



wwPDB EM Validation Summary Report ⓘ

Mar 12, 2026 – 09:53 AM UTC

PDB ID : 8SR8 / pdb_00008sr8
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:

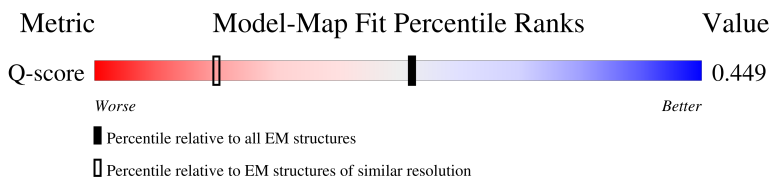
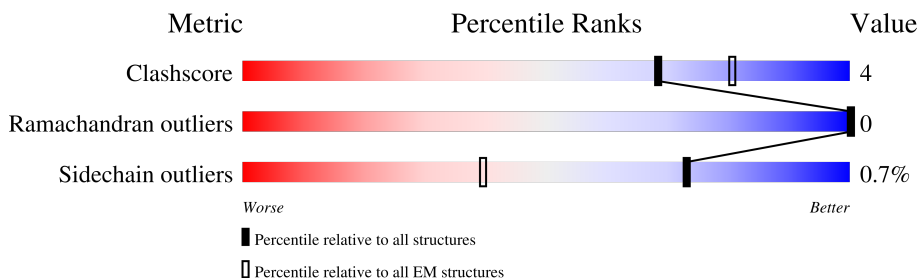
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10695 (2.27 - 3.27)

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	<p>26% (red), 83% (green), 7% (yellow), 9% (grey)</p>
1	B	1494	<p>25% (red), 83% (green), 7% (yellow), 9% (grey)</p>
1	C	1494	<p>26% (red), 83% (green), 7% (yellow), 9% (grey)</p>
1	D	1494	<p>25% (red), 83% (green), 7% (yellow), 9% (grey)</p>

2 Entry composition [i](#)

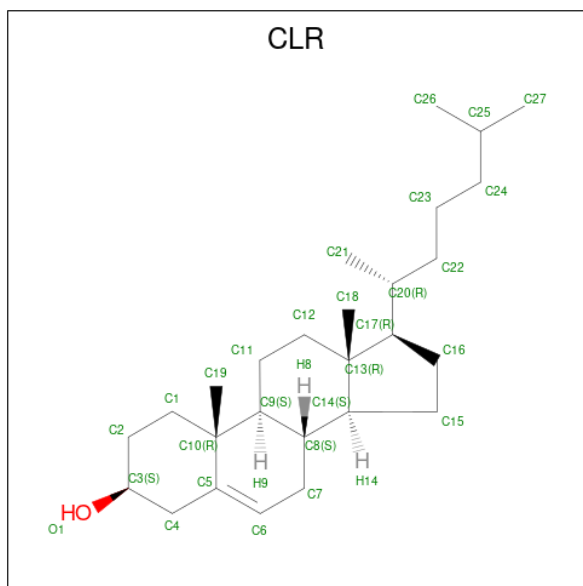
There are 2 unique types of molecules in this entry. The entry contains 39248 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: CLR) (formula: C₂₇H₄₆O) (labeled as "Ligand of Interest" by depositor).

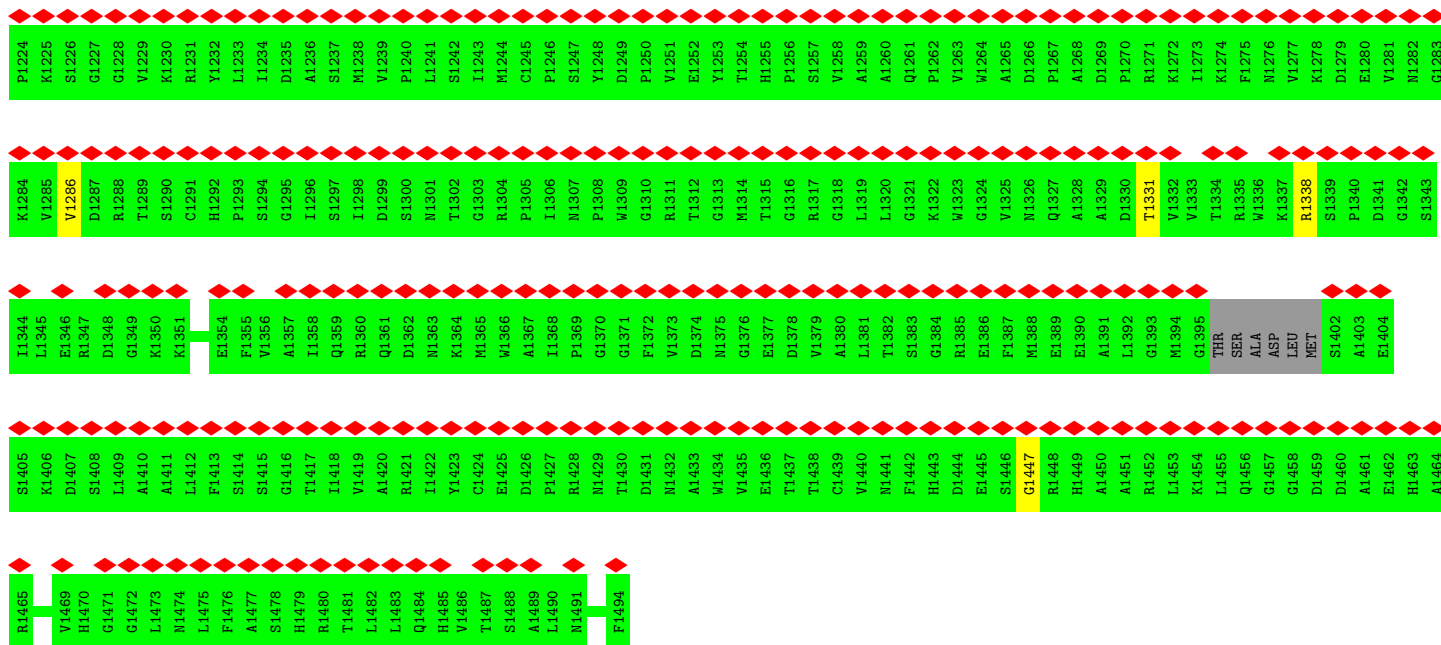


Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
2	A	1	Total 28	C 27	O 1	0
2	A	1	Total 28	C 27	O 1	0

