



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Dec 24, 2017 – 11:08 PM EST

PDB ID : 6F0L
EMDB ID: : EMD-3960
Title : S. cerevisiae MCM double hexamer bound to duplex DNA
Authors : Abid Ali, F.; Pye, V.E.; Douglas, M.E.; Locke, J.; Nans, A.; Diffley, J.F.X.;
Costa, A.
Deposited on : 2017-11-20
Resolution : 4.77 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

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030736

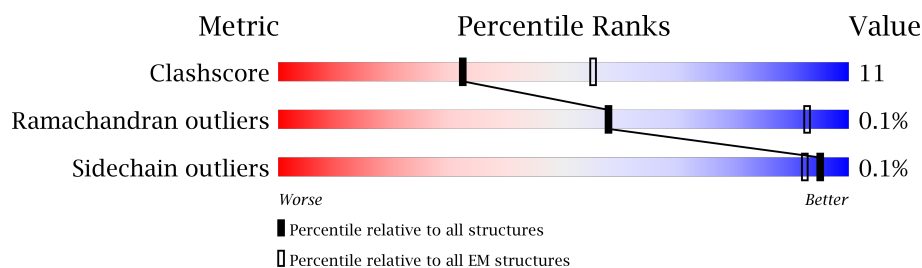
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.77 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.






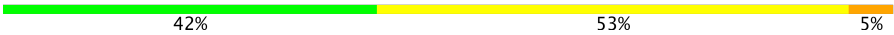
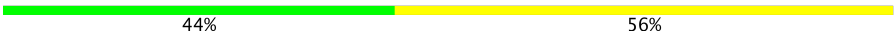
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

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	59% 10% 31%
1	A	868	59% 10% 31%
2	3	971	51% 10% 39%
2	B	971	51% 10% 39%
3	4	933	55% 14% 31%
3	C	933	55% 14% 31%
4	5	775	63% 18% • 18%
4	D	775	64% 17% • 18%
5	6	1017	50% 10% 40%

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Mol	Chain	Length	Quality of chain
5	E	1017	
6	7	845	
6	F	845	
7	X	62	
8	Y	62	

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
9	ADP	3	1001	-	-	X	-
9	ADP	5	1001	-	-	X	-
9	ADP	B	1001	-	-	X	-
9	ADP	D	1001	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 61818 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 licensing factor MCM2.

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

- Molecule 2 is a protein called DNA replication licensing factor MCM3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	596	Total	C	N	O	S	0	0
			4670	2941	834	882	13		
2	B	596	Total	C	N	O	S	0	0
			4670	2941	834	882	13		

- Molecule 3 is a protein called DNA replication licensing factor MCM4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	642	Total	C	N	O	S	0	0
			5083	3194	878	983	28		
3	C	642	Total	C	N	O	S	0	0
			5083	3194	878	983	28		

- Molecule 4 is a protein called Minichromosome maintenance protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	5	634	Total	C	N	O	S	0	0
			4975	3121	855	974	25		
4	D	634	Total	C	N	O	S	0	0
			4975	3121	855	974	25		

- Molecule 5 is a protein called DNA replication licensing factor MCM6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	6	615	Total	C	N	O	S	0	0
			4731	2979	837	895	20		
5	E	615	Total	C	N	O	S	0	0
			4731	2979	837	895	20		

- Molecule 6 is a protein called DNA replication licensing factor MCM7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	7	687	Total	C	N	O	S	0	0
			5411	3408	938	1035	30		
6	F	687	Total	C	N	O	S	0	0
			5411	3408	938	1035	30		

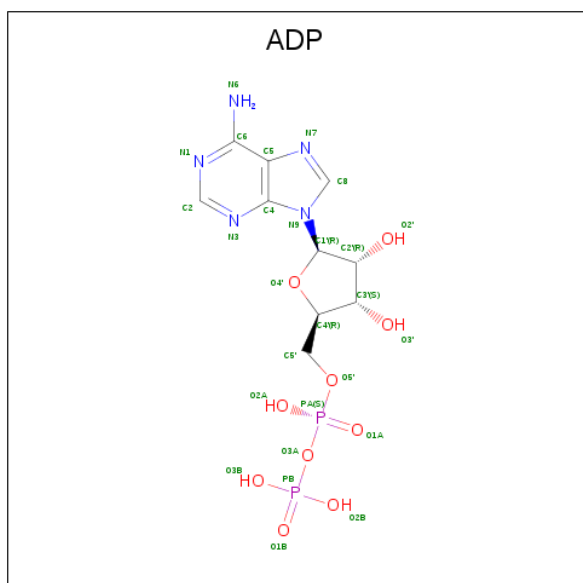
- Molecule 7 is a DNA chain called DNA (62-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	X	62	Total	C	N	O	P	0	0
			1270	604	233	371	62		

- Molecule 8 is a DNA chain called DNA (62-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Y	62	Total	C	N	O	P	0	0
			1272	605	232	373	62		

