



wwPDB EM Validation Summary Report ⓘ

Mar 20, 2026 – 01:33 AM UTC

PDB ID : 9LXE / pdb_00009lxe
EMDB ID : EMD-63475
Title : Structure of compacted DNA-free MCM DH at 3.9 Angstroms resolution
Authors : Liu, Y.; Lu, P.; Yang, M.; Gao, H.; Yu, H.
Deposited on : 2025-02-18
Resolution : 3.96 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:

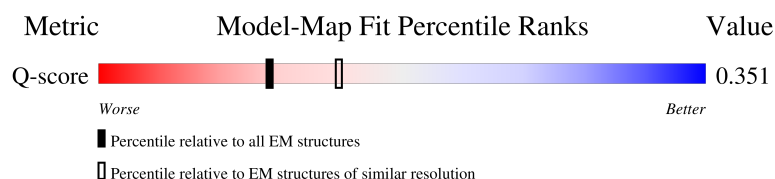
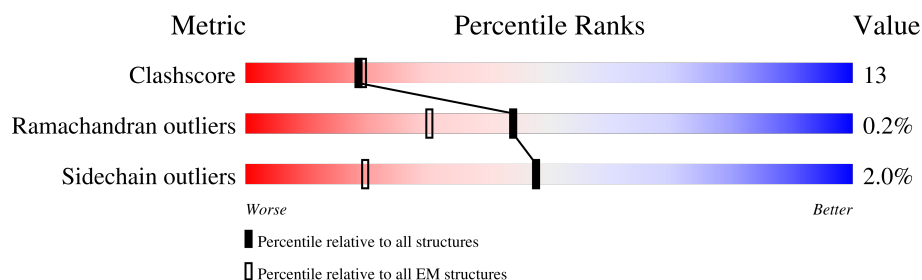
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

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

The reported resolution of this entry is 3.96 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.





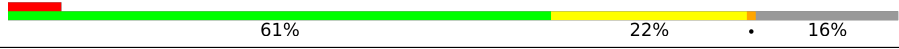



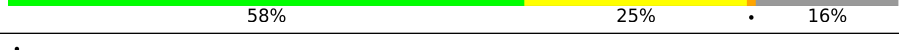
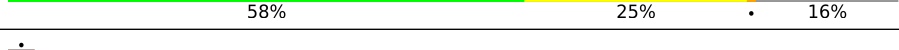
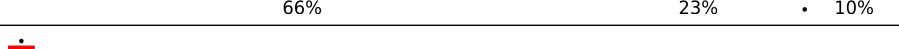
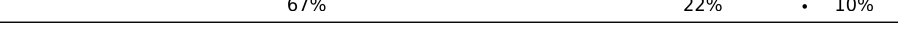
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7646 (3.46 - 4.46)

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	904	
1	D	904	
2	3	853	
2	B	853	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	C	853	
2	E	853	
3	4	863	
3	F	863	
4	5	734	
4	H	734	
5	6	821	
5	G	821	
6	7	719	
6	A	719	

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 66132 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	709	Total	C	N	O	S	0	0
			5628	3537	1005	1054	32		
1	D	709	Total	C	N	O	S	0	0
			5628	3537	1005	1054	32		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	629	Total	C	N	O	S	0	0
			4922	3077	863	956	26		
2	B	73	Total	C	N	O	S	0	0
			575	359	98	115	3		
2	C	73	Total	C	N	O	S	0	0
			575	359	98	115	3		
2	E	629	Total	C	N	O	S	0	0
			4922	3077	863	956	26		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	724	Total	C	N	O	S	0	0
			5753	3620	1013	1092	28		
3	F	724	Total	C	N	O	S	0	0
			5753	3620	1013	1092	28		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	5	678	Total	C	N	O	S	0	0
			5322	3346	948	990	38		
4	H	678	Total	C	N	O	S	0	0
			5322	3346	948	990	38		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
5	601	ALA	ASP	conflict	UNP P33992
5	602	LEU	ARG	conflict	UNP P33992
5	603	LEU	ARG	conflict	UNP P33992
5	604	ALA	SER	conflict	UNP P33992
5	652	THR	ALA	conflict	UNP P33992
H	601	ALA	ASP	conflict	UNP P33992
H	602	LEU	ARG	conflict	UNP P33992
H	603	LEU	ARG	conflict	UNP P33992
H	604	ALA	SER	conflict	UNP P33992
H	652	THR	ALA	conflict	UNP P33992

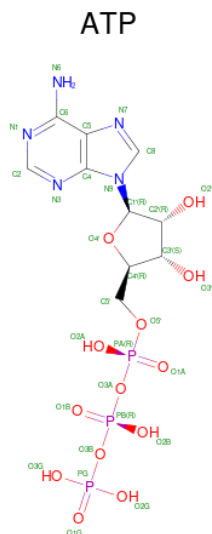
- Molecule 5 is a protein called DNA replication licensing factor MCM6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	6	693	Total	C	N	O	S	0	0
			5586	3516	985	1058	27		
5	G	693	Total	C	N	O	S	0	0
			5586	3516	985	1058	27		

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

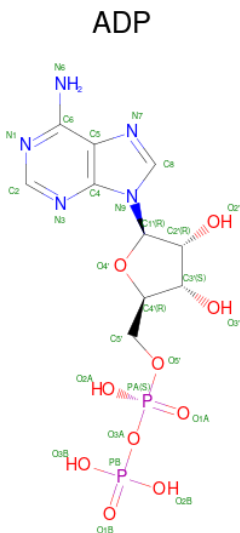
Mol	Chain	Residues	Atoms					AltConf	Trace
6	7	649	Total	C	N	O	S	0	0
			5141	3212	918	979	32		
6	A	649	Total	C	N	O	S	0	0
			5141	3212	918	979	32		

- Molecule 7 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					AltConf
7	2	1	Total 31	C 10	N 5	O 13	P 3	0
7	D	1	Total 31	C 10	N 5	O 13	P 3	0

- Molecule 8 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					AltConf
8	3	1	Total 27	C 10	N 5	O 10	P 2	0
8	4	1	Total 27	C 10	N 5	O 10	P 2	0

Continued on next page...

Continued from previous page...

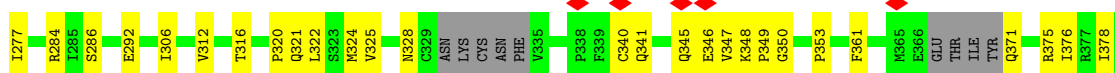
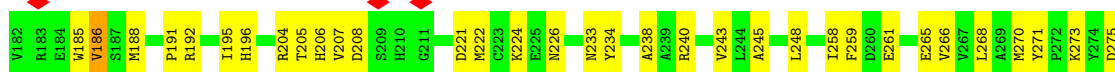
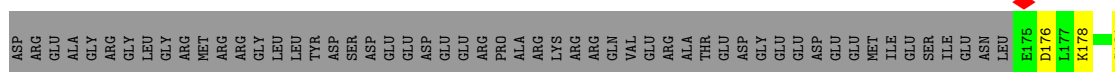
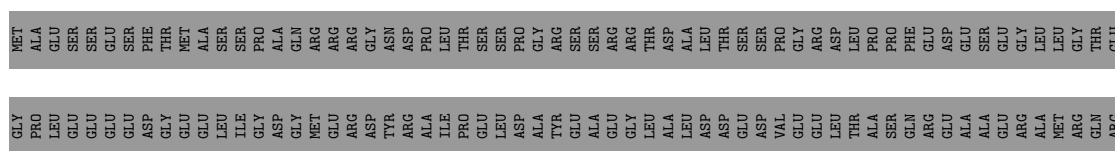
Mol	Chain	Residues	Atoms					AltConf
8	6	1	Total	C	N	O	P	0
			27	10	5	10	2	
8	7	1	Total	C	N	O	P	0
			27	10	5	10	2	
8	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
8	E	1	Total	C	N	O	P	0
			27	10	5	10	2	
8	F	1	Total	C	N	O	P	0
			27	10	5	10	2	
8	G	1	Total	C	N	O	P	0
			27	10	5	10	2	

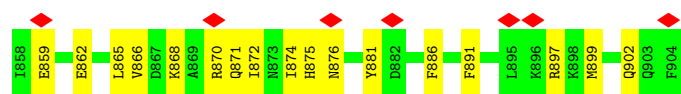
3 Residue-property plots

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

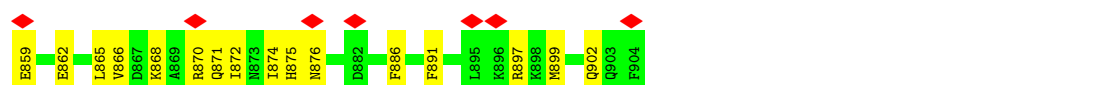
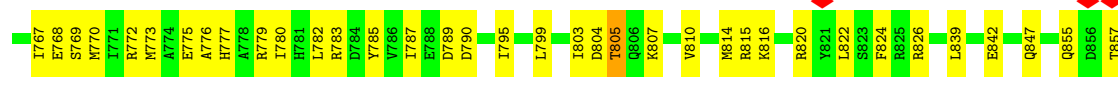
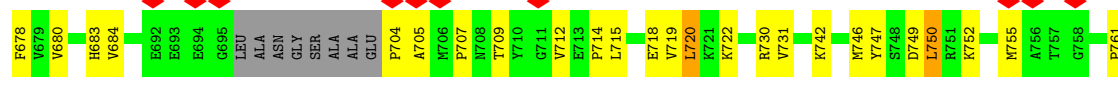
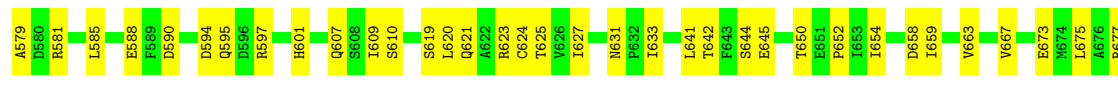
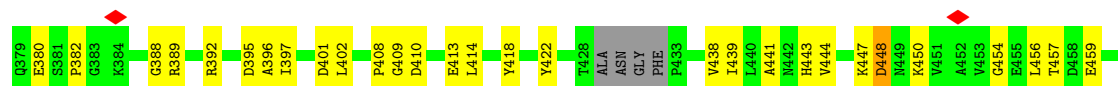
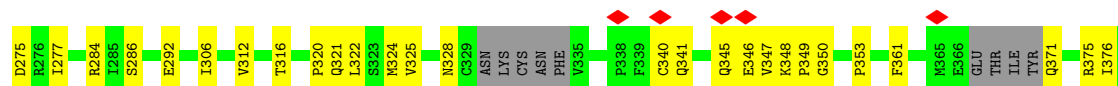
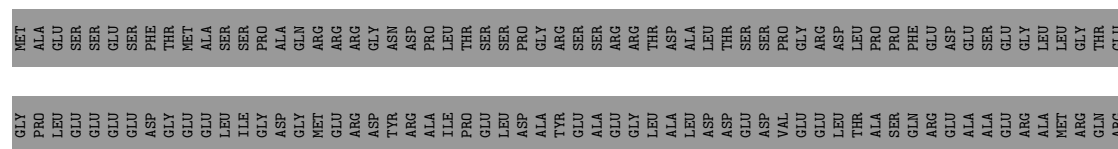
Chain 2:





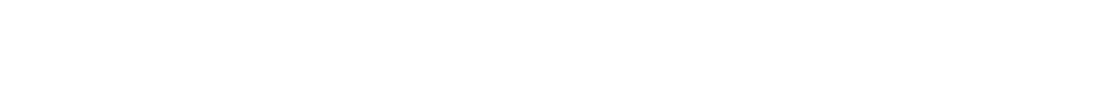
• Molecule 1: DNA replication licensing factor MCM2

Chain D: 52% 26% 22%



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

Chain 3: 48% 24% 26%







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

• Molecule 3: DNA replication licensing factor MCM4

Chain 4: 

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

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

ALA GLN LYS LEU VAL ASP LEU GLN ASP GLY ALA ALA THR D138 K149 L150 G154 T155 D156 K163 L170 Q171 D175 P176 L177 A178 K179 E180 E181 E182 N183 V184 G185 I188 E190 P191 L192 Y193 M194 V202 I203 A240 F245 L254

A285 L286 K267 R272 P276 L282 T284 V289 L290 R291 M299 Q300 E301 A302 C306 Q307 V308 H311 V315 D318 R319 R321 L322 A323 E324 C328 G329 H335 S336 H341 N342 R343 L345 I352 K353 E356 P362 Q365 H375

V390 R400 N401 P403 R404 V405 V418 R422 A426 K427 R428 L429 M430 G431 L432 S442 E443 K444 R445 V446 K455 P456 D457 E460 L461 L462 I470 Y471 D475 I476 L480 L481 L482 F485 T488 R489 K490 E503 I506 G509 G510 D511

S515 L526 Y532 T533 S534 G535 G537 G538 S539 A540 G542 L543 T544 A545 D550 P551 T553 R554 T560 V564 L565 S566 D567 N568 D574 E575 F576 D577 K578 M579 N580 T583 R584 S585 V586 L587 I598 A599 K600 S612 W624 N625 P626 T629 T630

