



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 12:44 AM UTC

PDB ID : 6XKV / pdb_00006xkv
EMDB ID : EMD-22226
Title : R. capsulatus cyt bc1 with both FeS proteins in b position (CIII2 b-b)
Authors : Steimle, S.; Van Eeuwen, T.; Ozturk, Y.; Kim, H.J.; Braitbard, M.; Selamoglu, N.; Garcia, B.A.; Schneidman-Duhovny, D.; Murakami, K.; Daldal, F.
Deposited on : 2020-06-27
Resolution : 3.50 Å(reported)
Based on initial model : 6XI0

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:

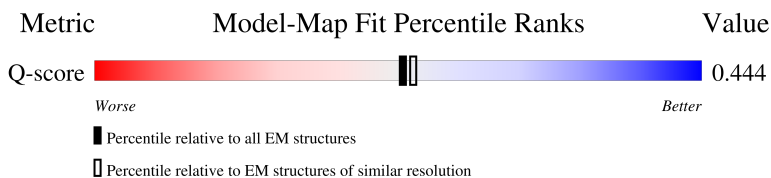
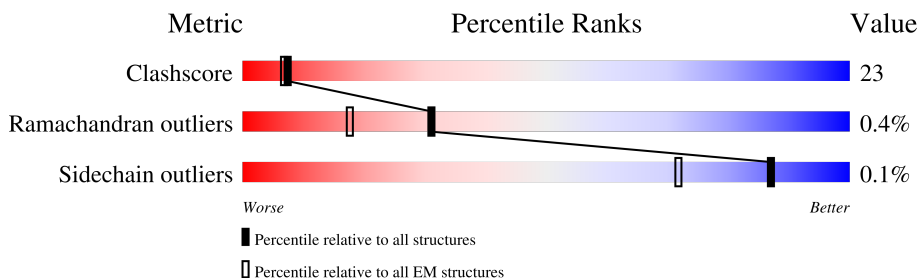
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.50 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	13950 (3.00 - 4.00)

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	C	437	 7% 76% 20% ..
1	P	437	 7% 75% 21% ..
2	D	279	 14% 63% 19% • 16%
2	Q	279	 13% 65% 18% • 16%

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Mol	Chain	Length	Quality of chain
3	E	191	75% 47% 47% • 5%
3	R	191	74% 49% 46% • 5%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13079 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 Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	423	Total	C	N	O	S	0	0
			3244	2186	519	525	14		
1	P	423	Total	C	N	O	S	0	0
			3244	2186	519	525	14		

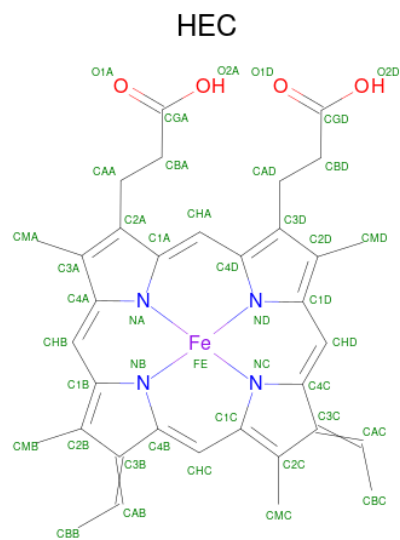
- Molecule 2 is a protein called Cytochrome c1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	235	Total	C	N	O	S	0	0
			1801	1148	301	337	15		
2	Q	235	Total	C	N	O	S	0	0
			1794	1144	300	335	15		

- Molecule 3 is a protein called Ubiquinol-cytochrome c reductase iron-sulfur subunit.

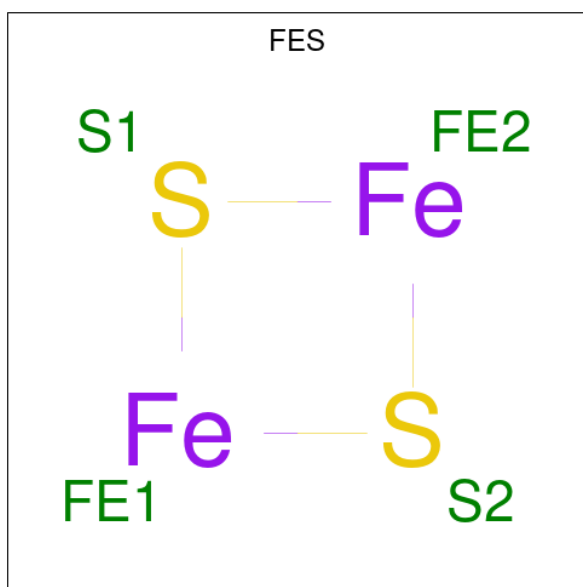
Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	181	Total	C	N	O	S	0	0
			1365	855	246	256	8		
3	R	181	Total	C	N	O	S	0	0
			1365	855	246	256	8		

- Molecule 4 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



Mol	Chain	Residues	Atoms					AltConf
4	C	1	Total 43	C 34	Fe 1	N 4	O 4	0
4	C	1	Total 43	C 34	Fe 1	N 4	O 4	0
4	D	1	Total 43	C 34	Fe 1	N 4	O 4	0
4	P	1	Total 43	C 34	Fe 1	N 4	O 4	0
4	P	1	Total 43	C 34	Fe 1	N 4	O 4	0
4	Q	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 5 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).

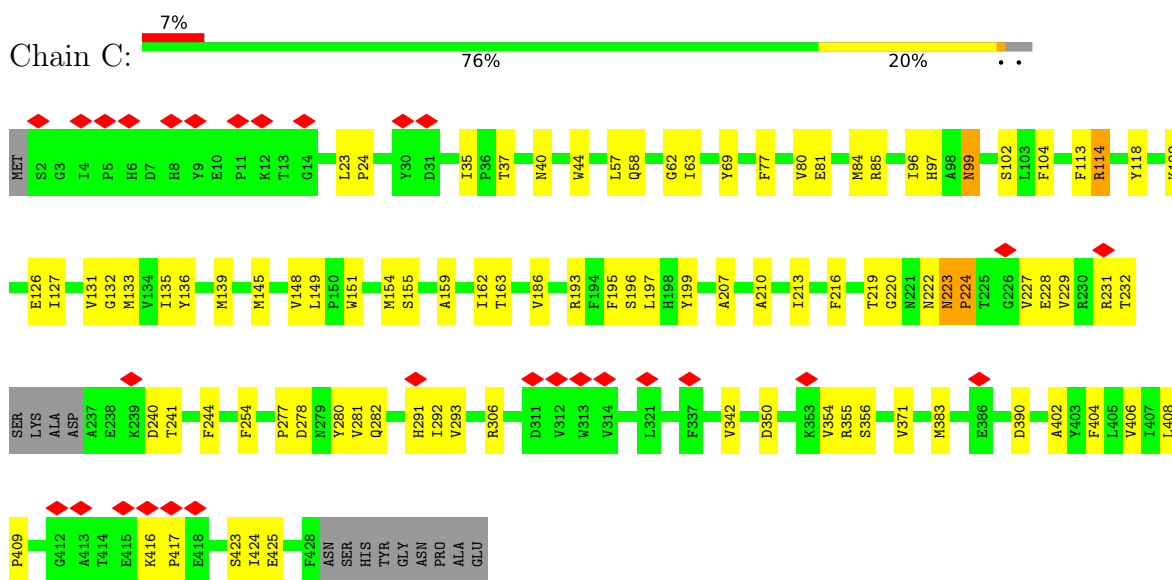


Mol	Chain	Residues	Atoms			AltConf
5	E	1	Total	Fe	S	0
			4	2	2	
5	R	1	Total	Fe	S	0
			4	2	2	

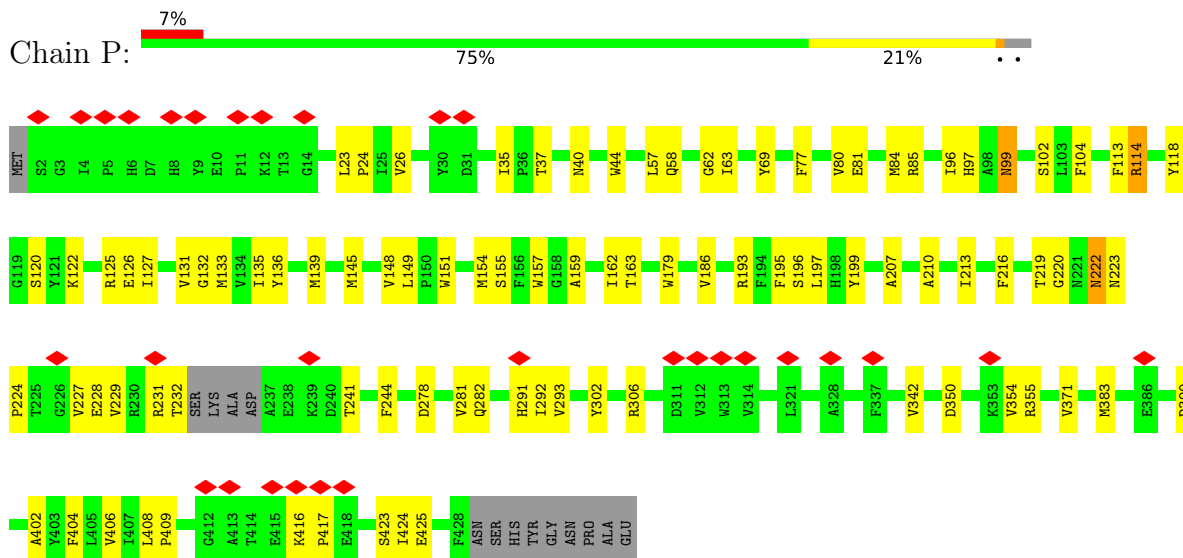
3 Residue-property plots

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.