- Molecule 9 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

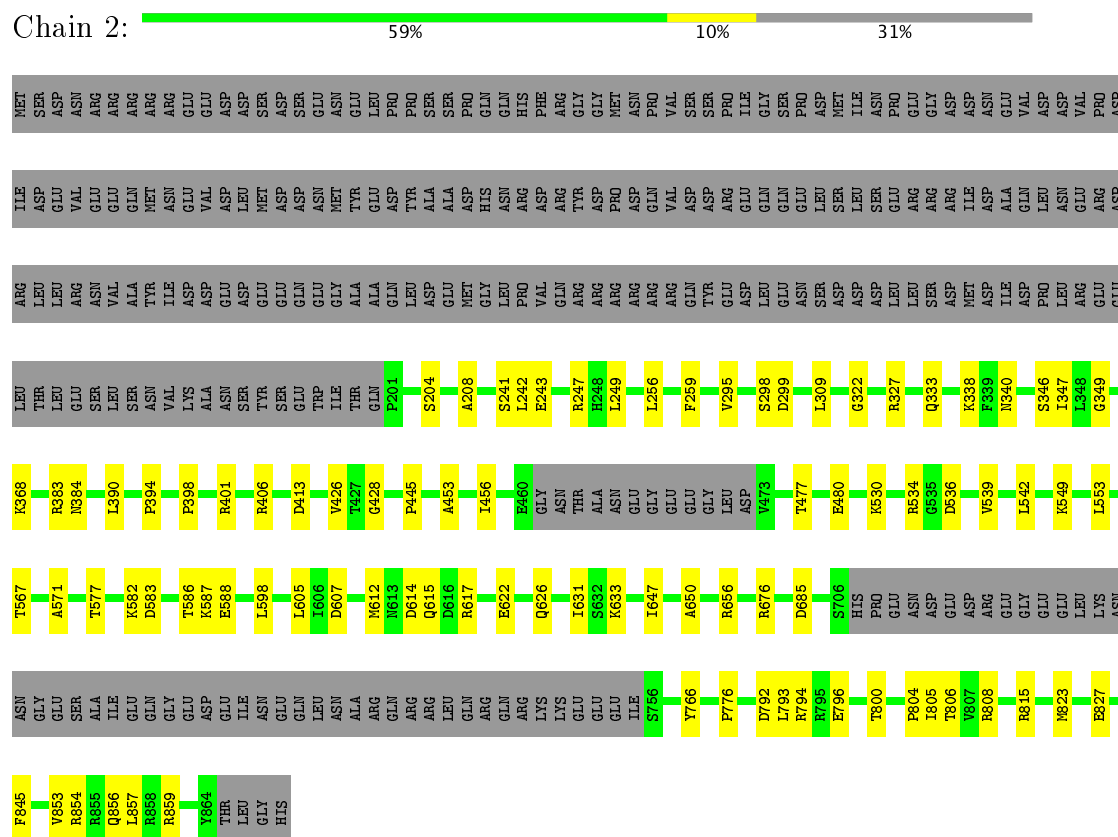


Mol	Chain	Residues	Atoms					AltConf
9	3	1	Total	C	N	O	P	0
			27	10	5	10	2	
9	5	1	Total	C	N	O	P	0
			27	10	5	10	2	
9	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
9	D	1	Total	C	N	O	P	0
			27	10	5	10	2	

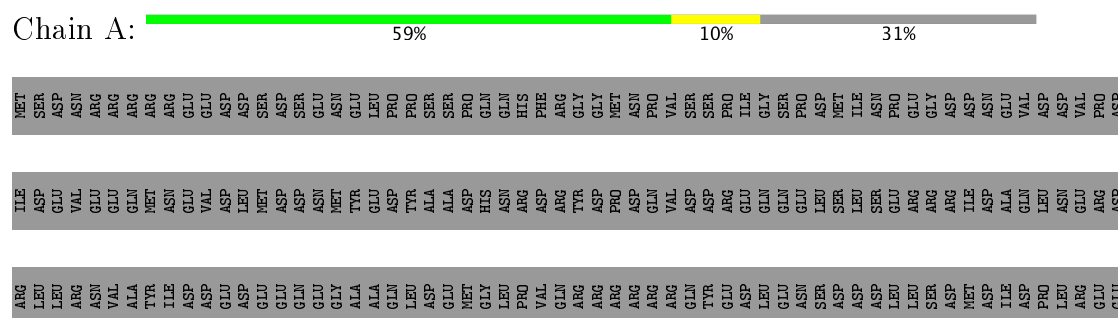
3 Residue-property plots

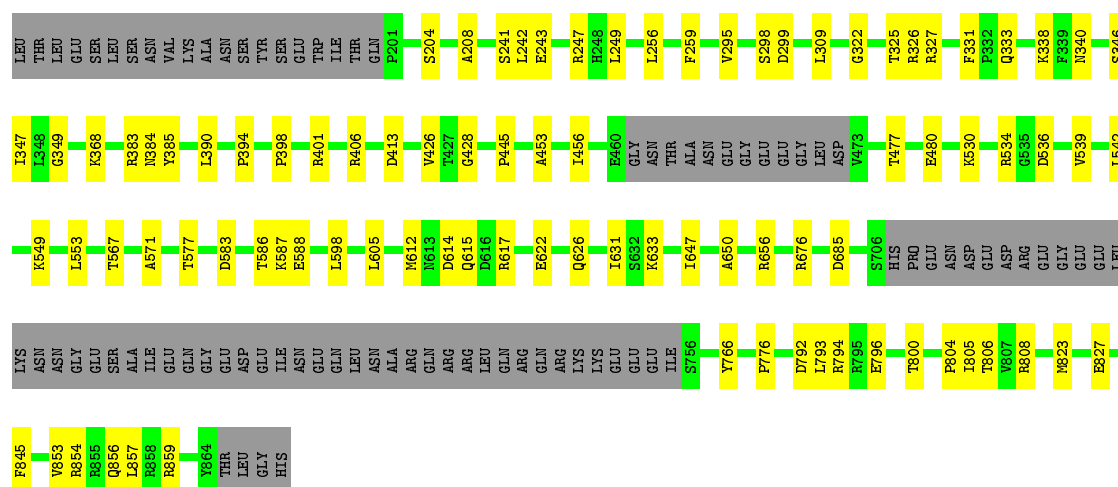
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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 licensing factor MCM2