I634 L646 I647 Q654 R661 L662 A663 L666 V667 A668 Y671 E674 A677 E678 E679 E680 L687 Y690 I698 M699 P700 R701 L702 D705 A706 L710 Y714 M717 R718 K719 I720 G721 S722 R723 R724 G725 M726 S727 W728 A729 Y730 L734 E735

I738 E742 A743 H744 V747 V753 D757 V758 K762 L769 S772 P776 R777 V781 I785 L786 T787 G789 M790 S791 A792 R795 K796 R797 E803 A804 L805 L808 I809 L810 S811 K812 G813 T814 P816 A817 L818 K819 Y820 Q821 Q822 L823 F824 E825

R828 G829 D832 I833 A834 I835 T836 K837 D838 M839 F840 E841 E842 R845 A846 L847 A848 D849 D850 D851 F852 L853 T854 V855 T856 G857 K858 T859 V860 R861 L862 L863

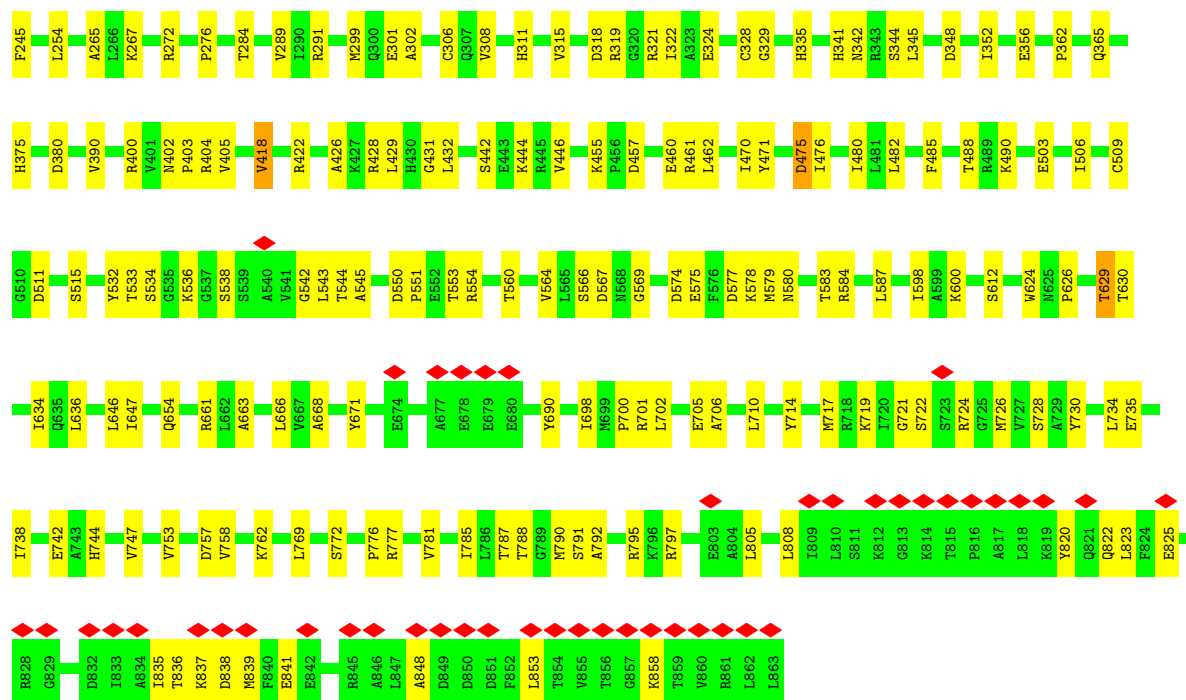
• Molecule 3: DNA replication licensing factor MCM4

Chain F: 

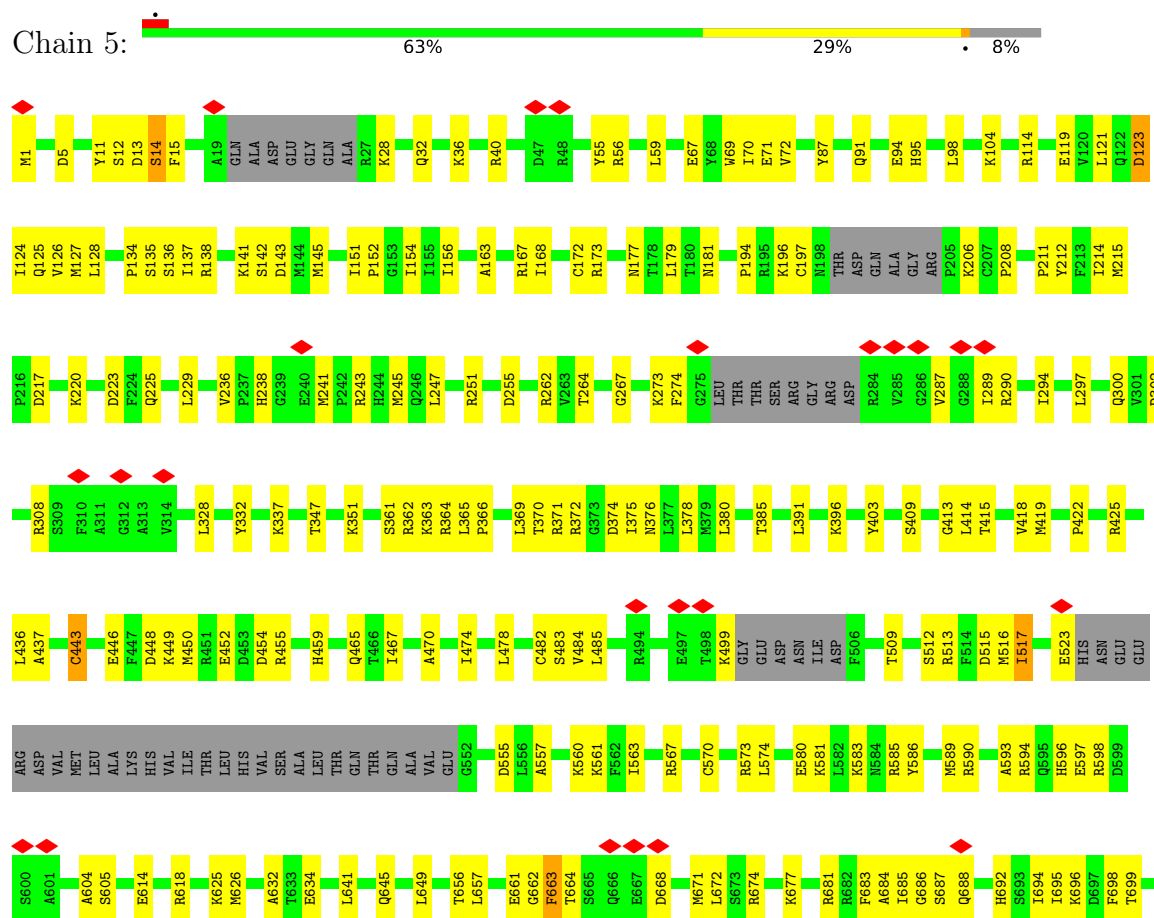
MET SER PRO ALA GLN THR PRO ARG GLY ARG GLN ARG ALA THR PRO ALA GLN THR ASP PHE ARG ASP VAL SER GLU ASP MET VAL SER THR SER THR ARG ARG GLY VAL GLU LEU GLN THR PRO MET VAL PRO THR SER GLN ARG PRO GLY VAL ASP LEU GLN

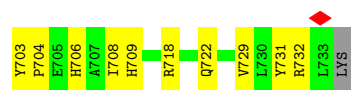
SER PRO ALA GLN THR PRO ARG GLY ARG GLN ARG ALA THR PRO ALA GLN THR ASP PHE ARG ASP VAL SER SER ASP MET VAL SER THR SER THR ARG ARG GLY VAL GLU LEU GLN THR PRO MET VAL PRO THR SER GLN ARG PRO GLY VAL ASP LEU GLN

ALA GLN LYS LEU VAL ASP LEU GLN ASP GLY ALA ALA THR D138 K149 L150 V151 I152 W153 G154 T155 D156 K163 L170 Q171 I174 D175 A178 K179 E180 E181 E182 V184 G185 I188 T189 E190 P191 L192 Y193 M194 V202 I203 A240



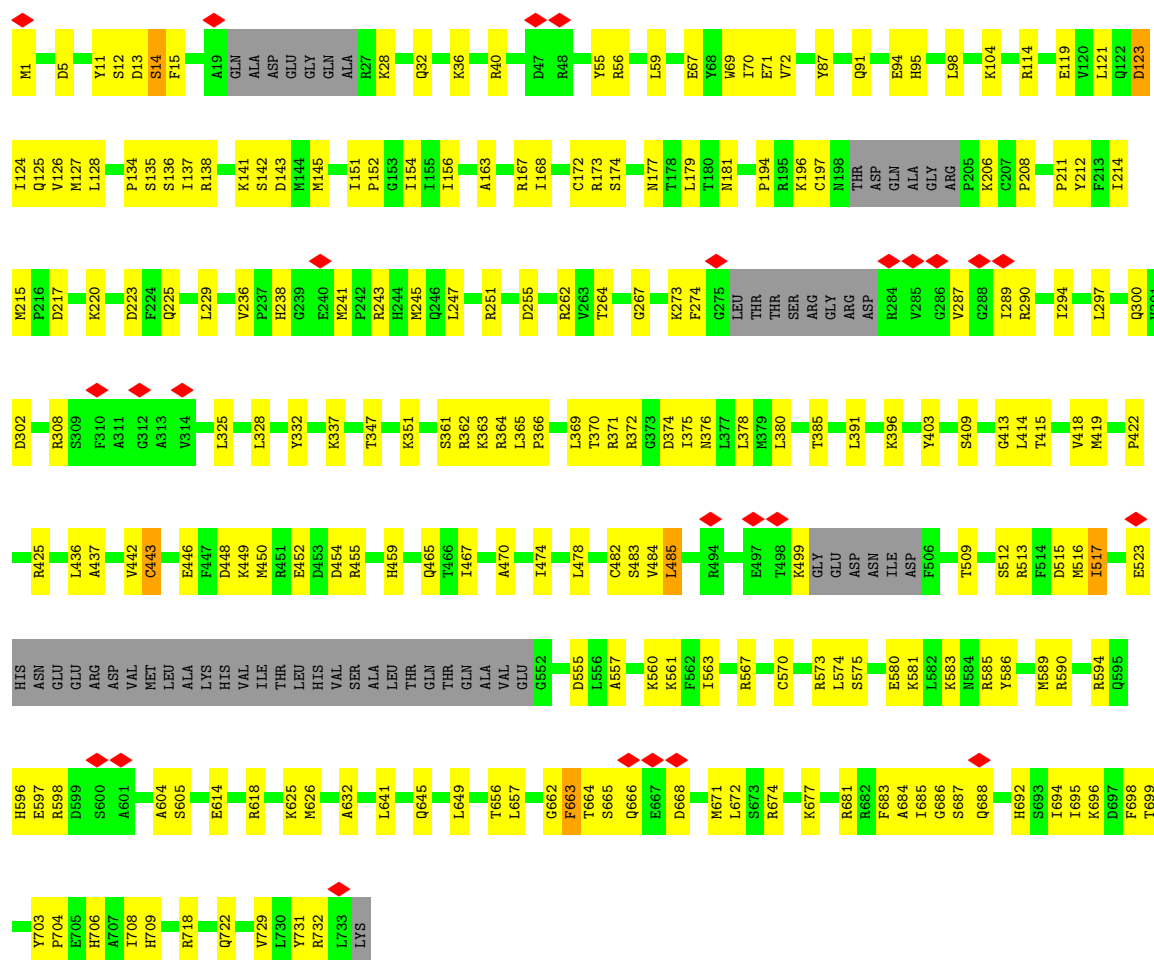
• Molecule 4: DNA replication licensing factor MCM5





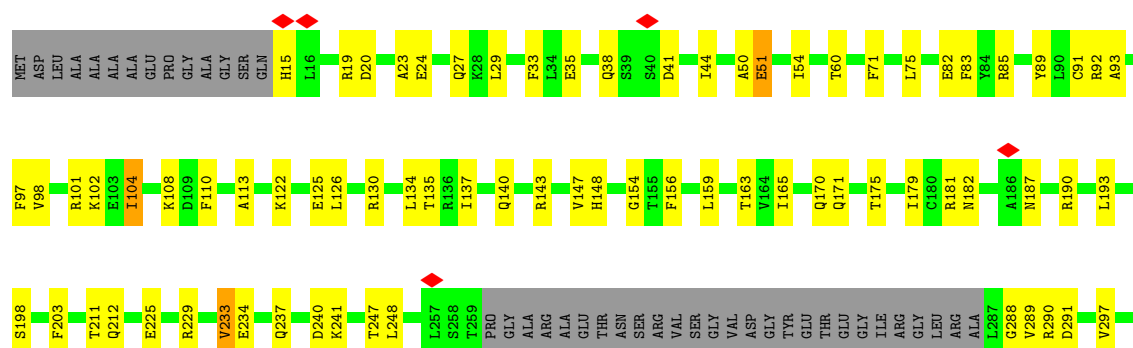
• Molecule 4: DNA replication licensing factor MCM5

