



# wwPDB EM Validation Summary Report ⓘ

Jan 14, 2025 – 03:02 PM JST

PDB ID : 8YEZ  
EMDB ID : EMD-39205  
Title : Human PIEZO1  
Authors : Zhang, M.F.  
Deposited on : 2024-02-23  
Resolution : 3.30 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](mailto: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>.

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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 : 1.8.5 (274361), CSD as541be (2020)  
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) : 2.40

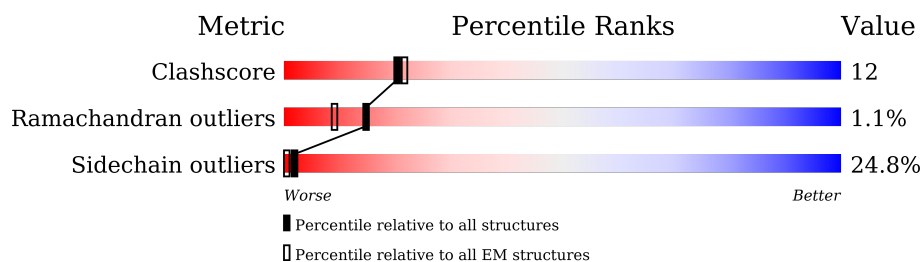
# 1 Overall quality at a glance

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)
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  $\geq 3$ , 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	2521	<p>10% 35% 13% . 49%</p>
1	B	2521	<p>11% 35% 13% . 49%</p>
1	C	2521	<p>10% 35% 13% . 49%</p>

## 2 Entry composition [i](#)

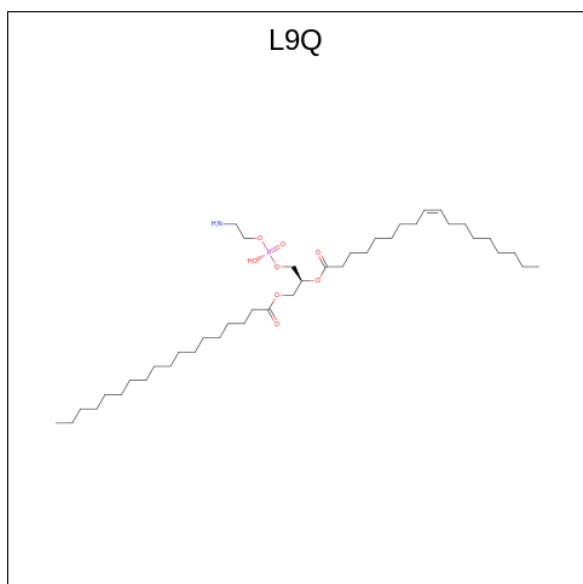
There are 2 unique types of molecules in this entry. The entry contains 31599 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Piezo-type mechanosensitive ion channel component 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1279	Total	C	N	O	S	0	0
			10431	6914	1725	1731	61		
1	B	1279	Total	C	N	O	S	0	0
			10431	6914	1725	1731	61		
1	C	1279	Total	C	N	O	S	0	0
			10431	6914	1725	1731	61		

- Molecule 2 is (1S)-2-{[(S)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-1-[(octadecanoyloxy)methyl]ethyl (9Z)-octadec-9-enoate (three-letter code: L9Q) (formula: C<sub>41</sub>H<sub>80</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
2	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
2	A	1	Total	C	N	O	P	0
			51	41	1	8	1	

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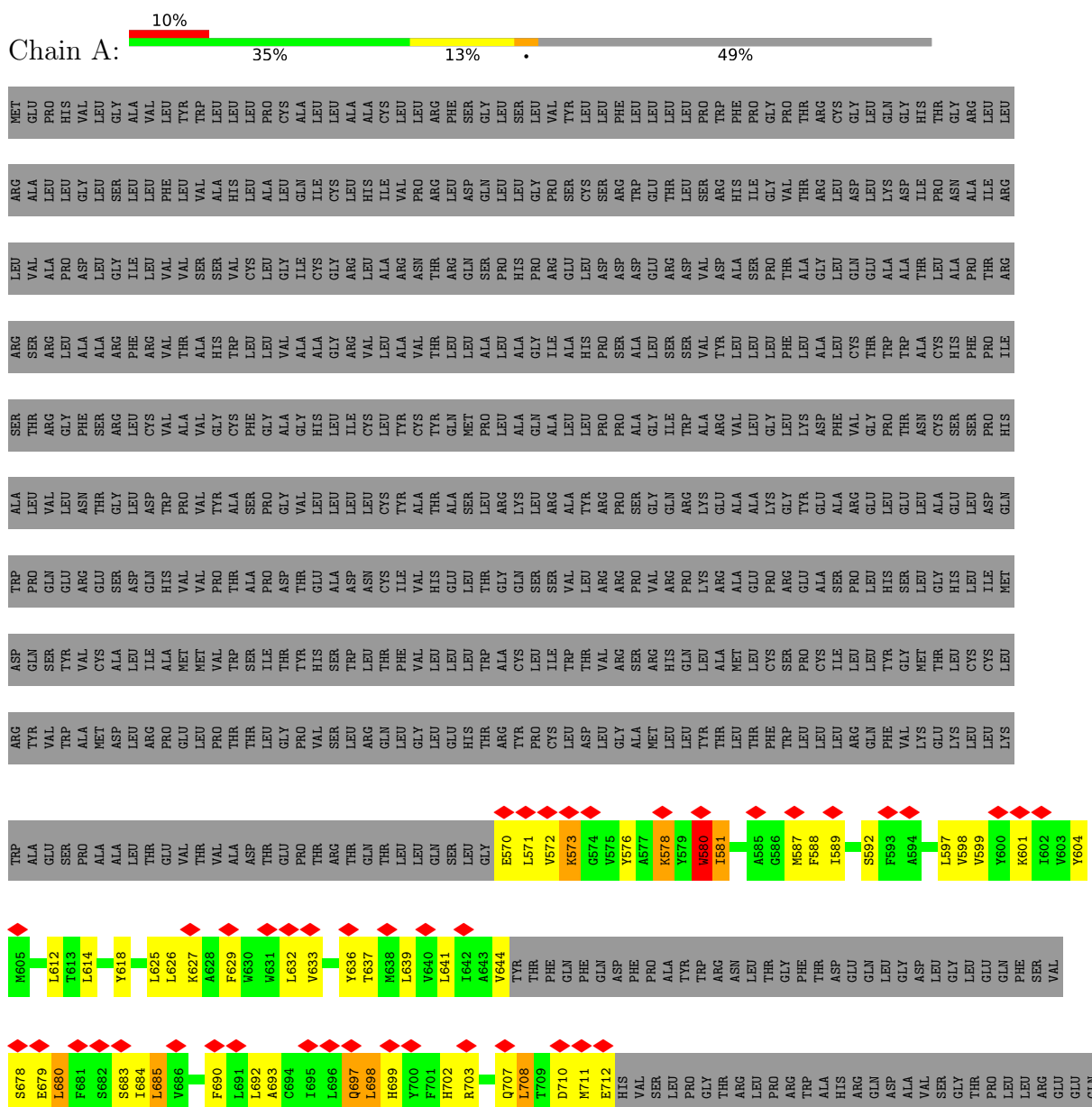
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Mol	Chain	Residues	Atoms					AltConf
2	B	1	Total	C	N	O	P	0
			51	41	1	8	1	
2	B	1	Total	C	N	O	P	0
			51	41	1	8	1	
2	C	1	Total	C	N	O	P	0
			51	41	1	8	1	

