



Full wwPDB EM Validation Report ⓘ

Oct 27, 2024 – 06:20 AM EDT

PDB ID : 7T3U
EMDB ID : EMD-25671
Title : IP3, ATP, and Ca²⁺ bound type 3 IP3 receptor in the inactive state
Authors : Schmitz, E.A.; Takahashi, H.; Karakas, E.
Deposited on : 2021-12-08
Resolution : 3.70 Å (reported)
Based on initial model : 6UQK

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

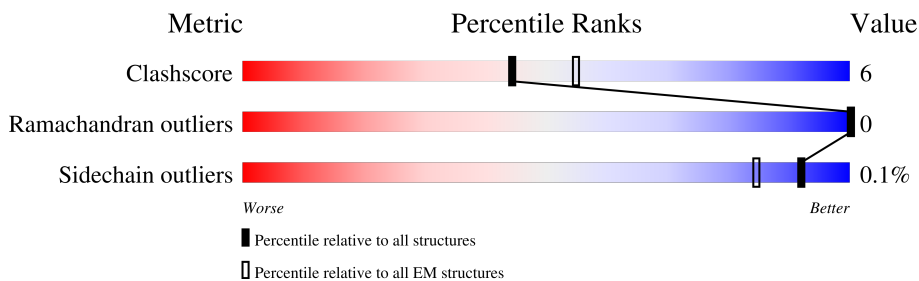
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	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	2633	
1	B	2633	
1	C	2633	
1	D	2633	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 44501 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.

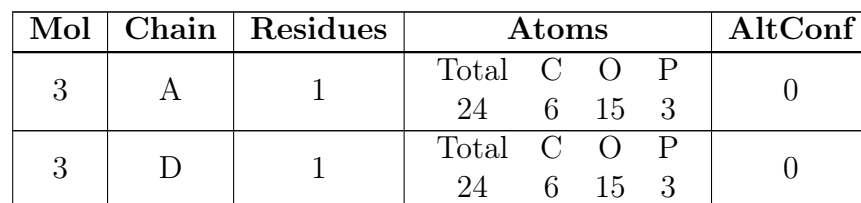
- Molecule 1 is a protein called Inositol 1,4,5-trisphosphate receptor type 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2020	Total	C	N	O	S	0	0
			12132	7515	2262	2326	29		
1	B	1662	Total	C	N	O	S	0	0
			10375	6470	1906	1968	31		
1	C	1575	Total	C	N	O	S	0	0
			9741	6073	1791	1849	28		
1	D	2012	Total	C	N	O	S	0	0
			12073	7474	2252	2316	31		

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total	Zn	0
			1	1	
2	B	1	Total	Zn	0
			1	1	
2	C	1	Total	Zn	0
			1	1	
2	D	1	Total	Zn	0
			1	1	

- Molecule 3 is D-MYO-INOSITOL-1,4,5-TRIPHOSPHATE (three-letter code: I3P) (formula: C₆H₁₅O₁₅P₃) (labeled as "Ligand of Interest" by depositor).



- # ATP

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



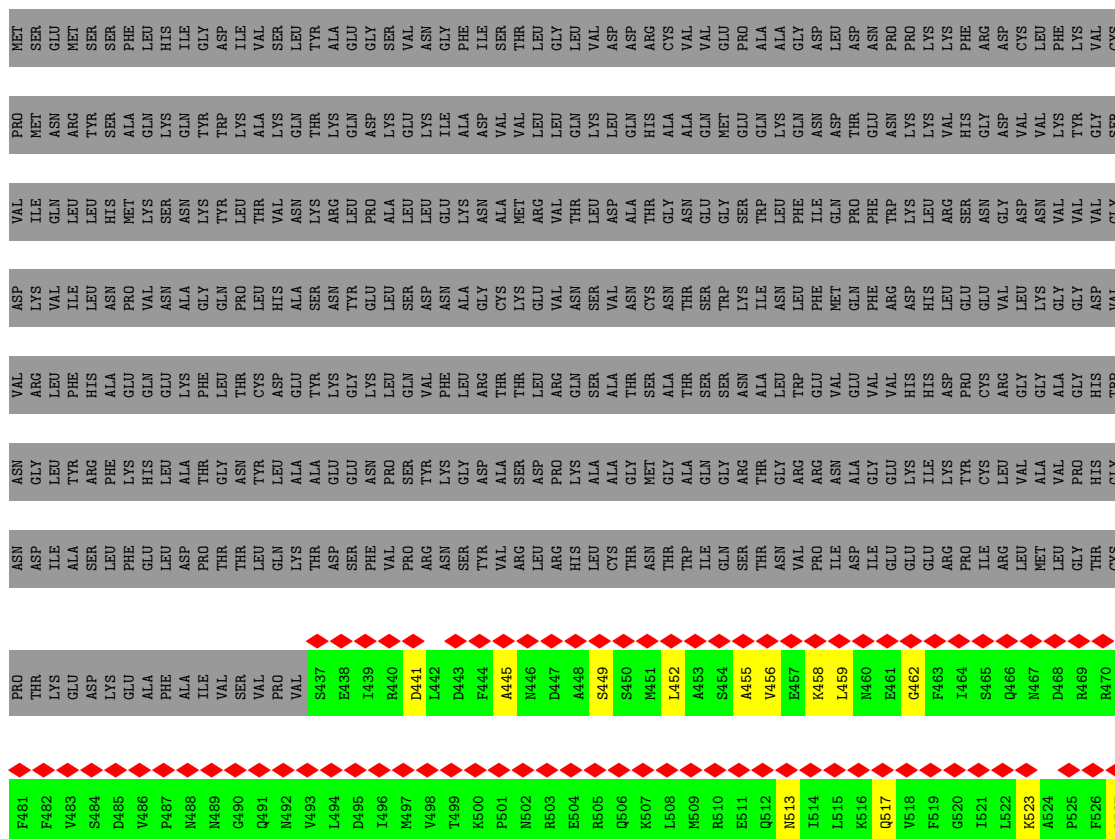
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Mol	Chain	Residues	Atoms					AltConf
4	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	D	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Ca	0
			1	1	
5	B	1	Total	Ca	0
			1	1	
5	C	1	Total	Ca	0
			1	1	
5	D	1	Total	Ca	0
			1	1	

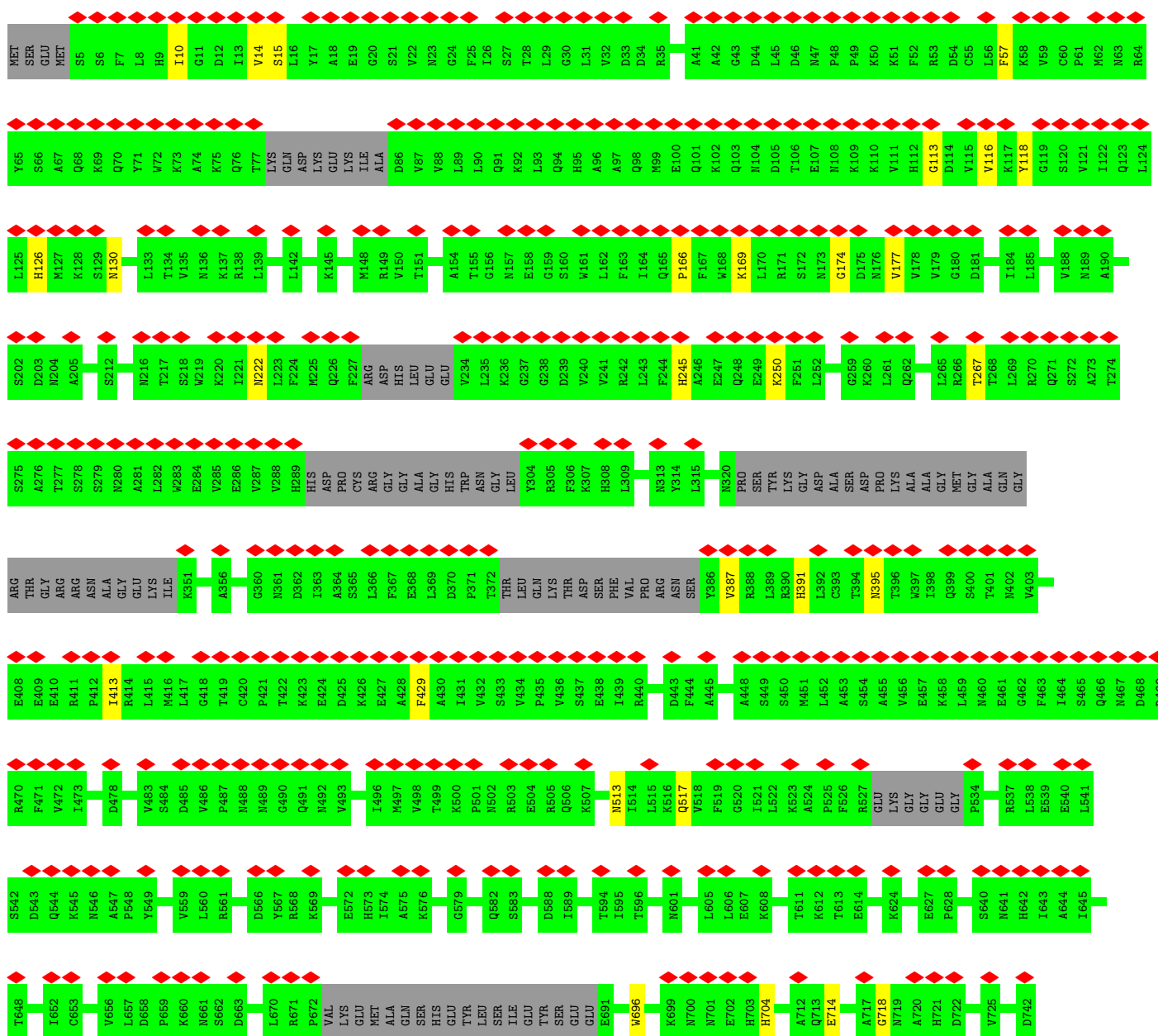




A1291	T1292	H1293	G1294	R1295	L1296	A1237	G1238	N1239	P1240	G1241	N1242	Q1243	A1244	L1245	L1246	H1247	K1248	H1249	L1250	H1251	L1252	F1253	L1254	T1255	P1256	G1257	L1258	L1259	E1260	A1261	E1262	T1263	M1264	Q1265	H1266	I1267	F1268	L1269	M1270	N1271	Y1272	Q1273	C1275	S1276	E1277	L1278	S1279	E1280	P1281	V1282	L1283	Q1284	H1285	V1286	H1288	L1289	L1290		
F1231	L1232	Q1233	K1234	F1235	C1236	A1237	G1238	N1239	P1240	G1241	N1242	Q1243	A1244	L1245	L1246	H1247	K1248	H1249	L1250	H1251	L1252	F1253	L1254	T1255	P1256	G1257	L1258	L1259	E1260	A1261	E1262	T1263	M1264	Q1265	H1266	I1267	F1268	L1269	M1270	N1271	Y1272	Q1273	C1275	S1276	E1277	L1278	S1279	E1280	P1281	V1282	L1283	Q1284	H1285	V1286	H1288	L1289	L1290		
Q1170	I1171	V1172	K1173	G1174	I1175	L1176	E1177	R1178	L1179	M1180	K1181	M1182	G1183	GLY	VAL	GLY	GLY	Q1188	M1189	R1190	K1191	K1192	R1196	L1197	K1198	M1199	M1200	D1201	A1202	H1203	K1204	V1205	M1206	PRO	L1207	D1208	L1209	L1210	Q1211	I1212	P1213	Y1214	D1215	K1216	G1217	D1218	A1219	K1220	M1221	M1222	E1223	I1224	L1225	R1226	Y1227	L1228	H1229	Q1230	
K1108	V1109	I1110	K1111	S1112	E1113	L1114	D1115	R1116	L1117	M1120	K1123	SER	GLU	LEU	THR	VAL	ASP	LYS	LYS	GLY	SER	GLY	LYS	GLY	GLY	GLU	GLU	VAL	ALA	LYS	ASP	LYS	LYS	GLU	ARG	PRO	THR	ASP	GLU	GLY	PHE	LEU	HIS	PRO	PRO	GLY	GLU	LYS	SER	SER	N1168	Y1169							
S1043	M1044	L1045	E1046	V1047	D1048	D1049	E1050	G1051	G1052	R1053	M1054	F1055	L1056	I1060	H1061	L1062	T1063	M1064	L1065	D1066	Y1067	A1068	P1069	L1070	G1073	A1074	L1075	L1078	F1079	F1082	S1083	Q1084	R1085	Q1086	E1087	A1088	M1089	H1090	T1091	F1092	K1093	Q1094	V1095	Q1096	L1097	L1098	I1099	S1100	A1101	Q1102	D1103	V1104	E1105	N1106	Y1107				
L983	D984	Y985	R986	S988	Y989	L990	L991	S992	V993	F994	K995	K996	E997	F998	VAL	GLU	VAL	PHE	PRO	ASP	GLY	ALA	ALA	ASP	GLY	THR	ALA	PRO	ALA	ASP	PHE	GLU	THR	ALA	ASN	L1025	D1026	R1027	I1028	G1029	E1030	Q1031	A1032	E1033	A1034	M1035	F1036	G1037	VAL	GLY	LYS	THR	SER						
K858	L859	T860	F861	V864	S865	L866	H868	N869	L870	I871	Y872	F873	G874	F875	Y876	S877	F878	S879	E880	L881	L882	R883	L884	T885	R886	T887	L888	G890	I891	R892	D893	C894	VAL	GLN	PRO	GLY	PRO	ALA	MET	LEU	GLN	ALA	TYR	GLU	ASP	PRO	GLY	LYS	ASN	VAL	ARG	SER	ILE	GLN					
F799	A800	R801	L802	W803	T804	E805	I806	P807	T808	A809	I810	Y811	I812	K813	D814	Y815	D816	S817	N818	L819	N820	ALA	SER	ARG	ASP	ASP	LYS	N828	K829	F830	A831	N832	T833	M834	E835	F836	V837	E838	D839	Y840	L841	N842	N843	V844	V845	S846	E847	A848	V849	P850	F851	A852	N853	E854	E855	K856	N857		
M724	V725	L726	S727	T728	Y729	R730	Y731	Q732	D742	Y745	L746	A747	I748	D749	E750	I751	S752	Q753	Q754	L755	G756	V757	D758	L759	I760	F761	L762	C763	M764	A765	D766	E767	M768	L769	P770	F771	D772	L773	R774	A775	C778	H779	M781	V784	H785	V786	P790	Q791	E792	L793	V794	T795	P796						
I664	L665	I666	R667	T668	E669	L670	R671	P672	VAL	L75	GLU	MET	ALA	GLN	HIS	GLU	TYR	LEU	SER	ILE	GLU	TYR	GLU	E691	V692	W693	L694	T695	W696	T697	D698	K699	N700	N701	E702	H703	H704	E705	K706	S707	V708	R709	Q710	L711	L712	Q713	E714	A715	R716	A717	G718	N719	A720	H721	D722	E723			
N601	N602	R603	K604	L605	L606	E607	K608	H609	I610	T611	K612	T613	E614	V615	E616	T617	F618	V619	S620	L621	V622	H623	K624	N625	R626	E627	P628	R629	F630	N570	D632	Y633	L634	V639	S640	N641	H642	I643	A644	I645	P646	V647	T648	Q649	E650	L651	I652	C653	K654	C655	V656	L657	D658	P659	K660	N661	S662	D663	
L541	S542	D543	Q544	K545	N546	A547	P548	Y549	Q550	H551	M552	F553	R554	L555	C556	Y557	R558	V559	L560	R561	H562	S563	Q564	S565	D566	Y567	P568	R569	K569	N570	Q571	E572	H573	I574	A575	K576	Q577	F578	G579	M580	M581	Q582	S583	Q584	I585	G586	Y587	D588	I589	L590	A591	E592	D593	T594	I595	T596	A597	L598	H600



- Molecule 1: Inositol 1,4,5-trisphosphate receptor type 3





V2508	L2511	L2523	K2530	L2534	E2544	R2545	D2546	K2547	F2548	D2549	K2560	L2574	V2575	R2576	V2577	Y2583	A2591	Q2592	M2593	N2598	L2599	V2611	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK	UNK
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	198441	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.911	Depositor
Minimum map value	-1.171	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.038	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	397.44, 397.44, 397.44	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.828, 0.828, 0.828	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: I3P, ATP, ZN, CA

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	0.24	0/12209	0.43	0/16761
1	B	0.24	0/10458	0.43	0/14326
1	C	0.24	0/9822	0.42	0/13474
1	D	0.24	0/12149	0.43	0/16677
All	All	0.24	0/44638	0.43	0/61238

There are no bond length outliers.

