



wwPDB EM Validation Summary Report ⓘ

Mar 23, 2026 – 01:31 PM UTC

PDB ID : 6BQ1 / pdb_00006bq1
EMDB ID : EMD-7129
Title : Human PI4KIIIa lipid kinase complex
Authors : Lees, J.A.; Zhang, Y.; Oh, M.; Schauder, C.M.; Yu, X.; Baskin, J.; Dobbs, K.;
Notarangelo, L.D.; Camilli, P.D.; Walz, T.; Reinisch, K.M.
Deposited on : 2017-11-27
Resolution : 3.60 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

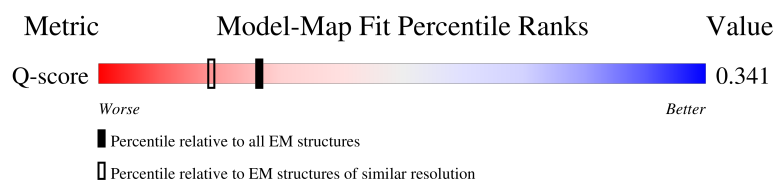
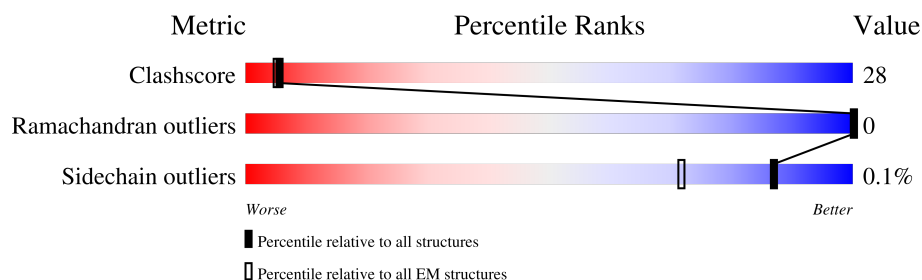
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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.



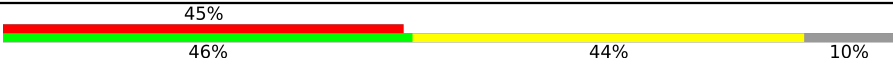
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12797 (3.10 - 4.10)

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	1647	14% 59% 31% 8%
2	B	863	37% 52% 32% 16%
2	F	863	35% 50% 34% 16%
3	C	292	44% 43% 47% 10%

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Mol	Chain	Length	Quality of chain
3	G	292	
4	E	1648	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	E4S	E	2201	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 37217 atoms, of which 54 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 Phosphatidylinositol 4-kinase III alpha (PI4KA).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1509	Total	C	N	O	S	0	0
			10673	6767	1872	1972	62		

- Molecule 2 is a protein called Tetratricopeptide repeat protein 7B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	728	Total	C	N	O	S	0	0
			5774	3670	1007	1065	32		
2	F	728	Total	C	N	O	S	0	0
			5774	3670	1007	1065	32		

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	MET	-	expression tag	UNP Q86TV6
B	-18	TYR	-	expression tag	UNP Q86TV6
B	-17	PRO	-	expression tag	UNP Q86TV6
B	-16	TYR	-	expression tag	UNP Q86TV6
B	-15	ASP	-	expression tag	UNP Q86TV6
B	-14	VAL	-	expression tag	UNP Q86TV6
B	-13	PRO	-	expression tag	UNP Q86TV6
B	-12	ASP	-	expression tag	UNP Q86TV6
B	-11	TYR	-	expression tag	UNP Q86TV6
B	-10	ALA	-	expression tag	UNP Q86TV6
B	-9	ALA	-	expression tag	UNP Q86TV6
B	-8	ILE	-	expression tag	UNP Q86TV6
B	-7	ALA	-	expression tag	UNP Q86TV6
B	-6	GLY	-	expression tag	UNP Q86TV6
B	-5	ALA	-	expression tag	UNP Q86TV6
B	-4	PRO	-	expression tag	UNP Q86TV6
B	-3	ASP	-	expression tag	UNP Q86TV6
B	-2	LEU	-	expression tag	UNP Q86TV6
B	-1	LYS	-	expression tag	UNP Q86TV6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	0	LEU	-	expression tag	UNP Q86TV6
F	-19	MET	-	expression tag	UNP Q86TV6
F	-18	TYR	-	expression tag	UNP Q86TV6
F	-17	PRO	-	expression tag	UNP Q86TV6
F	-16	TYR	-	expression tag	UNP Q86TV6
F	-15	ASP	-	expression tag	UNP Q86TV6
F	-14	VAL	-	expression tag	UNP Q86TV6
F	-13	PRO	-	expression tag	UNP Q86TV6
F	-12	ASP	-	expression tag	UNP Q86TV6
F	-11	TYR	-	expression tag	UNP Q86TV6
F	-10	ALA	-	expression tag	UNP Q86TV6
F	-9	ALA	-	expression tag	UNP Q86TV6
F	-8	ILE	-	expression tag	UNP Q86TV6
F	-7	ALA	-	expression tag	UNP Q86TV6
F	-6	GLY	-	expression tag	UNP Q86TV6
F	-5	ALA	-	expression tag	UNP Q86TV6
F	-4	PRO	-	expression tag	UNP Q86TV6
F	-3	ASP	-	expression tag	UNP Q86TV6
F	-2	LEU	-	expression tag	UNP Q86TV6
F	-1	LYS	-	expression tag	UNP Q86TV6
F	0	LEU	-	expression tag	UNP Q86TV6

- Molecule 3 is a protein called Protein FAM126A.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	264	Total	C	N	O	S	0	0
			2091	1357	338	383	13		
3	G	264	Total	C	N	O	S	0	0
			2091	1357	338	383	13		

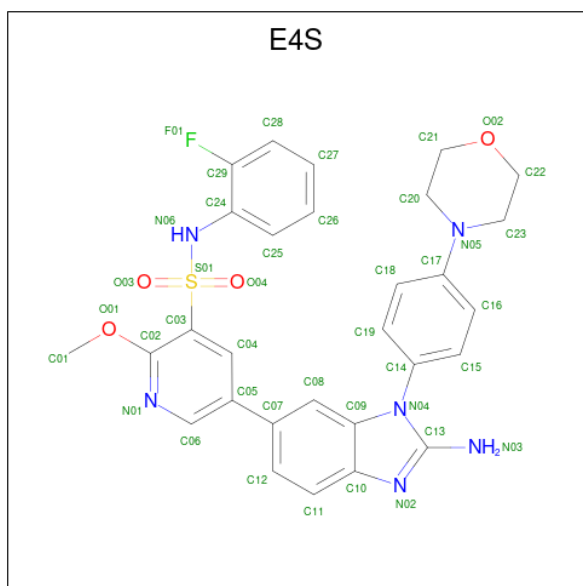
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	expression tag	UNP Q9BYI3
C	-1	PRO	-	expression tag	UNP Q9BYI3
C	0	GLY	-	expression tag	UNP Q9BYI3
C	1	SER	-	expression tag	UNP Q9BYI3
G	-2	GLY	-	expression tag	UNP Q9BYI3
G	-1	PRO	-	expression tag	UNP Q9BYI3
G	0	GLY	-	expression tag	UNP Q9BYI3
G	1	SER	-	expression tag	UNP Q9BYI3

