



wwPDB EM Validation Summary Report ⓘ

Oct 19, 2024 – 05:14 PM EDT

PDB ID : 8SR8
EMDB ID : EMD-40722
Title : Cryo-EM structure of TRPM2 chanzyme in the presence of EDTA (apo state)
Authors : Huang, Y.; Kumar, S.; Lu, W.; Du, J.
Deposited on : 2023-05-05
Resolution : 2.77 Å (reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

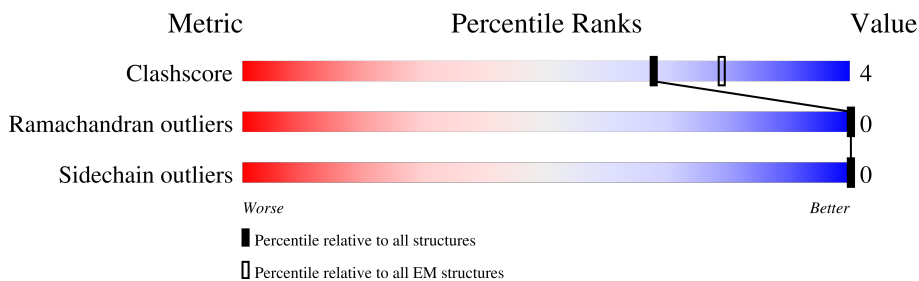
EMDB validation analysis : 0.0.1.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.77 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	1494	
1	B	1494	
1	C	1494	
1	D	1494	

2 Entry composition [i](#)

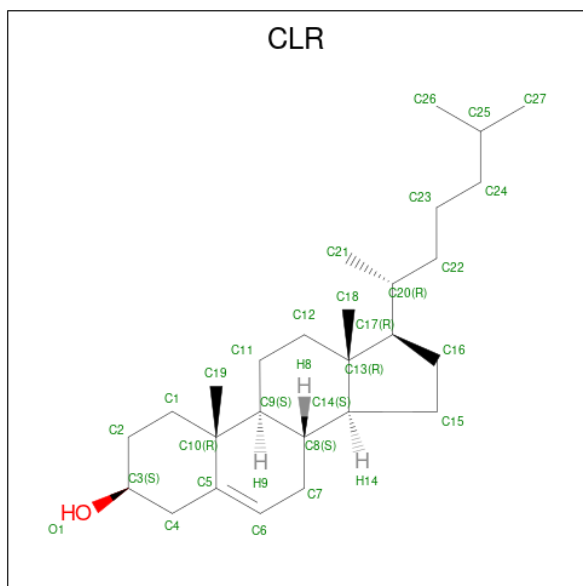
There are 2 unique types of molecules in this entry. The entry contains 39248 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 TRPM2 chanzyme.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1353	Total 9728	C 6248	N 1692	O 1739	S 49	0	0
1	B	1353	Total 9728	C 6248	N 1692	O 1739	S 49	0	0
1	C	1353	Total 9728	C 6248	N 1692	O 1739	S 49	0	0
1	D	1353	Total 9728	C 6248	N 1692	O 1739	S 49	0	0

- Molecule 2 is CHOLESTEROL (three-letter code: CLR) (formula: C₂₇H₄₆O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
2	A	1	Total 28	C 27	O 1	0
2	A	1	Total 28	C 27	O 1	0

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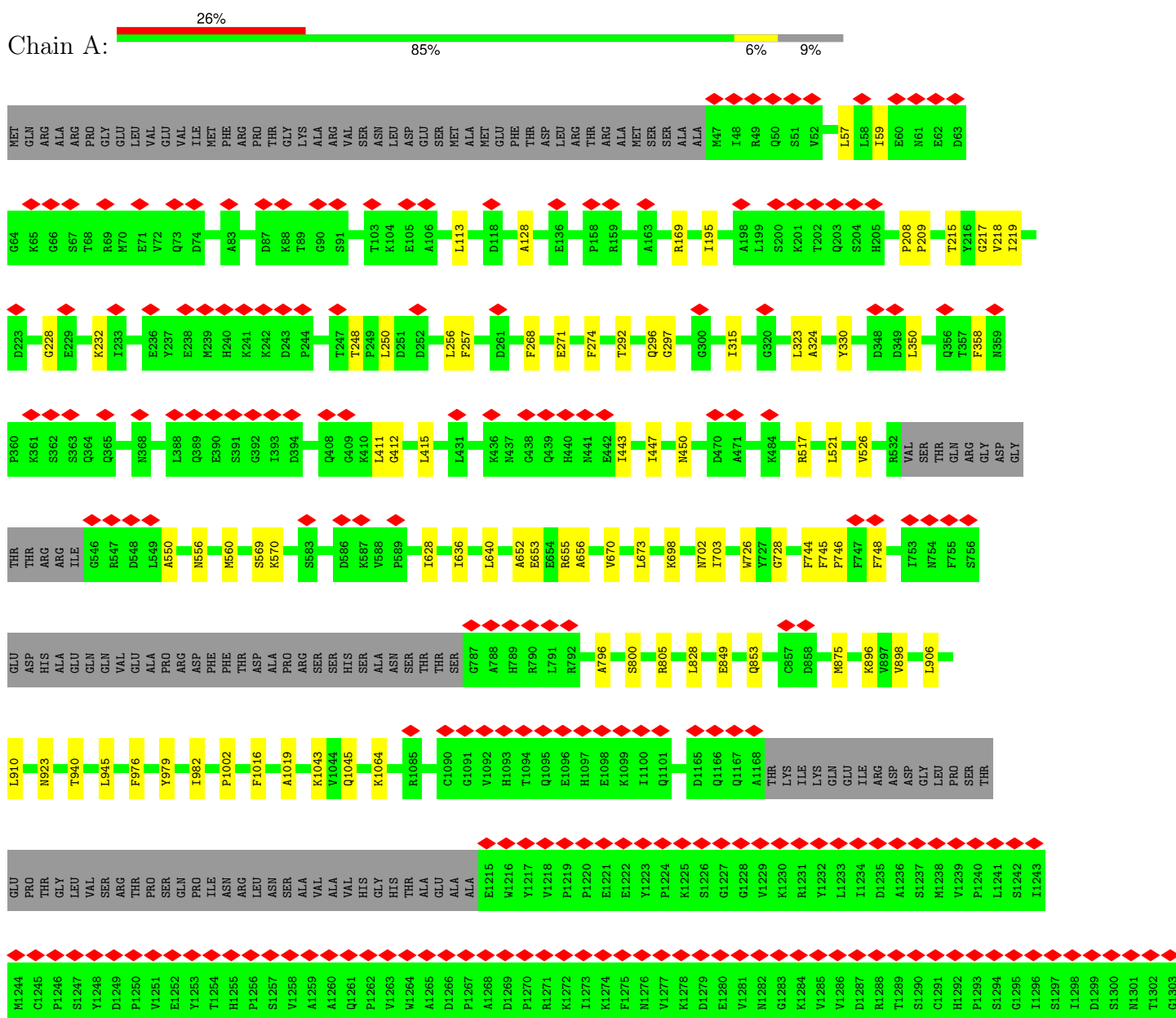
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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
2	A	1	28	27	1	0
2	B	1	28	27	1	0
2	B	1	28	27	1	0
2	B	1	28	27	1	0
2	C	1	28	27	1	0
2	C	1	28	27	1	0
2	C	1	28	27	1	0
2	D	1	28	27	1	0
2	D	1	28	27	1	0
2	D	1	28	27	1	0