There are no bond angle outliers.

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	12132	0	8448	112	0
1	B	10375	0	7682	134	0
1	C	9741	0	7105	120	0
1	D	12073	0	8390	129	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	24	0	9	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	24	0	9	0	0
4	A	31	0	12	1	0
4	B	31	0	12	1	0
4	C	31	0	12	1	0
4	D	31	0	12	2	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
All	All	44501	0	31691	474	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 6.

All (474) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2297:VAL:HG21	1:D:2327:ILE:HD11	1.33	1.06
1:C:2297:VAL:HG21	1:C:2327:ILE:HD11	1.40	1.00
1:D:1740:LEU:HD21	1:D:1749:ILE:HG22	1.47	0.95
1:A:2297:VAL:HG21	1:A:2327:ILE:HD11	1.51	0.92
1:B:1934:VAL:HG21	1:B:1988:LEU:HD13	1.55	0.89
1:A:2066:GLN:NE2	1:A:2070:LEU:HD11	1.90	0.86
1:B:1968:ASP:OD1	1:B:2019:SER:OG	1.97	0.82
1:C:1373:ALA:O	1:C:1377:GLU:N	2.14	0.81
1:C:2575:VAL:O	1:C:2583:TYR:OH	1.99	0.80
1:B:2166:SER:OG	1:B:2604:ARG:NH1	2.15	0.80
1:C:2155:LEU:O	1:C:2159:THR:OG1	1.99	0.79
1:D:1725:GLN:NE2	1:D:1759:HIS:O	2.17	0.78
1:B:1747:GLU:OE2	1:B:1792:ARG:NH1	2.17	0.78
1:C:1728:LEU:O	1:C:1732:GLY:N	2.16	0.78
1:C:1650:HIS:O	1:C:1654:LEU:CB	2.33	0.75
1:D:2155:LEU:O	1:D:2159:THR:OG1	2.04	0.74
1:B:2155:LEU:O	1:B:2159:THR:OG1	2.06	0.73
1:B:1933:ASN:O	1:B:1937:VAL:HG23	1.89	0.72
1:A:2066:GLN:O	1:A:2070:LEU:HD12	1.88	0.72
1:B:1492:GLN:O	1:B:1496:THR:N	2.23	0.72
1:D:1650:HIS:O	1:D:1654:LEU:CB	2.37	0.72
1:A:2362:VAL:HG21	1:D:2511:LEU:HD11	1.72	0.71
1:C:1603:GLU:O	1:C:1607:LYS:N	2.23	0.71
1:D:877:SER:O	1:D:881:LEU:N	2.22	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:802:LEU:O	1:C:806:ILE:N	2.23	0.71
1:B:1526:ILE:O	1:B:1530:ALA:N	2.24	0.70
1:B:2468:HIS:HB3	1:B:2479:ILE:HG21	1.74	0.70
1:B:1945:THR:O	1:B:1949:GLN:N	2.25	0.69
1:A:2468:HIS:HB3	1:A:2479:ILE:HG21	1.74	0.69
1:C:2511:LEU:HD11	1:D:2362:VAL:HG21	1.72	0.69
1:A:2155:LEU:HD22	1:A:2178:LEU:HD11	1.75	0.69
1:B:1909:GLN:HE22	1:B:1913:ILE:HD11	1.58	0.69
1:D:1449:ALA:O	1:D:1453:SER:N	2.25	0.69
1:B:1740:LEU:HD21	1:B:1749:ILE:HG22	1.73	0.69
1:A:1478:ALA:O	1:A:1482:SER:N	2.26	0.69
1:B:1914:MET:CE	1:B:1937:VAL:HG22	2.23	0.69
1:A:2362:VAL:CG2	1:D:2511:LEU:HD11	2.23	0.68
1:D:1974:ILE:O	1:D:1993:LYS:NZ	2.26	0.68
1:C:1680:GLY:O	1:C:1684:ASN:N	2.27	0.68
1:D:2575:VAL:O	1:D:2583:TYR:OH	2.06	0.68
1:C:2511:LEU:HD11	1:D:2362:VAL:CG2	2.24	0.68
1:B:2123:GLN:OE1	1:B:2135:GLN:NE2	2.28	0.67
1:A:2511:LEU:HD21	1:B:2362:VAL:HG23	1.77	0.67
1:B:2511:LEU:HD11	1:C:2362:VAL:HG21	1.75	0.67
1:C:870:LEU:O	1:C:874:GLY:N	2.28	0.67
1:A:1101:ALA:O	1:A:1104:VAL:N	2.28	0.66
1:B:1740:LEU:HD22	1:B:1753:SER:HB3	1.77	0.66
1:B:1740:LEU:HD22	1:B:1753:SER:CB	2.25	0.66
1:A:1650:HIS:O	1:A:1654:LEU:CB	2.43	0.66
1:A:1738:CYS:O	1:A:1742:THR:HG22	1.94	0.66
1:B:2015:ARG:NH1	1:B:2015:ARG:O	2.28	0.66
1:B:2511:LEU:HD11	1:C:2362:VAL:CG2	2.25	0.66
1:C:2468:HIS:HB3	1:C:2479:ILE:HG21	1.77	0.66
1:B:1960:VAL:HG23	1:B:1961:THR:HG23	1.76	0.66
1:D:1960:VAL:HG23	1:D:1961:THR:HG23	1.78	0.66
1:C:2511:LEU:HD13	1:D:2358:VAL:CG1	2.26	0.66
1:C:801:ARG:O	1:C:1098:LEU:N	2.29	0.66
1:D:1897:ASN:OD1	1:D:1898:LYS:N	2.29	0.66
1:A:2163:GLU:OE1	1:A:2163:GLU:N	2.29	0.65
1:D:2468:HIS:HB3	1:D:2479:ILE:HG21	1.79	0.65
1:C:2557:GLU:OE2	1:C:2561:LEU:HD12	1.97	0.65
1:B:1987:ASP:OD1	1:B:1988:LEU:N	2.30	0.65
1:B:2501:PHE:CE2	1:B:2506:ILE:HD11	2.32	0.65
1:A:1338:ASP:O	1:A:1342:LEU:N	2.29	0.64
1:C:2015:ARG:O	1:C:2015:ARG:NH1	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2160:GLU:OE2	1:B:2530:LYS:NZ	2.29	0.64
1:A:2064:ASN:OD1	1:A:2065:LYS:N	2.31	0.64
1:D:751:ILE:O	1:D:755:LEU:N	2.29	0.64
1:D:1933:ASN:O	1:D:1937:VAL:HG23	1.98	0.64
1:A:320:ASN:N	1:A:351:LYS:O	2.31	0.64
1:A:2155:LEU:O	1:A:2159:THR:OG1	2.15	0.64
1:C:2005:GLU:O	1:C:2007:ARG:N	2.31	0.63
1:B:2211:LEU:HD22	1:B:2285:LEU:HD22	1.80	0.63
1:B:2511:LEU:HD13	1:C:2358:VAL:CG1	2.29	0.63
1:D:387:VAL:N	1:D:429:PHE:O	2.31	0.63
1:C:707:SER:O	1:C:711:LEU:N	2.31	0.62
1:D:802:LEU:O	1:D:806:ILE:N	2.30	0.62
1:D:391:HIS:O	1:D:395:ASN:N	2.33	0.62
1:A:1887:ASP:OD1	1:A:1888:LEU:N	2.32	0.61
1:B:2476:VAL:HG22	1:B:2480:LEU:HD13	1.81	0.61
1:C:2544:GLU:N	1:C:2544:GLU:OE1	2.33	0.61
1:A:2557:GLU:OE1	1:A:2557:GLU:N	2.33	0.61
1:A:2544:GLU:OE1	1:A:2544:GLU:N	2.33	0.61
1:C:2059:GLN:OE1	1:C:2062:ARG:NH2	2.34	0.61
1:D:756:GLY:O	1:D:760:ILE:N	2.33	0.61
1:B:1875:ARG:O	1:B:1879:LEU:HD23	2.01	0.61
1:C:645:ILE:O	1:C:649:GLN:N	2.29	0.61
1:A:2478:ASP:OD1	1:B:2471:ARG:NH2	2.35	0.60
1:A:1867:VAL:HG23	1:A:1868:LEU:HD22	1.81	0.60
1:B:1741:ILE:HG22	1:B:1788:VAL:HG11	1.82	0.60
1:B:1911:LEU:HB2	1:B:1940:THR:HG21	1.82	0.60
1:A:1960:VAL:HG23	1:A:1961:THR:HG23	1.83	0.60
1:B:1914:MET:HE1	1:B:1937:VAL:HG22	1.83	0.60
1:D:2467:ASN:OD1	1:D:2471:ARG:NH1	2.33	0.60
1:D:1741:ILE:HG21	1:D:1785:PHE:HE1	1.67	0.59
1:D:1912:ASP:OD2	1:D:1964:SER:OG	2.19	0.59
1:C:1930:ASN:O	1:C:1934:VAL:HG13	2.00	0.59
1:D:245:HIS:N	1:D:250:LYS:O	2.34	0.59
1:D:1761:LEU:HD13	1:D:1880:LEU:HD12	1.83	0.59
1:A:1734:THR:HG23	1:A:1772:PHE:CD1	2.37	0.59
1:C:751:ILE:O	1:C:755:LEU:N	2.34	0.59
1:C:2020:LEU:HD12	1:C:2020:LEU:O	2.01	0.59
1:C:2484:SER:OG	1:D:2401:ARG:NH1	2.35	0.59
1:A:2358:VAL:CG1	1:D:2511:LEU:HD13	2.32	0.59
1:C:1978:ILE:CD1	1:C:1989:VAL:HG23	2.32	0.59
1:D:2364:ARG:HD2	1:D:2523:LEU:HD11	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1789:LEU:O	1:A:1793:MET:N	2.36	0.59
1:D:2269:ILE:HD12	1:D:2285:LEU:HD11	1.85	0.59
1:D:1387:CYS:O	1:D:1391:LEU:N	2.35	0.58
1:D:2015:ARG:O	1:D:2015:ARG:NH1	2.35	0.58
1:A:245:HIS:O	1:A:249:GLU:N	2.36	0.58
1:B:1757:ALA:HB1	1:B:1876:PHE:CE1	2.37	0.58
1:B:1930:ASN:O	1:B:1934:VAL:HG13	2.03	0.58
1:B:1793:MET:CE	1:B:1903:LEU:HD22	2.34	0.58
1:B:2364:ARG:HD2	1:B:2523:LEU:HD11	1.84	0.58
1:D:14:VAL:N	1:D:57:PHE:O	2.36	0.58
1:D:1734:THR:HG22	1:D:1775:LEU:HD13	1.86	0.58
1:D:2172:PHE:CD2	1:D:2599:LEU:HD21	2.38	0.58
1:B:2059:GLN:OE1	1:B:2062:ARG:NH2	2.37	0.58
1:C:445:ALA:O	1:C:449:SER:N	2.30	0.58
1:D:1965:ASN:O	1:D:1969:ILE:HD12	2.03	0.58
1:D:2530:LYS:O	1:D:2534:LEU:HD23	2.04	0.58
1:B:1288:HIS:O	1:B:1292:THR:N	2.32	0.58
1:A:193:PRO:O	1:A:213:VAL:N	2.37	0.57
1:B:2598:ASN:OD1	1:B:2599:LEU:N	2.38	0.57
1:C:1977:ASP:OD1	1:C:1978:ILE:N	2.38	0.57
1:C:1978:ILE:HD12	1:C:1989:VAL:HG23	1.84	0.57
1:D:1785:PHE:O	1:D:1788:VAL:HG12	2.03	0.57
1:A:10:ILE:N	1:A:114:ASP:O	2.35	0.57
1:A:1783:GLU:OE1	1:A:1897:ASN:ND2	2.38	0.57
1:D:1933:ASN:O	1:D:1933:ASN:ND2	2.37	0.57
1:D:2026:VAL:HG21	1:D:2070:LEU:HD22	1.85	0.57
1:C:781:MET:O	1:C:786:VAL:N	2.33	0.57
1:D:1934:VAL:HG21	1:D:1988:LEU:HD13	1.86	0.57
1:B:1974:ILE:O	1:B:1993:LYS:NZ	2.34	0.57
1:B:1974:ILE:CD1	1:B:2000:LEU:HD12	2.35	0.57
1:D:696:TRP:O	1:D:704:HIS:CB	2.53	0.57
1:D:1447:ASP:O	1:D:1451:VAL:N	2.35	0.57
1:D:1741:ILE:HG23	1:D:1750:PHE:CE1	2.39	0.57
1:B:2007:ARG:NE	1:B:2012:ASN:OD1	2.36	0.57
1:C:2560:LYS:NZ	4:C:2702:ATP:O3A	2.37	0.57
1:B:1909:GLN:NE2	1:B:1913:ILE:HD11	2.20	0.56
1:A:1741:ILE:HG21	1:A:1785:PHE:CE1	2.40	0.56
1:D:794:VAL:N	1:D:872:TYR:O	2.37	0.56
1:A:1968:ASP:OD1	1:A:2019:SER:OG	2.20	0.56
1:D:1101:ALA:O	1:D:1104:VAL:N	2.34	0.56
1:D:2476:VAL:HG22	1:D:2480:LEU:CD1	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1741:ILE:HG23	1:B:1750:PHE:CE1	2.41	0.56
1:C:1933:ASN:O	1:C:1937:VAL:HG23	2.05	0.56
1:C:513:ASN:O	1:C:517:GLN:N	2.35	0.56
1:A:2543:LEU:HD23	1:A:2548:PHE:CE1	2.40	0.56
1:C:877:SER:O	1:C:881:LEU:N	2.35	0.56
1:D:2017:LEU:HD23	1:D:2020:LEU:HD11	1.88	0.56
1:A:2358:VAL:HG12	1:D:2511:LEU:HD13	1.88	0.56
1:D:1659:GLU:HA	1:D:1749:ILE:HD11	1.88	0.55
1:D:2598:ASN:OD1	1:D:2599:LEU:N	2.40	0.55
1:B:1744:THR:HG21	1:B:1749:ILE:HG21	1.88	0.55
1:B:2474:GLY:O	1:C:2471:ARG:NH1	2.40	0.55
1:C:853:ASN:O	1:C:857:ASN:N	2.36	0.55
1:C:2211:LEU:HD22	1:C:2285:LEU:HD22	1.88	0.55
1:A:1505:THR:O	1:A:1509:LEU:N	2.35	0.55
1:C:2543:LEU:HD23	1:C:2548:PHE:CZ	2.41	0.55
1:D:2468:HIS:HB3	1:D:2479:ILE:HD13	1.89	0.55
1:D:1895:GLN:OE1	1:D:1901:TYR:N	2.40	0.54
1:B:1740:LEU:HD21	1:B:1749:ILE:CG2	2.38	0.54
1:C:781:MET:O	1:C:785:HIS:N	2.41	0.54
1:C:2200:ARG:O	1:C:2204:TRP:NE1	2.40	0.54
1:C:2543:LEU:HD23	1:C:2548:PHE:CE1	2.43	0.54
1:C:1732:GLY:O	1:C:1736:LEU:N	2.38	0.54
1:D:2059:GLN:OE1	1:D:2062:ARG:NH1	2.40	0.54
1:A:2376:ALA:HB2	1:A:2508:VAL:HG11	1.90	0.54
1:A:1971:THR:HG23	1:A:2020:LEU:HB3	1.89	0.54
1:C:458:LYS:O	1:C:462:GLY:N	2.41	0.54
1:C:1908:LEU:HD11	1:C:1966:GLY:HA3	1.91	0.53
1:C:523:LYS:O	1:C:527:ARG:N	2.39	0.53
1:C:2163:GLU:OE2	1:C:2164:GLN:NE2	2.42	0.53
1:D:267:THR:N	1:D:413:ILE:O	2.40	0.53
1:D:1777:MET:HE2	1:D:1777:MET:HA	1.90	0.53
1:A:1910:PHE:CE2	1:A:1936:LEU:HD21	2.43	0.53
1:A:1965:ASN:O	1:A:1968:ASP:N	2.40	0.53
1:B:1977:ASP:OD1	1:B:1978:ILE:N	2.42	0.53
1:B:2574:LEU:HA	1:B:2577:VAL:HG12	1.91	0.53
1:C:2376:ALA:HB2	1:C:2508:VAL:HG11	1.90	0.53
1:B:2359:ILE:O	1:B:2363:THR:HG22	2.08	0.53
1:C:696:TRP:O	1:C:704:HIS:N	2.42	0.53
1:A:1933:ASN:O	1:A:1937:VAL:HG23	2.08	0.53
1:A:1970:ILE:HA	1:A:1973:LEU:HD12	1.90	0.53
1:C:2184:TRP:NE1	1:C:2302:GLY:O	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1871:GLN:HB3	1:B:1872:PRO:HD3	1.91	0.53
1:B:1908:LEU:HD11	1:B:1966:GLY:HA3	1.91	0.53
1:A:525:PRO:O	1:A:536:VAL:N	2.39	0.53
1:B:1527:ARG:O	1:B:1530:ALA:HB3	2.09	0.53
1:C:2501:PHE:CE2	1:C:2506:ILE:HD11	2.44	0.53
1:A:2066:GLN:CD	1:A:2070:LEU:HD11	2.28	0.53
1:B:1876:PHE:CZ	1:B:1880:LEU:HD11	2.44	0.53
1:C:1790:HIS:O	1:C:1794:LYS:N	2.41	0.53
1:D:513:ASN:O	1:D:517:GLN:N	2.34	0.52
1:A:391:HIS:O	1:A:395:ASN:N	2.38	0.52
1:C:1641:GLY:O	1:C:1645:SER:N	2.39	0.52
1:B:1974:ILE:HD12	1:B:2000:LEU:HD12	1.90	0.52
1:D:714:GLU:O	1:D:718:GLY:N	2.40	0.52
1:B:2511:LEU:HD13	1:C:2358:VAL:HG12	1.92	0.52
1:A:1954:GLU:N	1:A:1954:GLU:OE1	2.42	0.52
1:B:2476:VAL:HG22	1:B:2480:LEU:CD1	2.40	0.52
1:A:1904:VAL:HG23	1:A:1947:TYR:HD2	1.75	0.52
1:A:2160:GLU:OE2	1:A:2530:LYS:NZ	2.40	0.52
1:C:1615:SER:O	1:C:1619:ASP:N	2.40	0.52
1:B:1740:LEU:HD23	1:B:1740:LEU:C	2.30	0.52
1:B:2501:PHE:CZ	1:B:2506:ILE:HD11	2.45	0.52
1:B:2560:LYS:NZ	4:B:2702:ATP:O3A	2.43	0.51
1:C:816:ASP:O	1:C:820:ASN:N	2.42	0.51
1:C:1934:VAL:HG11	1:C:1981:LEU:HD21	1.91	0.51
1:A:1876:PHE:CE1	1:A:1880:LEU:HD11	2.44	0.51
1:B:2511:LEU:HD22	1:C:2358:VAL:HG13	1.92	0.51
1:C:760:ILE:O	1:C:764:MET:N	2.44	0.51
1:C:2511:LEU:HD13	1:D:2358:VAL:HG12	1.92	0.51
1:A:2155:LEU:CD2	1:A:2178:LEU:HD11	2.39	0.51
1:B:2504:VAL:HG12	1:B:2504:VAL:O	2.11	0.51
1:C:2543:LEU:HD21	1:C:2610:LEU:HD22	1.92	0.51
1:D:1770:LYS:HA	1:D:1770:LYS:HE2	1.91	0.51
1:A:1785:PHE:O	1:A:1788:VAL:HG12	2.11	0.51
1:B:1793:MET:HE2	1:B:1903:LEU:HD22	1.92	0.51
1:D:1741:ILE:HG23	1:D:1750:PHE:HE1	1.76	0.51
1:A:2376:ALA:O	1:A:2380:VAL:HG23	2.11	0.50
1:B:1373:ALA:O	1:B:1377:GLU:N	2.44	0.50
1:A:1734:THR:HG22	1:A:1775:LEU:HD13	1.93	0.50
1:B:1985:ARG:HE	1:B:1988:LEU:HD12	1.76	0.50
1:D:1876:PHE:CE1	1:D:1880:LEU:HD11	2.46	0.50
1:D:2376:ALA:HB2	1:D:2508:VAL:HG11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1960:VAL:HG13	1:A:2003:LEU:HD22	1.92	0.50
1:D:166:PRO:O	1:D:169:LYS:N	2.43	0.50
