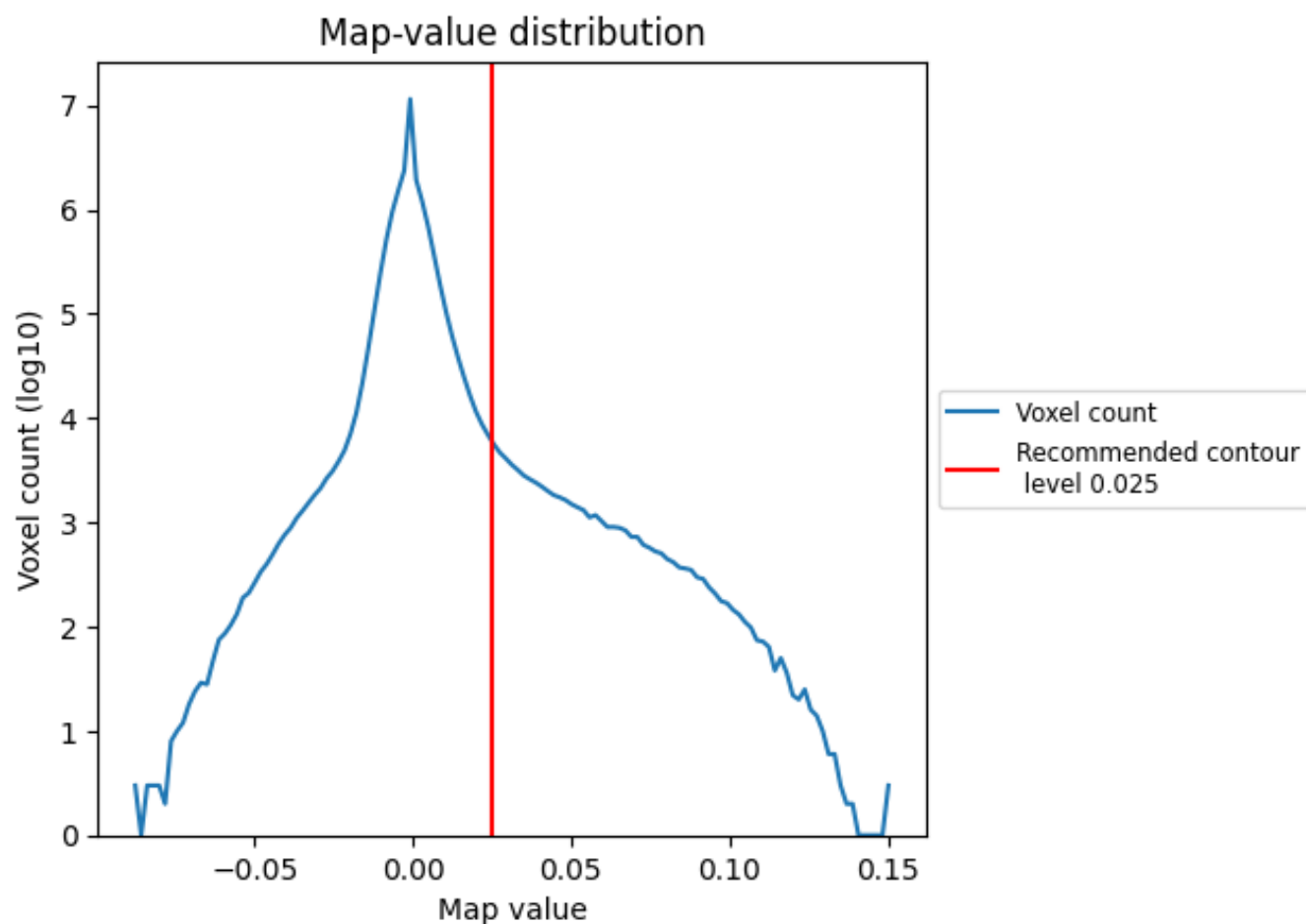
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