### 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: Piezo-type mechanosensitive ion channel component 1

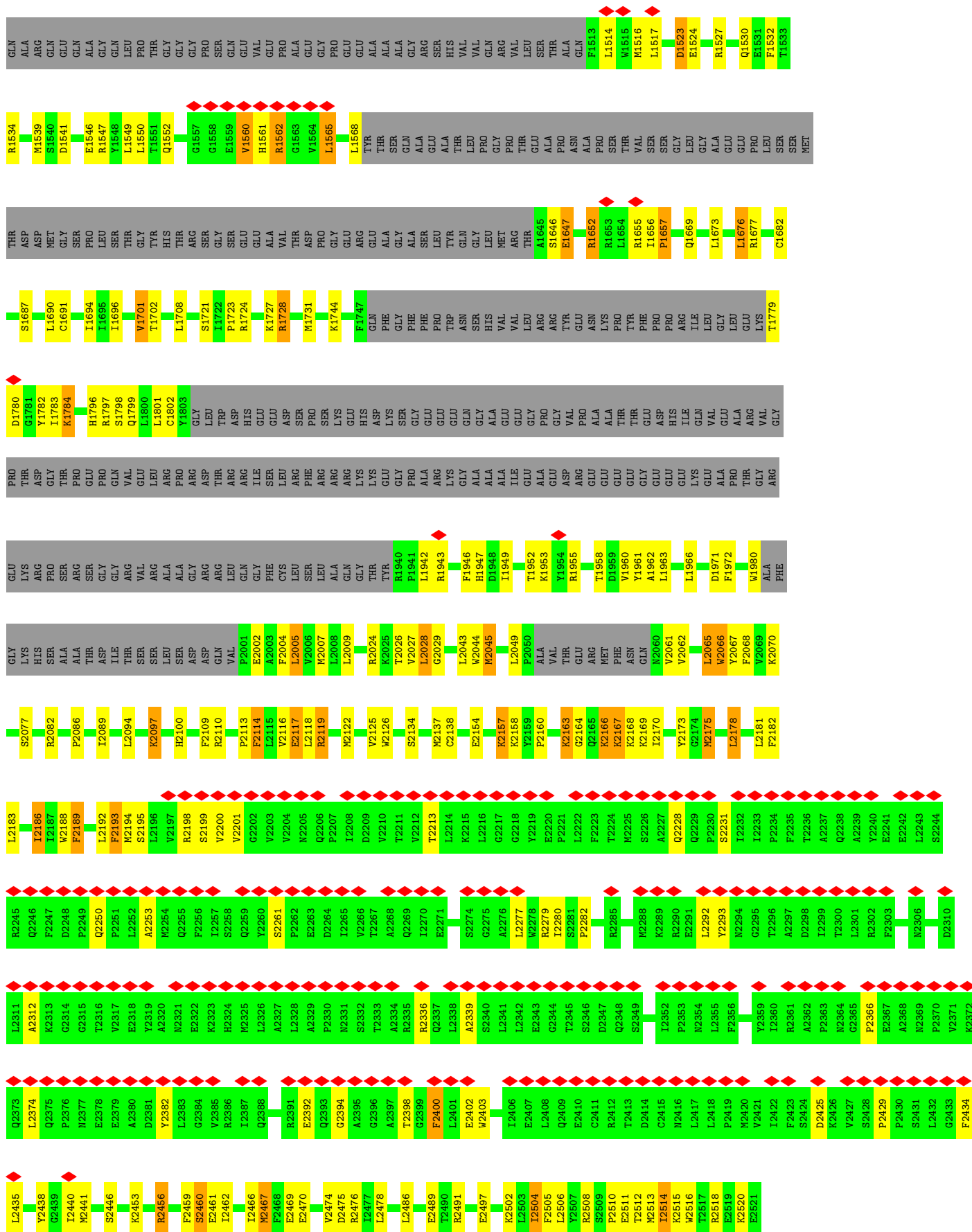














R0082	SER	ALA	PRO	GLY	C1691	GLY	D1541	GLU	K1334	VAL	GLU	PRO	ASP
P2086	ALA	THR	ARG	PRO	I1694	SER	E1546	GLN	S1335	PHE	ALA	PRO	TYR
I2089	ASP	THR	SER	GLU	I1695	LEU	R1547	GLY		GLU	LEU	LEU	TRP
L2094	ILE	ASP	GLY	PRO	I1696	THR	Y1548	LEU	H1338	GLN	GLY	TRP	ARG
K2097	THR	ARG	VAL	VAL	M1700	GLY	L1549	PRO	F1339	MET	PRO	SER	TRP
H2100	SER	ALA	GLU	GLU	V1701	THR	L1550	THR	R1340	GLN	ASN	ARG	ALA
F2109	SER	ALA	LEU	ARG	T1702	HIS	T1551	GLY	R1341	THR	VAL	ALA	VAL
R2110	ASP	ARG	ASP	ARG	L1708	THR	Q1552	GLY	I1342	GLY	ASN	ALA	ARG
P2113	VAL	ARG	THR	THR	L1709	SER	G1557	PRO	S1346	CYS	MET	VAL	PRO
F2114	GLN	ARG	ARG	GLY	V1710	SER	F1558	GLN	L1347	TRP	VAL	ASN	THR
L2115	GLU	ARG	GLU	GLY	P1723	GLU	V1560	GLU	L1350	ILE	PHE	ASN	VAL
V2116	GLU	ILE	GLU	GLU	R1724	GLU	H1561	VAL	K1351	GLN	ALA	SER	ALA
E2117	ASP	SER	GLU	VAL	K1727	ALA	R1562	PRO	M1354	LEU	CYS	LEU	LEU
L2118	SER	LEU	ASP	THR	R1728	THR	G1563	ALA	R1356	SER	ARG	ILE	ARG
R2119	PRO	ARG	SER	ASP	M1731	ASP	V1564	GLU	K1360	VAL	GLY	TRP	LEU
M2122	GLN	ARG	GLY	GLY	K1744	GLY	L1565	PRO	K1363	CYS	TYR	TYR	TYR
V2125	THR	LYS	THR	LYS	F1747	ALA	L1568	ALA	D1370	TYR	PHE	PHE	PHE
W2126	TYR	LYS	PHE	GLN		ALA	THR	VAL	ARG	ARG	ARG	ARG	ARG
S2134	GLY	GLY	GLY	GLY		ALA	SER	GLN	THR	ASP	ALA	ALA	ALA
L2137	ALA	PRO	PHE	LEU		SER	ALA	ARG	ARG	PRO	PRO	PRO	ASN
C2138	GLU	GLU	PHE	THR		THR	GLU	HIS	ARG	GLY	GLY	GLY	ASN
E2154	GLY	GLY	THR	VAL		GLN	PRO	VAL	GLY	TYR	GLY	GLY	S1096
K2157	ALA	ALA	VAL	ALA		THR	PRO	ALA	ASP	MET	GLY	GLY	L1099
Y2159	GLU	GLY	VAL	GLU		LEU	ALA	SER	THR	ASP	LEU	LEU	I1100
P2160	VAL	PRO	ARG	GLY		ARG	ASN	THR	GLY	ASP	ASP	ASP	D1102
K2163	THR	ASP	GLY	THR		THR	PRO	GLY	GLY	GLN	GLY	GLY	F1103
G2164	GLU	ARG	GLU	ALA		ALA	ALA	GLN	LYS	ASP	ASP	ASP	L1104
Q2165	ARG	GLU	ALA	GLY		LEU	ALA	SER	PRO	GLY	GLY	GLY	L1106
K2166	MET	GLU	ALA	GLY		LEU	ALA	THR	GLY	PRO	VAL	VAL	Q1112
K2167	PHE	GLU	THR	GLY		ARG	ALA	THR	GLY	GLY	GLY	GLY	E1119
K2168	ASN	GLU	THR	THR		THR	PRO	GLY	GLY	GLY	GLY	GLY	R1120
K2169	GLN	GLY	THR	GLY		THR	ASN	GLN	GLY	GLY	GLY	GLY	T1121
I2170	LEU	GLY	ASP	GLY		THR	ALA	ALA	ASP	GLY	GLY	GLY	GLY
Y2173	V2061	GLY	PRO	HIS		THR	ALA	THR	GLY	PRO	PRO	TRP	TRP
G2174	V2062	ILE	ARG	ILE		THR	LEU	GLY	I1285	VAL	GLY	GLN	GLN
M2175	L2065	LYS	GLY	GLN		THR	ALA	ASN	I1286	GLY	GLY	GLY	ARG
L2178	W2066	ALA	VAL	GLY		THR	ALA	ALA	A1283	GLY	GLY	MET	MET
L2181	Y2067	ALA	GLY	GLY		THR	GLY	GLY	G1284	GLY	GLY	GLY	ALA
F2182	F2068	THR	PRO	ARG		THR	PRO	VAL	N1221	ASP	GLY	GLY	ALA
L2183	F2069	GLY	GLY	GLY		THR	LEU	GLY	I1222	GLY	GLY	GLY	GLY
I2184	K2070	ARG	GLY	LYS		THR	SER	GLY	L1226	LEU	VAL	ASN	VAL
A2185	S2077	LYS	THR	LYS		THR	THR	GLY	I1227	LEU	L1232	THR	THR
		ARG	ARG	ARG		THR	ASP	GLY	L1228	ALA	L1233	ASP	ASP
			ASP	ASP		THR	ASP	GLY	S1229	ALA	S1233	ARG	LEU
						THR	ASP	GLY	N1229	ALA	L1237	ARG	ALA
						THR	ASP	GLY	L1230	GLY	T1317	TRP	CYS
						THR	ASP	GLY	M1231	GLY	R1323	TRP	LEU
						THR	ASP	GLY	M1232	GLY	L1327	TRP	LEU
						THR	ASP	GLY	L1233	GLY	L1327	TRP	LEU
						THR	ASP	GLY	L1234	GLY	L1327	TRP	LEU
						THR	ASP	GLY	L1235	GLY	L1327	TRP	LEU
						THR	ASP	GLY	L1236	GLY	L1327	TRP	LEU
						THR	ASP	GLY	L1237	GLY	L1327	TRP	LEU
						THR	ASP	GLY	L1238	GLY	L1327	TRP	LEU
						THR	ASP	GLY	L1239	GLY	L1327	TRP	LEU
						THR	ASP	GLY	L1240	GLY	L1327	TRP	LEU
						THR	ASP	GLY	L1241	GLY	L1327	TRP	LEU
						THR	ASP	GLY	L1242	GLY	L1327	TRP	LEU
						THR	ASP	GLY	L1243	GLY	L1327	TRP	LEU
						THR	ASP	GLY	L1244	GLY	L1327	TRP	LEU
						THR	ASP	GLY	L1245	GLY	L1327	TRP	LEU
						THR	ASP	GLY	L1246	GLY	L1327	TRP	LEU
						THR	ASP	GLY	L1247	GLY	L1327	TRP	LEU
						THR	ASP	GLY	L1248	GLY	L1327	TRP	LEU
						THR	ASP	GLY	L1249	GLY	L1327	TRP	LEU
						THR	ASP	GLY	L1250	GLY	L1327	TRP	LEU
						THR	ASP	GLY	L1251	GLY	L1327	TRP	LEU
						THR	ASP	GLY	L1252	GLY	L1327	TRP	LEU
						THR	ASP	GLY	L1253	GLY	L1327	TRP	LEU
						THR	ASP	GLY	L1254	GLY	L1327	TRP	LEU
						THR	ASP	GLY	L1255	GLY	L1327	TRP	LEU
						THR	ASP	GLY	L1256	GLY	L1327	TRP	LEU
						THR	ASP	GLY	L1257	GLY	L1327	TRP	LEU
						THR	ASP	GLY	L1258	GLY	L1327	TRP	LEU
						THR	ASP	GLY	L1259	GLY	L1327	TRP	LEU
						THR	ASP	GLY	L1260	GLY	L1327	TRP	LEU
						THR	ASP	GLY	L1261	GLY	L1327	TRP	LEU
						THR	ASP	GLY	L1262	GLY	L1327	TRP	LEU
						THR	ASP	GLY	L1263	GLY	L1327	TRP	LEU
						THR	ASP	GLY	L1264	GLY	L1327	TRP	LEU
						THR	ASP	GLY	L1265	GLY	L1327	TRP	LEU
						THR	ASP	GLY	L1266	GLY	L1327	TRP	LEU
						THR	ASP	GLY	L1267	GLY	L1327	TRP	LEU
						THR	ASP	GLY	L1268	GLY	L1327	TRP	LEU
						THR	ASP	GLY	L1269	GLY	L1327	TRP	LEU
						THR	ASP	GLY	L1270	GLY	L1327	TRP	LEU
						THR	ASP	GLY	L1271	GLY	L1327	TRP	LEU
						THR	ASP	GLY	L1272	GLY	L1327	TRP	LEU
						THR	ASP	GLY	L1273	GLY	L1327	TRP	LEU
						THR	ASP	GLY	L1274	GLY	L1327	TRP	LEU
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						THR	ASP	GLY	L1276	GLY	L1327	TRP	LEU
						THR	ASP	GLY	L1277	GLY	L1327	TRP	LEU
						THR	ASP	GLY	L1278	GLY	L1327	TRP	LEU
						THR	ASP	GLY	L1279	GLY	L1327	TRP	LEU
						THR	ASP	GLY	L1280	GLY	L1327	TRP	LEU
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						THR	ASP	GLY	L1282	GLY	L1327	TRP	LEU
						THR	ASP	GLY	L1283	GLY	L1327	TRP	LEU
						THR	ASP	GLY	L1284	GLY	L1327	TRP	LEU
						THR	ASP	GLY	L1285	GLY	L1327	TRP	LEU
						THR	ASP	GLY	L1286	GLY	L1327	TRP	LEU
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						THR	ASP	GLY	L1288	GLY	L1327	TRP	LEU
						THR	ASP	GLY	L1289	GLY	L1327	TRP	LEU
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						THR	ASP	GLY	L1297	GLY	L1327	TRP	LEU
						THR	ASP	GLY	L1298	GLY	L1327	TRP	LEU
						THR	ASP	GLY	L1299	GLY	L1327	TRP	LEU
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						THR	ASP	GLY	L1303	GLY	L1327	TRP	LEU
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						THR	ASP	GLY	L1313	GLY	L1327	TRP	LEU
						THR	ASP	GLY	L1314	GLY	L1327	TRP	LEU
						THR	ASP	GLY	L1315	GLY	L1327	TRP	LEU
						THR	ASP	GLY	L1316	GLY	L1327	TRP	LEU
						THR	ASP						