1:A:1734:THR:HG23	1:A:1772:PHE:HD1	1.77	0.50
1:C:1635:TYR:O	1:C:1639:GLU:N	2.45	0.50
1:A:2504:VAL:HG12	1:A:2504:VAL:O	2.11	0.49
1:B:2021:ARG:HA	1:B:2021:ARG:NE	2.27	0.49
1:C:2504:VAL:HG12	1:C:2504:VAL:O	2.12	0.49
1:A:1934:VAL:HG21	1:A:1988:LEU:HD22	1.95	0.49
1:B:1930:ASN:OD1	1:B:1933:ASN:N	2.45	0.49
1:A:671:ARG:O	1:A:691:GLU:N	2.45	0.49
1:B:481:PHE:O	1:B:485:ASP:N	2.46	0.49
1:C:2033:TYR:O	1:C:2047:ARG:NH1	2.45	0.49
1:A:1741:ILE:HG21	1:A:1785:PHE:HE1	1.78	0.49
1:D:2153:HIS:CE1	1:D:2157:THR:HG21	2.47	0.49
1:C:2278:ILE:O	1:C:2280:PRO:HD2	2.13	0.49
1:A:2511:LEU:HD21	1:B:2362:VAL:CG2	2.42	0.49
1:B:1740:LEU:HD22	1:B:1753:SER:OG	2.11	0.49
1:A:267:THR:N	1:A:413:ILE:O	2.37	0.49
1:C:714:GLU:O	1:C:718:GLY:N	2.40	0.49
1:C:1930:ASN:OD1	1:C:1933:ASN:N	2.45	0.49
1:A:853:ASN:O	1:A:857:ASN:N	2.43	0.49
1:A:1930:ASN:O	1:A:1934:VAL:HG13	2.13	0.49
1:B:1734:THR:HG22	1:B:1775:LEU:HD13	1.95	0.49
1:A:1904:VAL:HG23	1:A:1947:TYR:CD2	2.48	0.48
1:A:1910:PHE:HE2	1:A:1936:LEU:HD21	1.78	0.48
1:A:2501:PHE:CE2	1:A:2506:ILE:HD11	2.47	0.48
1:A:2275:TYR:HD2	1:A:2276:LEU:HD12	1.78	0.48
1:C:455:ALA:O	1:C:459:LEU:N	2.38	0.48
1:D:1911:LEU:HB2	1:D:1940:THR:HG21	1.94	0.48
1:D:2504:VAL:HG12	1:D:2504:VAL:O	2.13	0.48
1:A:1761:LEU:HD11	1:A:1772:PHE:CE2	2.48	0.48
1:C:1232:LEU:O	1:C:1236:CYS:N	2.47	0.48
1:B:2007:ARG:NH2	1:B:2009:ASP:OD2	2.46	0.48
1:B:2571:PHE:HE2	1:B:2590:VAL:HG21	1.79	0.48
1:C:1903:LEU:HA	1:C:1906:GLU:HG3	1.96	0.48
1:B:622:VAL:O	1:B:626:ARG:N	2.38	0.48
1:B:1757:ALA:HB1	1:B:1876:PHE:HE1	1.77	0.48
1:C:1871:GLN:HB3	1:C:1872:PRO:HD3	1.96	0.48
1:B:2575:VAL:O	1:B:2583:TYR:OH	2.15	0.48
1:C:1924:LEU:HD23	1:C:1924:LEU:H	1.79	0.48
1:B:2022:PRO:HB3	1:B:2067:LEU:HD13	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:118:TYR:O	1:D:174:GLY:N	2.46	0.48
1:A:2468:HIS:CB	1:A:2479:ILE:HD13	2.44	0.47
1:A:2571:PHE:HE2	1:A:2590:VAL:HG21	1.78	0.47
1:B:1741:ILE:HG22	1:B:1788:VAL:CG1	2.43	0.47
1:B:2014:GLU:O	1:B:2018:ILE:HG12	2.14	0.47
1:D:1904:VAL:HG21	1:D:1955:ASN:OD1	2.15	0.47
1:D:2022:PRO:HB3	1:D:2067:LEU:HD13	1.95	0.47
1:A:2200:ARG:O	1:A:2204:TRP:NE1	2.47	0.47
1:B:1761:LEU:HD13	1:B:1880:LEU:HD12	1.96	0.47
1:B:1770:LYS:O	1:B:1774:ASN:ND2	2.47	0.47
1:D:2020:LEU:HD12	1:D:2020:LEU:O	2.14	0.47
1:B:1949:GLN:HA	1:B:2002:ALA:HB1	1.95	0.47
1:B:2018:ILE:O	1:B:2021:ARG:NH1	2.47	0.47
1:C:1912:ASP:O	1:C:1916:GLY:N	2.48	0.47
1:D:1897:ASN:ND2	1:D:1899:THR:O	2.48	0.47
1:A:1881:CYS:SG	1:A:1892:LEU:HD12	2.55	0.47
1:B:1971:THR:HG23	1:B:2020:LEU:HB3	1.96	0.47
1:B:2045:SER:N	1:B:2048:GLU:OE2	2.48	0.47
1:A:1949:GLN:HA	1:A:2002:ALA:HB1	1.97	0.47
1:B:1797:GLN:NE2	1:B:1906:GLU:O	2.48	0.47
1:D:1784:ARG:O	1:D:1787:LYS:HB3	2.15	0.47
1:B:1725:GLN:OE1	1:B:1765:ASN:ND2	2.43	0.47
1:C:2017:LEU:O	1:C:2021:ARG:NH2	2.48	0.47
1:D:2070:LEU:O	1:D:2070:LEU:HD23	2.15	0.47
1:A:1790:HIS:O	1:A:1794:LYS:N	2.47	0.46
1:B:508:LEU:O	1:B:512:GLN:N	2.48	0.46
1:D:1442:GLU:O	1:D:1446:LEU:N	2.48	0.46
1:D:1740:LEU:HD23	1:D:1740:LEU:O	2.15	0.46
1:A:2476:VAL:HG22	1:A:2480:LEU:CD1	2.45	0.46
1:D:1914:MET:CE	1:D:1937:VAL:HG22	2.46	0.46
1:A:1373:ALA:O	1:A:1377:GLU:N	2.48	0.46
1:A:1904:VAL:HG21	1:A:1955:ASN:OD1	2.16	0.46
1:C:1910:PHE:CE2	1:C:1936:LEU:HD21	2.50	0.46
1:D:1725:GLN:HB3	1:D:1768:ILE:HD11	1.98	0.46
1:A:2016:ILE:HG22	1:A:2020:LEU:CD2	2.45	0.46
1:B:2017:LEU:HD23	1:B:2020:LEU:HD11	1.98	0.46
1:C:1757:ALA:HB1	1:C:1876:PHE:CE1	2.50	0.46
1:C:2151:THR:OG1	1:C:2181:GLU:OE2	2.33	0.46
1:A:2540:ILE:HD11	1:A:2565:MET:CB	2.45	0.46
1:A:2543:LEU:HD23	1:A:2548:PHE:CZ	2.51	0.46
1:B:2017:LEU:O	1:B:2021:ARG:NH1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1934:VAL:CG2	1:C:1988:LEU:HD22	2.46	0.46
1:A:2278:ILE:O	1:A:2280:PRO:HD2	2.16	0.46
1:C:1876:PHE:CZ	1:C:1880:LEU:HD11	2.51	0.46
1:C:1953:HIS:NE2	1:C:2006:SER:O	2.45	0.46
1:D:1950:GLY:O	1:D:1952:CYS:N	2.49	0.46
1:A:2163:GLU:OE2	1:A:2164:GLN:NE2	2.49	0.46
1:C:2513:PHE:CZ	1:C:2517:ILE:HD11	2.51	0.46
1:A:2598:ASN:OD1	1:A:2599:LEU:N	2.49	0.46
1:B:1741:ILE:HG23	1:B:1750:PHE:CD1	2.51	0.46
1:A:1725:GLN:NE2	1:A:1759:HIS:O	2.48	0.45
1:A:2135:GLN:HB2	1:A:2608:MET:HE1	1.98	0.45
1:B:2485:LYS:NZ	1:C:2453:ARG:O	2.29	0.45
1:B:2278:ILE:O	1:B:2280:PRO:HD2	2.16	0.45
1:D:1338:ASP:O	1:D:1342:LEU:N	2.40	0.45
1:A:1761:LEU:HD11	1:A:1772:PHE:HE2	1.81	0.45
1:B:1876:PHE:O	1:B:1880:LEU:HD13	2.16	0.45
1:C:1971:THR:HG23	1:C:2020:LEU:HB3	1.99	0.45
1:D:2549:ASP:OD1	1:D:2549:ASP:O	2.35	0.45
1:C:441:ASP:O	1:C:445:ALA:N	2.42	0.45
1:C:2058:LEU:HD23	1:C:2071:LEU:CD2	2.47	0.45
1:A:2560:LYS:NZ	4:A:2703:ATP:O2G	2.27	0.45
1:C:1934:VAL:HG11	1:C:1981:LEU:CD2	2.47	0.45
1:D:2163:GLU:OE2	1:D:2164:GLN:NE2	2.49	0.45
1:D:2468:HIS:CB	1:D:2479:ILE:HD13	2.47	0.45
1:D:2507:ILE:O	1:D:2511:LEU:N	2.48	0.45
1:D:1762:ASP:OD1	1:D:1763:GLY:N	2.49	0.45
1:D:1875:ARG:CZ	1:D:1879:LEU:HD21	2.46	0.45
1:D:2398:GLU:N	1:D:2398:GLU:OE1	2.50	0.45
1:B:2589:TYR:CZ	1:B:2593:MET:HE3	2.52	0.45
1:D:1877:LEU:HD13	1:D:1947:TYR:OH	2.16	0.45
1:D:2560:LYS:NZ	4:D:2703:ATP:O2G	2.26	0.45
1:B:2054:TYR:CE2	1:B:2058:LEU:HD11	2.52	0.44
1:C:2476:VAL:HG22	1:C:2480:LEU:CD1	2.48	0.44
1:D:1232:LEU:O	1:D:1236:CYS:N	2.50	0.44
1:D:2278:ILE:O	1:D:2280:PRO:HD2	2.18	0.44
1:B:1994:ASP:OD1	1:B:2052:ASN:ND2	2.49	0.44
1:B:2144:CYS:HA	1:B:2182:MET:CE	2.47	0.44
1:D:1871:GLN:HB2	1:D:1872:PRO:HD3	1.99	0.44
1:D:2328:LEU:C	1:D:2328:LEU:HD23	2.38	0.44
1:B:1793:MET:HE1	1:B:1903:LEU:HD22	1.99	0.44
1:C:780:LEU:O	1:C:784:VAL:N	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2054:TYR:HE1	1:C:2058:LEU:HD11	1.83	0.44
1:D:1772:PHE:O	1:D:1776:MET:SD	2.76	0.44
1:B:1754:ILE:O	1:B:1758:ILE:HG12	2.18	0.44
1:B:1925:LEU:HD11	1:B:1972:ALA:CB	2.47	0.44
1:B:1788:VAL:HG22	1:B:1788:VAL:O	2.17	0.44
1:D:2299:SER:O	1:D:2303:ASN:N	2.51	0.44
1:A:168:TRP:N	1:A:182:LYS:O	2.51	0.44
1:D:2269:ILE:HD11	1:D:2285:LEU:HD21	2.00	0.44
1:C:2268:LEU:C	1:C:2268:LEU:HD23	2.38	0.44
1:A:2400:ASP:O	1:D:2481:ARG:NH1	2.48	0.44
1:B:2268:LEU:HD23	1:B:2268:LEU:C	2.39	0.44
1:C:1026:ASP:O	1:C:1029:GLY:N	2.51	0.43
1:D:2467:ASN:O	1:D:2471:ARG:NH1	2.51	0.43
1:C:1338:ASP:O	1:C:1342:LEU:N	2.38	0.43
1:C:1926:GLY:HA2	1:C:1978:ILE:HG23	2.00	0.43
1:C:1974:ILE:CD1	1:C:2000:LEU:HD12	2.48	0.43
1:A:1784:ARG:O	1:A:1787:LYS:HB3	2.19	0.43
1:A:1965:ASN:O	1:A:1969:ILE:HD12	2.18	0.43
1:A:2359:ILE:O	1:A:2363:THR:HG22	2.19	0.43
1:A:2574:LEU:HA	1:A:2577:VAL:HG12	2.00	0.43
1:B:2144:CYS:HA	1:B:2182:MET:HE3	1.99	0.43
1:A:2465:VAL:HG22	1:A:2476:VAL:HG21	2.01	0.43
1:B:1741:ILE:HG23	1:B:1750:PHE:HE1	1.83	0.43
1:D:10:ILE:O	1:D:113:GLY:N	2.41	0.43
1:A:308:HIS:O	1:A:312:GLY:N	2.48	0.43
1:C:1987:ASP:OD1	1:C:1988:LEU:N	2.52	0.43
1:D:1719:SER:O	1:D:1723:ALA:N	2.42	0.43
1:B:1871:GLN:OE1	1:B:1939:GLN:HG3	2.19	0.43
1:B:2364:ARG:CD	1:B:2523:LEU:HD11	2.49	0.43
1:D:1067:TYR:O	1:D:1071:VAL:N	2.47	0.43
1:A:1876:PHE:O	1:A:1880:LEU:HD13	2.19	0.43
1:B:1727:ARG:O	1:B:1731:GLU:HG2	2.19	0.43
1:B:1750:PHE:O	1:B:1753:SER:OG	2.30	0.43
1:C:1773:HIS:CB	1:C:1888:LEU:HD21	2.49	0.43
1:D:1742:THR:O	1:D:1784:ARG:NH1	2.52	0.43
1:D:1876:PHE:CE1	1:D:1880:LEU:CD1	3.02	0.43
1:C:1720:ALA:O	1:C:1723:ALA:N	2.52	0.42
1:A:1908:LEU:HD11	1:A:1966:GLY:HA3	2.01	0.42
1:B:1650:HIS:O	1:B:1654:LEU:CB	2.67	0.42
1:C:452:LEU:O	1:C:456:VAL:N	2.37	0.42
1:A:1744:THR:HG22	1:A:1746:ASN:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1880:LEU:HD23	1:B:1888:LEU:HD22	2.01	0.42
1:D:2140:VAL:HG23	1:D:2140:VAL:O	2.19	0.42
1:D:2546:ASP:OD1	1:D:2547:LYS:N	2.52	0.42
1:D:2575:VAL:HG13	1:D:2591:ALA:HB2	2.01	0.42
1:A:1737:VAL:HG12	1:A:1756:LEU:HD23	2.01	0.42
1:A:1950:GLY:O	1:A:1952:CYS:N	2.46	0.42
1:C:1606:LEU:O	1:C:1609:LEU:N	2.53	0.42
1:C:2054:TYR:CE2	1:C:2071:LEU:HD11	2.54	0.42
1:D:126:HIS:O	1:D:130:ASN:N	2.48	0.42
1:A:2130:ASP:OD1	1:A:2132:SER:OG	2.26	0.42
1:A:2145:GLN:HA	1:A:2145:GLN:OE1	2.20	0.42
1:A:2468:HIS:HB3	1:A:2479:ILE:HD13	2.01	0.42
1:B:2215:ILE:HG23	1:B:2282:LEU:CD1	2.49	0.42
1:D:2574:LEU:HA	1:D:2577:VAL:HG12	2.01	0.42
1:A:2021:ARG:CZ	1:A:2021:ARG:HA	2.49	0.42
1:B:1938:ILE:HG23	1:B:1995:ASN:OD1	2.19	0.42
1:B:2278:ILE:C	1:B:2280:PRO:HD2	2.40	0.42
1:D:2560:LYS:NZ	4:D:2703:ATP:O3A	2.53	0.42
1:B:1758:ILE:HD11	1:B:1876:PHE:HB2	2.02	0.42
1:B:1925:LEU:HD11	1:B:1972:ALA:HB1	2.01	0.42
1:B:2376:ALA:HB2	1:B:2508:VAL:CG1	2.50	0.42
1:C:2135:GLN:HB2	1:C:2608:MET:HE1	2.02	0.42
1:C:2501:PHE:CZ	1:C:2506:ILE:HD11	2.54	0.42
1:C:2577:VAL:HG22	1:C:2577:VAL:O	2.20	0.42
1:D:841:LEU:O	1:D:845:VAL:N	2.53	0.42
1:D:1952:CYS:O	1:D:1953:HIS:HB2	2.20	0.42
1:B:1929:ILE:CG2	1:B:1934:VAL:HG12	2.50	0.41
1:B:2058:LEU:HD12	1:B:2071:LEU:HD21	2.01	0.41
1:C:1970:ILE:HA	1:C:1973:LEU:HD12	2.02	0.41
1:D:1970:ILE:HD12	1:D:1999:LEU:HD23	2.02	0.41
1:B:2020:LEU:HD12	1:B:2020:LEU:O	2.20	0.41
1:C:2519:THR:O	1:C:2523:LEU:HD13	2.19	0.41
1:A:1895:GLN:NE2	1:A:1901:TYR:O	2.53	0.41
1:A:1734:THR:HG23	1:A:1772:PHE:CE1	2.54	0.41
1:A:1925:LEU:HD23	1:A:1925:LEU:H	1.85	0.41
1:A:2501:PHE:CZ	1:A:2506:ILE:HD11	2.55	0.41
1:B:1914:MET:HE3	1:B:1937:VAL:HG22	2.00	0.41
1:B:2604:ARG:HE	1:B:2605:MET:HG2	1.85	0.41
1:B:1406:ILE:O	1:B:1410:LYS:N	2.41	0.41
1:B:1934:VAL:CG2	1:B:1988:LEU:HD13	2.38	0.41
1:B:1945:THR:HG22	1:B:1949:GLN:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1745:LYS:HE3	1:D:1745:LYS:HA	2.02	0.41
1:D:2184:TRP:NE1	1:D:2302:GLY:O	2.49	0.41
1:D:2544:GLU:OE1	1:D:2544:GLU:N	2.47	0.41
1:B:2200:ARG:O	1:B:2204:TRP:NE1	2.53	0.41
1:D:2163:GLU:CD	1:D:2164:GLN:HE21	2.24	0.41
1:A:2294:ILE:O	1:A:2298:VAL:HG23	2.21	0.41
1:B:2483:PRO:O	1:C:2399:VAL:HG12	2.20	0.41
1:B:2541:CYS:O	1:B:2604:ARG:NH2	2.53	0.41
1:C:1910:PHE:CZ	1:C:1936:LEU:HD21	2.56	0.41
1:C:2058:LEU:HD23	1:C:2071:LEU:HD23	2.03	0.41
1:A:1776:MET:HE2	1:A:1782:SER:HA	2.03	0.41
1:A:2293:LYS:O	1:A:2297:VAL:HG23	2.20	0.41
1:B:1871:GLN:CB	1:B:1872:PRO:HD3	2.50	0.41
1:B:1974:ILE:HD12	1:B:2000:LEU:CD1	2.51	0.41
1:D:1740:LEU:HD22	1:D:1753:SER:HB3	2.01	0.41
1:D:2593:MET:SD	1:D:2598:ASN:ND2	2.93	0.41
1:B:2151:THR:OG1	1:B:2181:GLU:OE2	2.39	0.41
1:C:2140:VAL:O	1:C:2140:VAL:HG23	2.20	0.41
1:C:2574:LEU:HA	1:C:2577:VAL:HG12	2.03	0.41
1:D:1788:VAL:O	1:D:1788:VAL:HG22	2.20	0.41
1:D:2295:VAL:O	1:D:2298:VAL:HG12	2.20	0.41
1:D:116:VAL:O	1:D:177:VAL:N	2.41	0.41
1:A:1754:ILE:HG21	1:A:1872:PRO:HB2	2.03	0.40
1:A:2323:HIS:O	1:A:2327:ILE:HG13	2.21	0.40
1:B:2140:VAL:O	1:B:2140:VAL:HG23	2.21	0.40
1:C:1960:VAL:HG23	1:C:1961:THR:HG23	2.03	0.40
1:D:1741:ILE:HG22	1:D:1788:VAL:HG11	2.03	0.40
1:D:1914:MET:HE3	1:D:1937:VAL:HG22	2.02	0.40
1:D:2014:GLU:O	1:D:2018:ILE:HG13	2.21	0.40
1:C:2295:VAL:O	1:C:2298:VAL:HG12	2.21	0.40
1:C:1865:THR:O	1:C:1865:THR:HG22	2.20	0.40
1:C:1911:LEU:HB2	1:C:1940:THR:HG21	2.03	0.40
1:D:2476:VAL:HG22	1:D:2480:LEU:HD11	2.02	0.40
1:C:1871:GLN:OE1	1:C:1939:GLN:HG3	2.21	0.40
1:D:15:SER:O	1:D:222:ASN:N	2.54	0.40
1:B:2131:ARG:NH2	1:B:2600:ASP:OD2	2.55	0.40
1:B:2398:GLU:OE1	1:B:2398:GLU:N	2.55	0.40
1:C:2051:HIS:O	1:C:2055:ILE:HG12	2.22	0.40
1:C:2212:ALA:O	1:C:2216:ASN:ND2	2.54	0.40
1:D:1725:GLN:OE1	1:D:1765:ASN:ND2	2.49	0.40