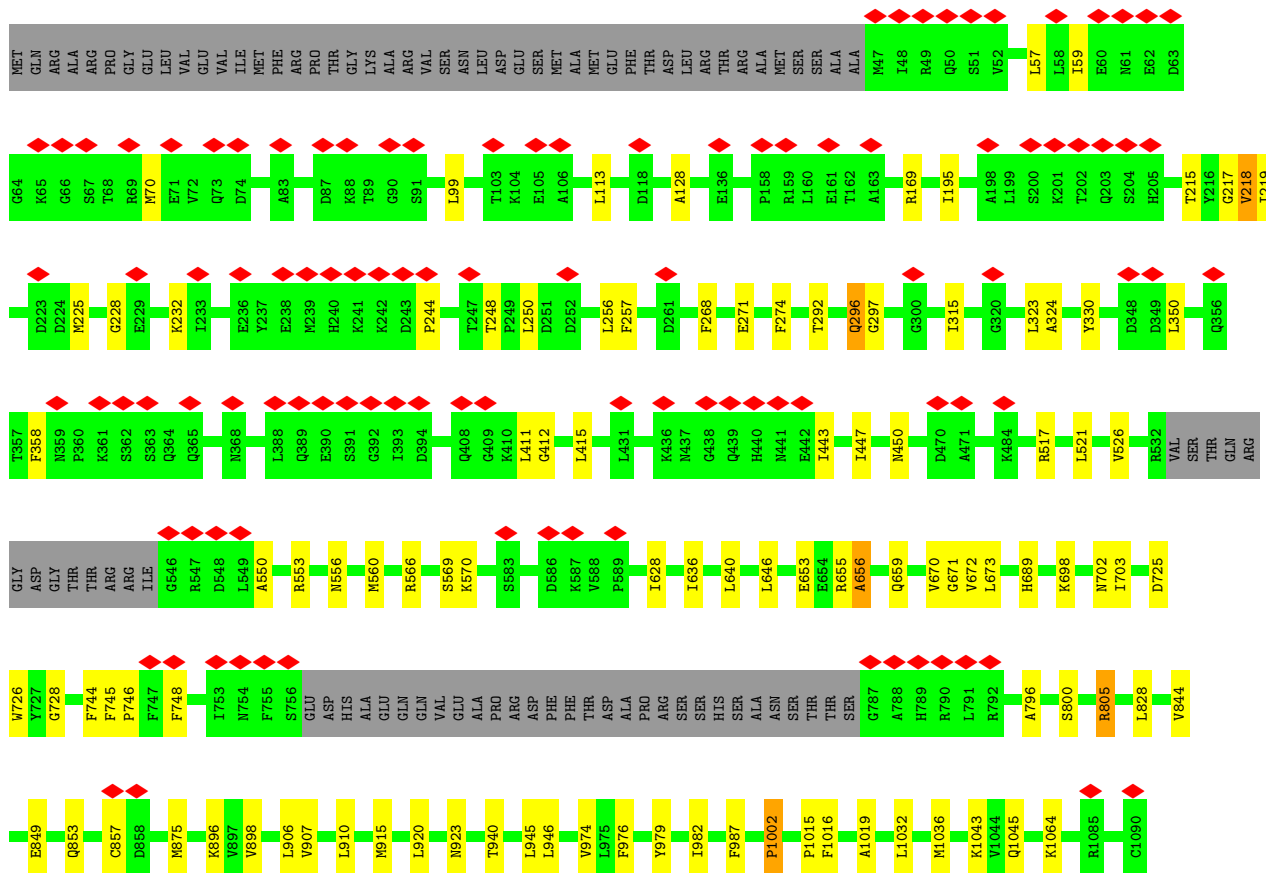
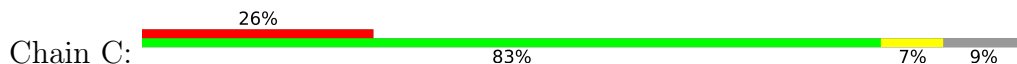
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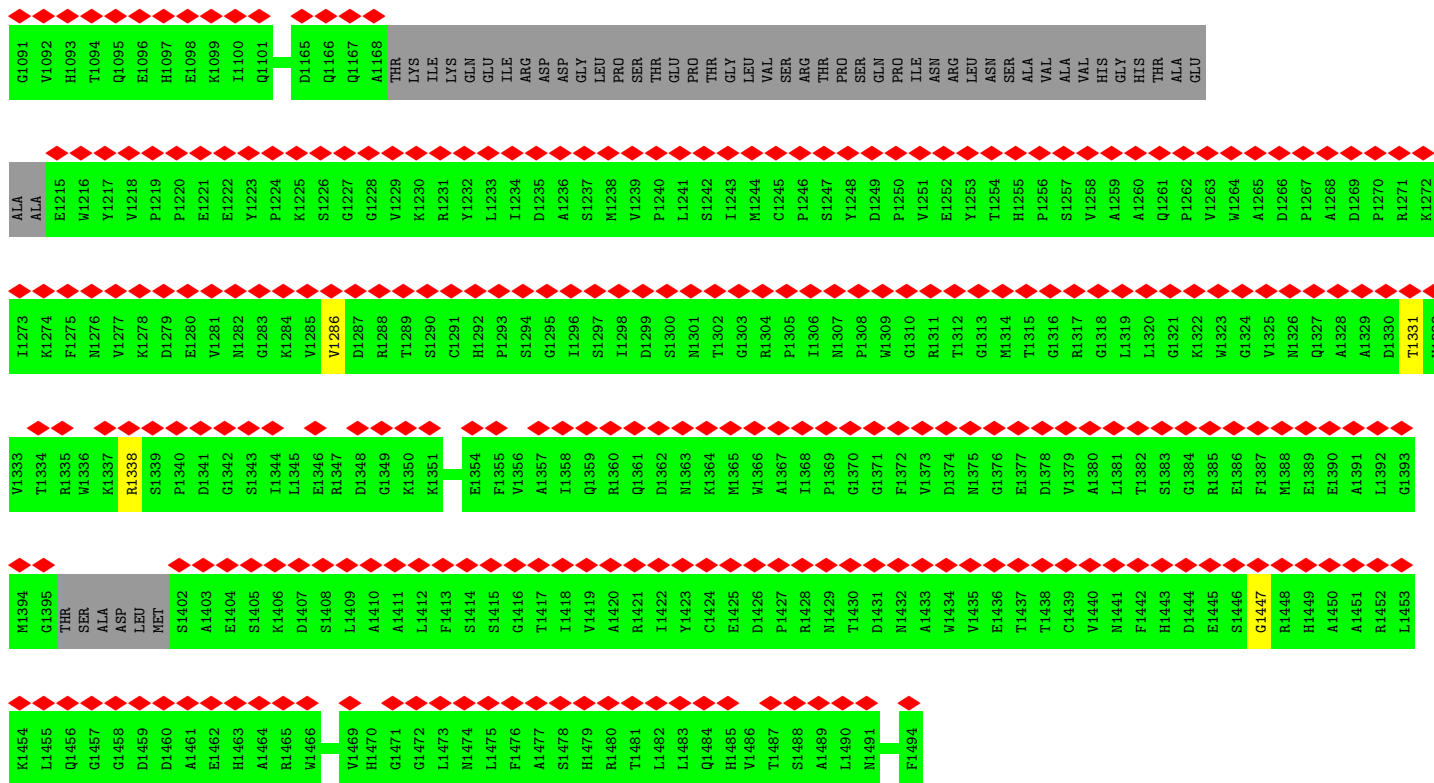
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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
2	A	1	28	27	1	0
2	B	1	28	27	1	0
2	B	1	28	27	1	0
2	B	1	28	27	1	0
2	C	1	28	27	1	0
2	C	1	28	27	1	0
2	C	1	28	27	1	0
2	D	1	28	27	1	0
2	D	1	28	27	1	0
2	D	1	28	27	1	0

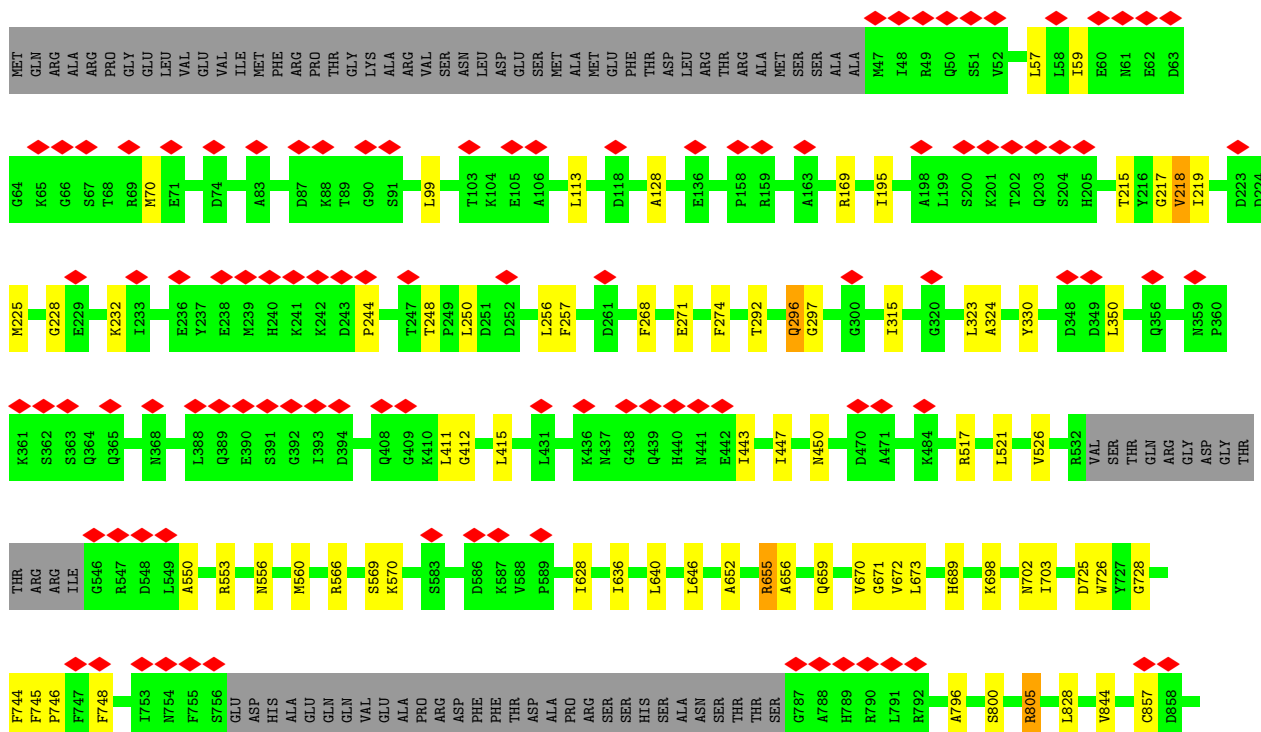
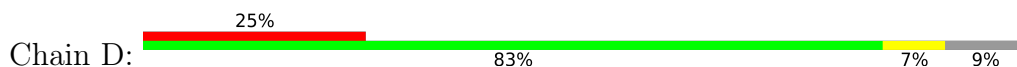


