



wwPDB EM Validation Summary Report ⓘ

Mar 29, 2026 – 04:08 AM UTC

PDB ID : 5V8F / pdb_00005v8f
EMDB ID : EMD-8540
Title : Structural basis of MCM2-7 replicative helicase loading by ORC-Cdc6 and Cdt1
Authors : Yuan, Z.; Riera, A.; Bai, L.; Sun, J.; Spanos, C.; Chen, Z.A.; Barbon, M.; Rappsilber, J.; Stillman, B.; Speck, C.; Li, H.
Deposited on : 2017-03-21
Resolution : 3.90 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

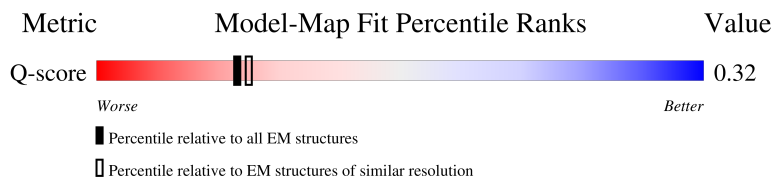
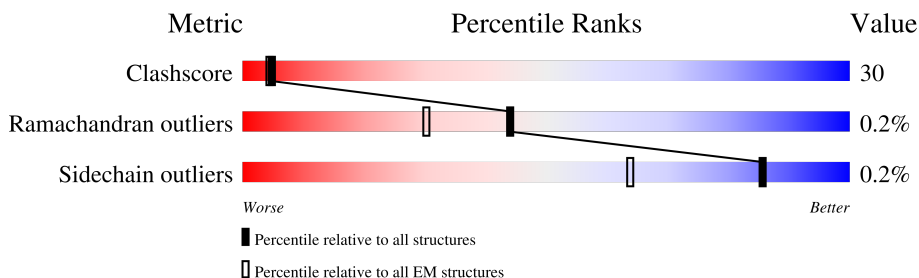
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8855 (3.40 - 4.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	2	868	21% 37% 32% 31%
2	3	971	60% 34% 33% 33%
3	4	933	17% 39% 40% 21%
4	5	775	75% 37% 37% 25%

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Mol	Chain	Length	Quality of chain
5	6	1017	
6	7	800	
7	8	604	
8	9	513	
9	A	913	
10	B	620	
11	C	616	
12	E	479	
13	D	529	
14	F	435	
15	M	39	
16	N	39	

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
17	AGS	2	2001	-	-	X	-
17	AGS	6	1101	-	-	X	-
17	AGS	7	2001	-	-	X	-

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 59586 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
			4735	2970	863	887	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	654	Total	C	N	O	S	0	0
			5134	3241	905	972	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	741	Total	C	N	O	S	0	0
			5891	3677	1030	1154	30		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	5	580	Total	C	N	O	S	0	0
			4527	2852	781	873	21		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	6	692	Total	C	N	O	S	0	0
			5512	3484	956	1048	24		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	7	725	Total	C	N	O	S	0	0
			5726	3610	990	1094	32		

- Molecule 7 is a protein called Cell division cycle protein CDT1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	8	519	Total	C	N	O	S	0	0
			4156	2644	715	778	19		

- Molecule 8 is a protein called Cell division control protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	9	373	Total	C	N	O	S	0	0
			2982	1914	497	554	17		

- Molecule 9 is a protein called Origin recognition complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	A	425	Total	C	N	O	S	0	0
			3399	2170	576	635	18		

- Molecule 10 is a protein called Origin recognition complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	B	328	Total	C	N	O	S	0	0
			2698	1747	448	487	16		

- Molecule 11 is a protein called Origin recognition complex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	C	544	Total	C	N	O	S	0	0
			4508	2911	743	838	16		

- Molecule 12 is a protein called Origin recognition complex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	E	422	Total	C	N	O	S	0	0
			3458	2253	549	643	13		

- Molecule 13 is a protein called Origin recognition complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	D	456	Total	C	N	O	S	0	0
			3698	2366	626	693	13		

- Molecule 14 is a protein called Origin recognition complex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	F	157	Total	C	N	O	S	0	0
			1315	846	222	235	12		

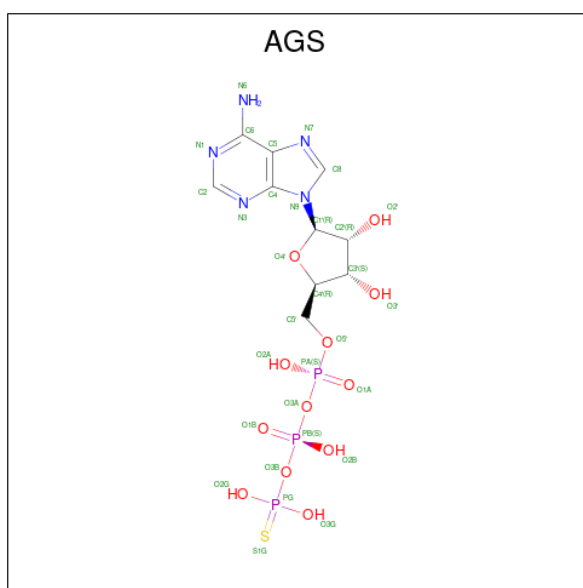
- Molecule 15 is a DNA chain called DNA (39-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
15	M	39	Total	C	N	O	P	0	0
			795	383	127	246	39		

- Molecule 16 is a DNA chain called DNA (39-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
16	N	39	Total	C	N	O	P	0	0
			804	382	161	222	39		

- Molecule 17 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$).

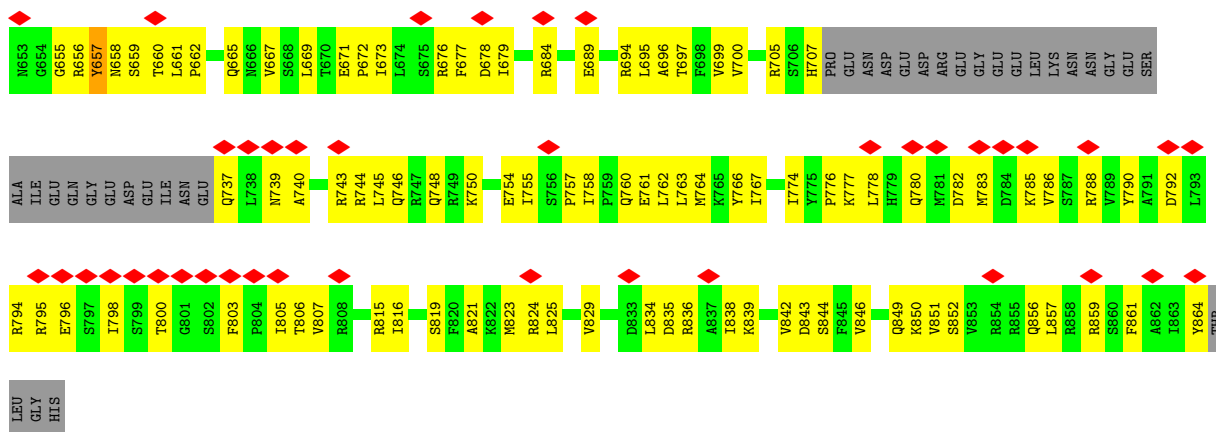


Mol	Chain	Residues	Atoms					AltConf	
17	2	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
17	4	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
17	6	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
17	7	1	Total 31	C 10	N 5	O 12	P 3	S 1	0

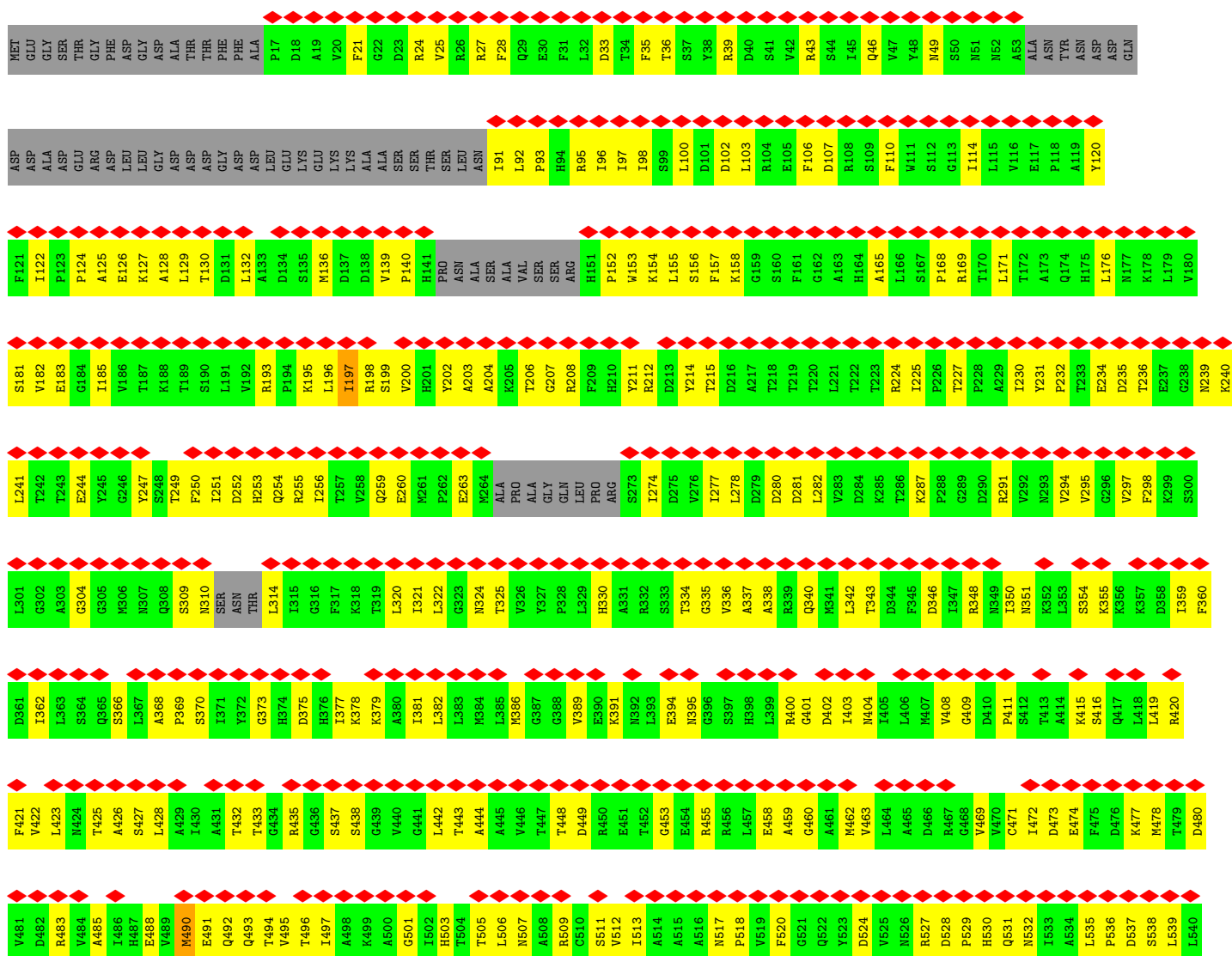
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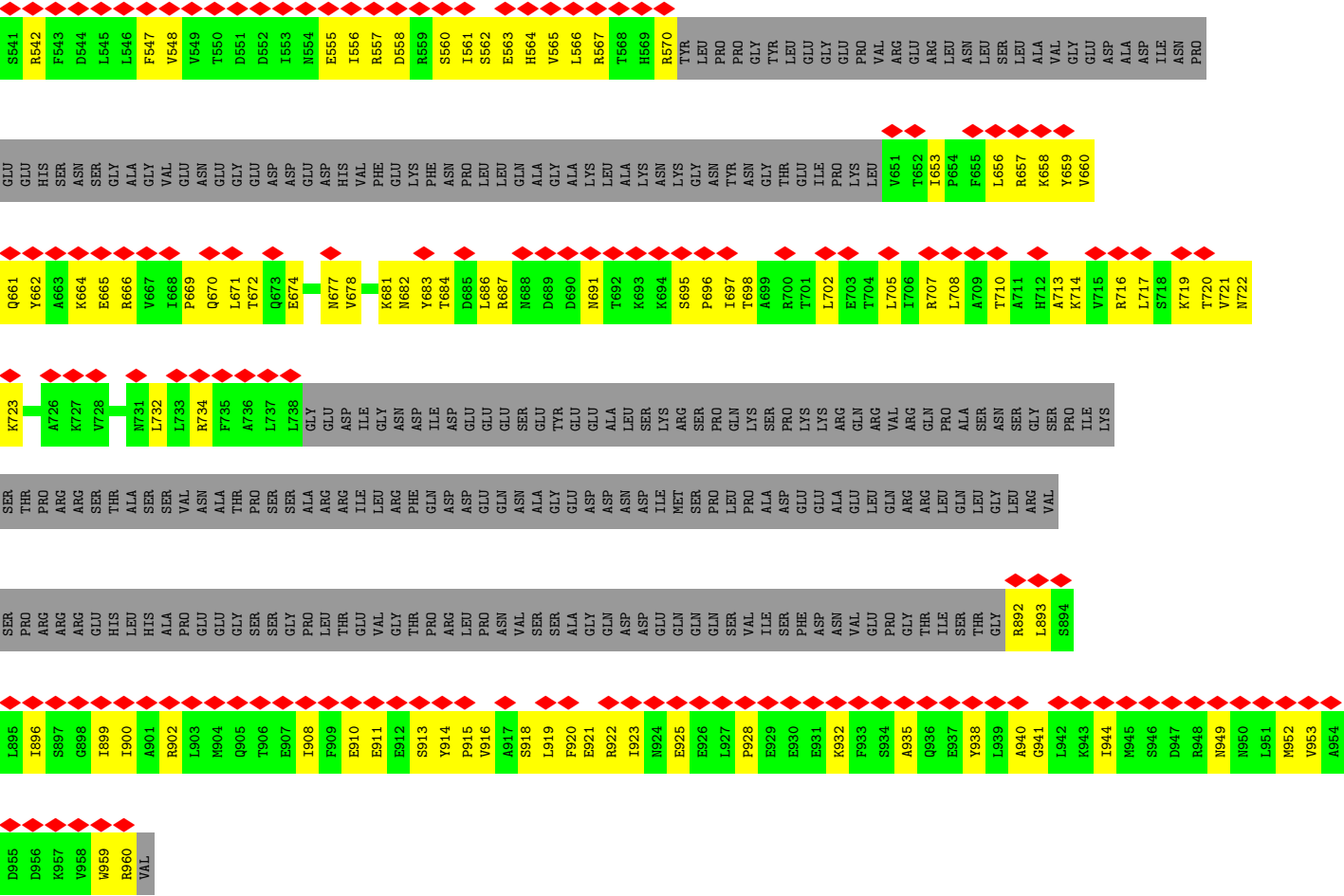
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Mol	Chain	Residues	Atoms						AltConf
17	9	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
17	A	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
17	E	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
17	D	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	

