



Full wwPDB EM Validation 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 Full wwPDB EM Validation 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.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

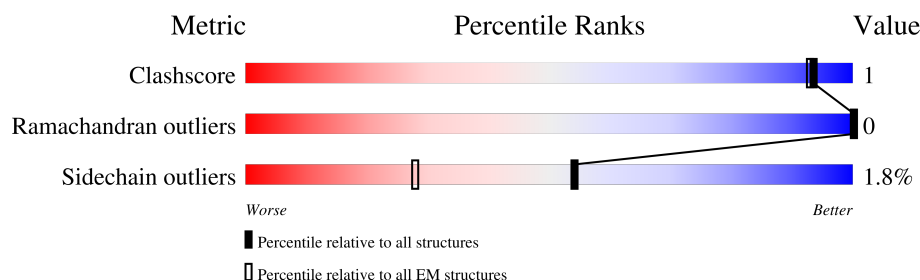
1 Overall quality at a glance

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.

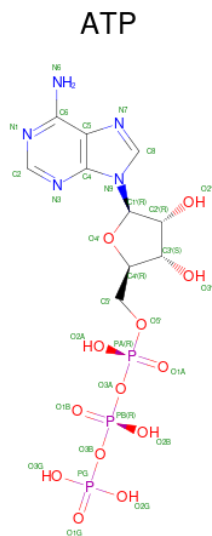
- Molecule 1 is a protein called ATP-binding protein Avs4.

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: C₁₀H₁₆N₅O₁₃P₃) (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

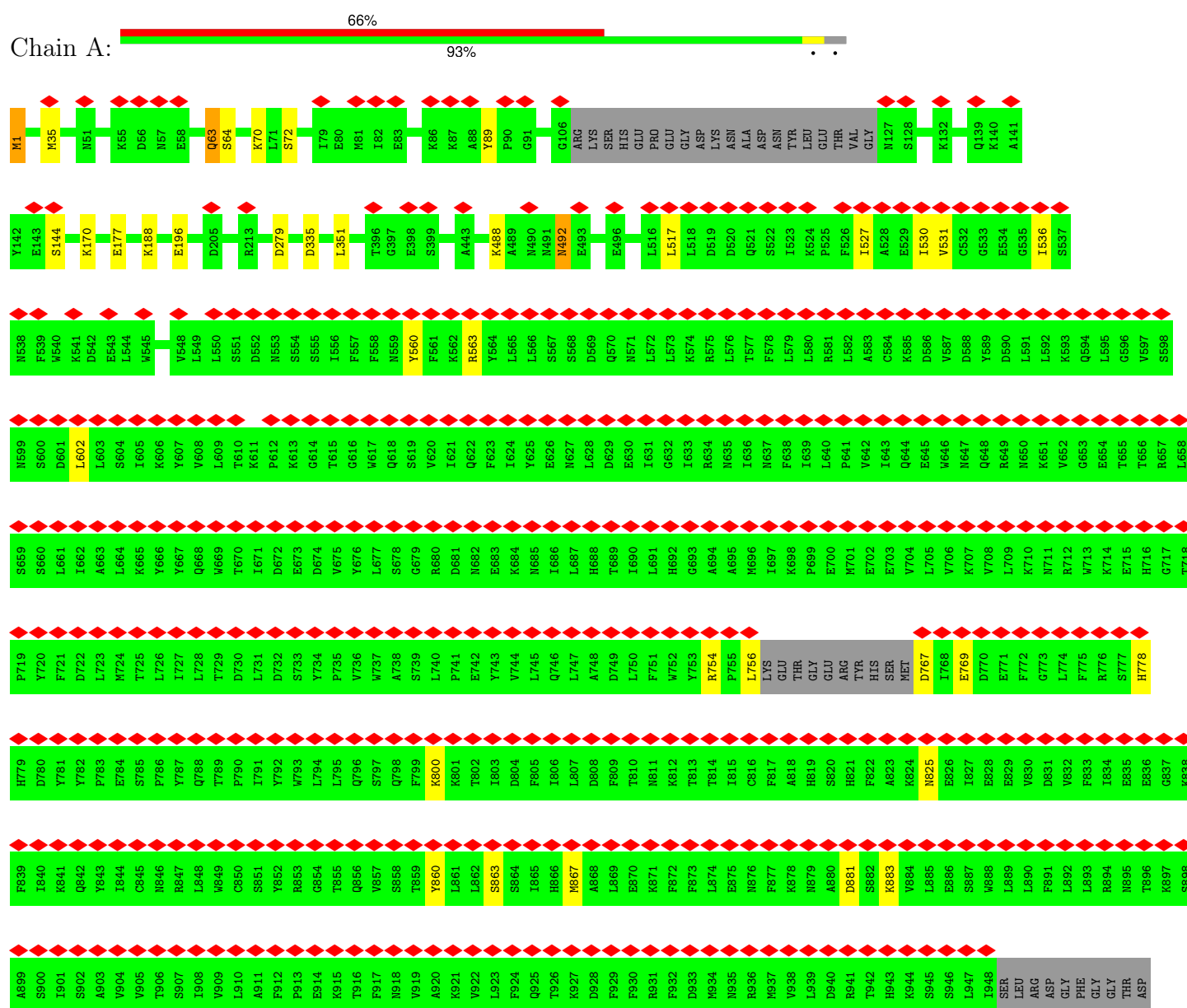
- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

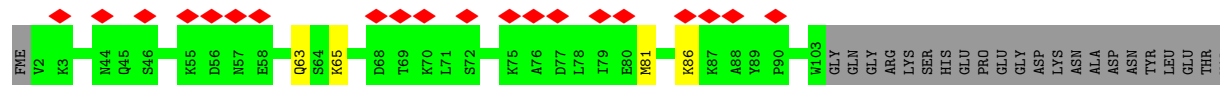
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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



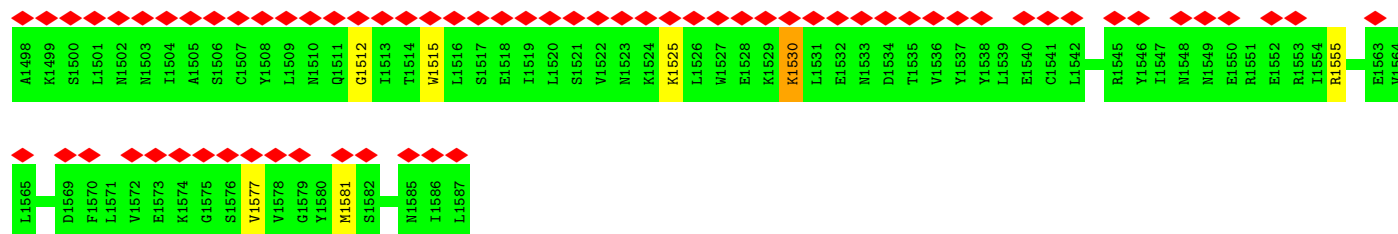
D1569	F1570	L1571	V1572	E1573	K1574	G1575	S1576	V1577	V1578	G1579	Y1580	M1581	S1582		N1585	I1586	L1587
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Chain B:

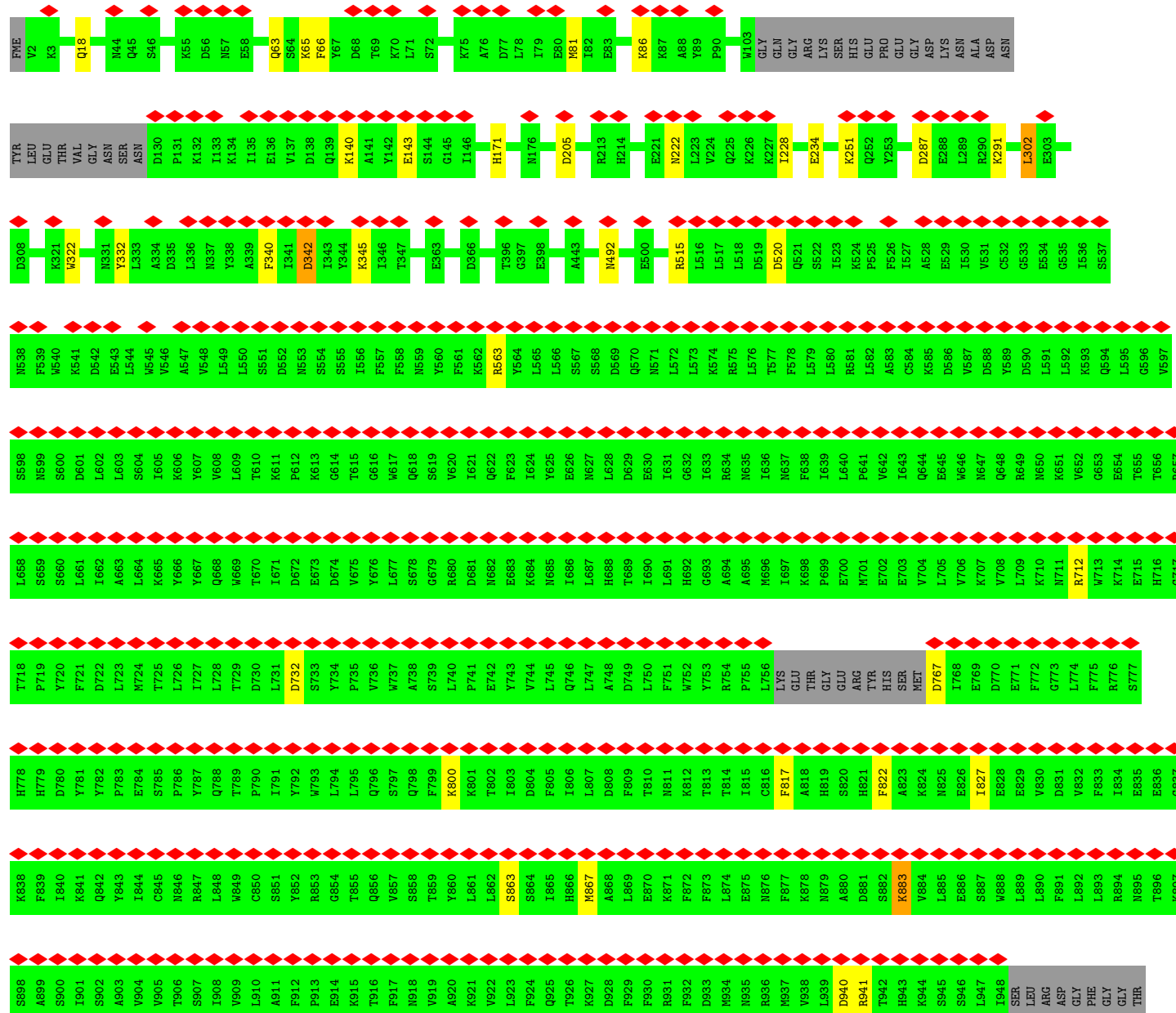
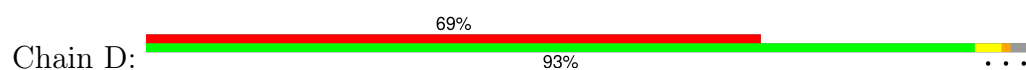