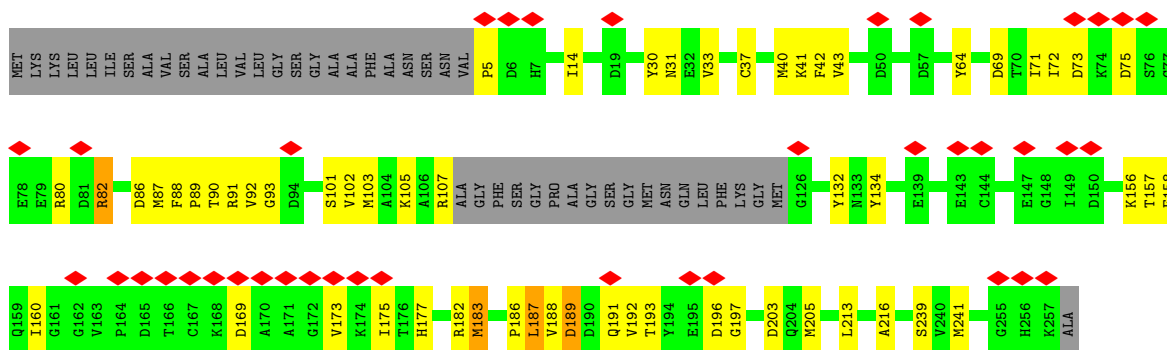
• Molecule 1: Cytochrome b



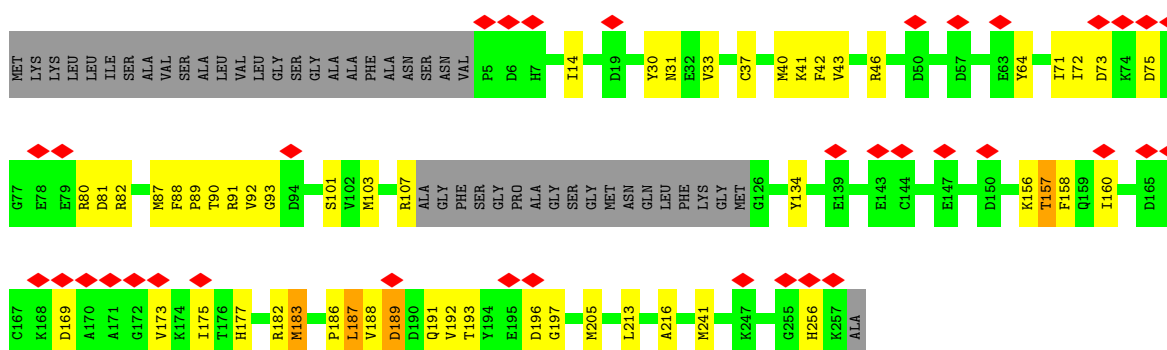
• Molecule 1: Cytochrome b



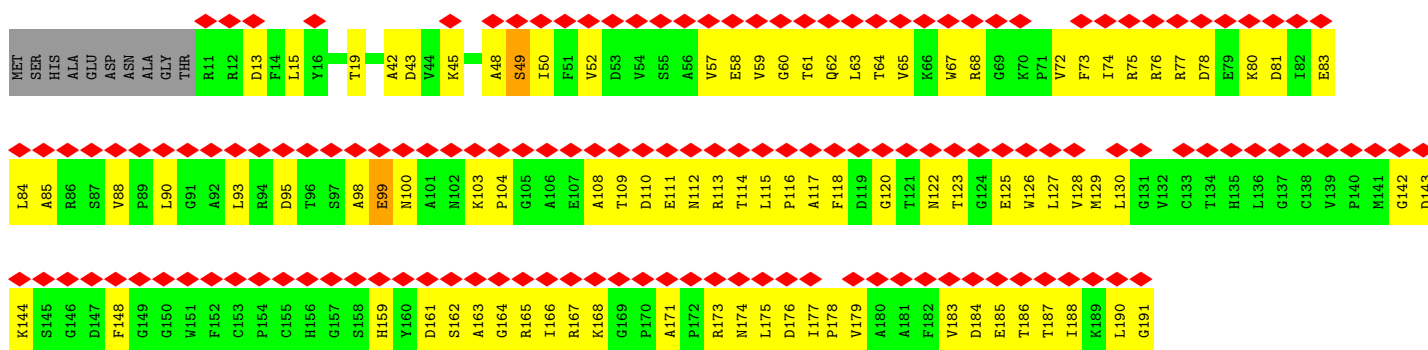
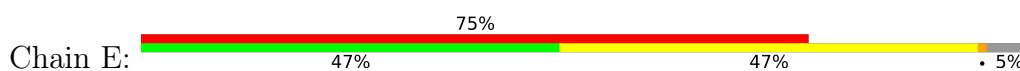
• Molecule 2: Cytochrome c1



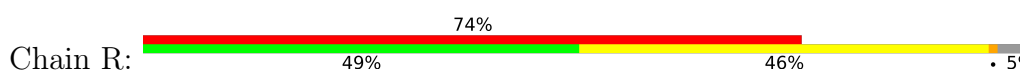
• Molecule 2: Cytochrome c1



• Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit



• Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit



D143	K144	S145	G146	D147	F148	G149	G150	W151	F152	C153	P154	C155	H156	G157	S158	H159	Y160	D161	S162	A163	G164	R165	I166	R167	K168	G169	P170	A171	P172	R173	N174	L175	D176	I177	P178	V179	A180	A181	F182	V183	D184	E185	T186	T187	I188	K189	L190	G191	E192	D193	S194	G195	P196	C197	H198	G199	P200	C201	H202	G203	P204	G205	E206	A207	I208	L209	P210	C211	H212	G213	P214	G215	E216	A217	I218	L219	P220	C221	H222	G223	P224	G225	E226	A227	I228	L229	P230	C231	H232	G233	P234	G235	E236	A237	I238	L239	P240	C241	H242	G243	P244	G245	E246	A247	I248	L249	P250	C251	H252	G253	P254	G255	E256	A257	I258	L259	P260	C261	H262	G263	P264	G265	E266	A267	I268	L269	P270	C271	H272	G273	P274	G275	E276	A277	I278	L279	P280	C281	H282	G283	P284	G285	E286	A287	I288	L289	P290	C291	H292	G293	P294	G295	E296	A297	I298	L299	P300	C301	H302	G303	P304	G305	E306	A307	I308	L309	P310	C311	H312	G313	P314	G315	E316	A317	I318	L319	P320	C321	H322	G323	P324	G325	E326	A327	I328	L329	P330	C331	H332	G333	P334	G335	E336	A337	I338	L339	P340	C341	H342	G343	P344	G345	E346	A347	I348	L349	P350	C351	H352	G353	P354	G355	E356	A357	I358	L359	P360	C361	H362	G363	P364	G365	E366	A367	I368	L369	P370	C371	H372	G373	P374	G375	E376	A377	I378	L379	P380	C381	H382	G383	P384	G385	E386	A387	I388	L389	P390	C391	H392	G393	P394	G395	E396	A397	I398	L399	P400	C401	H402	G403	P404	G405	E406	A407	I408	L409	P410	C411	H412	G413	P414	G415	E416	A417	I418	L419	P420	C421	H422	G423	P424	G425	E426	A427	I428	L429	P430	C431	H432	G433	P434	G435	E436	A437	I438	L439	P440	C441	H442	G443	P444	G445	E446	A447	I448	L449	P450	C451	H452	G453	P454	G455	E456	A457	I458	L459	P460	C461	H462	G463	P464	G465	E466	A467	I468	L469	P470	C471	H472	G473	P474	G475	E476	A477	I478	L479	P480	C481	H482	G483	P484	G485	E486	A487	I488	L489	P490	C491	H492	G493	P494	G495	E496	A497	I498	L499	P500	C501	H502	G503	P504	G505	E506	A507	I508	L509	P510	C511	H512	G513	P514	G515	E516	A517	I518	L519	P520	C521	H522	G523	P524	G525	E526	A527	I528	L529	P530	C531	H532	G533	P534	G535	E536	A537	I538	L539	P540	C541	H542	G543	P544	G545	E546	A547	I548	L549	P550	C551	H552	G553	P554	G555	E556	A557	I558	L559	P560	C561	H562	G563	P564	G565	E566	A567	I568	L569	P570	C571	H572	G573	P574	G575	E576	A577	I578	L579	P580	C581	H582	G583	P584	G585	E586	A587	I588	L589	P590	C591	H592	G593	P594	G595	E596	A597	I598	L599	P600	C601	H602	G603	P604	G605	E606	A607	I608	L609	P610	C611	H612	G613	P614	G615	E616	A617	I618	L619	P620	C621	H622	G623	P624	G625	E626	A627	I628	L629	P630	C631	H632	G633	P634	G635	E636	A637	I638	L639	P640	C641	H642	G643	P644	G645	E646	A647	I648	L649	P650	C651	H652	G653	P654	G655	E656	A657	I658	L659	P660	C661	H662	G663	P664	G665	E666	A667	I668	L669	P670	C671	H672	G673	P674	G675	E676	A677	I678	L679	P680	C681	H682	G683	P684	G685	E686	A687	I688	L689	P690	C691	H692	G693	P694	G695	E696	A697	I698	L699	P700	C701	H702	G703	P704	G705	E706	A707	I708	L709	P710	C711	H712	G713	P714	G715	E716	A717	I718	L719	P720	C721	H722	G723	P724	G725	E726	A727	I728	L729	P730	C731	H732	G733	P734	G735	E736	A737	I738	L739	P740	C741	H742	G743	P744	G745	E746	A747	I748	L749	P750	C751	H752	G753	P754	G755	E756	A757	I758	L759	P760	C761	H762	G763	P764	G765	E766	A767	I768	L769	P770	C771	H772	G773	P774	G775	E776	A777	I778	L779	P780	C781	H782	G783	P784	G785	E786	A787	I788	L789	P790	C791	H792	G793	P794	G795	E796	A797	I798	L799	P800	C801	H802	G803	P804	G805	E806	A807	I808	L809	P810	C811	H812	G813	P814	G815	E816	A817	I818	L819	P820	C821	H822	G823	P824	G825	E826	A827	I828	L829	P830	C831	H832	G833	P834	G835	E836	A837	I838	L839	P840	C841	H842	G843	P844	G845	E846	A847	I848	L849	P850	C851	H852	G853	P854	G855	E856	A857	I858	L859	P860	C861	H862	G863	P864	G865	E866	A867	I868	L869	P870	C871	H872	G873	P874	G875	E876	A877	I878	L879	P880	C881	H882	G883	P884	G885	E886	A887	I888	L889	P890	C891	H892	G893	P894	G895	E896	A897	I898	L899	P900	C901	H902	G903	P904	G905	E906	A907	I908	L909	P910	C911	H912	G913	P914	G915	E916	A917	I918	L919	P920	C921	H922	G923	P924	G925	E926	A927	I928	L929	P930	C931	H932	G933	P934	G935	E936	A937	I938	L939	P940	C941	H942	G943	P944	G945	E946	A947	I948	L949	P950	C951	H952	G953	P954	G955	E956	A957	I958	L959	P960	C961	H962	G963	P964	G965	E966	A967	I968	L969	P970	C971	H972	G973	P974	G975	E976	A977	I978	L979	P980	C981	H982	G983	P984	G985	E986	A987	I988	L989	P990	C991	H992	G993	P994	G995	E996	A997	I998	L999	P1000	C1001	H1002	G1003	P1004	G1005	E1006	A1007	I1008	L1009	P1010	C1011	H1012	G1013	P1014	G1015	E1016	A1017	I1018	L1019	P1020	C1021	H1022	G1023	P1024	G1025	E1026	A1027	I1028	L1029	P1030	C1031	H1032	G1033	P1034	G1035	E1036	A1037	I1038	L1039	P1040	C1041	H1042	G1043	P1044	G1045	E1046	A1047	I1048	L1049	P1050	C1051	H1052	G1053	P1054	G1055	E1056	A1057	I1058	L1059	P1060	C1061	H1062	G1063	P1064	G1065	E1066	A1067	I1068	L1069	P1070	C1071	H1072	G1073	P1074	G1075	E1076	A1077	I1078	L1079	P1080	C1081	H1082	G1083	P1084	G1085	E1086	A1087	I1088	L1089	P1090	C1091	H1092	G1093	P1094	G1095	E1096	A1097	I1098	L1099	P1100	C1101	H1102	G1103	P1104	G1105	E1106	A1107	I1108	L1109	P1110	C1111	H1112	G1113	P1114	G1115	E1116	A1117	I1118	L1119	P1120	C1121	H1122	G1123	P1124	G1125	E1126	A1127	I1128	L1129	P1130	C1131	H1132	G1133	P1134	G1135	E1136	A1137	I1138	L1139	P1140	C1141	H1142	G1143	P1144	G1145	E1146	A1147	I1148	L1149	P1150	C1151	H1152	G1153	P1154	G1155	E1156	A1157	I1158	L1159	P1160	C1161	H1162	G1163	P1164	G1165	E1166	A1167	I1168	L1169	P1170	C1171	H1172	G1173	P1174	G1175	E1176	A1177	I1178	L1179	P1180	C1181	H1182	G1183	P1184	G1185	E1186	A1187	I1188	L1189	P1190	C1191	H1192	G1193	P1194	G1195	E1196	A1197	I1198	L1199	P1200	C1201	H1202	G1203	P1204	G1205	E1206	A1207	I1208	L1209	P1210	C1211	H1212	G1213	P1214	G1215	E1216	A1217	I1218	L1219	P1220	C1221	H1222	G1223	P1224	G1225	E1226	A1227	I1228	L1229	P1230	C1231	H1232	G1233	P1234	G1235	E1236	A1237	I1238	L1239	P1240	C1241	H1242	G1243	P1244	G1245	E1246	A1247	I1248	L1249	P1250	C1251	H1252	G1253	P1254	G1255	E1256	A1257	I1258	L1259	P1260	C1261	H1262	G1263	P1264	G1265	E1266	A1267	I1268	L1269	P1270	C1271	H1272	G1273	P1274	G1275	E1276	A1277	I1278	L1279	P1280	C1281	H1282	G1283	P1284	G1285	E1286	A1287	I1288	L1289	P1290	C1291	H1292	G1293	P1294	G1295	E1296	A1297	I1298	L1299	P1300	C1301	H1302	G1303	P1304	G1305	E1306	A1307	I1308	L1309	P1310	C1311	H1312	G1313	P1314	G1315	E1316	A1317	I1318	L1319	P1320	C1321	H1322	G1323	P1324	G1325	E1326	A1327	I1328	L1329	P1330	C1331	H1332	G1333	P1334	G1335	E1336	A1337	I1338	L1339	P1340	C1341	H1342	G1343	P1344	G1345	E1346	A1347	I1348	L1349	P1350	C1351	H1352	G1353	P1354	G1355	E1356	A1357	I1358	L1359	P1360	C1361	H1362	G1363	P1364	G1365	E1366	A1367	I1368	L1369	P1370	C1371	H1372	G1373	P1374	G1375	E1376	A1377	I1378	L1379	P1380	C1381	H1382	G1383	P1384	G1385	E1386	A1387	I1388	L1389	P1390	C1391	H1392	G1393	P1394	G1395	E1396	A1397	I1398	L1399	P1400	C1401	H1402	G1403	P1404	G1405	E1406	A1407	I1408	L1409	P1410	C1411	H1412	G1413	P1414	G1415	E1416	A1417	I1418	L1419	P1420	C1421	H1422	G1423	P1424	G1425	E1426	A1427	I1428	L1429	P1430	C1431	H1432	G1433	P1434	G1435	E1436	A1437	I1438	L1439	P1440	C1441	H1442	G1443	P1444	G1445	E1446	A1447	I1448	L1449	P1450	C1451	H1452	G1453	P1454	G1455	E1456	A1457	I1458	L1459	P1460	C1461	H1462	G1463	P1464	G1465	E1466	A1467	I1468	L1469	P1470	C1471	H1472	G1473	P1474	G1475	E1476	A1477	I1478	L1479	P1480	C1481	H1482	G1483	P1484	G1485	E1486	A1487	I1488	L1489	P1490	C1491	H1492	G1493	P1494	G1495	E1496	A1497	I1498	L1499	P1500	C1501	H1502	G1503	P1504	G1505	E1506	A1507	I1508	L1509	P1510	C1511	H1512	G1513	P1514	G1515	E1516	A1517	I1518	L1519	P1520	C1521	H1522	G1523	P1524	G1525	E1526	A1527	I1528	L1529	P1530	C1531	H1532	G1533	P1534	G1535	E1536	A1537	I1538	L1539	P1540	C1541	H1542	G1543	P1544	G1545	E1546	A1547	I1548	L1549	P1550	C1551	H1552	G1553	P1554	G1555	E1556	A1557	I1558	L1559	P1560	C1561	H1562	G1563	P1564	G1565	E1566	A1567	I1568	L1569	P1570	C1571	H1572	G1573	P1574	G1575	E1576	A1577	I1578	L1579	P1580	C1581	H1582	G1583	P1584	G1585	E1586	A1587	I1588	L1589	P1590	C1591	H1592	G1593	P1594	G1595	E1596	A1597	I1598	L1599	P1600	C1601	H1602	G1603	P1604	G1605	E1606	A1607	I1608	L1609	P1610	C1611	H1612	G161
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	37710	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.244	Depositor
Minimum map value	-0.162	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.048	Depositor
Map size ($\text{\AA}$)	326.4, 326.4, 326.4	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.36, 1.36, 1.36	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: HEC, FES

