



## wwPDB EM Validation Summary Report ⓘ

Sep 28, 2024 – 09:57 AM EDT

PDB ID : 5U8S  
EMDB ID : EMD-8518  
Title : Structure of eukaryotic CMG helicase at a replication fork  
Authors : Li, H.; Li, B.; Georgescu, R.; Yuan, Z.; Santos, R.; Sun, J.; Zhang, D.; Yurieva, O.; O'Donnell, M.E.  
Deposited on : 2016-12-14  
Resolution : 6.10 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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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

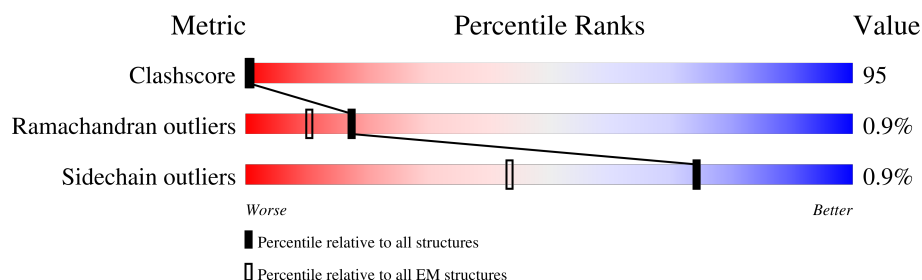
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 6.10 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.






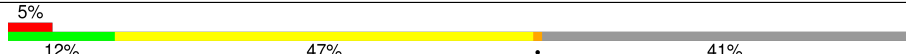
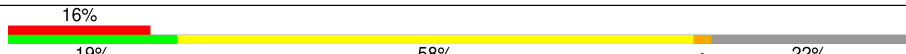
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 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	208	
2	B	213	
3	C	194	
4	D	294	
5	E	650	
6	F	26	
7	G	14	
8	2	868	

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Mol	Chain	Length	Quality of chain
9	3	971	
10	4	933	
11	5	775	
12	6	1017	
13	7	845	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	ATP	2	901	-	-	X	-
14	ATP	5	801	-	-	X	-

## 2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 41018 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA replication complex GINS protein PSF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	208	Total	C	N	O	S	0	0
			1696	1065	290	331	10		

- Molecule 2 is a protein called DNA replication complex GINS protein PSF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	181	Total	C	N	O	S	0	0
			1513	978	261	270	4		

- Molecule 3 is a protein called DNA replication complex GINS protein PSF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	159	Total	C	N	O	S	0	0
			1288	843	207	232	6		

- Molecule 4 is a protein called DNA replication complex GINS protein SLD5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	221	Total	C	N	O	S	0	0
			1820	1159	300	348	13		

- Molecule 5 is a protein called Cell division control protein 45.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	553	Total	C	N	O	S	0	0
			4482	2862	763	844	13		

- Molecule 6 is a DNA chain called DNA (26-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	26	Total	C	N	O	P	0	0
			527	257	76	168	26		

- Molecule 7 is a DNA chain called DNA (5'-D(P\*AP\*TP\*CP\*GP\*AP\*TP\*CP\*GP\*AP\*TP\*CP\*GP\*AP\*T)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	14	Total	C	N	O	P	0	0
			287	137	52	84	14		

- Molecule 8 is a protein called DNA replication licensing factor MCM2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	2	602	Total	C	N	O	S	0	0
			4707	2969	841	880	17		

- Molecule 9 is a protein called DNA replication licensing factor MCM3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	3	591	Total	C	N	O	S	0	0
			4638	2925	828	872	13		

- Molecule 10 is a protein called DNA replication licensing factor MCM4.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	4	682	Total	C	N	O	S	0	0
			5410	3397	946	1039	28		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	469	VAL	LYS	conflict	UNP P30665
4	470	SER	VAL	conflict	UNP P30665

- Molecule 11 is a protein called Minichromosome maintenance protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	5	597	Total	C	N	O	S	0	0
			4688	2946	808	910	24		

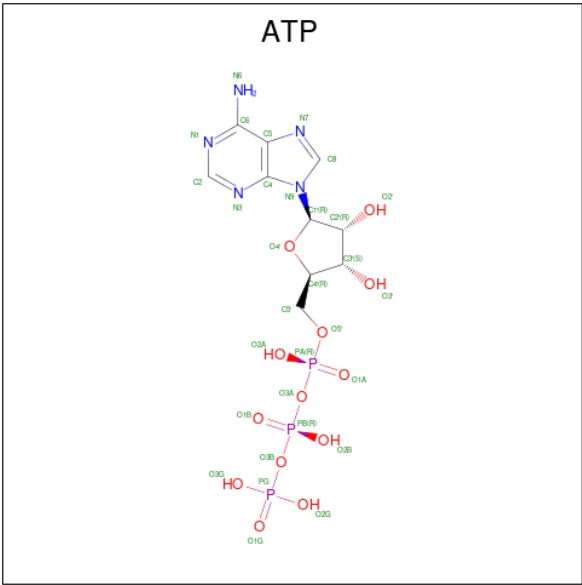
- Molecule 12 is a protein called DNA replication licensing factor MCM6.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	6	604	Total	C	N	O	S	0	0
			4649	2929	822	878	20		

- Molecule 13 is a protein called DNA replication licensing factor MCM7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	7	663	5220	3290	904	996	30	0	0

- Molecule 14 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).

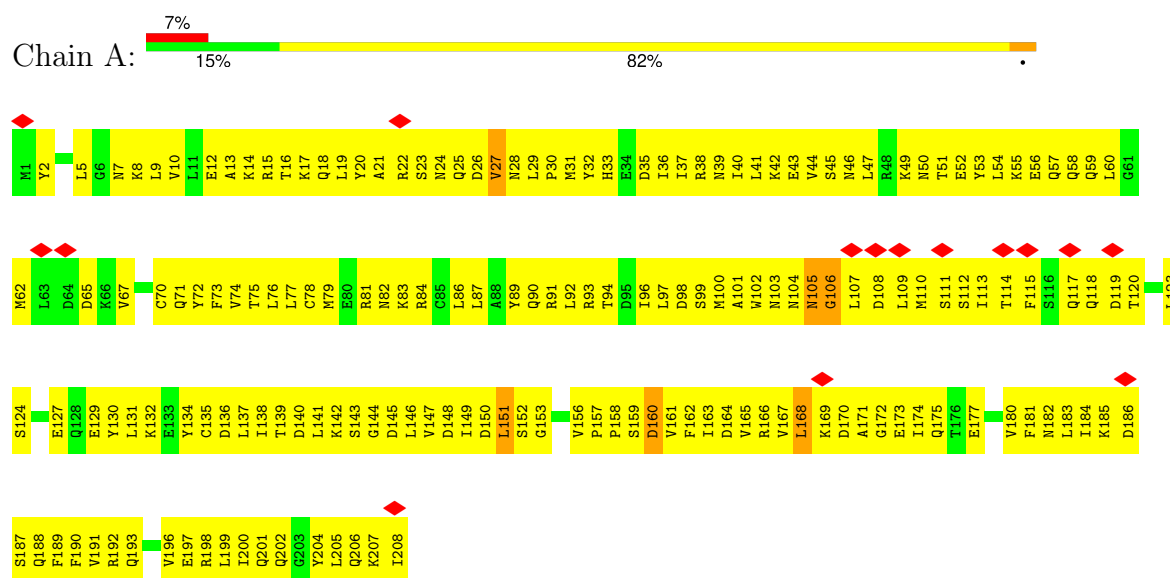


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
14	2	1	31	10	5	13	3	0
14	3	1	31	10	5	13	3	0
14	5	1	31	10	5	13	3	0

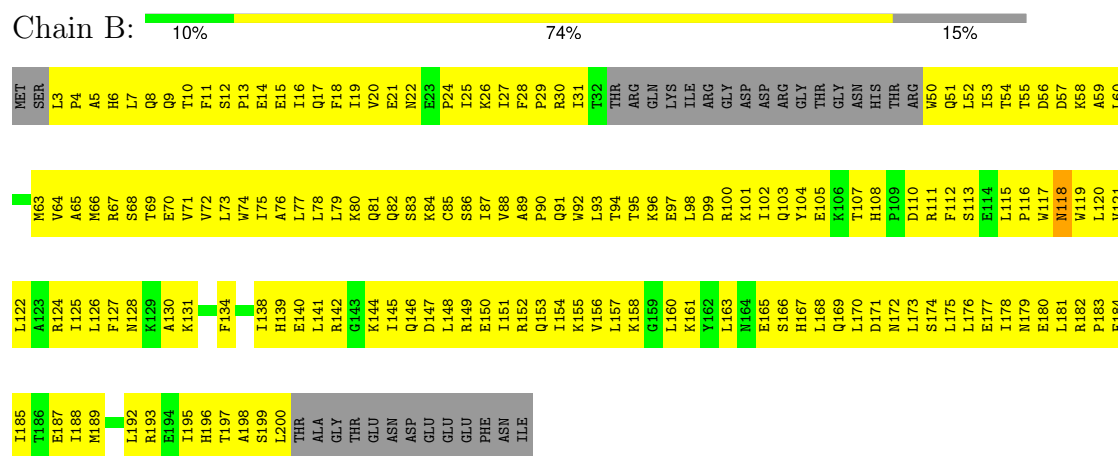
### 3 Residue-property plots

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: DNA replication complex GINS protein PSF1