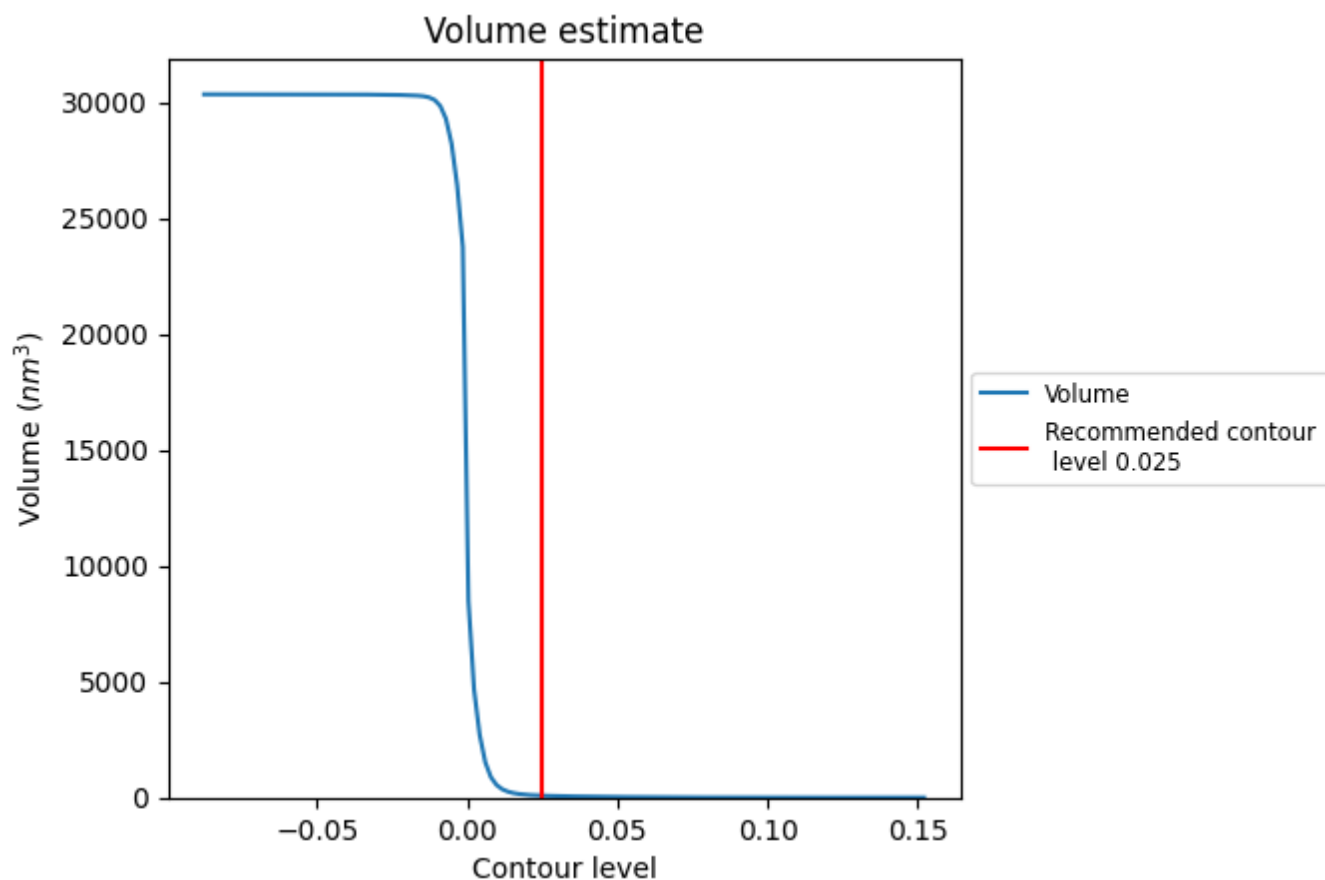
This section contains the results of statistical analysis of the map.

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.

