



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:59 PM BST

PDB ID : 3JA8
EMDB ID: : EMD-6338
Title : Cryo-EM structure of the MCM2-7 double hexamer
Authors : Li, N.; Zhai, Y.; Zhang, Y.; Li, W.; Yang, M.; Lei, J.; Tye, B.K.; Gao, N.
Deposited on : 2015-05-09
Resolution : 3.80 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

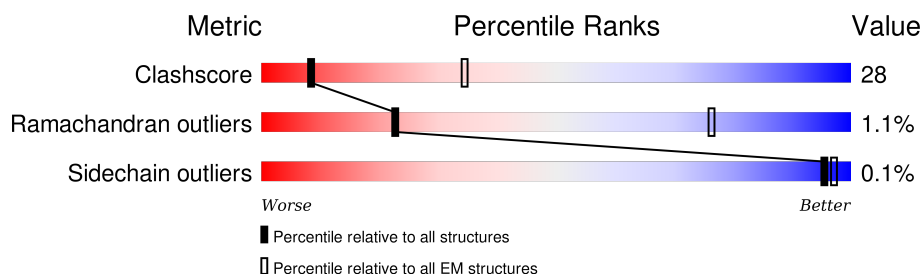
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	2	868	37% 32% • 31%
2	3	971	31% 30% • 38%
3	4	933	34% 34% • 31%
4	5	775	45% 36% 18%
5	6	1017	32% 28% • 39%
6	7	845	42% 38% • 18%

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
7	ADP	6	2001	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 29838 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 Minichromosome Maintenance 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	603	Total	C	N	O	S	0	0
			4714	2974	842	881	17		

- Molecule 2 is a protein called Minichromosome Maintenance 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	605	Total	C	N	O	S	0	0
			4745	2990	846	896	13		

- Molecule 3 is a protein called Minichromosome Maintenance 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	640	Total	C	N	O	S	0	0
			5081	3194	879	981	27		

- Molecule 4 is a protein called Minichromosome Maintenance 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	5	633	Total	C	N	O	S	0	0
			4962	3112	855	971	24		

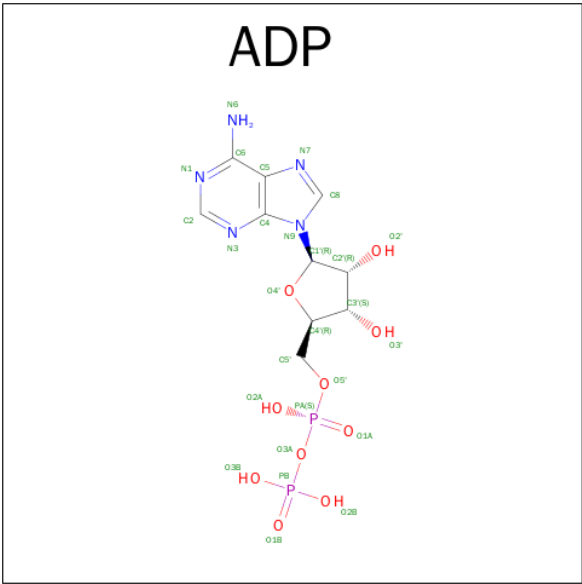
- Molecule 5 is a protein called Minichromosome Maintenance 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	6	616	Total	C	N	O	S	0	0
			4742	2985	841	896	20		

- Molecule 6 is a protein called Minichromosome Maintenance 7.