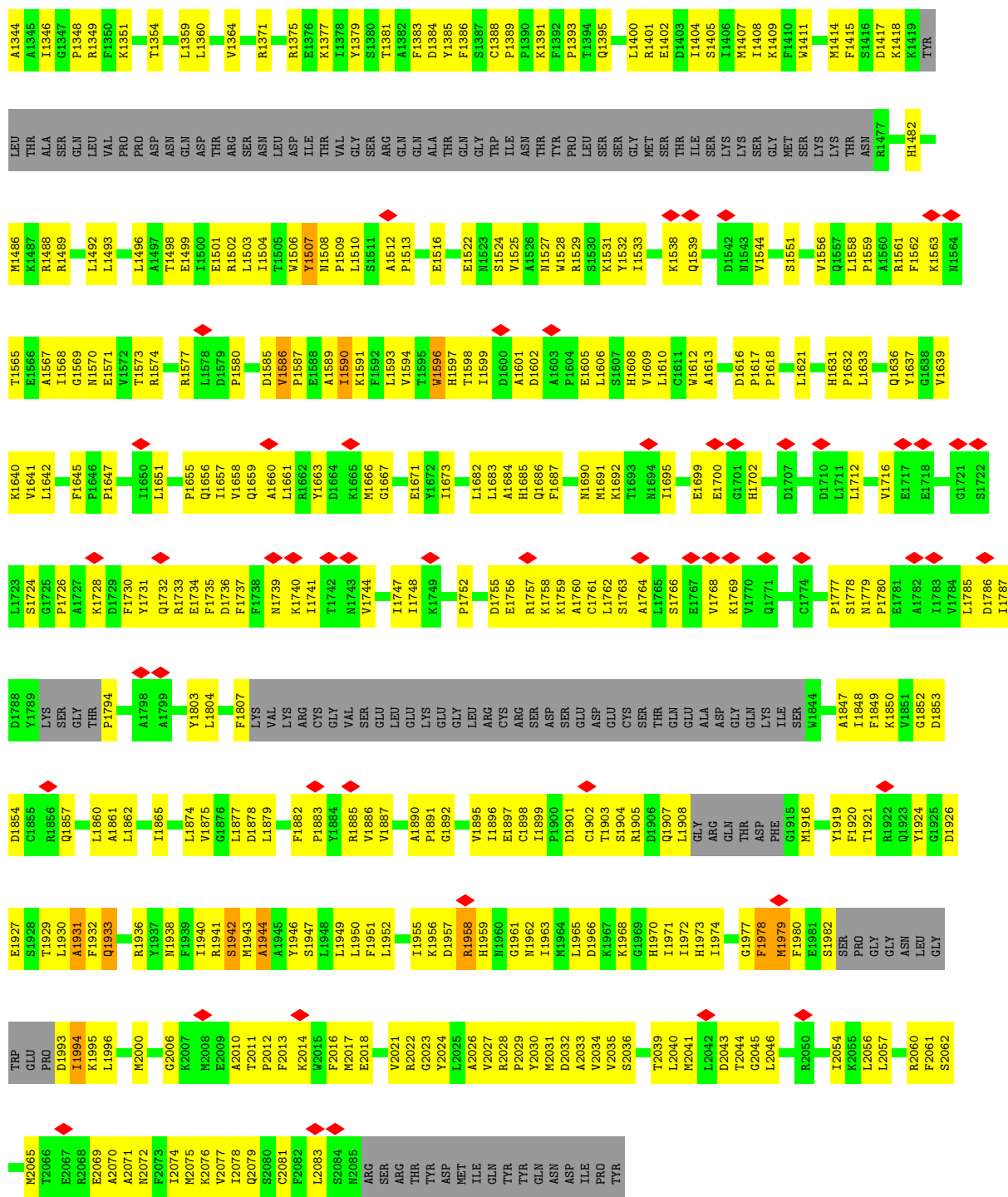
- Molecule 4 is a protein called Phosphatidylinositol 4-kinase III alpha (PI4KA).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	1510	Total	C	N	O	S	0	0
			10678	6770	1873	1973	62		

- Molecule 5 is 5-{2-amino-1-[4-(morpholin-4-yl)phenyl]-1H-benzimidazol-6-yl}-N-(2-fluorophenyl)-2-methoxypyridine-3-sulfonamide (CCD ID: E4S) (formula: C₂₉H₂₇FN₆O₄S).

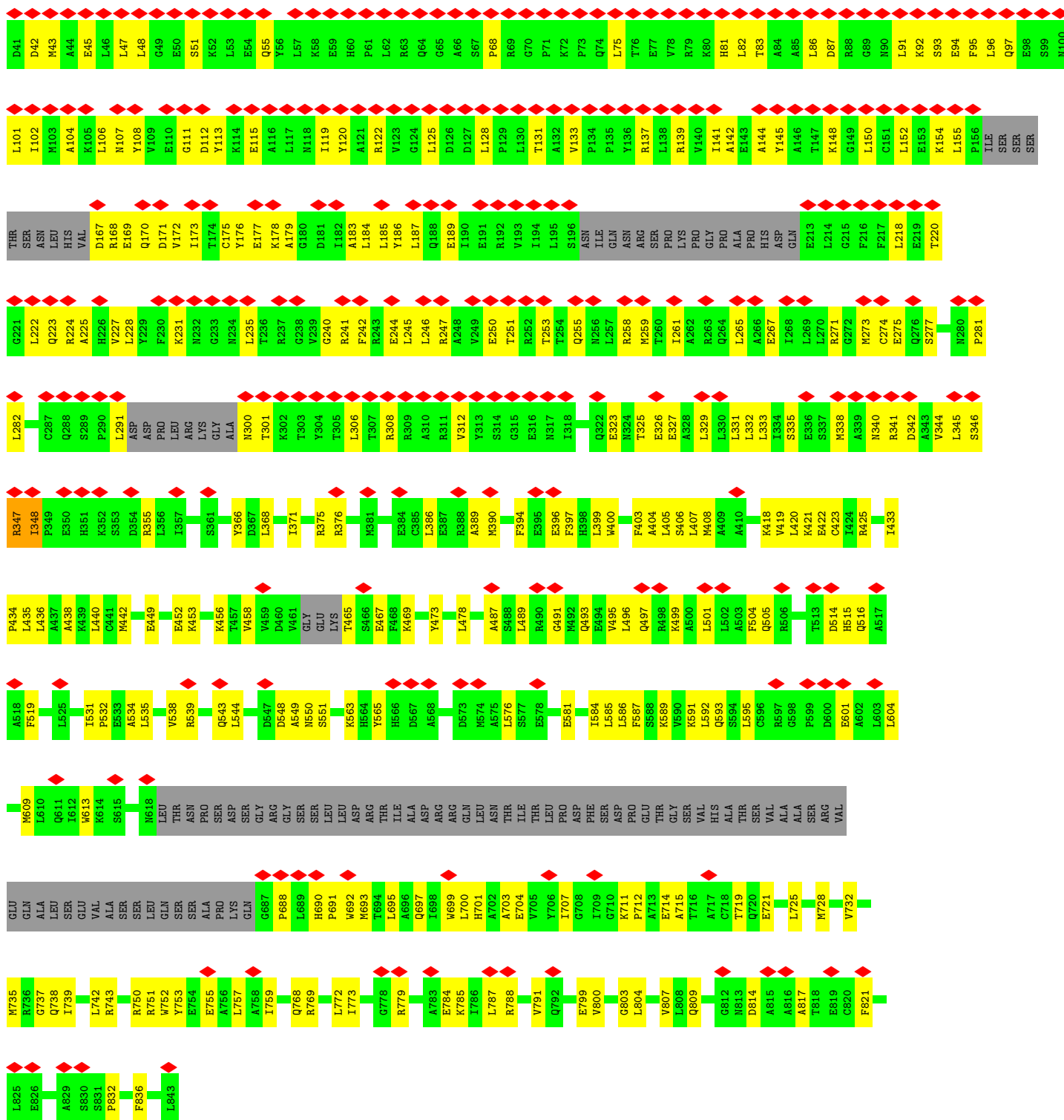


Mol	Chain	Residues	Atoms							AltConf
5	A	1	Total	C	F	H	N	O	S	0
			68	29	1	27	6	4	1	
5	E	1	Total	C	F	H	N	O	S	0
			68	29	1	27	6	4	1	

