



wwPDB EM Validation Summary Report ⓘ

Aug 4, 2026 – 08:54 PM EDT

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:

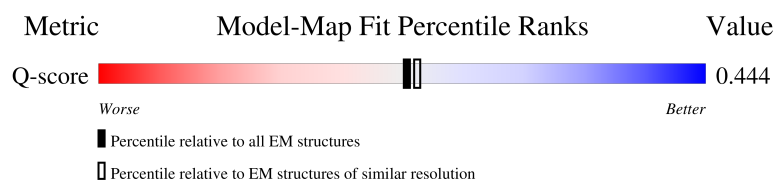
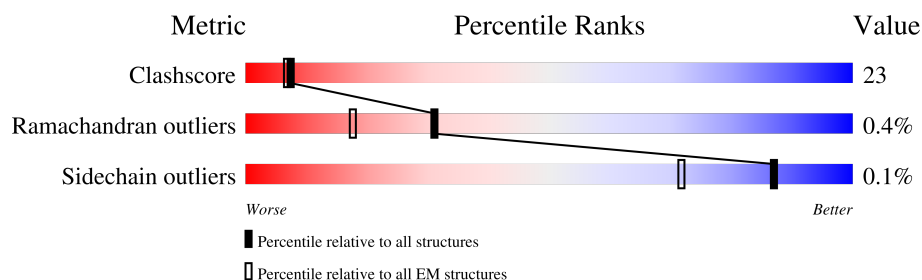
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.50

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	
1	P	437	
2	D	279	
2	Q	279	

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Mol	Chain	Length	Quality of chain
3	E	191	
3	R	191	

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
4	HEC	C	502	X	-	-	-
4	HEC	D	501	X	-	-	-
4	HEC	P	502	X	-	-	-
4	HEC	Q	501	X	-	-	-

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		

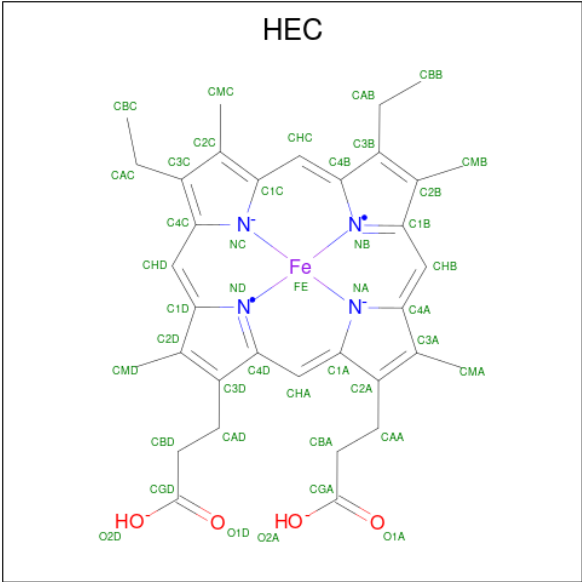
- Molecule 2 is a protein called Cytochrome c1.

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.

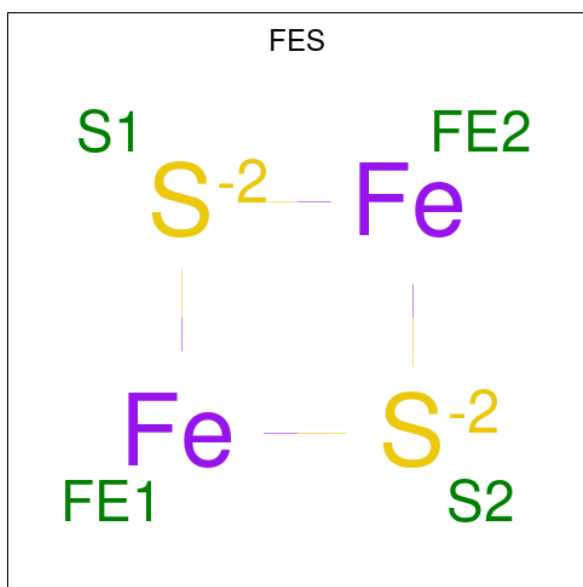
Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	181	Total	C	N	O	S	0	0
			1365	855	246	256	8		
3	R	181	Total	C	N	O	S	0	0
			1365	855	246	256	8		

- Molecule 4 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



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

- Molecule 5 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).

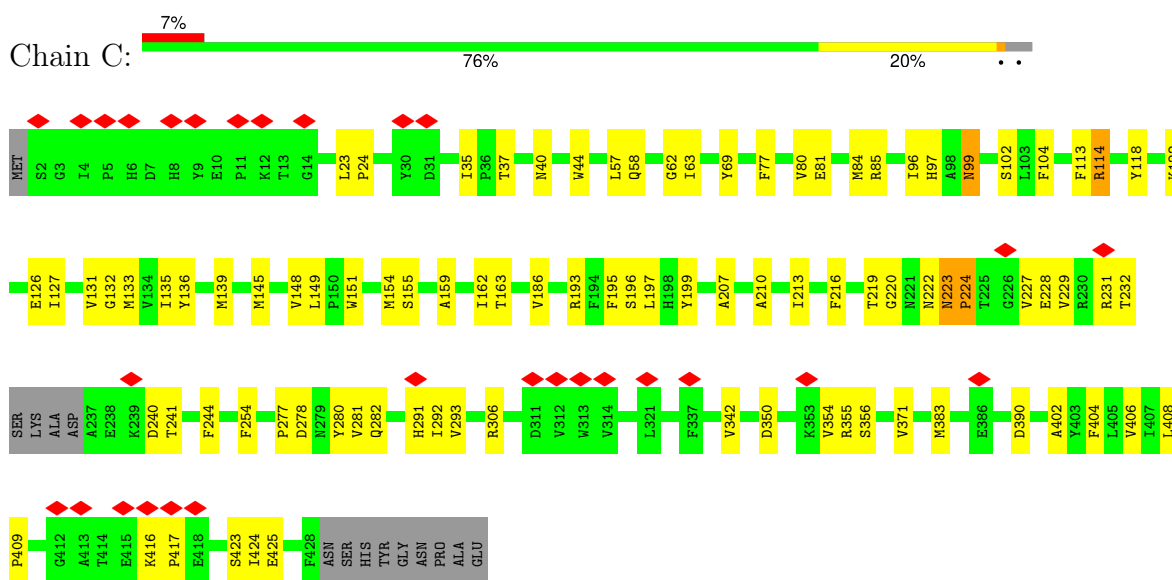


Mol	Chain	Residues	Atoms			AltConf
5	E	1	Total	Fe	S	0
			4	2	2	
5	R	1	Total	Fe	S	0
			4	2	2	

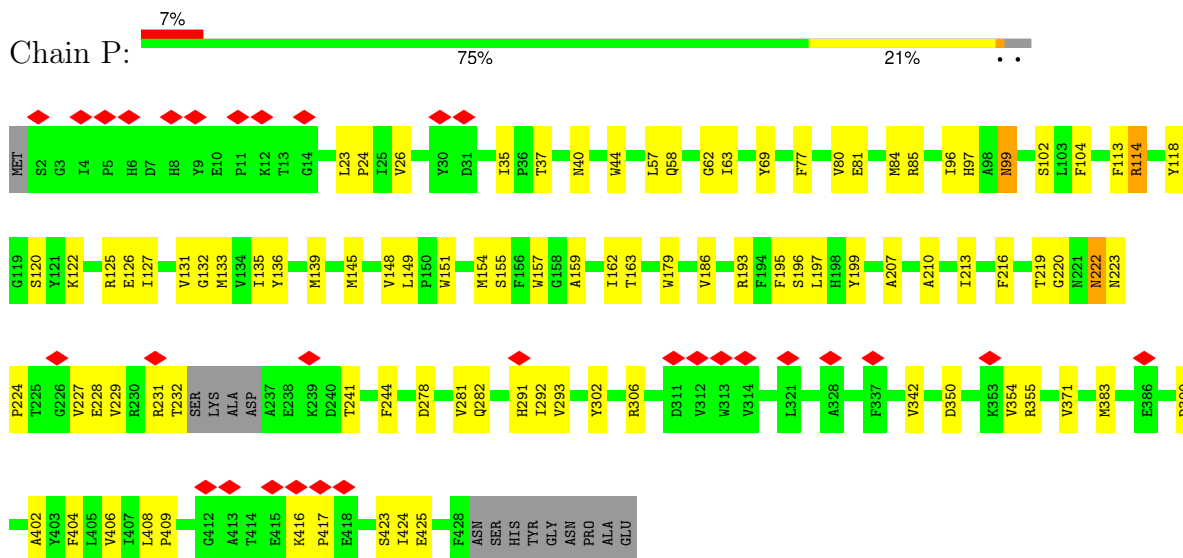
3 Residue-property plots

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.