GLY	ASN	SER	ASN	D130	P131	K132	I133	K134	I135	E136	V137	D138	Q139	K140	A141	Y142	E143	S144	G145	I146	H171	N176	D205	R213	H214	L219	H220	E221	N222	L223	V224	Q225	K226	K227	I228	E234	K244	E248	Q252	Y253	D287	E288	L289	R290	K291	L302	E303													
D308	K311	K321	W322	N331	Y332	K333	A334	D335	V346	L336	N337	Y338	A339	F340	I341	D342	I343	Y344	K345	I346	T347	E357	E363	D366	T396	G397	E398	M492	E500	R515	L516	L517	L518	D519	D520	Q521	S522	I523	K524	P525	F526	I527	A528	E529	I530	C532	G533	E534	G535											
I536	S537	N538	F539	W540	K541	D542	E543	L544	W545	D335	A547	V548	L549	L550	S551	D552	N553	S554	S555	I556	F557	F558	N559	Y560	F561	K562	Y564	L565	L566	S567	S568	D569	Q570	N571	L572	L573	K574	R575	L576	T577	F578	L579	L580	L581	L582	A583	C584	K585	D586	V587	D588	Y589	D590	L591	L592	Q594	L595			
G596	V597	S598	N599	D601	L602	L603	L604	I605	K606	V607	V608	L609	T610	K611	P612	K613	G614	T615	G616	W617	Q618	S619	V620	I621	Q622	F623	I624	Y625	E626	N627	L628	D629	E630	I631	G632	I633	R634	N635	I636	N637	F638	I639	L640	P641	V642	I643	Q644	E645	W646	N647	Q648	R649	N650	K651	V652	G653	E654	T655		
T656	R657	L658	S659	S660	L661	I662	A663	L664	K665	Y666	V667	W668	W669	T670	I671	D672	E673	D674	V675	V676	S677	Q678	S679	R680	I681	N682	K683	K684	N685	I686	L687	H688	T689	I690	L691	H692	G693	A694	A695	M696	I697	K698	P699	E700	M701	E702	E703	V704	L705	V706	V707	V708	L709	K710	N711	R712	W713	K714	E715	
H716	G717	T718	P719	Y720	F721	D722	L723	W724	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	TYR	HIS	SER	MET	D767	I768	E769	D770	E771	F772	G773	L774	F775	
R776	S777	H778	H779	D780	Y781	D782	P783	E784	S785	P786	Q787	Q788	T789	P790	I791	Y792	W793	L794	L795	Q796	Q797	Q798	F799	K800	K801	T802	L803	D804	F805	L806	L807	D808	F809	T810	N811	K812	T813	T814	L815	C816	F817	A818	H819	S820	H821	F822	A823	K824	N825	E826	I827	E828	E829	V830	D831	V832	F833	I834	E835	
E836	G837	K838	F839	I840	K841	Q842	Y843	I844	C845	M846	R847	L848	W849	C850	S851	Y852	R853	G854	T855	Q856	V857	S858	T859	Y860	L861	L862	S863	S864	T865	H866	N867	A868	L869	E870	K871	F872	L874	E875	N876	F877	K878	N879	A880	D881	S882	K883	W884	L885	E886	S887	N888	L889	L890	F891	L892	L893	R894	N895		
T896	K897	S898	A899	S900	I901	S902	A903	V904	N905	T906	S907	I908	V909	L910	A911	P912	P913	E914	K915	T916	F917	N918	V919	A920	K921	V922	L923	F924	Q925	T926	K927	D928	F929	P930	R931	P932	D933	N934	N935	R936	N937	V938	L939	D940	R941	T942	H943	K944	S945	S946	L947	T948	SER	LEU	ARG	ASP	GLY	PHE	GLY	
GLY	THR	ASP	TYR	ARG	N961	S962	L963	H964	E965	E966	D967	R968	K969	A971	C972	D973	D974	V975	H976	R977	N978	T979	Y980	L981	E982	N983	L984	A985	L986	H987	Q988	Q989	I990	F991	R992	S993	E994	N995	V996	T997	E998	K999	D1000	A1001	I1002	E1003	R1004	Q1005	Q1006	V1007	L1008	V1009	D1010	I1011	F1012	A1013	K1014	Y1015		
Y1016	N1017	Q1018	L1019	P1020	D1021	E1022	A1023	Q1024	E1025	T1026	E1027	D1028	A1029	K1030	T1031	W1032	R1033	L1034	C1035	L1036	A1037	R1038	M1039	L1040	R1041	R1042	K1043	M1044	K1045	I1046	T1047	T1048	K1049	E1050	K1051	D1052	E1053	G1054	I1055	E1056	I1057	S1058	F1059	M1060	P1061	E1062	I1063	D1064	P1065	K1066	L1067	Q1068	K1069	Y1070	S1071	E1072	K1073	A1074	I1075	
K1076	K1077	N1078	S1079	E1080	H1081	M1082	K1083	Y1084	V1085	T1086	L1087	L1088	K1089	W1090	A1091	S1092	Y1093	K1094	R1095	E1096	K1097	D1098	E1099	R1100	Y1101	K1102	N1103	Y1104	K1105	M1106	Y1107	E1108	D1109	N1110	P1111	Q1112	I1113	A1114	L1115	Q1116	E1117	T1118	K1119	E1120	I1121	I1122	K1123	K1124	L1125	N1126	E1127	K1128	G1129	G1130	E1131	D1132	E1133	R1134	L1135	
L1136	N1137	G1138	N1139	I1140	P1141	A1142	D1143	V1144	C1145	S1146	V1147	L1148	L1149	L1150	D1151	F1152	F1153	N1154	Q1155	L1156	N1157	N1158	E1159	E1160	R1161	E1162	Y1163	K1164	K1165	D1166	Y1167	V1168	L1169	A1170	Y1171	S1172	K1173	L1174	P1175	L1176	K1177	E1178	G1179	Y1180	N1181	Y1182	Q1183	V1184	I1185	D1186	G1187	T1188	T1189	S1190	A1191	I1192	S1193	A1194	L1195	





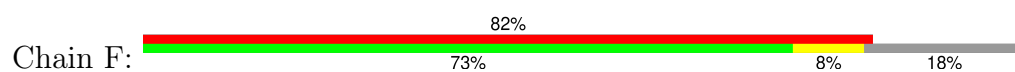
• Molecule 1: ATP-binding protein Avs4



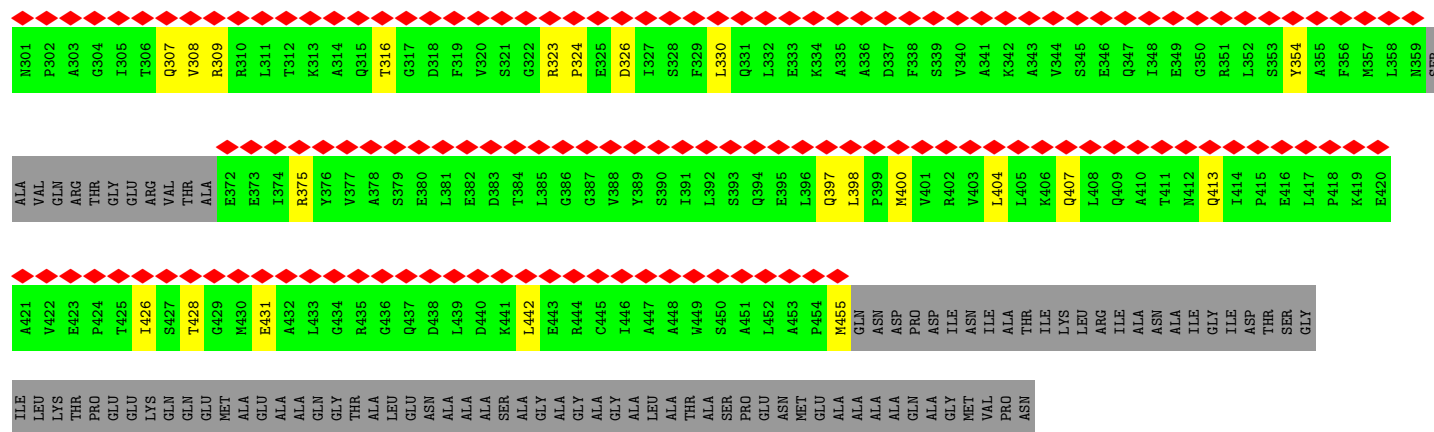
- Molecule 2: Portal protein

ILE	A421	ALA	N301	D241	V181	M121	Q61
LEU	V422	VAL	P302	A242	T182	Y122	A62
LYS	E423	GLN	A303	A243	T183	I123	V63
THR	P424	ARG	G304	Y244	D184	E124	G64
GLU	T425	THR	I305	P245	K185	S125	A65
GLU	T426	GLU	T306	V246	T186	N126	R66
GLN	S427	VAL	Q307	D247	A187	S127	G67
GLN	T428	THR	V308	A248	Y188	Y128	L68
GLU	G429	ALA	R309	C249	A189	R129	N69
MET	M430	E372	R310	P250	A190	V130	N70
ALA	E431	E373	L311	Y251	L191	T131	L71
GLU	A432	I374	T312	I252	P192	L132	A72
ALA	L433	R375	K313	P253	E193	F133	S73
GLN	L434	Y376	A314	V254	D194	E134	K74
GLY	G434	V377	Q315	R255	V195	T135	L75
THR	R435	A378	T316	M256	R196	L136	M76
LEU	G436	S379	G317	V257	N197	K137	L77
GLU	Q437	E380	L318	R258	A198	Q138	A78
ASN	D438	L381	F319	I259	M199	L139	L79
ALA	L439	E382	V320	D260	D200	V140	F80
ALA	D440	D383	S321	G261	S201	V141	P81
SER	K441	T384	G322	E262	G202	A142	M82
GLY	L442	L385	R323	S263	Q203	G143	Q83
ALA	E443	G386	P324	Y264	E204	N144	T84
GLY	R444	G387	E325	G265	H205	A145	M85
ALA	C445	V388	D326	R266	K206	L146	M86
GLY	T446	Y389	I327	S267	G207	L147	K87
LEU	A447	S390	S328	Y268	D208	Y148	L88
ALA	A448	I391	F329	C269	E209	I149	T89
THR	W449	L392	L330	E270	M210	P150	I90
ALA	S450	S393	Q331	E271	I211	E151	S91
SER	A451	Q394	L332	Y272	D212	P152	E92
PRO	L452	E395	E333	L273	V213	F93	F93
GLU	A453	L396	K334	G274	Y214	G154	E94
MET	P454	Q397	A335	D275	T215	A155	A95
ALA	M455	L398	A336	L276	H216	Y156	K96
ALA	GLN	P399	D337	R277	I217	N157	Q97
ALA	ASN	M400	F338	S278	Y218	P158	L98
ALA	ASP	V401	S339	L279	L219	M159	V99
GLN	PRO	R402	V340	E280	D220	K160	A100
ALA	ASP	V403	A341	N281	E221	L161	Q101
ILE	ASN	L404	K342	L282	E222	Y162	P102
VAL	ILE	L405	A343	Q283	G224	R163	A103
ALA	THR	K406	V344	E284	G224	L164	E104
ILE	ILE	Q407	S345	A285	E225	S165	L105
LEU	LEU	L408	E346	I286	Y226	S166	A106
THR	ARG	Q409	Q347	V287	L227	Y167	K107
ALA	ILE	A410	I348	K288	K228	V168	V108
ASN	ASN	T411	E349	M289	Y229	V169	E109
ALA	ALA	M412	G350	S290	E230	Q170	E110
ILE	GLY	Q413	R351	M291	E231	G171	G111
GLY	ILE	I414	L352	I292	I231	D172	L112
ASP	THR	P415	S353	S293	D233	A173	S113
SER	SER	E416	Y354	A294	G234	F174	M114
GLY	GLY	L417	A355	K295	V235	G175	V115
		P418	F356	V296	E236	T176	E116
		K419	M357	I297	V237	V177	R117
		E420	L358	G298	D238	L178	I118
			N359	L299	G239	Q179	L119
			SER	V300	T240	T180	M120

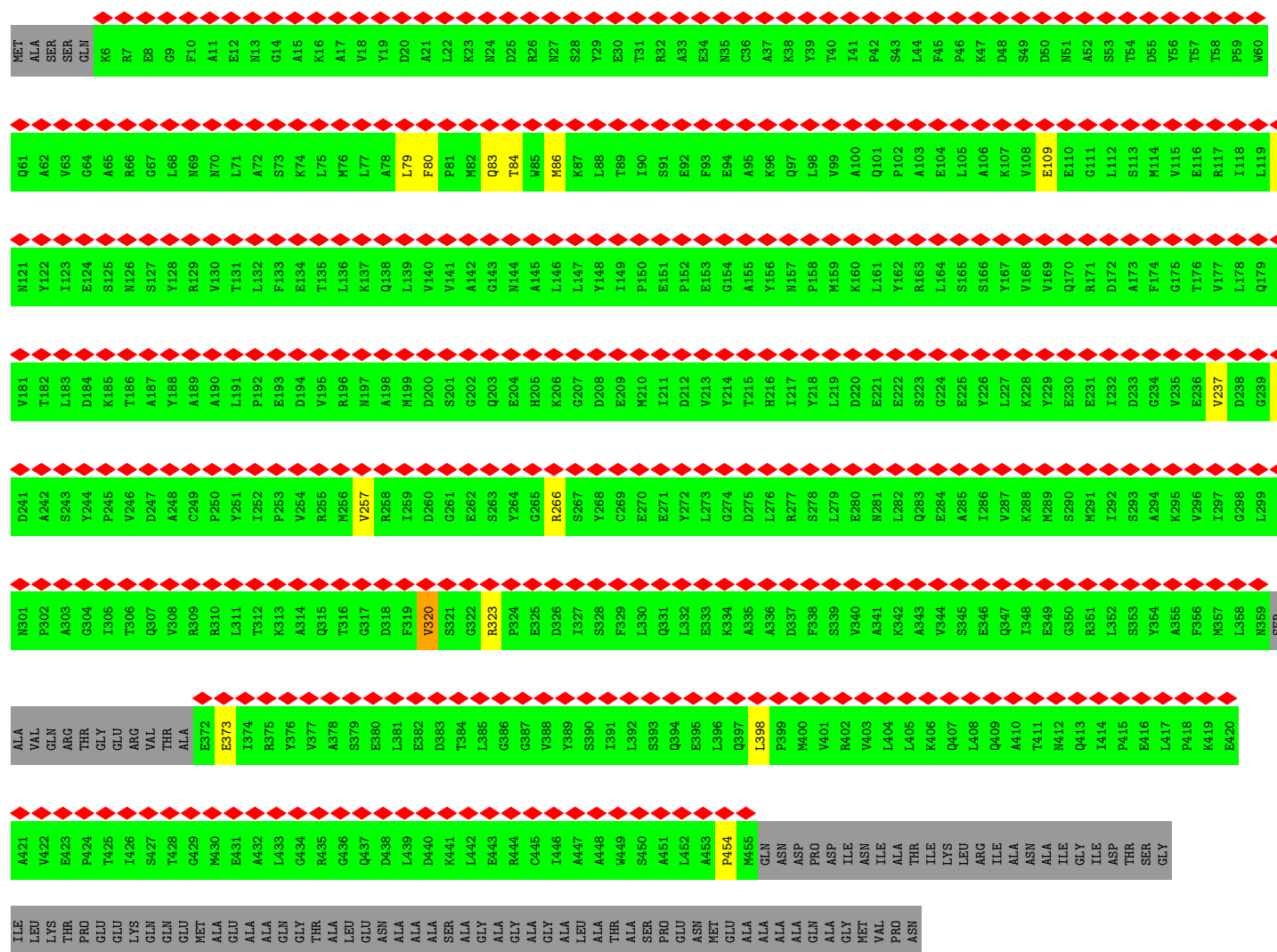
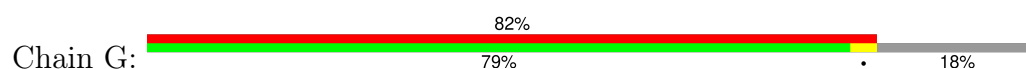
• Molecule 2: Portal protein