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	1964/2633 (75%)	1875 (96%)	89 (4%)	0	100	100
1	B	1614/2633 (61%)	1560 (97%)	54 (3%)	0	100	100
1	C	1535/2633 (58%)	1469 (96%)	66 (4%)	0	100	100
1	D	1956/2633 (74%)	1866 (95%)	90 (5%)	0	100	100
All	All	7069/10532 (67%)	6770 (96%)	299 (4%)	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	609/2329 (26%)	609 (100%)	0	100	100
1	B	613/2329 (26%)	613 (100%)	0	100	100
1	C	555/2329 (24%)	555 (100%)	0	100	100
1	D	605/2329 (26%)	603 (100%)	2 (0%)	91	94
All	All	2382/9316 (26%)	2380 (100%)	2 (0%)	92	96

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	1933	ASN
1	D	2592	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1797	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 8 are monoatomic - leaving 6 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	$\# Z > 2$
4	ATP	A	2703	-	28,33,33	0.64	0	34,52,52	0.91	1 (2%)
3	I3P	A	2702	-	24,24,24	1.34	3 (12%)	39,39,39	0.84	0
4	ATP	D	2703	-	28,33,33	0.64	0	34,52,52	0.92	1 (2%)
4	ATP	B	2702	-	28,33,33	0.64	0	34,52,52	0.92	1 (2%)
3	I3P	D	2702	-	24,24,24	1.34	3 (12%)	39,39,39	0.85	1 (2%)
4	ATP	C	2702	-	28,33,33	0.63	0	34,52,52	0.90	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
4	ATP	A	2703	-	-	9/18/38/38	0/3/3/3
3	I3P	A	2702	-	-	2/15/39/39	0/1/1/1
4	ATP	D	2703	-	-	9/18/38/38	0/3/3/3
4	ATP	B	2702	-	-	10/18/38/38	0/3/3/3
3	I3P	D	2702	-	-	3/15/39/39	0/1/1/1
4	ATP	C	2702	-	-	5/18/38/38	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2702	I3P	P4-O4	3.29	1.65	1.59
3	D	2702	I3P	P5-O5	3.29	1.65	1.59
3	A	2702	I3P	P5-O5	3.26	1.65	1.59
3	D	2702	I3P	P4-O4	3.26	1.65	1.59
3	A	2702	I3P	P1-O1	3.23	1.65	1.59
3	D	2702	I3P	P1-O1	3.21	1.65	1.59

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2702	ATP	C5-C6-N6	2.35	123.89	120.31
4	A	2703	ATP	C5-C6-N6	2.34	123.88	120.31
4	D	2703	ATP	C5-C6-N6	2.32	123.85	120.31
4	C	2702	ATP	C5-C6-N6	2.32	123.84	120.31
3	D	2702	I3P	P1-O1-C1	-2.07	117.92	123.43

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2703	ATP	PB-O3B-PG-O2G
4	A	2703	ATP	C5'-O5'-PA-O1A
4	A	2703	ATP	C5'-O5'-PA-O3A
4	B	2702	ATP	PB-O3B-PG-O2G
4	B	2702	ATP	C5'-O5'-PA-O3A
4	C	2702	ATP	PB-O3B-PG-O2G
4	D	2703	ATP	PB-O3B-PG-O2G
4	D	2703	ATP	C5'-O5'-PA-O1A
4	B	2702	ATP	O4'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	D	2703	ATP	O4'-C4'-C5'-O5'
4	A	2703	ATP	O4'-C4'-C5'-O5'
4	C	2702	ATP	O4'-C4'-C5'-O5'
4	C	2702	ATP	PB-O3B-PG-O1G
4	B	2702	ATP	C3'-C4'-C5'-O5'
4	A	2703	ATP	PB-O3A-PA-O1A
3	A	2702	I3P	C3-C4-O4-P4
4	A	2703	ATP	PA-O3A-PB-O2B
4	D	2703	ATP	PA-O3A-PB-O2B
4	B	2702	ATP	C5'-O5'-PA-O1A
4	B	2702	ATP	PA-O3A-PB-O2B
4	C	2702	ATP	PA-O3A-PB-O1B
4	D	2703	ATP	PB-O3A-PA-O2A
3	D	2702	I3P	C5-O5-P5-O53
3	A	2702	I3P	C5-C4-O4-P4
3	D	2702	I3P	C5-O5-P5-O51
4	B	2702	ATP	PB-O3B-PG-O1G
4	D	2703	ATP	PB-O3B-PG-O1G
4	A	2703	ATP	PB-O3B-PG-O3G
4	B	2702	ATP	PB-O3B-PG-O3G
4	A	2703	ATP	PA-O3A-PB-O1B
4	A	2703	ATP	PB-O3A-PA-O2A
4	B	2702	ATP	PB-O3A-PA-O1A
4	B	2702	ATP	PB-O3A-PA-O2A
4	C	2702	ATP	PA-O3A-PB-O2B
4	D	2703	ATP	C3'-C4'-C5'-O5'
3	D	2702	I3P	C1-O1-P1-O13
4	D	2703	ATP	PA-O3A-PB-O1B
4	D	2703	ATP	PB-O3A-PA-O1A