3 Residue-property plots

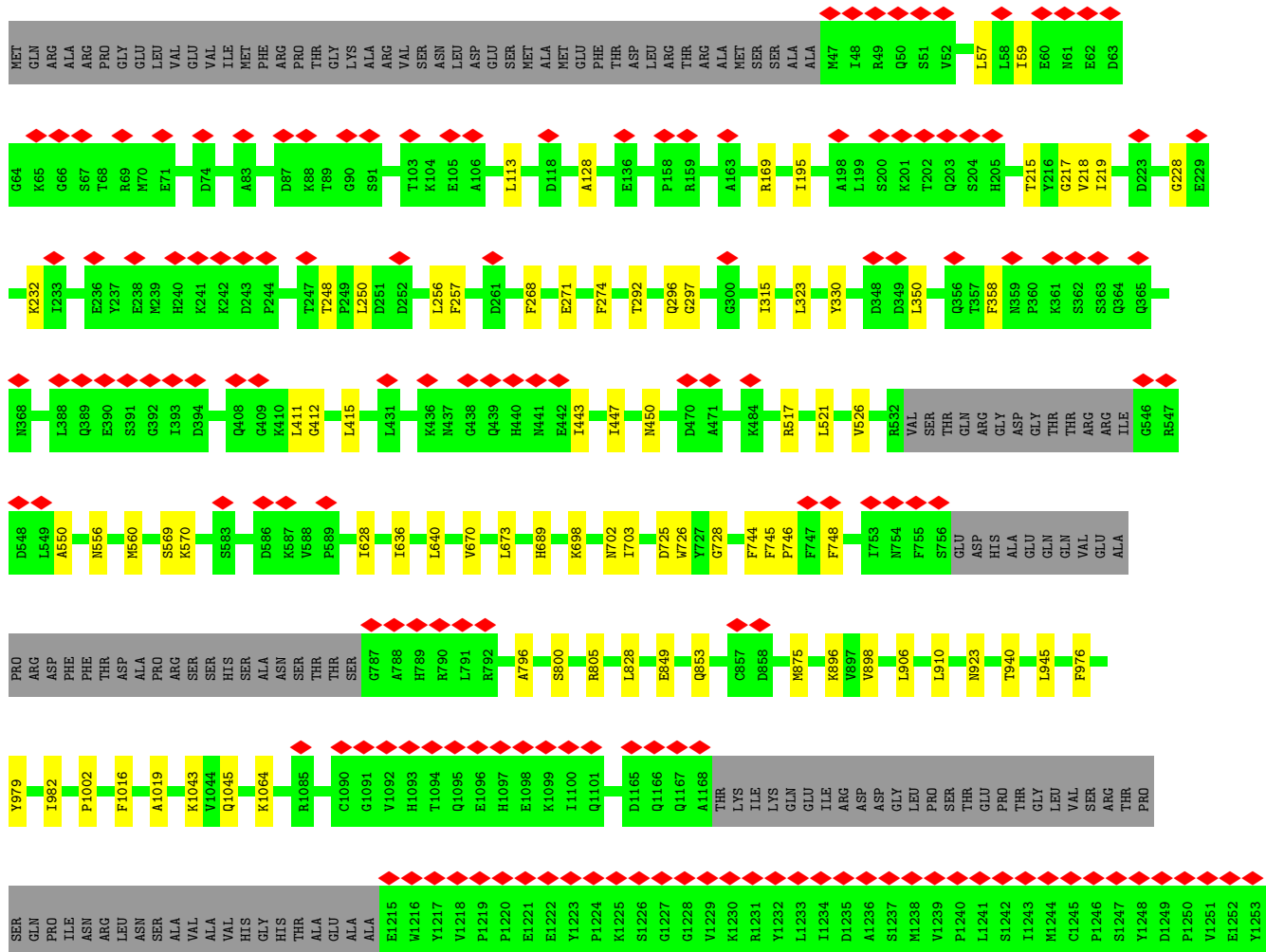
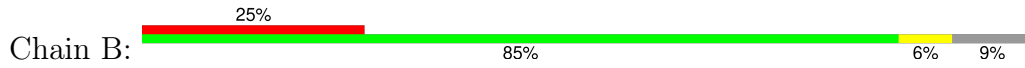
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: TRPM2 chanzyme



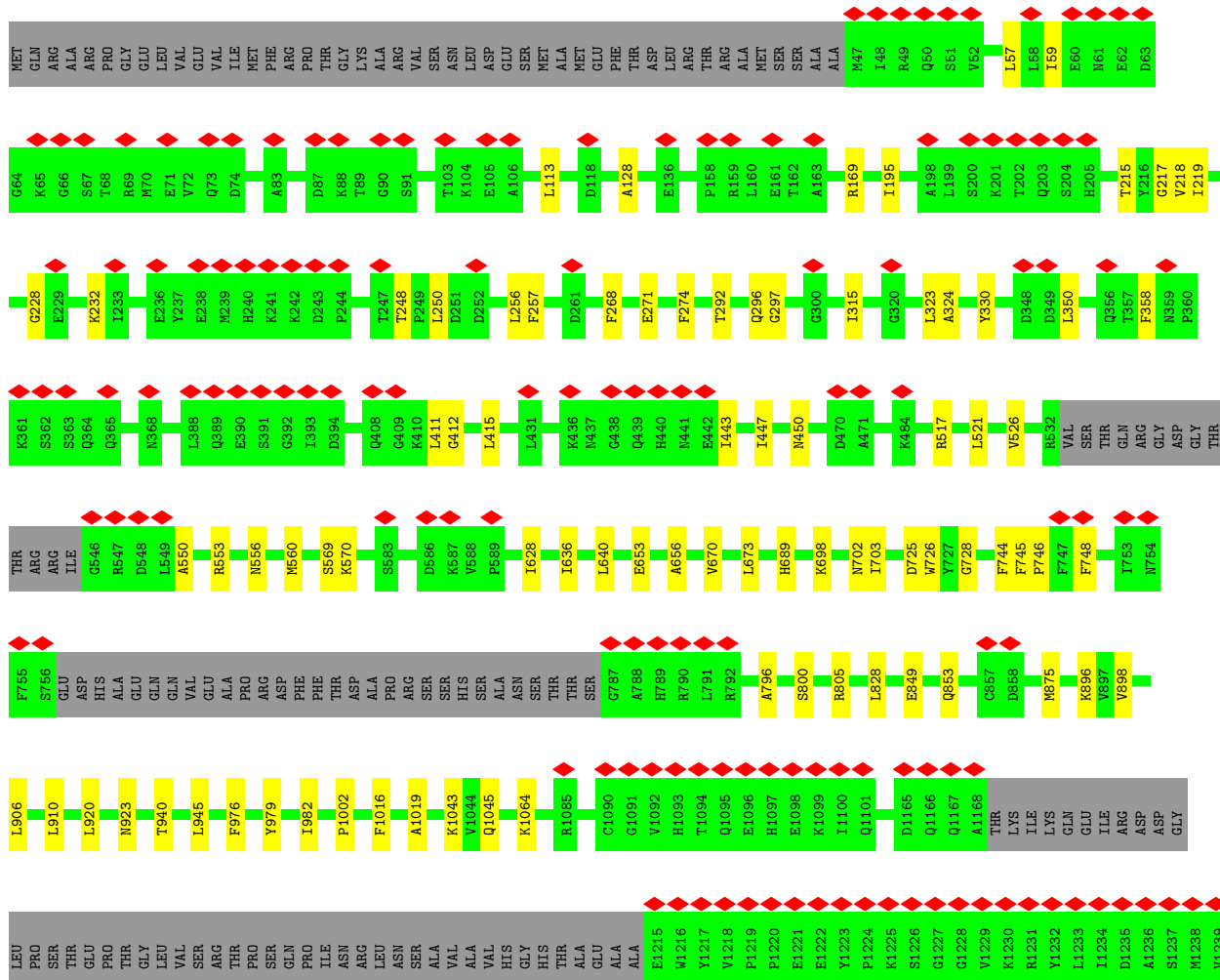
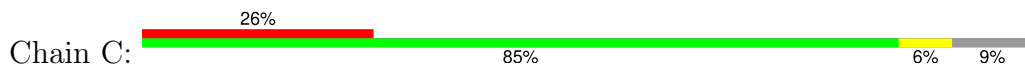


● Molecule 1: TRPM2 chanzyme



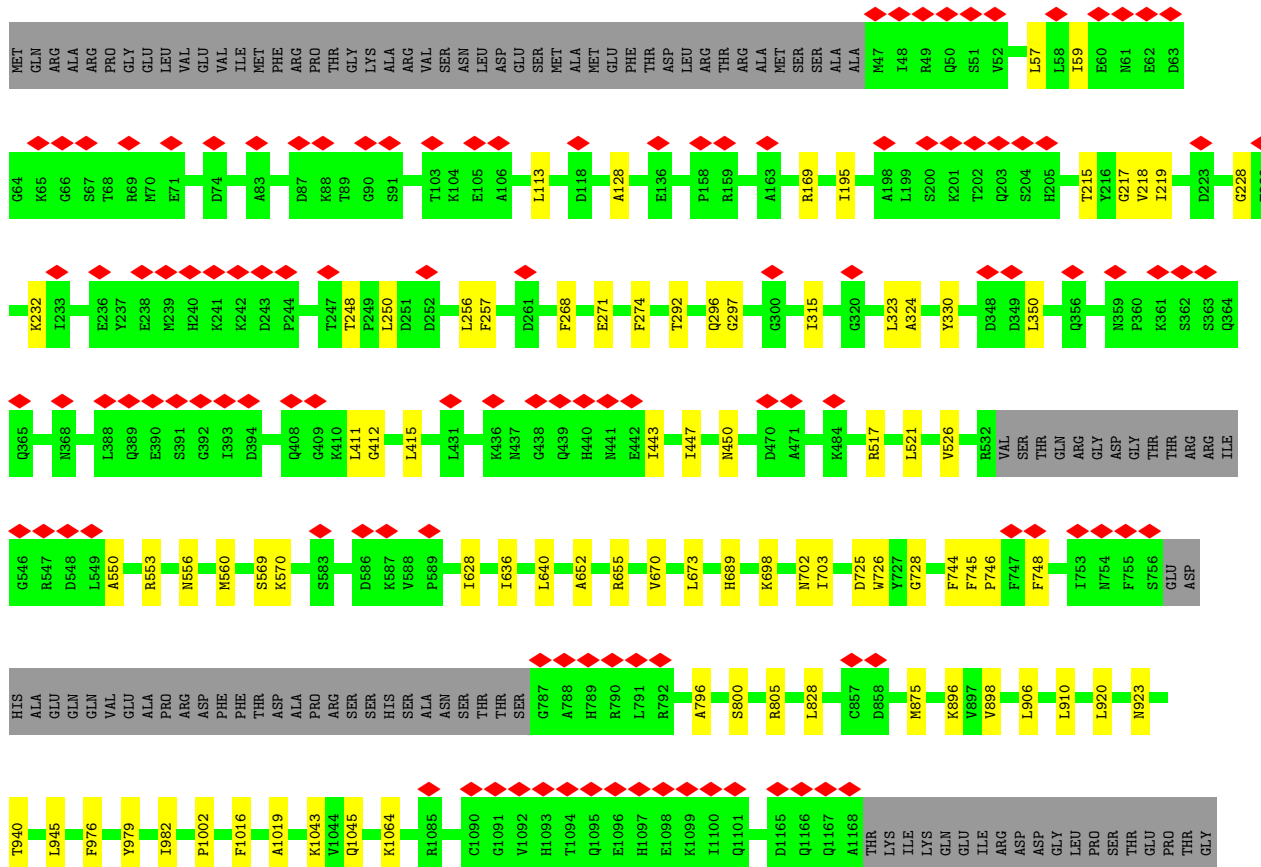
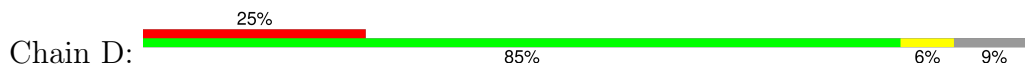