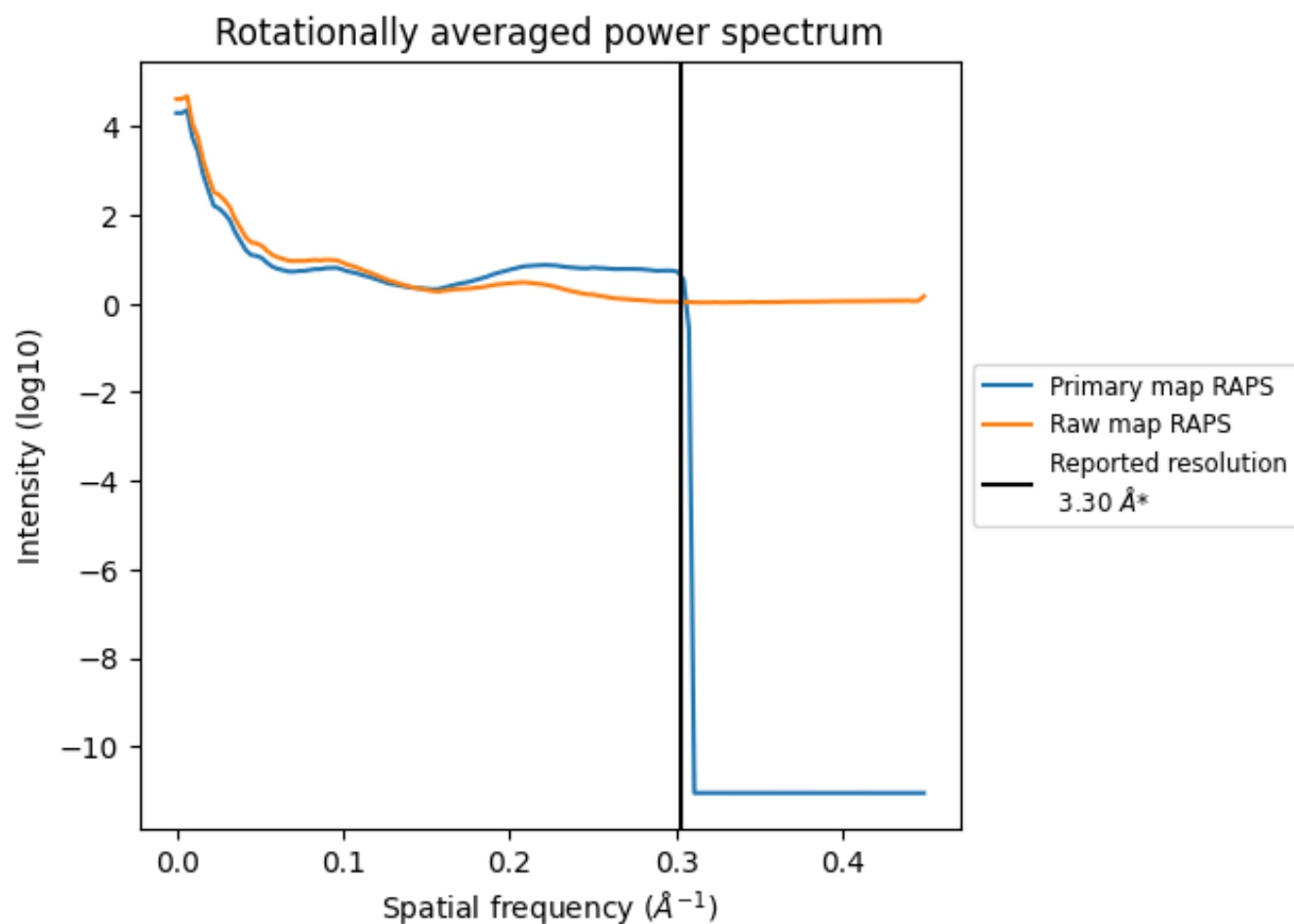
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 82 nm³; this corresponds to an approximate mass of 74 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

