wwPDB EM Validation Summary Report (i)

Oct 5, 2026 – 12:50 PM JST

PDB ID	:	9X4M / pdb_00009x4m
EMDB ID	:	EMD-66553
Title	:	Sld3-CTD Docking on Mcm4-NTD-A
Authors	:	Yu, D.; Huo, Y.; Dang, S.; Zhai, Y.
Deposited on	:	2025-10-11
Resolution	:	3.15 Å(reported)
Based on initial model	:	.

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:

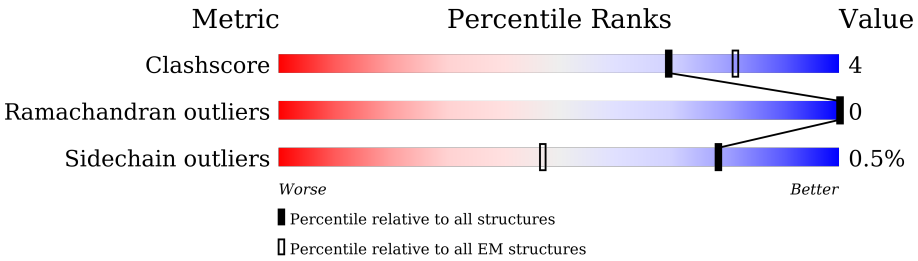
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using 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)	:	2.51

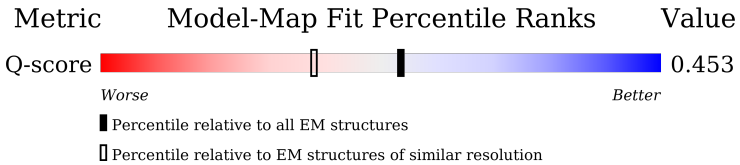
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.15 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	14486 (2.65 - 3.65)

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	868	65% 8% 28%
1	B	868	63% 9% 28%
2	3	971	58% 7% 35%
2	C	971	61% 5% 35%

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Mol	Chain	Length	Quality of chain
3	4	933	64% 7% 28%
3	D	933	63% 9% 28%
4	5	775	76% 9% 15%
4	E	775	75% 9% 15%
5	6	1017	57% 7% 36%
5	F	1017	58% 5% 37%
6	7	845	76% 7% 17%
6	G	845	74% 8% 18%
7	X	668	98%

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 62405 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	628	4970	3133	883	935	19	0	0
1	B	628	4970	3133	883	935	19	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	3	636	4983	3140	888	942	13	0	0
2	C	636	4978	3137	888	940	13	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	669	5316	3334	917	1035	30	0	0
3	D	670	5323	3339	918	1036	30	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	5	658	5145	3228	882	1010	25	0	0
4	E	657	5137	3222	881	1009	25	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	650	5143	3236	898	983	26	0	0
5	F	638	5052	3184	884	959	25	0	0

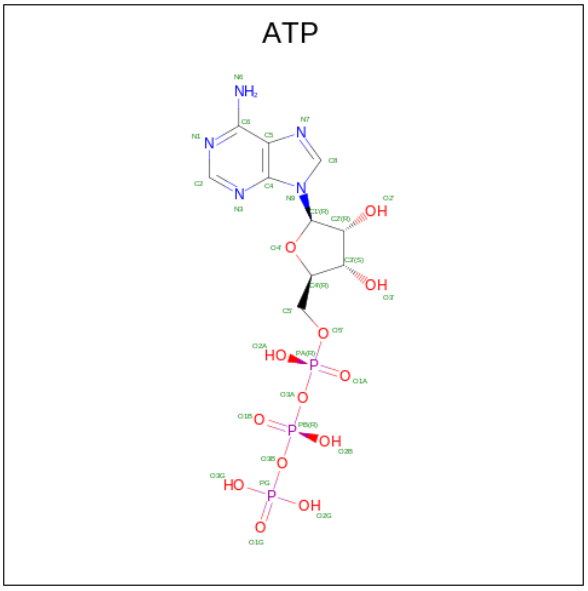
- Molecule 6 is a protein called DNA replication licensing factor MCM7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	7	699	5505	3463	952	1059	31	0	0
6	G	694	5467	3440	947	1049	31	0	0

- Molecule 7 is a protein called DNA replication regulator SLD3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	X	12	102	63	21	17	1	0	0

- Molecule 8 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
8	2	1	31	10	5	13	3	0
8	4	1	31	10	5	13	3	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
8	7	1	31	10	5	13	3	0
8	B	1	31	10	5	13	3	0
8	D	1	31	10	5	13	3	0
8	G	1	31	10	5	13	3	0

- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
9	2	1	1	1	0
9	3	1	1	1	0
9	4	1	1	1	0
9	5	1	1	1	0
9	7	1	1	1	0
9	B	1	1	1	0
9	C	1	1	1	0
9	D	1	1	1	0
9	E	1	1	1	0
9	G	1	1	1	0

- Molecule 10 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
10	2	1	1	1	0
10	4	1	1	1	0
10	5	1	1	1	0

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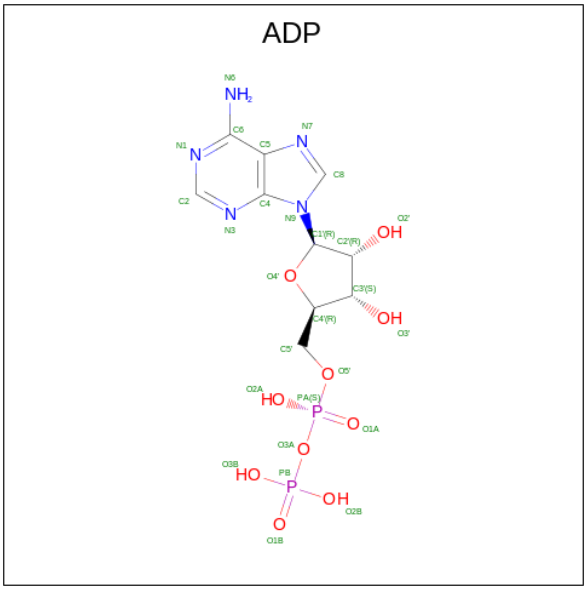
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
10	6	1	1	1	0
			Total	Zn	
10	7	1	1	1	0
			Total	Zn	
10	B	1	1	1	0
			Total	Zn	
10	D	1	1	1	0
			Total	Zn	
10	E	1	1	1	0
			Total	Zn	
10	F	1	1	1	0
			Total	Zn	
10	G	1	1	1	0

- Molecule 11 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



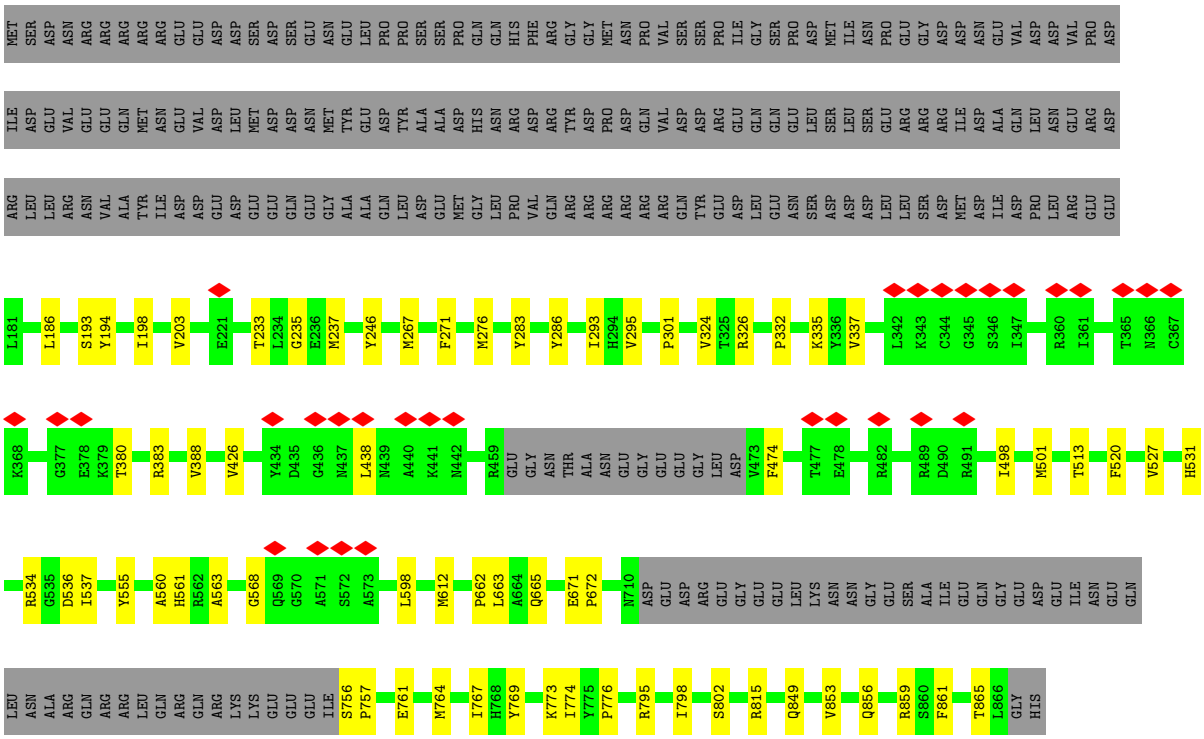
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
11	3	1	27	10	5	10	2	0
			Total	C	N	O	P	
11	5	1	27	10	5	10	2	0
			Total	C	N	O	P	
11	C	1	27	10	5	10	2	0
			Total	C	N	O	P	
11	E	1	27	10	5	10	2	0

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.

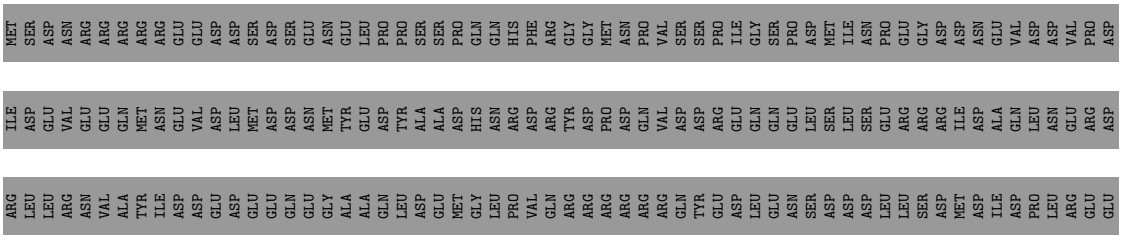
• Molecule 1: DNA replication licensing factor MCM2

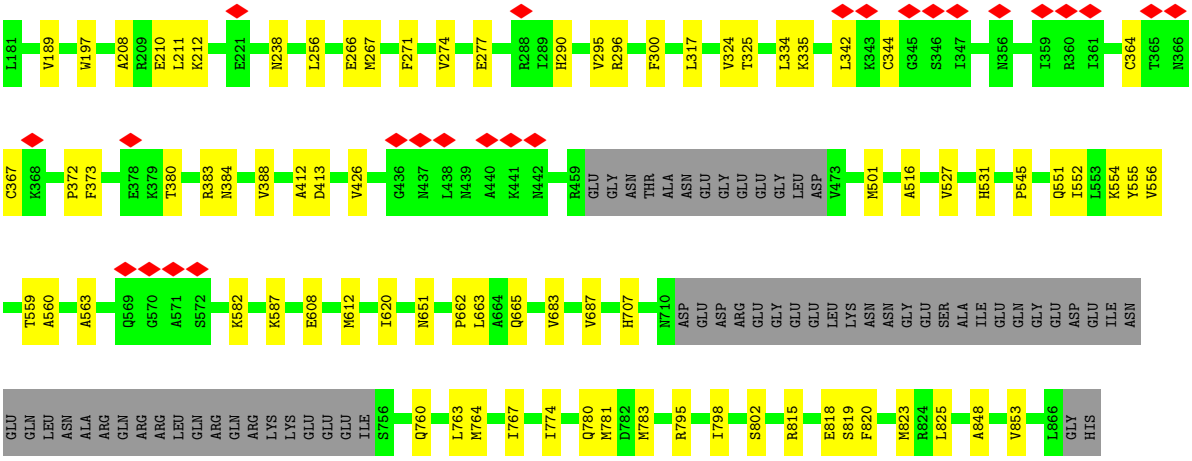
Chain 2:



• Molecule 1: DNA replication licensing factor MCM2

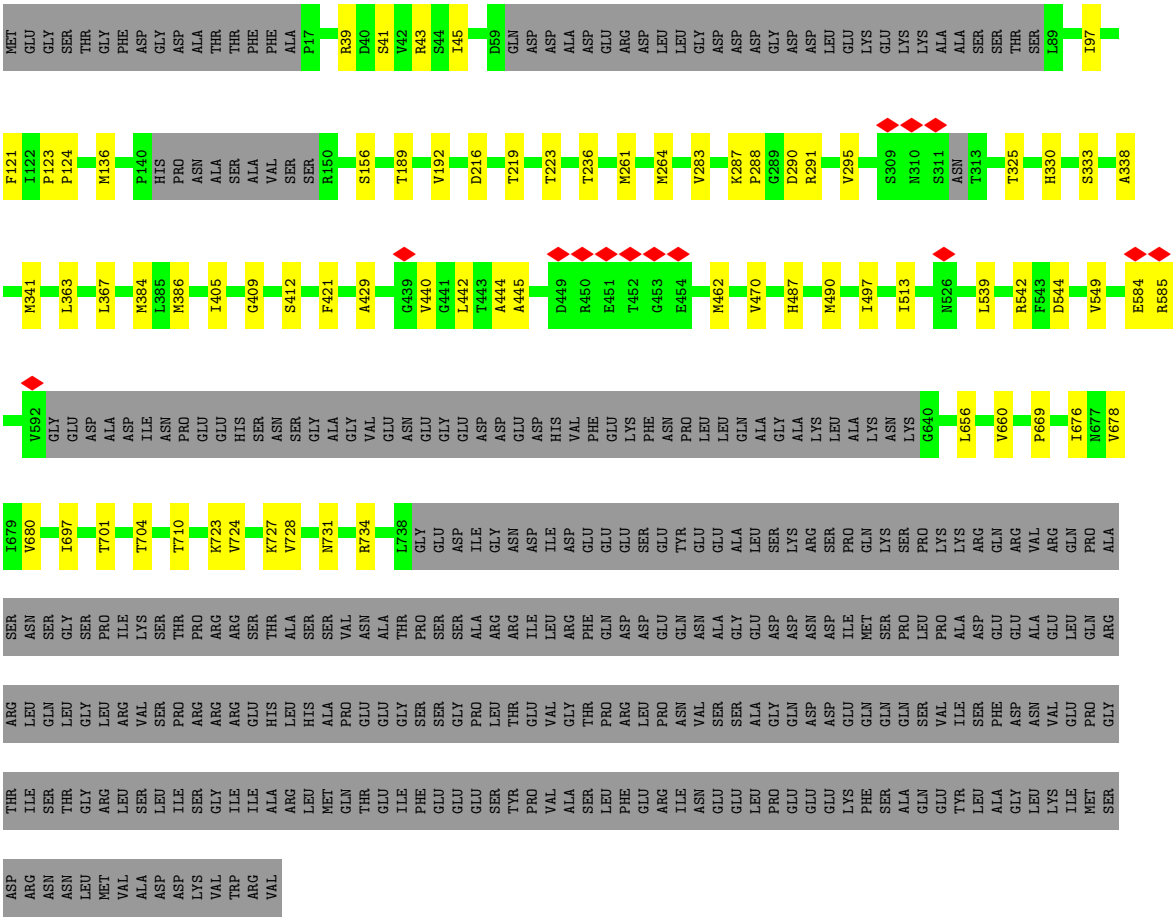
Chain B:





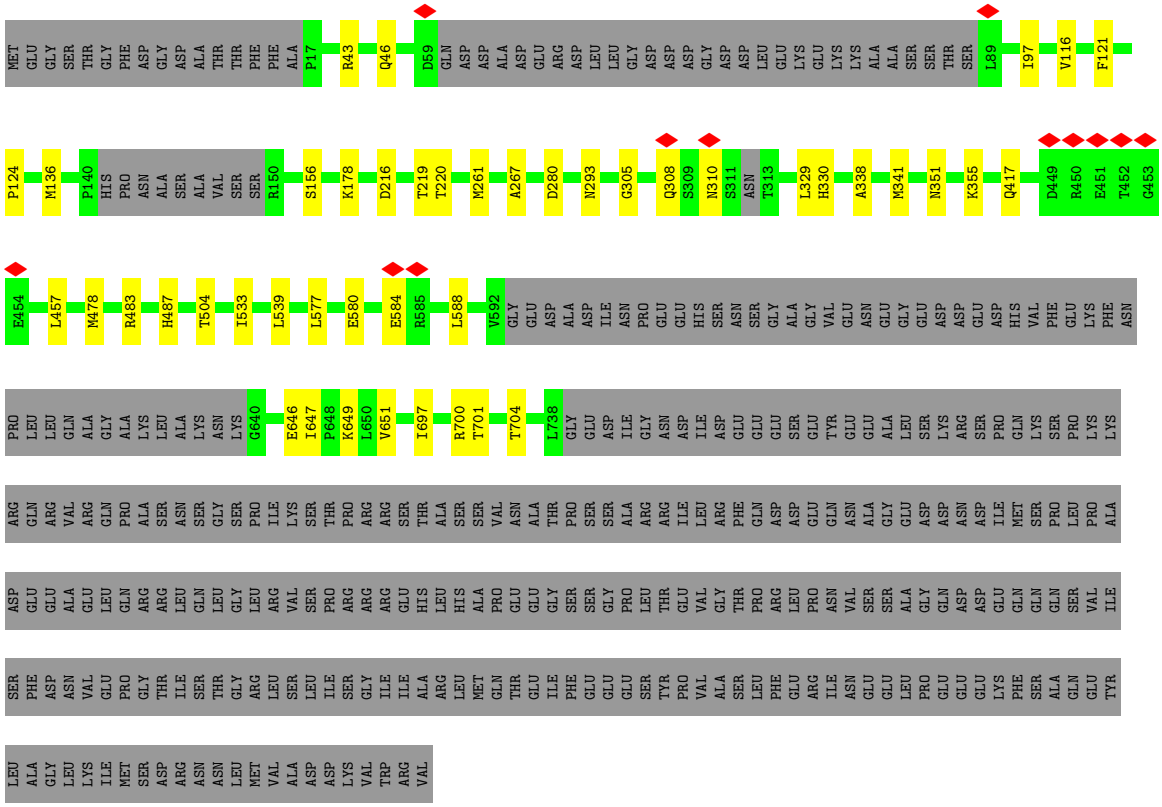
- Molecule 2: DNA replication licensing factor MCM3

Chain 3:



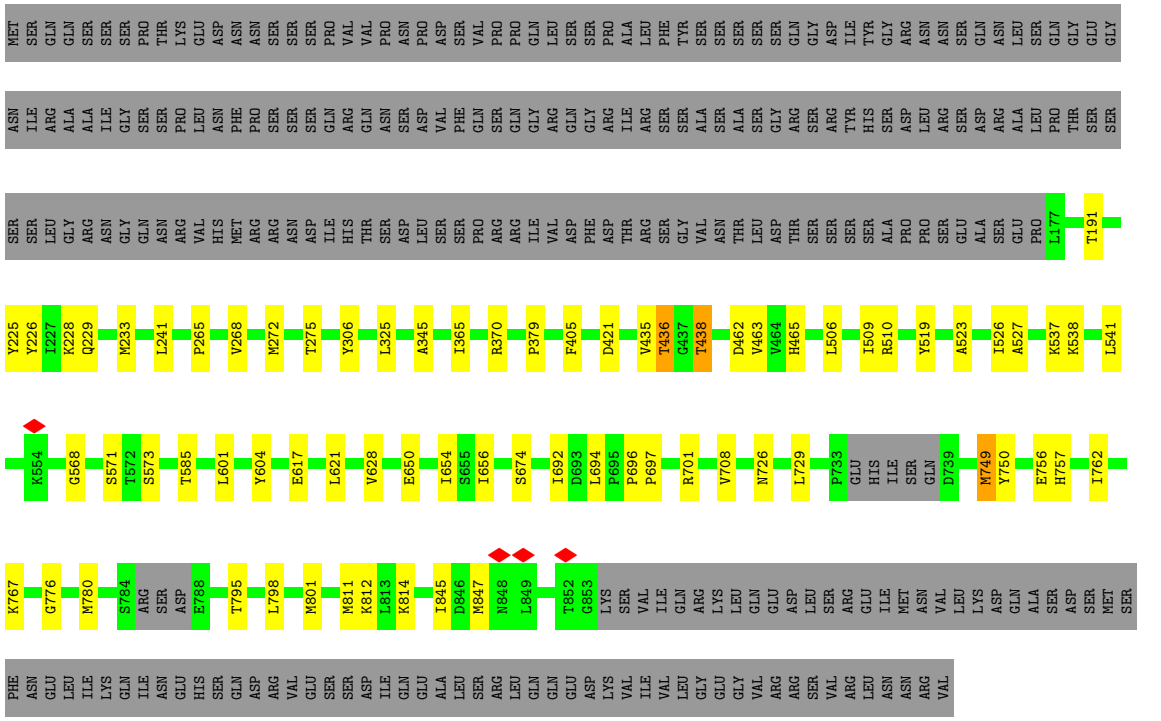
- Molecule 2: DNA replication licensing factor MCM3

Chain C:



• Molecule 3: DNA replication licensing factor MCM4

Chain 4: 64% 7% 28%



• Molecule 3: DNA replication licensing factor MCM4

Chain D: 63% 9% 28%

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

ASN ILE ARG ALA ALA ILE GLY SER SER PRO LEU ASN PHE PRO SER SER SER GLN ARG GLN ASN SER ASP VAL PHE GLN SER GLN GLY ARG GLN GLY ARG ILE ARG SER SER ALA SER ALA SER GLY ARG SER ARG TYR HIS SER ASP LEU ARG SER ASP ARG ALA LEU PRO THR SER SER

SER SER LEU GLY ARG ASN GLY GLN ASN ARG VAL HIS MET ARG ARG ASN ASP ILE HIS THR SER ASP LEU SER SER PRO ARG ARG ILE VAL ASP PHE ASP THR ARG SER GLY VAL ASN THR LEU ASP THR SER SER SER SER ALA PRO PRO SER GLU ALA SER GLU P176 Y225 Q229

P265 V268 I269 M272 D273 M280 Y301 Y306 N307 V308 M314 R315 E316 L317 D323 N327 V344 A345 C349 D353 A357 I365 P368 C371 E378 S381 M382 P412 H413 L417 V435 T436 R449 D471 M486

R499 D505 L506 A507 K508 I509 R510 E511 E532 L533 K550 S573 A598 L601 T602 A603 Y604 E617 A620 L621 T641 H646 E647 V648 M649 E650 V688 I692 P697 L709 N726 L727 Y728 L729 P733 GLU HIS ILE SER GLN D739 Y750

E756 H757 I758 H759 P760 M777 S784 ARG SER ASP E788 K789 A793 Q797 M801 M811 E818 L819 E820 I833 K834 D835 T838 N848 L849 V850 Q851 T852 G853 LYS SER VAL ILE GLN ARG LYS LEU GLN GLU ASP LEU SER ARG GLU ILE MET ASN VAL LEU LYS

ASP GLN ALA SER ASP SER MET SER PHE ASN GLU LEU ILE LYS GLN ILE ASN GLU HIS SER GLN ASP ARG VAL GLU SER SER ASP ILE GLN GLU ALA LEU SER ARG LEU GLN GLN GLU ASP LYS VAL ILE VAL LEU GLY GLU GLY VAL ARG ARG SER VAL ARG LEU ASN ASN ARG VAL

- Molecule 4: Minichromosome maintenance protein 5

Chain 5: 76% 9% 15%

MET S2 P12 T62 I69 Y76 D85 P88 I101 L104 A110 ASN ASN ASN ASP LYS ASP PRO GLU ASN THR SER MET ASP THR ASP SER LEU LEU L129 I138 T169 T177 M182 C183 H188 T189 T190 S191 F197 T200 T201 G202 N203

T204 V205 P208 E216 S217 E218 S219 A222 N223 GLU SER ASN ILE GLY ASP GLU SER THR K233 Y241 I244 D252 L256 V265 P266 V267 G268 E269 M270 P271 M276 L282 I300 K304 ASN GLY ALA GLY SER GLY ARG SER GLY GLY GLY GLY ASN GLY GLY

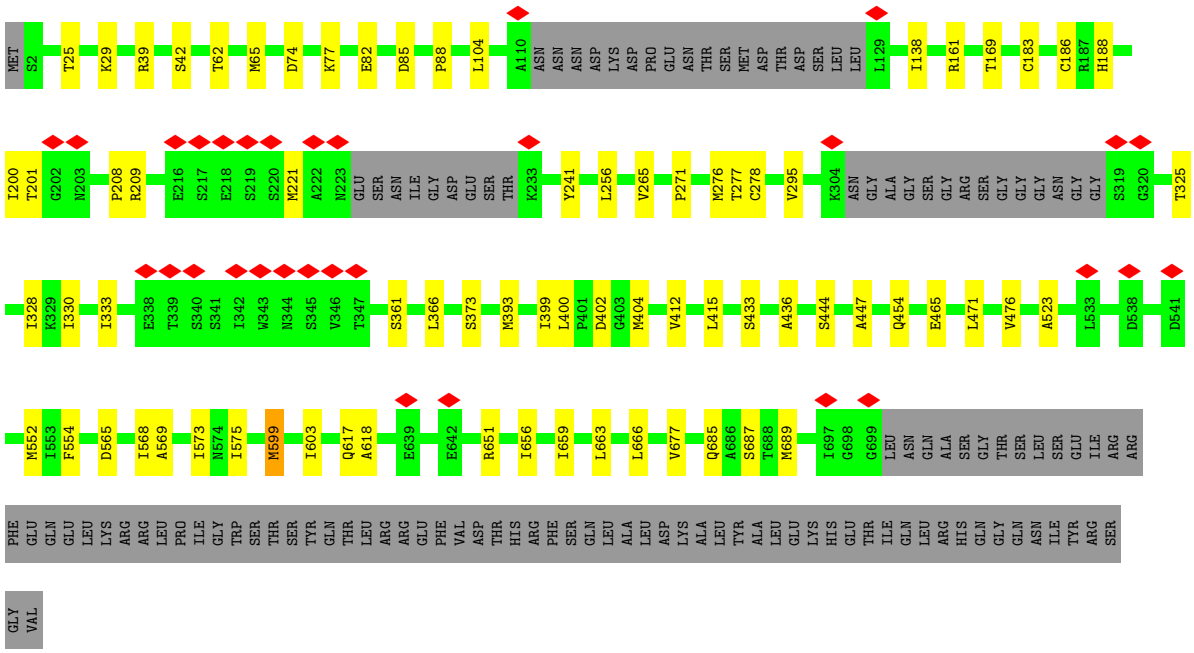
S319 I328 K329 I330 D336 V337 E338 T339 S340 S341 I342 W343 N344 S361 L366 A375 I378 F379 M393 I399 M404 G416 A421 S433 A436 S444 A447 M469 M485 I493 E498 I526 Y527 G528 R529 D532 L533 D541

F554 I555 V556 H560 Q586 E589 C606 R607 P616 E620 E639 S640 T641 E642 I650 K665 Q685 A686 S687 T688 M689 I697 G698 G699 L700 ASN GLN ALA SER GLY THR SER LEU SER GLU ILE ARG ARG PHE GLU GLN GLU LEU LYS ARG ARG LEU PRO

ILE GLY TRP SER THR SER TYR GLN THR LEU ARG ARG GLU PHE VAL ASP THR HIS ARG PHE SER GLN LEU ALA LEU ASP LYS ALA LEU TYR ALA LEU GLU LYS HIS GLU THR ILE GLN LEU ARG HIS GLN GLY GLN ASN ILE TYR ARG SER GLY VAL

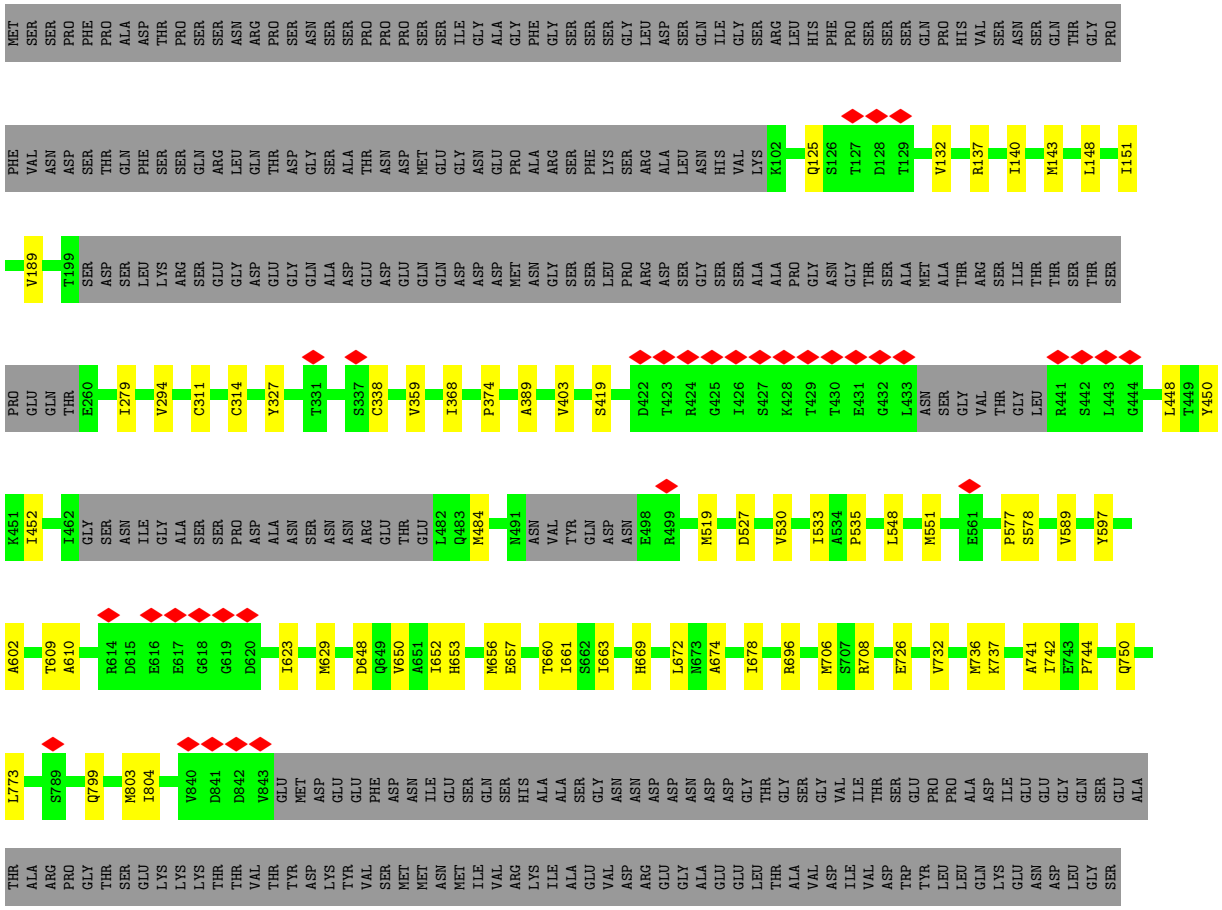
- Molecule 4: Minichromosome maintenance protein 5

