



wwPDB EM Validation Summary Report ⓘ

Dec 10, 2022 – 11:17 pm GMT

PDB ID : 6R9G
EMDB ID : EMD-4770
Title : Structural basis of transcription inhibition by the DNA mimic Ocr protein of bacteriophage T7
Authors : Ye, F.Z.; Zhang, X.D.
Deposited on : 2019-04-03
Resolution : 3.70 Å(reported)

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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.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

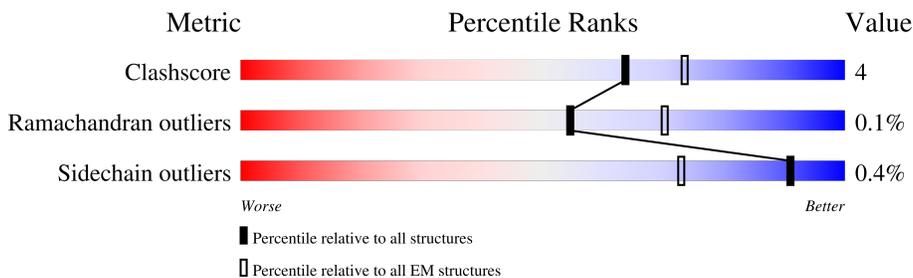
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	329	
1	B	329	
2	C	1342	
3	D	1407	
4	E	80	
5	F	117	
5	G	117	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 25944 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 DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	230	Total	C	N	O	S	0	0
			1765	1100	308	351	6		
1	B	231	Total	C	N	O	S	0	0
			1743	1090	301	346	6		

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	1341	Total	C	N	O	S	0	0
			10112	6334	1735	2006	37		

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	1334	Total	C	N	O	S	0	0
			10051	6297	1777	1934	43		

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	75	Total	C	N	O	S	0	0
			572	351	110	109	2		

- Molecule 5 is a protein called Overcome classical restriction gp0.3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	G	104	Total	C	N	O	S	0	0
			849	534	131	179	5		
5	F	106	Total	C	N	O	S	0	0
			852	530	136	182	4		

E181	R182	I183	A184	Y185	N186	V187	E188	A189	A190	R191	V192	E193	Q194	R195	T196	D197	L198	D199	K200	L201	V202	I203	E204	M205	E206	T207	N208	G209	T210	I211	D212	P213	E214	E215	A216	I217	R218	R219	A220	A221	T222	I223	L224	A225	E226	Q227	L228	E229	A230	F231	D232	L233	R235	ASP	VAL	ARG	GLN	PRO
GLU	VAL	LYS	GLY	LYS	VAL	PRO	PHE	ASP	ARG	PRO	ILE	LEU	LEU	LEU	ARG	PRO	MET	ARG	VAL	ASP	LEU	ASP	LEU	ASP	LEU	ASP	ASN	LEU	ILE	HIS	TVR	ILE	GLY	ASP	VAL	GLN	ARG	THR	GLU	VAL	LEU	LEU	LEU	LYS	THR	PRO	ASN	LEU	GLY	LYS	LYS	SER	LEU					
THR	GLU	ILE	LYS	ASP	VAL	LEU	SER	LEU	LEU	ILE	MET	ARG	LEU	ASP	LEU	ASN	TRP	PRO	ALA	ALA	ALA	ASP	GLU	THR	VAL	ARG	SER	ILE	ALA	ALA	ASP	GLU	THR	VAL	ARG	THR	GLU	VAL	LEU	LEU	LEU	LYS	THR	PRO	ASN	LEU	GLY	LYS	LYS	SER	LEU							

● Molecule 2: DNA-directed RNA polymerase subunit beta



M1	V2	Y3	S4	Y5	T6	E7	K8	R9	R10	I11	R12	K13	D14	F15	G16	K17	R18	P19	Q20	V21	L22	D23	V24	P25	Y26	L27	L28	S29	I30	Q31	L32	D33	S34	F35	Q36	K37	F38	I39	E40	Q41	D42	P43	E44	G45	Q46	Y47	G48	L49	E50	A51	A52	F53	R54	S55	V56	F57	P58	I59	Q60	
S61	Y62	S63	G64	N65	S66	E67	L68	Q69	Y70	M71	S72	Y73	R74	L75	G76	E77	P78	V79	F80	D81	V82	Q83	E84	C85	Q86	I87	R88	G89	V90	T91	Y92	L93	S94	A94	P95	L96	R97	F98	I99	L100	R101	L102	V103	I104	Y105	E106	R107	E108	A109	P110	E111	G112	T113	V114	K115	D116	I117	K118	E119	Q120
E121	V122	Y123	M124	G125	E126	I127	P128	L129	M130	T131	D132	N133	G134	L135	F136	V137	I138	N139	G140	D81	T141	E142	R143	V144	I145	A146	S147	Q148	L149	H150	R151	S152	P153	G154	V155	F156	R157	D158	S159	L160	K161	G162	K163	T164	H165	E166	S167	G168	K169	V170	L171	Y172	A173	V174	R175	I176	I177	P178	Y179	R180
G181	S182	V183	L184	S185	F186	E187	F188	L189	P190	K191	D192	N193	L194	F195	V196	R197	I198	D199	R200	R201	E202	K203	L204	P205	A206	T207	L208	I209	L210	R211	A212	L213	N214	Y215	T216	F157	E218	Q219	L220	L221	D222	L223	F224	F225	E226	K227	V228	L229	F230	E231	L232	R233	D234	N235	K236	V237	L238	Q239	M239	E240
L241	V242	P243	E244	R245	L246	R247	G248	E249	T250	A251	S252	F253	D254	I255	E256	A257	N258	G259	K260	V261	V262	V263	E264	K265	G266	R267	R268	I269	T270	A271	R272	H273	L274	R275	Q276	L277	E278	K279	D280	D281	V282	K283	L284	I285	E286	V287	P288	V289	L290	Y291	L292	A293	G294	K295	V296	V297	A298	K299	D300	
Y301	L302	D303	E304	S305	T306	G307	E308	L309	L310	C311	A312	A313	N314	M315	E316	L317	S318	L319	D320	L321	L322	A323	K324	L325	S326	Q327	S328	G329	H330	K331	R332	I333	E334	T335	L336	F337	T338	N339	D340	L341	D342	H343	G344	F345	Y346	T347	S348	E349	T350	L351	R352	V353	D354	G355	P356	T356	N357	D358	R359	L360
S361	A362	L363	V364	E365	L366	Y367	R368	K369	K370	R371	P372	G373	E374	P375	P376	T377	R378	E379	A380	A381	E382	S383	L384	F385	S386	N387	L388	F389	F390	S391	E392	D393	R394	Y395	D396	L397	S398	A399	V400	G401	R402	M403	L404	F405	N406	R407	S408	L409	L410	R411	E412	E413	L414	E415	G416	S417	Q418	L419	L420	
S421	K422	D423	D424	D425	L426	D427	V428	M429	K430	K431	L432	L433	D434	L435	R436	M437	G438	K439	G440	E441	V442	D443	D444	L445	F446	H447	L448	G449	N450	R451	R452	L453	F454	R455	D456	G457	E458	M459	A460	E461	N462	Q463	F464	R465	V466	G467	L468	V469	P470	R471	E472	R473	G474	V475	P476	D476	E477	R478	L479	S480
L481	G482	D483	L484	D485	T486	L487	M488	P489	Q490	D491	M492	L493	M494	A495	K496	P497	S498	A500	A501	V502	R503	E504	F505	F506	G507	S508	S509	L511	S512	F513	L514	S515	D516	Q517	N518	N519	P520	L521	S522	E523	I524	F525	H526	K527	R528	S529	P530	L531	S531	A532	L533	G534	P535	D536	G537	L538	T539	R540		
E541	R542	A543	G544	F545	E546	V547	M548	D549	V550	H551	P552	T553	H554	Y555	G556	R557	V558	C559	P560	I561	E562	T563	P564	E565	G566	P567	N568	G570	L571	I572	M573	R574	L575	S576	Y577	Y578	A579	Q580	T581	N582	E583	Y584	G585	F586	L587	E588	T589	P590	Y591	R592	K593	G594	T595	D596	G597	V598	Y599	T600		