● Molecule 1: TRPM2 chanzyme





• Molecule 1: TRPM2 chanzyme



LEU	E1215	Y1248	P1308	P1369	N1429	M1491	VAL	E1216	D1249	G1370	T1430	F1494	SER	E1217	P1250	W1309	G1371	D1430		ARG	E1218	V1251	G1310	F1372	D1431		THR	E1219	E1252	R1311	D1374	N1432		PRO	E1220	Y1253	G1312	D1374	A1433		SER	E1221	T1254	M1314	N1375	W1434		GLN	E1222	H1255	T1315	G1376	V1435		ILE	E1223	T1256	G1316	E1377	E1436		ASN	E1224	H1257	G1317	D1378	T1437		ARG	E1225	S1258	R1317	D1378	T1438		LEU	E1226	V1258	G1318	V1379	C1439		ASN	E1227	A1259	L1319	A1380	V1440		VAL	E1228	A1260	L1320	L1381	N1441		ALA	E1229	Q1261	G1321	T1382	F1442		ALA	E1230	P1262	K1322	S1383	H1443		VAL	E1231	V1263	W1323	G1384	D1444		HIS	E1232	H1264	W1324	R1385	E1445		GLY	E1233	A1265	V1325	E1386	S1446		HIS	E1234	D1266	M1326	F1387	G1447		THR	E1235	P1267	Q1327	M1388	R1448		ALA	E1236	A1268	A1328	E1389	H1449		GLU	E1237	D1269	A1329	E1390	A1450		ALA	E1238	P1270	D1330	A1391	A1451		ALA	E1239	K1271	T1331	L1392	R1452			E1240	K1272	V1332	G1393	L1453			E1241	I1273	W1333	M1394	K1454			E1242	K1274	T1334	G1395	L1455			E1243	F1275	R1335	THR	Q1456			E1244	N1276	R1336	SER	G1457			E1245	E1222	W1337	ALA	G1458			E1246	Y1227	K1337	ASP	D1459			E1247	K1278	R1338	LEU	D1460			E1248	K1278	S1339	MET	D1461			E1249	D1279	P1340	S1402	A1462			E1250	E1280	S1340	A1403	H1463			E1251	G1227	D1341	E1404	A1464			E1252	N1282	G1342	S1405	R1465			E1253	G1283	S1343	S1406				E1254	K1284	I1344	K1406				E1255	V1285	L1345	D1407				E1256	V1286	E1346	S1408				E1257	V1286	R1347	L1409				E1258	D1287	D1348	A1410				E1259	R1288	G1349	A1411				E1260	T1289	K1350	L1412				E1261	S1290	K1351	F1413				E1262	C1291	E1354	S1414				E1263	H1292	F1355	S1415				E1264	P1293	V1356	G1416				E1265	S1294	V1357	T1417				E1266	G1295	I1357	I1418				E1267	I1296	Q1359	V1419				E1268	S1297	R1360	A1420				E1269	I1298	D1361	R1421				E1270	I1298	D1362	T1422				E1271	S1300	M1363	Y1423				E1272	N1301	K1364	C1424				E1273	T1302	M1365	E1425				E1274	G1303	W1366	D1426				E1275	P1305	A1367	P1427				E1276	I1306	I1368	R1428				E1277							E1278							E1279							E1280							E1281							E1282							E1283							E1284							E1285							E1286							E1287							E1288							E1289							E1290							E1291							E1292							E1293							E1294							E1295							E1296							E1297							E1298							E1299							E1300							E1301							E1302							E1303							E1304							E1305							E1306					
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	168854	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	54	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	65.751	Depositor
Minimum map value	-26.704	Depositor
Average map value	0.181	Depositor
Map value standard deviation	1.441	Depositor
Recommended contour level	9	Depositor
Map size (\AA)	356.32, 356.32, 356.32	wwPDB
Map dimensions	340, 340, 340	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.048, 1.048, 1.048	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CLR

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	0.54	0/9943	0.79	0/13558
1	B	0.54	0/9943	0.79	0/13558
1	C	0.54	0/9943	0.79	0/13558
1	D	0.54	0/9943	0.79	0/13558
All	All	0.54	0/39772	0.79	0/54232

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 [i](#)

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	9728	0	8895	67	0
1	B	9728	0	8895	67	0
1	C	9728	0	8895	68	0
1	D	9728	0	8895	69	0
2	A	84	0	138	5	0
2	B	84	0	138	4	0
2	C	84	0	138	3	0
2	D	84	0	138	5	0
All	All	39248	0	36132	272	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 272 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:875:MET:HE1	1:B:910:LEU:CD2	2.01	0.91
1:D:875:MET:CE	1:D:910:LEU:CD2	2.49	0.91
1:A:875:MET:CE	1:A:910:LEU:CD2	2.49	0.91
1:B:875:MET:CE	1:B:910:LEU:CD2	2.49	0.90
1:C:875:MET:CE	1:C:910:LEU:CD2	2.49	0.90

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	1343/1494 (90%)	1305 (97%)	38 (3%)	0	100	100
1	B	1343/1494 (90%)	1305 (97%)	38 (3%)	0	100	100
1	C	1343/1494 (90%)	1305 (97%)	38 (3%)	0	100	100
1	D	1343/1494 (90%)	1305 (97%)	38 (3%)	0	100	100
All	All	5372/5976 (90%)	5220 (97%)	152 (3%)	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	868/1276 (68%)	868 (100%)	0	100	100
1	B	868/1276 (68%)	868 (100%)	0	100	100
1	C	868/1276 (68%)	868 (100%)	0	100	100
1	D	868/1276 (68%)	868 (100%)	0	100	100
All	All	3472/5104 (68%)	3472 (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. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1045	GLN
1	C	296	GLN
1	D	296	GLN
1	A	1045	GLN
1	A	296	GLN

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](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 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	$\# Z > 2$
2	CLR	D	6003	-	31,31,31	0.30	0	48,48,48	0.38	0
2	CLR	D	6002	-	31,31,31	0.30	0	48,48,48	0.55	0
2	CLR	A	1502	-	31,31,31	0.31	0	48,48,48	0.43	0
2	CLR	A	1503	-	31,31,31	0.30	0	48,48,48	0.55	0
2	CLR	A	1501	-	31,31,31	0.30	0	48,48,48	0.38	0
2	CLR	C	1503	-	31,31,31	0.30	0	48,48,48	0.55	0
2	CLR	B	1502	-	31,31,31	0.32	0	48,48,48	0.43	0
2	CLR	C	1502	-	31,31,31	0.32	0	48,48,48	0.43	0
2	CLR	B	1503	-	31,31,31	0.30	0	48,48,48	0.55	0
2	CLR	C	1501	-	31,31,31	0.30	0	48,48,48	0.38	0
2	CLR	B	1501	-	31,31,31	0.30	0	48,48,48	0.38	0
2	CLR	D	6001	-	31,31,31	0.31	0	48,48,48	0.43	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CLR	D	6003	-	-	7/10/68/68	0/4/4/4
2	CLR	D	6002	-	-	5/10/68/68	0/4/4/4
2	CLR	A	1502	-	-	6/10/68/68	0/4/4/4
2	CLR	A	1503	-	-	5/10/68/68	0/4/4/4
2	CLR	A	1501	-	-	7/10/68/68	0/4/4/4
2	CLR	C	1503	-	-	5/10/68/68	0/4/4/4
2	CLR	B	1502	-	-	5/10/68/68	0/4/4/4
2	CLR	C	1502	-	-	5/10/68/68	0/4/4/4
2	CLR	B	1503	-	-	5/10/68/68	0/4/4/4
2	CLR	C	1501	-	-	7/10/68/68	0/4/4/4
2	CLR	B	1501	-	-	7/10/68/68	0/4/4/4
2	CLR	D	6001	-	-	6/10/68/68	0/4/4/4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 70 torsion outliers are listed below:

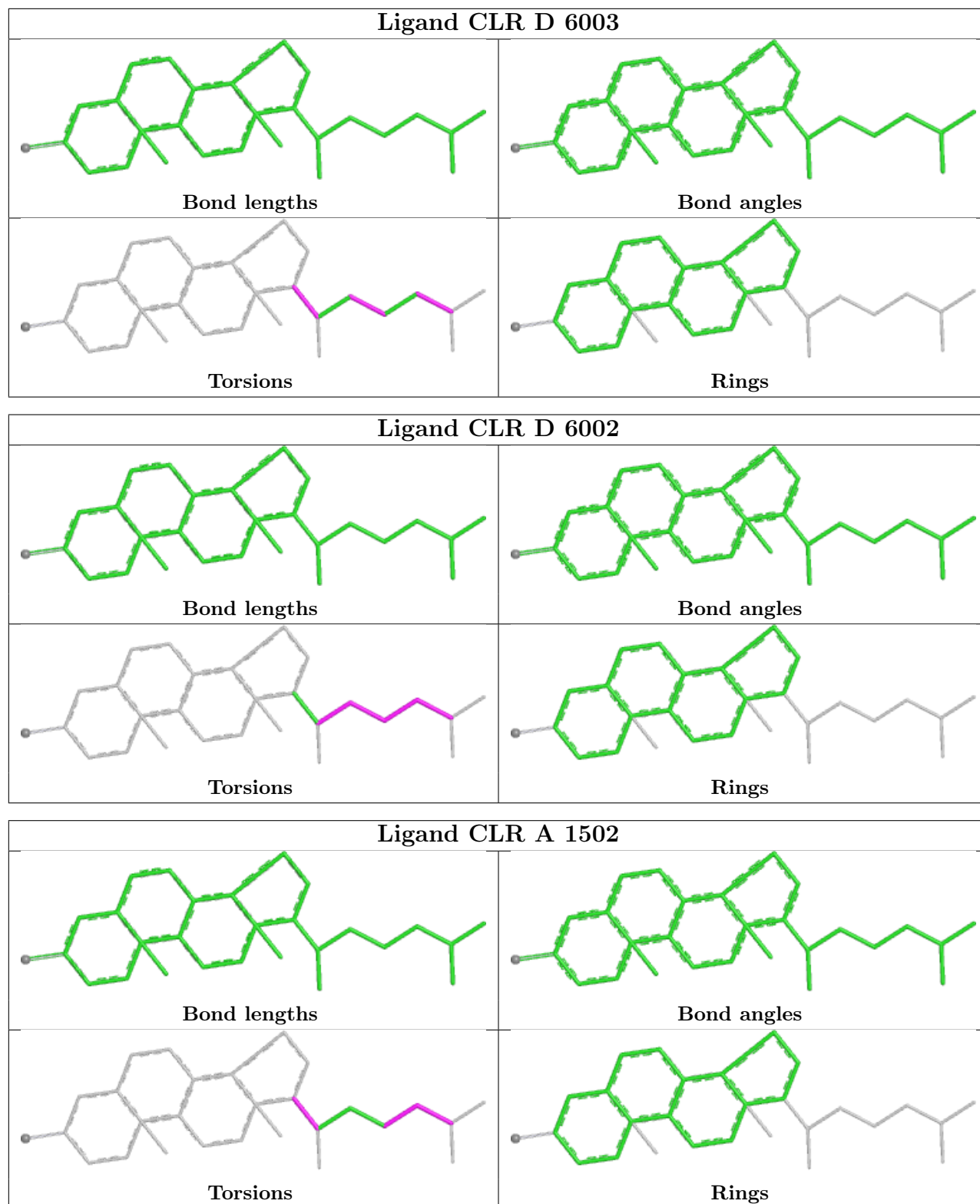
Mol	Chain	Res	Type	Atoms
2	A	1501	CLR	C13-C17-C20-C22
2	B	1501	CLR	C13-C17-C20-C22
2	C	1501	CLR	C13-C17-C20-C22
2	D	6003	CLR	C13-C17-C20-C22
2	A	1501	CLR	C13-C17-C20-C21

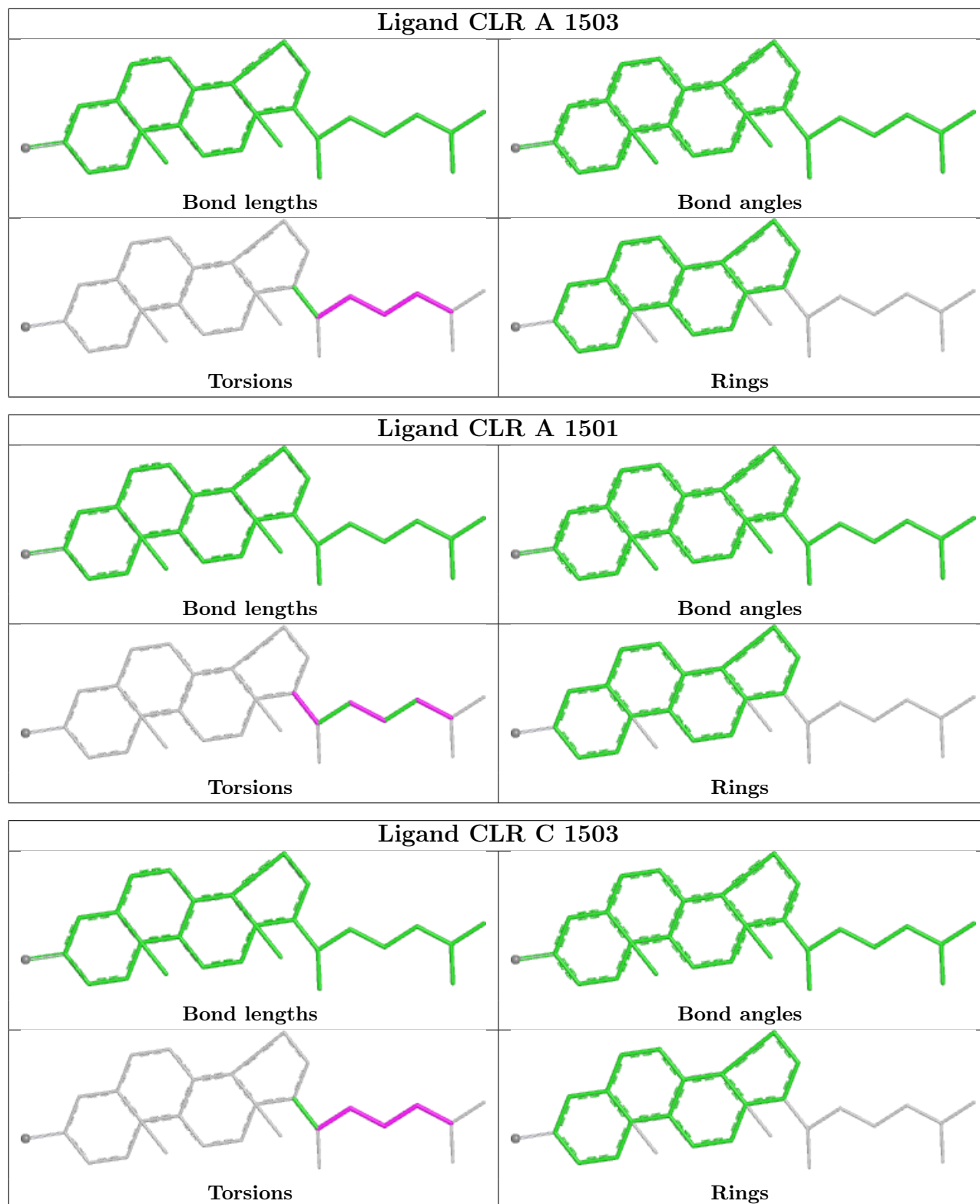
There are no ring outliers.