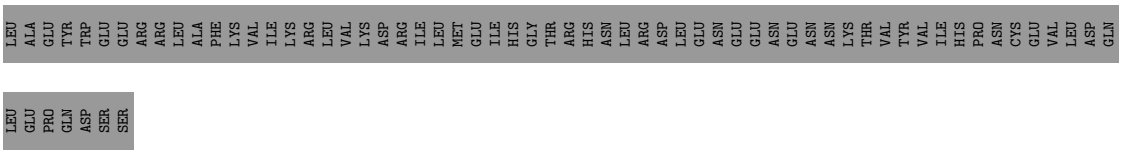
Chain E: 75% 9% 15%



- Molecule 5: DNA replication licensing factor MCM6

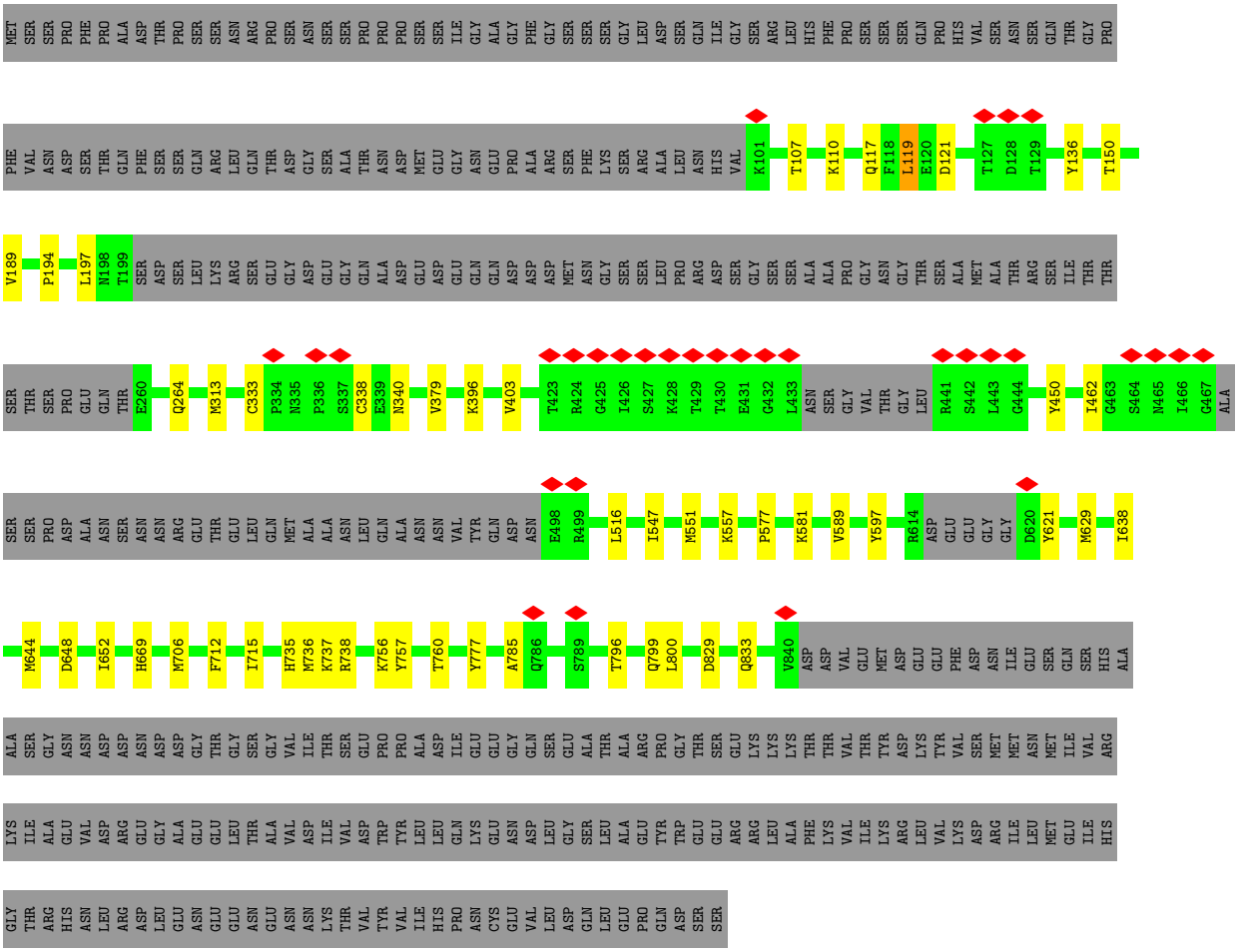
Chain 6:





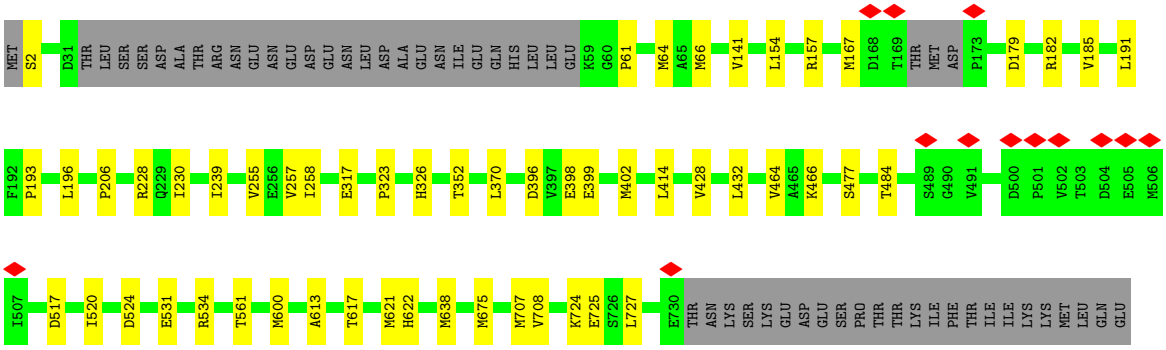
• Molecule 5: DNA replication licensing factor MCM6

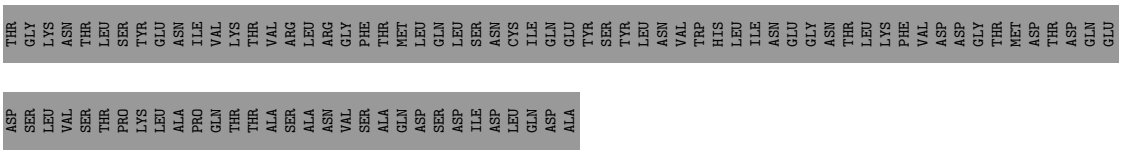
Chain F:



• Molecule 6: DNA replication licensing factor MCM7

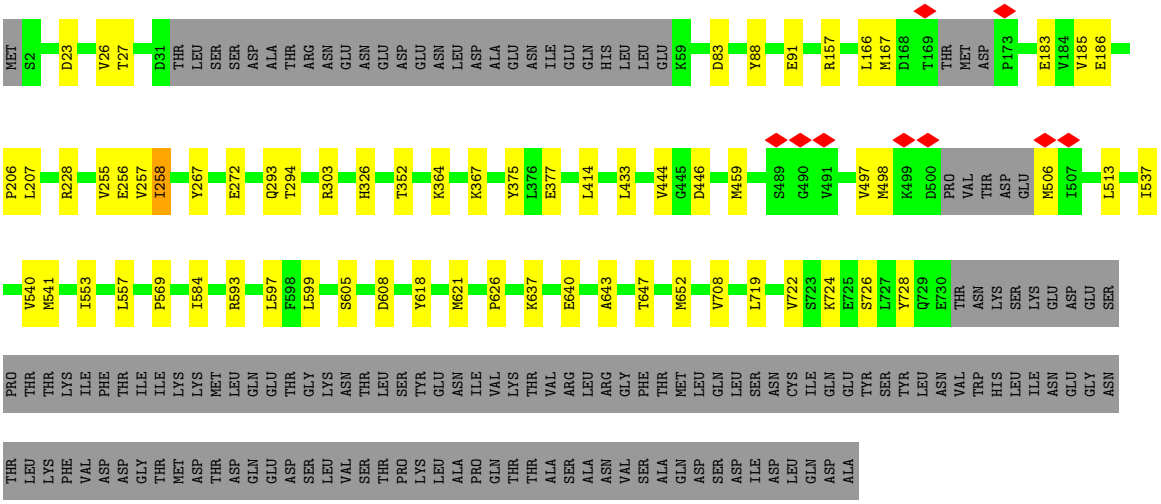
Chain 7:





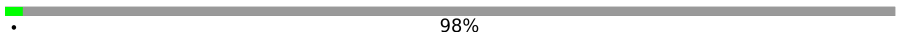
• Molecule 6: DNA replication licensing factor MCM7

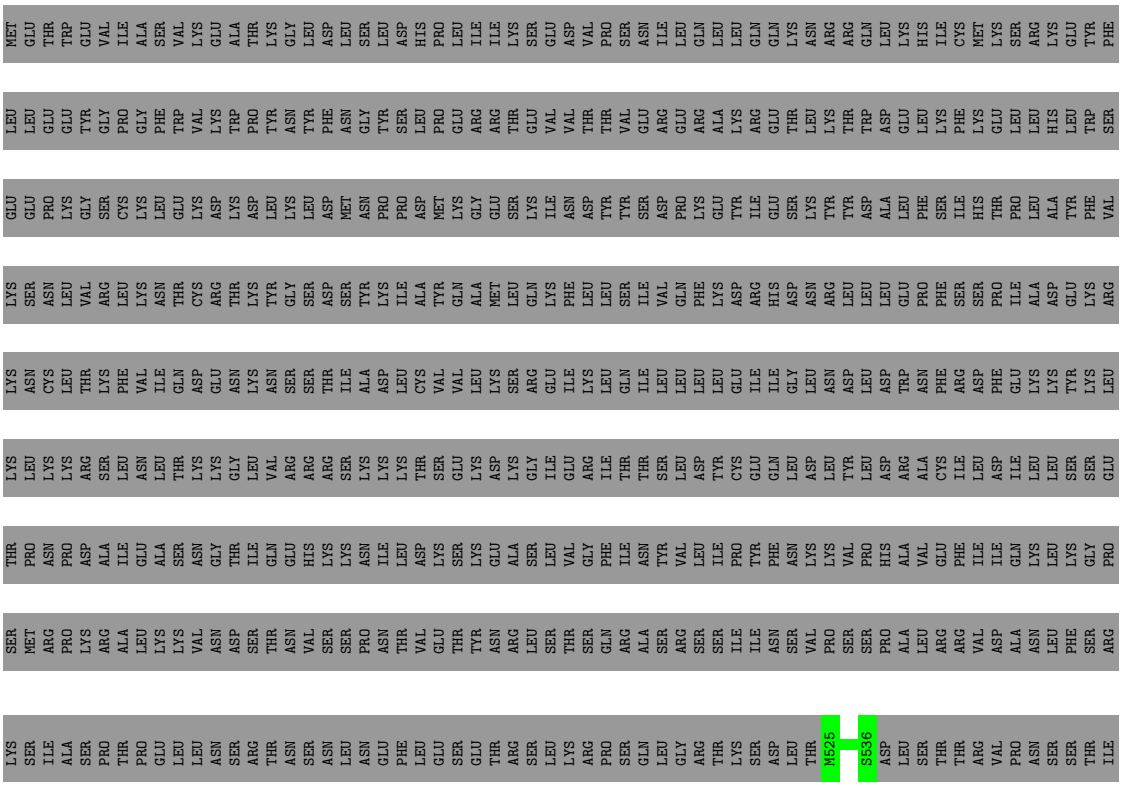
Chain G:



• Molecule 7: DNA replication regulator SLD3

Chain X:





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

PRO ASN LYS LYS ALA GLN LEU GLN SER ILE ILE GLU SER PRO LEU ASN PHE LYS ASP ASP ASP THR HIS GLU GLY ARG LYS ASN THR SER ASN ILE THR SER THR PRO THR ASN LYS PRO PRO GLU ASN SER SER LYS ARG ARG VAL ARG ARG ARG LEU PHE ALA PRO GLU SER THR

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	144373	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.894	Depositor
Minimum map value	-0.302	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.031	Depositor
Recommended contour level	0.154	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, ZN, MG

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	0.12	0/5057	0.31	0/6834
1	B	0.13	0/5057	0.33	0/6834
2	3	0.13	0/5069	0.30	0/6875
2	C	0.14	0/5064	0.31	1/6868 (0.0%)
3	4	0.14	0/5392	0.32	1/7289 (0.0%)
3	D	0.13	0/5400	0.32	0/7300
4	5	0.13	0/5219	0.33	0/7058
4	E	0.14	0/5211	0.33	0/7047
5	6	0.14	0/5223	0.33	0/7046
5	F	0.13	0/5132	0.31	0/6921
6	7	0.14	0/5590	0.31	0/7554
6	G	0.14	0/5550	0.31	0/7496
7	X	0.12	0/103	0.33	0/135
All	All	0.13	0/63067	0.32	2/85257 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	4	421	ASP	CB-CA-C	-5.68	110.04	116.63
2	C	280	ASP	CB-CA-C	-5.18	110.19	117.23

There are no chirality outliers.

There are no planarity outliers.

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	4970	0	5026	40	0
1	B	4970	0	5026	45	0
2	3	4983	0	5046	43	0
2	C	4978	0	5041	24	0
3	4	5316	0	5366	45	0
3	D	5323	0	5373	48	0
4	5	5145	0	5199	44	0
4	E	5137	0	5189	47	0
5	6	5143	0	5167	50	0
5	F	5052	0	5095	30	0
6	7	5505	0	5565	30	0
6	G	5467	0	5531	40	0
7	X	102	0	102	0	0
8	2	31	0	12	0	0
8	4	31	0	12	2	0
8	7	31	0	12	0	0
8	B	31	0	12	0	0
8	D	31	0	12	1	0
8	G	31	0	12	0	0
9	2	1	0	0	0	0
9	3	1	0	0	0	0
9	4	1	0	0	0	0
9	5	1	0	0	0	0
9	7	1	0	0	0	0
9	B	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	G	1	0	0	0	0
10	2	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	B	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
10	G	1	0	0	0	0
11	3	27	0	12	2	0
11	5	27	0	12	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	C	27	0	12	2	0
11	E	27	0	12	0	0
All	All	62405	0	62846	453	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 4.

