



wwPDB EM Validation Summary Report ⓘ

Mar 10, 2026 – 04:32 AM UTC

PDB ID : 8ZU8 / pdb_00008zu8
EMDB ID : EMD-60481
Title : Human PIEZO1-A1988V
Authors : Zhang, M.F.
Deposited on : 2024-06-08
Resolution : 3.90 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

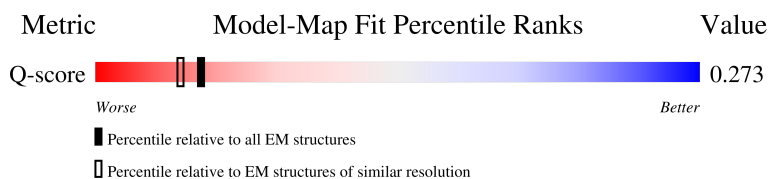
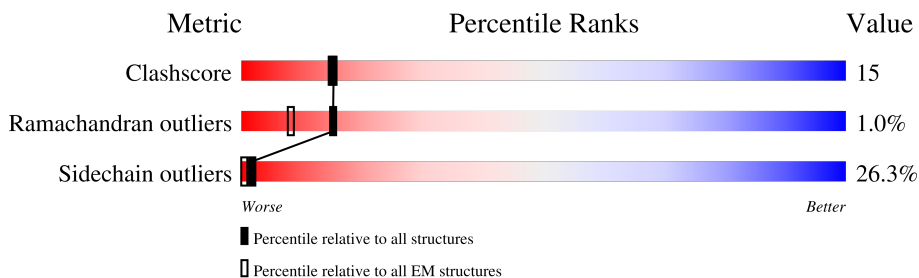
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 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	8855 (3.40 - 4.40)

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	1952	
1	B	1952	
1	C	1952	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 31401 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.

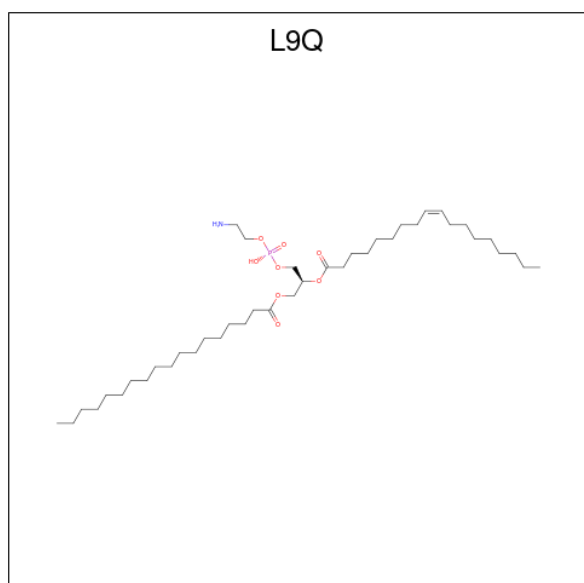
- Molecule 1 is a protein called Piezo-type mechanosensitive ion channel component 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1279	Total	C	N	O	S	0	0
			10418	6910	1721	1726	61		
1	B	1279	Total	C	N	O	S	0	0
			10418	6910	1721	1726	61		
1	C	1279	Total	C	N	O	S	0	0
			10412	6907	1718	1726	61		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1988	VAL	ALA	engineered mutation	UNP Q92508
B	1988	VAL	ALA	engineered mutation	UNP Q92508
C	1988	VAL	ALA	engineered mutation	UNP Q92508

- Molecule 2 is (1S)-2-[[[(S)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy]-1-[(octadecanoyloxymethyl)ethyl (9Z)-octadec-9-enoate (CCD ID: L9Q) (formula: C₄₁H₈₀NO₈P) (labeled as "Ligand of Interest" by depositor).

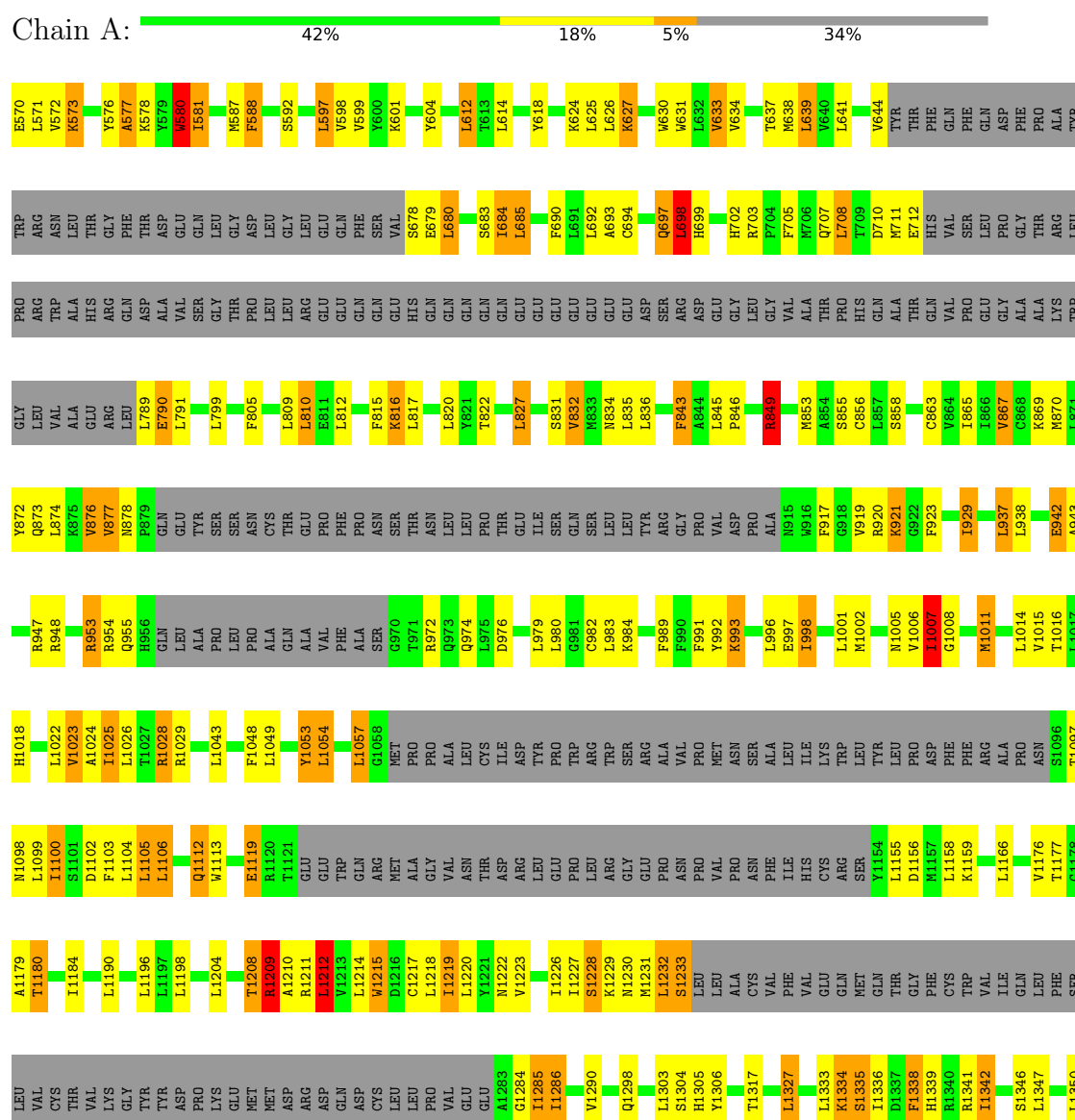


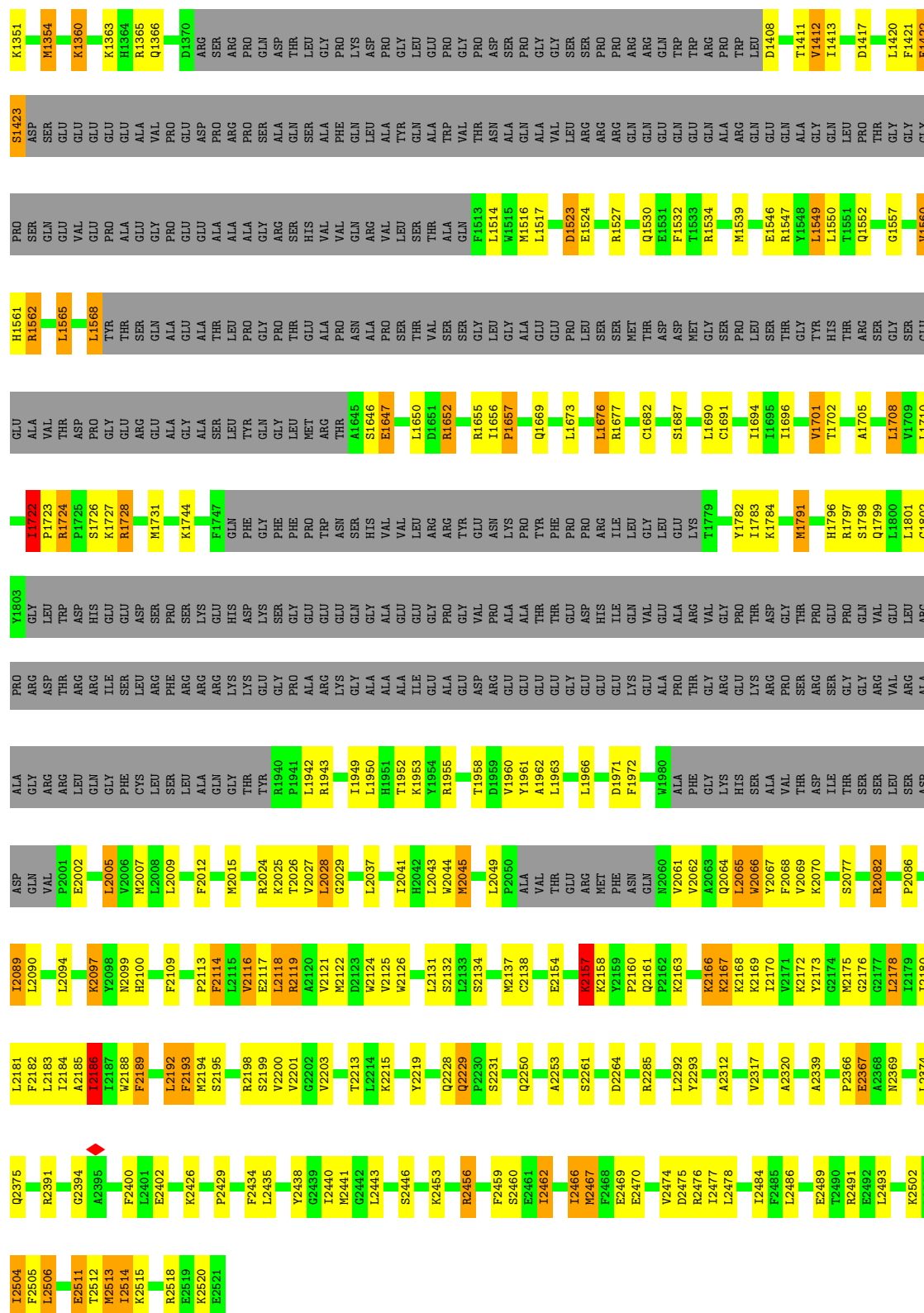
Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total 51	C 41	N 1	O 8	P 1	0
2	B	1	Total 51	C 41	N 1	O 8	P 1	0
2	C	1	Total 51	C 41	N 1	O 8	P 1	0