● Molecule 1: TRPM2 chanzyme





• Molecule 1: TRPM2 chanzyme



H875	H896	H897	H898	L906	L907	L910	H915	L920	H923	T940	L945	L946	V974	L975	F976	H979	I982	F987	T1001	P1002	P1015	F1016	A1019	L1032	M1036	K1043	V1044	Q1045	K1064	R1085	C1090	G1091	V1092	H1093	T1094	Q1095	E1096	H1097																					
E1098	K1099	I1100	Q1101	D1165	Q1166	Q1167	A1168	THR	LYS	ILE	LYS	GLN	GLU	ILE	ARG	ASP	ASP	GLY	LEU	PRO	SER	THR	THR	GLN	ILE	ASN	ARG	LEU	ASN	ALA	VAL	ALA	VAL	HIS	HIS	THR	ALA	GLU	ALA	ALA	E1215	W1216	Y1217	V1218	P1219														
P1220	E1221	E1222	Y1223	P1224	K1225	S1226	G1227	G1228	V1229	K1230	R1231	Y1232	L1233	I1234	D1235	A1236	S1237	M1238	V1239	P1240	L1241	S1242	I1243	M1244	C1245	P1246	S1247	Y1248	D1249	P1250	V1251	E1252	Y1253	T1254	H1255	P1256	S1257	V1258	A1259	A1260	Q1261	P1262	V1263	A1264	M1265	D1266	P1267	A1268	D1269	P1270	R1271	I1272	I1273	K1274	F1275	M1276	V1277	K1278	D1279
E1280	V1281	N1282	G1283	V1284	V1285	V1286	D1287	R1288	T1289	S1290	C1291	H1292	P1293	S1294	G1295	I1296	S1297	I1298	D1299	S1300	N1301	T1302	G1303	R1304	P1305	I1306	N1307	P1308	M1309	G1310	R1311	T1312	G1313	M1314	T1315	G1316	R1317	G1318	L1319	L1320	G1321	K1322	M1323	G1324	M1325	N1326	Q1327	A1328	A1329	D1330	T1331	V1332	V1333	T1334	R1335	M1336	K1337	R1338	S1339
P1340	D1341	G1342	S1343	I1344	L1345	E1346	R1347	D1348	G1349	K1350	K1351	E1354	F1355	V1356	A1357	I1358	Q1359	R1360	Q1361	D1362	M1363	K1364	M1365	W1366	A1367	I1368	P1369	G1370	G1371	F1372	V1373	D1374	M1375	G1376	E1377	D1378	V1379	A1380	L1381	T1382	S1383	G1384	R1385	E1386	F1387	M1388	E1389	E1390	A1391	L1392	G1393	M1394	G1395	THR	SER	ALA	ASP	LEU	
MET	S1402	A1403	E1404	S1405	K1406	D1407	S1408	L1409	A1410	A1411	L1412	F1413	S1414	S1415	G1416	T1417	I1418	V1419	A1420	R1421	I1422	Y1423	C1424	E1425	D1426	P1427	R1428	N1429	T1430	D1431	N1432	A1433	W1434	V1435	E1436	T1437	T1438	C1439	V1440	N1441	F1442	H1443	D1444	E1445	S1446	G1447	R1448	H1449	A1450	A1451	R1452	L1453	K1454	L1455	Q1456	G1457	G1458	D1459	D1460
A1461	E1462	H1463	A1464	R1465	V1469	H1470	G1471	G1472	L1473	N1474	L1475	F1476	A1477	S1478	H1479	R1480	T1481	L1482	L1483	Q1484	H1485	V1486	T1487	S1488	A1489	L1490	N1491	F1494																															

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	0.64	0/9943	1.20	26/13558 (0.2%)
1	B	0.64	0/9943	1.20	26/13558 (0.2%)
1	C	0.64	0/9943	1.20	26/13558 (0.2%)
1	D	0.64	0/9943	1.20	26/13558 (0.2%)
All	All	0.64	0/39772	1.20	104/54232 (0.2%)

There are no bond length outliers.

The worst 5 of 104 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1002	PRO	N-CA-C	7.46	123.91	113.53
1	B	1002	PRO	N-CA-C	7.46	123.91	113.53
1	C	1002	PRO	N-CA-C	7.46	123.91	113.53
1	D	1002	PRO	N-CA-C	7.46	123.91	113.53
1	A	1286	VAL	CB-CA-C	6.30	120.52	110.82

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	69	0
1	B	9728	0	8895	68	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	9728	0	8895	71	0
1	D	9728	0	8895	72	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	281	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 281 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:C:875:MET:HE3	1:C:910:LEU:HD21	1.44	0.98
1:A:875:MET:HE3	1:A:910:LEU:HD21	1.44	0.98
1:C:875:MET:HE3	1:C:910:LEU:CD2	1.96	0.96
1:B:875:MET:HE3	1:B:910:LEU:CD2	1.96	0.95
1:D:875:MET:HE3	1:D:910:LEU:HD21	1.44	0.95

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%)	862 (99%)	6 (1%)	76	90
1	B	868/1276 (68%)	862 (99%)	6 (1%)	76	90
1	C	868/1276 (68%)	863 (99%)	5 (1%)	78	91
1	D	868/1276 (68%)	862 (99%)	6 (1%)	76	90
All	All	3472/5104 (68%)	3449 (99%)	23 (1%)	73	90

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	646	LEU
1	D	70	MET
1	C	915	MET
1	D	566	ARG
1	B	70	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 54 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	296	GLN
1	C	957	GLN
1	D	957	GLN
1	C	307	GLN
1	C	677	HIS

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	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	1501	-	31,31,31	0.30	0	48,48,48	0.38	0
2	CLR	A	1501	-	31,31,31	0.30	0	48,48,48	0.38	0
2	CLR	C	1502	-	31,31,31	0.32	0	48,48,48	0.43	0
2	CLR	D	6002	-	31,31,31	0.30	0	48,48,48	0.55	0
2	CLR	D	6003	-	31,31,31	0.30	0	48,48,48	0.38	0
2	CLR	A	1502	-	31,31,31	0.31	0	48,48,48	0.43	0
2	CLR	D	6001	-	31,31,31	0.31	0	48,48,48	0.43	0
2	CLR	B	1501	-	31,31,31	0.30	0	48,48,48	0.38	0
2	CLR	A	1503	-	31,31,31	0.30	0	48,48,48	0.55	0
2	CLR	B	1503	-	31,31,31	0.30	0	48,48,48	0.55	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CLR	C	1503	-	-	5/10/68/68	0/4/4/4
2	CLR	B	1502	-	-	5/10/68/68	0/4/4/4

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

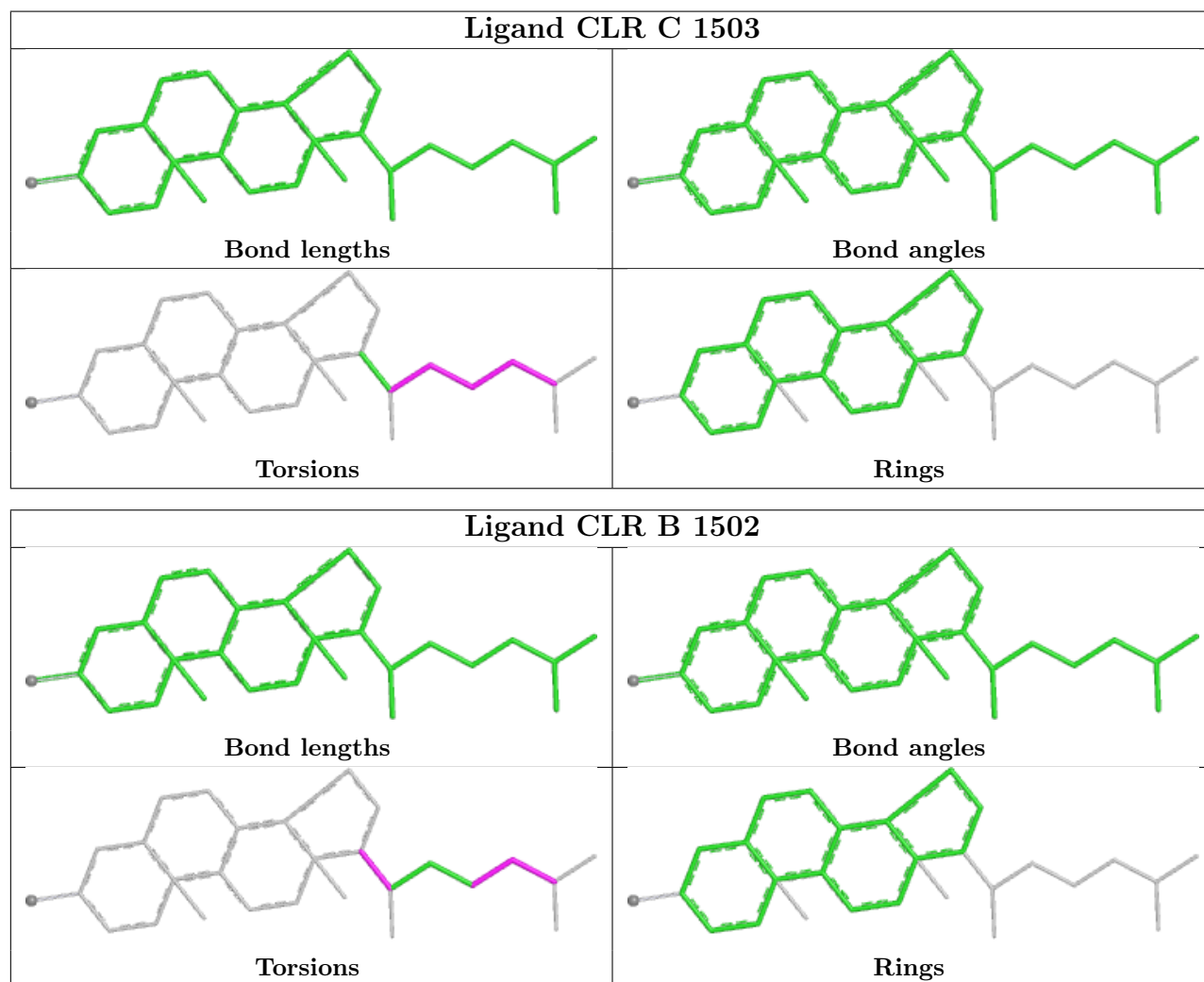
Mol	Chain	Res	Type	Atoms
2	A	1501	CLR	C13-C17-C20-C22
2	B	1501	CLR	C13-C17-C20-C22
2	C	1501	CLR	C13-C17-C20-C22
2	D	6003	CLR	C13-C17-C20-C22
2	A	1501	CLR	C13-C17-C20-C21