The worst 5 of 453 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)
5:6:484:MET:HE3	5:6:484:MET:H	1.45	0.82
3:D:314:MET:HG3	3:D:317:LEU:HD12	1.63	0.81
2:3:384:MET:HE1	2:3:513:ILE:HB	1.66	0.76
5:6:419:SER:HB2	5:6:448:LEU:HD11	1.68	0.75
6:7:167:MET:HE2	4:E:104:LEU:HB3	1.71	0.72

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	622/868 (72%)	613 (99%)	9 (1%)	0	100	100
1	B	622/868 (72%)	608 (98%)	14 (2%)	0	100	100
2	3	626/971 (64%)	614 (98%)	12 (2%)	0	100	100
2	C	626/971 (64%)	619 (99%)	7 (1%)	0	100	100
3	4	663/933 (71%)	649 (98%)	14 (2%)	0	100	100
3	D	664/933 (71%)	653 (98%)	11 (2%)	0	100	100
4	5	650/775 (84%)	640 (98%)	10 (2%)	0	100	100
4	E	649/775 (84%)	642 (99%)	7 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	6	640/1017 (63%)	627 (98%)	13 (2%)	0	100	100
5	F	628/1017 (62%)	615 (98%)	13 (2%)	0	100	100
6	7	693/845 (82%)	685 (99%)	8 (1%)	0	100	100
6	G	686/845 (81%)	679 (99%)	7 (1%)	0	100	100
7	X	10/668 (2%)	10 (100%)	0	0	100	100
All	All	7779/11486 (68%)	7654 (98%)	125 (2%)	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	552/770 (72%)	550 (100%)	2 (0%)	84	84
1	B	552/770 (72%)	548 (99%)	4 (1%)	76	80
2	3	550/835 (66%)	550 (100%)	0	100	100
2	C	549/835 (66%)	546 (100%)	3 (0%)	81	82
3	4	605/848 (71%)	601 (99%)	4 (1%)	76	80
3	D	606/848 (72%)	604 (100%)	2 (0%)	86	85
4	5	588/688 (86%)	584 (99%)	4 (1%)	76	80
4	E	587/688 (85%)	584 (100%)	3 (0%)	81	82
5	6	568/886 (64%)	566 (100%)	2 (0%)	84	84
5	F	559/886 (63%)	556 (100%)	3 (0%)	81	82
6	7	618/753 (82%)	614 (99%)	4 (1%)	78	81
6	G	613/753 (81%)	611 (100%)	2 (0%)	86	85
7	X	12/628 (2%)	12 (100%)	0	100	100
All	All	6959/10188 (68%)	6926 (100%)	33 (0%)	78	82

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	F	119	LEU
5	F	379	VAL
6	G	258	ILE
6	7	66	MET
5	6	726	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 49 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	531	GLN
3	D	582	HIS
2	C	670	GLN
3	D	242	ASN
3	D	666	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 30 ligands modelled in this entry, 20 are monoatomic - leaving 10 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	$\#\|Z\| > 2$
8	ATP	G	2001	9	29,33,33	0.31	0	44,52,52	0.51	0
8	ATP	2	2001	9	29,33,33	0.29	0	44,52,52	0.49	1 (2%)
8	ATP	B	2001	9	29,33,33	0.29	0	44,52,52	0.48	1 (2%)
8	ATP	7	2001	9	29,33,33	0.30	0	44,52,52	0.50	1 (2%)
8	ATP	D	2001	9	29,33,33	0.31	0	44,52,52	0.50	1 (2%)
11	ADP	5	2001	9	27,29,29	1.35	4 (14%)	42,45,45	2.01	9 (21%)
11	ADP	E	2001	9	27,29,29	1.34	4 (14%)	42,45,45	1.95	10 (23%)
11	ADP	3	2001	9	27,29,29	1.35	4 (14%)	42,45,45	1.96	10 (23%)
11	ADP	C	2001	9	27,29,29	1.35	4 (14%)	42,45,45	1.97	10 (23%)
8	ATP	4	2001	9	29,33,33	0.29	0	44,52,52	0.47	0

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
8	ATP	G	2001	9	-	3/22/38/38	0/3/3/3
8	ATP	2	2001	9	-	5/22/38/38	0/3/3/3
8	ATP	B	2001	9	-	4/22/38/38	0/3/3/3
8	ATP	7	2001	9	-	1/22/38/38	0/3/3/3
8	ATP	D	2001	9	-	4/22/38/38	0/3/3/3
11	ADP	5	2001	9	-	7/16/32/32	0/3/3/3
11	ADP	E	2001	9	-	8/16/32/32	0/3/3/3
11	ADP	3	2001	9	-	4/16/32/32	0/3/3/3
11	ADP	C	2001	9	-	3/16/32/32	0/3/3/3
8	ATP	4	2001	9	-	3/22/38/38	0/3/3/3

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	3	2001	ADP	C5-C4	4.50	1.47	1.39
11	5	2001	ADP	C5-C4	4.49	1.47	1.39
11	C	2001	ADP	C5-C4	4.39	1.47	1.39
11	E	2001	ADP	C5-C4	4.39	1.47	1.39
11	C	2001	ADP	C5-C6	2.66	1.48	1.41

The worst 5 of 43 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	5	2001	ADP	C5-C4-N3	-6.35	118.47	126.75
11	C	2001	ADP	C5-C4-N3	-6.06	118.85	126.75
11	3	2001	ADP	C5-C4-N3	-6.04	118.87	126.75
11	E	2001	ADP	C5-C4-N3	-6.01	118.91	126.75
11	5	2001	ADP	N3-C4-N9	4.99	135.31	127.08

There are no chirality outliers.

5 of 42 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	2	2001	ATP	PB-O3B-PG-O2G
8	2	2001	ATP	C5'-O5'-PA-O3A
8	4	2001	ATP	PB-O3B-PG-O2G
8	B	2001	ATP	PB-O3B-PG-O2G
11	3	2001	ADP	PA-O3A-PB-O2B

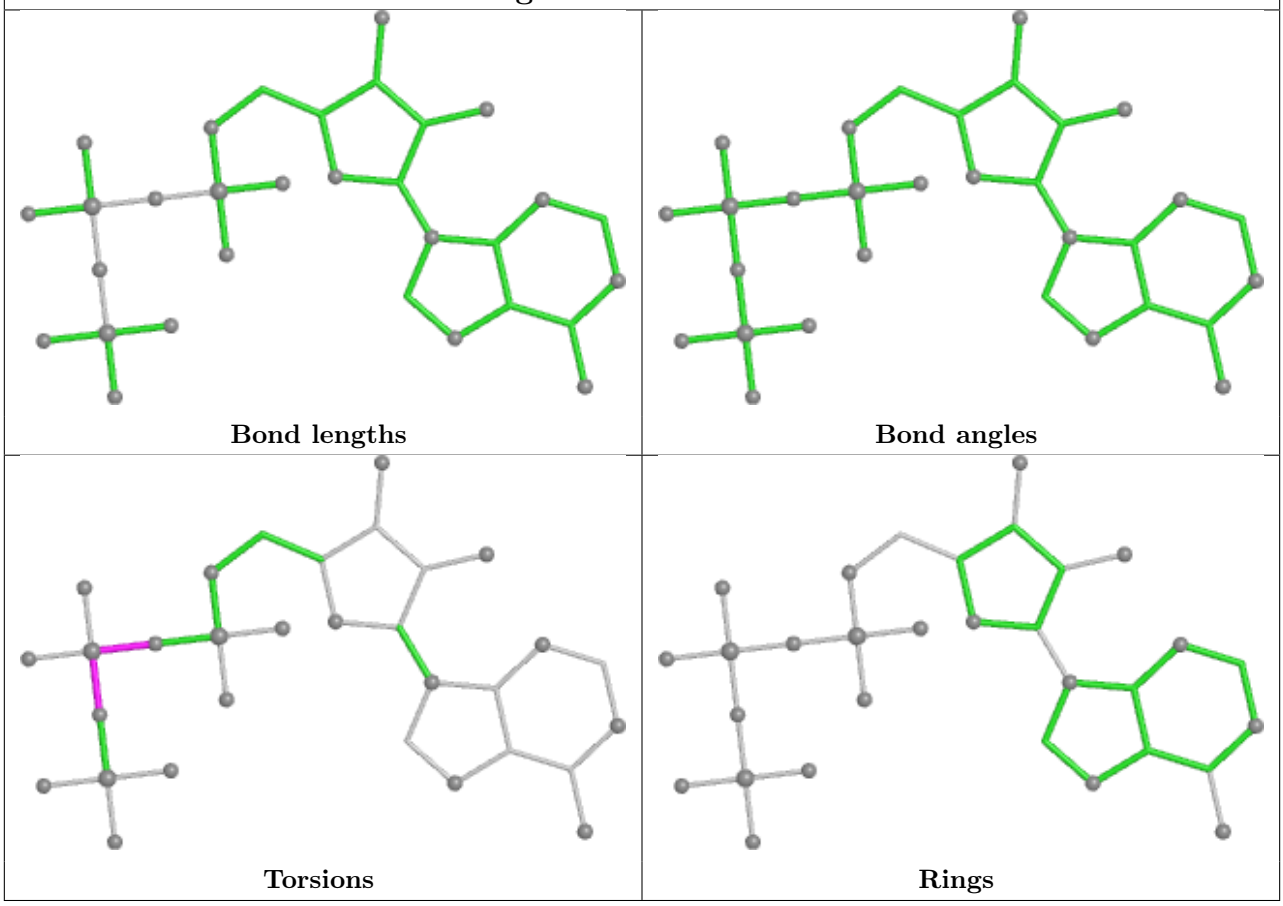
There are no ring outliers.

5 monomers are involved in 10 short contacts:

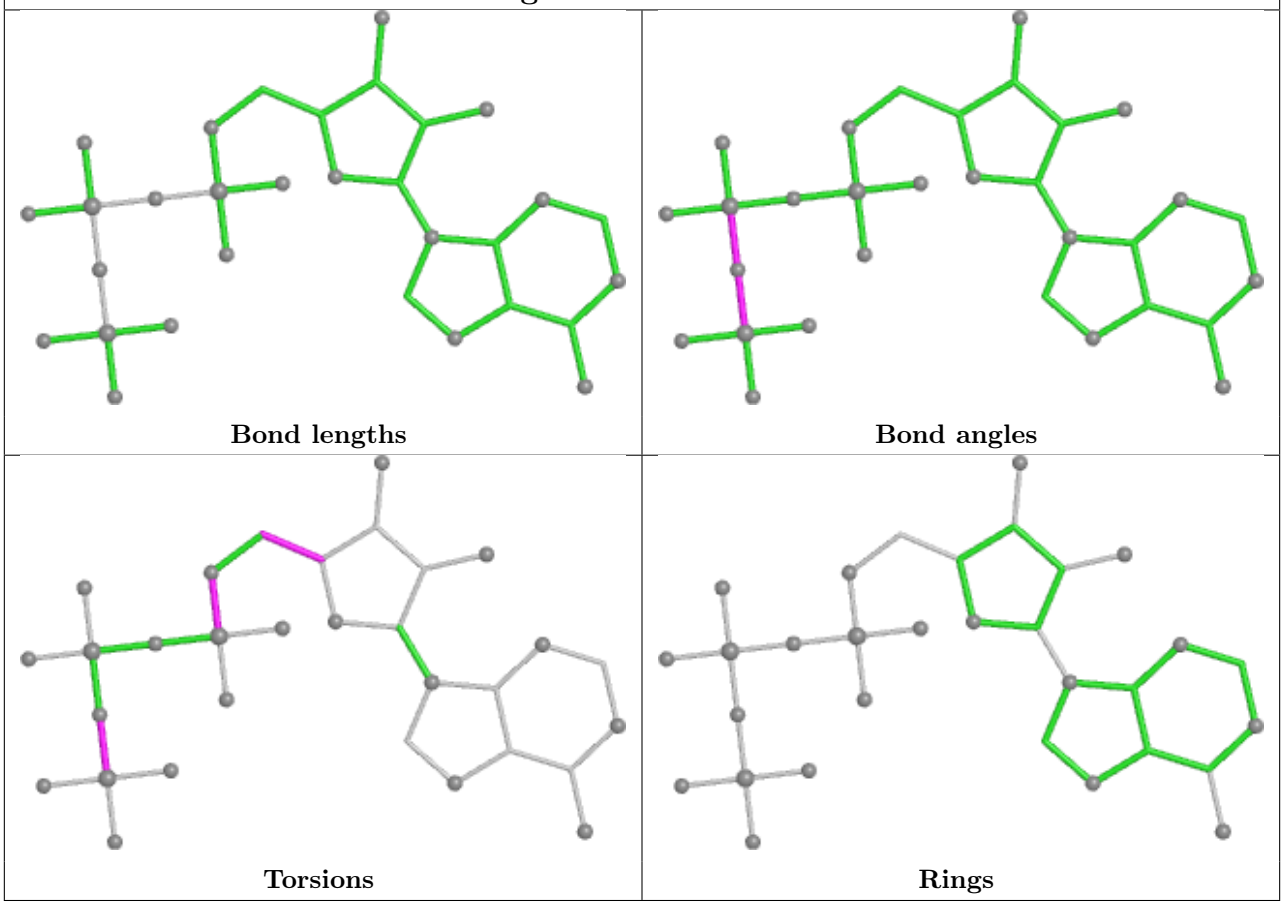
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	2001	ATP	1	0
11	5	2001	ADP	3	0
11	3	2001	ADP	2	0
11	C	2001	ADP	2	0
8	4	2001	ATP	2	0

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.