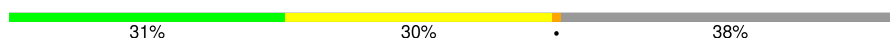
Mol	Chain	Residues	Atoms					AltConf	Trace
6	7	689	Total	C	N	O	S	0	0
			5432	3419	940	1042	31		

- Molecule 7 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					AltConf
7	2	1	Total	C	N	O	P	0
			27	10	5	10	2	
7	3	1	Total	C	N	O	P	0
			27	10	5	10	2	
7	4	1	Total	C	N	O	P	0
			27	10	5	10	2	
7	5	1	Total	C	N	O	P	0
			27	10	5	10	2	
7	6	1	Total	C	N	O	P	0
			27	10	5	10	2	
7	7	1	Total	C	N	O	P	0
			27	10	5	10	2	

Chain 3:



MET	GLU	GLY	SER	THR	GLY	PHE	ASP	GLY	ALA	THR	T13
LYS	GLU	LYS	LYS	ALA	SER	THR	SER	LEU	ASN	T191	T191
K154	K158	K159	S160	A163	H164	R169	T170	T171	T172	A173	T173
E237	Q238	R239	R240	L241	T242	T243	T244	T245	T246	T247	T248
R332	S333	V336	A337	L342	F345	D346	I347	R348	N349	I350	N351
L418	L419	R420	F421	V422	T425	A426	S427	A428	A429	L430	T433
H437	E438	F441	V442	T445	A446	S447	S448	S449	S450	S451	S452
V565	L566	H569	R570	T571	L572	L573	L574	L575	L576	L577	L578
ASN	PRO	LEU	GLN	ALA	GLY	PRO	LYS	LEU	GLY	GLY	GLY
K693	K694	S695	P696	T697	L698	L699	R700	T701	L702	L703	L704
L705	L706	L707	L708	L709	L710	L711	L712	L713	L714	L715	L716
L717	L718	L719	L720	L721	L722	L723	L724	L725	L726	L727	L728
L729	L730	L731	L732	L733	L734	L735	L736	L737	L738	L739	L740
L741	L742	L743	L744	L745	L746	L747	L748	L749	L750	L751	L752
L753	L754	L755	L756	L757	L758	L759	L760	L761	L762	L763	L764
L765	L766	L767	L768	L769	L770	L771	L772	L773	L774	L775	L776
L777	L778	L779	L780	L781	L782	L783	L784	L785	L786	L787	L788
L789	L790	L791	L792	L793	L794	L795	L796	L797	L798	L799	L800
L801	L802	L803	L804	L805	L806	L807	L808	L809	L810	L811	L812
L813	L814	L815	L816	L817	L818	L819	L820	L821	L822	L823	L824
L825	L826	L827	L828	L829	L830	L831	L832	L833	L834	L835	L836
L837	L838	L839	L840	L841	L842	L843	L844	L845	L846	L847	L848
L849	L850	L851	L852	L853	L854	L855	L856	L857	L858	L859	L860
L861	L862	L863	L864	L865	L866	L867	L868	L869	L870	L871	L872
L873	L874	L875	L876	L877	L878	L879	L880	L881	L882	L883	L884
L885	L886	L887	L888	L889	L890	L891	L892	L893	L894	L895	L896
L897	L898	L899	L900	L901	L902	L903	L904	L905	L906	L907	L908
L909	L910	L911	L912	L913	L914	L915	L916	L917	L918	L919	L920
L921	L922	L923	L924	L925	L926	L927	L928	L929	L930	L931	L932
L933	L934	L935	L936	L937	L938	L939	L940	L941	L942	L943	L944
L945	L946	L947	L948	L949	L950	L951	L952	L953	L954	L955	L956
L957	L958	L959	L960	L961	L962	L963	L964	L965	L966	L967	L968
L969	L970	L971	L972	L973	L974	L975	L976	L977	L978	L979	L980
L981	L982	L983	L984	L985	L986	L987	L988	L989	L990	L991	L992
L993	L994	L995	L996	L997	L998	L999	L1000	L1001	L1002	L1003	L1004
L1005	L1006	L1007	L1008	L1009	L1010	L1011	L1012	L1013	L1014	L1015	L1016
L1017	L1018	L1019	L1020	L1021	L1022	L1023	L1024	L1025	L1026	L1027	L1028
L1029	L1030	L1031	L1032	L1033	L1034	L1035	L1036	L1037	L1038	L1039	L1040
L1041	L1042	L1043	L1044	L1045	L1046	L1047	L1048	L1049	L1050	L1051	L1052
