



## wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Feb 2, 2017 – 06:56 PM EST

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/EMDataBank EM Map/Model Validation Summary Report  
for a publicly released PDB/EMDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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) : rb-20028442

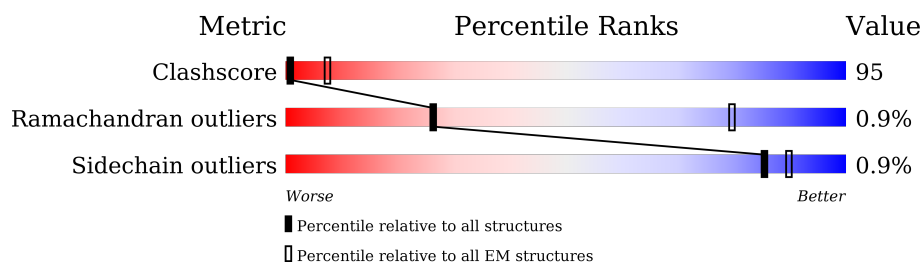
# 1 Overall quality at a glance

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.






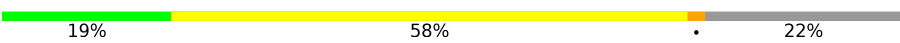
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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  $\geq 3$ , 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	A	208	15% 82% .
2	B	213	10% 74% 15%
3	C	194	12% 70% 18%
4	D	294	13% 60% . 25%
5	E	650	16% 68% 15%
6	F	26	27% 73%
7	G	14	7% 93%
8	2	868	12% 56% . 31%
9	3	971	13% 47% . 39%

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Mol	Chain	Length	Quality of chain
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		

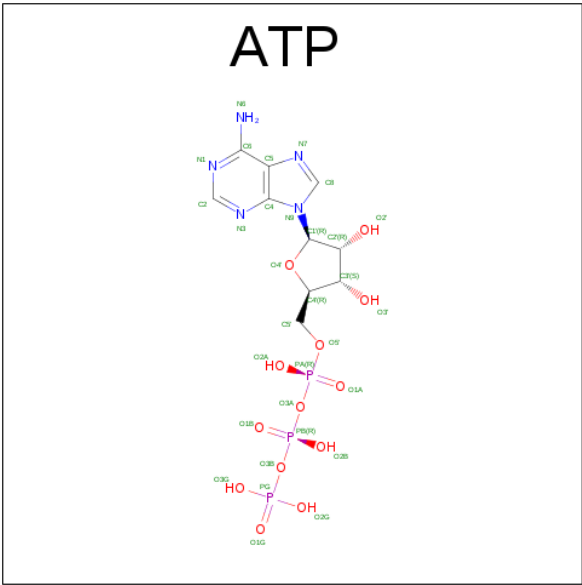
- Molecule 12 is a protein called DNA replication licensing factor MCM6.

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

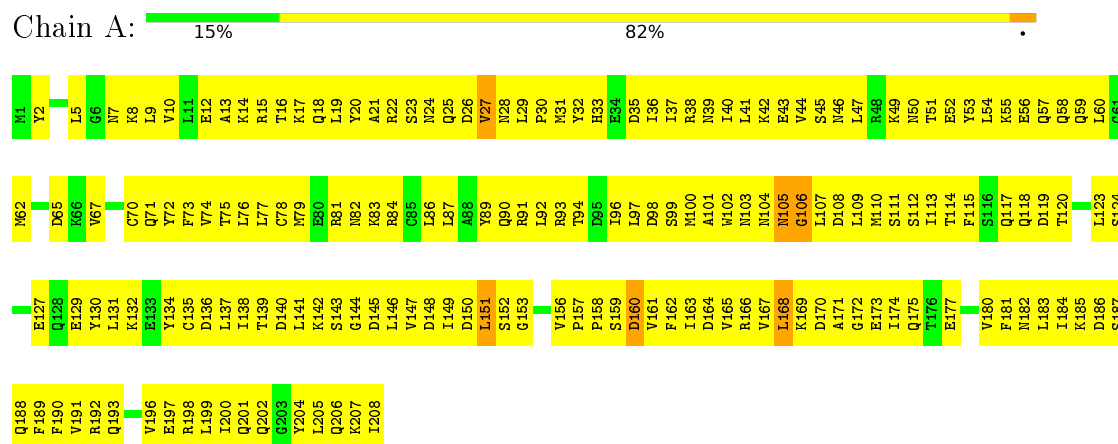
- Molecule 14 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



