



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 09:07 PM UTC

PDB ID : 6U5W / pdb_00006u5w
EMDB ID : EMD-20658
Title : Electron cryomicroscopy structure of C. albicans FAS in the KS-stalled state
Authors : Lou, J.W.; Mazhab-Jafari, M.T.
Deposited on : 2019-08-28
Resolution : 3.30 Å (reported)
Based on initial model : 2UV8

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

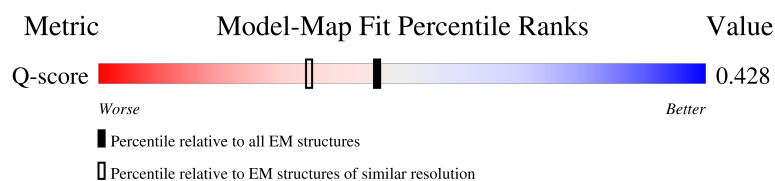
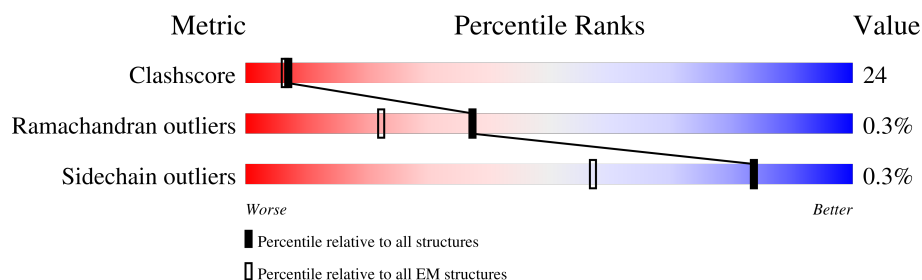
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 (2.80 - 3.80)

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	1722	21% 50% 33% 17%
2	B	2037	51% 54% 46%

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
3	NAP	A	1901	-	-	X	-
3	NAP	B	2102	-	-	X	-
4	FMN	B	2101	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 27482 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 Fatty acid synthase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1435	Total	C	N	O	S	0	0
			11309	7178	1895	2190	46		

There are 173 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ILE	deletion	UNP P43098
A	?	-	PRO	deletion	UNP P43098
A	?	-	ASP	deletion	UNP P43098
A	?	-	GLU	deletion	UNP P43098
A	?	-	PRO	deletion	UNP P43098
A	?	-	VAL	deletion	UNP P43098
A	?	-	LYS	deletion	UNP P43098
A	?	-	ALA	deletion	UNP P43098
A	?	-	ASN	deletion	UNP P43098
A	?	-	LEU	deletion	UNP P43098
A	?	-	LEU	deletion	UNP P43098
A	?	-	ILE	deletion	UNP P43098
A	?	-	HIS	deletion	UNP P43098
A	?	-	VAL	deletion	UNP P43098
A	?	-	LEU	deletion	UNP P43098
A	?	-	VAL	deletion	UNP P43098
A	?	-	ALA	deletion	UNP P43098
A	?	-	GLN	deletion	UNP P43098
A	?	-	LYS	deletion	UNP P43098
A	?	-	LEU	deletion	UNP P43098
A	?	-	LYS	deletion	UNP P43098
A	?	-	LYS	deletion	UNP P43098
A	?	-	PRO	deletion	UNP P43098
A	?	-	LEU	deletion	UNP P43098
A	?	-	ASP	deletion	UNP P43098
A	?	-	ALA	deletion	UNP P43098
A	?	-	VAL	deletion	UNP P43098
A	?	-	PRO	deletion	UNP P43098

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	MET	deletion	UNP P43098
A	?	-	THR	deletion	UNP P43098
A	?	-	LYS	deletion	UNP P43098
A	?	-	ALA	deletion	UNP P43098
A	?	-	ILE	deletion	UNP P43098
A	?	-	LYS	deletion	UNP P43098
A	?	-	ASP	deletion	UNP P43098
A	?	-	LEU	deletion	UNP P43098
A	?	-	VAL	deletion	UNP P43098
A	?	-	ASN	deletion	UNP P43098
A	?	-	GLY	deletion	UNP P43098
A	?	-	LYS	deletion	UNP P43098
A	?	-	SER	deletion	UNP P43098
A	?	-	THR	deletion	UNP P43098
A	?	-	VAL	deletion	UNP P43098
A	?	-	GLN	deletion	UNP P43098
A	?	-	ASN	deletion	UNP P43098
A	?	-	GLU	deletion	UNP P43098
A	?	-	ILE	deletion	UNP P43098
A	?	-	LEU	deletion	UNP P43098
A	?	-	GLY	deletion	UNP P43098
A	?	-	ASP	deletion	UNP P43098
A	?	-	LEU	deletion	UNP P43098
A	?	-	GLY	deletion	UNP P43098
A	?	-	LYS	deletion	UNP P43098
A	?	-	GLU	deletion	UNP P43098
A	?	-	PHE	deletion	UNP P43098
A	?	-	GLY	deletion	UNP P43098
A	?	-	SER	deletion	UNP P43098
A	?	-	THR	deletion	UNP P43098
A	?	-	PRO	deletion	UNP P43098
A	?	-	GLU	deletion	UNP P43098
A	?	-	LYS	deletion	UNP P43098
A	?	-	PRO	deletion	UNP P43098
A	?	-	GLU	deletion	UNP P43098
A	?	-	ASP	deletion	UNP P43098
A	?	-	THR	deletion	UNP P43098
A	?	-	PRO	deletion	UNP P43098
A	?	-	LEU	deletion	UNP P43098
A	?	-	GLU	deletion	UNP P43098
A	?	-	GLU	deletion	UNP P43098
A	?	-	LEU	deletion	UNP P43098

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ALA	deletion	UNP P43098
A	?	-	GLU	deletion	UNP P43098
A	?	-	GLN	deletion	UNP P43098
A	?	-	PHE	deletion	UNP P43098
A	?	-	GLN	deletion	UNP P43098
A	?	-	ASP	deletion	UNP P43098
A	?	-	SER	deletion	UNP P43098
A	?	-	PHE	deletion	UNP P43098
A	?	-	SER	deletion	UNP P43098
A	?	-	GLY	deletion	UNP P43098
A	?	-	GLN	deletion	UNP P43098
A	?	-	LEU	deletion	UNP P43098
A	?	-	GLY	deletion	UNP P43098
A	?	-	LYS	deletion	UNP P43098
A	?	-	THR	deletion	UNP P43098
A	?	-	SER	deletion	UNP P43098
A	?	-	THR	deletion	UNP P43098
A	?	-	SER	deletion	UNP P43098
A	?	-	LEU	deletion	UNP P43098
A	?	-	ILE	deletion	UNP P43098
A	?	-	GLY	deletion	UNP P43098
A	?	-	ARG	deletion	UNP P43098
A	?	-	LEU	deletion	UNP P43098
A	?	-	MET	deletion	UNP P43098
A	?	-	SER	deletion	UNP P43098
A	?	-	SER	deletion	UNP P43098
A	?	-	LYS	deletion	UNP P43098
A	?	-	MET	deletion	UNP P43098
A	?	-	PRO	deletion	UNP P43098
A	?	-	GLY	deletion	UNP P43098
A	?	-	GLY	deletion	UNP P43098
A	?	-	PHE	deletion	UNP P43098
A	?	-	SER	deletion	UNP P43098
A	?	-	ILE	deletion	UNP P43098
A	?	-	THR	deletion	UNP P43098
A	?	-	THR	deletion	UNP P43098
A	?	-	ALA	deletion	UNP P43098
A	?	-	ARG	deletion	UNP P43098
A	?	-	LYS	deletion	UNP P43098
A	?	-	TYR	deletion	UNP P43098
A	?	-	LEU	deletion	UNP P43098
A	?	-	GLU	deletion	UNP P43098

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	SER	deletion	UNP P43098
A	?	-	ARG	deletion	UNP P43098
A	?	-	PHE	deletion	UNP P43098
A	?	-	GLY	deletion	UNP P43098
A	?	-	LEU	deletion	UNP P43098
A	?	-	GLY	deletion	UNP P43098
A	?	-	ALA	deletion	UNP P43098
A	?	-	GLY	deletion	UNP P43098
A	?	-	ARG	deletion	UNP P43098
A	?	-	GLN	deletion	UNP P43098
A	?	-	ASP	deletion	UNP P43098
A	?	-	SER	deletion	UNP P43098
A	?	-	VAL	deletion	UNP P43098
A	?	-	LEU	deletion	UNP P43098
A	?	-	LEU	deletion	UNP P43098
A	?	-	MET	deletion	UNP P43098
A	?	-	ALA	deletion	UNP P43098
A	?	-	LEU	deletion	UNP P43098
A	?	-	THR	deletion	UNP P43098
A	?	-	ASN	deletion	UNP P43098
A	?	-	GLU	deletion	UNP P43098
A	?	-	PRO	deletion	UNP P43098
A	?	-	ALA	deletion	UNP P43098
A	?	-	ASN	deletion	UNP P43098
A	?	-	ARG	deletion	UNP P43098
A	?	-	LEU	deletion	UNP P43098
A	?	-	GLY	deletion	UNP P43098
A	?	-	SER	deletion	UNP P43098
A	?	-	GLU	deletion	UNP P43098
A	?	-	ALA	deletion	UNP P43098
A	?	-	ASP	deletion	UNP P43098
A	?	-	ALA	deletion	UNP P43098
A	?	-	LYS	deletion	UNP P43098
A	?	-	THR	deletion	UNP P43098
A	?	-	PHE	deletion	UNP P43098
A	?	-	PHE	deletion	UNP P43098
A	?	-	ASP	deletion	UNP P43098
A	?	-	GLY	deletion	UNP P43098
A	?	-	ILE	deletion	UNP P43098
A	?	-	ALA	deletion	UNP P43098
A	?	-	GLN	deletion	UNP P43098
A	?	-	LYS	deletion	UNP P43098