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	C	0.37	0/3363	0.61	7/4617 (0.2%)
1	P	0.37	0/3363	0.62	8/4617 (0.2%)
2	D	0.28	0/1846	0.60	6/2500 (0.2%)
2	Q	0.28	0/1839	0.59	5/2492 (0.2%)
3	E	0.34	0/1395	0.65	1/1895 (0.1%)
3	R	0.35	0/1395	0.67	1/1895 (0.1%)
All	All	0.34	0/13201	0.62	28/18016 (0.2%)

There are no bond length outliers.

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	222	ASN	N-CA-C	9.92	121.69	111.07
3	R	49	SER	N-CA-C	9.39	124.97	110.42
3	E	49	SER	N-CA-C	8.48	121.47	110.53
2	D	183	MET	CA-C-N	-8.09	112.04	120.38
2	D	183	MET	C-N-CA	-8.09	112.04	120.38

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	C	3244	0	3072	93	0
1	P	3244	0	3072	98	0
2	D	1801	0	1722	84	0
2	Q	1794	0	1709	80	0
3	E	1365	0	1340	138	0
3	R	1365	0	1340	131	0
4	C	86	0	64	15	0
4	D	43	0	30	5	0
4	P	86	0	64	16	0
4	Q	43	0	30	5	0
5	E	4	0	0	0	0
5	R	4	0	0	0	0
All	All	13079	0	12443	592	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 23.

The worst 5 of 592 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:40:ASN:O	1:C:224:PRO:HG2	1.44	1.18
2:D:188:VAL:HG12	2:D:189:ASP:H	0.98	1.14
3:R:183:VAL:HB	3:R:187:THR:HB	1.30	1.12
2:Q:188:VAL:HG12	2:Q:189:ASP:H	0.98	1.11
3:E:183:VAL:HB	3:E:187:THR:HB	1.31	1.11

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	C	419/437 (96%)	352 (84%)	65 (16%)	2 (0%)	24 57

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	P	419/437 (96%)	352 (84%)	66 (16%)	1 (0%)	43	74
2	D	231/279 (83%)	197 (85%)	34 (15%)	0	100	100
2	Q	231/279 (83%)	197 (85%)	34 (15%)	0	100	100
3	E	179/191 (94%)	141 (79%)	36 (20%)	2 (1%)	11	43
3	R	179/191 (94%)	140 (78%)	37 (21%)	2 (1%)	11	43
All	All	1658/1814 (91%)	1379 (83%)	272 (16%)	7 (0%)	31	62

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	99	GLU
3	R	99	GLU
3	E	144	LYS
3	R	144	LYS
1	C	223	ASN

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	C	300/360 (83%)	299 (100%)	1 (0%)	86	83
1	P	301/360 (84%)	301 (100%)	0	100	100
2	D	184/220 (84%)	184 (100%)	0	100	100
2	Q	182/220 (83%)	182 (100%)	0	100	100
3	E	142/149 (95%)	142 (100%)	0	100	100
3	R	142/149 (95%)	142 (100%)	0	100	100
All	All	1251/1458 (86%)	1250 (100%)	1 (0%)	87	87

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	224	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
3	R	100	ASN
3	E	122	ASN
1	P	221	ASN
3	E	17	HIS
1	P	68	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 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	$\# Z > 2$
4	HEC	C	502	1	46,50,50	1.87	8 (17%)	58,82,82	1.06	2 (3%)
4	HEC	C	501	1	46,50,50	1.87	8 (17%)	58,82,82	1.11	4 (6%)
5	FES	E	501	3	0,4,4	-	-	-		
4	HEC	Q	501	2	46,50,50	1.85	6 (13%)	58,82,82	1.69	3 (5%)
4	HEC	P	501	1	46,50,50	1.86	8 (17%)	58,82,82	1.11	4 (6%)
5	FES	R	501	3	0,4,4	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	HEC	D	501	2	46,50,50	1.85	6 (13%)	58,82,82	1.69	3 (5%)
4	HEC	P	502	1	46,50,50	1.88	8 (17%)	58,82,82	1.07	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
4	HEC	C	502	1	-	7/14/54/54	-
4	HEC	C	501	1	-	8/14/54/54	-
5	FES	E	501	3	-	-	0/1/1/1
4	HEC	Q	501	2	-	6/14/54/54	-
4	HEC	P	501	1	-	8/14/54/54	-
5	FES	R	501	3	-	-	0/1/1/1
4	HEC	D	501	2	-	6/14/54/54	-
4	HEC	P	502	1	-	7/14/54/54	-

The worst 5 of 44 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	502	HEC	CAB-C3B	6.43	1.55	1.35
4	P	502	HEC	CAB-C3B	6.42	1.55	1.35
4	D	501	HEC	CAC-C3C	6.34	1.55	1.35
4	Q	501	HEC	CAC-C3C	6.33	1.55	1.35
4	C	502	HEC	CAC-C3C	6.31	1.55	1.35

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	501	HEC	CBB-CAB-C3B	-7.73	111.99	127.43
4	Q	501	HEC	CBB-CAB-C3B	-7.72	112.00	127.43
4	D	501	HEC	CBC-CAC-C3C	-6.34	114.77	127.43
4	Q	501	HEC	CBC-CAC-C3C	-6.33	114.79	127.43
4	D	501	HEC	C4D-ND-C1D	3.29	111.18	105.82

There are no chirality outliers.