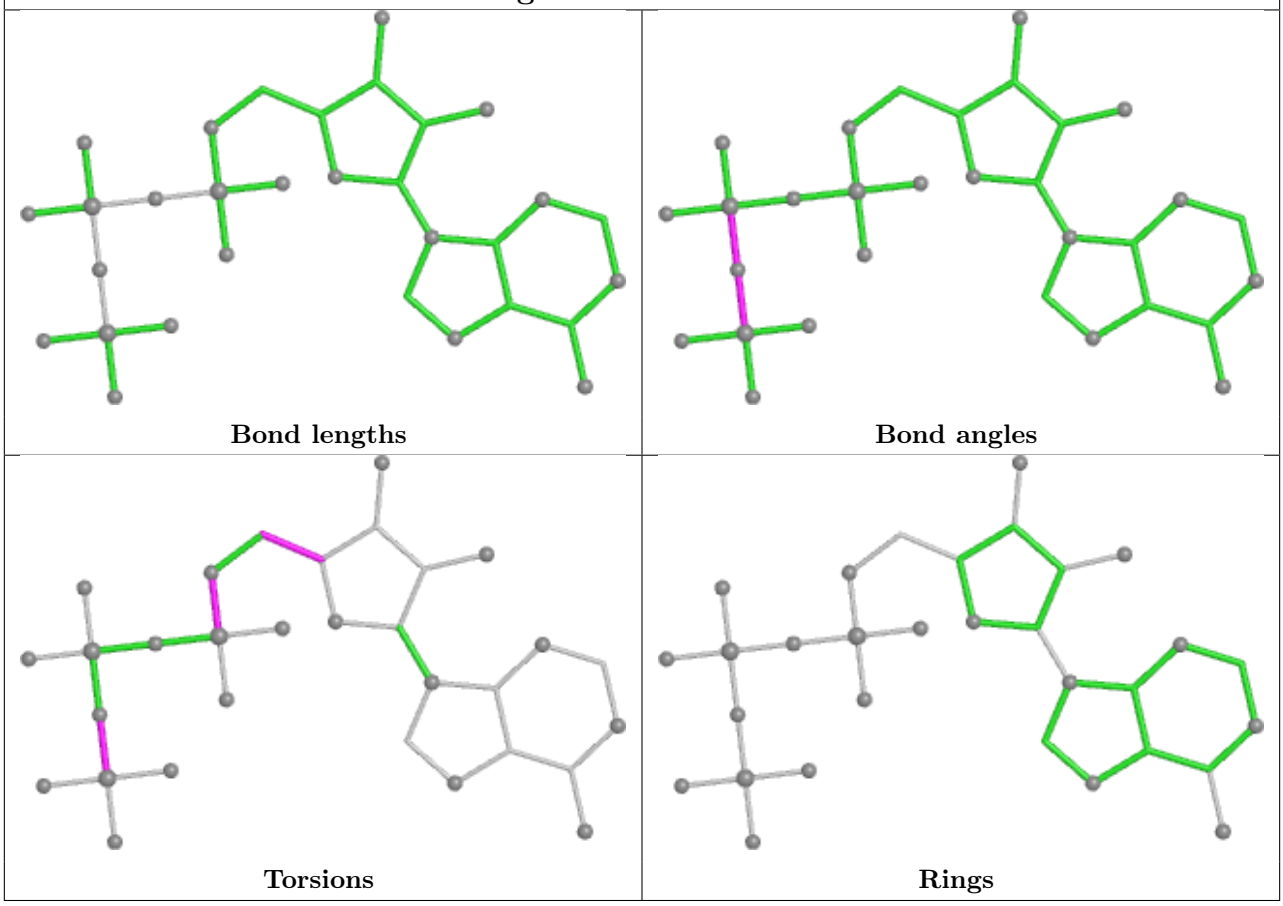
Ligand ATP G 2001



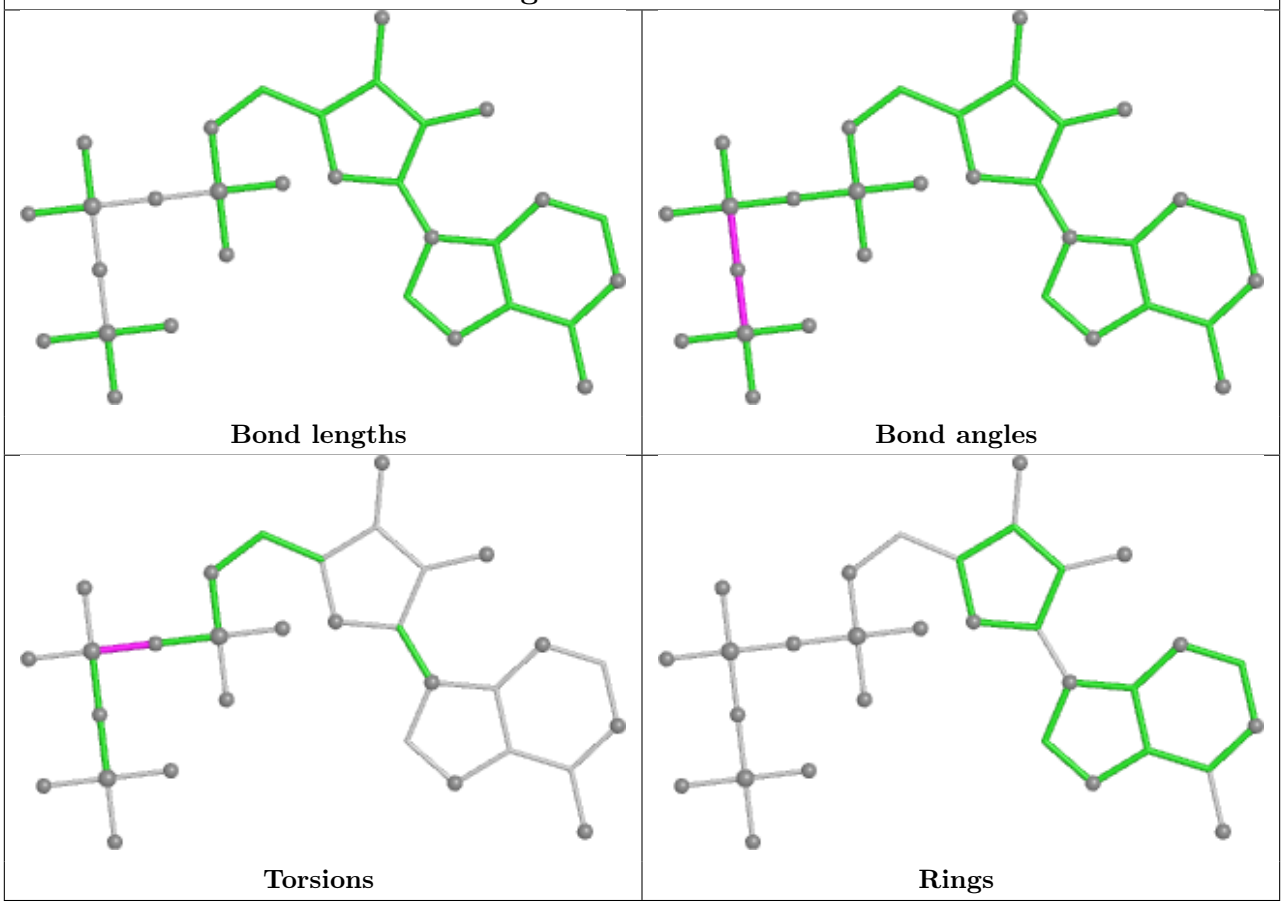
Ligand ATP 2 2001



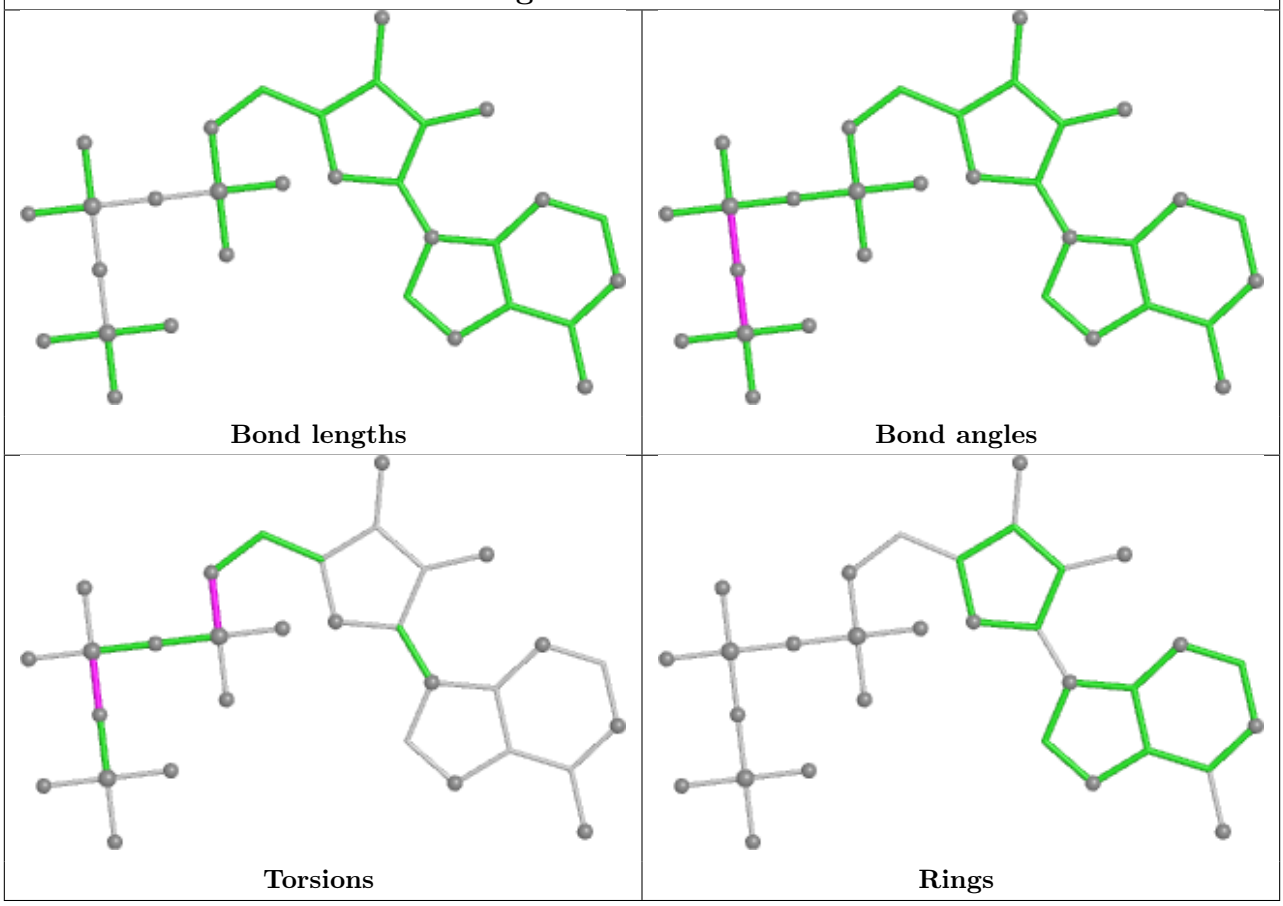
Ligand ATP B 2001



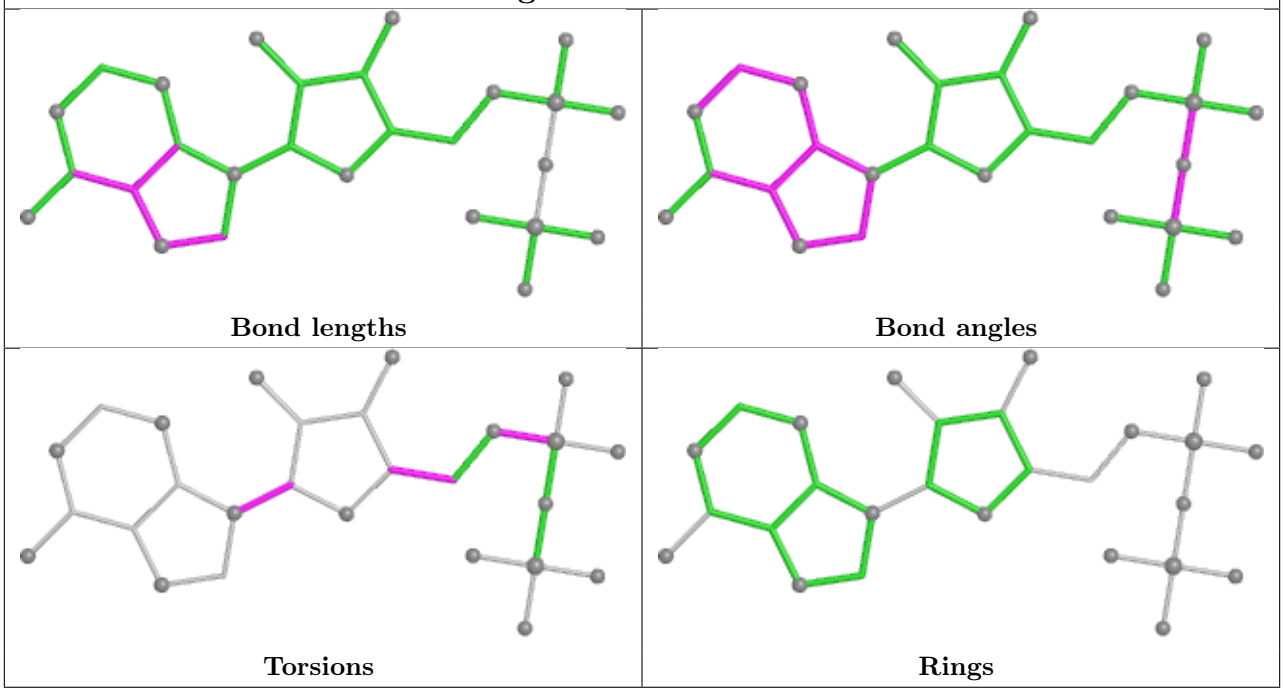
Ligand ATP 7 2001

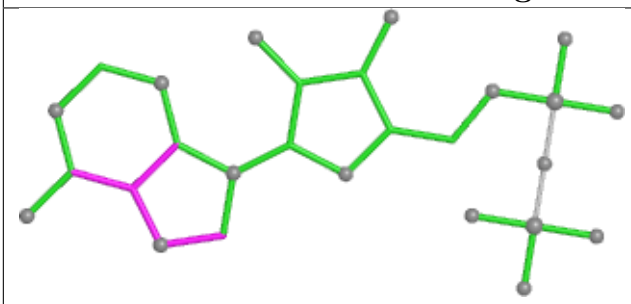
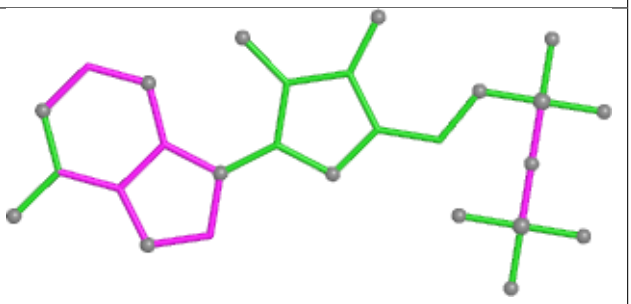
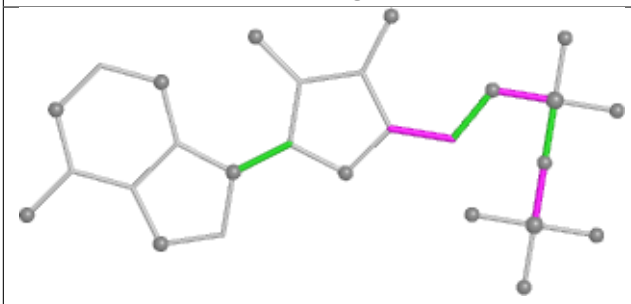
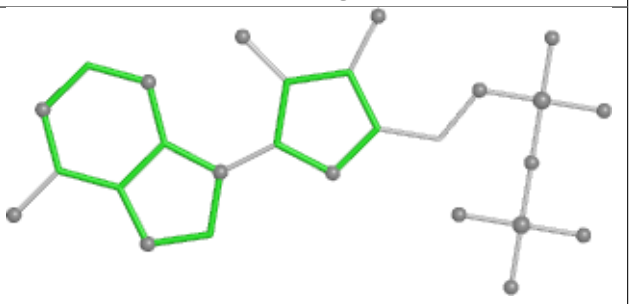


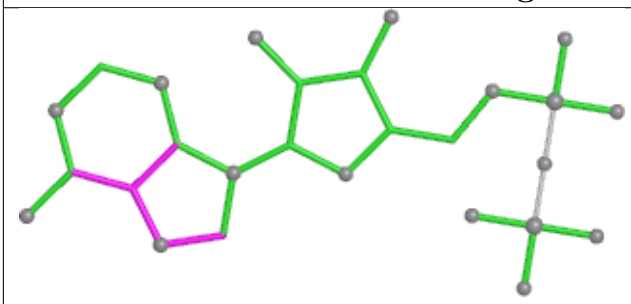
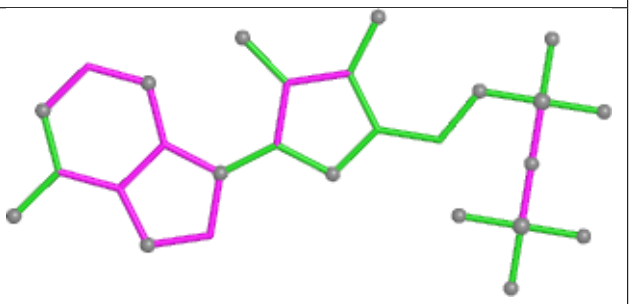
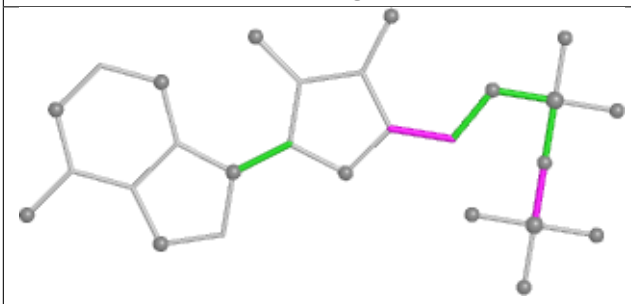
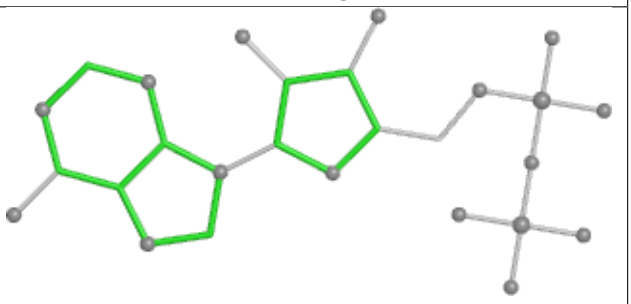
Ligand ATP D 2001