#### • Molecule 2: DNA replication complex GINS protein PSF2

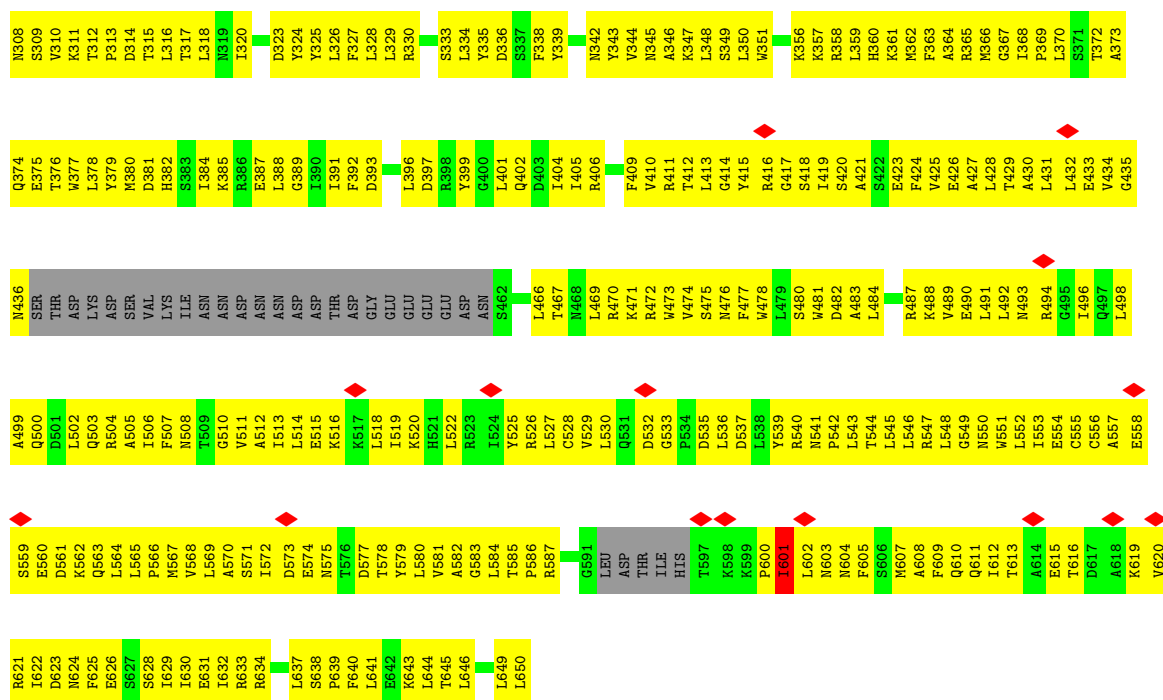


#### • Molecule 3: DNA replication complex GINS protein PSF3

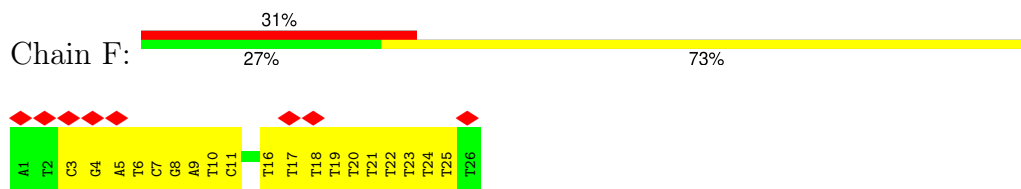


MET	GLY	Y3	Y4	Y5	Y6	Y7	Y8	Y9	Y10	Y11	Y12	Y13	Y14	Y15	Y16	Y17	Y18	Y19	Y20	Y21	Y22	Y23	Y24	Y25	Y26	Y27	Y28	Y29	Y30	Y31	Y32	Y33	Y34	Y35	Y36	Y37	Y38	Y39	Y40	Y41	Y42	Y43	Y44	Y45	Y46	Y47	Y48	Y49	Y50	Y51	Y52	Y53	Y54	Y55	Y56	Y57	Y58	Y59	Y60	Y61	Y62	Y63	Y64	Y65	Y66	Y67	Y68	Y69	Y70	Y71	Y72	Y73	Y74	Y75	Y76	Y77	Y78	Y79	Y80	Y81	Y82	Y83	Y84	Y85	Y86	Y87	Y88	Y89	Y90	Y91	Y92	Y93	Y94	Y95	Y96	Y97	Y98	Y99	Y100	Y101	Y102	Y103	Y104	Y105	Y106	Y107	Y108	Y109	Y110	Y111	Y112	Y113	Y114	Y115	Y116	Y117	Y118	Y119	Y120	Y121	Y122	Y123	Y124	Y125	Y126	Y127	Y128	Y129	Y130	Y131	Y132	Y133	Y134	Y135	Y136	Y137	Y138	Y139	Y140	Y141	Y142	Y143	Y144	Y145	Y146	Y147	Y148	Y149	Y150	Y151	Y152	Y153	Y154	Y155	Y156	Y157	Y158	Y159	Y160	Y161	Y162	Y163	Y164	Y165	Y166	Y167	Y168	Y169	Y170	Y171	Y172	Y173	Y174	Y175	Y176	Y177	Y178	Y179	Y180	Y181	Y182	Y183	Y184	Y185	Y186	Y187	Y188	Y189	Y190	Y191	Y192	Y193	Y194	Y195	Y196	Y197	Y198	Y199	Y200	Y201	Y202	Y203	Y204	Y205	Y206	Y207	Y208	Y209	Y210	Y211	Y212	Y213	Y214	Y215	Y216	Y217	Y218	Y219	Y220	Y221	Y222	Y223	Y224	Y225	Y226	Y227	Y228	Y229	Y230	Y231	Y232	Y233	Y234	Y235	Y236	Y237	Y238	Y239	Y240	Y241	Y242	Y243	Y244	Y245	Y246	Y247	Y248	Y249	Y250	Y251	Y252	Y253	Y254	Y255	Y256	Y257	Y258	Y259	Y260	Y261	Y262	Y263	Y264	Y265	Y266	Y267	Y268	Y269	Y270	Y271	Y272	Y273	Y274	Y275	Y276	Y277	Y278	Y279	Y280	Y281	Y282	Y283	Y284	Y285	Y286	Y287	Y288	Y289	Y290	Y291	Y292	Y293	Y294	Y295	Y296	Y297	Y298	Y299	Y300	Y301	Y302	Y303	Y304	Y305	Y306	Y307	Y308	Y309	Y310	Y311	Y312	Y313	Y314	Y315	Y316	Y317	Y318	Y319	Y320	Y321	Y322	Y323	Y324	Y325	Y326	Y327	Y328	Y329	Y330	Y331	Y332	Y333	Y334	Y335	Y336	Y337	Y338	Y339	Y340	Y341	Y342	Y343	Y344	Y345	Y346	Y347	Y348	Y349	Y350	Y351	Y352	Y353	Y354	Y355	Y356	Y357	Y358	Y359	Y360	Y361	Y362	Y363	Y364	Y365	Y366	Y367	Y368	Y369	Y370	Y371	Y372	Y373	Y374	Y375	Y376	Y377	Y378	Y379	Y380	Y381	Y382	Y383	Y384	Y385	Y386	Y387	Y388	Y389	Y390	Y391	Y392	Y393	Y394	Y395	Y396	Y397	Y398	Y399	Y400	Y401	Y402	Y403	Y404	Y405	Y406	Y407	Y408	Y409	Y410	Y411	Y412	Y413	Y414	Y415	Y416	Y417	Y418	Y419	Y420	Y421	Y422	Y423	Y424	Y425	Y426	Y427	Y428	Y429	Y430	Y431	Y432	Y433	Y434	Y435	Y436	Y437	Y438	Y439	Y440	Y441	Y442	Y443	Y444	Y445	Y446	Y447	Y448	Y449	Y450	Y451	Y452	Y453	Y454	Y455	Y456	Y457	Y458	Y459	Y460	Y461	Y462	Y463	Y464	Y465	Y466	Y467	Y468	Y469	Y470	Y471	Y472	Y473	Y474	Y475	Y476	Y477	Y478	Y479	Y480	Y481	Y482	Y483	Y484	Y485	Y486	Y487	Y488	Y489	Y490	Y491	Y492	Y493	Y494	Y495	Y496	Y497	Y498	Y499	Y500	Y501	Y502	Y503	Y504	Y505	Y506	Y507	Y508	Y509	Y510	Y511	Y512	Y513	Y514	Y515	Y516	Y517	Y518	Y519	Y520	Y521	Y522	Y523	Y524	Y525	Y526	Y527	Y528	Y529	Y530	Y531	Y532	Y533	Y534	Y535	Y536	Y537	Y538	Y539	Y540	Y541	Y542	Y543	Y544	Y545	Y546	Y547	Y548	Y549	Y550	Y551	Y552	Y553	Y554	Y555	Y556	Y557	Y558	Y559	Y560	Y561	Y562	Y563	Y564	Y565	Y566	Y567	Y568	Y569	Y570	Y571	Y572	Y573	Y574	Y575	Y576	Y577	Y578	Y579	Y580	Y581	Y582	Y583	Y584	Y585	Y586	Y587	Y588	Y589	Y590	Y591	Y592	Y593	Y594	Y595	Y596	Y597	Y598	Y599	Y600	Y601	Y602	Y603	Y604	Y605	Y606	Y607	Y608	Y609	Y610	Y611	Y612	Y613	Y614	Y615	Y616	Y617	Y618	Y619	Y620	Y621	Y622	Y623	Y624	Y625	Y626	Y627	Y628	Y629	Y630	Y631	Y632	Y633	Y634	Y635	Y636	Y637	Y638	Y639	Y640	Y641	Y642	Y643	Y644	Y645	Y646	Y647	Y648	Y649	Y650	Y651	Y652	Y653	Y654	Y655	Y656	Y657	Y658	Y659	Y660	Y661	Y662	Y663	Y664	Y665	Y666	Y667	Y668	Y669	Y670	Y671	Y672	Y673	Y674	Y675	Y676	Y677	Y678	Y679	Y680	Y681	Y682	Y683	Y684	Y685	Y686	Y687	Y688	Y689	Y690	Y691	Y692	Y693	Y694	Y695	Y696	Y697	Y698	Y699	Y700	Y701	Y702	Y703	Y704	Y705	Y706	Y707	Y708	Y709	Y710	Y711	Y712	Y713	Y714	Y715	Y716	Y717	Y718	Y719	Y720	Y721	Y722	Y723	Y724	Y725	Y726	Y727	Y728	Y729	Y730	Y731	Y732	Y733	Y734	Y735	Y736	Y737	Y738	Y739	Y740	Y741	Y742	Y743	Y744	Y745	Y746	Y747	Y748	Y749	Y750	Y751	Y752	Y753	Y754	Y755	Y756	Y757	Y758	Y759	Y760	Y761	Y762	Y763	Y764	Y765	Y766	Y767	Y768	Y769	Y770	Y771	Y772	Y773	Y774	Y775	Y776	Y777	Y778	Y779	Y780	Y781	Y782	Y783	Y784	Y785	Y786	Y787	Y788	Y789	Y790	Y791	Y792	Y793	Y794	Y795	Y796	Y797	Y798	Y799	Y800	Y801	Y802	Y803	Y804	Y805	Y806	Y807	Y808	Y809	Y810	Y811	Y812	Y813	Y814	Y815	Y816	Y817	Y818	Y819	Y820	Y821	Y822	Y823	Y824	Y825	Y826	Y827	Y828	Y829	Y830	Y831	Y832	Y833	Y834	Y835	Y836	Y837	Y838	Y839	Y840	Y841	Y842	Y843	Y844	Y845	Y846	Y847	Y848	Y849	Y850	Y851	Y852	Y853	Y854	Y855	Y856	Y857	Y858	Y859	Y860	Y861	Y862	Y863	Y864	Y865	Y866	Y867	Y868	Y869	Y870	Y871	Y872	Y873	Y874	Y875	Y876	Y877	Y878	Y879	Y880	Y881	Y882	Y883	Y884	Y885	Y886	Y887	Y888	Y889	Y890	Y891	Y892	Y893	Y894	Y895	Y896	Y897	Y898	Y899	Y900	Y901	Y902	Y903	Y904	Y905	Y906	Y907	Y908	Y909	Y910	Y911	Y912	Y913	Y914	Y915	Y916	Y917	Y918	Y919	Y920	Y921	Y922	Y923	Y924	Y925	Y926	Y927	Y928	Y929	Y930	Y931	Y932	Y933	Y934	Y935	Y936	Y937	Y938	Y939	Y940	Y941	Y942	Y943	Y944	Y945	Y946	Y947	Y948	Y949	Y950	Y951	Y952	Y953	Y954	Y955	Y956	Y957	Y958	Y959	Y960	Y961	Y962	Y963	Y964	Y965	Y966	Y967	Y968	Y969	Y970	Y971	Y972	Y973	Y974	Y975	Y976	Y977	Y978	Y979	Y980	Y981	Y982	Y983	Y984	Y985	Y986	Y987	Y988	Y989	Y990	Y991	Y992	Y993	Y994	Y995	Y996	Y997	Y998	Y999	Y1000	Y1001	Y1002	Y1003	Y1004	Y1005	Y1006	Y1007	Y1008	Y1009	Y1010	Y1011	Y1012	Y1013	Y1014	Y1015	Y1016	Y1017	Y10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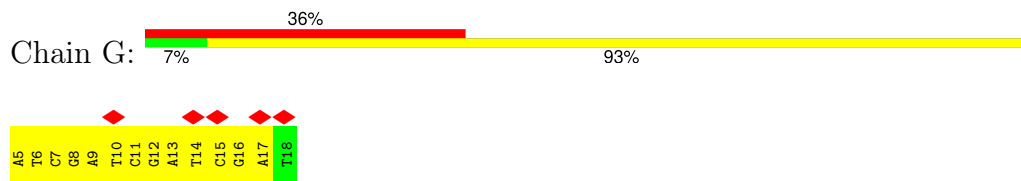