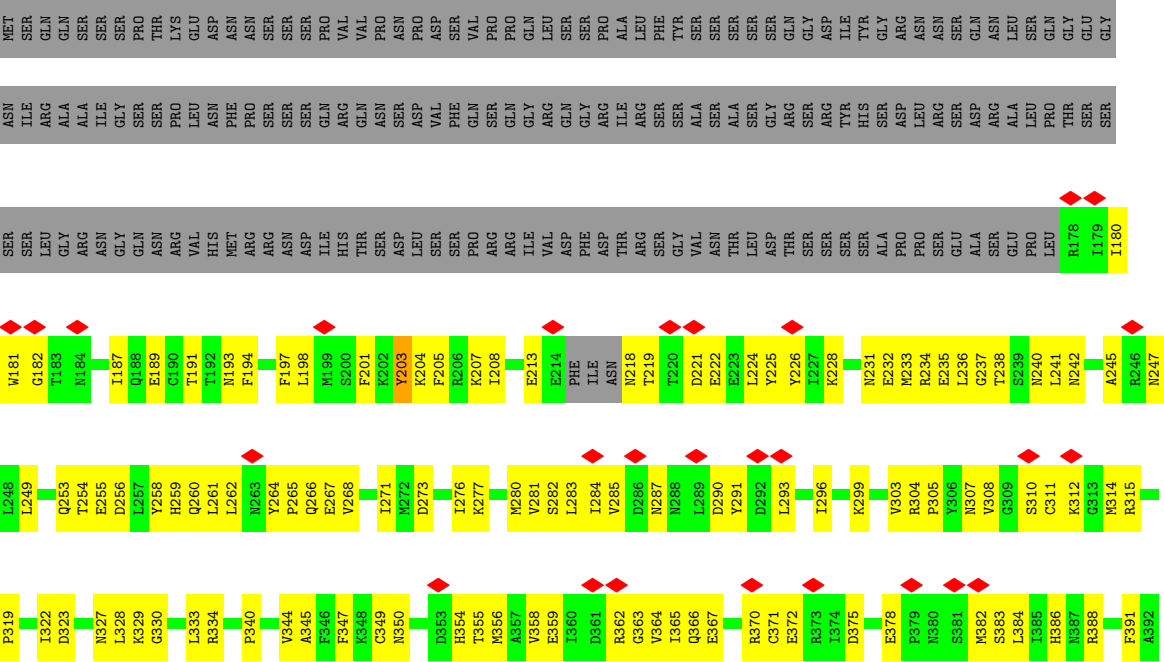


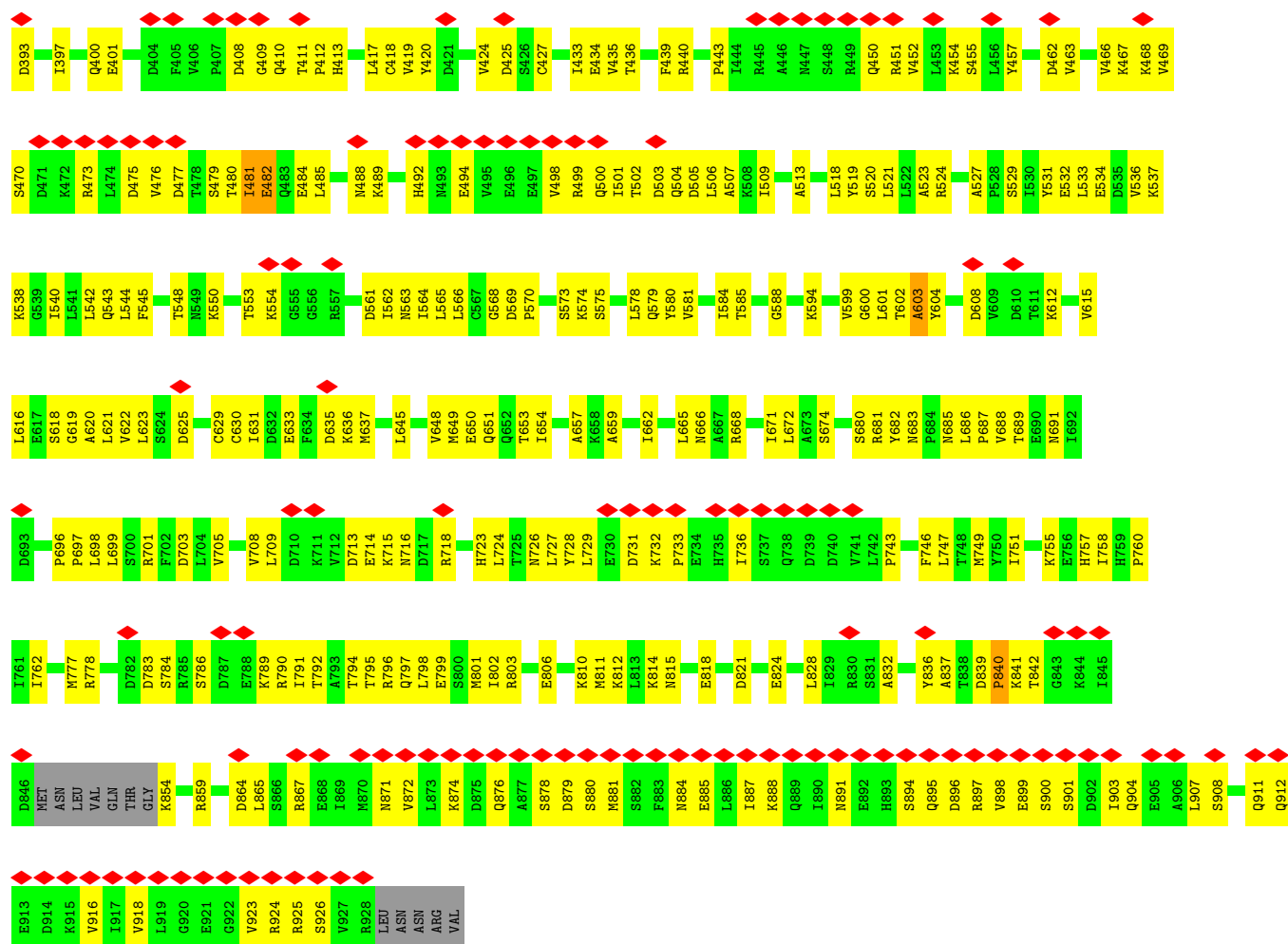
● Molecule 2: DNA replication licensing factor MCM3



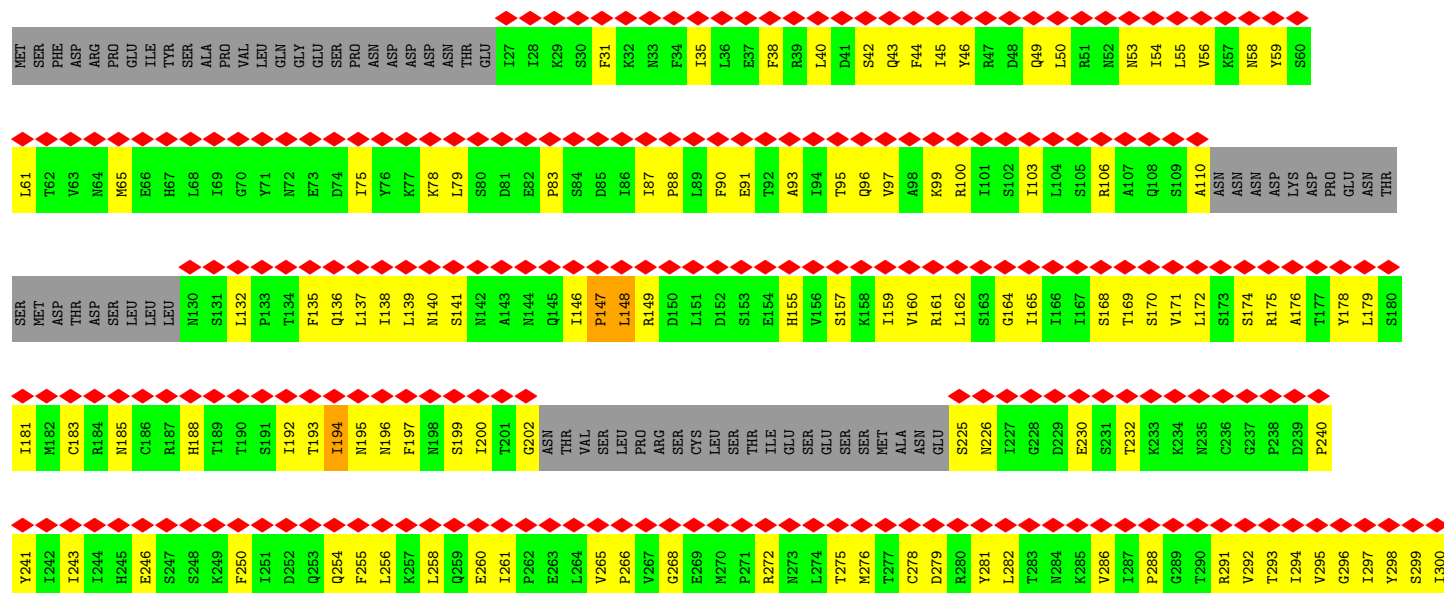
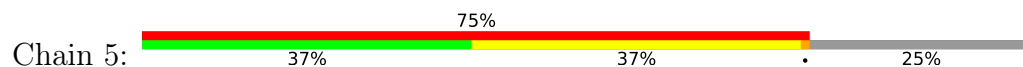


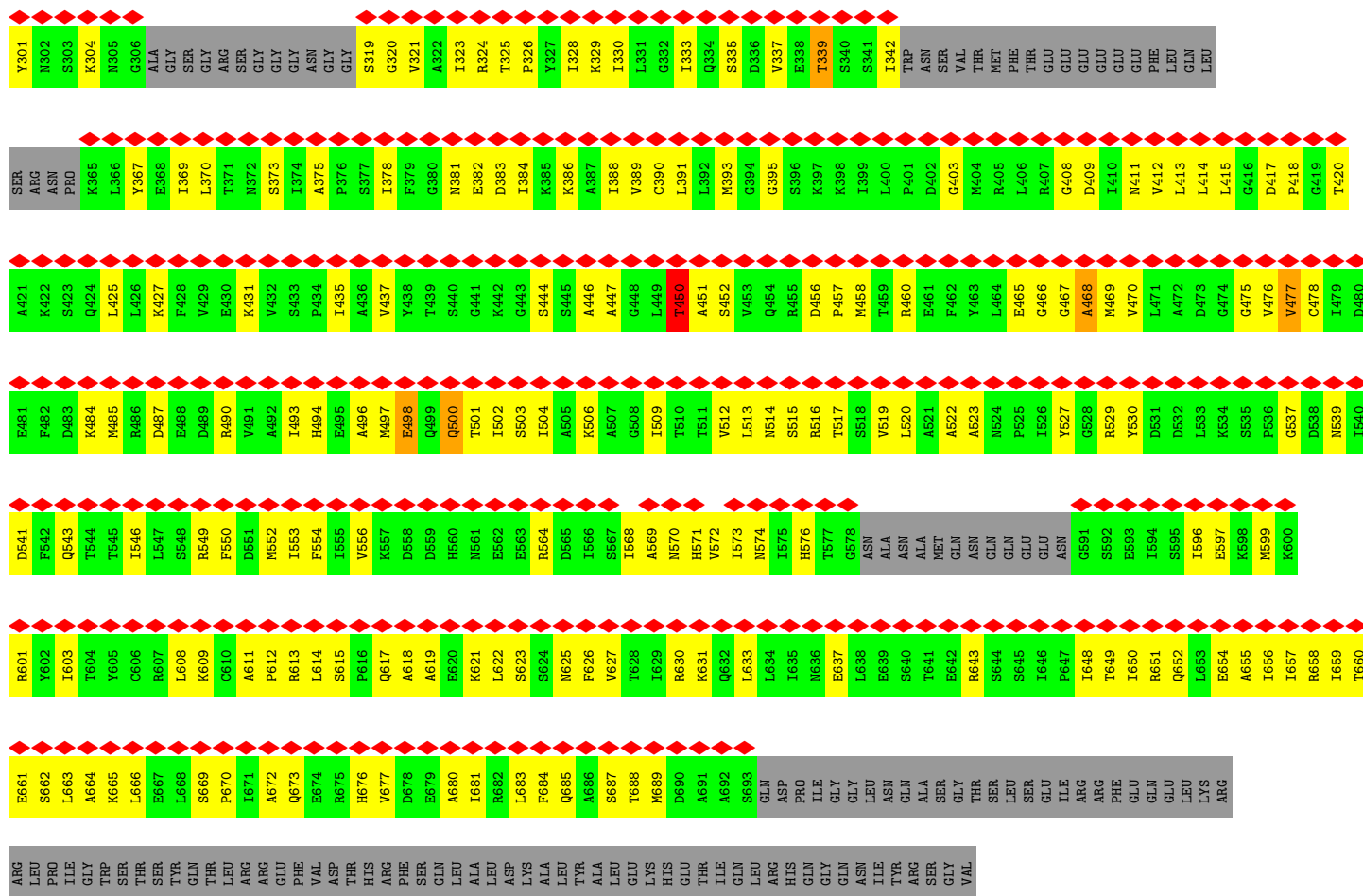
● Molecule 3: DNA replication licensing factor MCM4