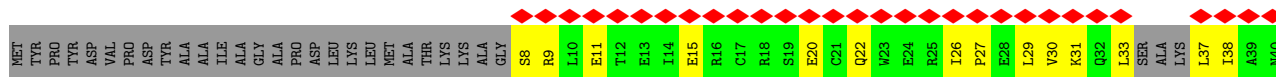


• Molecule 2: Tetratricopeptide repeat protein 7B

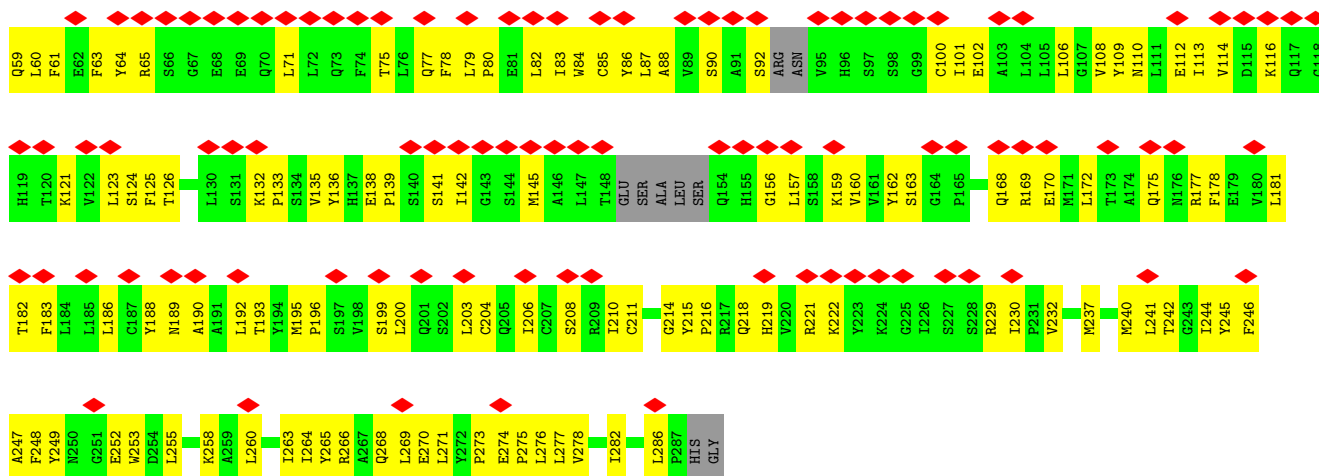




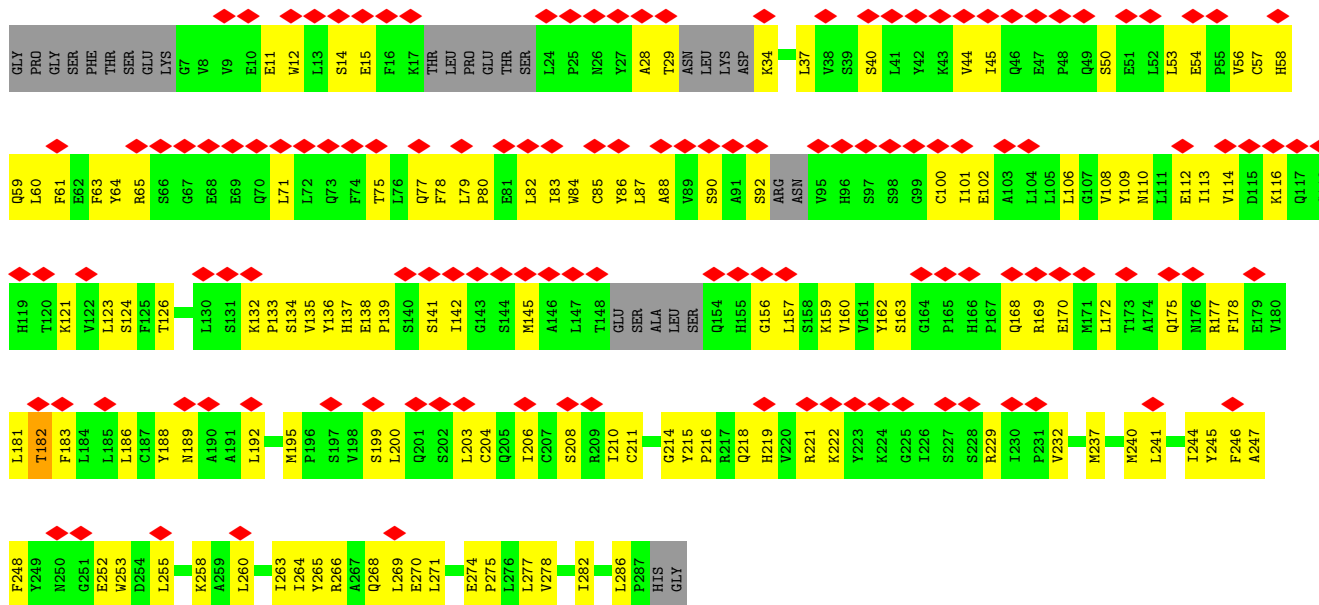
• Molecule 2: Tetratricopeptide repeat protein 7B



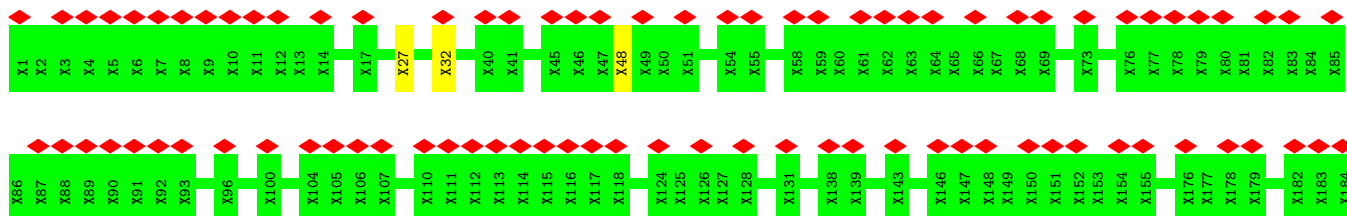




• Molecule 3: Protein FAM126A



• Molecule 4: Phosphatidylinositol 4-kinase III alpha (PI4KA)



X185	X191	X192	X193	X194	X197	X198	X199	X202	X203	X204	X205	X206	X207	X208	X209	X210	X214	X222	X223	X224	X225	X229	X230	X231	X232	X233	X234	X235	X236	X237	X238	X239	X240	X241	X242	X243	X248	X256	X274	X275	X278	X279	X286	X287	X290	X293								
X294	X304	X305	X306	X307	X308	X309	X328	X329	X330	X331	X337	X340	X341	X342	X343	X344	X347	X350	X358	X359	X360	X361	X362	X365	X366	X367	X368	X369	X370	X371	X374	X375	X378	X384	X385	X386	X399	X400	X403	X404	X408	X413	X414	X415										
X416	X417	X418	X419	X420	X421	X422	X437	X438	X443	X444	X449	X452	M933	Q934	I937	A938	V939	K942	F947	M950	M951	A952	D953	K954	A968	Q969	F970	L971	L972	N973	N974	F975	N976	H977	I978	H979	K980	R981	I982	R983	R984	D987	M1090	V1091	S1092	G1093								
M1010	L1011	D1012	L1013	L1014	Q1015	L1019	K1027	P1030	Y1031	Y1032	P1035	T1041	T1042	V1043	P1044	R1050	E1051	S1052	K1055	D1056	F1057	C1061	I1064	L1065	Q1066	E1067	A1068	M1069	K1070	V1071	A1072	V1075	T1076	K1077	L1080	Q1081	E1082	L1083	L1084	N1085	K1086	H1087	W1090	F1159	SER	GLY	THR							
L1094	S1095	Q1096	H1097	T1098	Q1099	L1100	M1101	A1102	A1103	T1104	L1108	H1109	F1110	A1111	G1112	Y1113	N1114	K1115	L1116	M1117	T1118	T1119	A1122	T1123	G1124	L1125	S1126	E1127	R1128	P1129	A1130	C1131	V1132	A1133	K1134	D1135	Y1136	S1137	M1140	A1141	S1142	L1143	N1144	L1145	R1146	Y1149	V1153	Y1154	R1158	F1159	SER	GLY	THR	
THR	GLY	GLN	MET	SER	D1168	H1185	P1186	T1190	Q1191	A1192	M1193	F1194	L1196	T1197	A1198	T1201	K1204	D1205	P1208	Q1269	L1210	L1211	H1212	R1213	L1214	C1215	W1216	M1221	H1225	G1226	M1227	L1231	A1232	C1233	W1234	L1237	L1238	D1242	G1243	V1246	P1247	F1248	M1249	P1348	E1251	A1255								
M1258	L1259	V1260	Q1262	K1263	F1264	G1265	L1266	F1267	P1276	L1277	E1281	V1292	T1293	H1294	H1295	Y1296	L1297	W1298	I1299	F1301	L1302	L1303	Q1304	R1305	F1306	D1315	Q1316	V1317	F1320	S1321	Q1325	S1329	L1330	N1331	I1332	M1339	R1340	H1341	V1343	A1344	A1345	L1346	G1347	P1348	F1350	K1351								
T1354	L1359	L1360	V1364	M1367	T1369	I1370	L1371	H1372	V1373	L1374	E1376	K1377	I1378	Y1379	S1380	T1381	F1382	F1383	D1384	Y1385	F1386	S1387	C1388	P1389	P1390	K1391	F1392	P1393	T1394	Q1395	L1400	R1401	E1402	D1403	I1404	S1405	T1406	M1407	I1408	K1409	F1410	W1411	M1414	F1415	S1416	D1417	K1418	K1419	TYR	LEU	THR			
ALA	SER	GLN	LEU	VAL	PRO	PRO	ASP	ASN	GLN	ASP	THR	ARG	SER	ASN	LEU	ASP	ILE	THR	VAL	GLY	SER	ARG	GLN	ALA	THR	GLN	ALA	THR	GLY	SER	THR	ILE	SER	LYS	LYS	LYS	THR	ASN	R1477	H1482	M1486	K1487												
R1488	R1489	L1492	L1493	L1496	A1497	T1498	A1499	I1500	E1501	R1502	L1503	I1504	T1505	W1506	Y1507	N1508	P1509	L1510	S1511	A1512	P1513	E1516	E1522	N1523	S1524	V1525	A1526	P1527	W1528	R1529	S1530	K1531	Y1532	I1533	K1538	Q1539	V1544	S1551	V1556	Q1557	L1558	P1559	A1560	R1561	F1562	K1563	N1564	T1565	F1566	A1567	I1568			
G1569	N1570	E1571	V1572	R1573	R1574	R1577	L1578	D1579	P1580	D1585	V1586	P1587	E1588	A1589	I1590	K1591	F1592	L1593	V1594	T1595	W1596	H1597	T1598	I1599	D1600	A1601	L1602	A1603	P1604	E1605	L1606	S1607	H1608	M1609	L1610	C1611	W1612	A1613	D1616	P1617	P1618	L1621	F1624	S1625	H1631	P1632	L1633	Q1636	Y1637	G1638	V1639	K1640		
V1641	L1642	R1643	S1644	F1645	P1646	P1647	L1651	P1655	Q1656	T1657	V1658	A1659	K1660	L1661	R1662	Y1663	M1666	G1667	R1670	E1671	Y1672	I1673	L1682	L1683	A1684	H1685	E1686	P1687	M1690	M1691	C1691	K1692	I1695	Y1696	L1697	D1698	E1699	V1700	G1701	H1702	D1707	D1710	L1711	L1712	V1716	E1717	Y1718	T1720	L1723					
S1724	G1725	P1726	A1727	K1728	D1729	F1730	Y1731	Q1732	R1733	E1734	F1735	F1736	F1737	F1738	N1739	K1740	I1741	T1742	N1743	V1744	I1747	I1748	K1749	P1752	K1753	L1754	D1755	E1756	R1757	K1758	K1759	A1760	C1761	L1762	S1763	A1764	L1765	S1766	E1767	V1768	K1769	V1770	Q1771	C1774	P1777	S1778	N1779	P1780	E1781	A1782	I1783	D1786	I1787	D1788