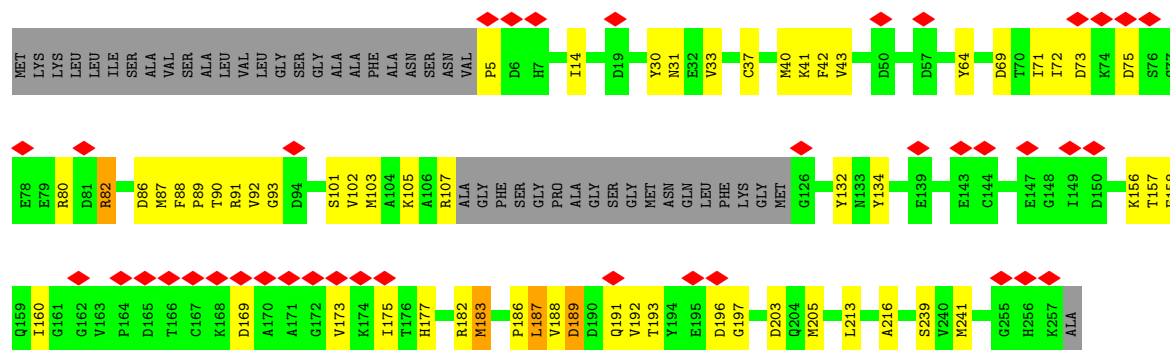
- Molecule 1: Cytochrome b



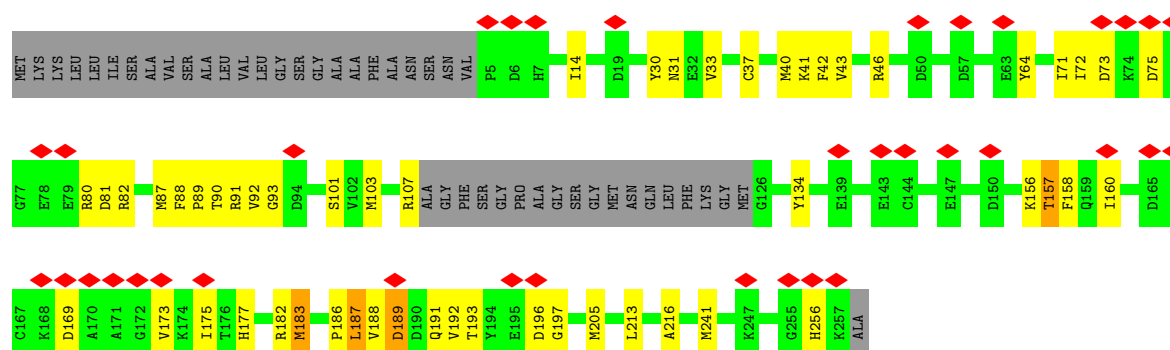
- Molecule 1: Cytochrome b



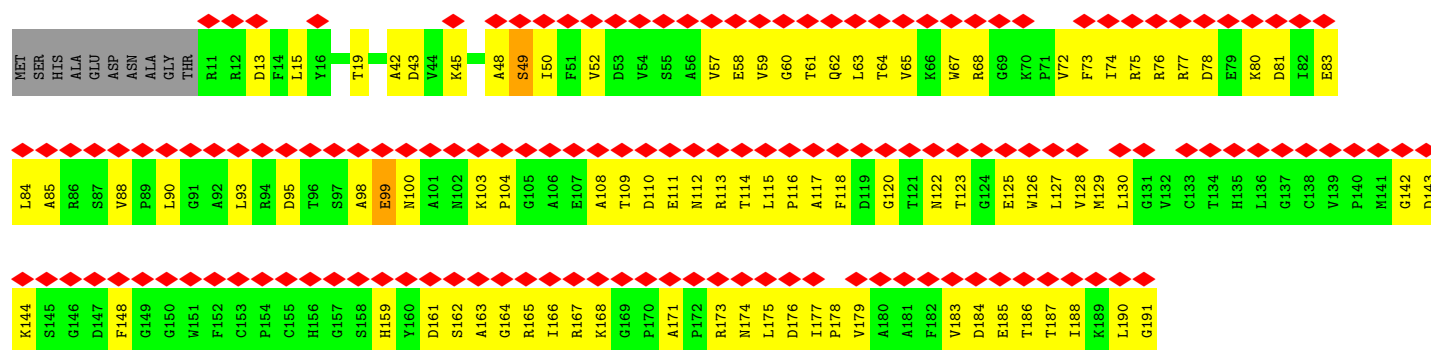
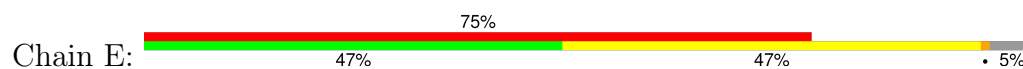
- Molecule 2: Cytochrome c1



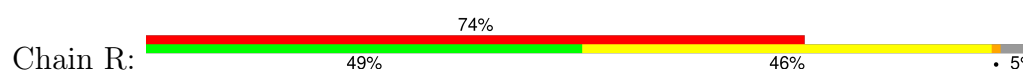
• Molecule 2: Cytochrome c1



• 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	P194	C195	H196	G197	S198	H199	Y200	D201	S202	A203	G204	R205	I206	R207	K208	G209	P210	A211	P212	R213	N214	L215	D216	I217	P218	V219	A220	A221	F222	V223	D224	E225	T226	T227	I228	K229	L230	G231	E232	D233	P234	C235	H236	G237	S238	H239	Y240	D241	S242	A243	G244	R245	I246	R247	K248	G249	P250	A251	P252	R253	N254	L255	D256	I257	P258	V259	A260	A261	F262	V263	D264	E265	T266	T267	I268	K269	L270	G271	E272	D273	P274	C275	H276	G277	S278	H279	Y280	D281	S282	A283	G284	R285	I286	R287	K288	G289	P290	A291	P292	R293	N294	L295	D296	I297	P298	V299	A300	A301	F302	V303	D304	E305	T306	T307	I308	K309	L310	G311	E312	D313	P314	C315	H316	G317	S318	H319	Y320	D321	S322	A323	G324	R325	I326	R327	K328	G329	P330	A331	P332	R333	N334	L335	D336	I337	P338	V339	A340	A341	F342	V343	D344	E345	T346	T347	I348	K349	L350	G351	E352	D353	P354	C355	H356	G357	S358	H359	Y360	D361	S362	A363	G364	R365	I366	R367	K368	G369	P370	A371	P372	R373	N374	L375	D376	I377	P378	V379	A380	A381	F382	V383	D384	E385	T386	T387	I388	K389	L390	G391	E392	D393	P394	C395	H396	G397	S398	H399	Y400	D401	S402	A403	G404	R405	I406	R407	K408	G409	P410	A411	P412	R413	N414	L415	D416	I417	P418	V419	A420	A421	F422	V423	D424	E425	T426	T427	I428	K429	L430	G431	E432	D433	P434	C435	H436	G437	S438	H439	Y440	D441	S442	A443	G444	R445	I446	R447	K448	G449	P450	A451	P452	R453	N454	L455	D456	I457	P458	V459	A460	A461	F462	V463	D464	E465	T466	T467	I468	K469	L470	G471	E472	D473	P474	C475	H476	G477	S478	H479	Y480	D481	S482	A483	G484	R485	I486	R487	K488	G489	P490	A491	P492	R493	N494	L495	D496	I497	P498	V499	A500	A501	F502	V503	D504	E505	T506	T507	I508	K509	L510	G511	E512	D513	P514	C515	H516	G517	S518	H519	Y520	D521	S522	A523	G524	R525	I526	R527	K528	G529	P530	A531	P532	R533	N534	L535	D536	I537	P538	V539	A540	A541	F542	V543	D544	E545	T546	T547	I548	K549	L550	G551	E552	D553	P554	C555	H556	G557	S558	H559	Y560	D561	S562	A563	G564	R565	I566	R567	K568	G569	P570	A571	P572	R573	N574	L575	D576	I577	P578	V579	A580	A581	F582	V583	D584	E585	T586	T587	I588	K589	L590	G591	E592	D593	P594	C595	H596	G597	S598	H599	Y600	D601	S602	A603	G604	R605	I606	R607	K608	G609	P610	A611	P612	R613	N614	L615	D616	I617	P618	V619	A620	A621	F622	V623	D624	E625	T626	T627	I628	K629	L630	G631	E632	D633	P634	C635	H636	G637	S638	H639	Y640	D641	S642	A643	G644	R645	I646	R647	K648	G649	P650	A651	P652	R653	N654	L655	D656	I657	P658	V659	A660	A661	F662	V663	D664	E665	T666	T667	I668	K669	L670	G671	E672	D673	P674	C675	H676	G677	S678	H679	Y680	D681	S682	A683	G684	R685	I686	R687	K688	G689	P690	A691	P692	R693	N694	L695	D696	I697	P698	V699	A700	A701	F702	V703	D704	E705	T706	T707	I708	K709	L710	G711	E712	D713	P714	C715	H716	G717	S718	H719	Y720	D721	S722	A723	G724	R725	I726	R727	K728	G729	P730	A731	P732	R733	N734	L735	D736	I737	P738	V739	A740	A741	F742	V743	D744	E745	T746	T747	I748	K749	L750	G751	E752	D753	P754	C755	H756	G757	S758	H759	Y760	D761	S762	A763	G764	R765	I766	R767	K768	G769	P770	A771	P772	R773	N774	L775	D776	I777	P778	V779	A780	A781	F782	V783	D784	E785	T786	T787	I788	K789	L790	G791	E792	D793	P794	C795	H796	G797	S798	H799	Y800	D801	S802	A803	G804	R805	I806	R807	K808	G809	P810	A811	P812	R813	N814	L815	D816	I817	P818	V819	A820	A821	F822	V823	D824	E825	T826	T827	I828	K829	L830	G831	E832	D833	P834	C835	H836	G837	S838	H839	Y840	D841	S842	A843	G844	R845	I846	R847	K848	G849	P850	A851	P852	R853	N854	L855	D856	I857	P858	V859	A860	A861	F862	V863	D864	E865	T866	T867	I868	K869	L870	G871	E872	D873	P874	C875	H876	G877	S878	H879	Y880	D881	S882	A883	G884	R885	I886	R887	K888	G889	P890	A891	P892	R893	N894	L895	D896	I897	P898	V899	A900	A901	F902	V903	D904	E905	T906	T907	I908	K909	L910	G911	E912	D913	P914	C915	H916	G917	S918	H919	Y920	D921	S922	A923	G924	R925	I926	R927	K928	G929	P930	A931	P932	R933	N934	L935	D936	I937	P938	V939	A940	A941	F942	V943	D944	E945	T946	T947	I948	K949	L950	G951	E952	D953	P954	C955	H956	G957	S958	H959	Y960	D961	S962	A963	G964	R965	I966	R967	K968	G969	P970	A971	P972	R973	N974	L975	D976	I977	P978	V979	A980	A981	F982	V983	D984	E985	T986	T987	I988	K989	L990	G991	E992	D993	P994	C995	H996	G997	S998	H999	Y1000	D1001	S1002	A1003	G1004	R1005	I1006	R1007	K1008	G1009	P1010	A1011	P1012	R1013	N1014	L1015	D1016	I1017	P1018	V1019	A1020	A1021	F1022	V1023	D1024	E1025	T1026	T1027	I1028	K1029	L1030	G1031	E1032	D1033	P1034	C1035	H1036	G1037	S1038	H1039	Y1040	D1041	S1042	A1043	G1044	R1045	I1046	R1047	K1048	G1049	P1050	A1051	P1052	R1053	N1054	L1055	D1056	I1057	P1058	V1059	A1060	A1061	F1062	V1063	D1064	E1065	T1066	T1067	I1068	K1069	L1070	G1071	E1072	D1073	P1074	C1075	H1076	G1077	S1078	H1079	Y1080	D1081	S1082	A1083	G1084	R1085	I1086	R1087	K1088	G1089	P1090	A1091	P1092	R1093	N1094	L1095	D1096	I1097	P1098	V1099	A1100	A1101	F1102	V1103	D1104	E1105	T1106	T1107	I1108	K1109	L1110	G1111	E1112	D1113	P1114	C1115	H1116	G1117	S1118	H1119	Y1120	D1121	S1122	A1123	G1124	R1125	I1126	R1127	K1128	G1129	P1130	A1131	P1132	R1133	N1134	L1135	D1136	I1137	P1138	V1139	A1140	A1141	F1142	V1143	D1144	E1145	T1146	T1147	I1148	K1149	L1150	G1151	E1152	D1153	P1154	C1155	H1156	G1157	S1158	H1159	Y1160	D1161	S1162	A1163	G1164	R1165	I1166	R1167	K1168	G1169	P1170	A1171	P1172	R1173	N1174	L1175	D1176	I1177	P1178	V1179	A1180	A1181	F1182	V1183	D1184	E1185	T1186	T1187	I1188	K1189	L1190	G1191	E1192	D1193	P1194	C1195	H1196	G1197	S1198	H1199	Y1200	D1201	S1202	A1203	G1204	R1205	I1206	R1207	K1208	G1209	P1210	A1211	P1212	R1213	N1214	L1215	D1216	I1217	P1218	V1219	A1220	A1221	F1222	V1223	D1224	E1225	T1226	T1227	I1228	K1229	L1230	G1231	E1232	D1233	P1234	C1235	H1236	G1237	S1238	H1239	Y1240	D1241	S1242	A1243	G1244	R1245	I1246	R1247	K1248	G1249	P1250	A1251	P1252	R1253	N1254	L1255	D1256	I1257	P1258	V1259	A1260	A1261	F1262	V1263	D1264	E1265	T1266	T1267	I1268	K1269	L1270	G1271	E1272	D1273	P1274	C1275	H1276	G1277	S1278	H1279	Y1280	D1281	S1282	A1283	G1284	R1285	I1286	R1287	K1288	G1289	P1290	A1291	P1292	R1293	N1294	L1295	D1296	I1297	P1298	V1299	A1300	A1301	F1302	V1303	D1304	E1305	T1306	T1307	I1308	K1309	L1310	G1311	E1312	D1313	P1314	C1315	H1316	G1317	S1318	H1319	Y1320	D1321	S1322	A1323	G1324	R1325	I1326	R1327	K1328	G1329	P1330	A1331	P1332	R1333	N1334	L1335	D1336	I1337	P1338	V1339	A1340	A1341	F1342	V1343	D1344	E1345	T1346	T1347	I1348	K1349	L1350	G1351	E1352	D1353	P1354	C1355	H1356	G1357	S1358	H1359	Y1360	D1361	S1362	A1363	G1364	R1365	I1366	R1367	K1368	G1369	P1370	A1371	P1372	R1373	N1374	L1375	D1376	I1377	P1378	V1379	A1380	A1381	F1382	V1383	D1384	E1385	T1386	T1387	I1388	K1389	L1390	G1391	E1392	D1393	P1394	C1395	H1396	G1397	S1398	H1399	Y1400	D1401	S1402	A1403	G1404	R1405	I1406	R1407	K1408	G1409	P1410	A1411	P1412	R1413	N1414	L1415	D1416	I1417	P1418	V1419	A1420	A1421	F1422	V1423	D1424	E1425	T1426	T1427	I1428	K1429	L1430	G1431	E1432	D1433	P1434	C1435	H1436	G1437	S1438	H1439	Y1440	D1441	S1442	A1443	G1444	R1445	I1446	R1447	K1448	G1449	P1450	A1451	P1452	R1453	N1454	L1455	D1456	I1457	P1458	V1459	A1460	A1461	F1462	V1463	D1464	E1465	T1466	T1467	I1468	K1469	L1470	G1471	E1472	D1473	P1474	C1475	H1476	G1477	S1478	H1479	Y1480	D1481	S1482	A1483	G1484	R1485	I1486	R1487	K1488	G1489	P1490	A1491	P1492	R1493	N1494	L1495	D1496	I1497	P1498	V1499	A1500	A1501	F1502	V1503	D1504	E1505	T1506	T1507	I1508	K1509	L1510	G1511	E1512	D1513	P1514	C1515	H1516	G1517	S1518	H1519	Y1520	D1521	S1522	A1523	G1524	R1525	I1526	R1527	K1528	G1529	P1530	A1531	P1532	R1533	N1534	L1535	D1536	I1537	P1538	V1539	A1540	A1541	F1542	V1543	D1544	E1545	T1546	T1547	I1548	K1549	L1550	G1551	E1552	D1553	P1554	C1555	H1556	G1557	S1558	H1559	Y1560	D1561	S1562	A1563	G1564	R1565	I1566	R1567	K1568	G1569	P1570	A1571	P1572	R1573	N1574	L1575	D1576	I1577	P1578	V1579	A1580	A1581	F1582	V1583	D1584	E1585	T1586	T1587	I1588	K1589	L1590	G1591	E1592	D1593	P1594	C1595	H1596	G1597	S1598	H1599	Y1600	D1601	S1602	A1603	G1604	R1605	I1606	R1607	K1608	G160
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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 [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	C	419/437 (96%)	352 (84%)	65 (16%)	2 (0%)	24 57