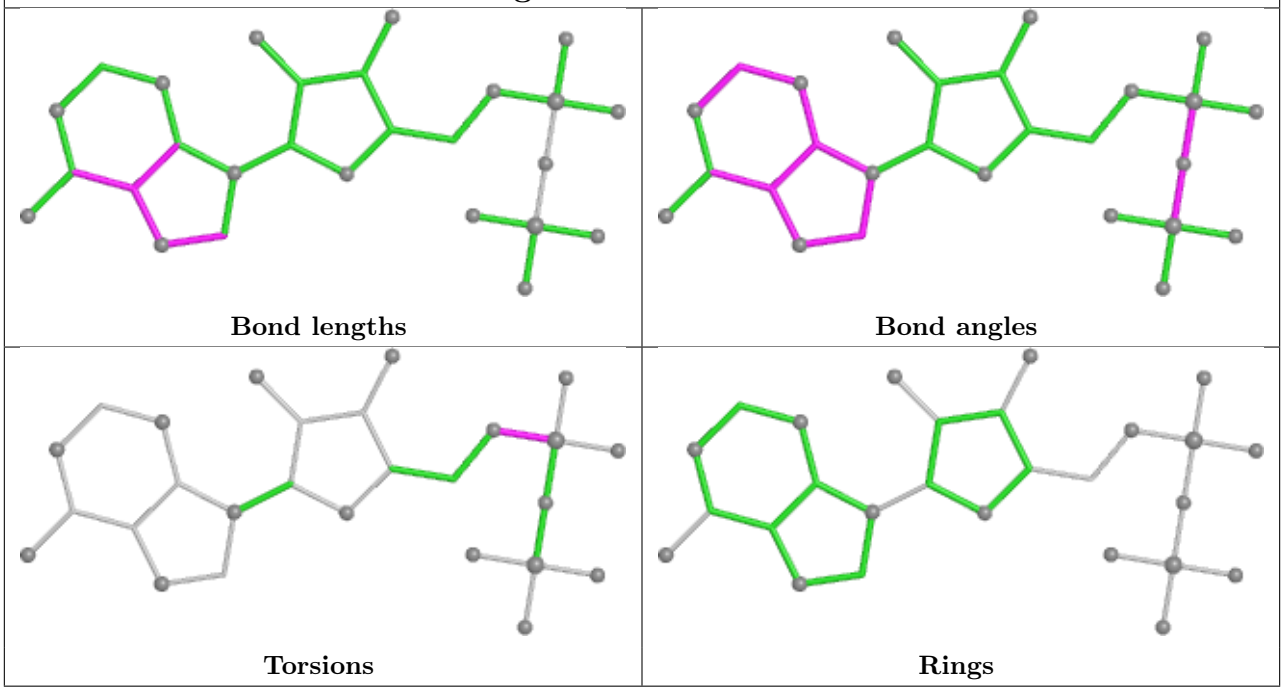
Ligand ADP 5 2001



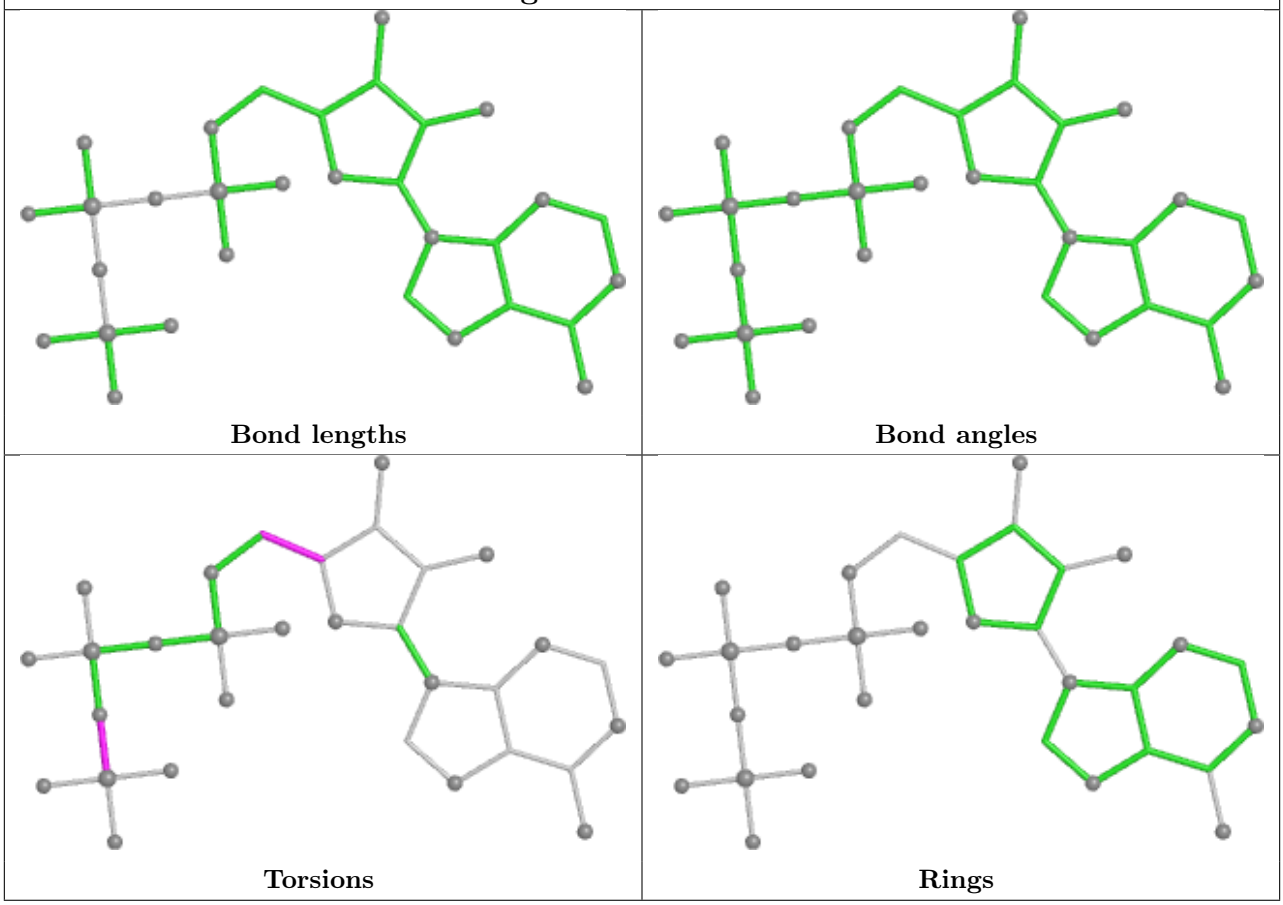
Ligand ADP E 2001	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP 3 2001	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP C 2001



Ligand ATP 4 2001



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.

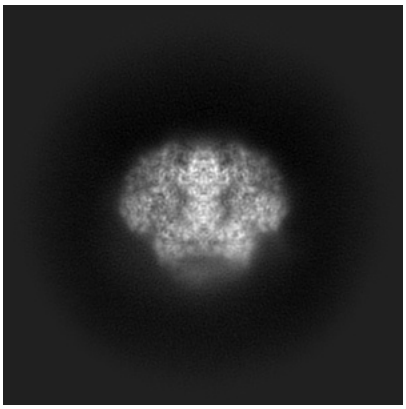
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-66553. These allow visual inspection of the internal detail of the map and identification of artifacts.

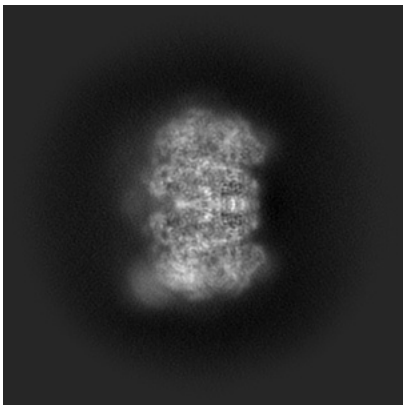
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

6.1.1 Primary map



X



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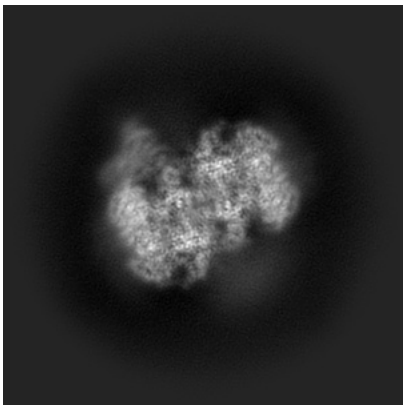
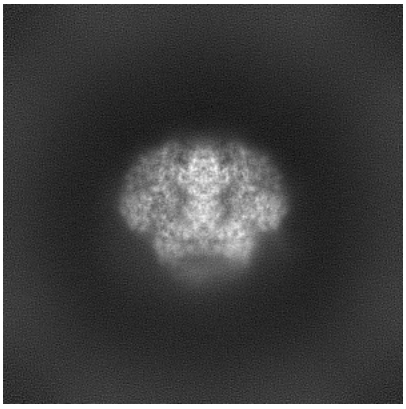


Z

6.1.2 Raw map



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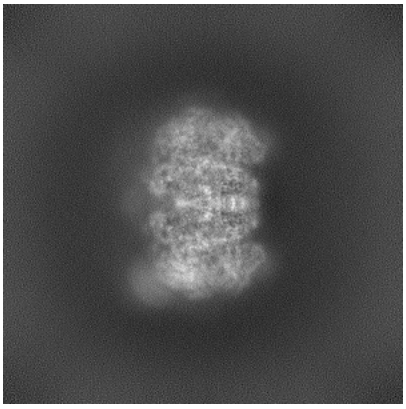

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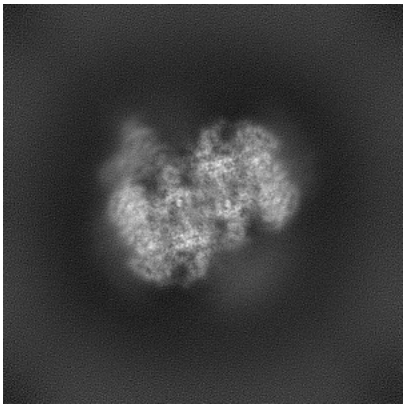
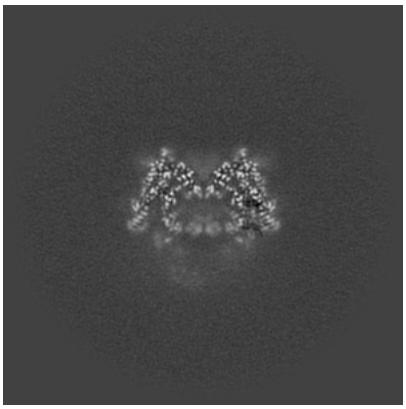


Z

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

6.2 Central slices (i)

6.2.1 Primary map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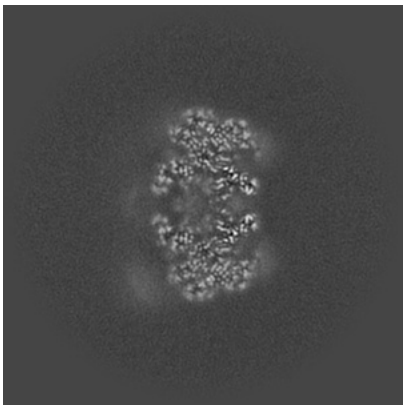
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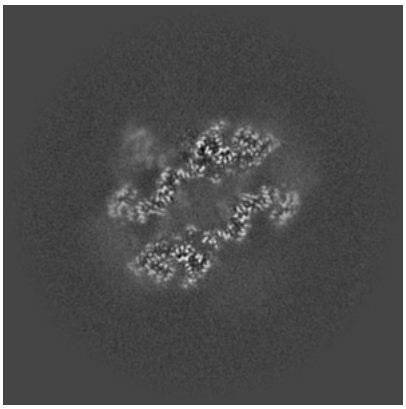
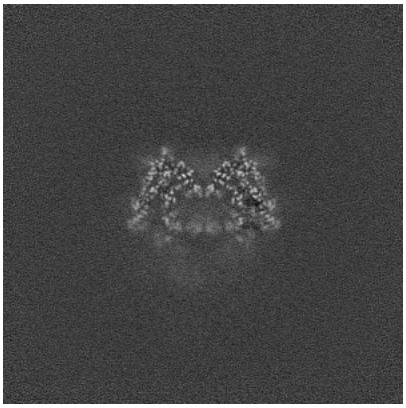
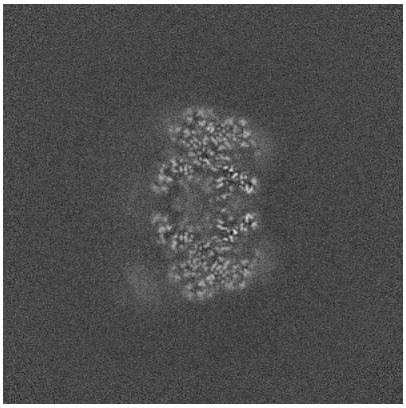
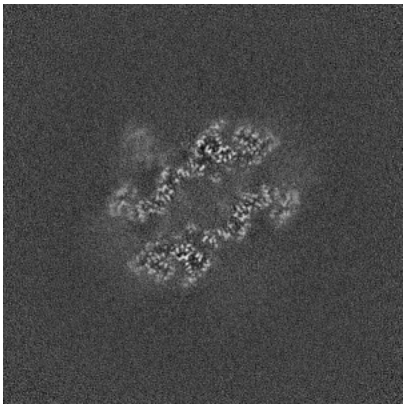

Z Index: 200

6.2.2 Raw map


X Index: 200

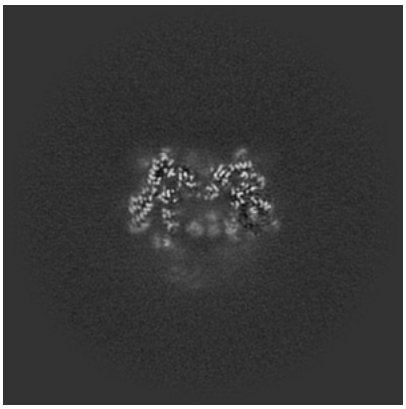

Y Index: 200


Z Index: 200

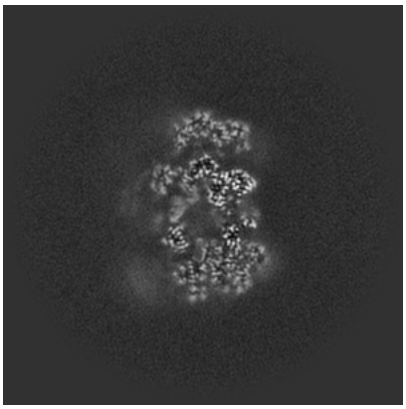
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