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	64104	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	47	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	3700	Depositor
Magnification	38461	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.287	Depositor
Minimum map value	-0.167	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	416.0, 416.0, 416.0	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3, 1.3, 1.3	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: E4S

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	0.39	0/8500	0.65	21/11506 (0.2%)
2	B	0.27	0/5877	0.44	4/7948 (0.1%)
2	F	0.27	0/5877	0.46	6/7948 (0.1%)
3	C	0.23	0/2140	0.45	1/2903 (0.0%)
3	G	0.23	0/2140	0.43	0/2903
4	E	0.39	0/8500	0.65	15/11506 (0.1%)
All	All	0.33	0/33034	0.56	47/44714 (0.1%)

There are no bond length outliers.

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	1994	ILE	N-CA-C	11.60	123.31	110.21
4	E	1979	MET	N-CA-C	9.46	121.19	111.07
4	E	1702	HIS	N-CA-C	-9.12	101.34	111.28
4	E	1586	VAL	CB-CA-C	-8.17	105.69	114.35
1	A	1586	VAL	CB-CA-C	-8.01	105.86	114.35

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	10673	0	8799	634	0
2	B	5774	0	5852	267	0
2	F	5774	0	5852	279	0
3	C	2091	0	2096	158	0
3	G	2091	0	2096	136	0
4	E	10678	0	8800	635	0
5	A	41	27	0	3	0
5	E	41	27	0	3	0
All	All	37163	54	33495	1951	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 28.

The worst 5 of 1951 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:1932:PHE:CZ	1:A:1936:ARG:HD3	1.30	1.60
4:E:1696:TYR:CD1	4:E:1701:GLY:HA2	1.34	1.58
4:E:1860:LEU:HD22	4:E:1979:MET:CE	1.50	1.40
1:A:1404:ILE:HD12	1:A:1507:TYR:CE2	1.55	1.40
1:A:1932:PHE:CE2	1:A:1936:ARG:HD3	1.55	1.38

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	1019/1647 (62%)	949 (93%)	70 (7%)	0	100	100
2	B	714/863 (83%)	691 (97%)	23 (3%)	0	100	100
2	F	714/863 (83%)	692 (97%)	22 (3%)	0	100	100
3	C	254/292 (87%)	242 (95%)	12 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	G	254/292 (87%)	242 (95%)	12 (5%)	0	100	100
4	E	1019/1648 (62%)	951 (93%)	68 (7%)	0	100	100
All	All	3974/5605 (71%)	3767 (95%)	207 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	901/1022 (88%)	900 (100%)	1 (0%)	88	87
2	B	616/727 (85%)	616 (100%)	0	100	100
2	F	616/727 (85%)	616 (100%)	0	100	100
3	C	236/260 (91%)	236 (100%)	0	100	100
3	G	236/260 (91%)	235 (100%)	1 (0%)	84	81
4	E	901/1022 (88%)	899 (100%)	2 (0%)	87	85
All	All	3506/4018 (87%)	3502 (100%)	4 (0%)	87	87

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1994	ILE
4	E	1929	THR
4	E	1955	ILE
3	G	182	THR

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

Mol	Chain	Res	Type
2	F	508	HIS
2	F	540	GLN
3	G	175	GLN

Continued on next page...

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Mol	Chain	Res	Type
2	B	508	HIS
2	B	446	HIS

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 ⓘ

2 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	$\# Z > 2$
5	E4S	A	2201	-	45,46,46	4.46	27 (60%)	64,67,67	3.00	23 (35%)
5	E4S	E	2201	-	45,46,46	4.67	28 (62%)	64,67,67	3.06	25 (39%)

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
5	E4S	A	2201	-	-	10/25/33/33	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	E4S	E	2201	-	-	9/25/33/33	0/6/6/6

The worst 5 of 55 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	2201	E4S	C24-C29	11.36	1.52	1.39
5	A	2201	E4S	C24-C29	11.15	1.52	1.39
5	E	2201	E4S	C04-C03	-8.83	1.24	1.39
5	A	2201	E4S	C27-C28	8.38	1.53	1.38
5	E	2201	E4S	C27-C28	8.34	1.53	1.38

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	2201	E4S	O04-S01-O03	-14.56	101.83	119.52
5	A	2201	E4S	O04-S01-O03	-13.93	102.60	119.52
5	E	2201	E4S	N03-C13-N04	8.44	132.16	122.10
5	A	2201	E4S	N03-C13-N04	7.87	131.48	122.10
5	A	2201	E4S	C10-C09-N04	-6.51	100.42	105.25

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2201	E4S	C03-C02-O01-C01
5	A	2201	E4S	N01-C02-O01-C01
5	A	2201	E4S	C02-C03-S01-N06
5	A	2201	E4S	C24-N06-S01-C03
5	E	2201	E4S	C03-C02-O01-C01

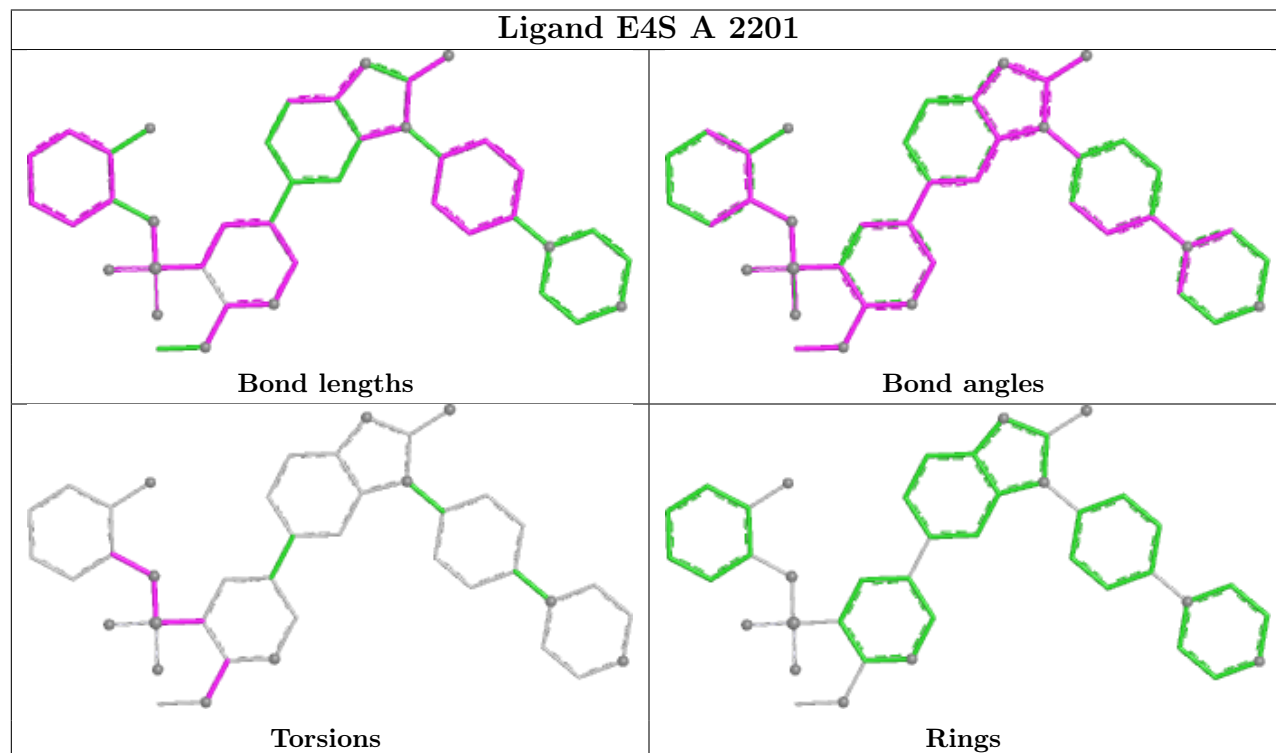
There are no ring outliers.