5 of 42 torsion outliers are listed below:

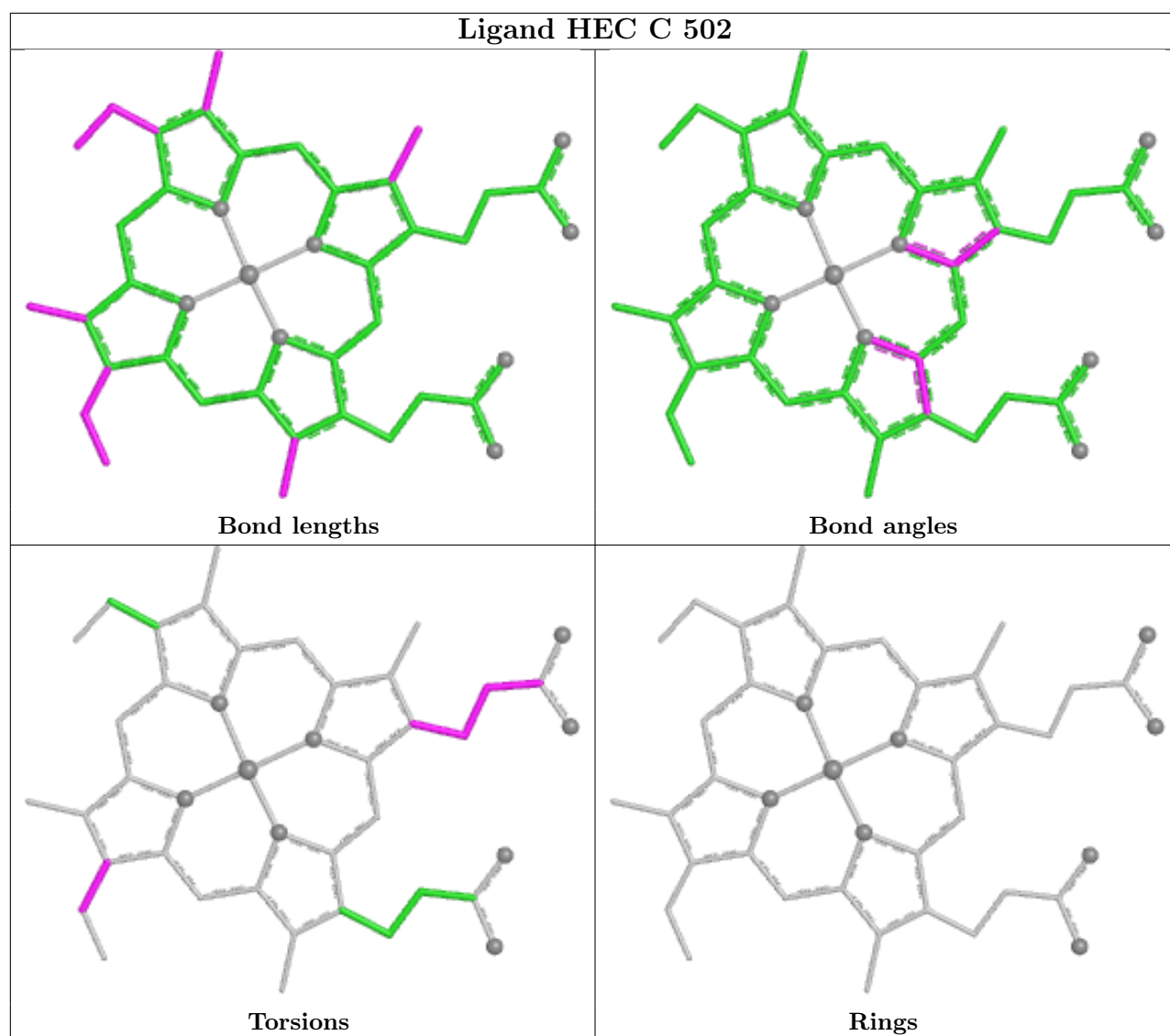
Mol	Chain	Res	Type	Atoms
4	C	501	HEC	C2B-C3B-CAB-CBB
4	C	501	HEC	C4B-C3B-CAB-CBB
4	C	501	HEC	C2C-C3C-CAC-CBC
4	C	501	HEC	C4C-C3C-CAC-CBC
4	C	502	HEC	C2C-C3C-CAC-CBC

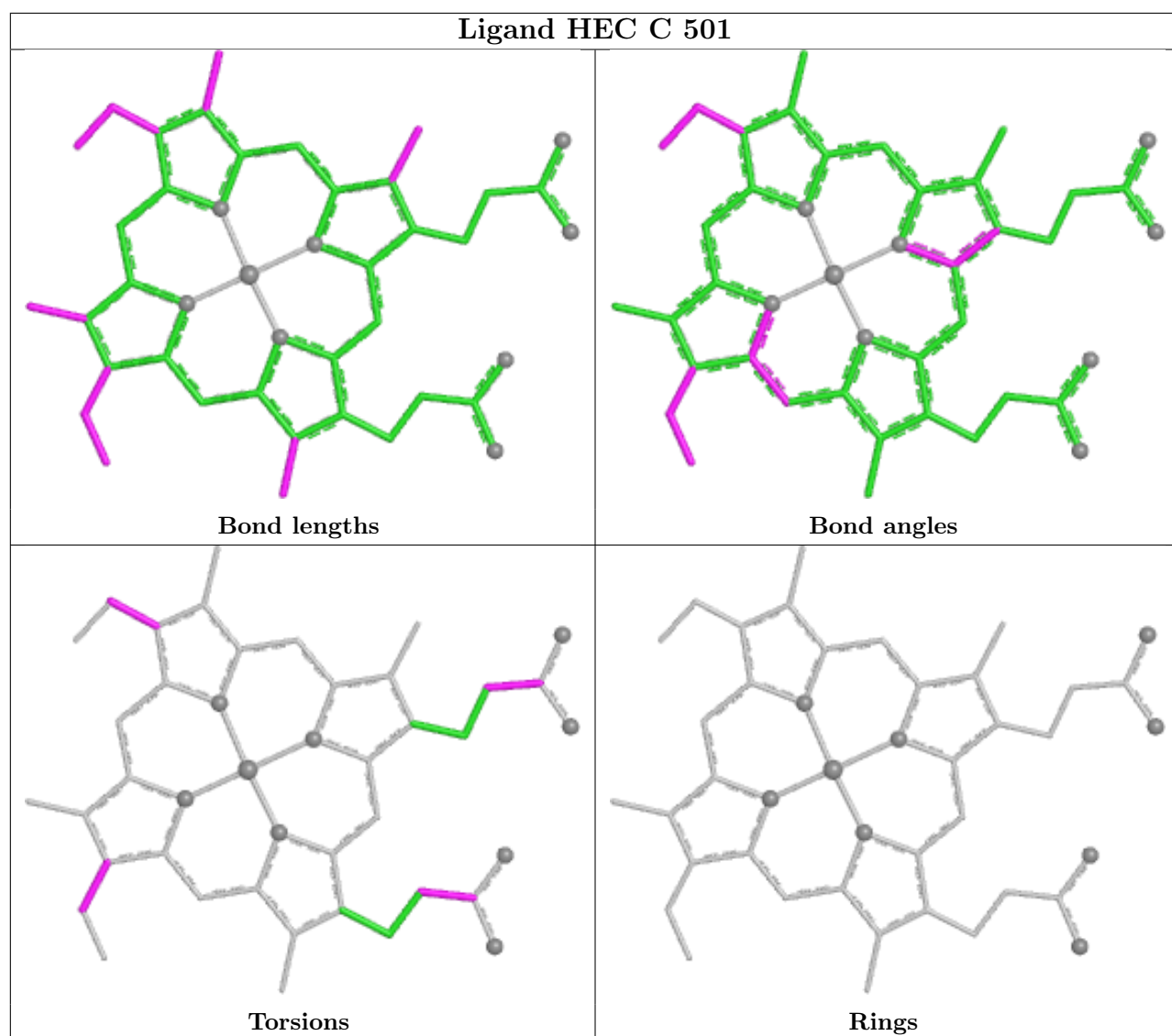
There are no ring outliers.

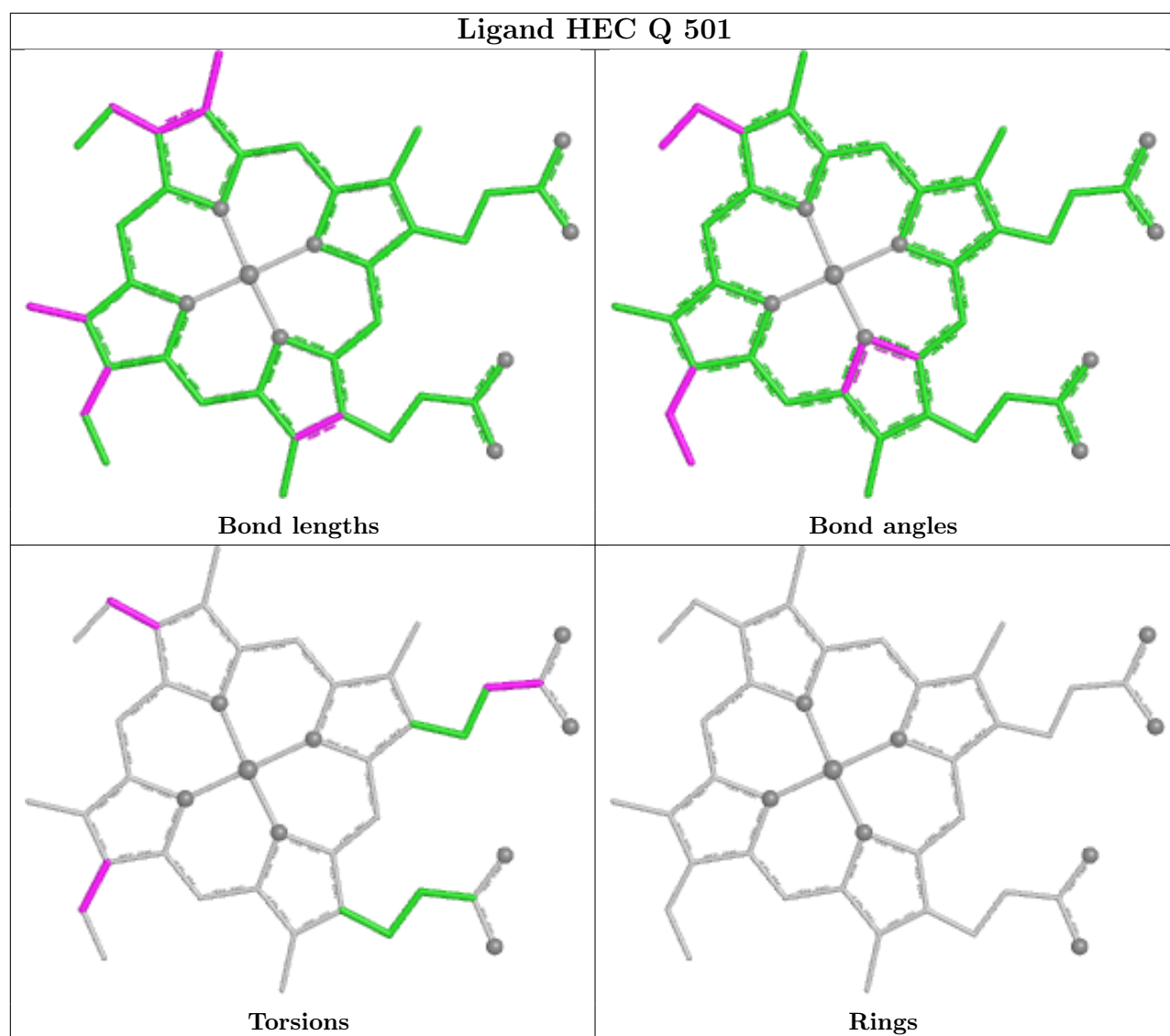
6 monomers are involved in 41 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	502	HEC	3	0
4	C	501	HEC	12	0
4	Q	501	HEC	5	0
4	P	501	HEC	13	0
4	D	501	HEC	5	0
4	P	502	HEC	3	0