### 3 Residue-property plots

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

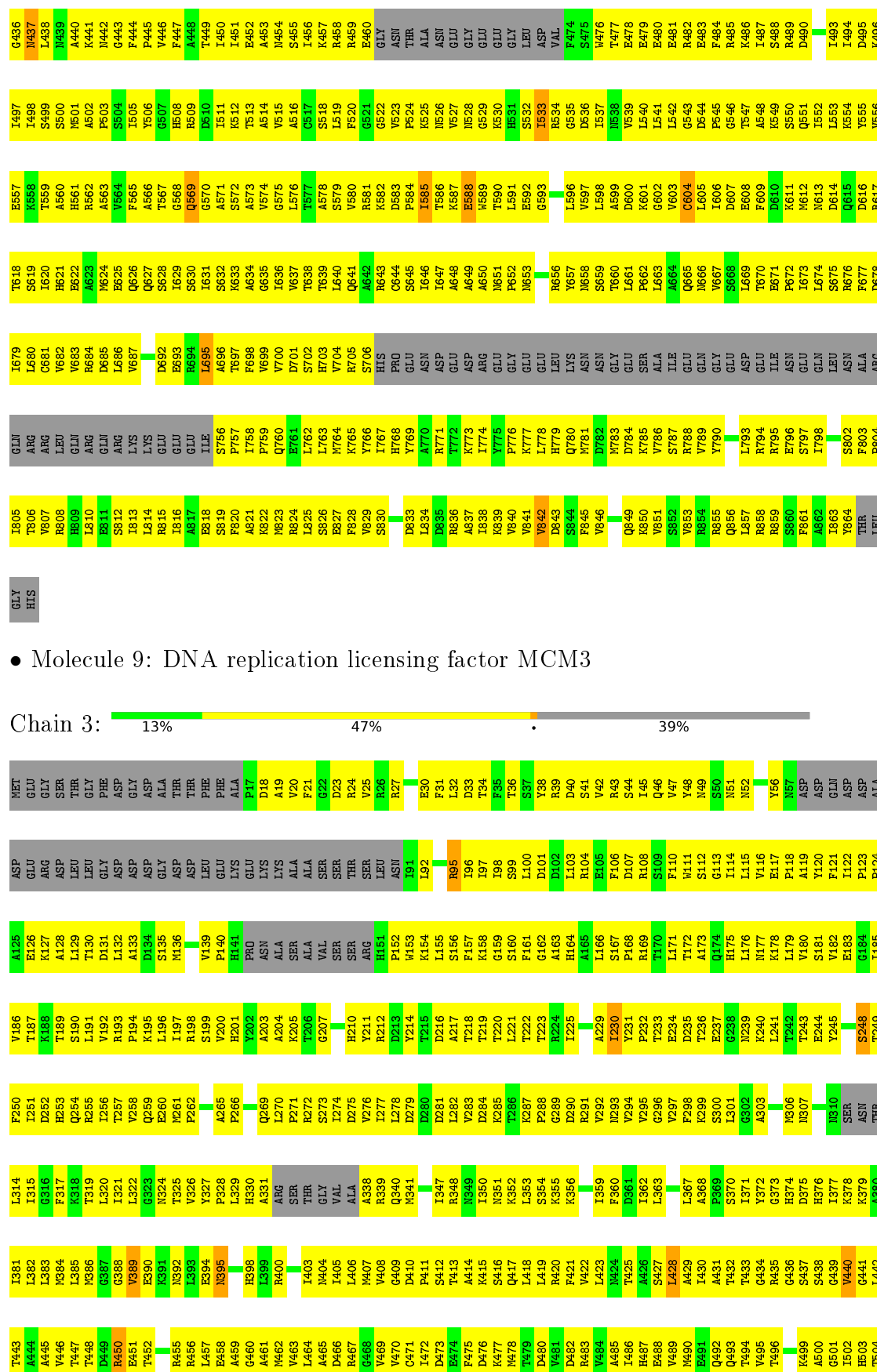
- Molecule 1: DNA replication complex GINS protein PSF1











