wwPDB EM Validation Summary Report (i)

Mar 8, 2026 – 10:00 AM UTC

PDB ID	:	7W1Y / pdb_00007w1y
EMDB ID	:	EMD-32258
Title	:	Human MCM double hexamer bound to natural DNA duplex (polyAT/polyTA)
Authors	:	Li, J.; Dong, J.; Dang, S.; Zhai, Y.
Deposited on	:	2021-11-21
Resolution	:	2.59 Å(reported)
Based on initial model	:	3JA8

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 (i) 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 (i)) were used in the production of this report:

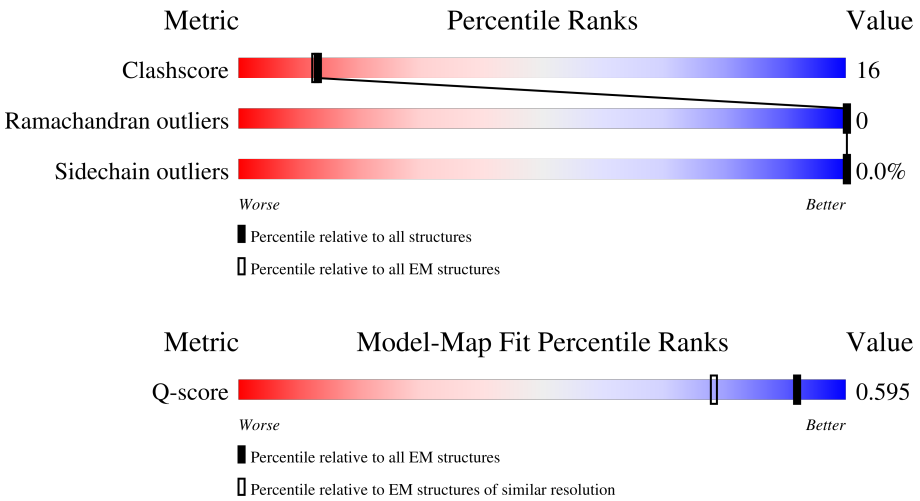
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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 (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.59 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	7741 (2.09 - 3.09)

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 <=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	904	5% 53% 25% 22%
1	A	904	• 52% 26% 22%
2	3	853	• 58% 18% 24%
2	B	853	• 59% 17% 24%

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Mol	Chain	Length	Quality of chain
3	4	863	55% 21% 24%
3	C	863	56% 20% 25%
4	5	734	13% 73% 24%
4	D	734	11% 72% 24%
5	6	821	5% 62% 25% 13%
5	E	821	64% 23% 13%
6	7	719	64% 24% 12%
6	F	719	65% 25% 11%
7	O	98	8% 20% 71% 8%
8	S	98	12% 16% 71% 10%

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 68655 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
			Total	C	N	O	S		
1	2	706	5591	3517	999	1043	32	0	0
1	A	702	5556	3499	991	1034	32	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	3	650	5080	3174	892	988	26	0	0
2	B	651	5100	3189	896	989	26	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	4	653	5187	3265	925	971	26	0	0
3	C	651	5184	3262	924	972	26	0	0

- Molecule 4 is a protein called DNA replication licensing factor MCM5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	5	710	5500	3451	979	1033	37	0	0
4	D	705	5474	3438	974	1024	38	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	6	716	5726	3593	1018	1088	27	0	0
5	E	711	5694	3575	1011	1081	27	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	7	636	5065	3170	905	958	32	1	0
6	F	643	5102	3189	911	970	32	1	0

- Molecule 7 is a DNA chain called DNA (49-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
7	O	49	2009	980	343	588	98	49	0

- Molecule 8 is a DNA chain called DNA (49-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
8	S	49	2009	980	343	588	98	49	0

- Molecule 9 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
9	2	1	1	1	0
9	4	1	1	1	0
9	5	1	1	1	0
9	6	1	1	1	0
9	7	1	1	1	0
9	A	1	1	1	0
9	C	1	1	1	0

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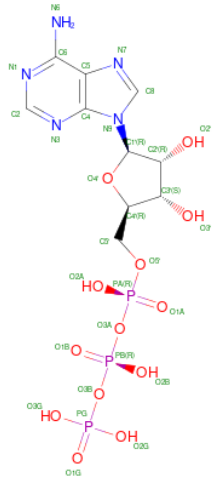
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
9	D	1	1	1	0
9	E	1	1	1	0
9	F	1	1	1	0

- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
10	2	1	1	1	0
10	3	1	1	1	0
10	4	1	1	1	0
10	5	1	1	1	0
10	6	1	1	1	0
10	7	1	1	1	0
10	A	1	1	1	0
10	B	1	1	1	0
10	C	1	1	1	0
10	D	1	1	1	0
10	E	1	1	1	0
10	F	1	1	1	0

- Molecule 11 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

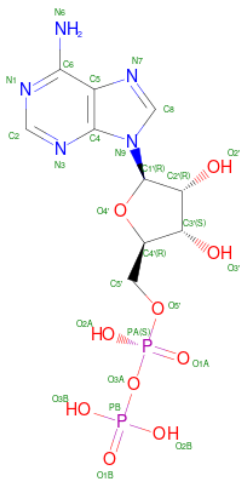
ATP



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
11	2	1	31	10	5	13	3	0
11	3	1	31	10	5	13	3	0
11	4	1	31	10	5	13	3	0
11	7	1	31	10	5	13	3	0
11	A	1	31	10	5	13	3	0
11	B	1	31	10	5	13	3	0
11	C	1	31	10	5	13	3	0
11	F	1	31	10	5	13	3	0

- Molecule 12 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

ADP



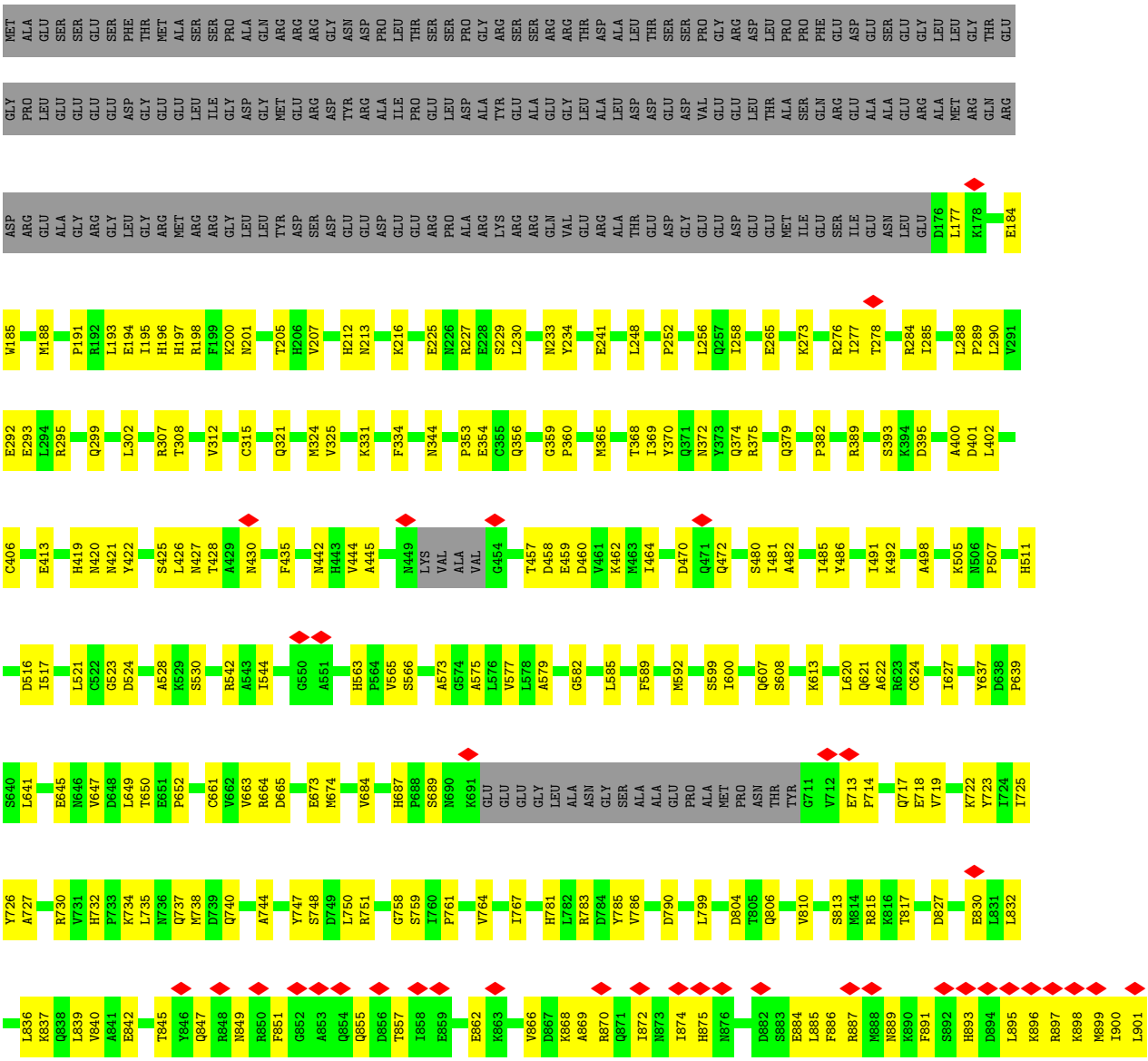
Mol	Chain	Residues	Atoms					AltConf
12	5	1	Total	C	N	O	P	0
			27	10	5	10	2	
12	6	1	Total	C	N	O	P	0
			27	10	5	10	2	
12	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
12	E	1	Total	C	N	O	P	0
			27	10	5	10	2	

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

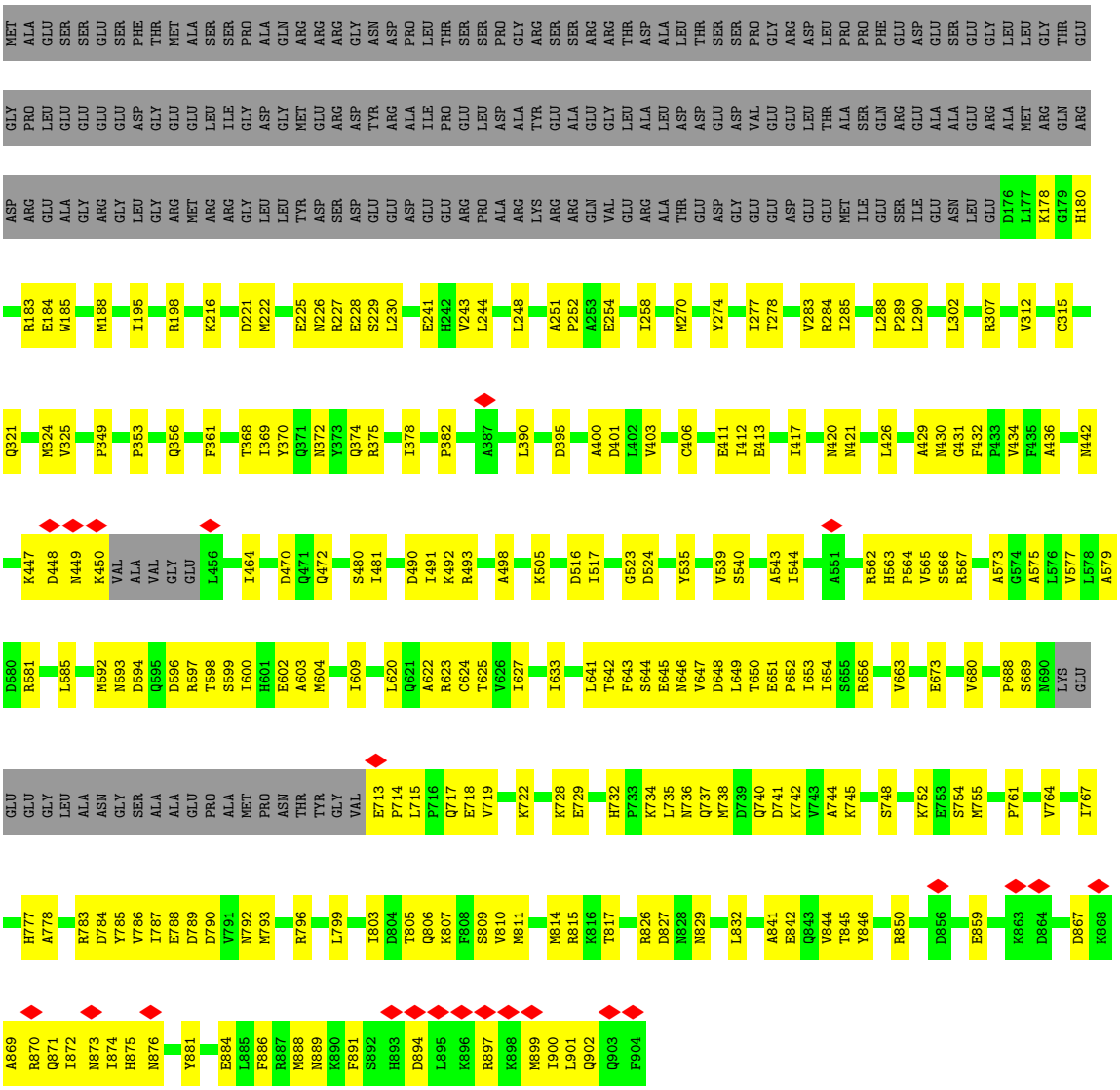
- Molecule 1: DNA replication licensing factor MCM2

Chain 2: 5% 53% 25% 22%



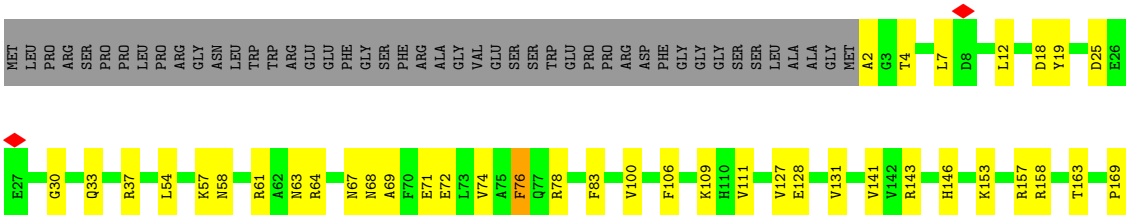
• Molecule 1: DNA replication licensing factor MCM2

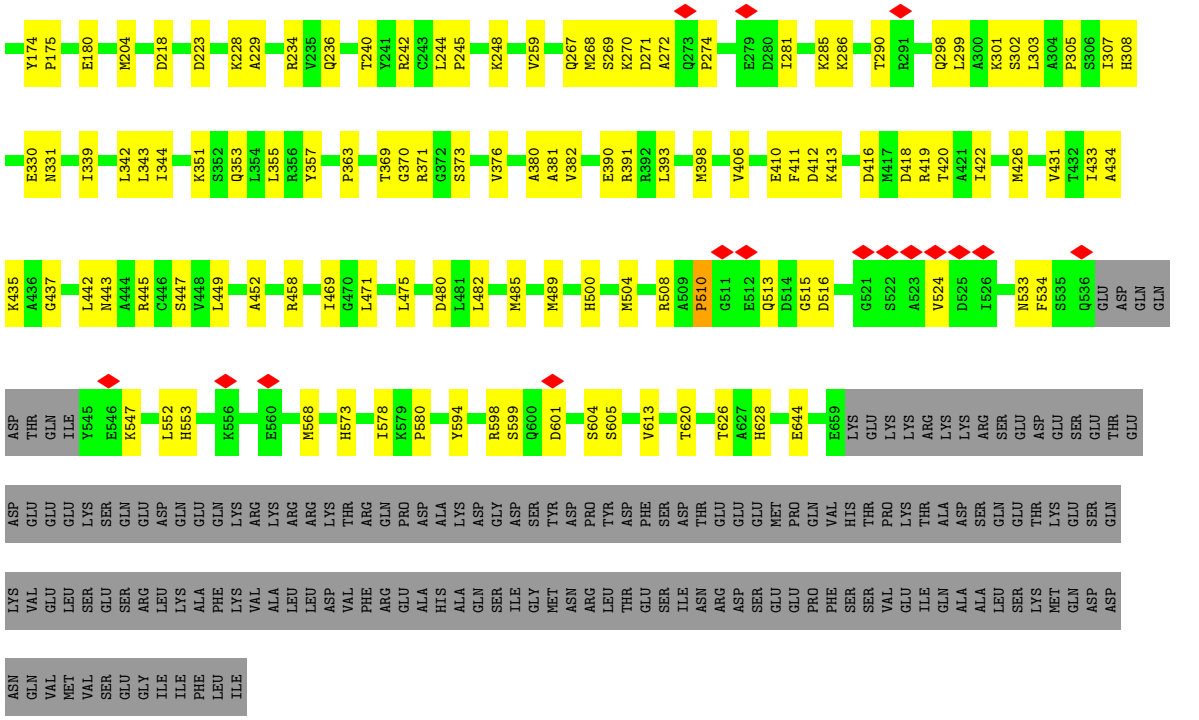
Chain A:



• Molecule 2: Isoform 2 of DNA replication licensing factor MCM3

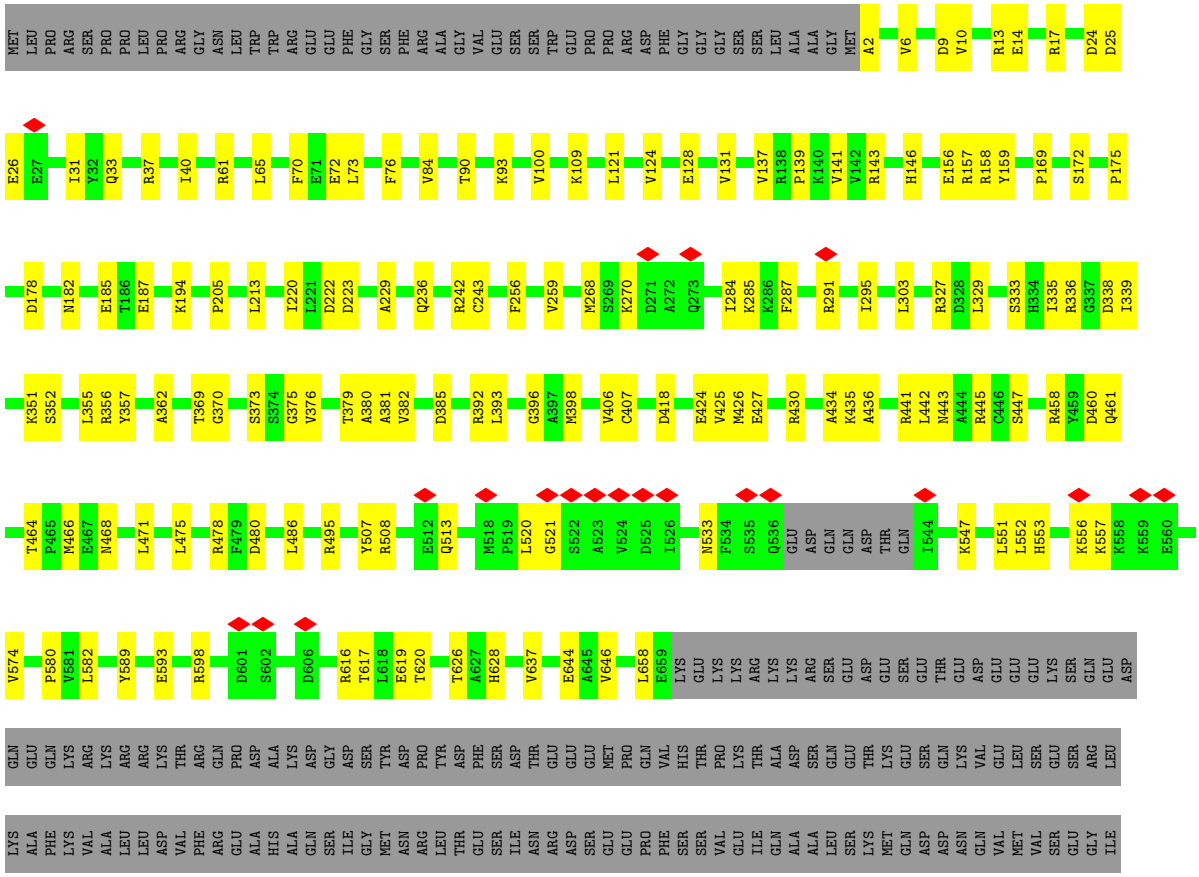
Chain 3:





- Molecule 2: Isoform 2 of DNA replication licensing factor MCM3

Chain B:



ILE PHE LEU ILE

- Molecule 3: DNA replication licensing factor MCM4

Chain 4:

MET SER SER PRO ALA SER THR PRO SER ARG ARG GLY SER ARG ARG GLY ARG ALA THR PRO ALA GLN THR PRO ARG SER GLU ASP ALA ARG SER SER PRO SER GLN ARG ARG ARG GLY GLU ASP SER THR SER THR GLY GLU LEU GLN PRO MET PRO THR SER PRO GLY VAL ASP LEU GLN

SER PRO ALA ALA GLN ASP VAL LEU PHE SER SER PRO PRO GLN MET HIS SER SER ALA ILE PRO LEU ASP PHE ASP VAL SER SER PRO LEU THR TYR GLY THR PRO SER SER ARG VAL GLU GLY THR PRO ARG SER GLY V107 R108 G109 V112 D117 L125 S131 ASP GLY ALA

ALA ALA GLU ASP ILE VAL ALA SER GLU GLN SER LEU GLY GLN K149 I152 W153 V157 Q167 R168 R172 F173 I174 D175 P176 L177 A178 E181 E182 N183 I188 T189 E190 P191 M194 Q195 E199 P206 N221 R224 Q225 L226 I227 Q231 F237 D238 M239

A240 V241 N242 E243 I244 R248 Y249 I253 H256 Q257 V260 F263 N270 M271 R272 Q281 I290 R291 L295 M299 A302 M317 D318 R319 I322 A323 E324 P325 S326 T334 H335 L339 D348 K349 Q350 M351 I352 K353 L354 Q355 D360 T366

P367 H368 T369 V370 I371 L372 V379 V388 N389 G392 R400 R404 V405 I419 H420 Y421 R422 K423 T424 D425 H430 E434 K439 Y459 E460 R461 A465 L466 A467 I470 Y471 E472 K478 G487 T488 R489 K490 D491 F492 S493 H494 T495 G496 R497 R501

I504 S515 K516 L519 R529 G542 L543 Y546 V547 M548 K549 E552 T553 R554 Q555 L556 Q559 T560 G561 A562 L563 V564 G569 E581 R584 V590 M591 E592 Q593 Q594 T595 L596 S597 I598 A599 K600 A601 G602 I603 I604 C605 Q606 N618 P619 I620 E621 S622

K628 I631 E632 Q635 D645 L649 L650 L651 D652 P653 Q654 D655 A668 L669 Y670 Y671 Q672 S673 GLU GLU GLN ALA GLU GLU GLU L681 L682 K688 D689 Y690 E705 I711 Y714 R718 S722 V727 Y730 Q733 L734 E735 S736 R739 E742

A743 H744 V747 S750 N751 K752 V753 E754 D757 E760 R763 A768 L769 T774 D775 P776 R777 I780 I783 SER ILE LEU THR THR GLY MET SER ALA THR SER ARG LYS ARG LYS GLU GLU LEU ALA GLU ALA LEU LYS LYS LEU ILE LEU SER LYS GLY LYS THR

PRO ALA LEU LYS TYR GLN GLN LEU PHE GLU ASP ILE ARG GLY GLN SER ASP ILE ALA ILE THR LYS ASP MET PHE GLU GLU ALA LEU ARG ALA LEU ALA ASP ASP ASP PHE LEU THR VAL THR GLY LYS THR VAL ARG LEU LEU

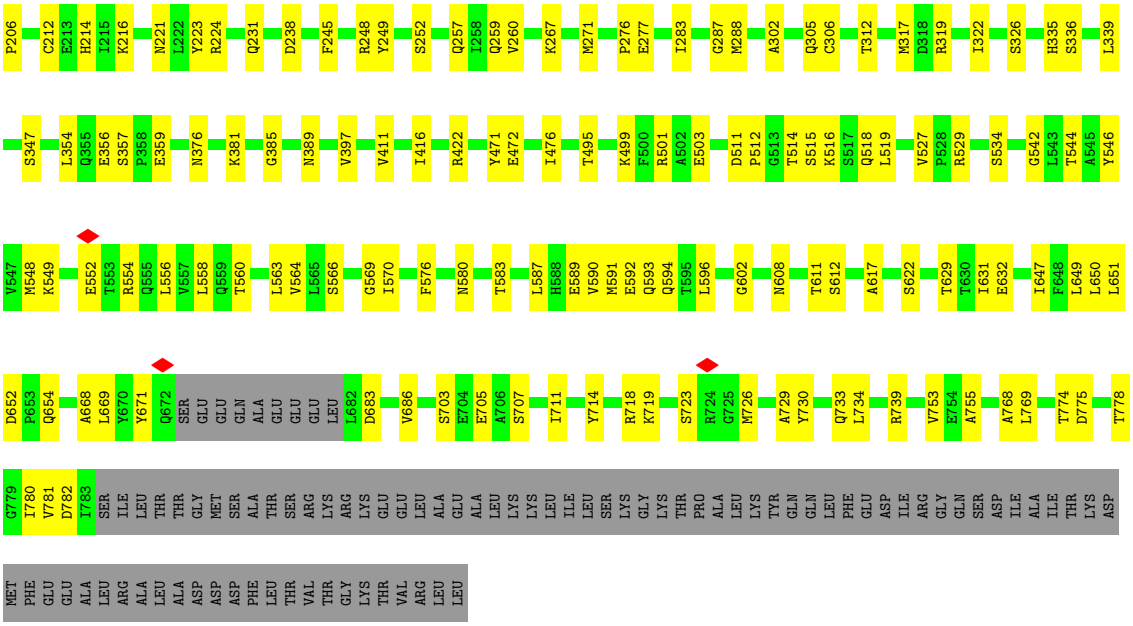
- Molecule 3: DNA replication licensing factor MCM4

Chain C:

MET SER SER PRO ALA SER THR PRO SER ARG ARG GLY SER ARG ARG GLY ARG ALA THR PRO ALA GLN THR PRO ARG SER GLU ASP ALA ARG SER SER PRO SER GLN ARG ARG ARG GLY GLU ASP SER THR SER THR GLY GLU LEU GLN PRO MET PRO THR SER PRO GLY VAL ASP LEU GLN

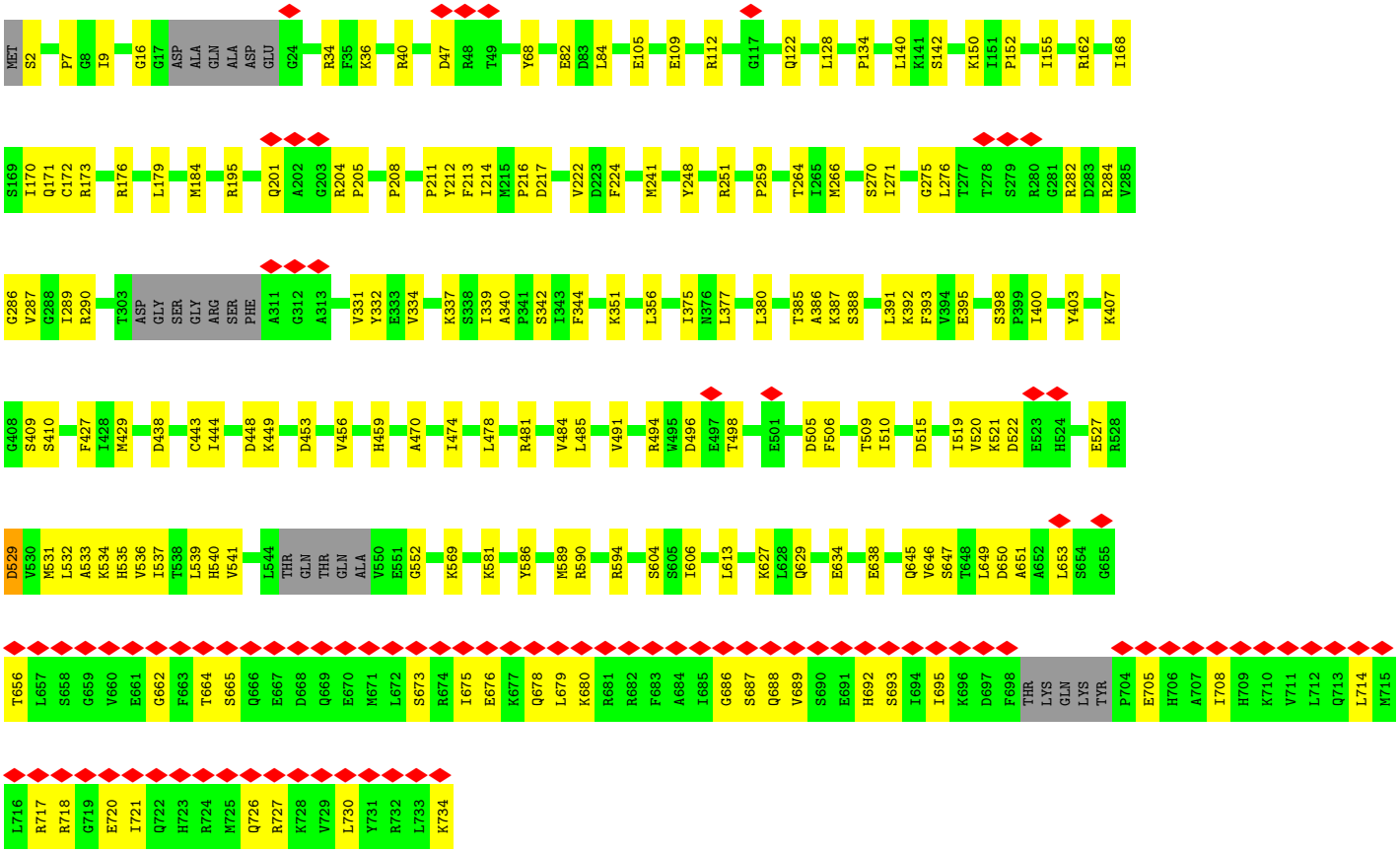
SER PRO ALA ALA GLN ASP VAL LEU PHE SER SER PRO PRO GLN MET HIS SER SER ALA ILE PRO LEU ASP PHE ASP VAL SER SER PRO LEU THR TYR GLY THR PRO SER SER ARG VAL GLU GLY THR PRO ARG SER GLY V107 R108 G109 V112 R115 P116 D117 L125 Q126 V127

S131 ASP GLY ALA ALA ALA GLU ASP ILE VAL ALA SER GLU GLN SER LEU GLY GLN K149 I152 W153 G154 T155 N158 A161 N165 R168 Q171 L177 A178 K179 E180 E181 E182 N183 V184 G185 I186 D187 I188 T189 E190 P191 L192 Y193 M194 Q195 R196 L197 I203 G204 E205