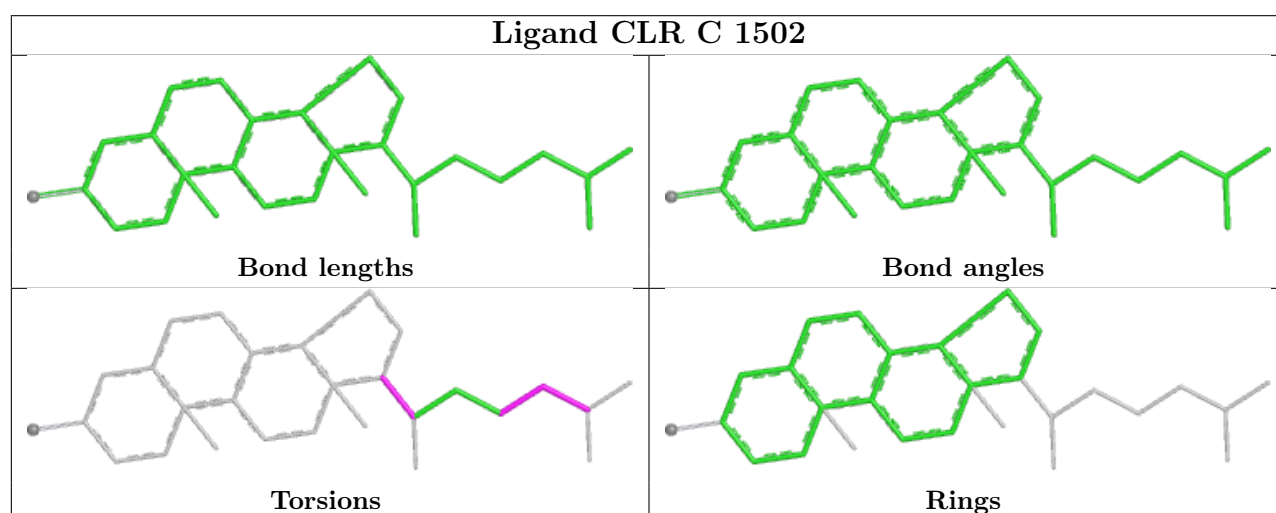
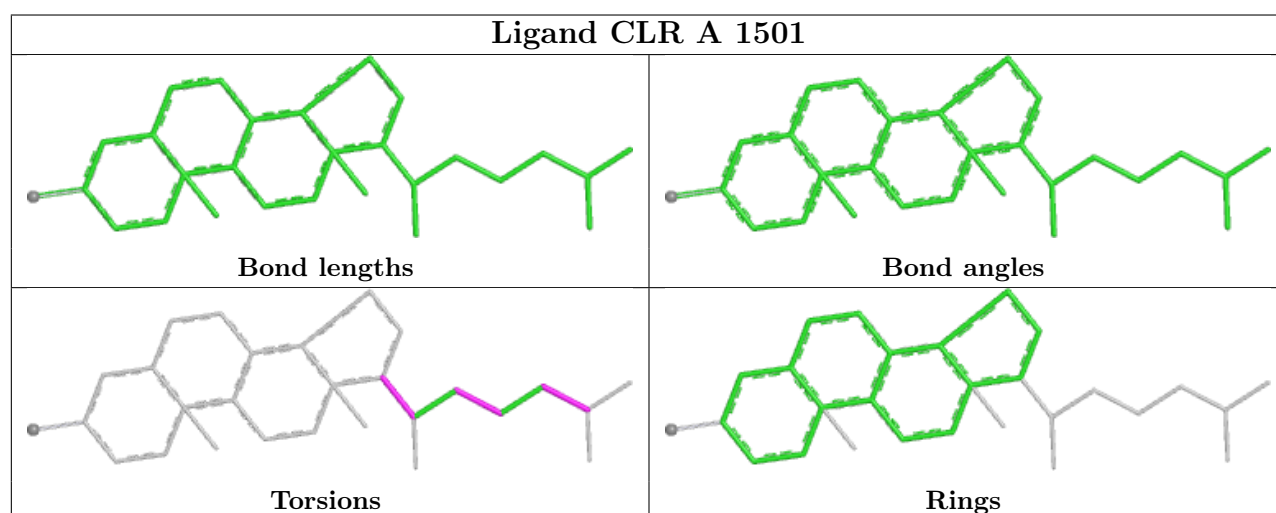
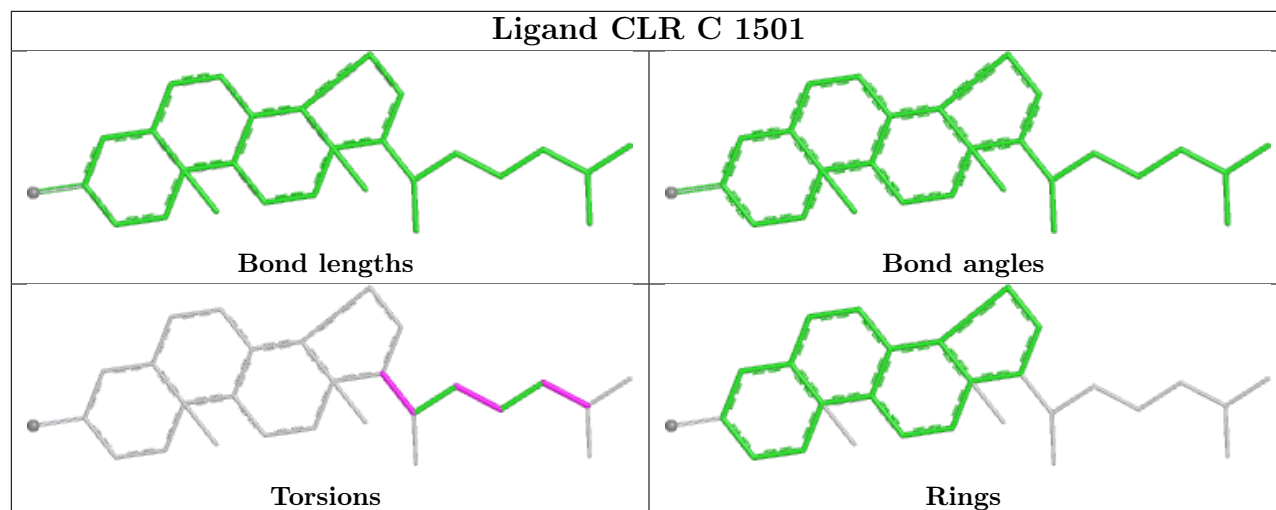
There are no ring outliers.

