



wwPDB EM Validation Summary Report ⓘ

Oct 28, 2024 – 07:40 AM EDT

PDB ID : 8DGF
EMDB ID : EMD-27422
Title : Avs4 bound to phage PhiV-1 portal
Authors : Wilkinson, M.E.; Gao, L.; Strecker, J.; Makarova, K.S.; Macrae, R.K.; Koonin, E.V.; Zhang, F.
Deposited on : 2022-06-23
Resolution : 2.90 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

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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.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

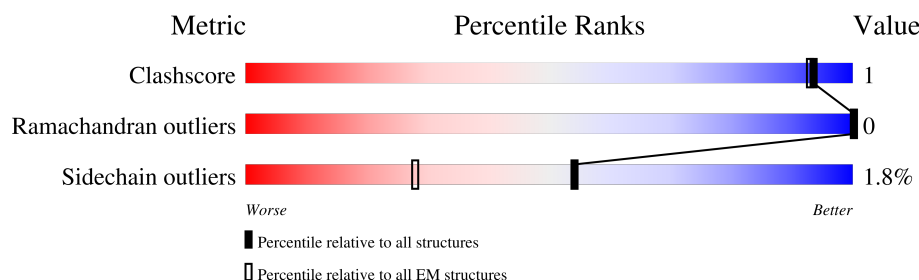
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	1587	<div> <div>66%</div> <div>93%</div> <div>• •</div> </div>
1	B	1587	<div> <div>69%</div> <div>92%</div> <div>• • •</div> </div>
1	C	1587	<div> <div>66%</div> <div>94%</div> <div>• •</div> </div>
1	D	1587	<div> <div>69%</div> <div>93%</div> <div>• • •</div> </div>
2	E	535	<div> <div>82%</div> <div>76%</div> <div>5%</div> <div>18%</div> </div>
2	F	535	<div> <div>82%</div> <div>73%</div> <div>8%</div> <div>18%</div> </div>
2	G	535	<div> <div>82%</div> <div>79%</div> <div>•</div> <div>18%</div> </div>
2	H	535	<div> <div>82%</div> <div>74%</div> <div>7%</div> <div>18%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 64958 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 ATP-binding protein Avs4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1541	Total	C	N	O	S	0	0
			12805	8291	2104	2370	40		
1	B	1534	Total	C	N	O	S	0	0
			12756	8265	2094	2358	39		
1	C	1541	Total	C	N	O	S	0	0
			12805	8291	2104	2370	40		
1	D	1534	Total	C	N	O	S	0	0
			12756	8265	2094	2358	39		

- Molecule 2 is a protein called Portal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	438	Total	C	N	O	S	0	0
			3427	2165	565	678	19		
2	F	438	Total	C	N	O	S	0	0
			3427	2165	565	678	19		
2	G	438	Total	C	N	O	S	0	0
			3427	2165	565	678	19		
2	H	438	Total	C	N	O	S	0	0
			3427	2165	565	678	19		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total 31	C 10	N 5	O 13	P 3	0
3	B	1	Total 31	C 10	N 5	O 13	P 3	0
3	C	1	Total 31	C 10	N 5	O 13	P 3	0
3	D	1	Total 31	C 10	N 5	O 13	P 3	0

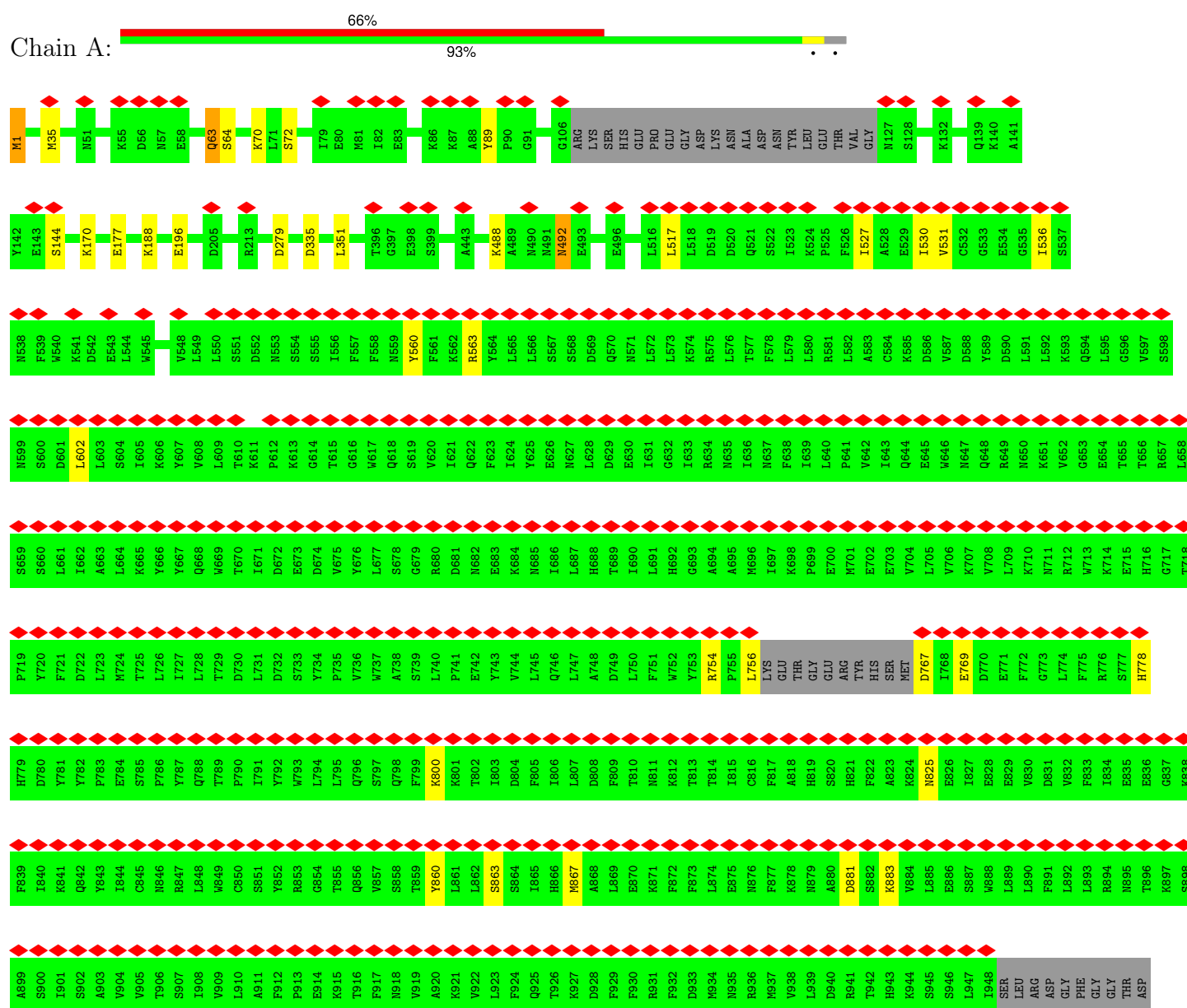
- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
4	A	1	Total Mg 1 1	0
4	B	1	Total Mg 1 1	0
4	C	1	Total Mg 1 1	0
4	D	1	Total Mg 1 1	0

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.

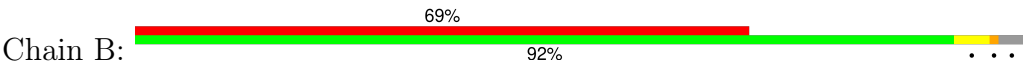
• Molecule 1: ATP-binding protein Avs4



TYR	ARG	L1019	S1079	M1139	Y1139	L1259	D1319	T1379	C1439	L1499	S1500	D1441	N1502	N1503	I1504	A1505	S1506	C1507	V1508	L1509	M1510	Q1511	G1512	T1513	T1514	W1515	L1516	S1517	E1518	I1519	L1520	P1461	V1462	K1463	E1464	N1465	S1466	W1467	G1468	W1469	K1530	L1531	E1532	N1533	D1534	T1535	V1536	Y1537	Y1538	L1539	E1540	C1541	L1542	R1543	Y1546	I1547	N1548	N1549	E1550	R1551	E1552	R1553	I1554	R1555	E1563	V1564	L1565
		P1020	H1081	P1141	N1201	P1261	H1321	H1381	D1441	L1499	L1501	D1442	N1502	N1503	I1504	A1505	S1506	C1507	V1508	L1509	M1510	Q1511	G1512	T1513	T1514	W1515	L1516	S1517	E1518	I1519	L1520	P1461	V1462	K1463	E1464	N1465	S1466	W1467	G1468	W1469	K1530	L1531	E1532	N1533	D1534	T1535	V1536	Y1537	Y1538	L1539	E1540	C1541	L1542	R1543	Y1546	I1547	N1548	N1549	E1550	R1551	E1552	R1553	I1554	R1555	E1563	V1564	L1565
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		R1041	Y1101	R1161	H1221	I1282	K1341	S1401	P1461	S1517	S1518	E1519	L1520</																																																						

D1569	F1570	L1571	V1572	E1573	K1574	G1575	S1576	V1577	V1578	G1579	Y1580	M1581	S1582	N1585	I1586	L1587
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● Molecule 1: ATP-binding protein Avs4