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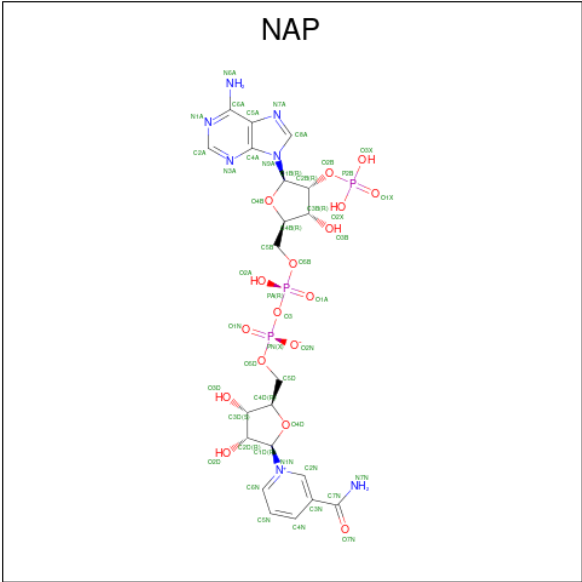
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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	TYR	deletion	UNP P43098
A	?	-	ALA	deletion	UNP P43098
A	?	-	SER	deletion	UNP P43098
A	?	-	SER	deletion	UNP P43098
A	?	-	ALA	deletion	UNP P43098
A	?	-	GLY	deletion	UNP P43098
A	?	-	ILE	deletion	UNP P43098
A	?	-	SER	deletion	UNP P43098
A	?	-	LEU	deletion	UNP P43098
A	350	VAL	SER	conflict	UNP P43098
A	351	ASP	ARG	conflict	UNP P43098
A	353	ASN	LYS	conflict	UNP P43098
A	354	LYS	GLN	conflict	UNP P43098
A	356	ALA	LEU	conflict	UNP P43098
A	813	THR	PRO	conflict	UNP P43098
A	1066	LYS	GLN	conflict	UNP P43098
A	1123	VAL	ILE	conflict	UNP P43098
A	1444	GLU	LYS	conflict	UNP P43098
A	1742	SER	ASN	conflict	UNP P43098

- Molecule 2 is a protein called Fatty acid synthase subunit beta.

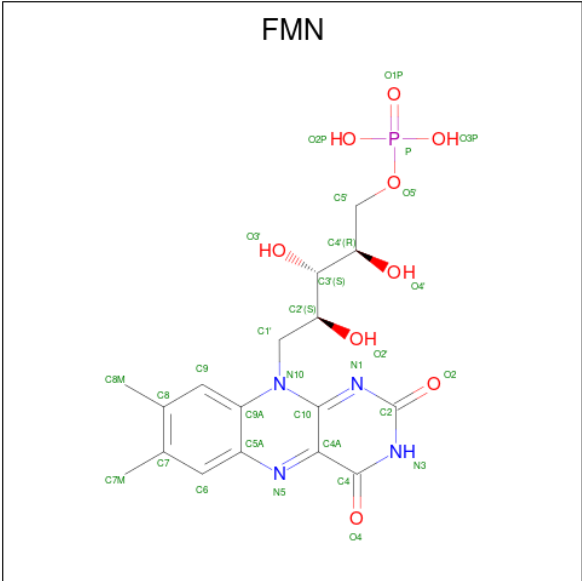
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	2033	Total	C	N	O	S	0	0
			16046	10286	2662	3044	54		

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			48	21	7	17	3	
3	B	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 4 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).