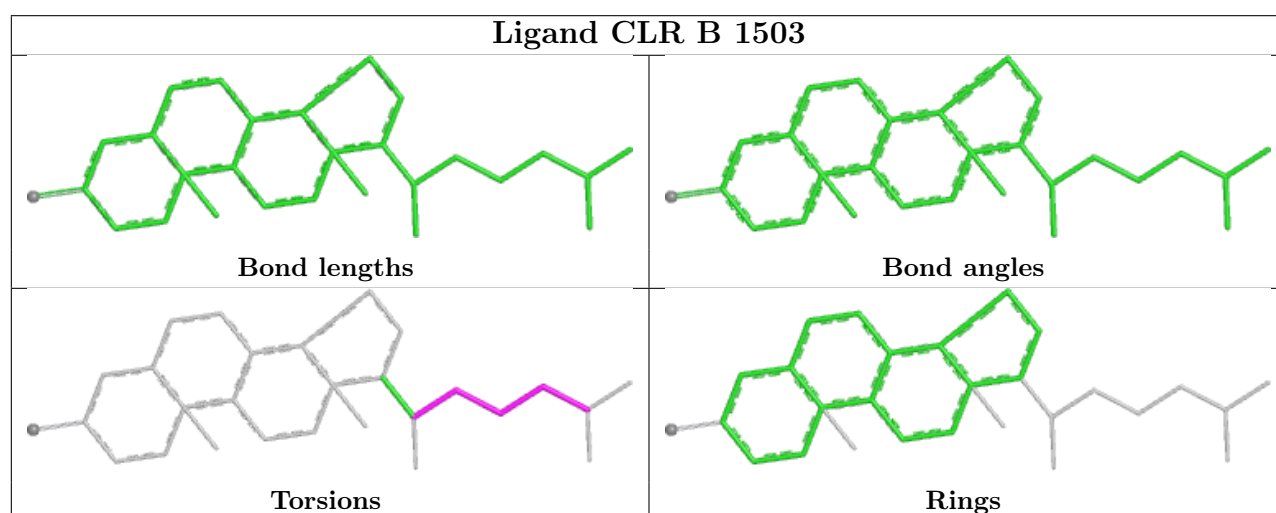
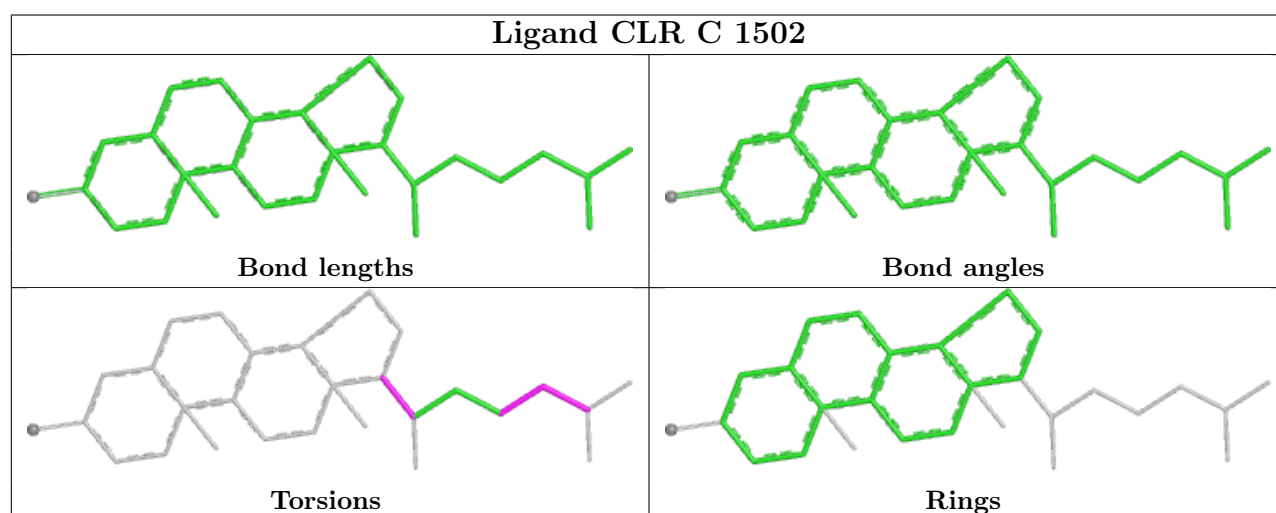
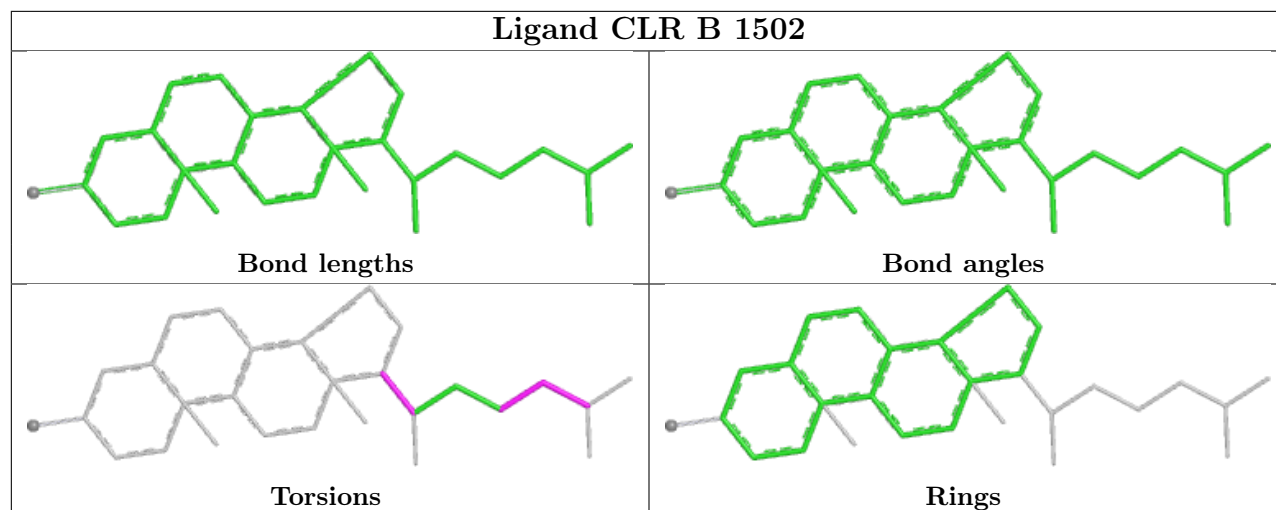
11 monomers are involved in 17 short contacts:

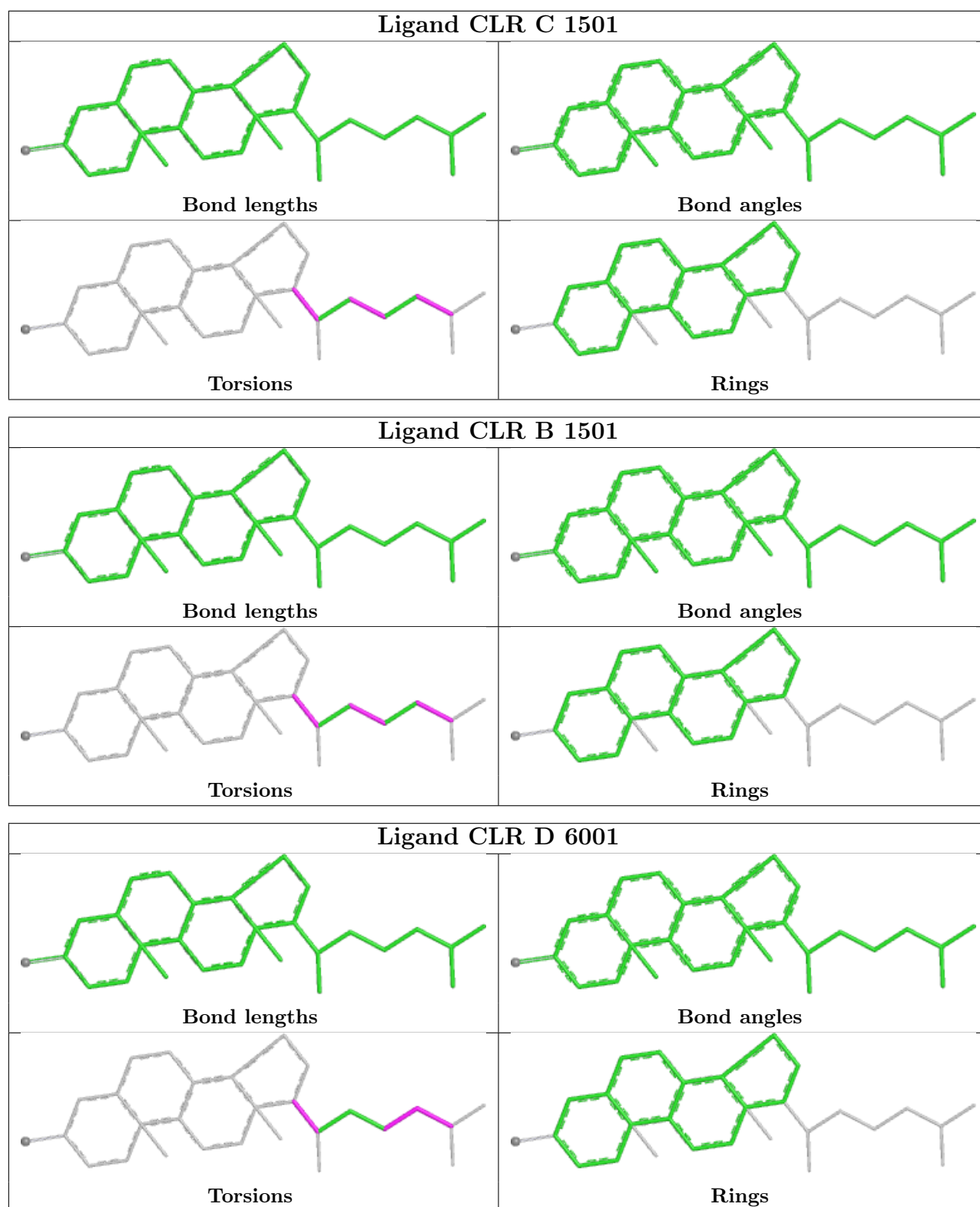
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	6003	CLR	2	0
2	D	6002	CLR	2	0
2	A	1502	CLR	1	0
2	A	1503	CLR	2	0
2	A	1501	CLR	2	0
2	C	1503	CLR	1	0
2	C	1502	CLR	1	0
2	B	1503	CLR	2	0
2	C	1501	CLR	1	0
2	B	1501	CLR	2	0
2	D	6001	CLR	1	0

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

There are no chain breaks in this entry.

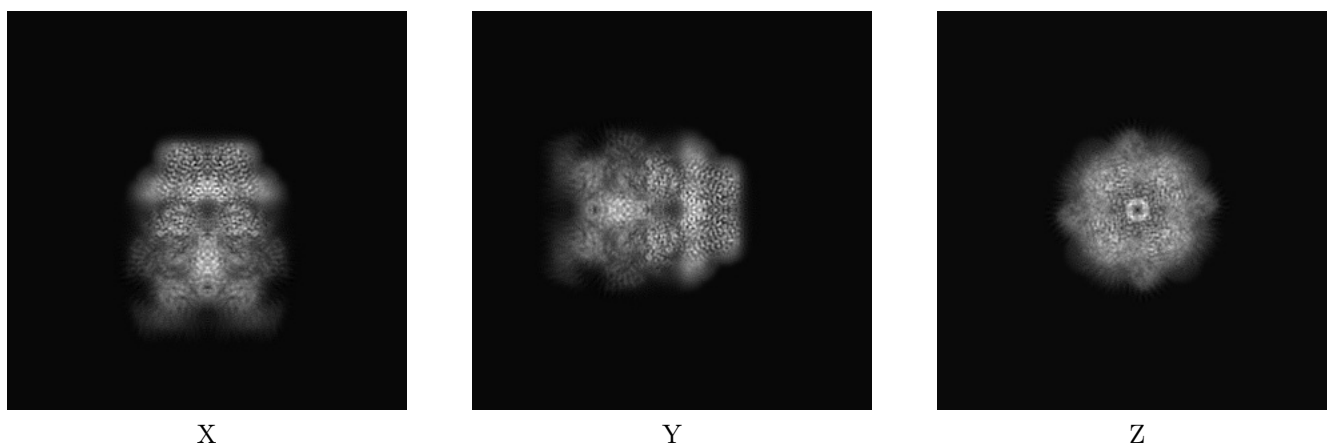
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40722. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections [i](#)