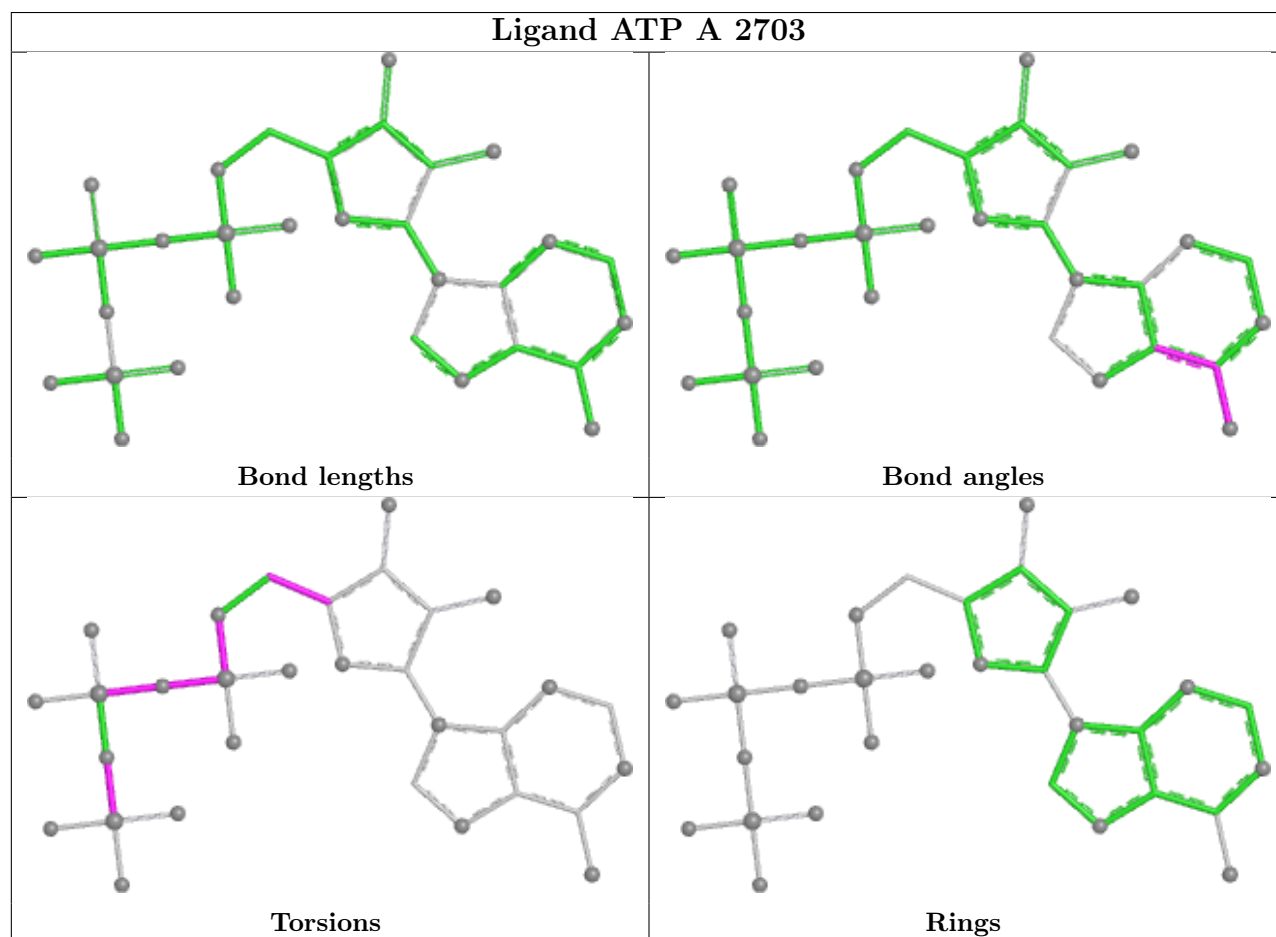
There are no ring outliers.

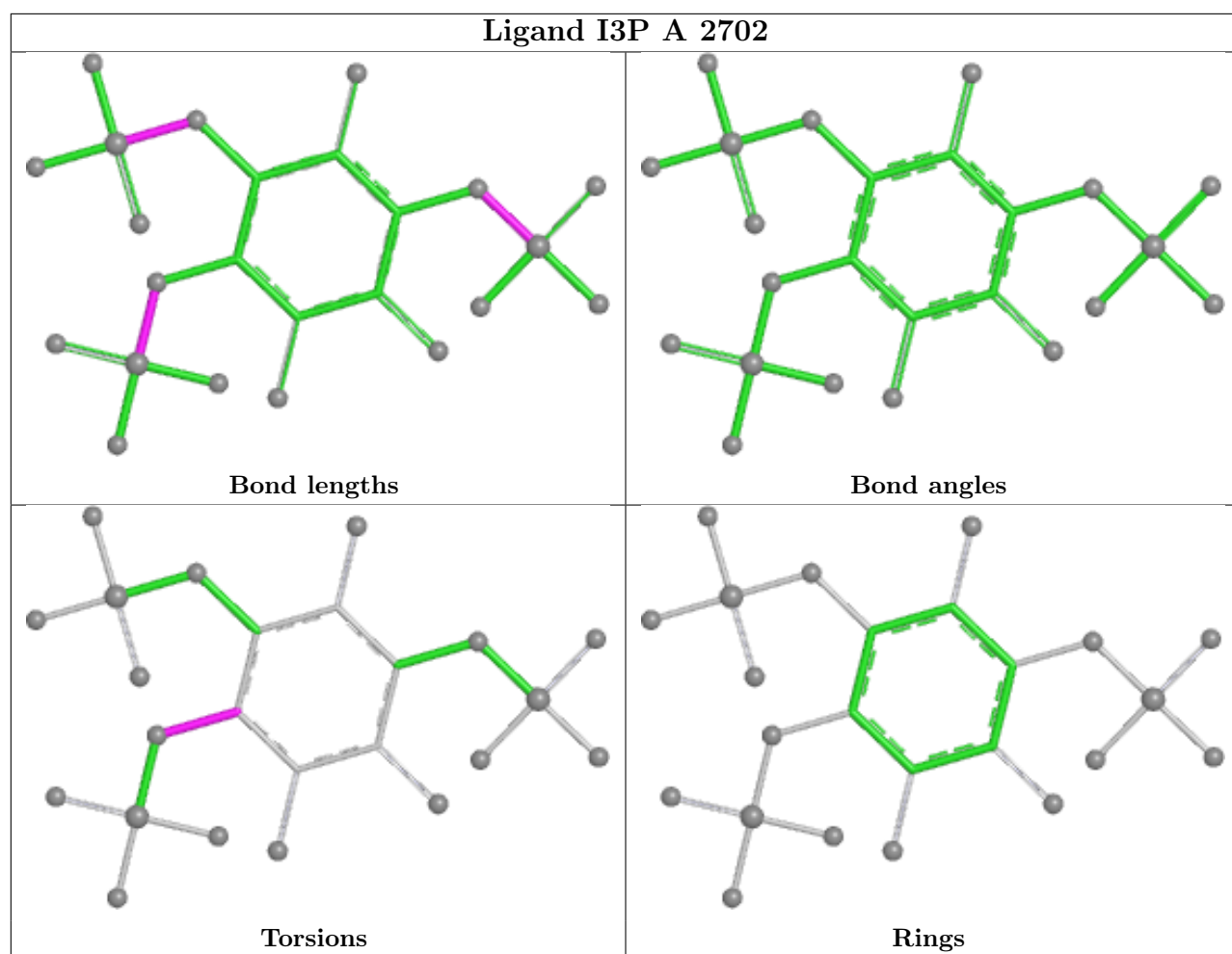
4 monomers are involved in 5 short contacts:

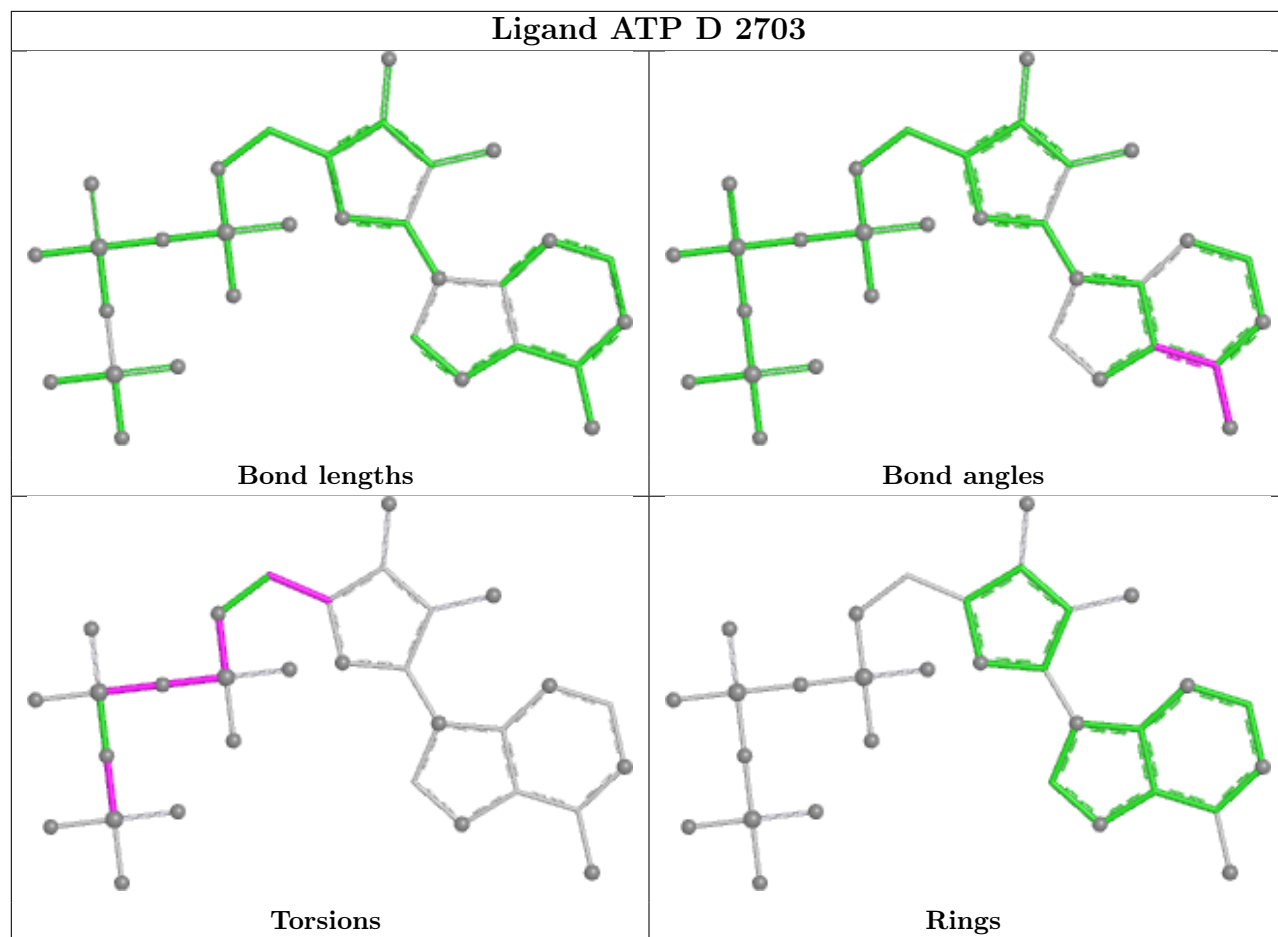
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2703	ATP	1	0
4	D	2703	ATP	2	0
4	B	2702	ATP	1	0
4	C	2702	ATP	1	0

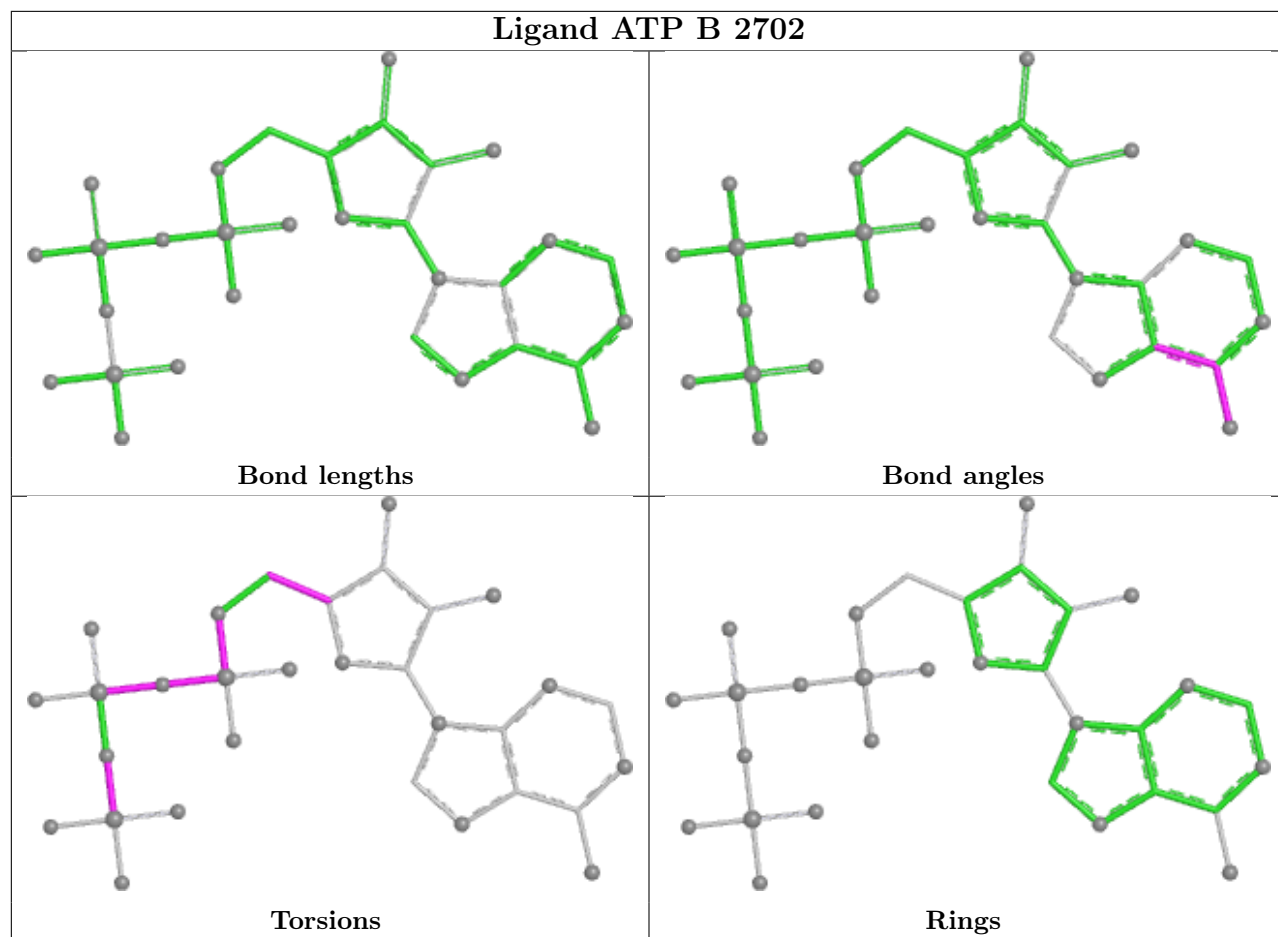
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