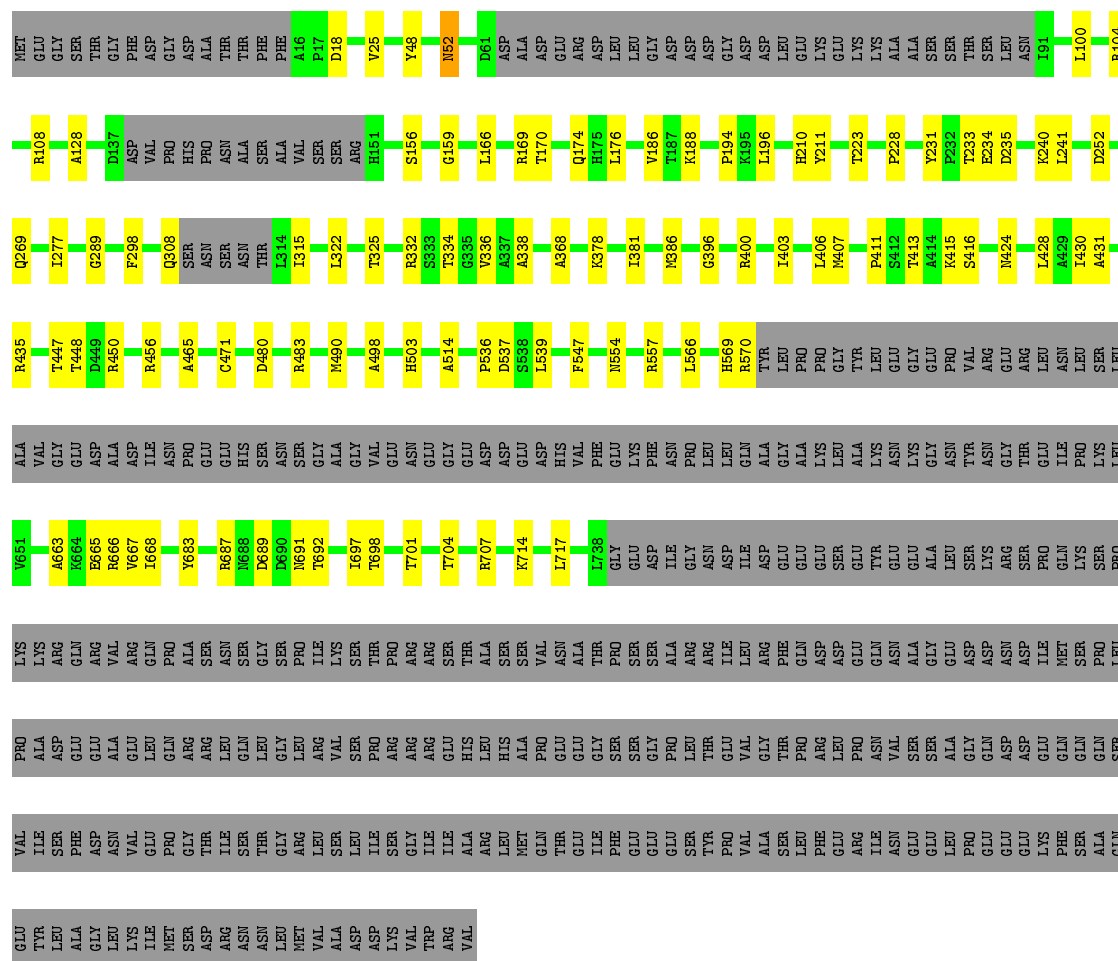
- Molecule 1: DNA replication licensing factor MCM2