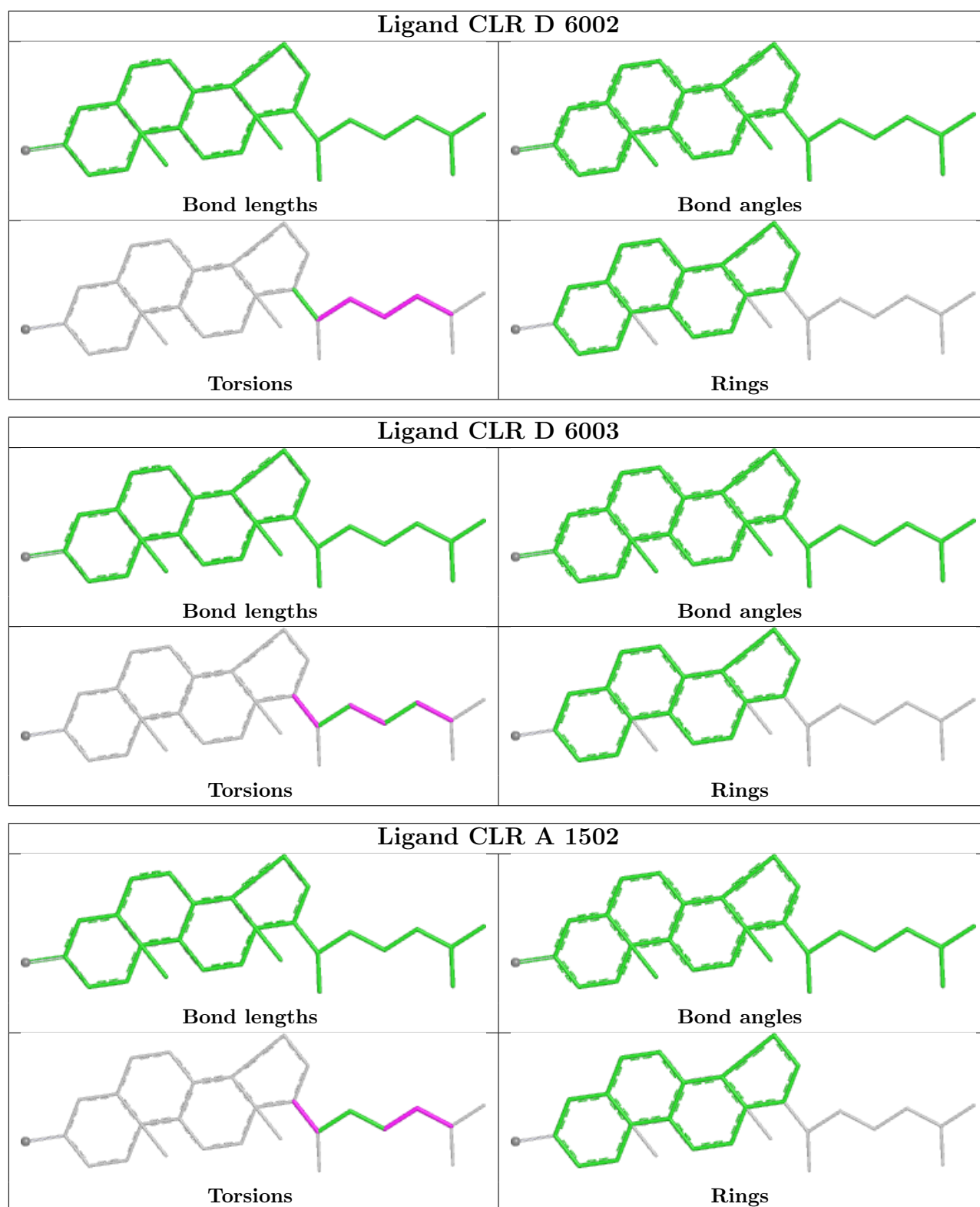
11 monomers are involved in 17 short contacts:

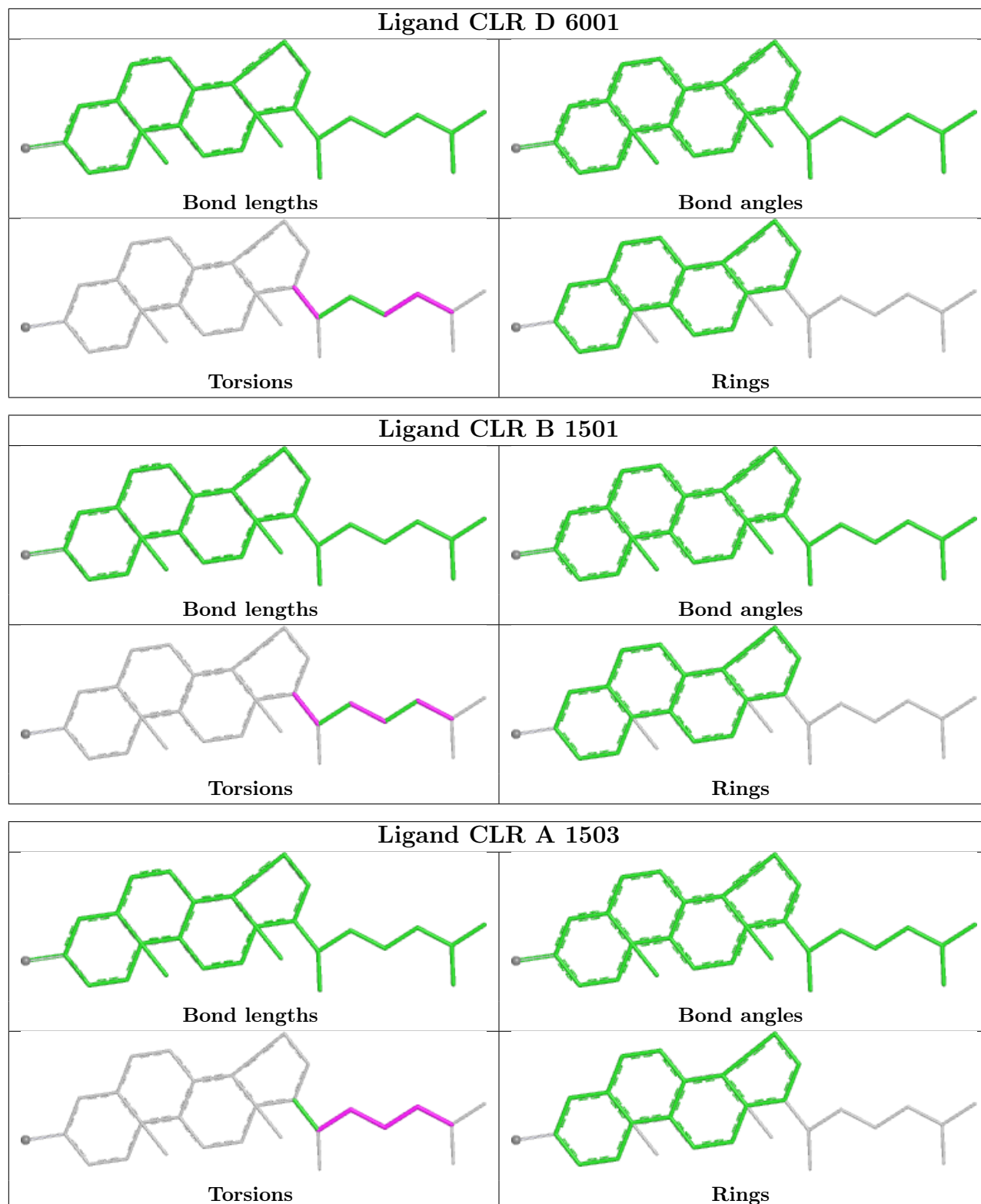
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1503	CLR	1	0
2	C	1501	CLR	1	0
2	A	1501	CLR	2	0
2	C	1502	CLR	1	0
2	D	6002	CLR	2	0
2	D	6003	CLR	2	0
2	A	1502	CLR	1	0
2	D	6001	CLR	1	0
2	B	1501	CLR	2	0
2	A	1503	CLR	2	0
2	B	1503	CLR	2	0

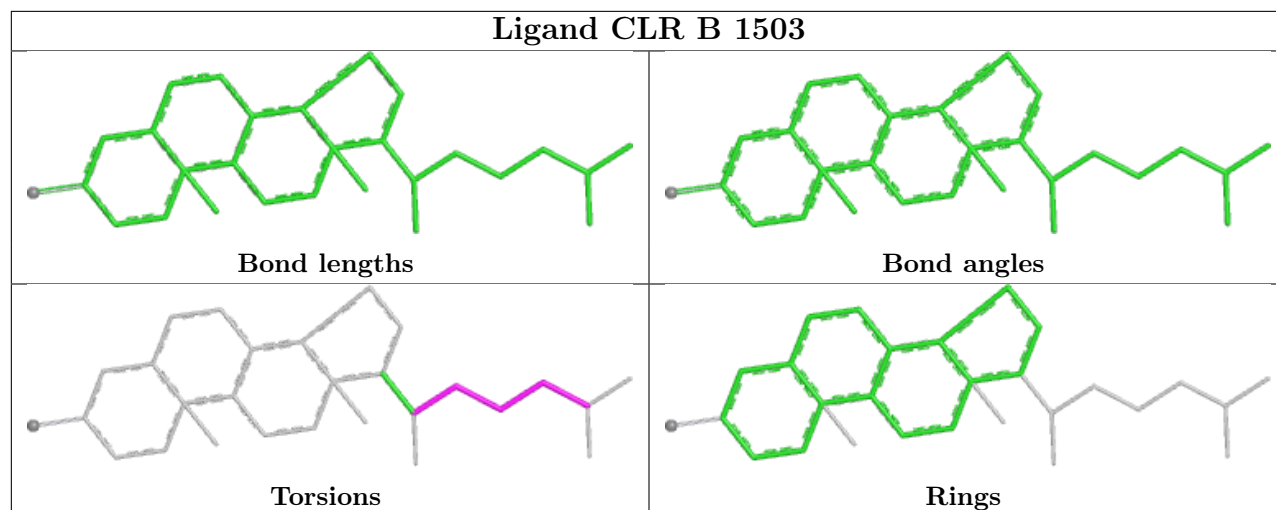
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