Chain H: 63% 29% 8%

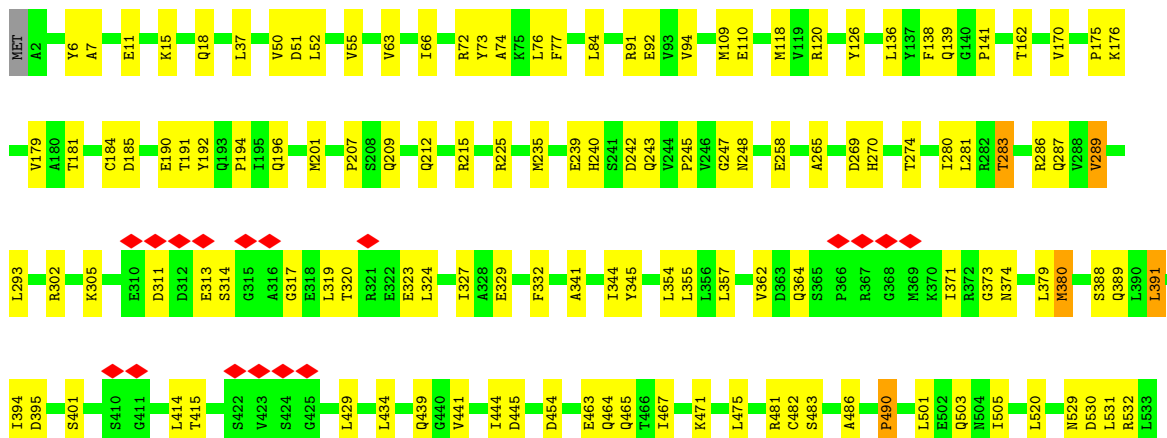
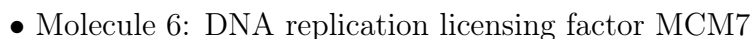


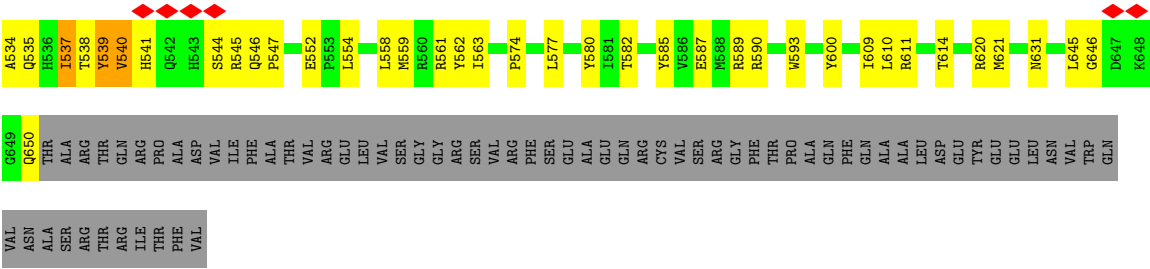
• Molecule 5: DNA replication licensing factor MCM6

Chain 6: 58% 25% 16%









4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	242055	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.006	Depositor
Minimum map value	-0.940	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.055	Depositor
Recommended contour level	0.241	Depositor
Map size (\AA)	430.91998, 430.91998, 430.91998	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.0773, 1.0773, 1.0773	Depositor

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	2	0.12	0/5730	0.35	0/7731
1	D	0.12	0/5730	0.35	0/7731
2	3	0.16	0/4997	0.38	0/6750
2	B	0.13	0/580	0.41	0/776
2	C	0.13	0/580	0.41	0/776
2	E	0.16	0/4997	0.37	0/6750
3	4	0.16	0/5848	0.38	0/7898
3	F	0.15	0/5848	0.37	0/7898
4	5	0.12	0/5406	0.33	0/7257
4	H	0.12	0/5406	0.33	0/7257
5	6	0.13	0/5676	0.34	0/7654
5	G	0.13	0/5676	0.34	0/7654
6	7	0.13	0/5222	0.34	0/7049
6	A	0.13	0/5222	0.33	0/7049
All	All	0.14	0/66918	0.35	0/90230

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
2	E	0	1
6	7	0	1
6	A	0	1
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	3	83	PHE	Peptide
6	7	645	LEU	Peptide
6	A	645	LEU	Peptide
2	E	83	PHE	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	5628	0	5638	163	0
1	D	5628	0	5638	162	0
2	3	4922	0	4954	158	0
2	B	575	0	579	22	0
2	C	575	0	579	22	0
2	E	4922	0	4954	159	0
3	4	5753	0	5820	133	0
3	F	5753	0	5820	129	0
4	5	5322	0	5409	176	0
4	H	5322	0	5409	178	0
5	6	5586	0	5619	151	0
5	G	5586	0	5619	154	0
6	7	5141	0	5180	132	0
6	A	5141	0	5180	122	0
7	2	31	0	12	3	0
7	D	31	0	12	3	0
8	3	27	0	12	0	0
8	4	27	0	12	0	0
8	6	27	0	12	1	0
8	7	27	0	12	5	0
8	A	27	0	12	5	0
8	E	27	0	12	0	0
8	F	27	0	12	0	0
8	G	27	0	12	1	0
All	All	66132	0	66518	1725	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 13.

The worst 5 of 1725 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)
4:5:196:LYS:HD2	6:A:215:ARG:HH22	1.06	1.12
6:7:215:ARG:HH22	4:H:196:LYS:HD2	1.06	1.12
4:5:143:ASP:OD1	5:G:15:HIS:HB2	1.72	0.90
1:2:715:LEU:HD11	1:2:720:LEU:HD13	1.55	0.89
1:D:715:LEU:HD11	1:D:720:LEU:HD13	1.55	0.88

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	699/904 (77%)	623 (89%)	76 (11%)	0	100	100
1	D	699/904 (77%)	623 (89%)	76 (11%)	0	100	100
2	3	625/853 (73%)	542 (87%)	79 (13%)	4 (1%)	21	56
2	B	71/853 (8%)	68 (96%)	3 (4%)	0	100	100
2	C	71/853 (8%)	68 (96%)	3 (4%)	0	100	100
2	E	625/853 (73%)	543 (87%)	78 (12%)	4 (1%)	21	56
3	4	720/863 (83%)	649 (90%)	70 (10%)	1 (0%)	48	81
3	F	720/863 (83%)	649 (90%)	71 (10%)	0	100	100
4	5	666/734 (91%)	606 (91%)	60 (9%)	0	100	100
4	H	666/734 (91%)	606 (91%)	60 (9%)	0	100	100
5	6	685/821 (83%)	639 (93%)	46 (7%)	0	100	100
5	G	685/821 (83%)	639 (93%)	46 (7%)	0	100	100
6	7	647/719 (90%)	608 (94%)	37 (6%)	2 (0%)	36	69

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	A	647/719 (90%)	609 (94%)	36 (6%)	2 (0%)	36	69
All	All	8226/11494 (72%)	7472 (91%)	741 (9%)	13 (0%)	44	75

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	4	190	GLU
2	3	69	ALA
2	3	70	PHE
2	3	84	VAL
6	7	530	ASP

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	2	622/781 (80%)	612 (98%)	10 (2%)	55	69
1	D	622/781 (80%)	612 (98%)	10 (2%)	55	69
2	3	542/742 (73%)	529 (98%)	13 (2%)	43	63
2	B	65/742 (9%)	62 (95%)	3 (5%)	24	48
2	C	65/742 (9%)	62 (95%)	3 (5%)	24	48
2	E	542/742 (73%)	529 (98%)	13 (2%)	43	63
3	4	636/753 (84%)	625 (98%)	11 (2%)	53	68
3	F	636/753 (84%)	626 (98%)	10 (2%)	55	69
4	5	577/624 (92%)	568 (98%)	9 (2%)	55	69
4	H	577/624 (92%)	568 (98%)	9 (2%)	55	69
5	6	627/724 (87%)	612 (98%)	15 (2%)	43	63
5	G	627/724 (87%)	612 (98%)	15 (2%)	43	63
6	7	560/619 (90%)	547 (98%)	13 (2%)	44	64
6	A	560/619 (90%)	548 (98%)	12 (2%)	47	65
All	All	7258/9970 (73%)	7112 (98%)	146 (2%)	48	66

5 of 146 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	F	475	ASP
4	H	517	ILE
3	F	666	LEU
5	G	466	ASP
5	6	247	THR

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

Mol	Chain	Res	Type
6	A	212	GLN
4	H	713	GLN
1	D	356	GLN
4	H	479	ASN
5	G	196	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](#)

10 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
8	ADP	G	901	-	28,29,29	1.41	4 (14%)	43,45,45	1.89	8 (18%)
8	ADP	7	801	-	28,29,29	1.37	4 (14%)	43,45,45	1.82	10 (23%)
7	ATP	D	1001	-	32,33,33	0.37	0	48,52,52	0.39	0
8	ADP	E	901	-	28,29,29	1.40	4 (14%)	43,45,45	1.85	7 (16%)
8	ADP	A	801	-	28,29,29	1.37	4 (14%)	43,45,45	1.82	10 (23%)
7	ATP	2	1001	-	32,33,33	0.37	0	48,52,52	0.39	0
8	ADP	F	901	-	28,29,29	1.41	4 (14%)	43,45,45	1.90	8 (18%)
8	ADP	6	901	-	28,29,29	1.41	4 (14%)	43,45,45	1.89	8 (18%)
8	ADP	3	901	-	28,29,29	1.40	4 (14%)	43,45,45	1.85	7 (16%)
8	ADP	4	901	-	28,29,29	1.41	4 (14%)	43,45,45	1.90	8 (18%)

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	ADP	G	901	-	-	4/16/32/32	0/3/3/3
8	ADP	7	801	-	-	3/16/32/32	0/3/3/3
7	ATP	D	1001	-	-	5/22/38/38	0/3/3/3
8	ADP	E	901	-	-	2/16/32/32	0/3/3/3
8	ADP	A	801	-	-	3/16/32/32	0/3/3/3
7	ATP	2	1001	-	-	5/22/38/38	0/3/3/3
8	ADP	F	901	-	-	3/16/32/32	0/3/3/3
8	ADP	6	901	-	-	4/16/32/32	0/3/3/3
8	ADP	3	901	-	-	2/16/32/32	0/3/3/3
8	ADP	4	901	-	-	3/16/32/32	0/3/3/3

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	6	901	ADP	C5-C4	4.77	1.47	1.39
8	G	901	ADP	C5-C4	4.77	1.47	1.39
8	4	901	ADP	C5-C4	4.77	1.47	1.39
8	F	901	ADP	C5-C4	4.77	1.47	1.39
8	3	901	ADP	C5-C4	4.72	1.47	1.39

The worst 5 of 66 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	4	901	ADP	C5-C4-N3	-6.55	117.70	126.72
8	F	901	ADP	C5-C4-N3	-6.55	117.70	126.72
8	6	901	ADP	C5-C4-N3	-6.44	117.84	126.72
8	G	901	ADP	C5-C4-N3	-6.44	117.84	126.72
8	3	901	ADP	C5-C4-N3	-6.17	118.22	126.72

There are no chirality outliers.

5 of 34 torsion outliers are listed below:

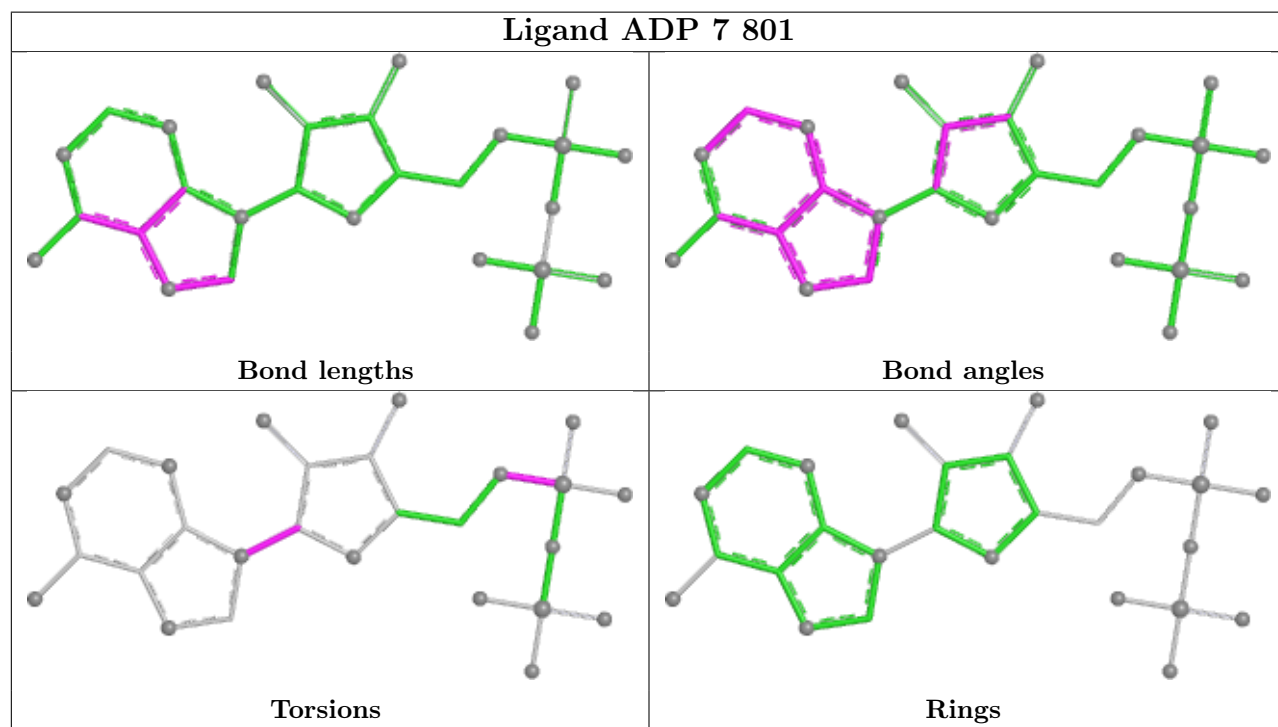
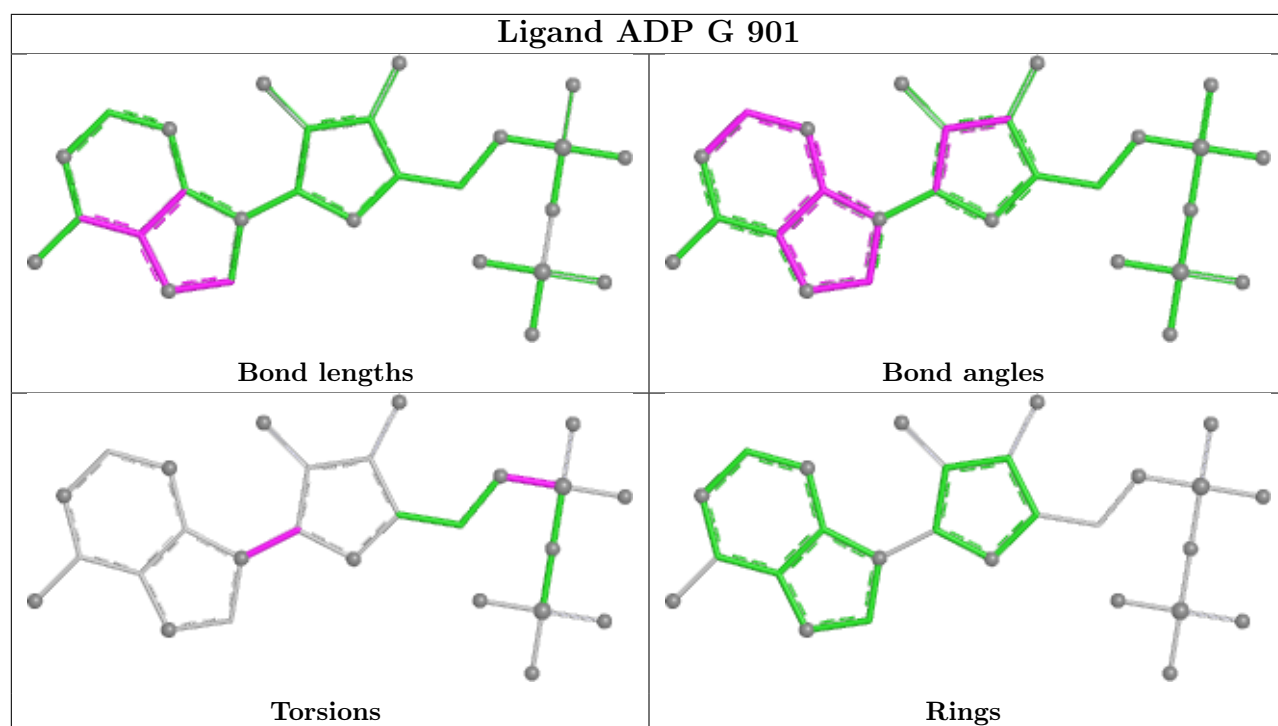
Mol	Chain	Res	Type	Atoms
7	2	1001	ATP	C5'-O5'-PA-O3A
7	D	1001	ATP	C5'-O5'-PA-O3A
8	4	901	ADP	C5'-O5'-PA-O1A
8	6	901	ADP	C5'-O5'-PA-O1A
8	7	801	ADP	C5'-O5'-PA-O1A

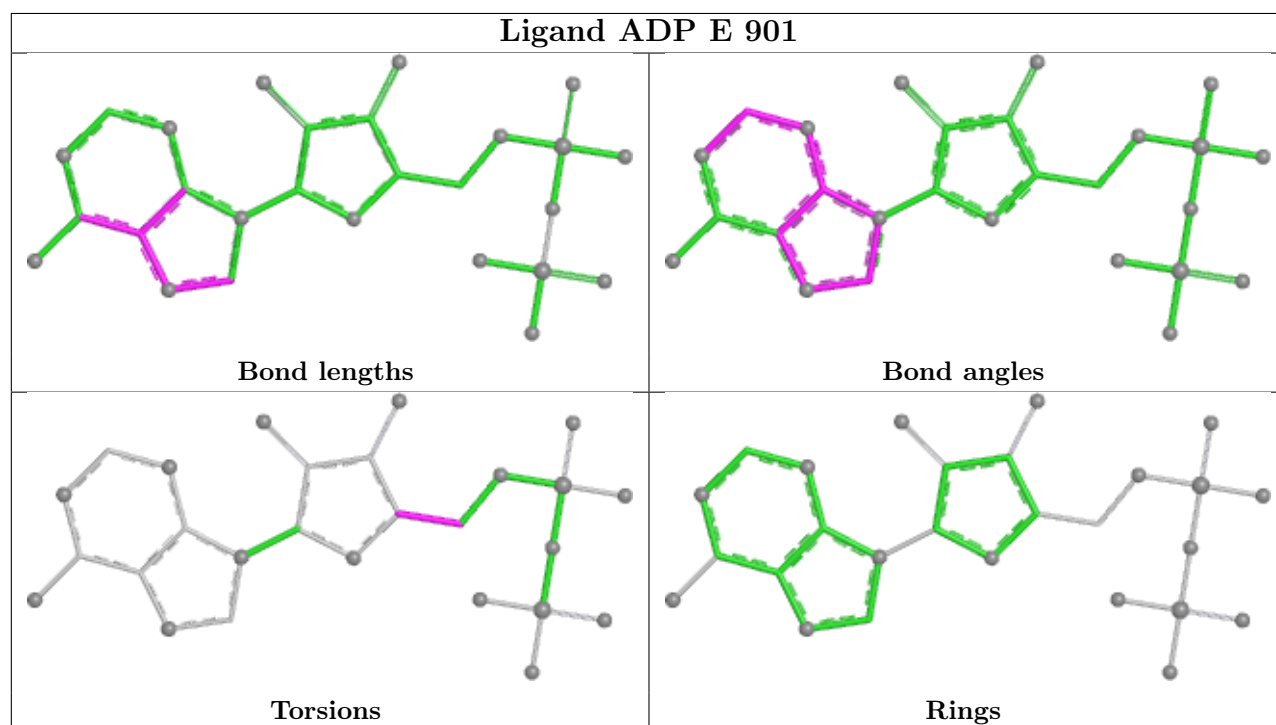
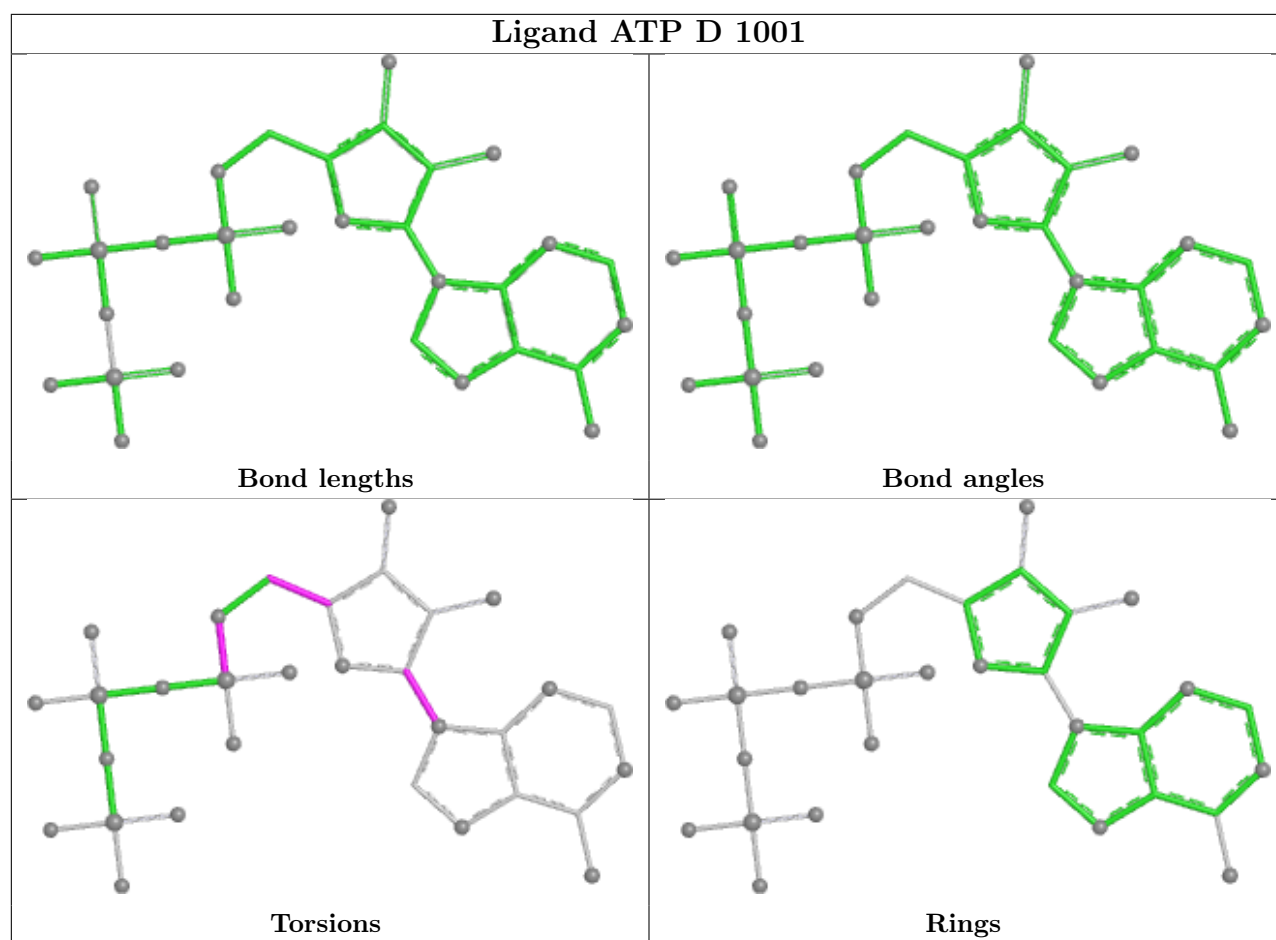
There are no ring outliers.