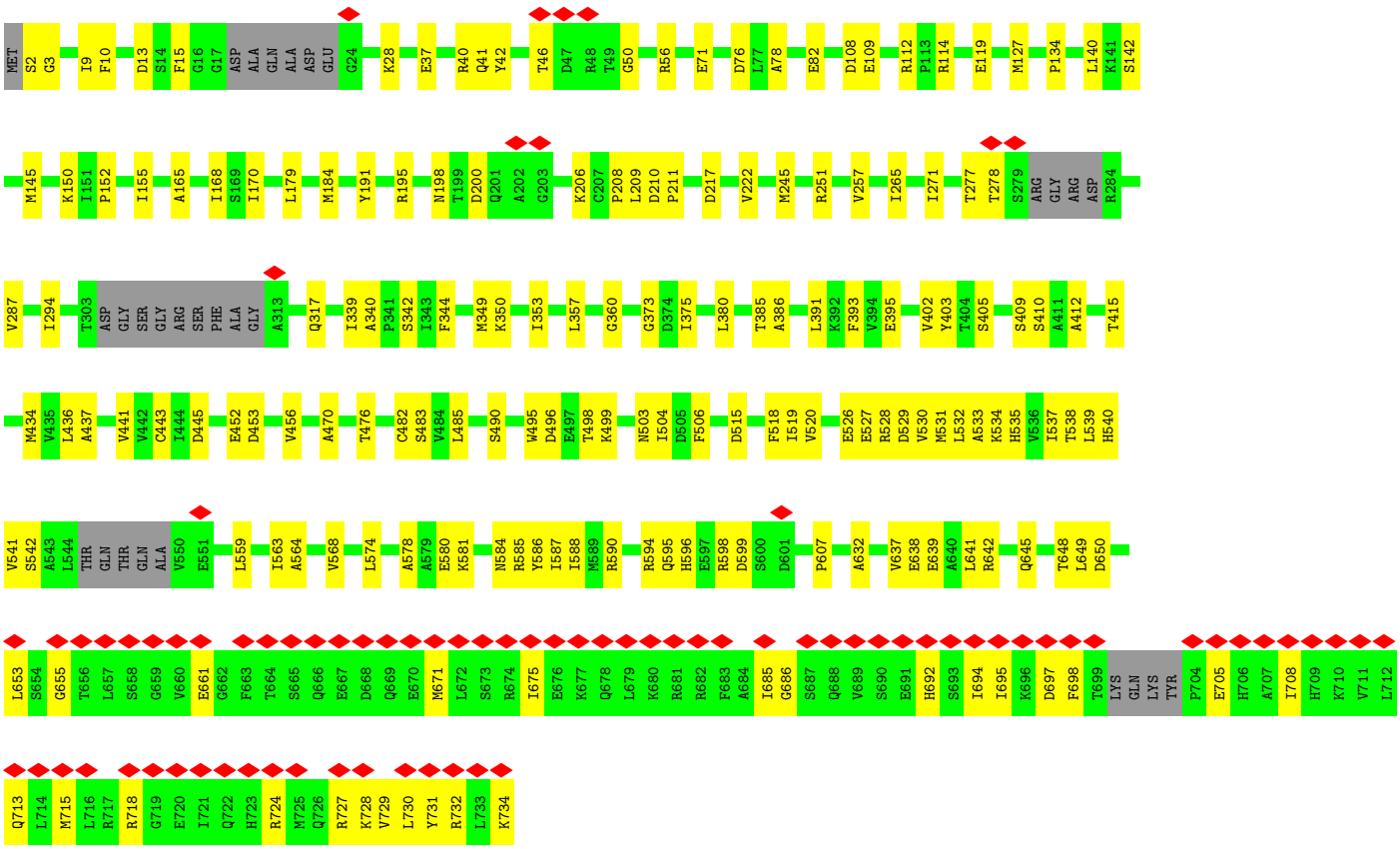
- Molecule 4: DNA replication licensing factor MCM5

Chain 5:



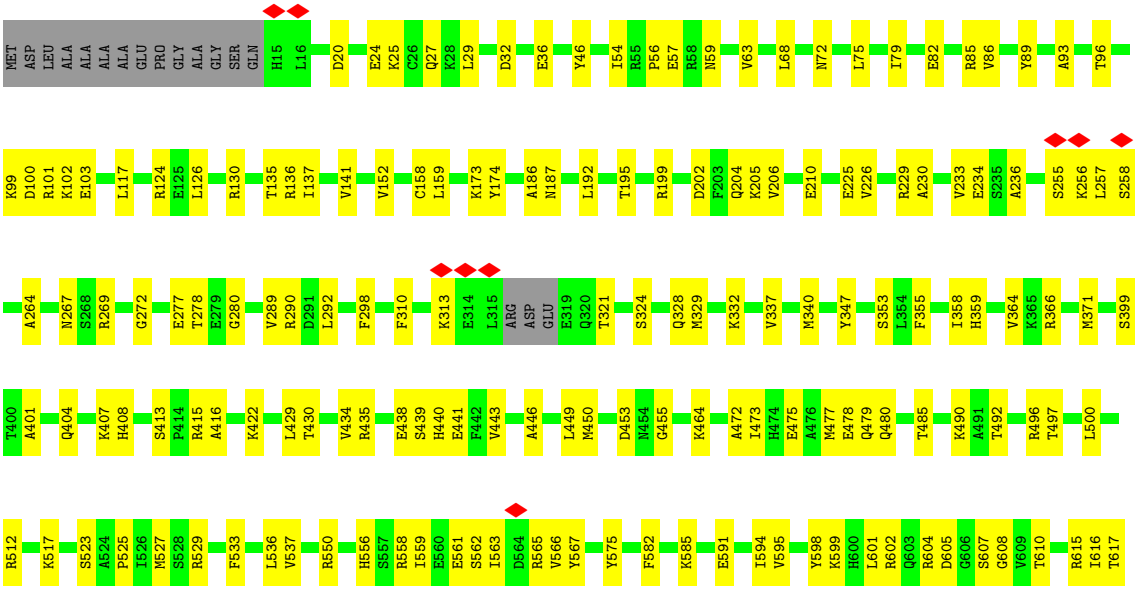
- Molecule 4: DNA replication licensing factor MCM5

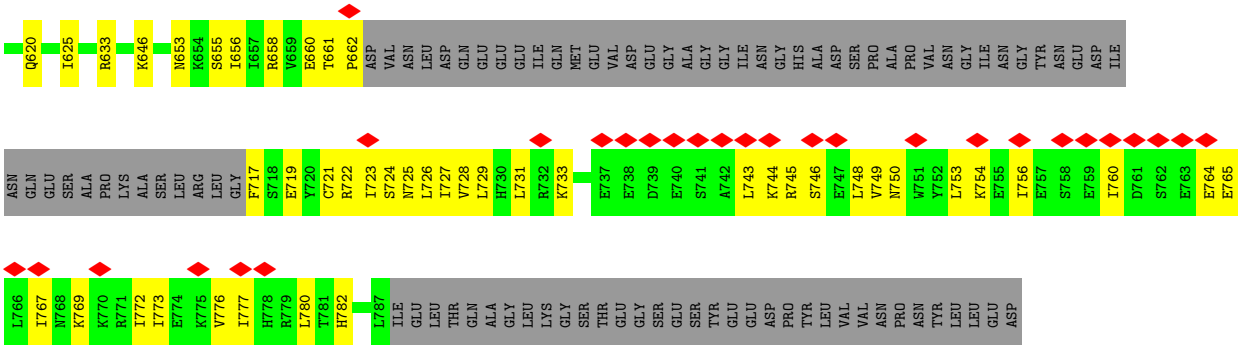
Chain D:



- Molecule 5: DNA replication licensing factor MCM6

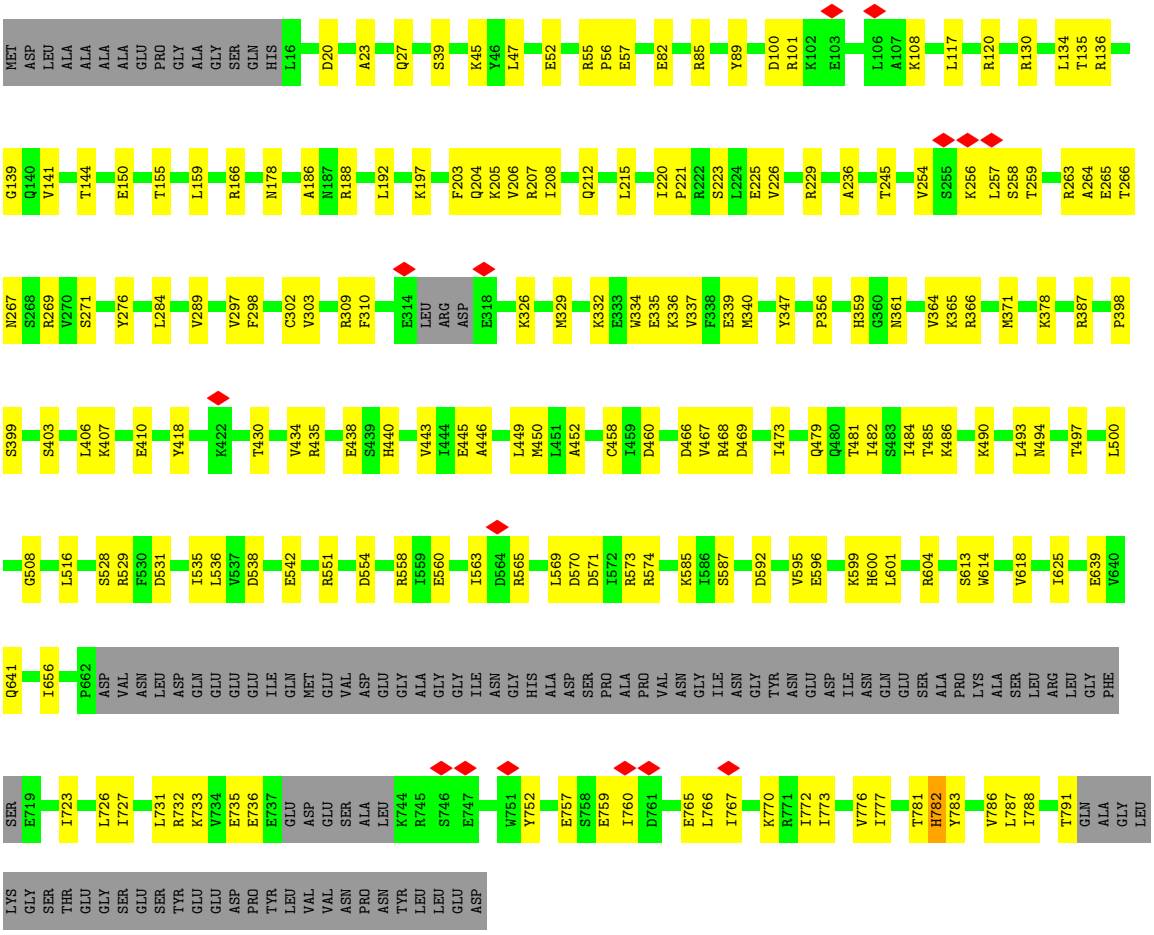
Chain 6:





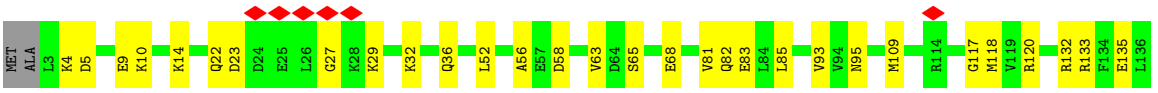
• Molecule 5: DNA replication licensing factor MCM6

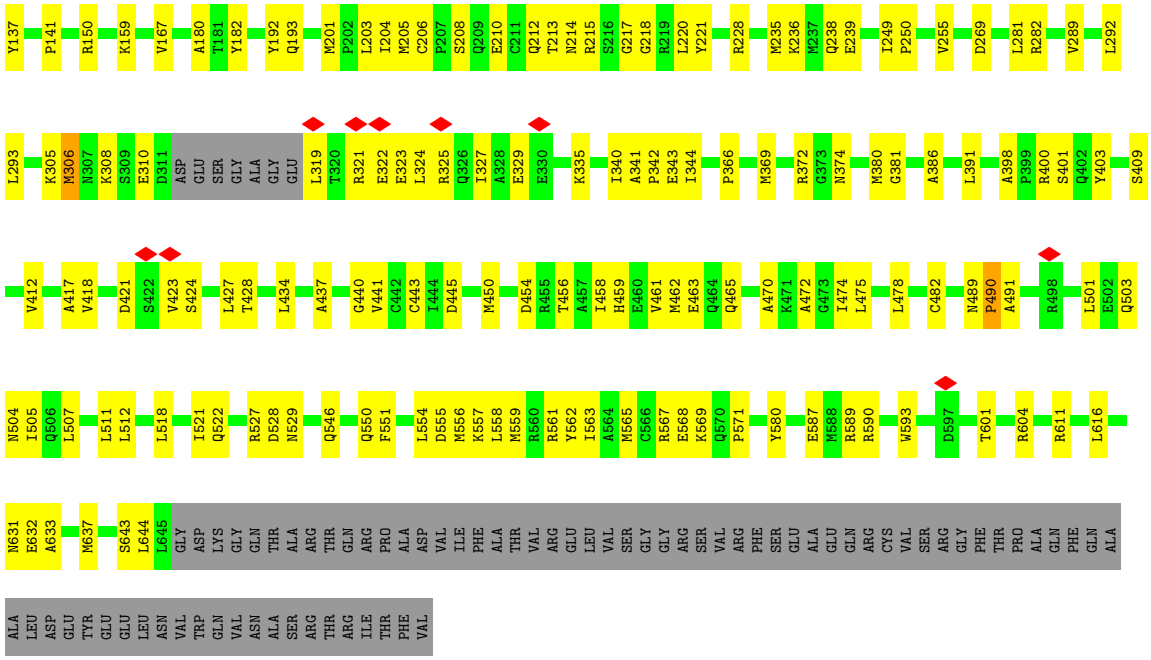
Chain E:



• Molecule 6: DNA replication licensing factor MCM7

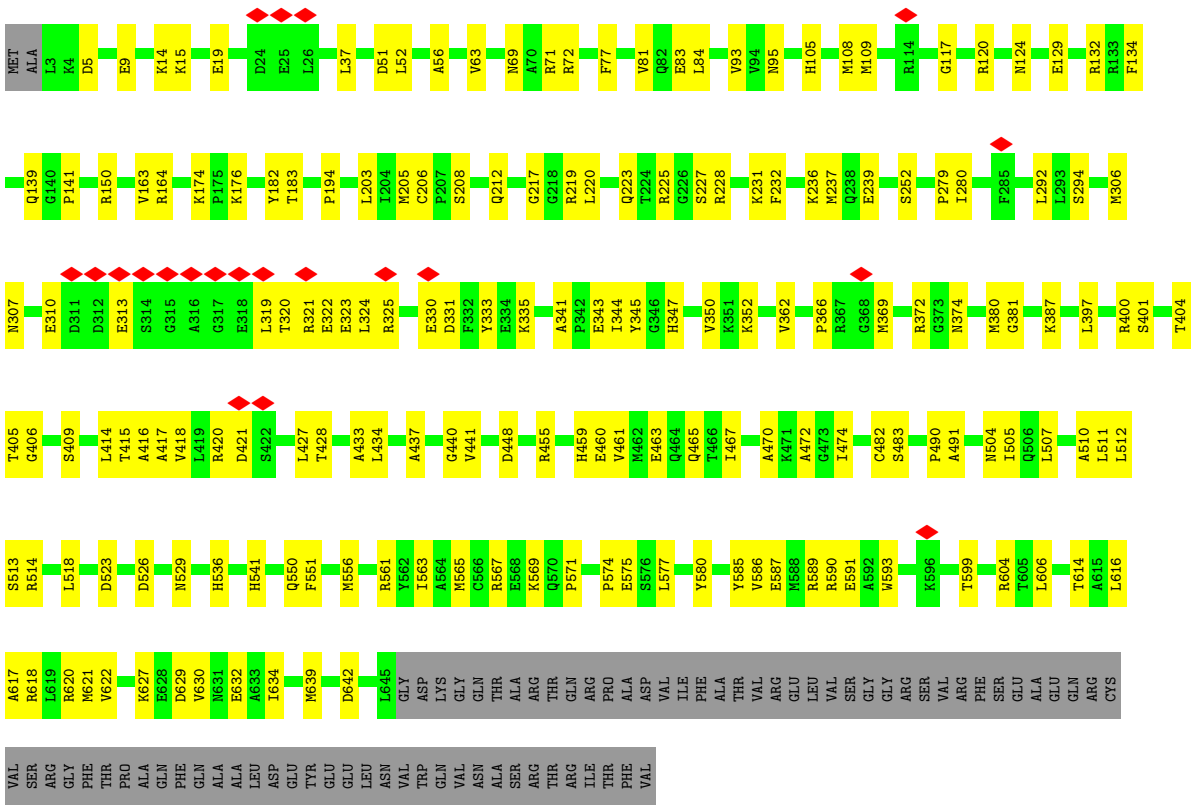
Chain 7:





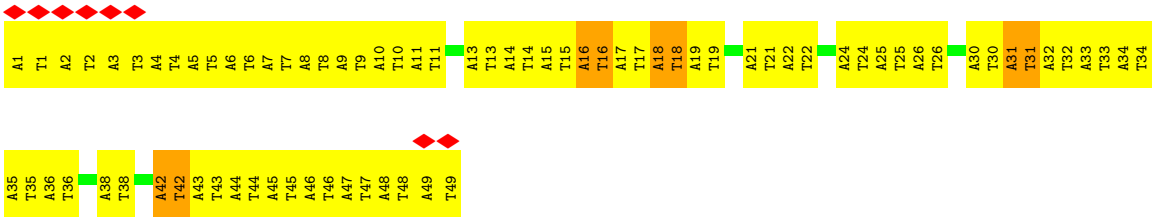
- Molecule 6: DNA replication licensing factor MCM7

Chain F:



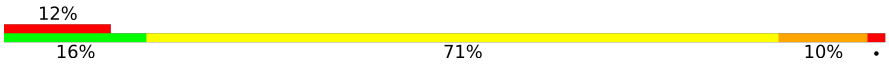
- Molecule 7: DNA (49-MER)

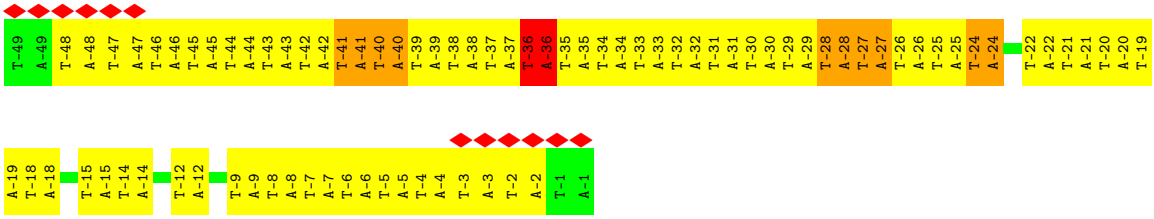
Chain O:



- Molecule 8: DNA (49-MER)

Chain S:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	329847	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 ($e^-/Å^2$)	51.78	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	4.638	Depositor
Minimum map value	-2.141	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.115	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	423.99997, 423.99997, 423.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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: ADP, ATP, MG, ZN

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	0.51	0/5693	0.54	0/7686
1	A	0.51	0/5658	0.54	0/7640
2	3	0.58	0/5159	0.57	3/6970 (0.0%)
2	B	0.56	1/5179 (0.0%)	0.54	0/6993
3	4	0.59	0/5278	0.56	0/7137
3	C	0.57	0/5275	0.55	1/7131 (0.0%)
4	5	0.56	0/5585	0.57	1/7511 (0.0%)
4	D	0.55	0/5558	0.55	0/7472
5	6	0.51	0/5817	0.53	1/7845 (0.0%)
5	E	0.51	0/5783	0.52	0/7798
6	7	0.60	2/5145 (0.0%)	0.59	2/6946 (0.0%)
6	F	0.59	0/5183	0.56	0/7000
7	O	0.71	4/2204 (0.2%)	0.75	3/3279 (0.1%)
8	S	0.73	5/2204 (0.2%)	0.69	4/3279 (0.1%)
All	All	0.56	12/69721 (0.0%)	0.56	15/94687 (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
2	3	0	1
4	D	0	1
5	6	0	1
5	E	0	2
6	7	0	1
8	S	0	1
All	All	0	7

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	O	16[B]	DT	O3'-P	-13.03	1.41	1.61
8	S	-40[B]	DA	O3'-P	-7.30	1.50	1.61
8	S	-12[B]	DA	C1'-N9	-6.39	1.33	1.46
7	O	31[B]	DT	O3'-P	-5.64	1.52	1.61
7	O	42[A]	DA	C1'-N9	-5.51	1.35	1.46

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	3	510	PRO	CA-N-CD	-11.07	96.50	112.00
4	5	529	ASP	N-CA-C	-8.79	103.67	114.75
2	3	524	VAL	N-CA-C	-7.69	105.99	113.53
7	O	18[B]	DT	P-O5'-C5'	-6.58	110.13	120.00
7	O	16[B]	DT	P-O3'-C3'	6.47	129.91	120.20

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	3	76	PHE	Sidechain
5	6	229	ARG	Peptide
6	7	306	MET	Peptide
4	D	528	ARG	Peptide
5	E	229	ARG	Peptide

5.2 Too-close contacts (i)

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	5591	0	5588	192	0
1	A	5556	0	5552	177	0
2	3	5080	0	5086	134	0
2	B	5100	0	5130	109	0
3	4	5187	0	5230	145	0
3	C	5184	0	5231	139	0
4	5	5500	0	5523	154	0
4	D	5474	0	5516	149	0
5	6	5726	0	5748	173	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	5694	0	5726	155	0
6	7	5065	0	5111	144	0
6	F	5102	0	5129	133	0
7	O	2009	0	1113	112	0
8	S	2009	0	1110	177	0
9	2	1	0	0	0	0
9	4	1	0	0	0	0
9	5	1	0	0	0	0
9	6	1	0	0	0	0
9	7	1	0	0	0	0
9	A	1	0	0	0	0
9	C	1	0	0	0	0
9	D	1	0	0	0	0
9	E	1	0	0	0	0
9	F	1	0	0	0	0
10	2	1	0	0	0	0
10	3	1	0	0	0	0
10	4	1	0	0	0	0
10	5	1	0	0	0	0
10	6	1	0	0	0	0
10	7	1	0	0	0	0
10	A	1	0	0	0	0
10	B	1	0	0	0	0
10	C	1	0	0	0	0
10	D	1	0	0	0	0
10	E	1	0	0	0	0
10	F	1	0	0	0	0
11	2	31	0	12	5	0
11	3	31	0	12	3	0
11	4	31	0	12	2	0
11	7	31	0	12	1	0
11	A	31	0	12	1	0
11	B	31	0	12	1	0
11	C	31	0	12	2	0
11	F	31	0	12	0	0
12	5	27	0	12	3	0
12	6	27	0	12	3	0
12	D	27	0	12	1	0
12	E	27	0	12	0	0
All	All	68655	0	66937	1862	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 16.

The worst 5 of 1862 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)
8:S:-36[A]:DT:C6	8:S:-35[A]:DT:H72	1.23	1.67
8:S:-41[A]:DT:H1'	8:S:-40[A]:DT:C5	1.56	1.40
8:S:-48[A]:DT:H72	8:S:-47[A]:DT:O4	1.18	1.30
8:S:-36[A]:DT:C6	8:S:-35[A]:DT:C7	2.19	1.26
8:S:-41[A]:DT:H1'	8:S:-40[A]:DT:C6	1.72	1.23

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	700/904 (77%)	643 (92%)	57 (8%)	0	100	100
1	A	696/904 (77%)	646 (93%)	50 (7%)	0	100	100
2	3	646/853 (76%)	601 (93%)	45 (7%)	0	100	100
2	B	647/853 (76%)	613 (95%)	34 (5%)	0	100	100
3	4	647/863 (75%)	598 (92%)	49 (8%)	0	100	100
3	C	645/863 (75%)	602 (93%)	43 (7%)	0	100	100
4	5	700/734 (95%)	640 (91%)	60 (9%)	0	100	100
4	D	693/734 (94%)	649 (94%)	44 (6%)	0	100	100
5	6	710/821 (86%)	668 (94%)	42 (6%)	0	100	100
5	E	703/821 (86%)	666 (95%)	37 (5%)	0	100	100
6	7	633/719 (88%)	588 (93%)	45 (7%)	0	100	100
6	F	642/719 (89%)	601 (94%)	41 (6%)	0	100	100
All	All	8062/9788 (82%)	7515 (93%)	547 (7%)	0	100	100

There are no Ramachandran outliers to report.

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	615/781 (79%)	615 (100%)	0	100	100
1	A	610/781 (78%)	609 (100%)	1 (0%)	87	95
2	3	557/742 (75%)	557 (100%)	0	100	100
2	B	561/742 (76%)	561 (100%)	0	100	100
3	4	574/753 (76%)	574 (100%)	0	100	100
3	C	575/753 (76%)	575 (100%)	0	100	100
4	5	589/625 (94%)	589 (100%)	0	100	100
4	D	589/625 (94%)	589 (100%)	0	100	100
5	6	639/724 (88%)	639 (100%)	0	100	100
5	E	636/724 (88%)	636 (100%)	0	100	100
6	7	554/619 (90%)	554 (100%)	0	100	100
6	F	556/619 (90%)	556 (100%)	0	100	100
All	All	7055/8488 (83%)	7054 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	784	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 58 such sidechains are listed below:

Mol	Chain	Res	Type
5	6	72	ASN
6	F	212	GLN
1	A	226	ASN
5	E	212	GLN
3	C	608	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)

Of 34 ligands modelled in this entry, 22 are monoatomic - leaving 12 for Mogul analysis.

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	$\#\|Z\| > 2$
11	ATP	7	803	10	32,33,33	1.40	3 (9%)	48,52,52	1.81	11 (22%)
11	ATP	2	1003	10	32,33,33	1.34	3 (9%)	48,52,52	1.61	8 (16%)
11	ATP	F	803	10	32,33,33	1.36	5 (15%)	48,52,52	1.78	10 (20%)
12	ADP	D	803	10	28,29,29	1.42	5 (17%)	43,45,45	1.81	8 (18%)
11	ATP	B	1101	10	32,33,33	1.34	5 (15%)	48,52,52	1.78	8 (16%)
11	ATP	4	903	10	32,33,33	1.39	4 (12%)	48,52,52	1.71	11 (22%)
12	ADP	5	803	10	28,29,29	1.45	3 (10%)	43,45,45	1.76	8 (18%)
11	ATP	C	903	10	32,33,33	1.40	5 (15%)	48,52,52	1.73	8 (16%)
12	ADP	E	903	10	28,29,29	1.42	5 (17%)	43,45,45	1.83	10 (23%)
11	ATP	3	1101	10	32,33,33	1.38	3 (9%)	48,52,52	1.65	8 (16%)
12	ADP	6	903	10	28,29,29	1.42	3 (10%)	43,45,45	1.79	8 (18%)
11	ATP	A	1003	10	32,33,33	1.30	5 (15%)	48,52,52	1.75	7 (14%)

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
11	ATP	7	803	10	-	7/22/38/38	0/3/3/3
11	ATP	2	1003	10	-	6/22/38/38	0/3/3/3
11	ATP	F	803	10	-	0/22/38/38	0/3/3/3
12	ADP	D	803	10	-	4/16/32/32	0/3/3/3
11	ATP	B	1101	10	-	1/22/38/38	0/3/3/3
11	ATP	4	903	10	-	6/22/38/38	0/3/3/3
12	ADP	5	803	10	-	6/16/32/32	0/3/3/3
11	ATP	C	903	10	-	3/22/38/38	0/3/3/3
12	ADP	E	903	10	-	6/16/32/32	0/3/3/3
11	ATP	3	1101	10	-	6/22/38/38	0/3/3/3
12	ADP	6	903	10	-	2/16/32/32	0/3/3/3
11	ATP	A	1003	10	-	3/22/38/38	0/3/3/3

The worst 5 of 49 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	3	1101	ATP	C5-C4	4.41	1.47	1.39
11	4	903	ATP	C5-C4	4.37	1.46	1.39
12	6	903	ADP	C5-C4	4.36	1.46	1.39
11	7	803	ATP	C5-C4	4.32	1.46	1.39
12	5	803	ADP	C5-C4	4.32	1.46	1.39

The worst 5 of 105 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	C	903	ATP	C5-C4-N3	-5.82	118.70	126.72
11	A	1003	ATP	C5-C4-N3	-5.82	118.70	126.72
12	D	803	ADP	C5-C4-N3	-5.77	118.77	126.72
11	B	1101	ATP	C5-C4-N3	-5.76	118.78	126.72
12	E	903	ADP	C5-C4-N3	-5.61	119.00	126.72

There are no chirality outliers.

5 of 50 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	2	1003	ATP	O4'-C1'-N9-C8
11	2	1003	ATP	O4'-C1'-N9-C4
11	3	1101	ATP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
11	3	1101	ATP	O4'-C1'-N9-C8
11	3	1101	ATP	O4'-C1'-N9-C4

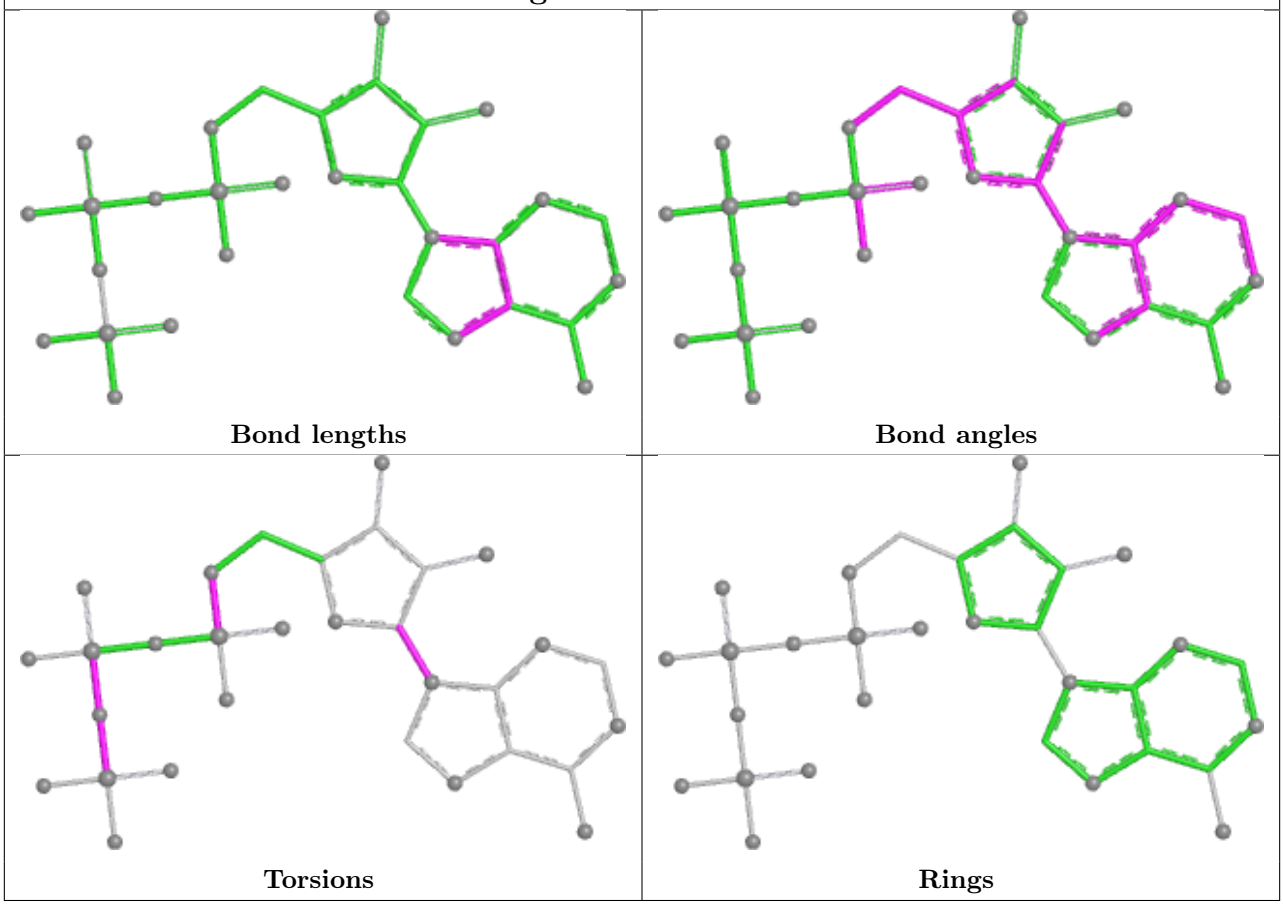
There are no ring outliers.