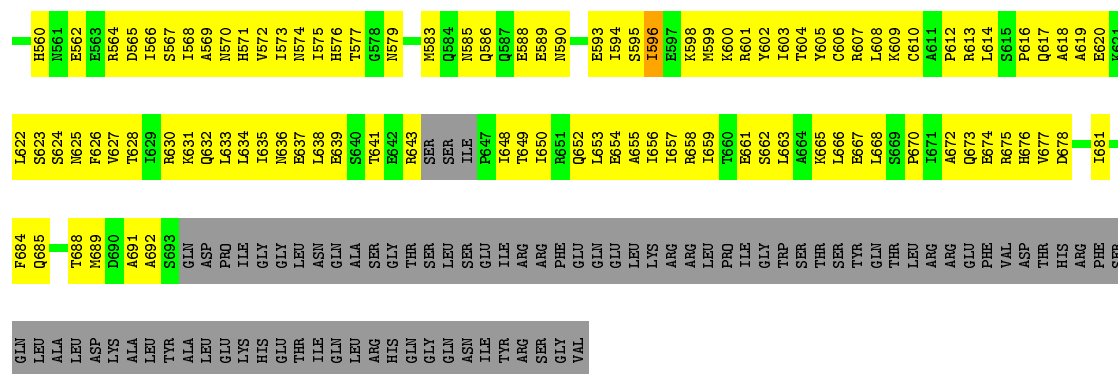


I903	H808	L747	P684	S624	Y558	ASN
I907	A809	M748	M685	D625	R559	GLU
S908	K810	M749	L686	G626	G560	VAL
R909		M750	P687	G627	D561	GLU
	L813	L751	M688	V628	L562	GLU
		S752	T689	C629	M663	V496
		Y753	R690	C630	L564	R499
	V816	A754	M691	L631	L565	Q500
	E818	K755	L692	D632	L566	L501
	L819	E756	D693	E633	C567	T502
	E820	H757	L694	F634	G568	D503
	D821	L758	P695	D635		Q504
V923		H759	P696	F636		D505
R924		T760	P697	M637	S571	L506
R925		E761	L698	S638	S573	
	A825	L762	L699	D639	K574	K508
R928		T763	S700	S640		L509
L929		E764	R701	T641	I577	
ASN		A765	F702	R642	L578	V512
ASN		H766	D703	S643	Q579	A513
ARG		K767	L704	V644	Y580	A514
VAL			V705	L645	V581	R515
				H646		E516
		L770	V708	E647	I584	D517
		V771	L709	F648	T585	L518
		H772	D710	M649	P586	Y519
		A773	K711	E650	R387	S520
		Y774	V712	Q651	G588	L521
		V775	D713	Q652	G589	L522
		G776	D714	T653		A523
		M777	E715	L654		R524
		K778	K715	S655	S592	
		L779	N716	F656	G593	S925
		NET	D717	L657	K594	L526
		GLY	R718	A657	A527	
		LYS	E719	K658		P528
		ASP	E720	A659		S529
		ILE	L721			L530
		ASP	A721	G660	G600	E531
		SER	K722	T661	L601	T602
		ASN	R723	L662	E603	E532
		SER	L724	T663	A604	L533
		LEU	E725	T664	Y604	E534
		GLU	N726	L665	I605	
		LYS	N726	L666		E535
		ARG	L727	M666	T606	V536
		ILE	O728	A667	R607	K537
		THR	L729	R668	K538	
		A733	E730	S669	V609	G539
		T734	ASP	S670	D610	L540
		T735	LVS	L671	T611	L541
		R736	P80	L672	K612	L542
		L737	GLU	A673	Q613	
		Q738	H1S	S674	L614	Q543
		L739	ILE	A675	V615	L544
		E739	SER	L676	L616	F545
		S900	GLN	P677	E617	G546
		M801	ASP			G547
		L802	ASP		S618	
		R803	ASP		G619	
		L804	V741	S680	A620	
		A805	L742	R681	L621	
		E806		V622	F552	
		L903				