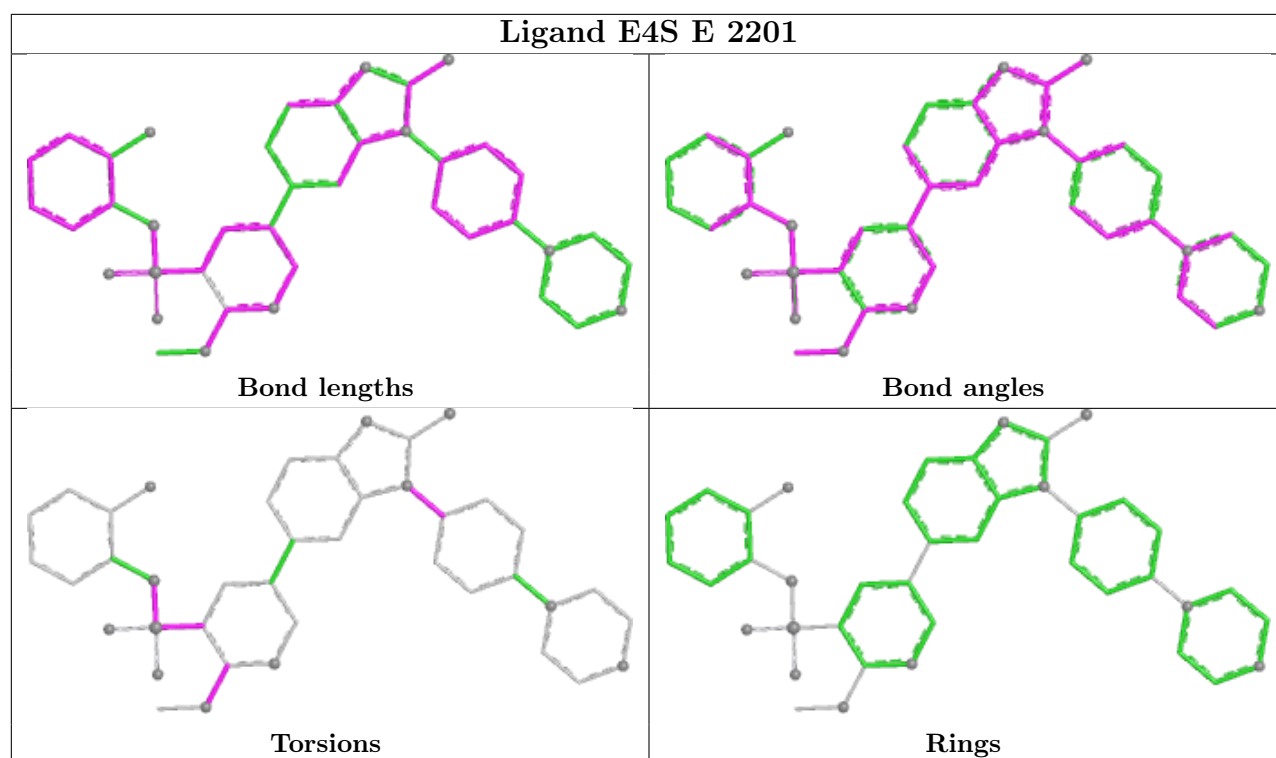
2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2201	E4S	3	0
5	E	2201	E4S	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	E	27
1	A	27

The worst 5 of 54 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	194:UNK	C	195:UNK	N	33.07
1	A	175:UNK	C	176:UNK	N	30.98
1	E	175:UNK	C	176:UNK	N	30.98
1	A	437:UNK	C	438:UNK	N	29.73
1	E	438:UNK	C	439:UNK	N	29.73

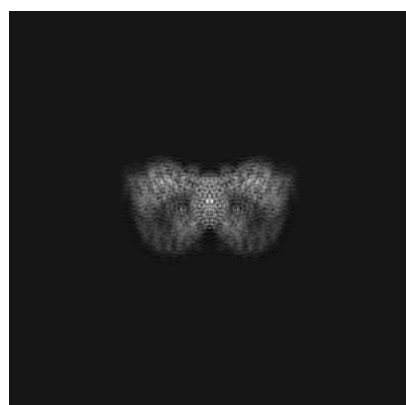
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7129. These allow visual inspection of the internal detail of the map and identification of artifacts.

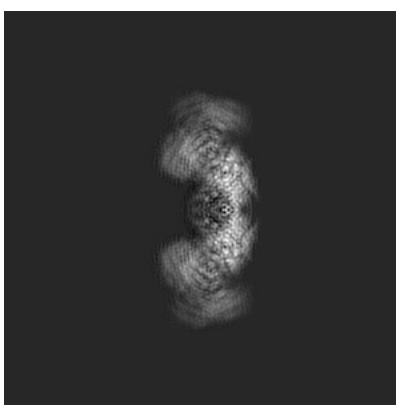
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

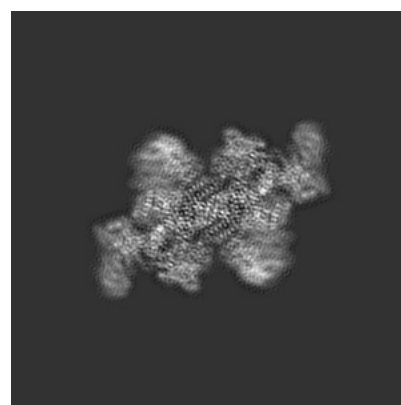
6.1.1 Primary map



X



Y



Z

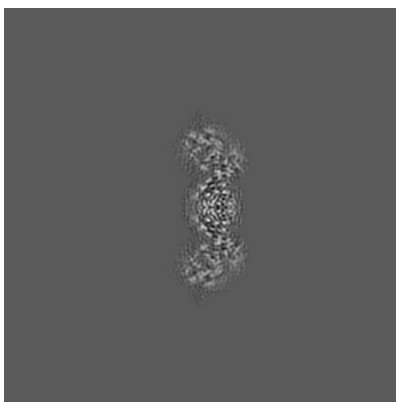
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

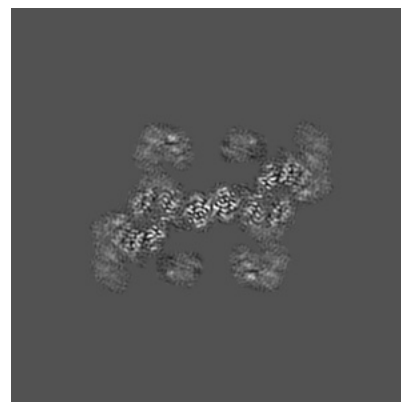
6.2.1 Primary map



X Index: 160



Y Index: 160

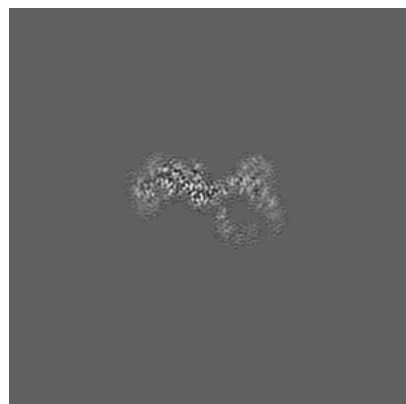


Z Index: 160

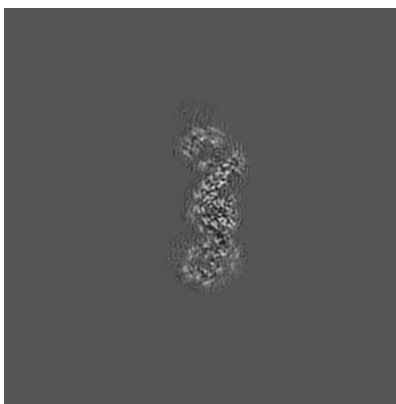
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

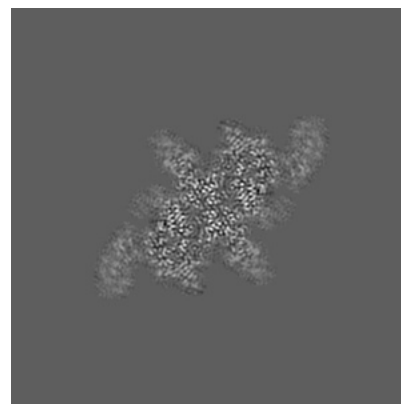
6.3.1 Primary map



X Index: 136



Y Index: 163

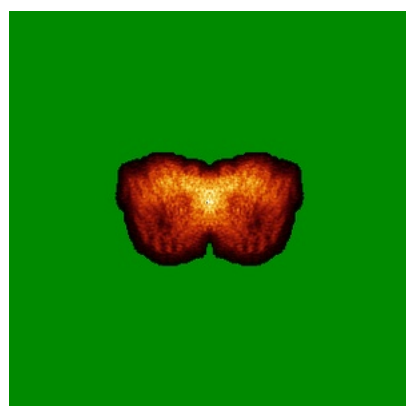


Z Index: 178

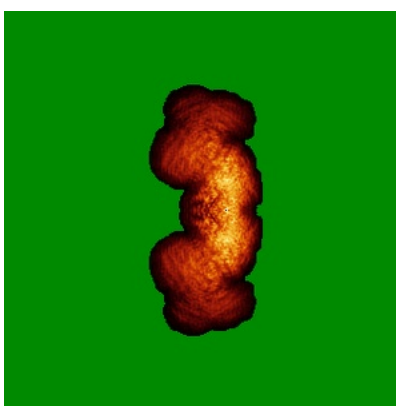
The images above show the largest variance slices of the map in three orthogonal directions.