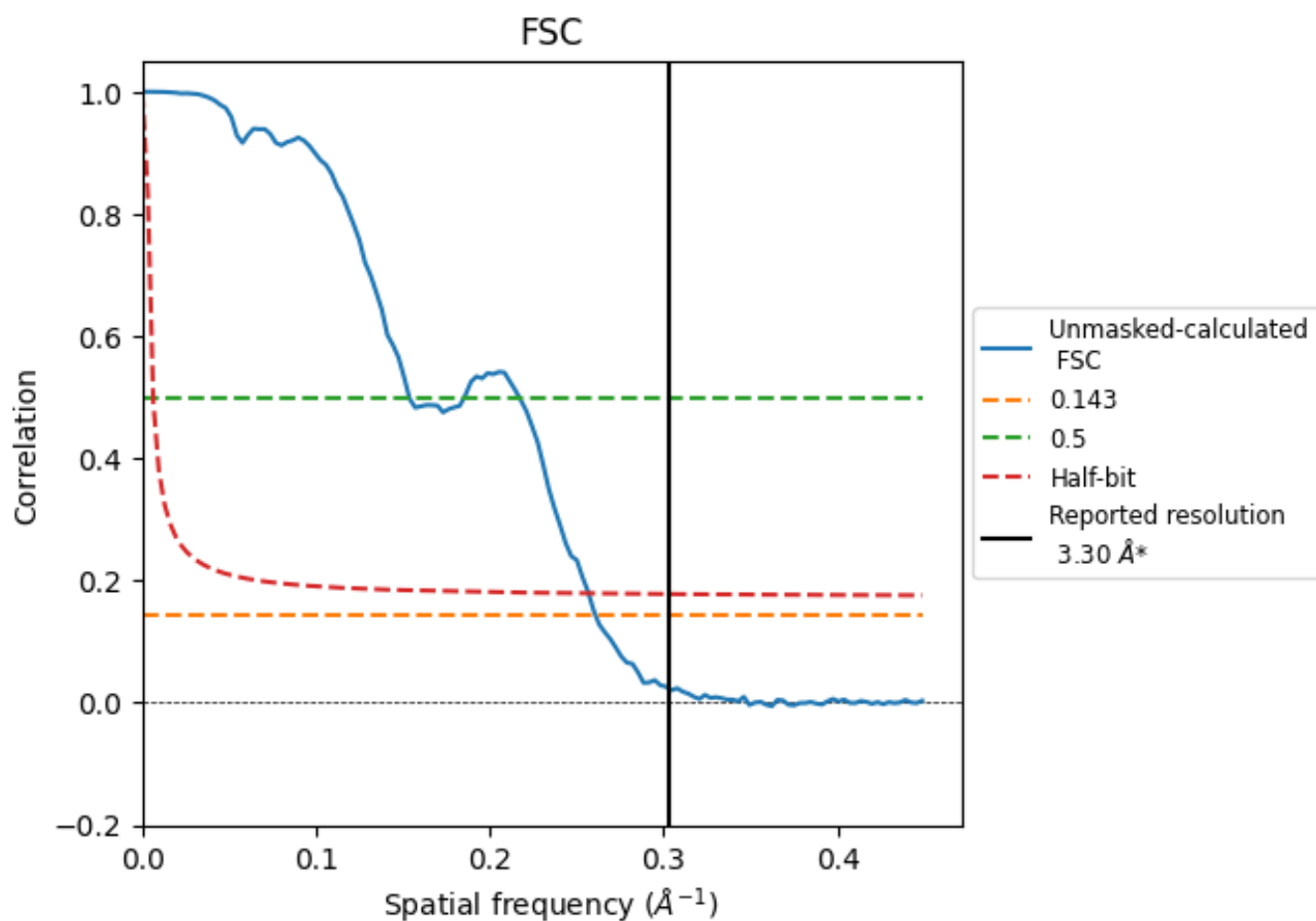


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

8 Fourier-Shell correlation [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 0.303 Å⁻¹

8.2 Resolution estimates [i](#)

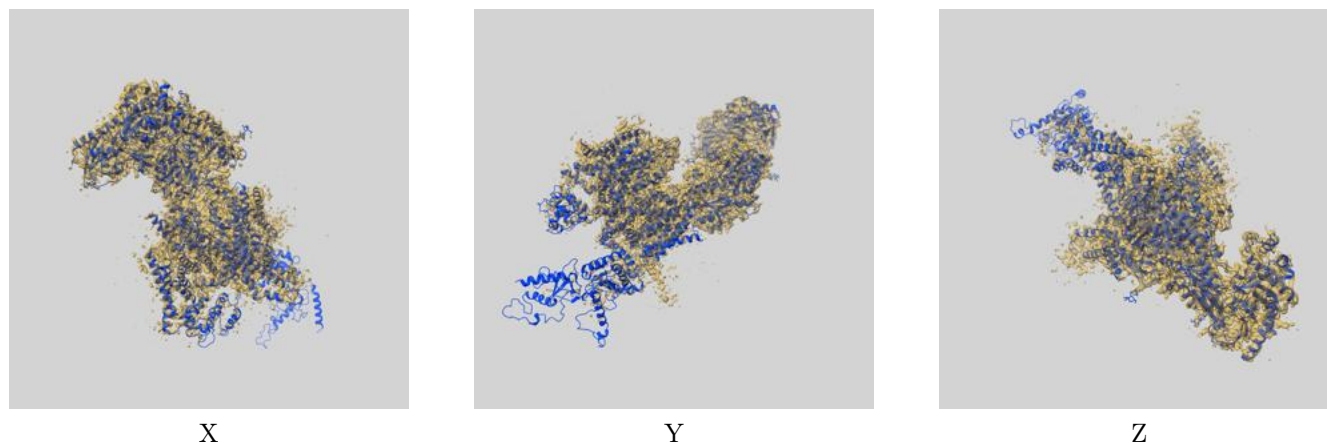
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.83	6.51	3.89