L1053	L1054	L1055	L1056	L1057	L1058	L1059	L1060	L1061	L1062	L1063	L1064
L1065	L1066	L1067	L1068	L1069	L1070	L1071	L1072	L1073	L1074	L1075	L1076
L1077	L1078	L1079	L1080	L1081	L1082	L1083	L1084	L1085	L1086	L1087	L1088
L1089	L1090	L1091	L1092	L1093	L1094	L1095	L1096	L1097	L1098	L1099	L1100
L1101	L1102	L1103	L1104	L1105	L1106	L1107	L1108	L1109	L1110	L1111	L1112
L1113	L1114	L1115	L1116	L1117	L1118	L1119	L1120	L1121	L1122	L1123	L1124
L1125	L1126	L1127	L1128	L1129	L1130	L1131	L1132	L1133	L1134	L1135	L1136
L1137	L1138	L1139	L1140	L1141	L1142	L1143	L1144	L1145	L1146	L1147	L1148
L1149	L1150	L1151	L1152	L1153	L1154	L1155	L1156	L1157	L1158	L1159	L1160
L1161	L1162	L1163	L1164	L1165	L1166	L1167	L1168	L1169	L1170	L1171	L1172
L1173	L1174	L1175	L1176	L1177	L1178	L1179	L1180	L1181	L1182	L1183	L1184
L1185	L1186	L1187	L1188	L1189	L1190	L1191	L1192	L1193	L1194	L1195	L1196
L1197	L1198	L1199	L1200	L1201	L1202	L1203	L1204	L1205	L1206	L1207	L1208
L1209	L1210	L1211	L1212	L1213	L1214	L1215	L1216	L1217	L1218	L1219	L1220
L1221	L1222	L1223	L1224	L1225	L1226	L1227	L1228	L1229	L1230	L1231	L1232
L1233	L1234	L1235	L1236	L1237	L1238	L1239	L1240	L1241	L1242	L1243	L1244
L1245	L1246	L1247	L1248	L1249	L1250	L1251	L1252	L1253	L1254	L1255	L1256
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L1269	L1270	L1271	L1272	L1273	L1274	L1275	L1276	L1277	L1278	L1279	L1280
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L1293	L1294	L1295	L1296	L1297	L1298	L1299	L1300	L1301	L1302	L1303	L1304
L1305	L1306	L1307	L1308	L1309	L1310	L1311	L1312	L1313	L1314	L1315	L1316
L1317	L1318	L1319	L1320	L1321	L1322	L1323	L1324	L1325	L1326	L1327	L1328
L1329	L1330	L1331	L1332	L1333	L1334	L1335	L1336	L1337	L1338	L1339	L1340
L1341	L1342	L1343	L1344	L1345	L1346	L1347	L1348	L1349	L1350	L1351	L1352
L1353	L1354	L1355	L1356	L1357	L1358	L1359	L1360	L1361	L1362	L1363	L1364
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L1377	L1378	L1379	L1380	L1381	L1382	L1383	L1384	L1385	L1386	L1387	L1388
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L1401	L1402	L1403	L1404	L1405	L1406	L1407	L1408	L1409	L1410	L1411	L1412
L1413	L1414	L1415	L1416	L1417	L1418	L1419	L1420	L1421	L1422	L1423	L1424
L1425	L1426	L1427	L1428	L1429	L1430	L1431	L1432	L1433	L1434	L1435	L1436
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L1449	L1450	L1451	L1452	L1453	L1454	L1455	L1456	L1457	L1458	L1459	L1460
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L1857	L1858	L1859	L1860	L1861	L1862	L1863	L1864	L1865	L1866	L1867	L1868
L1869	L1870	L1871	L1872	L1873	L1874	L1875	L1876	L1877	L1878	L1879	L1880
L1881	L1882	L1883	L1884	L1885	L1886	L1887	L1888	L1889	L1890	L1891	L1892
L1893	L1894	L1895	L1896	L1897	L1898	L1899	L1900	L1901	L1902	L1903	L1904
L1905	L1906	L1907	L1908	L1909	L1910	L1911	L1912	L1913	L1914	L1915	L1916
L1917	L1918	L1919	L1920	L1921	L1922	L1923	L				