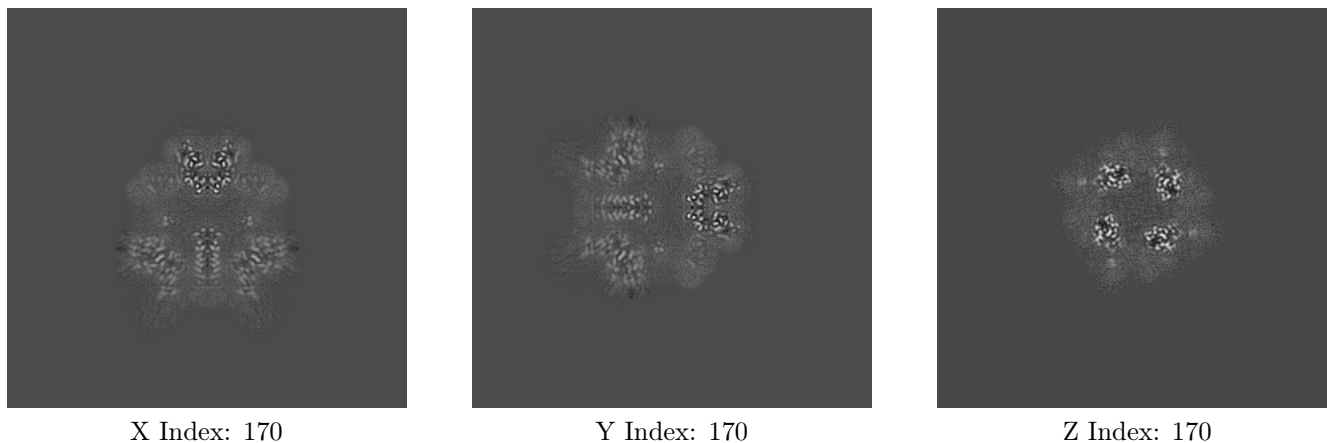
6.1.1 Primary map



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

6.2 Central slices [i](#)

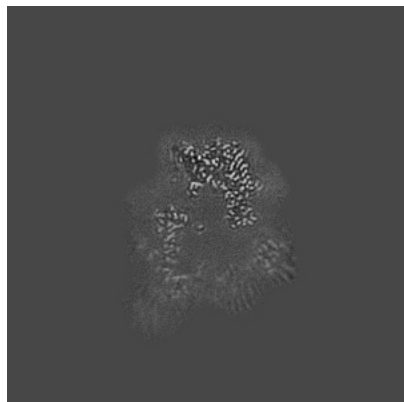
6.2.1 Primary map



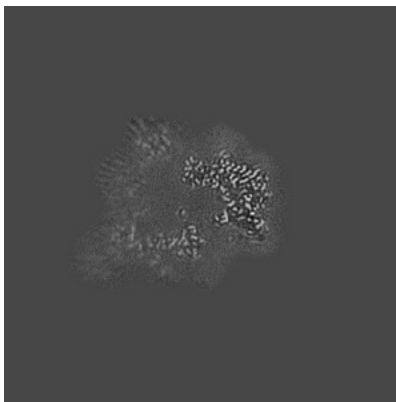
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

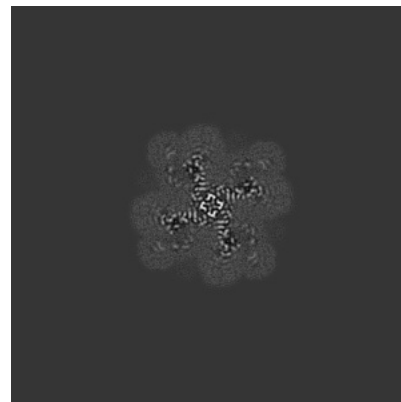
6.3.1 Primary map



X Index: 156



Y Index: 184

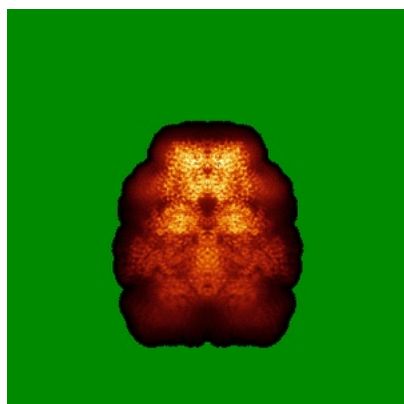


Z Index: 188

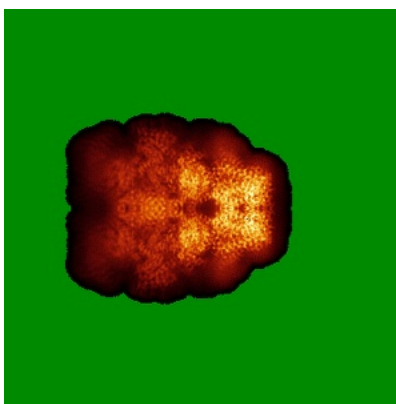
The images above show the largest variance slices of the map in three orthogonal directions.

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

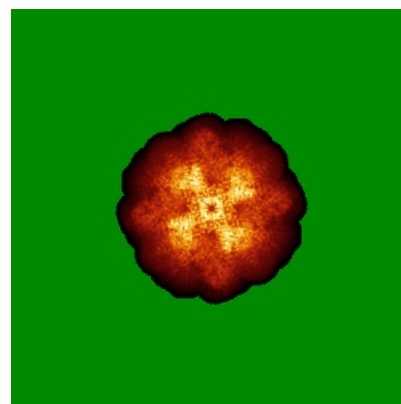
6.4.1 Primary map



X



Y

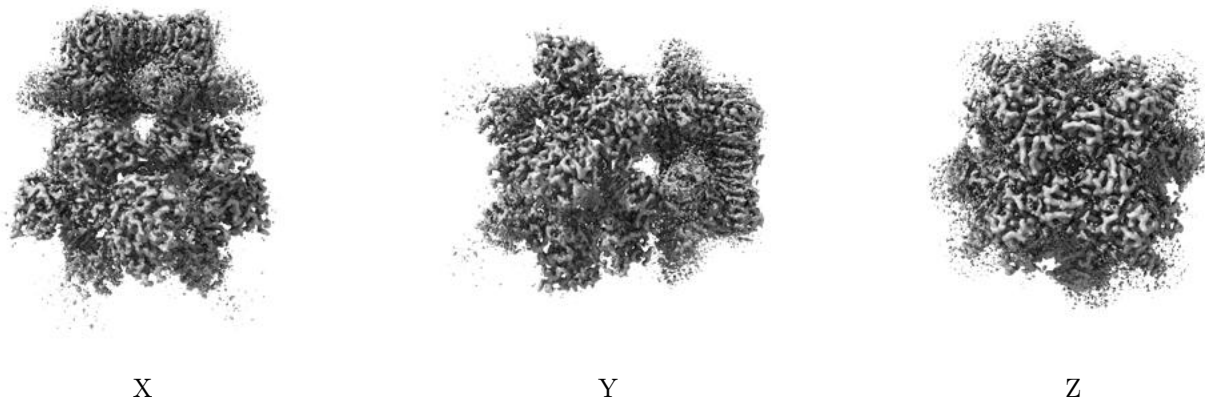


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 9.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

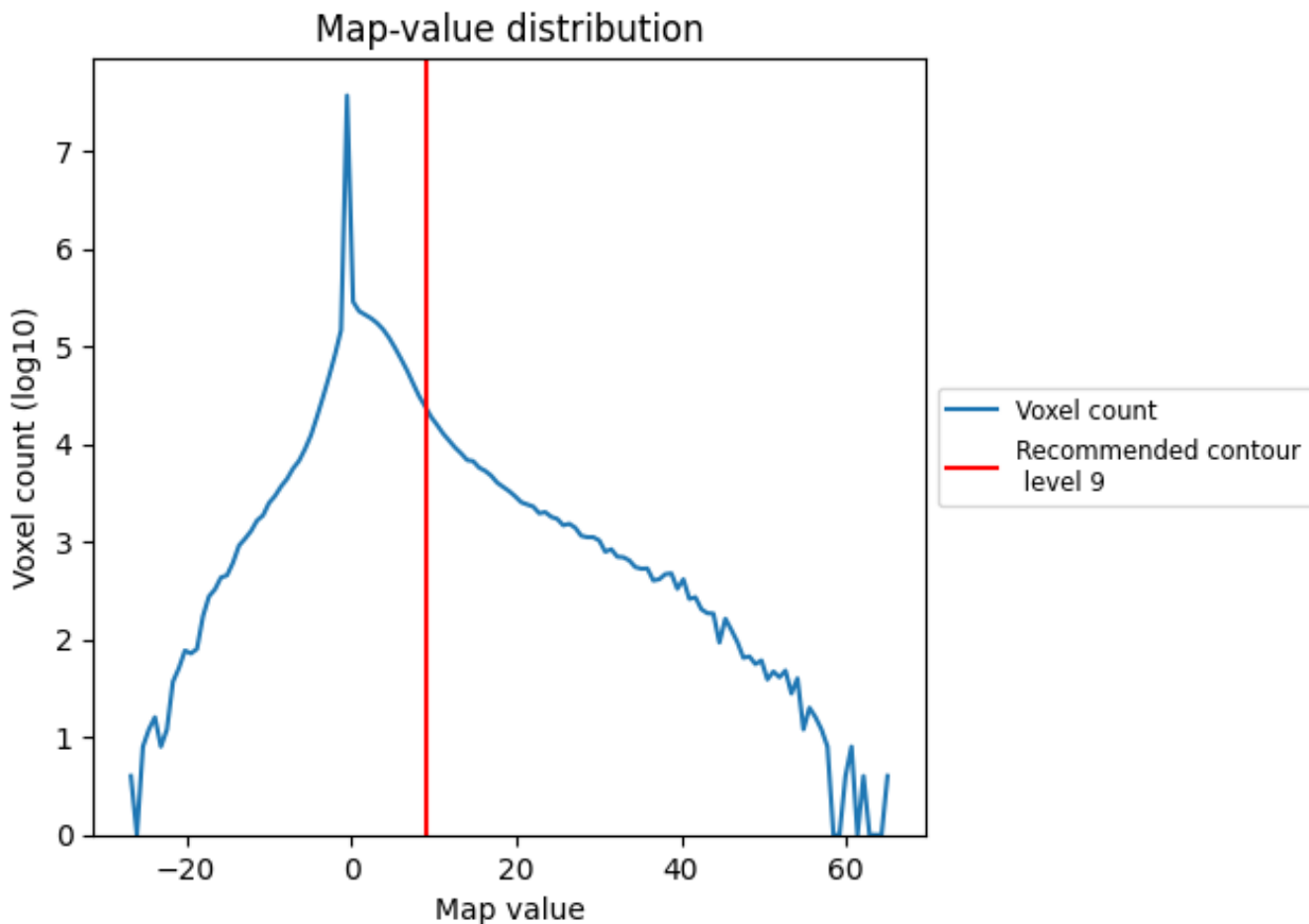
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