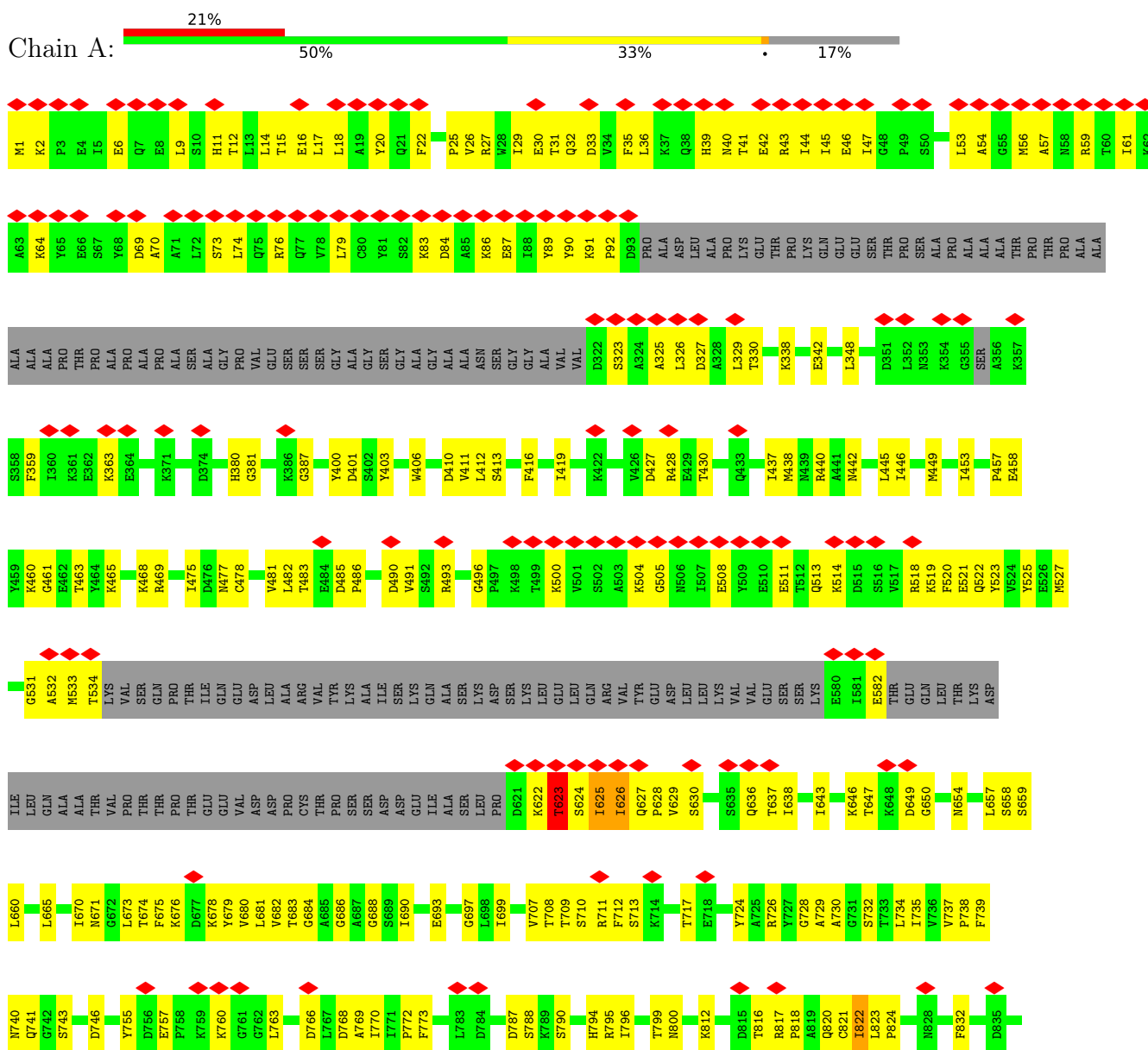


Mol	Chain	Residues	Atoms					AltConf
4	B	1	Total	C	N	O	P	0
			31	17	4	9	1	

3 Residue-property plots

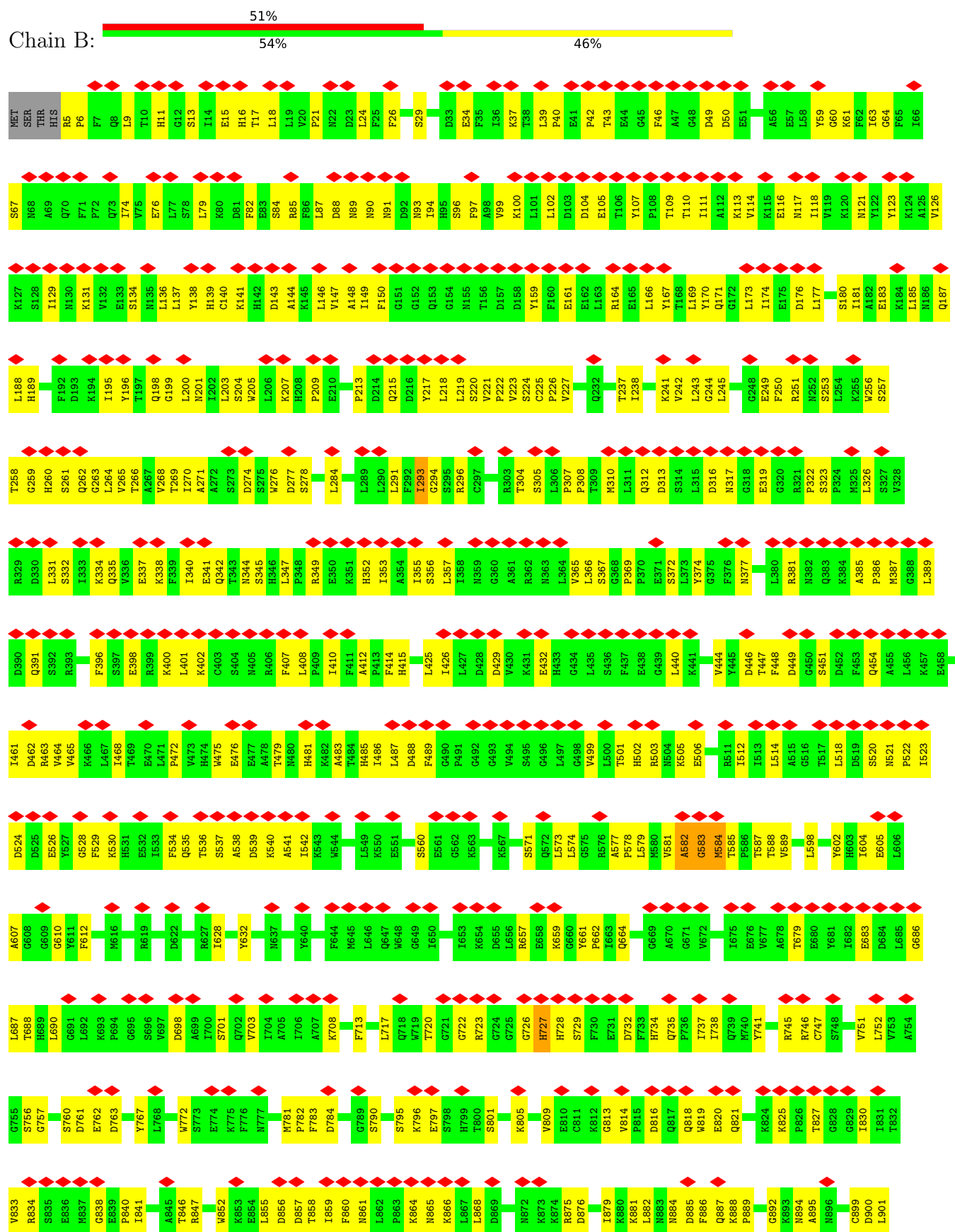
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Fatty acid synthase subunit alpha



[illegible]

• Molecule 2: Fatty acid synthase subunit beta



Q1698	L1635	S1574	E1510	D1441	V1367	A1304	I1235	D1173	Q1111	I1041	K980	Q902
N1699	P1636	I1575	E1511	V1442	M1368	T1305	L1236	K1174	V1112	H1042	Q981	E903
M1702	L1638	R1576	E1512	Q1443	M1369	L1306	E1237	K1175	E1115	H1043	L983	M904
E1703	I1639	A1577	S1513	F1444	Q1370	A1307	I1238	T1176	I1116	G1044	L982	T905
L1704	G1640	L1578	E1517	D1445	P1371	P1308	M1239	K1177	D1117	P1045	S984	Y906
E1641	L1704	V1579	M1518	V1446	K1374	M1309	E1240	K1178	D1117	V1046	E985	K907
T1705	E1641	E1580	A1519	L1447	L1375	D1310	D1241	K1179	S1118	A1047	E986	E908
L1706	A1642	E1581	L1375	T1448	V1376	F1311	R1242	T1180	E1119	S1048	D987	
H1707	E1643	V1582	I1520	F1449	E1377	I1313	R1245	A1181	L1120	Q1049	C988	L916
F1708	I1644	A1583	P1521	R1450	G1386	V1314	K1246	F1182	P1121	Y1050	D989	K920
G1709	E1645	A1584	L1522	C1451	I1382	I1315	I1247	E1183	M1222	K1053	F991	K921
K1712	Q1646	G1583	L1522	E1452	Y1383	G1316	E1248	T1184	Q1123	V1054	S922	S921
G1713	P1647	N1585	S1523	S1453	R1384	W1317	F1249	I1185	K1124	D1055	M993	H923
R1714	T1648	N1586	S1524	S1453	E1385	K1318	Y1250	K1186	E1125	E1056	L994	I926
T1715	T1649	V1587	G1525	K1456	G1386	I1321	W1251	G1187	W1126	P1057		D927
I1716	T1650	A1588	E1526	F1457		I1321		D1188	L1127	I1058	R997	D927
R1717	T1650	A1589	E1527	F1457	M1390	K1322	G1256	D1188	D1128	I1058	R997	V928
D1718	Y1651	A1589	E1527	K1458	M1390	K1322	G1256	D1188	L1128	I1058	R997	S929
W1719	V1652	R1590	L1528	S1459	Q1395	A1323	S1257	L1189	L1129	G1059	G999	L930
Y1720	F1653	V1591	T1529	A1460	F1396	I1324	S1258	L1190	L1130	D1060	Q999	R931
G1722	T1654	R1592	S1530	N1461	F1396	F1325	P1259	V1192	A1131	I1061	Q1000	R931
G1655	A1593	A1593	K1531	Y1462	R1399	P1326	P1260	V1193	G1132	L1062	K1001	N932
Q1656	F1594	F1594	A1532	Y1463	G1400	K1327	P1260	E1194	T1133	N1063	P1002	M933
G1657	C1596	C1596	E1532	S1464	G1400	S1328	Y1261	I1196	E1134	S1064	P1004	Y934
F1725	S1658	D1597	P1533		E1401	V1329	S1262	E1196	L1135	I1065	F1005	R939
E1726	Q1659	F1597	G1534	K1467	Y1402	V1329	Y1261	E1196	M1136	H1066	F1006	R940
T1727	M1536	F1598	T1535	T1468	E1401	D1330	N1263	E1197	W1137	E1067	P1007	
I1728	E1660	V1599	M1537	T1469	Y1402	G1331	D1264	V1198	L1138	K1075	V1008	E943
Q1661	Q1661	G1600	E1537	T1470	D1404	D1332	I1265	K1199	Q1139	E1076	L1009	R944
G1662	M1601	M1601	P1538	Q1471	Y1405	L1333	V1267	N1201	A1140		D1010	F945
M1663	V1602	V1602	Y1539	E1475	N1407	L1334	E1268	I1202	F1141	A1079	E1011	S948
G1664	L1603	P1604	A1540	L1476	T1408	K1335	K1269	I1203	I1142	G1080	R1012	A949
M1665	E1666	M1605	G1544	P1477	E1415	L1336	A1270	S1206	S1143	D1081	F1013	G950
L1667	L1667	D1606	D1545	T1478	T1415	V1337	I1271		T1144	E1082	E1014	T951
V1668	M1669	T1607	Y1546	K1479	E1415	L1339	L1272	E1209	R1146	E1082	F1015	L954
S1735	K1736	L1607	Y1546	E1480	P1416	L1339	G1273	H1210	I1147	S1083	F1016	L955
E1737	E1737	Q1609	Y1547	V1417	Q1417	N1341	D1274	R1211	Q1149	K1084	F1017	Q956
K1738	S1670	T1610	P1548	E1480	Q1417	G1342	E1275	T1212	G1150	V1087	K1018	N957
I1739	S1671	T1611	L1549	V1481	V1419	Y1343	L1276	A1213	S1151	V1088	K1019	F958
F1740	V1672	M1612	H1550	Q1483	A1420	K1344	T1277	D1214	K1152	E1089	D1020	N959
K1741	E1673	E1613	V1551	V1484	F1421	M1345	I1278	T1215	H1153	Y1090	S1021	Q960
D1742	A1674	L1613	S1552	G1485	K1422	I1346	I1278	T1215			L1022	L961
L1743	R1675	E1675	R1553	S1486	S1423	T1347	S1279	N1216	M1156	G1093	W1023	N962
D1744	V1677	V1677	V1554	V1487	A1424	A1349	F1286	P1217	P1157	K1094	Q1024	E963
E1745	E1678	L1618	F1555	K1425	K1425	E1348	T1287	V1218	L1158	K1095	S1025	P964
T1746	D1679	M1619	A1556	D1488	D1426	A1350	H1288	A1219	H1159	P1096	E1026	E965
K1680	K1680	G1620	A1557	E1490	L1437	P1351	A1289	P1221	D1160	A1097	D1027	Q966
				L1491	A1428	L1352	I1290	F1222	I1161	S1098	E1029	F967
				G1492	V1429	K1353	G1291	L1162	T1163	V1099	S1030	T968
												A969
												D970
												F971
												F972
												E973
												K974
												Q977