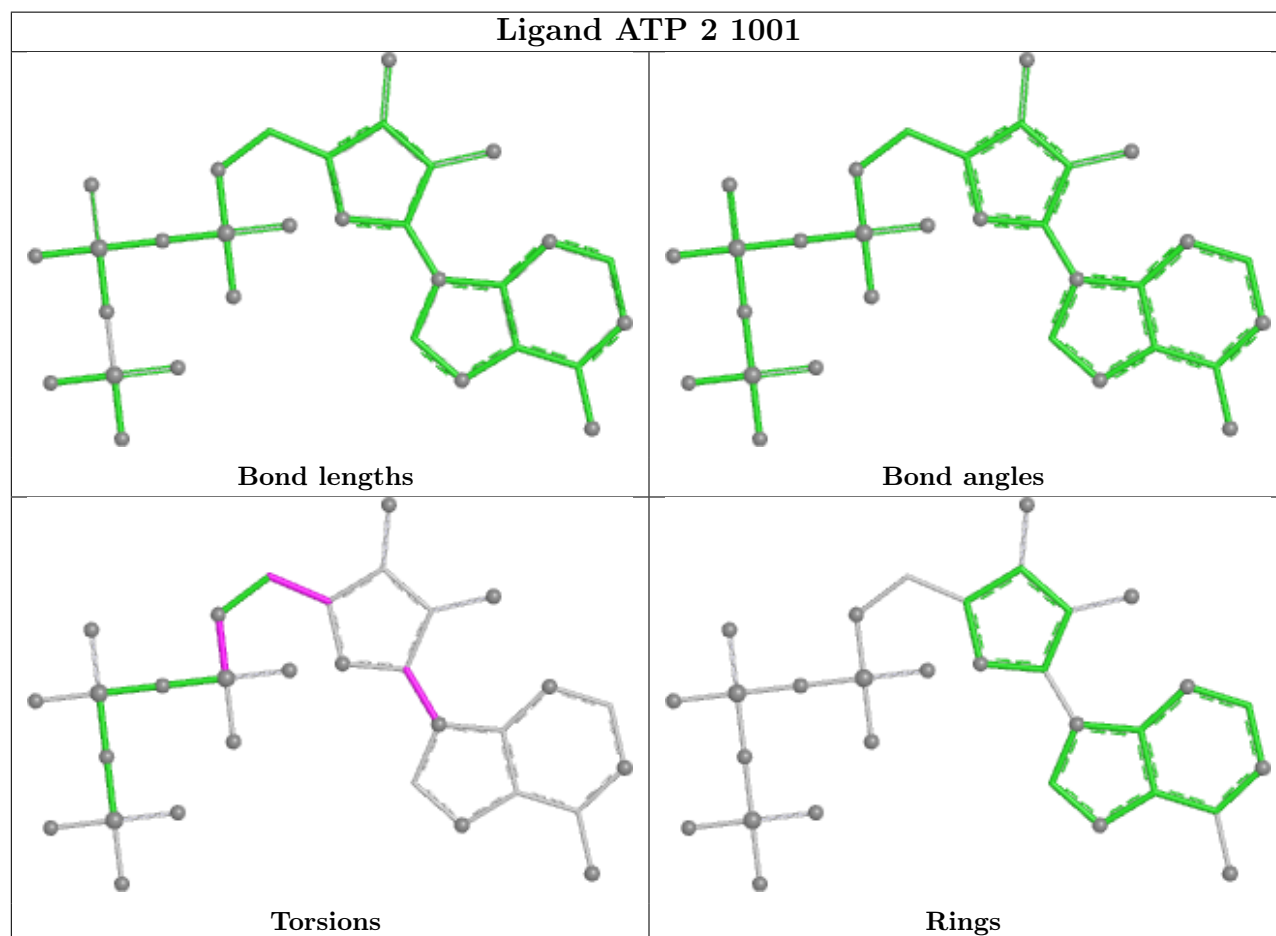
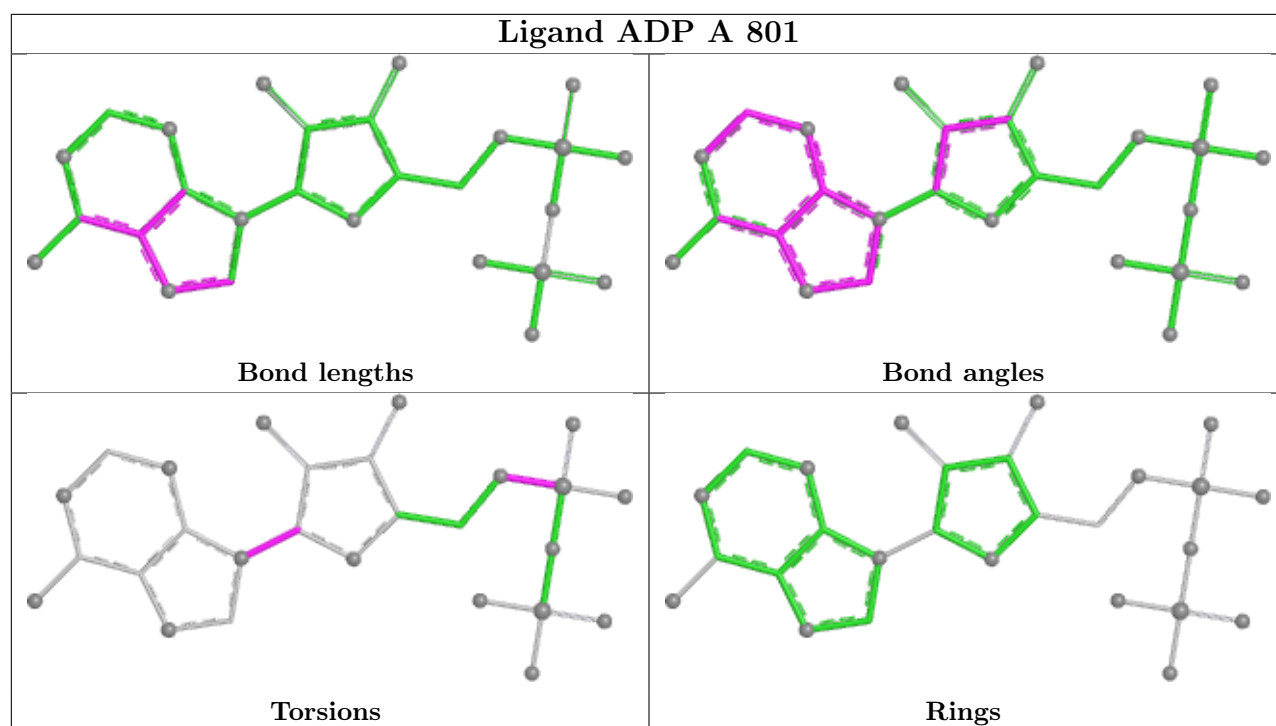
6 monomers are involved in 18 short contacts:

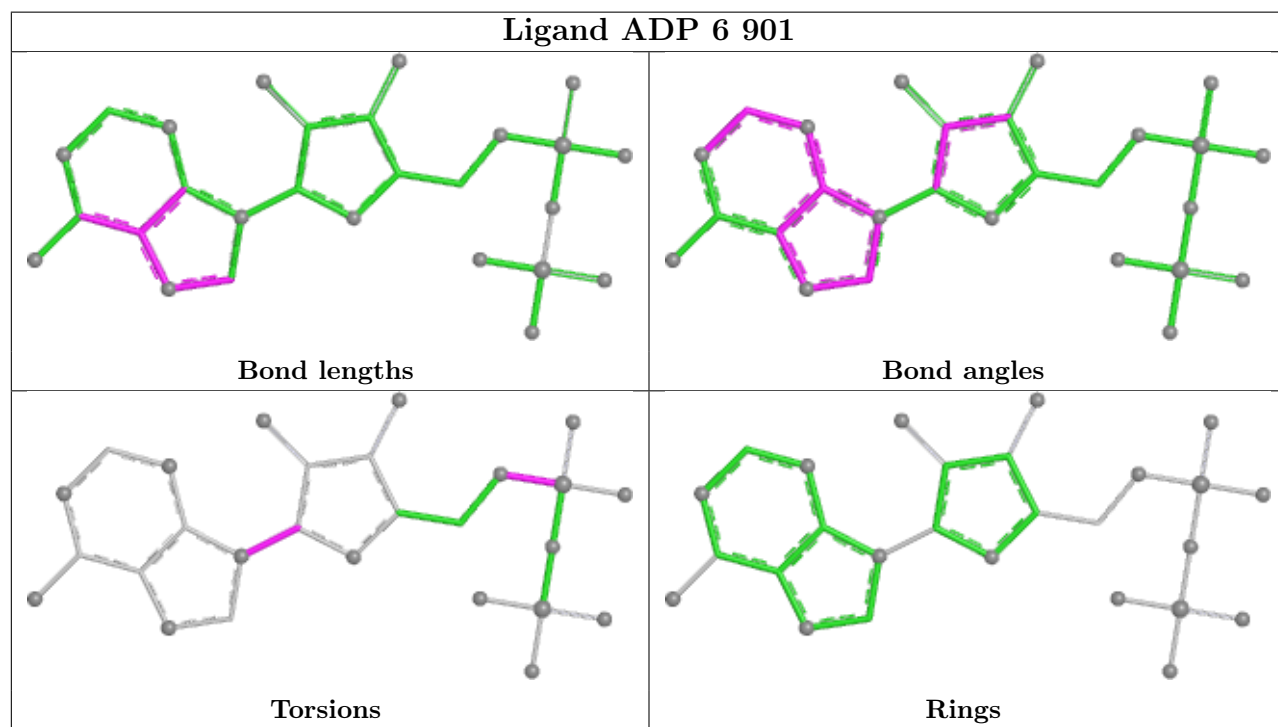
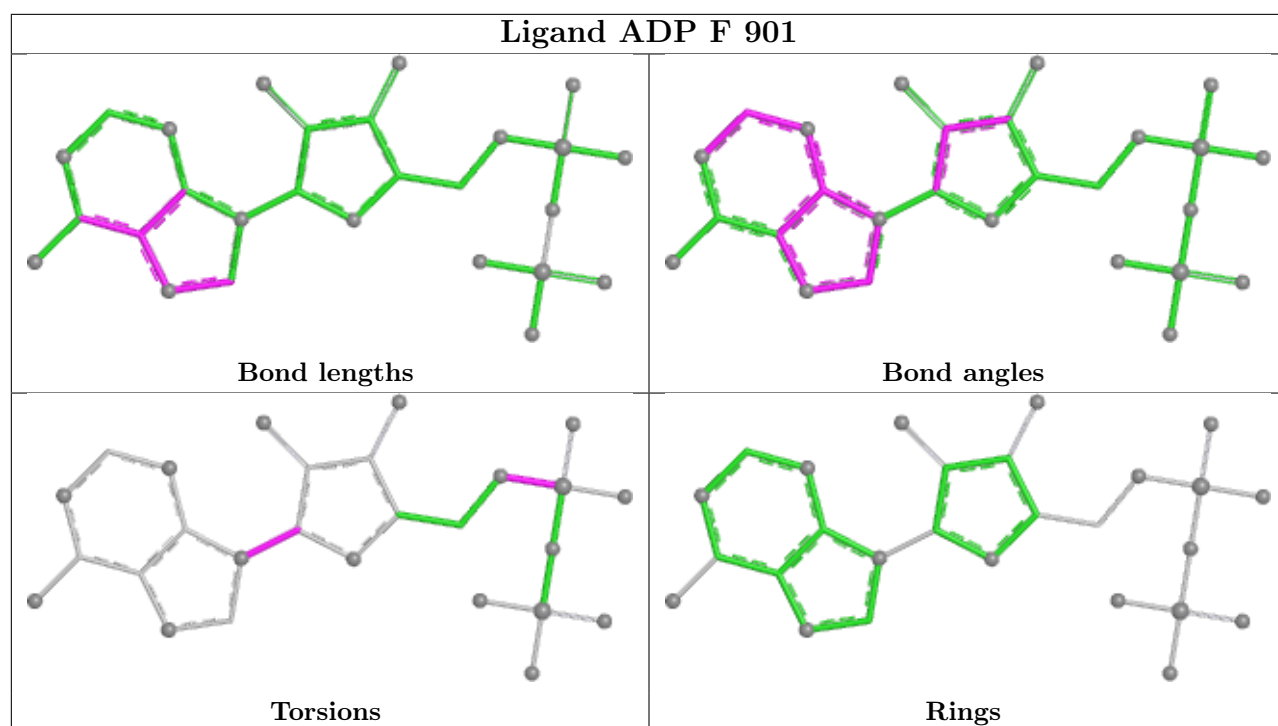
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	G	901	ADP	1	0
8	7	801	ADP	5	0
7	D	1001	ATP	3	0
8	A	801	ADP	5	0
7	2	1001	ATP	3	0
8	6	901	ADP	1	0

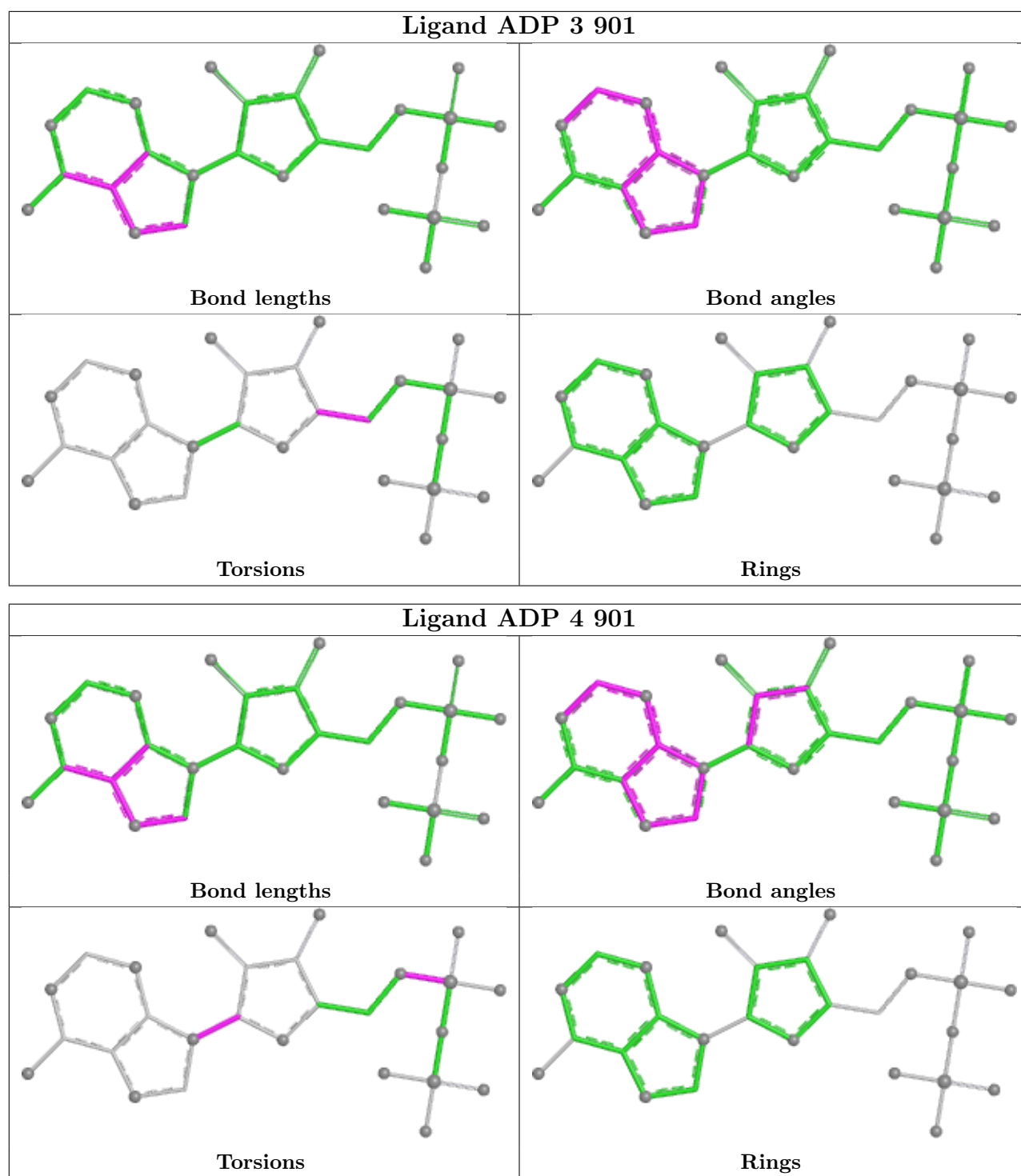
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

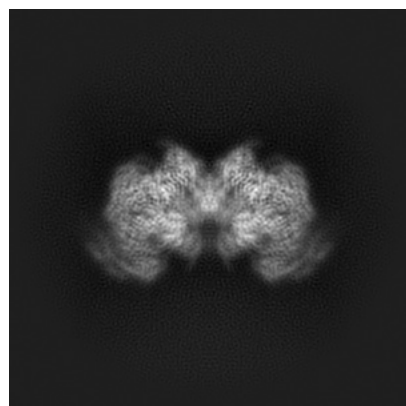
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-63475. These allow visual inspection of the internal detail of the map and identification of artifacts.