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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	$\# Z > 2$
5	FES	E	501	3	0,4,4	-	-	-		
5	FES	R	501	3	0,4,4	-	-	-		
4	HEC	Q	501	2	50,50,50	1.79	7 (14%)	68,82,82	1.24	3 (4%)
4	HEC	P	502	1	50,50,50	1.66	9 (18%)	68,82,82	1.41	9 (13%)
4	HEC	C	502	1	50,50,50	1.66	9 (18%)	68,82,82	1.41	9 (13%)
4	HEC	C	501	1	50,50,50	1.57	9 (18%)	68,82,82	1.39	9 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	HEC	P	501	1	50,50,50	1.57	9 (18%)	68,82,82	1.39	9 (13%)
4	HEC	D	501	2	50,50,50	1.80	7 (14%)	68,82,82	1.24	2 (2%)

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	FES	E	501	3	-	-	0/1/1/1
5	FES	R	501	3	-	-	0/1/1/1
4	HEC	Q	501	2	1/1/3/7	6/14/54/54	-
4	HEC	P	502	1	1/1/3/7	9/14/54/54	-
4	HEC	C	502	1	1/1/3/7	9/14/54/54	-
4	HEC	C	501	1	-	8/14/54/54	-
4	HEC	P	501	1	-	8/14/54/54	-
4	HEC	D	501	2	1/1/3/7	6/14/54/54	-

The worst 5 of 50 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	501	HEC	C3D-C2D	7.76	1.53	1.36
4	Q	501	HEC	C3D-C2D	7.68	1.53	1.36
4	C	502	HEC	FE-NB	5.96	2.13	1.94
4	P	502	HEC	FE-NB	5.94	2.13	1.94
4	D	501	HEC	FE-ND	5.12	2.10	1.94

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	501	HEC	C1D-ND-C4D	5.04	111.18	105.21
4	Q	501	HEC	C1D-ND-C4D	5.00	111.13	105.21
4	P	502	HEC	CBB-CAB-C3B	4.56	124.79	112.42
4	C	502	HEC	CBB-CAB-C3B	4.56	124.78	112.42
4	P	502	HEC	CBC-CAC-C3C	4.24	123.91	112.42

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	C	502	HEC	NA

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Mol	Chain	Res	Type	Atom
4	D	501	HEC	NA
4	P	502	HEC	NA
4	Q	501	HEC	NA

5 of 46 torsion outliers are listed below:

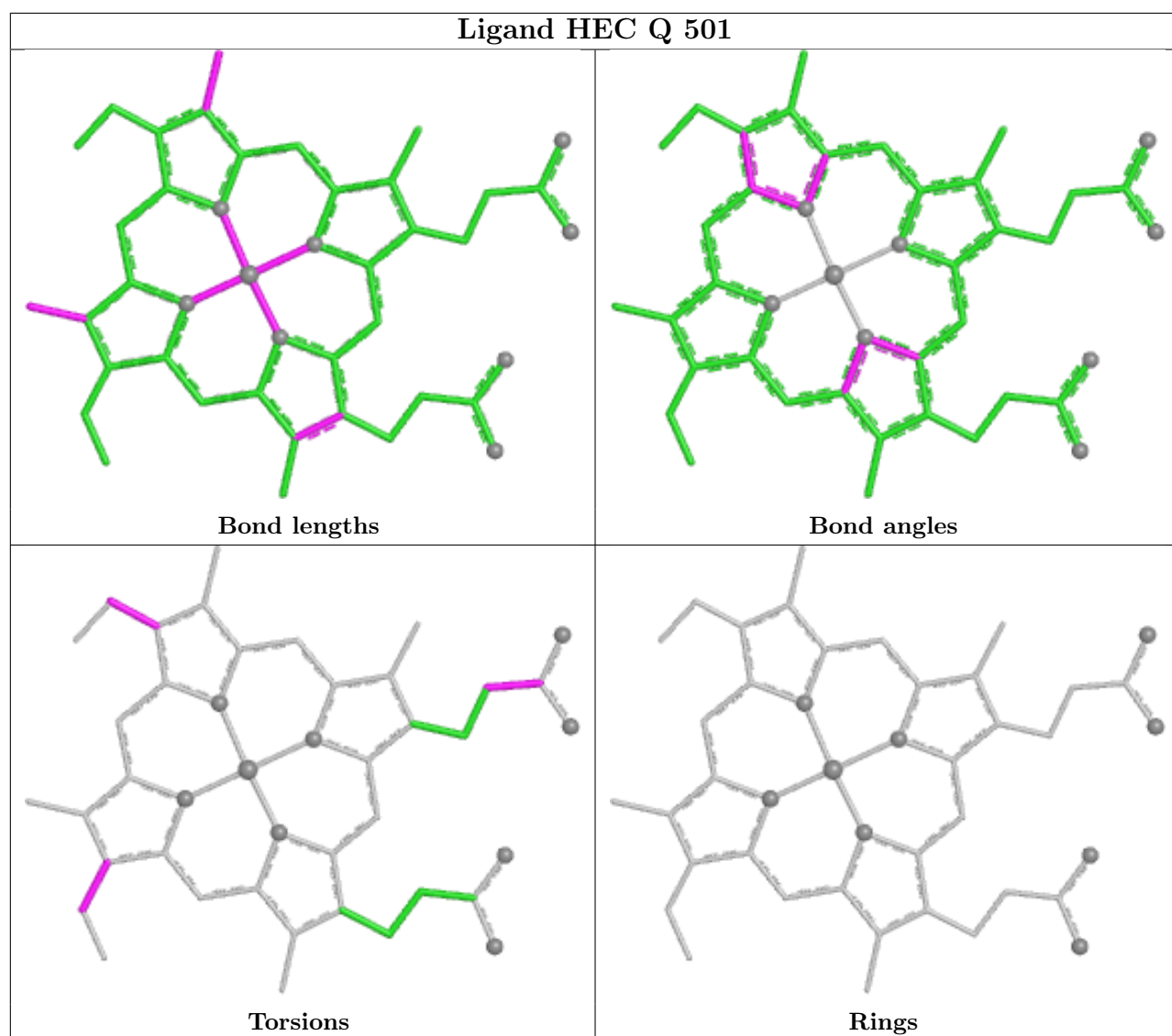
Mol	Chain	Res	Type	Atoms
4	C	501	HEC	C2C-C3C-CAC-CBC
4	P	501	HEC	C2C-C3C-CAC-CBC
4	C	501	HEC	C4B-C3B-CAB-CBB
4	P	501	HEC	C4B-C3B-CAB-CBB
4	C	501	HEC	C2B-C3B-CAB-CBB