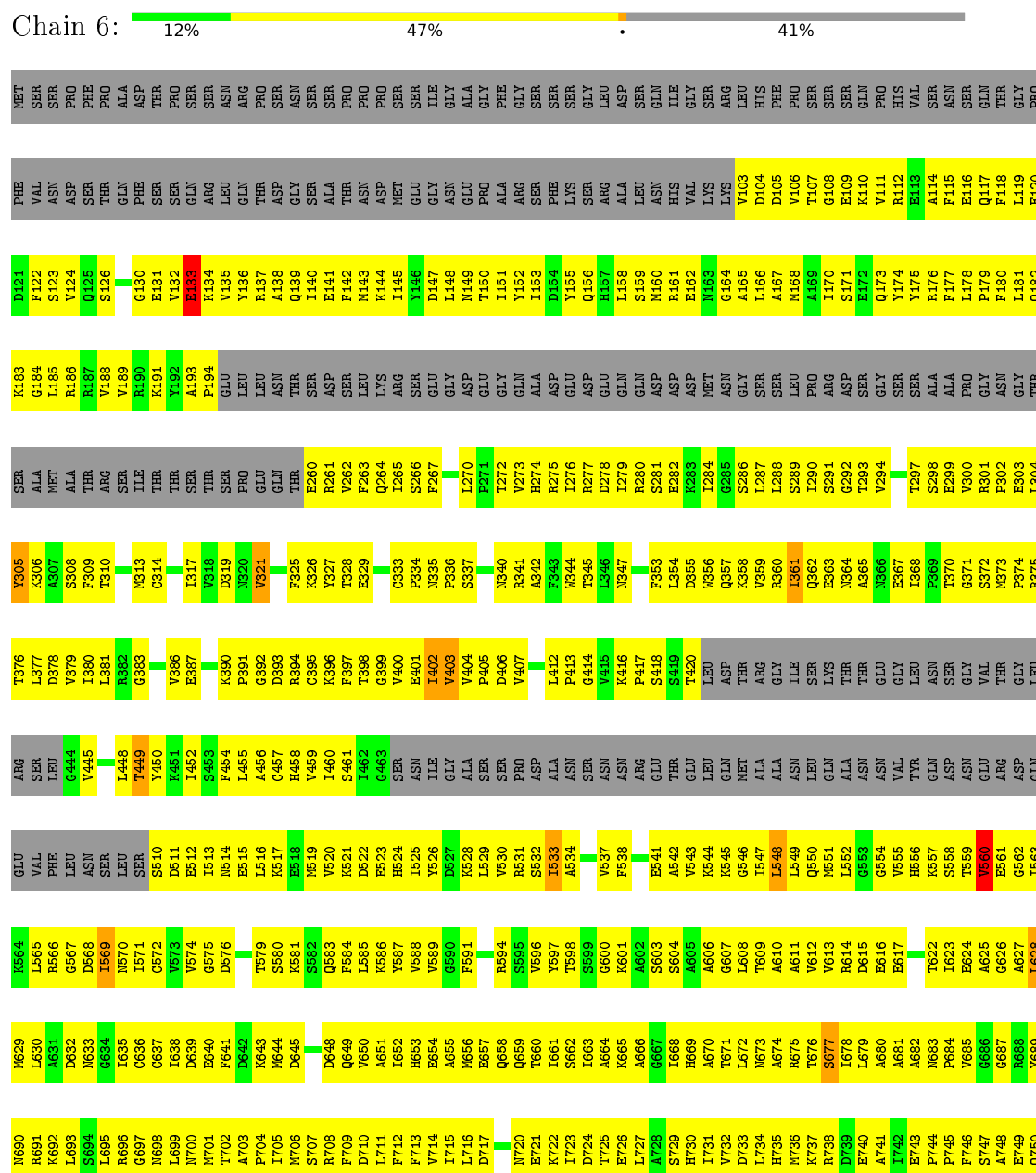
• Molecule 11: Minichromosome maintenance protein 5