P2006 F2007 E2008 L2009 T2010 T2011 E2012 Y2013 F2014 Q2015 S2016 T2017 Y2018 D2019 T2021 K2022 S2023 E2024 K2025 L2026 K2027 S2028 L2029 L2030 D2031 N2032 W2033 E2034 Q2035 Y2036 E2037	P1945 I1946 D1947 L1948 E1949 R1950 G1951 F1952 A1953 V1954 I1955 P1956 L1957 K1958 G1959 I1960 V1962 F1963 F1964 H1965 S1966 S1967 L1968 L1969 M1970 V1973 K1974 P1975 F1976 Q1977 R1978 F1979 L1980 C1981 K1982 I1984 P1985 K1986 S1987 S1988 V1989 K1990 P1991 Q1992 L1994 I1995 G1996 K1997 Y1998 P2000 N2001 L2002 T2003 K2004 K2005	Q1885 Y1886 V1887 A1888 A1889 G1890 D1891 L1892 R1893 A1894 L1895 D1896 T1897 L1898 T1899 M1900 V1901 L1902 M1903 V1904 L1905 K1906 I1907 M1908 K1909 D1910 I1911 I1912 V1913 K1914 L1915 Q1916 E1917 Q1918 M1919 S1920 I1921 E1922 K1923 V1924 K1925 E1926 H1927 L1928 Y1929 E1930 I1931 V1932 D1933 E1934 V1935 A1936 A1937 K1938 S1939 L1940 A1941 K1942 P1943 Q1944	T1825 M1826 Q1827 L1828 A1829 V1830 P1831 R1832 D1833 E1834 L1835 G1836 R1837 S1838 M1839 Y1840 G1841 M1842 V1843 A1844 L1845 M1846 P1847 S1848 R1849 V1850 S1851 A1852 T1853 F1854 D1855 D1856 S1857 A1858 L1859 R1860 F1861 V1862 V1863 D1864 E1865 L1866 A1867 M1868 K1869 T1870 K1871 L1872 L1873 L1874 E1875 I1876 V1877 M1878 Y1879 N1880 V1881 E1882 M1883 Q1884	S1760 A1761 T1762 Q1763 F1764 T1765 Q1766 P1767 A1768 L1769 T1770 L1771 M1772 E1773 Y1777 E1778 D1779 I1780 K1783 G1784 L1785 I1786 P1787 S1788 D1789 I1790 M1791 F1792 A1793 G1794 H1795 S1796 L1797 G1798 E1799 Y1800 L1803 S1804 S1805 L1806 A1807 M1808 V1809 M1810 P1811 I1812 E1813 S1814 L1815 D1816 V1817 V1818 V1819 R1822 G1823 M1824
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D3	Depositor
Number of particles used	24417	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE; CTFFIND4 within cryoSPARC2	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	43	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	1.942	Depositor
Minimum map value	-0.817	Depositor
Average map value	0.012	Depositor
Map value standard deviation	0.133	Depositor
Recommended contour level	0.704	Depositor
Map size ($\text{\AA}$)	373.12, 373.12, 373.12	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.51	1/11536 (0.0%)	0.54	0/15595
2	B	0.37	0/16415	0.48	3/22269 (0.0%)
All	All	0.43	1/27951 (0.0%)	0.51	3/37864 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	822	ILE	C-N	-5.44	1.25	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	74	ILE	N-CA-C	-5.44	107.49	111.90
2	B	1386	GLY	CA-C-N	-5.16	111.14	120.94
2	B	1386	GLY	C-N-CA	-5.16	111.14	120.94

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1301	GLY	Peptide

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	11309	0	11219	498	0
2	B	16046	0	16024	853	0
3	A	48	0	25	34	0
3	B	48	0	25	49	0
4	B	31	0	17	50	0
All	All	27482	0	27310	1312	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 24.

The worst 5 of 1312 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)
2:B:584:MET:HE2	4:B:2101:FMN:C7	1.23	1.64
2:B:584:MET:HB3	4:B:2101:FMN:C5A	1.29	1.61
1:A:712:PHE:CE1	1:A:717:THR:HG22	1.35	1.58
2:B:727:HIS:ND1	3:B:2102:NAP:C4N	1.79	1.45
2:B:727:HIS:ND1	3:B:2102:NAP:C3N	1.73	1.44

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	1427/1722 (83%)	1306 (92%)	115 (8%)	6 (0%)	30 60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	2031/2037 (100%)	1860 (92%)	168 (8%)	3 (0%)	48	75
All	All	3458/3759 (92%)	3166 (92%)	283 (8%)	9 (0%)	37	65

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	879	ALA
2	B	582	ALA
1	A	623	THR
1	A	876	LEU
2	B	727	HIS

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	1222/1445 (85%)	1215 (99%)	7 (1%)	78	81
2	B	1780/1784 (100%)	1777 (100%)	3 (0%)	87	88
All	All	3002/3229 (93%)	2992 (100%)	10 (0%)	84	86

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	293	ILE
2	B	584	MET
2	B	1667	LEU
1	A	660	LEU
1	A	876	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 44 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	959	ASN
2	B	1338	HIS

Continued on next page...

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Mol	Chain	Res	Type
2	B	960	GLN
2	B	1066	HIS
2	B	1688	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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
3	NAP	A	1901	-	50,52,52	1.17	4 (8%)	71,80,80	1.55	10 (14%)
4	FMN	B	2101	-	33,33,33	6.45	22 (66%)	48,50,50	1.35	6 (12%)
3	NAP	B	2102	-	50,52,52	1.16	4 (8%)	71,80,80	1.55	9 (12%)

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
3	NAP	A	1901	-	-	11/35/67/67	0/5/5/5
4	FMN	B	2101	-	-	5/18/18/18	0/3/3/3
3	NAP	B	2102	-	-	5/35/67/67	0/5/5/5

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	2101	FMN	C6-C7	13.57	1.58	1.39
4	B	2101	FMN	C6-C5A	12.37	1.58	1.40
4	B	2101	FMN	C9-C9A	12.34	1.59	1.39
4	B	2101	FMN	C9-C8	11.96	1.55	1.39
4	B	2101	FMN	O4-C4	9.98	1.42	1.23

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1901	NAP	C5A-C4A-N3A	-5.84	118.67	126.72
3	B	2102	NAP	C5A-C4A-N3A	-5.83	118.69	126.72
3	A	1901	NAP	N3A-C4A-N9A	4.58	134.96	127.17
3	B	2102	NAP	N3A-C4A-N9A	4.57	134.94	127.17
3	B	2102	NAP	C2A-N3A-C4A	3.71	120.88	111.83

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1901	NAP	C5B-O5B-PA-O1A
3	A	1901	NAP	C5D-O5D-PN-O3
3	A	1901	NAP	C5D-O5D-PN-O1N
3	A	1901	NAP	C5D-O5D-PN-O2N
3	B	2102	NAP	C5D-O5D-PN-O1N

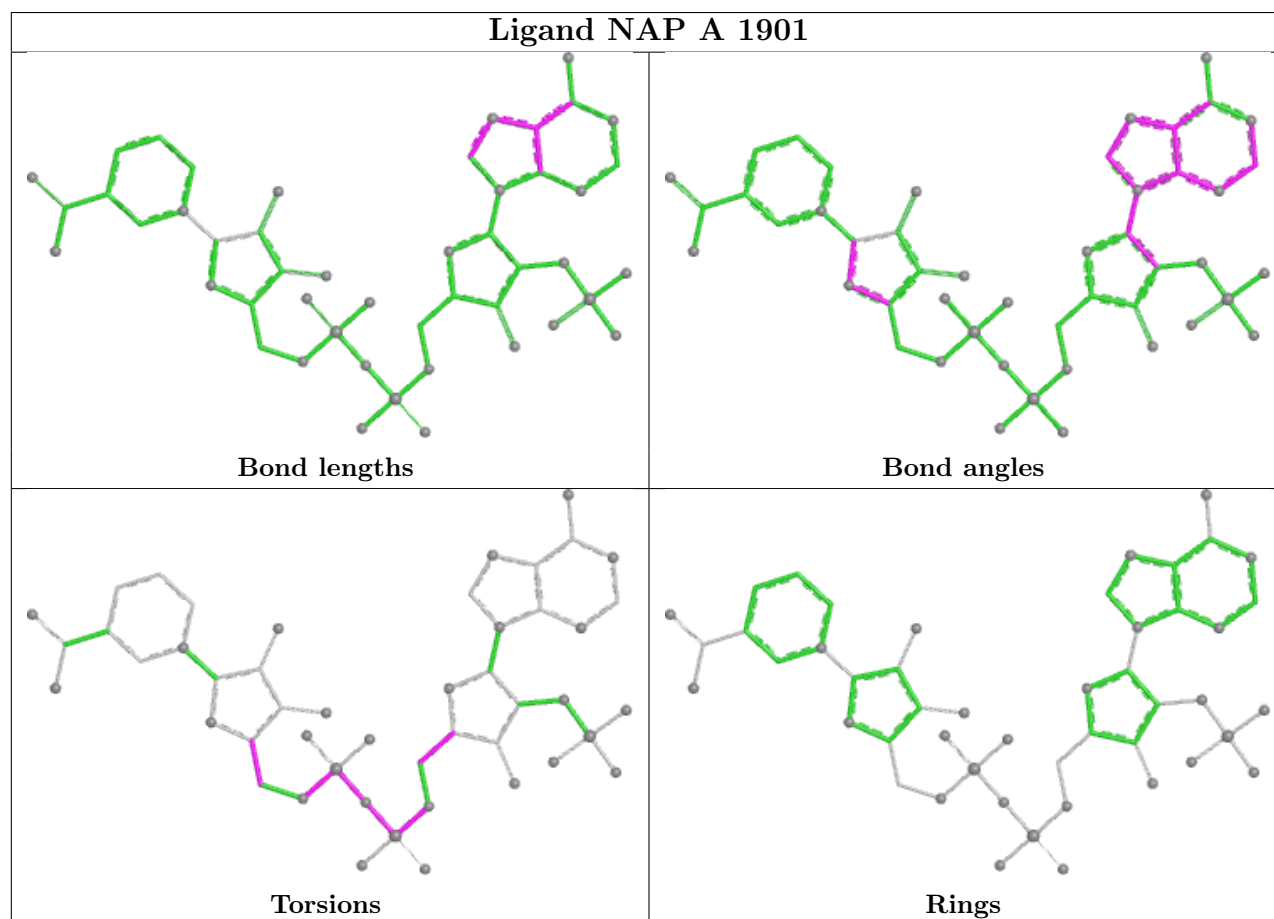
There are no ring outliers.