10 monomers are involved in 22 short contacts:

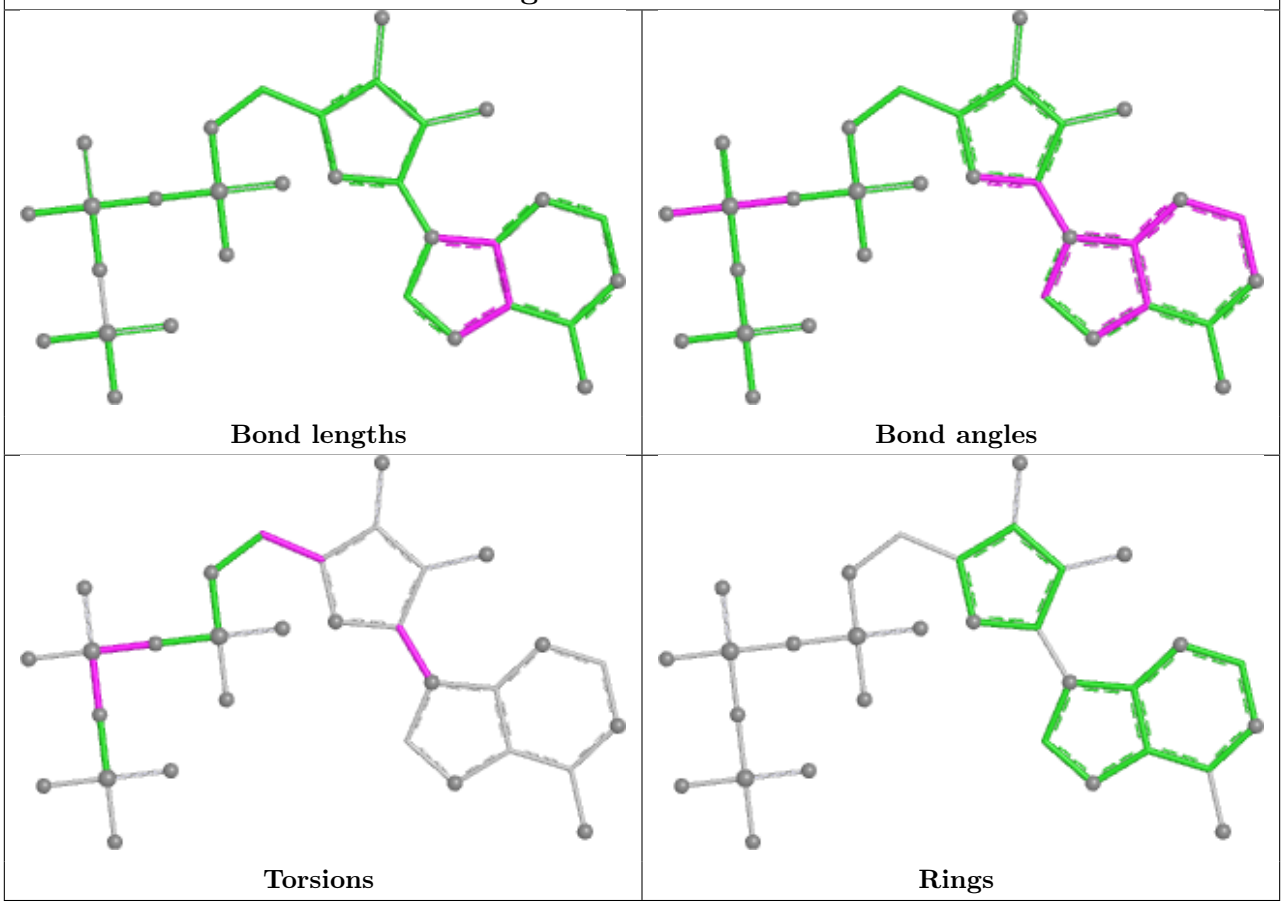
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	7	803	ATP	1	0
11	2	1003	ATP	5	0
12	D	803	ADP	1	0
11	B	1101	ATP	1	0
11	4	903	ATP	2	0
12	5	803	ADP	3	0
11	C	903	ATP	2	0
11	3	1101	ATP	3	0
12	6	903	ADP	3	0
11	A	1003	ATP	1	0

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 then 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.