Chain 5: 15% 61% 23%

K431	Y367	M305	I243	C183	MET	L61
V432	E368	GLY	I244	I184	ASP	T62
S433	I369	ALA	E245	N185	THR	V63
P434	I370	GLY	E246	C186	ASP	N64
I435	T371	SER	S247	R187	SER	N65
A436	N372	GLY	S248	H188	LEU	E66
V437	S373	ARG	E249	T189	LEU	H67
T438	I374	SER	F250	T190	LEU	L68
T439	A375	GLY	I251	S191	N130	T69
S440		GLY	D252	I192		G70
O441	I378	GLY	Q253	T193		V71
K442	F379	ASN	Q254	I194	T134	M72
G443		GLY	F255	N195	F135	E73
S444	E382	GLY	L256	N196	Q136	D74
A445	D383	S319	K257	F197	L137	I75
L446	I384	G320	L258	N198	I138	V76
V447	K385	V321	Q259	SER	L139	K77
L448	K386	A322	E260	I1E	H140	K78
L449	A387	I323	L261	T201	S141	L79
M514	L388	R324	P262	G202	N142	S80
N515	T389	T325	E263	N203	A143	
T516	C390	P326	L264	T204	N144	
A517	S452	C391	V265	V205	Q145	
V518	V453	L391	P266	S206	I146	
V519	Q454	L392	E267	L207	P147	
L520	R455	K329	E268	P208	L148	
A521	D456	I330	G269	T209	R149	
E522	P457	L331	M270	S210	D150	
A523	K397	G332	M271	C211	L151	
N524	K398	I333	P271	LEU	D152	
P525	L400	Q334	R272	SER	S153	
I526	E461		M273	THR	E154	
T527	P462	P401	L274	I1E	H155	
G528	K403	G338	T275	GLU	V156	
B529	L464	T339	M276	SER	S157	
Y530	E465	R405	T277	GLU	K158	
D531	G466	L406	C278	SER	I159	
E532	D467	R407	D279	THR	V160	
L533	A468	G408	E280	SER	R161	
		D409	Y281	MET	L162	
		ASN	L282	ALA	I101	
		SER	T283	ASN	S163	
		Y346		GLU	G164	
		N411	I287	SER	I165	
		V412	P288	ASN	I166	
		L413	G289	I1E	I167	
		L414	T290	GLY	S168	
		L415	R291	ASP	T169	
		G416	V292	GLU	S170	
		D417	S293	SER	V171	
		P418	I294	THR	L172	
		G419	F295	LYS	S173	
		T420	V296	LYS	S174	
		F421	G296		R175	
		A422	I297	N235	ASN	
		K423	Y298	C236	R176	
		S423	S299	G237	A176	
		S424	I300	P238	T177	
		L425	Y301	D239	L178	
		L426	T302	P240	L179	
		K427	N302	Y241	S180	
		F428	S303	T242	ASN	
		V429	V243	S244	THR	
		E430	T245		SER	



• Molecule 12: DNA replication licensing factor MCM6



THR	VAL	SER	D817	L751
	VAL	GLU	ASP	R753
	THR	PRO	THR	R752
	VAL	THR	PRO	R754
	ILE	LEU	ALA	R755
	HIS	LEU	ASP	R756
	PRO	GLN	ILE	R757
	ASN	LYS	GLU	R758
	PRO	CYS	GLU	R759
	ASP	GLU	ASN	R760
SER	VAL	GLN	ASP	R761
	LEU	LEU	SER	R762
	ASP	GLY	GLU	R763
	GLN	SER	ALA	R764
	LEU	LEU	THR	R765
	GLU	ALA	ALA	R766
	PRO	ARG	ARG	R767
	GLN	THR	PRO	R768
	ASP	THR	GLY	R769
	SER	GLU	THR	R770
SER	GLU	GLU	SER	R771
	ARG	GLU	ARG	R772
	ARG	LYS	THR	R773
	LEU	LYS	ASP	R774
	ALA	LYS	ASP	R775
	PRE	THR	ASP	R776
	LYS	THR	VAL	R777
	VAL	VAL	GLU	R778
	ILE	THR	MET	R779
	LYS	THR	ASP	R780
SER	ARG	ASP	GLU	R781
	LEU	LYS	GLU	R782
	VAL	THR	PHE	R783
	LYS	VAL	ASP	R791
	ASP	SER	ASN	R792
	ARG	MET	ILE	R793
	ILE	MET	GLU	R794
	LEU	ASN	SER	R795
	MET	MET	GLN	R796
	GLU	GLU	SER	R797
SER	ILE	VAL	HIS	R798
	HIS	ARG	ALA	R799
	GLY	LYS	ALA	R800
	THR	ILE	SER	R801
	ARG	GLU	GLY	R802
	HIS	GLU	ASN	R803
	ASN	VAL	ASN	R804
	LEU	ASP	ASP	R805
	ARG	ARG	ASP	R806
	ASP	GLU	ASN	R807
SER	LEU	GLY	ASP	R808
	GLU	ALA	ASP	R809
	ASN	GLU	GLY	R810
	GLU	GLU	THR	R811
	GLU	LEU	GLY	R812
	ASN	THR	SER	R813
	GLU	ALA	GLY	R814
	ASN	VAL	VAL	R815
	GLU	VAL	VAL	R816
	LYS	THR	ILE	R817