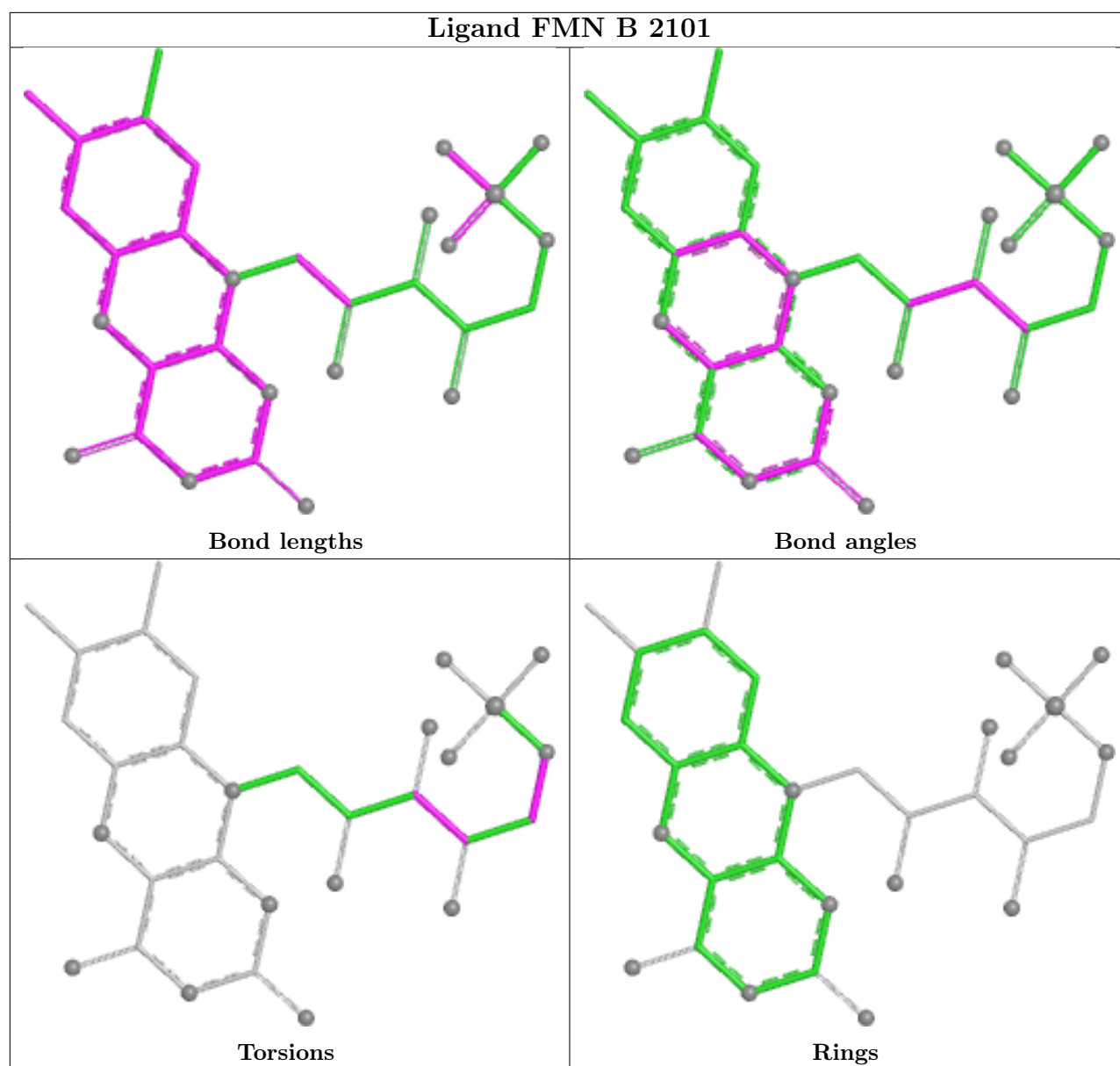
3 monomers are involved in 133 short contacts:

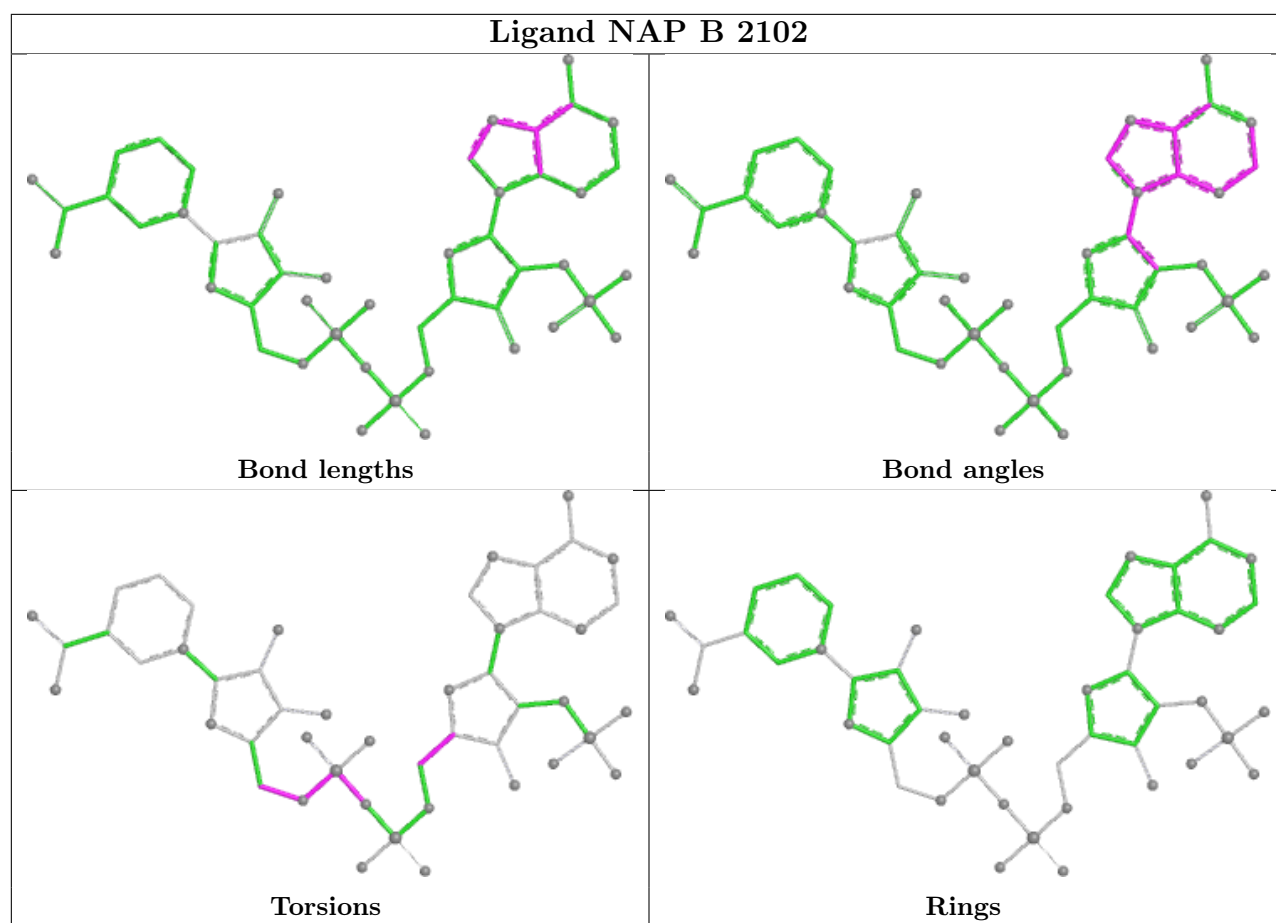
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1901	NAP	34	0
4	B	2101	FMN	50	0
3	B	2102	NAP	49	0

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.

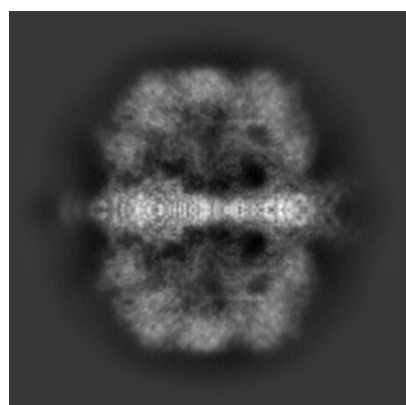
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20658. These allow visual inspection of the internal detail of the map and identification of artifacts.