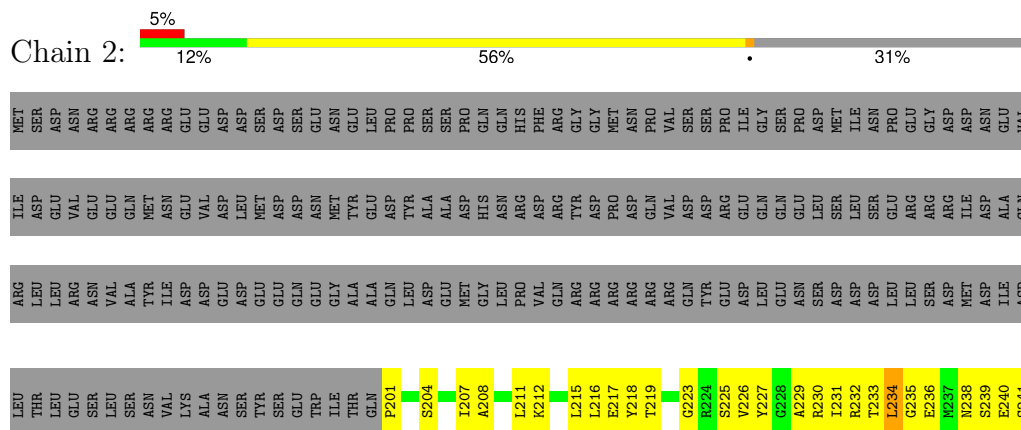
• Molecule 6: DNA (26-MER)

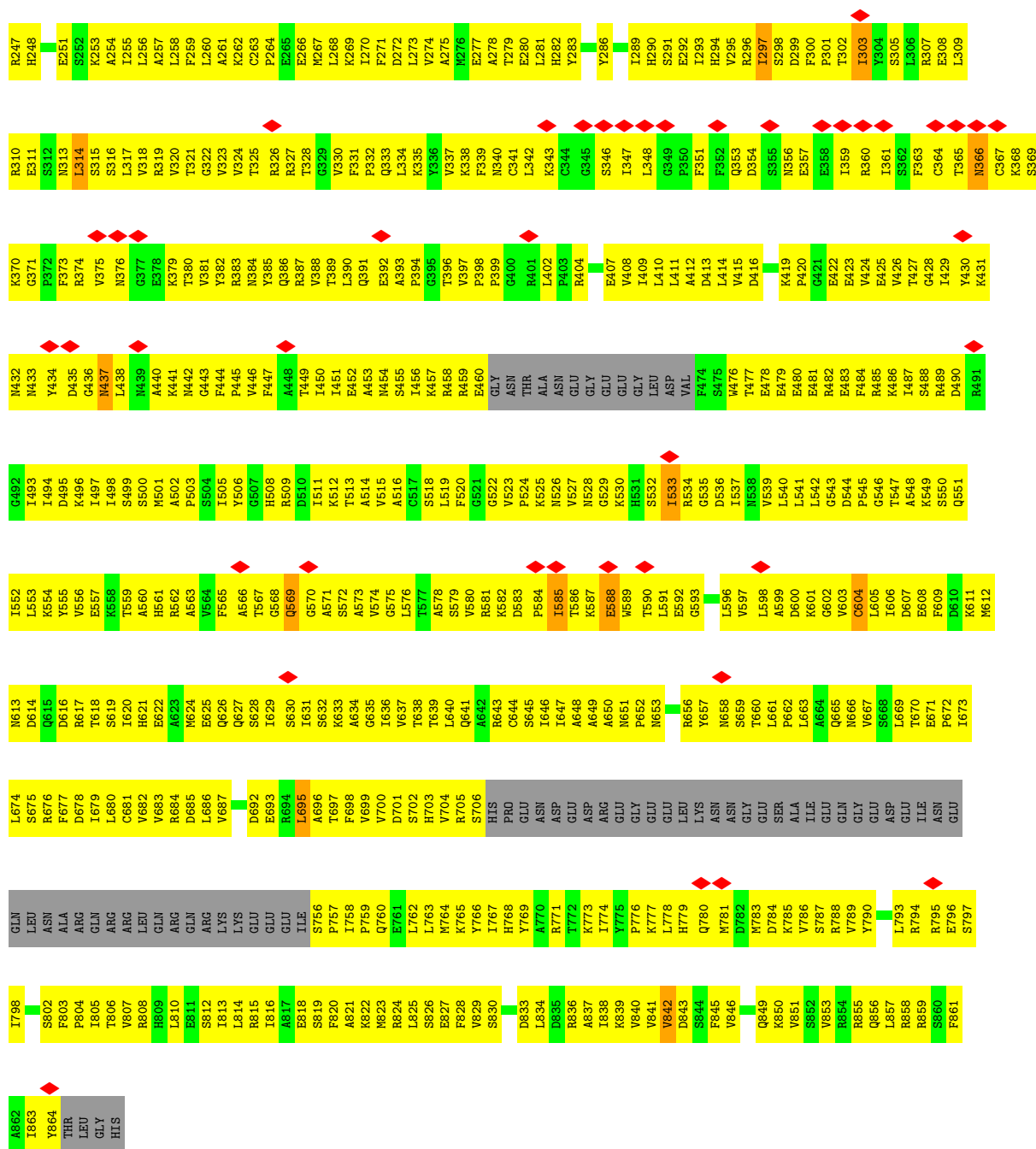


• Molecule 7: DNA (5'-D(P\*AP\*TP\*CP\*GP\*AP\*TP\*CP\*GP\*AP\*TP\*CP\*GP\*AP\*T)-3')