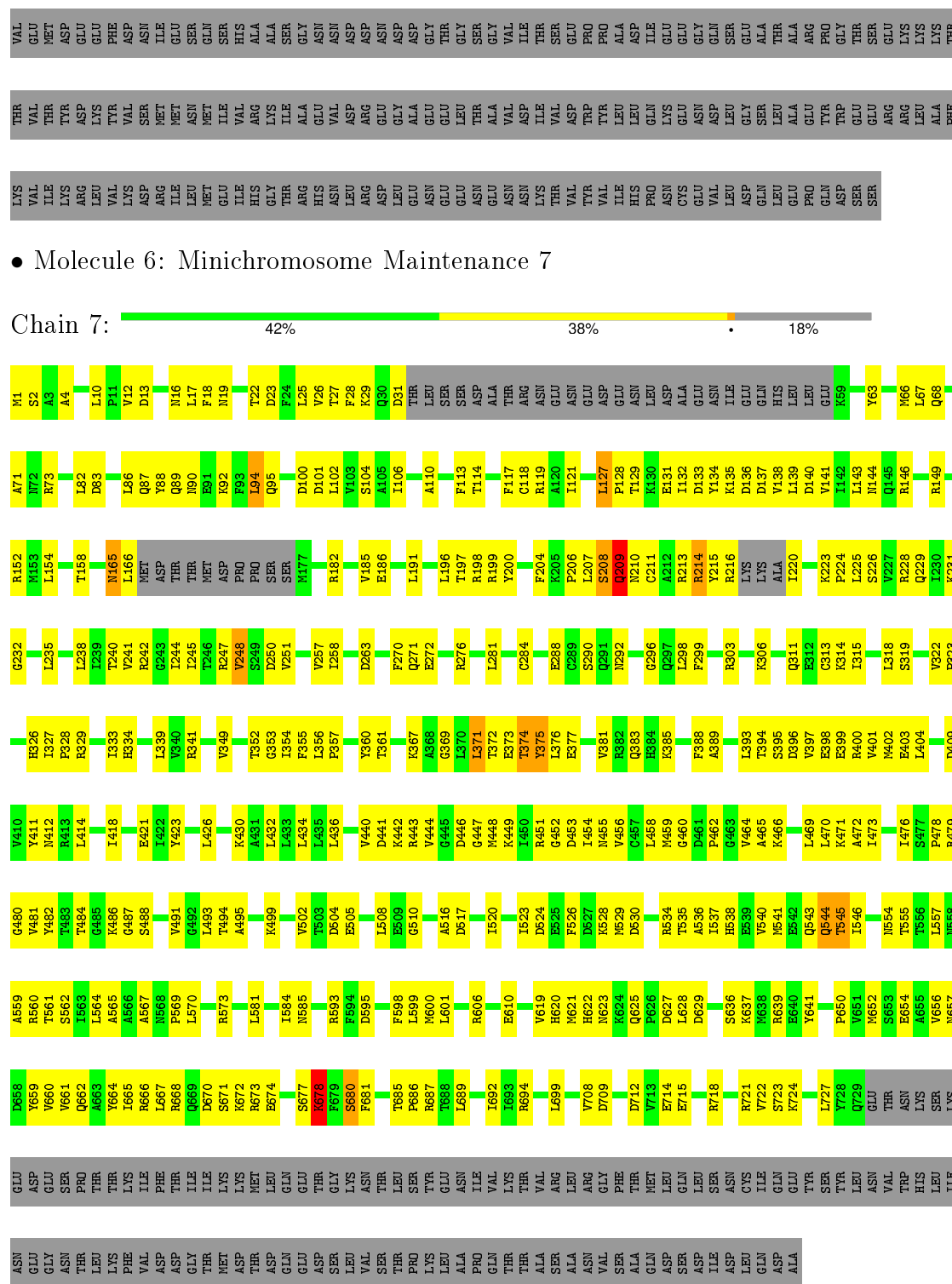
SER	M184	T254	V332	G409	T478	R559	V648	P733	M811	ALA
SER	M185	T257	L333	Q410	E482	Q560	M649	S737	R812	SER
LEU	S186	Y258	R334	T411	Q483	D561	E650	S737	L813	ASP
GLY	I187	Q259	P337	H412	Q484	I562	Q651	L742	M817	SER
ASN	Q188	D260	P340	S414	L485	N564	S655	P743	R818	SER
GLN	E189	L261	D341	T415	L486	L565	I656	F746	L819	PHE
ASN	C190	M262	M342	S416	K488	L566	A657	L747	E820	ASN
ARG	T191	M263	K343	L417	K489	C567	K658	L747	D821	GLU
VAL	N196	Y264	V344	V418	D490	G568	G659	I751	Q823	LEU
HIS	F197	P265	A345	V419	H492	D569	I662	I758	R827	LYS
MET	K202	Q266	F346	Y420	H493	P570	M666	I758	M827	GLN
ARG	Y203	E267	F347	D421	E494	T572	A667	H759	R830	ILE
ASN	R206	V268	F349	E422	E494	S573	R668	I760	R831	ASN
ASP		I269	C349	R428	V498	S575	S670	I762	A832	SER
ILE		I271	C352	D431	T502	L578	A675	E764	R833	SER
HIS		T275	R353	R432	D503		M676	K767	Y836	GLN
THR		I276	R354	I433	Q504	T585	P677	K767	A837	ASP
SER		E211	T355	E434	D505	P586	I678	E768	T838	ARG
LEU		R212	M356	V435	L506	R587	G679	E769	T839	VAL
ASP		M280	A357	T436			G680	L770	PRO	GLU
LEU		V281		G437	I509	S592	R681	R771	LYS	SER
SER		M284	I360	T438	R510	G593	V682	R772	THR	SER
PHE			R681	F439	E511	R594	V688	A773	GLY	ASP
ILE			R362	T442	V512			Y774	LYS	ILE