G2439	I2440	M2441	S2446	K2453	R2456	F2459	S2460	E2461	I2462	I2466	M2467	F2468	E2469	E2470	V2474	D2475	R2476	I2477	L2478	L2486	E2489	T2490	R2491	E2497	K2502	L2503	I2504	F2505	L2506	Y2507	R2508	S2509	P2510	E2511	T2512	M2513	I2514	K2515	W2516	T2517	R2518	E2519	K2520	E2521														
P2376	N2377	E2378	E2379	A2380	D2381	Y2382	L2383	G2384	V2385	R2386	I2387	Q2388	R2391	E2392	Q2393	G2394	A2395	G2396	A2397	T2398	G2399	F2400	L2401	E2402	W2403	I2406	E2407	L2408	Q2409	E2410	C2411	R2412	T2413	D2414	C2415	N2416	L2417	L2418	P2419	M2420	V2421	I2422	F2423	S2424	D2425	K2426	V2427	S2428	P2429	P2430	S2431	L2432	G2433	F2434	L2435	Y2438		
K2313	Q2314	G2315	T2316	V2317	E2318	Y2319	A2320	N2321	E2322	K2323	H2324	M2325	L2326	A2327	L2328	A2329	P2330	N2331	S2332	T2333	A2334	R2335	Y2336	Q2337	L2338	A2339	S2340	L2341	L2342	E2343	Q2344	T2345	S2346	D2347	Q2348	S2349	I2352	P2353	N2354	L2355	F2356	Y2359	A2362	P2363	N2364	G2365	P2366	E2367	A2368	N2369	P2370	V2371	K2372	Q2373	L2374	Q2375		
F2247	D2248	P2249	Q2250	P2251	L2252	A2253	M2254	Q2255	F2256	I2257	S2258	Q2259	Y2260	S2261	P2262	E2263	D2264	I2265	V2266	T2267	A2268	Q2269	I2270	E2271	S2274	G2275	A2276	L2277	W2278	R2279	I2280	S2281	P2282	R2285	M2288	K2289	E2290	E2291	L2292	Y2293	N2294	G2295	T2296	A2297	D2298	I2299	T2300	L2301	R2302	F2303	N2306	D2310	L2311	A2312				
T2186	T2187	W2188	F2189	L2192	F2193	K2194	S2195	L2196	V2197	R2198	S2199	V2200	V2201	G2202	V2203	V2204	N2205	Q2206	P2207	T2208	D2209	V2210	T2211	V2212	T2213	L2214	K2215	L2216	G2217	G2218	V2219	E2220	P2221	L2222	F2223	T2224	N2225	S2226	A2227	Q2228	Q2229	P2230	S2231	I2232	I2233	F2234	F2235	T2236	A2237	Q2238	A2239	Y2240	E2241	E2242	L2243	S2244	R2245	Q2246

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	161218	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI MORGAGNI	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.095	Depositor
Minimum map value	-0.712	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.1	Depositor
Map size ( $\text{\AA}$ )	543.36, 543.36, 543.36	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.849, 0.849, 0.849	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: L9Q

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	0.52	0/10690	0.65	3/14491 (0.0%)
1	B	0.52	0/10690	0.66	3/14491 (0.0%)
1	C	0.52	0/10690	0.66	3/14491 (0.0%)
All	All	0.52	0/32070	0.66	9/43473 (0.0%)

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	2425	ASP	CB-CG-OD1	5.77	123.50	118.30
1	B	2425	ASP	CB-CG-OD1	5.76	123.49	118.30
1	A	2425	ASP	CB-CG-OD1	5.76	123.48	118.30
1	A	2382	TYR	CB-CG-CD2	-5.51	117.70	121.00
1	C	2382	TYR	CB-CG-CD2	-5.50	117.70	121.00

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	10431	0	10666	285	0
1	B	10431	0	10666	275	0
1	C	10431	0	10666	283	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	153	0	237	9	0
2	B	102	0	158	6	0
2	C	51	0	79	1	0
All	All	31599	0	32472	770	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 12.

The worst 5 of 770 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:2193:PHE:HD1	1:A:2194:MET:N	1.11	1.44
1:B:2157:LYS:NZ	1:B:2157:LYS:CB	1.70	1.44
1:C:2193:PHE:HD1	1:C:2194:MET:N	1.11	1.42
1:A:2028:LEU:CD1	1:A:2028:LEU:C	1.78	1.41
1:B:2193:PHE:HD1	1:B:2194:MET:N	1.11	1.39

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	1249/2521 (50%)	1126 (90%)	109 (9%)	14 (1%)	12	40
1	B	1249/2521 (50%)	1128 (90%)	107 (9%)	14 (1%)	12	40
1	C	1249/2521 (50%)	1128 (90%)	107 (9%)	14 (1%)	12	40
All	All	3747/7563 (50%)	3382 (90%)	323 (9%)	42 (1%)	15	40

5 of 42 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1723	PRO
1	C	626	LEU
1	C	1723	PRO
1	A	1657	PRO
1	A	2429	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1116/2172 (51%)	839 (75%)	277 (25%)	0	2
1	B	1116/2172 (51%)	837 (75%)	279 (25%)	0	2
1	C	1116/2172 (51%)	842 (75%)	274 (25%)	0	2
All	All	3348/6516 (51%)	2518 (75%)	830 (25%)	2	2

5 of 830 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1797	ARG
1	C	636	TYR
1	C	2201	VAL
1	B	1971	ASP
1	B	1784	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	2228	GLN
1	C	977	GLN
1	C	699	HIS
1	C	1112	GLN
1	A	2064	GLN



### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

6 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	L9Q	A	2602	-	50,50,50	1.03	3 (6%)	53,55,55	1.17	4 (7%)
2	L9Q	A	2603	-	50,50,50	1.05	3 (6%)	53,55,55	1.10	3 (5%)
2	L9Q	C	2601	-	50,50,50	1.03	3 (6%)	53,55,55	1.17	4 (7%)
2	L9Q	B	2601	-	50,50,50	1.05	3 (6%)	53,55,55	1.10	3 (5%)
2	L9Q	B	2602	-	50,50,50	1.03	3 (6%)	53,55,55	1.17	4 (7%)
2	L9Q	A	2601	-	50,50,50	1.05	3 (6%)	53,55,55	1.10	3 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	L9Q	A	2602	-	-	37/54/54/54	-
2	L9Q	A	2603	-	-	33/54/54/54	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	L9Q	C	2601	-	-	37/54/54/54	-
2	L9Q	B	2601	-	-	33/54/54/54	-
2	L9Q	B	2602	-	-	37/54/54/54	-
2	L9Q	A	2601	-	-	33/54/54/54	-

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2601	L9Q	O3-C11	4.30	1.45	1.33
2	A	2601	L9Q	O3-C11	4.29	1.45	1.33
2	A	2603	L9Q	O3-C11	4.29	1.45	1.33
2	A	2602	L9Q	O2-C31	4.02	1.45	1.34
2	B	2602	L9Q	O2-C31	4.00	1.45	1.34

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2601	L9Q	O2-C31-C32	4.26	120.68	111.50
2	A	2602	L9Q	O2-C31-C32	4.25	120.66	111.50
2	B	2602	L9Q	O2-C31-C32	4.25	120.66	111.50
2	B	2601	L9Q	O2-C31-C32	3.94	120.00	111.50
2	A	2603	L9Q	O2-C31-C32	3.94	120.00	111.50

There are no chirality outliers.

5 of 210 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2601	L9Q	C4-O4P-P-O1P
2	A	2601	L9Q	O4P-C4-C5-N
2	A	2602	L9Q	C4-O4P-P-O1P
2	A	2602	L9Q	C4-O4P-P-O2P
2	A	2602	L9Q	C4-O4P-P-O3P

There are no ring outliers.

6 monomers are involved in 16 short contacts:

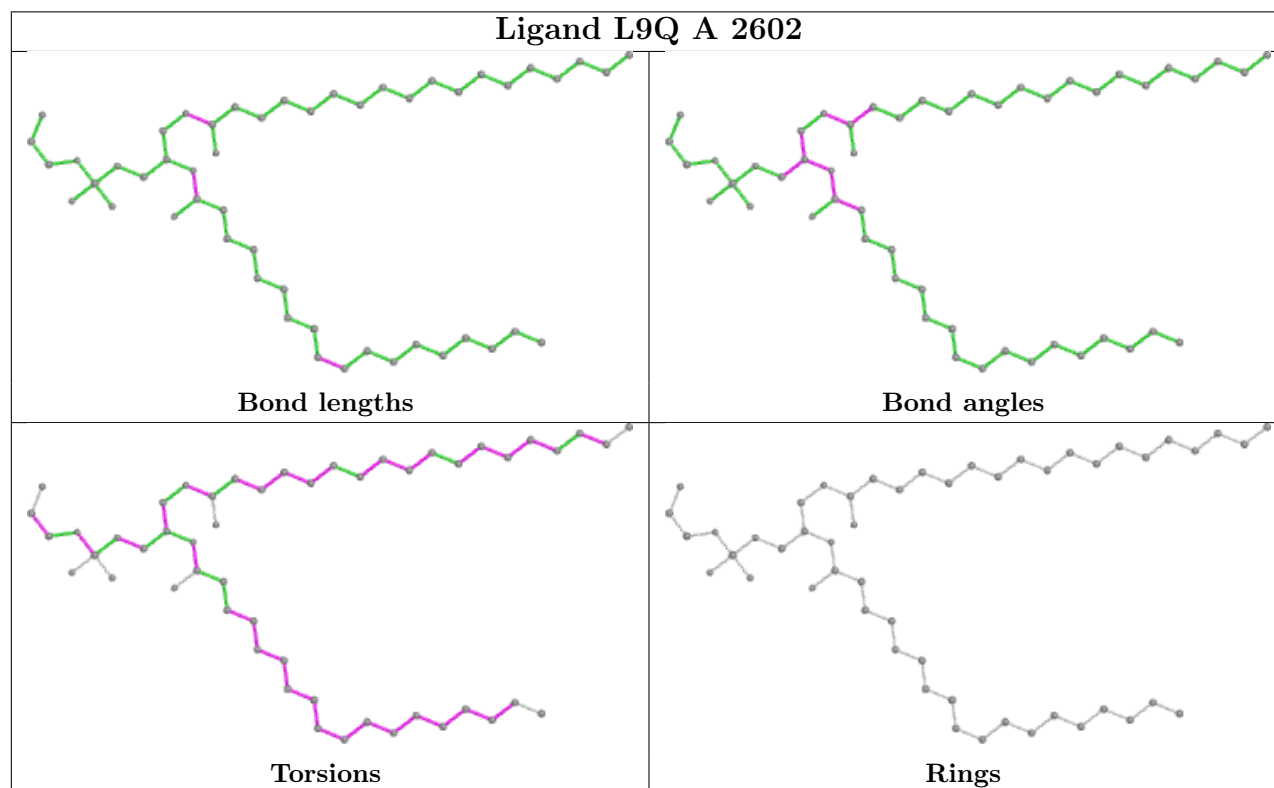
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2602	L9Q	4	0
2	A	2603	L9Q	2	0
2	C	2601	L9Q	1	0