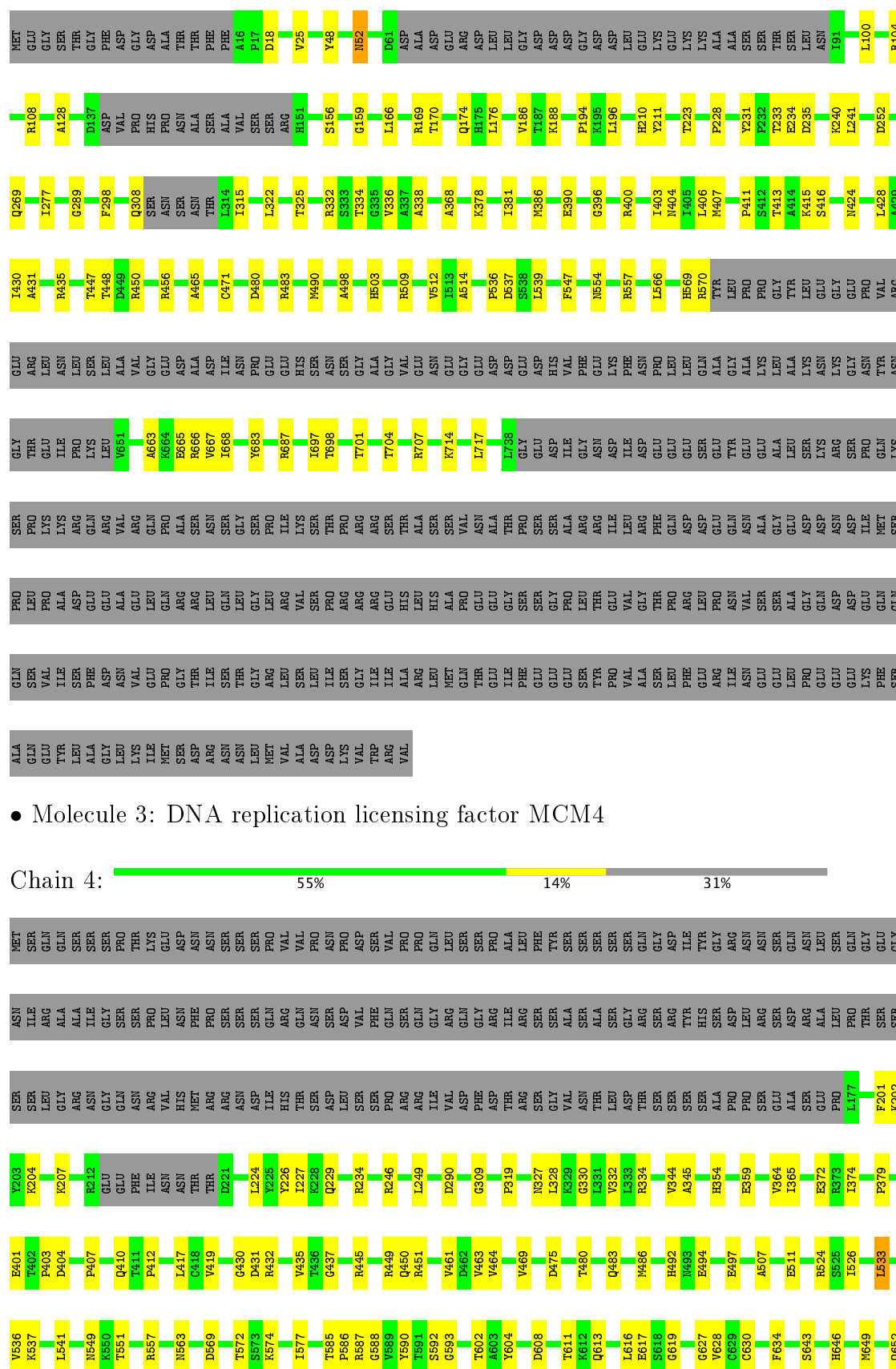
• Molecule 2: DNA replication licensing factor MCM3