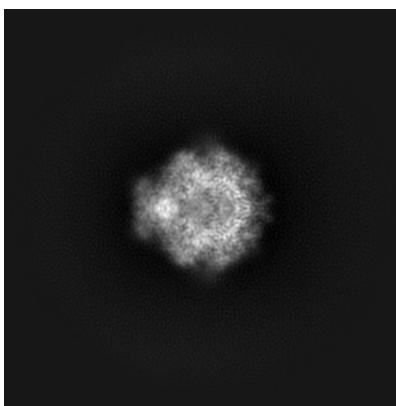
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

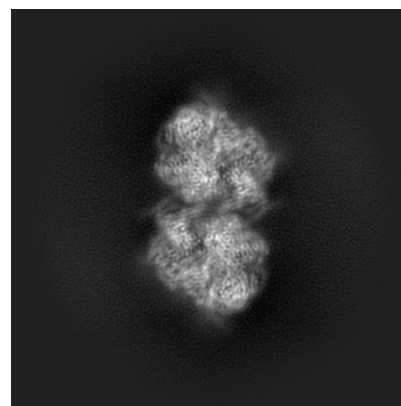
6.1.1 Primary map



X

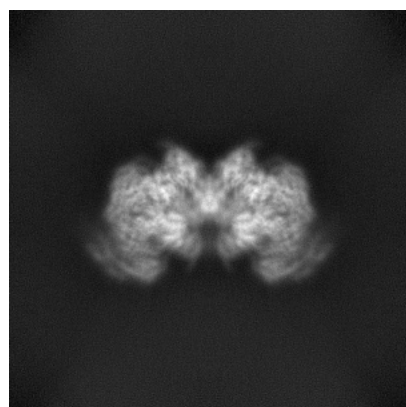


Y

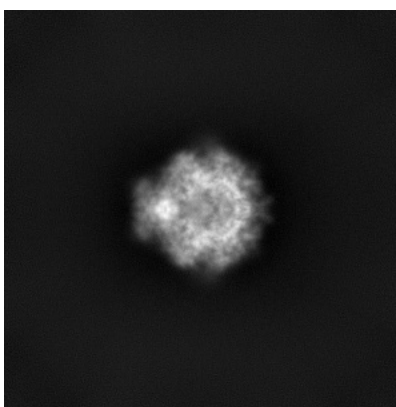


Z

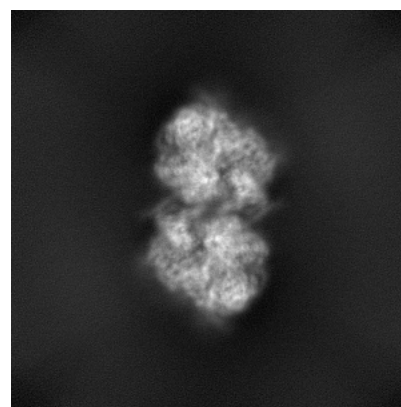
6.1.2 Raw map



X



Y

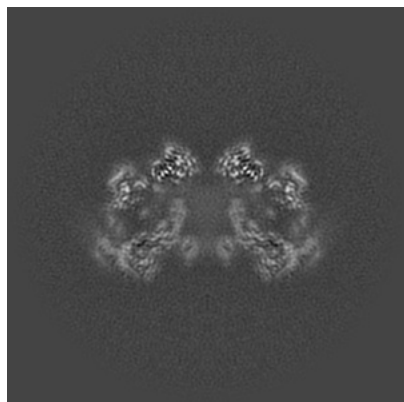


Z

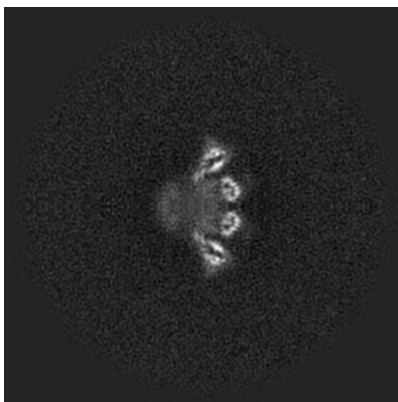
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

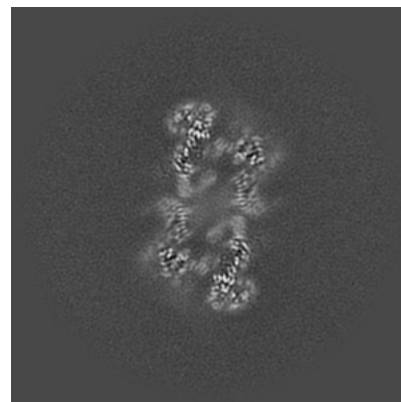
6.2.1 Primary map



X Index: 200

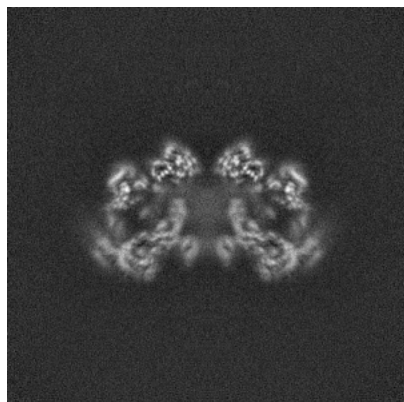


Y Index: 200



Z Index: 200

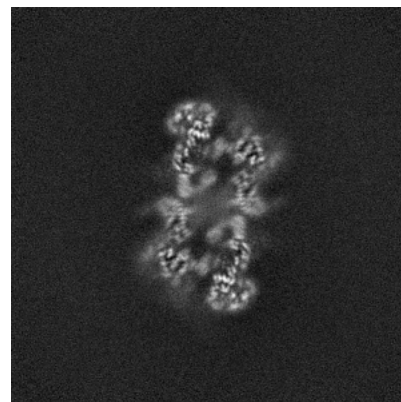
6.2.2 Raw map



X Index: 200



Y Index: 200

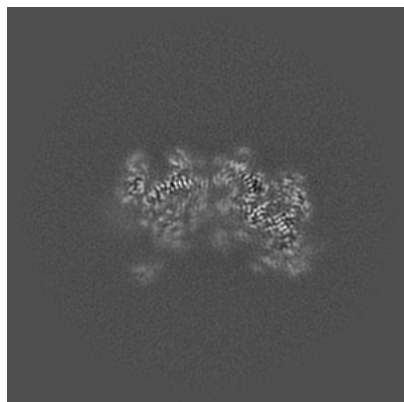


Z Index: 200

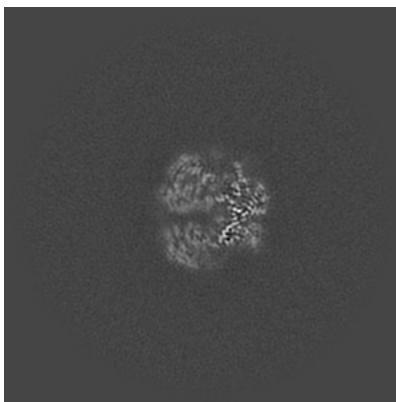
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

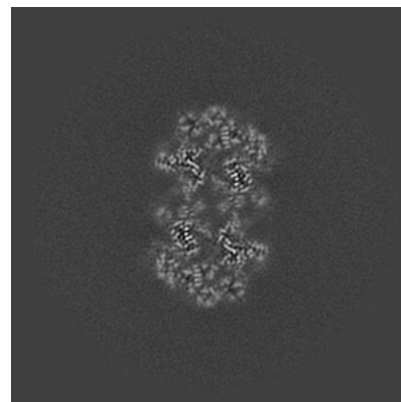
6.3.1 Primary map



X Index: 175

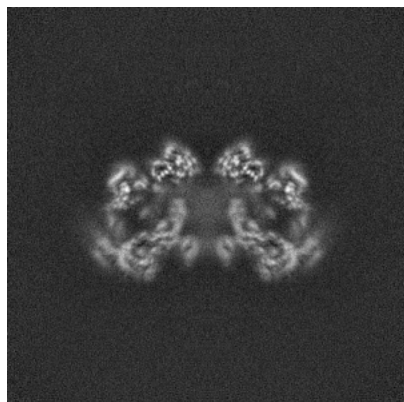


Y Index: 169

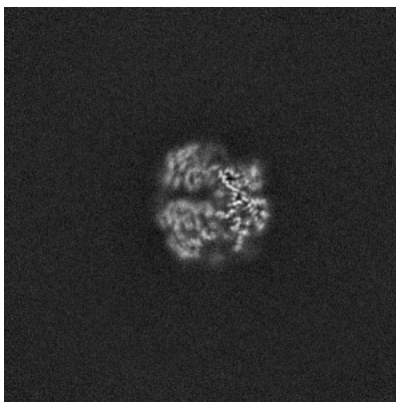


Z Index: 223

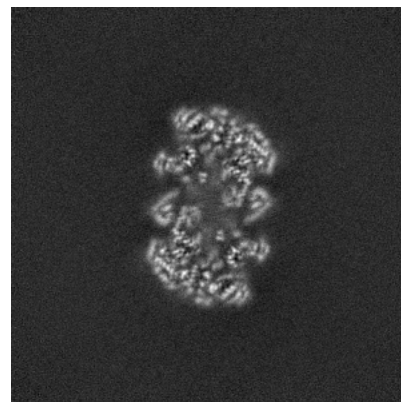
6.3.2 Raw map



X Index: 200



Y Index: 231

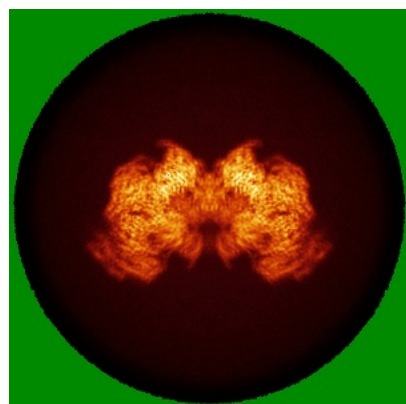


Z Index: 217

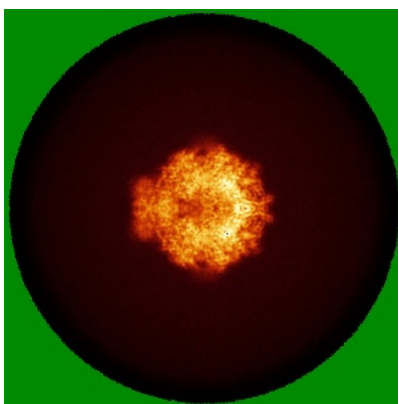
The images above show the largest variance slices of the map in three orthogonal directions.