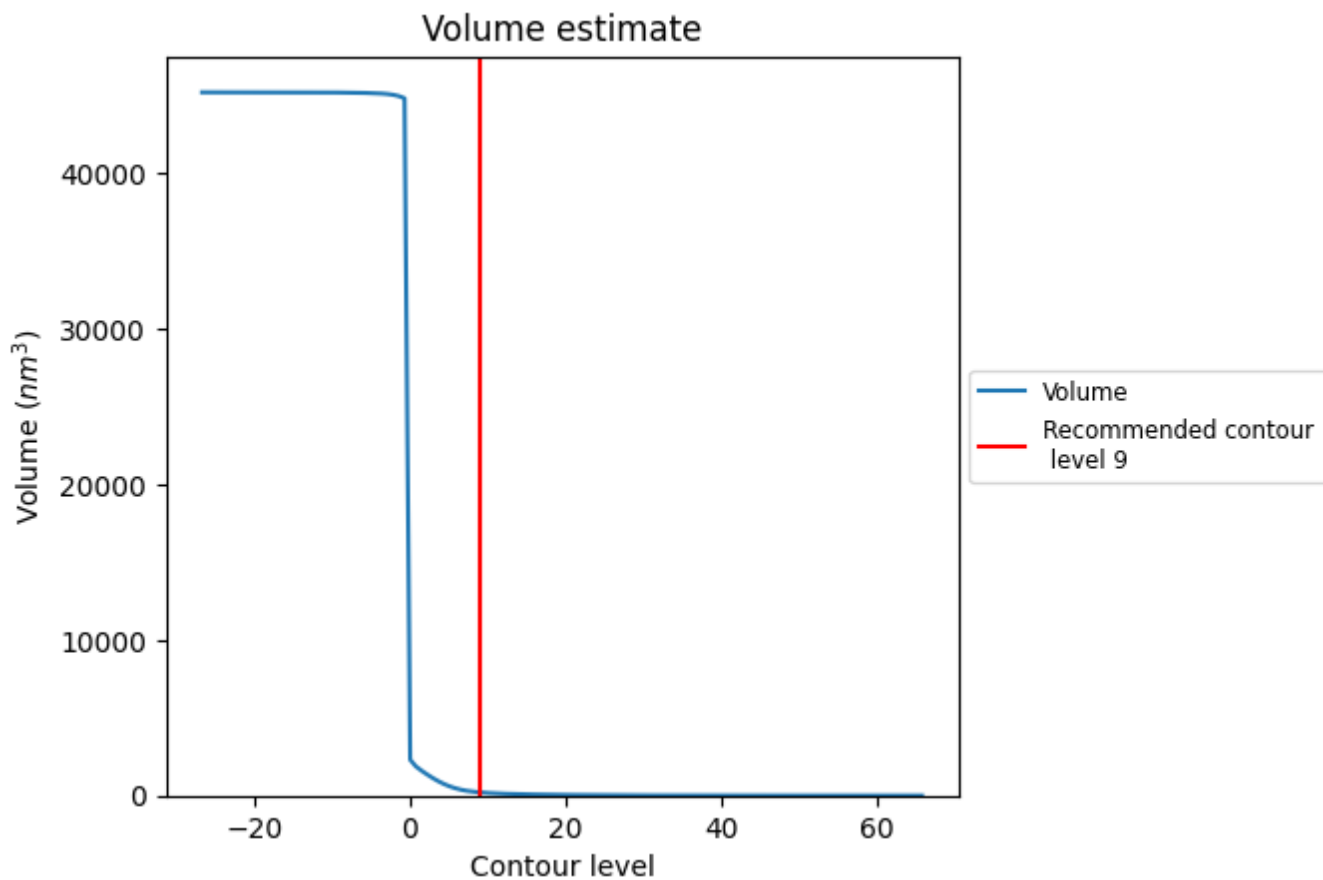
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

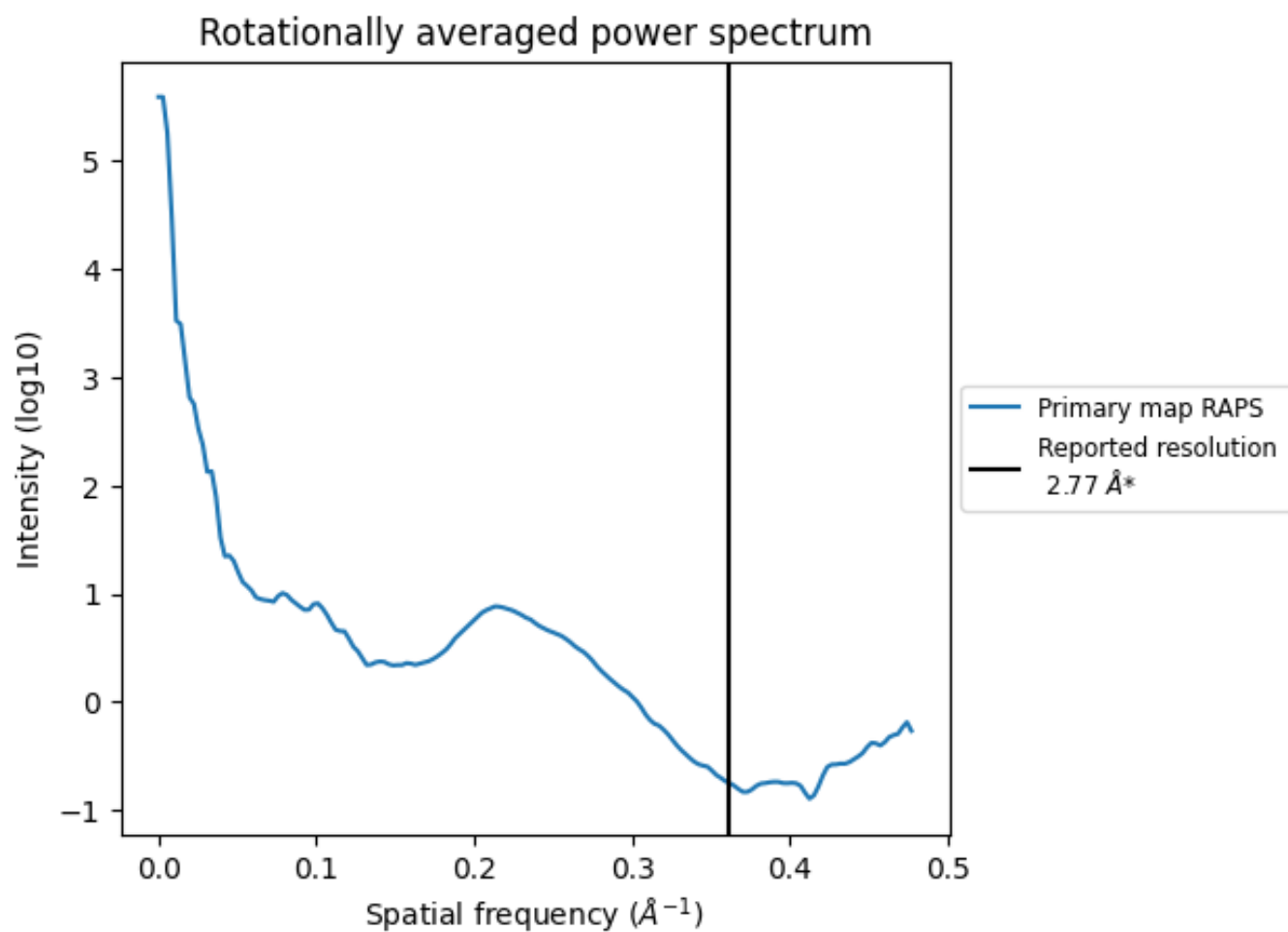
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 203 nm³; this corresponds to an approximate mass of 183 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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.361 Å⁻¹