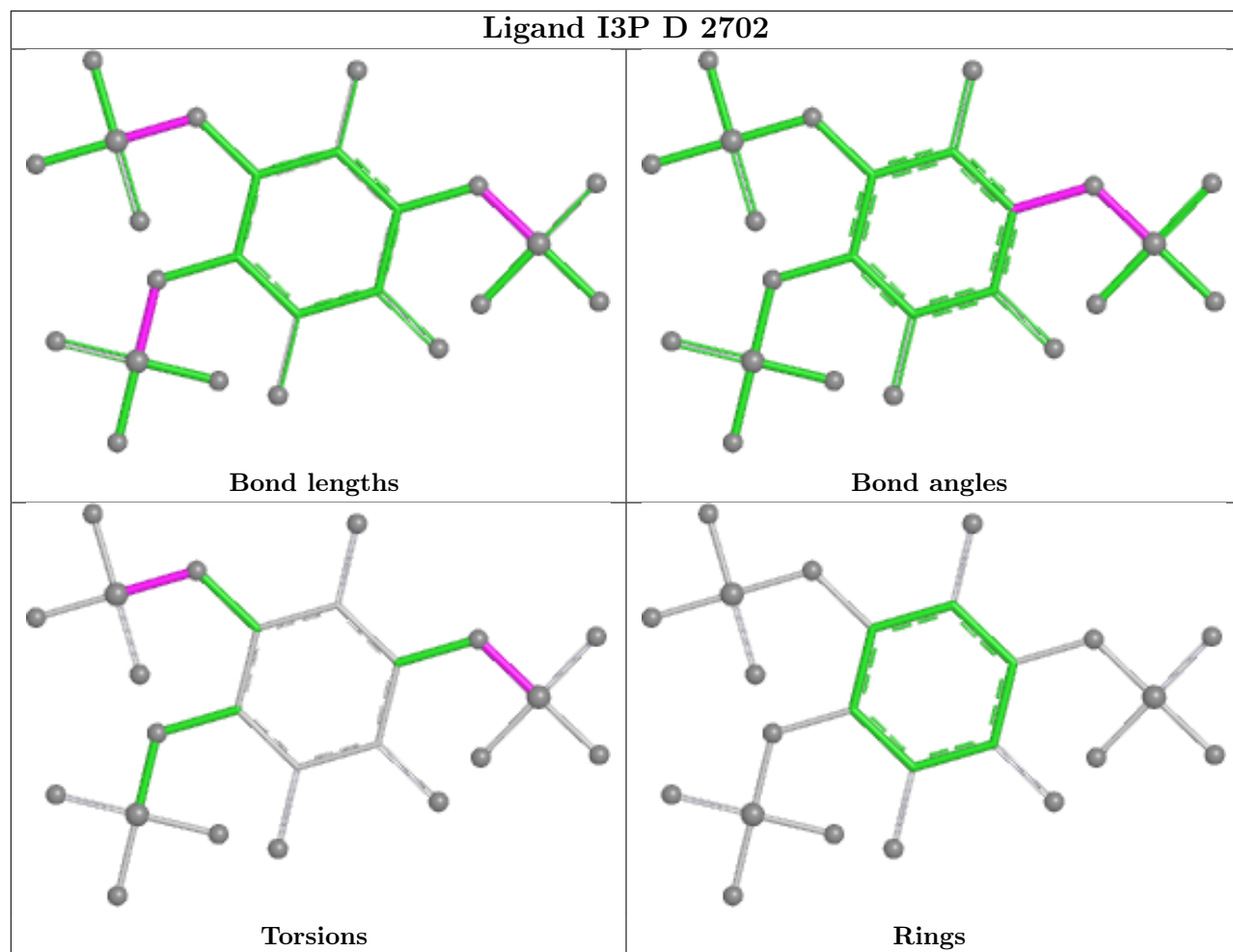
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

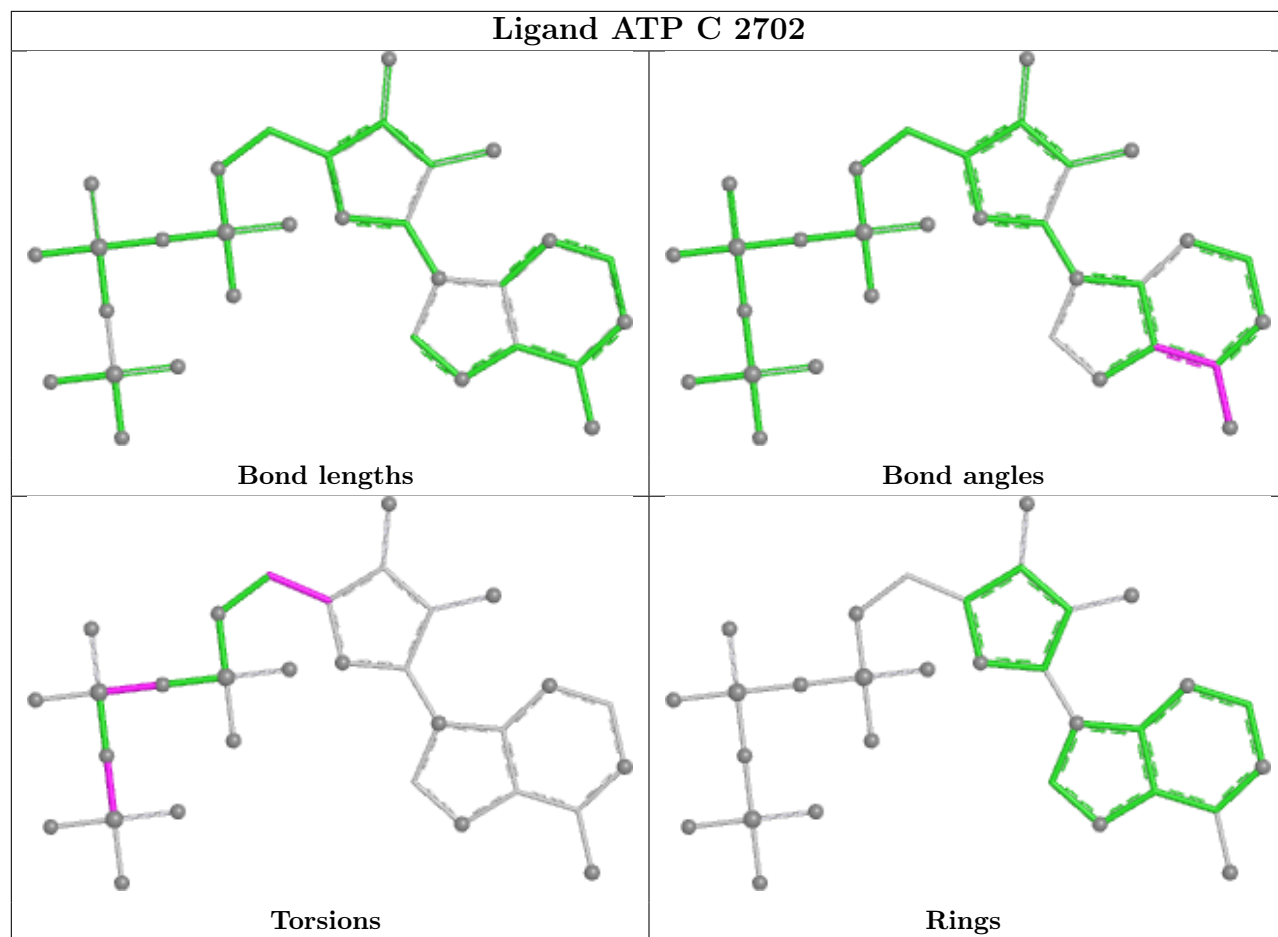












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

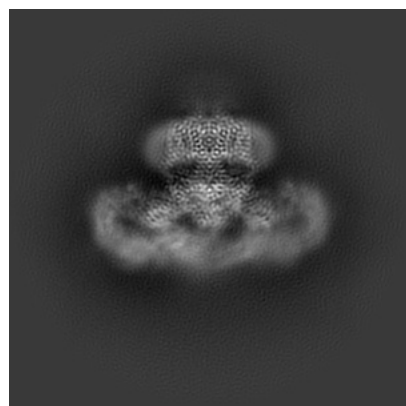
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25671. These allow visual inspection of the internal detail of the map and identification of artifacts.

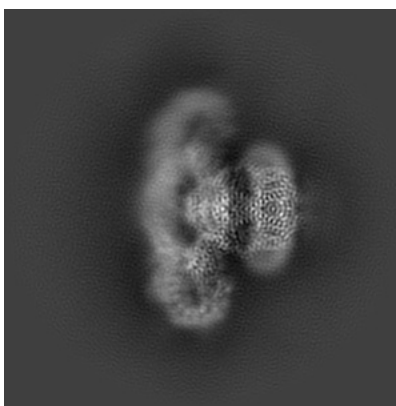
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

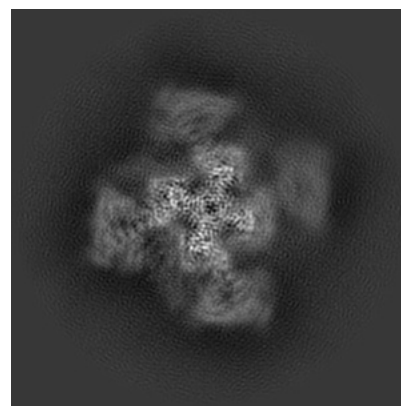
6.1.1 Primary map



X

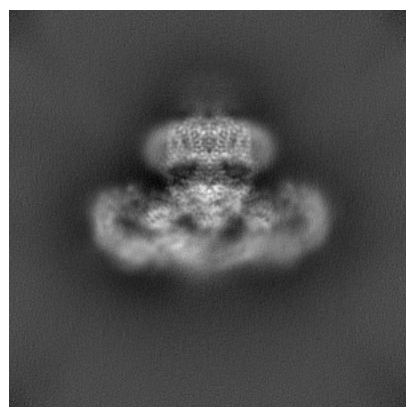


Y

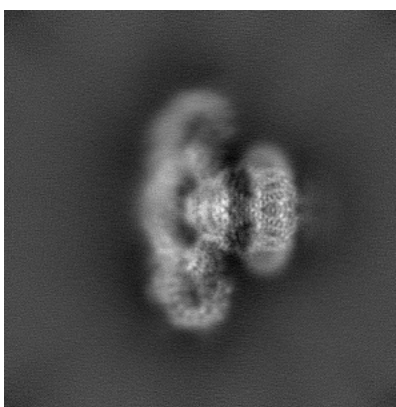


Z

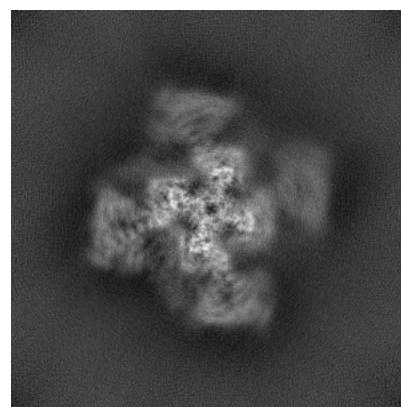
6.1.2 Raw map



X



Y

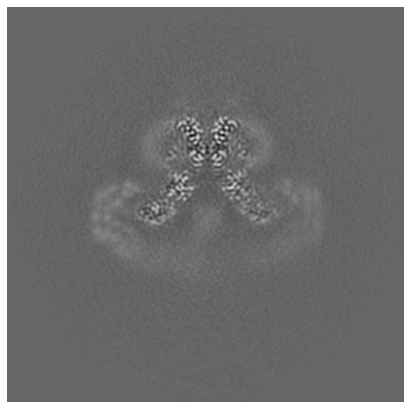


Z

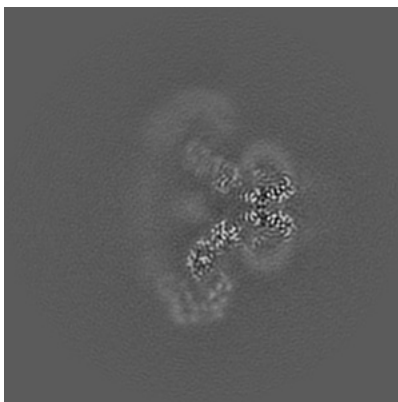
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

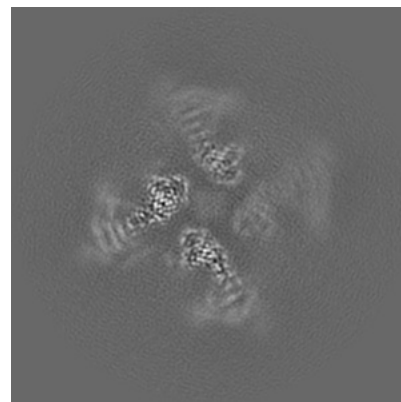
6.2.1 Primary map



X Index: 240

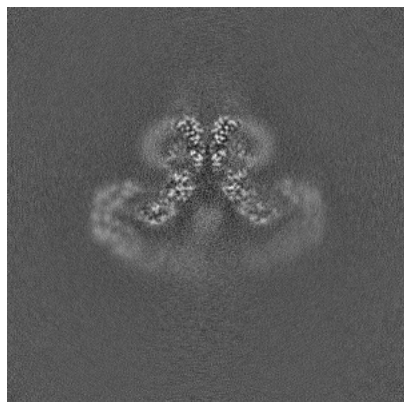


Y Index: 240

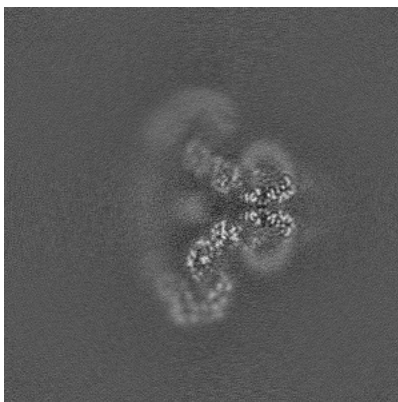


Z Index: 240

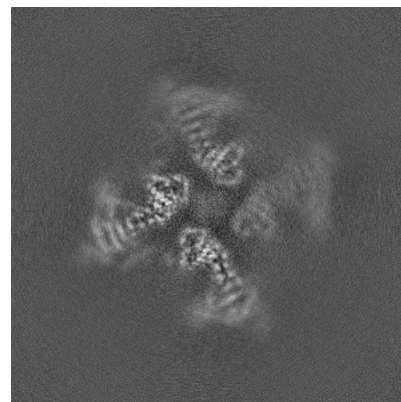
6.2.2 Raw map



X Index: 240



Y Index: 240

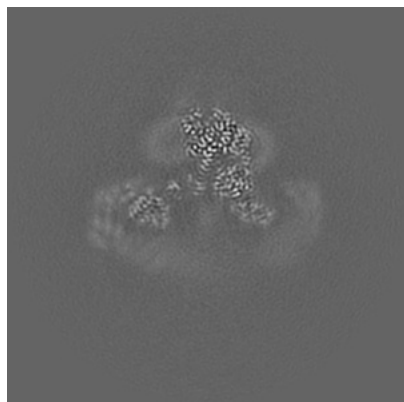


Z Index: 240

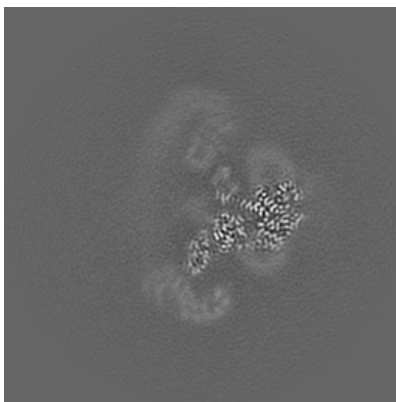
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

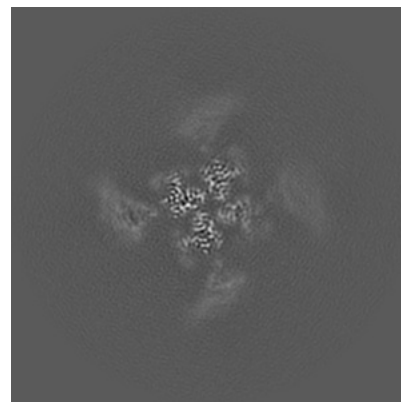
6.3.1 Primary map



X Index: 250

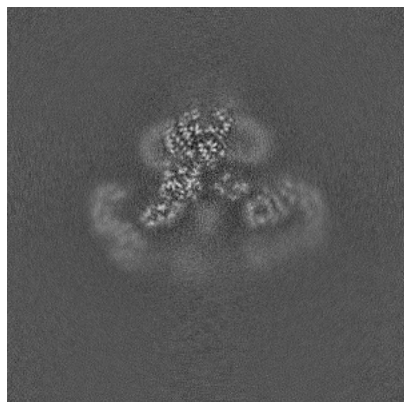


Y Index: 250

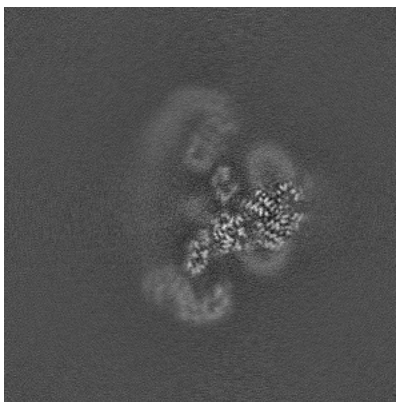


Z Index: 262

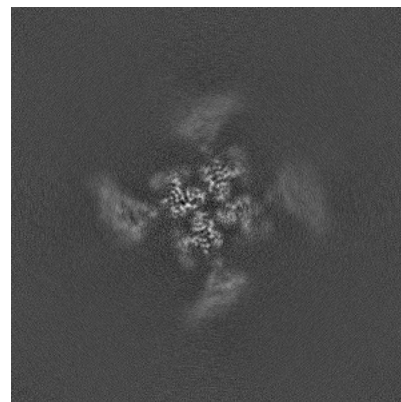
6.3.2 Raw map



X Index: 232



Y Index: 249

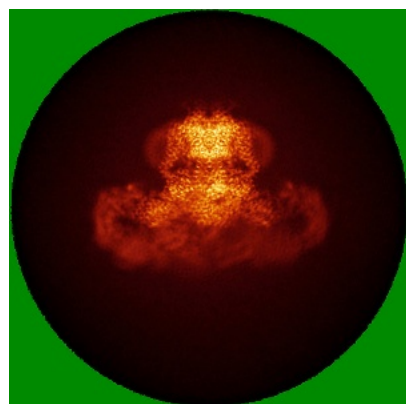


Z Index: 262

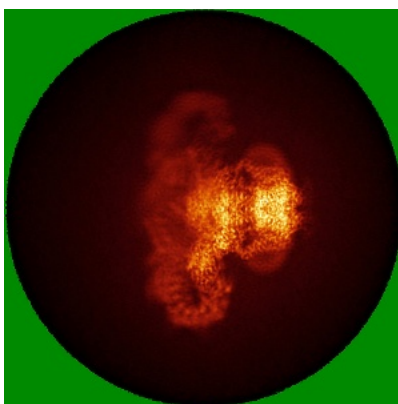
The images above show the largest variance slices of the map in three orthogonal directions.