F1323	D601
N1324	E602
V1325	I603
L1326	H604
L1327	Y605
K1328	L606
E1329	S607
I1330	A608
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N1336	G614
I1337	V615
E1338	I616
L1339	A617
E1340	Q618
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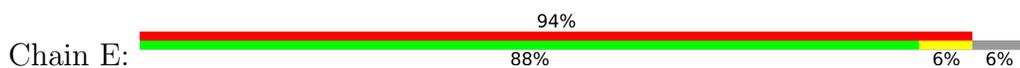
- Molecule 3: DNA-directed RNA polymerase subunit beta'



MET	LYS	ASP	LEU	LYS	PHE	LEU	LYS	ALA	GLN	THR	LYS	T14	E15	E16	F17	D18	A19	I20	K21	I22	A23	L24	A25	S26	P27	D28	M29	I30	R31	S32	W33	F35	G36	E37	V38	K39	K40	P41	E42	T43	I44	N45	Y46	R47	T48	F49	K50	P51	E52	R53	G55	L56	F57	C58	A59	R60										
I61	F62	G63	P64	V65	K66	D67	Y68	E69	C70	L71	C72	G73	K74	Y75	K76	R77	L78	K79	H80	R81	G82	V83	I84	C85	V86	K87	C88	G89	V90	E91	S92	V93	F95	T93	L94	Q94	T95	K96	V97	Q98	R99	E100	R101	M102	G103	H104	I105	I106	L107	A108	S109	P110	T111	A112	H113	I114	W115	F116	L117	K118	S119	L120				
P121	S122	R123	I124	G125	L126	L127	L128	M129	M130	P131	L132	R133	D134	I135	E136	R137	L138	L139	Y140	E142	S143	Y144	V145	V146	I147	E148	G149	G150	M151	T152	M153	L154	E155	R156	Q157	Q158	I159	L160	T161	E162	E163	Q164	Y165	L166	L167	A168	L169	E170	E171	F172	G173	D174	E175	F176	D177	A178	K179	M180								
G181	A182	E183	A184	I185	Q186	A187	L188	L189	K190	S191	M192	D193	L194	E195	Q196	E197	C198	E199	Q200	L201	R202	E203	E204	L205	L206	E207	T208	M209	S210	E211	T212	K213	R214	K215	K216	L217	T218	K219	R220	I221	K222	L223	L224	E225	A226	F227	V228	Q229	S230	G231	N232	K233	D234	E235	W236	M237	D177	L238	L239	T240						
L242	P243	V244	L245	P246	P247	D248	L249	R250	P251	L252	V253	P254	L255	D256	G257	G258	R259	F260	L261	T262	S263	D264	L265	L266	D267	L268	Y269	R270	R271	V272	I273	I274	N274	R275	N276	N277	R278	L279	K280	R281	L282	L283	D284	L285	A286	A287	P288	D289	L290	I291	V292	R293	N294	E295	K296	R297	M298	L299	Q300							
E301	A302	V303	D304	A305	L306	L307	D308	R309	G310	R311	R312	G313	A315	I316	T317	G318	S319	N320	K321	R322	P323	L324	K325	S326	L327	A328	D329	K330	I331	K332	G333	K334	Q335	G336	R337	F338	R339	Q340	N341	L342	L343	G344	K345	R346	V347	D348	Y349	R352	S353	V354	L355	T356	V357	G358	P359	Y360	L361									
R362	L363	H364	Q365	C366	G367	L368	P369	K370	K371	R372	A373	L374	E375	L376	F377	R378	P379	F380	I381	Y382	K384	L385	E386	R388	G389	L390	A391	T392	T393	I394	K395	A396	A397	K398	A400	V401	E402	R403	E404	E405	A406	V407	V408	W409	D410	I411	L412	D413	E414	V415	I416	R417	E418	H419	P420	V421										
L422	L423	N424	R425	A426	P427	T428	L429	H430	R431	L432	G433	I434	Q435	A436	F437	E438	V440	L441	L442	E443	C444	R445	A446	L447	Q448	L449	H450	P451	L452	V453	C454	A455	A456	Y457	N458	A459	D460	F461	D462	C463	D464	Q465	M466	A467	V468	H469	V470	P471	L472	T473	L474	E475	A476	Q477	L478	E479	A480	R481								
A482	L483	H484	H485	S486	T487	N488	H489	I490	L491	S492	P493	A494	H495	G496	E497	P498	I499	F500	V501	P502	S503	Q504	D505	V506	Y507	L508	G509	L510	Y511	Y512	M513	T514	R515	D516	C517	V518	N519	A520	K521	G522	G523	M524	M525	V526	L527	T528	G529	P530	K531	E532	A533	E534	R535	L536	Y537	R538	S539	G540	L541							
A542	S543	L544	H545	A546	R547	V548	K549	V550	R551	F552	T553	E554	Y555	E556	K557	D558	A559	M560	G561	E562	L563	V564	A565	K566	Y626	T627	G628	F629	A630	Y631	A632	A633	V634	S635	G575	R576	A577	I578	S638	V639	G640	M581	F582	D642	D643	M644	V645	K585	G586	P647	E648	K649	K650	H651	E652	I653	L654	Q594	R635	L596	G597	E658	K598	S639	G540	L601
S602	K603	M604	L605	M606	T607	C608	V609	R610	I611	L612	G613	L614	K615	P616	T617	V618	I619	F620	A621	D622	G623	L624	M625	Y626	T627	G628	F629	A630	Y631	A632	A633	V634	S635	G575	R576	A577	I578	S638	V639	G640	M581	F582	D642	D643	M644	V645	K585	G586	P647	E648	K649	K650	H651	E652	I653	L654	Q594	R635	L596	G597	E658	K598	S639	G540	L601	
A662	E663	I664	Q665	E666	Q667	F668	Q669	S670	G671	L672	V673	T674	A675	G676	E677	R678	Y679	M680	K681	V682	L683	D684	I685	W686	M747	A687	A688	A689	M690	D691	R692	V693	S694	K695	A696	M697	M698	I699	N700	L701	Q702	T703	E704	T705	V706	L707	E708	R709	D710	L711	Q712	E713	L714	K715	Q716	V717	S718	A719	N720	S721						
I722	Y723	M724	M725	E666	D727	S728	Q729	A730	R731	G732	S733	A734	A735	Q736	I737	R738	Q739	L740	A741	G742	M743	R744	G745	L746	M747	A748	K749	P750	D751	G752	S753	I754	I755	E756	T757	F758	I759	T760	A761	N762	F763	R764	E765	G766	L767	N768	V769	L770	Q771	Y772	F773	I774	S775	T776	H777	G778	A779	R780	K781							