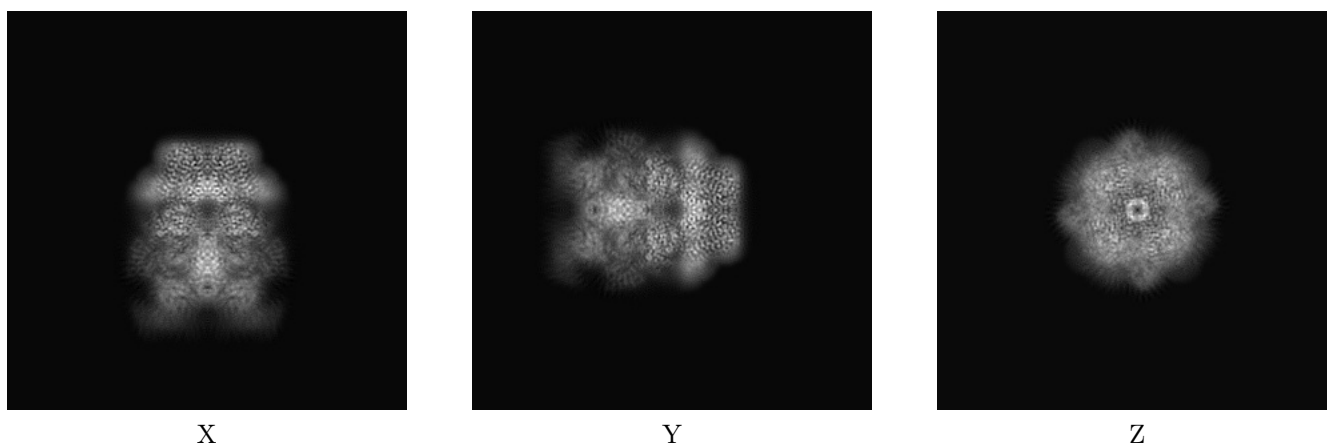
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-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](#)

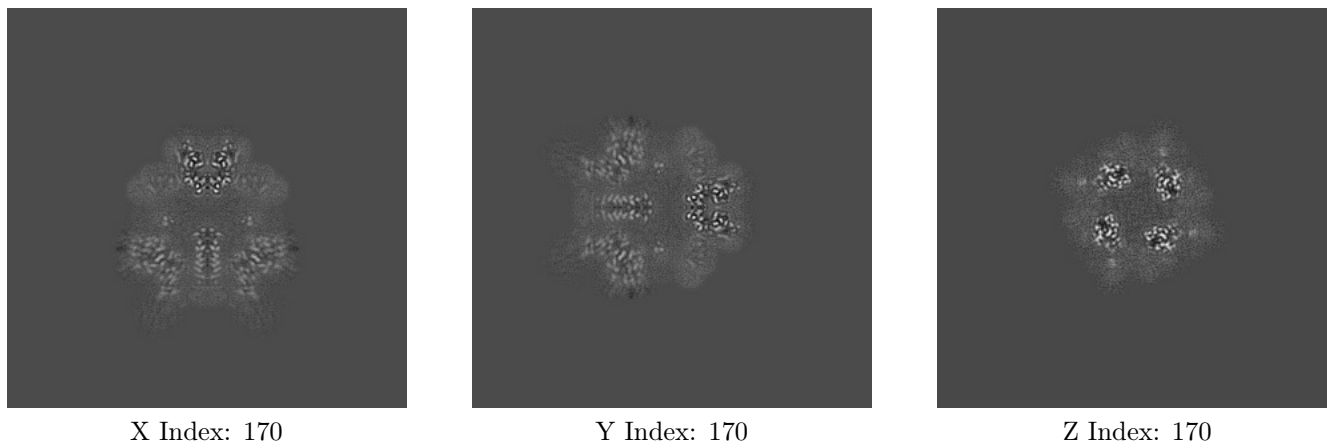
6.1.1 Primary map



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

6.2 Central slices [i](#)

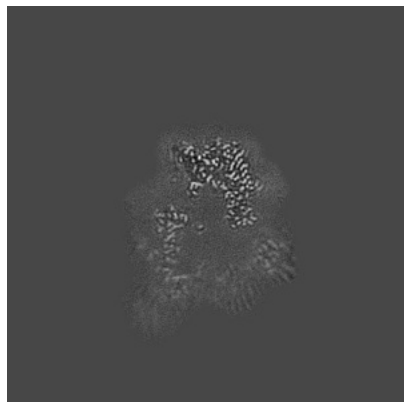
6.2.1 Primary map



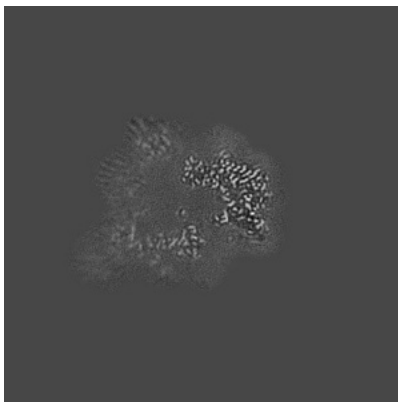
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

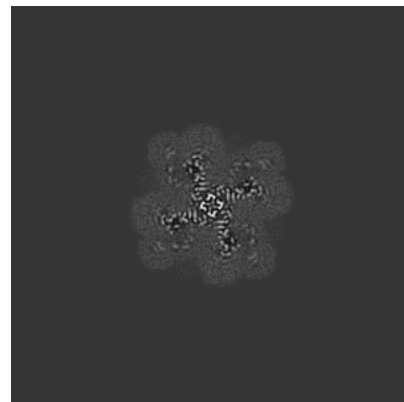
6.3.1 Primary map



X Index: 156



Y Index: 184

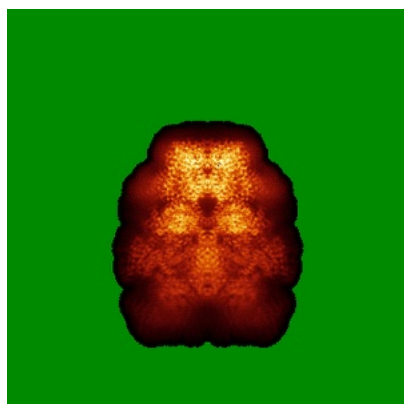


Z Index: 188

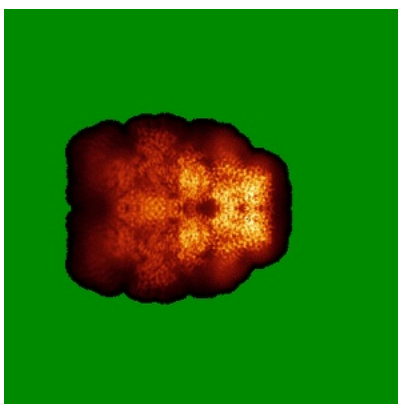
The images above show the largest variance slices of the map in three orthogonal directions.

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

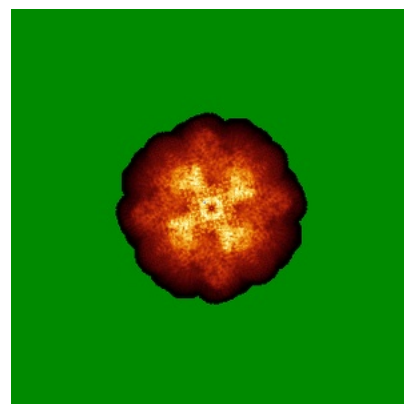
6.4.1 Primary map



X



Y

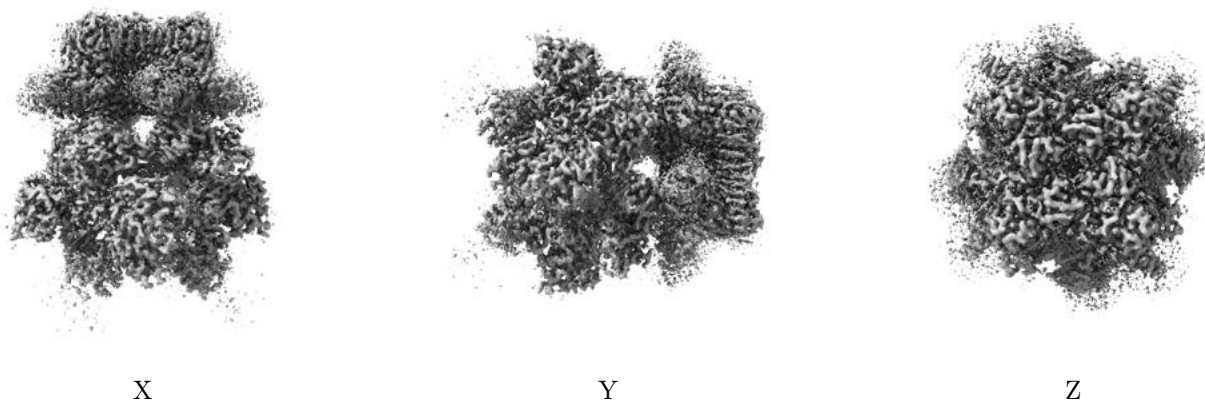


Z

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.

