Full wwPDB EM Validation Report

Aug 1, 2026 – 07:43 am BST

PDB ID	:	9RHL / pdb_00009rhl
EMDB ID	:	EMD-53972
Title	:	Phospho-DH bound by Sld3-MBD on ARS1 DNA
Authors	:	Puehringer, T.; Couves, E.C.; Costa, A.
Deposited on	:	2025-06-09
Resolution	:	3.10 Å(reported)

This is a Full wwPDB EM Validation 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:

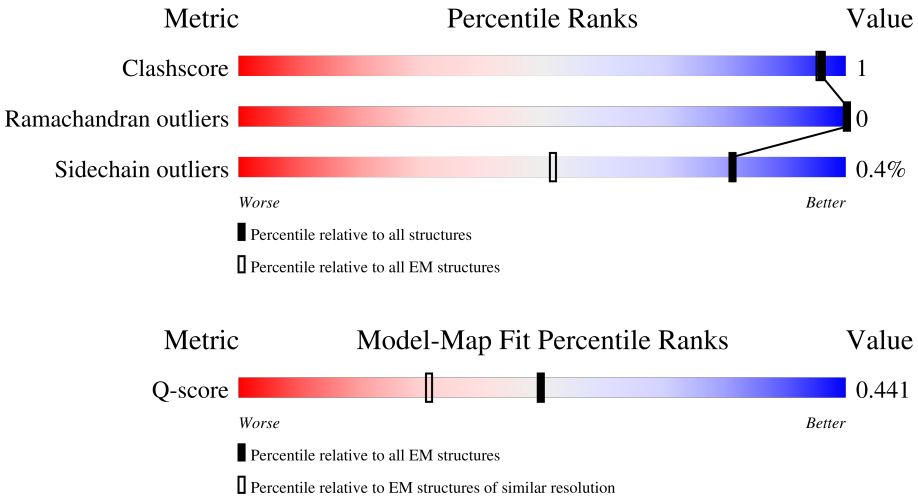
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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)	:	2.50

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 3.10 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	14724 (2.60 - 3.60)

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	23% 70% · 28%
1	a	868	24% 69% · 28%
2	3	1006	7% 62% · 37%
2	b	1006	7% 62% · 37%

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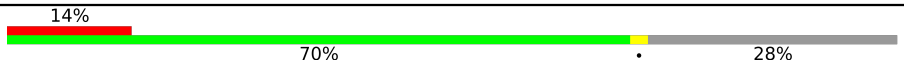
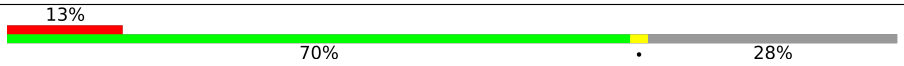
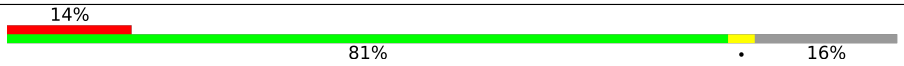
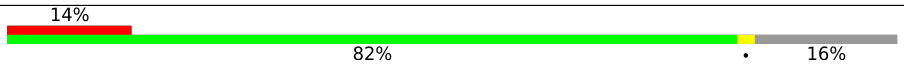
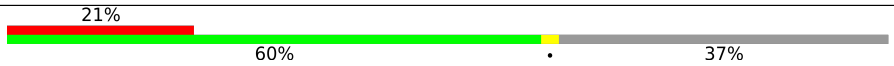
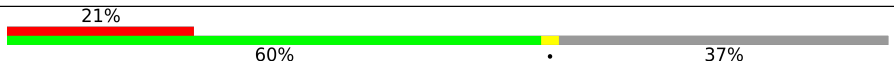
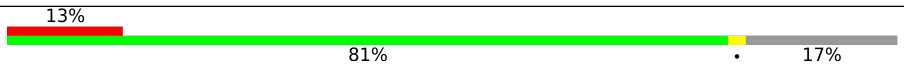
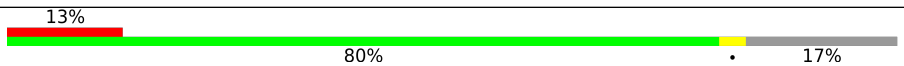
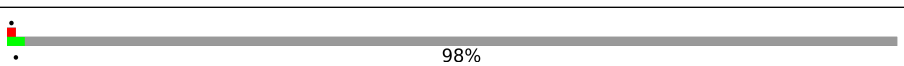
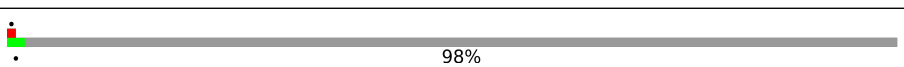
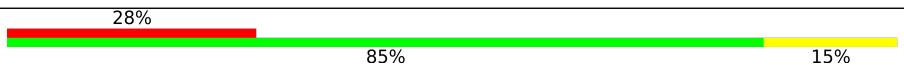
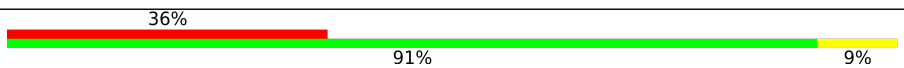
Mol	Chain	Length	Quality of chain
3	4	933	
3	c	933	
4	5	775	
4	d	775	
5	6	1017	
5	e	1017	
6	7	845	
6	f	845	
7	H	704	
7	I	704	
8	X	53	
9	Y	53	