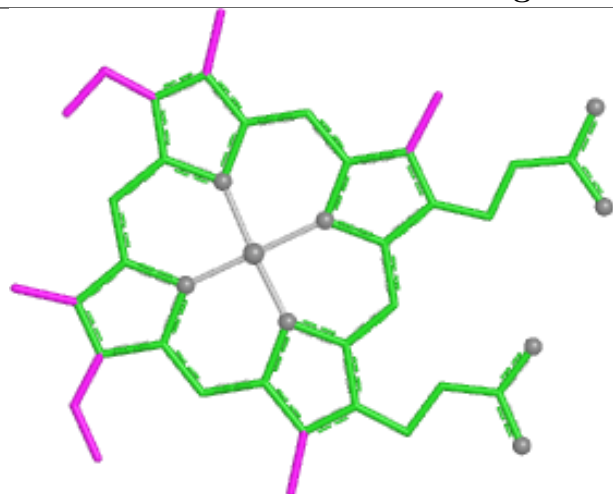
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



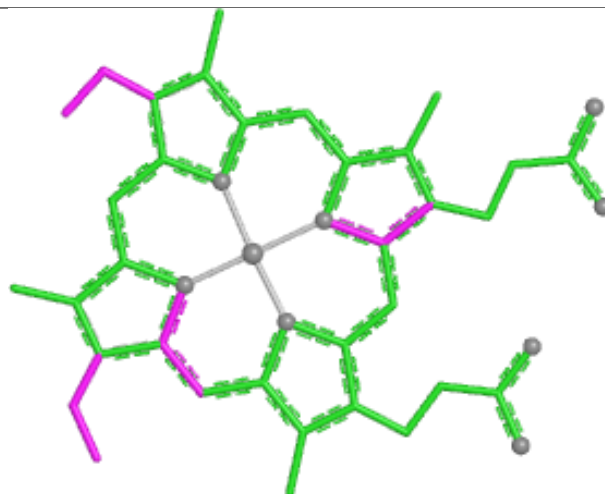




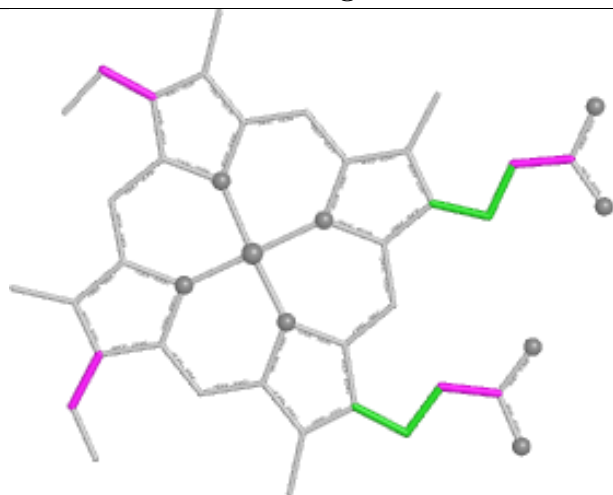
Ligand HEC P 501



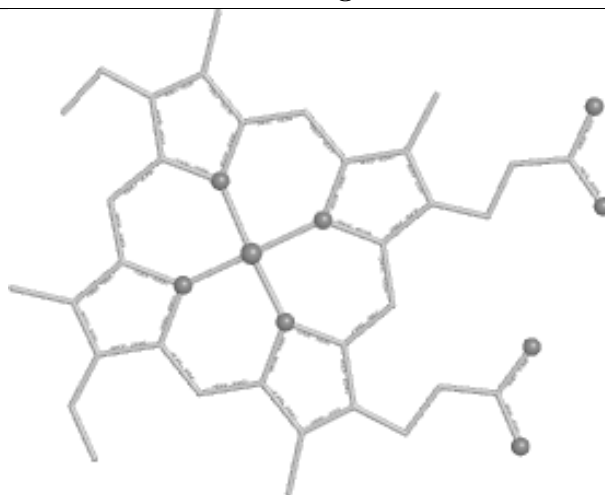
Bond lengths



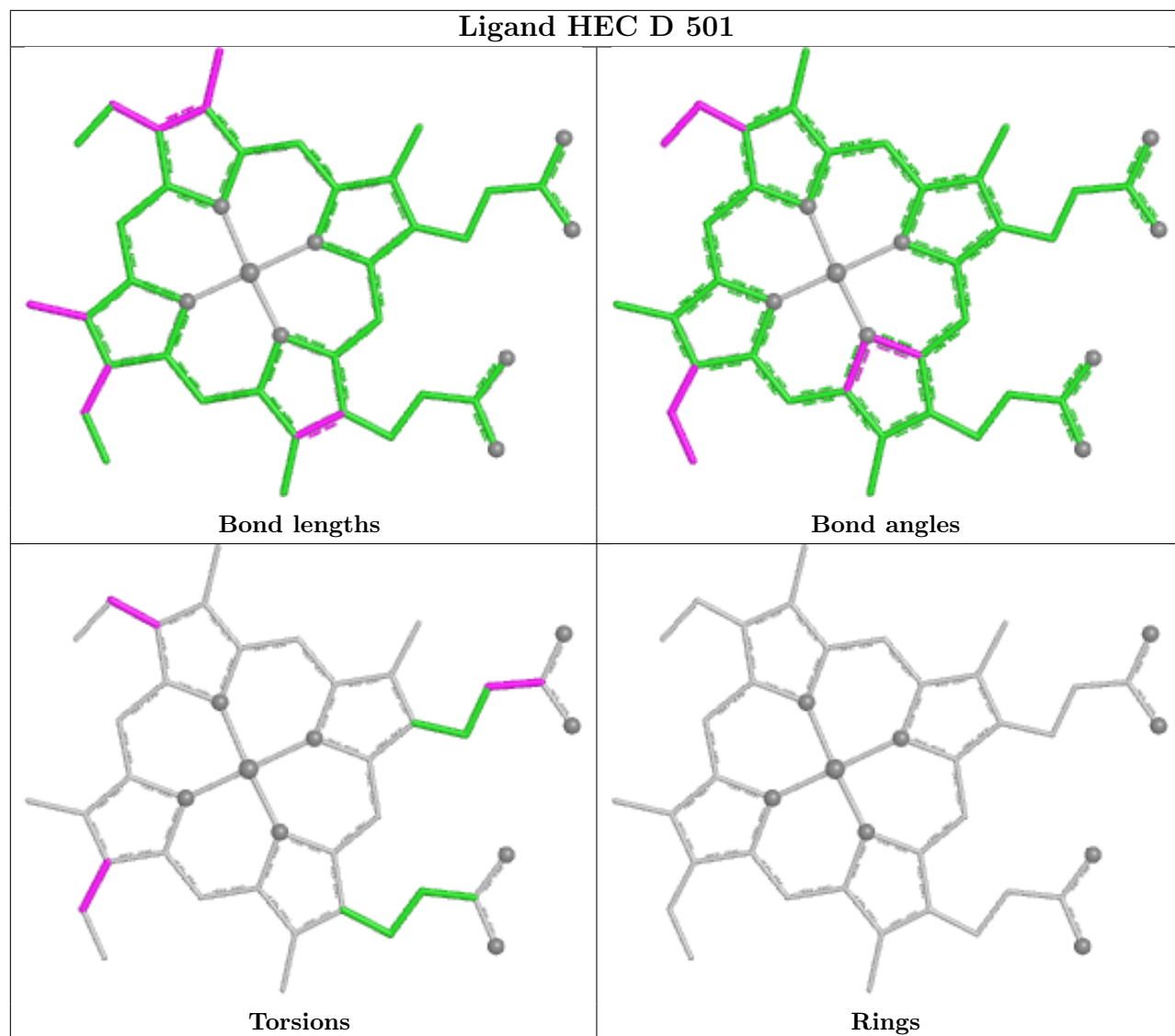
Bond angles

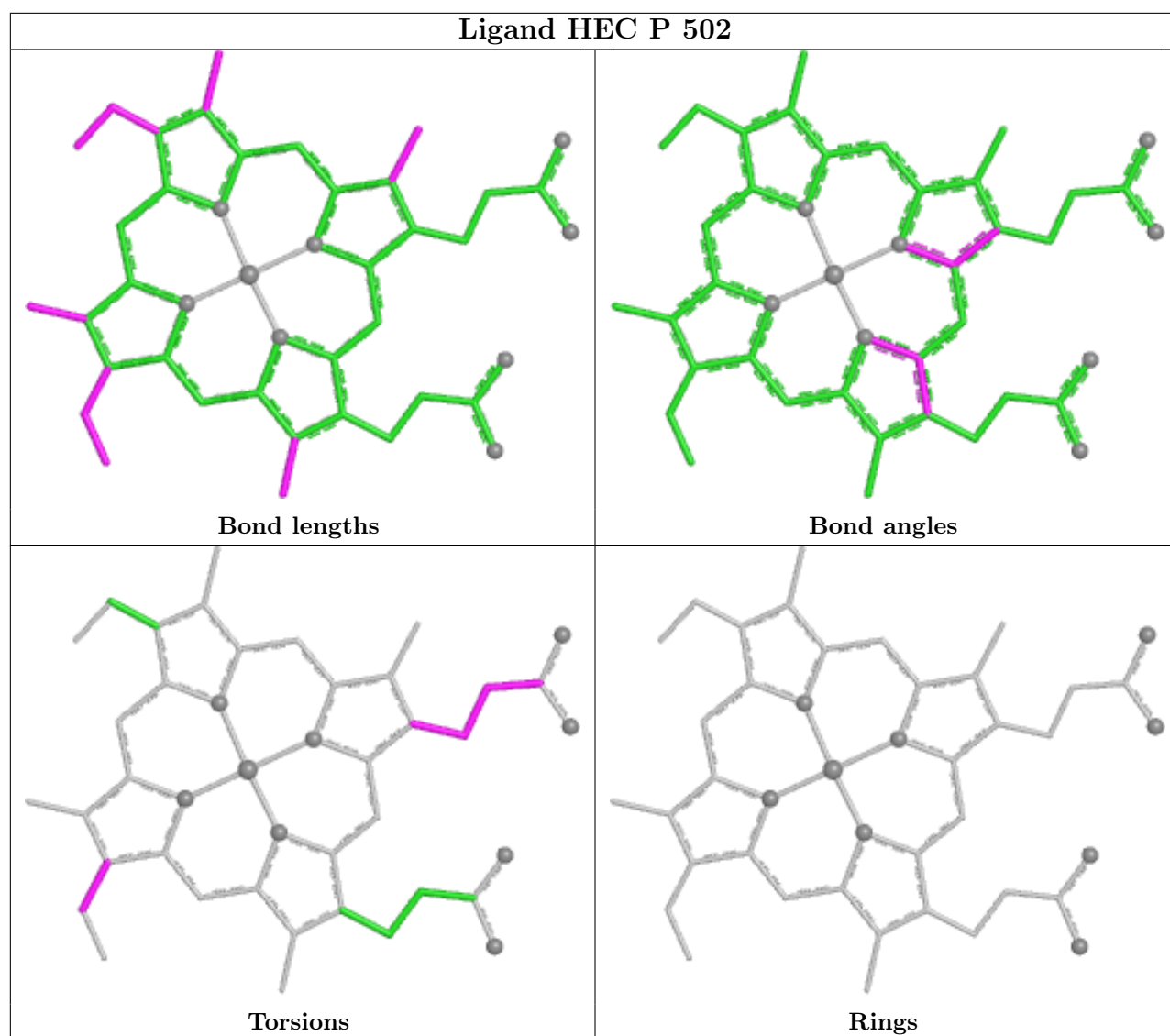


Torsions



Rings





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.

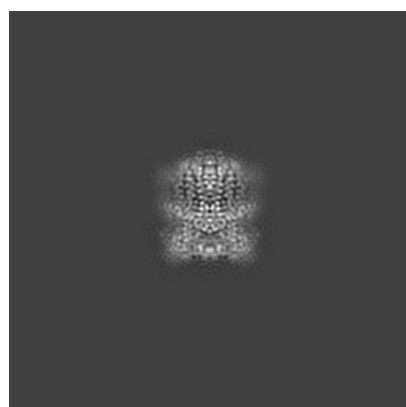
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22226. These allow visual inspection of the internal detail of the map and identification of artifacts.

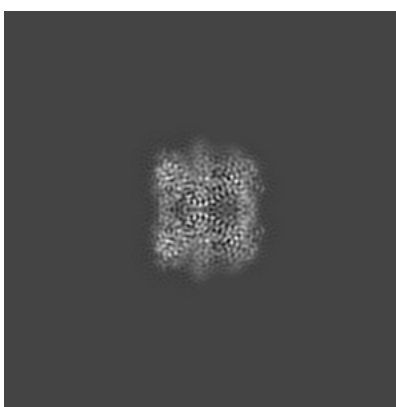
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

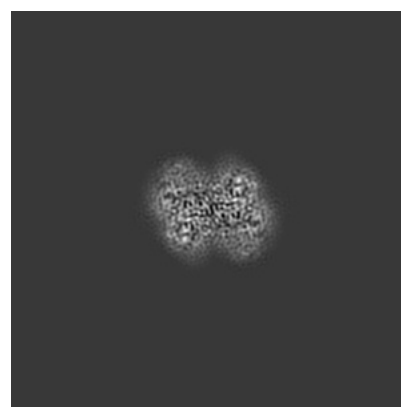
6.1.1 Primary map



X



Y

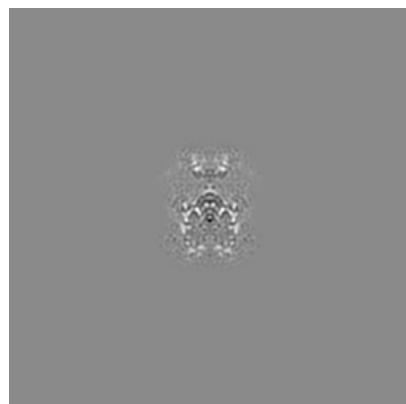