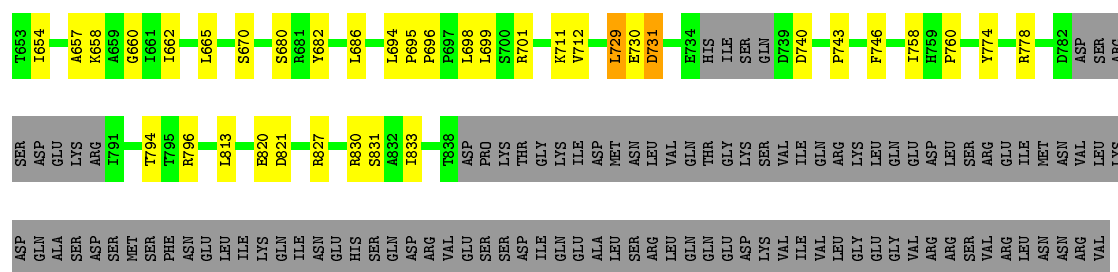
Chain 3: 51% 10% 39%



• Molecule 2: DNA replication licensing factor MCM3

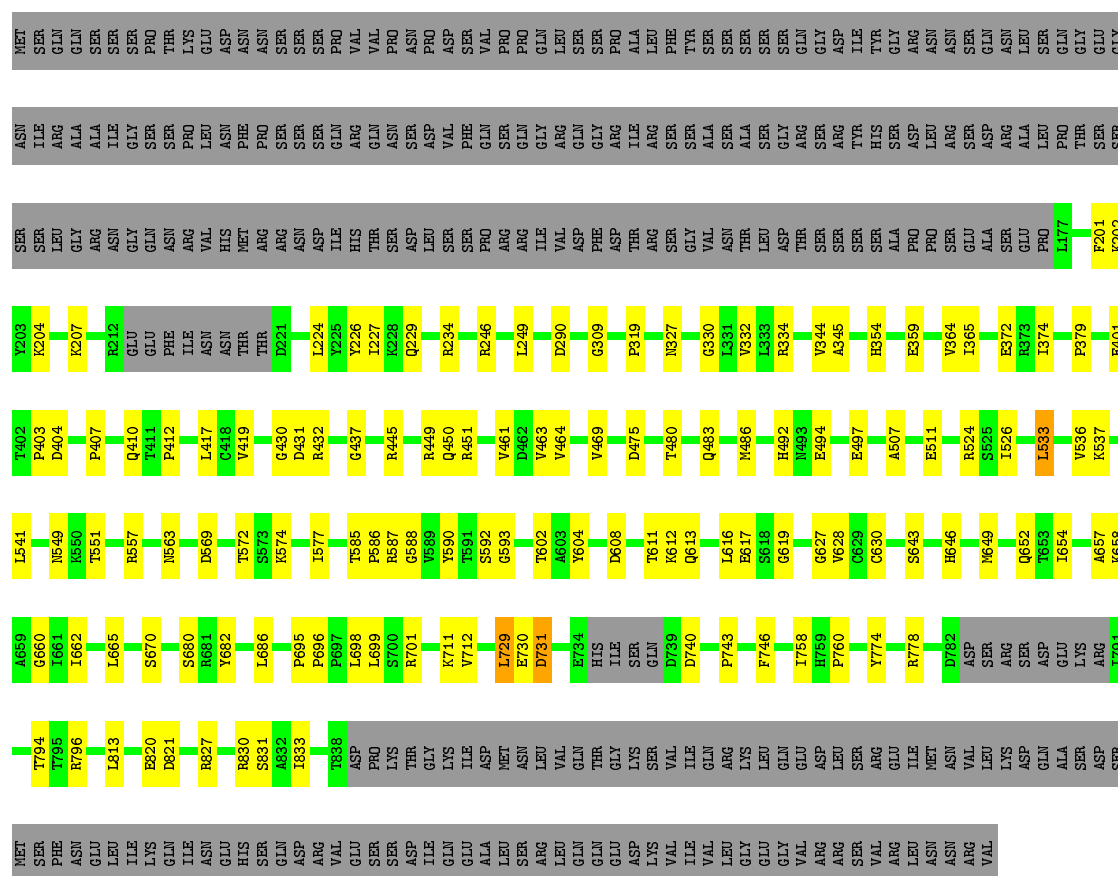
Chain B: 51% 10% 39%





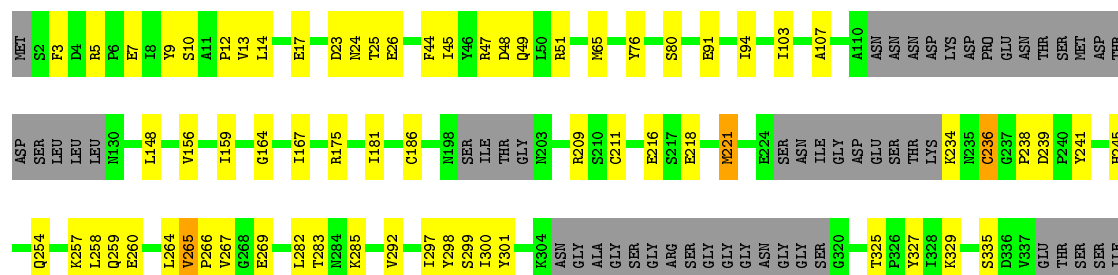
- Molecule 3: DNA replication licensing factor MCM4