ASN		D290	I365	T443	R515	A598	M691	M777	ALA	GLU
ARG		Y291	Q366	T444	P516	G600	I692	R778	ASP	ALA
THR		D292	Q366	R445	D517	L603	D693	K779	MET	LEU
VAL		L293	E367	R446	L519	A603	P695	GLY	VAL	SER
ASP		E297	R370	R447	S520	Y604	P696	ASP	THR	ARG
PHE		T298	C371	S448	L521		P697	ASP	GLY	GLU
ASP		T299	E372	L453	R524	V609	L698	SER	LYS	ASP
THR		F300	R373	K454		D610		ARG	LYS	LYS
ARG		Y301	C376	S455	A527	T611	R701	SER	SER	VAL
SER		X302	M377	L456			F702	VAL	VAL	VAL
GLY		V303	E378	L457	A527	B517	D703	ILE	ILE	ILE
VAL		R304	P305	L458	P528	S518	L712	LYS	GLN	VAL
LEU		Y306	N307	R458	S529	G619	D713	ARG	LYS	VAL
ASP		N307	N330	T459	I530	G619	E714	LEU	GLY	GLY
THR		V308	L384	V460	Y531	D625	E714	LEU	GLY	GLY
SER		G309		V461	E532		K715	GLN	GLY	GLY
SER				D462	E534	V628	D717	GLU	GLU	VAL
SER		K312		V463	R538	G629	D717	ASP	ARG	ARG
ALA		G313		R465	K537	G630	R718	LEU	SER	SER
PRO		R315		V466	K538	L633		SER	VAL	VAL
PRO		R318		V467	Q543	D632	A721	ARG	VAL	VAL
SER				LYS	L544		F722	GLU	ARG	ARG
SER		K324		S470	F545	D635	H723	ILE	LEU	LEU
ALA		L325		D471	G546	K636		ASN	ASN	ASN
GLY		I326		R472	G547	T641	L727	VAL	VAL	ARG
PRO		I327		R473	T548	R642	L728	LEU	LEU	VAL
L177		L248		L474		H646	E730	LYS	LYS	ASP
L178		L249		D475	R557			ASP	ASP	GLN
L179		A250		V476						
L180		Q253		D477						