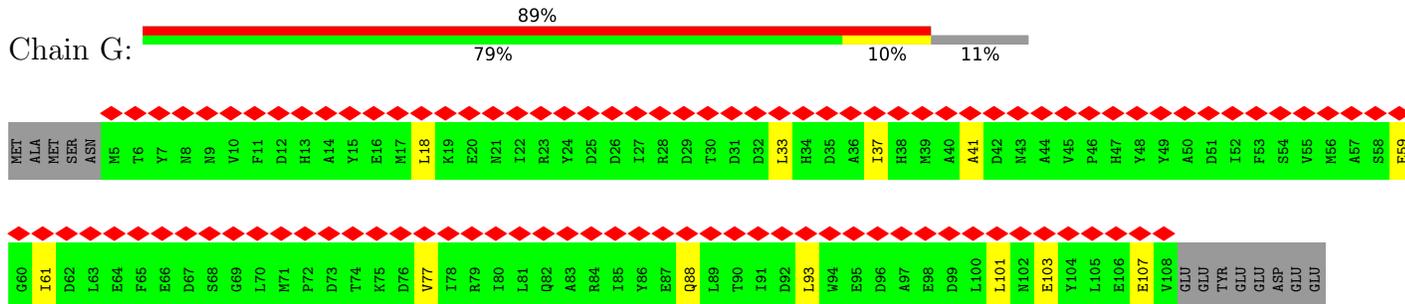
G782	L783	A784	D785	T786	A787	L788	K789	T790	K850	A791	N792	S793	G794	A854	Y795	L796	T797	R798	R799	L800	V801	D802	V803	A804	Q805	D806	L807	V808	V809	T810	E811	D812	D813	C814	G815	T816	H817	E818	G819	I820	M821	M822	T823	P824	V825	E826	E827	G828	G829	D830	V831	K832	E833	P834	L835	R836	D837	R838	L840	G841
R843	T844	A845	E846	D847	L848	L849	K850	P851	G852	T853	A854	D855	L856	L857	V858	P859	R860	N861	T862	S863	L864	H865	E866	Q867	W868	C869	D870	L871	L872	E873	E874	N875	S876	V877	D878	A879	V880	K881	V882	R883	S884	V885	V886	E887	C888	D889	T890	I891	F892	G893	V894	C895	A896	H897	C898	G899	R901			
D902	L903	A904	R905	G906	H907	L908	I909	N910	K911	G912	E913	A914	I915	G916	V917	I918	A919	A920	Q921	I922	G923	G924	E925	P926	Q927	T928	Q929	L930	T931	M932	R933	T934	F935	H936	I937	G938	G939	A940	A941	S942	R943	A944	A945	A946	E947	S948	S949	I950	Q951	V952	K953	N954	C955	G956	S957	I958	K959	L960	S961	
N962	V963	K964	S965	V966	V967	N968	S969	S970	G971	E972	L973	V974	I975	T976	S977	R978	N979	T980	E981	L982	K983	L984	I985	D986	E987	F988	G989	A990	R991	K992	E993	S994	V995	K996	V997	P998	G999	G1000	A1001	V1002	L1003	A1004	K1005	G1006	D1007	G1008	E1009	Q1010	V1011	A1012	G1013	G1014	E1015	T1016	V1017	A1018	N1019	W1020	D1021	
P1022	H1023	T1024	M1025	P1026	I1027	I1028	T1029	E1030	N1031	S1032	G1033	F1034	V1035	R1036	F1037	T1038	D1039	M1040	I1041	D1042	G1043	Q1044	T1045	I1046	T1047	R1048	Q1049	THR	ASP	GLU	LEU	THR	GLY	LEU	SER	S1058	L1059	V1060	V1061	L1062	D1063	I1124	A1064	E1066	R1067	THR	ALA	GLY	GLY	THR	LYS	ASP	LEU	R1075	P1076	A1077	L1078	K1079	I1080	V1081
D1082	A1083	Q1084	G1085	N1086	D1087	V1088	LEU	ILE	PRO	GLY	THR	ASP	MET	A1097	Q1098	V1099	F1100	L1101	P1102	G1103	K1104	I1105	I1106	V1107	Q1108	L1109	D1110	D1111	G1112	V1113	I1114	I1115	S1116	S1117	G1118	D1119	T1120	L1121	A1122	R1123	I1124	P1125	Q1126	GLU	GLY	THR	LYS	D1133	I1134	T1135	G1136	G1137	L1138	P1139	R1140	V1141				
A1142	D1143	L1144	F1145	E1146	A1147	R1148	R1149	P1150	K1151	E1152	P1153	A1154	I1155	L1156	A1157	E1158	I1159	S1160	G1161	I1162	S1163	S1164	F1165	G1166	K1167	E1168	T1169	K1170	G1171	K1172	R1173	R1174	L1175	V1176	I1177	P1178	T1179	V1180	D1181	G1182	S1183	D1184	P1185	V1186	E1187	E1188	M1189	I1190	P1191	K1192	W1193	R1194	Q1195	L1196	N1197	V1198	F1199	E1200	G1201	
E1202	R1203	V1204	E1205	R1206	G1207	D1208	V1209	I1210	S1211	D1212	G1213	P1214	E1215	A1216	P1217	H1218	D1219	I1220	L1221	L1222	L1223	R1224	V1225	V1226	H1227	A1228	V1229	T1230	R1231	Y1232	I1233	V1234	M1235	E1236	V1237	Q1238	D1239	V1240	Y1241	R1242	Q1244	G1245	V1246	K1247	I1248	M1249	D1250	K1251	H1252	I1253	E1254	L1255	I1256	V1257	R1258	Q1259	M1260	L1261		
R1262	K1263	A1264	T1265	V1266	M1268	A1269	R1330	S1270	S1271	S1272	D1273	F1274	L1275	E1276	G1277	E1278	Q1279	E1281	I1282	S1283	R1284	V1285	K1286	I1287	A1288	M1289	E1290	E1291	L1292	E1293	G1294	M1295	G1296	K1297	V1298	G1299	A1300	T1301	Y1302	S1303	R1304	D1305	L1306	L1307	G1308	I1309	T1310	K1311	A1312	S1313	L1314	A1315	T1316	E1317	F1318	I1320	S1321			
A1322	A1323	S1324	F1325	Q1326	E1327	T1328	T1329	R1330	V1331	L1332	T1333	E1334	A1335	A1336	V1337	A1338	G1339	K1340	R1341	D1342	E1343	L1344	R1345	G1346	L1347	K1348	E1349	M1350	V1351	I1352	V1353	G1354	R1355	L1356	I1357	P1358	A1359	G1360	T1361	G1362	A1364	Y1365	H1366	Q1367	D1368	R1369	M1370	R1371	R1372	R1373	A1374	A1375	G1376	GLU	ALA	PRO	ALA	ALA		
PRO	GLN	VAL	THR	ALA	GLU	ASP	ALA	SER	ALA	SER	LEU	ALA	ASN	ALA	GLY	GLY	GLY	SER	ASP	ASN	GLU																																							