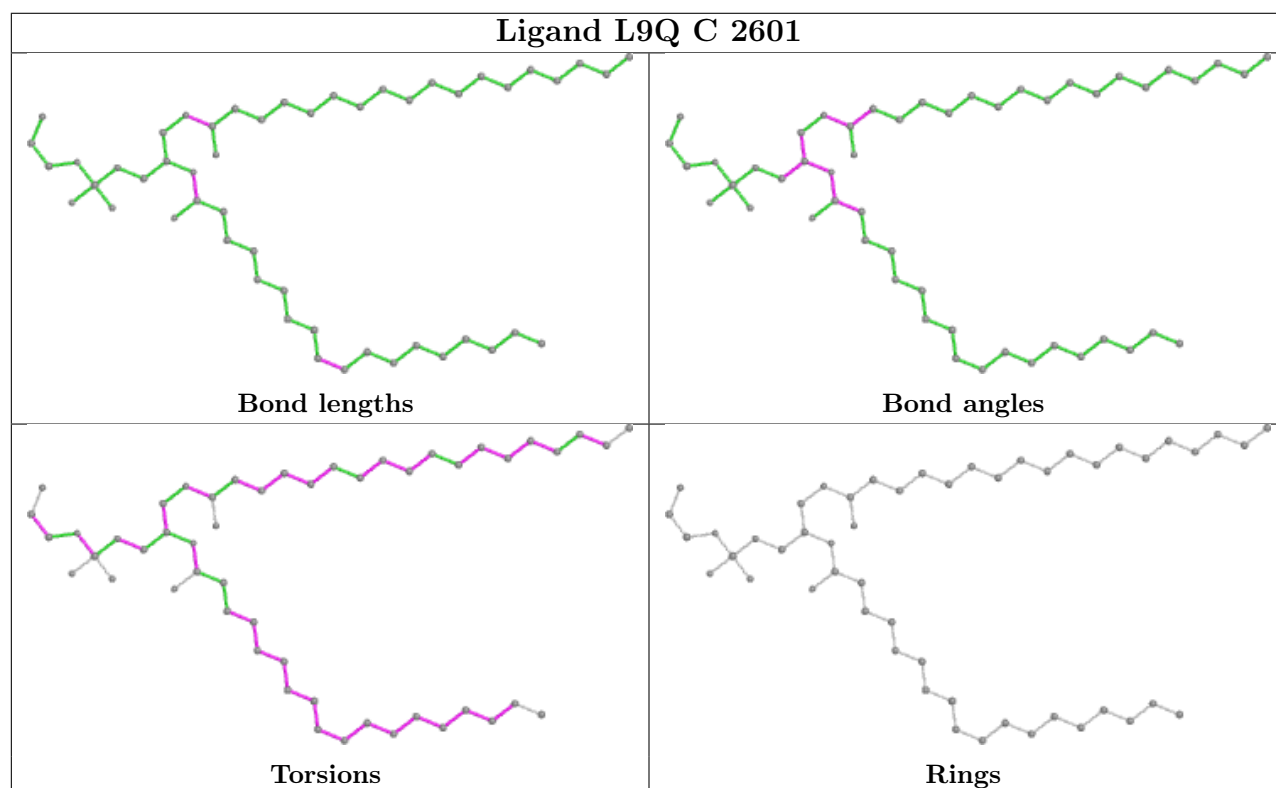
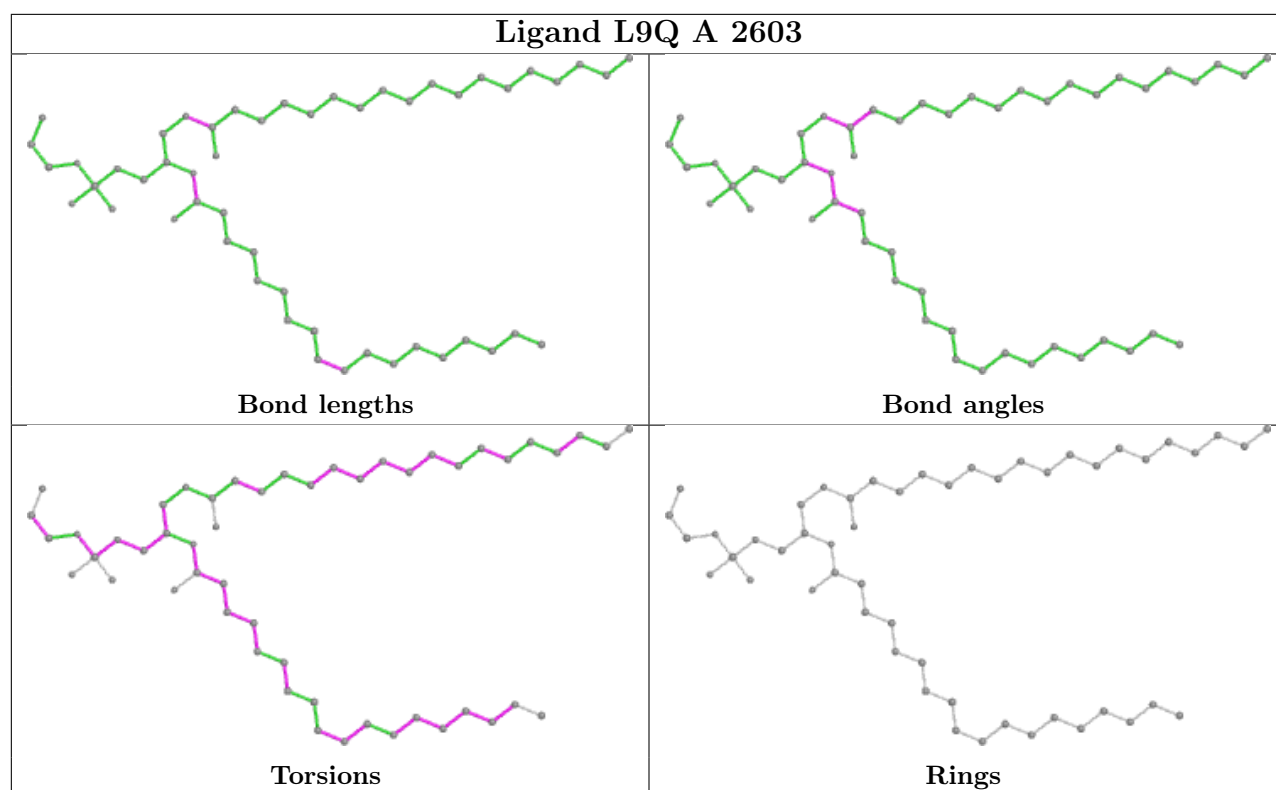
*Continued on next page...*

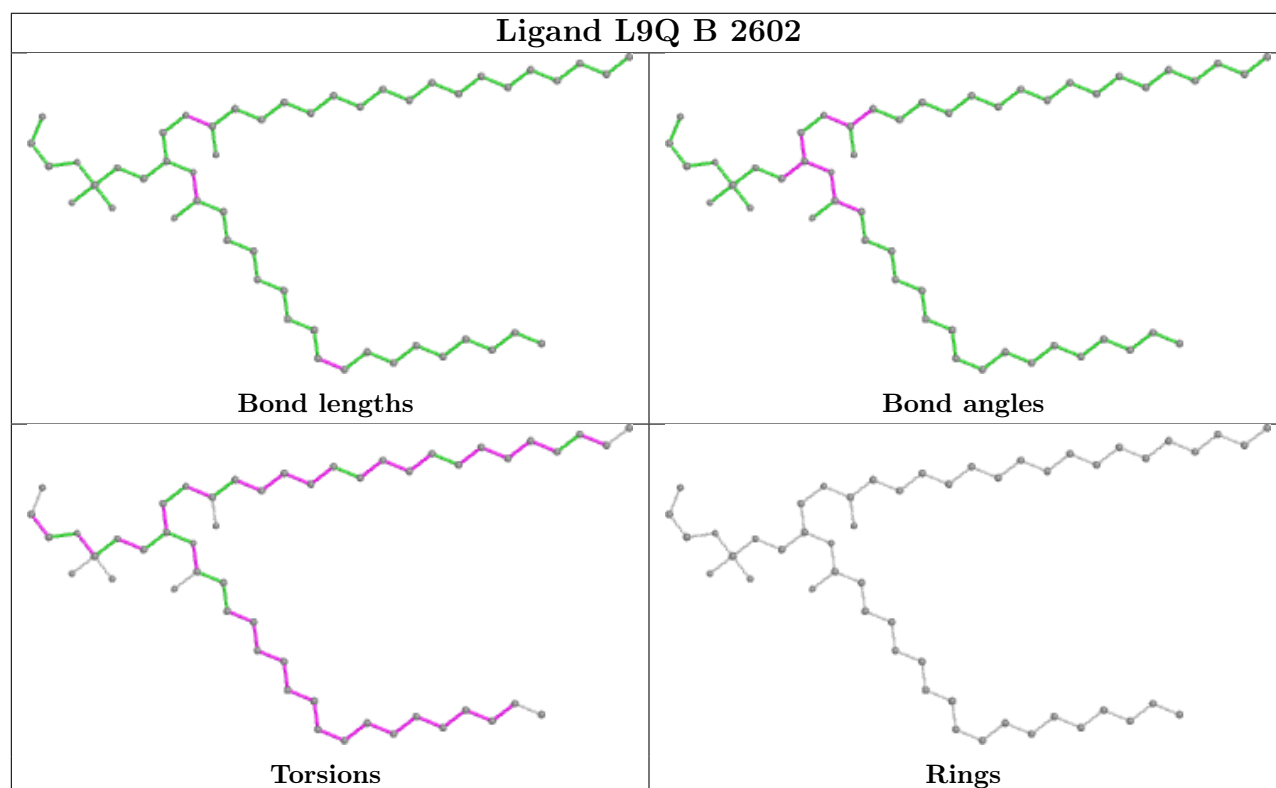
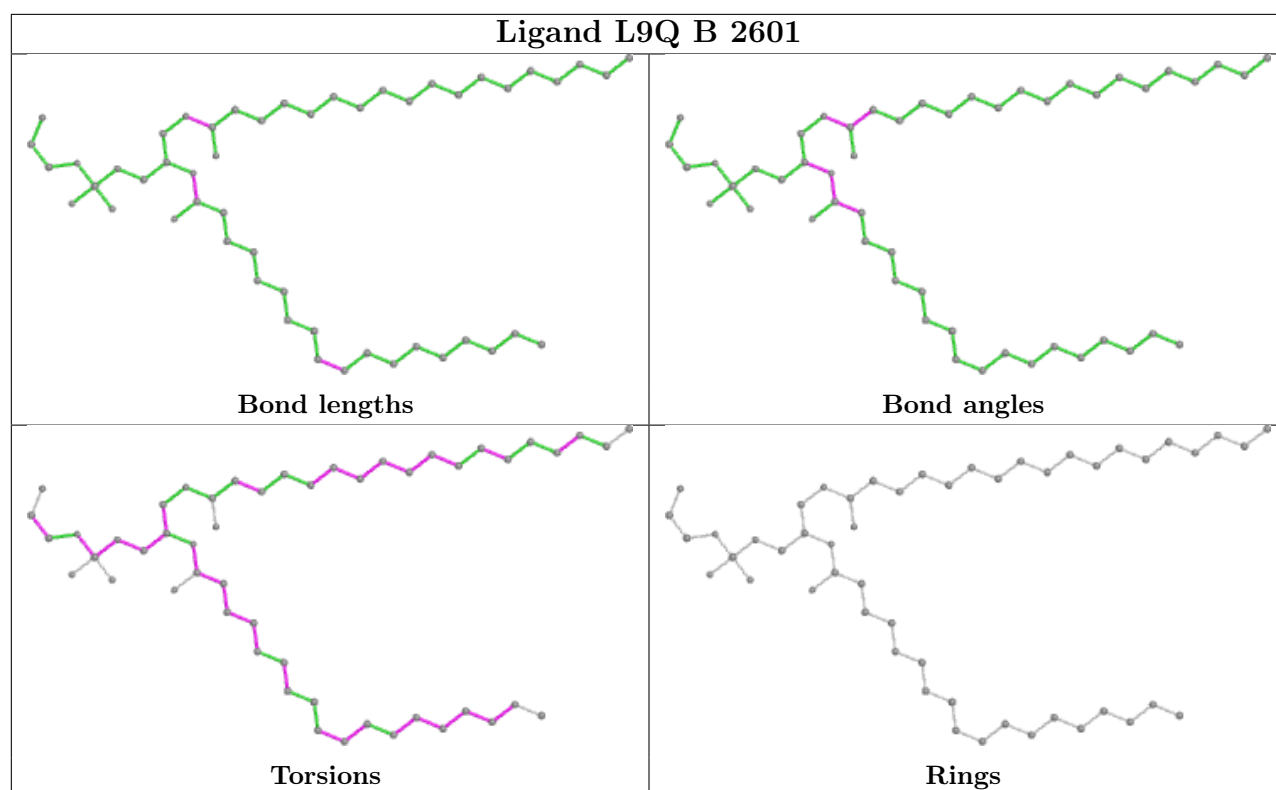
*Continued from previous page...*