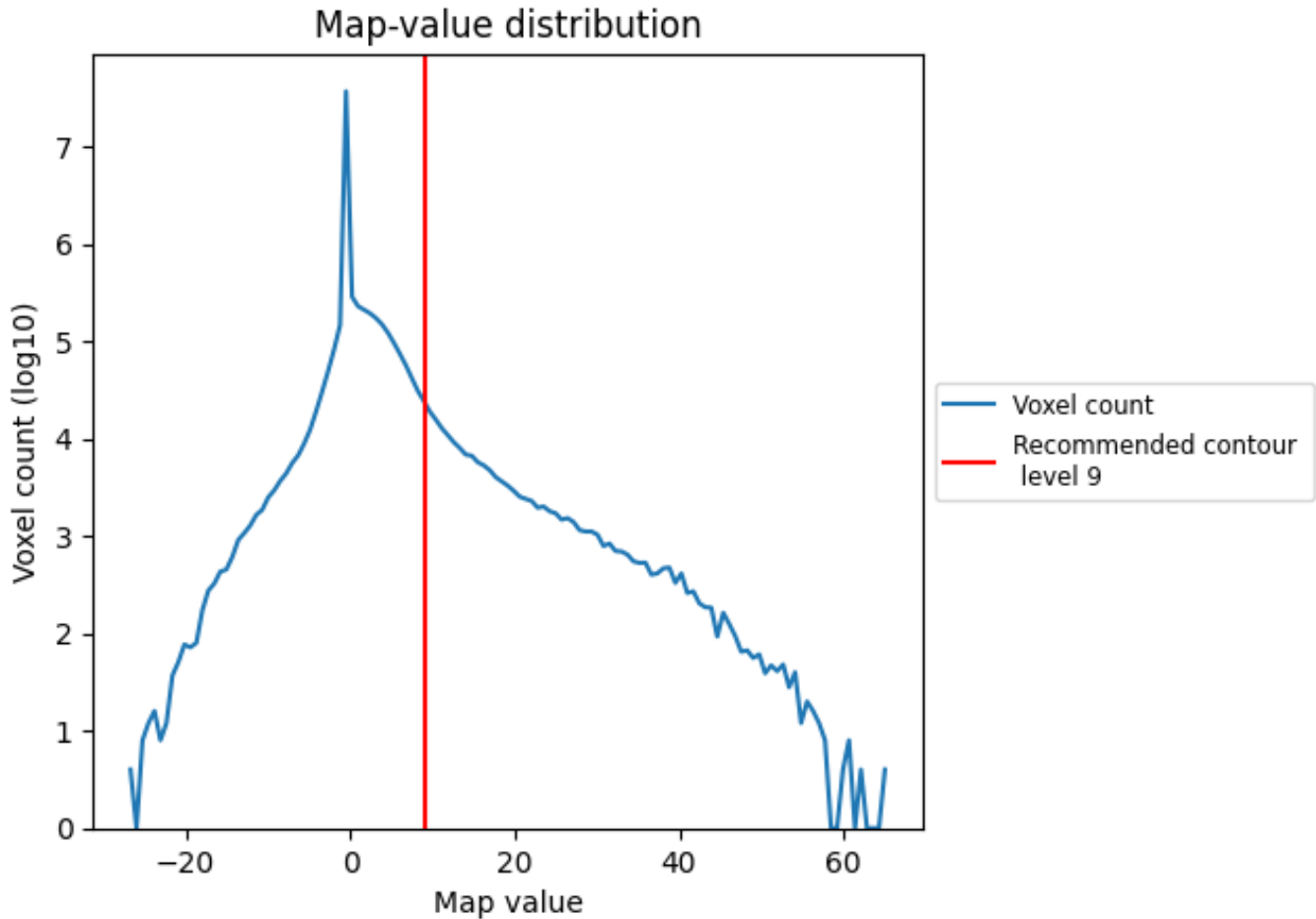
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

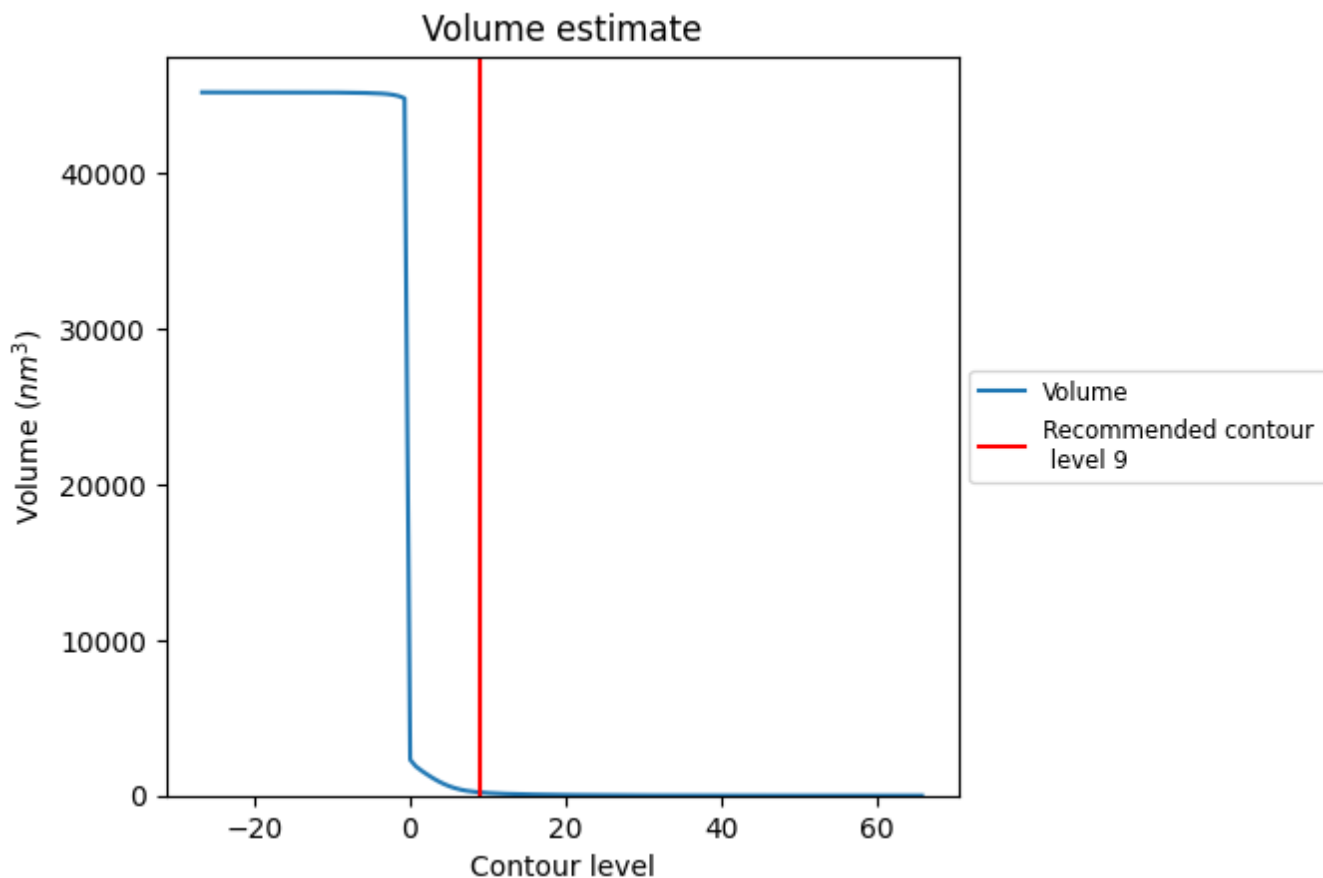
This section contains the results of statistical analysis of the map.

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.

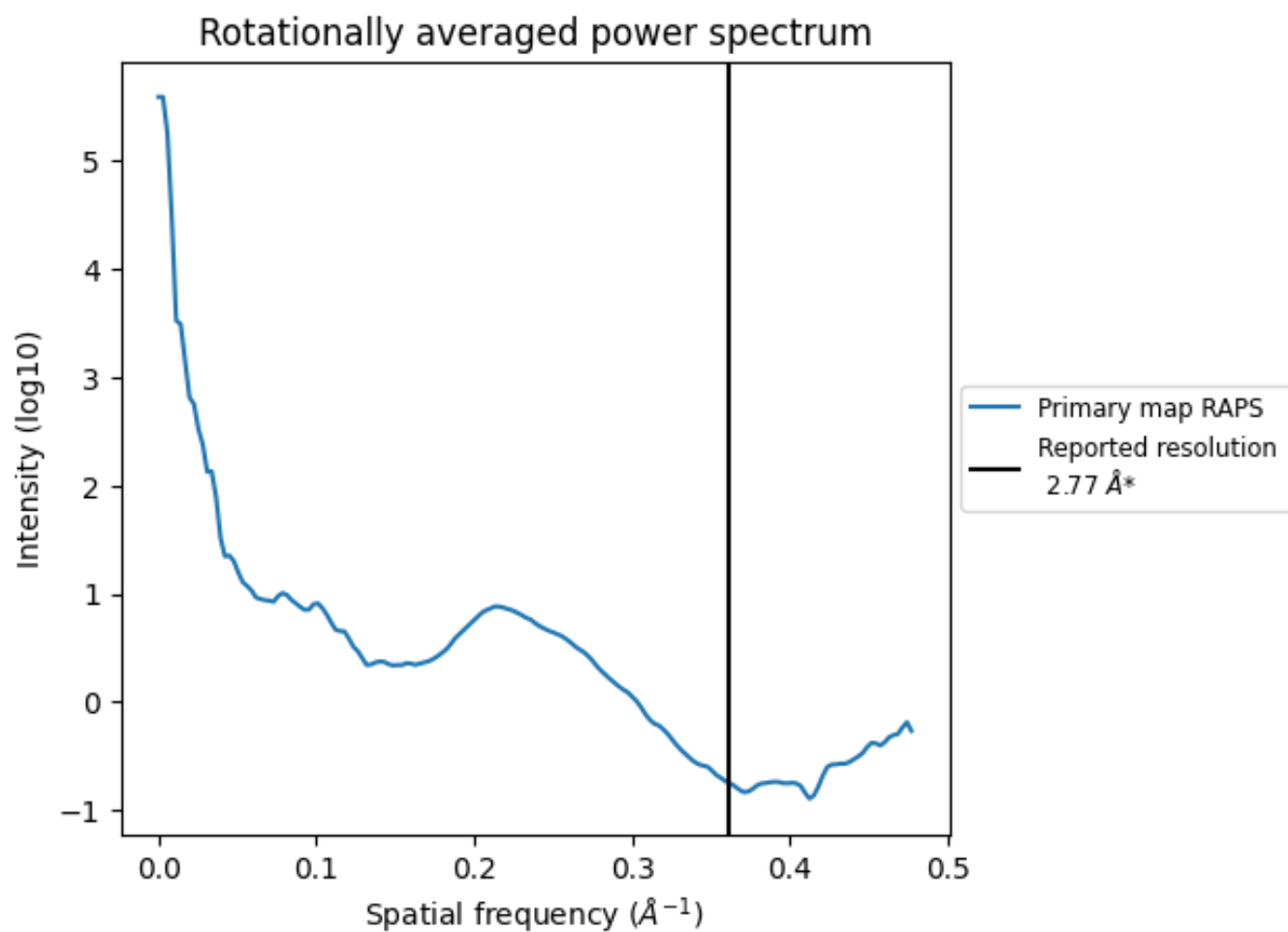
7.2 Volume estimate [i](#)