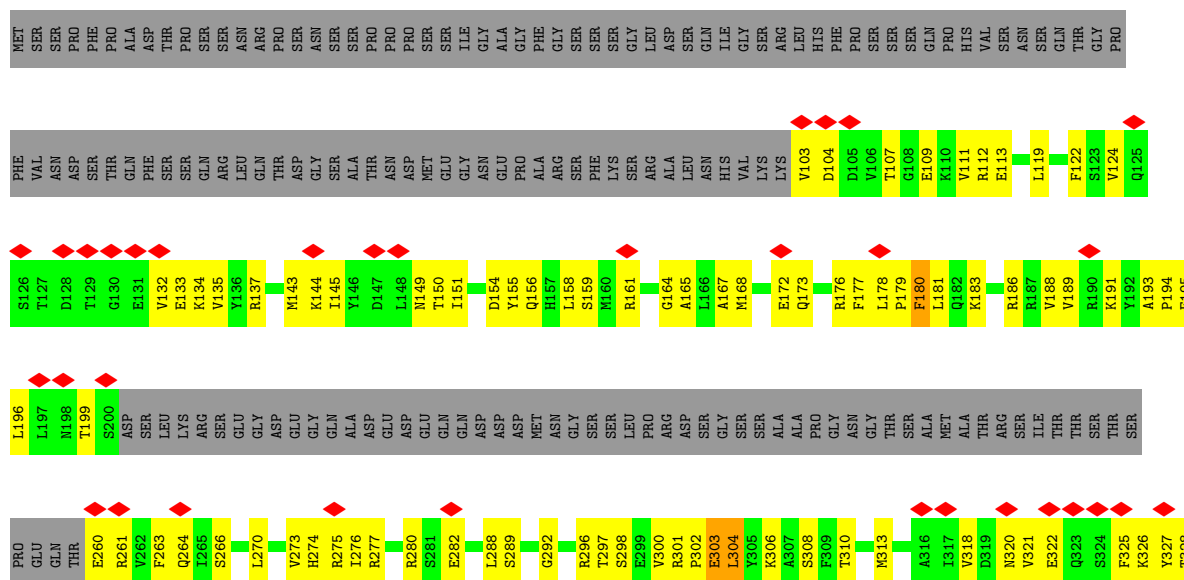


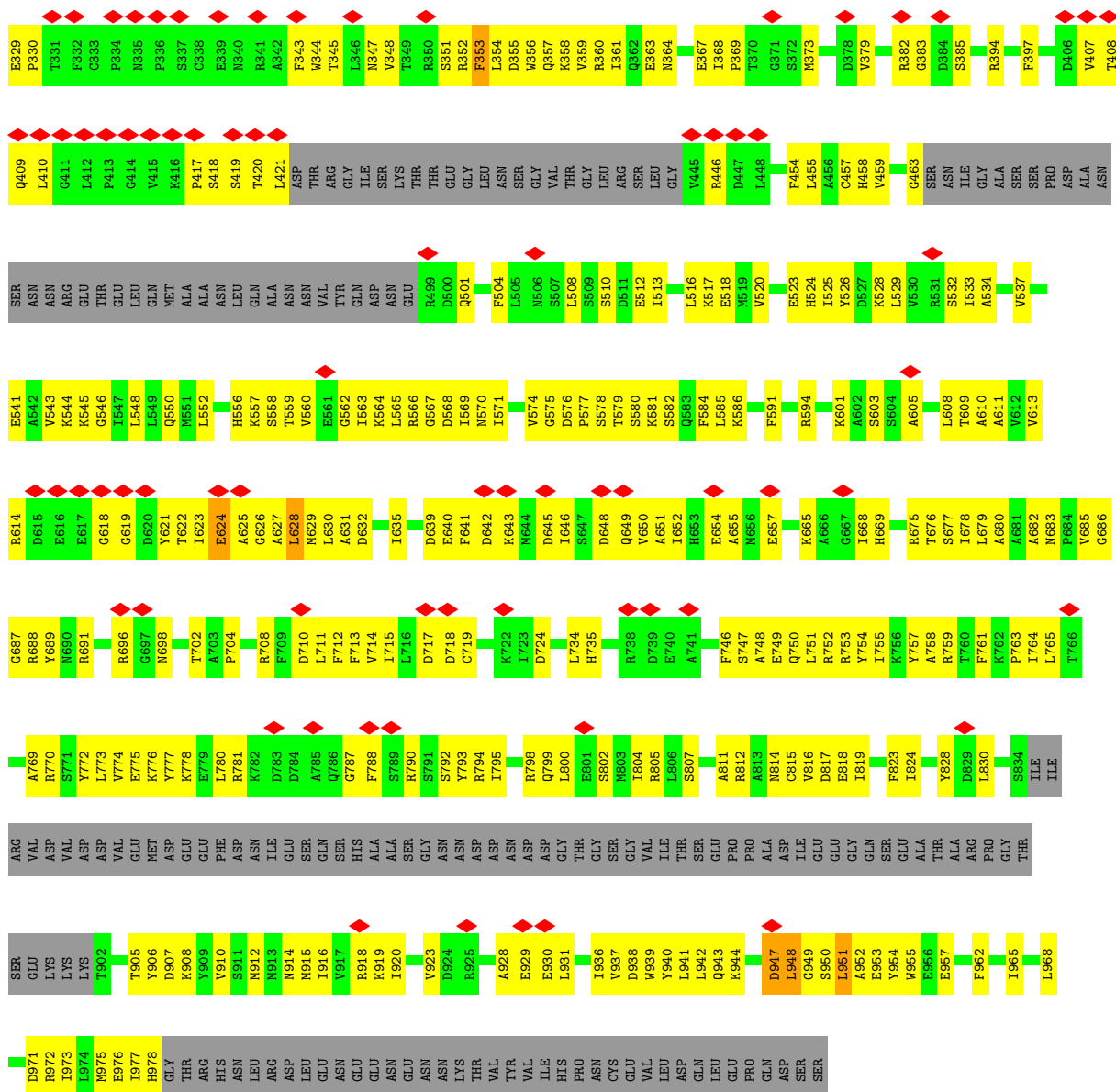
● Molecule 4: Minichromosome maintenance protein 5



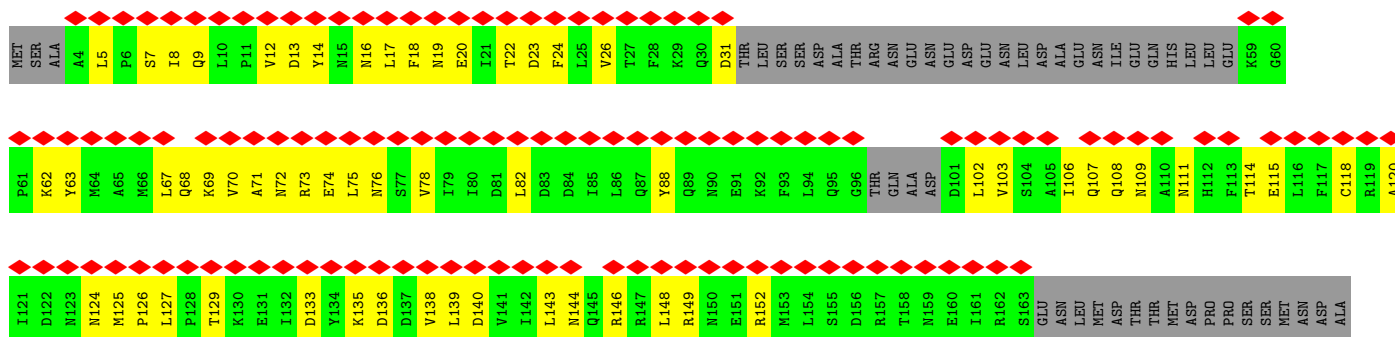


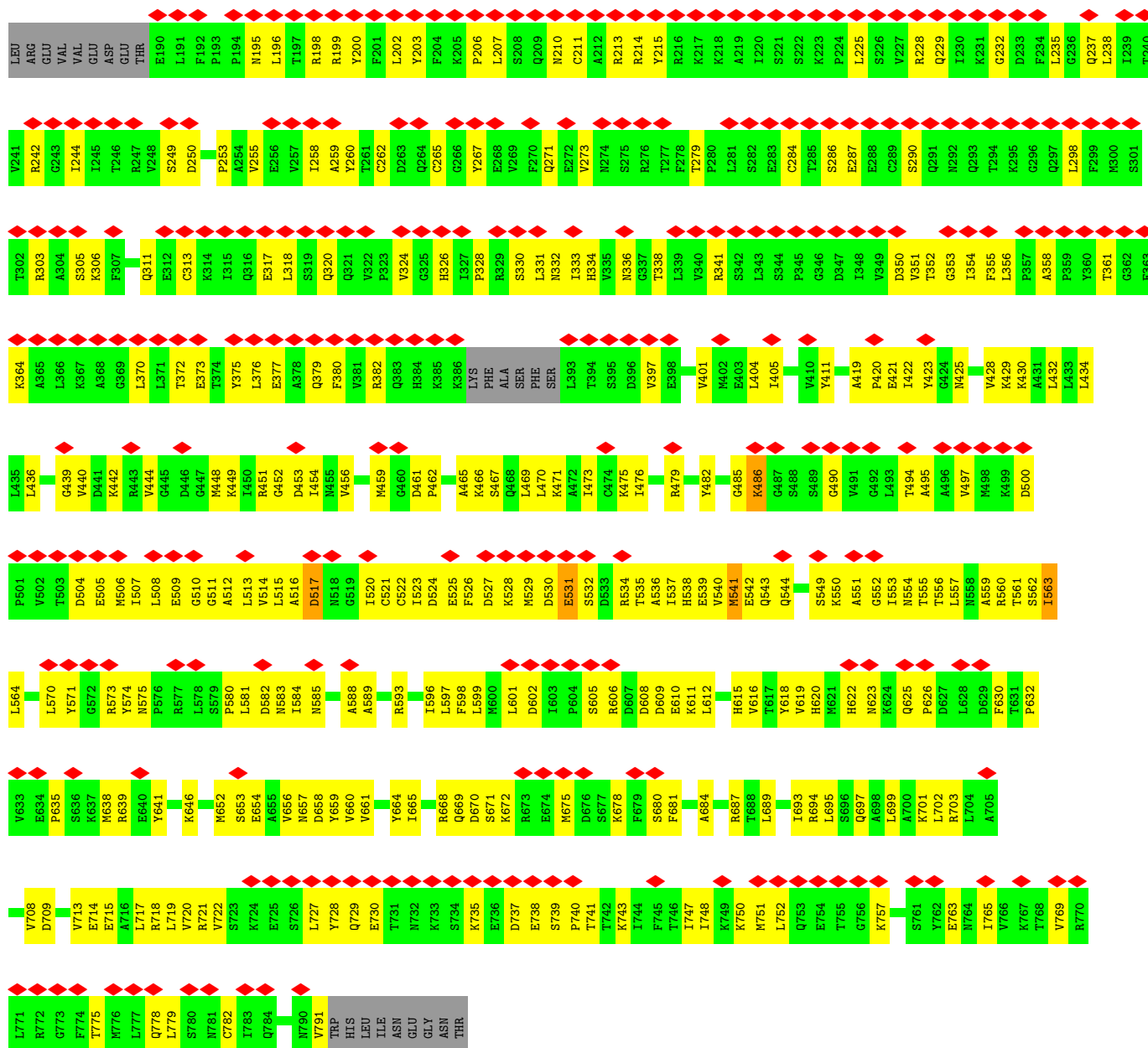
• Molecule 5: DNA replication licensing factor MCM6



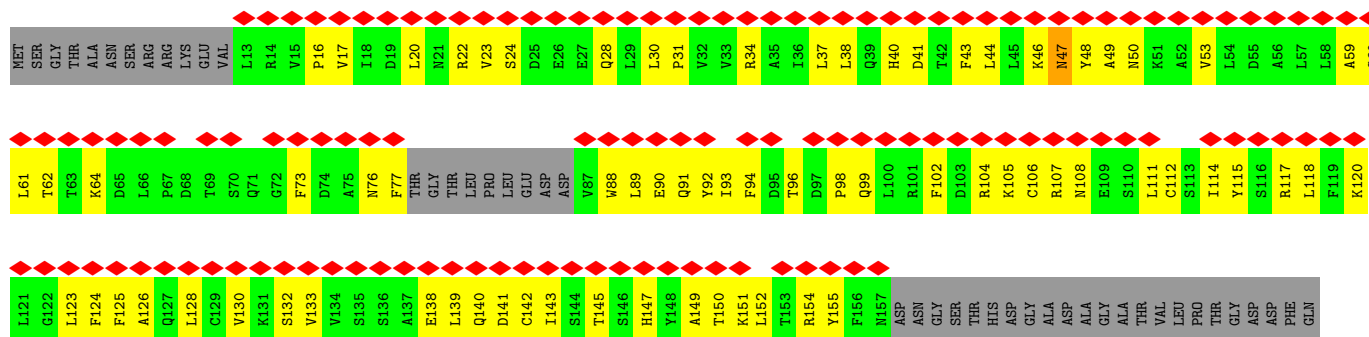


• Molecule 6: DNA replication licensing factor MCM7

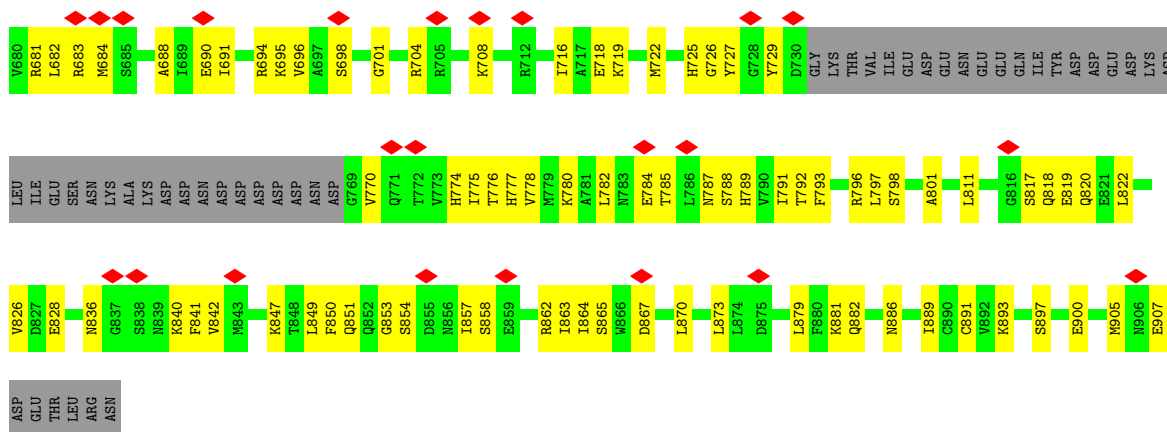




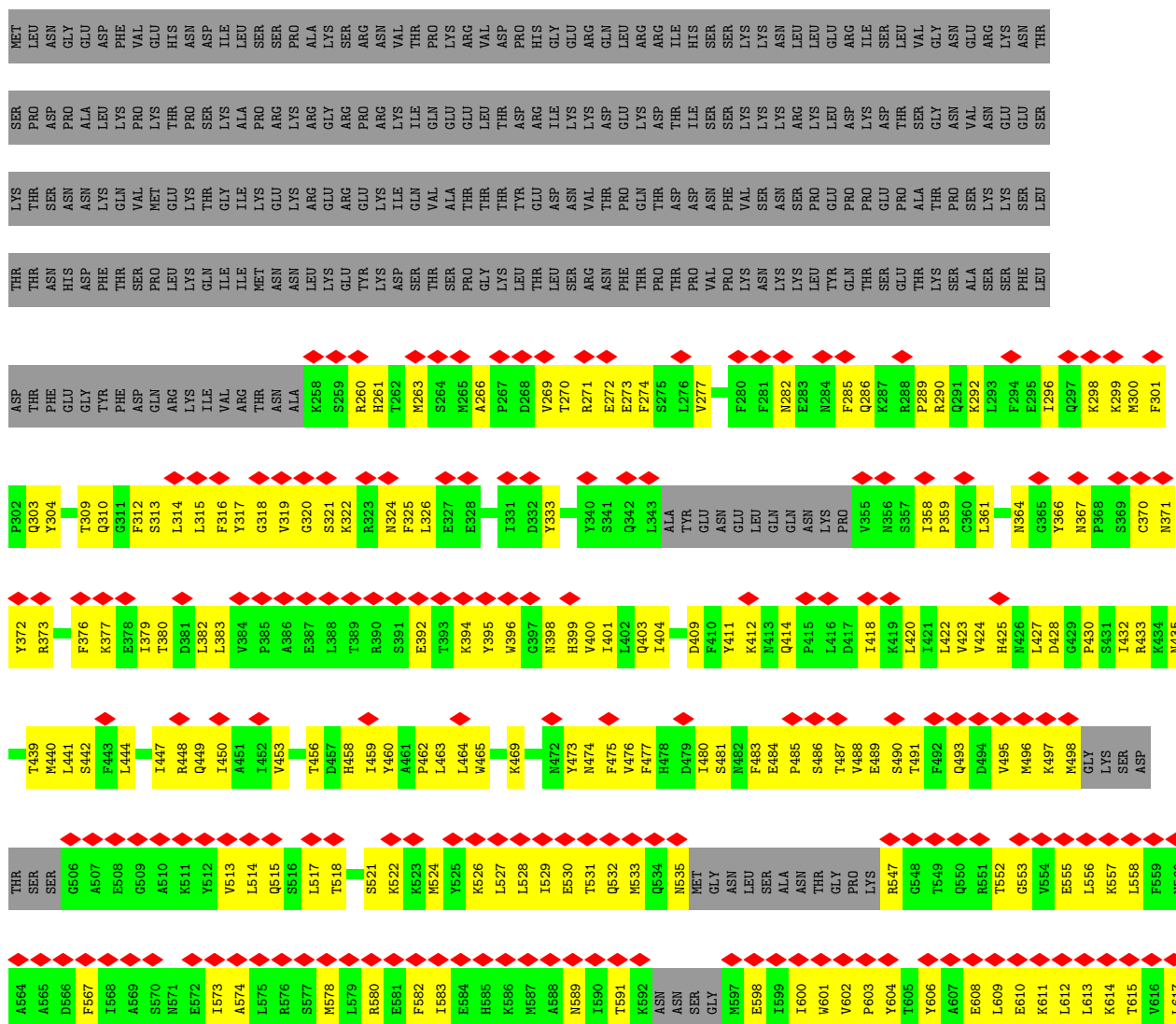
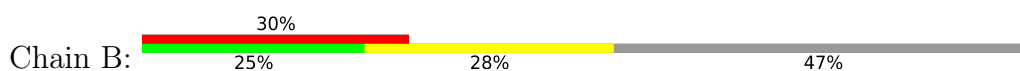
● Molecule 7: Cell division cycle protein CDT1