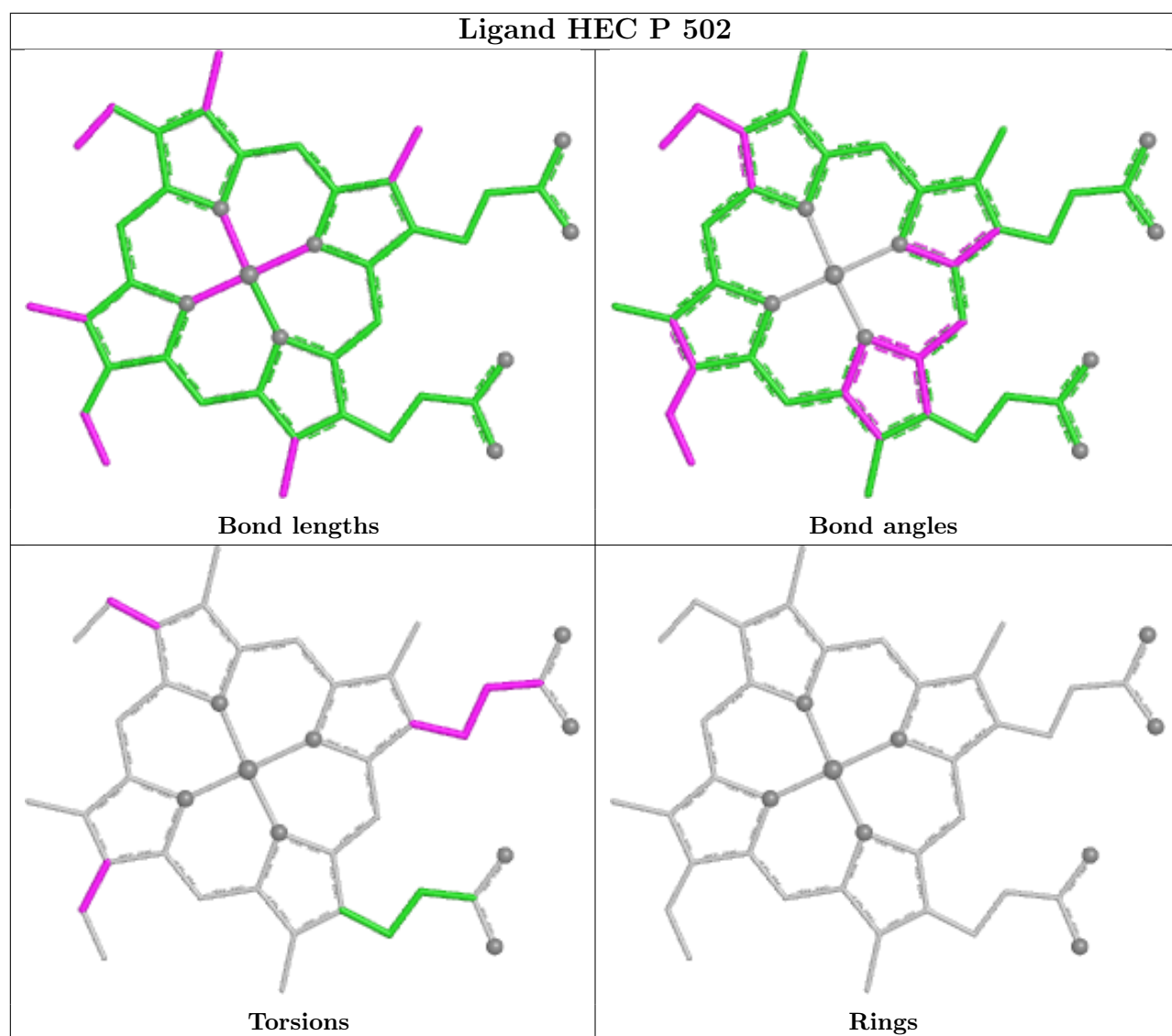
There are no ring outliers.

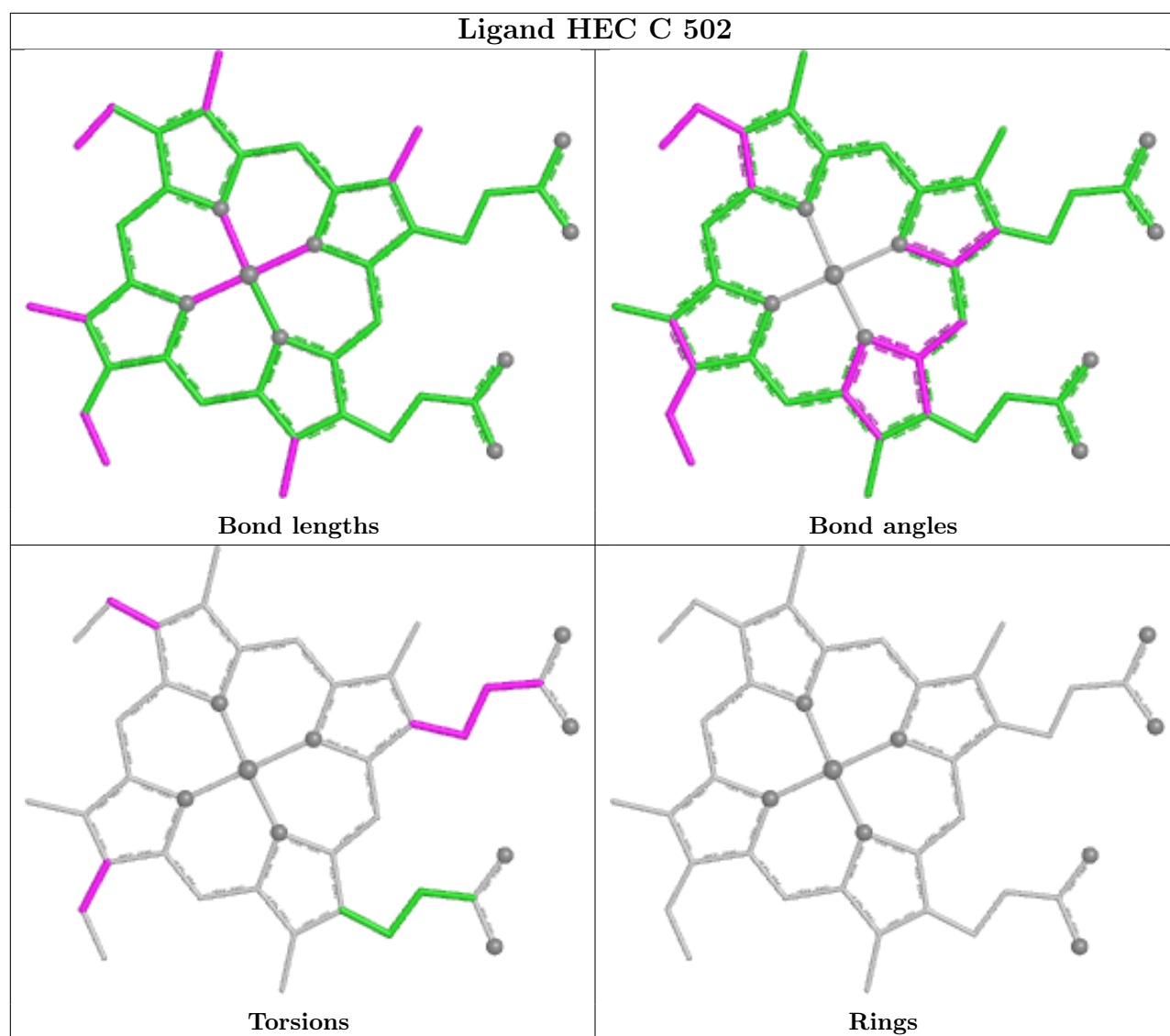
6 monomers are involved in 41 short contacts:

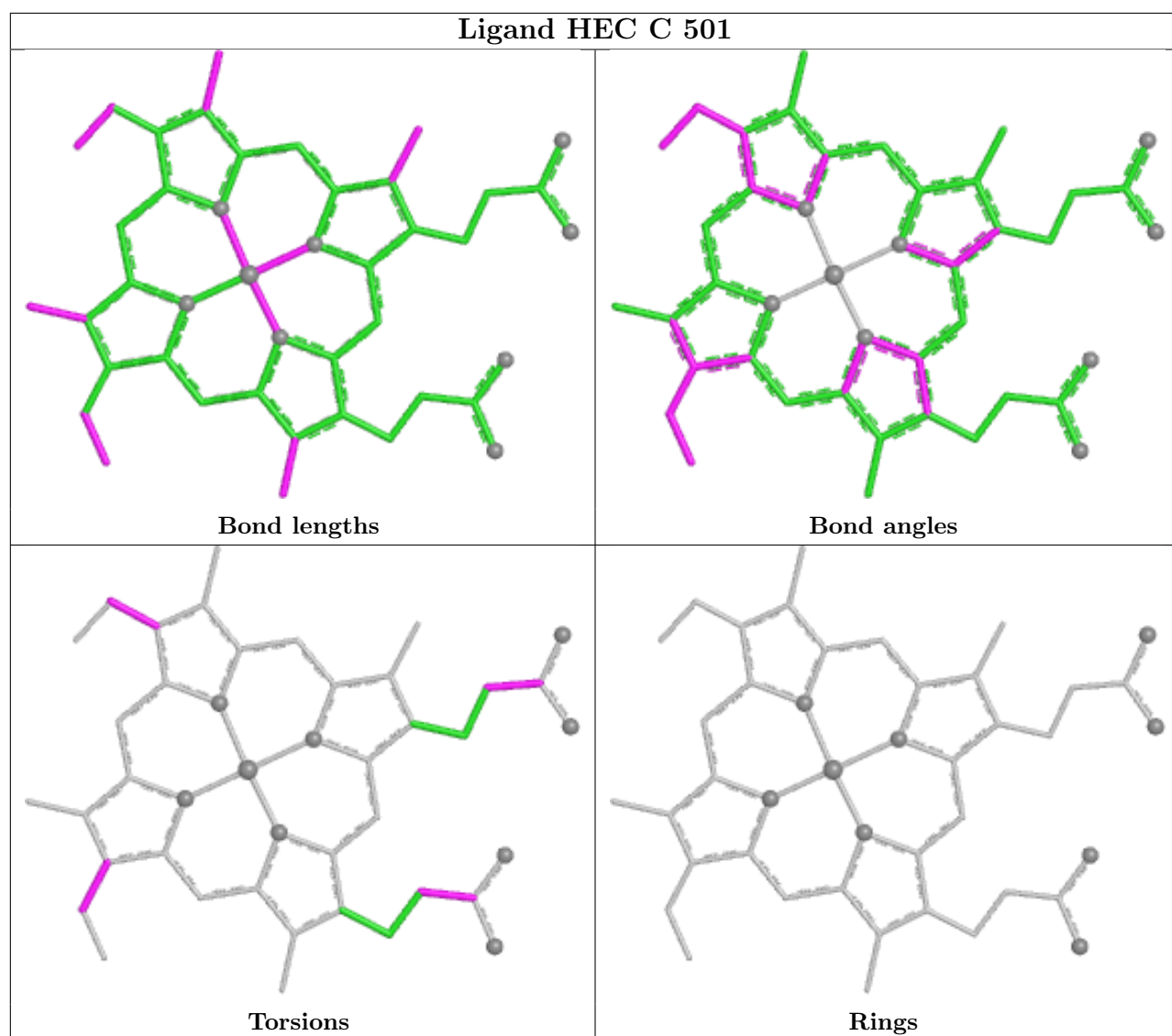
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	Q	501	HEC	5	0
4	P	502	HEC	3	0
4	C	502	HEC	3	0
4	C	501	HEC	12	0
4	P	501	HEC	13	0
4	D	501	HEC	5	0