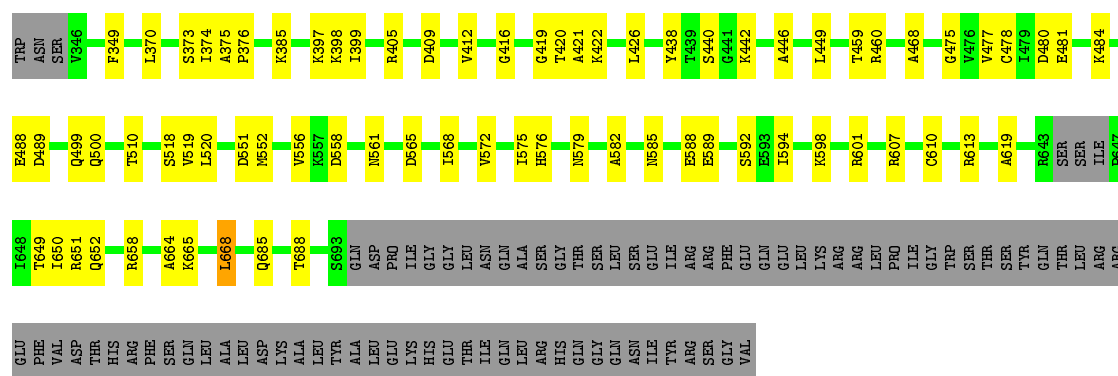
Chain C:  55% 14% 31%



- Molecule 4: Minichromosome maintenance protein 5

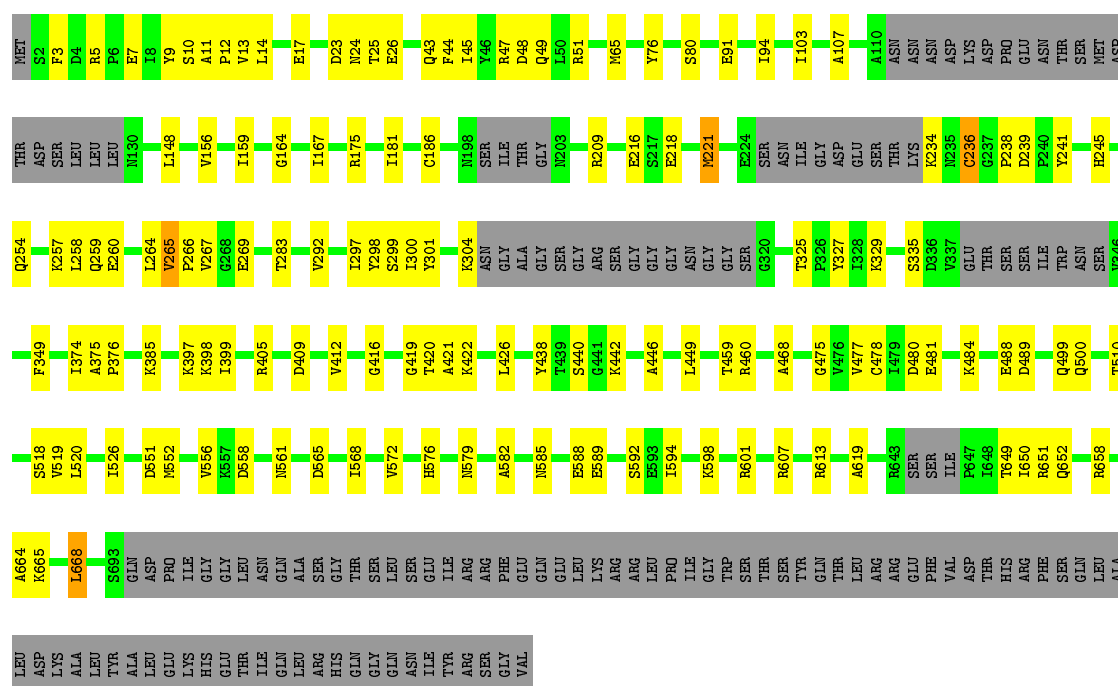
Chain 5:  63% 18% • 18%





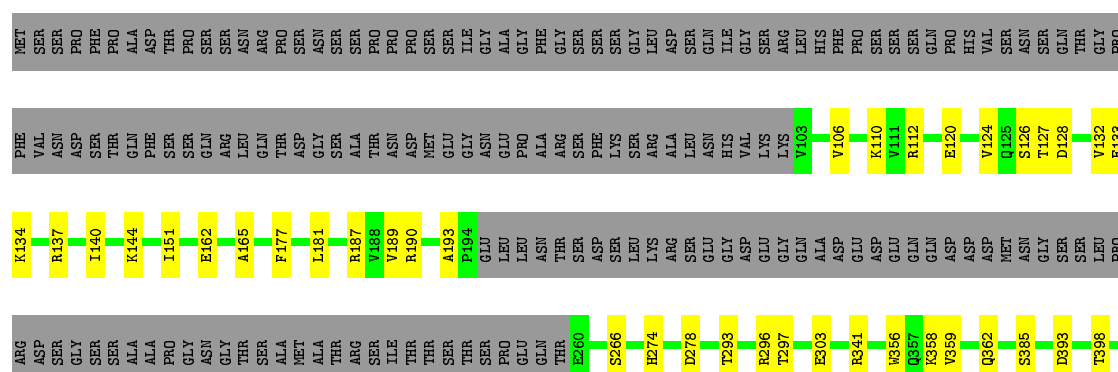
- Molecule 4: Minichromosome maintenance protein 5