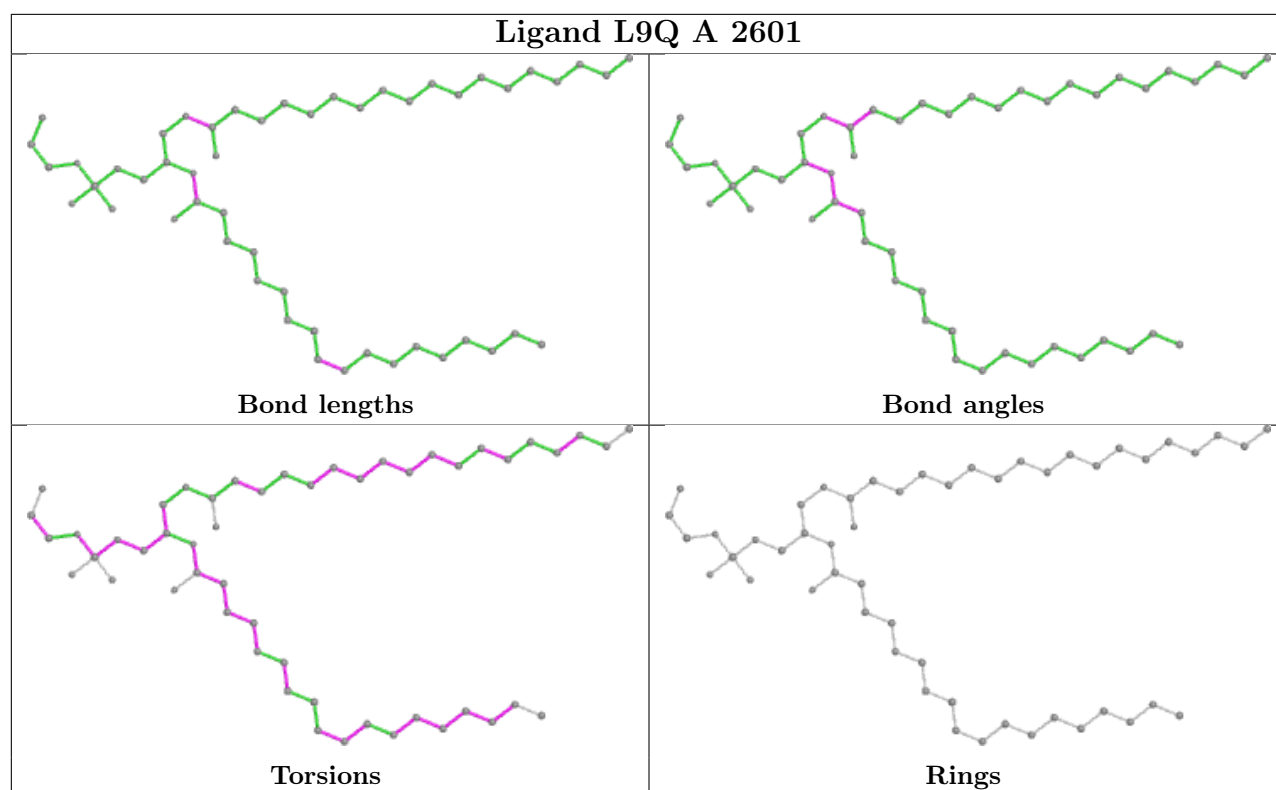
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2601	L9Q	3	0
2	B	2602	L9Q	3	0
2	A	2601	L9Q	3	0

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.

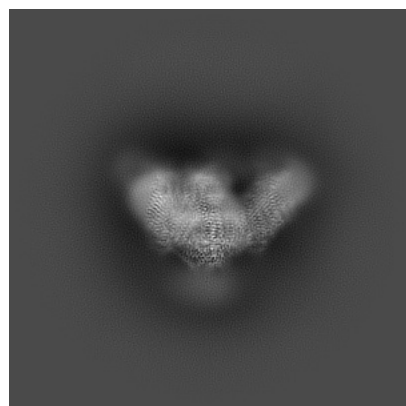
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39205. These allow visual inspection of the internal detail of the map and identification of artifacts.

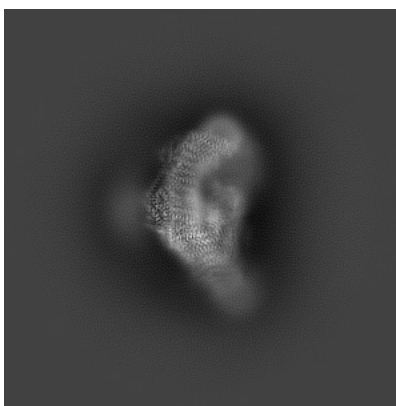
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