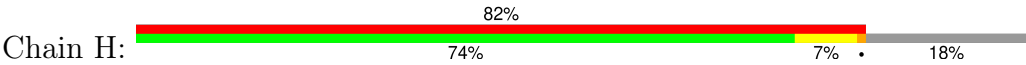
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	Q61	A62	V63	G64	A65	R66	G67	L68	N69	N70	L71	A72	S73	K74	L75	M76	L77	A78	L79	F80	P81	M82	Q83	T84	M85	M86	K87	L88	T89	I90	S91	E92	F93	E94	A95	K96	Q97	L98	V99	A100	Q101	P102	A103	E104	L105	A106	K107	V108	E109	E110	G111	L112	S113	M114	V115	E116	R117	I118	L119	M120
	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	N157	P158	M159	K160	L161	Y162	R163	L164	S165	S166	Y167	V168	V169	Q170	R171	D172	A173	F174	G175	T176	V177	L178	Q179	I180
	V181	T182	L183	D184	K185	T186	A187	Y188	A189	A190	L191	P192	F193	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	L222	S223	G224	E225	Y226	L227	K228	Y229	E230	E231	I232	D233	G234	V235	E236	V237	D238	G239	T240
	D241	A242	S243	Y244	P245	V246	D247	A248	C249	P250	Y251	I252	P253	V254	R255	M256	V257	R258	I259	D260	G261	E262	S263	Y264	G265	R266	S267	Y268	C269	E270	E271	Y272	L273	G274	D275	L276	R277	S278	L279	N280	N281	L282	Q283	E284	A285	I286	V287	K288	M289	S290	M291	I292	S293	A294	K295	V296	I297	G298	L299	V300



• Molecule 2: Portal protein



• Molecule 2: Portal protein



ILE	LEU	LYS	THR	PRO	GLU	GLU	LYS	GLN	GLN	GLU	MET	ALA	GLU	ALA	ALA	GLN	GLY	THR	ALA	LEU	GLU	ASN	ALA	ALA	ALA	SER	ALA	GLY	GLY	ALA	GLY	ASN	MET	GLU	ALA	ALA	ALA	ASP	PRO	ASP	ILE	ASN	ILE	ALA	ALA	THR	LYS	LEU	ARG	ILE	ALA	ASN	ALA	ILE	GLY	ASP	THR	SER	GLY
A421	V422	E423	P424	T425	GLU	GLU	I426	S427	T428	G429	M430	E431	A432	L433	G434	R435	G436	Q437	E380	D438	L439	D440	K441	L442	E443	G444	C445	I446	A447	S450	A451	L452	A453	P454	M455	GLN	ASN	ASP	PRO	ASP	ILE	ASN	ILE	ALA	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	M412	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	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

5.1 Standard geometry

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%)

All (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
2	F	257	VAL	CB-CG1	-5.43	1.41	1.52
2	E	324	PRO	CA-C	5.39	1.63	1.52

All (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
2	G	454	PRO	CA-CB-CG	-11.32	82.49	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	324	PRO	N-CD-CG	-10.84	86.94	103.20
2	E	324	PRO	CA-CB-CG	-10.32	84.40	104.00
2	G	398	LEU	CB-CG-CD2	-10.07	93.89	111.00
2	E	398	LEU	CB-CG-CD2	-9.63	94.63	111.00
1	B	342	ASP	CB-CG-OD1	8.81	126.23	118.30
1	D	342	ASP	CB-CG-OD1	8.80	126.22	118.30
2	H	383	ASP	CB-CG-OD2	8.77	126.19	118.30
2	H	398	LEU	CB-CG-CD2	-8.40	96.71	111.00
2	F	324	PRO	CA-N-CD	-8.37	99.78	111.50
2	H	324	PRO	CA-N-CD	-8.12	100.13	111.50
2	H	330	LEU	CB-CG-CD1	-8.02	97.37	111.00
2	H	330	LEU	CA-CB-CG	7.93	133.54	115.30
2	F	324	PRO	CA-CB-CG	-7.62	89.52	104.00
2	H	324	PRO	CA-CB-CG	-7.08	90.55	104.00
1	D	287	ASP	CB-CG-OD1	7.02	124.62	118.30
1	B	287	ASP	CB-CG-OD1	6.91	124.52	118.30
1	C	351	LEU	CA-CB-CG	6.86	131.08	115.30
2	H	199	MET	CG-SD-CE	6.84	111.14	100.20
1	D	302	LEU	CB-CG-CD1	-6.79	99.46	111.00
2	E	323	ARG	C-N-CD	6.68	142.43	128.40
1	A	351	LEU	CA-CB-CG	6.67	130.65	115.30
2	E	324	PRO	N-CD-CG	-6.66	93.22	103.20
2	F	398	LEU	CB-CG-CD1	6.63	122.28	111.00
1	C	1186	ASP	CB-CG-OD1	6.14	123.83	118.30
2	H	172	ASP	CB-CG-OD1	6.11	123.80	118.30
1	D	1064	ASP	CB-CG-OD1	6.10	123.79	118.30
2	F	172	ASP	CB-CG-OD1	6.10	123.79	118.30
1	A	1186	ASP	CB-CG-OD1	6.07	123.76	118.30
1	B	1186	ASP	CB-CG-OD1	6.05	123.75	118.30
1	C	1064	ASP	CB-CG-OD1	6.02	123.72	118.30
1	D	1186	ASP	CB-CG-OD1	6.02	123.72	118.30
1	A	1064	ASP	CB-CG-OD1	5.99	123.69	118.30
1	C	517	LEU	CA-CB-CG	5.97	129.04	115.30
1	A	517	LEU	CA-CB-CG	5.97	129.04	115.30
1	B	302	LEU	CB-CG-CD1	-5.95	100.89	111.00
1	B	1064	ASP	CB-CG-OD1	5.93	123.64	118.30
1	A	1098	ASP	CB-CG-OD1	5.92	123.62	118.30
1	C	1098	ASP	CB-CG-OD1	5.81	123.53	118.30
2	H	326	ASP	CB-CG-OD2	5.75	123.47	118.30
1	B	1569	ASP	CB-CG-OD2	5.72	123.45	118.30
2	E	320	VAL	CG1-CB-CG2	-5.63	101.89	110.90
1	D	1098	ASP	CB-CG-OD1	5.60	123.34	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1569	ASP	CB-CG-OD2	5.60	123.34	118.30
2	G	454	PRO	N-CA-CB	-5.59	96.45	102.60
1	B	1098	ASP	CB-CG-OD1	5.53	123.28	118.30
1	D	251	LYS	CD-CE-NZ	5.51	124.36	111.70
2	F	194	ASP	CB-CG-OD2	5.51	123.26	118.30
2	G	320	VAL	CG1-CB-CG2	-5.38	102.29	110.90
2	E	324	PRO	N-CA-CB	-5.36	96.70	102.60
2	H	330	LEU	CB-CG-CD2	5.34	120.07	111.00
1	A	881	ASP	CB-CG-OD1	5.29	123.06	118.30
2	G	454	PRO	CA-N-CD	-5.27	104.13	111.50
2	F	442	LEU	CA-CB-CG	5.24	127.36	115.30
2	F	404	LEU	CB-CG-CD1	-5.23	102.11	111.00
1	B	878	LYS	CD-CE-NZ	5.20	123.66	111.70
1	C	881	ASP	CB-CG-OD1	5.19	122.97	118.30
2	H	114	MET	CG-SD-CE	5.16	108.45	100.20
2	H	132	LEU	CA-CB-CG	-5.09	103.60	115.30
2	F	199	MET	CG-SD-CE	5.01	108.21	100.20

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	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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.

All (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
2:E:257:VAL:HG12	2:E:266:ARG:H	1.58	0.68
2:G:257:VAL:HG12	2:G:266:ARG:H	1.59	0.68
2:E:83:GLN:HG3	2:E:431:GLU:HG2	1.77	0.67
1:C:1026:THR:OG1	1:C:1027:GLU:OE2	2.13	0.66
2:H:83:GLN:HG3	2:H:431:GLU:HG2	1.78	0.66
1:D:515:ARG:NH2	1:D:520:ASP:OD2	2.30	0.64
1:A:1226:ALA:HB2	2:E:384:THR:HG23	1.81	0.63
2:F:83:GLN:HG3	2:F:431:GLU:HG2	1.82	0.62
1:B:1106:MET:SD	1:B:1106:MET:N	2.73	0.61
1:B:1462:TRP:O	2:F:375:ARG:NH2	2.34	0.61
1:D:1462:TRP:O	2:H:375:ARG:NH2	2.34	0.61
1:C:1027:GLU:OE2	1:C:1027:GLU:N	2.33	0.61
2:F:149:ILE:HD11	2:F:400:MET:HG3	1.83	0.60
1:D:302:LEU:HD11	1:D:332:TYR:CD1	2.37	0.60
1:B:302:LEU:HD11	1:B:332:TYR:CD1	2.37	0.59
1:D:1106:MET:N	1:D:1106:MET:SD	2.74	0.59
1:B:308:ASP:HA	1:B:311:LYS:HG3	1.83	0.59
2:H:315:GLN:HG2	2:H:318:ASP:HB2	1.85	0.58
1:A:1525:LYS:H	1:A:1525:LYS:HD2	1.69	0.58
2:F:308:VAL:HG22	2:F:309:ARG:HH21	1.69	0.58
1:C:1525:LYS:HD2	1:C:1525:LYS:H	1.69	0.58
2:E:237:VAL:O	2:E:240:THR:OG1	2.21	0.57
2:H:257:VAL:HG12	2:H:266:ARG:H	1.69	0.57
2:G:237:VAL:O	2:G:240:THR:OG1	2.22	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1359:ARG:HH11	1:B:1362:ARG:HD3	1.69	0.56
2:H:330:LEU:HG	2:H:334:LYS:HB2	1.87	0.56
2:F:118:ILE:HG21	2:F:413:GLN:HE21	1.72	0.55
2:H:330:LEU:HD12	2:H:333:GLU:HB3	1.88	0.55
2:H:152:PRO:HA	2:H:157:ASN:OD1	2.06	0.55
2:H:149:ILE:HD11	2:H:400:MET:HG3	1.88	0.55
1:A:196:GLU:OE1	1:A:196:GLU:N	2.40	0.54
1:C:196:GLU:N	1:C:196:GLU:OE2	2.40	0.54
1:D:302:LEU:HD21	1:D:332:TYR:CE1	2.43	0.54
2:F:118:ILE:HD13	2:F:413:GLN:NE2	2.23	0.53
2:H:309:ARG:HH12	2:H:313:LYS:HD3	1.74	0.53
1:A:1:FME:O1	1:D:171:HIS:ND1	2.43	0.52
1:B:1112:GLN:O	1:B:1116:GLN:HG3	2.09	0.52
1:D:1041:ARG:HE	2:H:316:THR:HG23	1.73	0.52
1:B:1525:LYS:H	1:B:1525:LYS:HE2	1.74	0.52
1:C:941:ARG:HB2	1:C:941:ARG:NH1	2.24	0.52
1:B:171:HIS:ND1	1:C:1:FME:O1	2.43	0.52
1:D:1112:GLN:O	1:D:1116:GLN:HG3	2.09	0.52
1:D:1525:LYS:HE2	1:D:1525:LYS:H	1.75	0.52
1:C:1469:TRP:CD1	2:G:373:GLU:HG3	2.45	0.51
1:A:1469:TRP:CD1	2:E:373:GLU:HG3	2.45	0.51
2:F:153:GLU:H	2:F:157:ASN:HD21	1.58	0.50
1:D:63:GLN:HG2	1:D:81:MET:SD	2.52	0.50
1:B:515:ARG:NH2	1:B:520:ASP:OD2	2.44	0.50
1:D:228:ILE:HG21	1:D:340:PHE:CZ	2.47	0.50
1:B:244:LYS:O	1:B:248:GLU:HG2	2.12	0.50
1:B:63:GLN:HG2	1:B:81:MET:SD	2.52	0.49
1:B:228:ILE:HG21	1:B:340:PHE:CZ	2.48	0.49
1:B:302:LEU:HD21	1:B:332:TYR:CE1	2.48	0.49
1:B:1059:PHE:HB2	2:F:296:VAL:HG13	1.95	0.48
2:F:297:ILE:HG22	2:F:330:LEU:HD23	1.94	0.48
1:A:1530:LYS:HA	1:A:1530:LYS:HE2	1.95	0.48
1:B:1134:ARG:HH11	1:B:1134:ARG:HB3	1.78	0.48
2:F:152:PRO:HA	2:F:157:ASN:ND2	2.29	0.48
1:A:825:ASN:HD22	2:E:54:THR:C	2.17	0.47
1:C:1530:LYS:HA	1:C:1530:LYS:HE2	1.95	0.47
2:F:80:PHE:CE2	2:F:397:GLN:HG2	2.49	0.47
2:F:118:ILE:HD13	2:F:413:GLN:HE22	1.80	0.47
2:F:80:PHE:HE2	2:F:397:GLN:HG2	1.78	0.47
1:A:530:ILE:HD12	1:A:536:ILE:HD13	1.96	0.47
2:H:302:PRO:HD3	2:H:326:ASP:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:291:LYS:HB3	1:B:322:TRP:CE3	2.50	0.46
1:D:1134:ARG:HB3	1:D:1134:ARG:HH11	1.79	0.46
2:F:151:GLU:HA	2:F:407:GLN:HE21	1.80	0.46
1:A:170:LYS:NZ	1:A:177:GLU:O	2.48	0.46
1:B:990:ILE:HG23	1:B:991:PHE:HD2	1.80	0.46
1:B:132:LYS:H	1:B:132:LYS:HE2	1.81	0.46
1:D:291:LYS:HB3	1:D:322:TRP:CE3	2.50	0.46
2:F:286:ILE:HA	2:F:289:MET:HE3	1.96	0.46
2:F:426:ILE:HG22	2:F:428:THR:HG23	1.98	0.46
2:H:117:ARG:NH1	2:H:121:ASN:HB2	2.24	0.46
1:B:65:LYS:HA	1:B:65:LYS:HD3	1.81	0.45
1:B:1041:ARG:HE	2:F:316:THR:HG23	1.81	0.45
2:H:80:PHE:CE2	2:H:397:GLN:HG2	2.51	0.45
2:G:84:THR:HA	2:G:120:MET:CE	2.46	0.45
1:A:754:ARG:HH12	1:A:756:LEU:HD23	1.81	0.45
1:C:1469:TRP:HD1	2:G:373:GLU:HG3	1.81	0.45
1:A:863:SER:O	1:A:867:MET:HG3	2.17	0.45
1:D:65:LYS:HD3	1:D:65:LYS:HA	1.82	0.45
1:D:205:ASP:OD2	1:D:205:ASP:N	2.50	0.45
1:C:170:LYS:NZ	1:C:177:GLU:O	2.50	0.45
1:B:1134:ARG:HB3	1:B:1134:ARG:NH1	2.32	0.44
1:D:1134:ARG:HB3	1:D:1134:ARG:NH1	2.32	0.44
1:D:1059:PHE:HB2	2:H:296:VAL:HG13	1.98	0.44
1:A:1081:HIS:HD1	1:A:1081:HIS:C	2.21	0.44
1:B:1287:ILE:HD12	1:B:1288:ASN:N	2.33	0.44
1:C:492:ASN:OD1	1:C:492:ASN:N	2.50	0.44
1:B:205:ASP:OD2	1:B:205:ASP:N	2.49	0.44
2:E:84:THR:HA	2:E:120:MET:CE	2.47	0.44
2:H:157:ASN:HD22	2:H:157:ASN:HA	1.53	0.44
2:G:79:LEU:HB3	2:G:80:PHE:CD2	2.52	0.44
1:B:1120:GLU:O	1:B:1123:LYS:HE2	2.18	0.43
1:A:778:HIS:CE1	1:A:860:TYR:HD1	2.36	0.43
1:A:1469:TRP:HD1	2:E:373:GLU:HG3	1.82	0.43
2:G:83:GLN:O	2:G:120:MET:HE1	2.18	0.43
1:D:1046:ILE:HD12	2:H:311:LEU:HB3	2.01	0.43
1:A:527:ILE:O	1:A:531:VAL:HG23	2.19	0.43
1:D:1359:ARG:NH1	1:D:1362:ARG:HD3	2.34	0.43
1:D:1524:LYS:HD2	1:D:1524:LYS:HA	1.78	0.43
2:F:307:GLN:OE1	2:F:309:ARG:HG2	2.18	0.43
2:E:79:LEU:HB3	2:E:80:PHE:CD2	2.53	0.43
2:H:295:LYS:HE3	2:H:334:LYS:NZ	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:883:LYS:HD3	1:C:883:LYS:N	2.34	0.42
2:H:77:LEU:HD12	2:H:77:LEU:HA	1.89	0.42
1:A:492:ASN:OD1	1:A:492:ASN:N	2.50	0.42
1:C:1099:GLU:O	1:C:1102:LYS:HG3	2.20	0.42
2:E:151:GLU:HA	2:E:152:PRO:HD3	1.90	0.42
2:H:151:GLU:HA	2:H:407:GLN:HE21	1.83	0.42
2:G:257:VAL:HG11	2:G:266:ARG:HB2	2.01	0.42
1:B:883:LYS:HD2	1:B:883:LYS:H	1.85	0.42
1:C:1577:VAL:O	1:C:1581:MET:HG3	2.20	0.42
1:D:863:SER:O	1:D:867:MET:HG3	2.20	0.42
1:D:883:LYS:H	1:D:883:LYS:HD2	1.85	0.42
1:D:1569:ASP:N	1:D:1569:ASP:OD1	2.53	0.42
2:G:83:GLN:OE1	2:G:84:THR:N	2.53	0.42
1:B:817:PHE:CE2	1:B:827:ILE:HD11	2.54	0.41
2:F:194:ASP:OD2	2:F:195:VAL:N	2.52	0.41
1:B:825:ASN:HD22	2:F:54:THR:C	2.23	0.41
1:B:1113:ILE:H	1:B:1113:ILE:HG12	1.70	0.41
1:C:3:LYS:HG2	1:C:4:PRO:HD2	2.02	0.41
1:A:1577:VAL:O	1:A:1581:MET:HG3	2.20	0.41
1:B:140:LYS:O	1:B:143:GLU:HG3	2.21	0.41
1:C:1081:HIS:HD1	1:C:1081:HIS:C	2.24	0.41
2:E:257:VAL:HG11	2:E:266:ARG:HB2	2.02	0.41
2:F:117:ARG:HH22	2:F:121:ASN:HD22	1.69	0.41
1:A:1512:GLY:HA2	1:A:1515:TRP:CE3	2.56	0.41
1:D:18:GLN:NE2	1:D:66:PHE:O	2.54	0.41
1:A:883:LYS:N	1:A:883:LYS:HD3	2.35	0.41
1:C:438:PHE:HE1	1:C:1555:ARG:HH12	1.68	0.41
1:A:990:ILE:HD11	2:E:311:LEU:HD13	2.03	0.41
1:C:1512:GLY:HA2	1:C:1515:TRP:CE3	2.56	0.41
1:B:863:SER:O	1:B:867:MET:HG3	2.21	0.41
1:C:1119:LYS:HA	1:C:1122:ILE:HG22	2.03	0.41
2:E:380:GLU:HA	2:E:384:THR:OG1	2.21	0.41
2:E:315:GLN:HG2	2:E:318:ASP:HB2	2.02	0.40
1:A:1099:GLU:O	1:A:1102:LYS:HG3	2.20	0.40
1:B:228:ILE:HD13	1:B:340:PHE:CZ	2.57	0.40
1:C:63:GLN:OE1	1:C:64:SER:N	2.54	0.40
1:A:70:LYS:NZ	1:A:72:SER:OG	2.54	0.40
1:A:769:GLU:HG2	1:A:778:HIS:CE1	2.57	0.40
1:D:140:LYS:O	1:D:143:GLU:HG3	2.20	0.40
1:D:817:PHE:CE2	1:D:827:ILE:HD11	2.56	0.40
2:E:381:LEU:O	2:E:385:LEU:HD23	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:398:LEU:HA	2:E:398:LEU:HD23	1.93	0.40
2:H:84:THR:HA	2:H:120:MET:HE3	2.04	0.40
1:A:63:GLN:OE1	1:A:64:SER:N	2.54	0.40
1:B:1569:ASP:N	1:B:1569:ASP:OD1	2.51	0.40