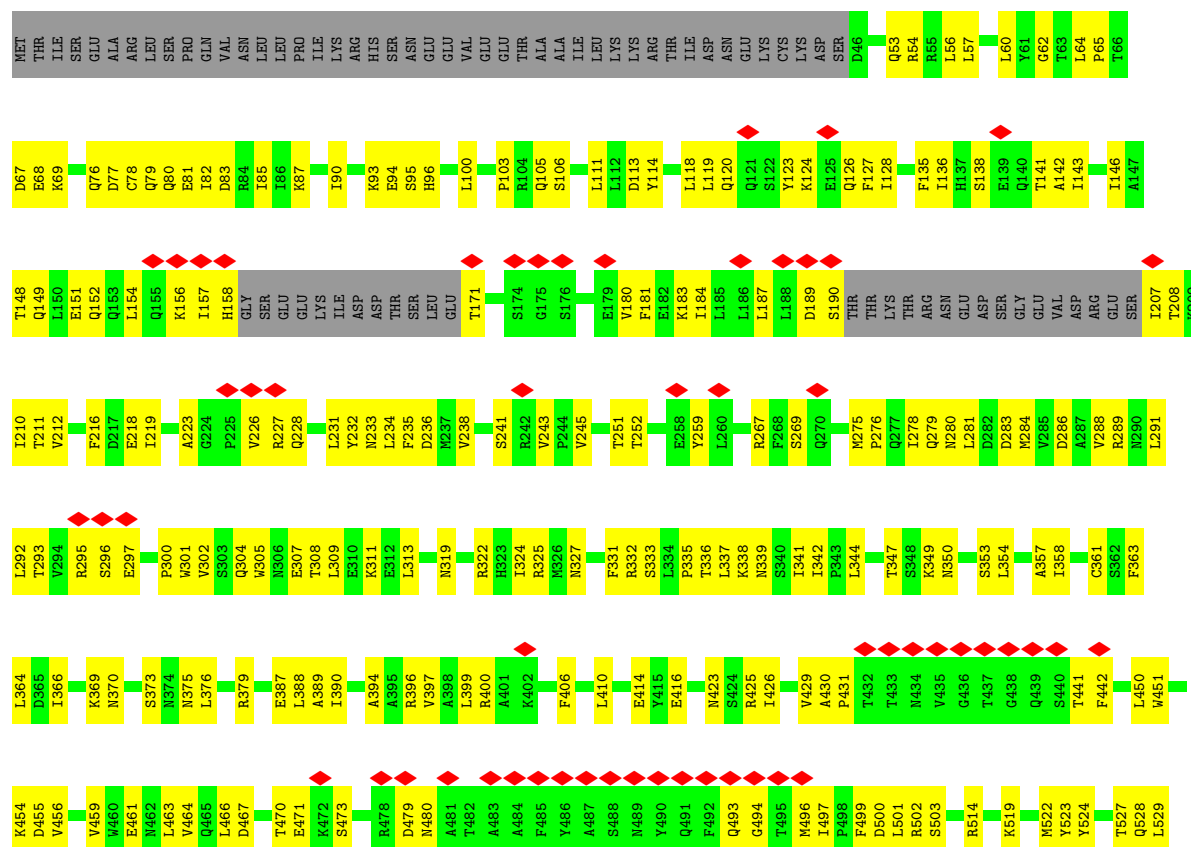
• Molecule 10: Origin recognition complex subunit 2



• Molecule 11: Origin recognition complex subunit 3



- Molecule 13: Origin recognition complex subunit 4



- Molecule 14: Origin recognition complex subunit 6



W421 W422 W423 W424 W425 W426 W427 W428 W429 W430	LEU THR GLU PRO LEU	D361 V362 I363 E364 C365 V366 K367 L368 V369 K370 E371 L372 I373 L374 G375 E376 K377 W378 F379 R380 D381 L382 K383 I384 R385 Y386 D387 D388 F389 ASP GLY ILE	K301 I302 V303 D304 E305 V306 K307 L308 N309 A310 S311 R312 L313 V314 C315 P316 W317 Q318 L319 V320 C321 G322 L323 V324 L325 N326 C327 T328 F329 I330 V331 F332 N333 E334 R335 R336 R337 K338 D339 P340 R341 I342 D343 H344 F345 I346 V347 S348 K349 M350 C351 S352 L353 M354 L356 T356 S357 K358 V359 D360	GLY THR GLN ASN LYS ALA VAL GLY LYS PRO GLN SER GLU LEU THR ALA ALA LEU LYS ARG GLY ILE PRO ASN	S271 L272 L273 V274 K275 K276 Y277 C278 K279 M280 T281 T282 E283 E284 I285 I286 R287 L288 C289 N290 D291 F292 E293 L294 R295 R296 E297 V298 A299 Y300
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Chain M: 23% 74% 77%

[illegible]

Chain N: 28% 67% 72%

A45	A46	A47	A48	A49	A50	A51	A52	A53	A54	A55	A56	A57	A58	A59	A60	A61	A62	A63	A64	A65	A66	A67	A68	A69	A70	A71	A72	A73	A74	A75	A76	A77	A78	A79	A80	A81	A82	A83
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	304288	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	0.108	Depositor
Minimum map value	-0.039	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.021	Depositor
Map size (Å)	258.56, 258.56, 258.56	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.01, 1.01, 1.01	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	2	0.31	2/4809 (0.0%)	0.52	4/6492 (0.1%)
2	3	0.21	0/5218	0.49	6/7063 (0.1%)
3	4	0.33	0/5968	0.55	1/8055 (0.0%)
4	5	0.19	0/4587	0.55	5/6193 (0.1%)
5	6	0.36	0/5601	0.55	6/7558 (0.1%)
6	7	0.22	0/5811	0.49	2/7848 (0.0%)
7	8	0.22	0/4232	0.52	1/5732 (0.0%)
8	9	0.20	0/3025	0.52	1/4070 (0.0%)
9	A	0.27	0/3448	0.43	0/4639
10	B	0.20	0/2756	0.41	0/3717
11	C	0.24	0/4605	0.41	0/6215
12	E	0.34	0/3540	0.47	3/4812 (0.1%)
13	D	0.34	0/3764	0.43	0/5092
14	F	0.16	0/1336	0.43	0/1798
15	M	0.23	0/886	0.45	0/1366
16	N	0.26	0/906	0.37	0/1395
All	All	0.27	2/60492 (0.0%)	0.49	29/82045 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	575	GLY	C-N	8.93	1.44	1.33
1	2	644	CYS	C-N	6.28	1.41	1.33

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	3	337	ALA	N-CA-C	7.53	119.49	111.28
7	8	47	ASN	N-CA-C	7.48	121.71	111.54
4	5	339	THR	N-CA-C	7.26	120.20	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	5	450	THR	N-CA-C	-7.19	97.53	108.96
4	5	468	ALA	N-CA-C	-7.10	103.54	111.28

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	4735	0	4759	307	0
2	3	5134	0	5181	340	0
3	4	5891	0	5933	404	0
4	5	4527	0	4641	294	0
5	6	5512	0	5530	473	0
6	7	5726	0	5814	382	0
7	8	4156	0	4225	334	0
8	9	2982	0	3107	201	0
9	A	3399	0	3475	183	0
10	B	2698	0	2713	199	0
11	C	4508	0	4465	250	0
12	E	3458	0	3465	178	0
13	D	3698	0	3755	172	0
14	F	1315	0	1353	64	0
15	M	795	0	448	46	0
16	N	804	0	436	61	0
17	2	31	0	12	11	0
17	4	31	0	12	8	0
17	6	31	0	12	10	0
17	7	31	0	12	11	0
17	9	31	0	12	5	0
17	A	31	0	12	7	0
17	D	31	0	12	5	0
17	E	31	0	12	6	0
All	All	59586	0	59396	3547	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 30.

The worst 5 of 3547 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)
6:7:541:MET:HG3	6:7:593:ARG:CD	1.45	1.46
6:7:541:MET:CG	6:7:593:ARG:HD3	1.50	1.39
4:5:470:VAL:HG22	4:5:513:LEU:CD2	1.52	1.39
5:6:977:ILE:HG22	5:6:978:HIS:CD2	1.57	1.38
5:6:394:ARG:HD3	5:6:594:ARG:CD	1.52	1.38

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	595/868 (68%)	526 (88%)	68 (11%)	1 (0%)	43	74
2	3	640/971 (66%)	562 (88%)	78 (12%)	0	100	100
3	4	735/933 (79%)	629 (86%)	102 (14%)	4 (0%)	24	59
4	5	568/775 (73%)	500 (88%)	64 (11%)	4 (1%)	18	53
5	6	682/1017 (67%)	606 (89%)	76 (11%)	0	100	100
6	7	715/800 (89%)	631 (88%)	83 (12%)	1 (0%)	48	80
7	8	509/604 (84%)	417 (82%)	89 (18%)	3 (1%)	21	55
8	9	365/513 (71%)	324 (89%)	40 (11%)	1 (0%)	36	69
9	A	413/913 (45%)	371 (90%)	42 (10%)	0	100	100
10	B	318/620 (51%)	293 (92%)	25 (8%)	0	100	100
11	C	536/616 (87%)	495 (92%)	41 (8%)	0	100	100
12	E	414/479 (86%)	384 (93%)	30 (7%)	0	100	100
13	D	450/529 (85%)	408 (91%)	42 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	F	153/435 (35%)	146 (95%)	7 (5%)	0	100	100
All	All	7093/10073 (70%)	6292 (89%)	787 (11%)	14 (0%)	44	74

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	4	603	ALA
4	5	500	GLN
8	9	232	ASN
3	4	481	ILE
7	8	142	CYS

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	510/770 (66%)	509 (100%)	1 (0%)	87	87
2	3	564/835 (68%)	564 (100%)	0	100	100
3	4	668/848 (79%)	667 (100%)	1 (0%)	88	89
4	5	516/688 (75%)	513 (99%)	3 (1%)	78	80
5	6	603/886 (68%)	599 (99%)	4 (1%)	76	78
6	7	644/714 (90%)	642 (100%)	2 (0%)	86	85
7	8	473/545 (87%)	472 (100%)	1 (0%)	87	87
8	9	341/470 (73%)	341 (100%)	0	100	100
9	A	376/812 (46%)	375 (100%)	1 (0%)	86	85
10	B	302/573 (53%)	302 (100%)	0	100	100
11	C	506/576 (88%)	506 (100%)	0	100	100
12	E	394/440 (90%)	394 (100%)	0	100	100
13	D	420/488 (86%)	419 (100%)	1 (0%)	87	87
14	F	151/406 (37%)	151 (100%)	0	100	100
All	All	6468/9051 (72%)	6454 (100%)	14 (0%)	85	87

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	6	304	LEU
5	6	353	PHE
13	D	231	LEU
7	8	263	TRP
9	A	486	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 135 such sidechains are listed below:

Mol	Chain	Res	Type
12	E	231	GLN
12	E	391	GLN
13	D	528	GLN
5	6	524	HIS
5	6	514	ASN

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](#)

8 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
17	AGS	4	2001	-	32,33,33	1.04	3 (9%)	45,52,52	0.92	1 (2%)
17	AGS	E	2001	-	32,33,33	1.06	3 (9%)	45,52,52	0.80	1 (2%)
17	AGS	D	2001	-	32,33,33	1.07	3 (9%)	45,52,52	1.05	1 (2%)
17	AGS	A	2001	-	32,33,33	0.84	3 (9%)	45,52,52	0.80	1 (2%)
17	AGS	2	2001	-	32,33,33	1.25	3 (9%)	45,52,52	0.95	1 (2%)
17	AGS	9	2001	-	32,33,33	0.72	2 (6%)	45,52,52	0.85	1 (2%)
17	AGS	7	2001	-	32,33,33	0.86	3 (9%)	45,52,52	0.84	1 (2%)
17	AGS	6	1101	-	32,33,33	2.04	6 (18%)	45,52,52	1.89	10 (22%)

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
17	AGS	4	2001	-	-	5/21/38/38	0/3/3/3
17	AGS	E	2001	-	-	9/21/38/38	0/3/3/3
17	AGS	D	2001	-	-	2/21/38/38	0/3/3/3
17	AGS	A	2001	-	-	9/21/38/38	0/3/3/3
17	AGS	2	2001	-	-	8/21/38/38	0/3/3/3
17	AGS	9	2001	-	-	5/21/38/38	0/3/3/3
17	AGS	7	2001	-	-	2/21/38/38	0/3/3/3
17	AGS	6	1101	-	-	1/21/38/38	0/3/3/3

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	6	1101	AGS	PG-S1G	7.98	2.08	1.90
17	6	1101	AGS	C5-C4	4.75	1.47	1.39
17	E	2001	AGS	PB-O3A	-3.83	1.55	1.59
17	2	2001	AGS	PB-O3B	-3.78	1.55	1.59
17	D	2001	AGS	PB-O3B	-3.69	1.55	1.59

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	D	2001	AGS	PB-O3B-PG	-6.41	109.70	133.17
17	6	1101	AGS	C5-C4-N3	-5.84	118.68	126.72
17	2	2001	AGS	PB-O3B-PG	-5.50	113.05	133.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	4	2001	AGS	PB-O3B-PG	-5.41	113.38	133.17
17	9	2001	AGS	PB-O3B-PG	-4.89	115.28	133.17

There are no chirality outliers.