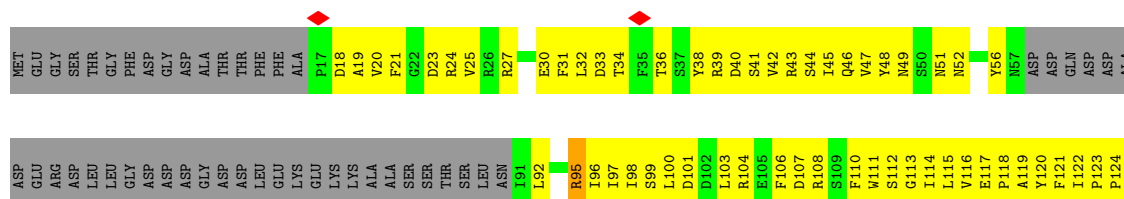
• Molecule 8: DNA replication licensing factor MCM2





● Molecule 9: DNA replication licensing factor MCM3

Chain 3: 13% 47% 39%







Chain 5: 







																																MET																																
P686	R687	T688	L689	L690	G691	L692	L693	R694	L695	S696	Q697	A698	L699	A700	K701	L702	R703	L704	A705	D706	M707	V708	D709	I710	D711	D712	V713	E714	E715	A716	L717	R718	L719	V720	R721	V722	S726	Q729	GLU	THR	ASN	LYS	SER	LYS	GLU	ASP	SER	PRO	THR	LYS	ILE	PHE	THR	ILE										
LYS	LYS	MET	GLN	GLU	THR	GLY	LYS	ASN	THR	LEU	SER	TYR	GLU	ASN	ILE	VAL	LYS	THR	VAL	ARG	LEU	ARG	GLY	PHE	THR	MET	LEU	GLN	LEU	SER	ASN	CYS	ILE	GLN	GLU	TYR	SER	TYR	LEU	ASN	VAL	TRP	HIS	LEU	ILE	ASN	GLY	ASN	THR	LEU	LYS	PHE	VAL	ASP	ASP	GLY	THR							
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																																ASP																																
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																																LEU																																
																																GLN																																
																																ASP																																
																																ALA																																



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	243796	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 ( $e^-/\text{\AA}^2$ )	10	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.079	Depositor
Minimum map value	-0.033	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	332.8, 332.8, 332.8	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3, 1.3, 1.3	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

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	0/1718	0.51	1/2314 (0.0%)
2	B	0.23	0/1545	0.47	0/2092
3	C	0.23	0/1320	0.41	0/1784
4	D	0.24	0/1853	0.48	0/2500
5	E	0.23	0/4563	0.45	0/6173
6	F	0.48	0/585	0.99	0/901
7	G	0.51	0/321	0.90	0/493
8	2	0.24	0/4787	0.52	1/6469 (0.0%)
9	3	0.23	0/4717	0.49	0/6393
10	4	0.25	0/5480	0.52	0/7395
11	5	0.24	0/4750	0.48	0/6412
12	6	0.24	0/4719	0.51	1/6373 (0.0%)
13	7	0.24	0/5299	0.51	1/7160 (0.0%)
All	All	0.25	0/41657	0.51	4/56459 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
4	D	0	1
9	3	0	1
10	4	0	2
12	6	0	3
13	7	0	1
All	All	0	9

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	7	369	GLY	N-CA-C	7.97	133.04	113.10
1	A	106	GLY	N-CA-C	7.29	131.32	113.10
8	2	366	ASN	C-N-CA	6.50	137.94	121.70
12	6	628	LEU	CA-CB-CG	5.26	127.39	115.30

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	3	428	LEU	Peptide
10	4	373	ARG	Peptide
10	4	408	ASP	Peptide
1	A	160	ASP	Peptide
4	D	258	VAL	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1696	0	1698	437	0
2	B	1513	0	1558	354	0
3	C	1288	0	1298	283	0
4	D	1820	0	1824	452	0
5	E	4482	0	4499	910	0
6	F	527	0	303	50	0
7	G	287	0	159	16	0
8	2	4707	0	4721	1026	0
9	3	4638	0	4701	925	0
10	4	5410	0	5491	980	0
11	5	4688	0	4748	992	0
12	6	4649	0	4589	1048	0
13	7	5220	0	5296	901	0
14	2	31	0	12	12	0
14	3	31	0	12	5	0
14	5	31	0	12	12	0
All	All	41018	0	40921	7794	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 95.

The worst 5 of 7794 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)
11:5:302:ASN:OD1	11:5:324:ARG:CZ	1.64	1.46
5:E:5:ILE:N	5:E:142:CYS:HG	1.30	1.26
13:7:94:LEU:HB2	13:7:95:GLN:HB2	1.21	1.19
13:7:680:SER:HB2	13:7:681:PHE:HA	1.22	1.19
11:5:303:SER:O	11:5:304:LYS:HG3	1.41	1.17

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	206/208 (99%)	182 (88%)	23 (11%)	1 (0%)	25	65
2	B	177/213 (83%)	160 (90%)	17 (10%)	0	100	100
3	C	151/194 (78%)	142 (94%)	9 (6%)	0	100	100
4	D	215/294 (73%)	193 (90%)	20 (9%)	2 (1%)	14	51
5	E	543/650 (84%)	490 (90%)	51 (9%)	2 (0%)	30	68
8	2	596/868 (69%)	535 (90%)	54 (9%)	7 (1%)	11	44
9	3	579/971 (60%)	528 (91%)	48 (8%)	3 (0%)	25	65
10	4	670/933 (72%)	594 (89%)	69 (10%)	7 (1%)	13	49
11	5	583/775 (75%)	549 (94%)	30 (5%)	4 (1%)	19	57
12	6	596/1017 (59%)	528 (89%)	58 (10%)	10 (2%)	7	36
13	7	653/845 (77%)	583 (89%)	60 (9%)	10 (2%)	8	40
All	All	4969/6968 (71%)	4484 (90%)	439 (9%)	46 (1%)	17	51

5 of 46 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	601	ILE
10	4	189	GLU
10	4	419	VAL
10	4	609	VAL
11	5	596	ILE

### 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	193/193 (100%)	190 (98%)	3 (2%)	58	73
2	B	171/198 (86%)	170 (99%)	1 (1%)	84	88
3	C	144/173 (83%)	144 (100%)	0	100	100
4	D	213/279 (76%)	211 (99%)	2 (1%)	75	83
5	E	499/586 (85%)	496 (99%)	3 (1%)	84	88
8	2	508/770 (66%)	502 (99%)	6 (1%)	67	79
9	3	512/835 (61%)	506 (99%)	6 (1%)	67	79
10	4	610/848 (72%)	606 (99%)	4 (1%)	81	87
11	5	534/688 (78%)	528 (99%)	6 (1%)	70	80
12	6	486/886 (55%)	482 (99%)	4 (1%)	79	85
13	7	585/753 (78%)	581 (99%)	4 (1%)	81	87
All	All	4455/6209 (72%)	4416 (99%)	39 (1%)	74	83

5 of 39 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	5	305	ASN
13	7	139	LEU
11	5	331	LEU
12	6	449	THR
13	7	396	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 50 such sidechains are listed below:

Mol	Chain	Res	Type
10	4	410	GLN
11	5	625	ASN
13	7	620	HIS
10	4	646	HIS
11	5	254	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](#)

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
14	ATP	5	801	-	28,33,33	1.02	2 (7%)	34,52,52	1.20	2 (5%)
14	ATP	2	901	-	28,33,33	1.01	2 (7%)	34,52,52	1.22	2 (5%)
14	ATP	3	1001	-	28,33,33	0.98	1 (3%)	34,52,52	1.19	2 (5%)

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
14	ATP	5	801	-	-	3/18/38/38	0/3/3/3
14	ATP	2	901	-	-	3/18/38/38	0/3/3/3
14	ATP	3	1001	-	-	2/18/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	2	901	ATP	PB-O3A	2.15	1.61	1.59
14	5	801	ATP	PB-O3A	2.15	1.61	1.59
14	5	801	ATP	PA-O3A	2.12	1.61	1.59
14	2	901	ATP	O4'-C1'	2.06	1.43	1.40
14	3	1001	ATP	PB-O3B	2.04	1.61	1.59

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	5	801	ATP	N3-C2-N1	-4.31	122.82	128.67
14	2	901	ATP	N3-C2-N1	-4.30	122.83	128.67
14	3	1001	ATP	N3-C2-N1	-4.16	123.02	128.67
14	5	801	ATP	C4-C5-N7	-2.63	106.55	109.34
14	3	1001	ATP	C4-C5-N7	-2.52	106.67	109.34