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: Piezo-type mechanosensitive ion channel component 1

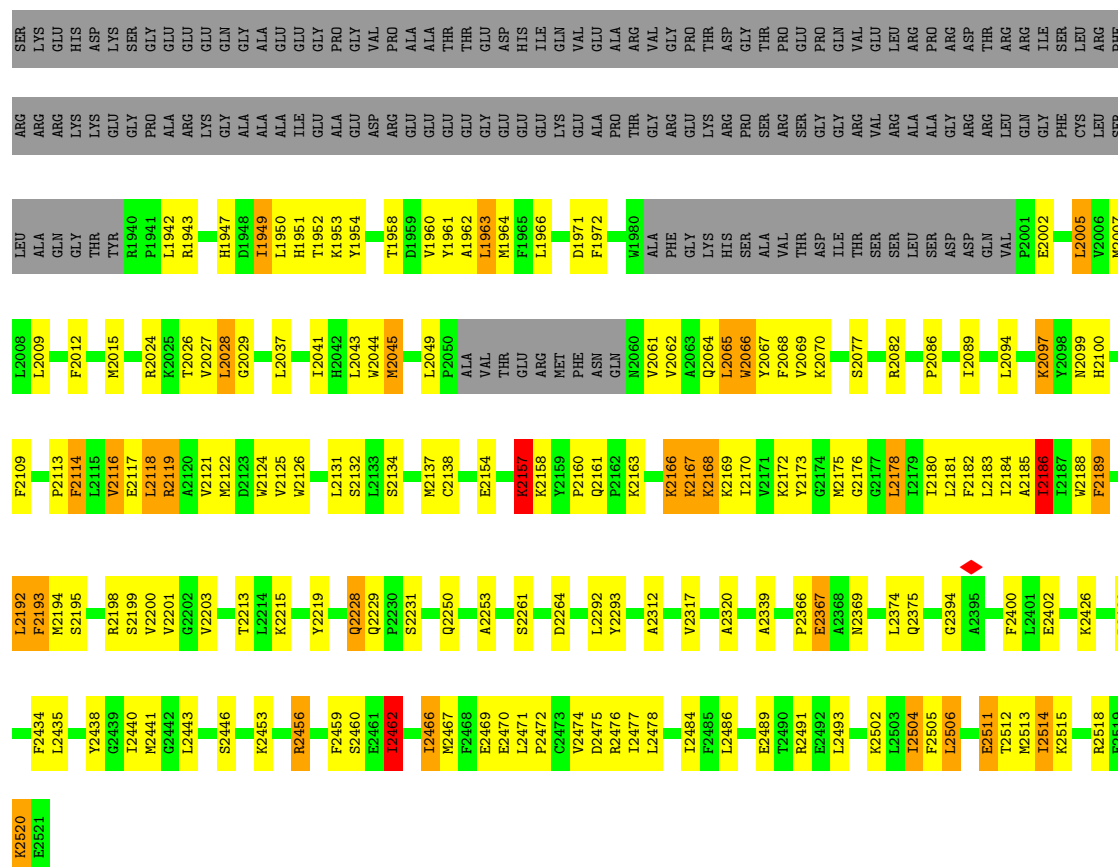




• Molecule 1: Piezo-type mechanosensitive ion channel component 1

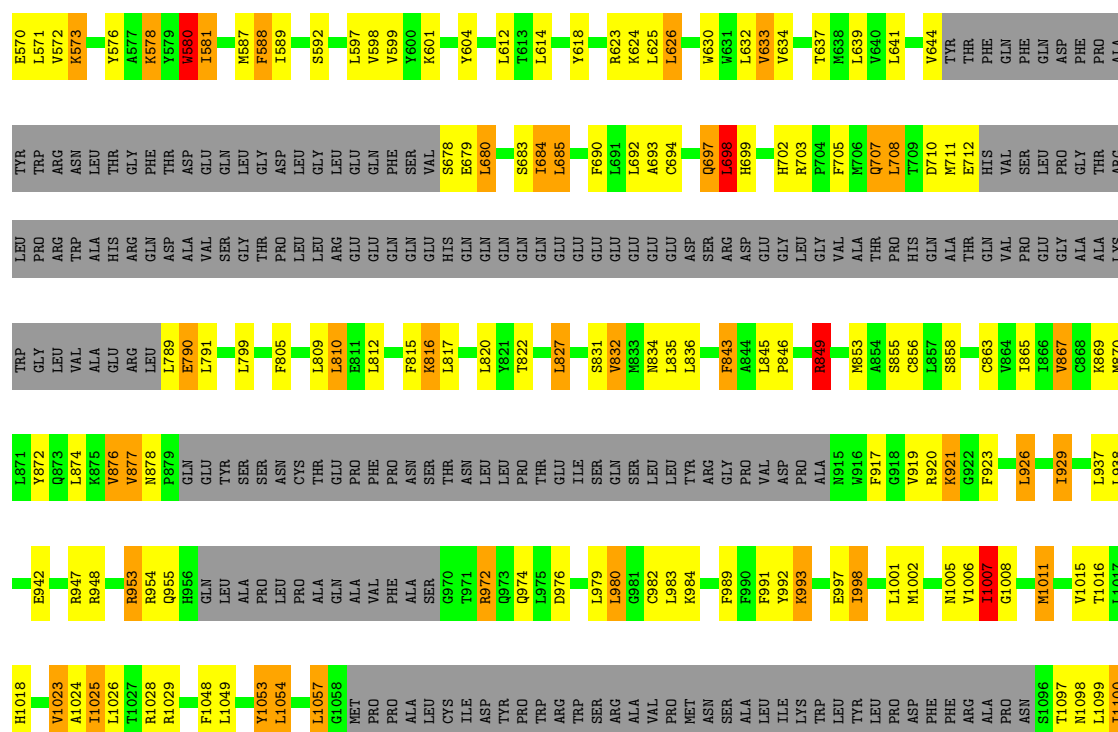
Chain B: 43% 17% 5% 34%

K1744	ALA	ALA	GLU	ASP	ARG	LYS	L1190	D1102	V1023	A943	Q873	LEU	ARG	TRP	E570
F1747	LEU	ALA	ALA	PRO	SER	GLY	L1199	F1103	A1024	R947	L874	VAL	TRP	ARG	L571
	TYR	ALA	ALA	PRO	ARG	MET	L1198	L1104	A1025	R948	K875	ALA	ASN	ASN	V572
	GLY	GLY	GLY	SER	GLN	ASP	L1204	L1105	I1026	R949	V877	ARG	LEU	THR	K573
	PRO	ARG	ARG	ALA	ASP	ASP	L1204	L1106	T1027	R953	N878	LEU	GLN	GLY	Y576
	THR	SER	SER	GLN	THR	ASP	T1208	Q1112	R1028	R954	P879	ASN	ASP	PHE	A577
	GLU	HIS	HIS	SER	LEU	GLN	R1209	W1113	R1029	Q955	G879	THR	THR	THR	K578
	ALA	VAL	VAL	PHE	GLY	ASP	R1209	E1119	F1048	R956	GLU	LEU	ALA	THR	K579
	PRO	VAL	GLN	GLN	PRO	CYS	R1211	A1210	A1210	R957	TYR	LEU	VAL	ASP	Y579
	ALA	ARG	ARG	LEU	LEU	LEU	R1212	R1120	L1049	GLN	GLY	GLY	SER	GLU	V580
	VAL	VAL	VAL	PRO	PRO	VAL	V1213	T1121	L1053	ALA	ASN	THR	GLN	GLN	I581
	LEU	LEU	LEU	VAL	GLY	VAL	L1214	GLU	L1054	PRO	SER	PRO	LEU	GLY	M587
	SER	THR	SER	GLY	GLY	GLY	W1215	TRP	L1057	LEU	CYS	LEU	LEU	ASP	F588
	THR	GLU	GLU	GLY	GLY	GLY	I1219	ARG	G1058	ALA	PHE	LEU	GLU	GLY	I589
	ALA	ALA	ALA	PRO	PRO	ALA	I1220	MET	G1058	VAL	ASN	PRO	GLN	GLU	S592
	VAL	VAL	VAL	ASP	ASP	GLY	I1226	ALA	PRO	PHE	ASN	VAL	GLN	GLN	L597
	GLY	GLY	F1513	THR	GLY	G1284	I1227	VAL	PRO	ALA	ASN	THR	GLN	PHE	V598
	SER	GLY	L1514	ASN	GLY	I1285	I1228	VAL	ALA	ALA	SER	LEU	GLN	SER	V599
	GLY	GLY	M1516	ALA	THR	V1290	K1229	THR	LEU	SER	THR	ALA	HIS	VAL	Y600
	ALA	ALA	L1517	ALA	GLY	Y1306	M1230	ASN	CYS	GLY	ASN	GLN	GLN	VAL	K601
	GLU	GLU	L1517	VAL	GLY	Q1298	M1231	ASP	ILE	T971	LEU	LEU	GLN	ASP	Y604
	PRO	PRO	D1523	LEU	SER	L1303	L1232	LEU	ASP	R972	LEU	ASP	GLN	GLY	Y604
	LEU	LEU	E1524	ARG	SER	S1304	S1233	LEU	TYR	Q973	PRO	PRO	GLN	GLN	L612
	SER	SER	R1527	ARG	PRO	H1305	S1233	GLU	TRP	Q974	THR	THR	GLN	GLN	L612
	MET	MET	L1527	GLN	ARG	Y1306	LEU	PRO	TRP	D976	GLU	GLU	GLU	GLU	L614
	THR	THR	Q1530	GLN	ARG	T1317	ALA	ARG	TRP	TRP	ILE	ILE	GLU	GLU	L614
	ASP	ASP	F1531	GLY	GLN	L1327	VAL	GLY	SER	L979	GLN	GLU	GLU	GLU	Y618
	ASP	ASP	F1532	GLN	TRP	L1327	VAL	GLY	ARG	L980	SER	GLU	GLU	GLU	Y618
	MET	MET	T1533	GLY	TRP	K1334	GLY	PRO	ALA	G981	LEU	GLU	GLU	GLU	K624
	GLY	GLY	R1534	ALA	ARG	S1335	VAL	ASN	VAL	C982	LEU	GLU	GLU	GLU	L625
	PRO	PRO	M1539	ALA	PRO	I1336	GLY	PRO	PRO	L983	TYR	ASP	ASP	ASP	L626
	LEU	LEU	E1546	GLN	LEU	T1337	MET	VAL	ASN	K984	ARG	SER	SER	ARG	K627
	SER	SER	R1547	GLY	LEU	D1337	GLN	ASN	SER	F989	GLY	ARG	ARG	ASP	W630
	THR	THR	Y1548	GLN	GLY	F1338	THR	PHE	ALA	F990	VAL	ASP	GLU	GLU	W630
	GLY	GLY	L1549	ALA	GLY	H1339	GLY	ILE	ILE	F991	ASP	GLY	GLY	GLY	V633
	TYR	TYR	L1550	GLY	GLY	R1340	PHE	HIS	ILE	Y992	PRO	LEU	LEU	LEU	V634
	HIS	HIS	L1550	GLN	GLN	R1341	CYS	CYS	LYS	K993	ALA	GLY	GLY	GLY	V634
	THR	THR	T1551	LEU	ASP	I1342	TRP	ARG	TRP	E997	N915	VAL	VAL	VAL	T637
	ARG	ARG	Q1552	PRO	ASP	L1346	VAL	SER	LEU	I998	W915	ALA	ALA	ALA	T637
	SER	SER	G1557	THR	GLY	L1347	ILE	GLY	TYR		W915	THR	THR	THR	W638
	GLY	GLY	L1557	GLY	GLY	L1420	GLN	L1154	LEU		F917	ALA	ALA	ALA	L639
	SER	SER	Y1560	GLY	GLY	F1421	LEU	D1155	LEU		G919	PRO	PRO	PRO	V640
	GLU	GLU	L1561	PRO	GLY	E1422	PHE	M1157	ASP	L1001	V919	C956	HIS	L708	L641
	ALA	ALA	R1562	SER	ASP	S1423	SER	L1158	PHE	M1002	R920	ASP	GLN	M710	
	VAL	VAL	L1565	GLN	SER	ASP	VAL	K1159	PHE	N1005	G922	ALA	ALA	M711	V644
	THR	THR	L1565	GLY	GLY	SER	CYS	L1166	ARG	V1006	G923	GLN	GLN	E712	
	ASP	ASP	L1568	VAL	GLY	GLY	THR	L1166	ALA	I1007	ASN	VAL	VAL	HIS	THR
	PRO	PRO	T1568	GLY	GLY	K1360	VAL	V1176	PRO	G1008	L926	GLY	GLY	VAL	PHE
	GLY	GLY	Y1568	ALA	GLY	K1363	VAL	T1177	ASP	M1011	V967	GLY	PRO	LEU	PHE
	THR	THR	H1564	PRO	THR	H1364	GLY	L1178	GLY	S1096	C968	ALA	GLY	GLY	ASP
	ARG	ARG	R1365	GLY	ALA	R1365	TYR	A1179	N1098	V1015	K969	ALA	THR	THR	PHE
	GLY	GLY	Q1366	VAL	VAL	Q1366	ASP	T1180	N1099	T1016	M870	LYS	ARG	ARG	PRO
	PRO	PRO	D1370	GLY	GLY	D1370	PRO	T1184	TYR	L1017	L871	TYR	LEU	LEU	ALA
	GLY	GLY		GLY	GLY					H1018	E942	GLY	PRO	PRO	TYR