5 of 41 torsion outliers are listed below:

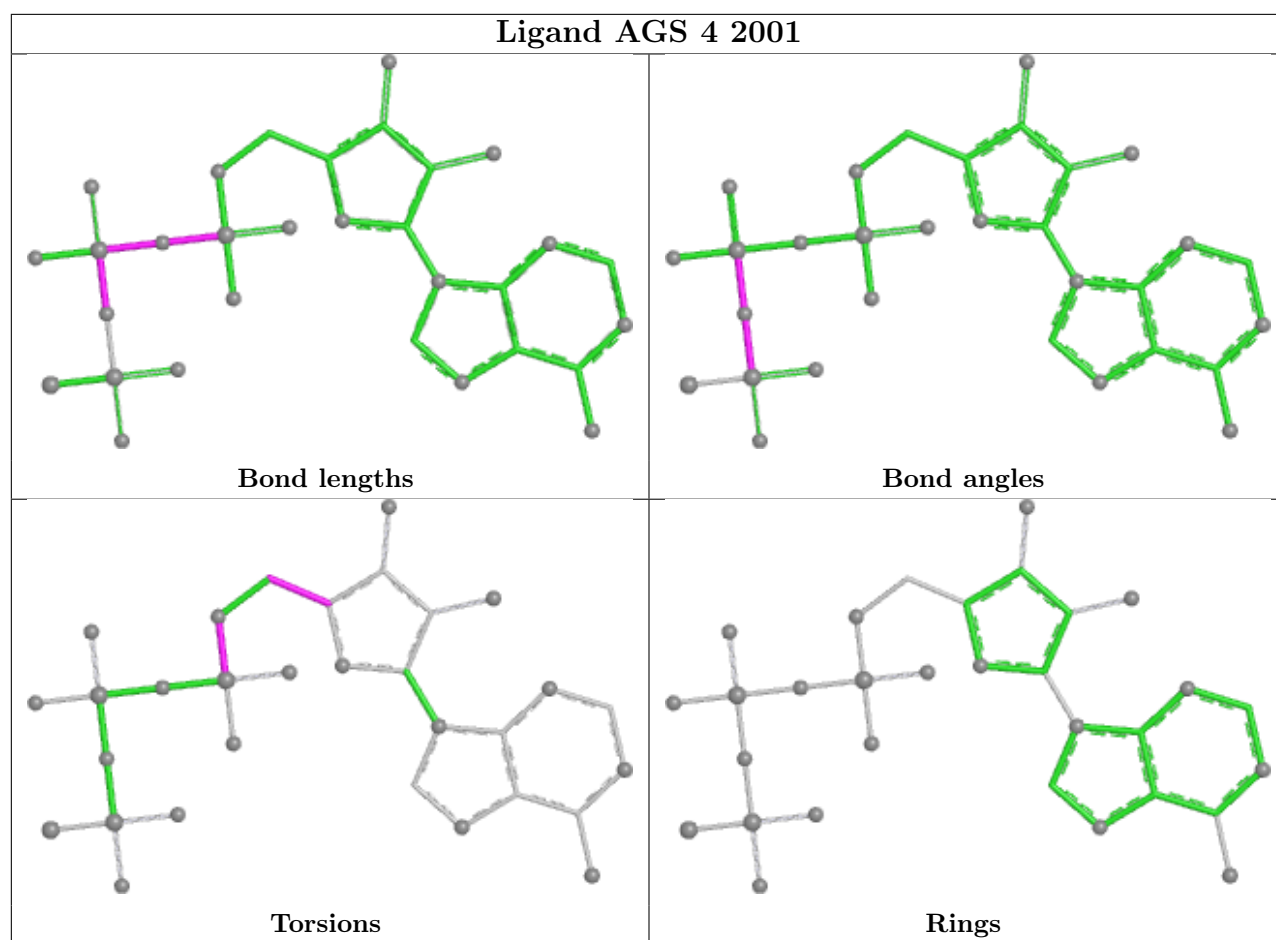
Mol	Chain	Res	Type	Atoms
17	2	2001	AGS	PB-O3B-PG-O2G
17	2	2001	AGS	PB-O3B-PG-O3G
17	2	2001	AGS	C5'-O5'-PA-O2A
17	2	2001	AGS	C5'-O5'-PA-O3A
17	4	2001	AGS	C5'-O5'-PA-O1A

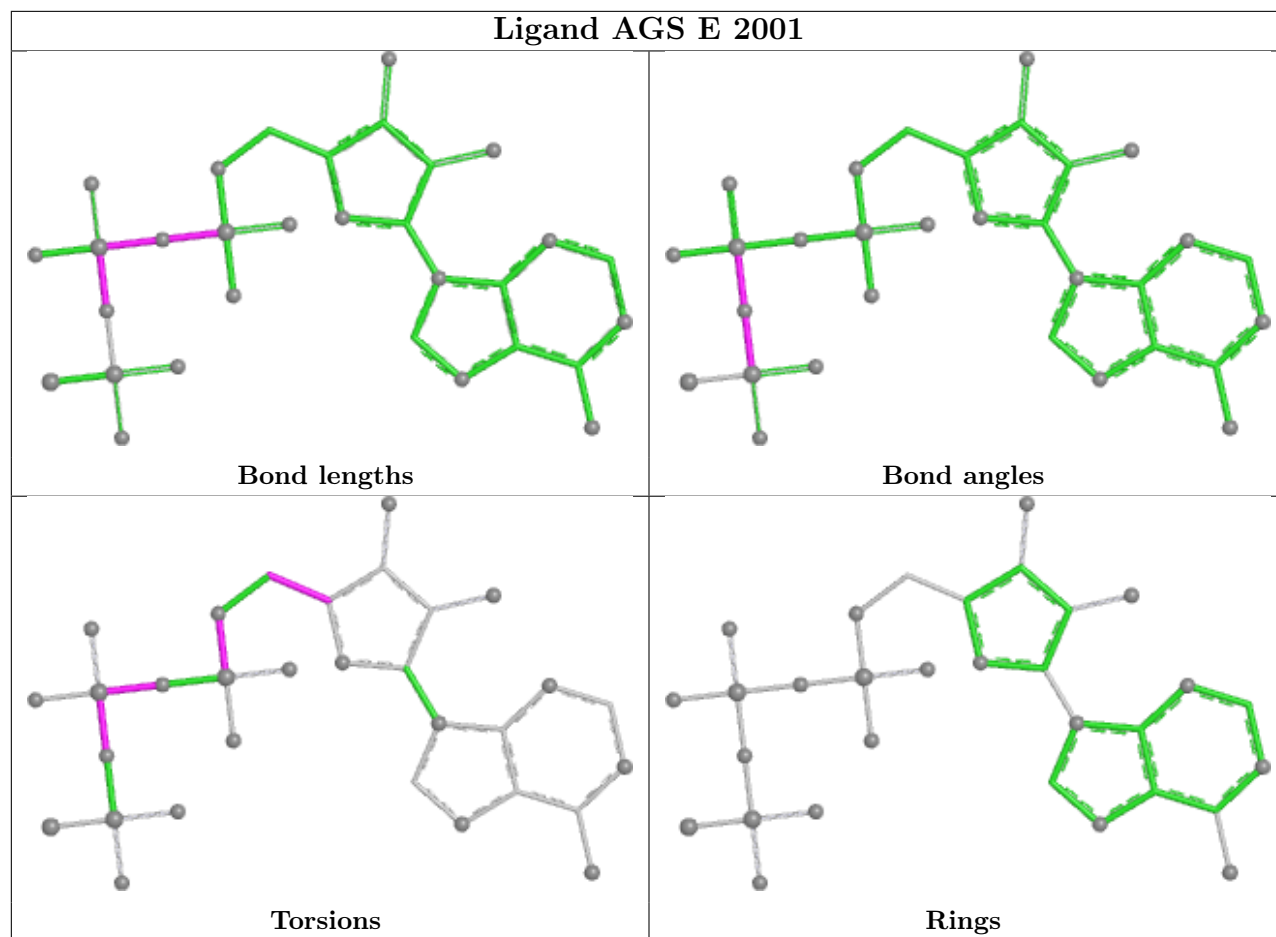
There are no ring outliers.

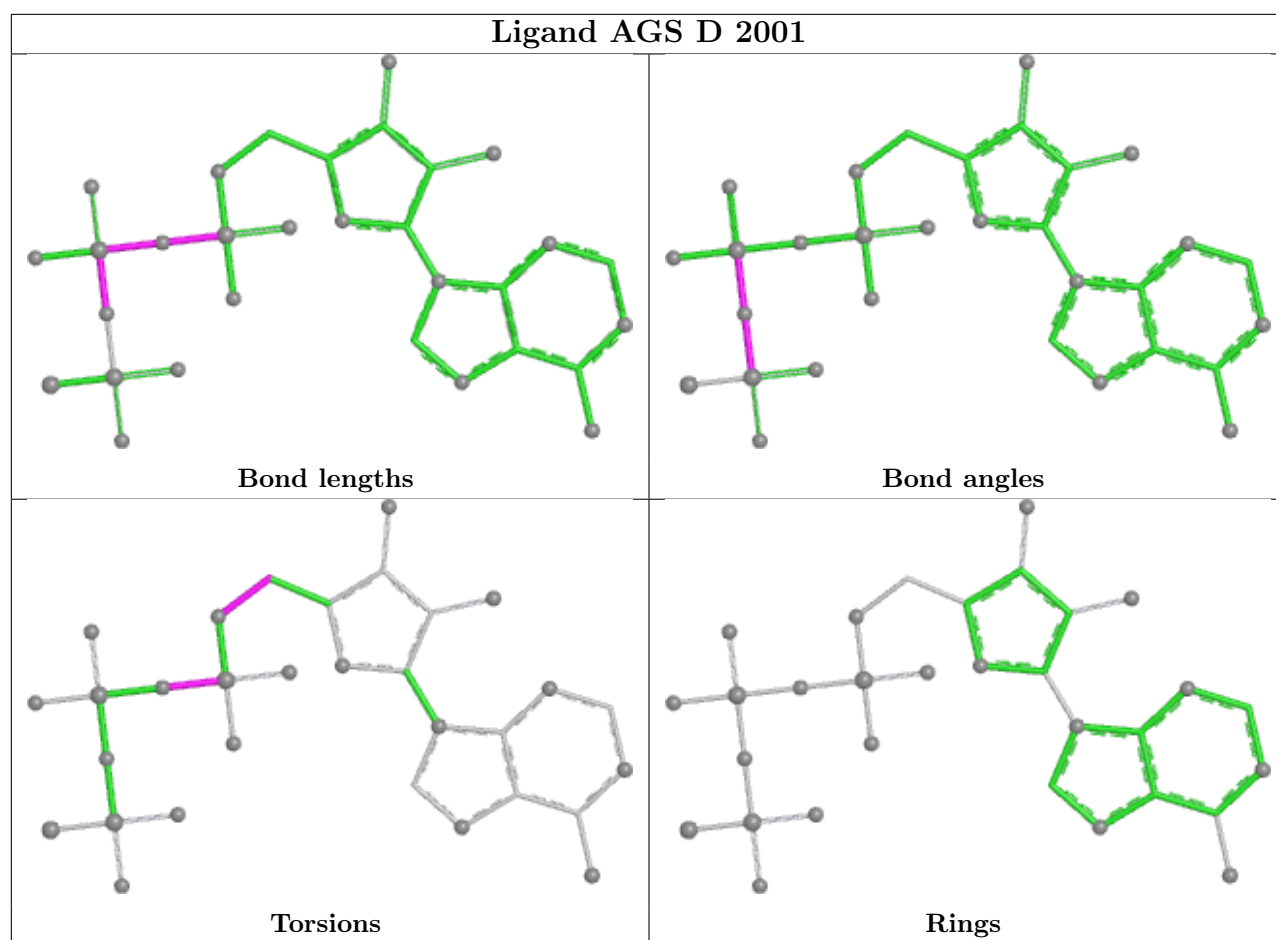
8 monomers are involved in 63 short contacts:

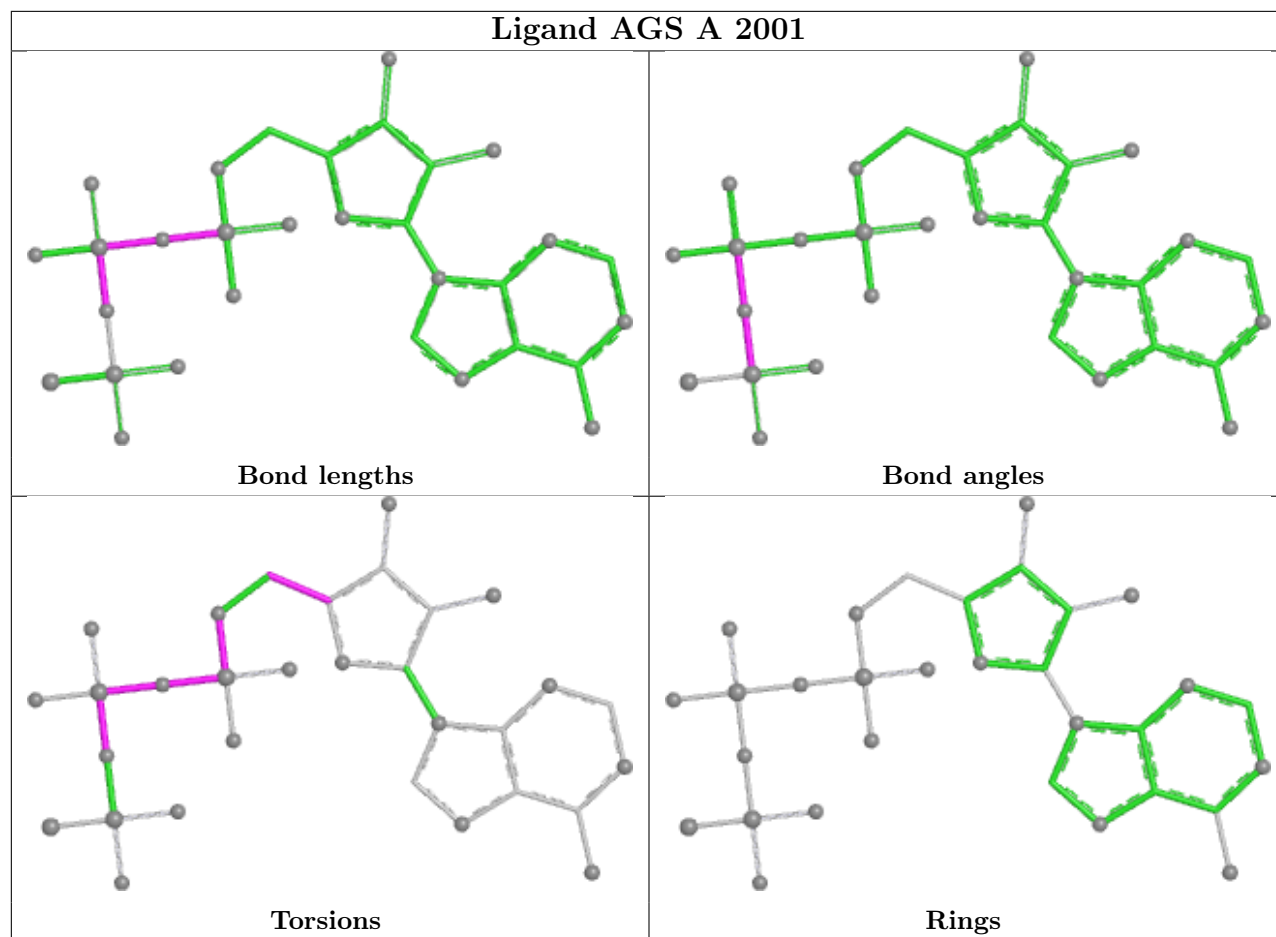
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	4	2001	AGS	8	0
17	E	2001	AGS	6	0
17	D	2001	AGS	5	0
17	A	2001	AGS	7	0
17	2	2001	AGS	11	0
17	9	2001	AGS	5	0
17	7	2001	AGS	11	0
17	6	1101	AGS	10	0