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

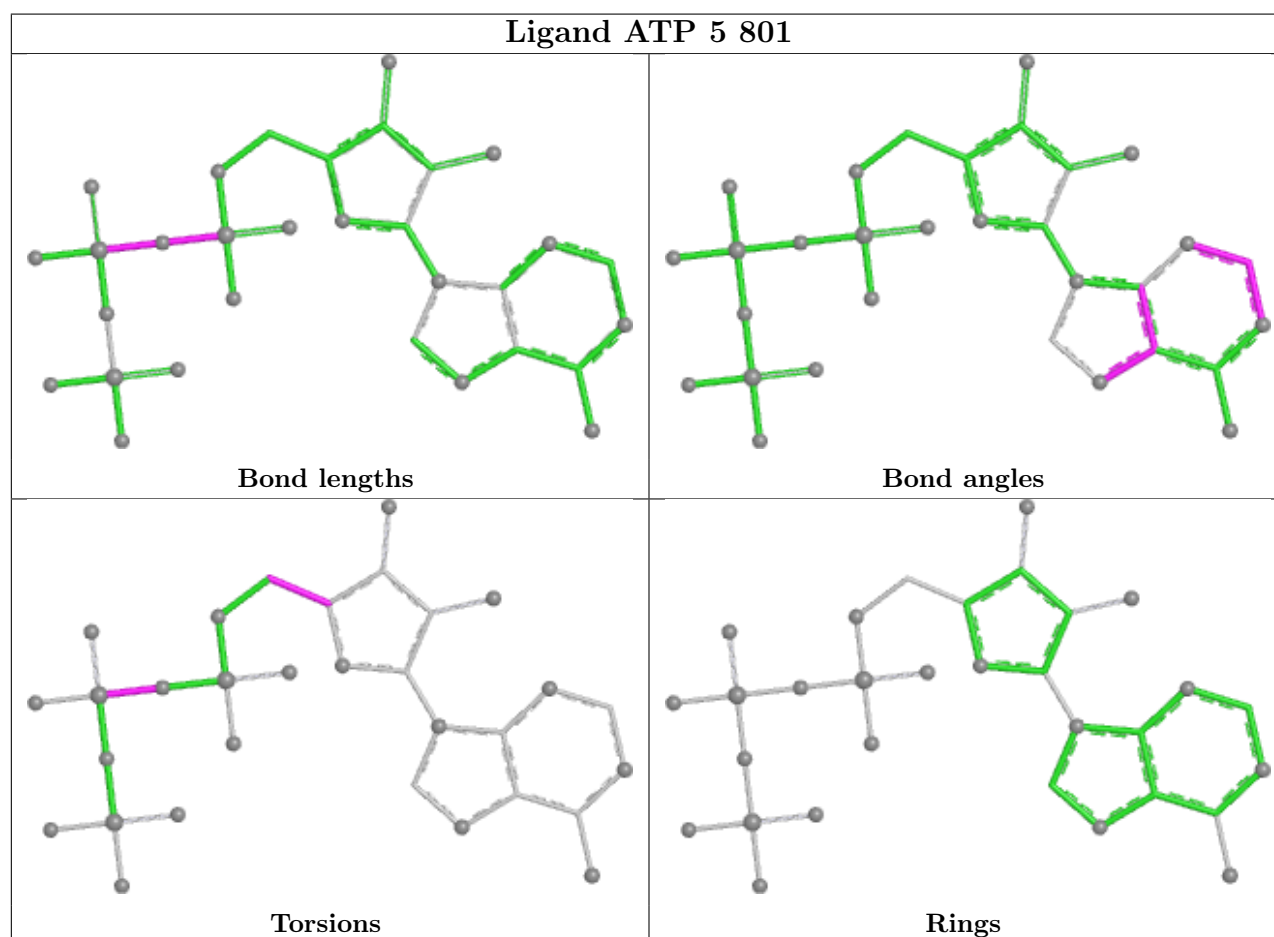
Mol	Chain	Res	Type	Atoms
14	2	901	ATP	C5'-O5'-PA-O1A
14	2	901	ATP	C5'-O5'-PA-O2A
14	2	901	ATP	C5'-O5'-PA-O3A
14	3	1001	ATP	PG-O3B-PB-O1B
14	5	801	ATP	PA-O3A-PB-O1B

There are no ring outliers.

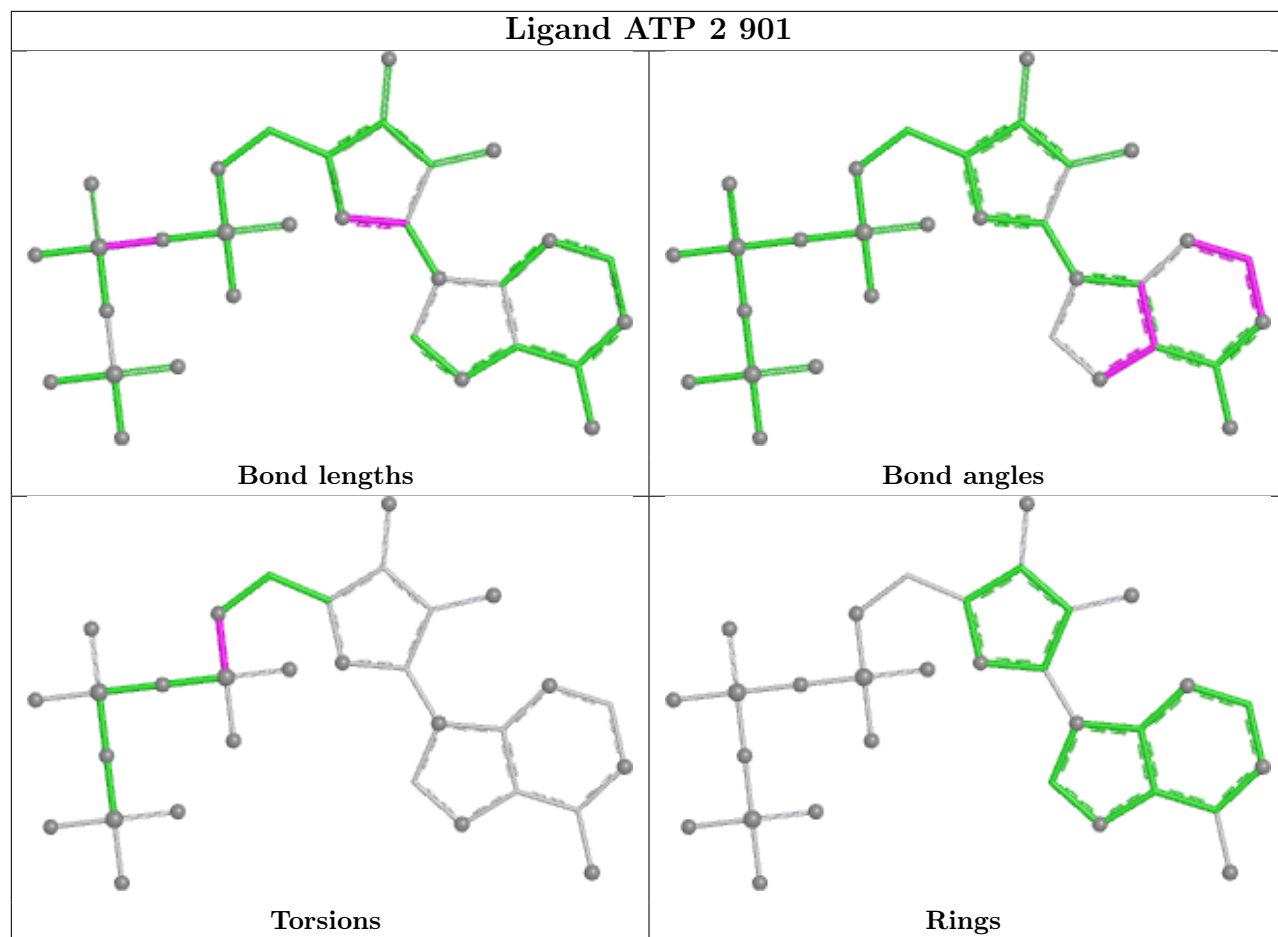
3 monomers are involved in 29 short contacts:

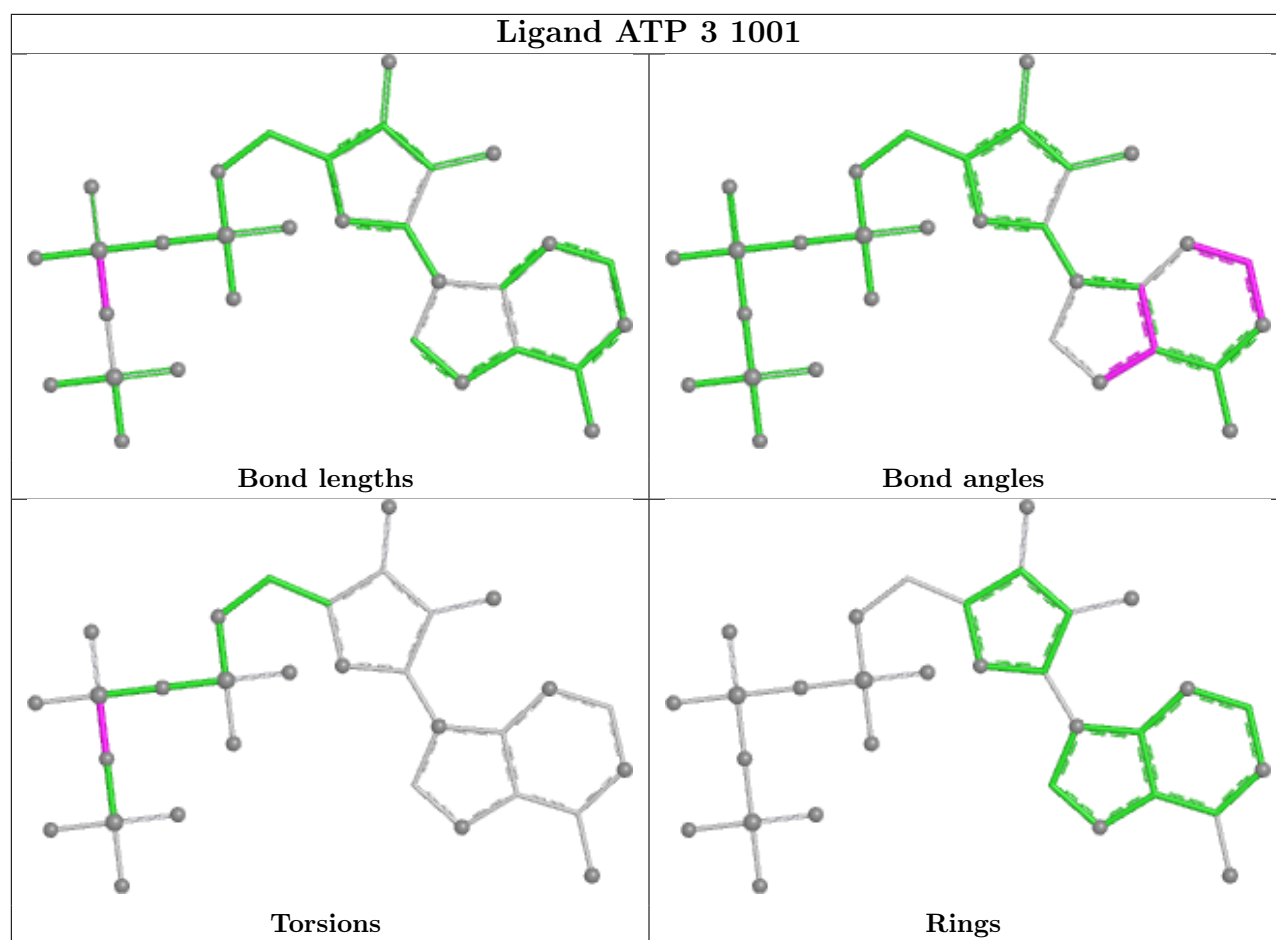
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	5	801	ATP	12	0
14	2	901	ATP	12	0
14	3	1001	ATP	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