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

Chain C: 43% 17% 5% 34%



F2434	M2194	P2113	L2008	LEU	ARG	SER	PRO	ALA	ALA	PRO	GLY	S1101
L2435	S2195	F2114	L2009	SER	PHE	LEU	PRO	GLY	GLU	GLU	ASP	D1102
Y2438	R2198	L2115	F2012	ALA	ARG	ALA	LYS	THR	ALA	ASP	LYS	F1103
G2439	S2199	E2116	M2015	GLN	ARG	LEU	HIS	PRO	ALA	ARG	GLY	L1104
T2440	V2200	L2118	R2024	THR	LYS	PHE	ASP	GLY	ALA	PRO	MET	L1105
M2441	V2201	K2120	K2025	TYR	GLY	GLY	LYS	PRO	GLY	GLY	MET	L1106
G2442	G2203	V2121	T2026	TYR	GLY	PHE	LYS	PRO	GLY	ASP	ASP	Q1112
L2443	G2202	D2123	V2027	P1941	ALA	PHE	GLY	LEU	THR	GLN	ASP	W1113
S2446	T2213	D2124	V2028	R1942	ALA	GLY	GLY	ALA	VAL	GLY	GLN	E1119
K2453	L2214	W2125	L2028	R1943	LYS	GLY	GLY	VAL	VAL	PRO	ASP	R1120
R2456	K2215	W2126	G2029	T1949	GLY	ASN	GLN	ASN	GLN	LYS	CYS	T1121
R2457	Y2219	L2131	L2037	H1950	ALA	SER	GLY	ALA	ARG	LEU	LEU	GLU
F2459	Q2228	S2132	T2041	H1951	ALA	GLY	ALA	PRO	VAL	PRO	TRP	GLU
S2460	Q2229	L2133	H2042	T1952	ALA	GLY	ALA	THR	LEU	TYR	GLY	TRP
E2461	P2230	S2134	L2043	R1953	ILE	GLY	GLY	VAL	SER	GLN	GLY	ARG
E2462	S2231	M2137	W2044	R1954	GLY	PRO	GLY	SER	GLN	THR	GLY	MET
T2466	Q2250	C2138	M2045	R1955	ALA	GLY	ARG	SER	ALA	TRP	GLY	ALA
M2467	A2253	E2154	L2049	T1958	ASP	VAL	GLY	GLY	GLN	VAL	GLY	GLY
E2469	S2261	K2157	P2050	D1959	GLY	ALA	THR	THR	ALA	GLY	ASP	ASN
E2470	S2261	K2158	VAL	Y1960	GLY	ALA	THR	GLY	GLY	GLY	ASP	VAL
T2471	D2264	T2159	GLY	Y1961	GLY	ALA	THR	GLY	GLY	GLY	ASP	ASN
P2472	D2264	T2160	GLY	A1962	GLY	ALA	THR	GLY	GLY	GLY	ASP	THR
C2473	R2285	Q2161	MET	L1966	GLY	ALA	THR	GLY	GLY	GLY	ASP	ASP
V2474	R2285	P2162	PHE	D1971	LYS	ILE	GLY	GLY	GLY	GLY	ARG	ARG
D2475	L2292	K2163	ASN	F1972	GLY	VAL	GLY	THR	GLY	GLY	GLY	GLY
R2476	Y2293	K2166	N2060	W1980	GLY	VAL	GLY	ASP	ASP	GLN	ALA	LEU
T2477	V2317	K2167	V2061	ALA	ALA	GLY	ALA	ASP	ASP	GLY	ALA	LEU
I2484	A2320	K2168	V2062	PHE	THR	ALA	ALA	GLY	GLY	TRP	VAL	GLY
F2485	A2320	K2169	A2063	GLY	ARG	VAL	VAL	GLY	GLY	ARG	VAL	GLY
L2486	A2339	T2170	Q2064	LYS	ARG	GLY	GLY	SER	PRO	ARG	PRO	GLY
E2489	A2339	V2171	L2065	HIS	GLY	PRO	PRO	LEU	LEU	TRP	GLY	GLY
T2490	P2366	K2172	W2066	SER	LYS	THR	THR	GLY	GLY	TRP	GLY	GLY
R2491	E2367	Y2173	Y2067	ALA	ALA	ASP	GLY	THR	THR	GLY	ILE	VAL
E2492	A2368	G2174	F2068	VAL	PRO	GLY	GLY	GLY	GLY	GLY	GLN	ILE
L2493	A2368	K2175	V2069	THR	SER	THR	THR	TYR	GLY	GLY	GLY	THR
K2502	N2369	G2176	K2070	ASP	ARG	PRO	GLY	HIS	THR	L1550	GLY	CYS
L2503	L2374	G2177	S2077	ILE	SER	GLY	GLY	ARG	LEU	T1951	LEU	ARG
L2504	Q2375	L2178	T2077	THR	GLY	PRO	GLY	GLY	PRO	Q1552	TRP	SER
F2505	R2391	T2180	R2082	SER	GLY	GLY	GLN	THR	THR	I1342	TRP	Y1154
L2506	R2391	L2181	S2086	LEU	ARG	VAL	VAL	SER	GLY	S1346	VAL	L1155
E2511	G2394	L2182	P2086	SER	ARG	LEU	GLY	GLY	GLY	F1421	ILE	D1156
T2512	A2395	L2183	I2089	ASP	ALA	ASP	ARG	GLY	GLY	E1422	GLN	M1157
M2513	A2395	L2184	L2094	ASP	GLY	PRO	ARG	GLY	GLY	S1423	LEU	L1158
L2514	F2400	T2185	L2094	GLN	GLY	PRO	ARG	VAL	GLY	ASP	PHE	K1159
K2515	L2401	T2186	K2097	VAL	ARG	ASP	THR	THR	VAL	M1354	SER	L1166
E2518	E2402	L2187	Y2096	P2001	ARG	ASP	THR	THR	CYS	K1360	VAL	V1176
E2519	K2426	V2188	H2100	E2002	LEU	THR	ARG	PRO	GLY	K1363	THR	T1177
K2520	P2429	F2189		L2005	GLN	ARG	ARG	GLY	GLY	H1364	VAL	G1178
		L2192		W2006	PHE	ILE	ILE	GLY	ALA	R1365	LYS	A1179
		F2193		M2007	SER	GLY	GLY	ARG	GLY	T1365	GLY	T1180
					LEU	ASP	ASP	GLU	VAL	Q1366	TYR	

EMD-60481

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	32000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TECNAI 10	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.525	Depositor
Minimum map value	-0.286	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.02	Depositor
Map size ($\text{\AA}$)	434.688, 434.688, 434.688	wwPDB
Map dimensions	512, 512, 512	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	0.74	2/10678 (0.0%)	0.98	52/14479 (0.4%)
1	B	0.74	1/10678 (0.0%)	0.98	50/14479 (0.3%)
1	C	0.74	1/10672 (0.0%)	0.98	50/14472 (0.3%)
All	All	0.74	4/32028 (0.0%)	0.98	152/43430 (0.3%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	577	ALA	C-O	-6.54	1.15	1.24
1	B	2099	ASN	CA-C	-5.62	1.50	1.53
1	C	2099	ASN	CA-C	-5.55	1.50	1.53
1	A	2099	ASN	CA-C	-5.50	1.50	1.53

The worst 5 of 152 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	684	ILE	N-CA-C	-10.51	103.39	111.90
1	B	684	ILE	N-CA-C	-10.48	103.41	111.90
1	A	684	ILE	N-CA-C	-10.47	103.42	111.90
1	A	1025	ILE	N-CA-C	-10.24	103.60	111.90
1	C	1025	ILE	N-CA-C	-10.22	103.62	111.90

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	10418	0	10650	354	0
1	B	10418	0	10650	343	0
1	C	10412	0	10639	338	0
2	A	51	0	79	20	0
2	B	51	0	79	20	0
2	C	51	0	79	19	0
All	All	31401	0	32176	946	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 15.