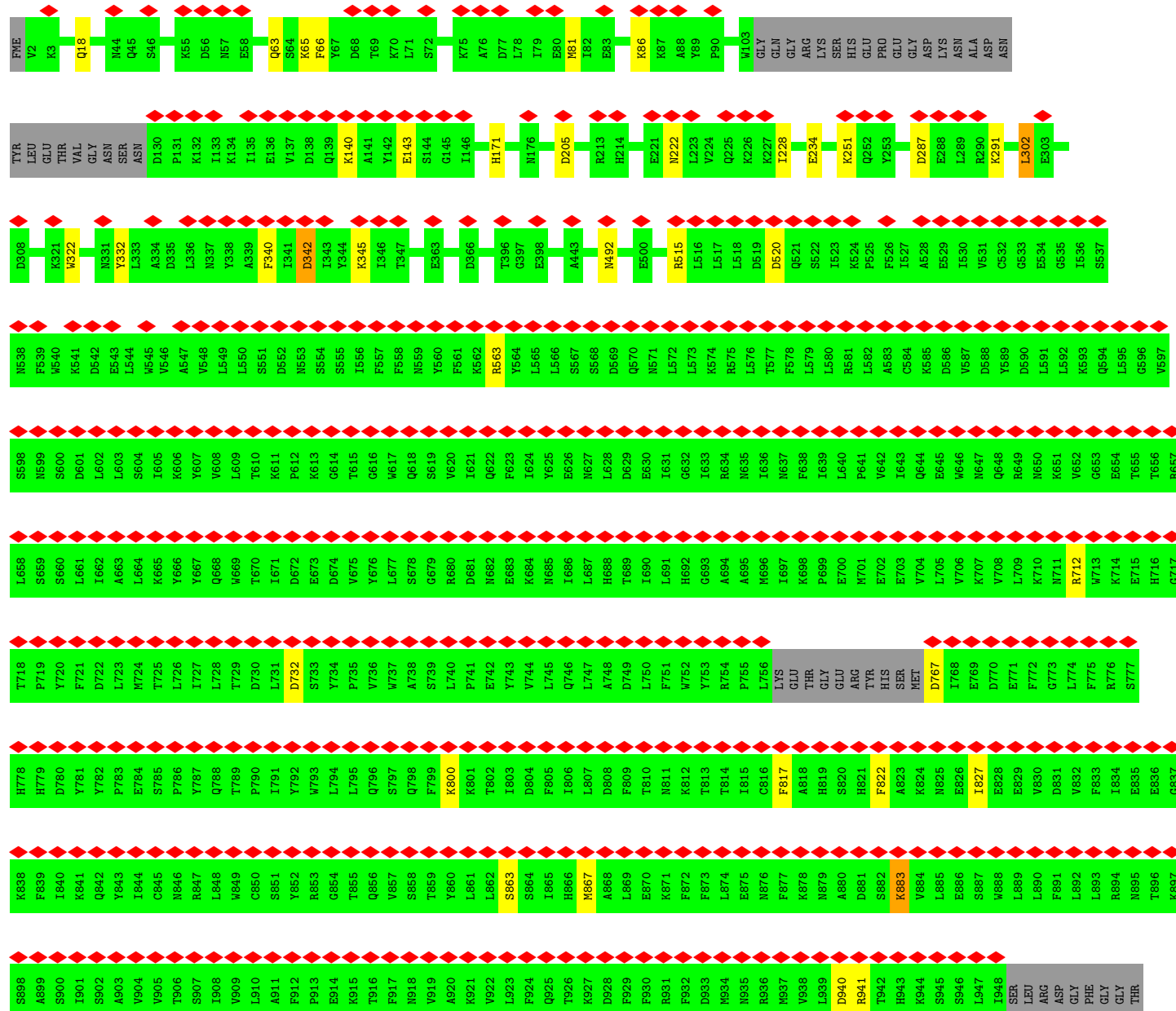
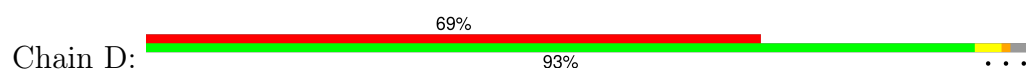
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L1136	K1076	Y1016	GLY	THR	ASP	TYR	ARG	T896	E836	R776	H716	T656	G596	I536	D308	GLY
N1137	K1077	N1017		K397	K397			K397	G337	S777	G717	R657	V597	S537		ASN
G1138	N1078	Q1018		S898	S898			S898	F338	H778	T718	L658	N598	F538	K311	SER
N1139	S1079	L1019		A899	A899			A899	F339	H779	P719	S659	N599	W540		ASN
T1140	E1080	P1020		S900	S900			S900	I840	D780	Y720	S660	S600	K321	W322	
P1141	H1081	D1021		I901	I901			I901	K941	Y781	F721	L661	D601	K641		
A1142	M1082	E1022		S902	S902			S902	Q842	Y782	D722	I662	L603	D542		
D1143	K1083	A1023		A903	A903			A903	Y843	P783	L723	A663	L603	E543	N331	
V1144	Y1084	Q1024		V904	V904			V904	I844	E784	M724	L664	S604	L544	Y332	
C1145	V1085	E1025		N905	N905			N905	C945	S785	T725	K665	I605	W545	L333	
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V1147	L1087	E1027		S907	S907			S907	R947	V787	I727	V667	V607	A547	L336	
L1148	K1088	A1028		I908	I908			I908	L948	Q788	L728	Q668	V608	V548	D138	
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A1151	A1091	T1031		A911	A911			A911	S951	I791	L731	I671	K611	S551	A141	
Y1152	S1092	W1032		P912	P912			P912	Y952	Y792	D732	D672	P612	D552	Y142	
F1153	Y1093	K1033		P913	P913			P913	R953	W793	S733	E673	K613	N553	E143	
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Q1155	R1095	C1035		K915	K915			K915	T955	L795	P735	V675	T615	S555	I146	
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K1097	A1037	A1037		F917	F917			F917	V957	S797	W737	L677	W617	F557		
D1098	R1038	R1038		N918	N918			N918	S958	Q798	A738	S678	Q618	F558		
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R1100	D1040	D1040		L981	L981			L981	Y960	K800	L740	R680	V620	Y560		
Y1101	R1041	R1041		K921	K921			K921	L861	T802	E742	D681	I621	F561		
E1162	K1102	K1042		V922	V922			V922	L862	T802	E742	N682	Q622	K562		
Y1163	M1103	K1043		N983	N983			N983	S863	I803	Y743	E683	F623	R563		
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Y1167	Y1107	T1047		Q988	Q988			Q988	N967	L807	L747	N627	S567	E221		
E1168	E1108	T1048		D928	D928			D928	A869	D808	A748	H688	L628	S568	N492	
L1169	D1109	K1049		F929	F929			F929	L869	F809	D749	T689	D629	D569		
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P1175	L1115	I1055		N935	N935			N935	E875	I815	P755	A695	N635	L518		
L1176	Q1116	E1056		R936	R936			R936	N876	C816	L756	M696	I636	L576		
K1177	E1117	I1057		N937	N937			N937	F877	F817	LYS	I697	N637	D520		
E1178	T1118	S1058		V938	V938			V938	K878	A818	GLU	K698	F638	Q521		
G1179	K1119	F1059		L939	L939			L939	N879	H819	GLY	P699	S522	E248		
Y1180	E1120	M1060		D940	D940			D940	A880	S820	GLU	E700	L640	Q252		
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Q1183	K1123	I1063		R943	R943			R943	K883	A823	HIS	V703	I643	K524		
V1184	K1124	D1064		K944	K944			K944	V884	K824	MET	W704	V642	F626		
K1185	L1125	P1065		S945	S945			S945	L885	N825	D767	E702	C584	F526		
D1186	N1126	K1066		S946	S946			S946	E886	E826	I768	V706	E645	L527		
G1187	E1127	L1067		L947	L947			L947	S987	I827	D770	V769	W646	A528		
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A1194	F1133	E1073		PHE	PHE			PHE	L893	F833	F775	K714	E654	E534		
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	L1135	I1075							N895	E835						

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T718	P719	Y720	D721	D722	L723	M724	T725	L726	I727	L728	T729	D730	L731	D732	S733	Y734	P735	V736	W737	A738	S739	L740	P741	E742	Y743	V744	L745	Q746	L747	A748	D749	L750	F751	W752	Y753	R754	P755	L756	LYS	GLU	THR	GLY	GLU	ARG	THR	HIS	SER	MET	D767	I768	E769	D770	E771	F772	G773	L774	F775	R776	S777		



• Molecule 1: ATP-binding protein Avs4

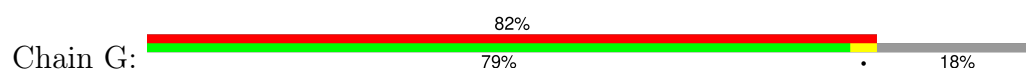


- Molecule 2: Portal protein



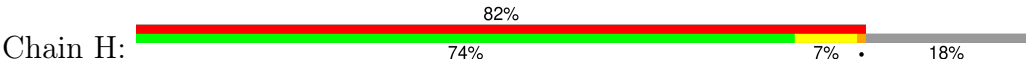
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A421	V422	E423	P424	T425	I426	S427	T428	G429	M430	E431	A432	L433	G434	R435	G436	Q437	D438	L439	D440	K441	L442	E443	R444	C445	I446	A447	A448	W449	S450	A451	L452	A453	M454	M455	GLN	ASN	ASP	PRO	GLN	ALA	GLY	ILE	ASN	ILE	ALA	THR	ILE	LYS	LEU	ARG	ILE	ALA	ASN	ALA	ILE	GLY	ILE	ASP	THR	SER	GLY
ALA	VAL	GLN	ARG	THR	GLY	GLU	VAL	THR	ALA	E372	E373	I374	R375	Y376	V377	A378	S379	E380	L381	E382	D383	T384	L385	G386	G387	V388	Y389	S390	I391	L392	S393	Q394	E395	L396	Q397	L398	P399	M400	V401	R402	V403	L404	L405	K406	Q407	L408	Q409	A410	T411	N412	Q413	I414	P415	E416	L417	P418	K419	E420			
N301	P302	A303	G304	I305	T306	Q307	V308	R309	R310	L311	T312	K313	A314	Q315	T316	G317	D318	F319	V320	S321	G322	R323	P324	E325	D326	I327	S328	F329	L330	Q331	L332	E333	K334	A335	A336	D337	F338	S339	V340	A341	K342	A343	V344	S345	Q347	I348	E349	G350	R351	L352	S353	Y354	A355	F356	M357	L358	N359	SER			

• Molecule 2: Portal protein



ILE	LEU	LYS	THR	PRO	GLU	GLU	GLN	GLN	GLU	MET	ALA	GLU	GLU	GLN	GLY	THR	ALA	GLU	GLU	ASN	ALA	ALA	SER	GLY	ALA	GLY	LEU	ALA	LEU	ALA	THR	ALA	SER	PRO	GLU	ASN	ASN	MET	GLU	ALA	ALA	ALA	ALA	GLN	ASN	ASP	PRO	GLN	ALA	ALA	GLY	GLY	ASN	MET	VAL	PRO	PRO	ASN						
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ALA	VAL	GLN	ARG	THR	GLY	GLU	ARG	VAL	THR	ALA	E372	E373	I374	R375	Y376	V377	A378	S379	E380	L381	E382	D383	T384	L385	G386	G387	V388	Y389	S390	I391	L392	S393	Q394	E395	L396	Q397	L398	P399	M400	V401	R402	V403	L404	L405	K406	Q407	L408	Q409	ALA	A410	T411	N412	Q413	I414	P415	E416	L417	P418	K419	E420				
N301	P302	A303	G304	I305	T306	Q307	V308	R309	R310	L311	T312	K313	A314	Q315	T316	G317	D318	F319	V320	S321	G322	R323	P324	E325	D326	I327	S328	F329	L330	Q331	L332	E333	K334	A335	A336	D337	F338	S339	V340	A341	K342	A343	V344	S345	E346	Q347	I348	E349	G350	R351	L352	S353	Y354	A355	F356	M357	L358	N359						
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V181	T182	L183	D184	K185	T186	A187	Y188	A189	A190	L191	P192	E193	D194	V195	R196	N197	A198	M199	D200	S201	G202	Q203	E204	H205	K206	G207	D208	E209	M210	I211	D212	V213	Y214	T215	H216	I217	Y218	L219	D220	E221	S223	G224	E225	Y226	L227	K228	Y229	E230	E231	I232	D233	G234	V235	E236	V237	D238	G239							
M121	Y122	I123	E124	N125	S126	S127	Y128	A129	V130	T131	L132	F133	E134	T135	L136	K137	Q138	L139	V140	V141	A142	G143	M144	N145	L146	L147	Y148	E149	P150	E151	P152	E153	G154	A155	Y156	M157	P158	M159	K160	L161	R163	L164	S165	S166	Y167	V168	V169	Q170	R171	D172	A173	F174	G175	T176	V177	L178	Q179							
Q61	A62	V63	G64	A65	R66	G67	L68	N69	M70	L71	A72	S73	K74	L75	M76	L77	A78	L79	F80	P81	M82	Q83	T84	W85	M86	K87	L88	T89	I90	S91	E92	F93	E94	A95	K96	Q97	L98	V99	A100	Q101	P102	A103	E104	L105	A106	K107	V108	E109	E110	G111	L112	S113	M114	V115	E116	R117	L118	L119						
NET	ALA	SER	GLN	K6	R7	E8	G9	F10	A11	E12	M13	G14	A15	K16	A17	V18	Y19	D20	A21	L22	K23	N24	D25	R26	N27	S28	Y29	E30	T31	R32	A33	E34	N35	C36	A37	K38	Y39	T40	I41	P42	S43	L44	F45	P46	K47	D48	S49	D50	M51	A52	S53	T54	D55	Y56	T57	T58	P59	W60						