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

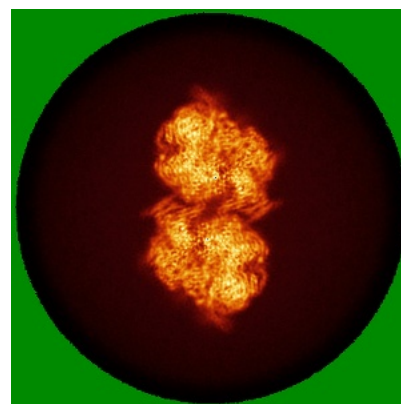
6.4.1 Primary map



X

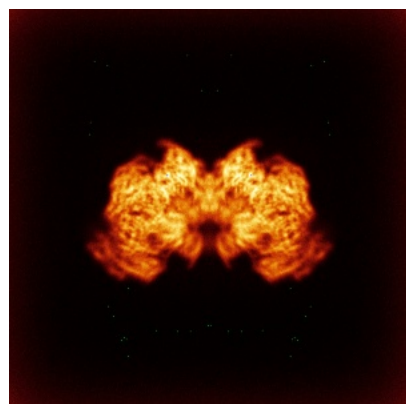


Y

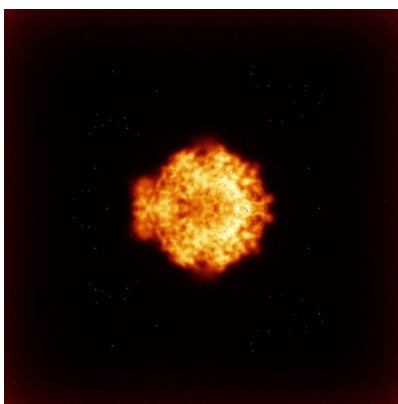


Z

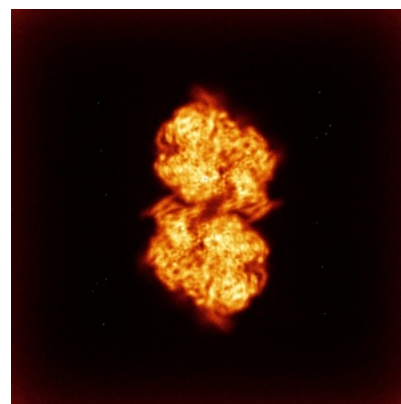
6.4.2 Raw map



X



Y

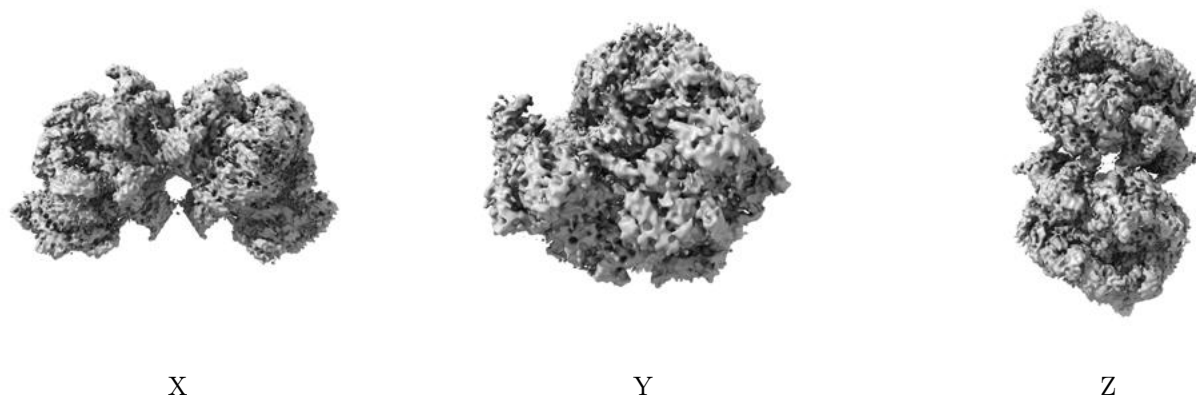


Z

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.

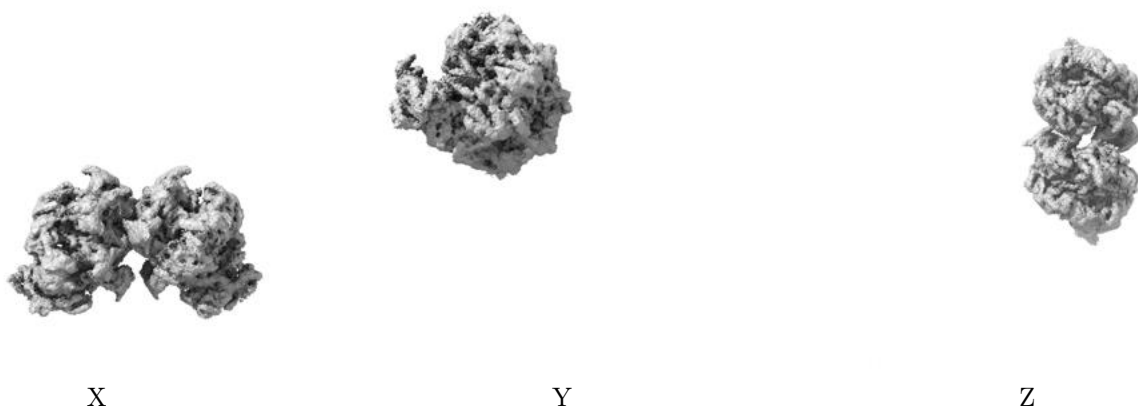
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.241. 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



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.

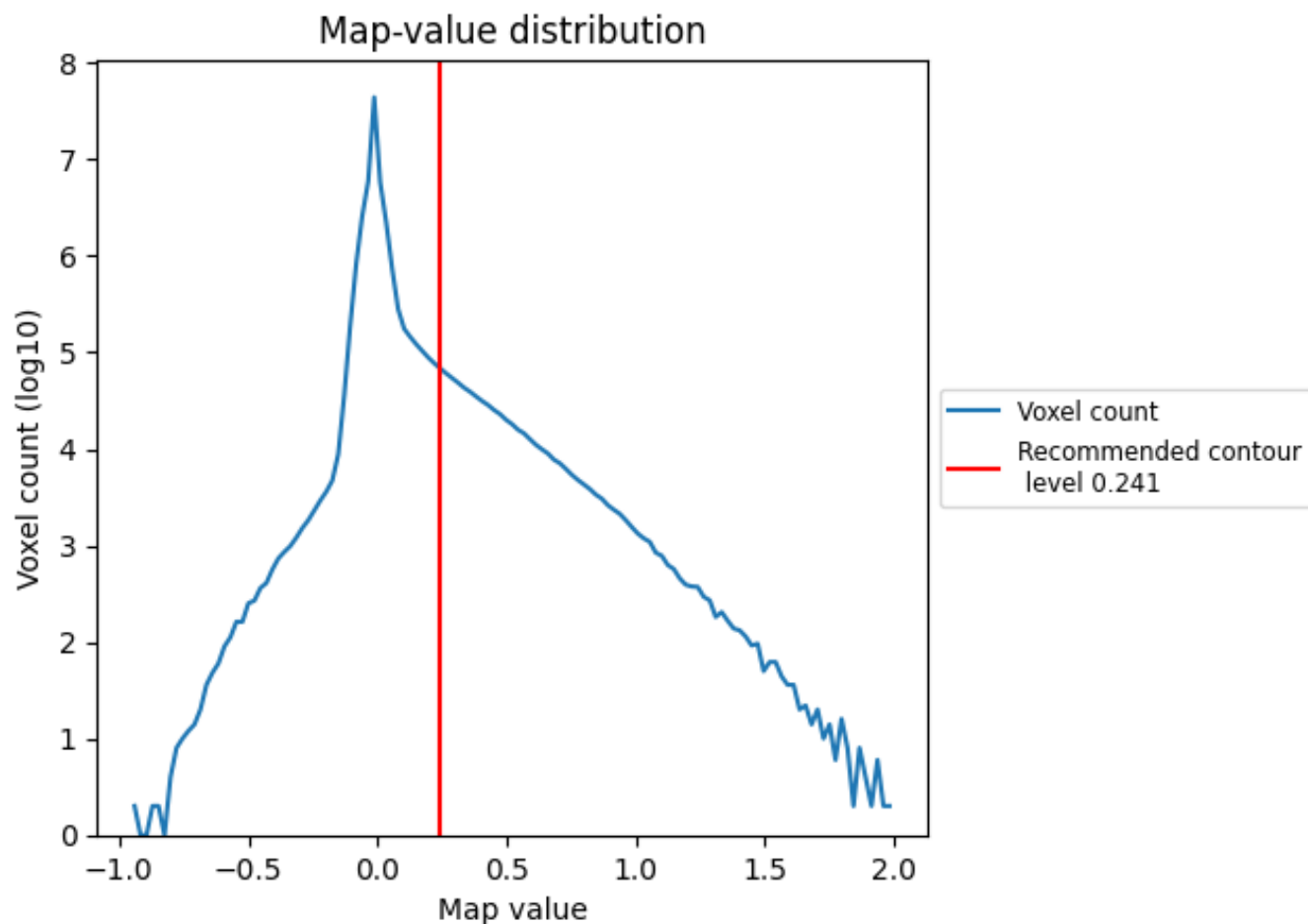
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

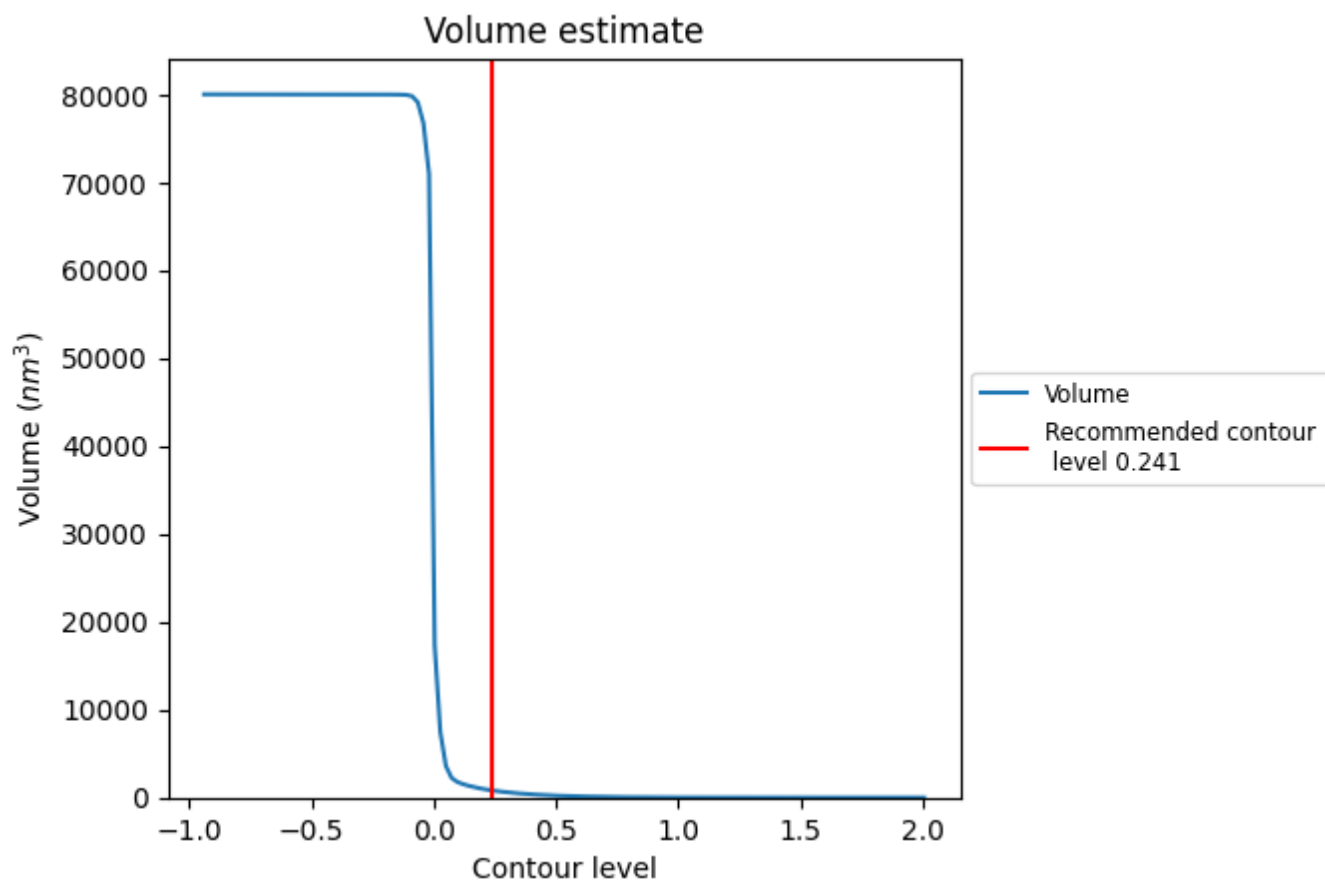
This section contains the results of statistical analysis of the map.

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.