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

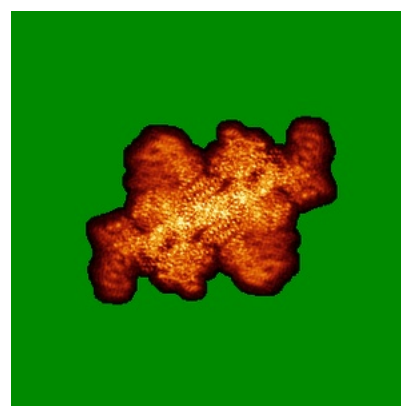
6.4.1 Primary map



X



Y

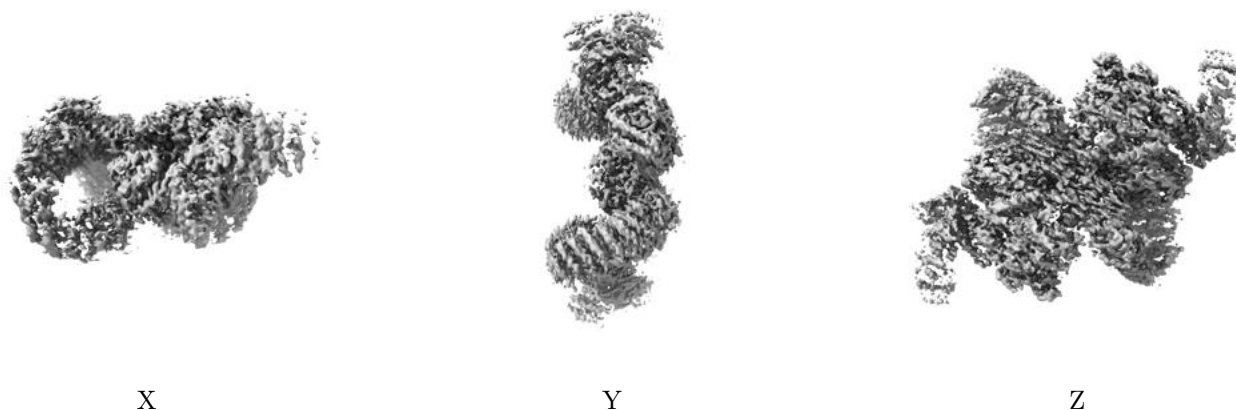


Z

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 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

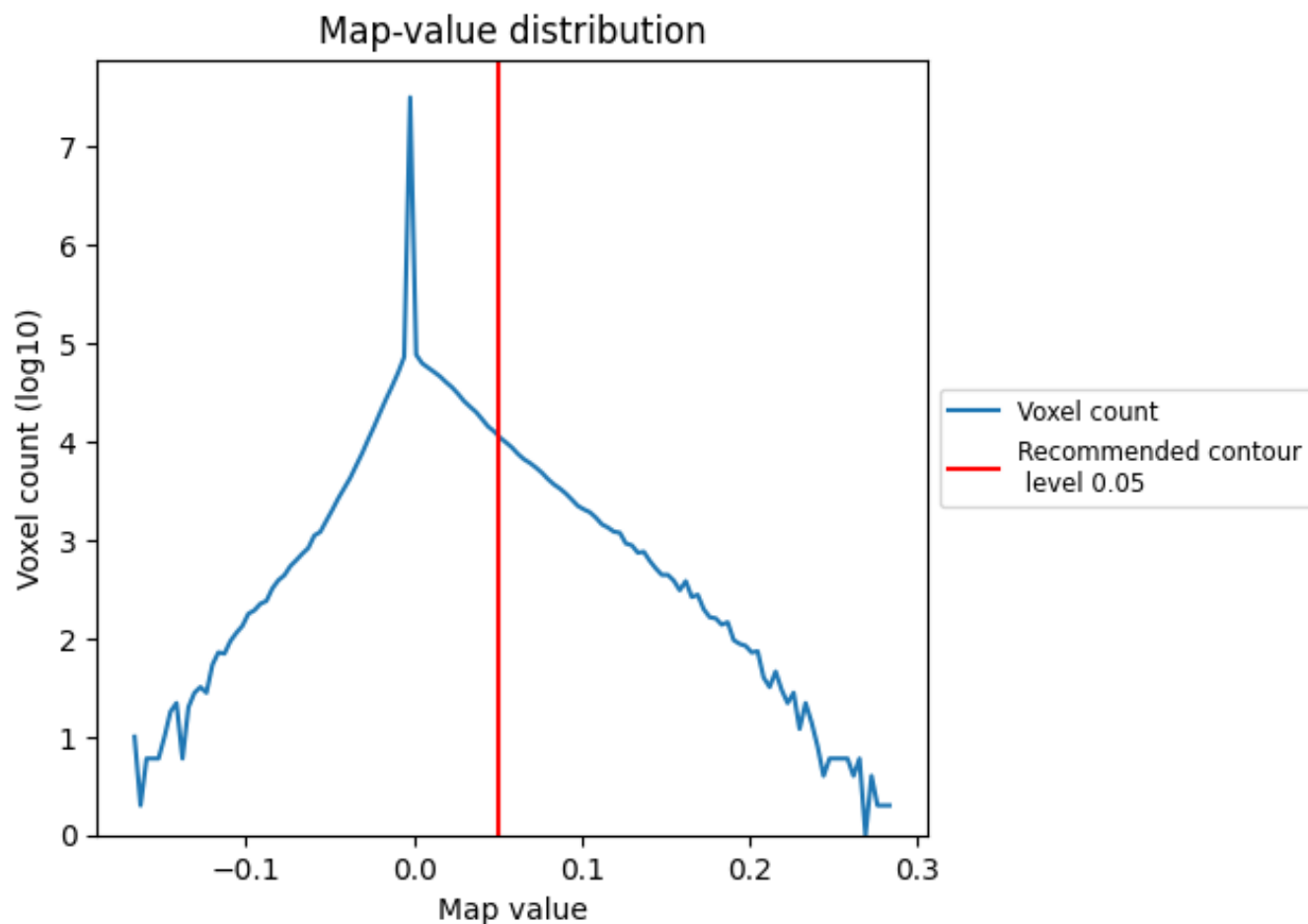
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

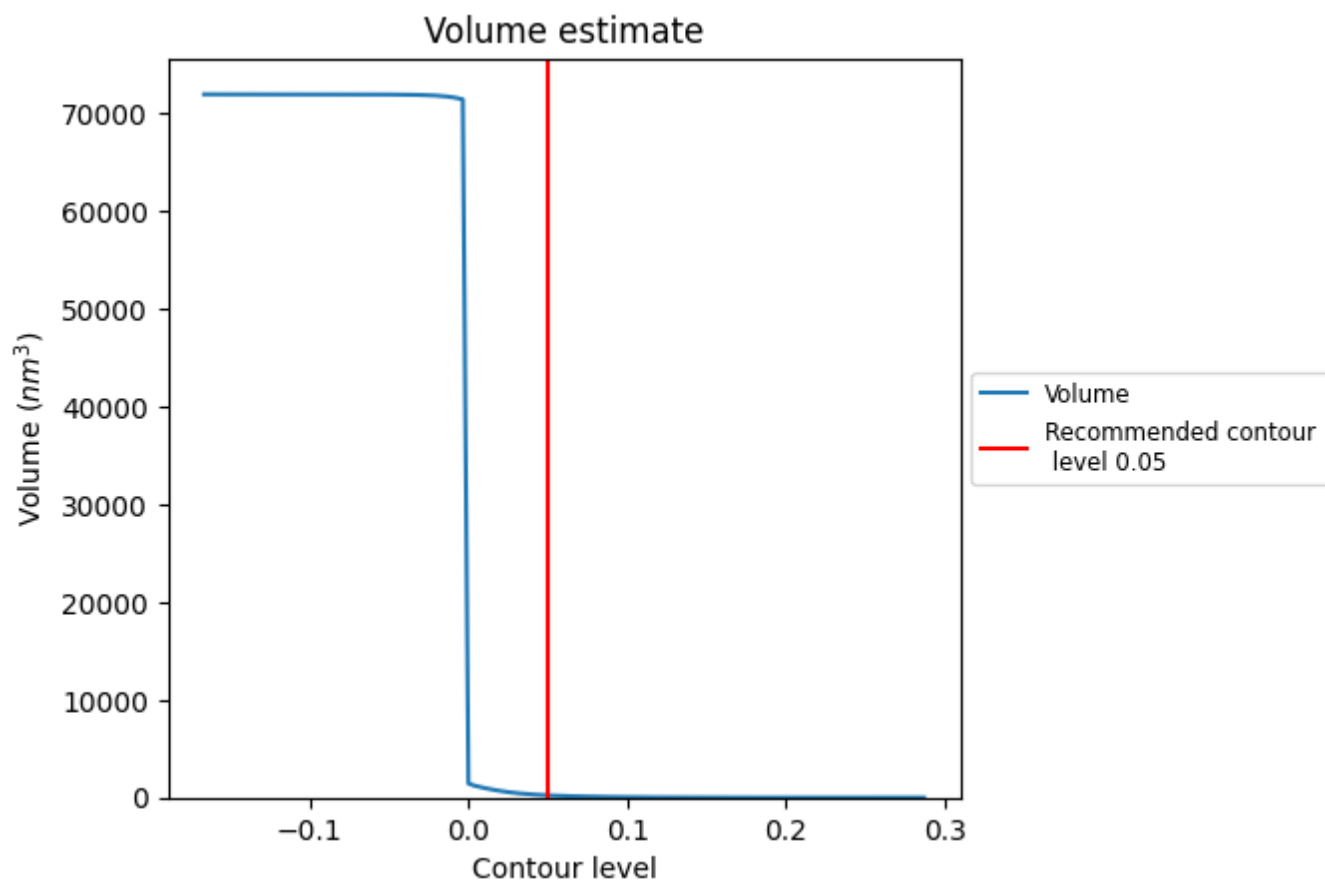
This section contains the results of statistical analysis of the map.