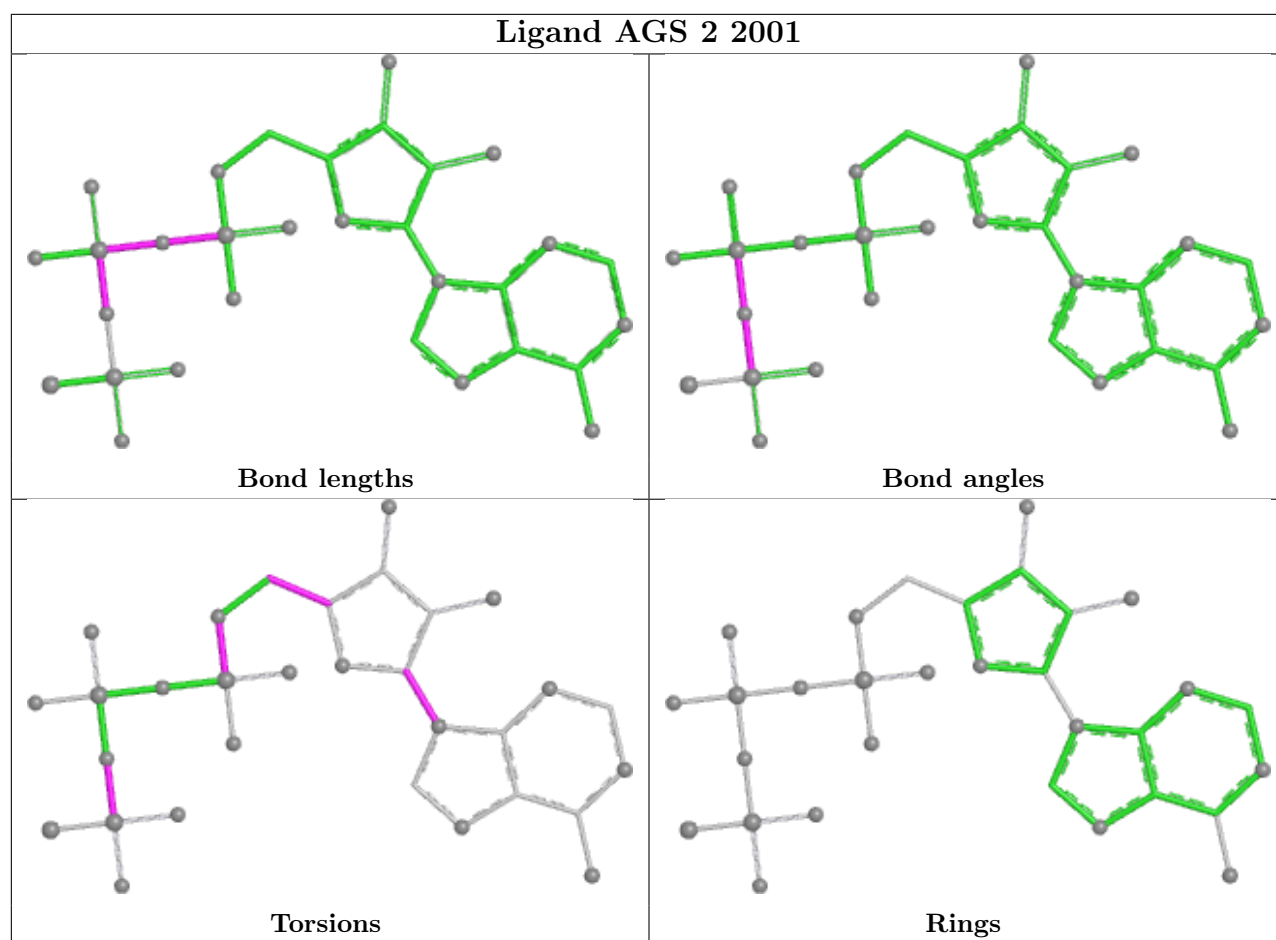
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

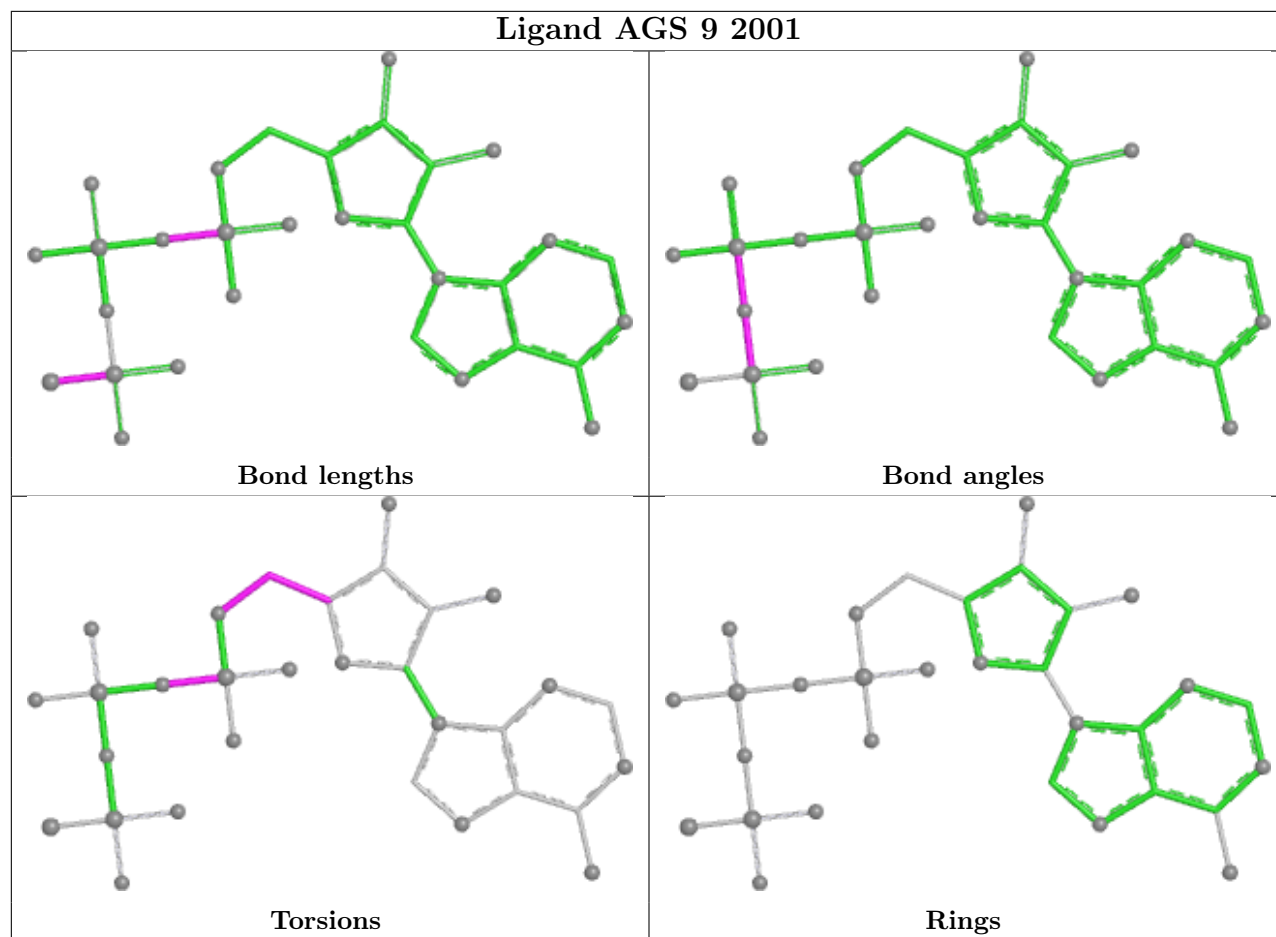


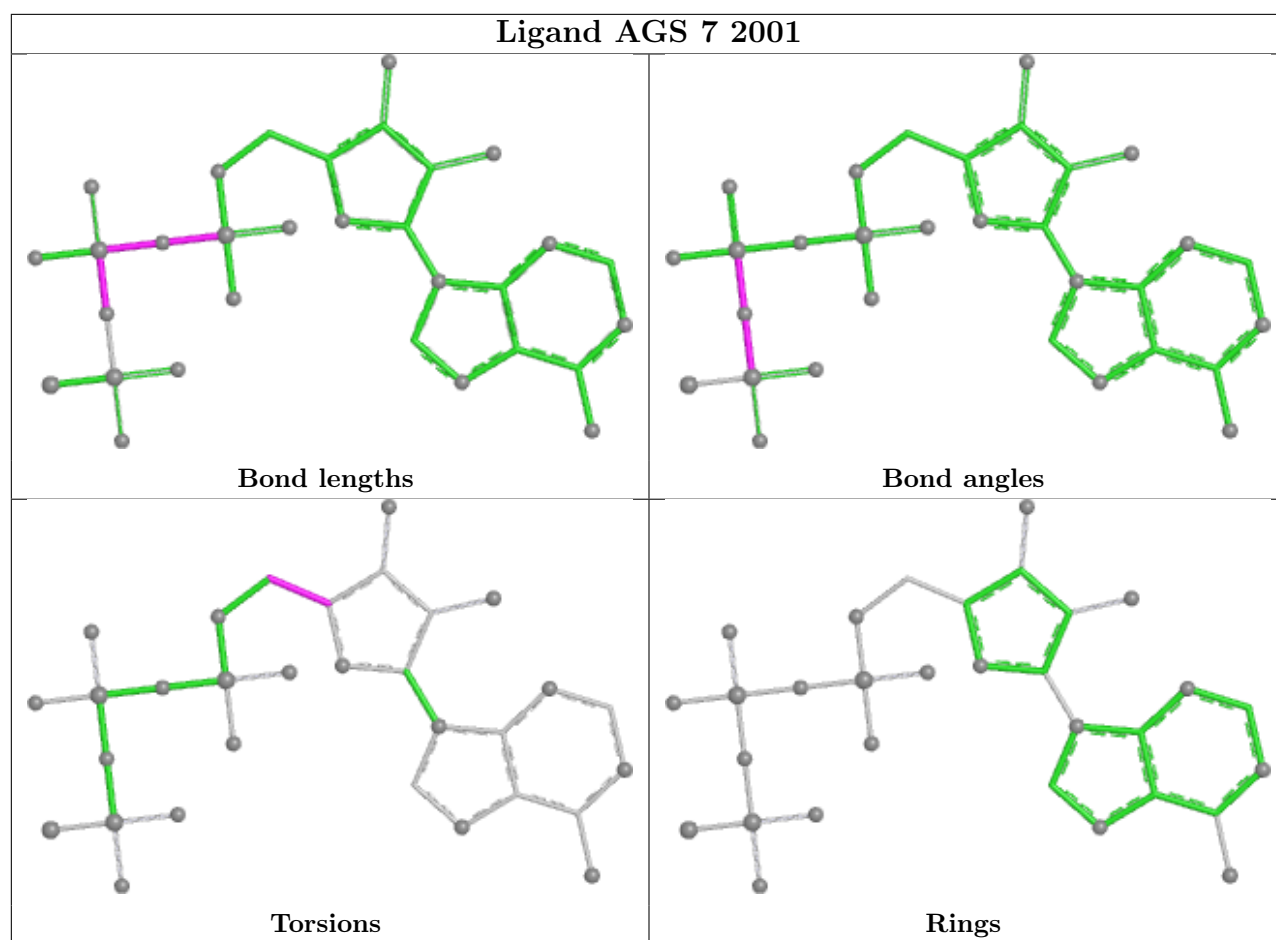


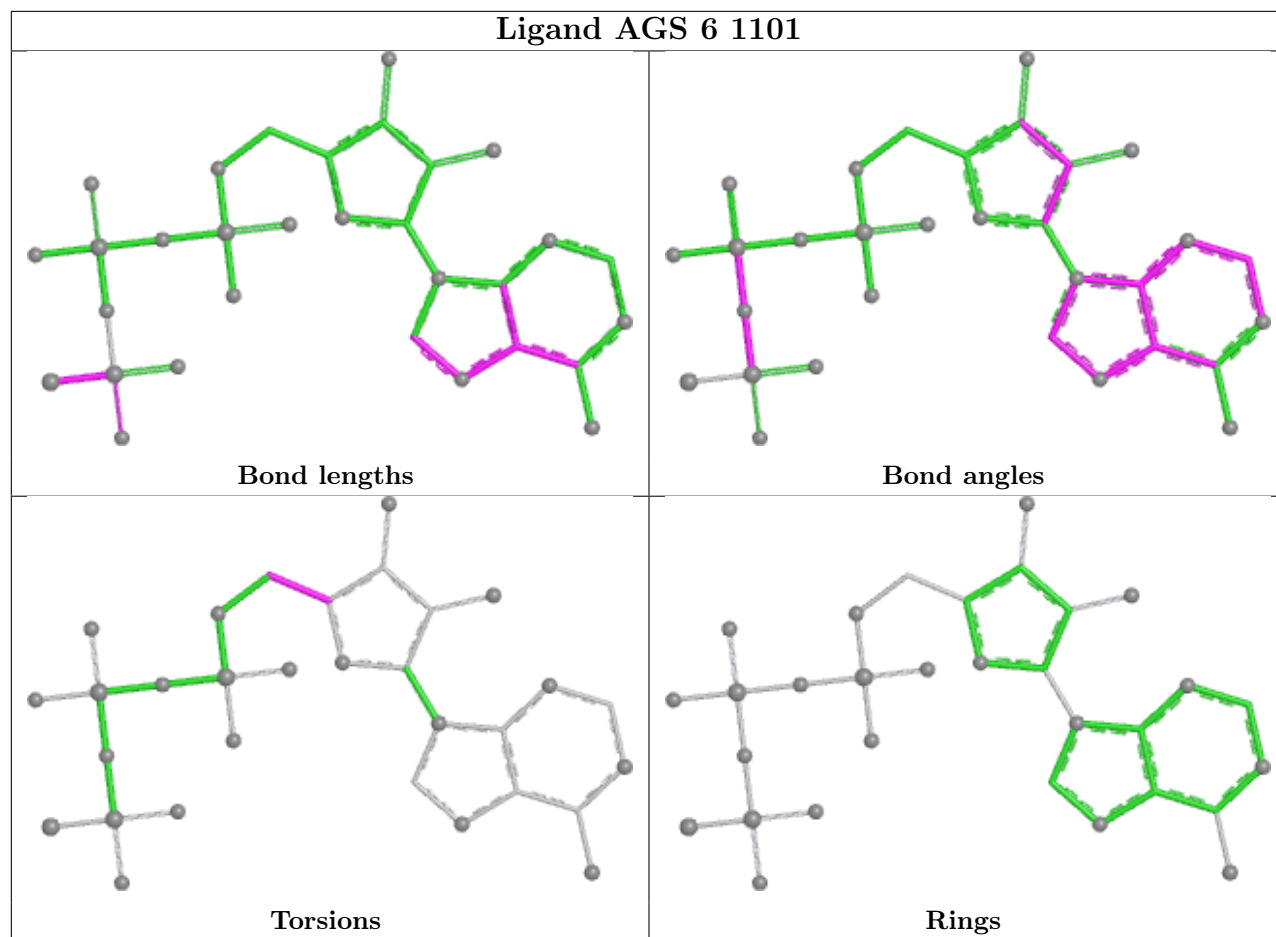












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

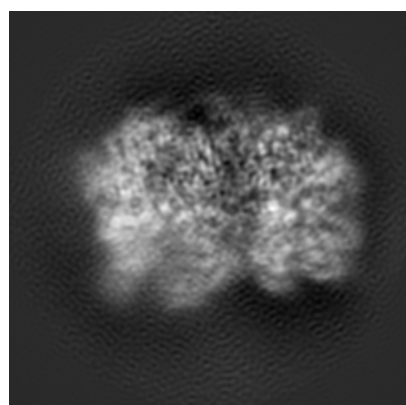
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8540. These allow visual inspection of the internal detail of the map and identification of artifacts.