Z

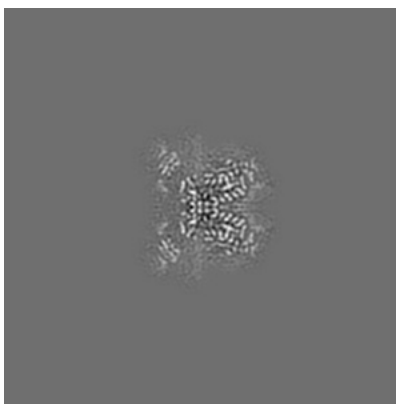
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

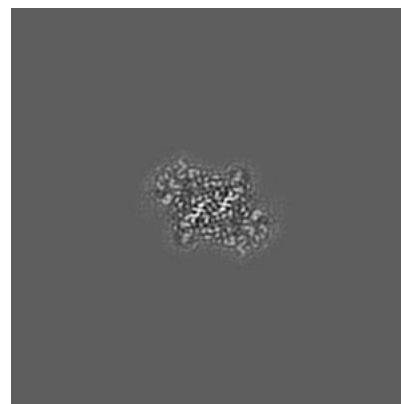
6.2.1 Primary map



X Index: 120



Y Index: 120

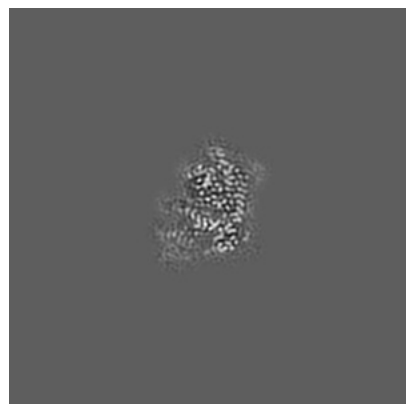


Z Index: 120

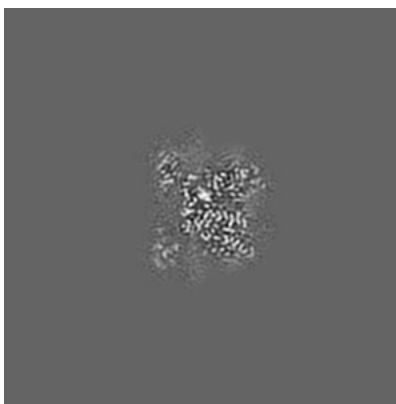
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

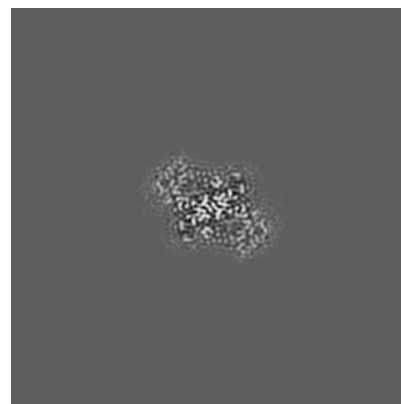
6.3.1 Primary map



X Index: 134



Y Index: 122

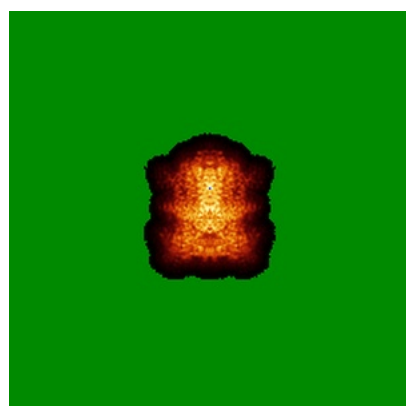


Z Index: 121

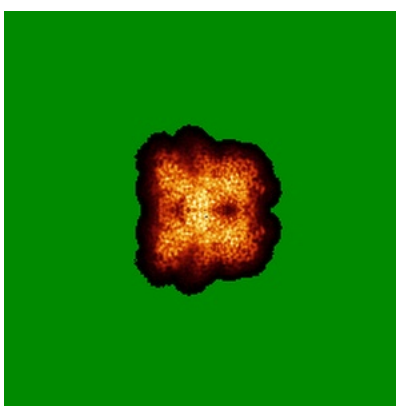
The images above show the largest variance slices of the map in three orthogonal directions.

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

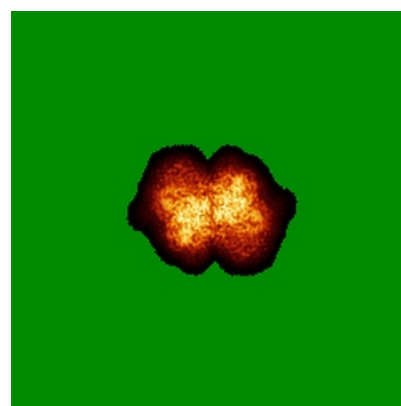
6.4.1 Primary map



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

This section was not generated.