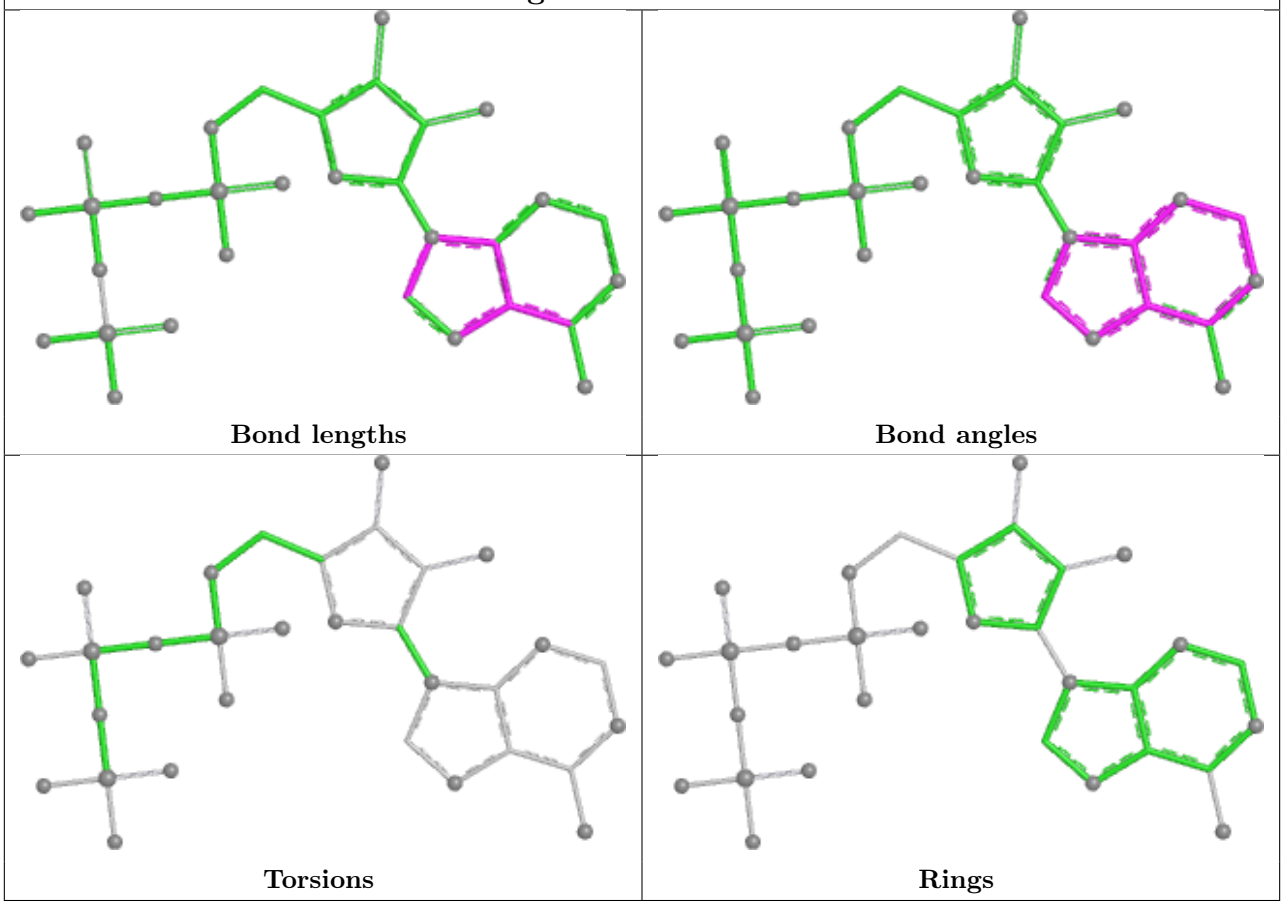
Ligand ATP 7 803



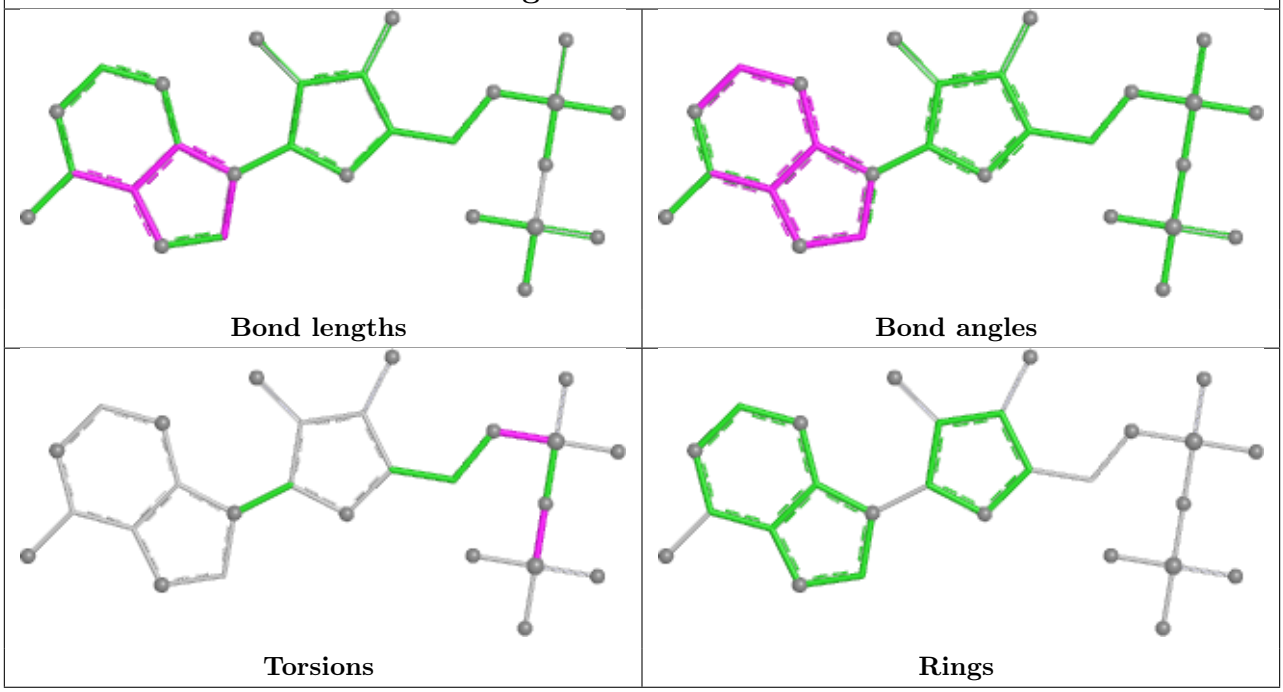
Ligand ATP 2 1003



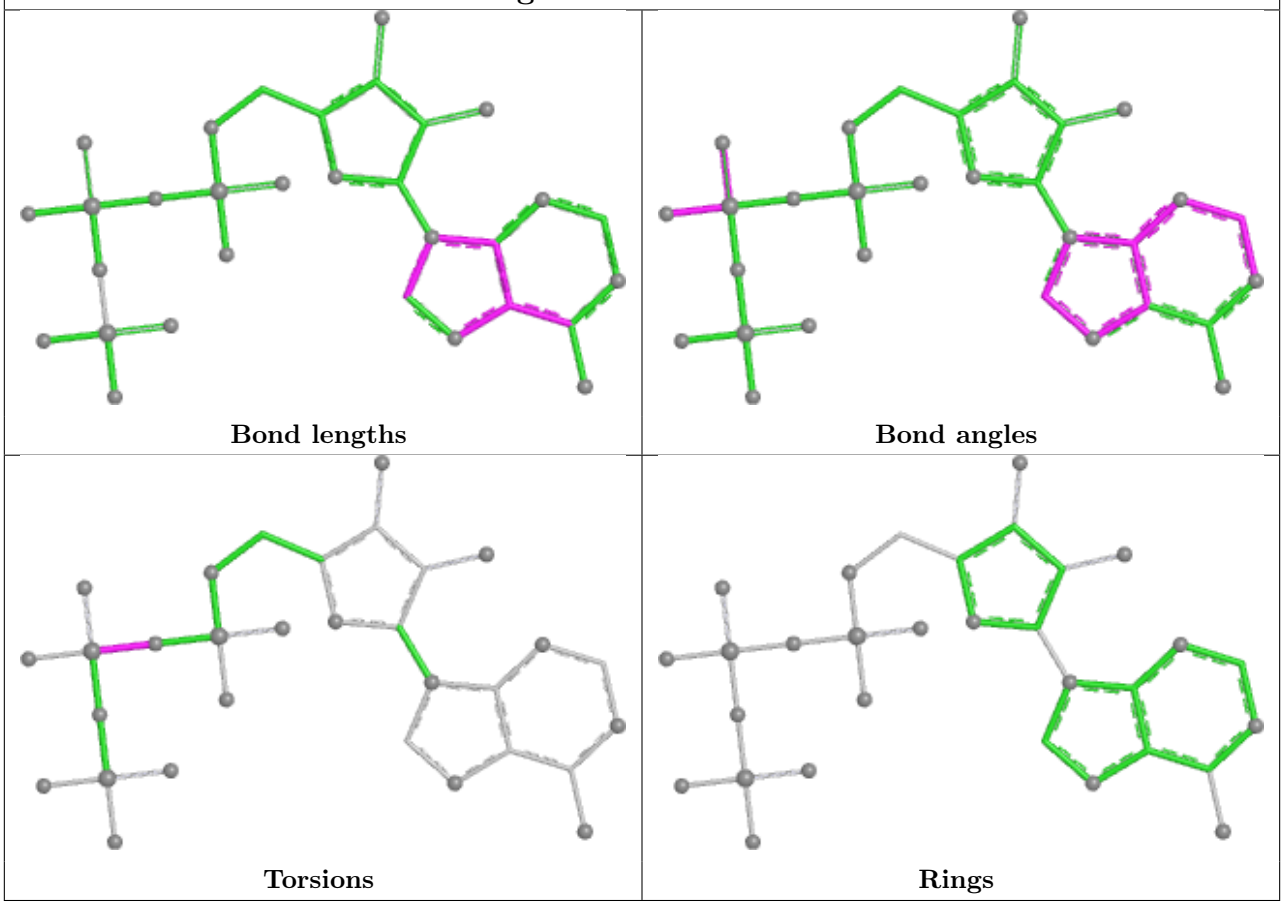
Ligand ATP F 803



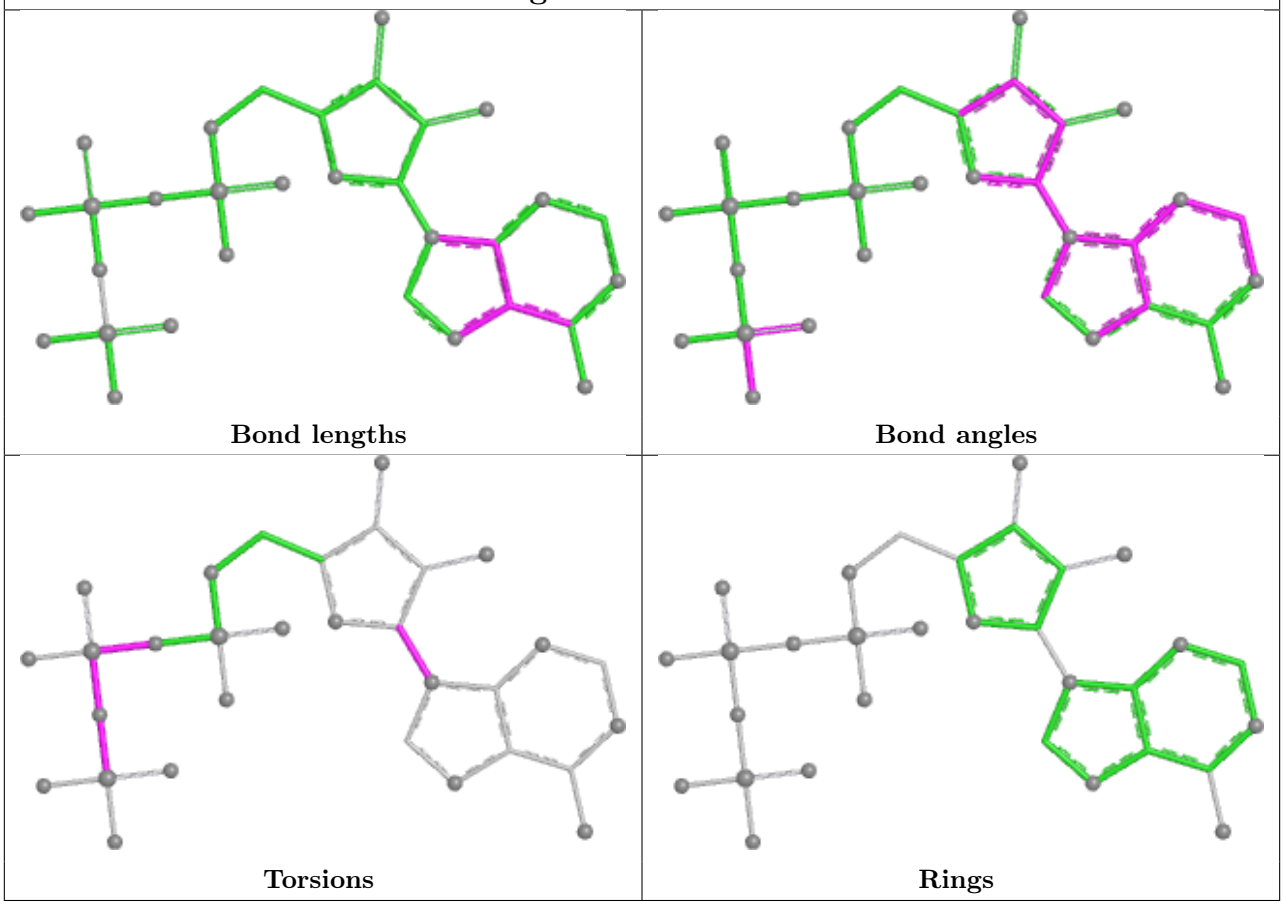
Ligand ADP D 803



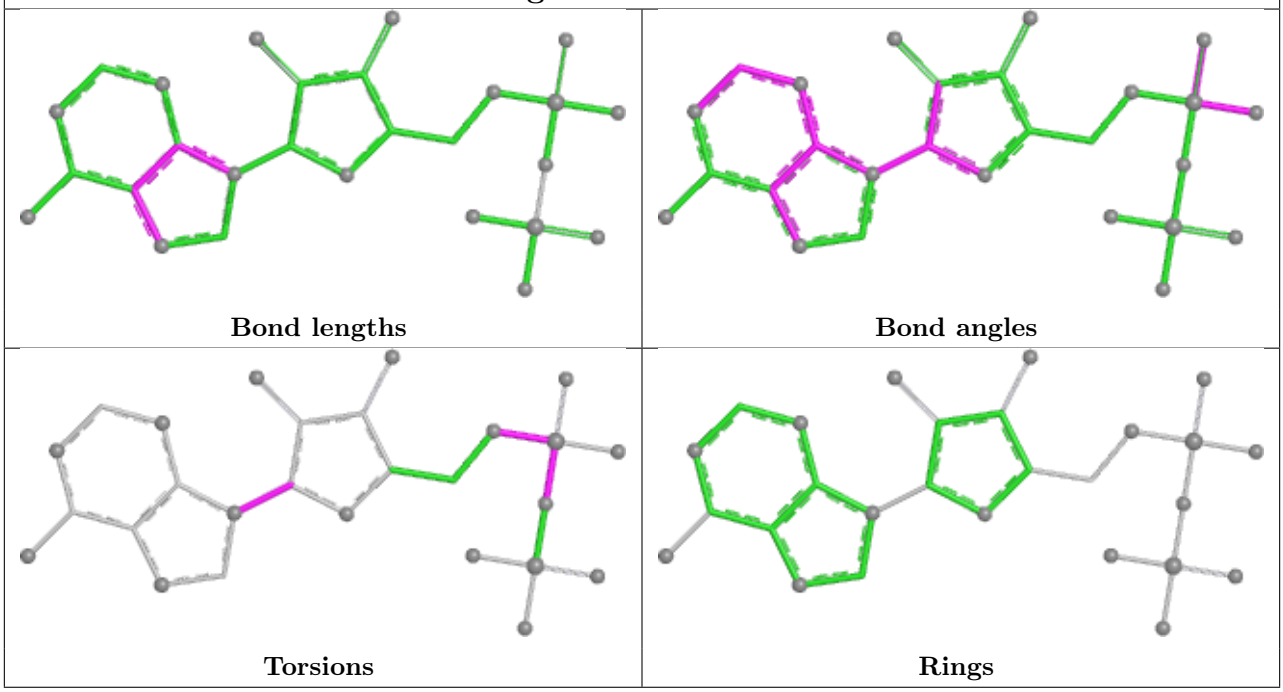
Ligand ATP B 1101



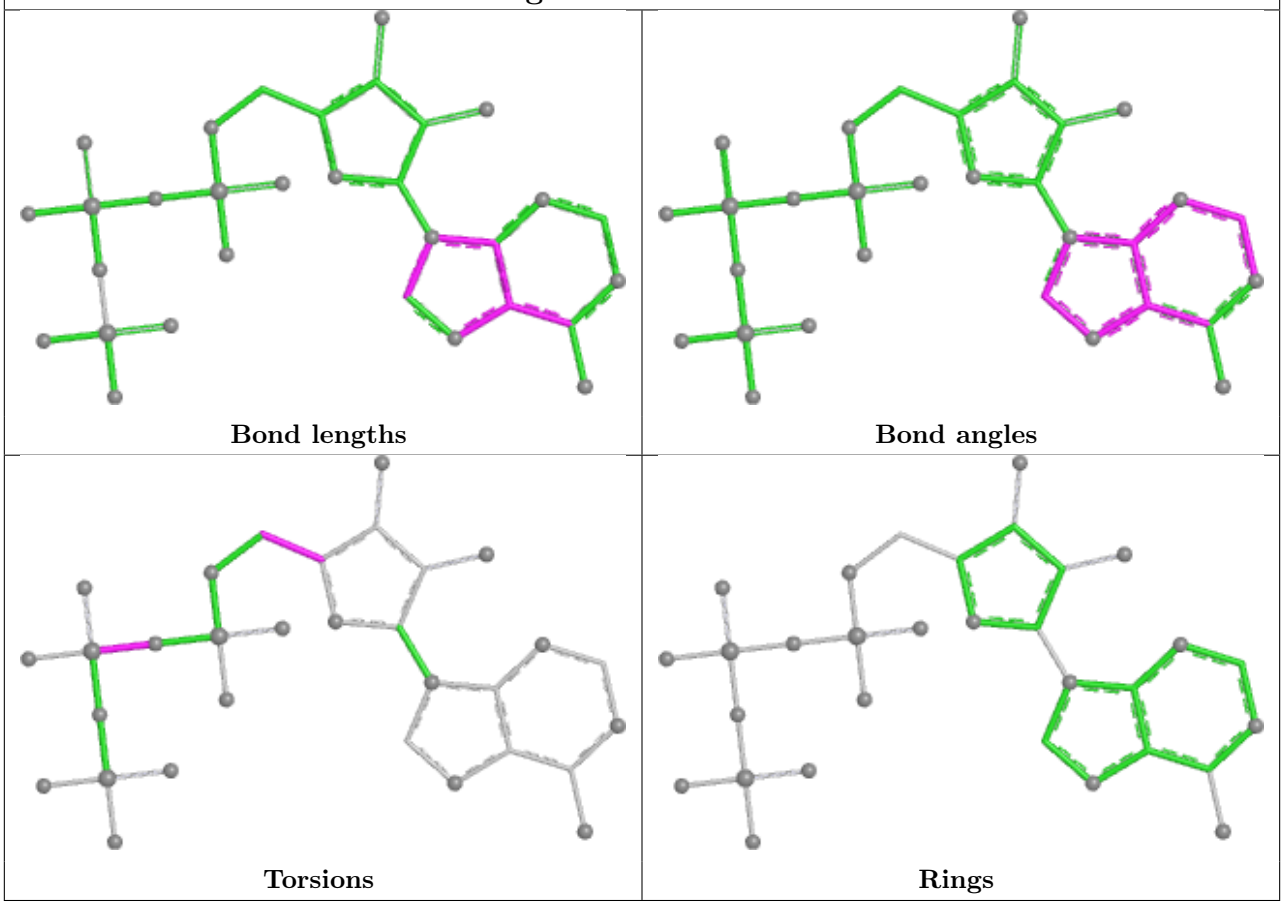
Ligand ATP 4 903



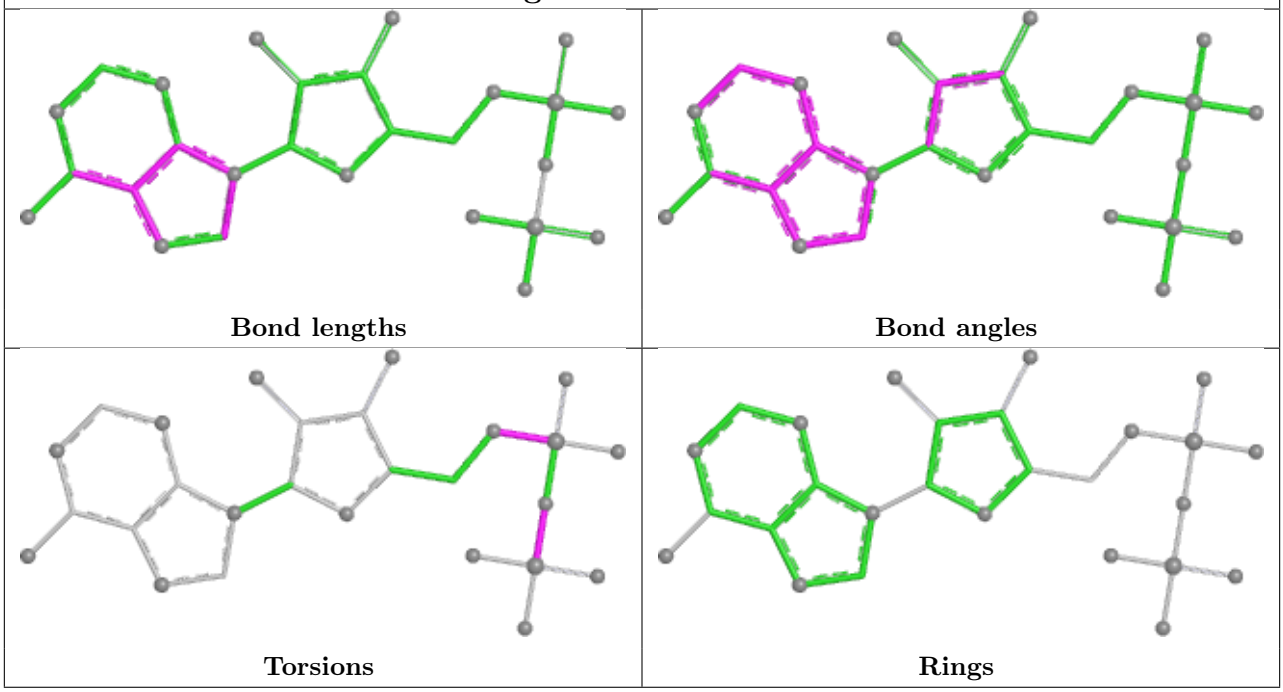
Ligand ADP 5 803



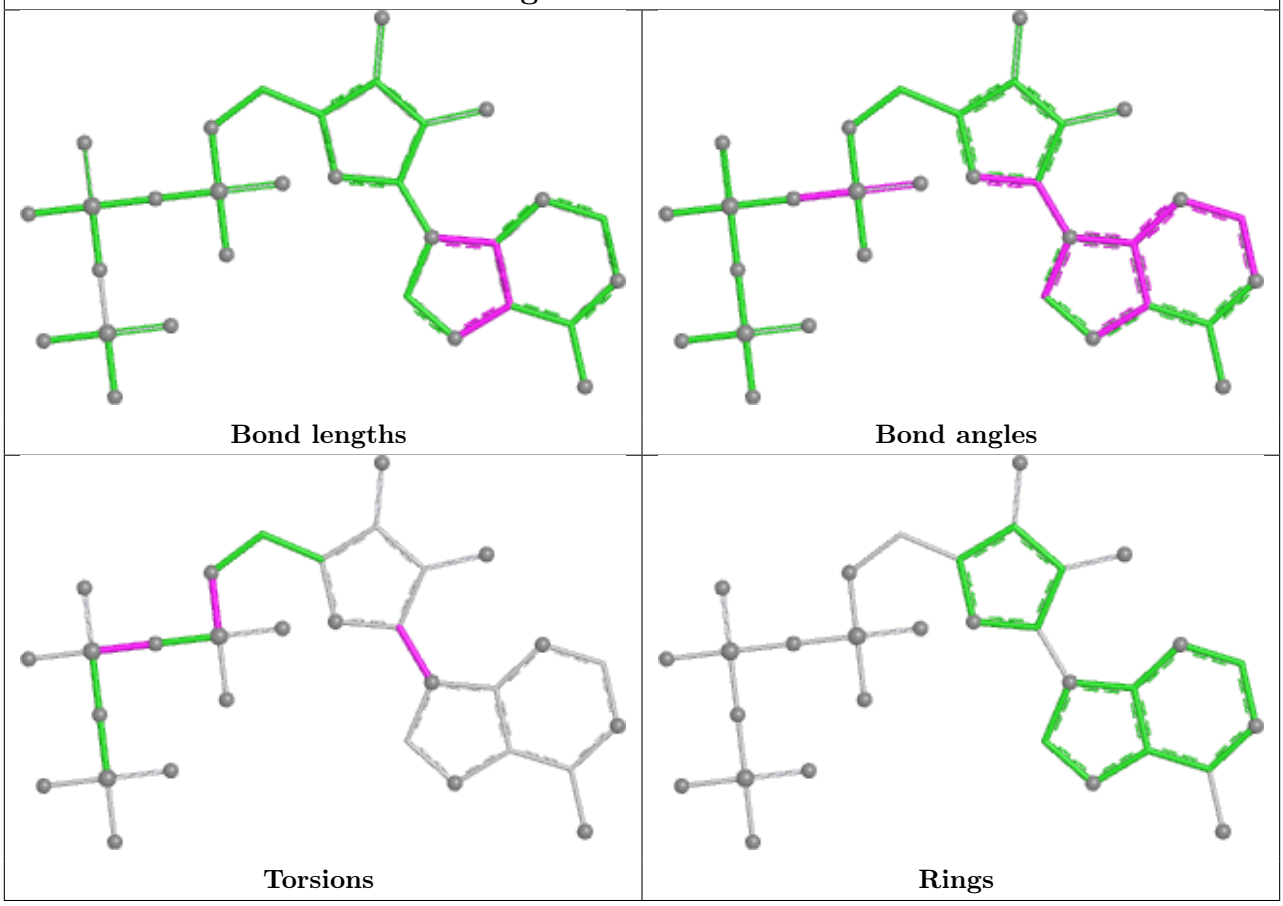
Ligand ATP C 903



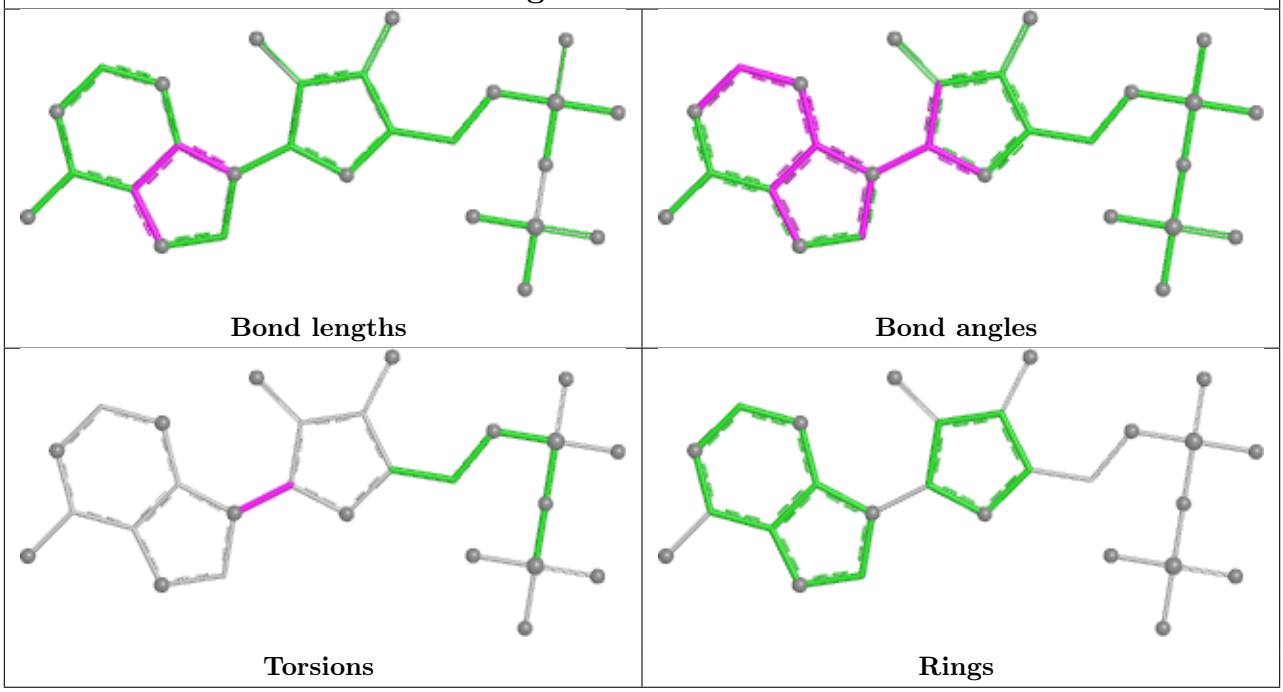
Ligand ADP E 903

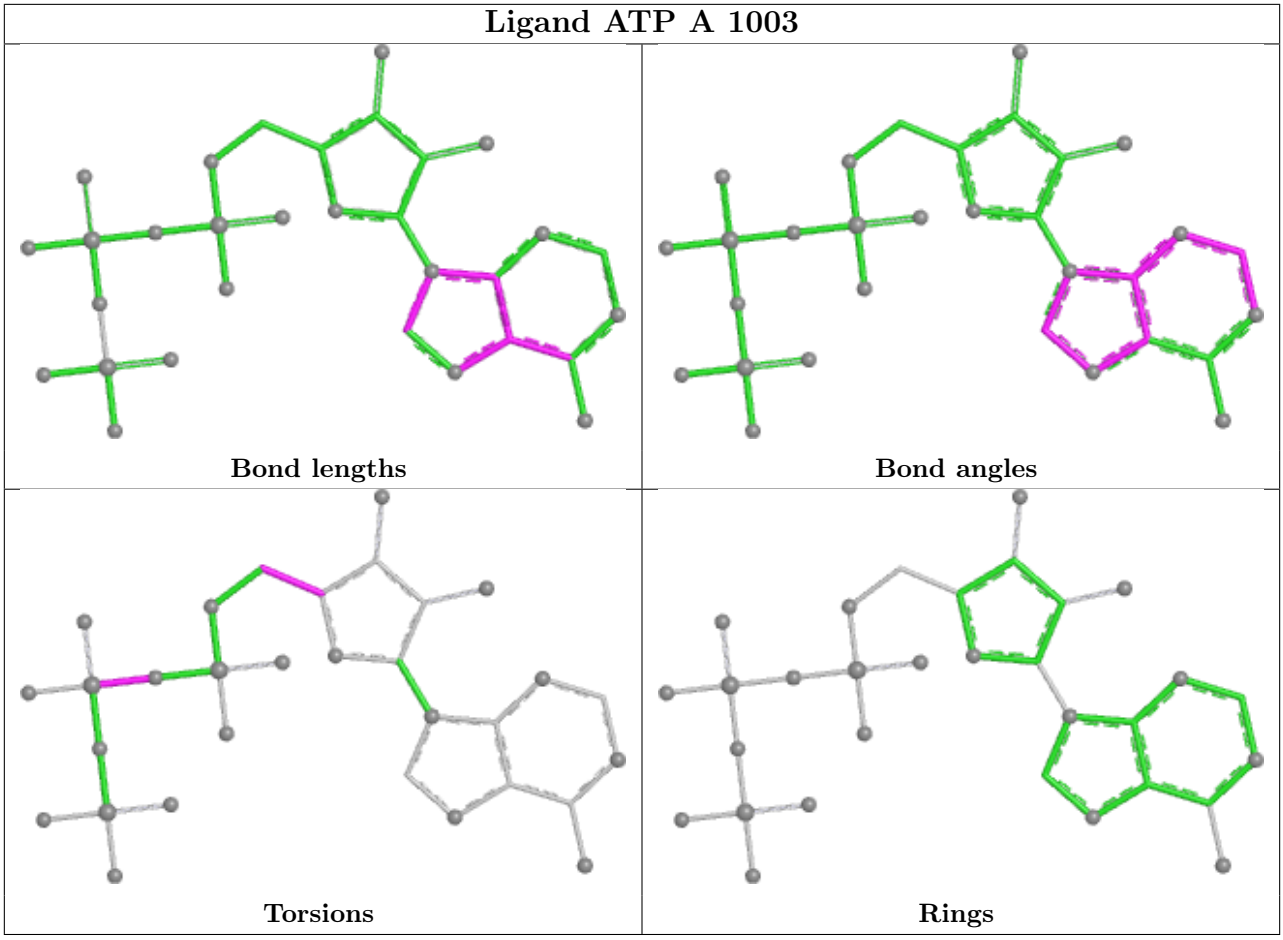


Ligand ATP 3 1101



Ligand ADP 6 903





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.

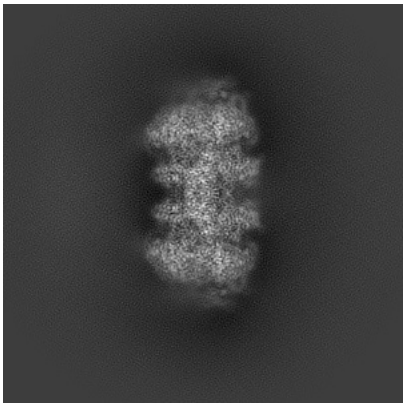
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-32258. These allow visual inspection of the internal detail of the map and identification of artifacts.

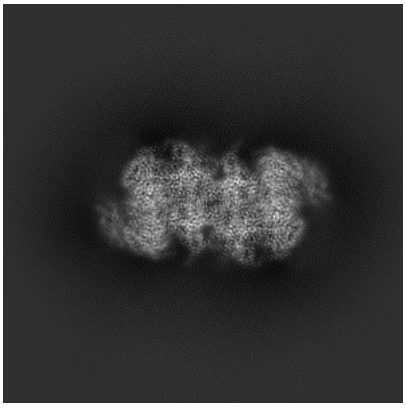
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

6.1.1 Primary map