• Molecule 2: Portal protein



ILE	LEU	LYS	THR	PRO	GLU	GLU	LYS	GLN	GLN	GLU	MET	ALA	GLU	ALA	GLN	GLY	THR	ALA	LEU	GLU	ASN	ALA	ALA	ALA	SER	GLY	GLY	ALA	GLY	LEU	ALA	THR	ALA	SER	PRO	GLU	ASN	MET	GLU	ALA	ALA	GLN	ASP	PRO	ASP	ILE	ASN	ILE	ALA	THR	LYS	LEU	ARG	ILE	ALA	ASN	ALA	ILE	GLY	ASP	THR	SER	GLY
A421	V422	E423	P424	T425	L426	S427	T428	G429	M430	E431	A432	L433	G434	R435	G436	Q437	D438	L439	D440	K441	L442	E443	G444	C445	I446	A447	A448	W449	S450	A451	L452	A453	P454	M455	GLN	ASN	ASP	PRO	ASP	ILE	ASN	ILE	ALA	THR	LYS	LEU	ARG	ILE	ALA	ASN	ALA	ILE	GLY	ASP	THR	SER	GLY						
VAL	ARG	THR	GLY	GLU	ARG	VAL	THR	ALA	E372	E373	I374	R375	Y376	V377	A378	S379	E380	L381	E382	D383	T384	L385	G386	G387	V388	Y389	S390	I391	L392	S393	Q394	E395	L396	Q397	L398	P399	M400	V401	R402	V403	L404	L405	K406	Q407	L408	Q409	A410	T411	N412	Q413	I414	P415	E416	L417	P418	K419	E420						
N301	P302	A303	G304	I305	T306	Q307	V308	R309	R310	L311	T312	K313	A314	Q315	T316	G317	D326	F319	V320	S321	G322	R323	P324	E325	D326	I327	S328	F329	L330	Q331	L332	E333	K334	A335	A336	D337	F338	S339	V340	A341	K342	A343	V344	S345	E346	Q347	T348	E349	G350	R351	L352	S353	Y354	A355	F356	M357	L358	N359	SER				
D241	A242	S243	Y244	P245	V246	D247	A248	C249	P250	Y251	T252	P253	V254	R255	M256	Y257	R258	I259	D260	G261	E262	S263	Y264	G265	R266	S267	Y268	C269	E270	E271	Y272	L273	G274	D275	L276	R277	S278	L279	E280	N281	L282	Q283	E284	A285	T286	V287	K288	M289	S290	M291	T292	S293	A294	K295	V296	T297	G298	L299	V300				
V181	T182	L183	D184	K185	T186	A187	Y188	A189	A190	L191	P192	E193	D194	V195	R196	N197	A198	M199	D200	S201	G202	Q203	E204	H205	K206	G207	D208	E209	M210	I211	D212	V213	Y214	T215	H216	I217	Y218	L219	D220	E221	S222	G224	E225	V226	L227	K228	Y229	E230	E231	T232	D233	G234	V235	E236	V237	D238	G239	T240					
N121	Y122	I123	E124	S125	N126	S127	Y128	R129	V130	T131	L132	F133	E134	T135	L136	K137	Q138	L139	V140	V141	A142	G143	N144	A145	L146	L147	Y148	I149	P150	E151	P152	E153	G154	A155	Y156	M157	P158	M159	K160	L161	Y162	R163	L164	S165	S166	Y167	V168	V169	Q170	R171	D172	A173	F174	G175	T176	V177	L178	Q179	I180				
Q61	A62	V63	G64	A65	R66	G67	L68	N69	N70	L71	A72	S73	K74	L75	M76	L77	A78	L79	F80	P81	M82	Q83	T84	W85	M86	K87	L88	T89	I90	S91	E92	F93	G94	A95	K96	Q97	L98	V99	A100	Q101	P102	A103	E104	L105	A106	K107	V108	E109	E110	G111	L112	S113	M114	V115	E116	R117	I118	L119	M120				

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	169977	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 ($e^-/\text{\AA}^2$)	31	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.138	Depositor
Minimum map value	-0.055	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	372.3703, 372.3703, 372.3703	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.034362, 1.034362, 1.034362	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: ATP, FME, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.39	0/13095	0.66	6/17695 (0.0%)
1	B	0.40	0/13056	0.67	8/17643 (0.0%)
1	C	0.39	0/13095	0.66	6/17695 (0.0%)
1	D	0.40	0/13056	0.66	8/17643 (0.0%)
2	E	0.73	3/3485 (0.1%)	0.89	8/4720 (0.2%)
2	F	0.48	2/3485 (0.1%)	0.80	10/4720 (0.2%)
2	G	0.54	1/3485 (0.0%)	0.81	6/4720 (0.1%)
2	H	0.47	1/3485 (0.0%)	0.82	13/4720 (0.3%)
All	All	0.44	7/66242 (0.0%)	0.70	65/89556 (0.1%)

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	324	PRO	CG-CD	-32.03	0.45	1.50
2	G	454	PRO	CG-CD	-19.71	0.85	1.50
2	F	324	PRO	CG-CD	-11.44	1.12	1.50
2	E	324	PRO	CB-CG	11.21	2.06	1.50
2	H	324	PRO	CG-CD	-10.89	1.14	1.50

The worst 5 of 65 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	324	PRO	CB-CG-CD	-27.29	0.07	106.50
2	G	454	PRO	N-CD-CG	-20.29	72.77	103.20
2	E	324	PRO	CA-N-CD	-15.21	90.20	111.50
2	F	398	LEU	CB-CG-CD2	-12.07	90.47	111.00
2	F	324	PRO	N-CD-CG	-11.55	85.88	103.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	12805	0	12724	25	0
1	B	12756	0	12683	32	0
1	C	12805	0	12724	22	0
1	D	12756	0	12683	26	0
2	E	3427	0	3400	16	0
2	F	3427	0	3400	22	0
2	G	3427	0	3400	9	0
2	H	3427	0	3400	21	0
3	A	31	0	12	0	0
3	B	31	0	12	0	0
3	C	31	0	12	0	0
3	D	31	0	12	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
All	All	64958	0	64462	156	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 1.

The worst 5 of 156 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:117:ARG:HH12	2:F:121:ASN:HB2	1.39	0.87
2:H:117:ARG:HH12	2:H:121:ASN:HB2	1.46	0.79
1:C:937:MET:HG2	1:C:941:ARG:HH12	1.51	0.76
1:A:1359:ARG:O	1:A:1359:ARG:NH1	2.25	0.69
1:C:1359:ARG:O	1:C:1359:ARG:NH1	2.26	0.69

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	A	1531/1587 (96%)	1499 (98%)	32 (2%)	0	100	100
1	B	1524/1587 (96%)	1490 (98%)	34 (2%)	0	100	100
1	C	1531/1587 (96%)	1501 (98%)	30 (2%)	0	100	100
1	D	1524/1587 (96%)	1490 (98%)	34 (2%)	0	100	100
2	E	434/535 (81%)	422 (97%)	12 (3%)	0	100	100
2	F	434/535 (81%)	422 (97%)	12 (3%)	0	100	100
2	G	434/535 (81%)	419 (96%)	15 (4%)	0	100	100
2	H	434/535 (81%)	425 (98%)	9 (2%)	0	100	100
All	All	7846/8488 (92%)	7668 (98%)	178 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1422/1461 (97%)	1400 (98%)	22 (2%)	60	85
1	B	1418/1461 (97%)	1393 (98%)	25 (2%)	54	82
1	C	1422/1461 (97%)	1400 (98%)	22 (2%)	60	85
1	D	1418/1461 (97%)	1390 (98%)	28 (2%)	50	79
2	E	370/435 (85%)	363 (98%)	7 (2%)	52	81
2	F	370/435 (85%)	361 (98%)	9 (2%)	44	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	G	370/435 (85%)	366 (99%)	4 (1%)	70	90
2	H	370/435 (85%)	361 (98%)	9 (2%)	44	76
All	All	7160/7584 (94%)	7034 (98%)	126 (2%)	54	82

5 of 126 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	492	ASN
2	F	326	ASP
1	D	234	GLU
2	F	323	ARG
2	H	86	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	825	ASN
1	B	825	ASN
2	F	157	ASN
2	F	413	GLN
2	H	205	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues 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
1	FME	A	1	1	8,9,10	1.02	0	8,9,11	2.53	2 (25%)
1	FME	C	1	1	8,9,10	1.02	0	8,9,11	2.62	2 (25%)

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
1	FME	A	1	1	-	6/7/9/11	-
1	FME	C	1	1	-	6/7/9/11	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1	FME	CA-N-CN	-5.49	114.38	122.82
1	A	1	FME	CA-N-CN	-5.30	114.67	122.82
1	C	1	FME	O1-CN-N	4.57	137.12	125.32
1	A	1	FME	O1-CN-N	4.42	136.74	125.32

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	O1-CN-N-CA
1	A	1	FME	O-C-CA-CB
1	C	1	FME	O1-CN-N-CA
1	C	1	FME	O-C-CA-CB
1	A	1	FME	CB-CG-SD-CE

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1	FME	1	0
1	C	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	ATP	A	1601	4	28,33,33	1.16	2 (7%)	34,52,52	0.64	1 (2%)
3	ATP	D	1601	4	28,33,33	1.34	2 (7%)	34,52,52	0.66	1 (2%)
3	ATP	C	1601	4	28,33,33	1.15	2 (7%)	34,52,52	0.64	1 (2%)
3	ATP	B	1601	4	28,33,33	1.34	2 (7%)	34,52,52	0.66	1 (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
3	ATP	A	1601	4	-	1/18/38/38	0/3/3/3
3	ATP	D	1601	4	-	0/18/38/38	0/3/3/3
3	ATP	C	1601	4	-	1/18/38/38	0/3/3/3
3	ATP	B	1601	4	-	0/18/38/38	0/3/3/3

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1601	ATP	PA-O3A	-5.52	1.53	1.59
3	B	1601	ATP	PA-O3A	-5.51	1.53	1.59
3	A	1601	ATP	PA-O3A	-3.64	1.55	1.59
3	C	1601	ATP	PA-O3A	-3.58	1.55	1.59
3	A	1601	ATP	PB-O3B	-3.04	1.56	1.59

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1601	ATP	C5-C6-N6	2.13	123.56	120.31
3	C	1601	ATP	C5-C6-N6	2.09	123.49	120.31
3	D	1601	ATP	C5-C6-N6	2.08	123.48	120.31
3	B	1601	ATP	C5-C6-N6	2.05	123.44	120.31

There are no chirality outliers.