*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 3.83 differs from the reported value 3.3 by more than 10 %

9 Map-model fit [i](#)

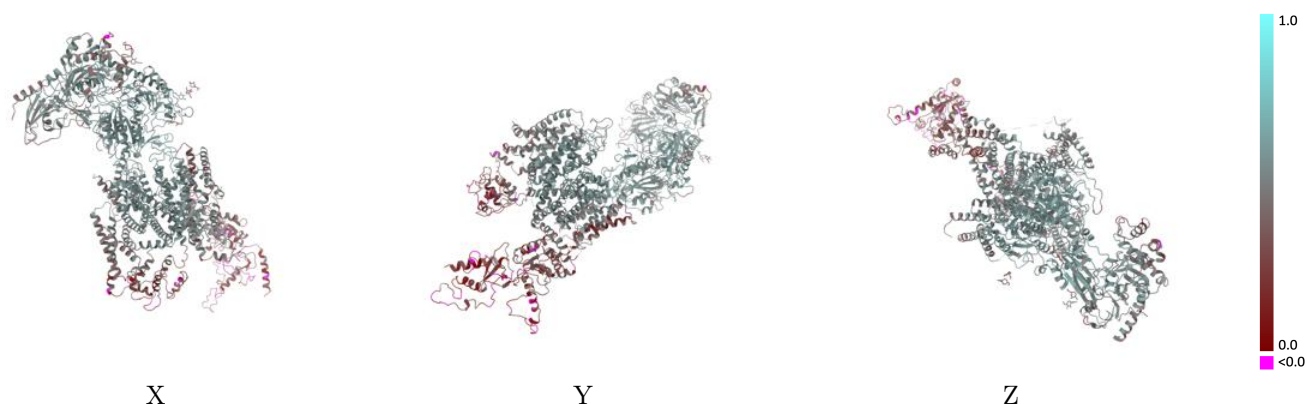
This section contains information regarding the fit between EMDB map EMD-27909 and PDB model 8E5B. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



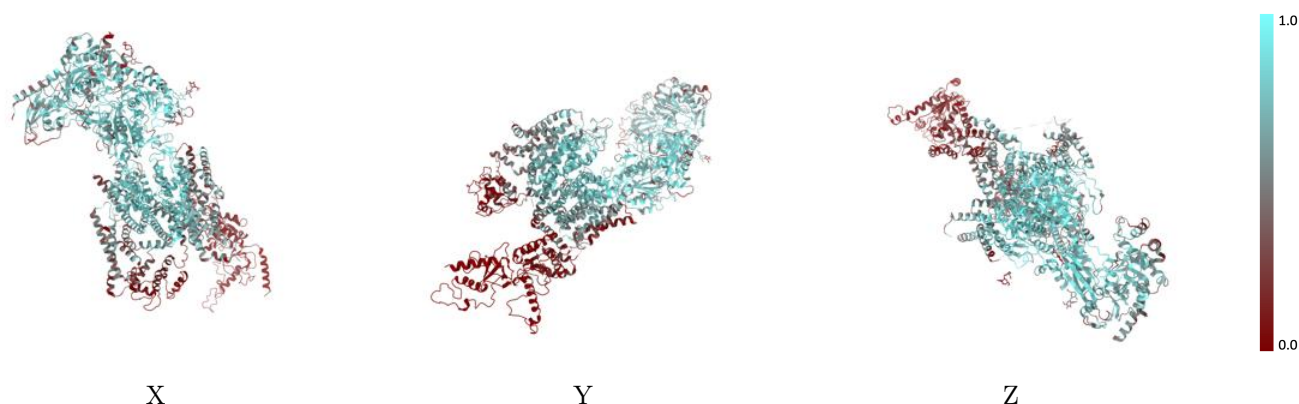
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