X



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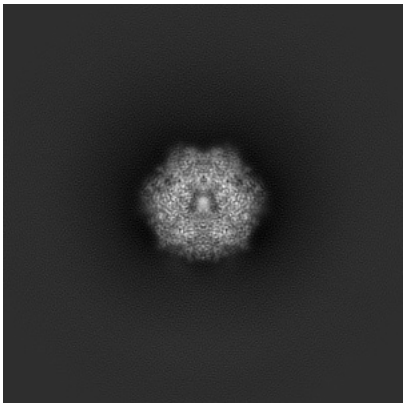
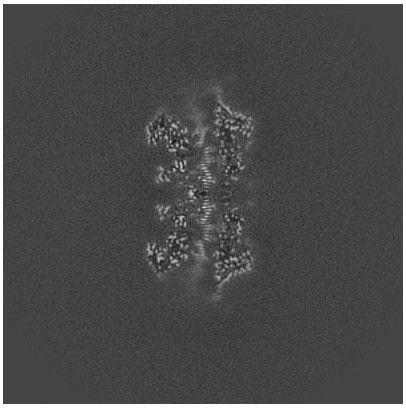


Z

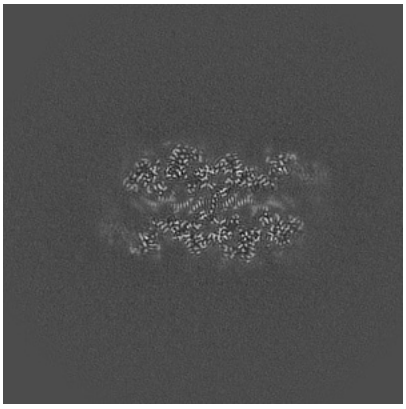
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map



X Index: 200



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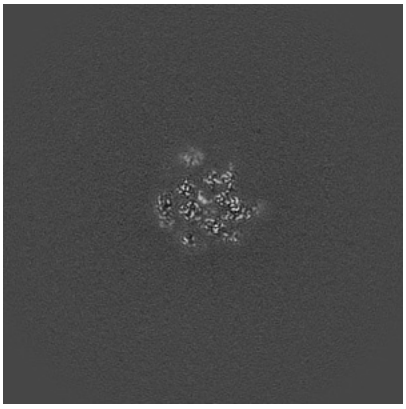
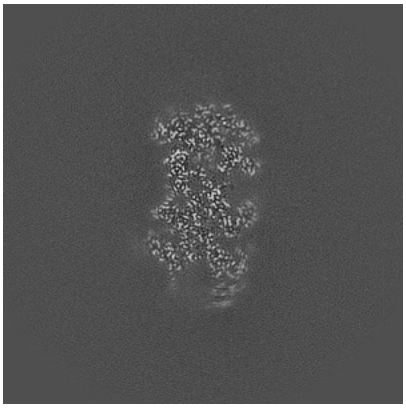


Z Index: 200

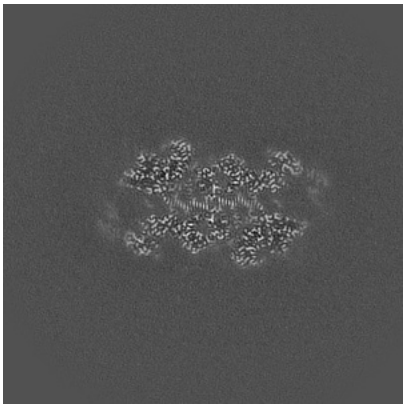
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

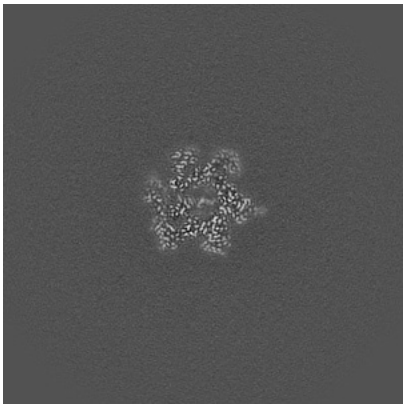
6.3.1 Primary map



X Index: 183



Y Index: 205

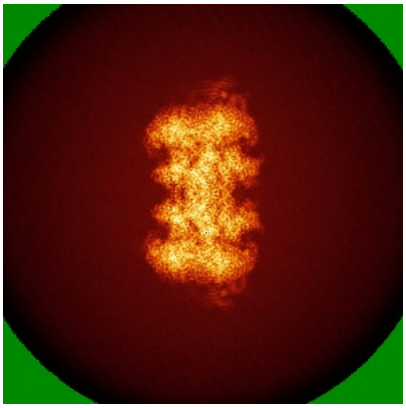


Z Index: 233

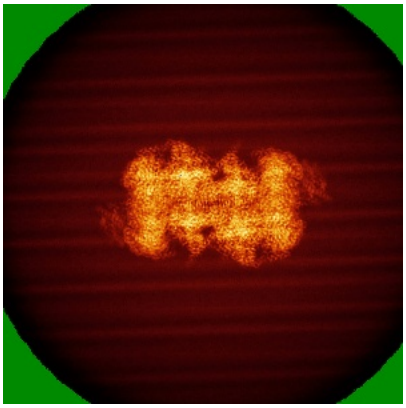
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

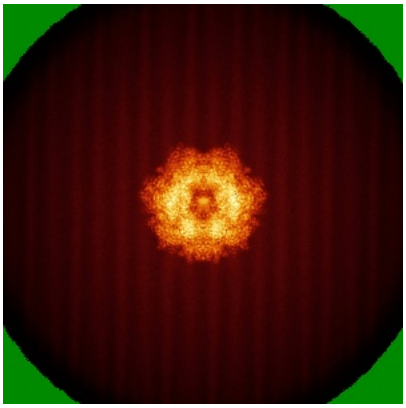
6.4.1 Primary map



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

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

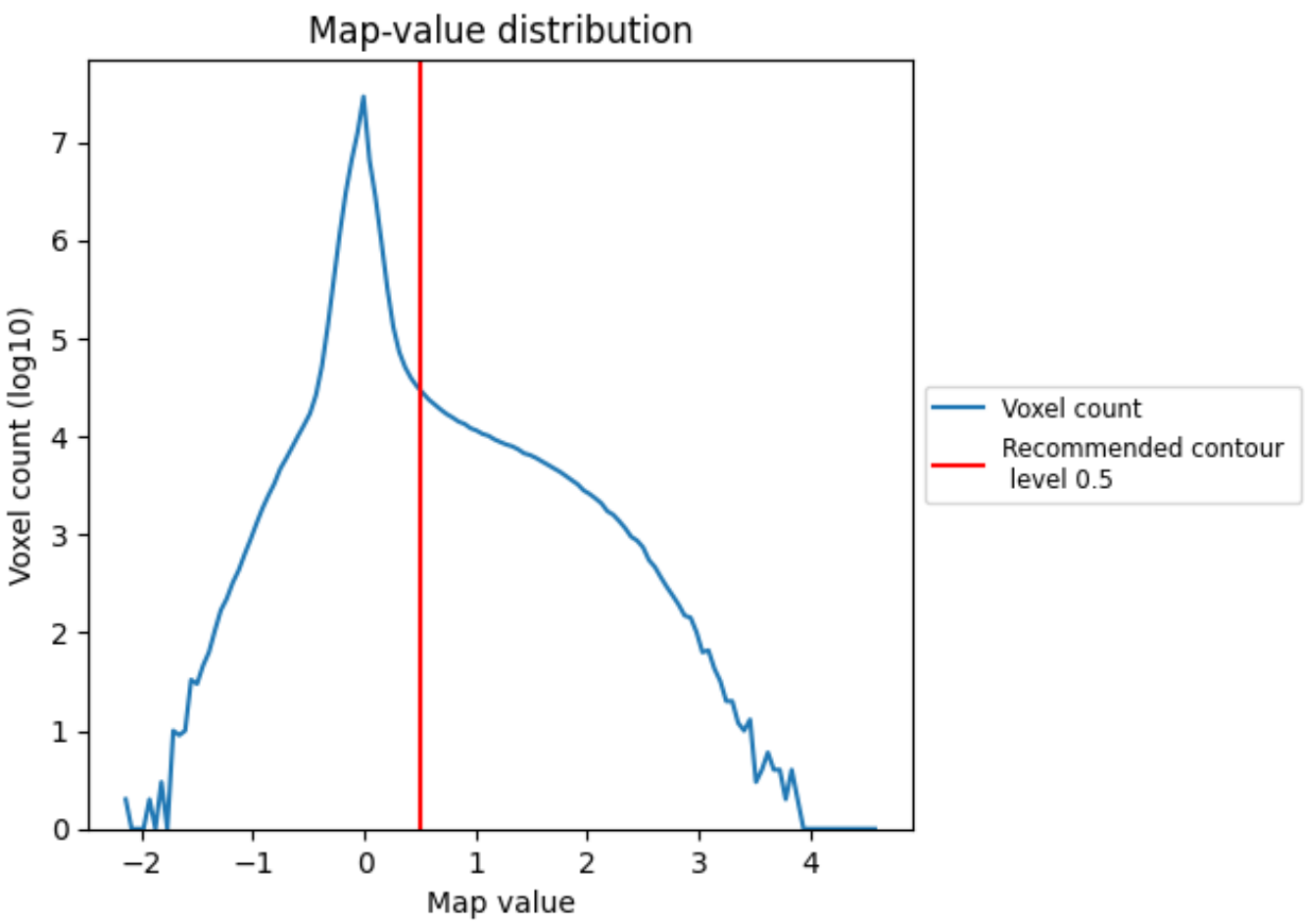
6.6 Mask visualisation (i)