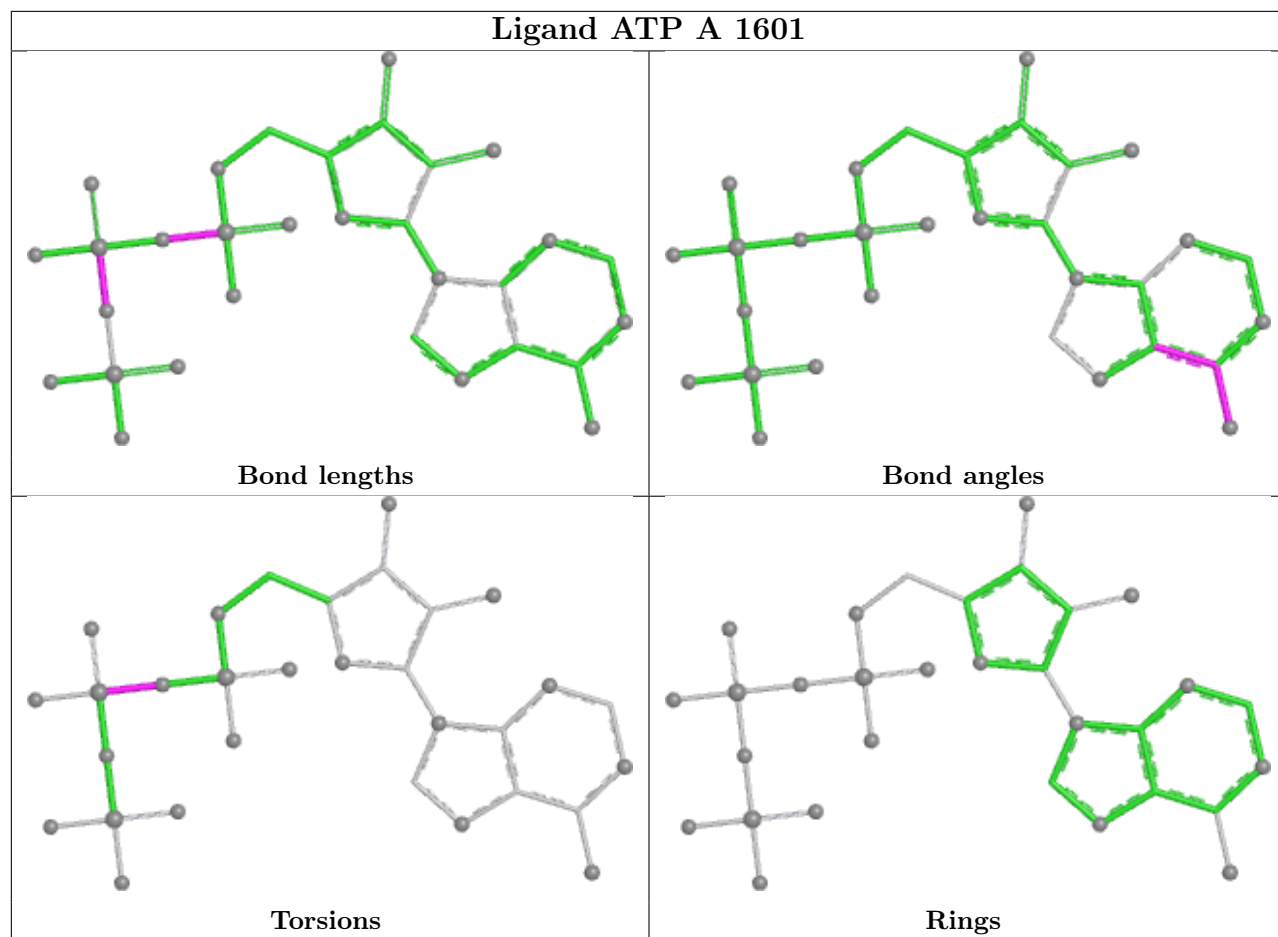
All (2) torsion outliers are listed below:

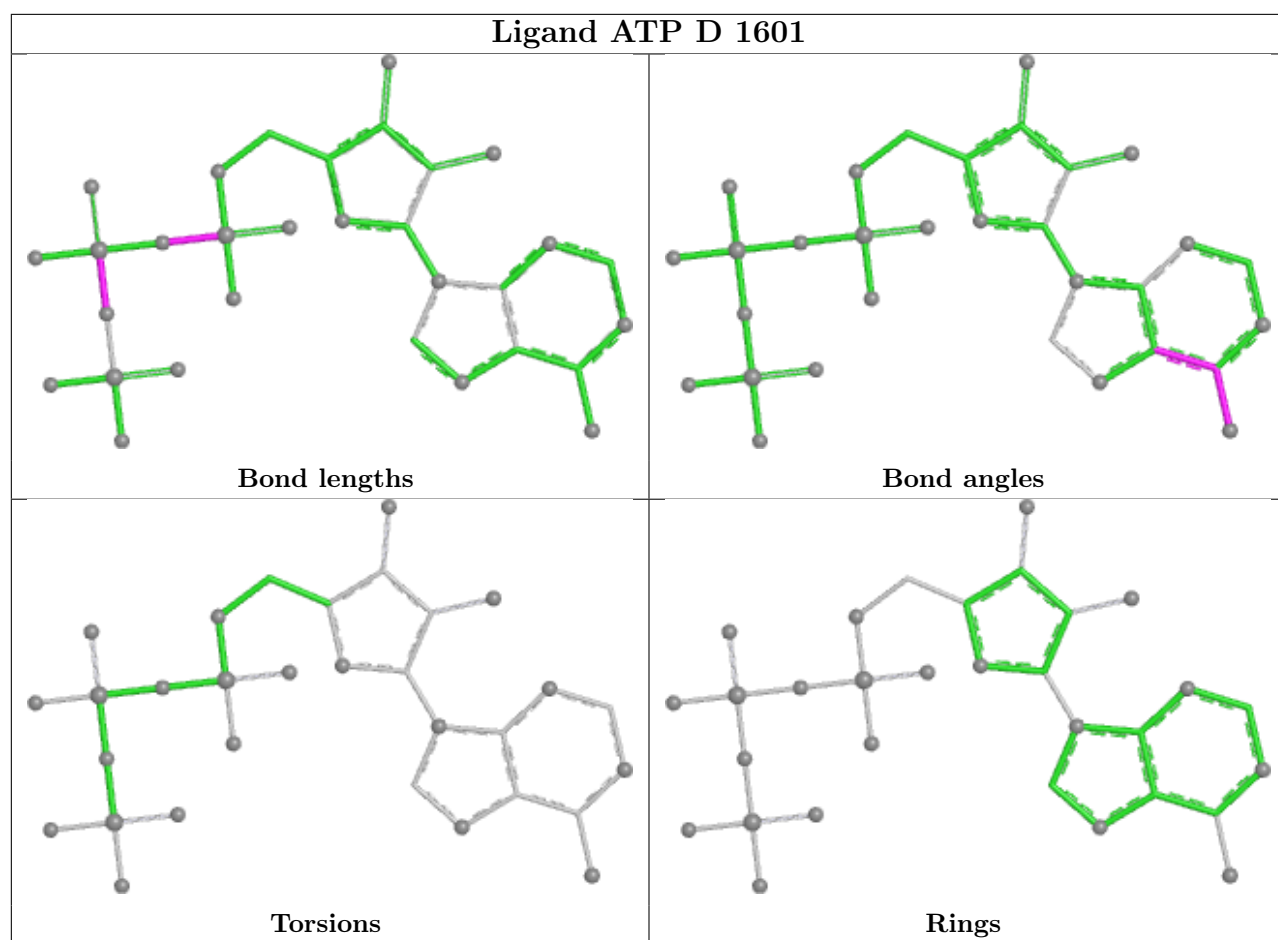
Mol	Chain	Res	Type	Atoms
3	A	1601	ATP	PA-O3A-PB-O2B
3	C	1601	ATP	PA-O3A-PB-O2B

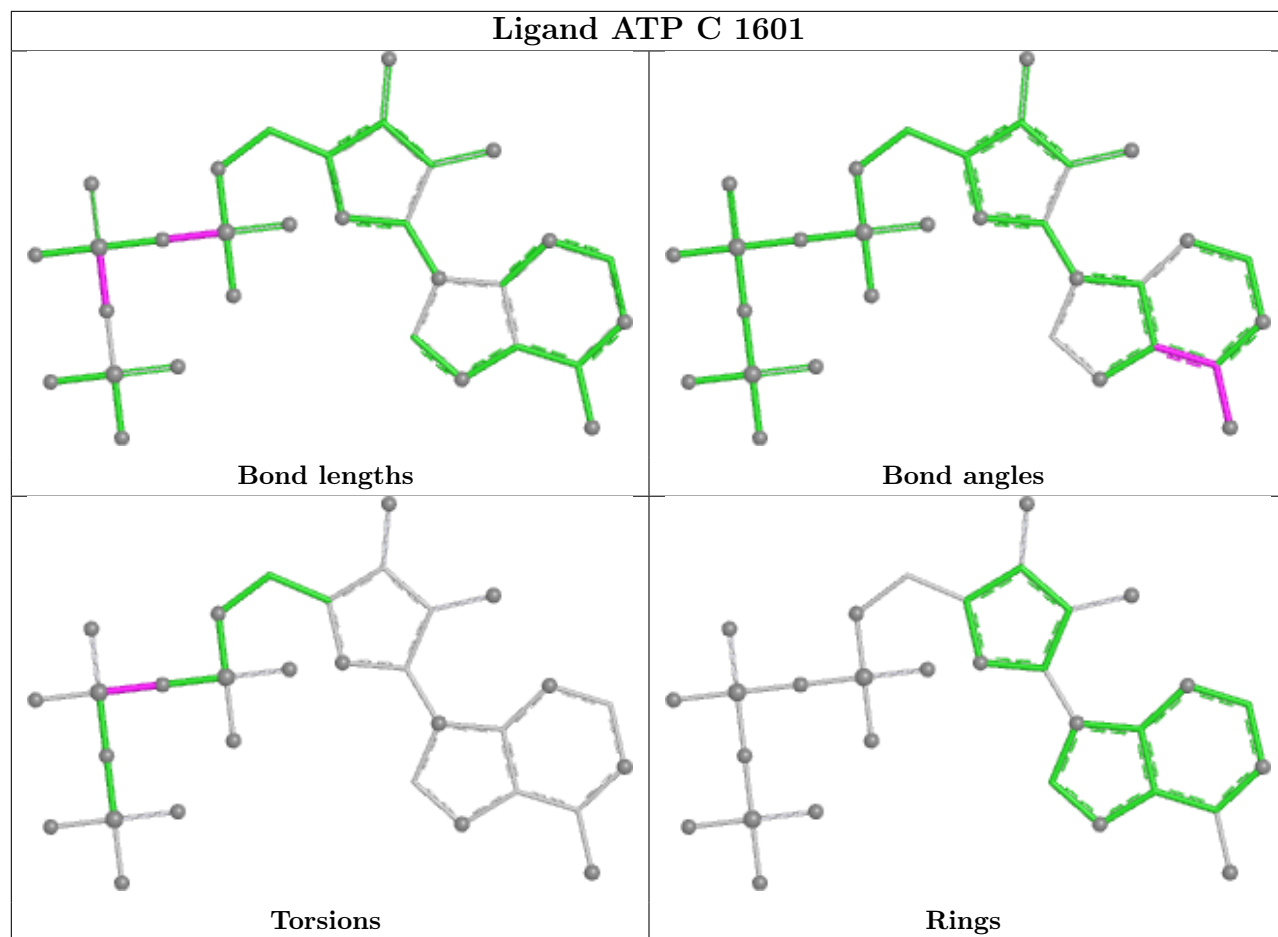
There are no ring outliers.