The worst 5 of 946 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:2157:LYS:CB	1:A:2157:LYS:NZ	1.70	1.45
1:C:2193:PHE:HD1	1:C:2194:MET:N	1.11	1.43
1:B:2193:PHE:HD1	1:B:2194:MET:N	1.11	1.42
1:C:2028:LEU:CD1	1:C:2028:LEU:C	1.78	1.42
1:B:2028:LEU:CD1	1:B:2028:LEU:C	1.78	1.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1249/1952 (64%)	1128 (90%)	109 (9%)	12 (1%)	12	45
1	B	1249/1952 (64%)	1126 (90%)	110 (9%)	13 (1%)	12	45
1	C	1249/1952 (64%)	1127 (90%)	110 (9%)	12 (1%)	12	45
All	All	3747/5856 (64%)	3381 (90%)	329 (9%)	37 (1%)	15	45

5 of 37 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1657	PRO
1	A	2429	PRO
1	B	1657	PRO
1	B	2429	PRO
1	C	1657	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	1113/1693 (66%)	819 (74%)	294 (26%)	0	3
1	B	1113/1693 (66%)	819 (74%)	294 (26%)	0	3
1	C	1112/1693 (66%)	823 (74%)	289 (26%)	0	3
All	All	3338/5079 (66%)	2461 (74%)	877 (26%)	2	3

5 of 877 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1568	LEU
1	B	2467	MET
1	C	2026	THR
1	B	1701	VAL
1	B	1565	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 66 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	1535	HIS
1	C	1699	HIS
1	C	2464	HIS
1	B	915	ASN
1	B	697	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 ⓘ

3 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	C	2601	-	50,50,50	1.08	3 (6%)	53,55,55	1.10	2 (3%)
2	L9Q	A	2601	-	50,50,50	1.08	3 (6%)	53,55,55	1.10	2 (3%)
2	L9Q	B	2601	-	50,50,50	1.08	3 (6%)	53,55,55	1.10	2 (3%)

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	C	2601	-	-	35/54/54/54	-
2	L9Q	A	2601	-	-	35/54/54/54	-
2	L9Q	B	2601	-	-	35/54/54/54	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2601	L9Q	O2-C31	4.44	1.46	1.34
2	C	2601	L9Q	O2-C31	4.44	1.46	1.34
2	B	2601	L9Q	O2-C31	4.43	1.46	1.34
2	C	2601	L9Q	O3-C11	4.19	1.45	1.33
2	A	2601	L9Q	O3-C11	4.19	1.45	1.33

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2601	L9Q	O2-C31-C32	4.68	121.60	111.48
2	A	2601	L9Q	O2-C31-C32	4.67	121.58	111.48
2	B	2601	L9Q	O2-C31-C32	4.67	121.58	111.48
2	A	2601	L9Q	O3-C11-C12	2.73	120.15	111.83
2	C	2601	L9Q	O3-C11-C12	2.72	120.14	111.83

There are no chirality outliers.

5 of 105 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2601	L9Q	C1-O3P-P-O1P
2	A	2601	L9Q	C1-O3P-P-O2P
2	A	2601	L9Q	C1-O3P-P-O4P
2	A	2601	L9Q	C32-C31-O2-C2
2	B	2601	L9Q	C1-O3P-P-O1P

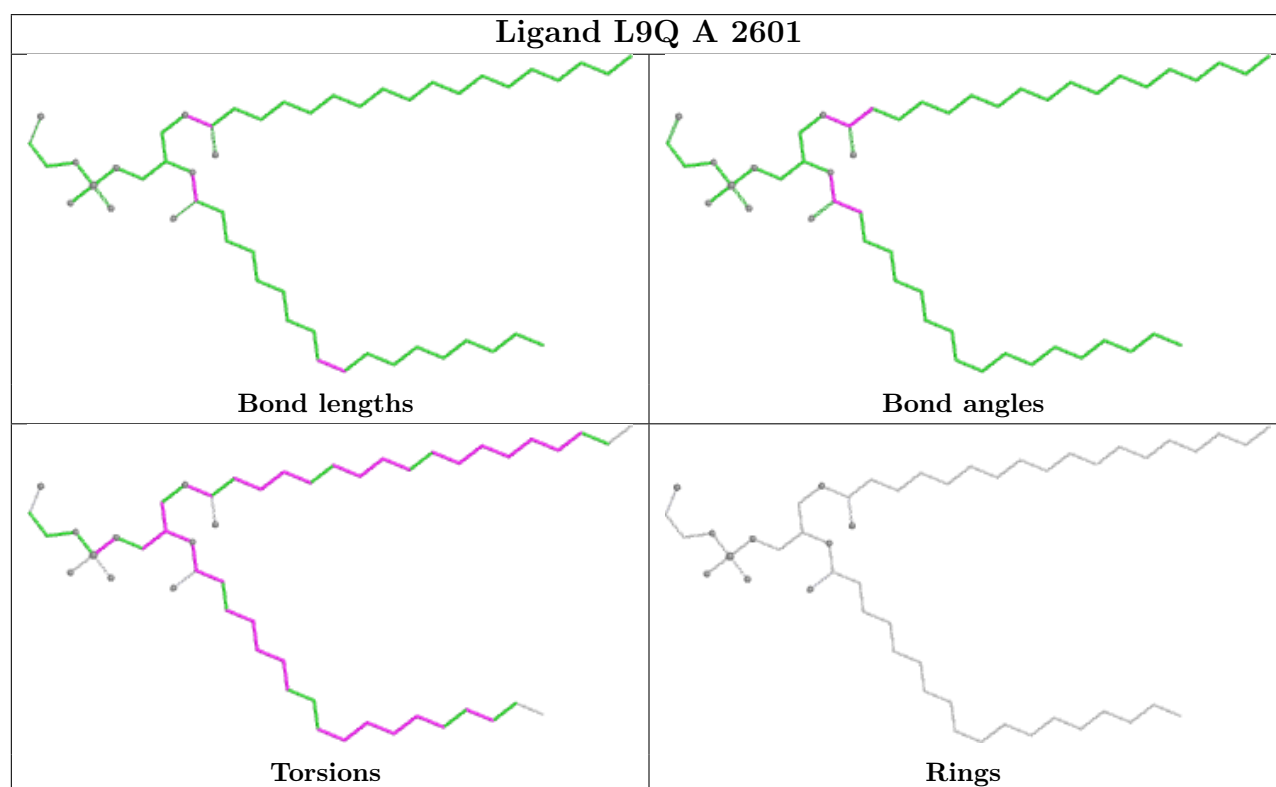
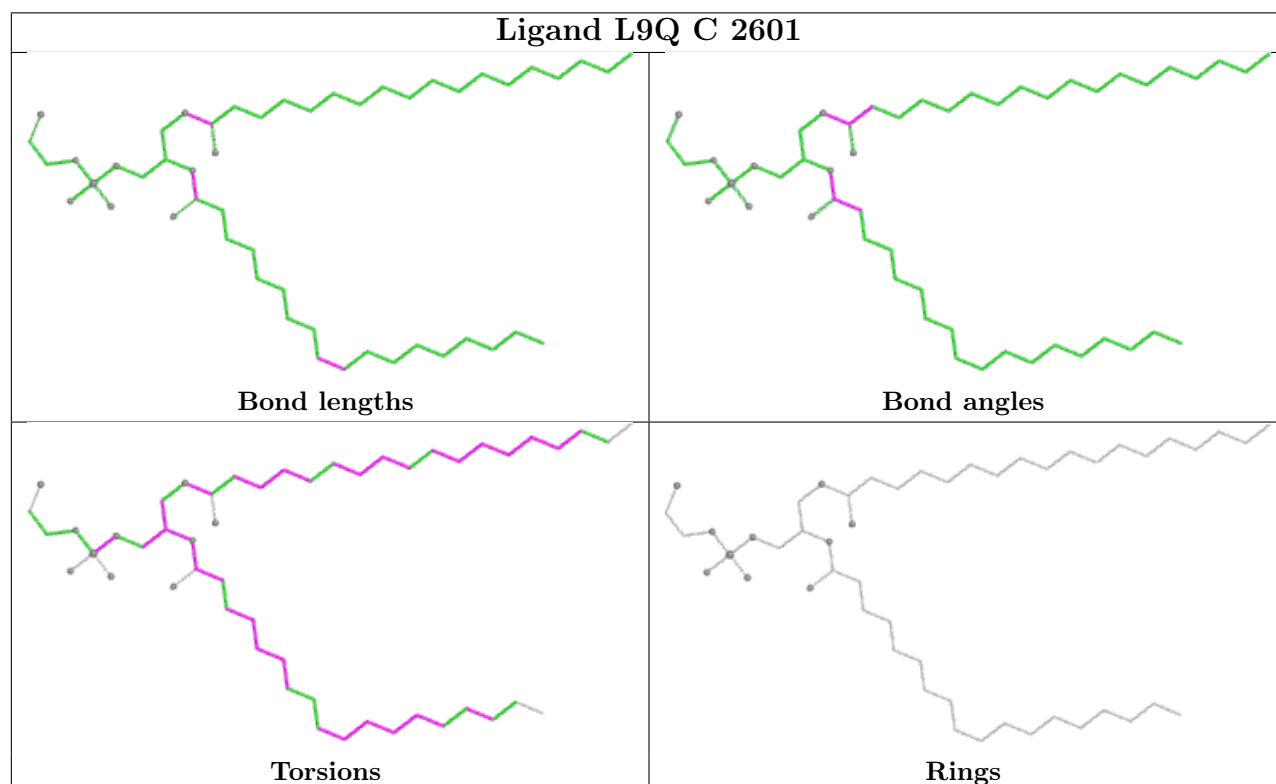
There are no ring outliers.