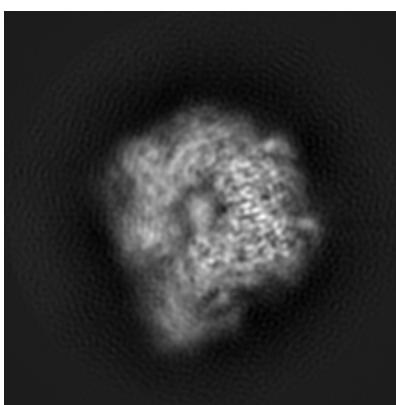
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

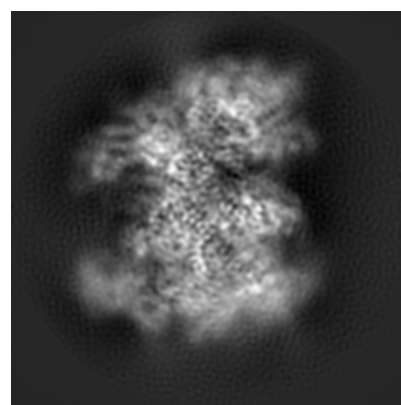
6.1.1 Primary map



X



Y

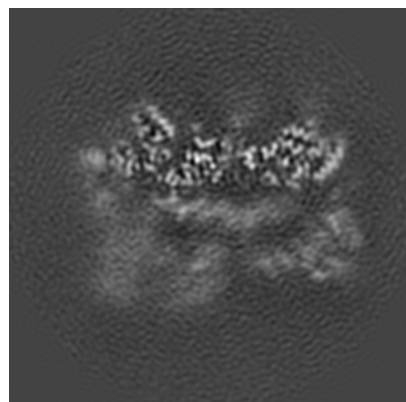


Z

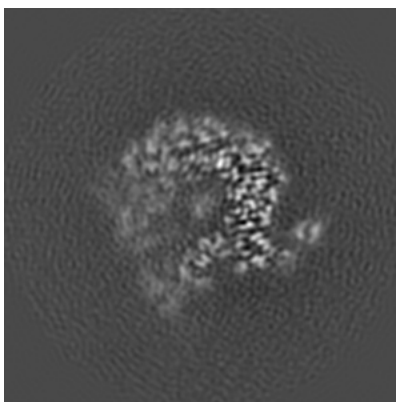
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

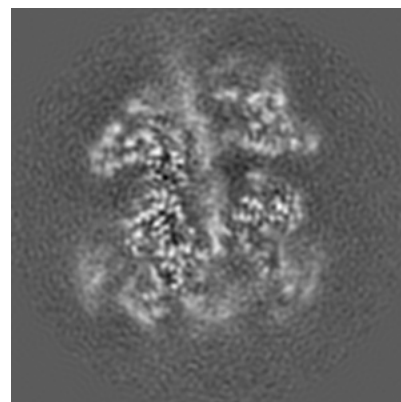
6.2.1 Primary map



X Index: 128



Y Index: 128

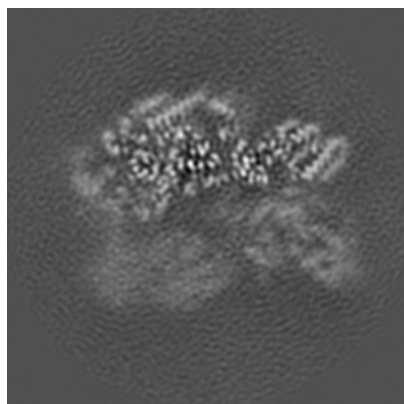


Z Index: 128

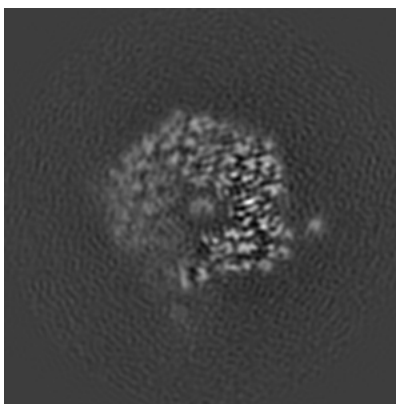
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

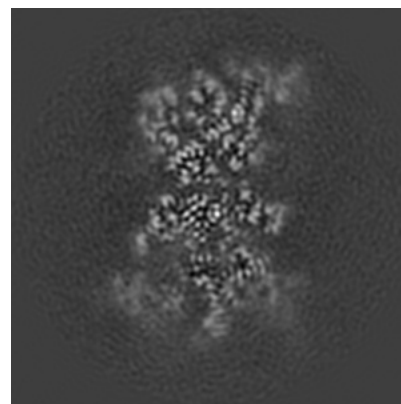
6.3.1 Primary map



X Index: 119



Y Index: 123

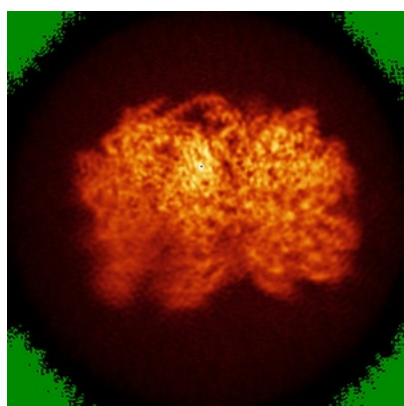


Z Index: 157

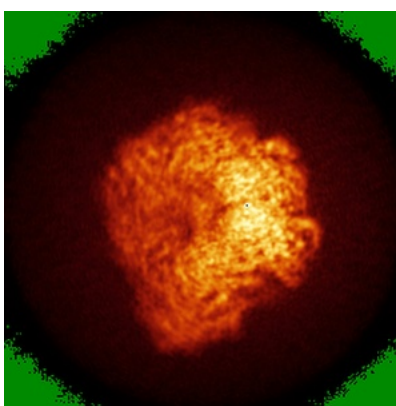
The images above show the largest variance slices of the map in three orthogonal directions.

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

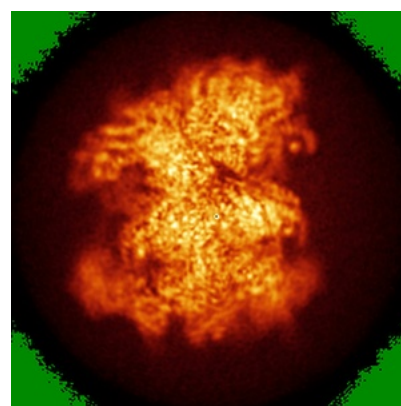
6.4.1 Primary map



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 0.021. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

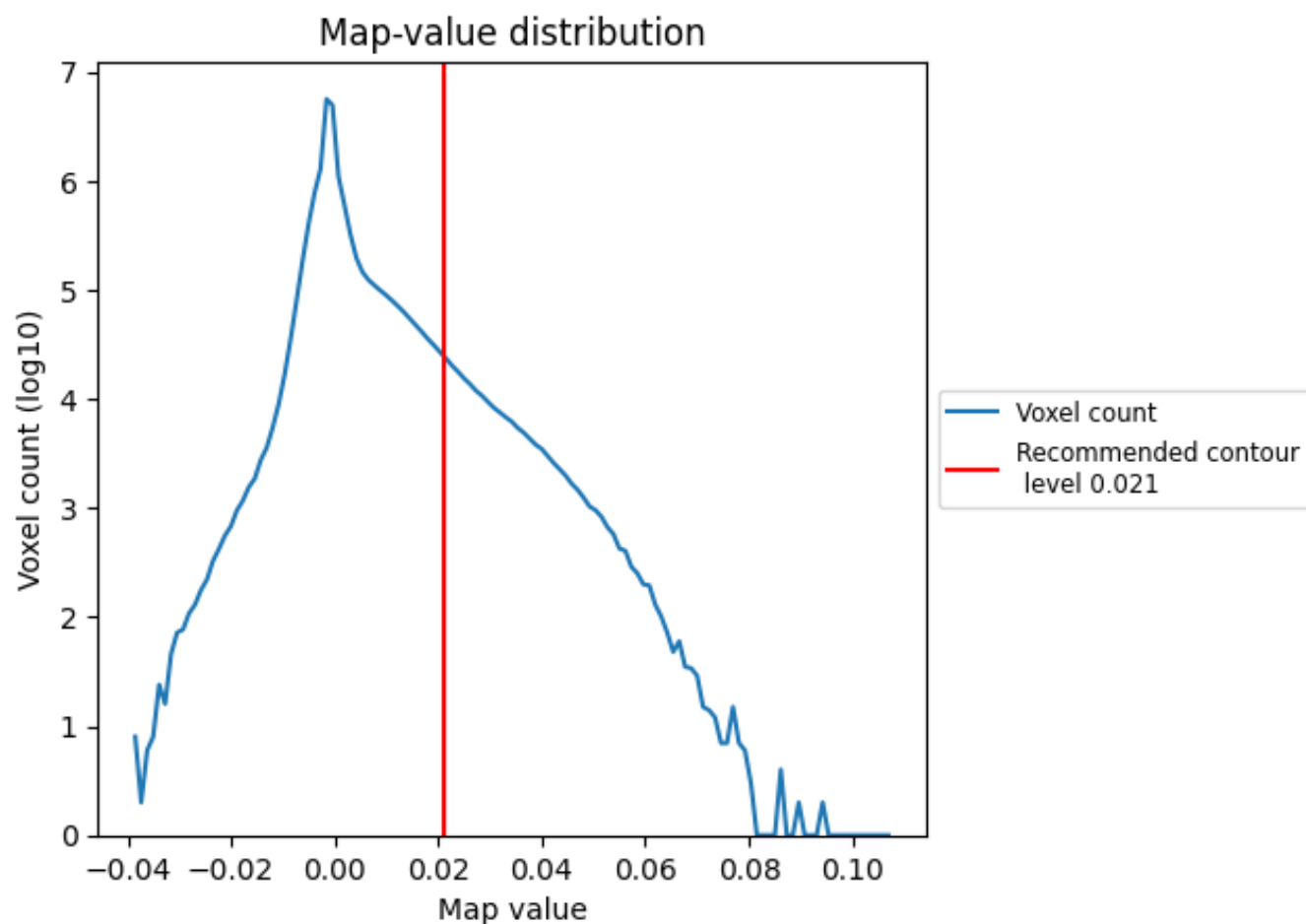
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

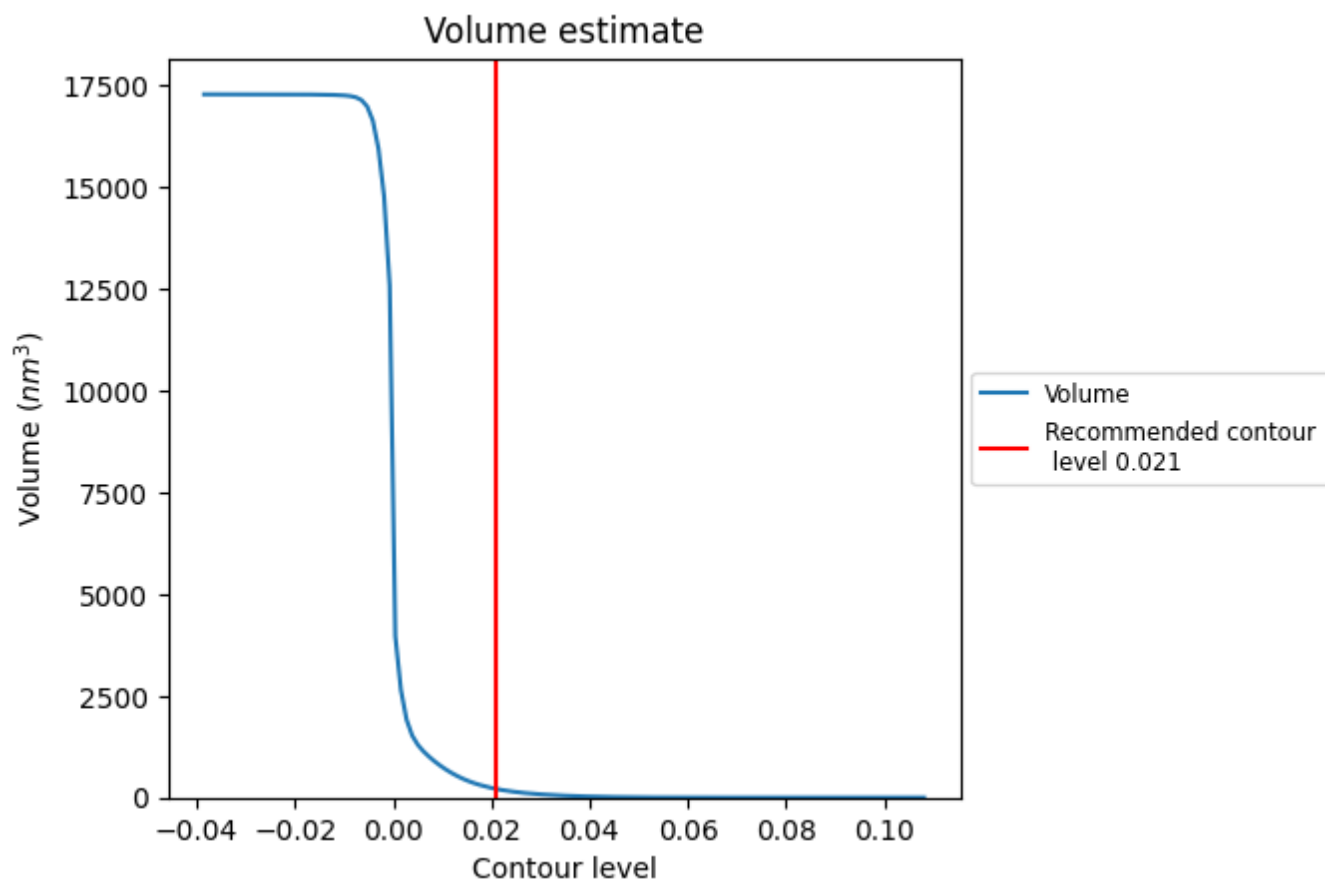
This section contains the results of statistical analysis of the map.