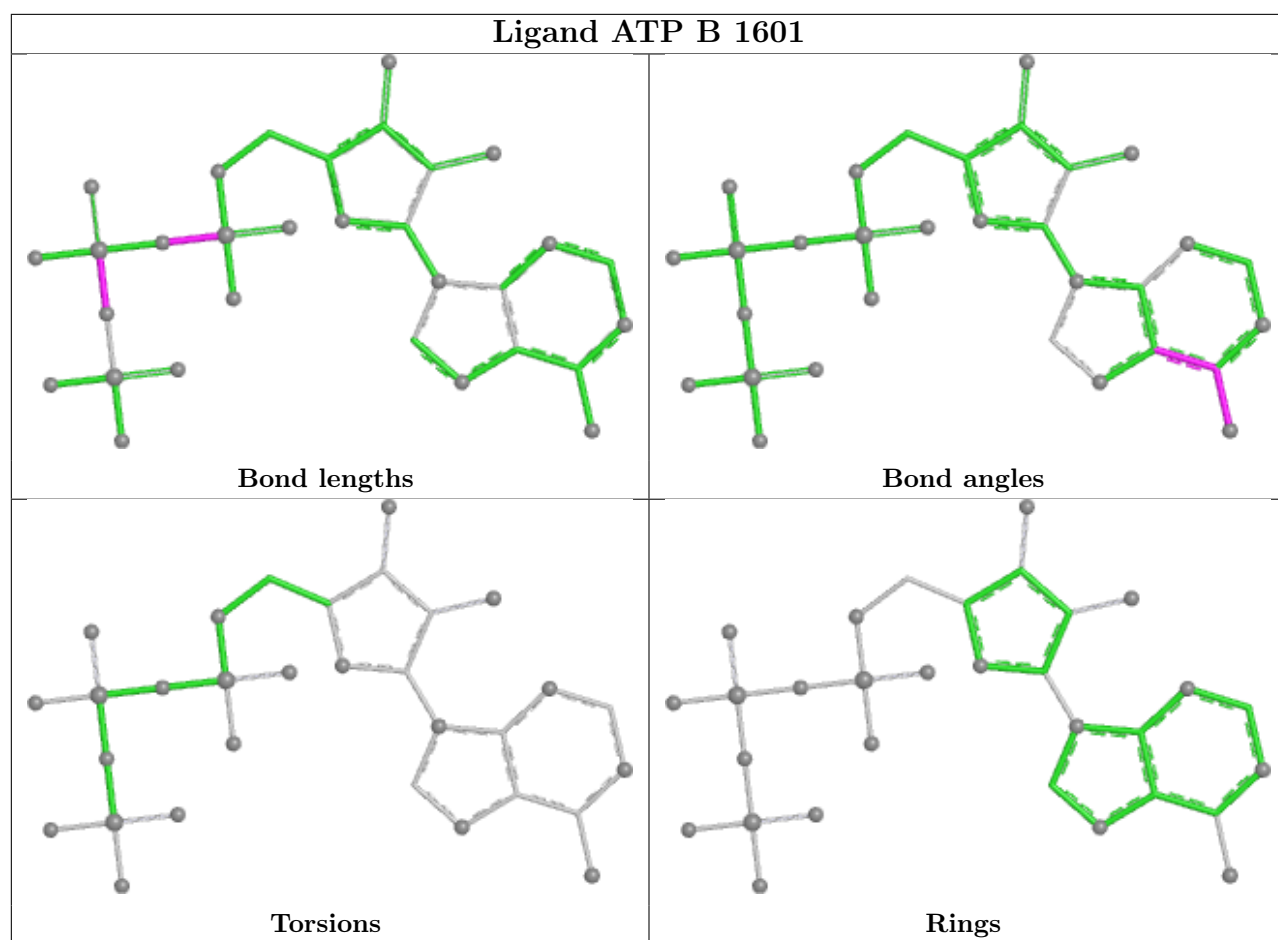
No monomer is involved in short contacts.

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.

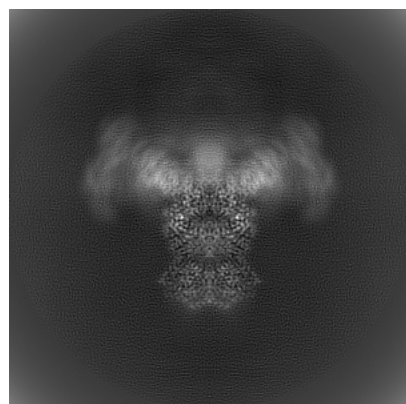
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27422. These allow visual inspection of the internal detail of the map and identification of artifacts.

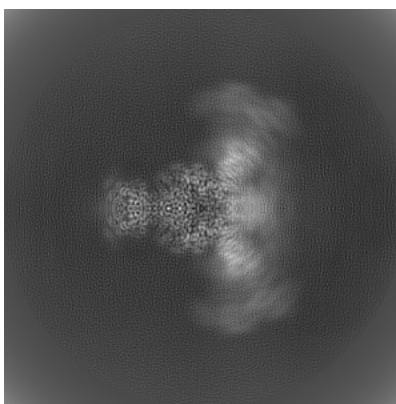
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

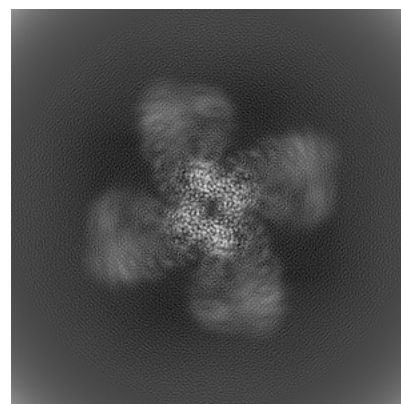
6.1.1 Primary map



X

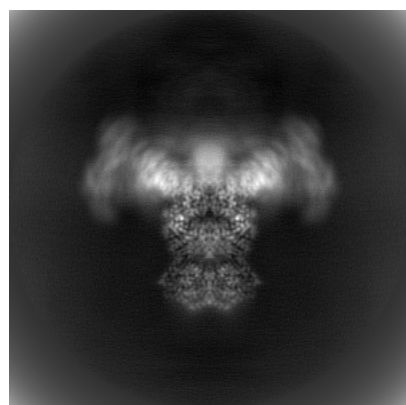


Y

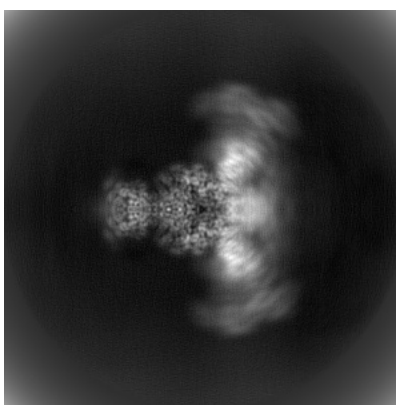


Z

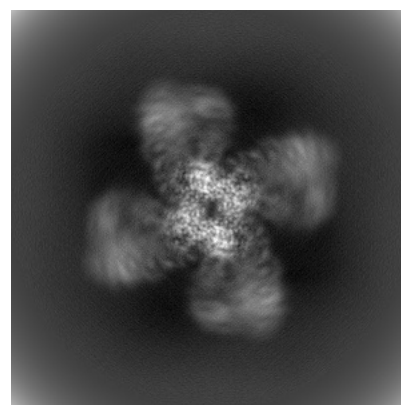
6.1.2 Raw map



X



Y

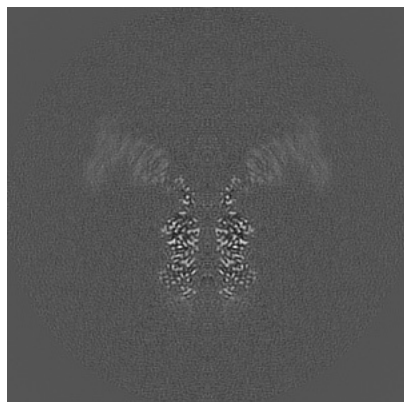


Z

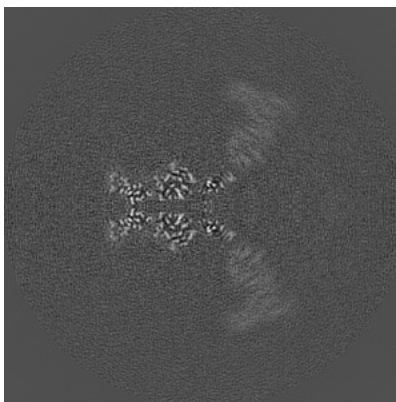
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

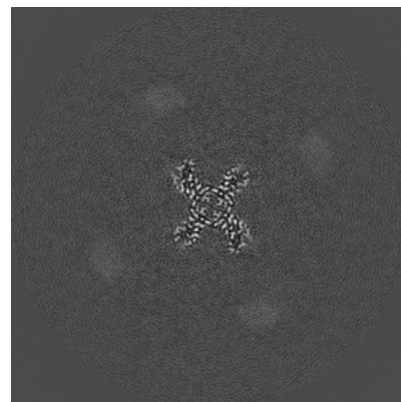
6.2.1 Primary map



X Index: 180

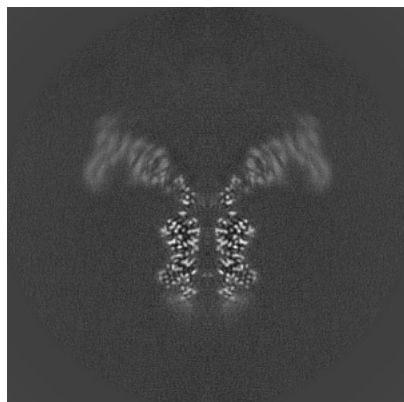


Y Index: 180

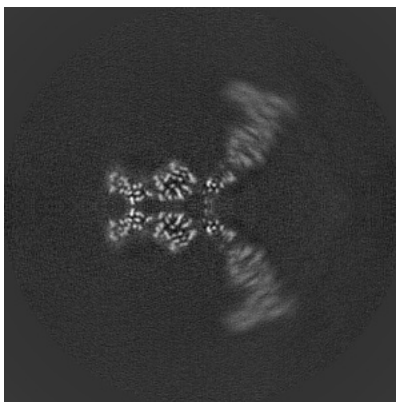


Z Index: 180

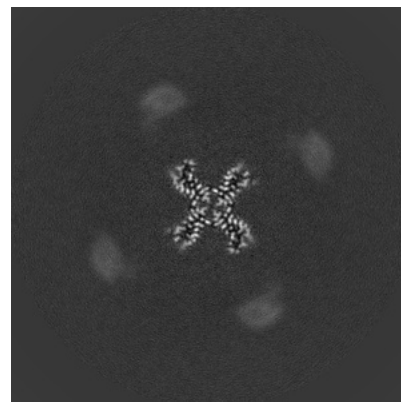
6.2.2 Raw map



X Index: 180



Y Index: 180

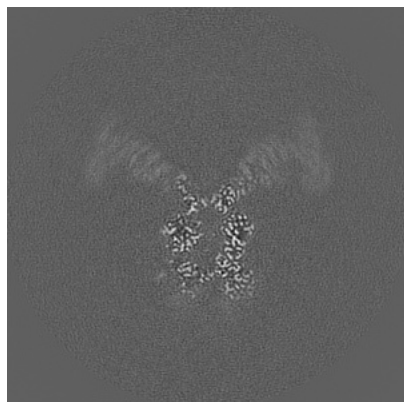


Z Index: 180

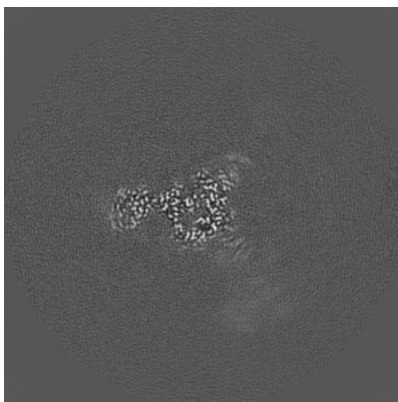
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