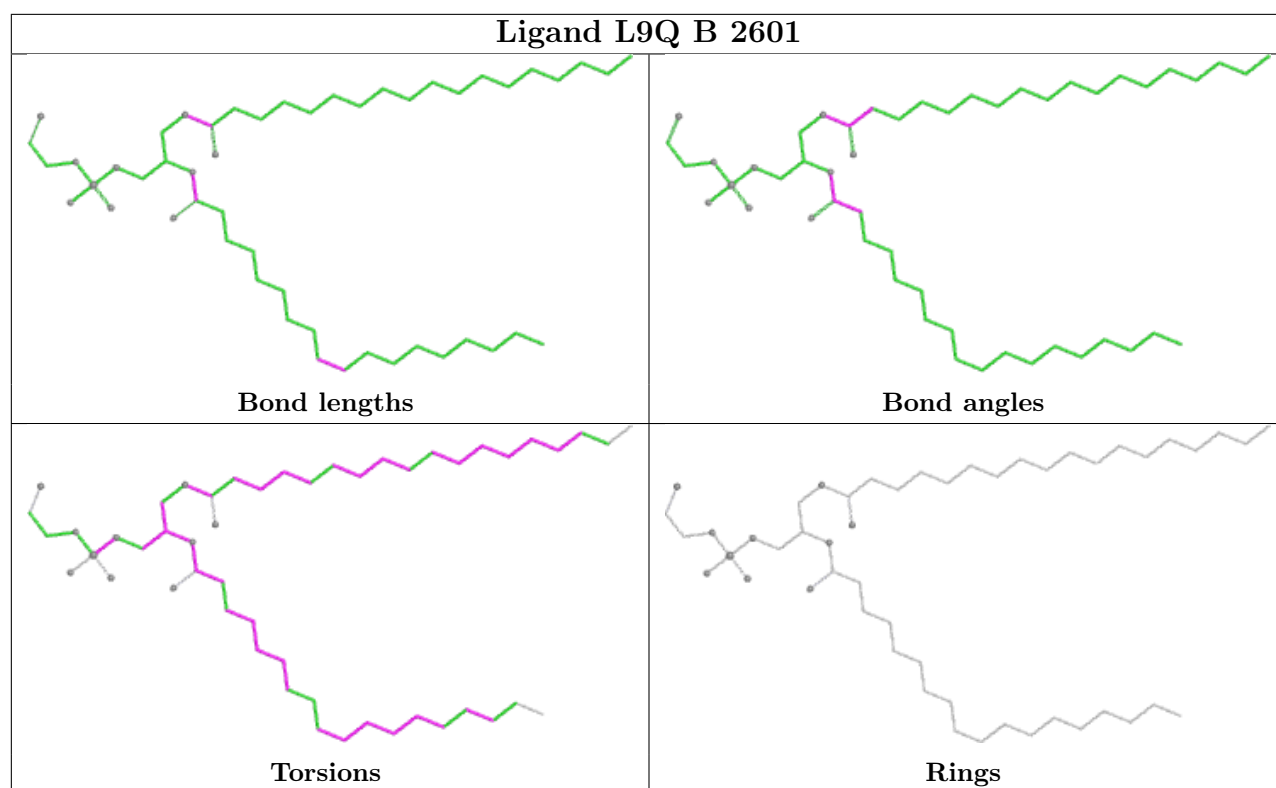
3 monomers are involved in 59 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2601	L9Q	19	0
2	A	2601	L9Q	20	0
2	B	2601	L9Q	20	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.

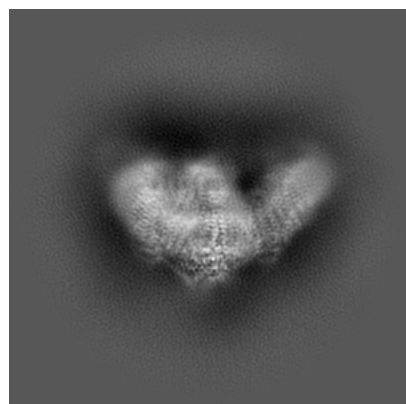
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60481. These allow visual inspection of the internal detail of the map and identification of artifacts.

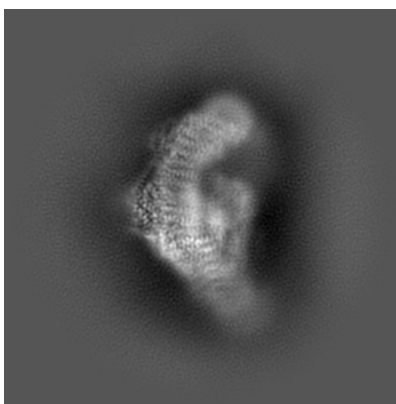
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

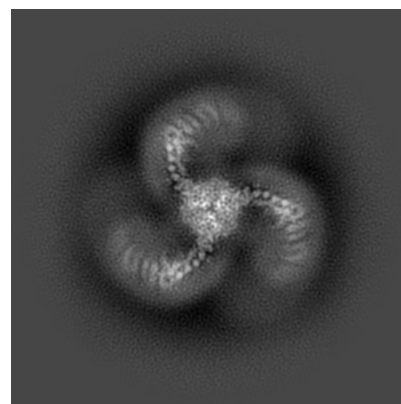
6.1.1 Primary map



X

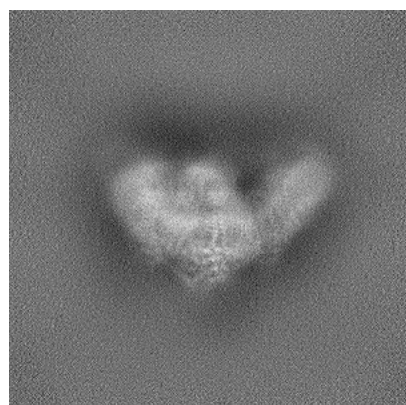


Y

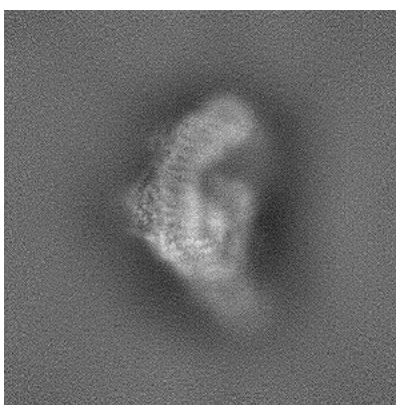


Z

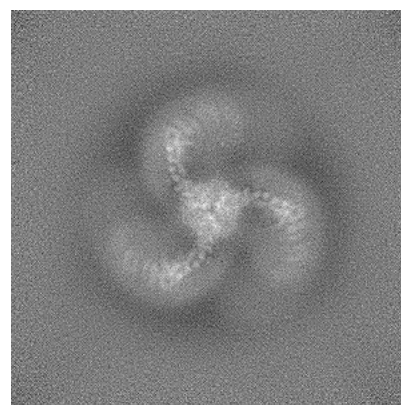
6.1.2 Raw map



X



Y

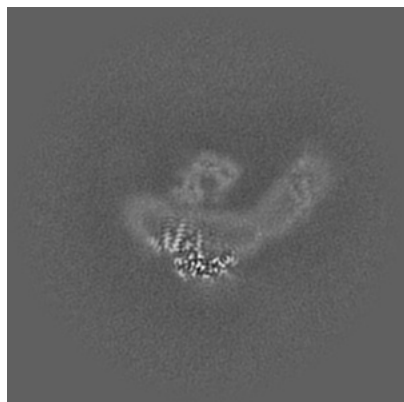


Z

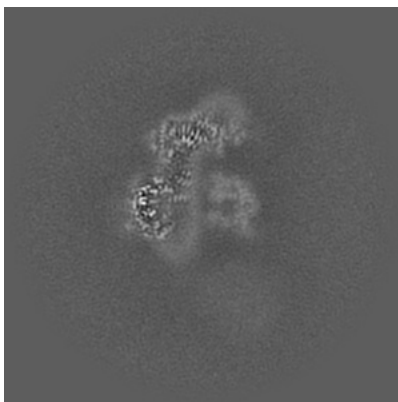
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

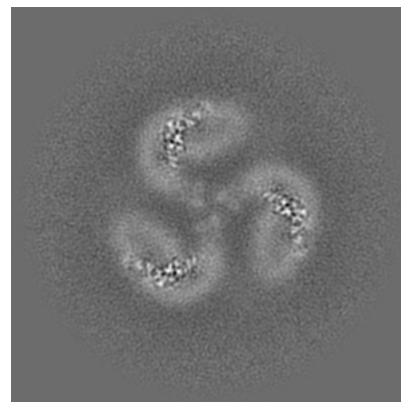
6.2.1 Primary map



X Index: 256



Y Index: 256

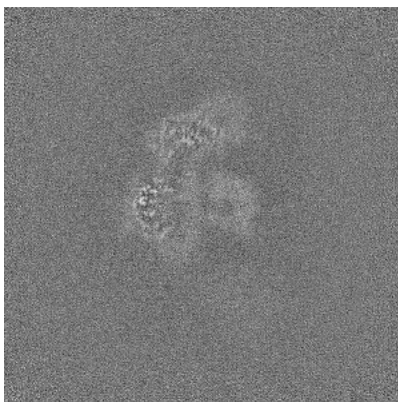


Z Index: 256

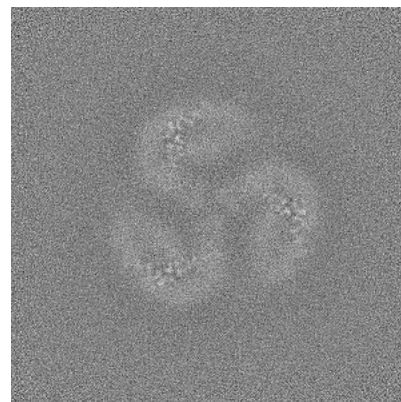
6.2.2 Raw map



X Index: 256



Y Index: 256

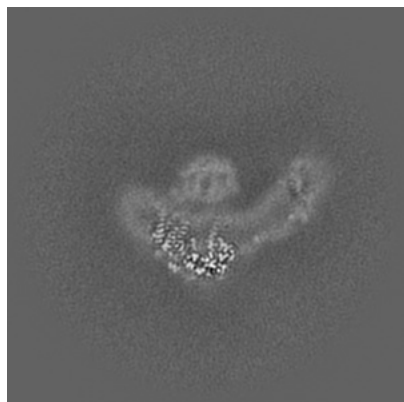


Z Index: 256

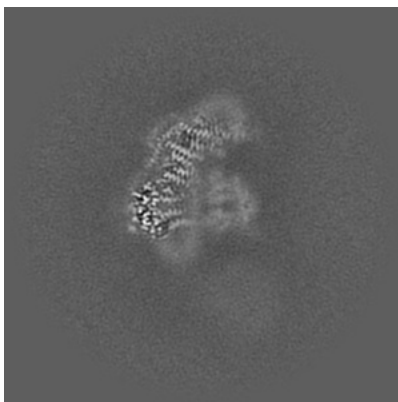
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