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 64409 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	623	Total	C	N	O	S	0	0
			4932	3109	877	927	19		
1	a	623	Total	C	N	O	S	0	0
			4932	3109	877	927	19		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	638	Total	C	N	O	S	0	0
			4994	3150	889	942	13		
2	b	638	Total	C	N	O	S	0	0
			4994	3150	889	942	13		

There are 70 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	-34	MET	-	initiating methionine	UNP P24279
3	-33	LYS	-	expression tag	UNP P24279
3	-32	ARG	-	expression tag	UNP P24279
3	-31	ARG	-	expression tag	UNP P24279
3	-30	TRP	-	expression tag	UNP P24279
3	-29	LYS	-	expression tag	UNP P24279
3	-28	LYS	-	expression tag	UNP P24279
3	-27	ASN	-	expression tag	UNP P24279
3	-26	PHE	-	expression tag	UNP P24279
3	-25	ILE	-	expression tag	UNP P24279
3	-24	ALA	-	expression tag	UNP P24279
3	-23	VAL	-	expression tag	UNP P24279
3	-22	SER	-	expression tag	UNP P24279
3	-21	ALA	-	expression tag	UNP P24279
3	-20	ALA	-	expression tag	UNP P24279
3	-19	ASN	-	expression tag	UNP P24279
3	-18	ARG	-	expression tag	UNP P24279

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Chain	Residue	Modelled	Actual	Comment	Reference
3	-17	PHE	-	expression tag	UNP P24279
3	-16	LYS	-	expression tag	UNP P24279
3	-15	LYS	-	expression tag	UNP P24279
3	-14	ILE	-	expression tag	UNP P24279
3	-13	SER	-	expression tag	UNP P24279
3	-12	SER	-	expression tag	UNP P24279
3	-11	SER	-	expression tag	UNP P24279
3	-10	GLY	-	expression tag	UNP P24279
3	-9	ALA	-	expression tag	UNP P24279
3	-8	LEU	-	expression tag	UNP P24279
3	-7	GLU	-	expression tag	UNP P24279
3	-6	ASN	-	expression tag	UNP P24279
3	-5	LEU	-	expression tag	UNP P24279
3	-4	TYR	-	expression tag	UNP P24279
3	-3	PHE	-	expression tag	UNP P24279
3	-2	GLN	-	expression tag	UNP P24279
3	-1	GLY	-	expression tag	UNP P24279
3	0	GLU	-	expression tag	UNP P24279
b	-34	MET	-	initiating methionine	UNP P24279
b	-33	LYS	-	expression tag	UNP P24279
b	-32	ARG	-	expression tag	UNP P24279
b	-31	ARG	-	expression tag	UNP P24279
b	-30	TRP	-	expression tag	UNP P24279
b	-29	LYS	-	expression tag	UNP P24279
b	-28	LYS	-	expression tag	UNP P24279
b	-27	ASN	-	expression tag	UNP P24279
b	-26	PHE	-	expression tag	UNP P24279
b	-25	ILE	-	expression tag	UNP P24279
b	-24	ALA	-	expression tag	UNP P24279
b	-23	VAL	-	expression tag	UNP P24279
b	-22	SER	-	expression tag	UNP P24279
b	-21	ALA	-	expression tag	UNP P24279
b	-20	ALA	-	expression tag	UNP P24279
b	-19	ASN	-	expression tag	UNP P24279
b	-18	ARG	-	expression tag	UNP P24279
b	-17	PHE	-	expression tag	UNP P24279
b	-16	LYS	-	expression tag	UNP P24279
b	-15	LYS	-	expression tag	UNP P24279
b	-14	ILE	-	expression tag	UNP P24279
b	-13	SER	-	expression tag	UNP P24279
b	-12	SER	-	expression tag	UNP P24279
b	-11	SER	-	expression tag	UNP P24279

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Chain	Residue	Modelled	Actual	Comment	Reference
b	-10	GLY	-	expression tag	UNP P24279
b	-9	ALA	-	expression tag	UNP P24279
b	-8	LEU	-	expression tag	UNP P24279
b	-7	GLU	-	expression tag	UNP P24279
b	-6	ASN	-	expression tag	UNP P24279
b	-5	LEU	-	expression tag	UNP P24279
b	-4	TYR	-	expression tag	UNP P24279
b	-3	PHE	-	expression tag	UNP P24279
b	-2	GLN	-	expression tag	UNP P24279
b	-1	GLY	-	expression tag	UNP P24279
b	0	GLU	-	expression tag	UNP P24279

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	672	Total	C	N	O	S	0	0
			5356	3357	926	1043	30		
3	c	672	Total	C	N	O	S	0	0
			5356	3357	926	1043	30		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	5	651	Total	C	N	O	S	0	0
			5097	3195	872	1005	25		
4	d	651	Total	C	N	O	S	0	0
			5097	3195	872	1005	25		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	6	637	Total	C	N	O	S	0	0
			5041	3174	879	963	25		
5	e	637	Total	C	N	O	S	0	0
			5041	3174	879	963	25		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	7	700	Total	C	N	O	S	0	0
			5513	3468	953	1060	32		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	700	Total	C	N	O	S	0	0
			5513	3468	953	1060	32		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	15	Total	C	N	O	S	0	0
			124	76	24	23	1		
7	I	15	Total	C	N	O	S	0	0
			124	76	24	23	1		