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.

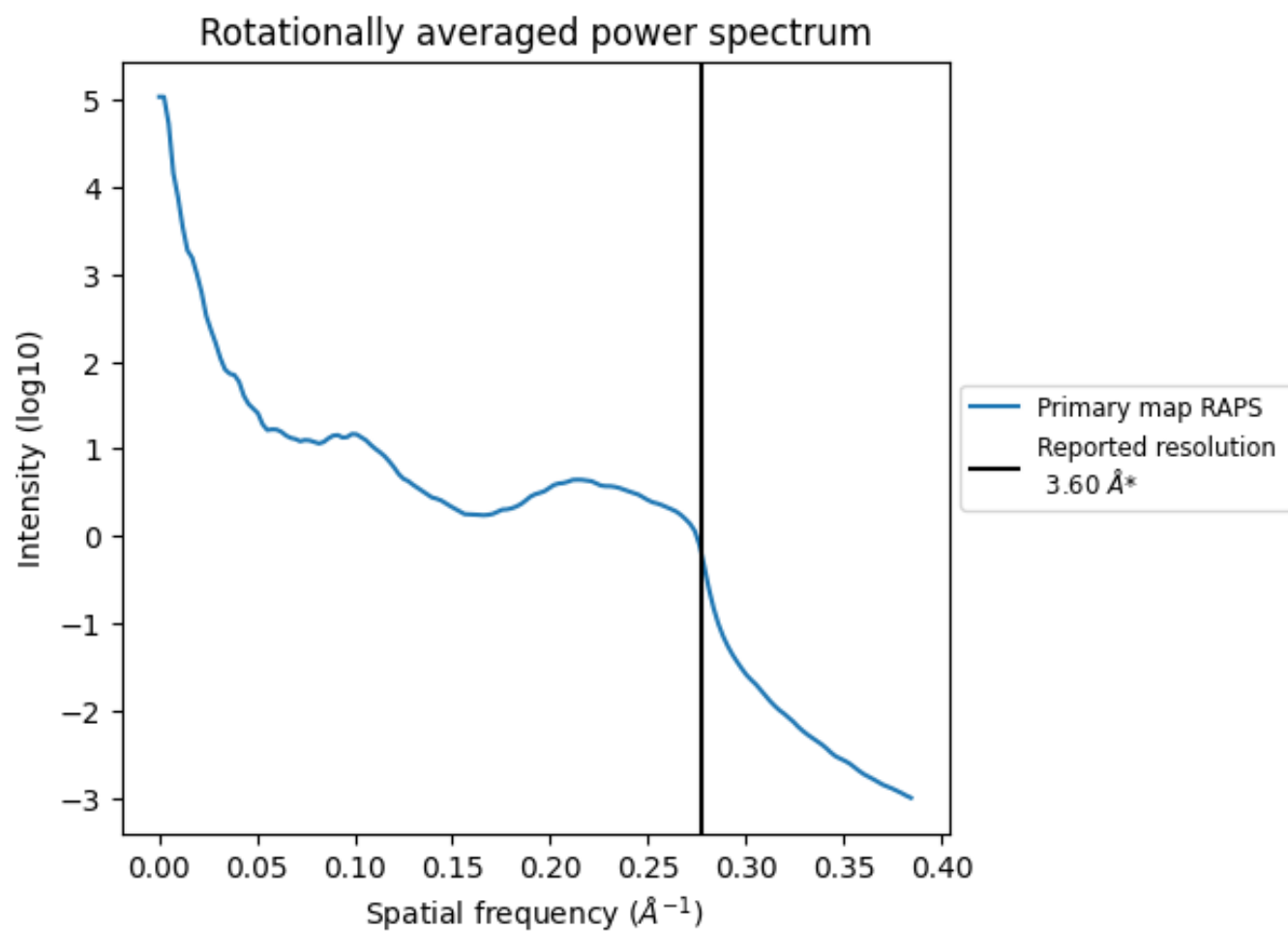
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 227 nm³; this corresponds to an approximate mass of 205 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 ⓘ

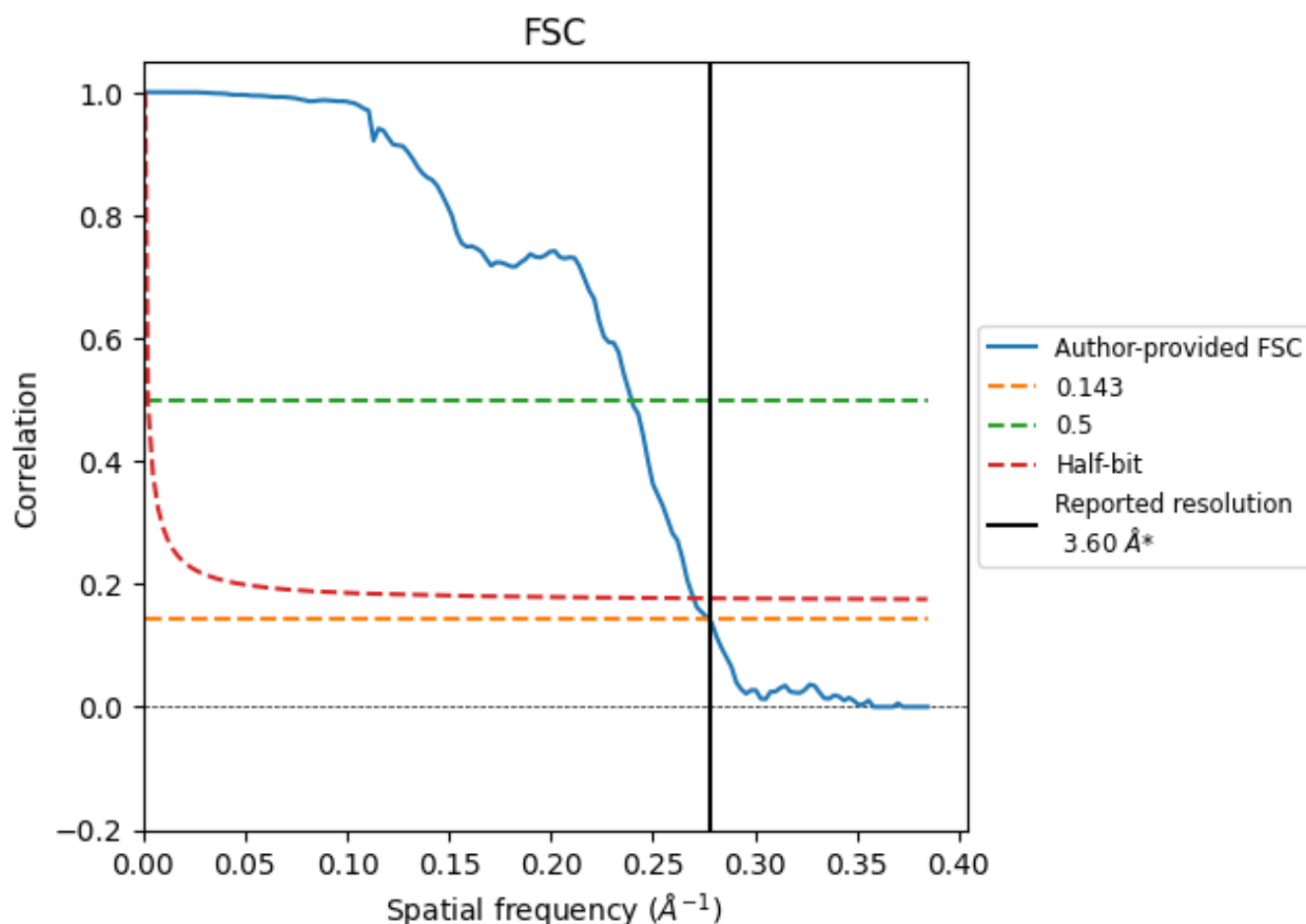


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

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 0.278 Å⁻¹

8.2 Resolution estimates [i](#)

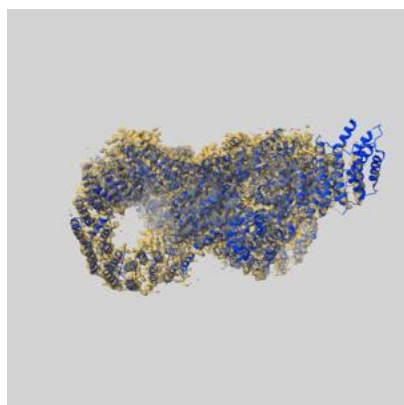
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.61	4.18	3.70
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