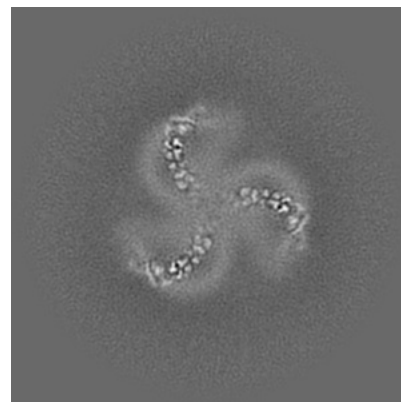
6.3.1 Primary map



X Index: 246

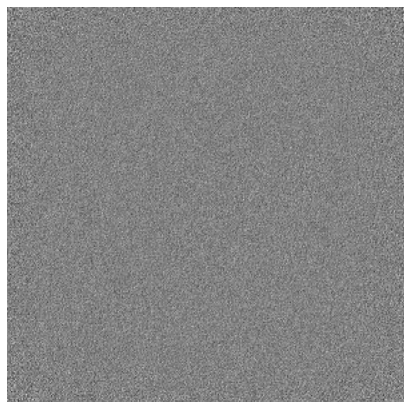


Y Index: 262

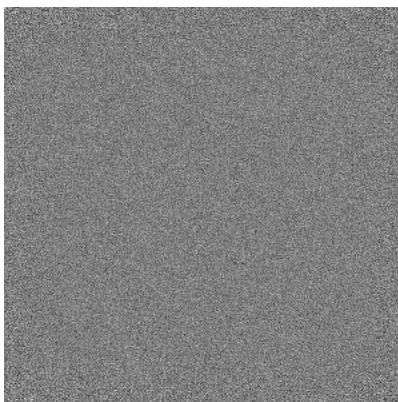


Z Index: 240

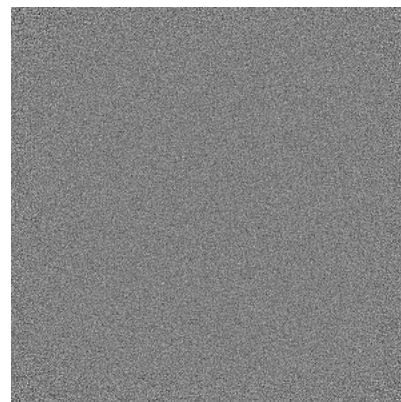
6.3.2 Raw map



X Index: 0



Y Index: 0

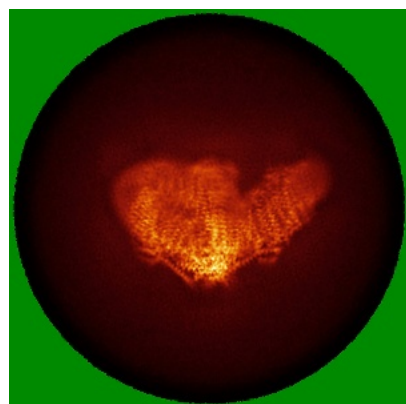


Z Index: 0

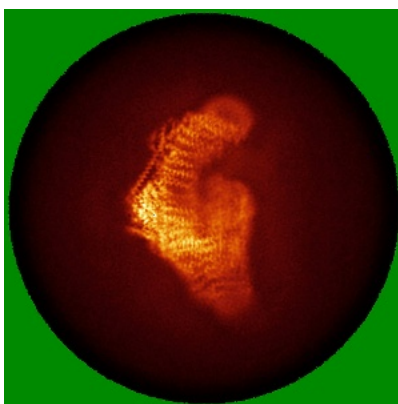
The images above show the largest variance slices of the map in three orthogonal directions.

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

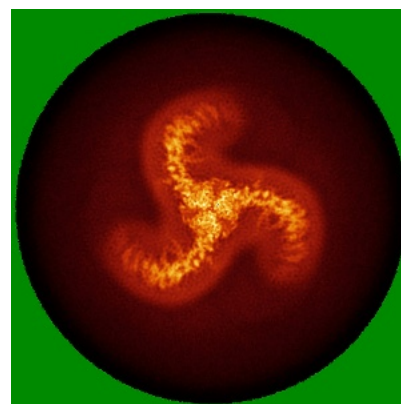
6.4.1 Primary map



X

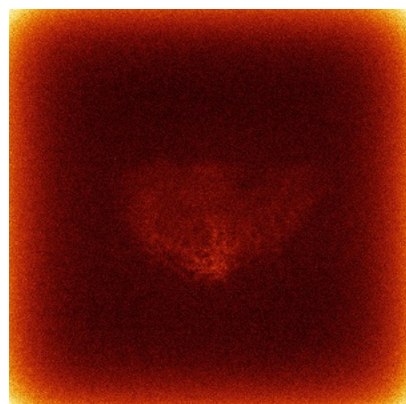


Y

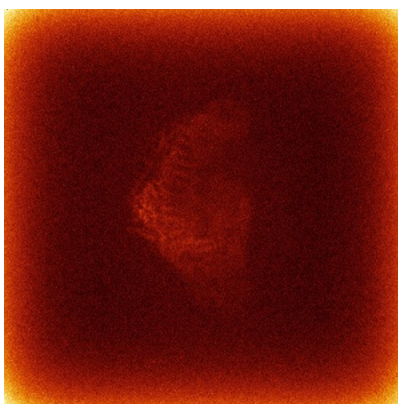


Z

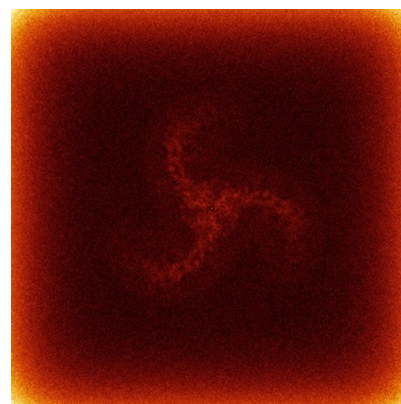
6.4.2 Raw map



X



Y

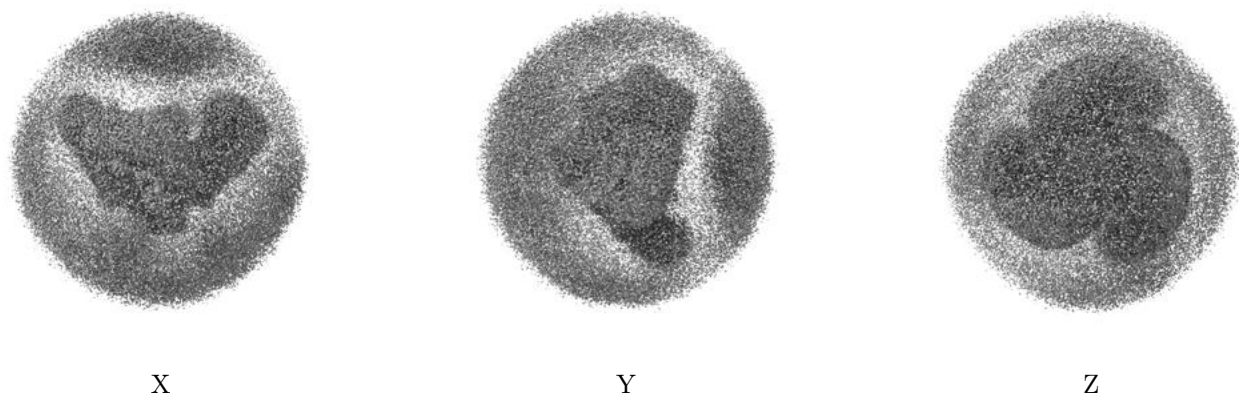


Z

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.

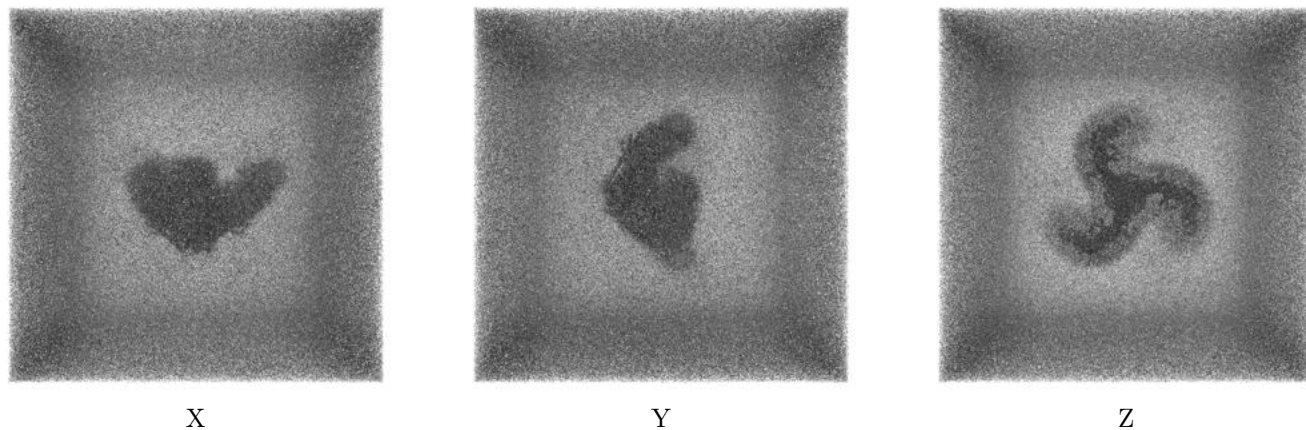
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. 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.