• Molecule 4: Minichromosome Maintenance 5

Chain 5:  45% 36% 18%

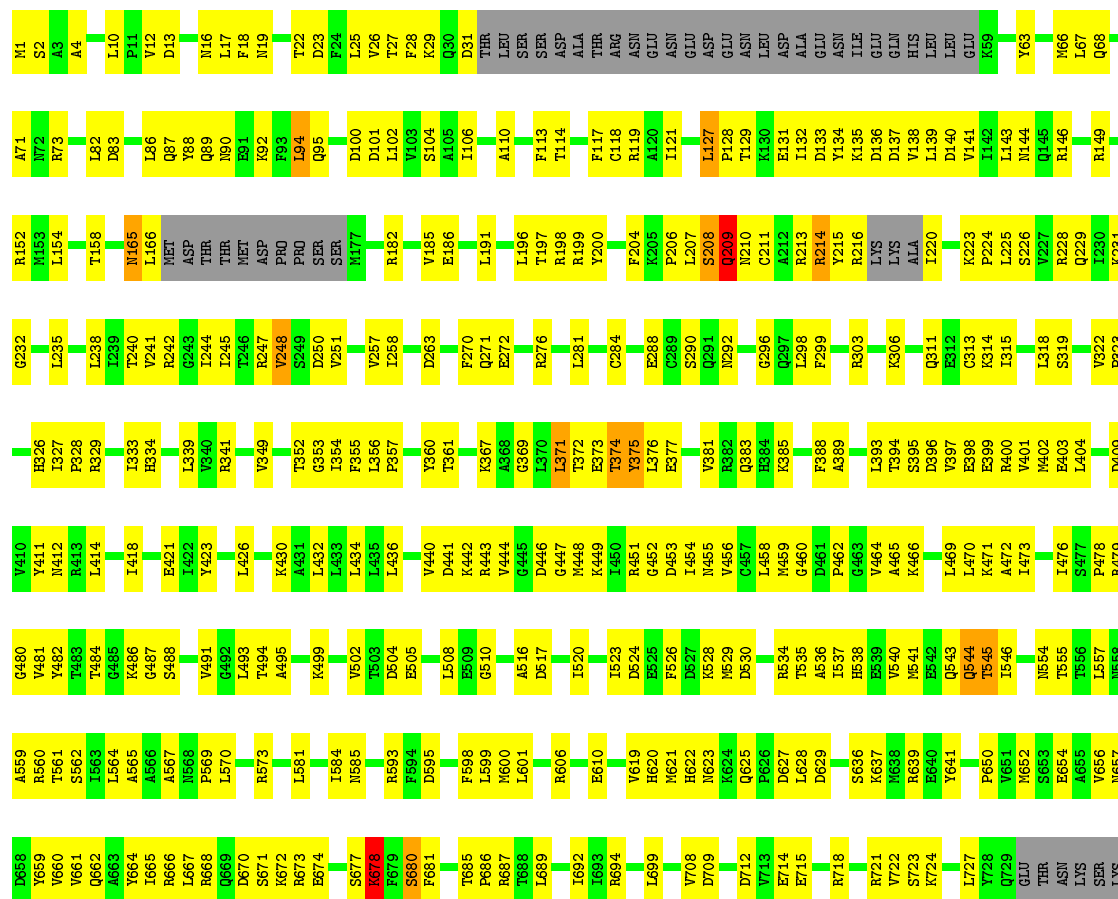
MET	T95	I194	V265	S345
S2	I101	N195	F266	F349
D4		N196	V267	
		F197	G268	
		N198	E269	
Q15	ASN	SER	M270	E356
G16	ASN	ILE	P271	F357
	ASN	T201	R272	N363
P19	ASN			
N20	LYS	T204	M276	L366
D21	ASP	V205	T277	I374
	PRO		C278	A375
T25	GLU	P208		P376
E26	ASN	R209	L282	S377
I27	THR	S210	V286	S377
I28	SER	C211	I287	F379
K29	MET	LEU		
S30	ASP	SER		
F31	THR	THR	T290	K385
	ASP	ILE	R291	K386
F34	SER	GLY		A387
I35	LEU	SER	T294	I388
	LEU	GLY	V295	V389
F38	LEU	SER		C390
	M130	SER	S299	I391
		MET	I300	L392
F44	L137	ALA	Y301	S396
I45	I138	ASN	S302	K397
Y46	GLN	GLY	S303	K398
R47	SER	SER	K304	
D48	S141	ILE	N305	
Q49	M142	GLY	G306	D402
L50	A143	GLY	ALA	G403
		P147	GLY	M404
N53	L148	R149	SER	R407
	R149	GLY	GLY	D409
T62	D150	THR	ARG	N411
	L151	LYS	SER	V412
N65	D152		GLY	L413
B66		H155	ASN	L414
H67	V156	V156	GLY	L415
L68	H155		S319	
I69			G320	T420
	I165			A421
E73	I166	S170		L425
D74		L172		L426
I75	V171	K77		K427
Y76	L172	L79		F428
K78				
L79	R175			V437
		Y178		Y438
I86		L179		T439
I87		S180		S440
P88	I181	I181		S341
L89		I261		I342
F90		T262		K441
E91		E263		K442
I92	R184			G443
T92		L264		
A93	T193			
I94				