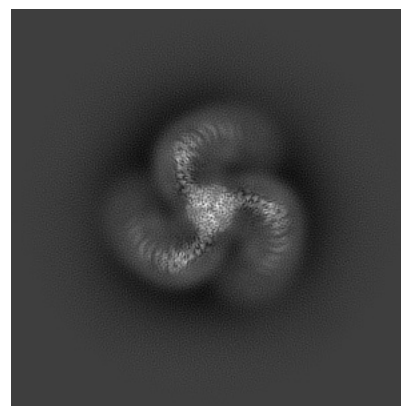
#### 6.1.1 Primary map



X

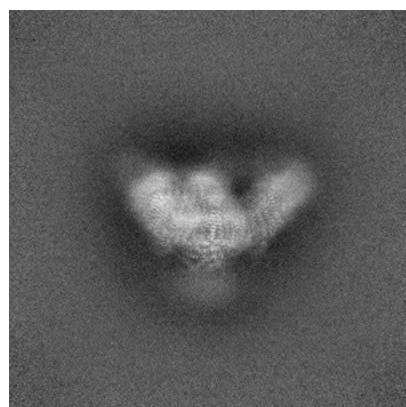


Y

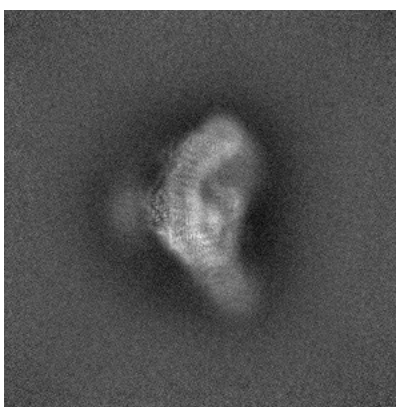


Z

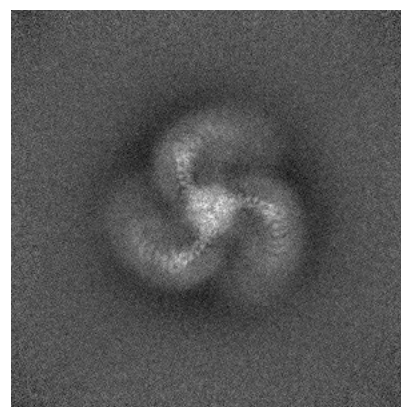
#### 6.1.2 Raw map



X



Y



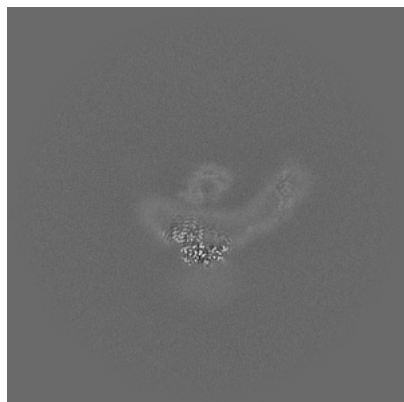
Z

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

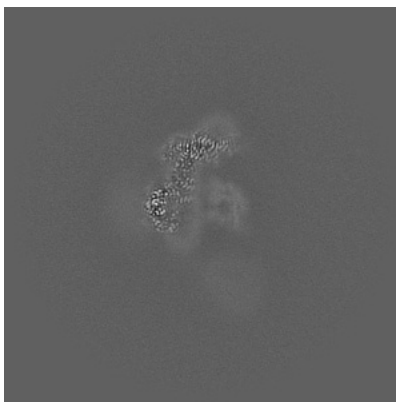


## 6.2 Central slices [i](#)

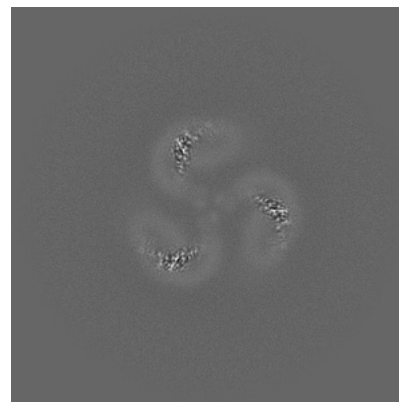
### 6.2.1 Primary map



X Index: 320

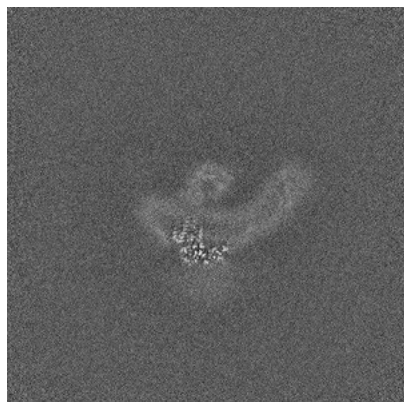


Y Index: 320

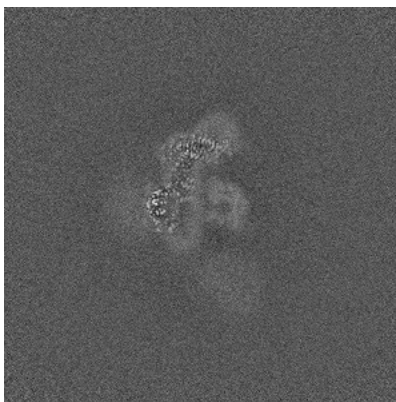


Z Index: 320

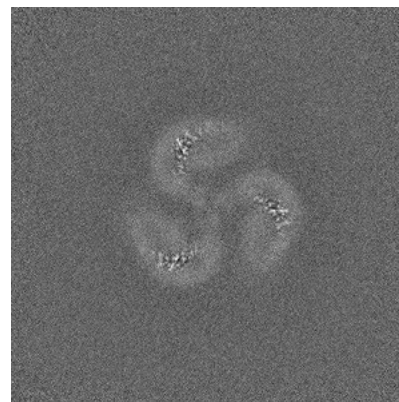
### 6.2.2 Raw map



X Index: 320



Y Index: 320



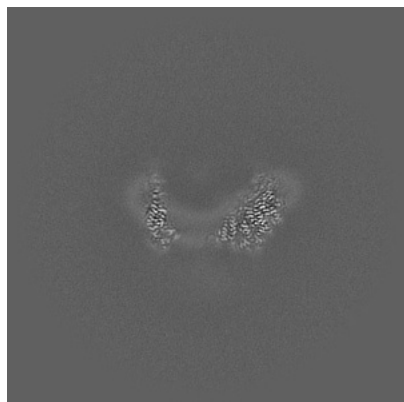
Z Index: 320

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

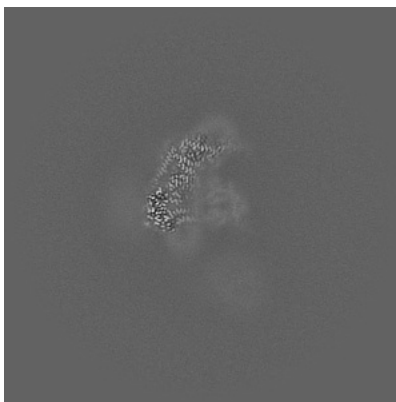


## 6.3 Largest variance slices [i](#)

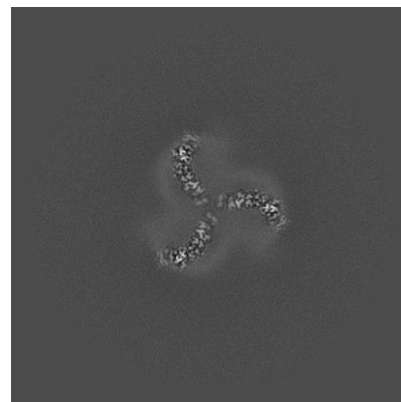
### 6.3.1 Primary map



X Index: 276

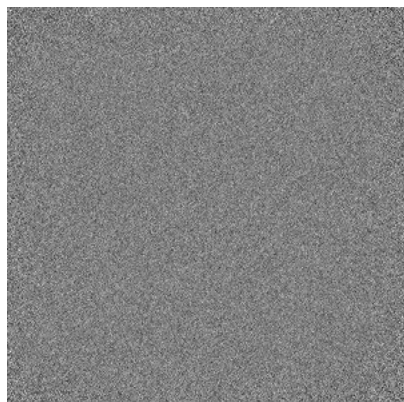


Y Index: 327

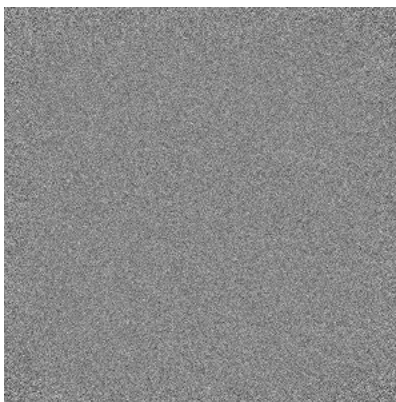


Z Index: 293

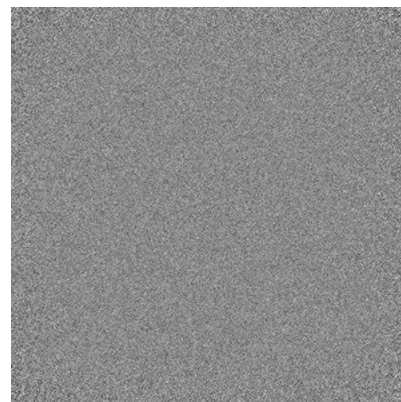
### 6.3.2 Raw map



X Index: 0



Y Index: 0

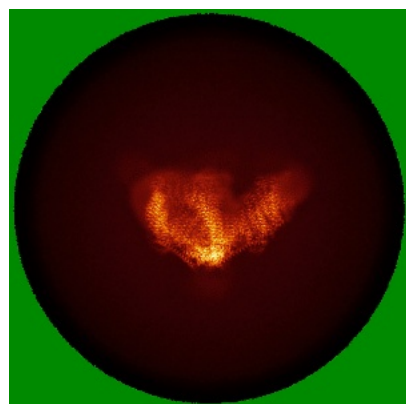


Z Index: 0

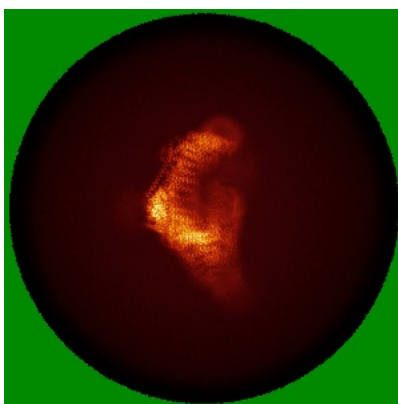
The images above show the largest variance slices of the map in three orthogonal directions.

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

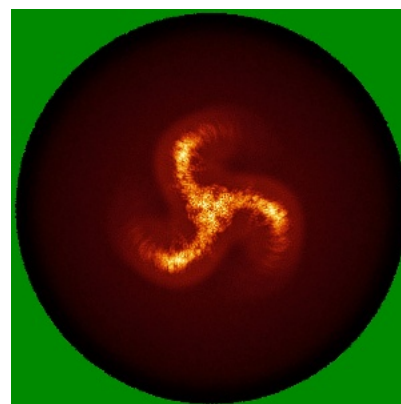
### 6.4.1 Primary map



X

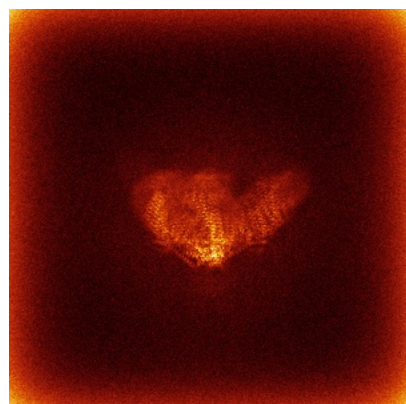


Y

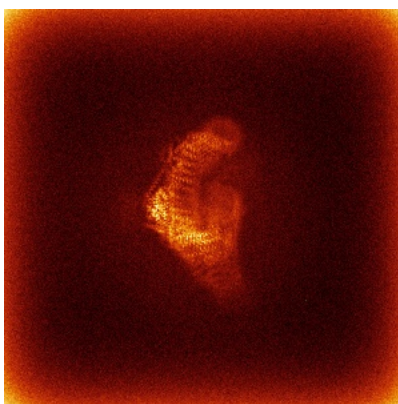


Z

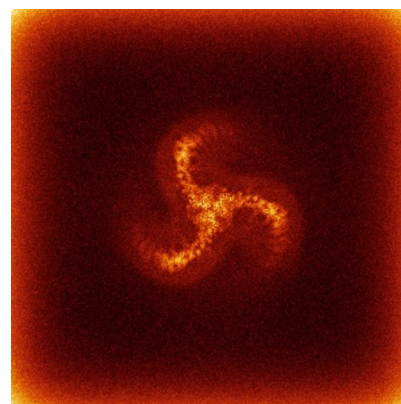
### 6.4.2 Raw map



X



Y

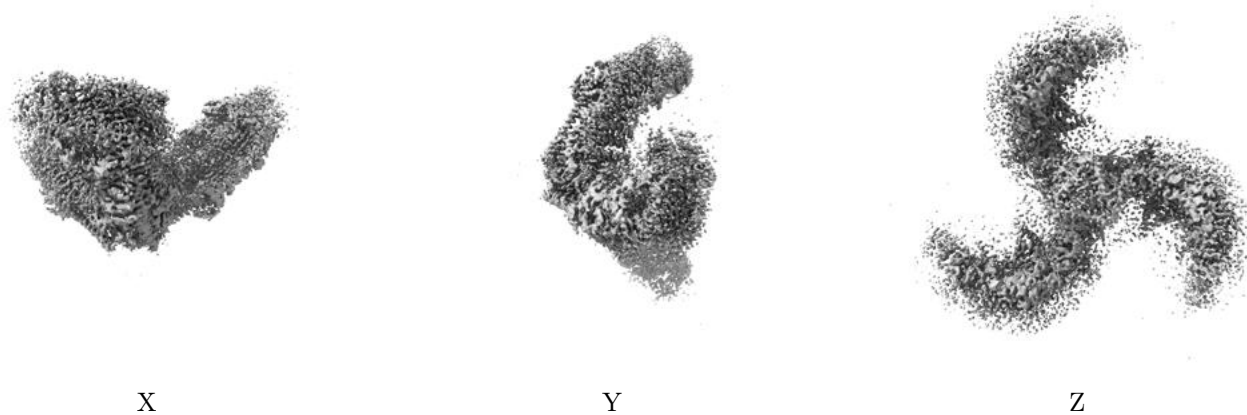


Z

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

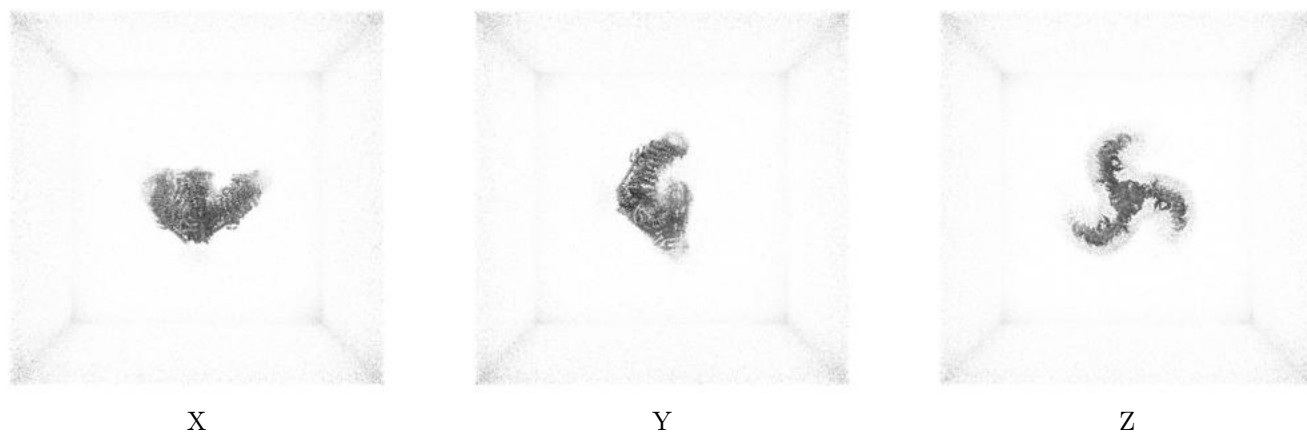
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