• Molecule 4: DNA-directed RNA polymerase subunit omega

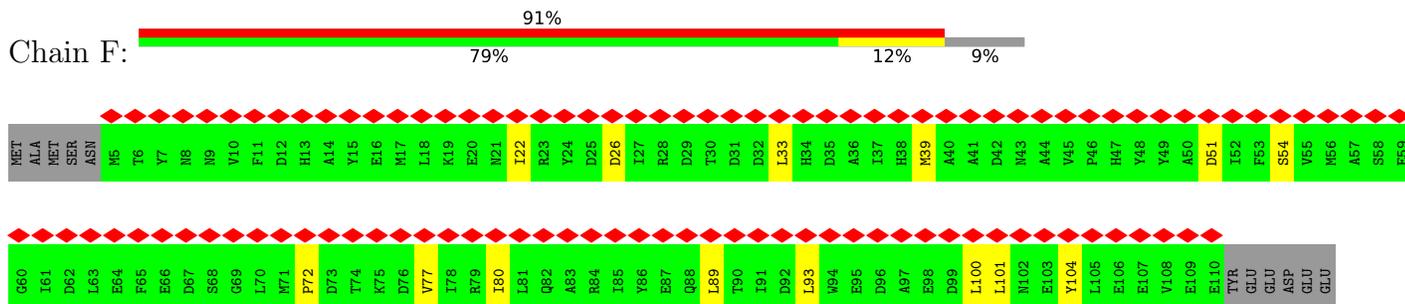


M1	A2	R3	V4	T5	V6	Q7	D8	A9	V10	E11	K12	I13	G14	M15	R16	F17	D18	L19	V20	L21	V22	A23	A24	R25	R26	A27	R28	Q29	M30	Q31	V32	G33	G34	K35	D36	P37	L38	V39	P40	E41	E42	M43	D44	K45	T46	T47	V48	I49	A50	L51	R52	E53	I54	E55	E56	G57	L58	I59	N60
N61	Q62	I63	L64	D65	V66	R67	E68	R69	Q70	E71	Q72	Q73	E74	GLU	ALA	ALA	GLY	LEU																																									

• Molecule 5: Overcome classical restriction gp0.3



• Molecule 5: Overcome classical restriction gp0.3



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	33646	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 ($e^-/\text{\AA}^2$)	49.53	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.220	Depositor
Minimum map value	-0.151	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	270.08, 270.08, 270.08	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.055, 1.055, 1.055	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.26	0/1786	0.52	0/2424
1	B	0.26	0/1764	0.57	0/2398
2	C	0.26	0/10263	0.53	0/13922
3	D	0.26	0/10187	0.51	0/13803
4	E	0.25	0/574	0.49	0/775
5	F	0.25	0/866	0.50	1/1177 (0.1%)
5	G	0.24	0/866	0.42	0/1178
All	All	0.26	0/26306	0.52	1/35677 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	26	ASP	CB-CG-OD1	5.19	122.97	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1765	0	1775	21	0
1	B	1743	0	1741	13	0
2	C	10112	0	9785	112	0
3	D	10051	0	10034	81	0
4	E	572	0	574	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	852	0	772	8	0
5	G	849	0	768	7	0
All	All	25944	0	25449	219	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 4.

The worst 5 of 219 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)
3:D:121:PRO:HD2	5:G:59:GLU:HG3	1.66	0.75
5:F:100:LEU:O	5:F:104:TYR:HB2	1.87	0.74
3:D:189:LEU:HD21	3:D:234:PRO:HB2	1.76	0.67
3:D:707:ILE:H	3:D:716:GLN:HG2	1.60	0.65
2:C:205:PRO:HG2	2:C:208:ILE:HG12	1.79	0.65

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	228/329 (69%)	220 (96%)	8 (4%)	0	100	100
1	B	229/329 (70%)	214 (93%)	13 (6%)	2 (1%)	17	54
2	C	1339/1342 (100%)	1226 (92%)	113 (8%)	0	100	100
3	D	1324/1407 (94%)	1198 (90%)	124 (9%)	2 (0%)	47	78
4	E	73/80 (91%)	66 (90%)	7 (10%)	0	100	100
5	F	104/117 (89%)	100 (96%)	4 (4%)	0	100	100
5	G	102/117 (87%)	100 (98%)	2 (2%)	0	100	100
All	All	3399/3721 (91%)	3124 (92%)	271 (8%)	4 (0%)	54	83

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	30	PRO
3	D	886	VAL
3	D	1183	SER
1	B	29	GLU

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	194/286 (68%)	193 (100%)	1 (0%)	88	94
1	B	189/286 (66%)	188 (100%)	1 (0%)	88	94
2	C	1057/1157 (91%)	1053 (100%)	4 (0%)	91	95
3	D	1048/1168 (90%)	1043 (100%)	5 (0%)	88	94
4	E	58/68 (85%)	58 (100%)	0	100	100
5	F	91/105 (87%)	91 (100%)	0	100	100
5	G	91/105 (87%)	91 (100%)	0	100	100
All	All	2728/3175 (86%)	2717 (100%)	11 (0%)	91	95

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	128	LEU
3	D	314	ARG
3	D	1268	ASN
3	D	320	ASN
2	C	1175	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
3	D	1023	HIS
3	D	1268	ASN

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Mol	Chain	Res	Type
3	D	320	ASN
3	D	341	ASN
3	D	504	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.