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	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 [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	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
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

All (126) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	MET
1	A	63	GLN
1	A	89	TYR
1	A	144	SER
1	A	188	LYS
1	A	279	ASP
1	A	335	ASP
1	A	488	LYS
1	A	492	ASN
1	A	560	TYR
1	A	563	ARG
1	A	602	LEU
1	A	767	ASP
1	A	800	LYS
1	A	1041	ARG
1	A	1052	ASP
1	A	1081	HIS
1	A	1123	LYS
1	A	1359	ARG
1	A	1362	ARG
1	A	1428	TRP
1	A	1530	LYS
1	B	86	LYS
1	B	132	LYS
1	B	222	ASN

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Mol	Chain	Res	Type
1	B	234	GLU
1	B	338	TYR
1	B	342	ASP
1	B	345	LYS
1	B	492	ASN
1	B	563	ARG
1	B	594	GLN
1	B	701	MET
1	B	712	ARG
1	B	767	ASP
1	B	800	LYS
1	B	883	LYS
1	B	940	ASP
1	B	1041	ARG
1	B	1095	ARG
1	B	1123	LYS
1	B	1289	LYS
1	B	1359	ARG
1	B	1360	GLU
1	B	1428	TRP
1	B	1518	GLU
1	B	1525	LYS
1	C	35	MET
1	C	63	GLN
1	C	89	TYR
1	C	144	SER
1	C	188	LYS
1	C	211	ASP
1	C	279	ASP
1	C	335	ASP
1	C	398	GLU
1	C	488	LYS
1	C	492	ASN
1	C	560	TYR
1	C	563	ARG
1	C	602	LEU
1	C	800	LYS
1	C	816	CYS
1	C	1041	ARG
1	C	1081	HIS
1	C	1123	LYS
1	C	1359	ARG

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Mol	Chain	Res	Type
1	C	1428	TRP
1	C	1530	LYS
1	D	86	LYS
1	D	222	ASN
1	D	234	GLU
1	D	342	ASP
1	D	345	LYS
1	D	492	ASN
1	D	563	ARG
1	D	712	ARG
1	D	732	ASP
1	D	767	ASP
1	D	800	LYS
1	D	822	PHE
1	D	883	LYS
1	D	940	ASP
1	D	941	ARG
1	D	1041	ARG
1	D	1044	MET
1	D	1095	ARG
1	D	1106	MET
1	D	1123	LYS
1	D	1272	HIS
1	D	1289	LYS
1	D	1359	ARG
1	D	1360	GLU
1	D	1428	TRP
1	D	1518	GLU
1	D	1524	LYS
1	D	1525	LYS
2	E	86	MET
2	E	210	MET
2	E	214	TYR
2	E	320	VAL
2	E	323	ARG
2	E	326	ASP
2	E	437	GLN
2	F	22	LEU
2	F	86	MET
2	F	114	MET
2	F	117	ARG
2	F	210	MET

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Mol	Chain	Res	Type
2	F	323	ARG
2	F	326	ASP
2	F	354	TYR
2	F	455	MET
2	G	86	MET
2	G	109	GLU
2	G	320	VAL
2	G	323	ARG
2	H	22	LEU
2	H	86	MET
2	H	114	MET
2	H	117	ARG
2	H	194	ASP
2	H	199	MET
2	H	210	MET
2	H	323	ARG
2	H	354	TYR

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 [i](#)

There are no RNA molecules in this entry.

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

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($^{\circ}$)	Ideal($^{\circ}$)
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.

All (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
1	C	1	FME	CB-CG-SD-CE
1	A	1	FME	N-CA-CB-CG
1	C	1	FME	N-CA-CB-CG
1	A	1	FME	CA-CB-CG-SD
1	C	1	FME	CA-CB-CG-SD
1	A	1	FME	C-CA-CB-CG
1	C	1	FME	C-CA-CB-CG

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

All (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
3	C	1601	ATP	PB-O3B	-3.01	1.56	1.59
3	D	1601	ATP	PB-O3B	-2.43	1.56	1.59
3	B	1601	ATP	PB-O3B	-2.42	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.

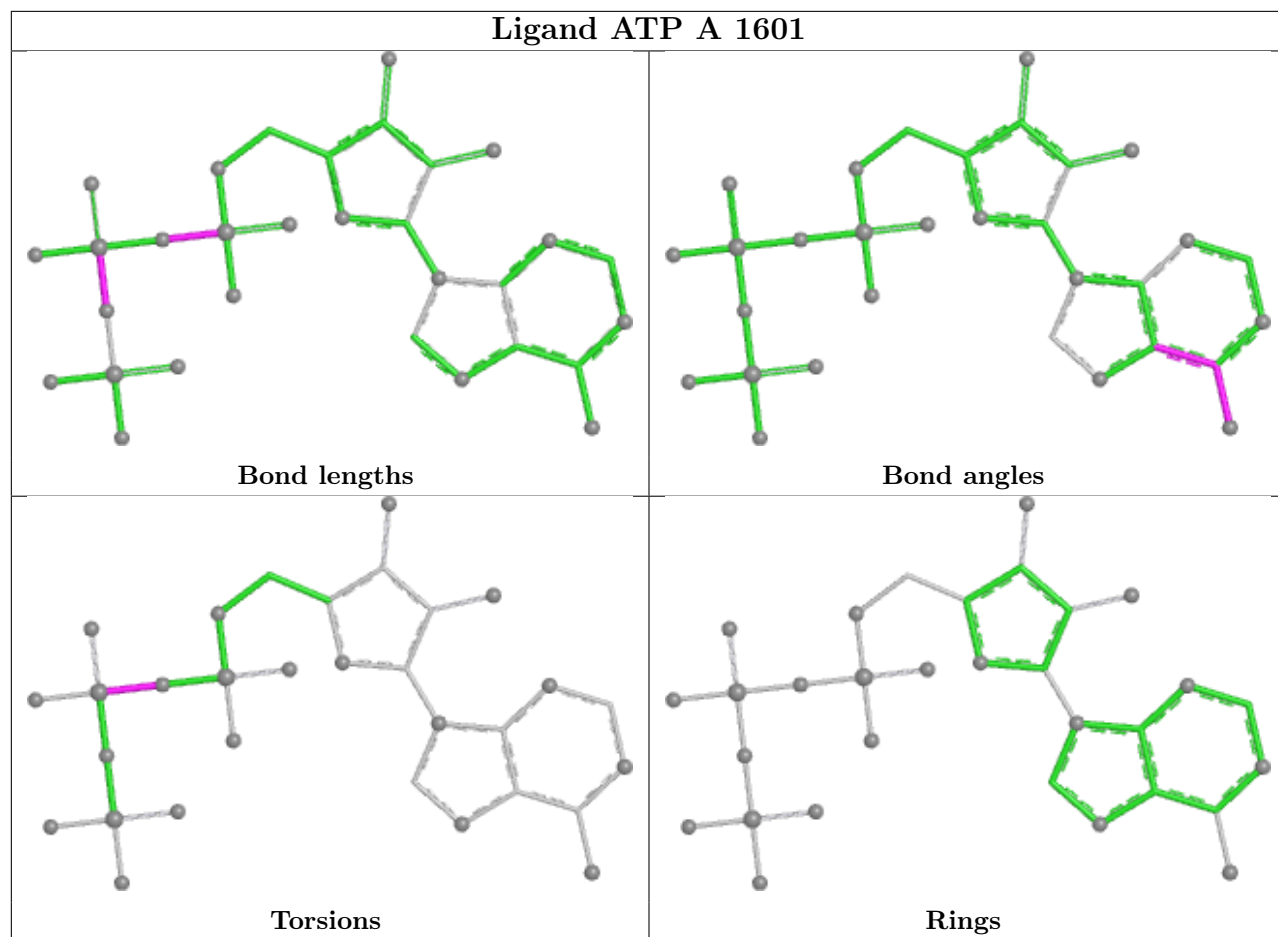
All (2) torsion outliers are listed below:

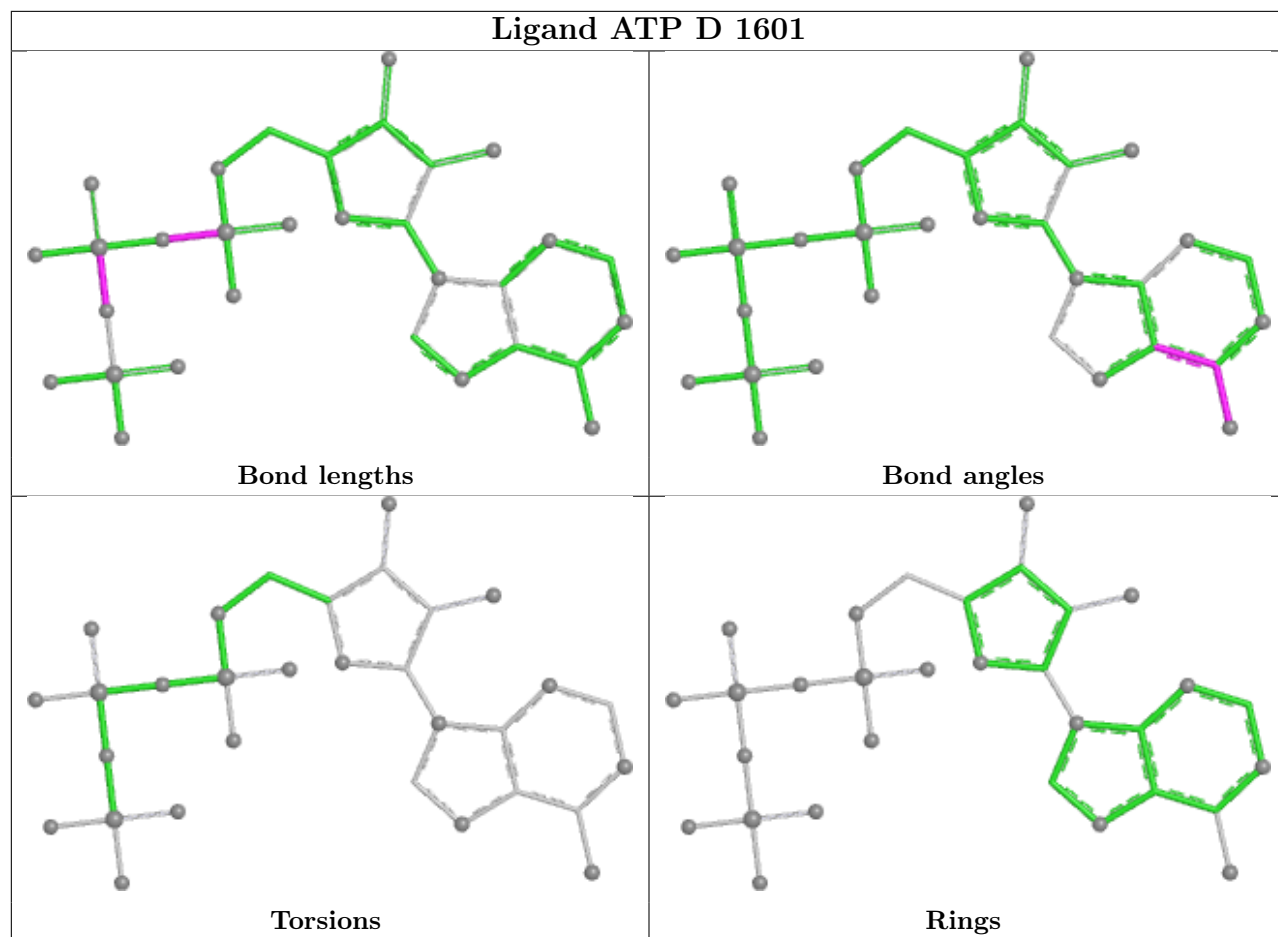
Mol	Chain	Res	Type	Atoms
3	A	1601	ATP	PA-O3A-PB-O2B
3	C	1601	ATP	PA-O3A-PB-O2B

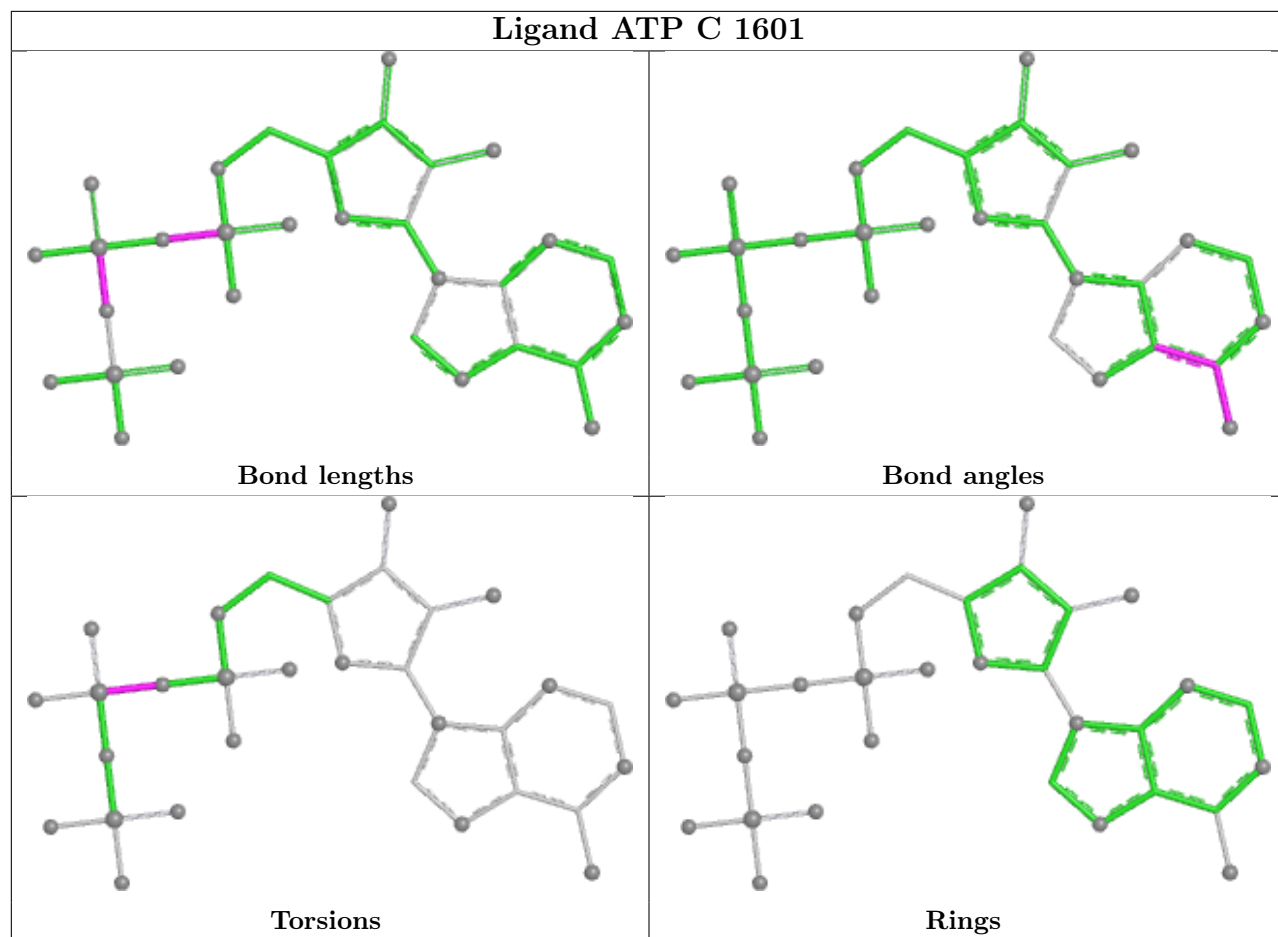
There are no ring outliers.

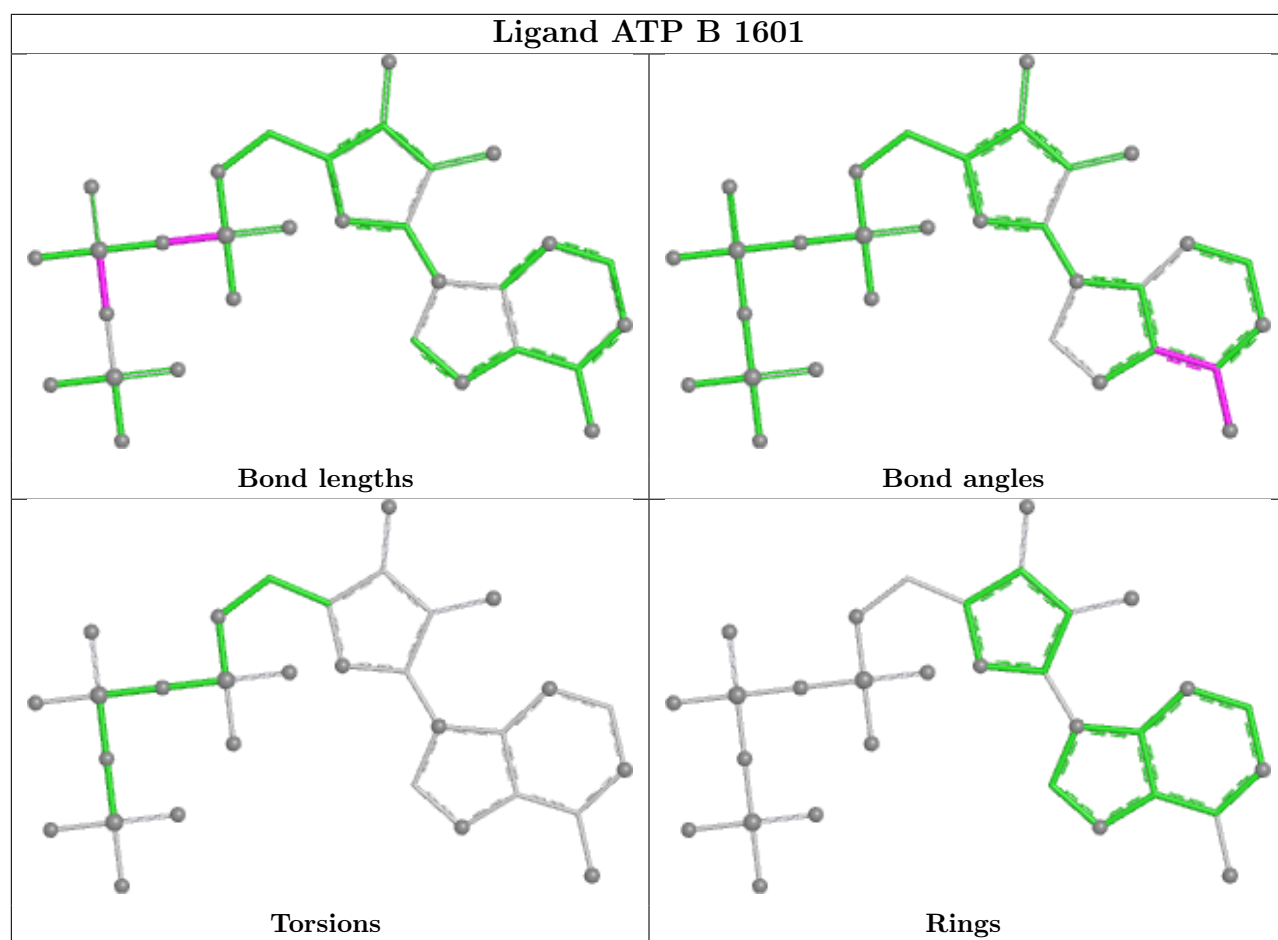
No monomer is involved in short contacts.

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.

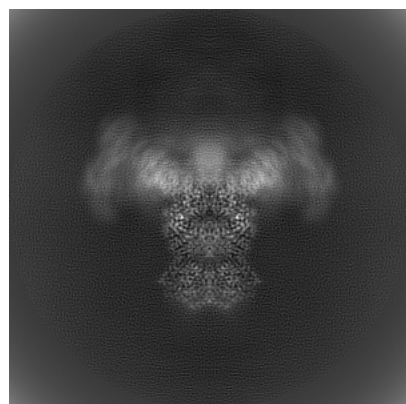
6 Map visualisation [i](#)

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.