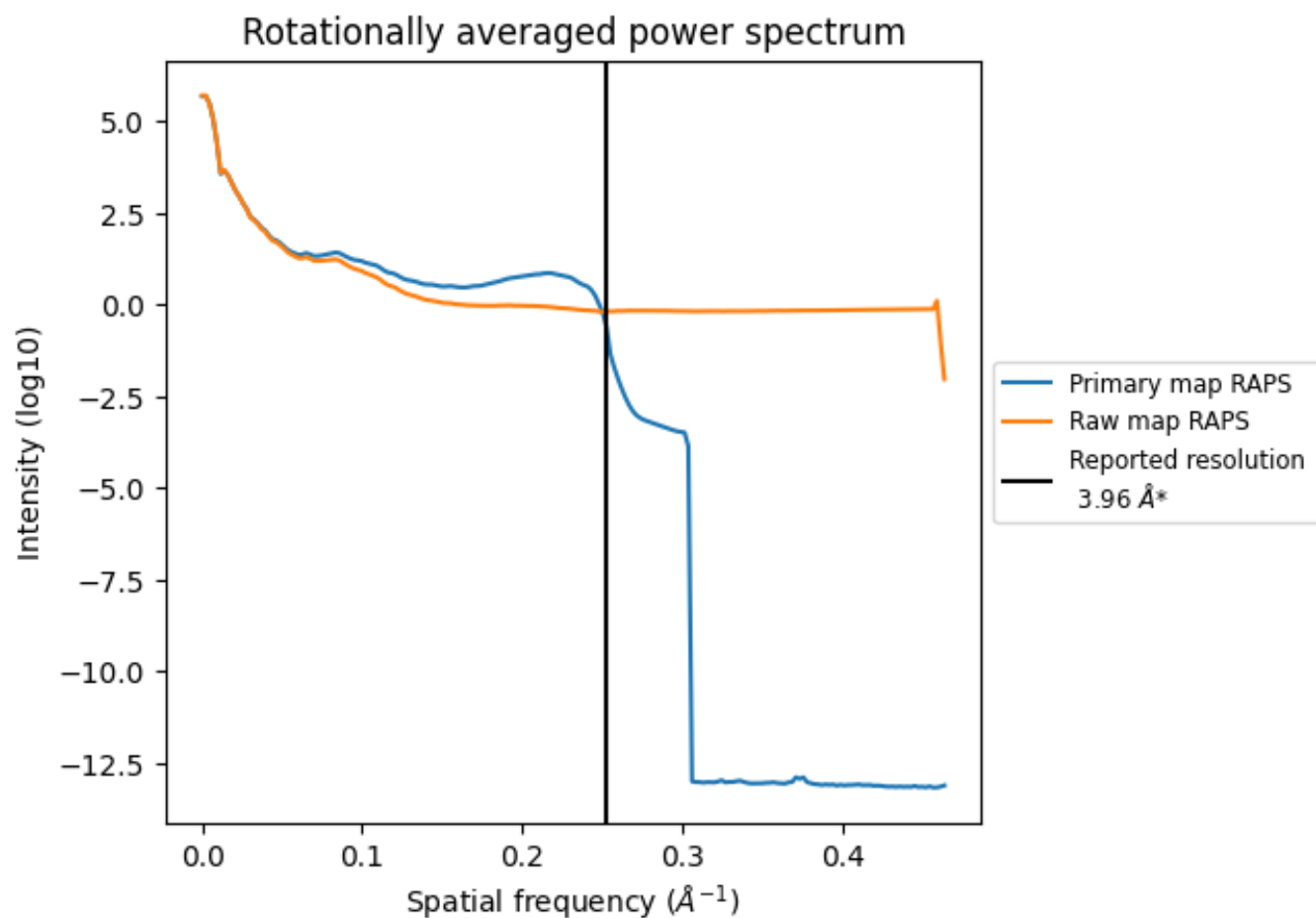
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 802 nm³; this corresponds to an approximate mass of 724 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 ⓘ

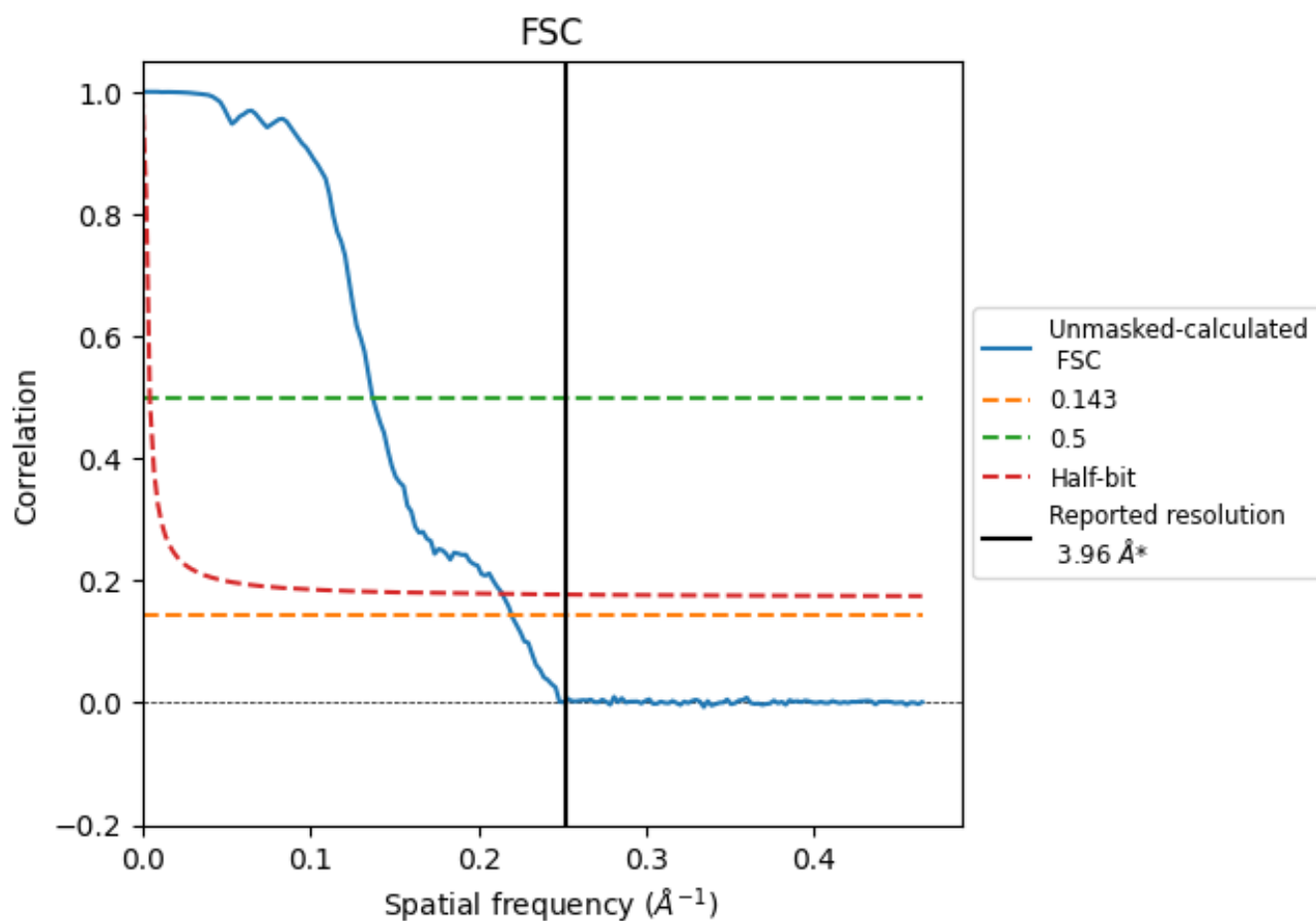


*Reported resolution corresponds to spatial frequency of 0.253 Å⁻¹

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 0.253 \AA^{-1}

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.96	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.55	7.29	4.67

*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 4.55 differs from the reported value 3.96 by more than 10 %

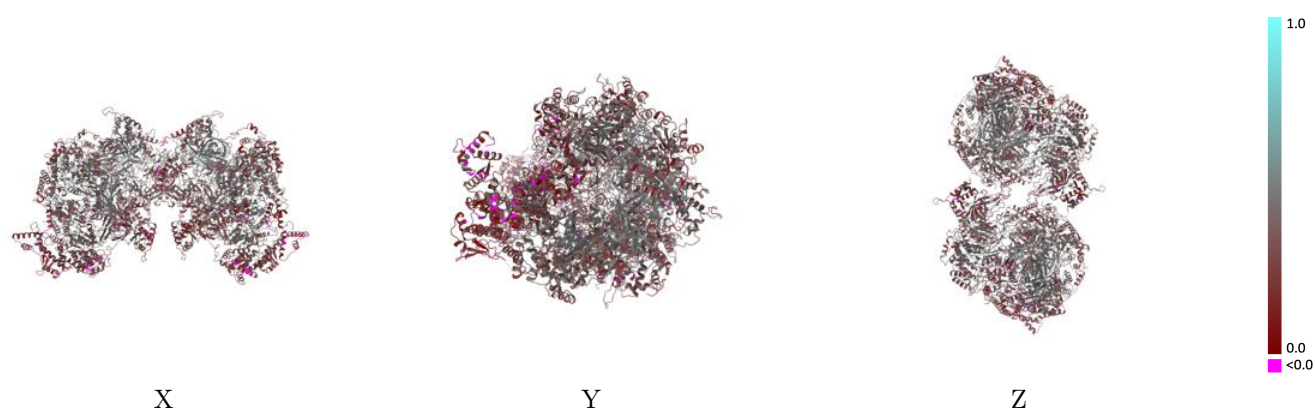
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-63475 and PDB model 9LXE. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)

This section was not generated.

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

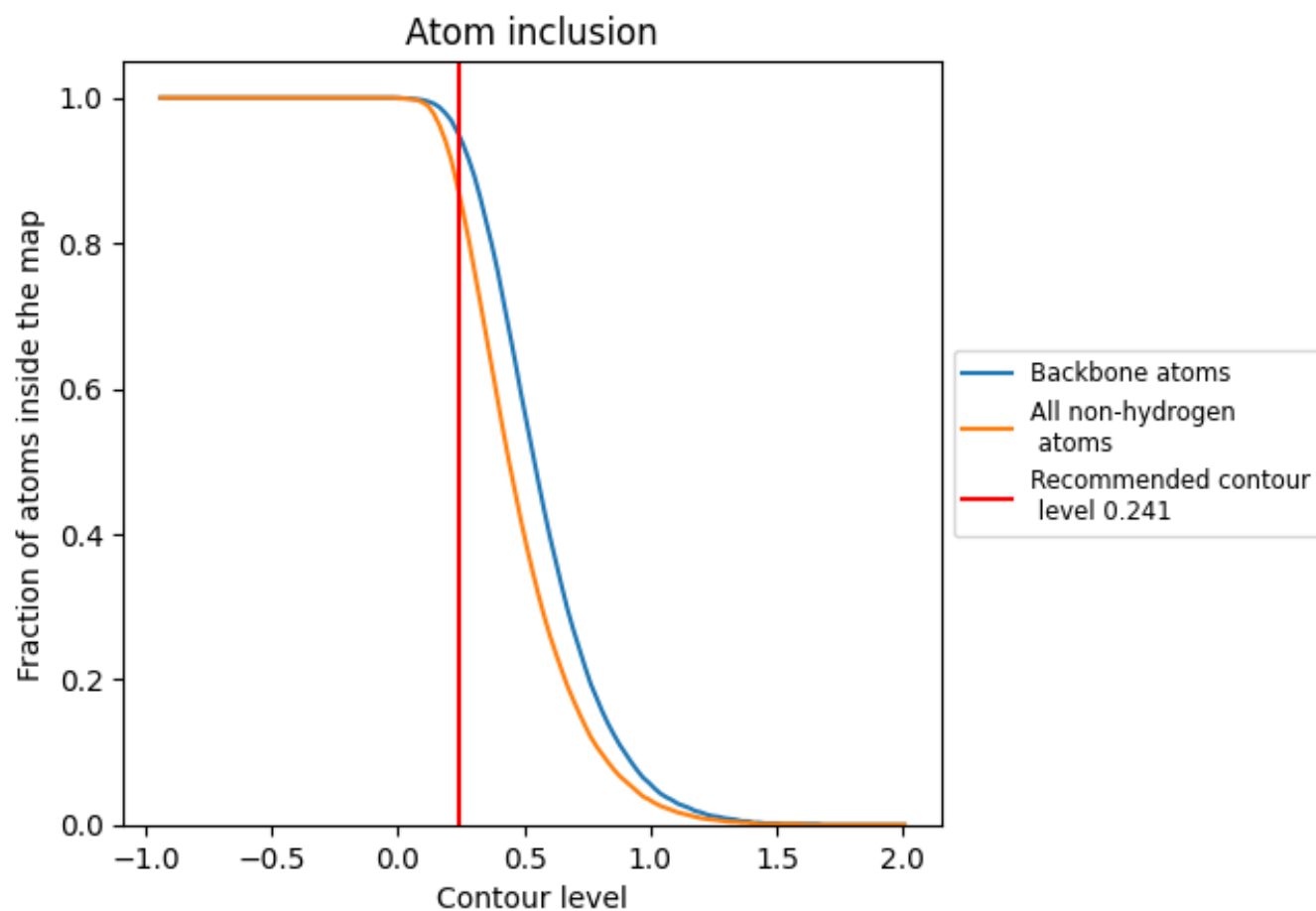


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.































9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 87% 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 (0.241) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8700	 0.3510
2	 0.8530	 0.2990
3	 0.8990	 0.3880
4	 0.8590	 0.3760
5	 0.8630	 0.3100
6	 0.8900	 0.3650
7	 0.8950	 0.3880
A	 0.8950	 0.3890
B	 0.5380	 0.2050
C	 0.5380	 0.2000
D	 0.8530	 0.3000
E	 0.8980	 0.3900
F	 0.8590	 0.3740
G	 0.8900	 0.3660
H	 0.8630	 0.3090