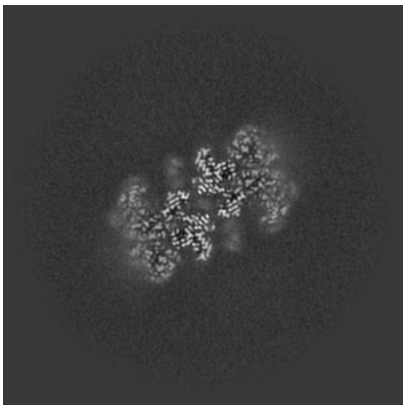
6.3.1 Primary map



X Index: 197

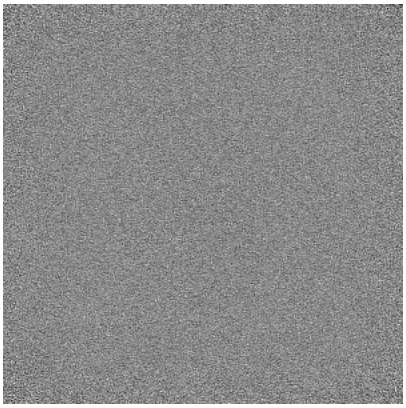


Y Index: 192

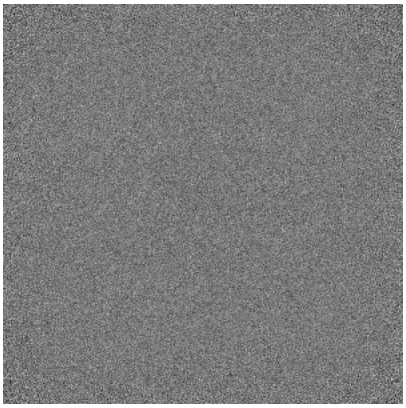


Z Index: 230

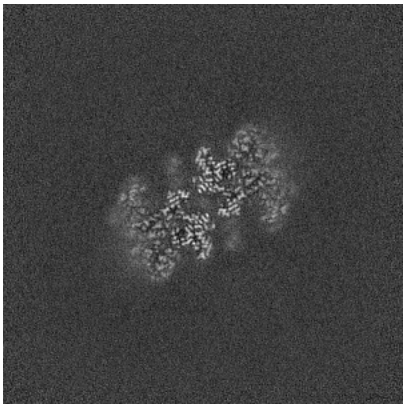
6.3.2 Raw map



X Index: 0



Y Index: 0

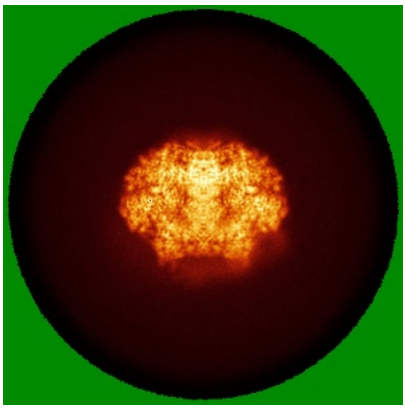


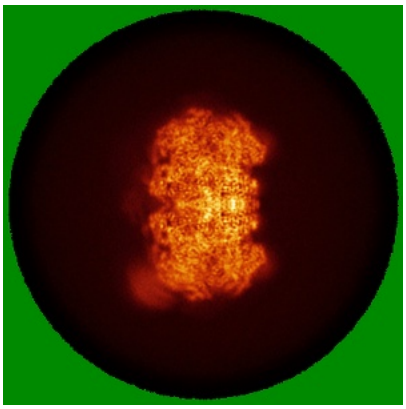
Z Index: 230

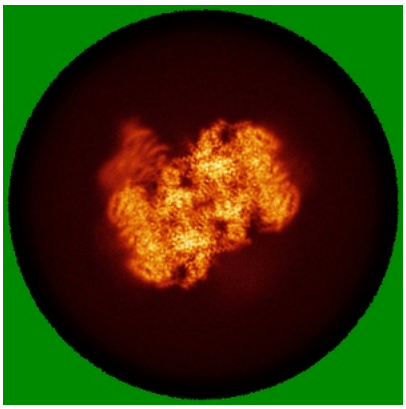
The images above show the largest variance slices of the map in three orthogonal directions.

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

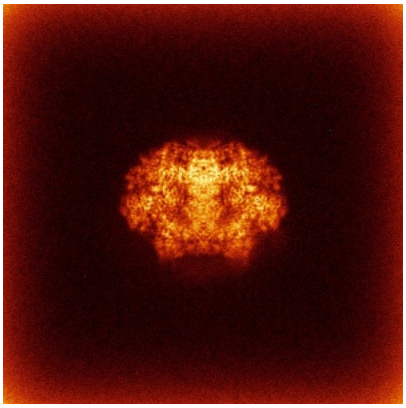
6.4.1 Primary map

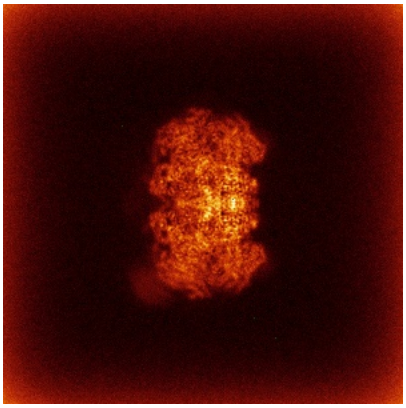

X

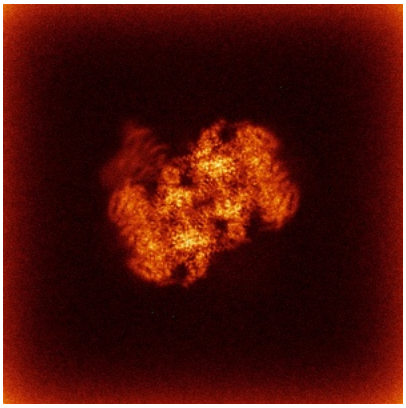

Y


Z

6.4.2 Raw 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.

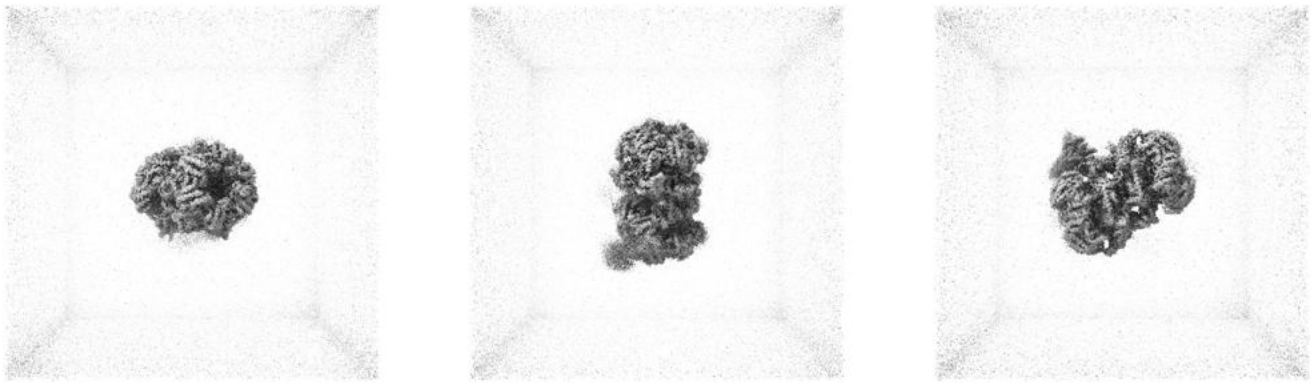
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.154. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

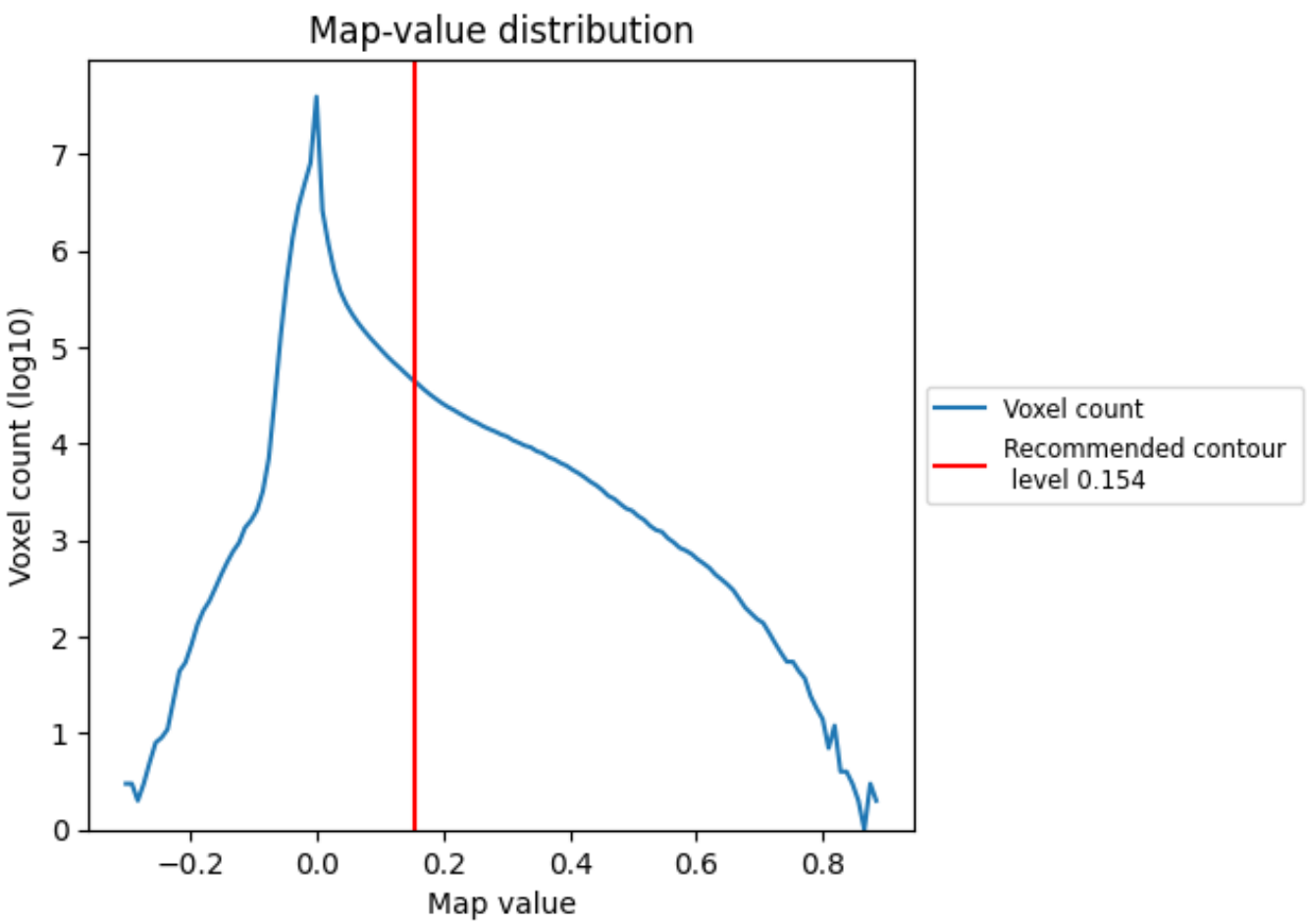
6.6 Mask visualisation (i)

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

7 Map analysis (i)

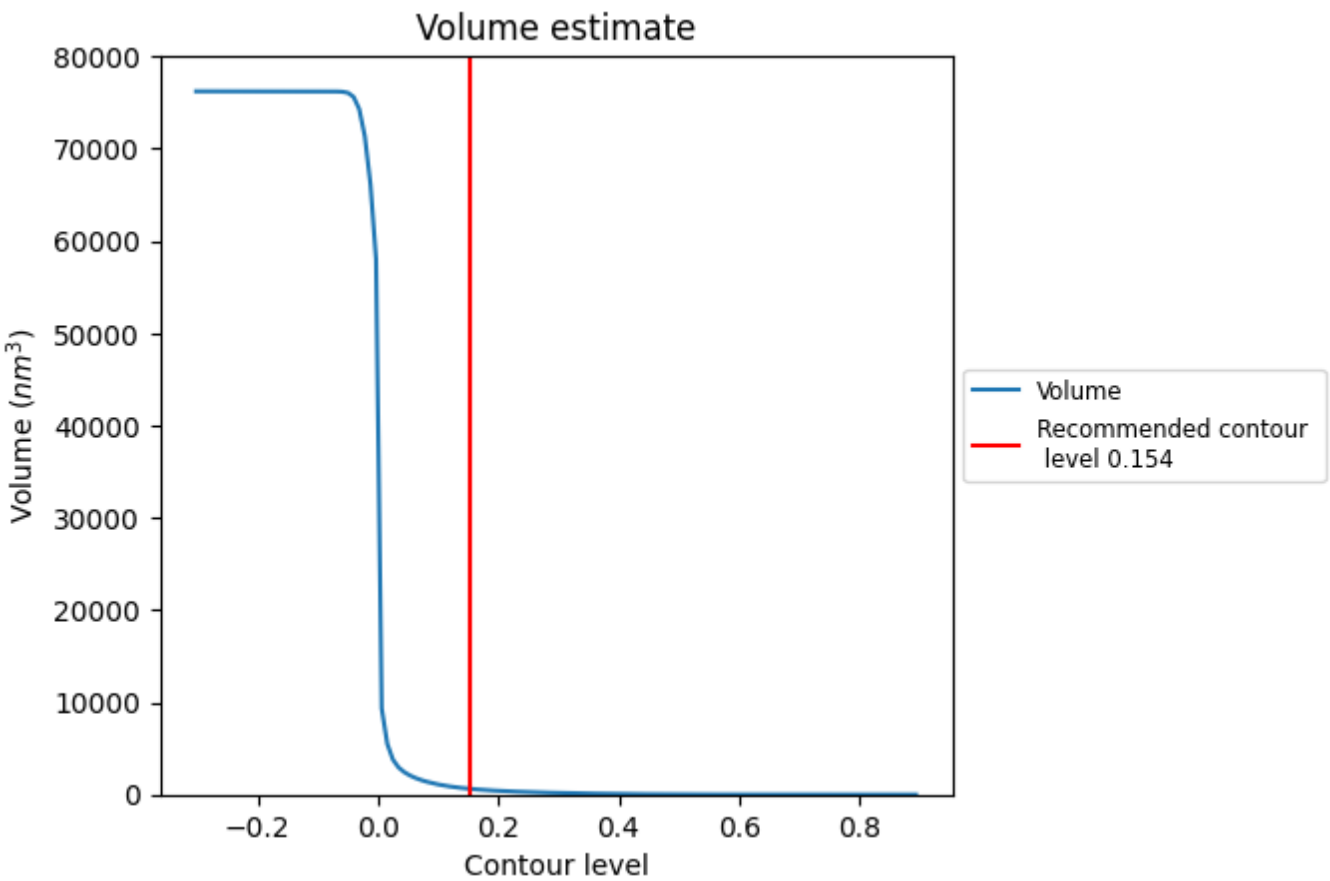
This section contains the results of statistical analysis of the map.

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.