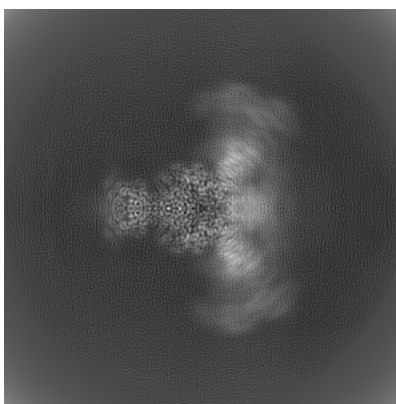
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

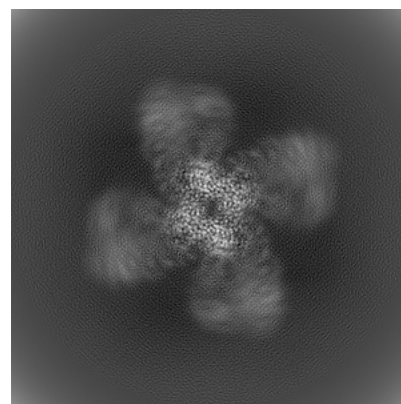
6.1.1 Primary map



X

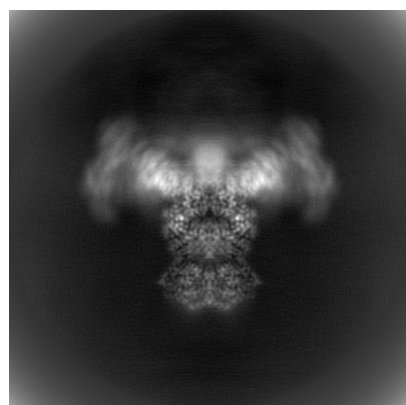


Y

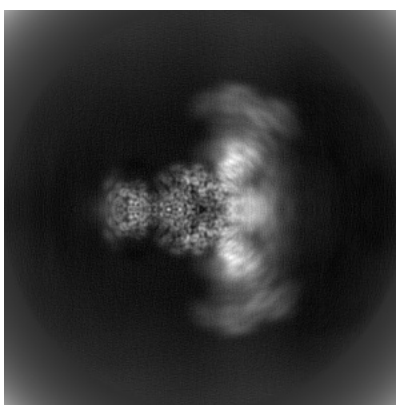


Z

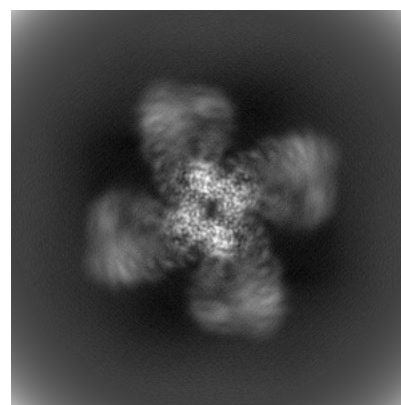
6.1.2 Raw map



X



Y

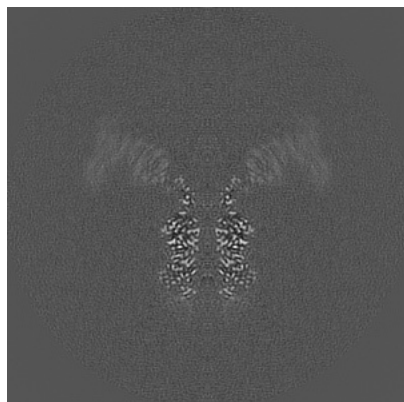


Z

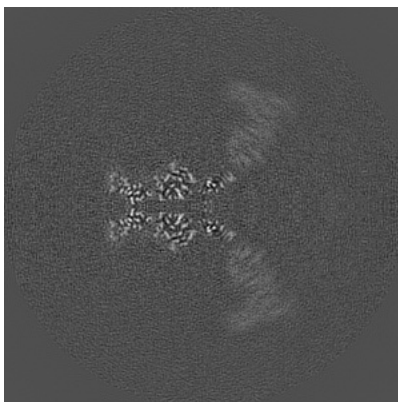
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

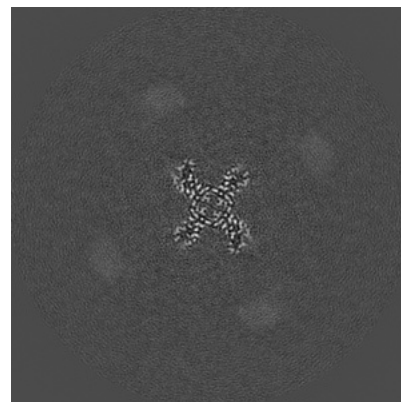
6.2.1 Primary map



X Index: 180

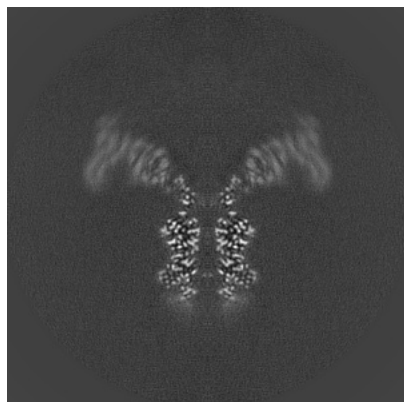


Y Index: 180

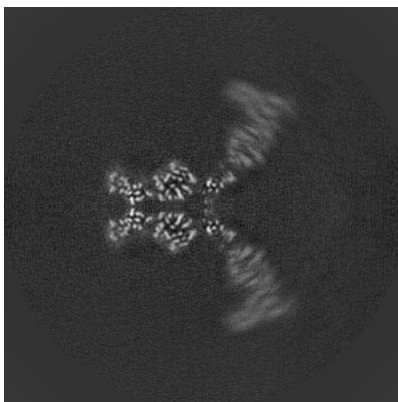


Z Index: 180

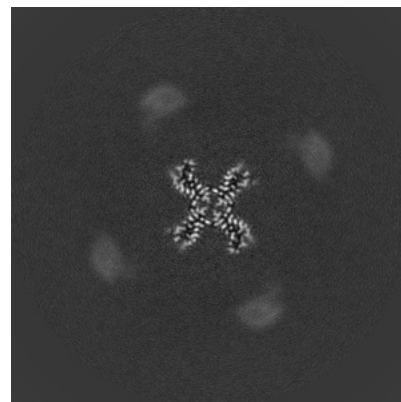
6.2.2 Raw map



X Index: 180



Y Index: 180

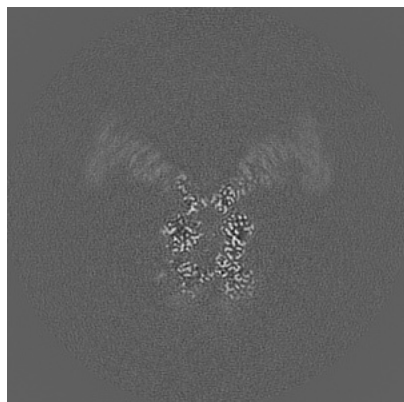


Z Index: 180

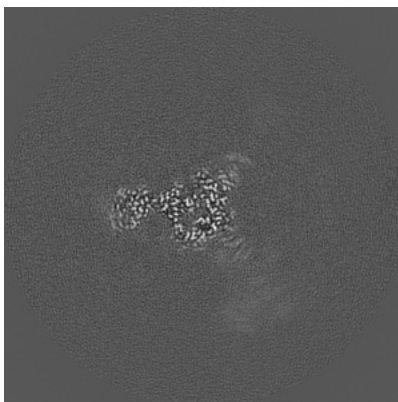
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

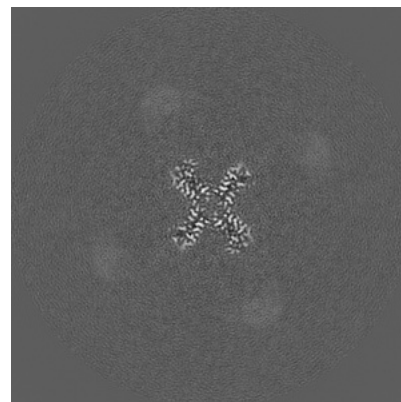
6.3.1 Primary map



X Index: 175

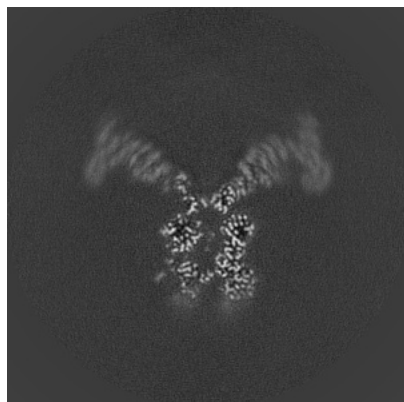


Y Index: 160

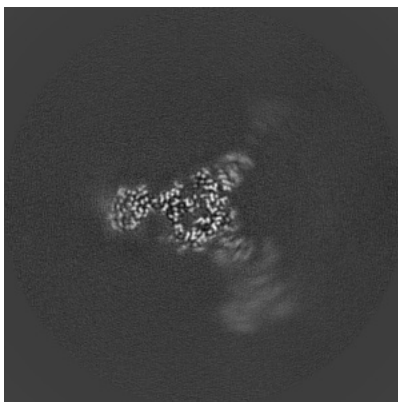


Z Index: 179

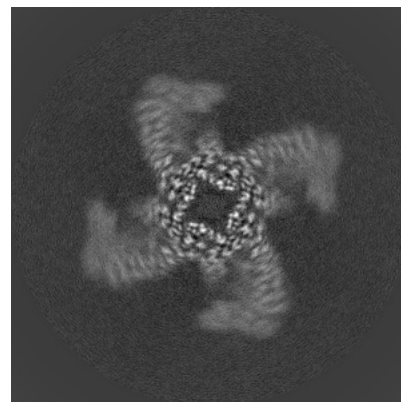
6.3.2 Raw map



X Index: 175



Y Index: 160

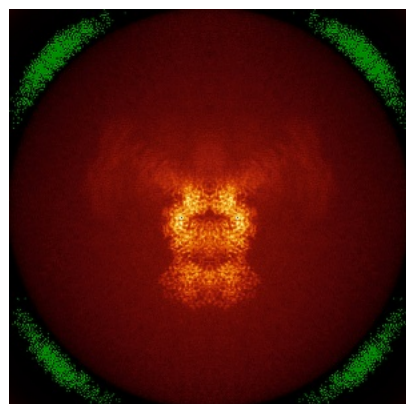


Z Index: 204

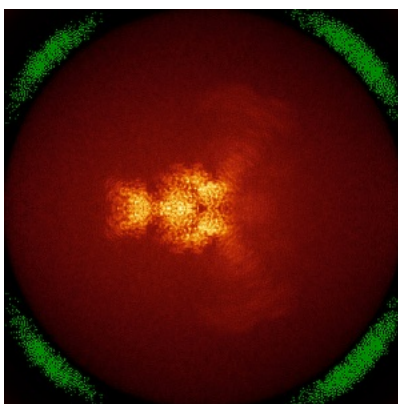
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

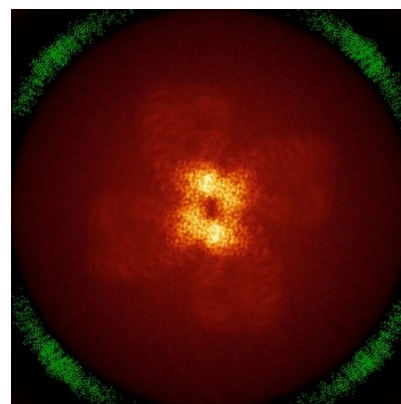
6.4.1 Primary map



X

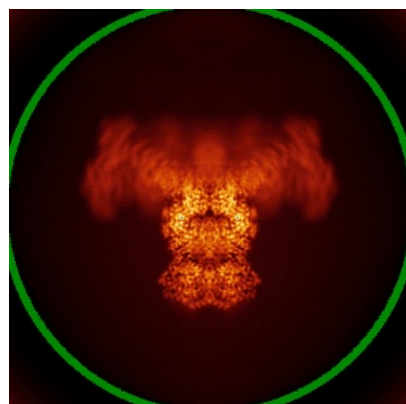


Y

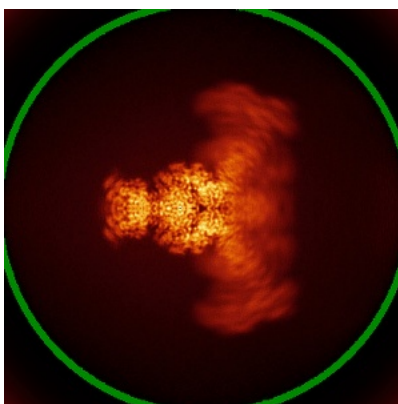


Z

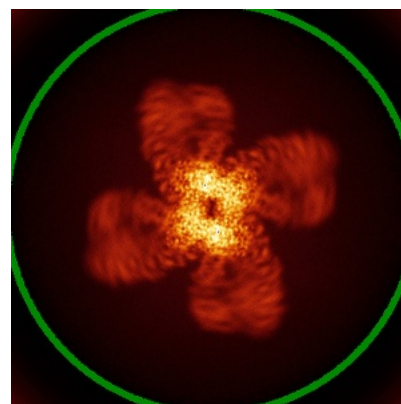
6.4.2 Raw map



X



Y

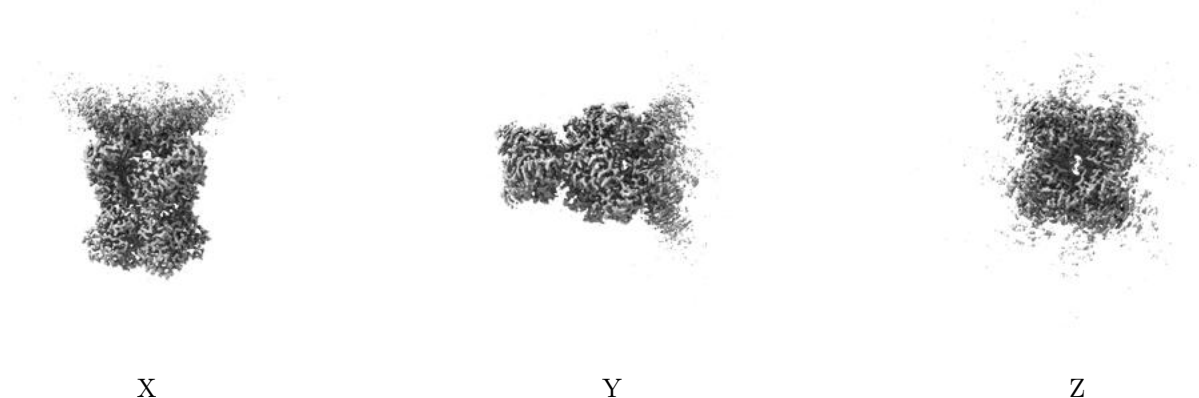


Z

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.