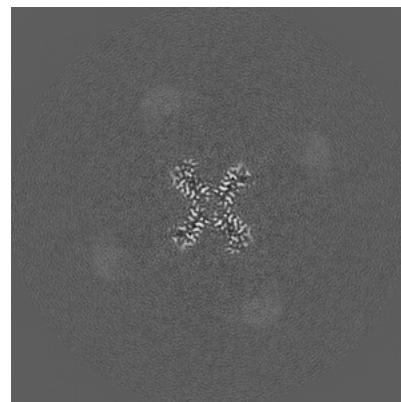
6.3.1 Primary map



X Index: 175

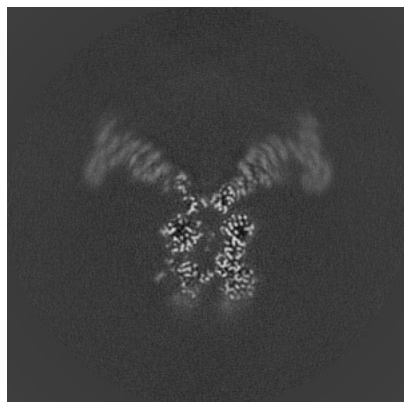


Y Index: 160

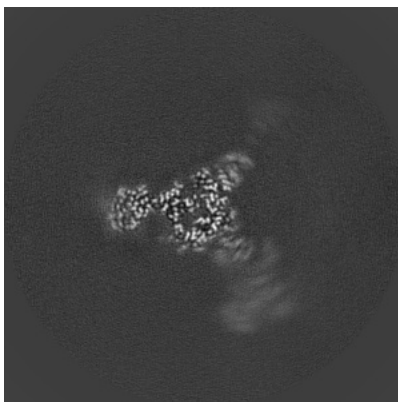


Z Index: 179

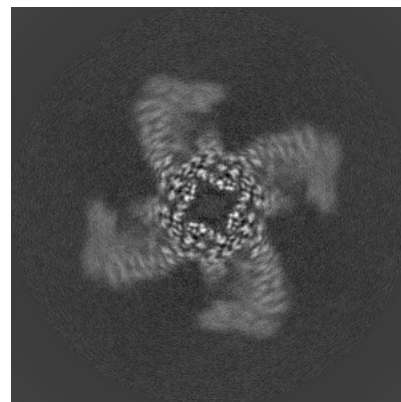
6.3.2 Raw map



X Index: 175



Y Index: 160

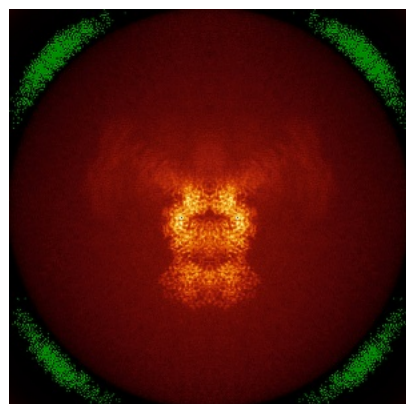


Z Index: 204

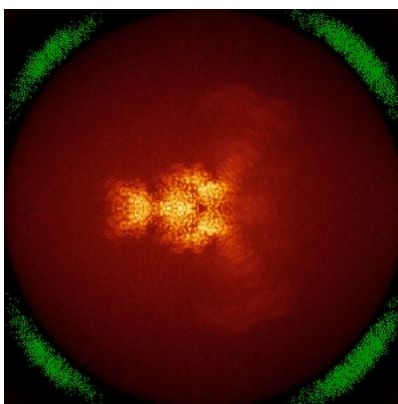
The images above show the largest variance slices of the map in three orthogonal directions.

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

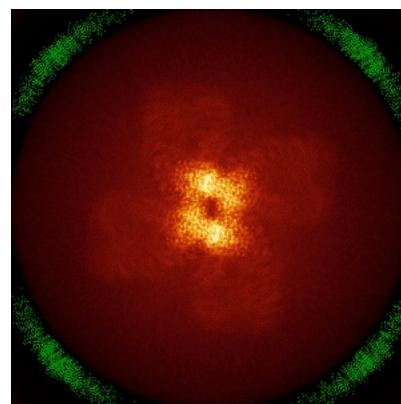
6.4.1 Primary map



X

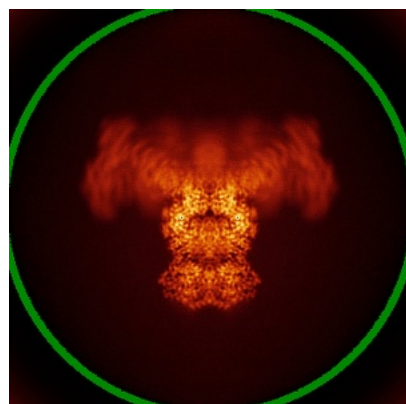


Y

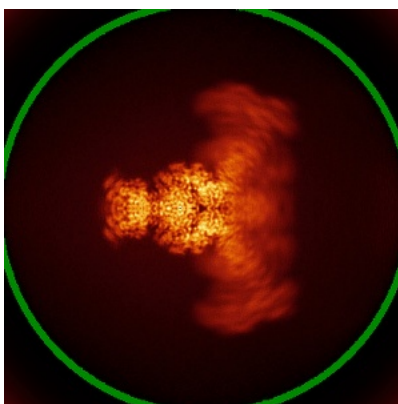


Z

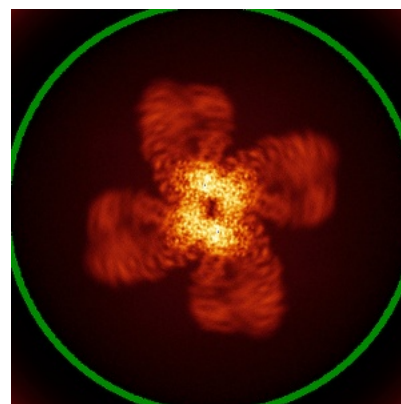
6.4.2 Raw map



X



Y

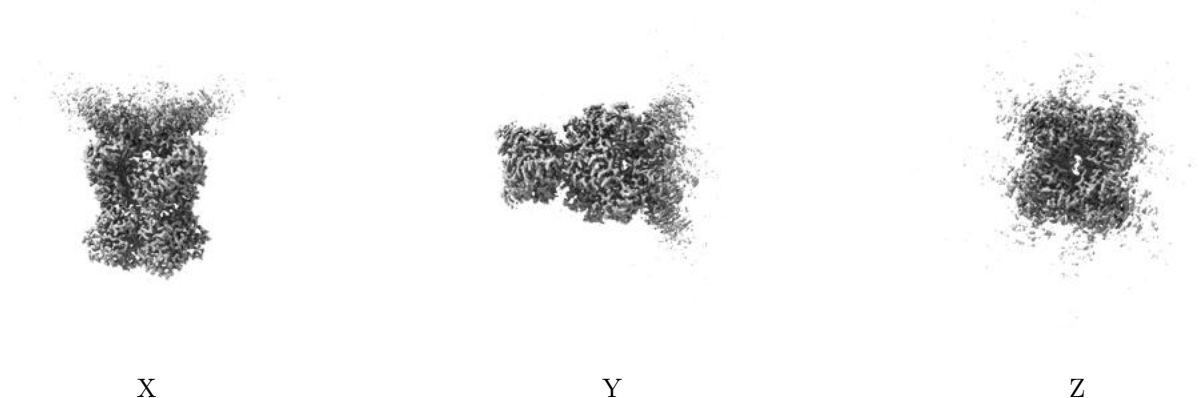


Z

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.

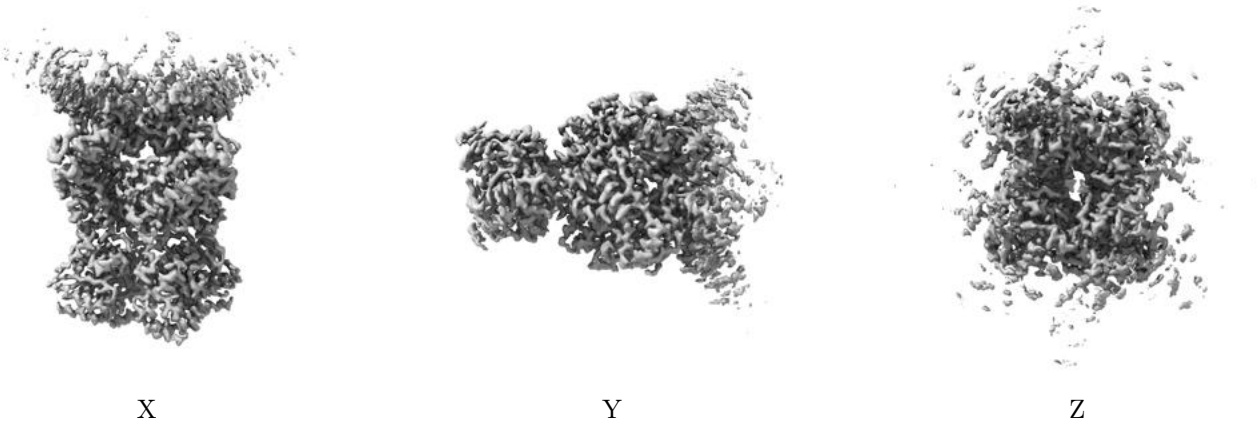
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

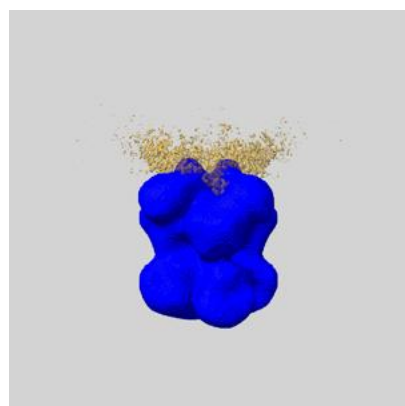
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

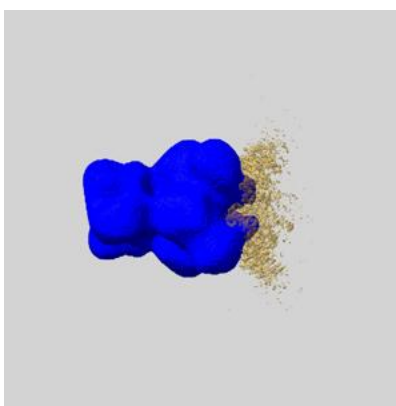
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

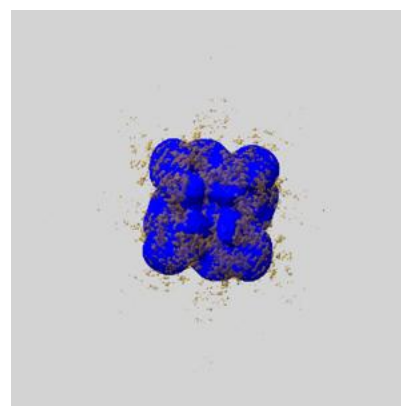
6.6.1 emd_27422_msk_1.map [i](#)