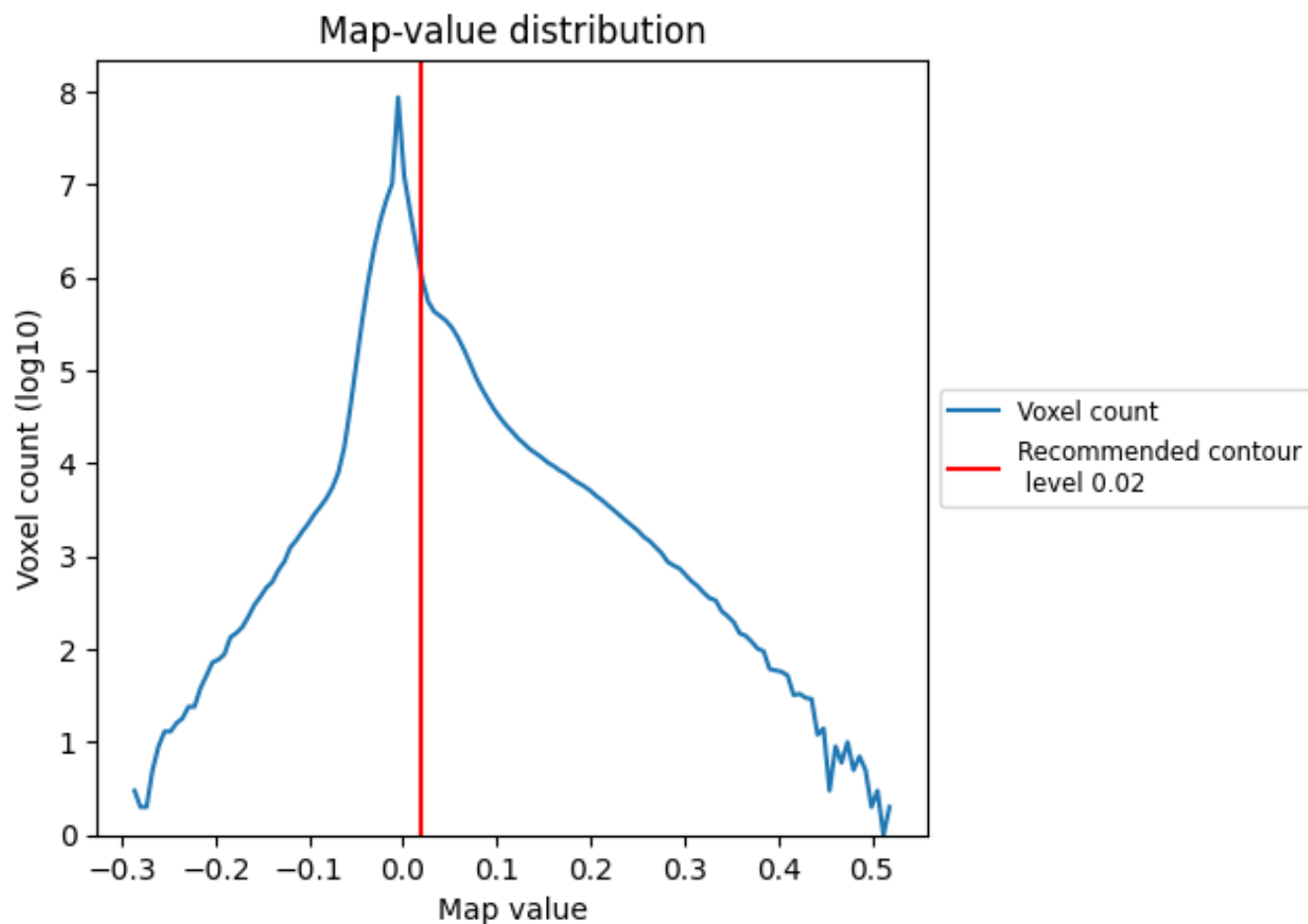
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

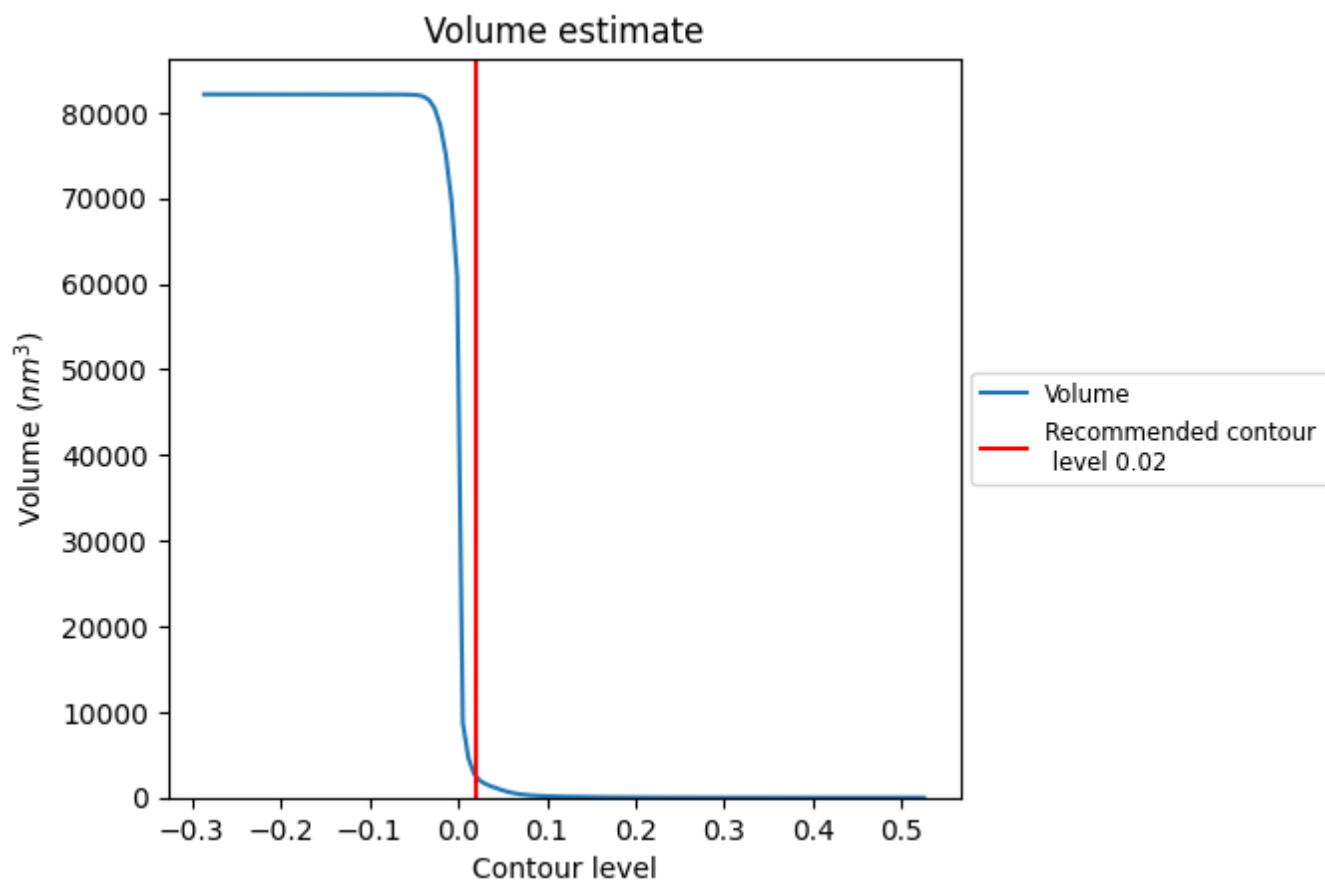
This section contains the results of statistical analysis of the map.

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.

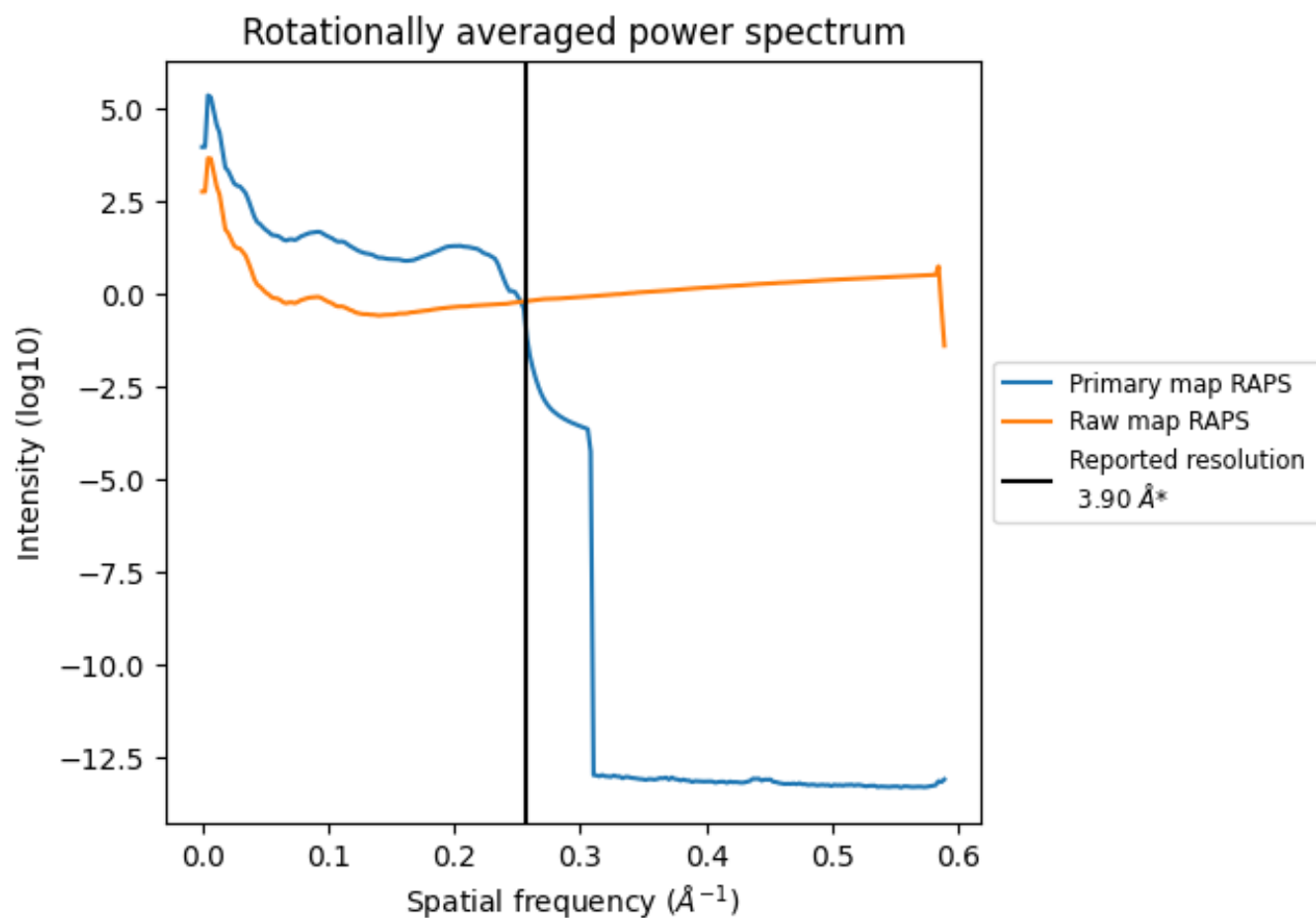
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2526 nm^3 ; this corresponds to an approximate mass of 2282 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 ⓘ