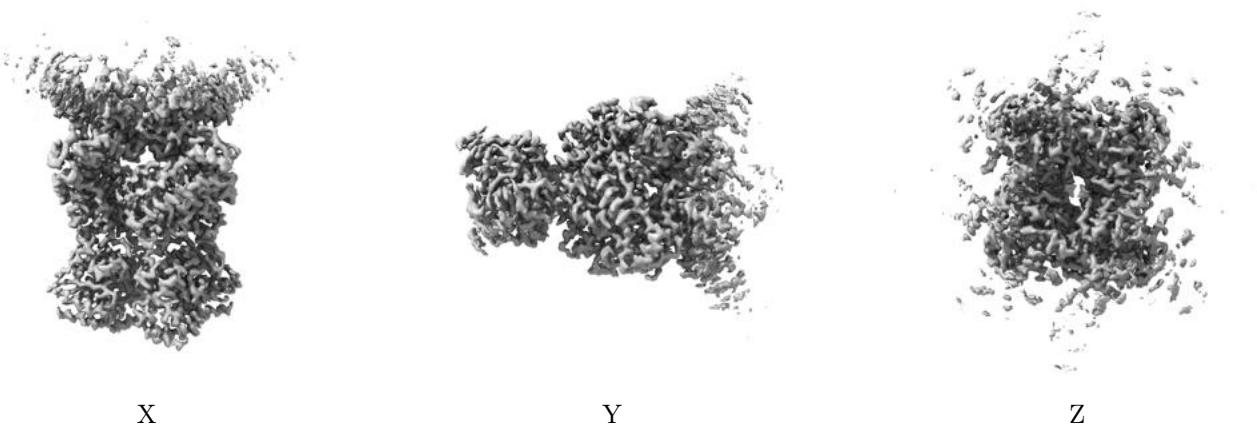
6.5 Orthogonal surface views [i](#)

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.

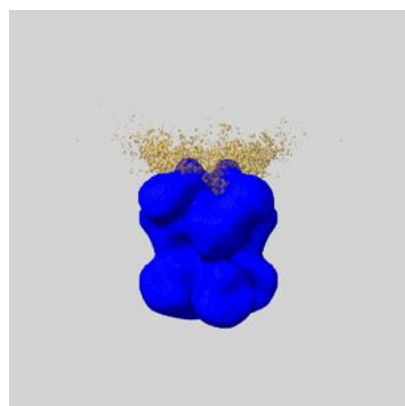
6.6 Mask visualisation [i](#)

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

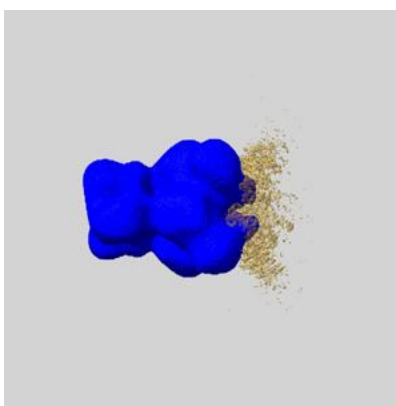
A mask typically either:

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

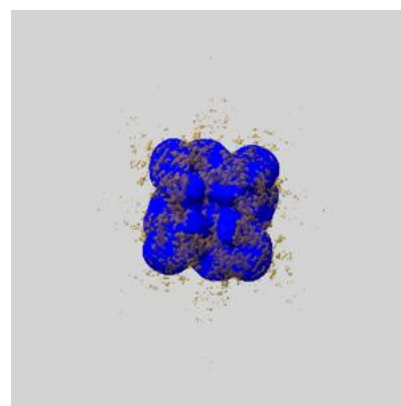
6.6.1 emd_27422_msk_1.map [i](#)



X



Y

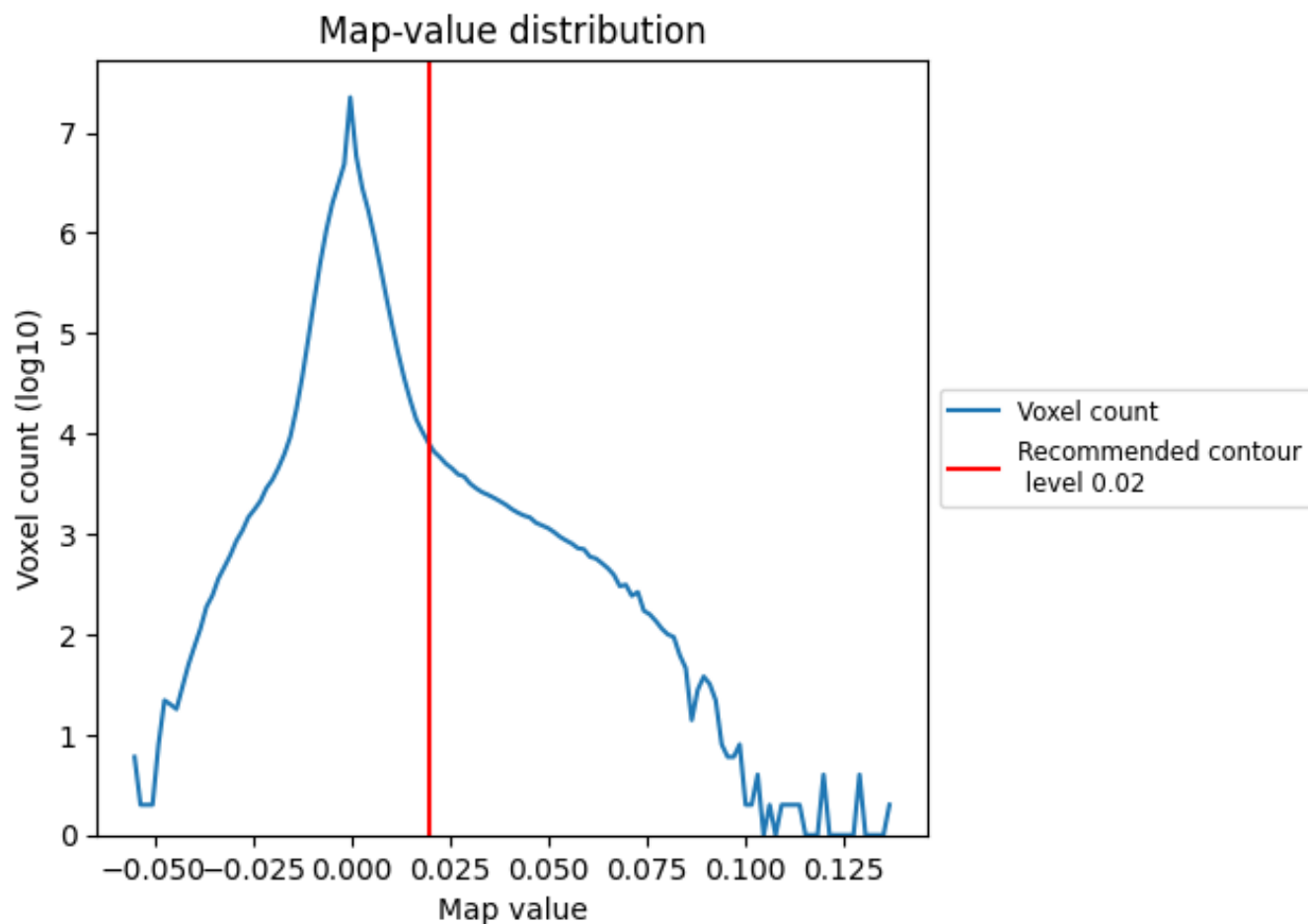


Z

7 Map analysis [i](#)

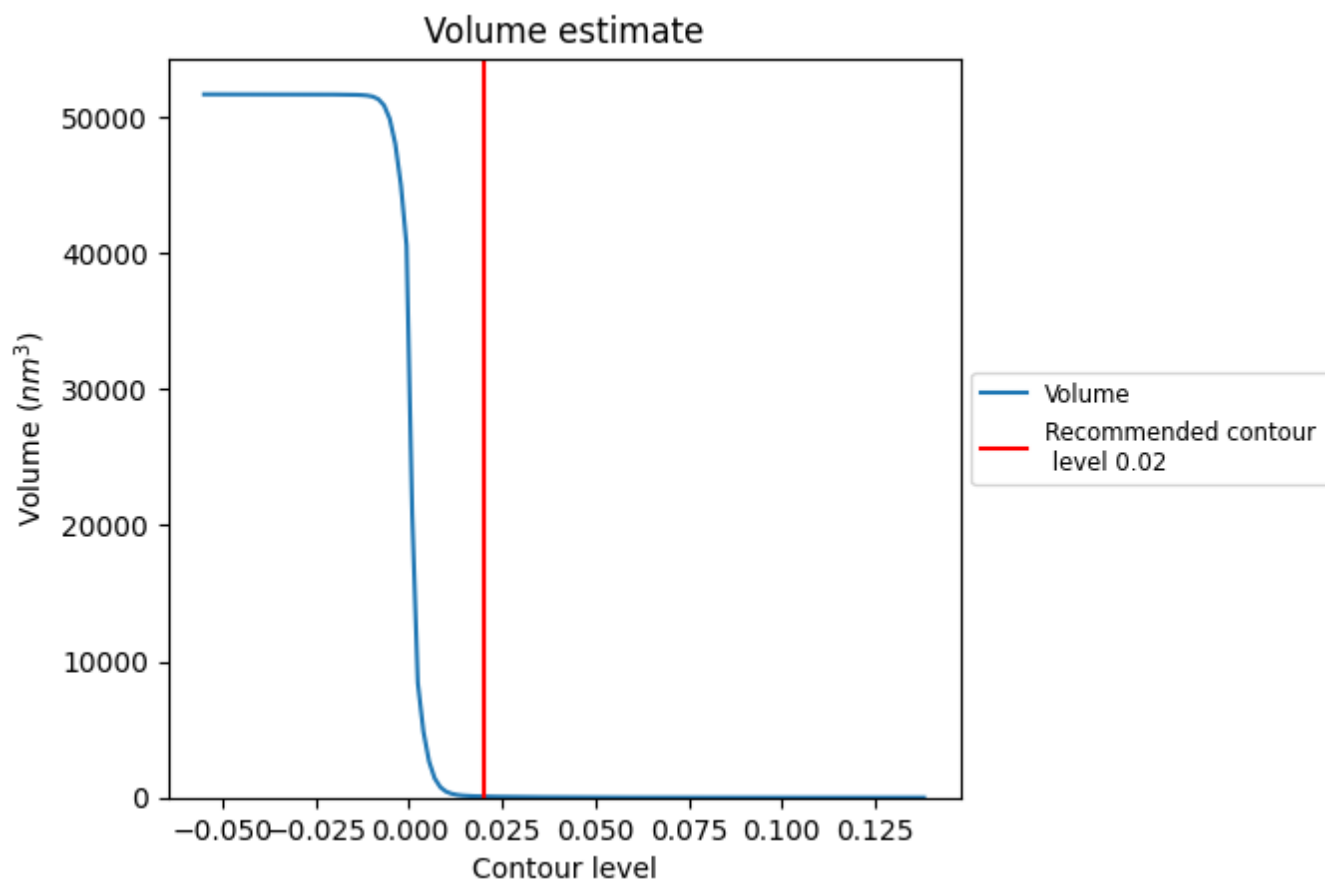
This section contains the results of statistical analysis of the map.

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.

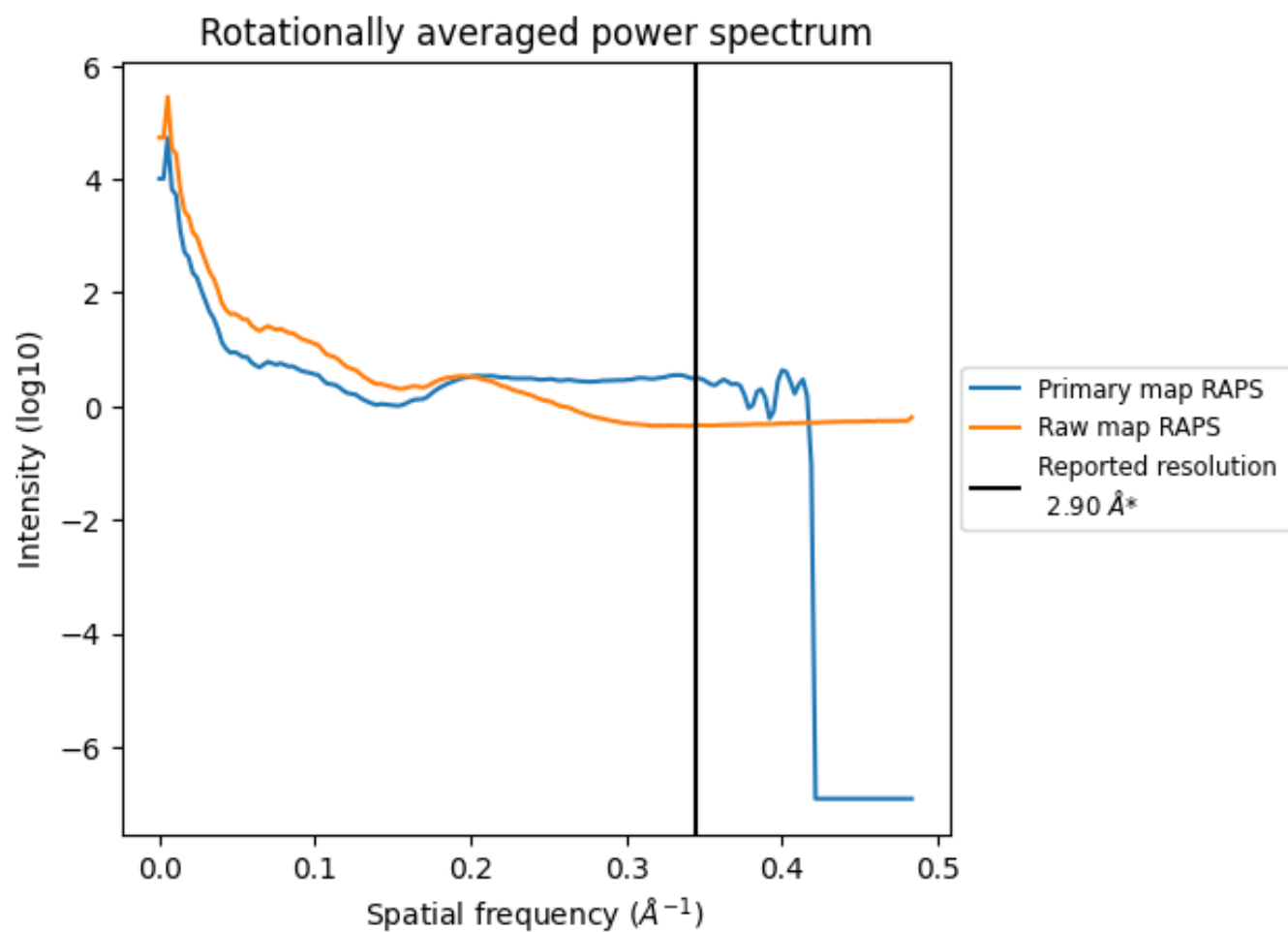
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 80 nm³; 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 ⓘ