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

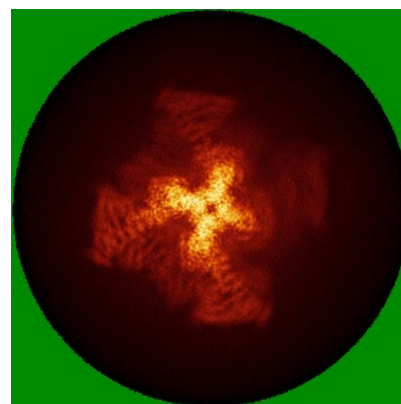
6.4.1 Primary map



X

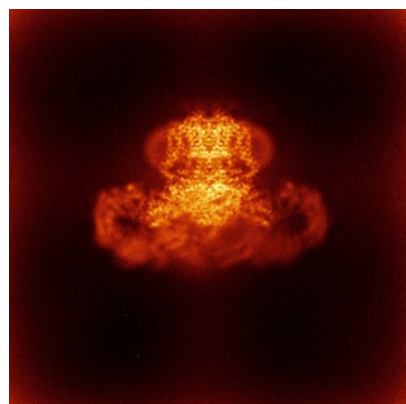


Y

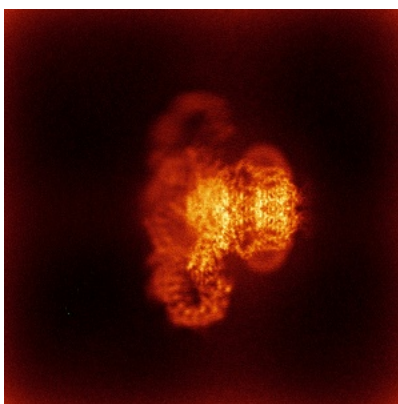


Z

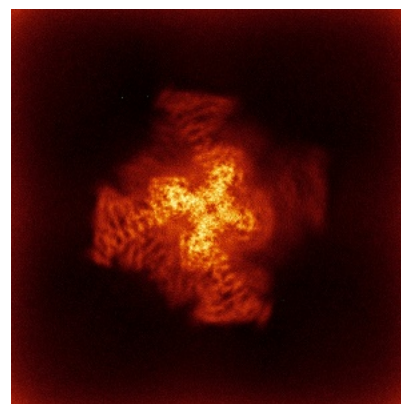
6.4.2 Raw map



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](#)

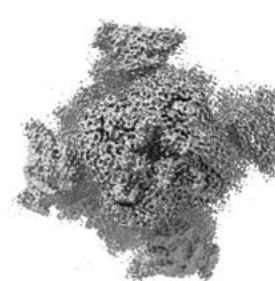
6.5.1 Primary map



X



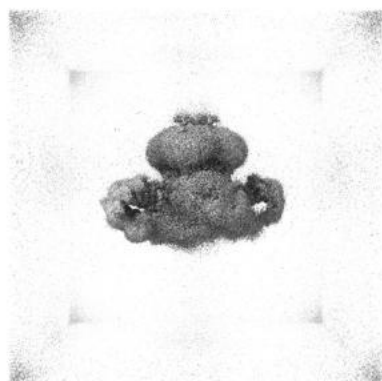
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.12. 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



X



Y



Z

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.

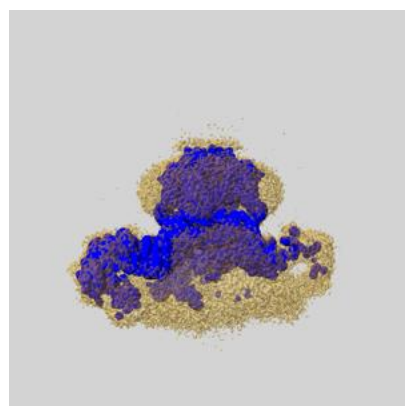
6.6 Mask visualisation [i](#)

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

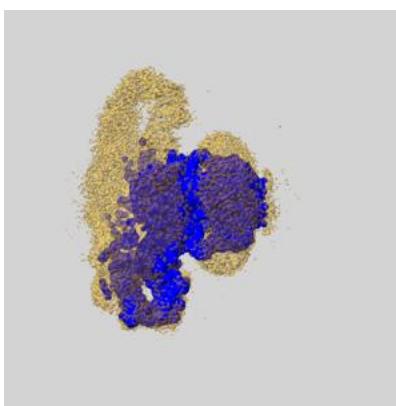
A mask typically either:

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

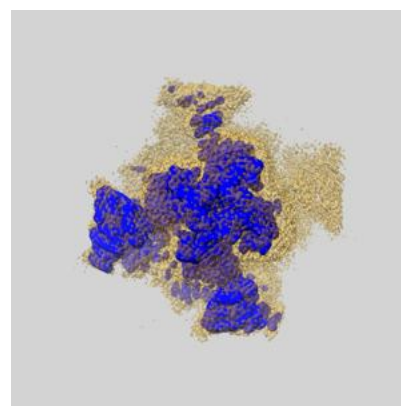
6.6.1 emd_25671_msk_1.map [i](#)



X



Y

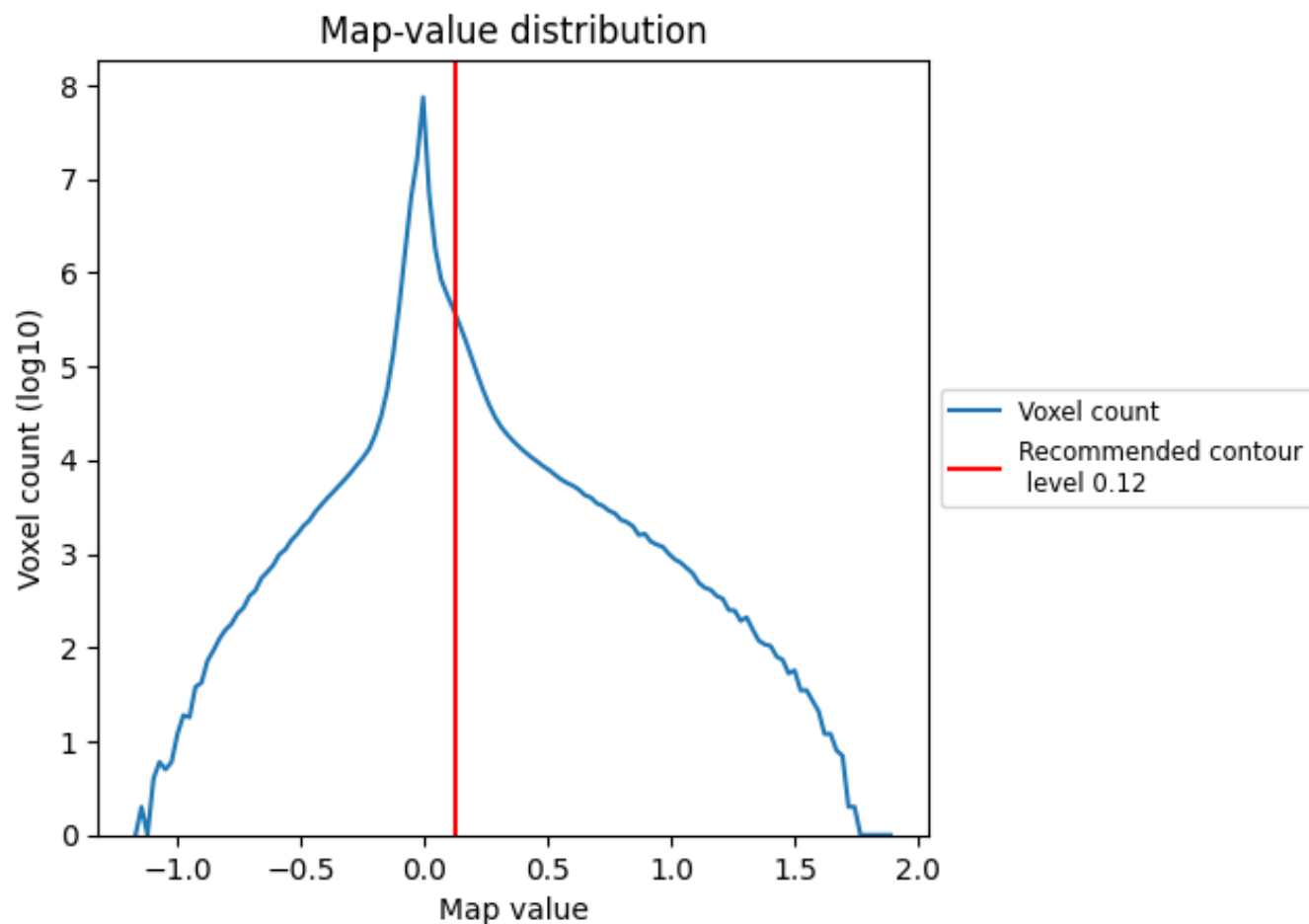


Z

7 Map analysis [i](#)

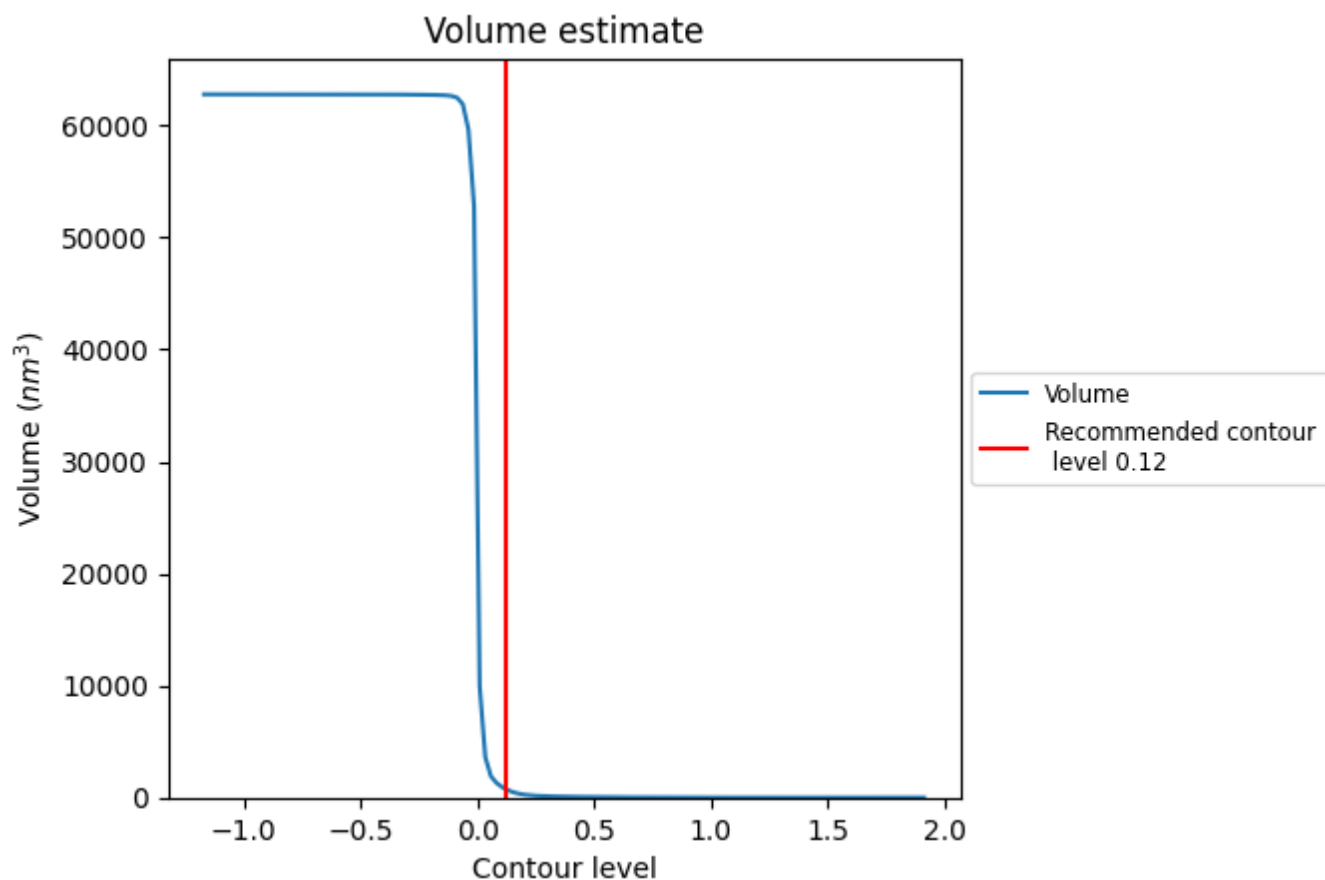
This section contains the results of statistical analysis of the map.

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.