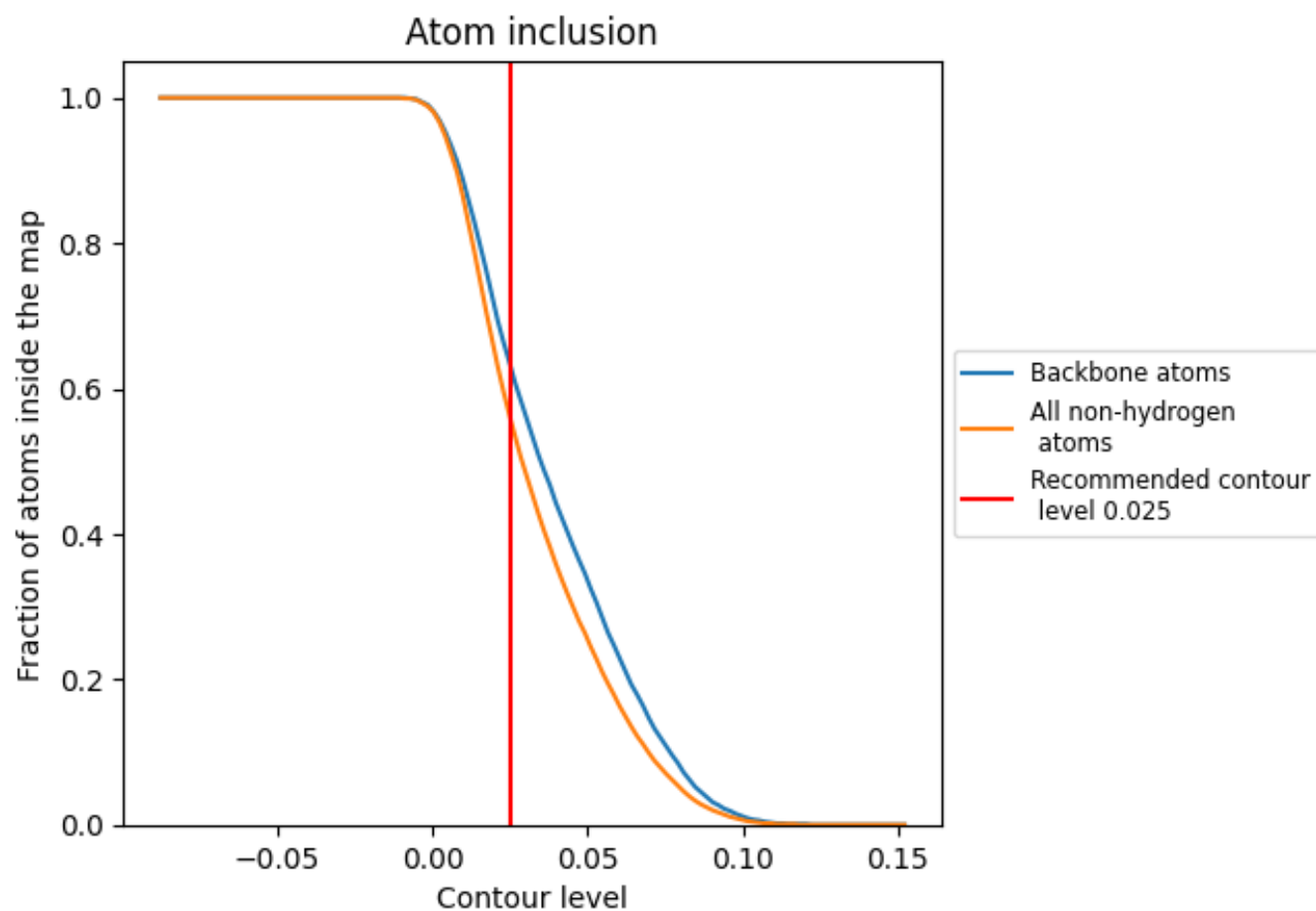
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.025).

9.4 Atom inclusion [i](#)



At the recommended contour level, 63% of all backbone atoms, 56% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5600	0.4670
A	0.5770	0.4800
B	0.3570	0.3880
C	0.0430	0.2340
D	0.7160	0.5310
E	0.1430	0.3180
F	0.5000	0.4650
G	0.3570	0.3770
H	0.4640	0.4610