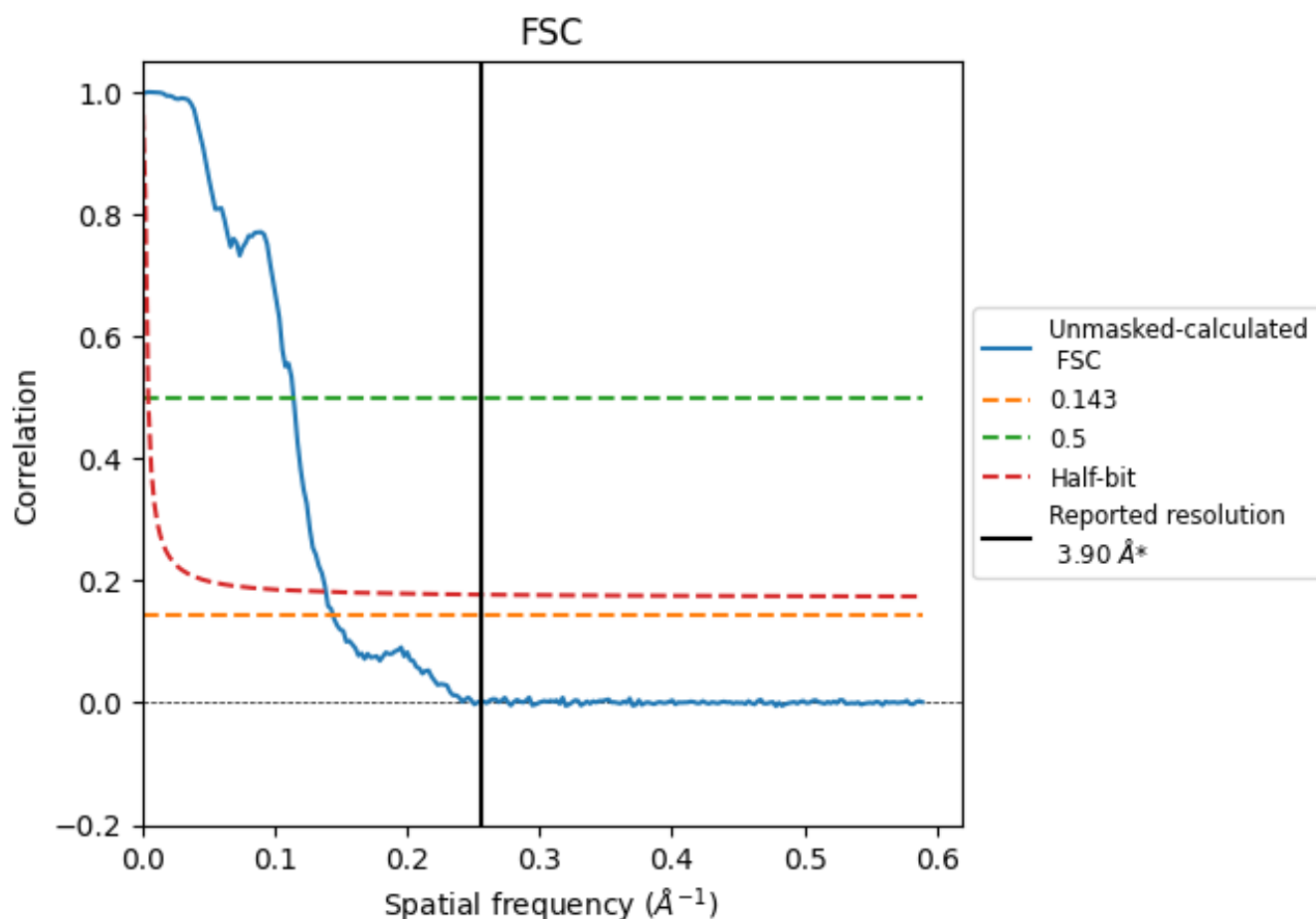


*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.94	8.76	7.21

*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 6.94 differs from the reported value 3.9 by more than 10 %

9 Map-model fit [i](#)

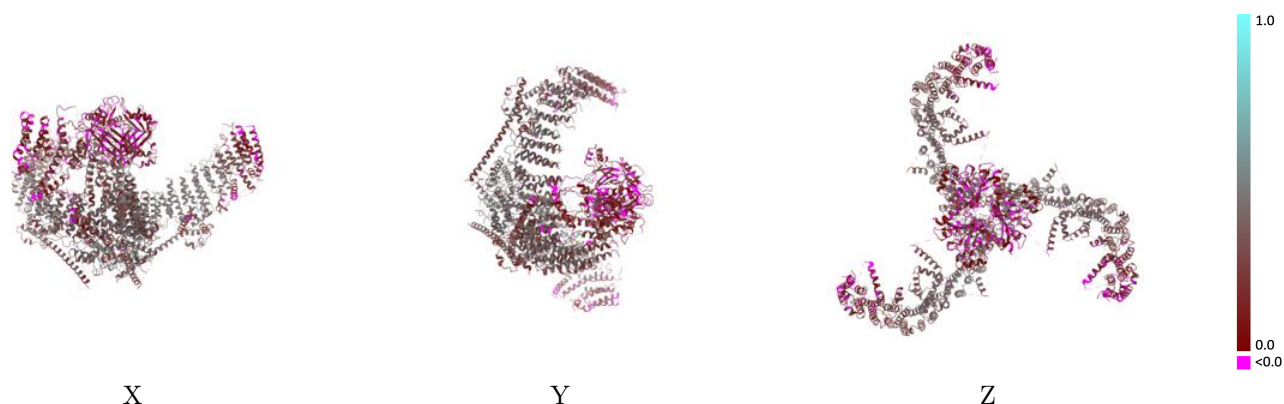
This section contains information regarding the fit between EMDB map EMD-60481 and PDB model 8ZU8. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

9.1 Map-model overlay [i](#)



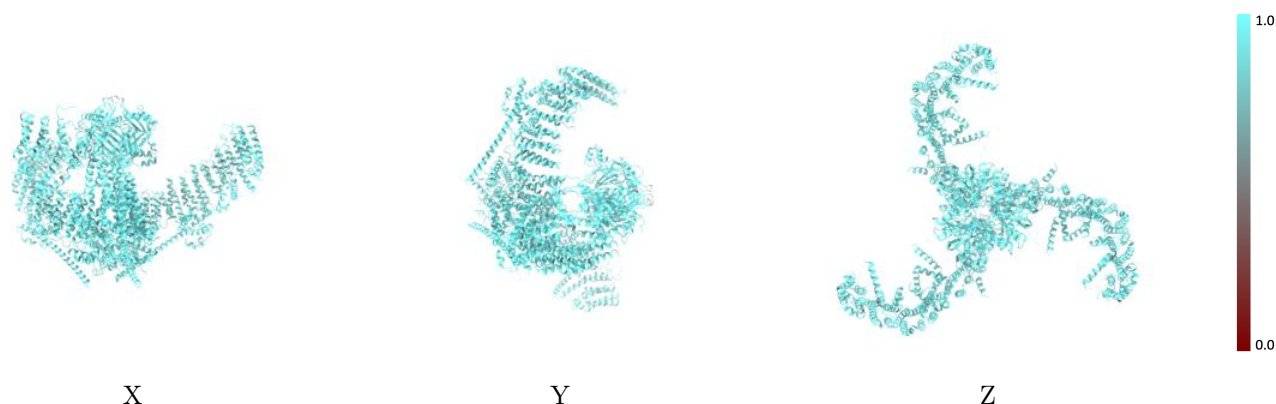
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



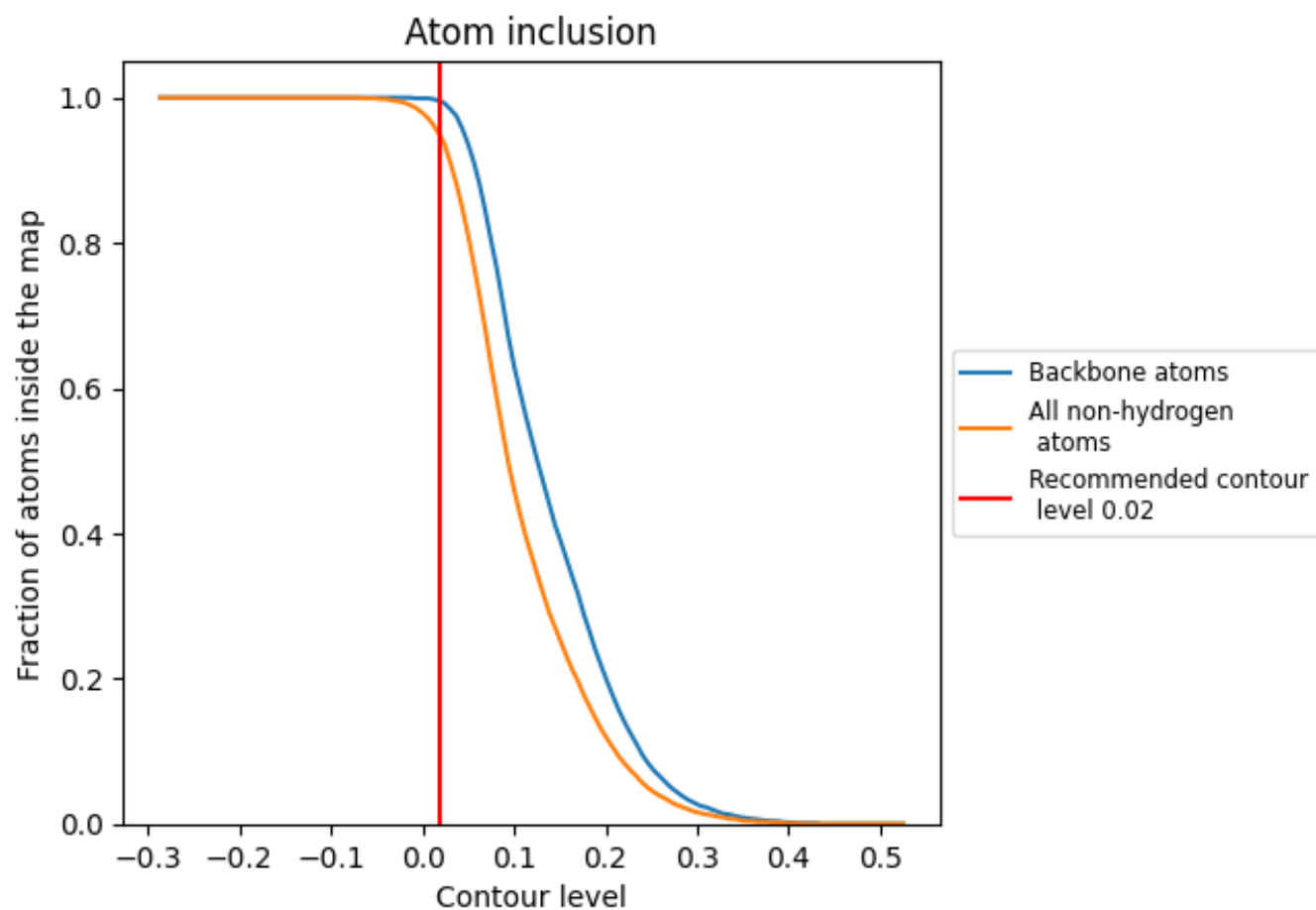
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 95% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9460	0.2730
A	0.9460	0.2730
B	0.9470	0.2720
C	0.9470	0.2730