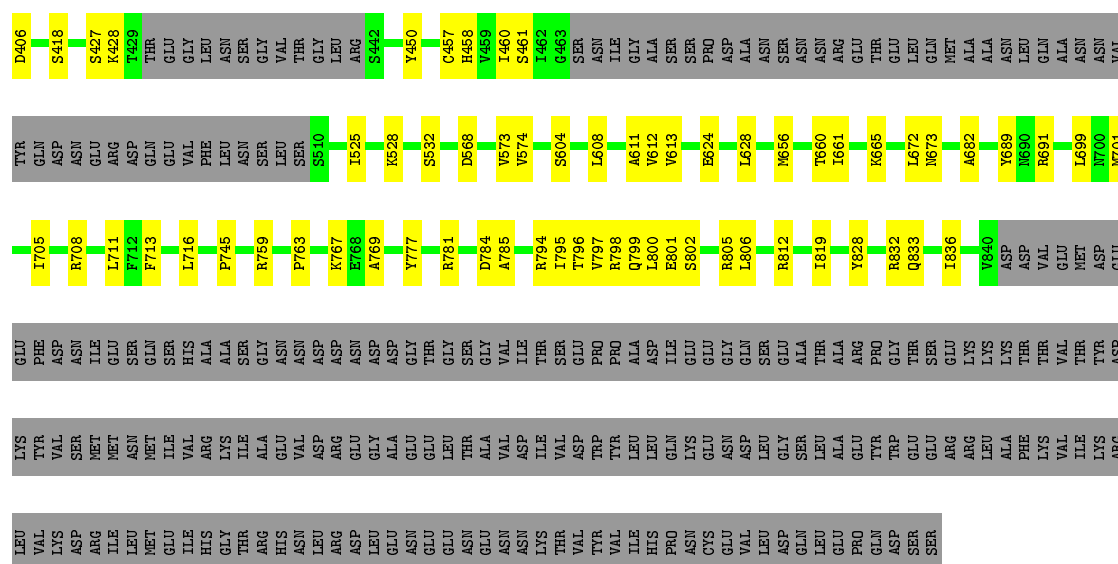
Chain D: 64% 17% 18%



- Molecule 5: DNA replication licensing factor MCM6

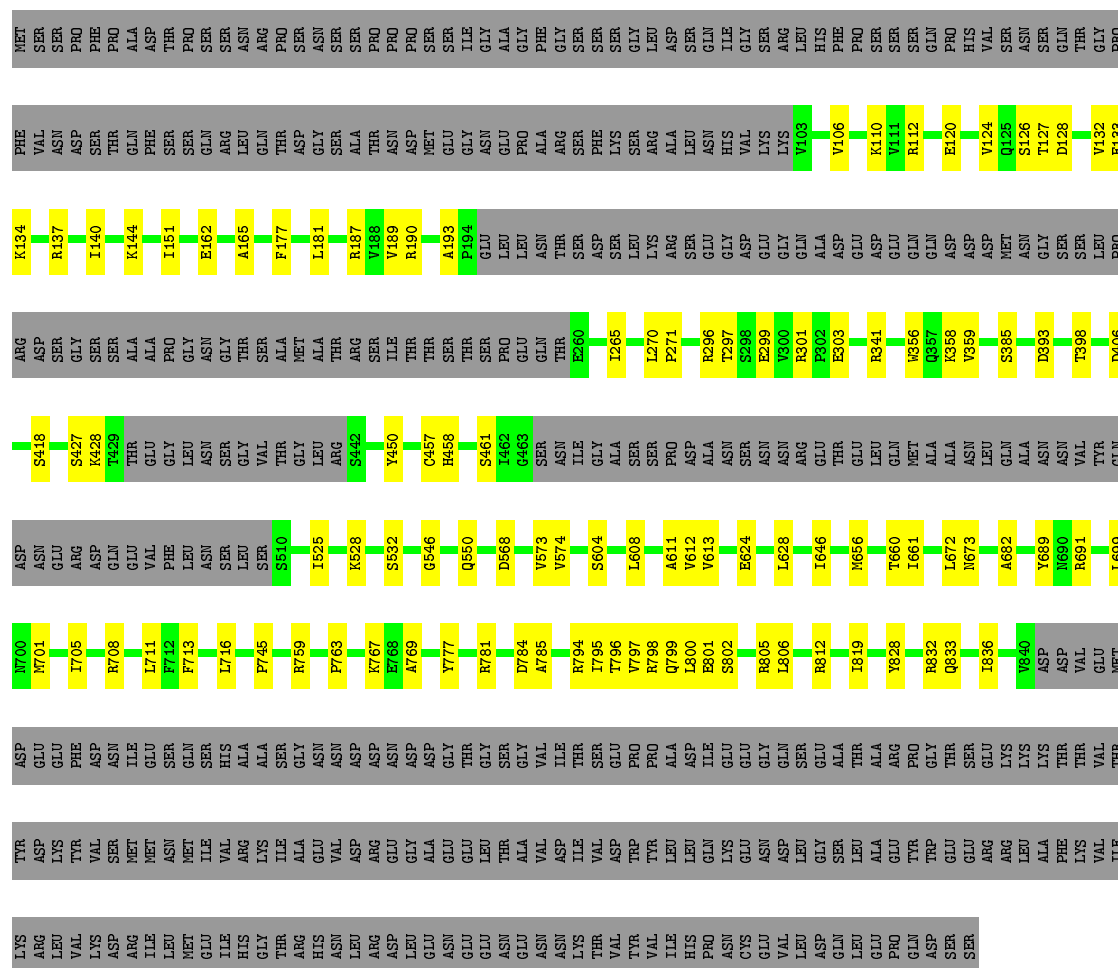
Chain 6: 50% 10% 40%



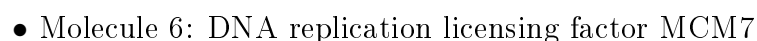


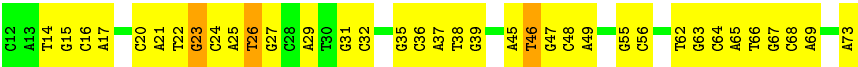
- Molecule 5: DNA replication licensing factor MCM6

Chain E:  50% 10% 40%

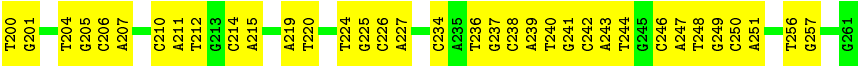


- Molecule 6: DNA replication licensing factor MCM7





● Molecule 8: DNA (62-MER)



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	52319	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 ($e^-/\text{\AA}^2$)	1.7	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (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	0.29	0/4794	0.57	0/6479
1	A	0.29	0/4794	0.57	0/6479
2	3	0.30	0/4748	0.55	0/6436
2	B	0.30	0/4748	0.55	0/6436
3	4	0.31	0/5155	0.64	5/6969 (0.1%)
3	C	0.31	0/5155	0.64	5/6969 (0.1%)
4	5	0.30	0/5043	0.57	3/6811 (0.0%)
4	D	0.30	0/5043	0.57	3/6811 (0.0%)
5	6	0.29	0/4801	0.56	0/6483
5	E	0.29	0/4801	0.56	0/6483
6	7	0.30	0/5493	0.58	1/7423 (0.0%)
6	F	0.30	0/5493	0.58	1/7423 (0.0%)
7	X	1.10	4/1423 (0.3%)	0.98	6/2191 (0.3%)
8	Y	0.49	0/1426	1.33	5/2199 (0.2%)
All	All	0.34	4/62917 (0.0%)	0.62	29/85592 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	X	24	DC	O3'-P	23.79	1.89	1.61
7	X	23	DG	O3'-P	22.60	1.88	1.61
7	X	25	DA	O3'-P	-13.61	1.44	1.61
7	X	26	DT	O3'-P	-8.87	1.50	1.61

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	Y	242	DC	O5'-P-OP2	-27.78	77.36	110.70
8	Y	242	DC	OP1-P-OP2	-26.44	79.94	119.60
8	Y	242	DC	O5'-P-OP1	17.37	131.54	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	Y	241	DG	OP1-P-O3'	-15.20	71.77	105.20
8	Y	241	DG	OP2-P-O3'	13.94	135.87	105.20

There are no chirality outliers.