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.

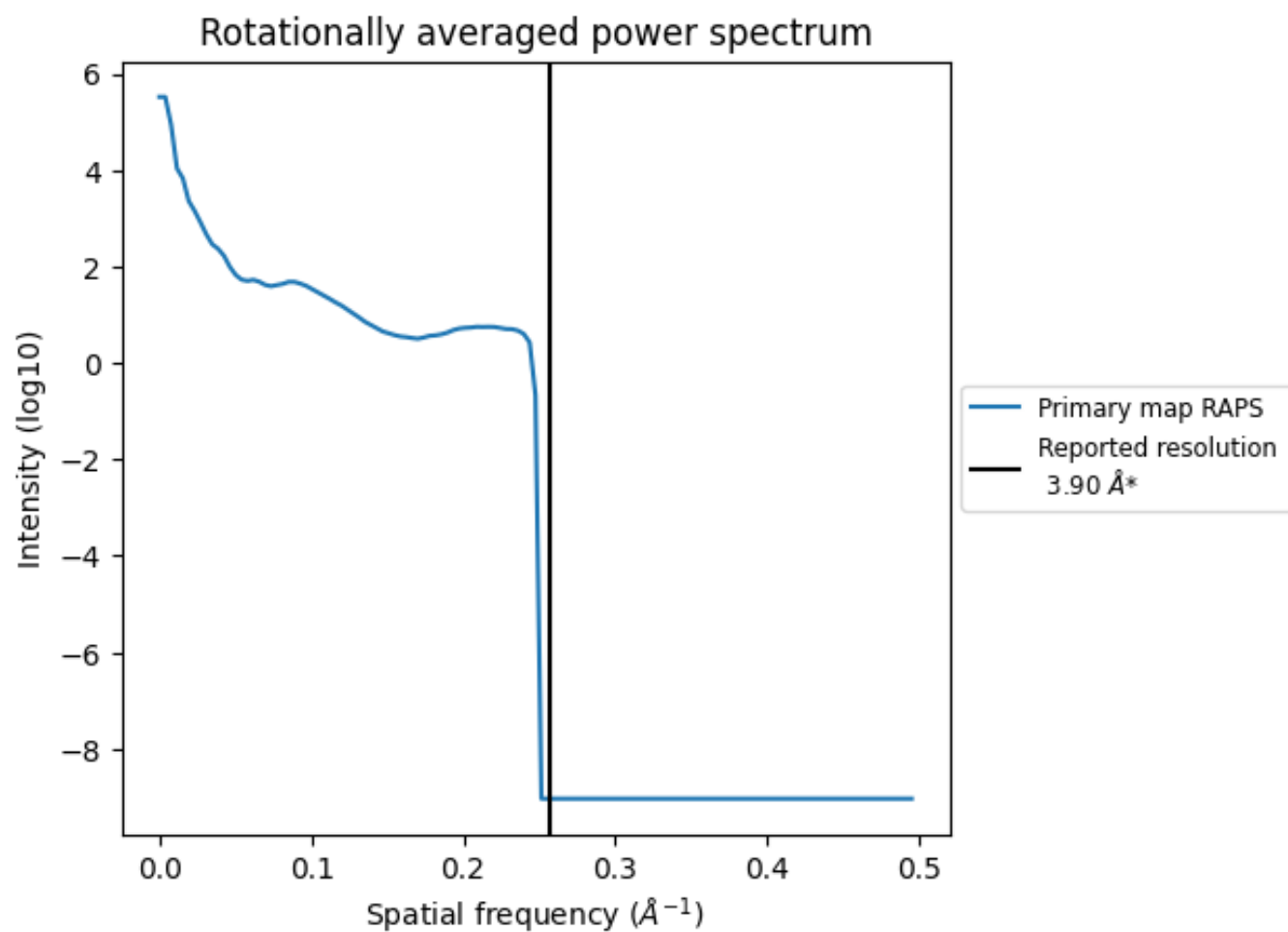
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 212 nm³; this corresponds to an approximate mass of 192 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 0.256 Å⁻¹

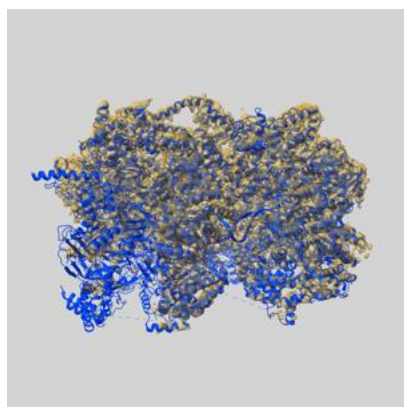
8 Fourier-Shell correlation

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

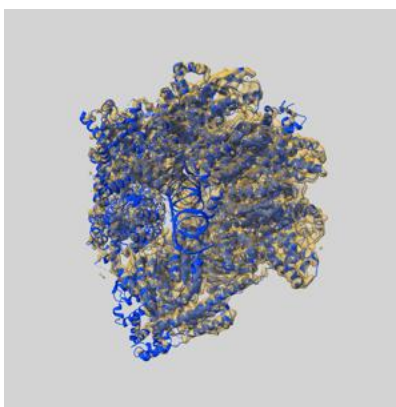
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8540 and PDB model 5V8F. Per-residue inclusion information can be found in section [3](#) on page [8](#).

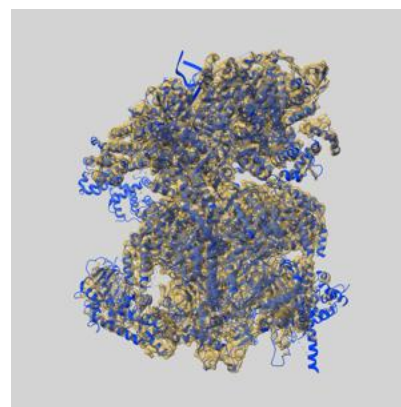
9.1 Map-model overlay [i](#)



X



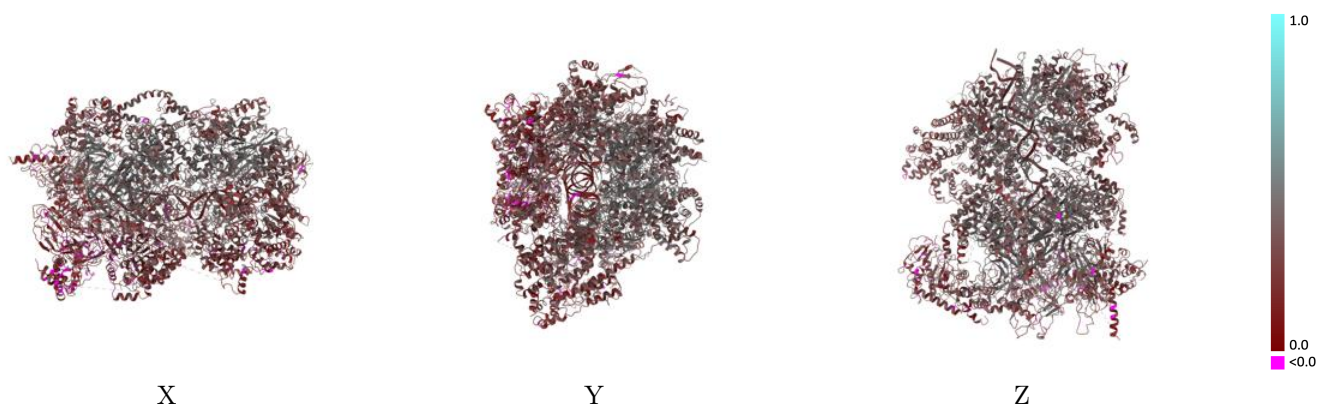
Y



Z

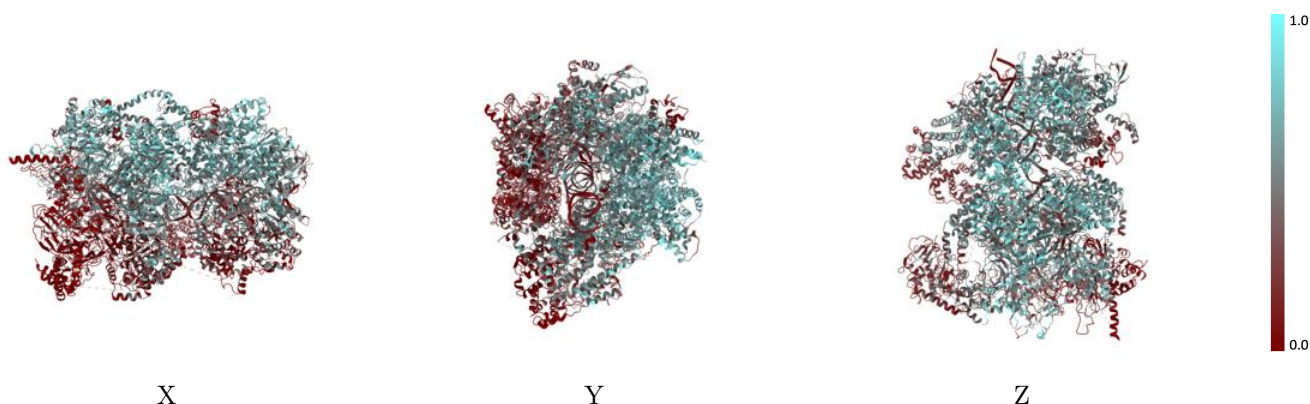
The images above show the 3D surface view of the map at the recommended contour level 0.021 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



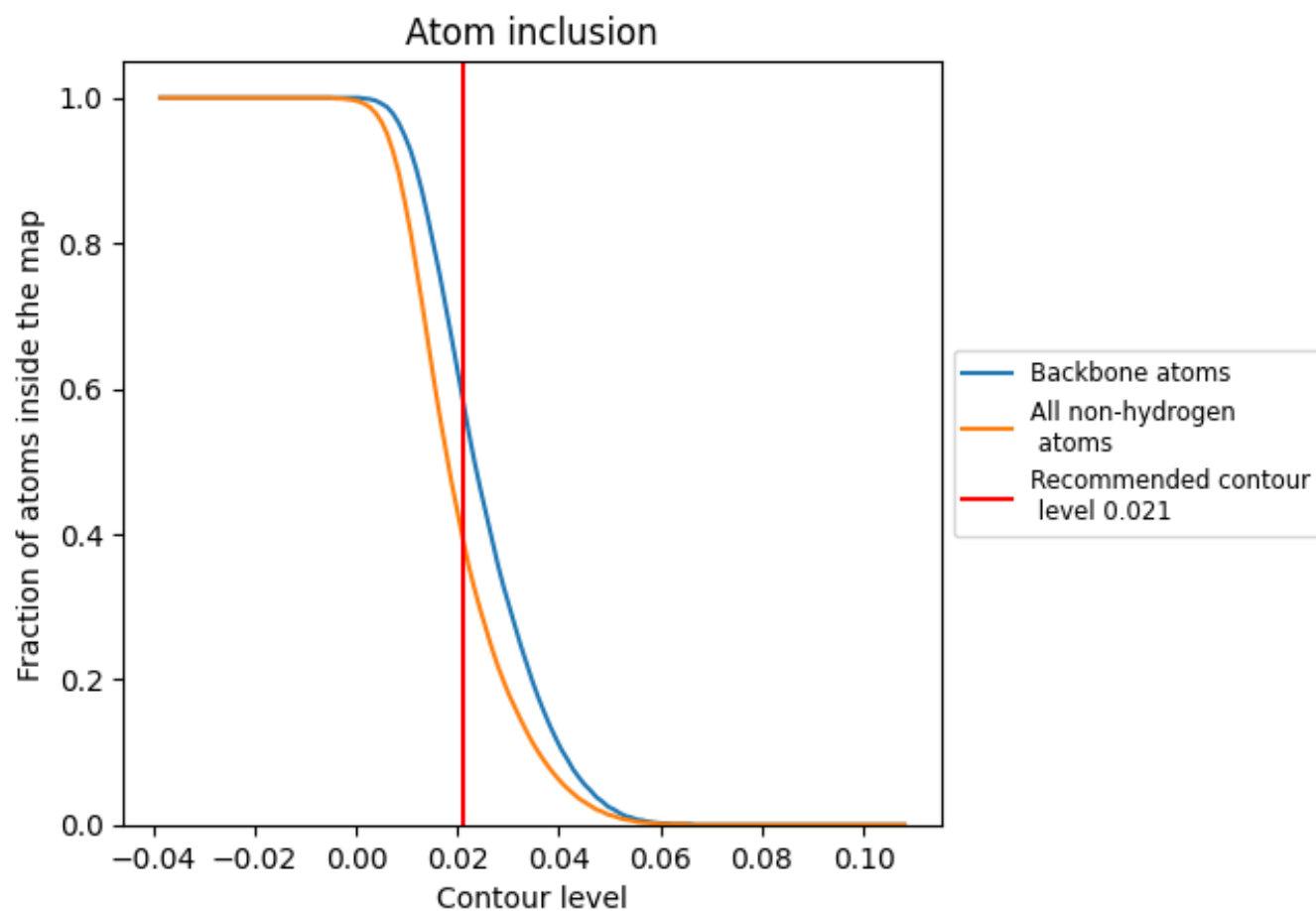
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.021).

9.4 Atom inclusion [i](#)



At the recommended contour level, 59% of all backbone atoms, 40% 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 (0.021) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.3950	0.3200
2	0.4980	0.3530
3	0.1360	0.2420
4	0.5640	0.3790
5	0.0100	0.1920
6	0.6200	0.3940
7	0.3220	0.3170
8	0.2970	0.2730
9	0.2610	0.2640
A	0.5310	0.3470
B	0.3450	0.2920
C	0.4190	0.3230
D	0.6330	0.4030
E	0.6470	0.4050
F	0.0390	0.2620
M	0.2630	0.2070
N	0.3540	0.2480

1.0

0.0

<0.0