● Molecule 6: Minichromosome Maintenance 7

Chain 7:  42% 38% • 18%



4 Experimental information

Property	Value	Source
Reconstruction method	Not provided	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	85365	Depositor
Resolution determination method	FSC 0.143	Depositor
CTF correction method	CTFFIND	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	22	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	22500	Depositor
Image detector	GATAN K2 (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP

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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	2	0.41	0/4794	0.64	2/6479 (0.0%)
2	3	0.48	0/4827	0.67	1/6545 (0.0%)
3	4	0.45	0/5154	0.67	4/6967 (0.1%)
4	5	0.46	0/5032	0.62	0/6799
5	6	0.40	0/4812	0.65	1/6497 (0.0%)
6	7	0.47	0/5514	0.65	3/7450 (0.0%)
All	All	0.45	0/30133	0.65	11/40737 (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	2	0	4
2	3	0	2
3	4	0	3
5	6	0	5
6	7	0	5
All	All	0	19

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	3	654	PRO	CA-N-CD	-8.68	99.35	111.50
5	6	399	GLY	N-CA-C	6.81	130.12	113.10
6	7	127	LEU	CA-CB-CG	6.30	129.79	115.30
6	7	209	GLN	N-CA-C	-6.27	94.06	111.00
3	4	243	LEU	CA-CB-CG	5.94	128.96	115.30

There are no chirality outliers.

5 of 19 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	2	367	CYS	Peptide
1	2	372	PRO	Peptide
1	2	436	GLY	Peptide
1	2	803	PHE	Peptide
2	3	172	THR	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	2	4714	0	4730	259	0
2	3	4745	0	4793	311	0
3	4	5081	0	5125	338	0
4	5	4962	0	4994	265	0
5	6	4742	0	4692	317	0
6	7	5432	0	5495	349	0
7	2	27	0	12	1	0
7	3	27	0	12	4	0
7	4	27	0	12	6	0
7	5	27	0	12	7	0
7	6	27	0	12	10	0
7	7	27	0	12	6	0
All	All	29838	0	29901	1676	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 28.