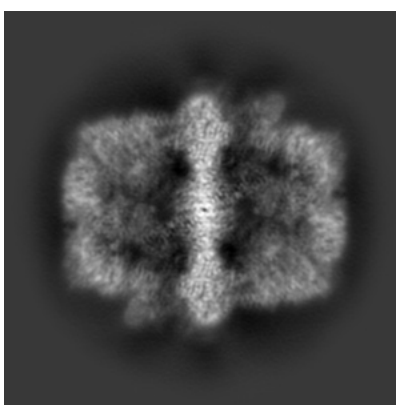
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

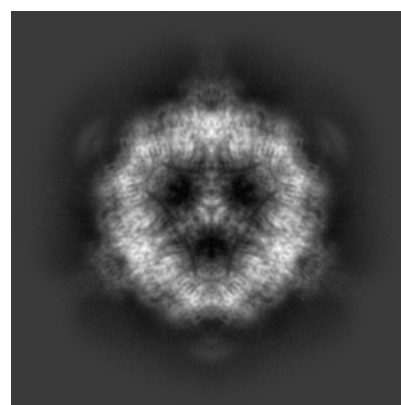
6.1.1 Primary map



X



Y

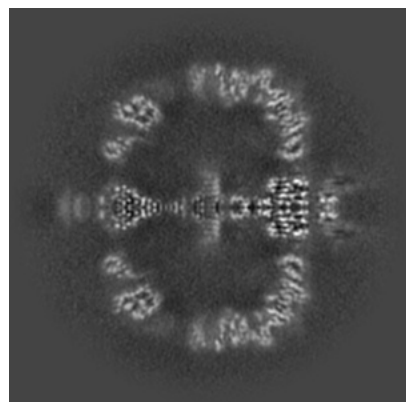


Z

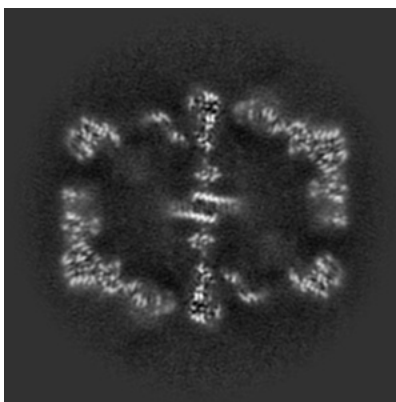
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

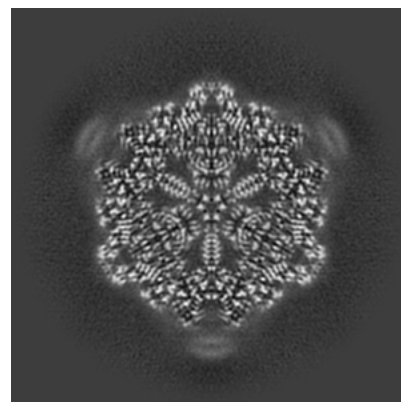
6.2.1 Primary map



X Index: 176



Y Index: 176

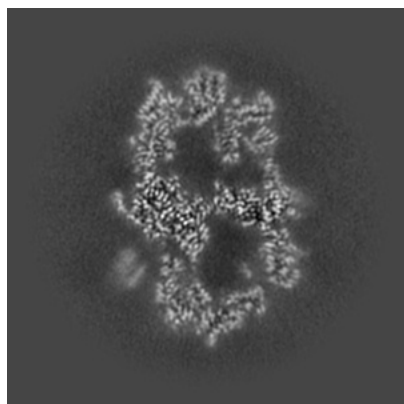


Z Index: 176

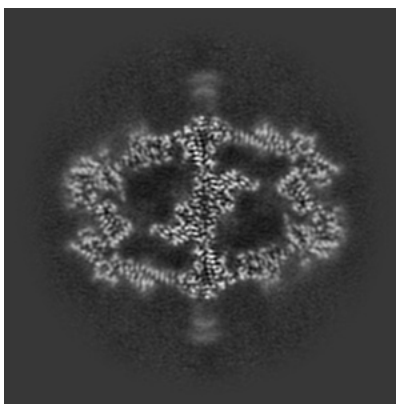
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

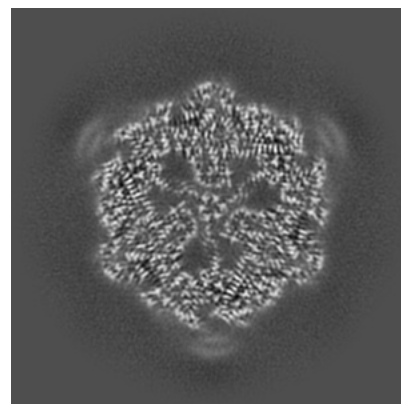
6.3.1 Primary map



X Index: 237



Y Index: 231

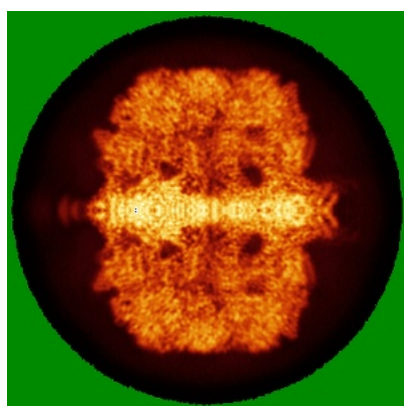


Z Index: 172

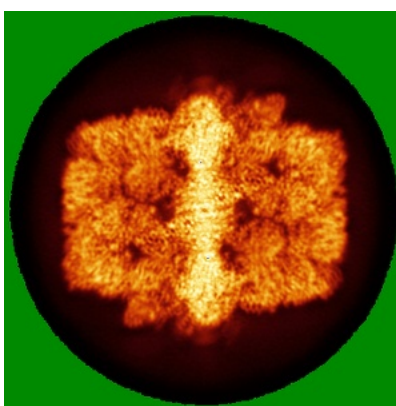
The images above show the largest variance slices of the map in three orthogonal directions.

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

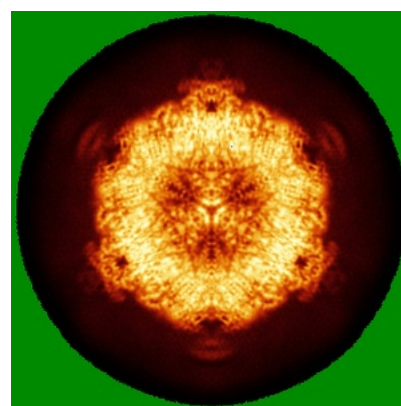
6.4.1 Primary map



X



Y

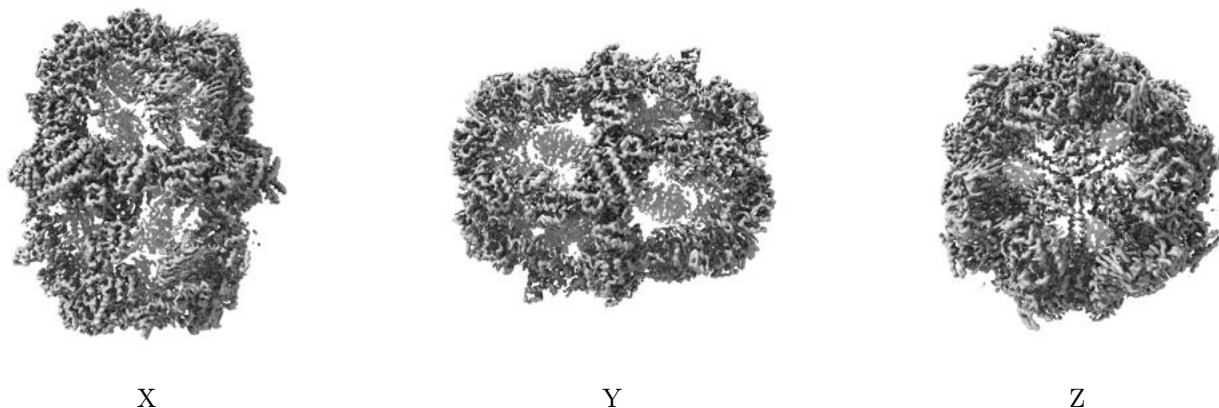


Z

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

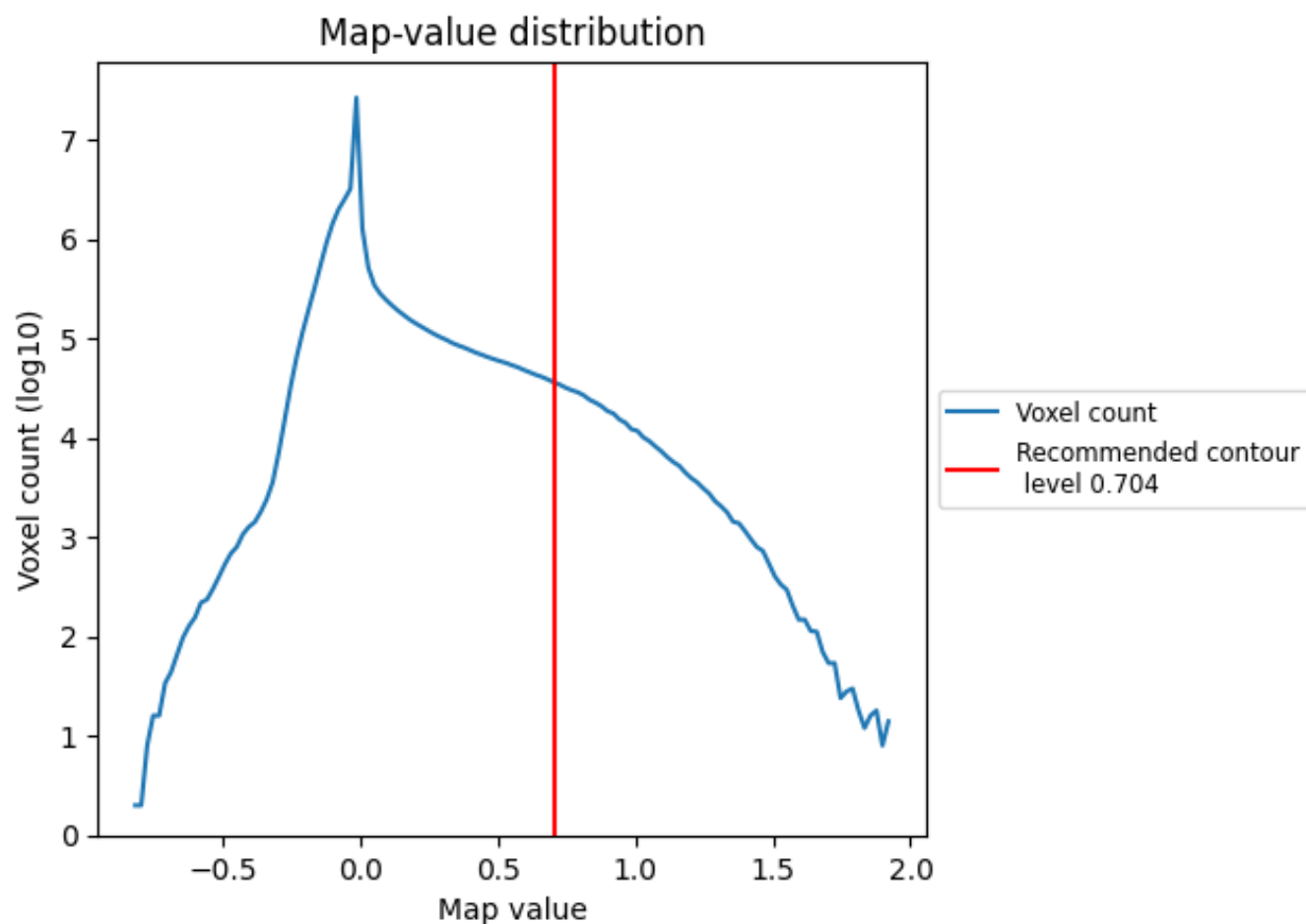
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