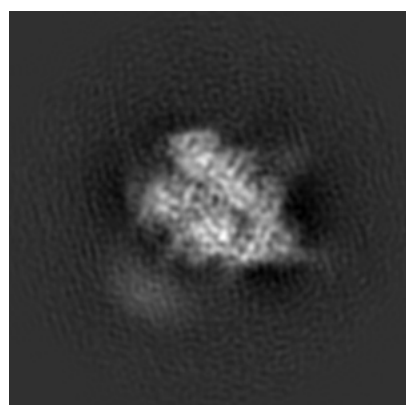
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8518. These allow visual inspection of the internal detail of the map and identification of artifacts.

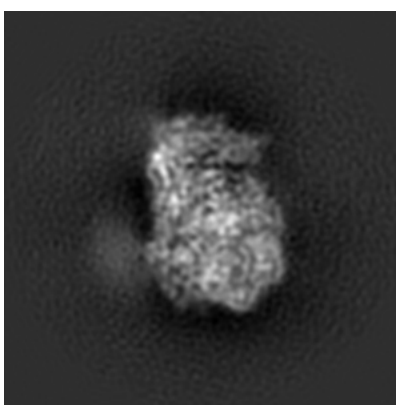
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

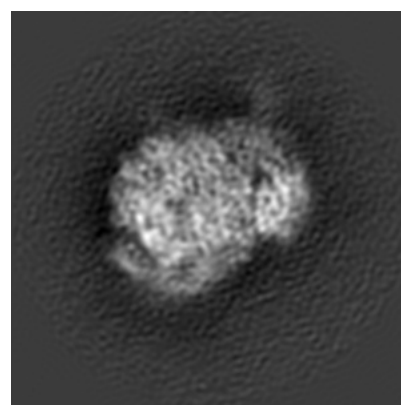
#### 6.1.1 Primary map



X



Y

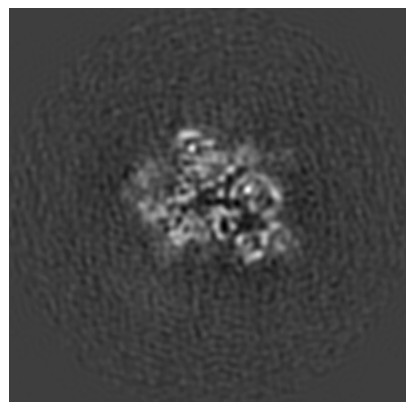


Z

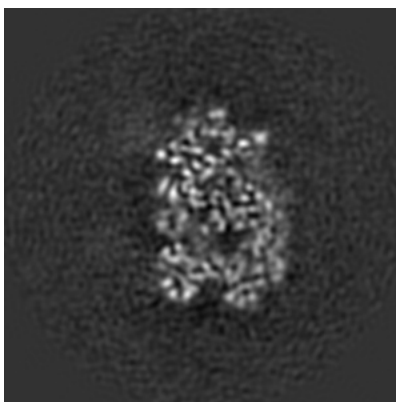
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

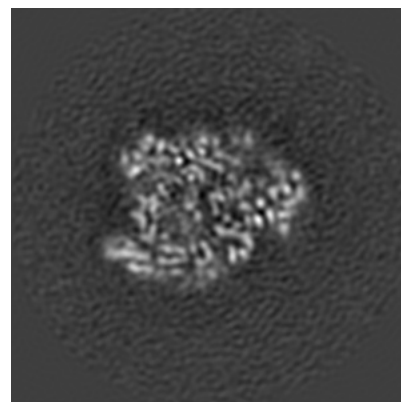
#### 6.2.1 Primary map



X Index: 128



Y Index: 128

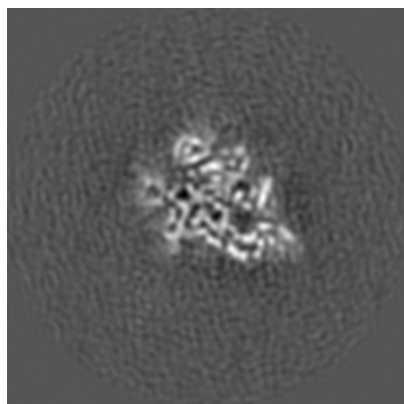


Z Index: 128

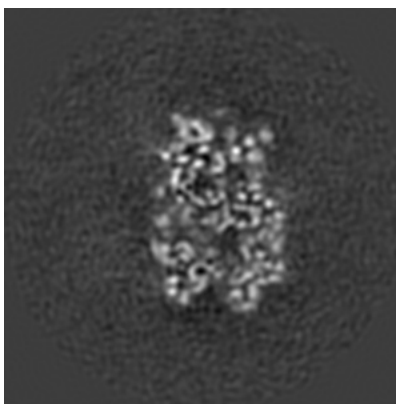
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

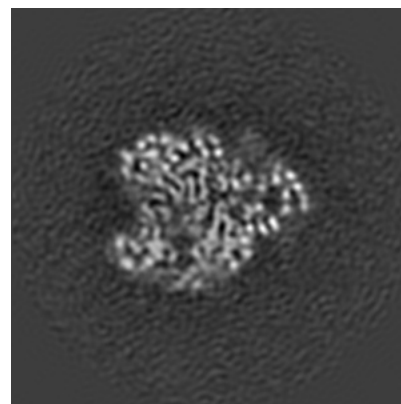
### 6.3.1 Primary map



X Index: 133



Y Index: 124

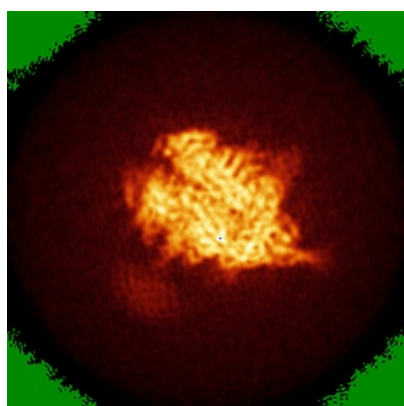


Z Index: 133

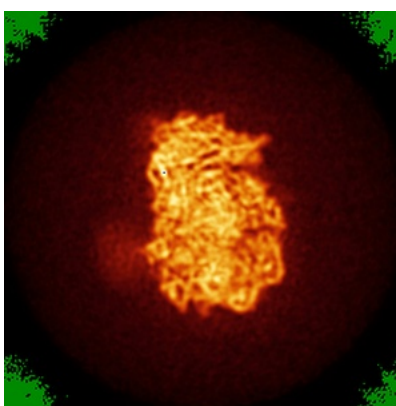
The images above show the largest variance slices of the map in three orthogonal directions.