- Molecule 13: DNA replication licensing factor MCM7

Chain 7:  19% 58% • 22%

A643	S579	L515	M448	K386	V324	T261	F201	D137	L67	M1
	P580	A516	K449	LPHS	G325	C262	L202	V138	K68	S2
	F581	D517	L450	PHE	H326	D263	Y203	L139	K69	
	D582	N518	R451	ALA	I327	D264	F204	D140	V70	L5
	N583	G519	K452	SER	P328	C265	K205	V441	A71	P6
	R649	I520	D453	PHE	R329	G266	P206	I142	N72	S7
	N585	C521	L454	SER	S330	T267	L207	L143	R73	I8
	L586	C522	M455	L393		E268	S208	N144	E74	
	P587	I523	V456	T394	I333	V269	Q209	R145	L75	D13
		D524	C457	S395	H334	F270	N210	R146	N76	Y14
L590		E525	L458	D396	V335	D271	C211	R147	S77	
L591		F526	M459	V397	N336	E272	A212	L148	V78	L17
	F594	D527	G460	E398	G337	V273	R213	R149	L79	F18
	D595	K528	D461	E399	T338		R214	N150	I80	N19
	D658	N529	P462	R400	L339	R276	Y215		D81	E20
	V596	G463	G463	V401	V340	T277	R216	M153	L82	I21
	M597	V464	V464	M402	R341	F278	LVS	L154		D23
	F598	A465	A465	E403	S342	T279	LVS		I85	D23
	L599	R534	K466	L404	L343	P280	ALA	R157	L86	F24
	N600	T535		L405	S344	L281	I220	T158	K87	L25
	L601	A536	L469	T406	P345	E282	S221	ASN	V88	V26
	D602	I537	L470	S407	G346	E283	S222	GLU	K89	T27
	H603	H538	K471	G403	D347	C284	K223	IIE	N90	F28
	P604	E539	A472	D409	I348	T285	P224	ARG	E91	
	S605	V540	I473	V410	V349	S286	L225	SER	K92	
	D606	M541	C474	Y411	D350	E287	S226	GLU	F93	THR
	H607	K475	K475	N412	V351	E288	V227	ASN	L94	LEU
	D608	G542	L476	R413	T352	C289	R228	LEU	D95	SER
	D609	O544	S477	L414	G353	S290	Q229	MET		SER
	E510	T545	P478	A415	I354	Q291	I230	ASP	D101	ASP
	H611	I546	R479	K416	F355	I292	K231	THR	L102	ALA
	L612	S547	G480	S417	L356		G232	THR	V103	THR
	H613	I548		L418	P357	D296	D233	MET	S104	ARG
	R679	S549	T484	A419	A358	G297	F234	ASP	A105	ASN
	B614	G485	G485	P420	P359	L298	L235	PRO	I106	GLU
	S680	A551	K486	E421	V360	F289	G236			ASN
	V616	G552		L422		P300	Q237	SER	A110	GLU
	H617					S301	L238	SER	H111	ASP
	T685	L553	S489	L426	F363	T302	L239	MET	H112	GLU
	V618	N554	G490	D427	K364	R303	T240	ASN	F113	ASN
	P686	T555	V491	V428	A365	A304	V241	ASP	T114	LEU
	H620	T556	G492	K429	L366	S305	R342	ALA	E115	ASP
	H622	L557	L493	K430	K367	R306	G243	LEU	L116	ALA
	H623	N558			A431	F307	T244	ARG	F117	GLU
	Q625	A559	V497	L432	G369	A309	T245	GLU	C118	ASN
		T561	H498	L433	L370	F310	R246	VAL	R119	IIE
	L628	S562	K499	L434	I371	R311	R247	VAL	A120	GLU
	D629	L563	D500	L435	T372	Q311	V248	GLU	I121	GLU
	F630	L564	P501	L436	E373	E312	S249	ASP		HIS
	H632	A565	V502	G437	F374	C313	V250		M124	LEU
	H633	A566	G439	G439	V375	R314	K252		P126	LEU
	V633	A567	D504	V440	L376	I315	P127		L128	GLU
		N568	E505			I316	K253		P128	K59
	S636	P569		D441		E317	V255		P129	G60
	H637		L508	K442	Q379	R318	V256			P61
	P638			R443	F380	L319	V257			K62
	R639			V444	V381	S319	E256			N63
	L704	N574		G445	R382	Q320	L258			R64
				G446	Q383	Q321	L268			
	V641	L513		D446	H384	V322	K260			
		L514		C412	E385	P322				
	L578									