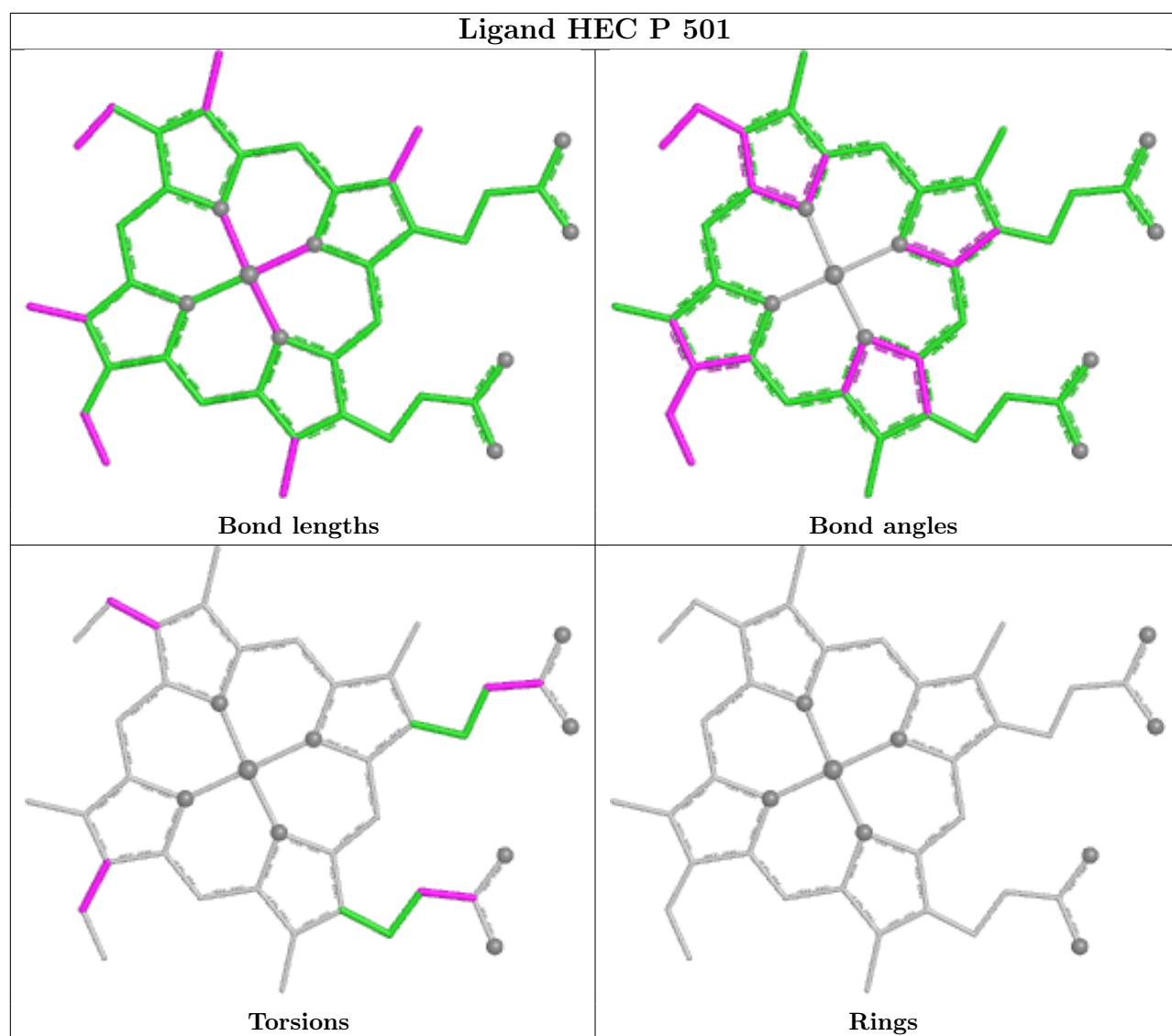
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

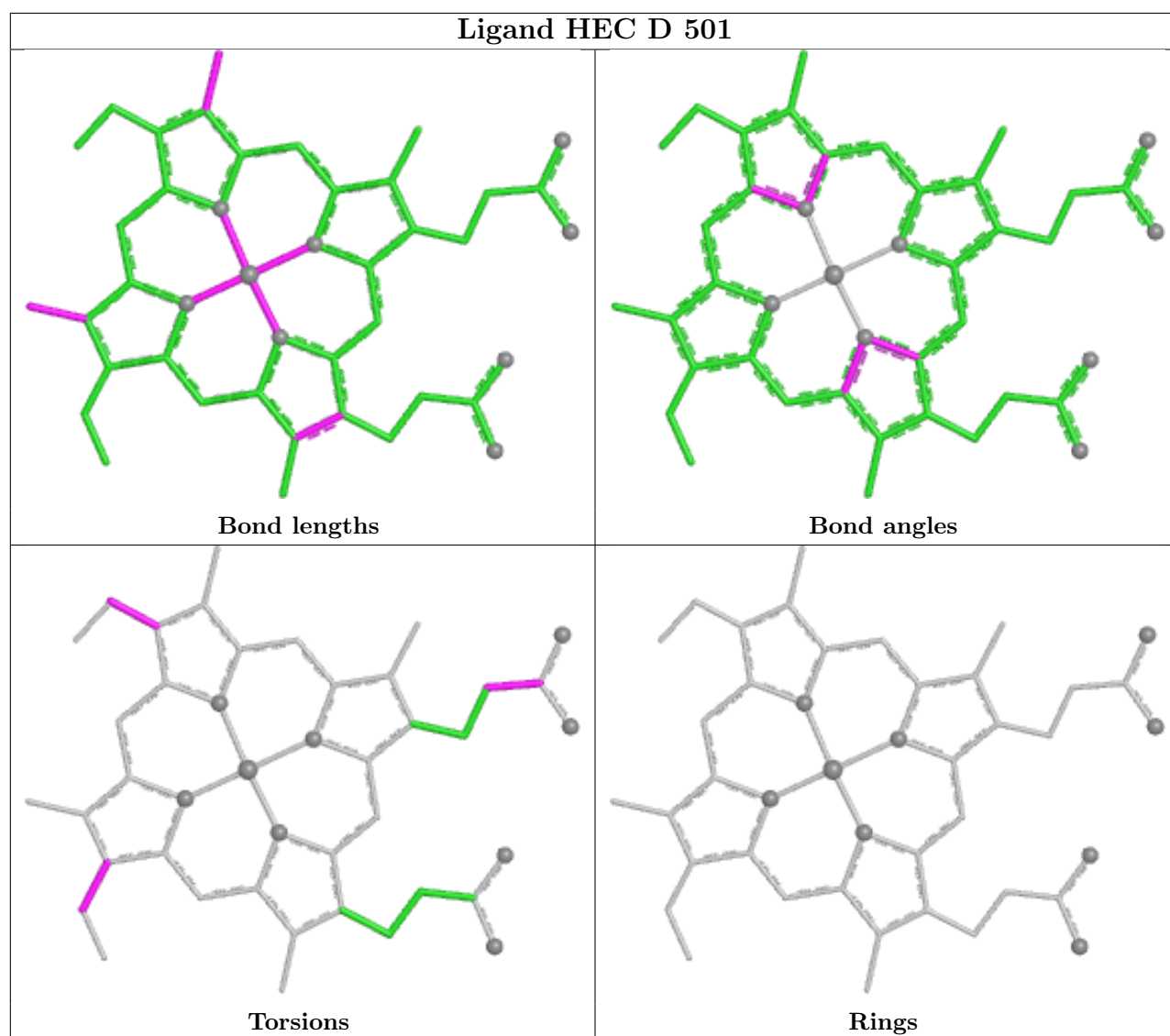












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

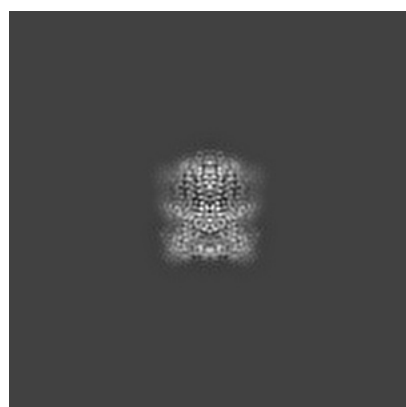
6 Map visualisation [i](#)

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

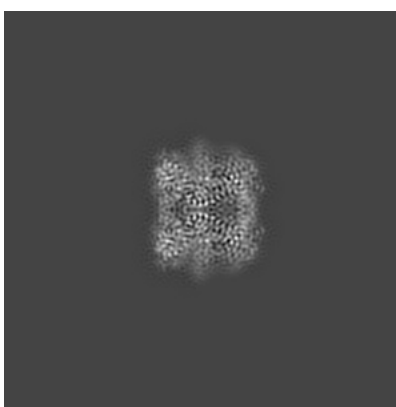
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