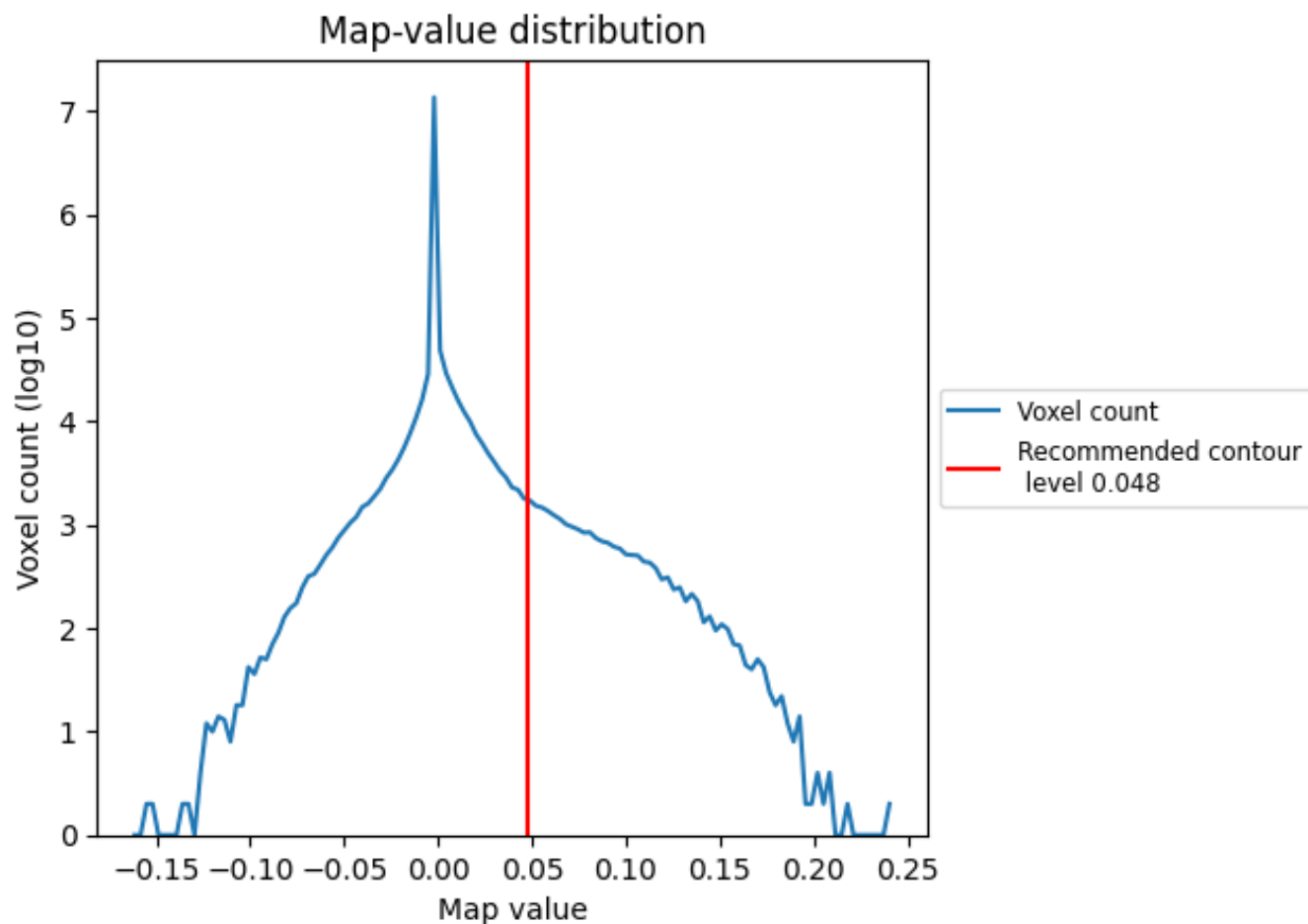
6.6 Mask visualisation

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

7 Map analysis [i](#)

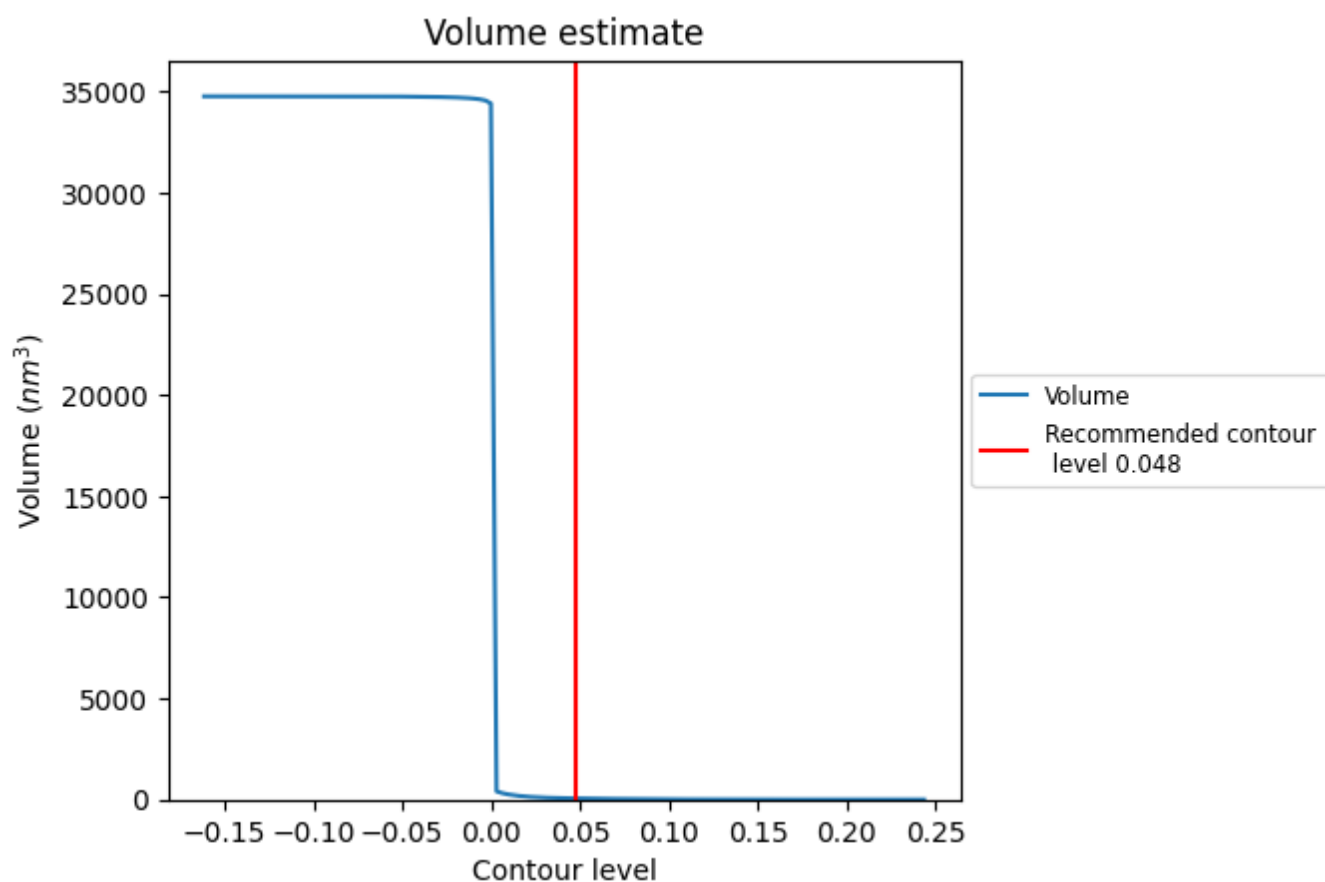
This section contains the results of statistical analysis of the map.

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.

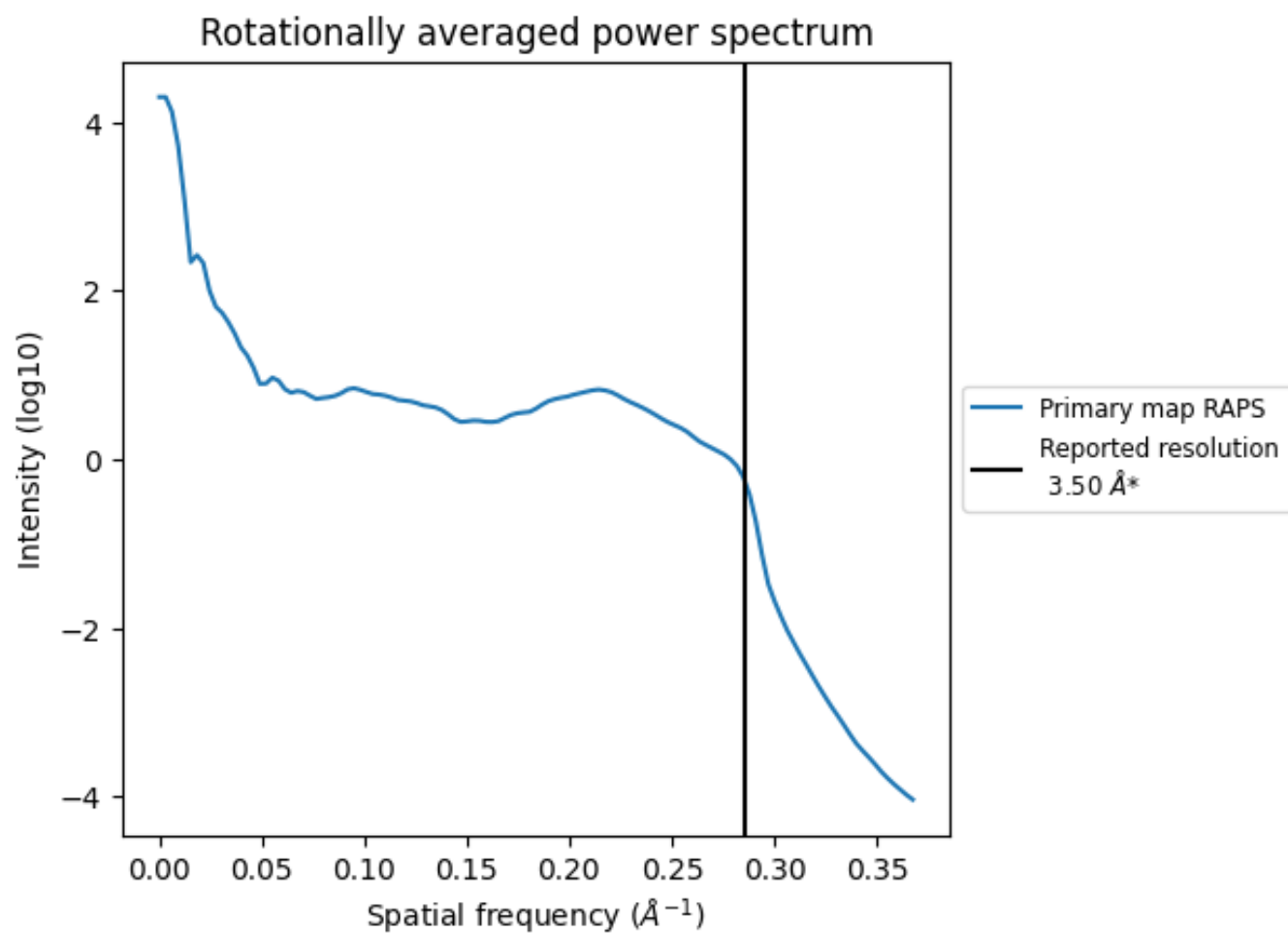
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 56 nm^3 ; this corresponds to an approximate mass of 51 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 ⓘ