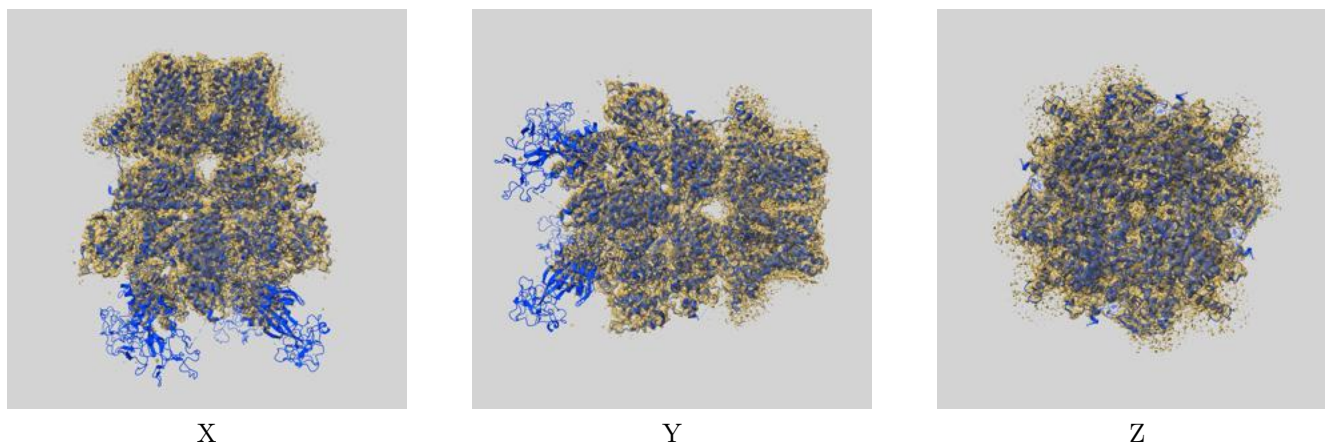
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

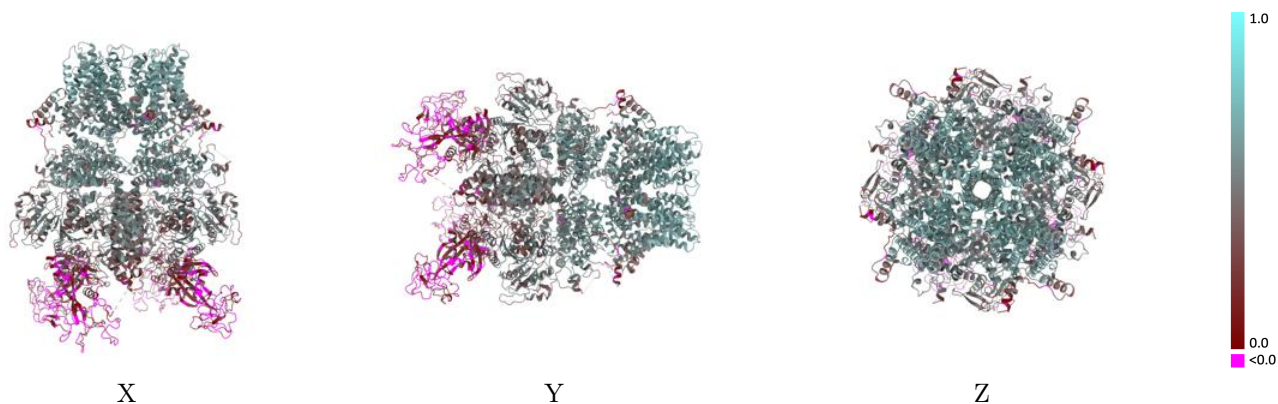
This section contains information regarding the fit between EMDB map EMD-40722 and PDB model 8SR8. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



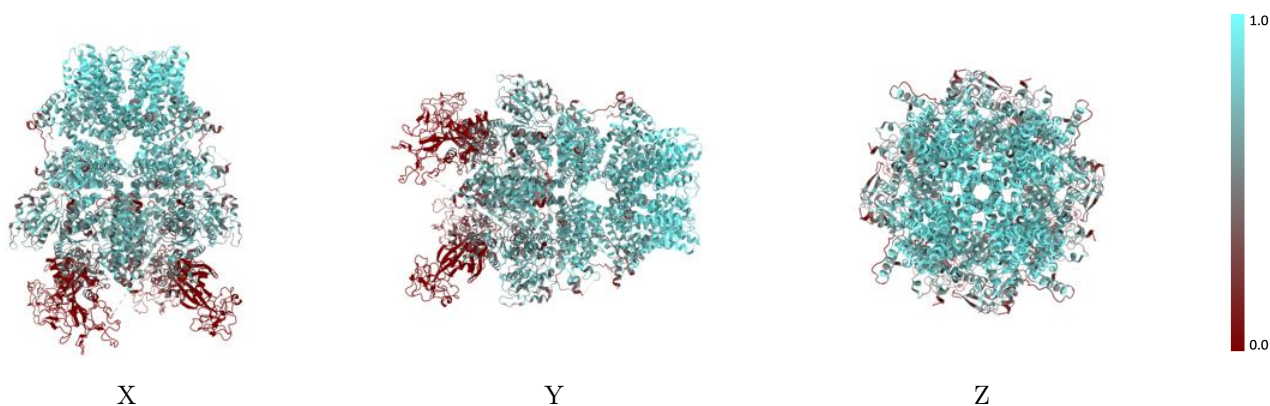
The images above show the 3D surface view of the map at the recommended contour level 9.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



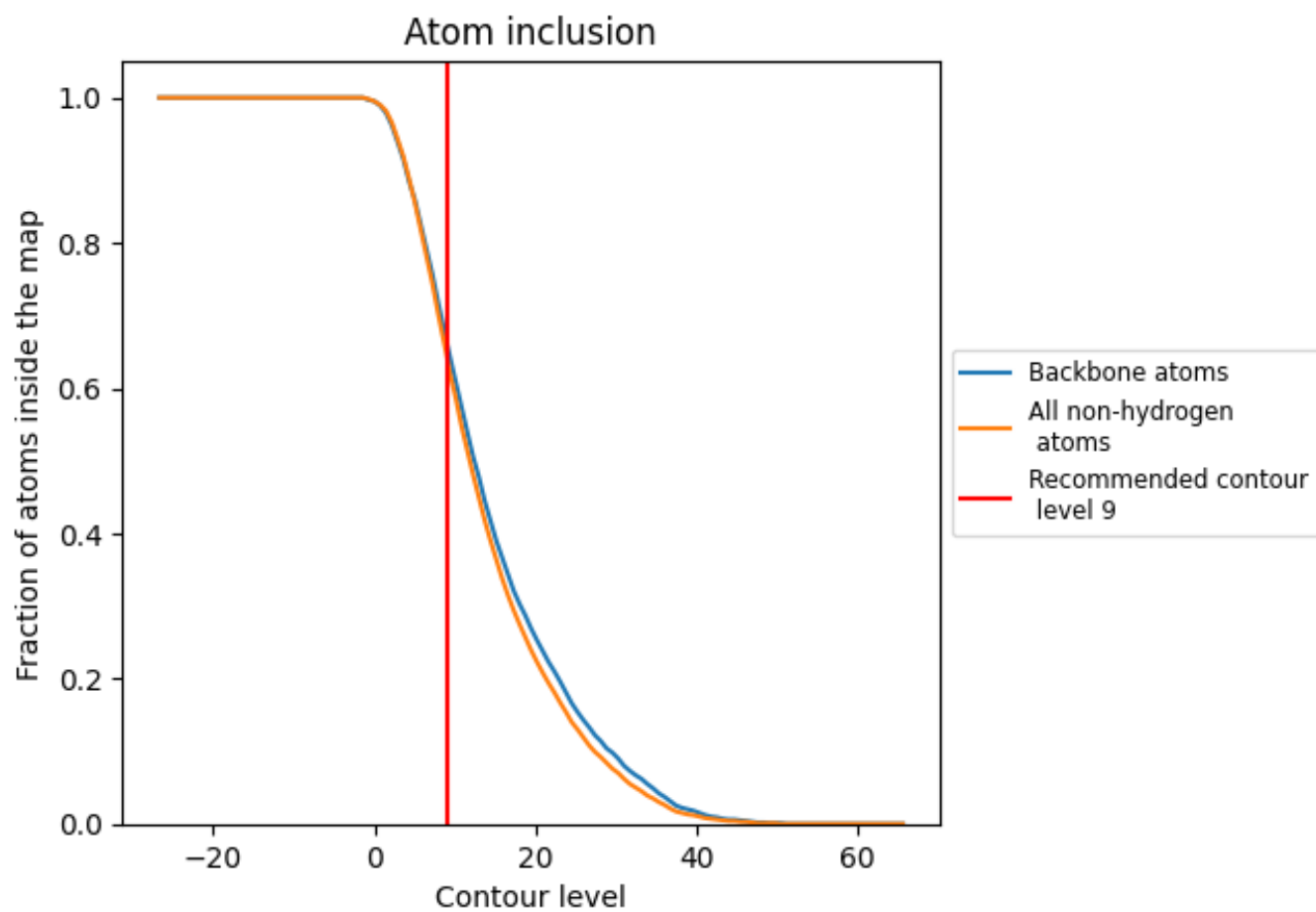
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (9).











9.4 Atom inclusion [i](#)



At the recommended contour level, 66% of all backbone atoms, 65% 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 (9) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6460	 0.4490
A	 0.6460	 0.4480
B	 0.6470	 0.4480
C	 0.6440	 0.4490
D	 0.6460	 0.4490