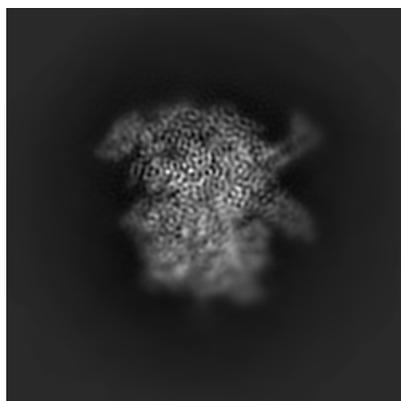
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4770. These allow visual inspection of the internal detail of the map and identification of artifacts.

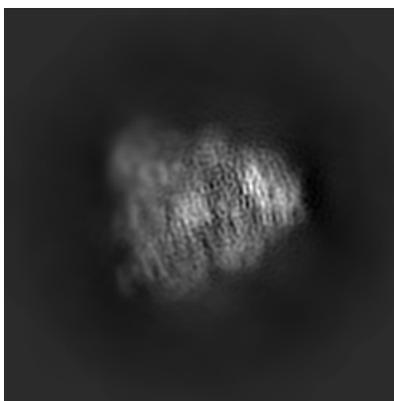
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

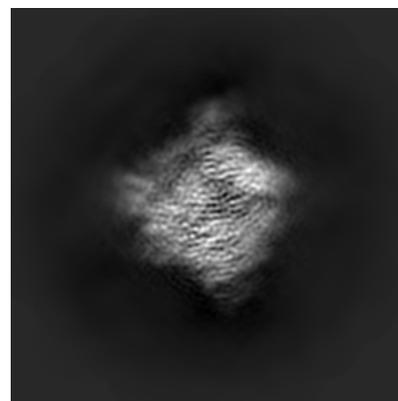
6.1.1 Primary map



X



Y

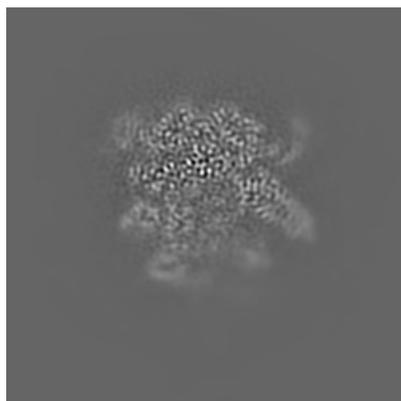


Z

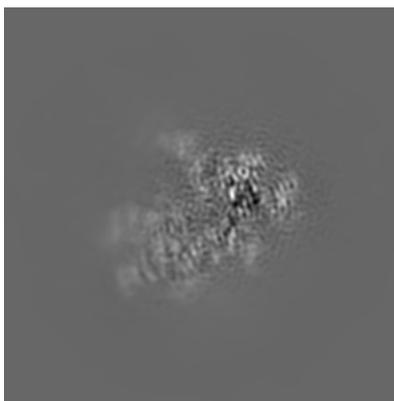
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

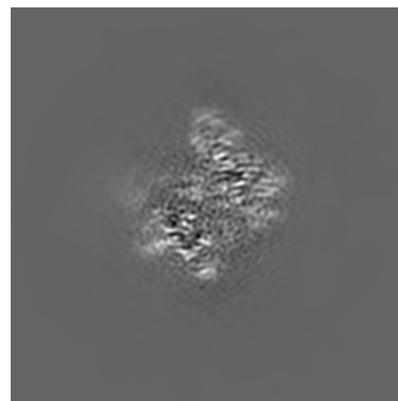
6.2.1 Primary map



X Index: 128



Y Index: 128

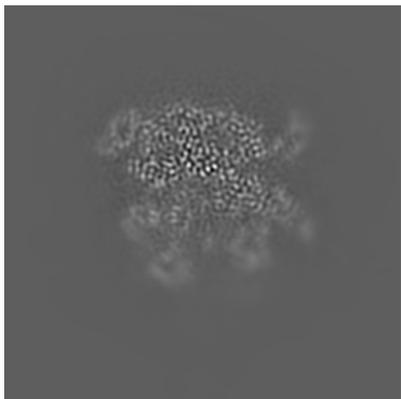


Z Index: 128

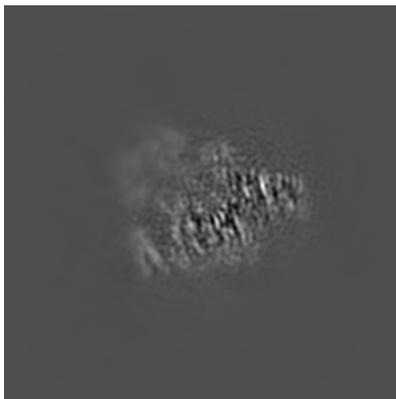
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