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

7 Map analysis (i)

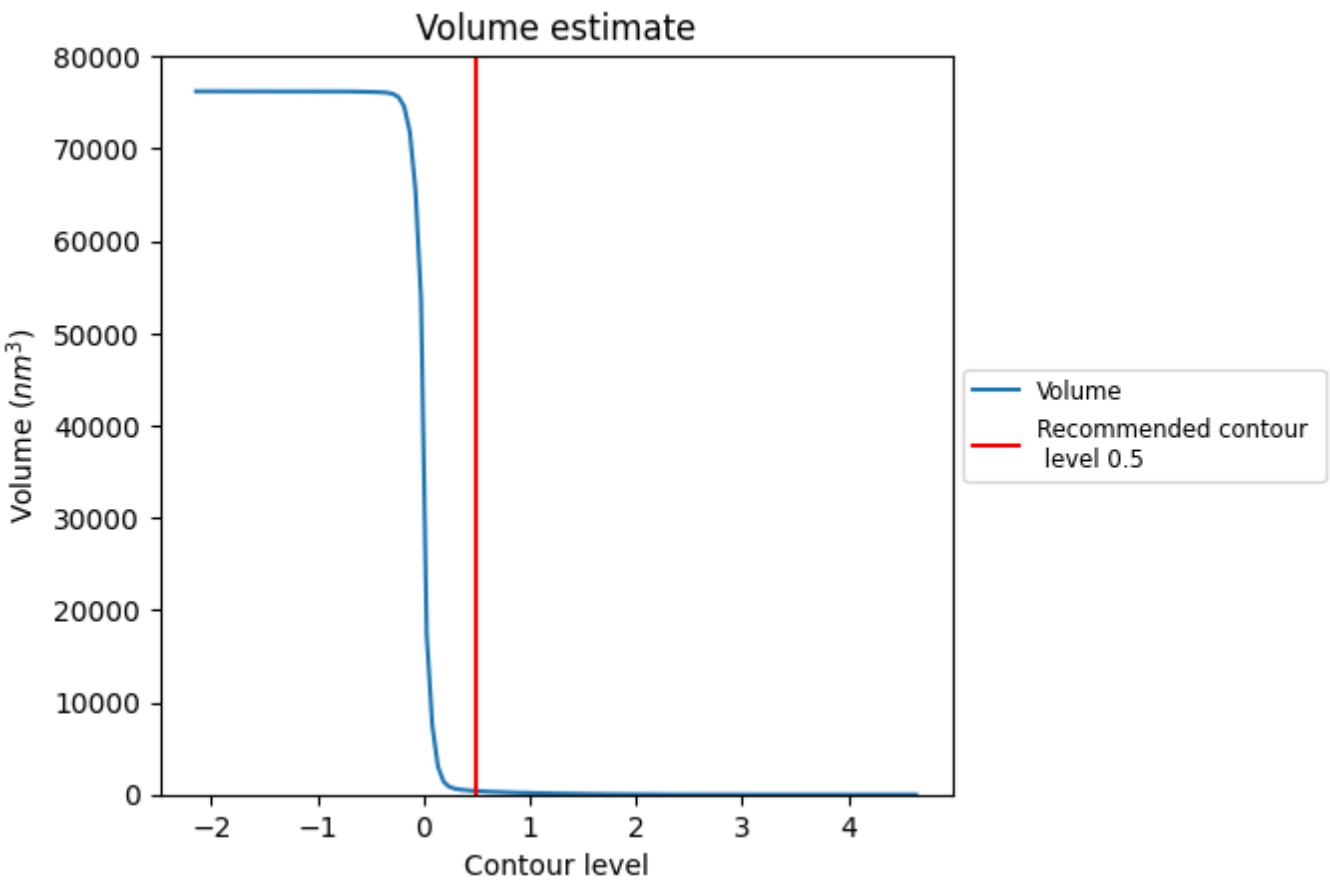
This section contains the results of statistical analysis of the map.

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.

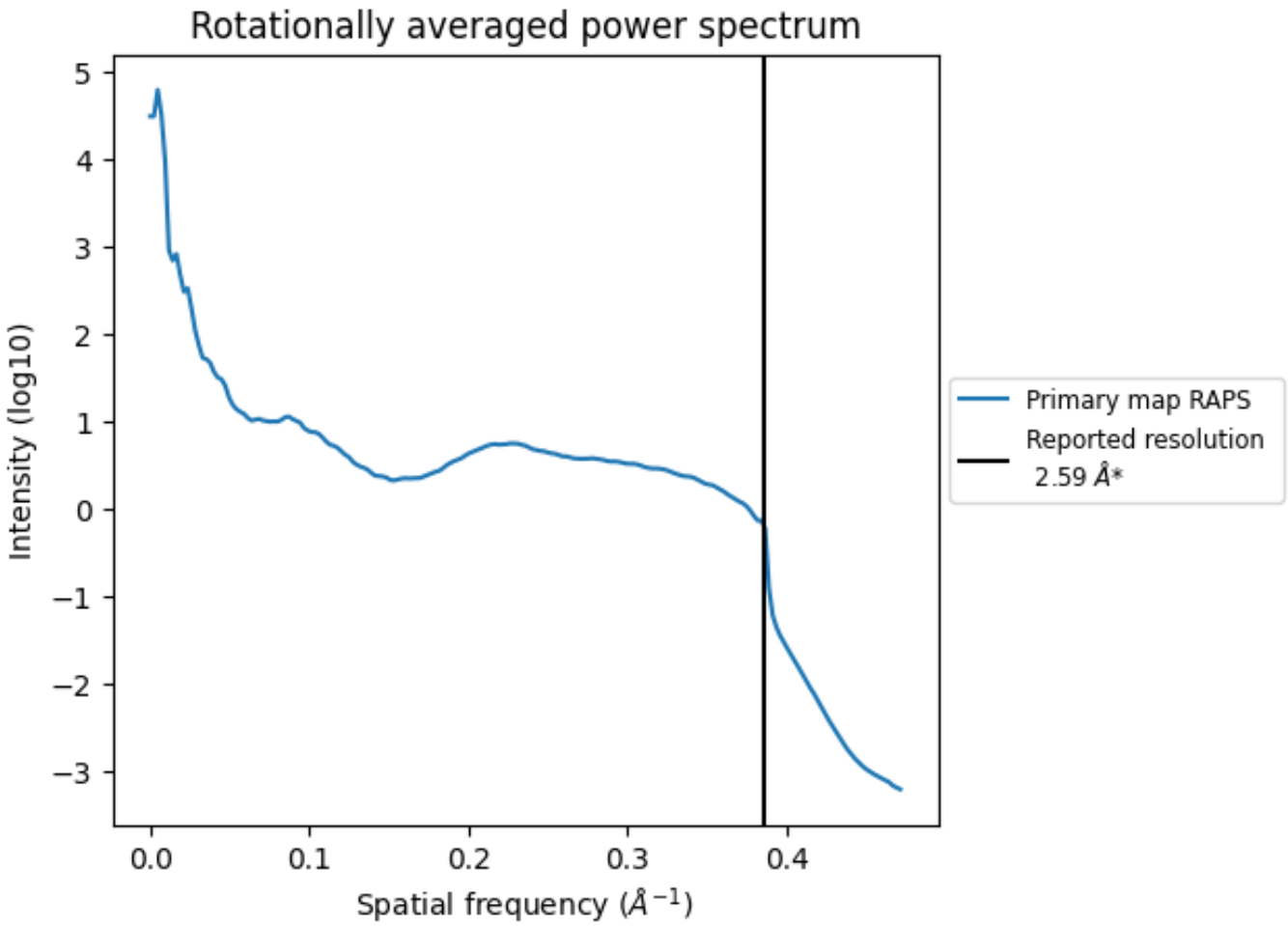
7.2 Volume estimate (i)



The volume at the recommended contour level is 385 nm^3; this corresponds to an approximate mass of 348 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 (i)



*Reported resolution corresponds to spatial frequency of 0.386 Å^{-1}

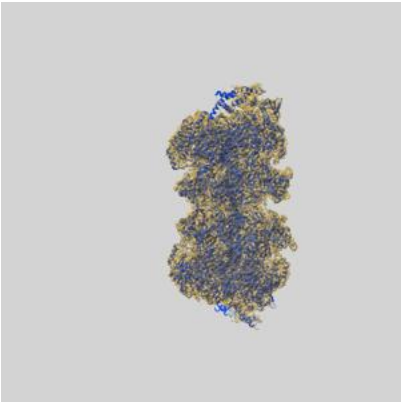
8 Fourier-Shell correlation (i)

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

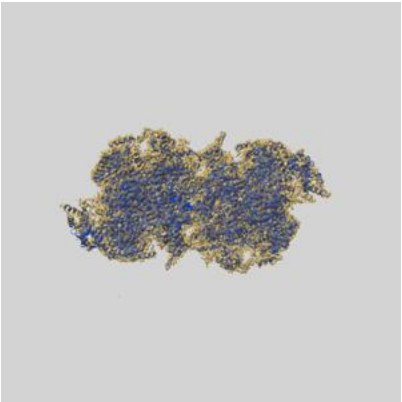
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-32258 and PDB model 7W1Y. Per-residue inclusion information can be found in section 3 on page 9.

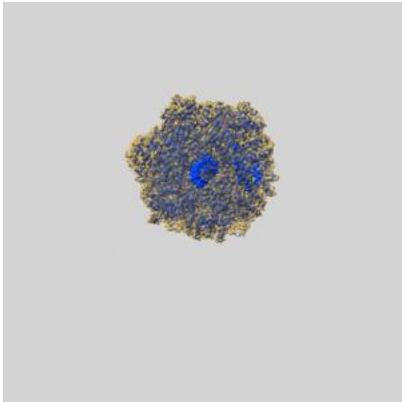
9.1 Map-model overlay (i)



X



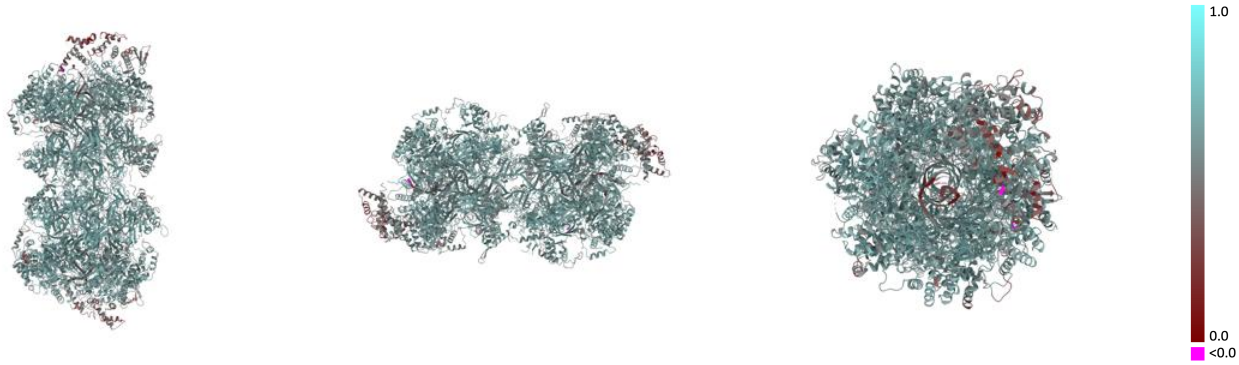
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.5 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.

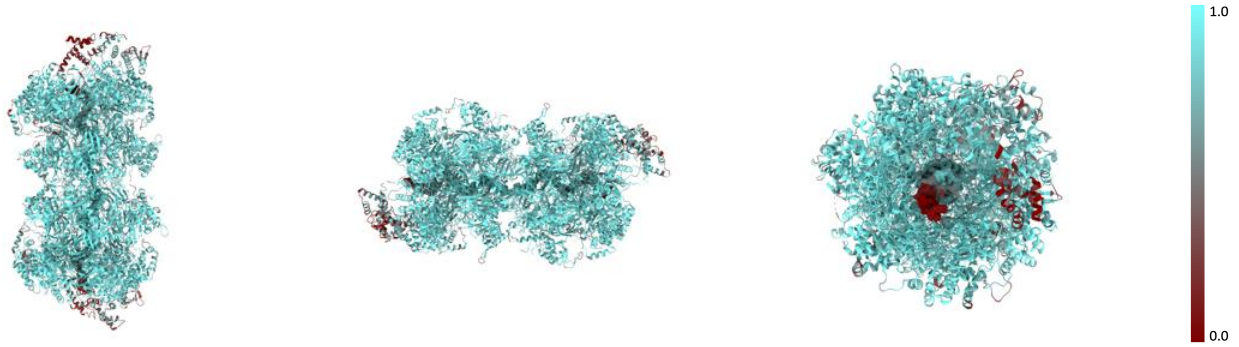
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

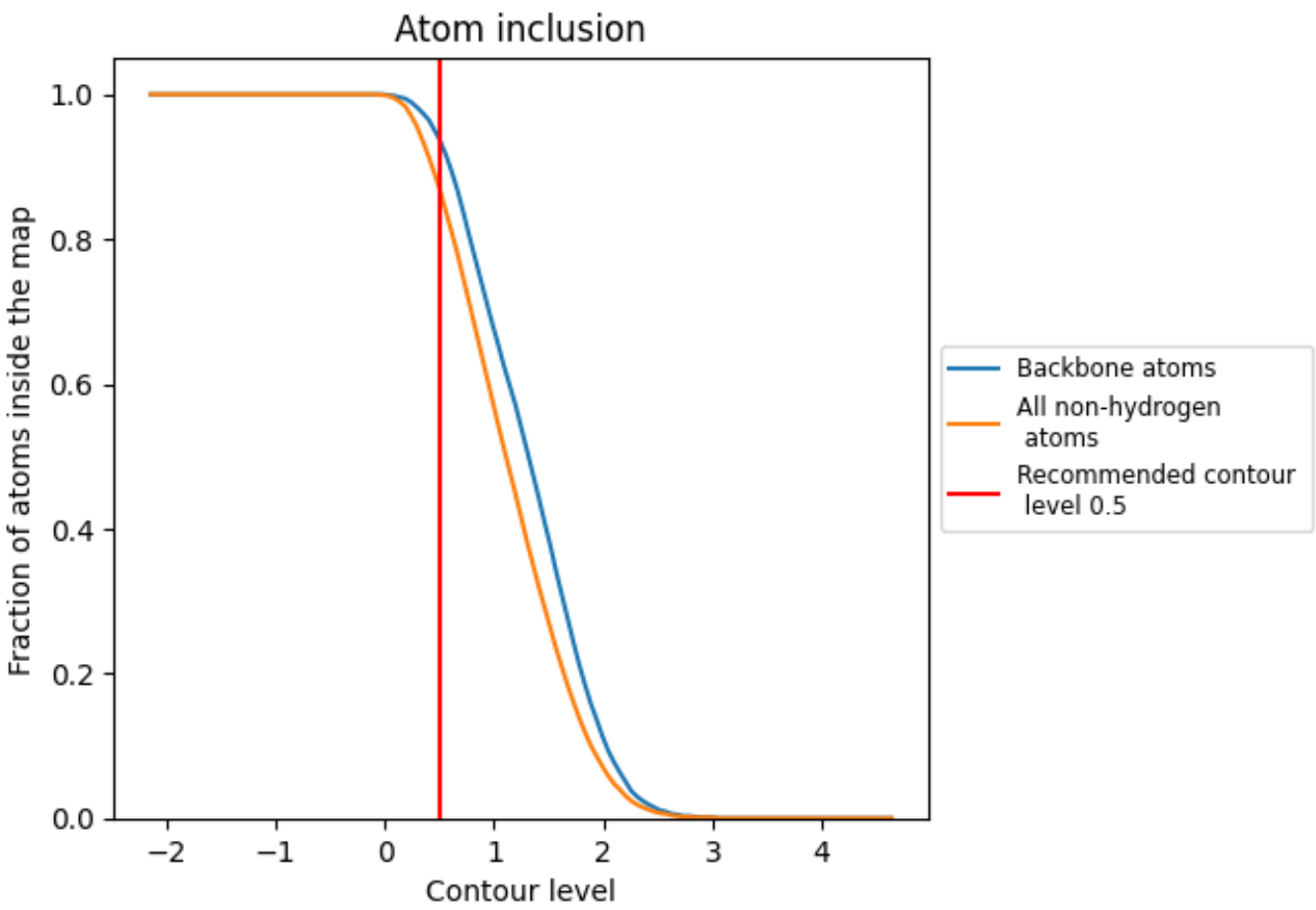
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.5).

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 87% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8700	0.5950
2	0.8420	0.5760
3	0.8930	0.6120
4	0.9100	0.6170
5	0.8110	0.5810
6	0.8530	0.5870
7	0.9060	0.6190
A	0.8570	0.5760
B	0.8890	0.6080
C	0.9130	0.6170
D	0.8300	0.5870
E	0.8720	0.5900
F	0.9030	0.6160
O	0.8220	0.5120
S	0.7670	0.5190