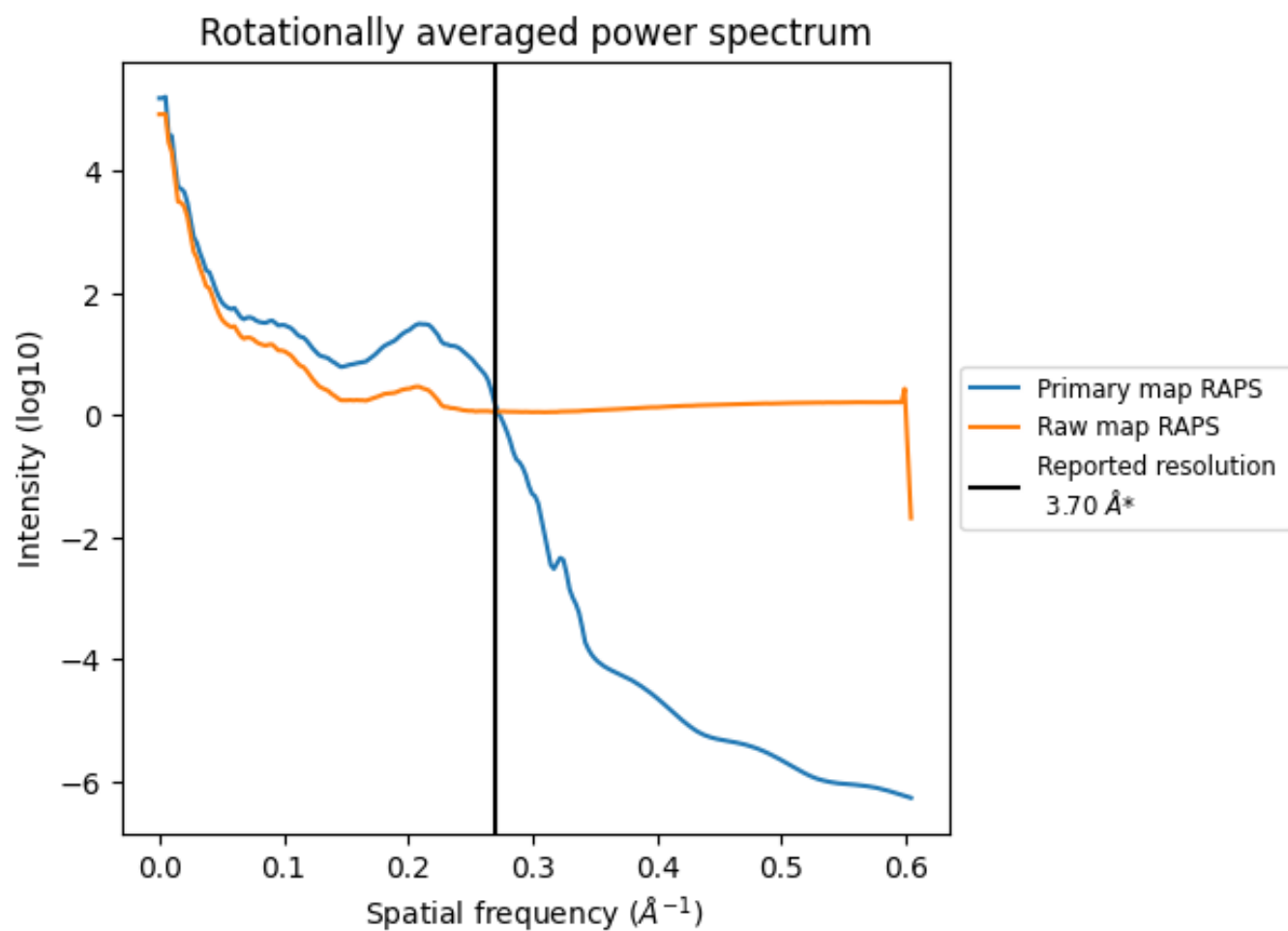
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 762 nm³; this corresponds to an approximate mass of 689 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 ⓘ

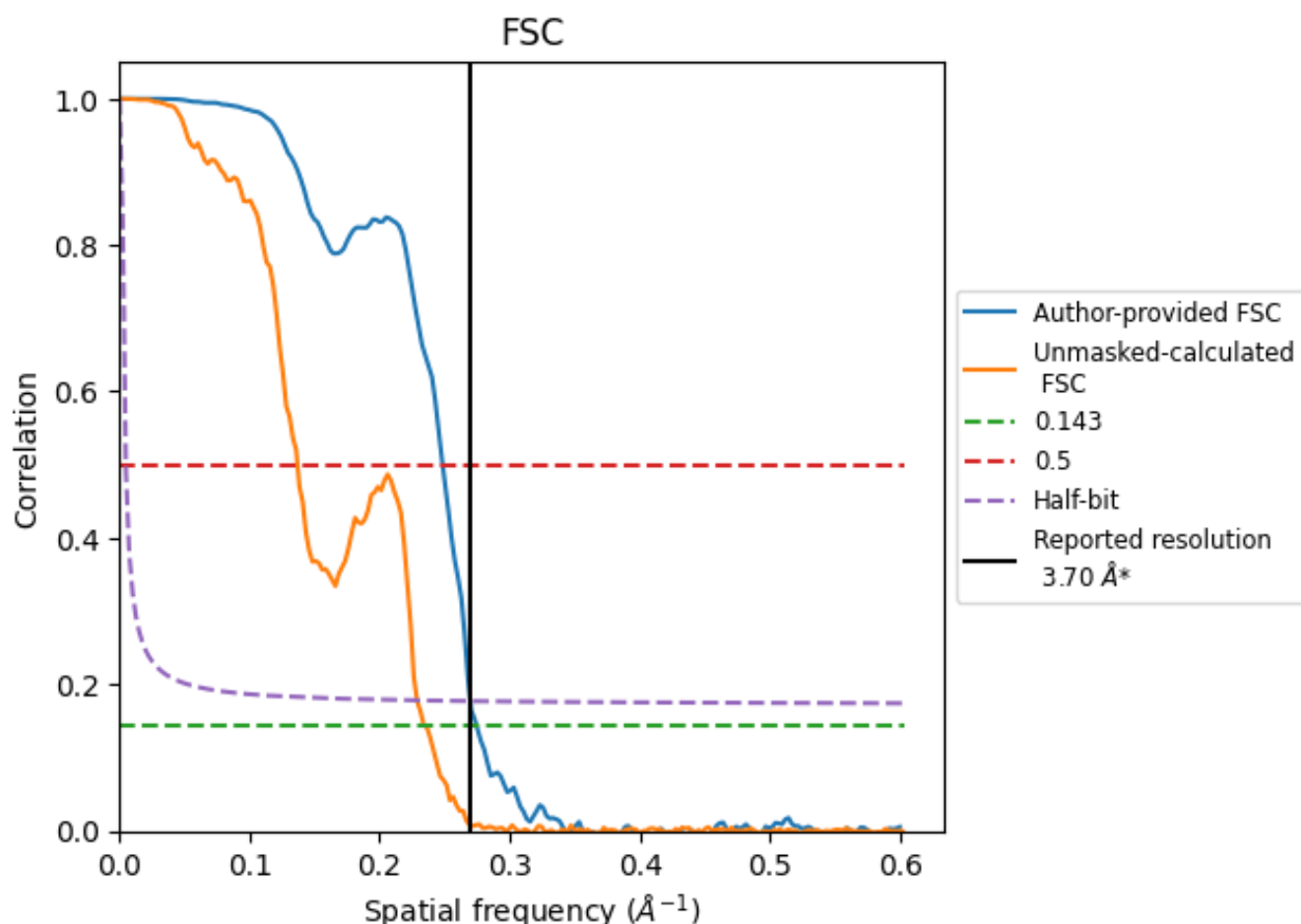


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

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 0.270 \AA^{-1}

8.2 Resolution estimates [i](#)

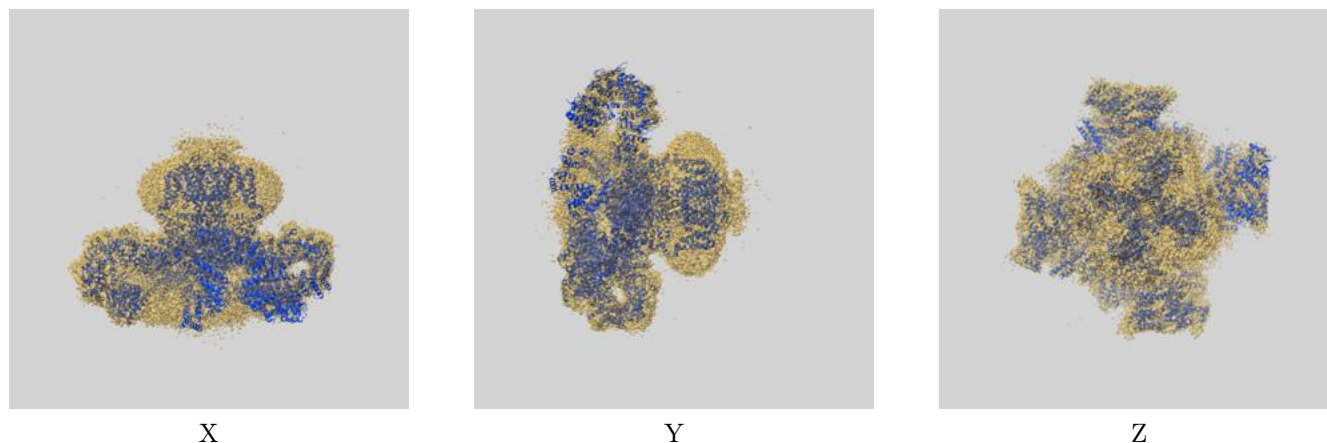
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.64	4.02	3.71
Unmasked-calculated*	4.26	7.30	4.37

*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 4.26 differs from the reported value 3.7 by more than 10 %

9 Map-model fit [i](#)

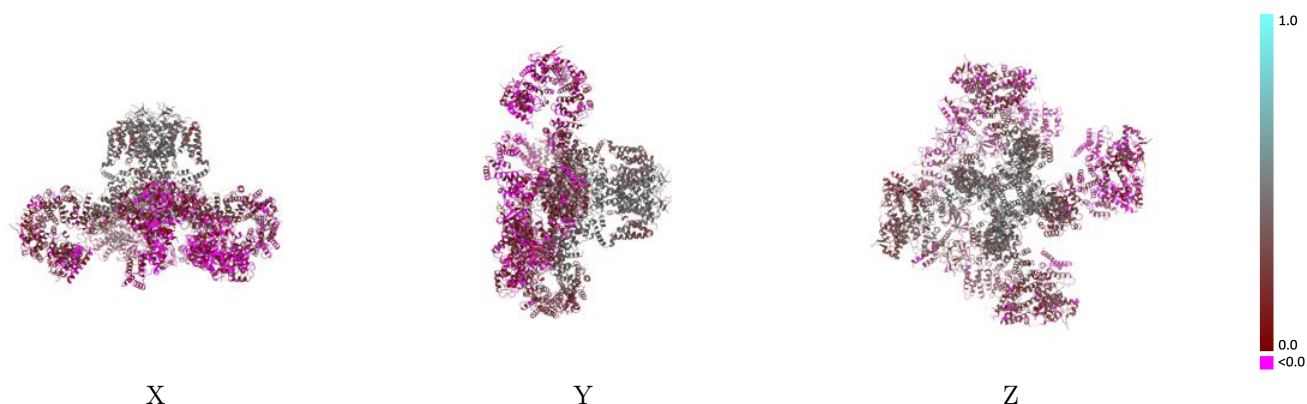
This section contains information regarding the fit between EMDB map EMD-25671 and PDB model 7T3U. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



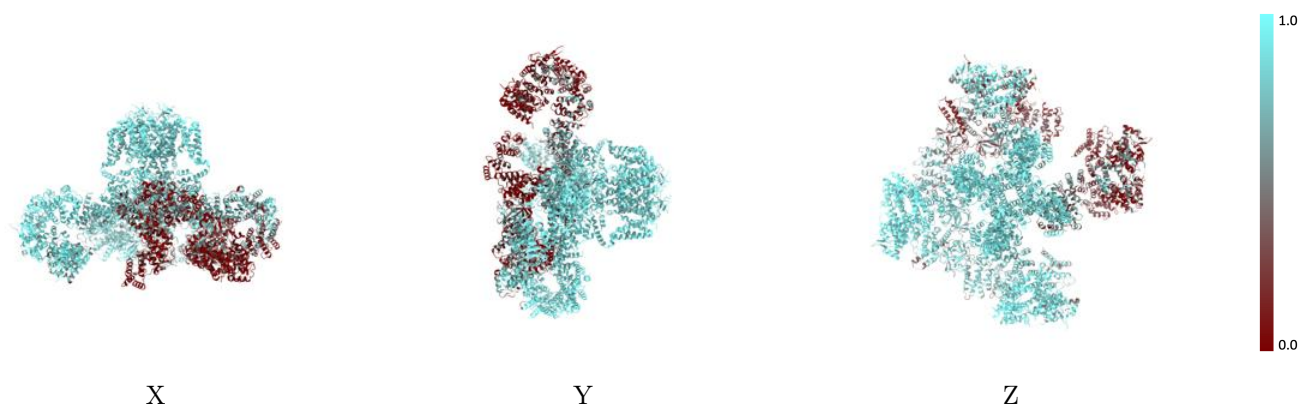
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



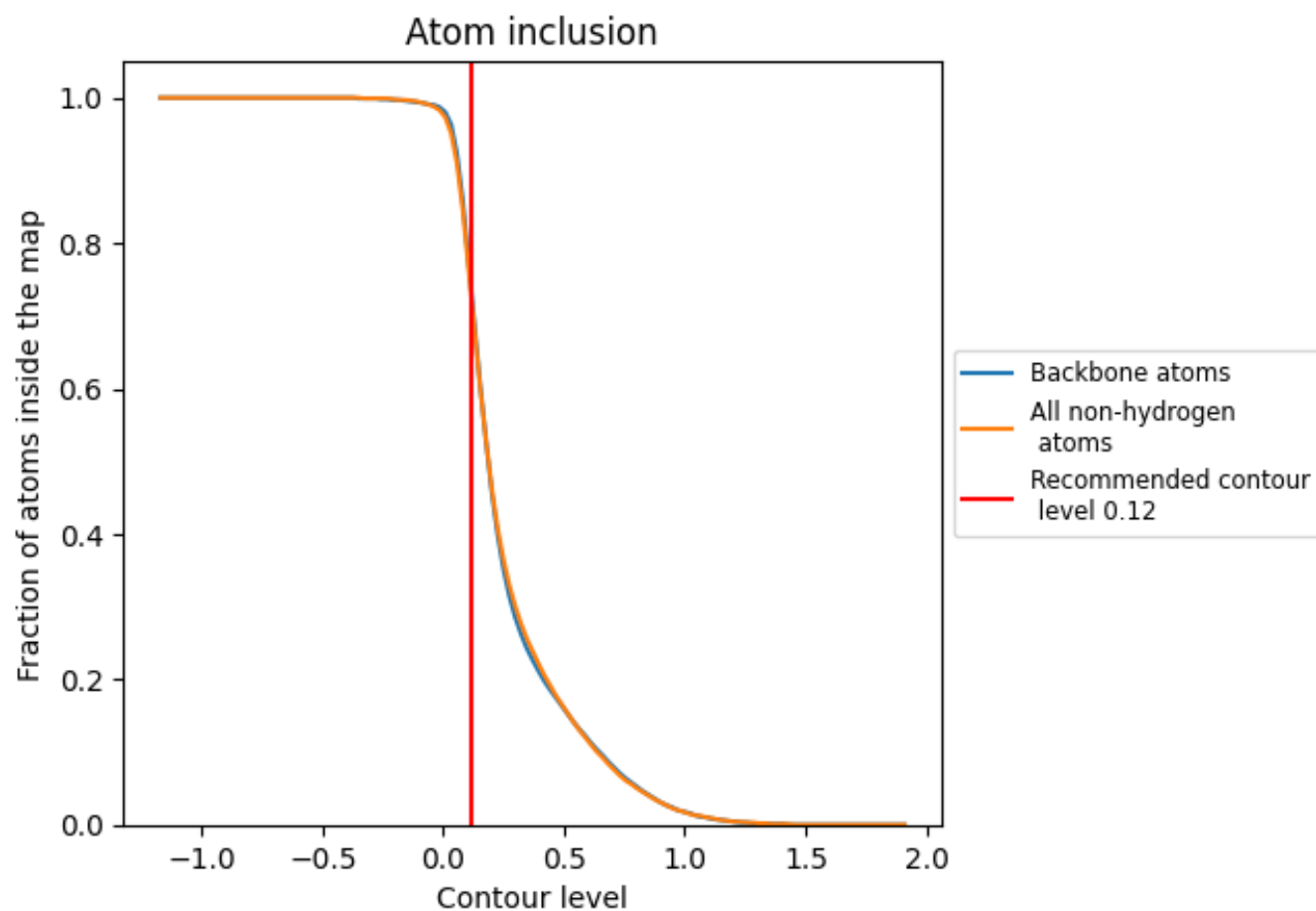
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.12).

9.4 Atom inclusion ⓘ



At the recommended contour level, 72% of all backbone atoms, 72% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7150	<div></div> 0.2550
A	<div></div> 0.8740	<div></div> 0.3140
B	<div></div> 0.8740	<div></div> 0.2900
C	<div></div> 0.4710	<div></div> 0.1810
D	<div></div> 0.6170	<div></div> 0.2230