The worst 5 of 1676 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:653:ILE:CD1	4:5:402:ASP:HB3	1.36	1.53
2:3:653:ILE:HD13	4:5:402:ASP:CB	1.55	1.36
2:3:652:THR:C	2:3:654:PRO:HD3	1.52	1.28
2:3:653:ILE:CD1	4:5:402:ASP:CB	2.11	1.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:214:ARG:HG3	6:7:215:TYR:C	1.64	1.14

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	2	597/868 (69%)	544 (91%)	47 (8%)	6 (1%)	19	66
2	3	595/971 (61%)	548 (92%)	40 (7%)	7 (1%)	16	63
3	4	632/933 (68%)	554 (88%)	71 (11%)	7 (1%)	17	65
4	5	621/775 (80%)	586 (94%)	32 (5%)	3 (0%)	34	77
5	6	608/1017 (60%)	547 (90%)	52 (9%)	9 (2%)	13	59
6	7	681/845 (81%)	619 (91%)	52 (8%)	10 (2%)	13	59
All	All	3734/5409 (69%)	3398 (91%)	294 (8%)	42 (1%)	23	65

5 of 42 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	4	189	GLU
3	4	609	VAL
4	5	596	ILE
5	6	317	ILE
6	7	26	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	2	509/770 (66%)	509 (100%)	0	100	100
2	3	523/835 (63%)	523 (100%)	0	100	100
3	4	573/848 (68%)	572 (100%)	1 (0%)	95	98
4	5	566/688 (82%)	566 (100%)	0	100	100
5	6	497/886 (56%)	497 (100%)	0	100	100
6	7	609/753 (81%)	608 (100%)	1 (0%)	95	98
All	All	3277/4780 (69%)	3275 (100%)	2 (0%)	95	98

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

Mol	Chain	Res	Type
3	4	442	ILE
6	7	214	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 59 such sidechains are listed below:

Mol	Chain	Res	Type
3	4	410	GLN
4	5	140	ASN
6	7	544	GLN
3	4	465	HIS
3	4	651	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

6 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
7	ADP	2	2001	-	24,29,29	0.95	1 (4%)	23,45,45	1.95	2 (8%)
7	ADP	3	2001	-	24,29,29	1.00	1 (4%)	23,45,45	1.71	1 (4%)
7	ADP	4	2001	-	24,29,29	0.96	1 (4%)	23,45,45	1.70	2 (8%)
7	ADP	5	2001	-	24,29,29	0.97	1 (4%)	23,45,45	1.73	2 (8%)
7	ADP	6	2001	-	24,29,29	1.00	1 (4%)	23,45,45	1.85	2 (8%)
7	ADP	7	2001	-	24,29,29	0.98	1 (4%)	23,45,45	1.69	1 (4%)

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
7	ADP	2	2001	-	-	0/12/32/32	0/3/3/3
7	ADP	3	2001	-	-	0/12/32/32	0/3/3/3
7	ADP	4	2001	-	-	0/12/32/32	0/3/3/3
7	ADP	5	2001	-	-	0/12/32/32	0/3/3/3
7	ADP	6	2001	-	-	0/12/32/32	0/3/3/3
7	ADP	7	2001	-	-	0/12/32/32	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	5	2001	ADP	C5-C4	2.82	1.46	1.40
7	4	2001	ADP	C5-C4	2.84	1.46	1.40
7	7	2001	ADP	C5-C4	2.88	1.47	1.40
7	2	2001	ADP	C5-C4	2.91	1.47	1.40
7	3	2001	ADP	C5-C4	2.92	1.47	1.40

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
7	2	2001	ADP	N3-C2-N1	-7.35	123.10	128.87
7	6	2001	ADP	N3-C2-N1	-6.81	123.52	128.87
7	3	2001	ADP	N3-C2-N1	-6.35	123.88	128.87
7	5	2001	ADP	N3-C2-N1	-6.32	123.91	128.87
7	7	2001	ADP	N3-C2-N1	-6.30	123.92	128.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	2	2001	ADP	1	0
7	3	2001	ADP	4	0
7	4	2001	ADP	6	0
7	5	2001	ADP	7	0
7	6	2001	ADP	10	0
7	7	2001	ADP	6	0

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.