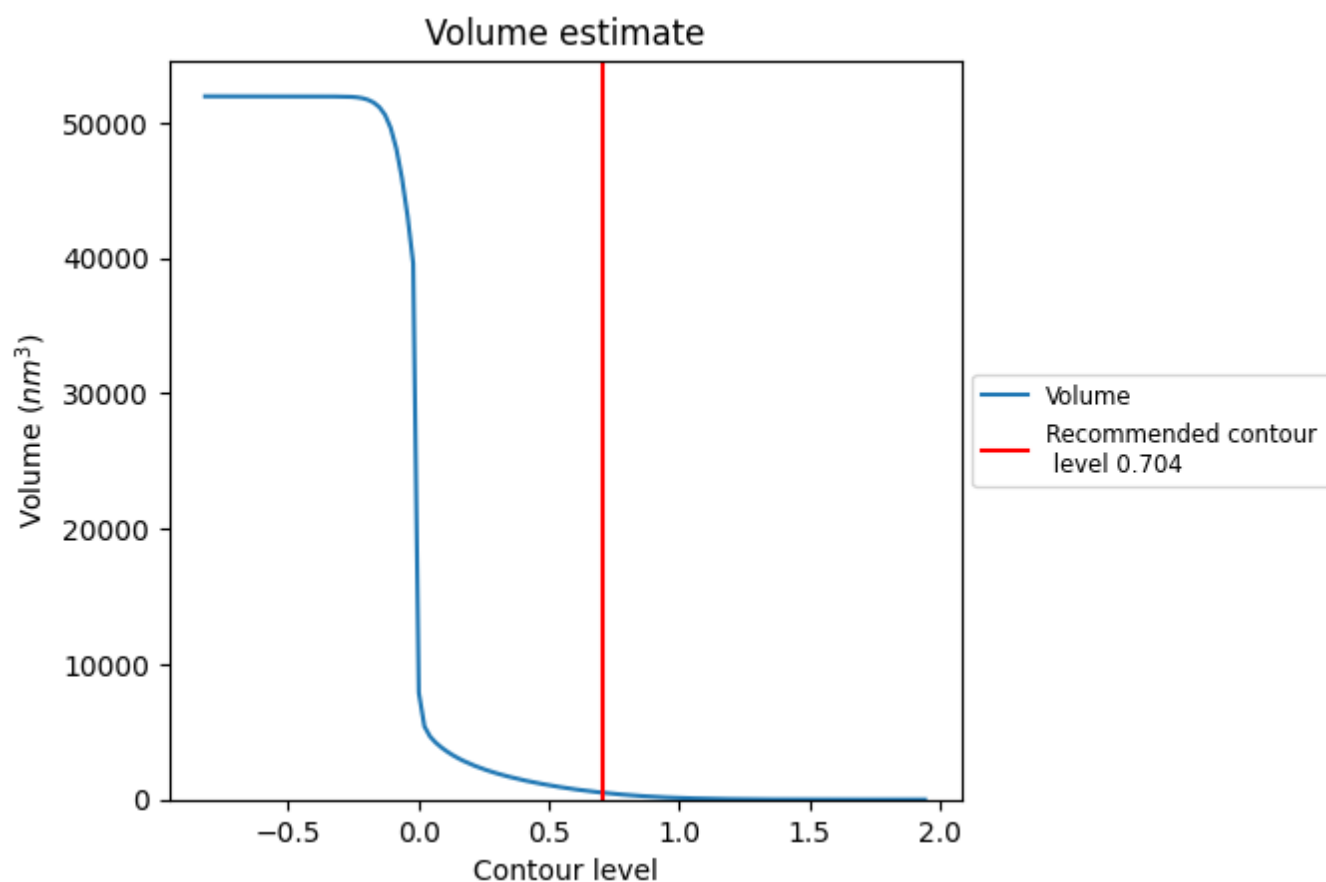
This section contains the results of statistical analysis of the map.

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.

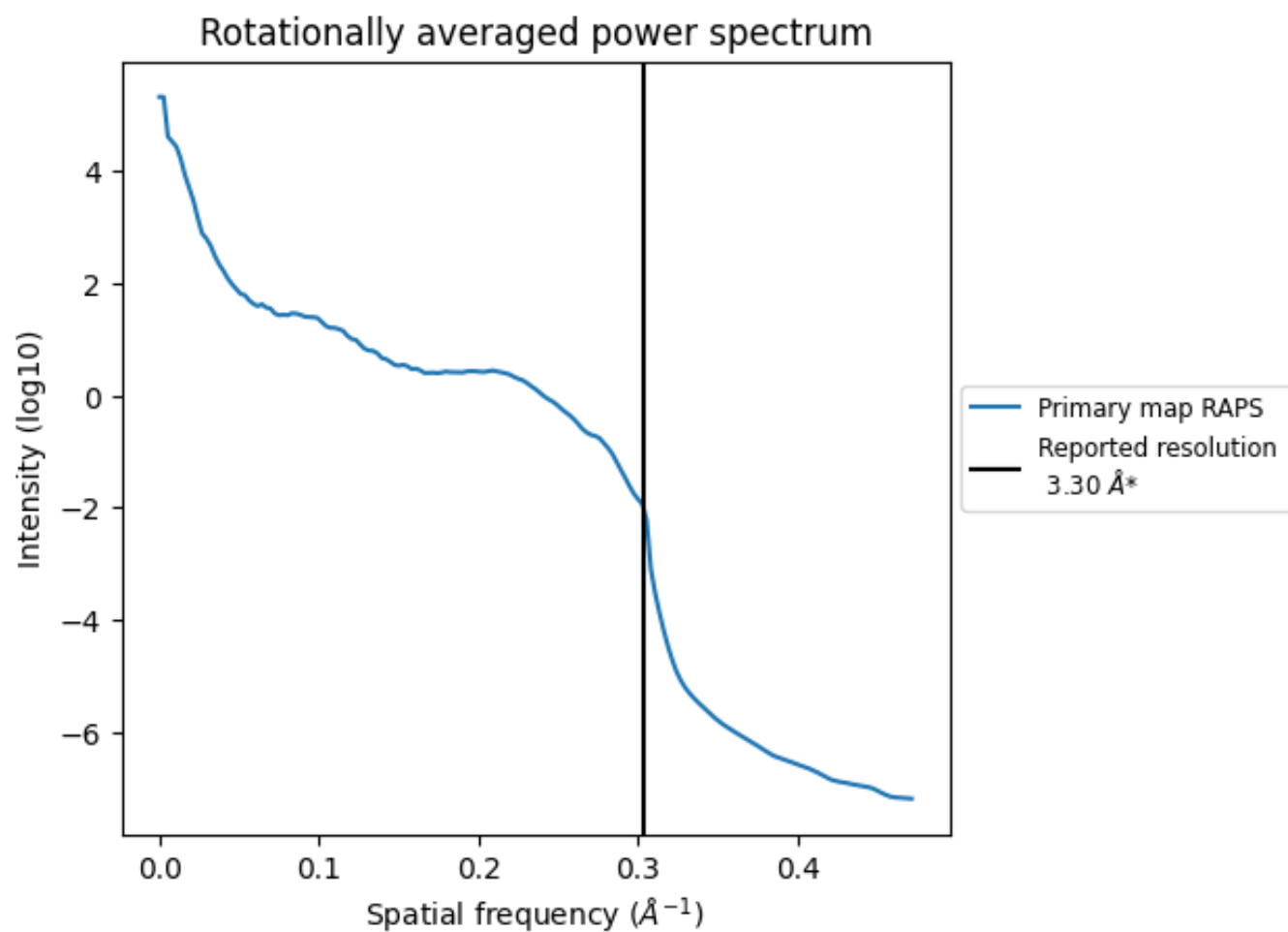
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 513 nm³; this corresponds to an approximate mass of 464 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⁻¹

8 Fourier-Shell correlation ⓘ

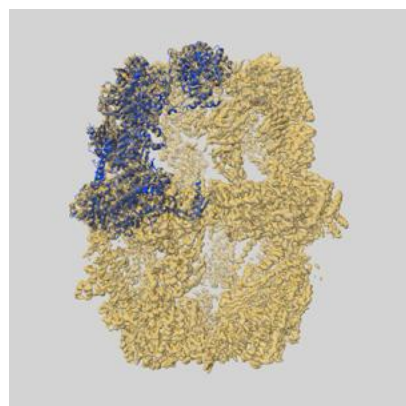
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

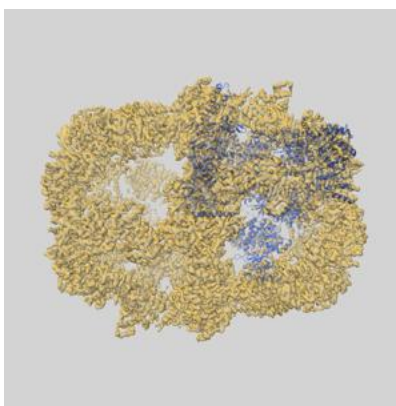
This section contains information regarding the fit between EMDB map EMD-20658 and PDB model 6U5W. Per-residue inclusion information can be found in section [3](#) on page [10](#).