X



Y

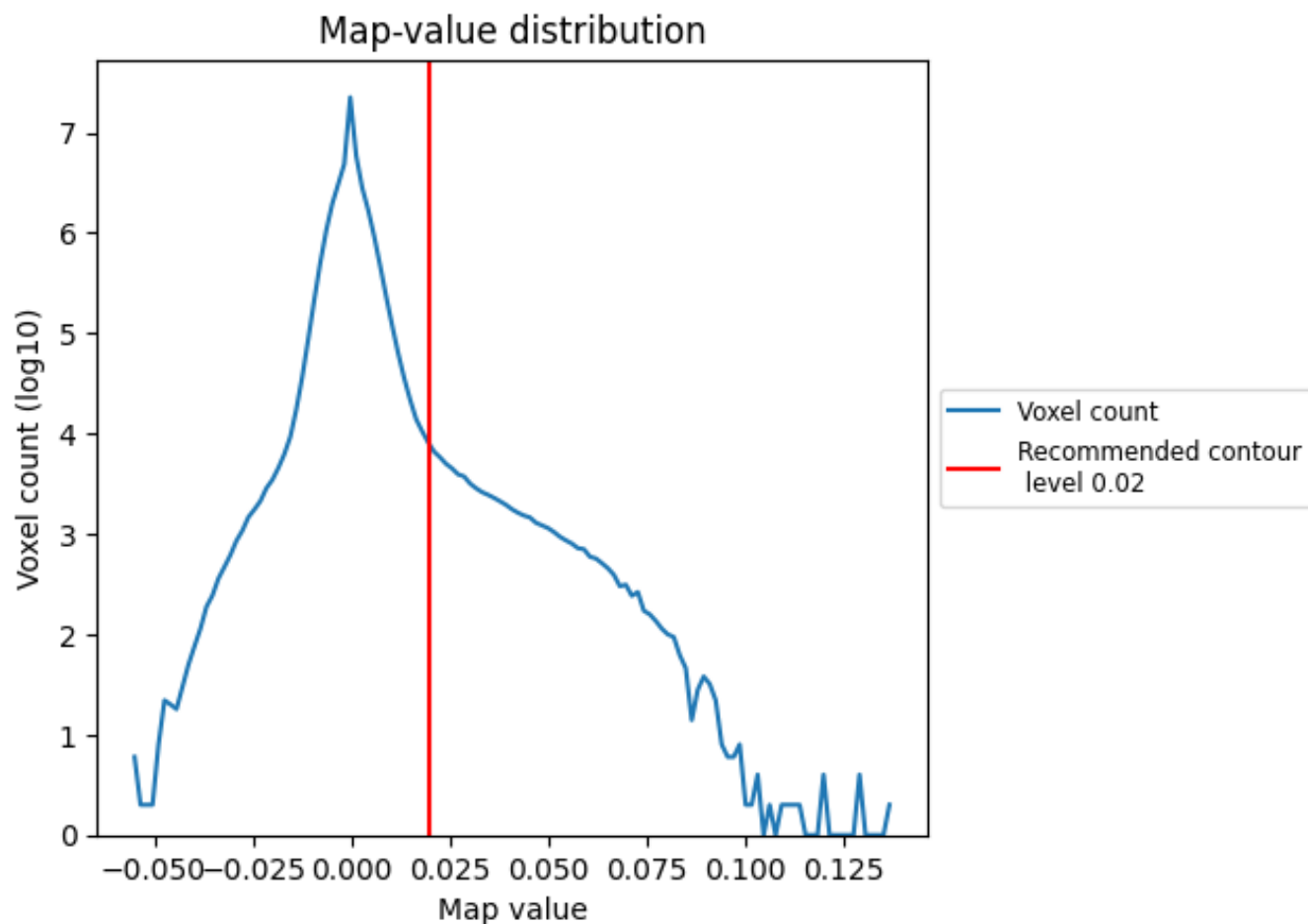


Z

7 Map analysis [i](#)

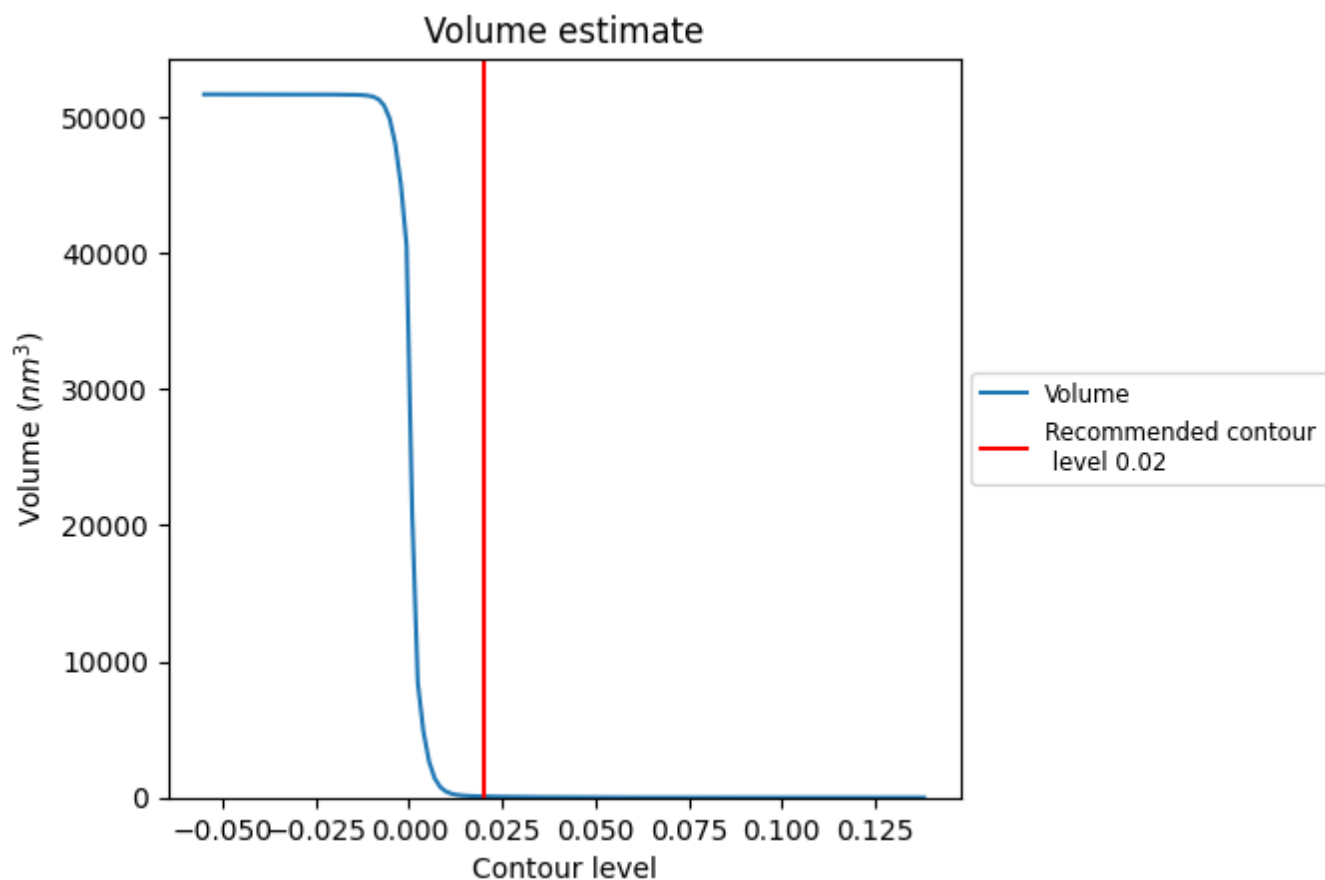
This section contains the results of statistical analysis of the map.

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.

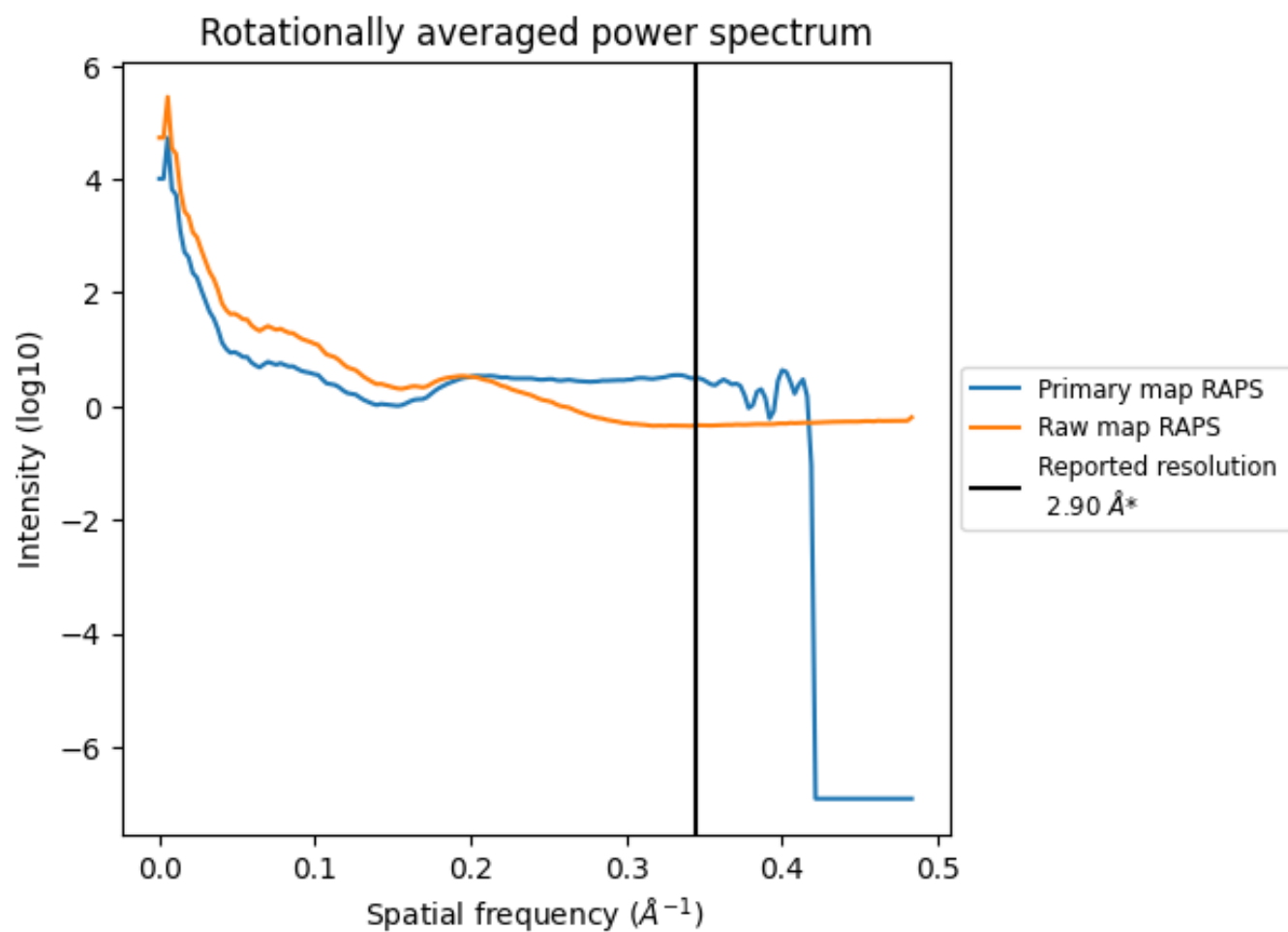
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 80 nm^3 ; this corresponds to an approximate mass of 73 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](#)