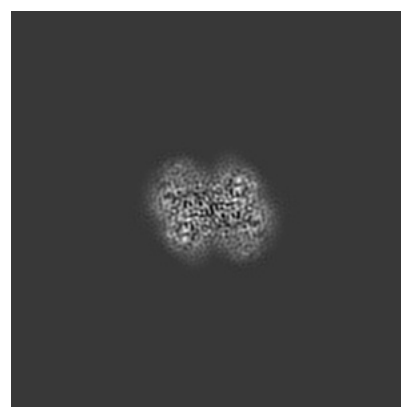
6.1.1 Primary map



X



Y

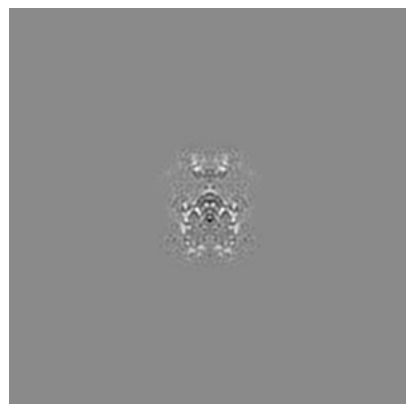


Z

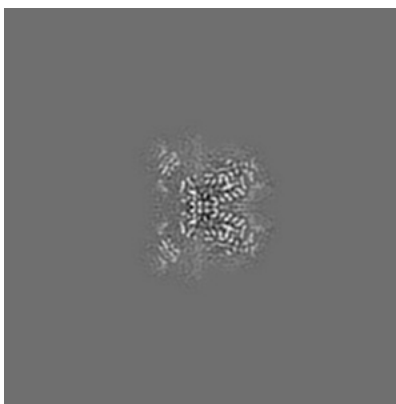
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

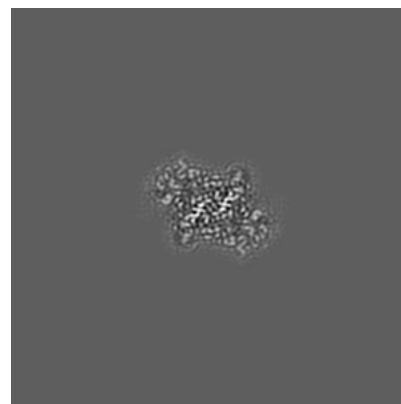
6.2.1 Primary map



X Index: 120



Y Index: 120

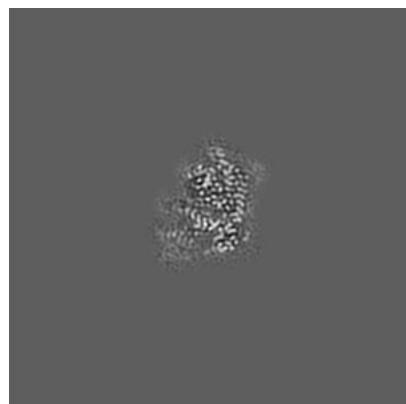


Z Index: 120

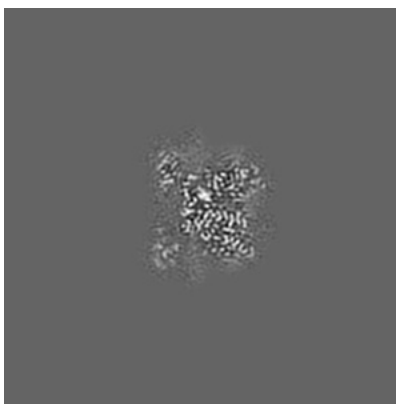
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

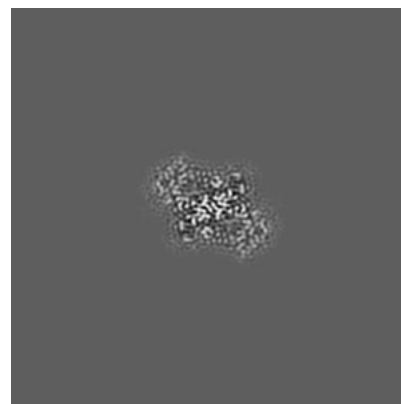
6.3.1 Primary map



X Index: 134



Y Index: 122

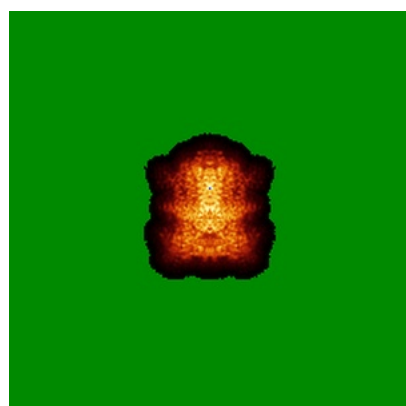


Z Index: 121

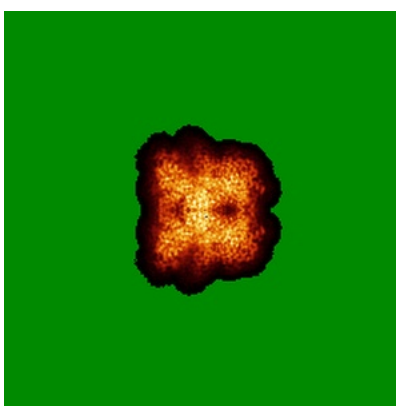
The images above show the largest variance slices of the map in three orthogonal directions.

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

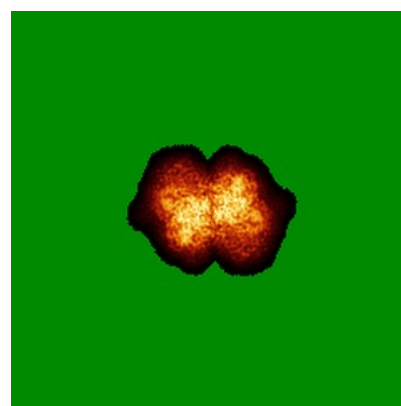
6.4.1 Primary map



X



Y

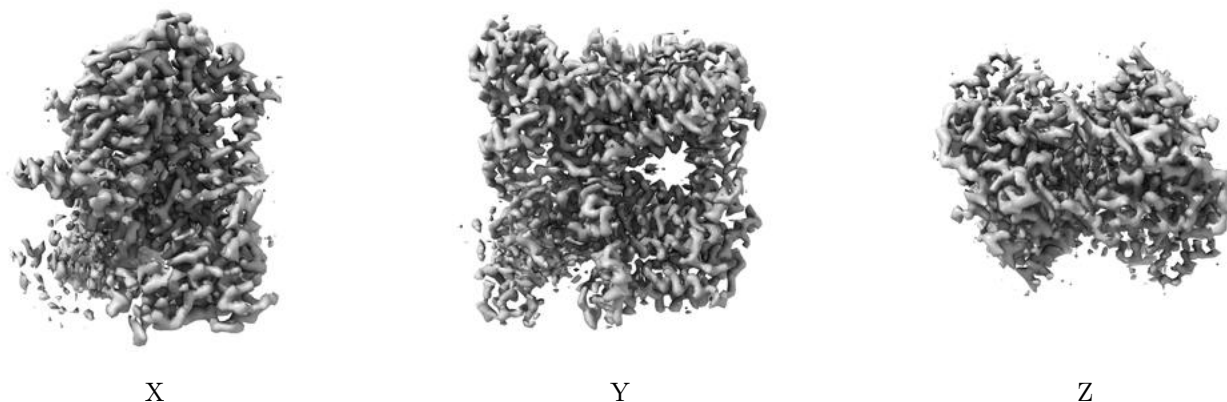


Z

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 [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.048. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

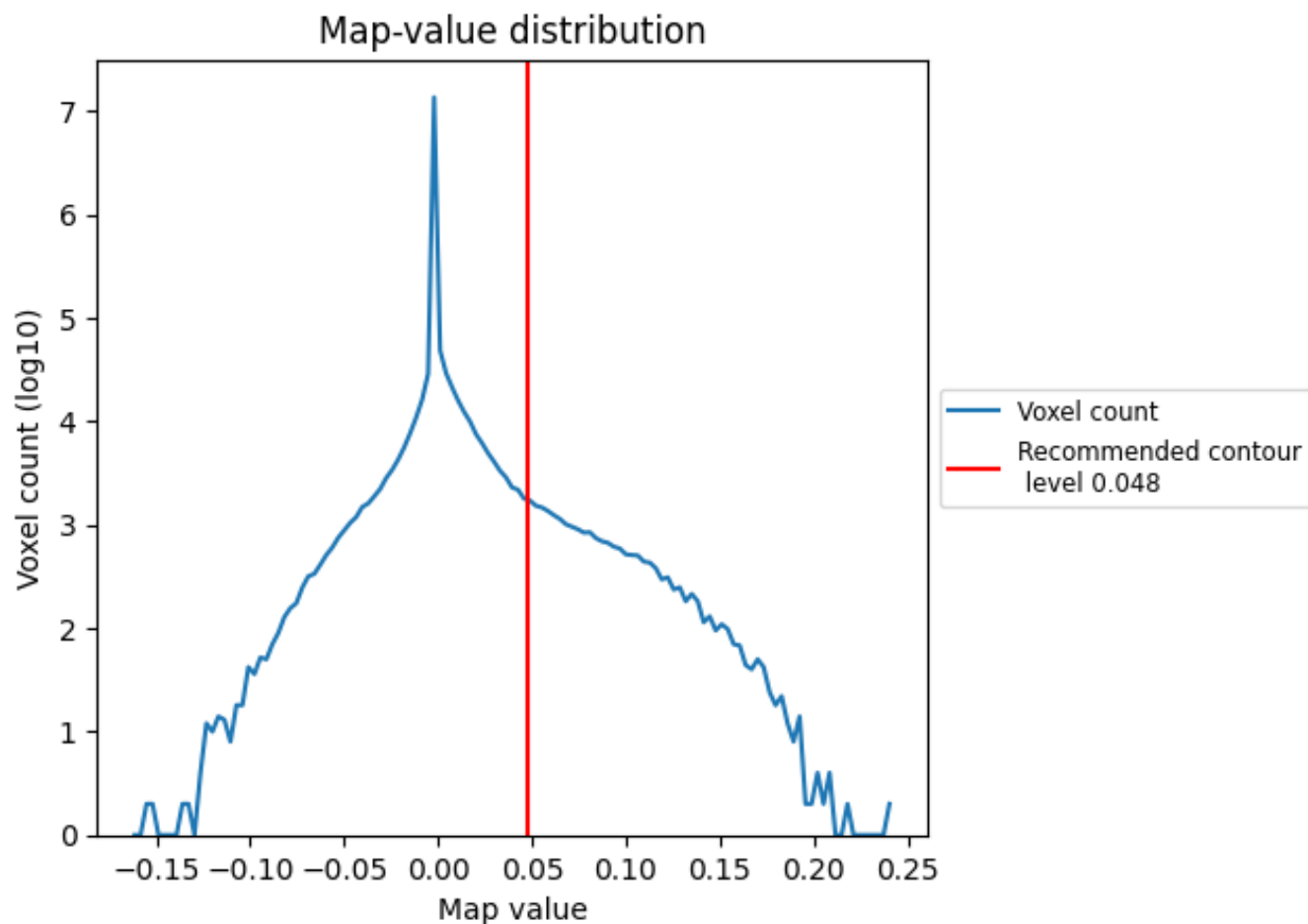
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