There are no planarity outliers.

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	4729	102	0
1	A	4714	0	4729	113	0
2	3	4670	0	4730	133	0
2	B	4670	0	4730	120	0
3	4	5083	0	5129	91	0
3	C	5083	0	5129	126	0
4	5	4975	0	5016	216	0
4	D	4975	0	5017	220	0
5	6	4731	0	4679	79	0
5	E	4731	0	4679	68	0
6	7	5411	0	5472	125	0
6	F	5411	0	5472	120	0
7	X	1270	0	699	100	0
8	Y	1272	0	699	72	0
9	3	27	0	12	35	0
9	5	27	0	12	33	0
9	B	27	0	12	34	0
9	D	27	0	12	32	0
All	All	61818	0	60957	1308	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 11.

The worst 5 of 1308 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)
2:3:231:TYR:HD2	4:D:221:MET:CE	1.02	1.67
2:3:231:TYR:CD2	4:D:221:MET:CE	1.75	1.62
6:7:292:ASN:HD21	4:D:25:THR:CG2	1.23	1.52
4:5:300:ILE:C	4:5:327:TYR:HE1	1.16	1.49
4:D:300:ILE:N	4:D:327:TYR:CE1	1.80	1.48

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%)	534 (89%)	63 (11%)	0	100	100
1	A	597/868 (69%)	533 (89%)	64 (11%)	0	100	100
2	3	586/971 (60%)	544 (93%)	42 (7%)	0	100	100
2	B	586/971 (60%)	544 (93%)	42 (7%)	0	100	100
3	4	634/933 (68%)	569 (90%)	63 (10%)	2 (0%)	44	81
3	C	634/933 (68%)	569 (90%)	63 (10%)	2 (0%)	44	81
4	5	620/775 (80%)	561 (90%)	58 (9%)	1 (0%)	51	84
4	D	620/775 (80%)	562 (91%)	57 (9%)	1 (0%)	51	84
5	6	607/1017 (60%)	549 (90%)	58 (10%)	0	100	100
5	E	607/1017 (60%)	548 (90%)	59 (10%)	0	100	100
6	7	679/845 (80%)	618 (91%)	61 (9%)	0	100	100
6	F	679/845 (80%)	618 (91%)	61 (9%)	0	100	100
All	All	7446/10818 (69%)	6749 (91%)	691 (9%)	6 (0%)	58	88

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	4	374	ILE

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Mol	Chain	Res	Type
3	C	374	ILE
4	5	266	PRO
4	D	266	PRO
3	4	731	ASP

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	2	509/770 (66%)	509 (100%)	0	100	100
1	A	509/770 (66%)	509 (100%)	0	100	100
2	3	514/835 (62%)	513 (100%)	1 (0%)	94	96
2	B	514/835 (62%)	513 (100%)	1 (0%)	94	96
3	4	573/848 (68%)	573 (100%)	0	100	100
3	C	573/848 (68%)	573 (100%)	0	100	100
4	5	567/688 (82%)	566 (100%)	1 (0%)	94	96
4	D	567/688 (82%)	566 (100%)	1 (0%)	94	96
5	6	496/886 (56%)	496 (100%)	0	100	100
5	E	496/886 (56%)	496 (100%)	0	100	100
6	7	605/753 (80%)	605 (100%)	0	100	100
6	F	605/753 (80%)	605 (100%)	0	100	100
All	All	6528/9560 (68%)	6524 (100%)	4 (0%)	95	97

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	3	52	ASN
4	5	221	MET
2	B	52	ASN
4	D	221	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such

sidechains are listed below:

Mol	Chain	Res	Type
3	4	354	HIS
3	C	354	HIS

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 ⓘ

4 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$
9	ADP	3	1001	-	25,29,29	1.02	1 (4%)	24,45,45	1.70	4 (16%)
9	ADP	5	1001	-	25,29,29	1.00	1 (4%)	24,45,45	1.70	3 (12%)
9	ADP	B	1001	-	25,29,29	1.02	1 (4%)	24,45,45	1.71	4 (16%)
9	ADP	D	1001	-	25,29,29	1.00	1 (4%)	24,45,45	1.70	3 (12%)

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
9	ADP	3	1001	-	-	0/12/32/32	0/3/3/3
9	ADP	5	1001	-	-	0/12/32/32	0/3/3/3
9	ADP	B	1001	-	-	0/12/32/32	0/3/3/3
9	ADP	D	1001	-	-	0/12/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	3	1001	ADP	C5-C4	2.98	1.47	1.40
9	B	1001	ADP	C5-C4	2.98	1.47	1.40
9	D	1001	ADP	C5-C4	3.03	1.47	1.40
9	5	1001	ADP	C5-C4	3.04	1.47	1.40

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	1001	ADP	N3-C2-N1	-6.10	123.54	128.86
9	3	1001	ADP	N3-C2-N1	-6.09	123.56	128.86
9	D	1001	ADP	N3-C2-N1	-5.67	123.92	128.86
9	5	1001	ADP	N3-C2-N1	-5.65	123.94	128.86
9	B	1001	ADP	C4-C5-N7	-2.47	107.03	109.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 134 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	3	1001	ADP	35	0
9	5	1001	ADP	33	0
9	B	1001	ADP	34	0
9	D	1001	ADP	32	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
7	X	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	X	34:DT	O3'	35:DG	P	3.37
1	X	24:DC	O3'	25:DA	P	1.89
1	X	23:DG	O3'	24:DC	P	1.88