SER	ALA	ASN	VAL	SER	ALA	GLN	ASP	SER	ASP	ILE	ASP	LEU	GLN	GLN	ASP	ALA
ARG	LEU	ARG	GLY	PHE	THR	MET	LEU	GLN	LEU	SER	ASN	CYS	ILE	GLN	GLU	TYR
GLU	THR	ASN	TRP	HIS	LYS	LEU	ILE	ASN	GLU	GLY	ASN	THR	LEU	LYS	PHE	VAL
ILE	ASP	ASP	GLY	THR	MET	ASP	THR	THR	ASP	GLN	GLU	ASP	SER	LEU	VAL	SER
THR	THR	ASP	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
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## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	243796	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	Depositor



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	A	0.24	0/1718	0.51	1/2314 (0.0%)
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%)
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
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
10	4	0	2
12	6	0	3
13	7	0	1
4	D	0	1
9	3	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%)	34	77
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%)	21	66
5	E	543/650 (84%)	490 (90%)	51 (9%)	2 (0%)	39	80
8	2	596/868 (69%)	535 (90%)	54 (9%)	7 (1%)	16	61
9	3	579/971 (60%)	528 (91%)	48 (8%)	3 (0%)	34	77
10	4	670/933 (72%)	594 (89%)	69 (10%)	7 (1%)	19	64
11	5	583/775 (75%)	549 (94%)	30 (5%)	4 (1%)	26	71
12	6	596/1017 (59%)	528 (89%)	58 (10%)	10 (2%)	11	55
13	7	653/845 (77%)	583 (89%)	60 (9%)	10 (2%)	13	57
All	All	4969/6968 (71%)	4484 (90%)	439 (9%)	46 (1%)	26	66

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%)	70	88
2	B	171/198 (86%)	170 (99%)	1 (1%)	90	95
3	C	144/173 (83%)	144 (100%)	0	100	100
4	D	213/279 (76%)	211 (99%)	2 (1%)	84	93
5	E	499/586 (85%)	496 (99%)	3 (1%)	90	95
8	2	508/770 (66%)	502 (99%)	6 (1%)	78	90
9	3	512/835 (61%)	506 (99%)	6 (1%)	78	90
10	4	610/848 (72%)	606 (99%)	4 (1%)	88	94
11	5	534/688 (78%)	528 (99%)	6 (1%)	80	91
12	6	486/886 (55%)	482 (99%)	4 (1%)	86	94
13	7	585/753 (78%)	581 (99%)	4 (1%)	88	94
All	All	4455/6209 (72%)	4416 (99%)	39 (1%)	85	93

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

Mol	Chain	Res	Type
9	3	395	ASN
10	4	188	GLN
13	7	291	GLN
9	3	450	ARG
9	3	510	CYS

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

Mol	Chain	Res	Type
9	3	351	ASN
10	4	354	HIS
13	7	379	GLN
9	3	688	ASN
10	4	260	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 ⓘ

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	2	901	-	26,33,33	0.96	1 (3%)	26,52,52	1.85	2 (7%)
14	ATP	3	1001	-	26,33,33	0.95	1 (3%)	26,52,52	1.79	1 (3%)
14	ATP	5	801	-	26,33,33	0.94	1 (3%)	26,52,52	1.83	2 (7%)

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	5	801	ATP	C5-C4	2.97	1.47	1.40
14	3	1001	ATP	C5-C4	2.98	1.47	1.40
14	2	901	ATP	C5-C4	3.10	1.47	1.40

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	5	801	ATP	N3-C2-N1	-7.70	122.82	128.87
14	2	901	ATP	N3-C2-N1	-7.69	122.83	128.87
14	3	1001	ATP	N3-C2-N1	-7.45	123.02	128.87
14	5	801	ATP	C2-N1-C6	2.04	122.41	118.77
14	2	901	ATP	C2-N1-C6	2.31	122.88	118.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 29 short contacts:

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