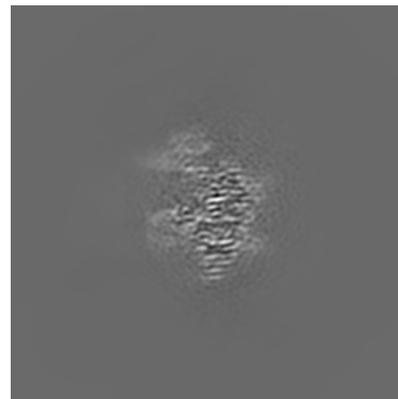
6.3.1 Primary map



X Index: 133



Y Index: 115



Z Index: 150

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

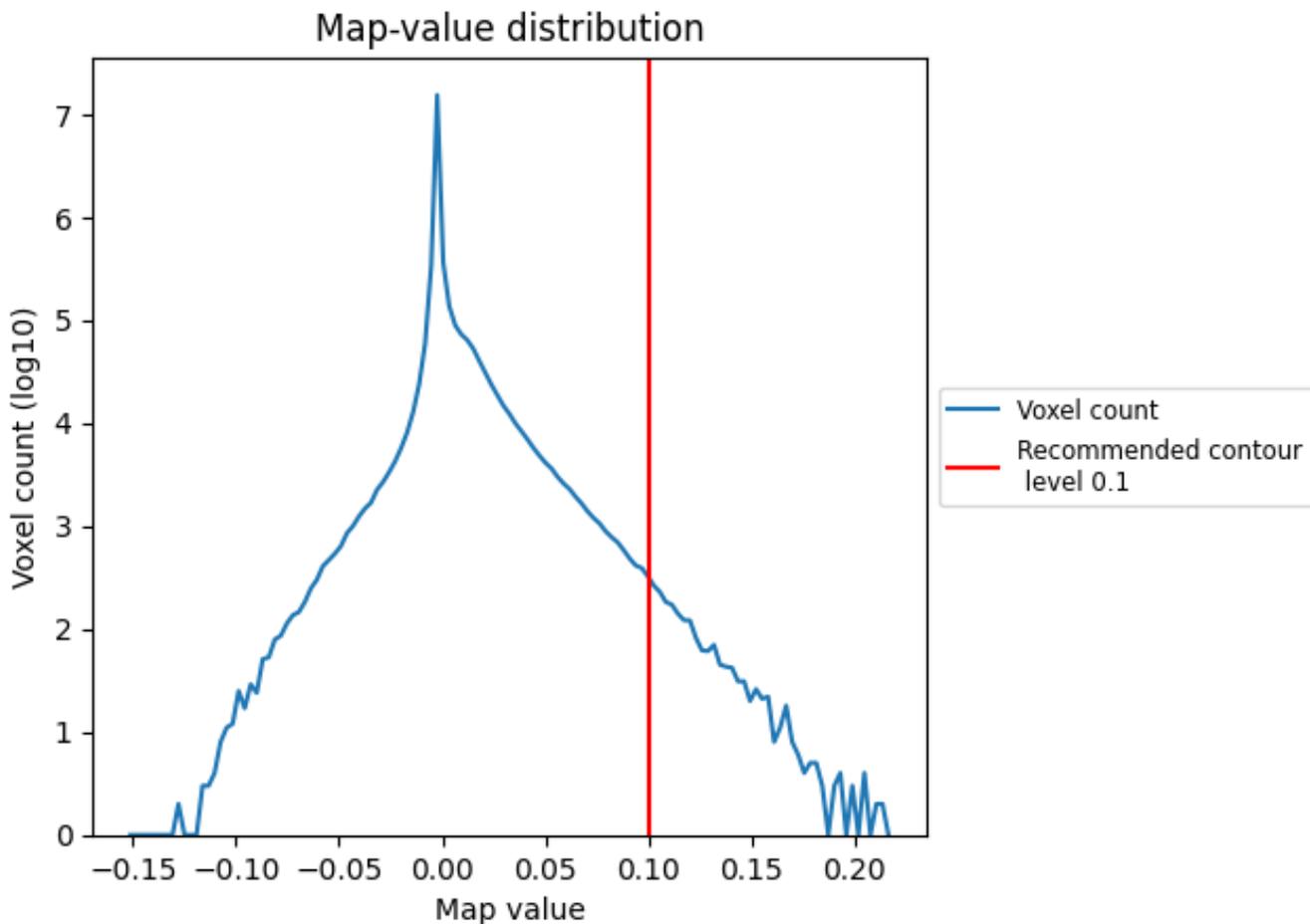
6.5 Mask visualisation

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

7 Map analysis [i](#)

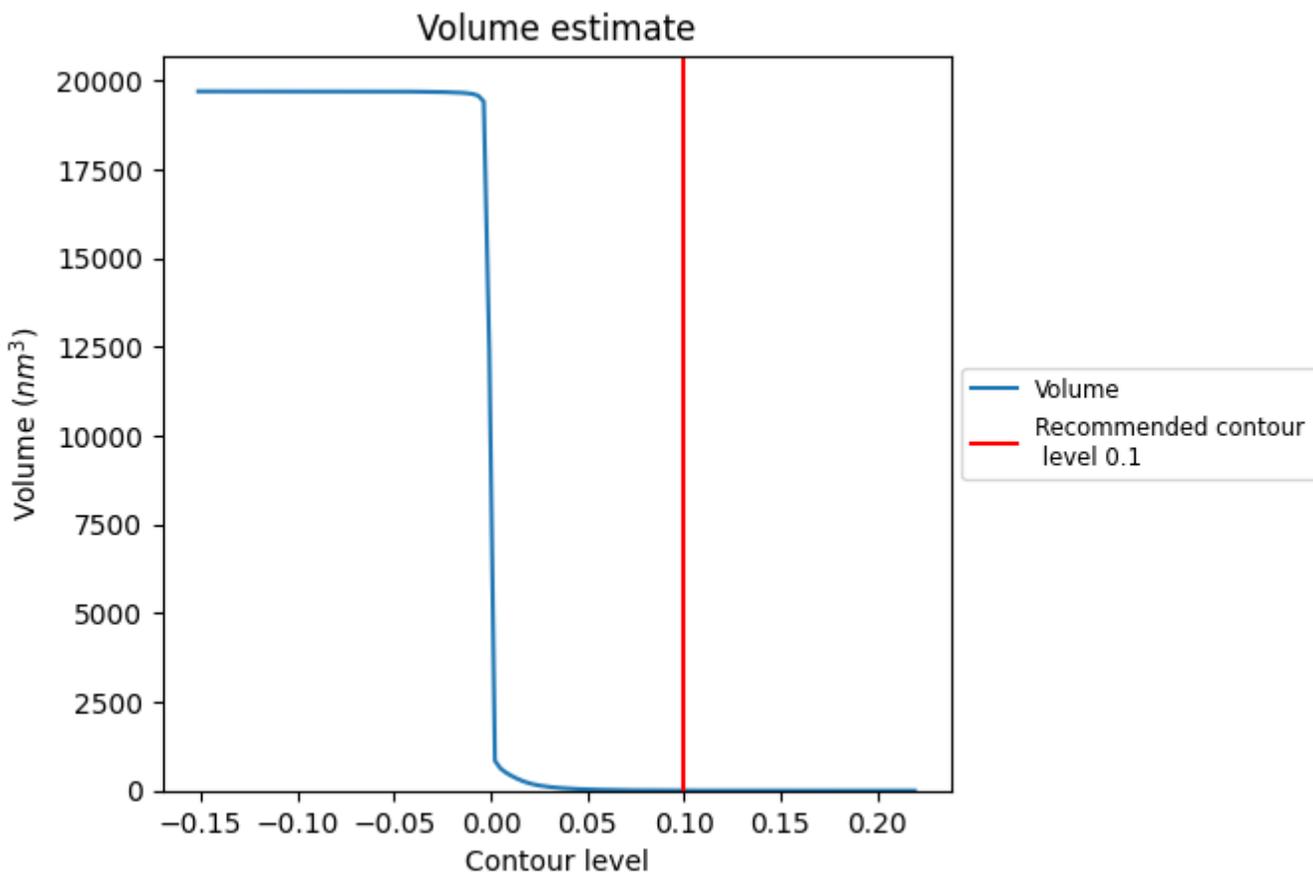
This section contains the results of statistical analysis of the map.

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.