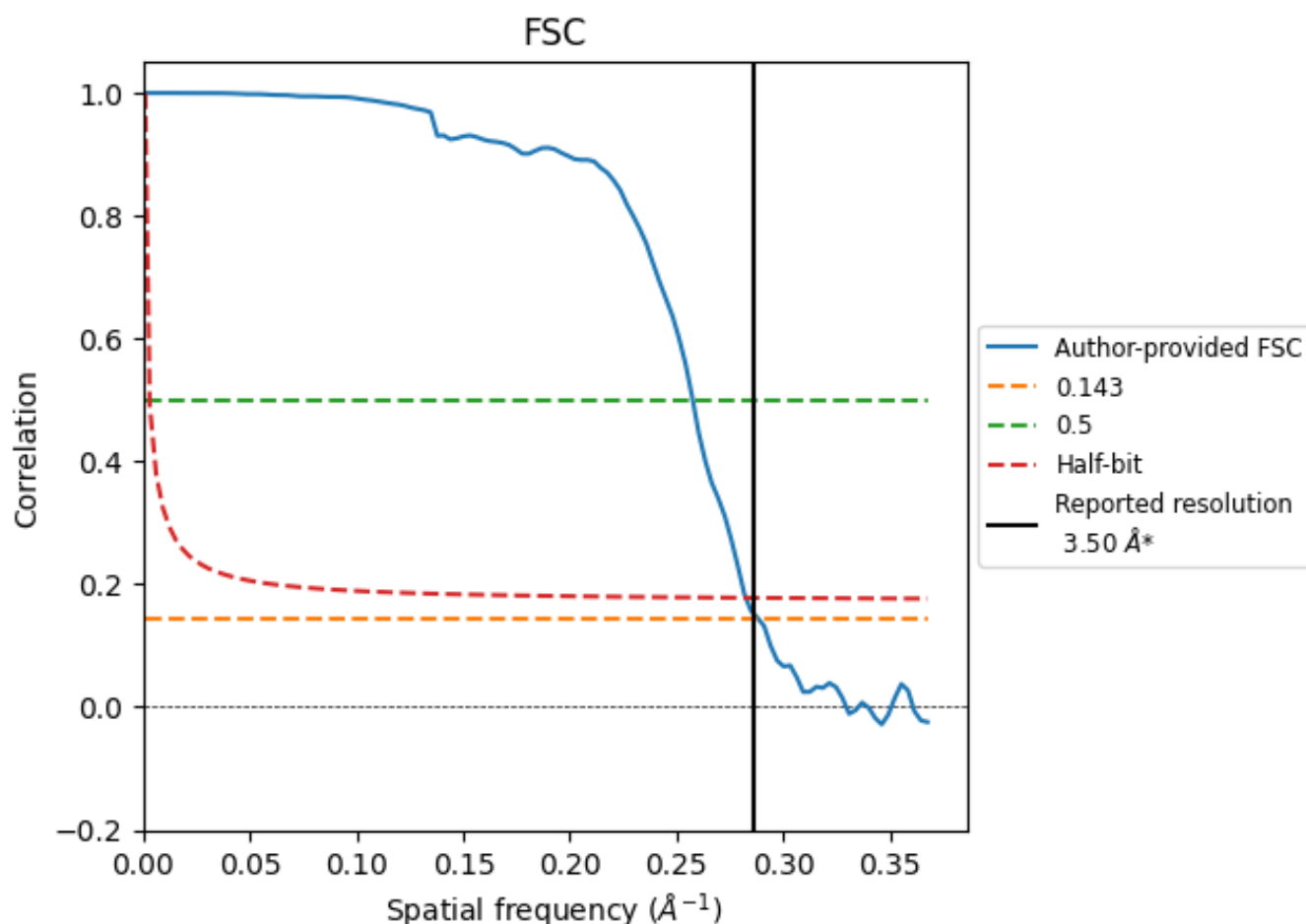


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

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 0.286 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.47	3.88	3.54
Unmasked-calculated*	-	-	-

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

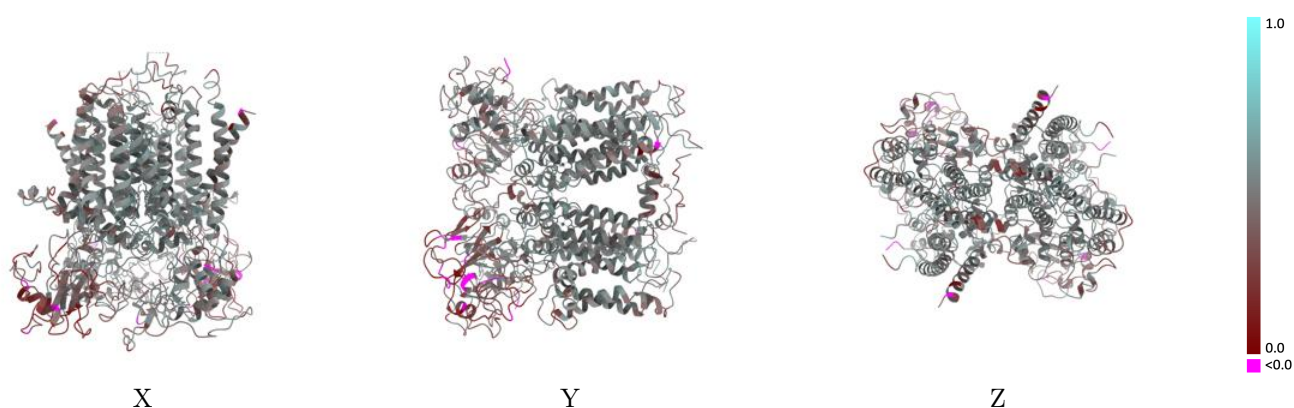
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-22226 and PDB model 6XKV. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)

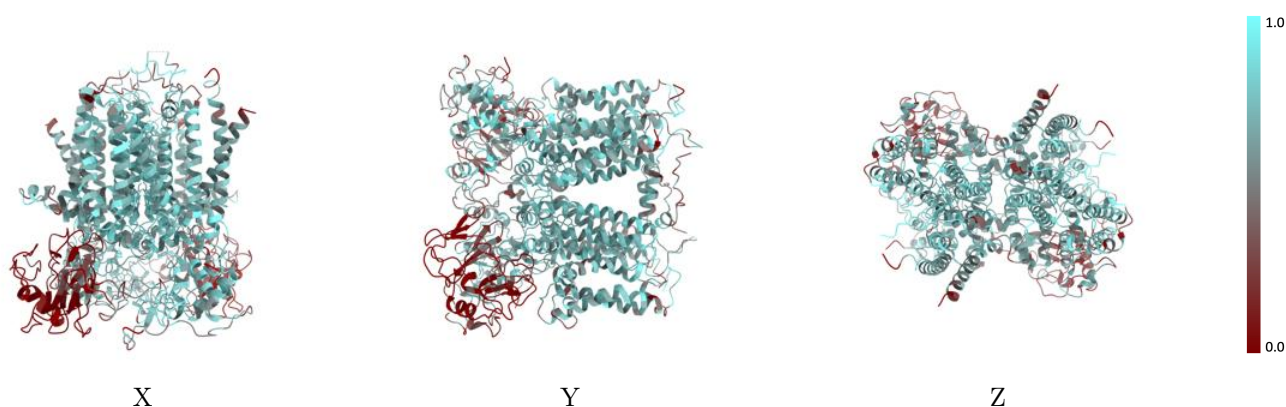
This section was not generated.

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



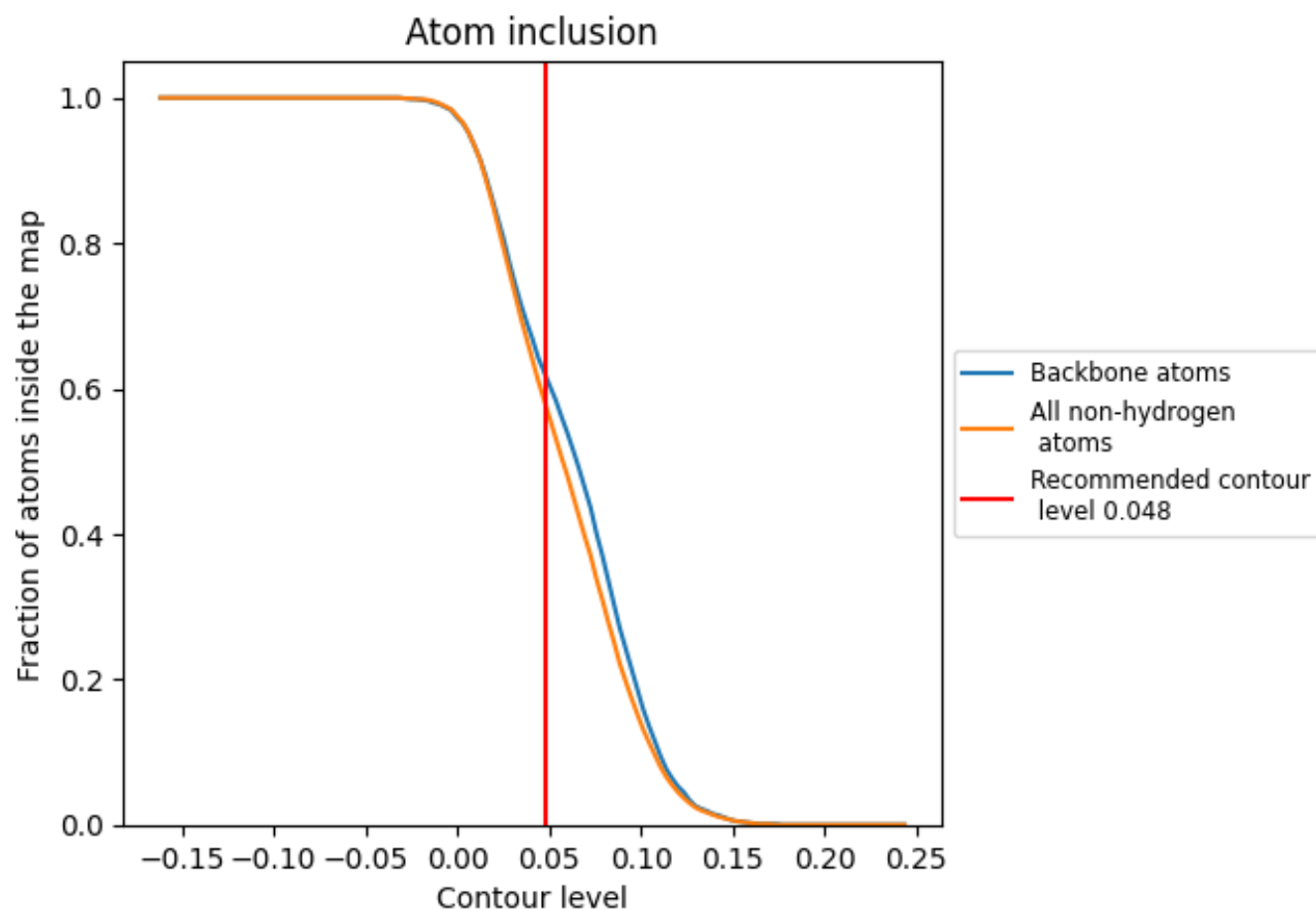
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.048).

9.4 Atom inclusion [i](#)



At the recommended contour level, 62% 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 (0.048) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5790	0.4440
C	0.7180	0.4930
D	0.6130	0.4560
E	0.1830	0.2820
P	0.7160	0.4950
Q	0.6190	0.4570
R	0.2060	0.3310

1.0

0.0

<0.0