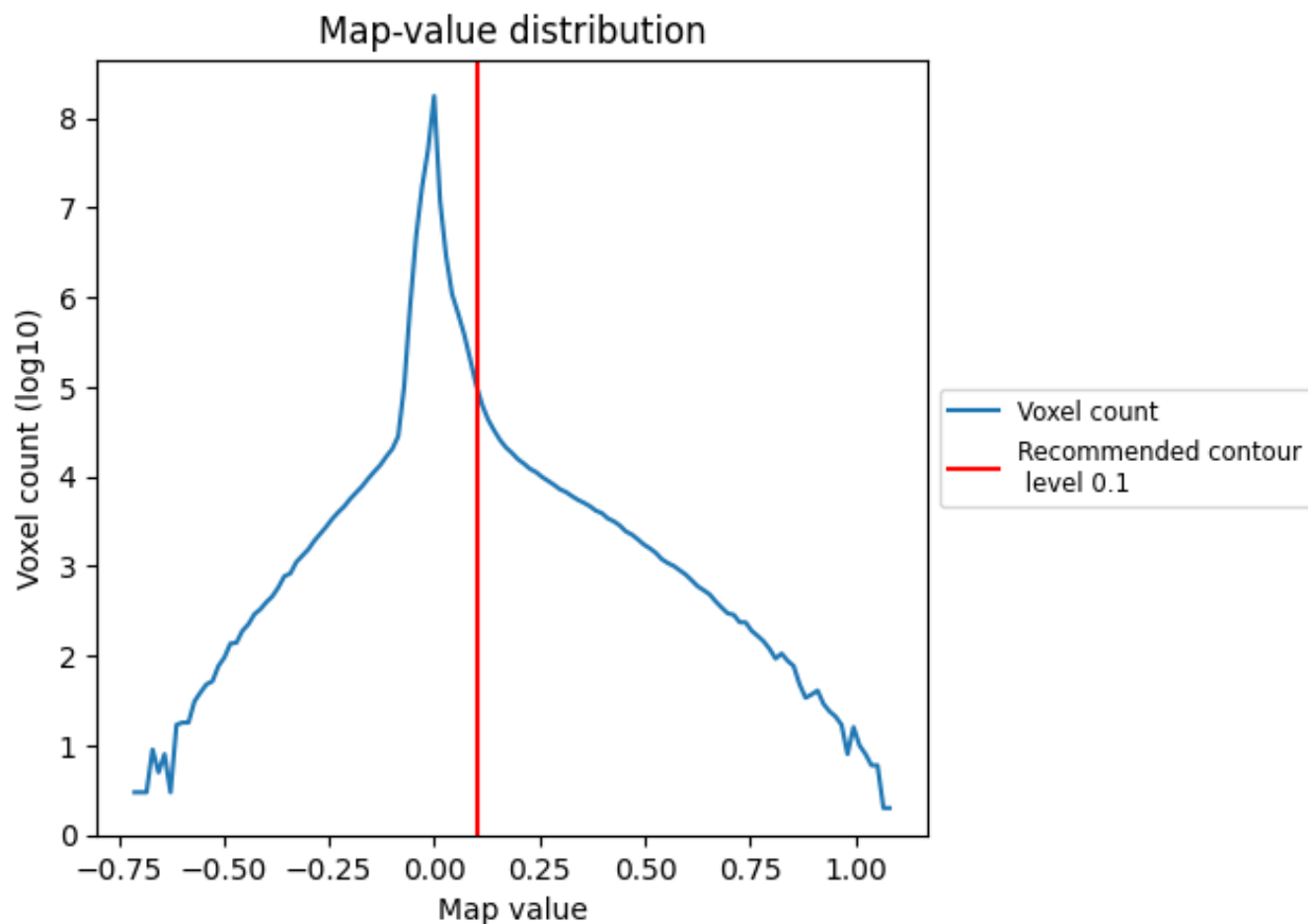
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

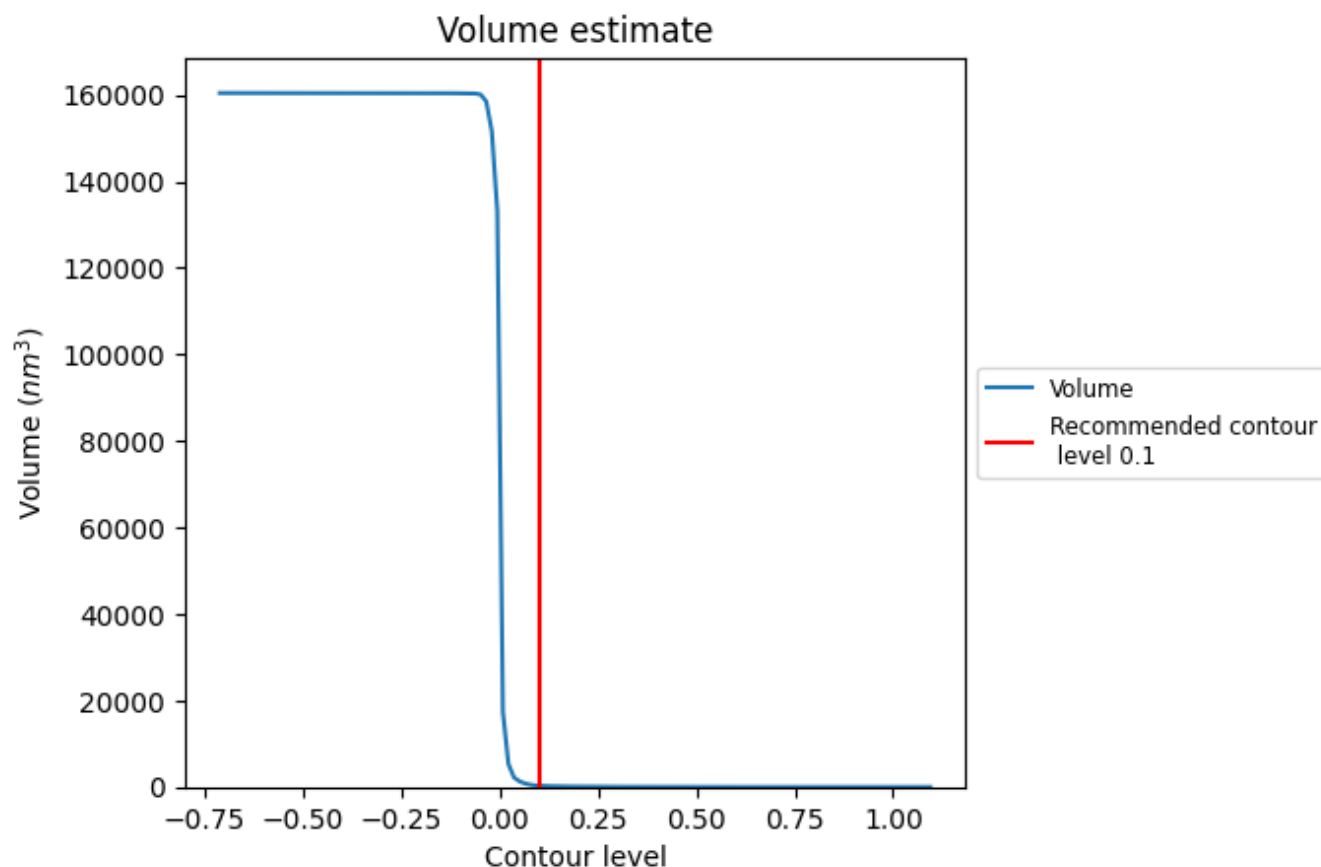
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

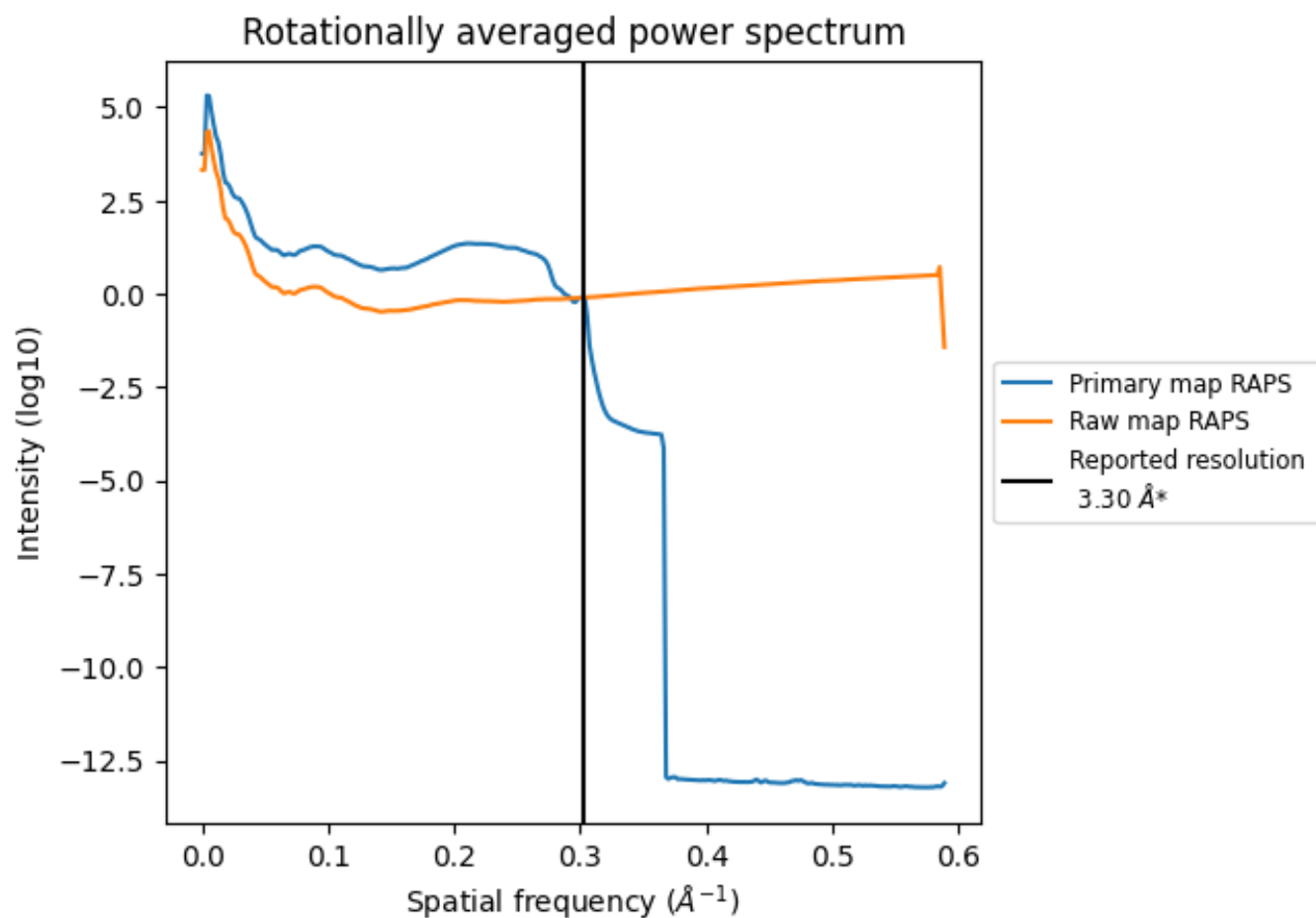
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 286  $\text{nm}^3$ ; this corresponds to an approximate mass of 258 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 ⓘ