9.1 Map-model overlays

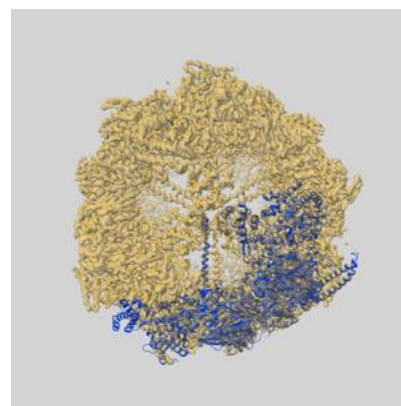
9.1.1 Map-model overlay [i](#)



X



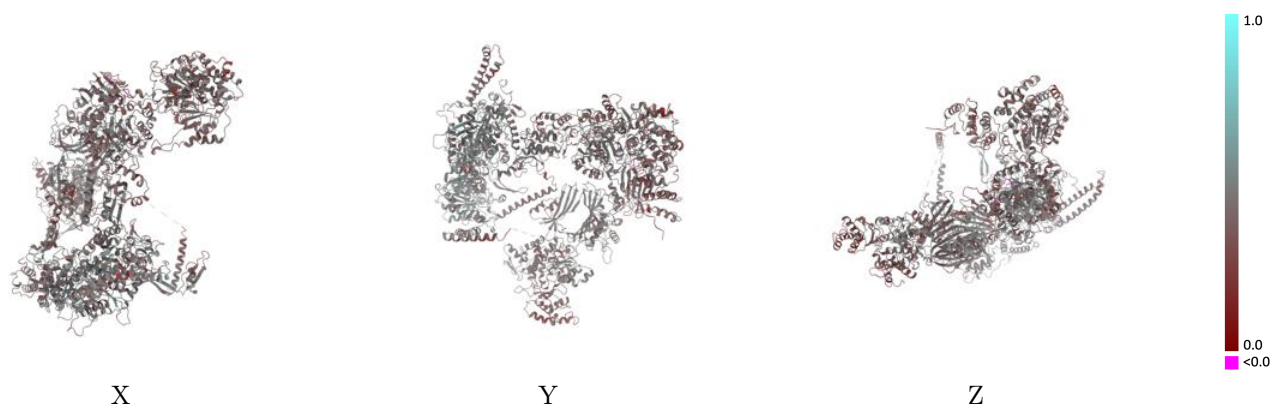
Y



Z

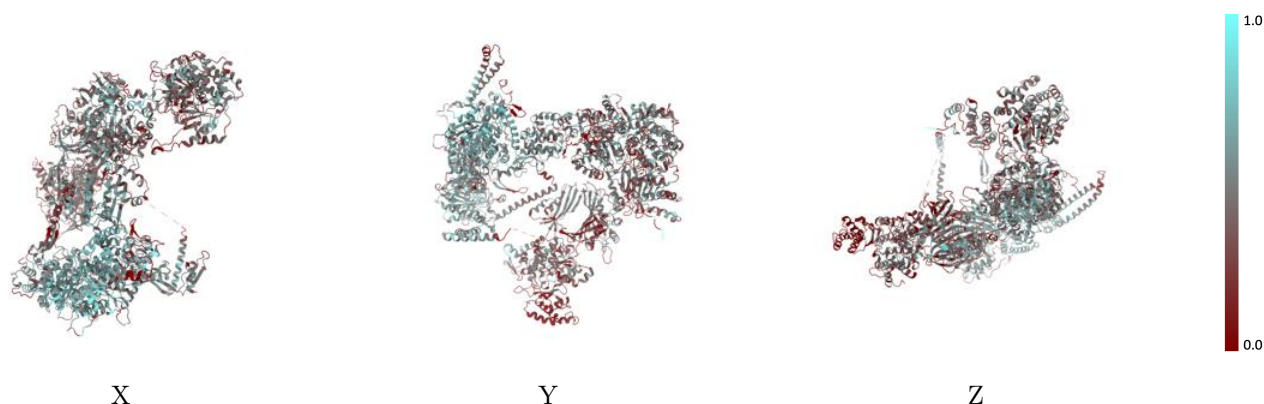
The images above show the 3D surface view of the map at the recommended contour level 0.704 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



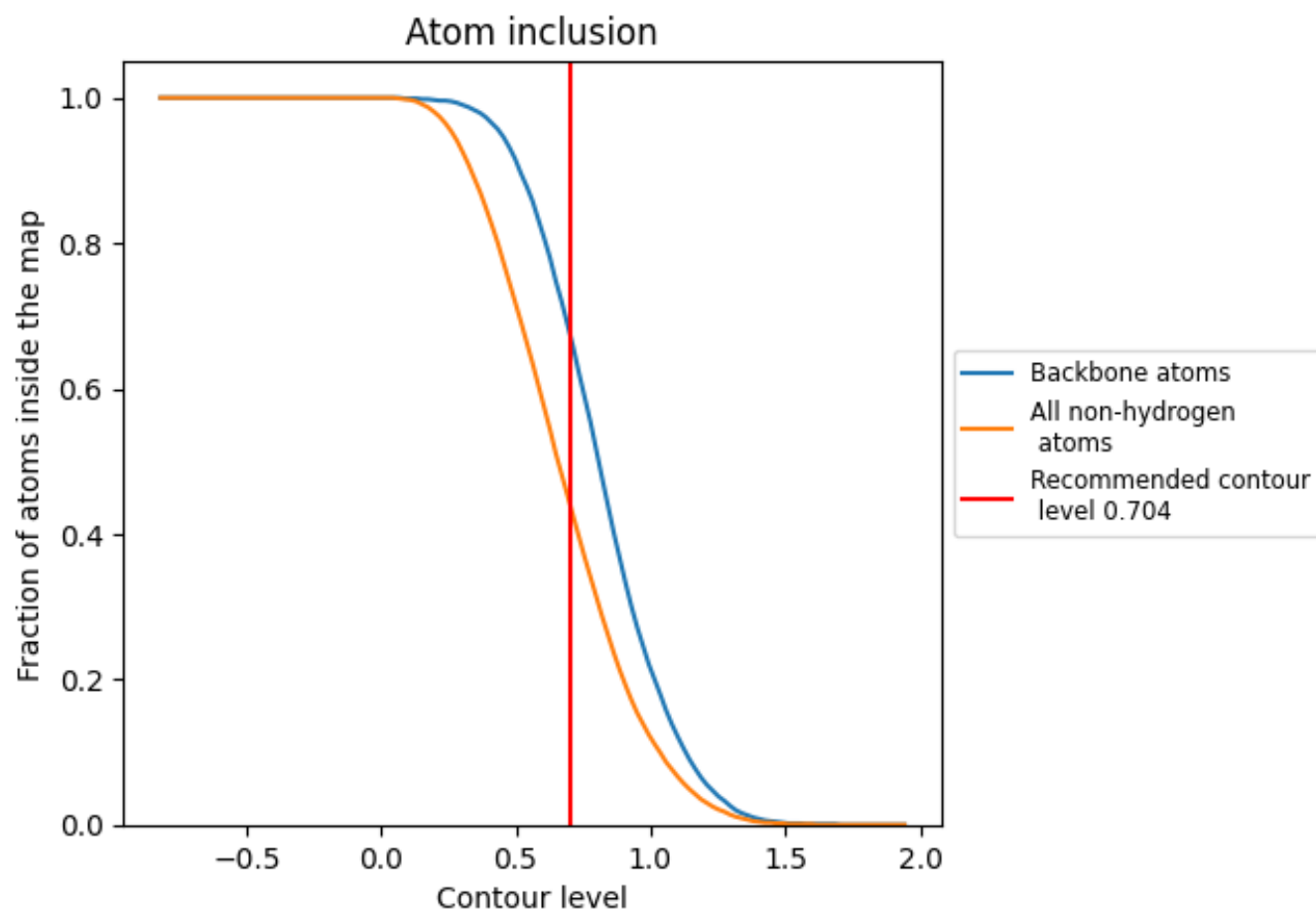
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.704).

9.4 Atom inclusion [i](#)



At the recommended contour level, 67% of all backbone atoms, 44% 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 (0.704) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4360	0.4280
A	0.5230	0.4560
B	0.3760	0.4080