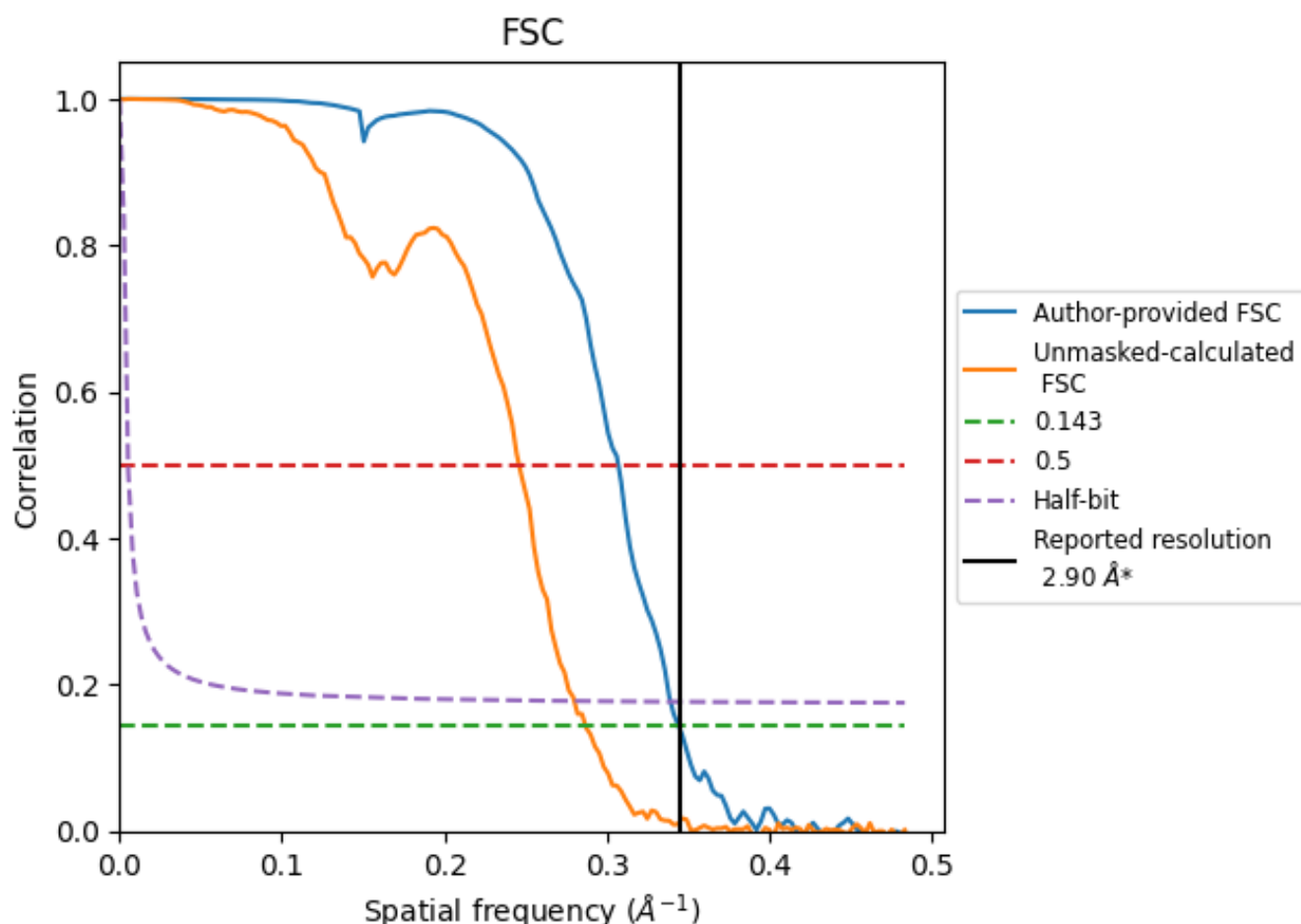


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

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 \AA^{-1}

8.2 Resolution estimates [i](#)

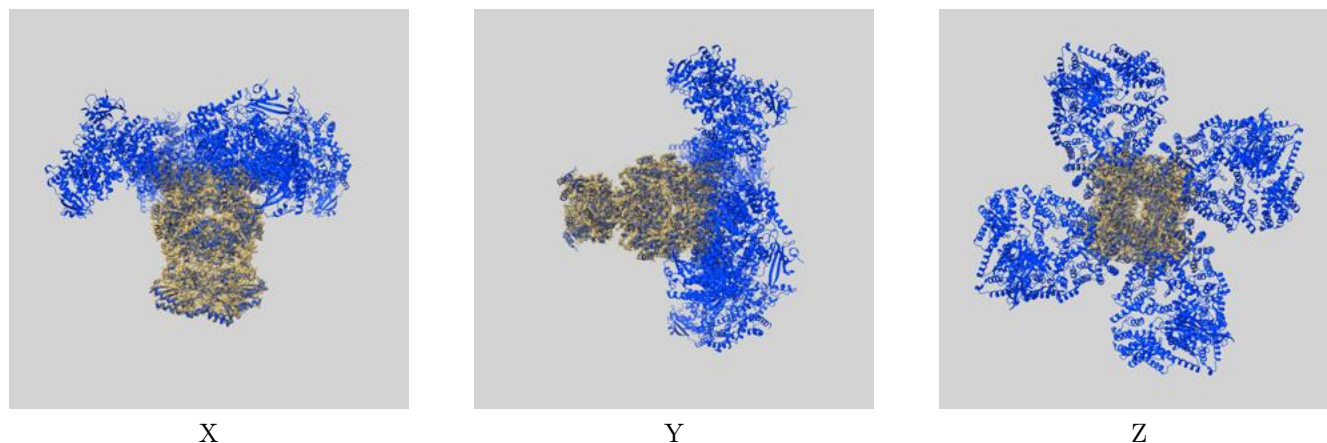
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.90	3.26	2.95
Unmasked-calculated*	3.48	4.07	3.57

*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](#)

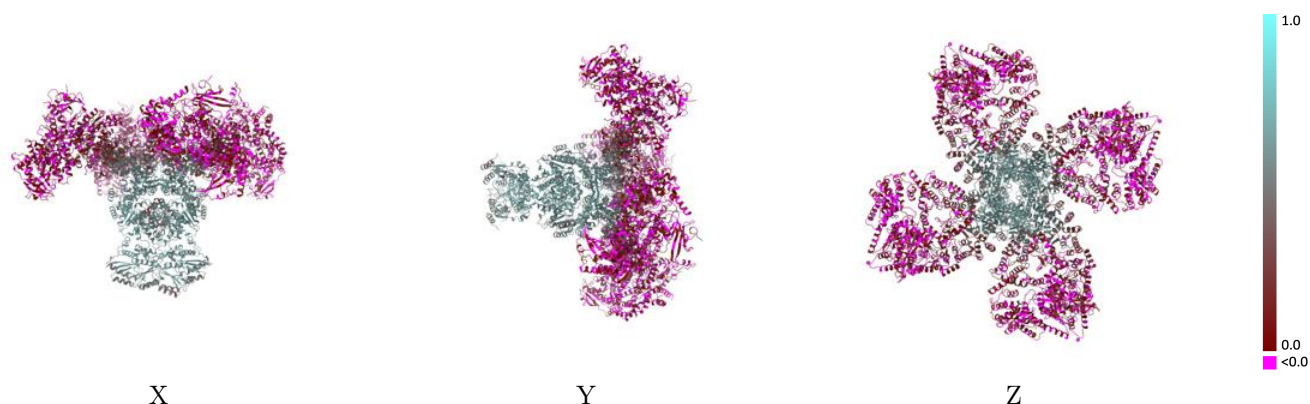
This section contains information regarding the fit between EMDB map EMD-27422 and PDB model 8DGF. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

9.1 Map-model overlay [i](#)



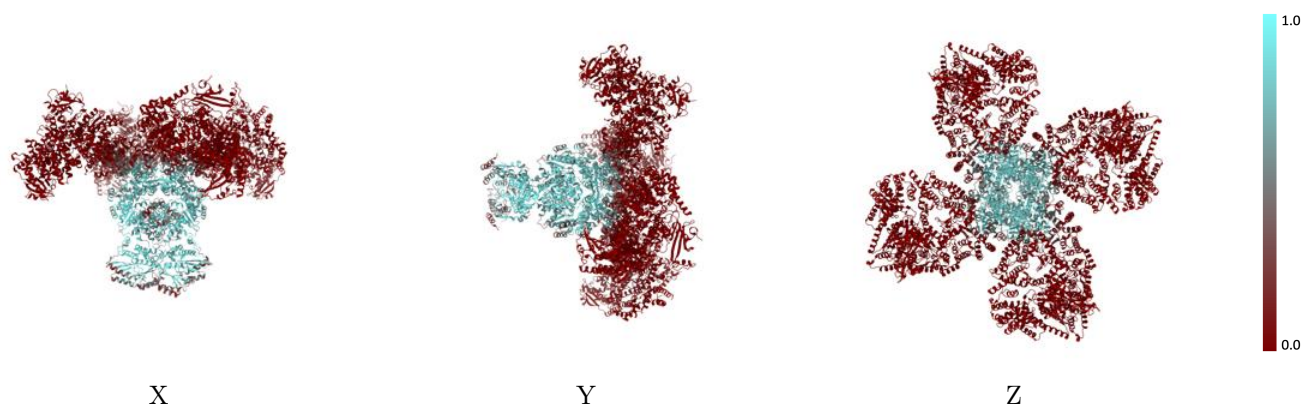
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



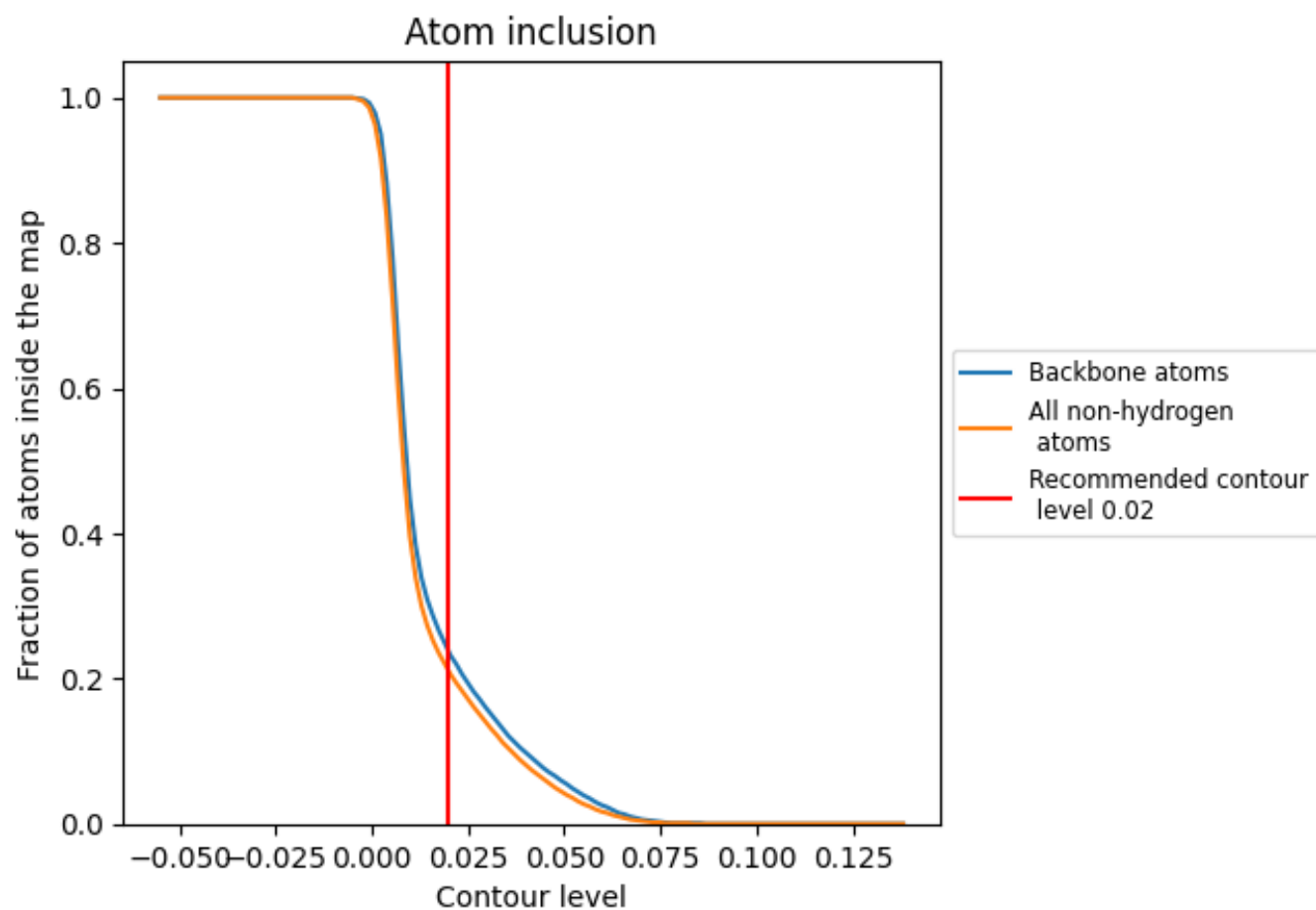
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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