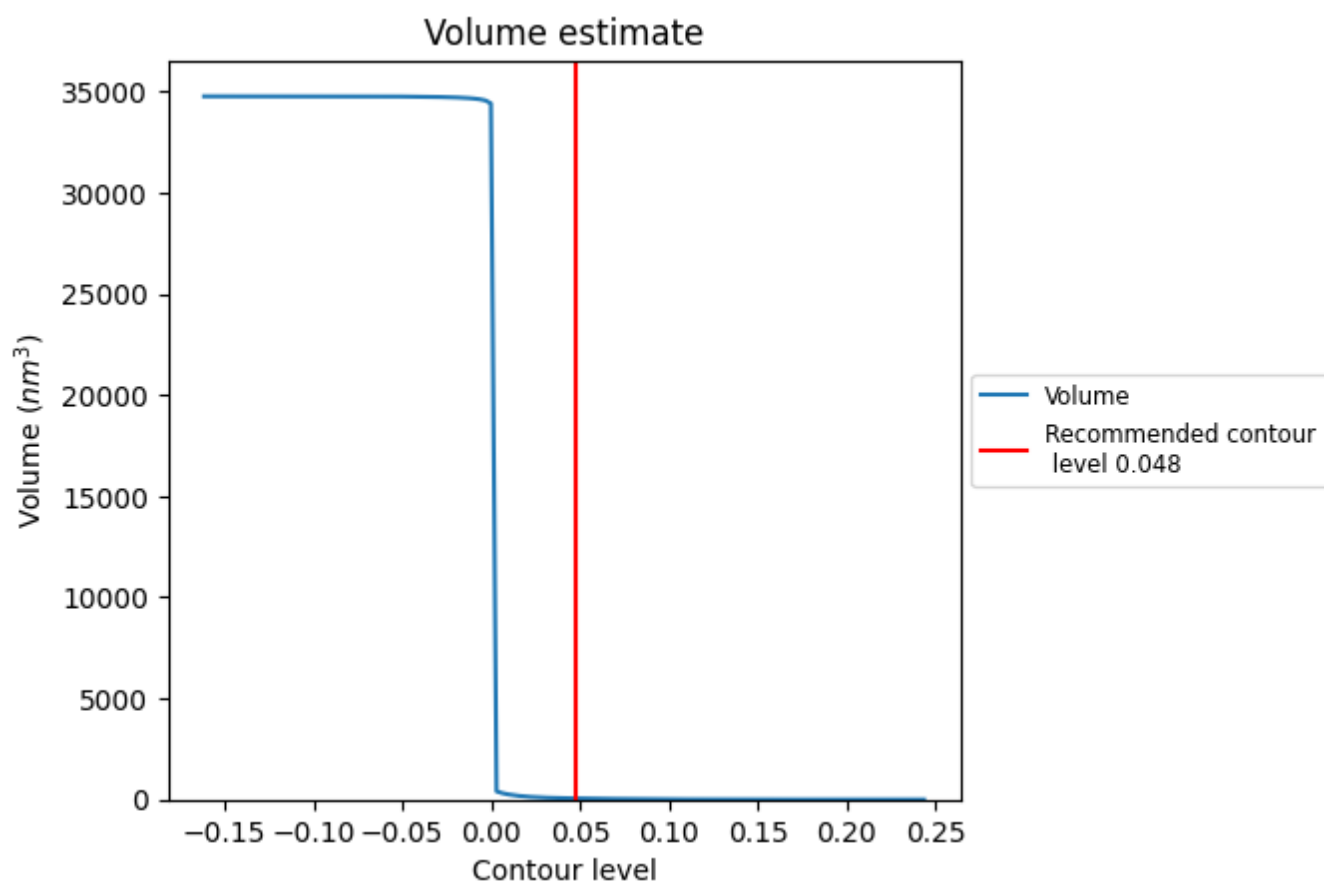
This section contains the results of statistical analysis of the map.

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.

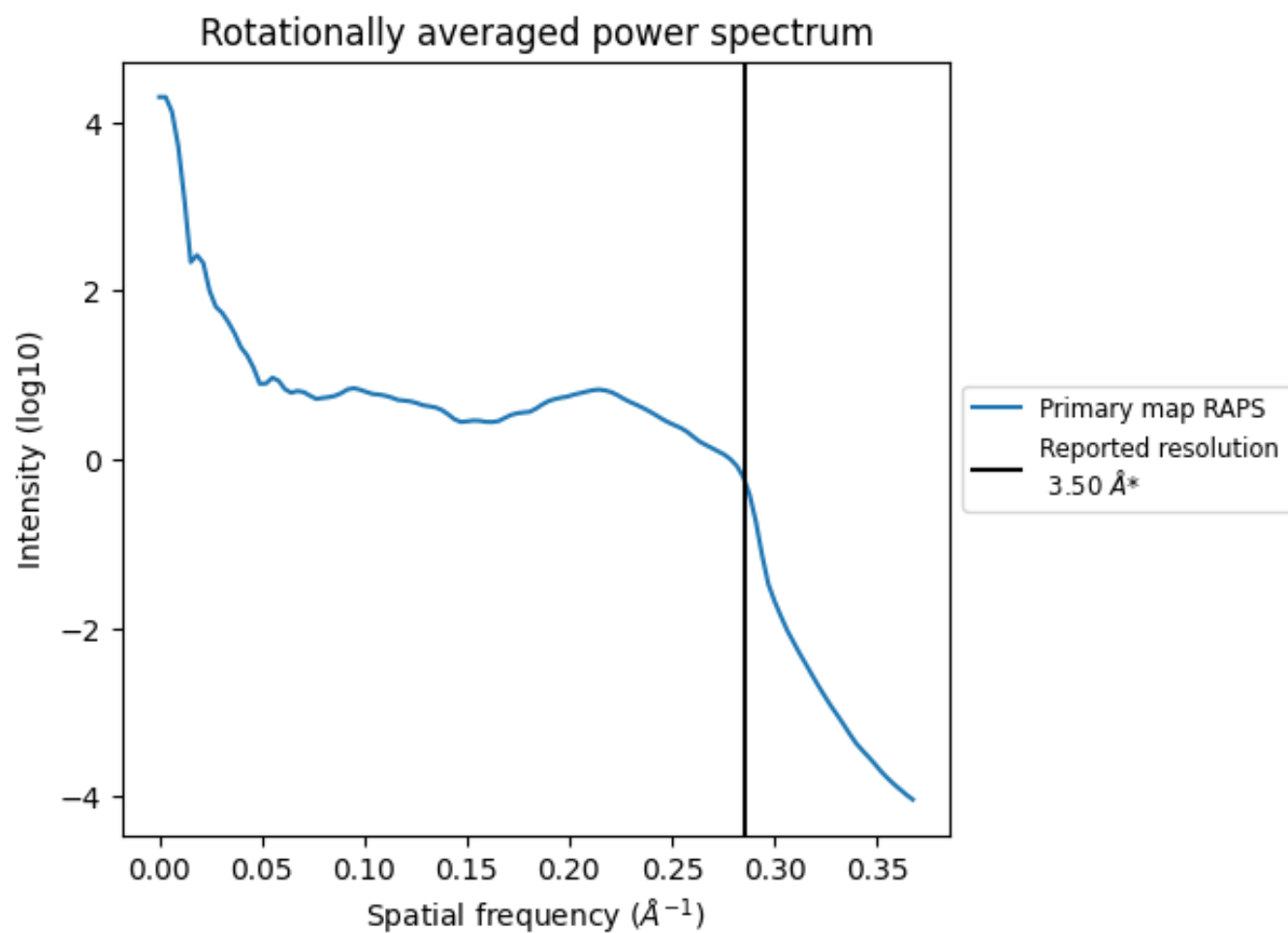
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 56 nm³; 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 ⓘ

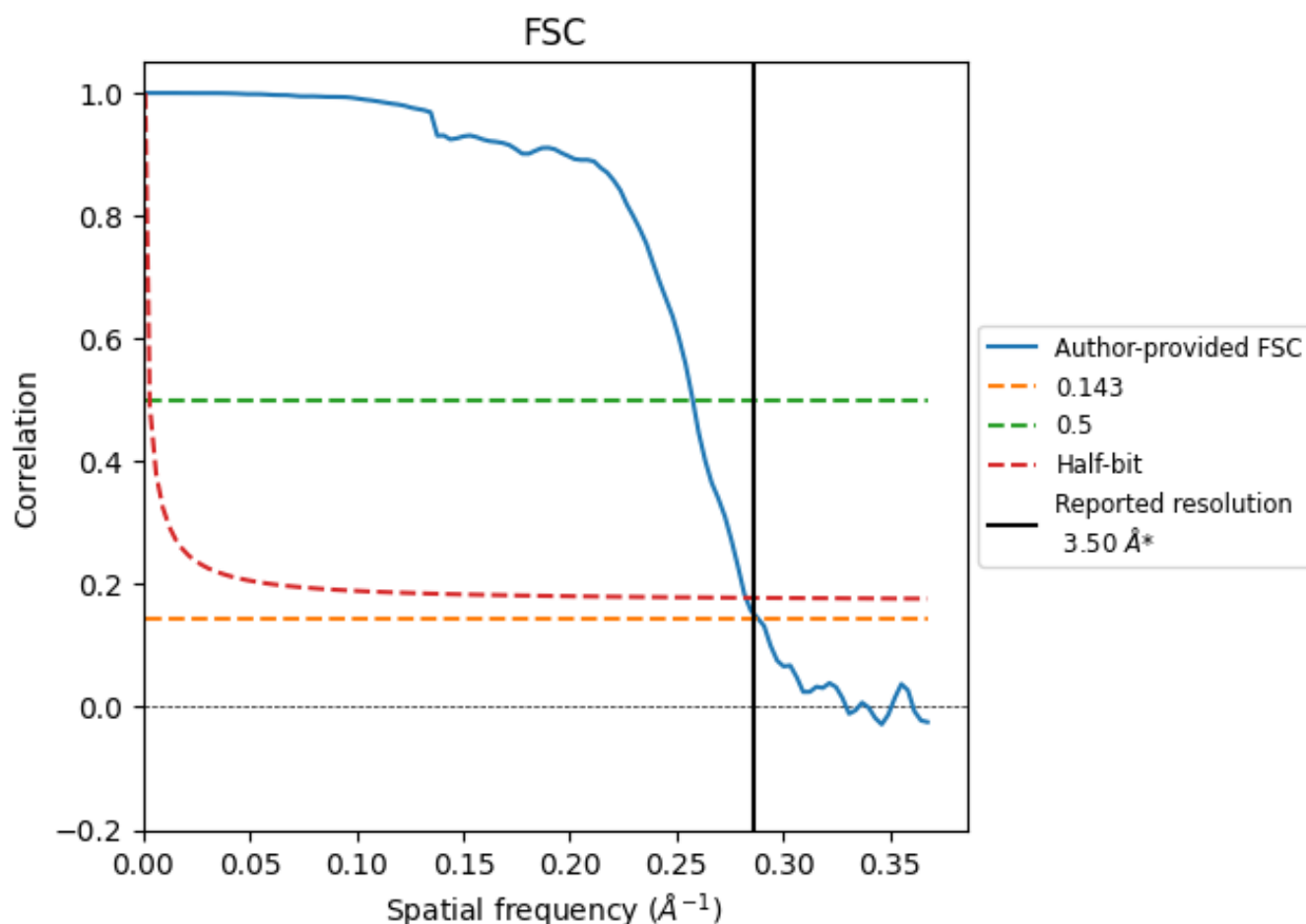


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

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](#)