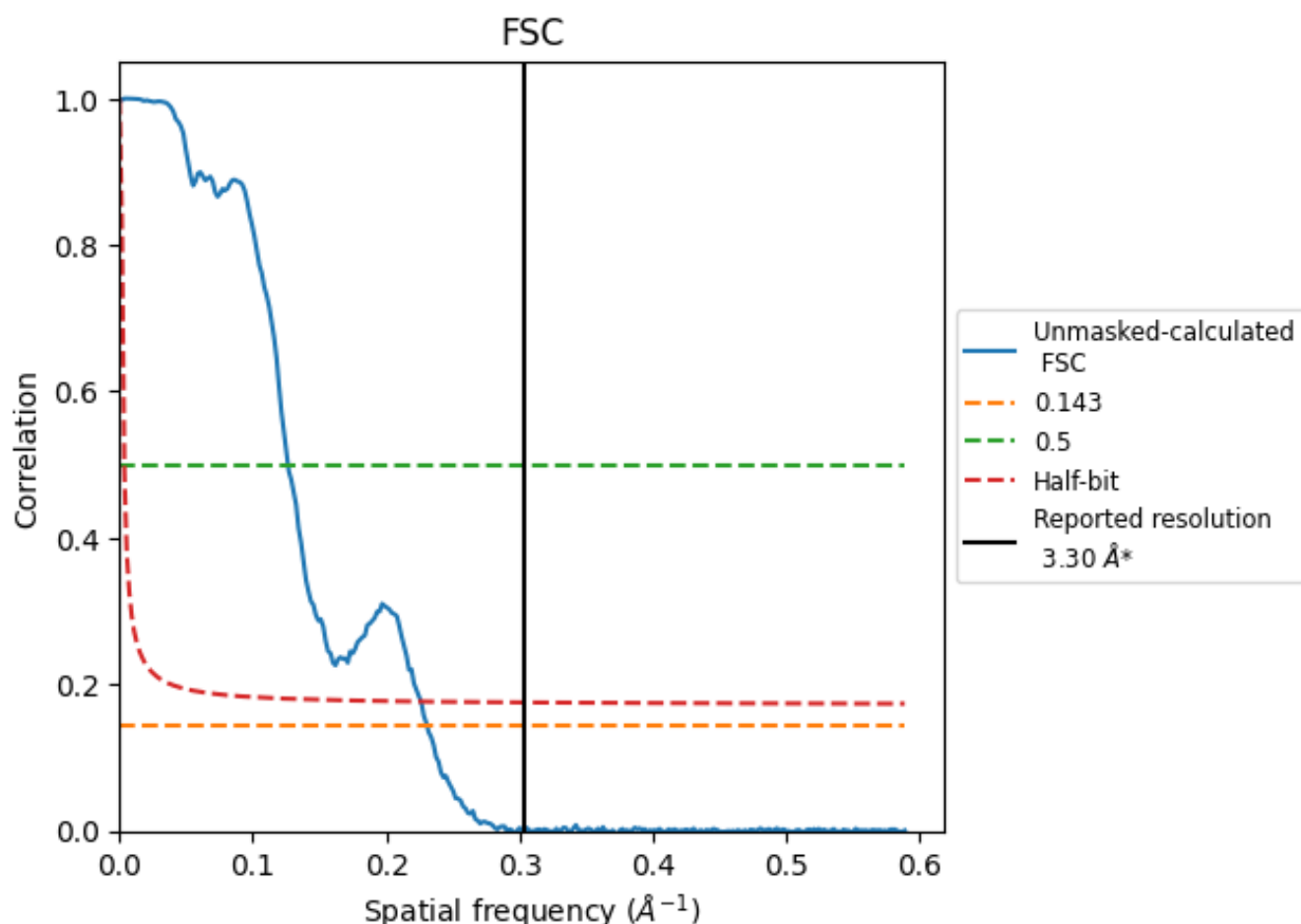


\*Reported resolution corresponds to spatial frequency of 0.303 Å<sup>-1</sup>

## 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<sup>-1</sup>

## 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*	4.34	7.91	4.42

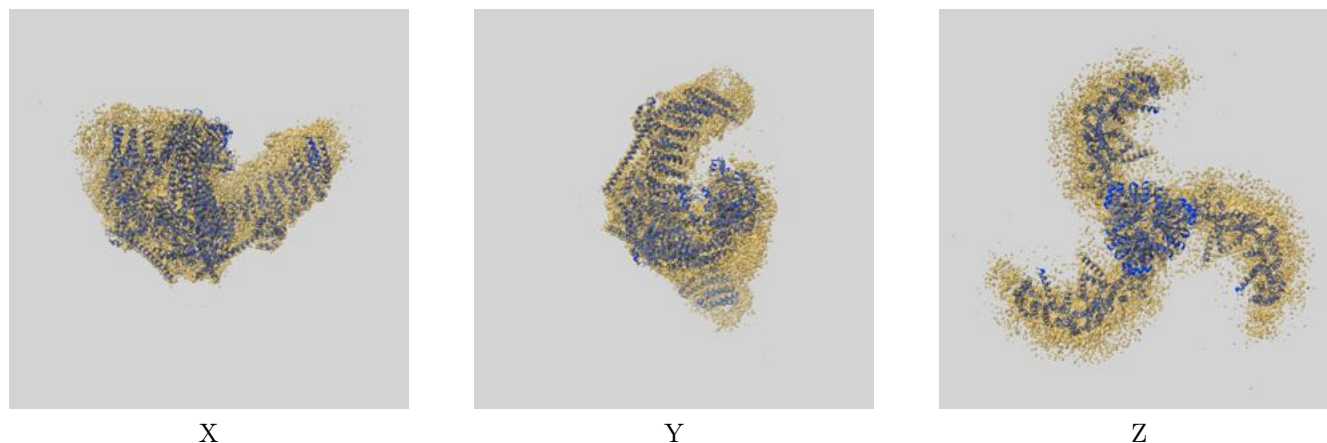
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.34 differs from the reported value 3.3 by more than 10 %



## 9 Map-model fit [i](#)

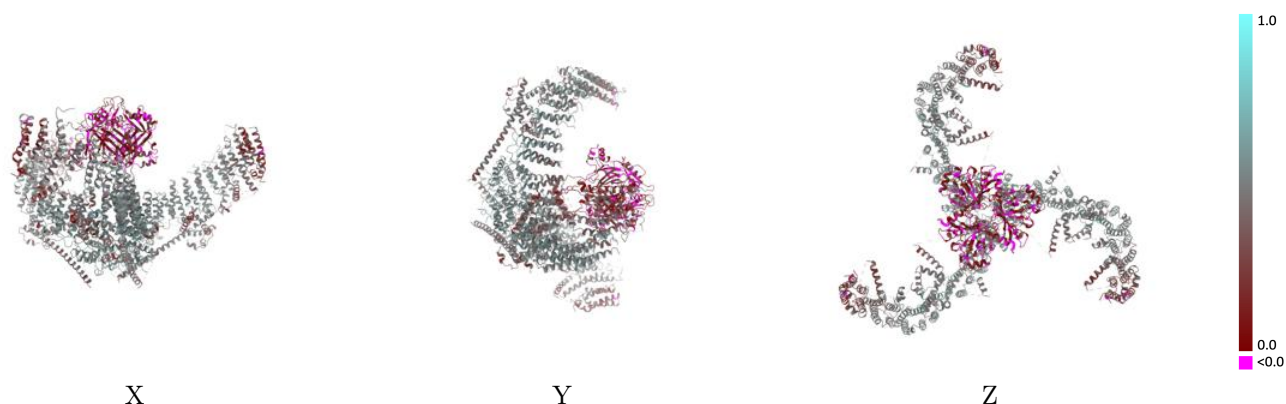
This section contains information regarding the fit between EMDB map EMD-39205 and PDB model 8YEZ. Per-residue inclusion information can be found in section [3](#) on page [5](#).

### 9.1 Map-model overlay [i](#)



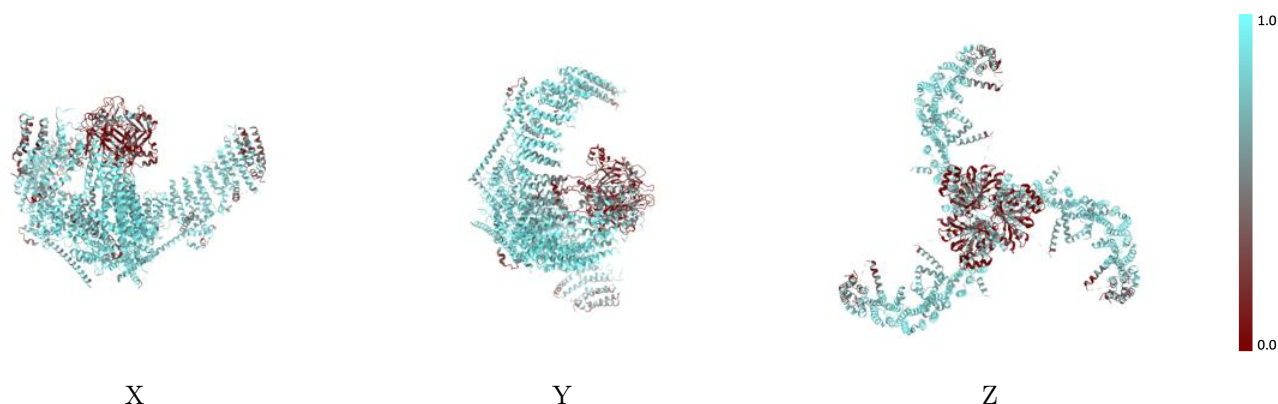
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



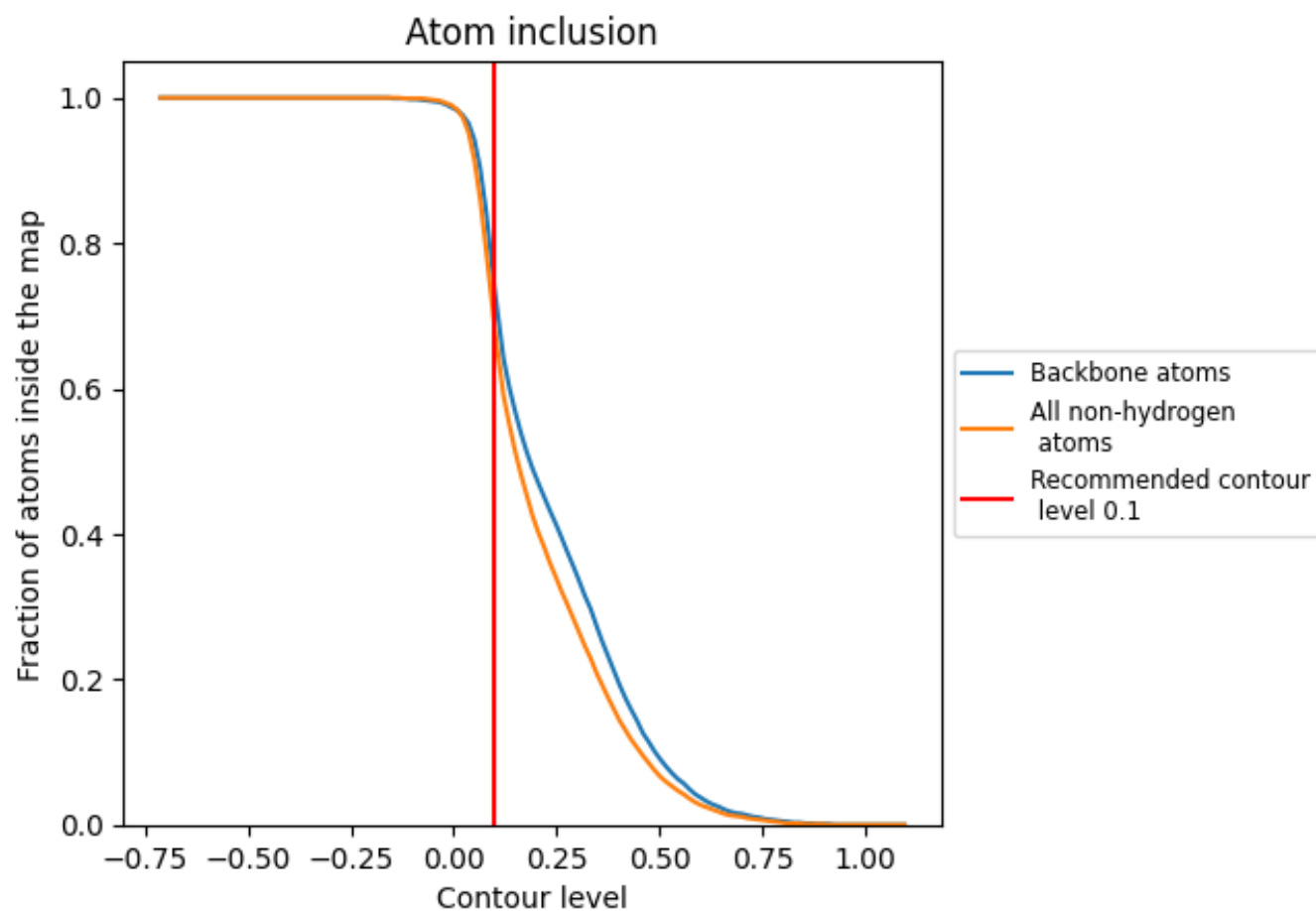
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.1).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 68% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6810	<div></div> 0.4010
A	<div></div> 0.6800	<div></div> 0.4000
B	<div></div> 0.6810	<div></div> 0.4010
C	<div></div> 0.6840	<div></div> 0.4010