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 \AA^{-1}

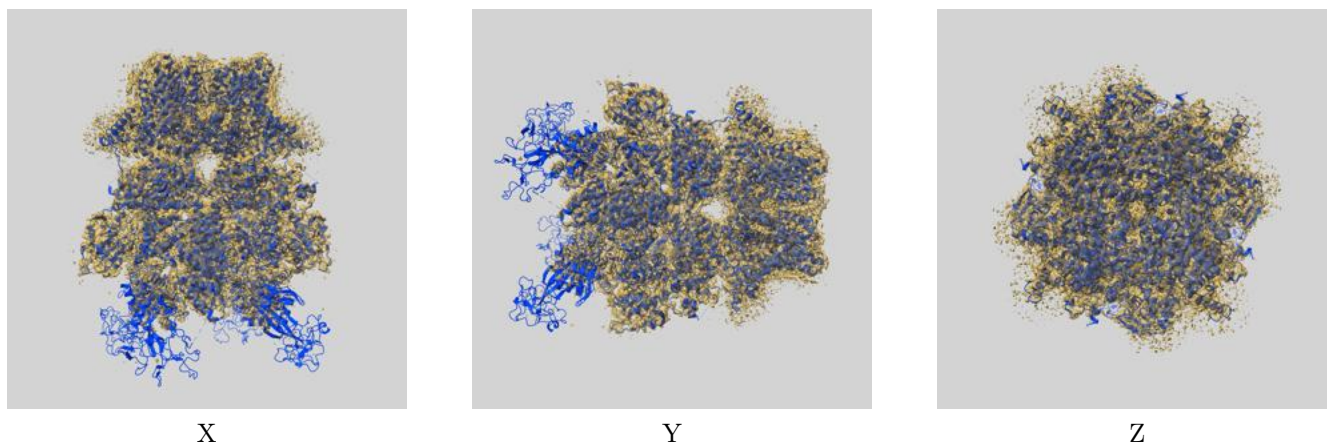
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

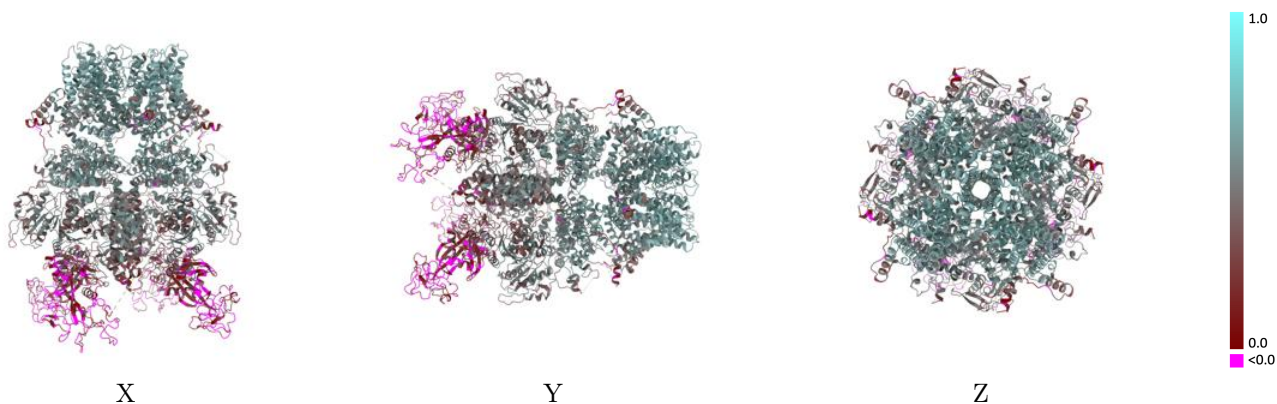
This section contains information regarding the fit between EMDB map EMD-40722 and PDB model 8SR8. Per-residue inclusion information can be found in section 3 on page 5.

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](#)

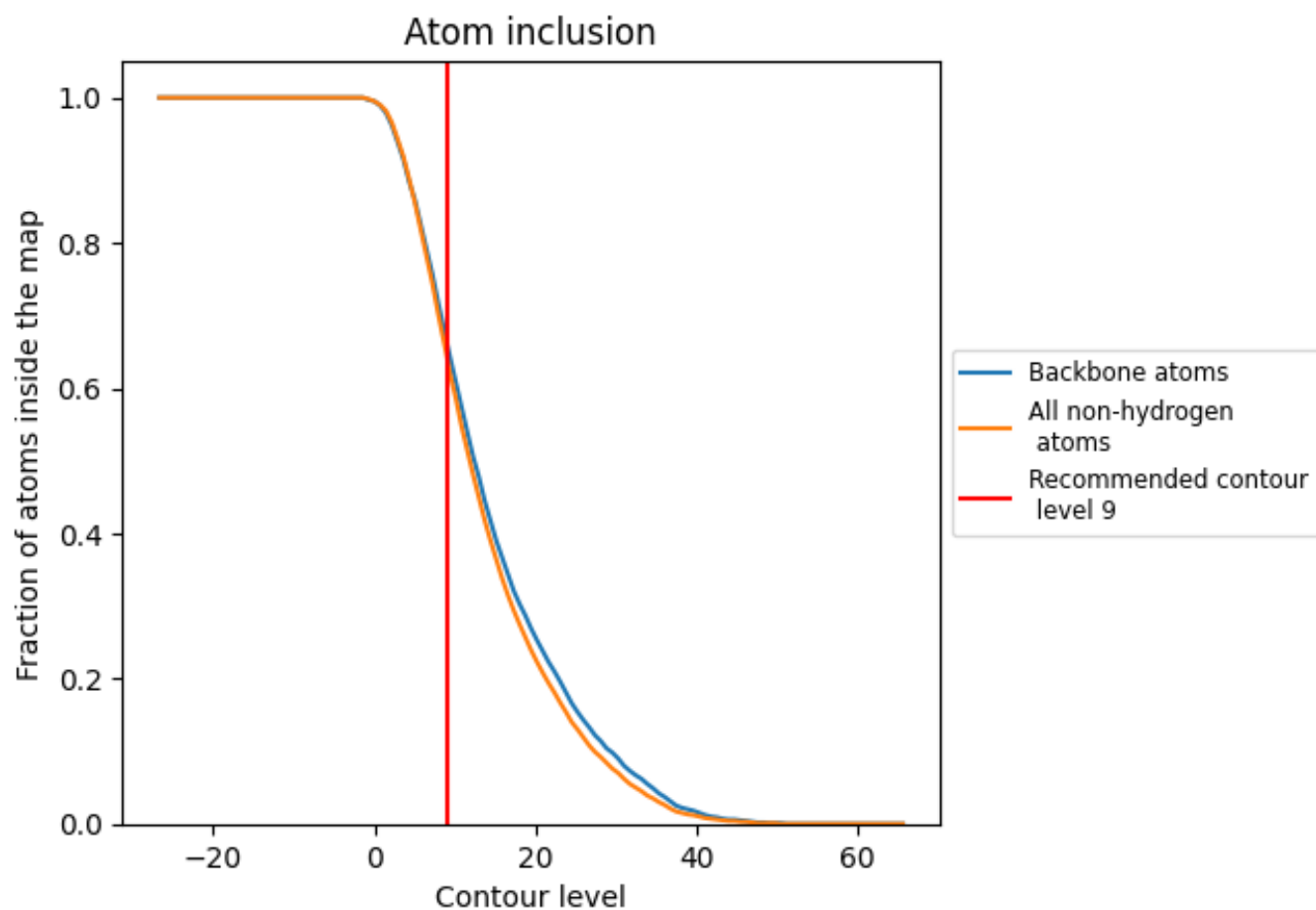


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.











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 [i](#)

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