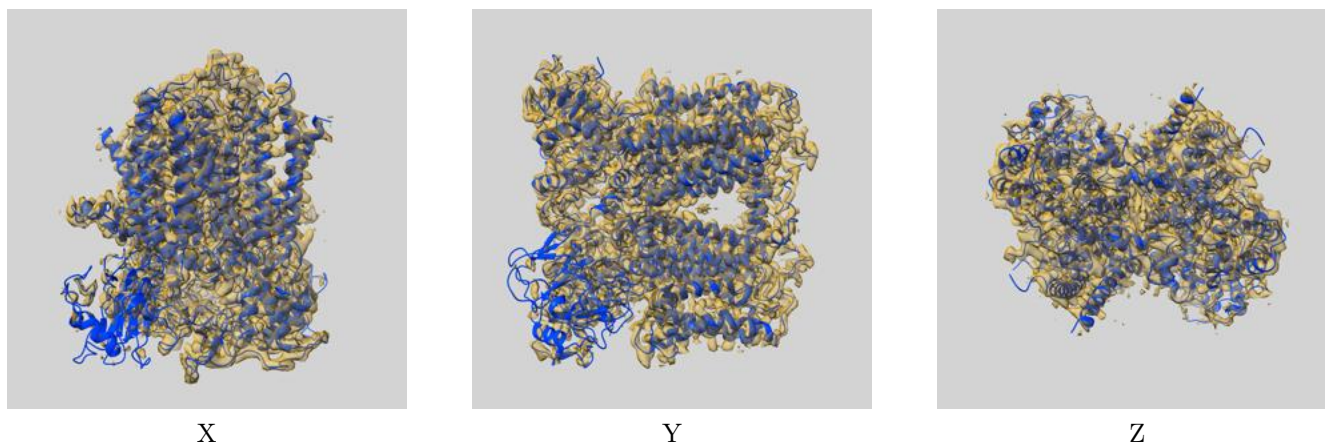
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.47	3.88	3.54
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

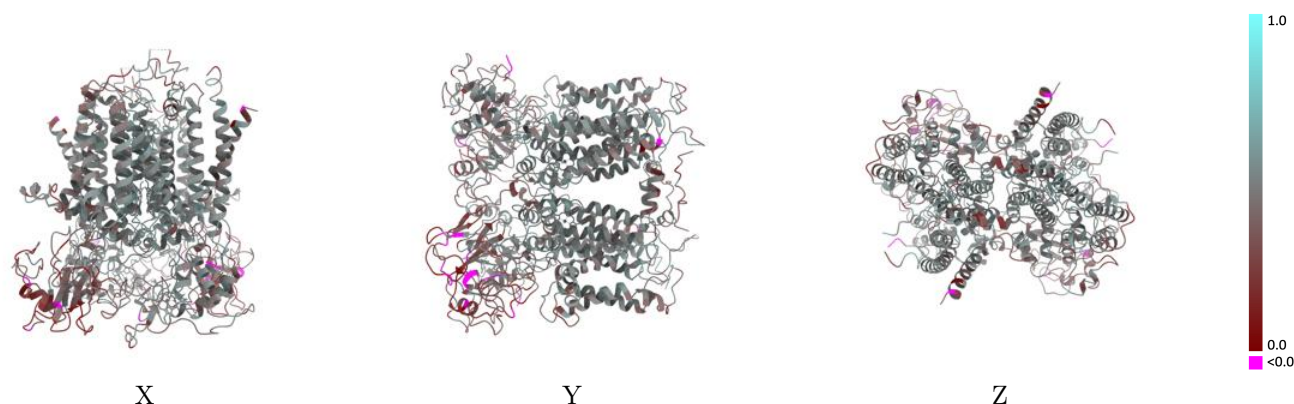
This section contains information regarding the fit between EMDB map EMD-22226 and PDB model 6XKV. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

9.1 Map-model overlay [i](#)



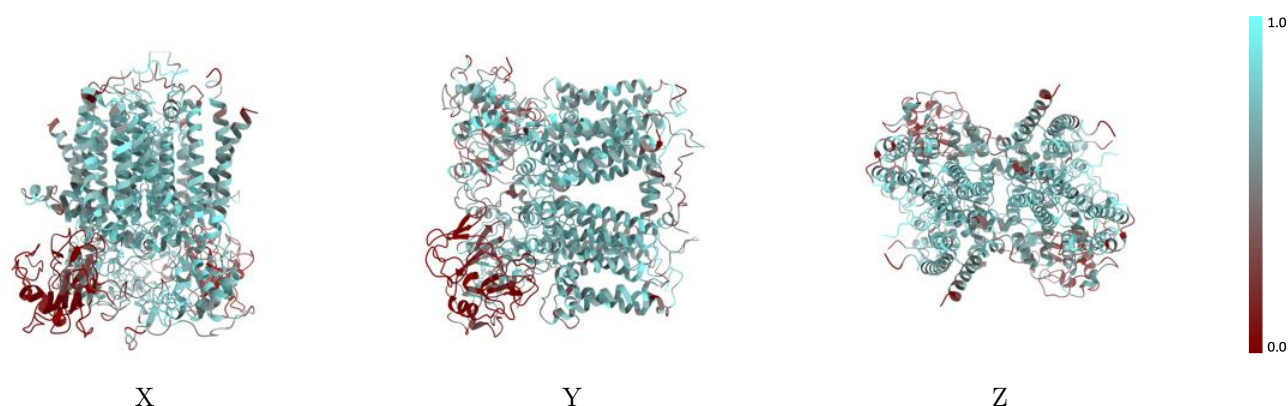
The images above show the 3D surface view of the map at the recommended contour level 0.048 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



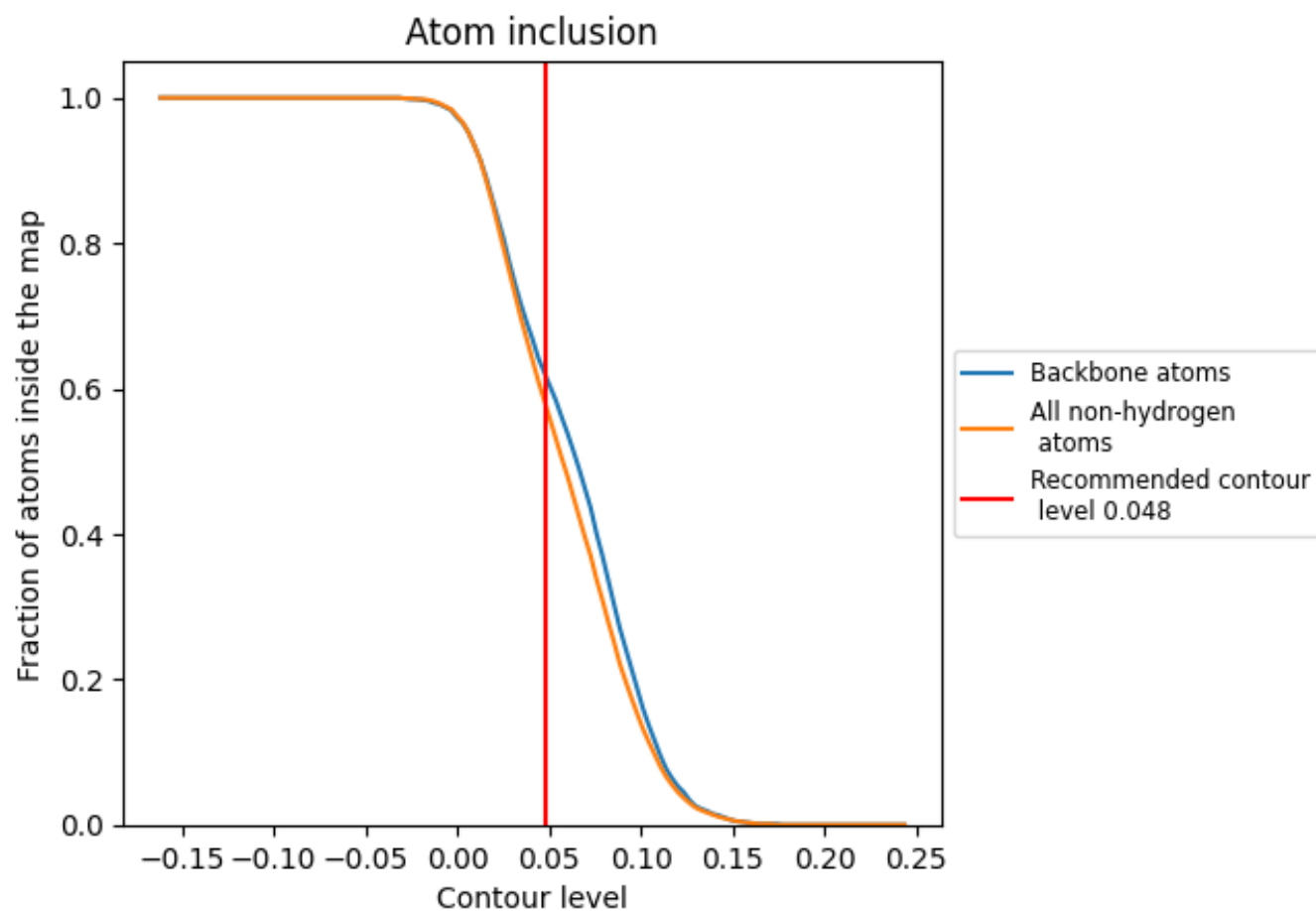
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.048).

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