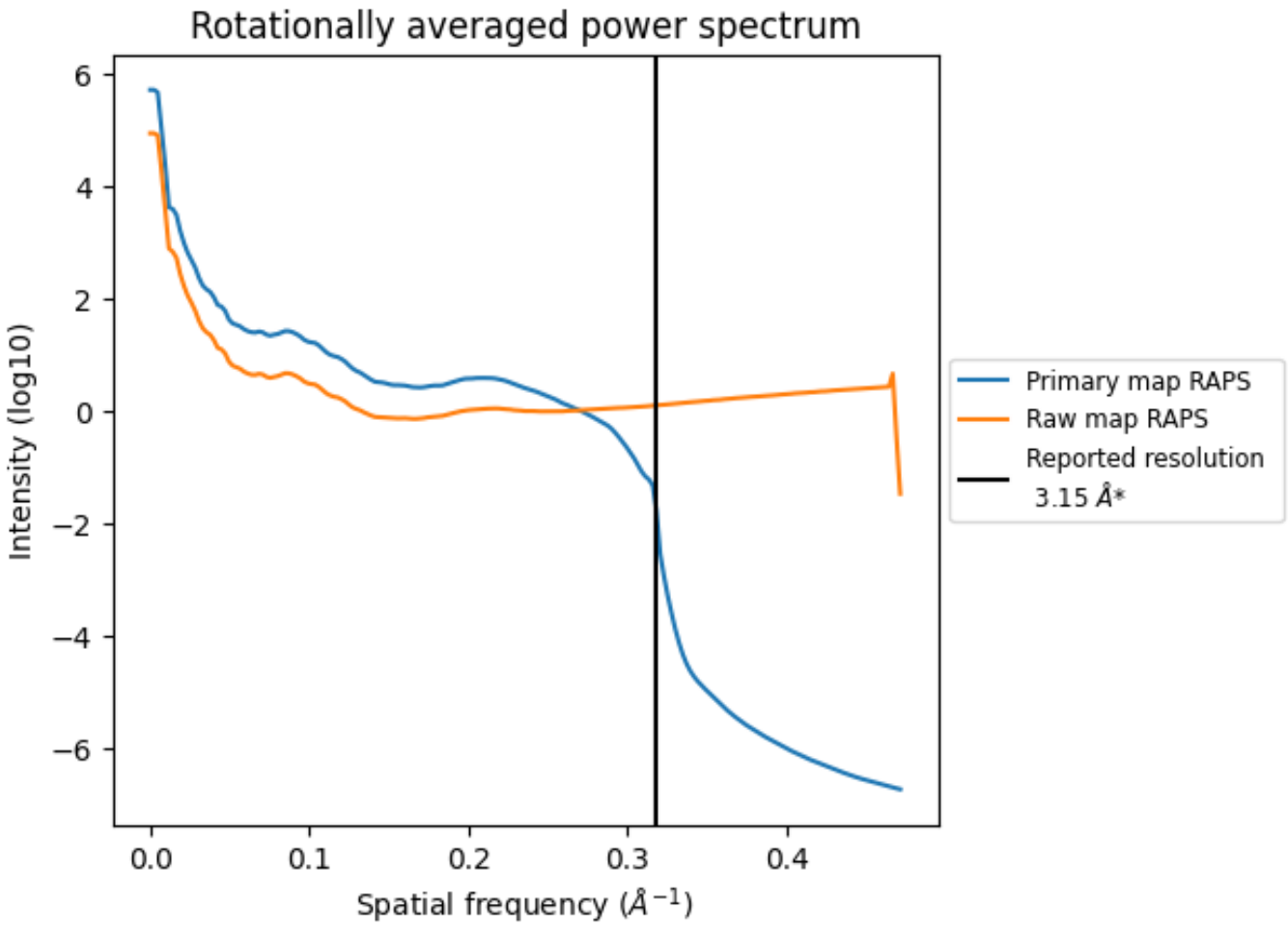
7.2 Volume estimate (i)



The volume at the recommended contour level is 615 nm^3; this corresponds to an approximate mass of 556 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)

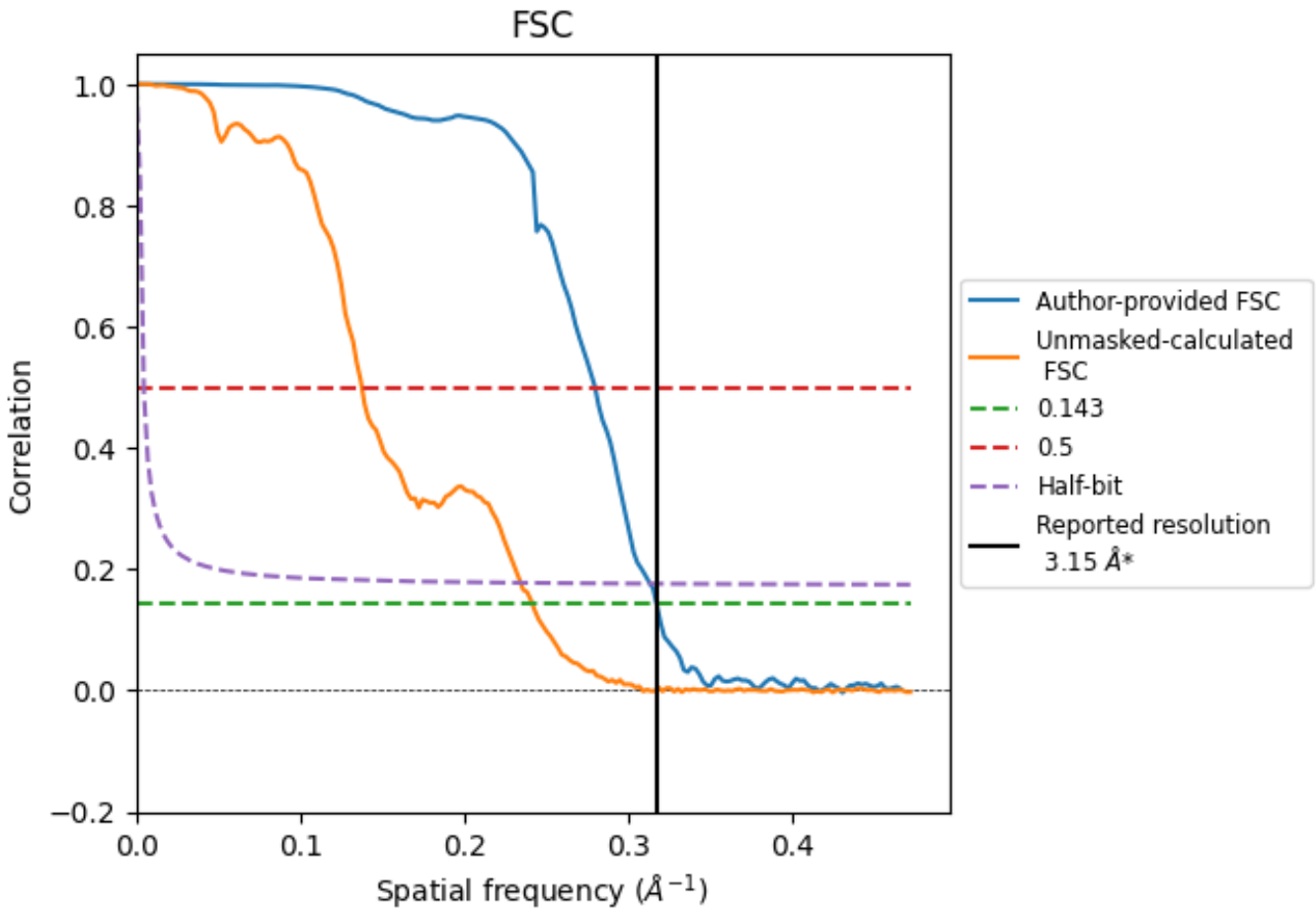


*Reported resolution corresponds to spatial frequency of 0.317 Å^{-1}

8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.317 Å^{-1}

8.2 Resolution estimates (i)

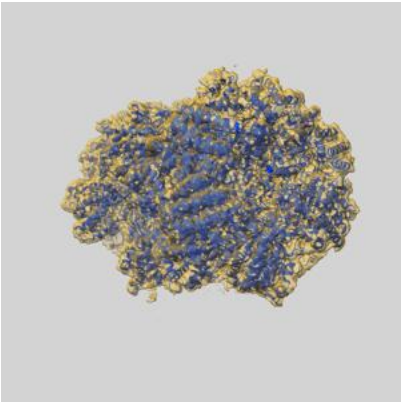
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.15	-	-
Author-provided FSC curve	3.15	3.58	3.19
Unmasked-calculated*	4.14	7.27	4.27

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.14 differs from the reported value 3.15 by more than 10 %

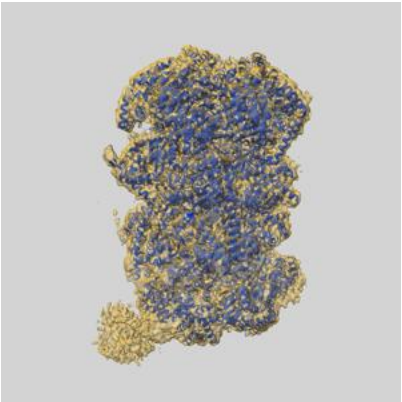
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-66553 and PDB model 9X4M. Per-residue inclusion information can be found in section 3 on page 8.

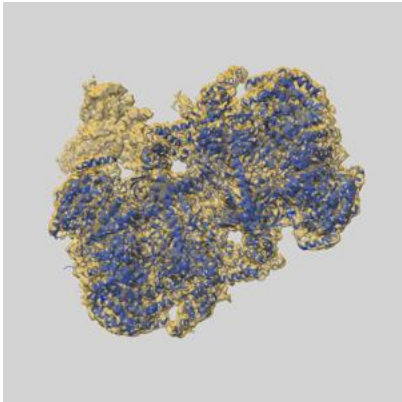
9.1 Map-model overlay (i)



X



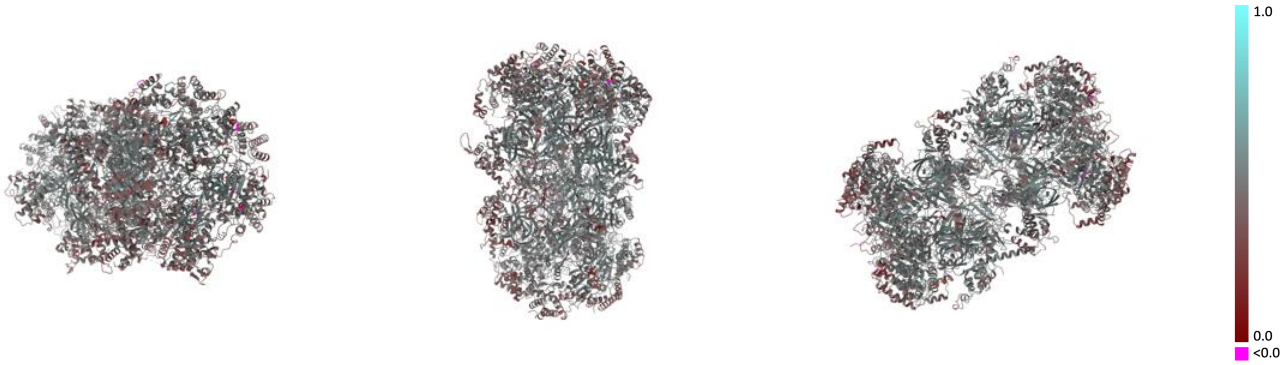
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.154 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.

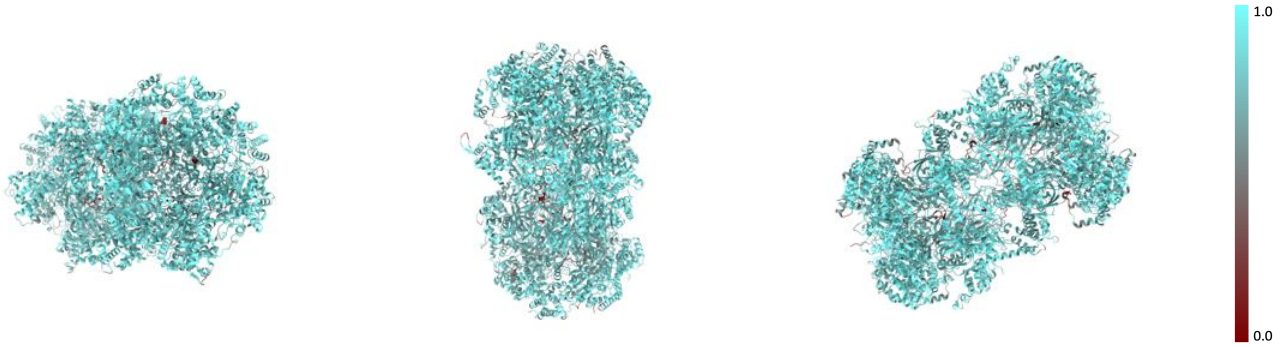
9.2 Q-score mapped to coordinate model (i)



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.

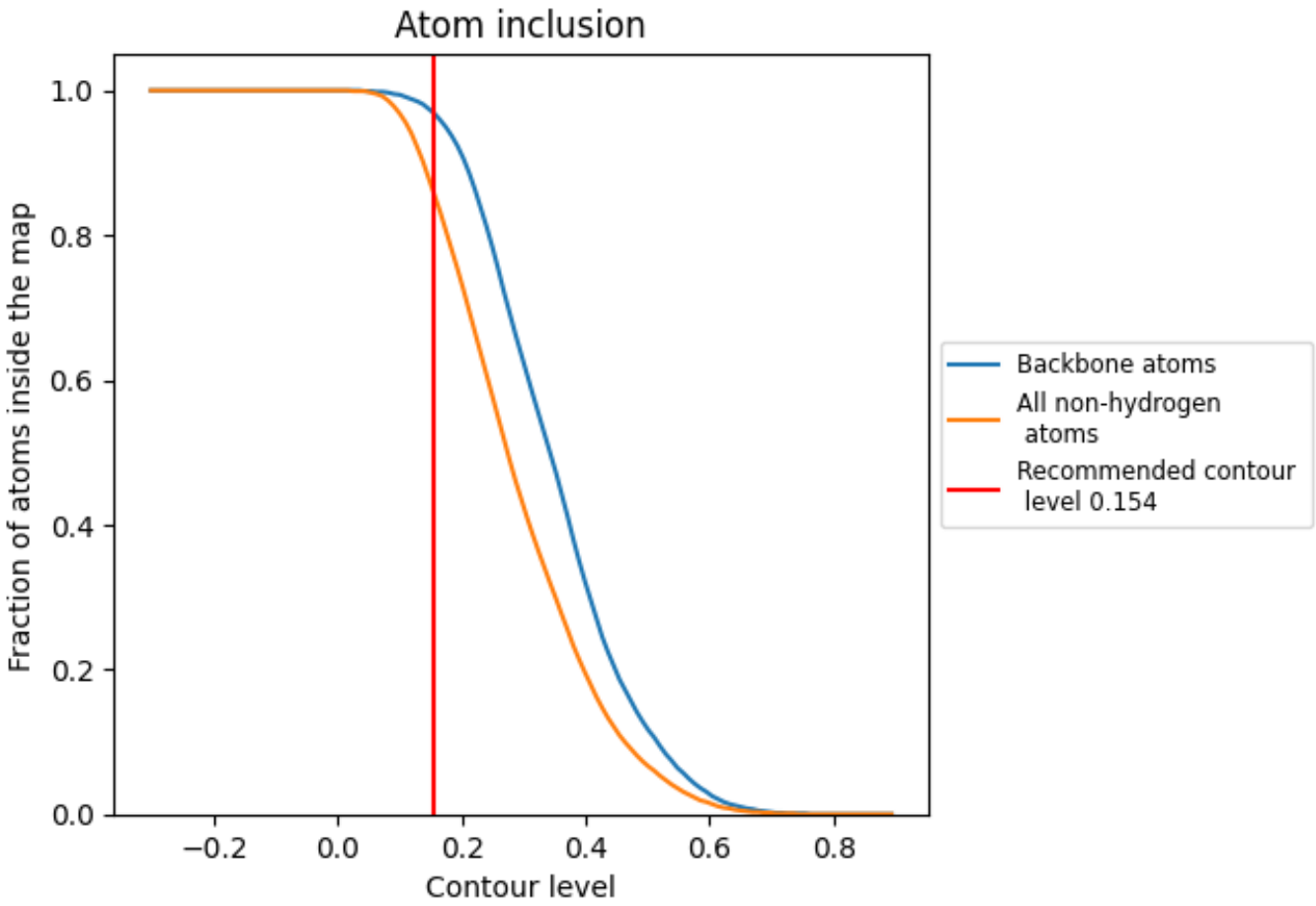
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.154).

9.4 Atom inclusion (i)



At the recommended contour level, 97% of all backbone atoms, 86% 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 (0.154) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8600	0.4530
2	0.8210	0.4180
3	0.8900	0.4770
4	0.8730	0.4650
5	0.8450	0.4500
6	0.8220	0.4290
7	0.8890	0.4730
B	0.8380	0.4260
C	0.8900	0.4780
D	0.8740	0.4640
E	0.8520	0.4500
F	0.8260	0.4330
G	0.8950	0.4680
X	0.9700	0.4540