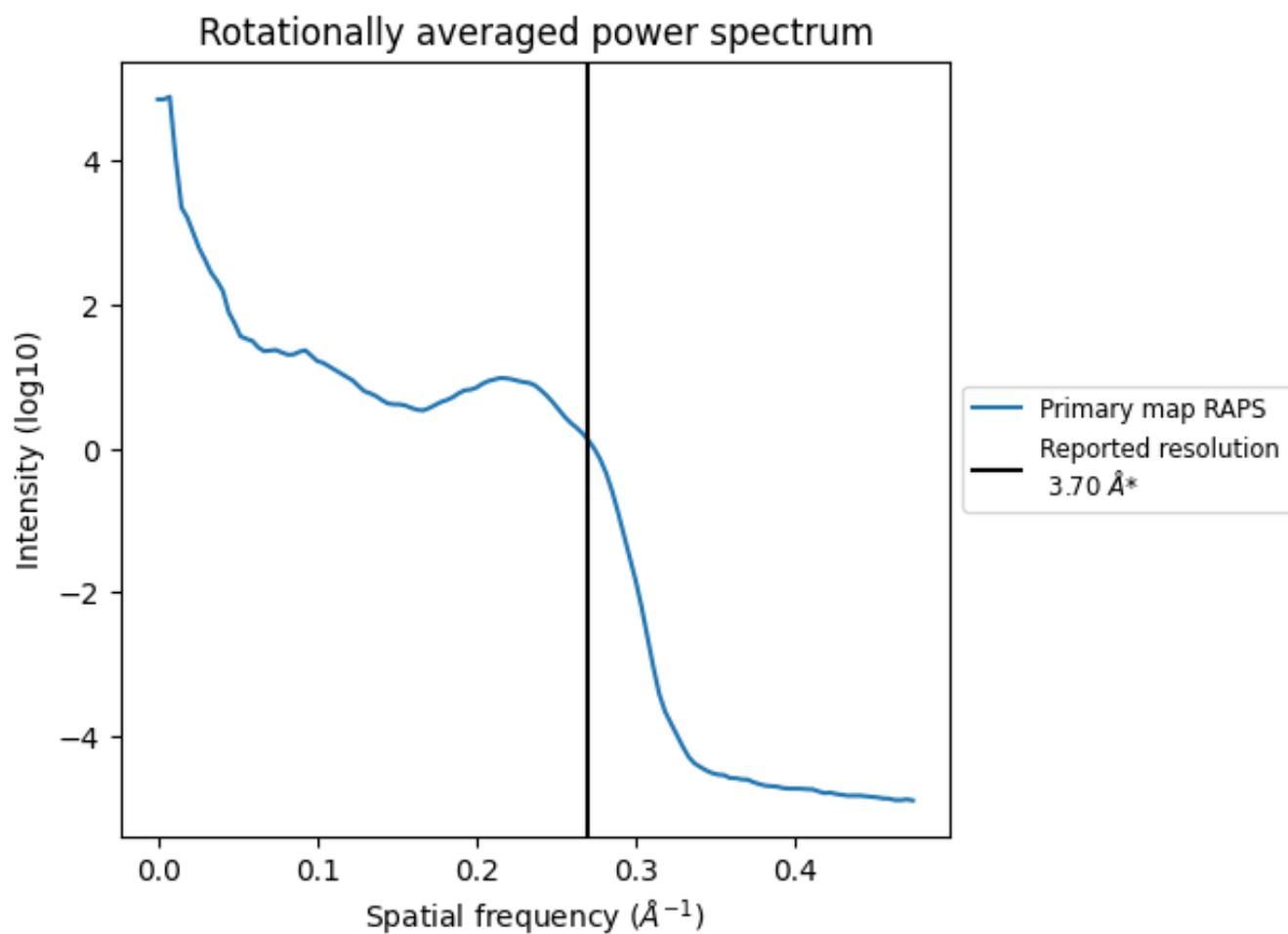
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3 nm³; this corresponds to an approximate mass of 2 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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

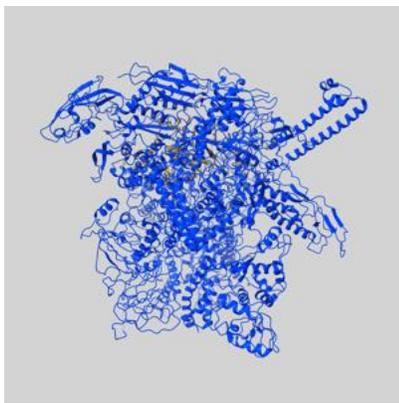
8 Fourier-Shell correlation

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

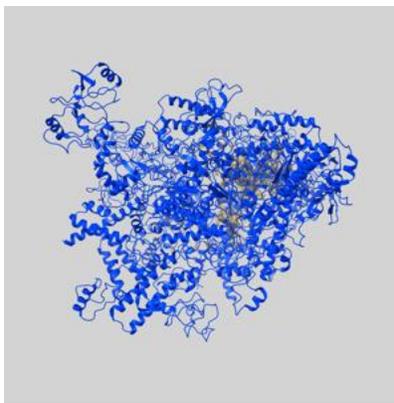
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-4770 and PDB model 6R9G. Per-residue inclusion information can be found in section 3 on page 4.

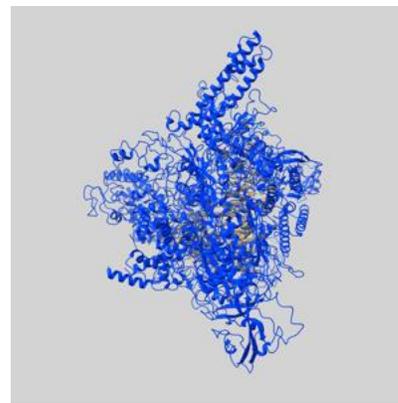
9.1 Map-model overlay [i](#)