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	669	GLU	-	expression tag	UNP P53135
H	670	ASN	-	expression tag	UNP P53135
H	671	LEU	-	expression tag	UNP P53135
H	672	TYR	-	expression tag	UNP P53135
H	673	PHE	-	expression tag	UNP P53135
H	674	GLN	-	expression tag	UNP P53135
H	675	GLY	-	expression tag	UNP P53135
H	676	TRP	-	expression tag	UNP P53135
H	677	SER	-	expression tag	UNP P53135
H	678	HIS	-	expression tag	UNP P53135
H	679	PRO	-	expression tag	UNP P53135
H	680	GLN	-	expression tag	UNP P53135
H	681	PHE	-	expression tag	UNP P53135
H	682	GLU	-	expression tag	UNP P53135
H	683	LYS	-	expression tag	UNP P53135
H	684	GLY	-	expression tag	UNP P53135
H	685	GLY	-	expression tag	UNP P53135
H	686	GLY	-	expression tag	UNP P53135
H	687	SER	-	expression tag	UNP P53135
H	688	GLY	-	expression tag	UNP P53135
H	689	GLY	-	expression tag	UNP P53135
H	690	GLY	-	expression tag	UNP P53135
H	691	SER	-	expression tag	UNP P53135
H	692	GLY	-	expression tag	UNP P53135
H	693	GLY	-	expression tag	UNP P53135
H	694	SER	-	expression tag	UNP P53135
H	695	SER	-	expression tag	UNP P53135
H	696	ALA	-	expression tag	UNP P53135

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Chain	Residue	Modelled	Actual	Comment	Reference
H	697	TRP	-	expression tag	UNP P53135
H	698	SER	-	expression tag	UNP P53135
H	699	HIS	-	expression tag	UNP P53135
H	700	PRO	-	expression tag	UNP P53135
H	701	GLN	-	expression tag	UNP P53135
H	702	PHE	-	expression tag	UNP P53135
H	703	GLU	-	expression tag	UNP P53135
H	704	LYS	-	expression tag	UNP P53135
I	669	GLU	-	expression tag	UNP P53135
I	670	ASN	-	expression tag	UNP P53135
I	671	LEU	-	expression tag	UNP P53135
I	672	TYR	-	expression tag	UNP P53135
I	673	PHE	-	expression tag	UNP P53135
I	674	GLN	-	expression tag	UNP P53135
I	675	GLY	-	expression tag	UNP P53135
I	676	TRP	-	expression tag	UNP P53135
I	677	SER	-	expression tag	UNP P53135
I	678	HIS	-	expression tag	UNP P53135
I	679	PRO	-	expression tag	UNP P53135
I	680	GLN	-	expression tag	UNP P53135
I	681	PHE	-	expression tag	UNP P53135
I	682	GLU	-	expression tag	UNP P53135
I	683	LYS	-	expression tag	UNP P53135
I	684	GLY	-	expression tag	UNP P53135
I	685	GLY	-	expression tag	UNP P53135
I	686	GLY	-	expression tag	UNP P53135
I	687	SER	-	expression tag	UNP P53135
I	688	GLY	-	expression tag	UNP P53135
I	689	GLY	-	expression tag	UNP P53135
I	690	GLY	-	expression tag	UNP P53135
I	691	SER	-	expression tag	UNP P53135
I	692	GLY	-	expression tag	UNP P53135
I	693	GLY	-	expression tag	UNP P53135
I	694	SER	-	expression tag	UNP P53135
I	695	SER	-	expression tag	UNP P53135
I	696	ALA	-	expression tag	UNP P53135
I	697	TRP	-	expression tag	UNP P53135
I	698	SER	-	expression tag	UNP P53135
I	699	HIS	-	expression tag	UNP P53135
I	700	PRO	-	expression tag	UNP P53135
I	701	GLN	-	expression tag	UNP P53135
I	702	PHE	-	expression tag	UNP P53135

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Chain	Residue	Modelled	Actual	Comment	Reference
I	703	GLU	-	expression tag	UNP P53135
I	704	LYS	-	expression tag	UNP P53135

- Molecule 8 is a DNA chain called DNA (53-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	X	53	Total	C	N	O	P	0	0
			1086	515	199	319	53		

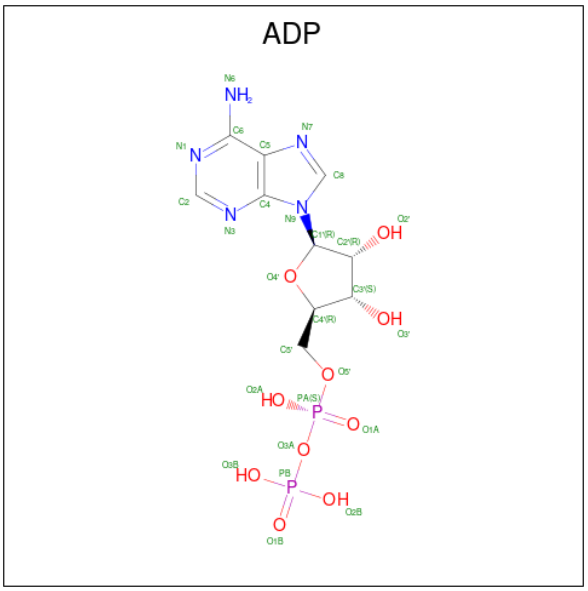
- Molecule 9 is a DNA chain called DNA (53-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Y	53	Total	C	N	O	P	0	0
			1087	515	202	317	53		