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

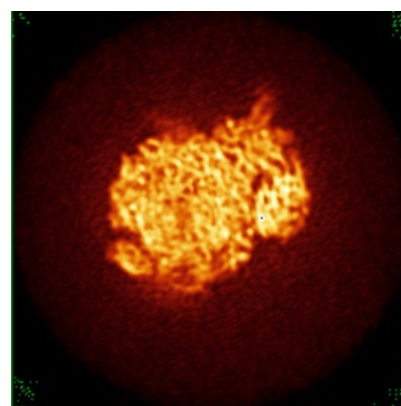
### 6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



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

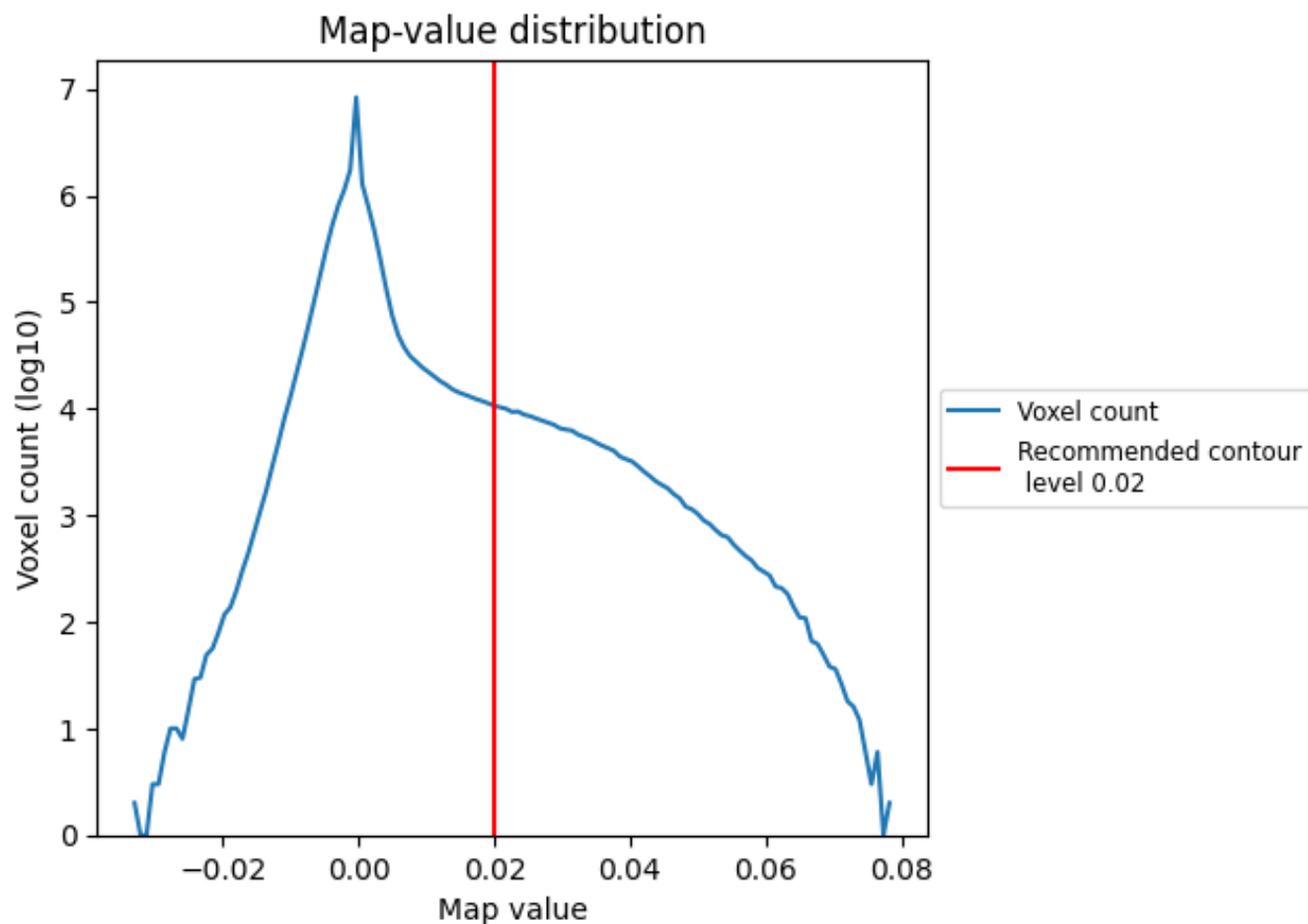
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

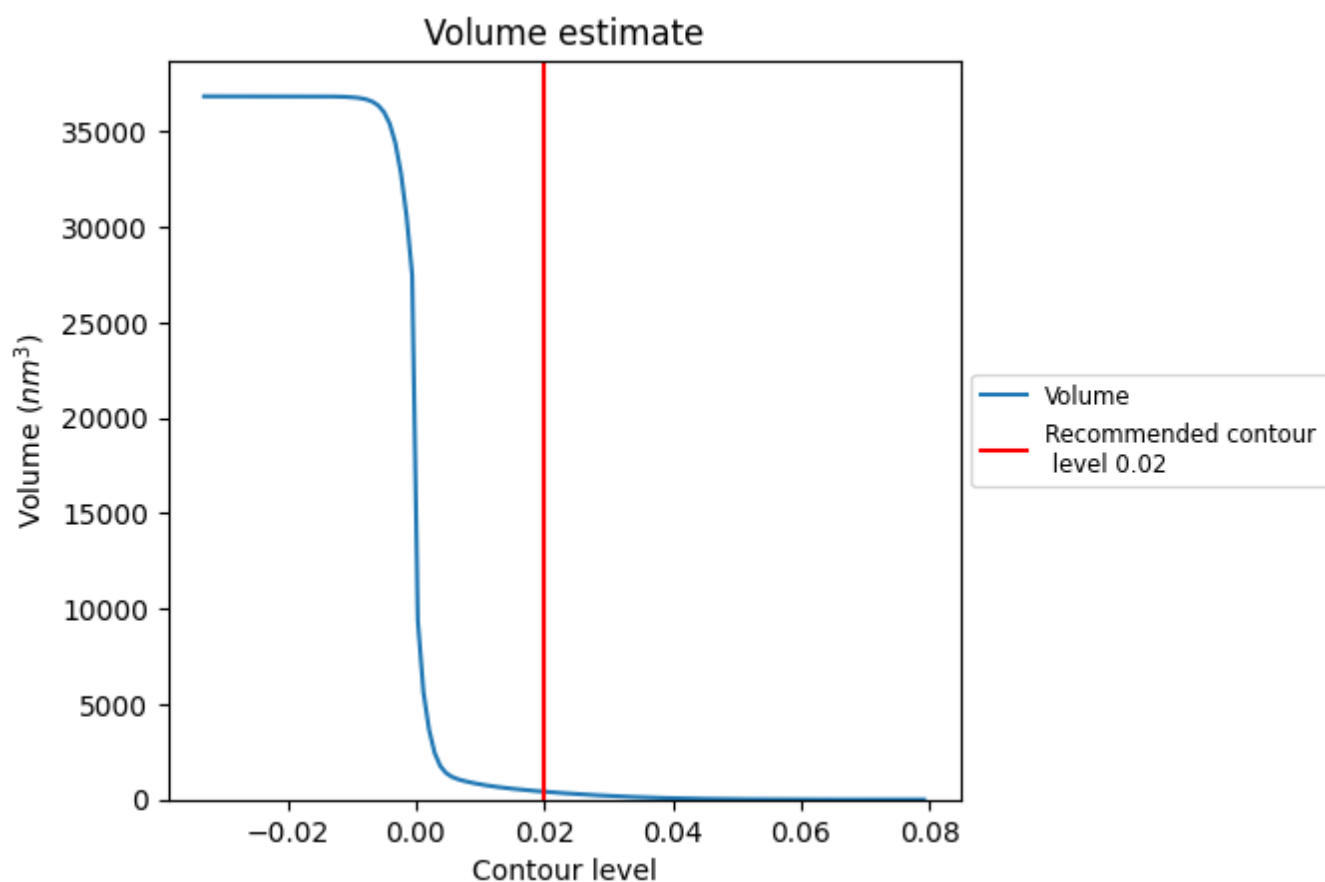
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

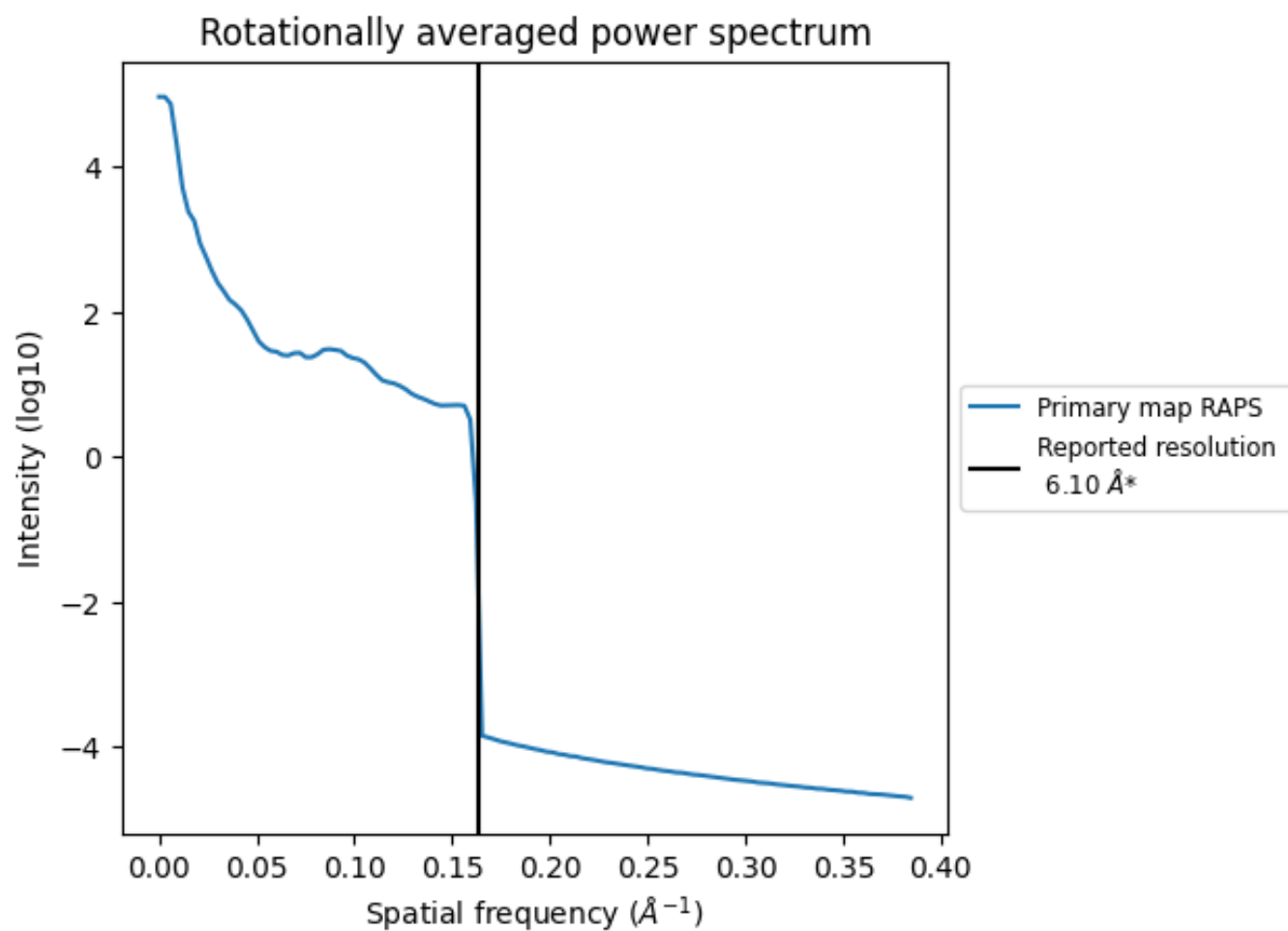
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 413  $\text{nm}^3$ ; this corresponds to an approximate mass of 373 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 0.164 Å<sup>-1</sup>