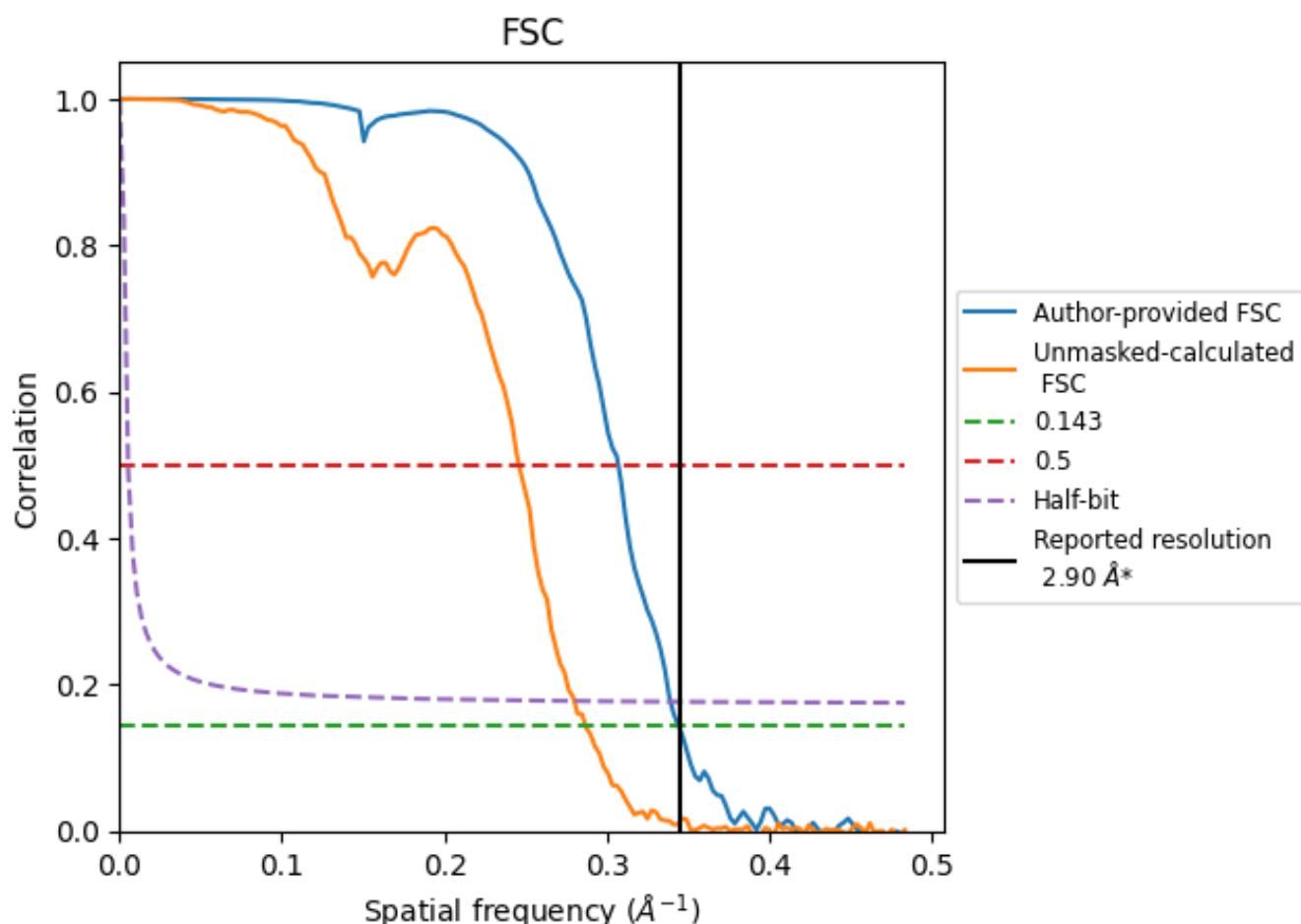


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

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 0.345 Å⁻¹

8.2 Resolution estimates [i](#)

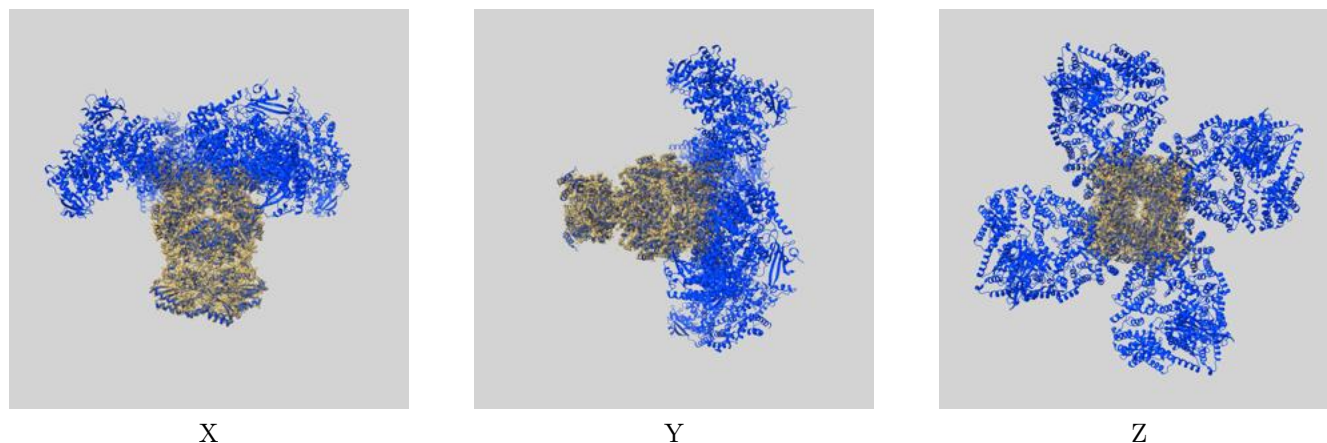
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.90	3.26	2.95
Unmasked-calculated*	3.48	4.07	3.57

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.48 differs from the reported value 2.9 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-27422 and PDB model 8DGF. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

9.1 Map-model overlay [i](#)



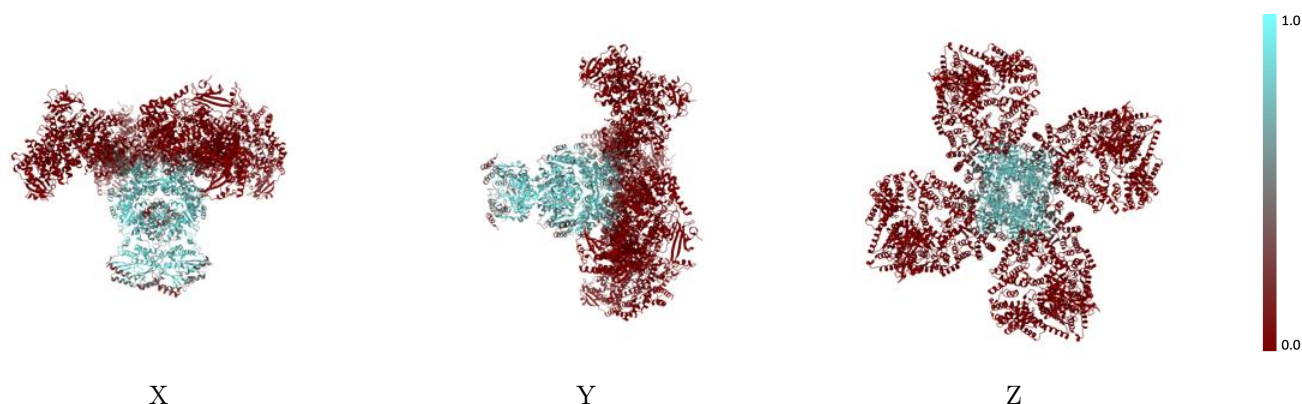
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



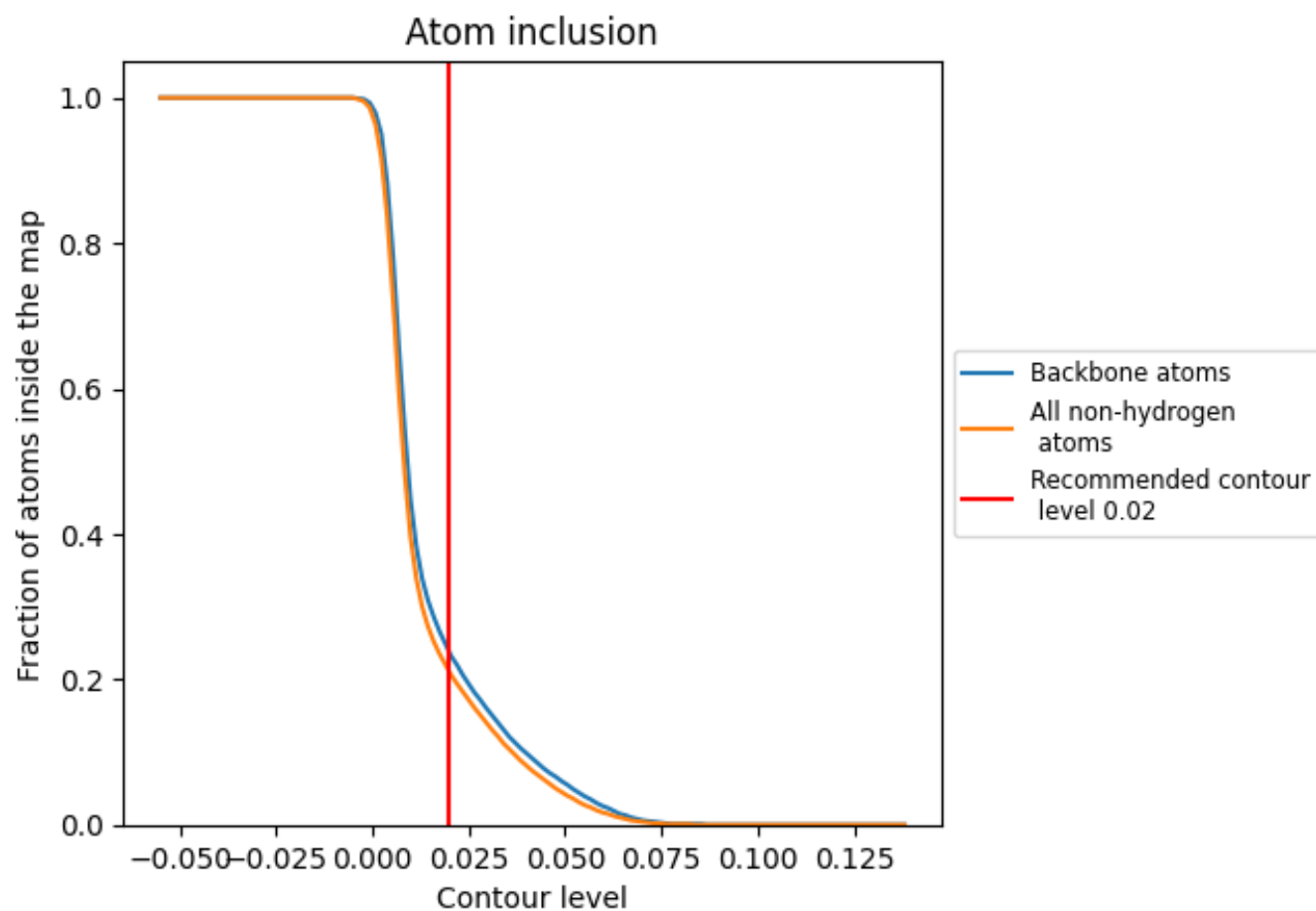
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

9.4 Atom inclusion ⓘ



At the recommended contour level, 24% of all backbone atoms, 21% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.2110	<div></div> 0.2340
A	<div></div> 0.2860	<div></div> 0.2990
B	<div></div> 0.2480	<div></div> 0.2640
C	<div></div> 0.2860	<div></div> 0.3000
D	<div></div> 0.2470	<div></div> 0.2650
E	<div></div> 0.0000	<div></div> 0.0570
F	<div></div> 0.0000	<div></div> 0.0470
G	<div></div> 0.0000	<div></div> 0.0570
H	<div></div> 0.0000	<div></div> 0.0470

1.0

0.0

<0.0