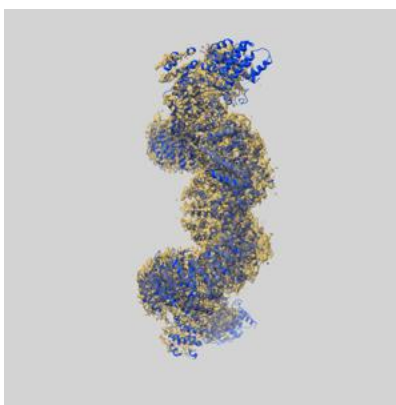
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-7129 and PDB model 6BQ1. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

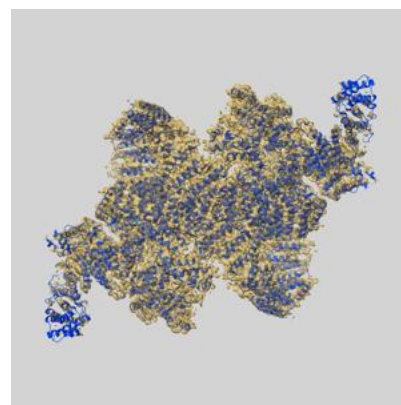
9.1 Map-model overlay [i](#)



X



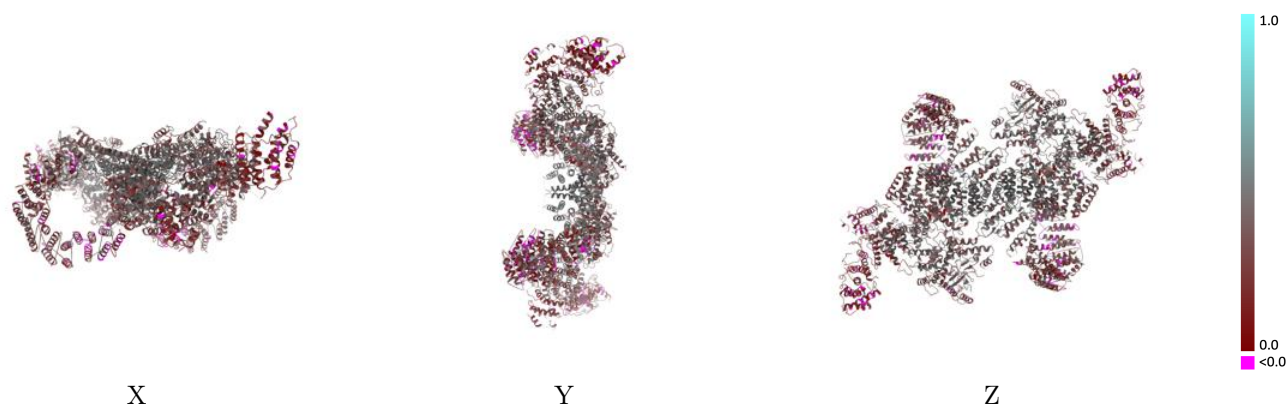
Y



Z

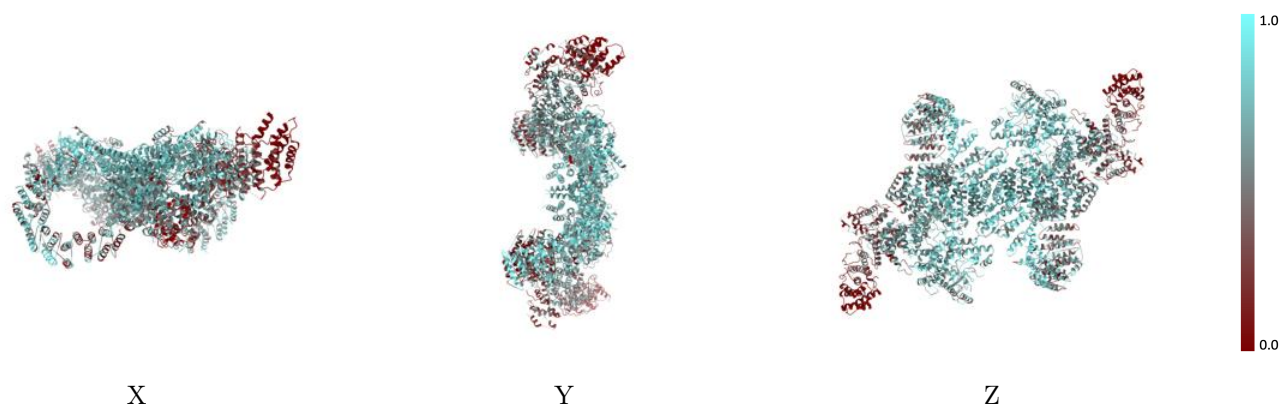
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



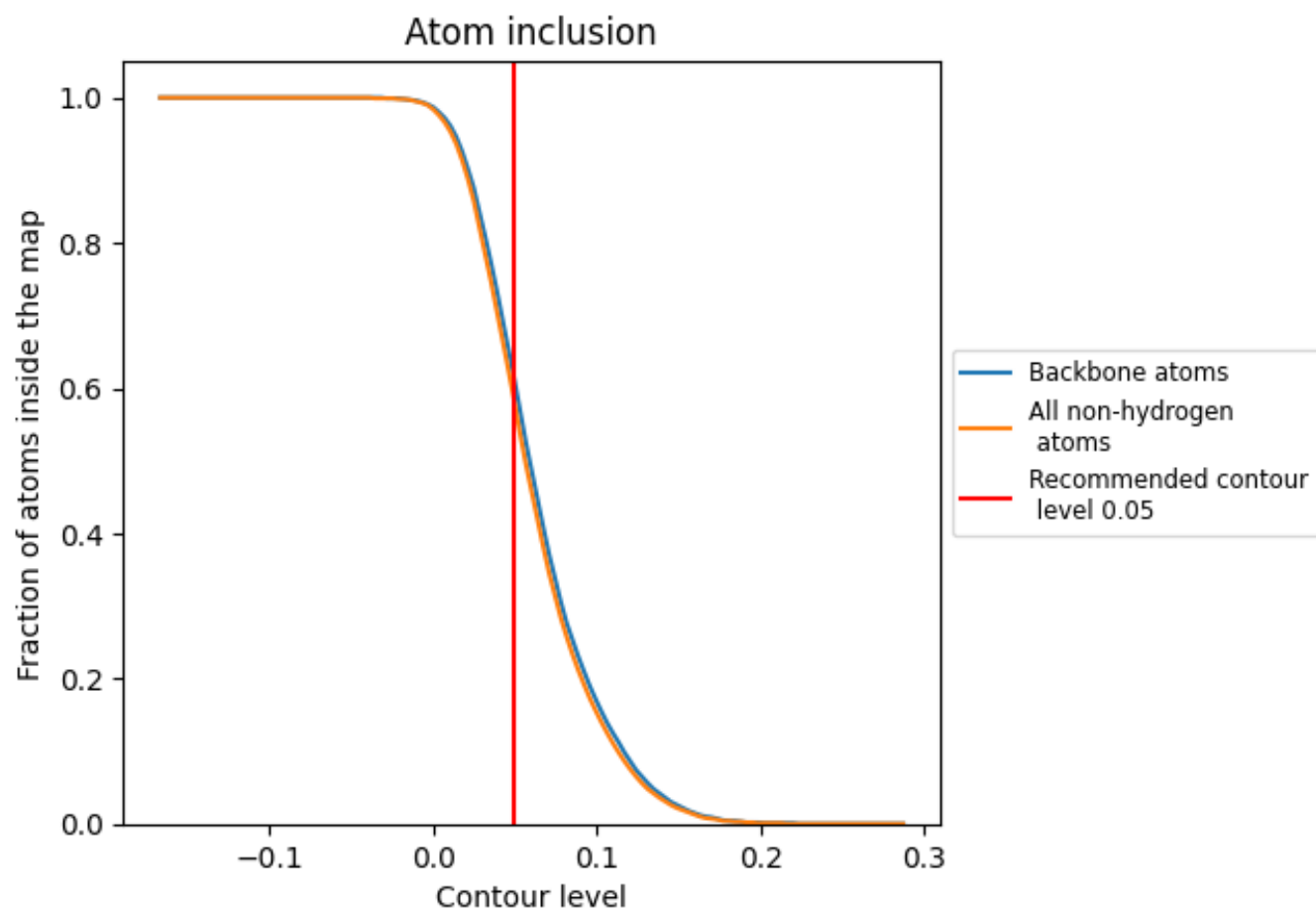
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.05).

9.4 Atom inclusion [i](#)



At the recommended contour level, 61% of all backbone atoms, 58% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5780	0.3410
A	0.6900	0.3680
B	0.4340	0.2940
C	0.3910	0.2800
E	0.7020	0.3820
F	0.4370	0.3040
G	0.3970	0.2830

1.0

0.0

<0.0