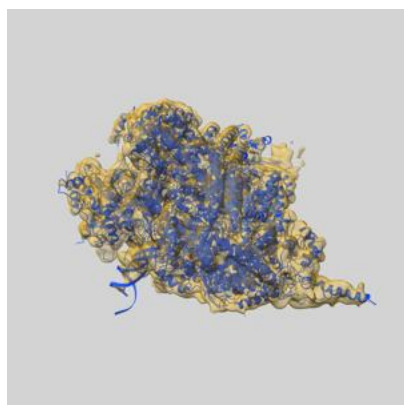
## 8 Fourier-Shell correlation

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

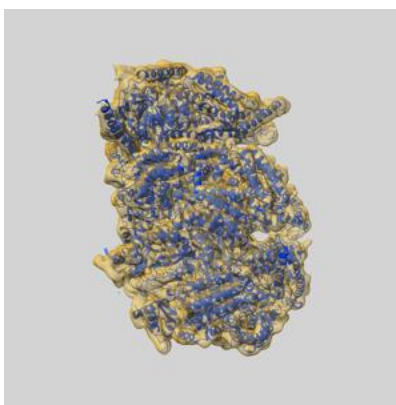
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8518 and PDB model 5U8S. Per-residue inclusion information can be found in section [3](#) on page [7](#).

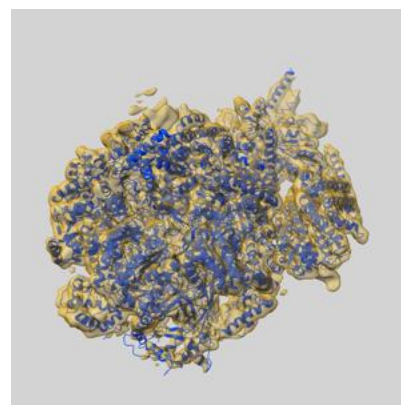
### 9.1 Map-model overlay [i](#)



X



Y



Z

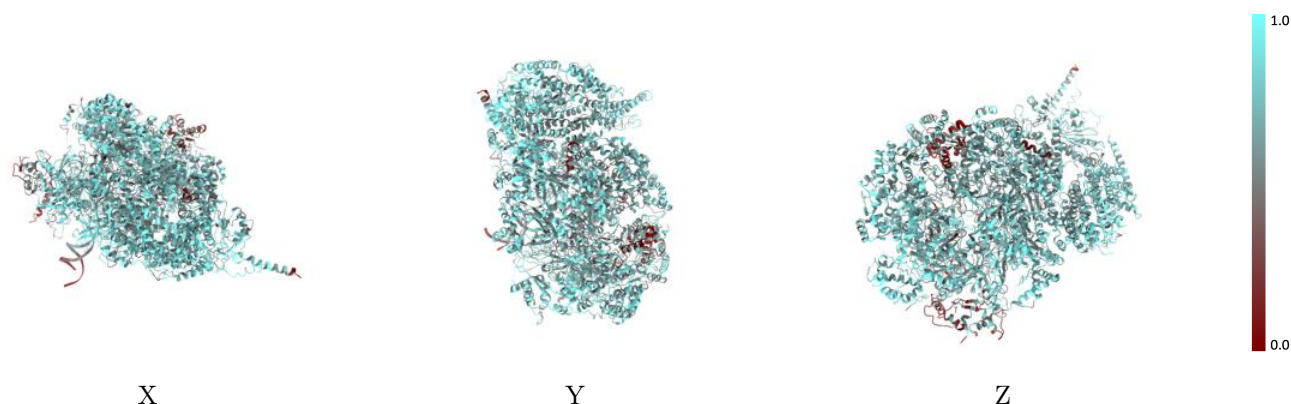
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



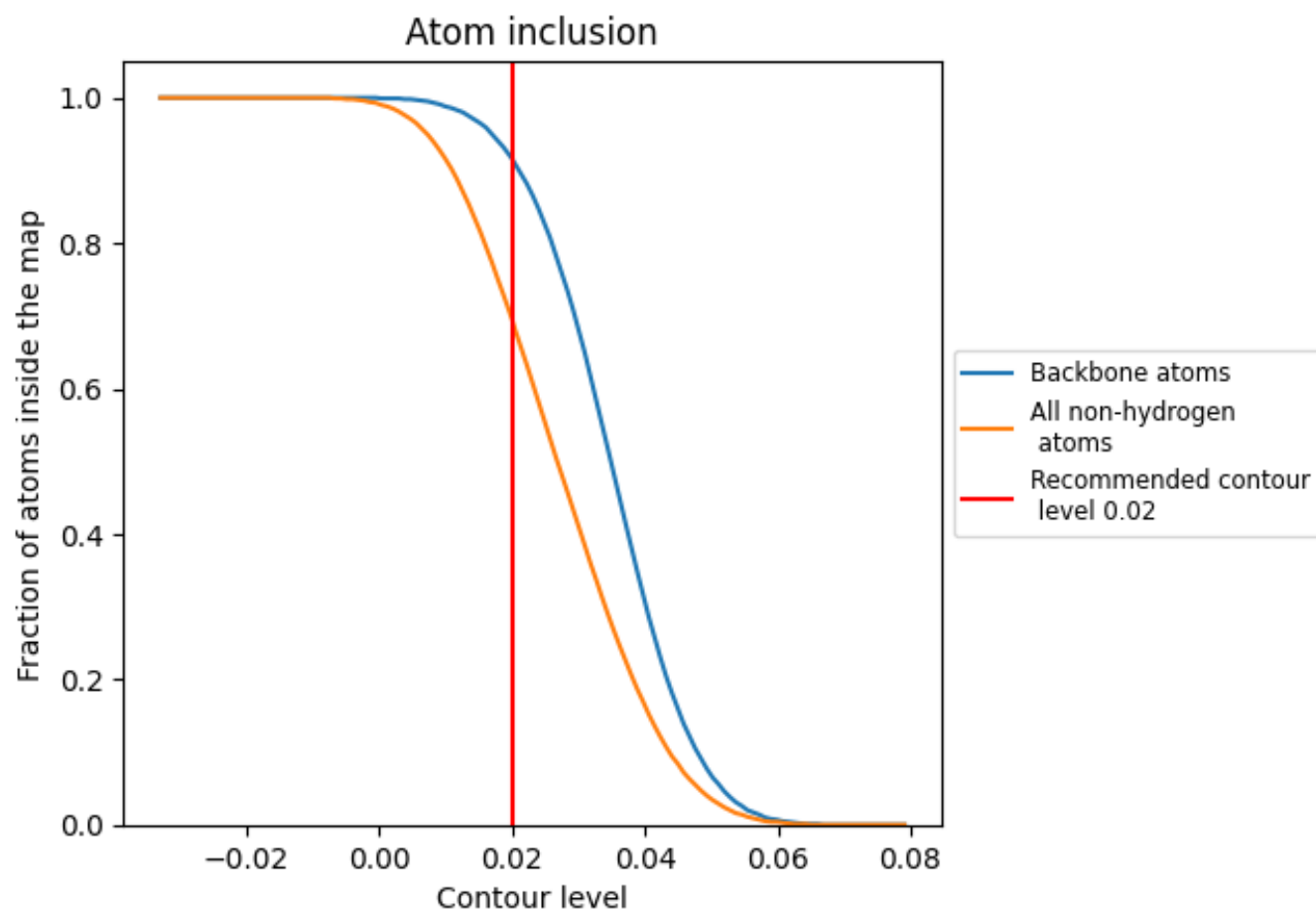
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).





























## 9.4 Atom inclusion ⓘ



At the recommended contour level, 92% of all backbone atoms, 70% 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	 0.6950	 0.1990
2	 0.7040	 0.1990
3	 0.7180	 0.2070
4	 0.6650	 0.1880
5	 0.6780	 0.2030
6	 0.7040	 0.2020
7	 0.6110	 0.1920
A	 0.6950	 0.1880
B	 0.7560	 0.2070
C	 0.7590	 0.2000
D	 0.7850	 0.1990
E	 0.7560	 0.2010
F	 0.5390	 0.2370
G	 0.4840	 0.2260