X



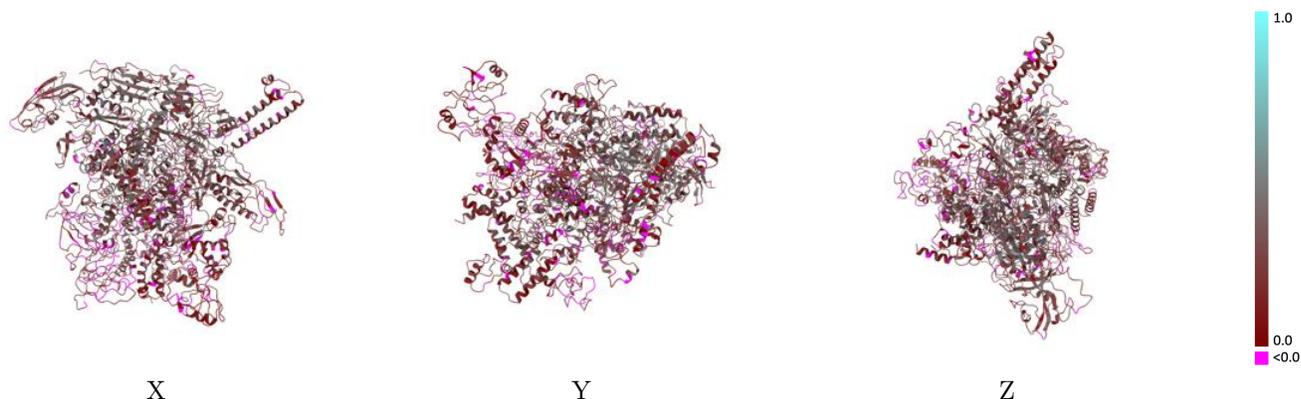
Y



Z

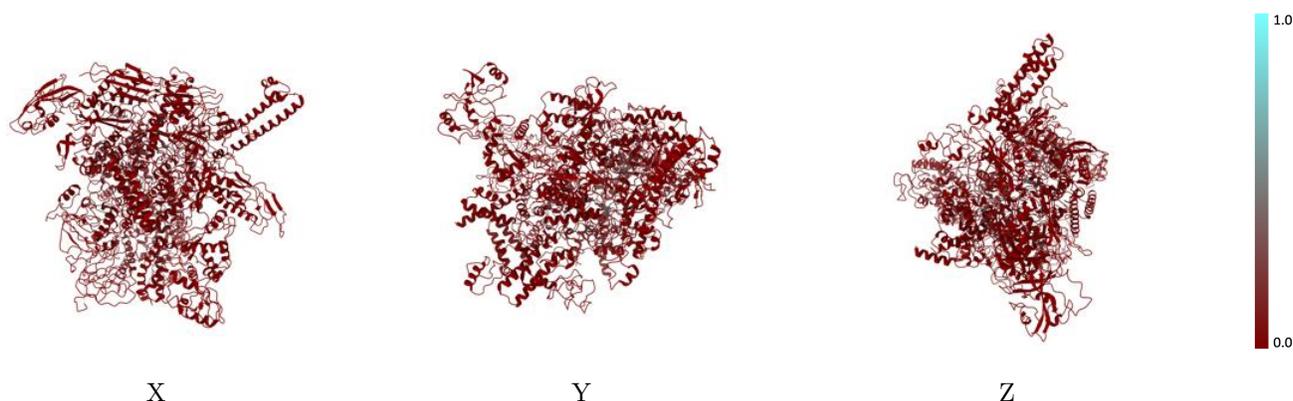
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



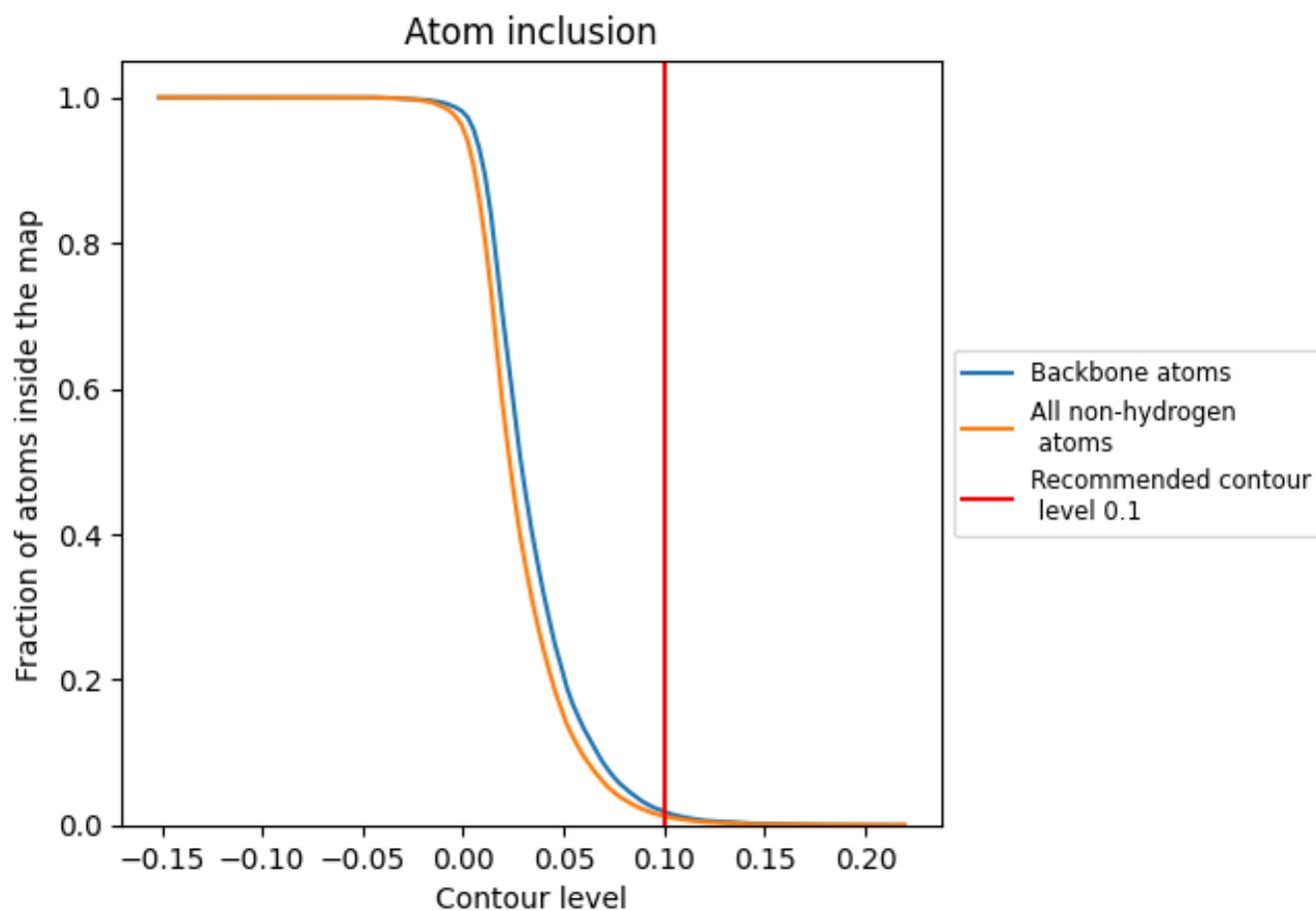
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 2% of all backbone atoms, 1% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.0125	 0.2250
A	 0.0058	 0.3070
B	 0.0029	 0.2760
C	 0.0166	 0.2340
D	 0.0141	 0.2030
E	 0.0000	 0.1290
F	 0.0000	 0.2230
G	 0.0000	 0.1720