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

Mol	Chain	Residues	Atoms		AltConf
10	2	1	Total	Zn	0
			1	1	
10	4	1	Total	Zn	0
			1	1	
10	5	1	Total	Zn	0
			1	1	
10	6	1	Total	Zn	0
			1	1	
10	7	1	Total	Zn	0
			1	1	
10	a	1	Total	Zn	0
			1	1	
10	c	1	Total	Zn	0
			1	1	
10	d	1	Total	Zn	0
			1	1	
10	e	1	Total	Zn	0
			1	1	
10	f	1	Total	Zn	0
			1	1	

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



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

- Molecule 12 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

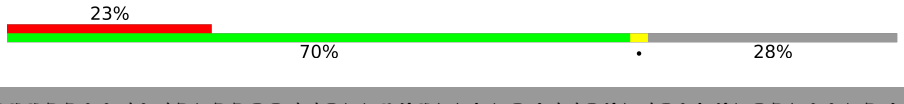
Mol	Chain	Residues	Atoms		AltConf
12	3	1	Total	Mg	0
			1	1	
12	5	1	Total	Mg	0
			1	1	
12	b	1	Total	Mg	0
			1	1	
12	d	1	Total	Mg	0
			1	1	

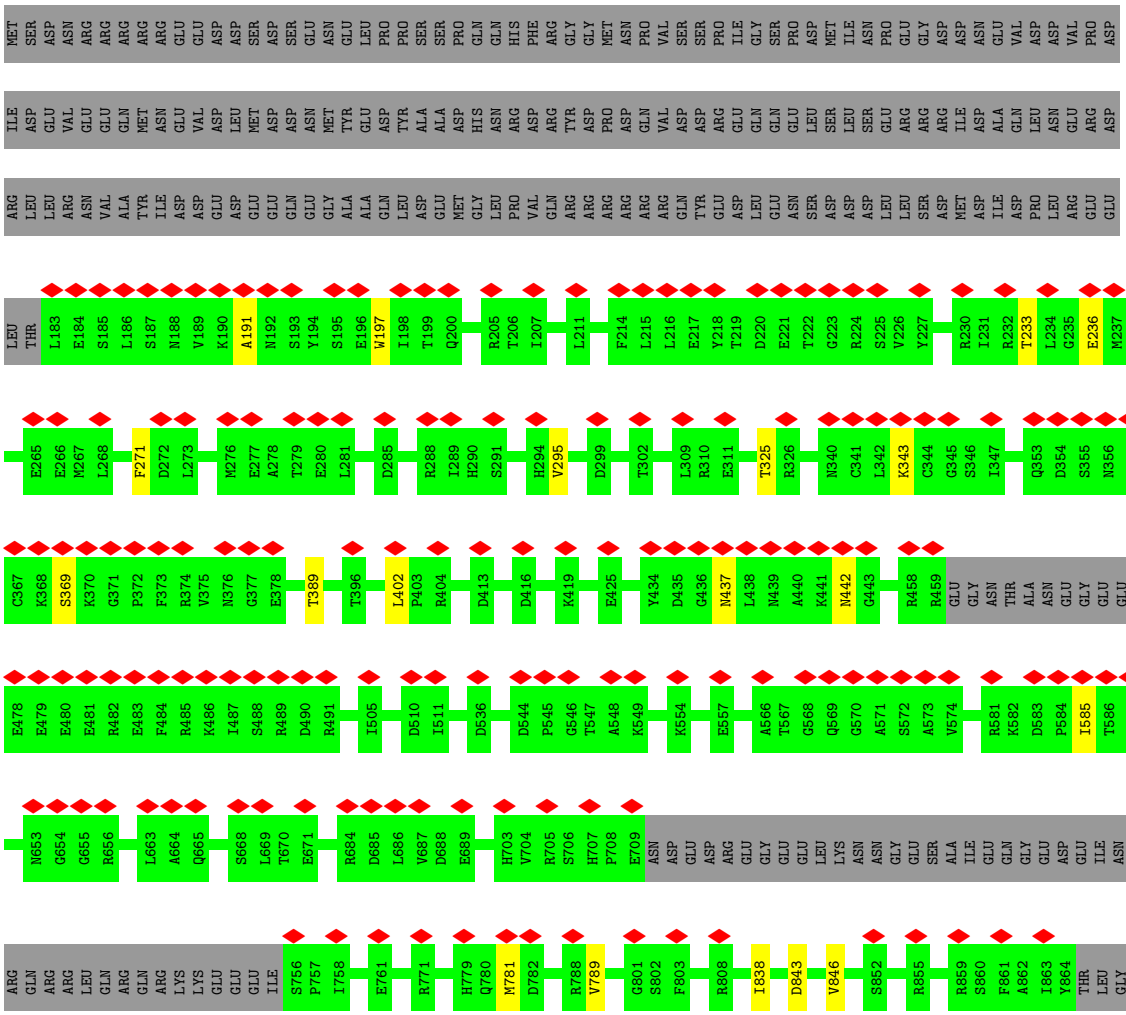
3 Residue-property plots (i)

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:

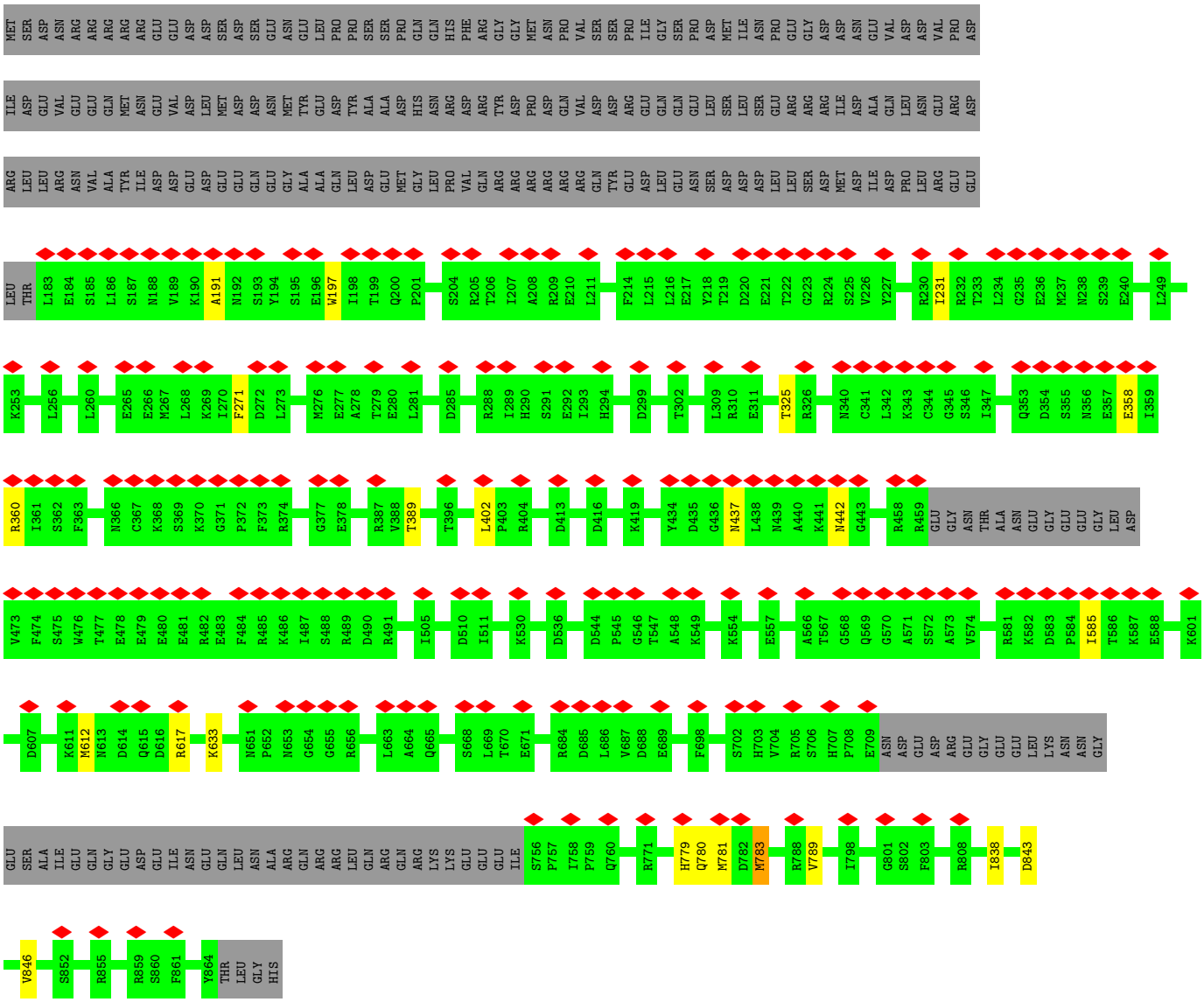




• Molecule 1: DNA replication licensing factor MCM2

Chain a:

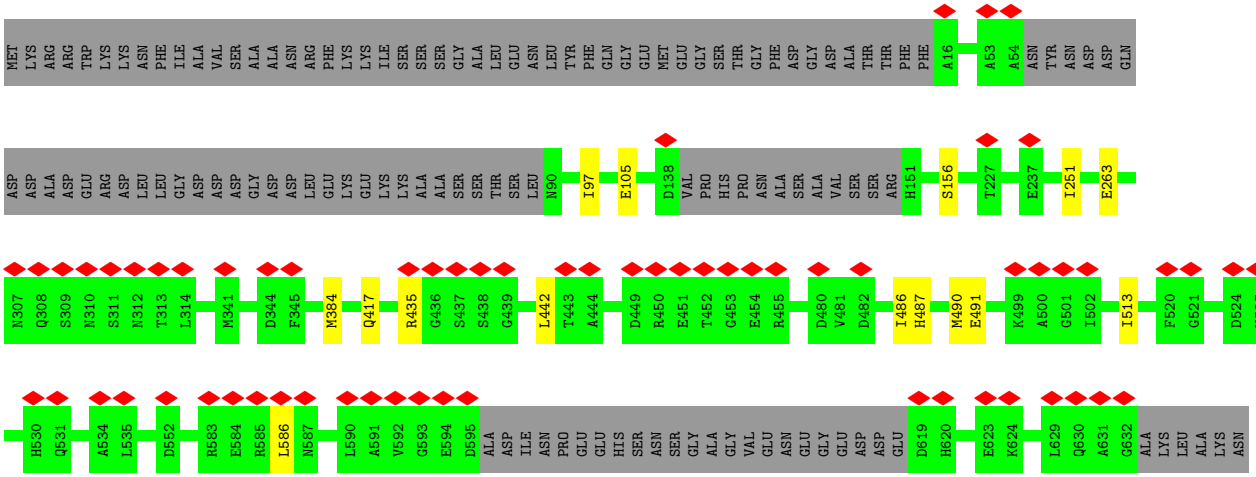


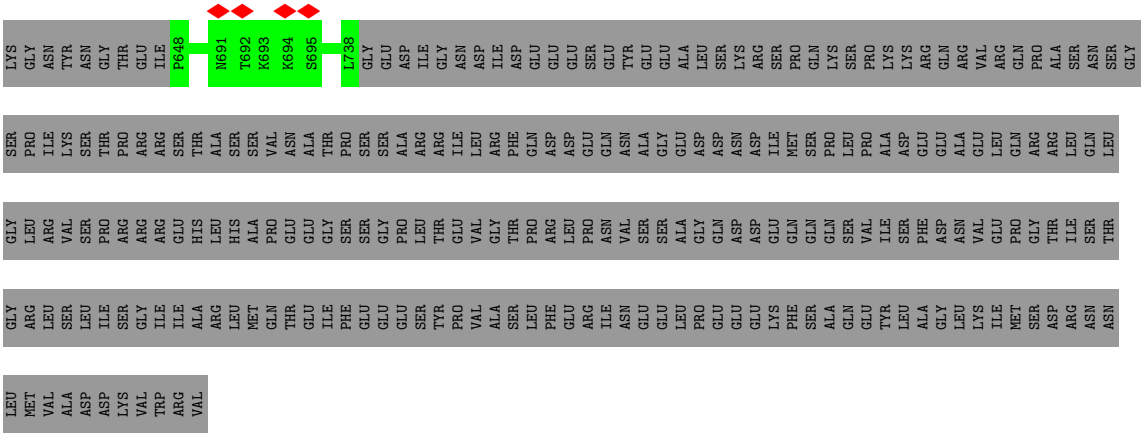


• Molecule 2: DNA replication licensing factor MCM3

Chain 3:



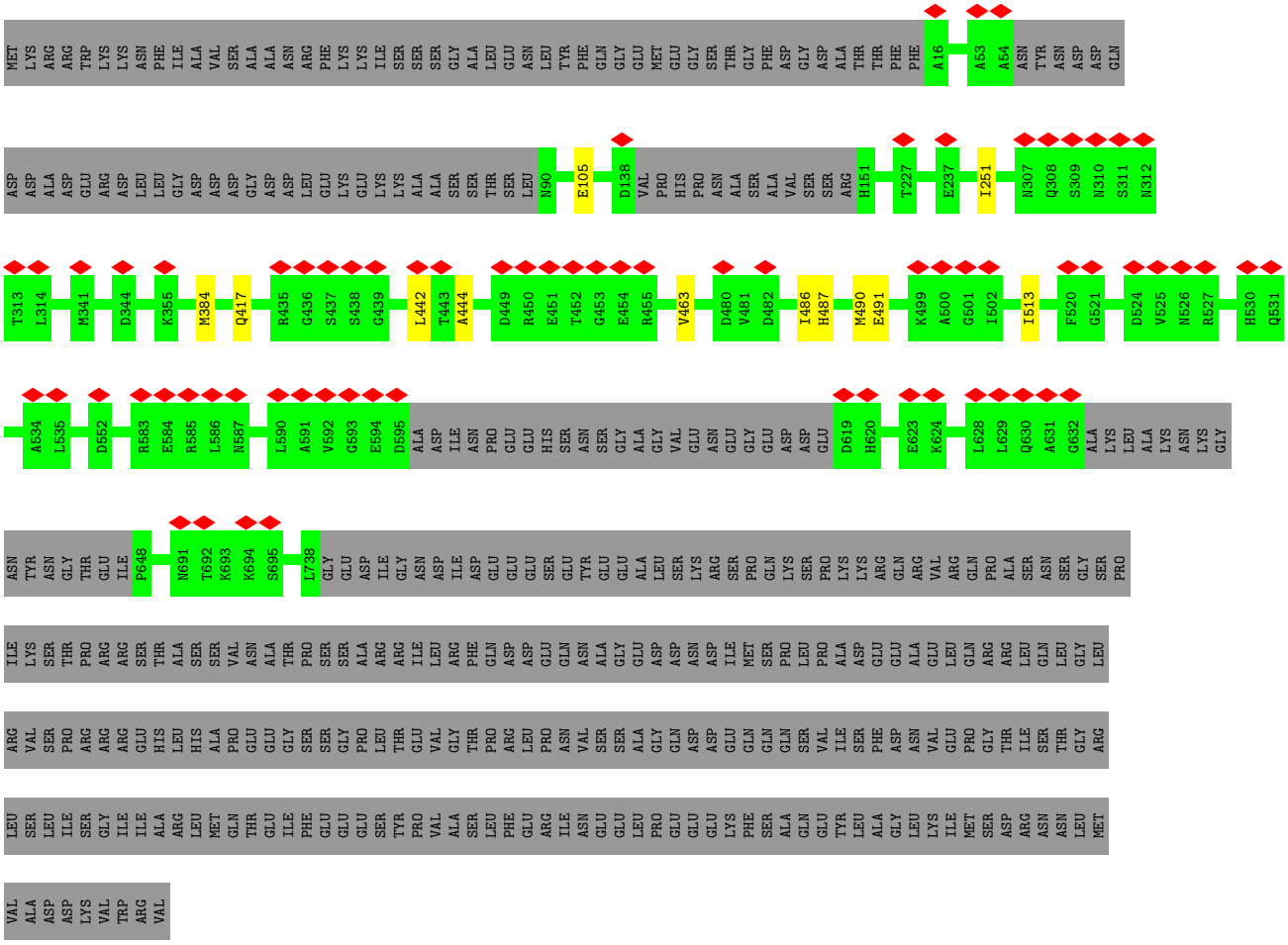




• Molecule 2: DNA replication licensing factor MCM3

Chain b:

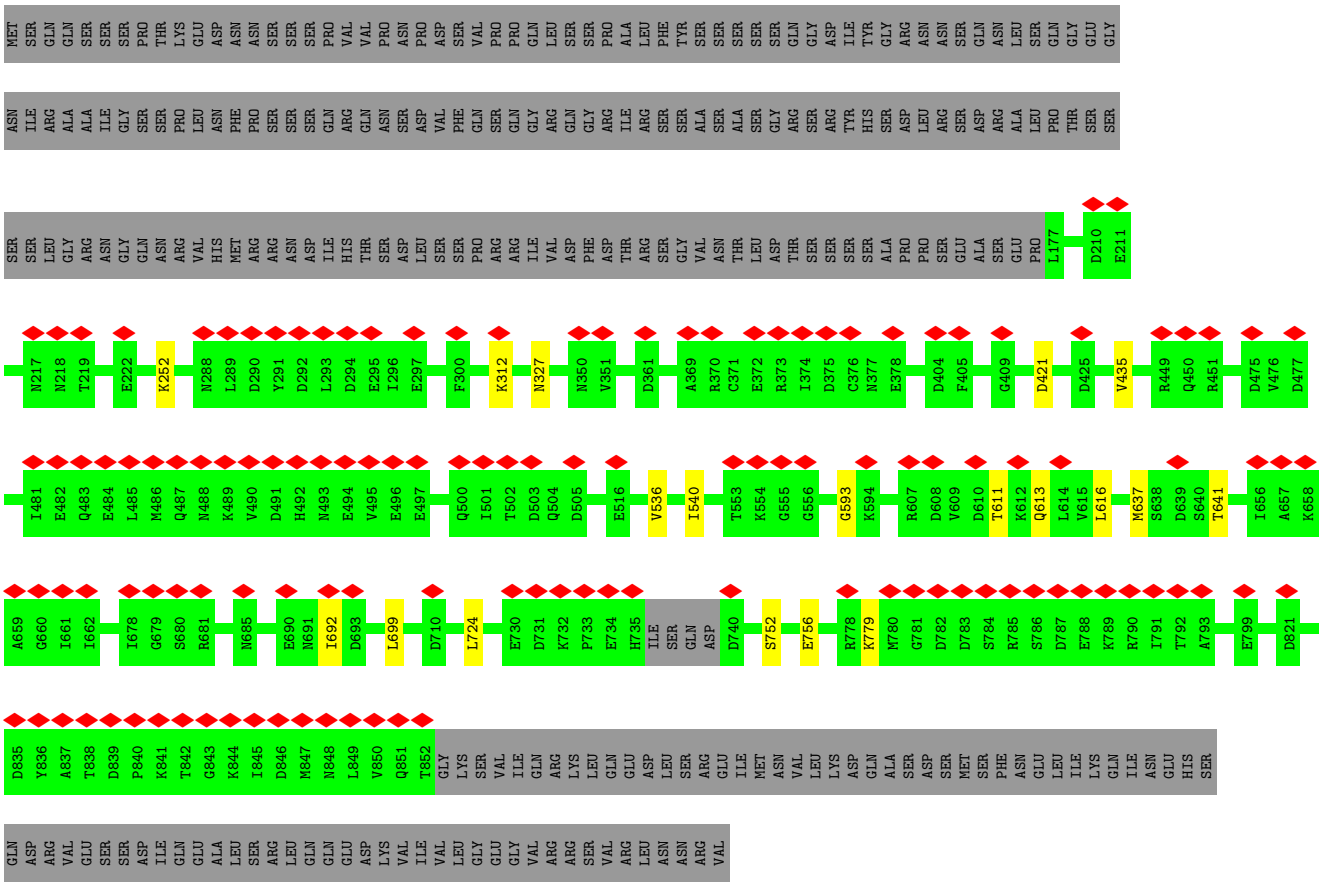




• Molecule 3: DNA replication licensing factor MCM4

Chain 4:

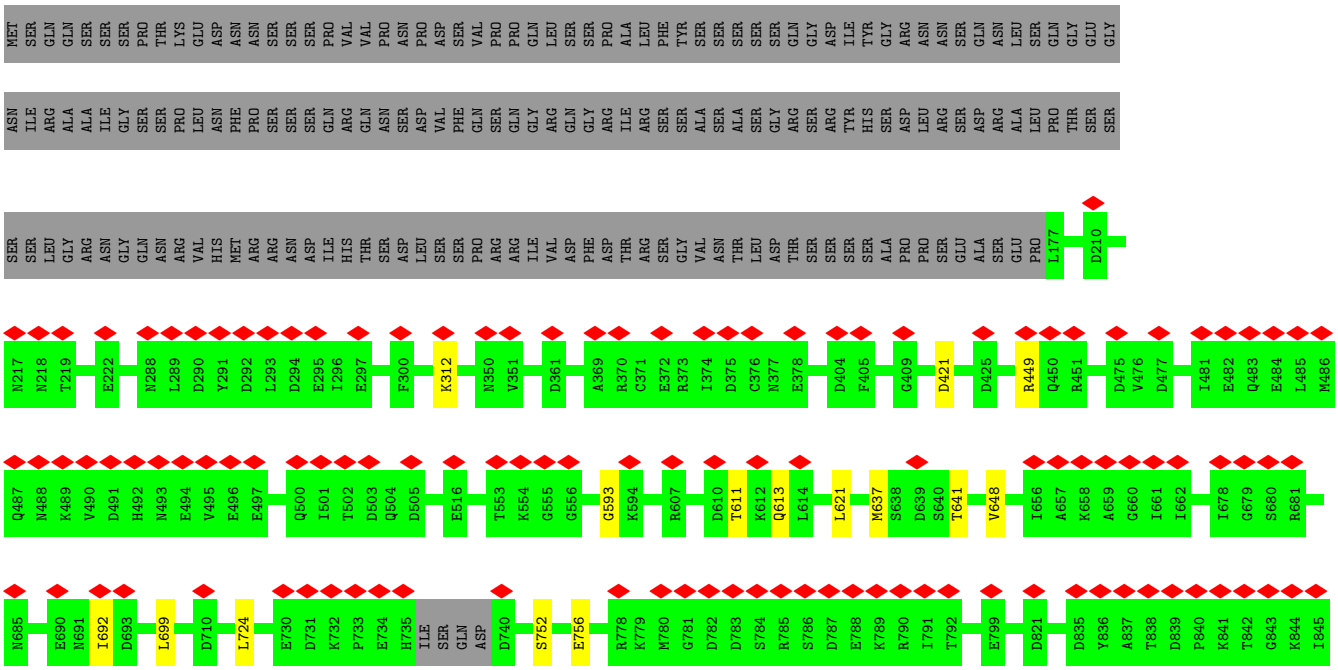


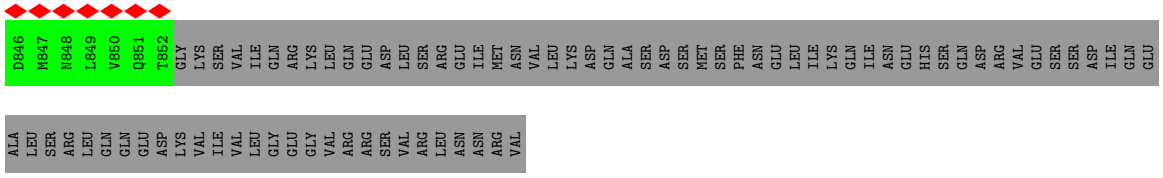


• Molecule 3: DNA replication licensing factor MCM4

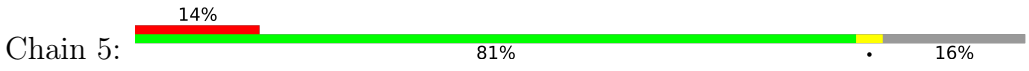
Chain c:

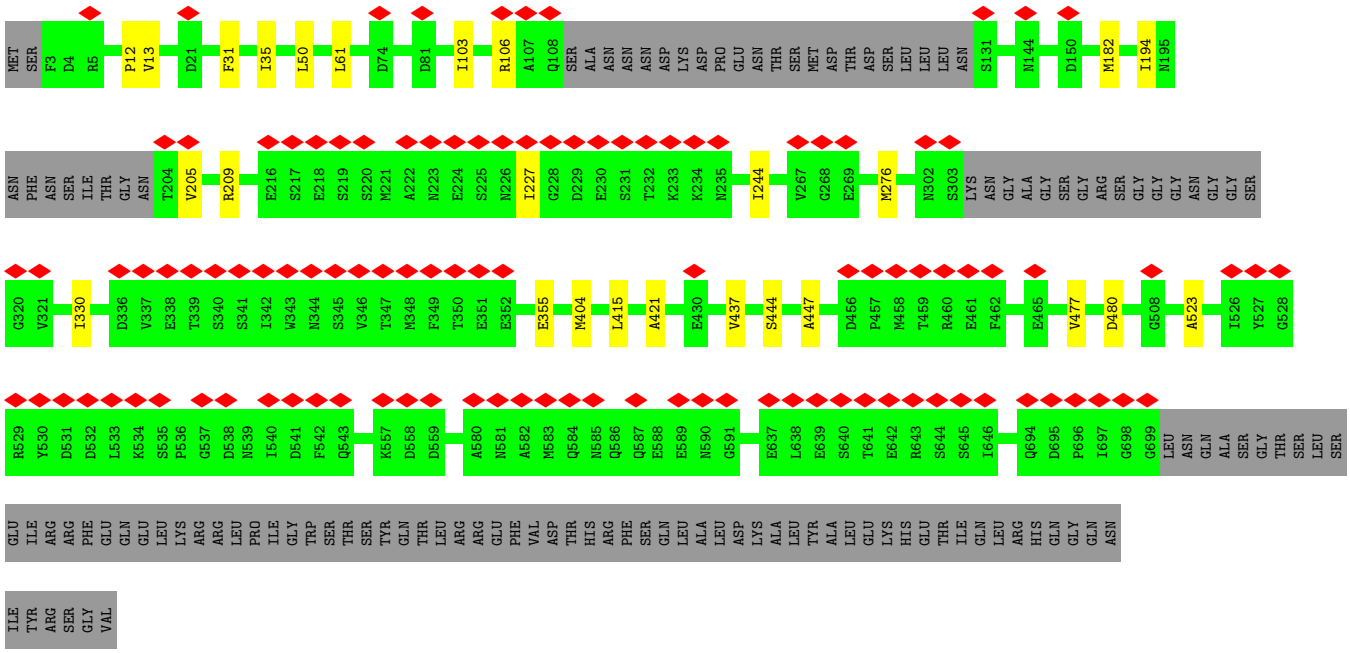




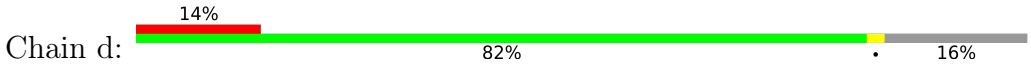


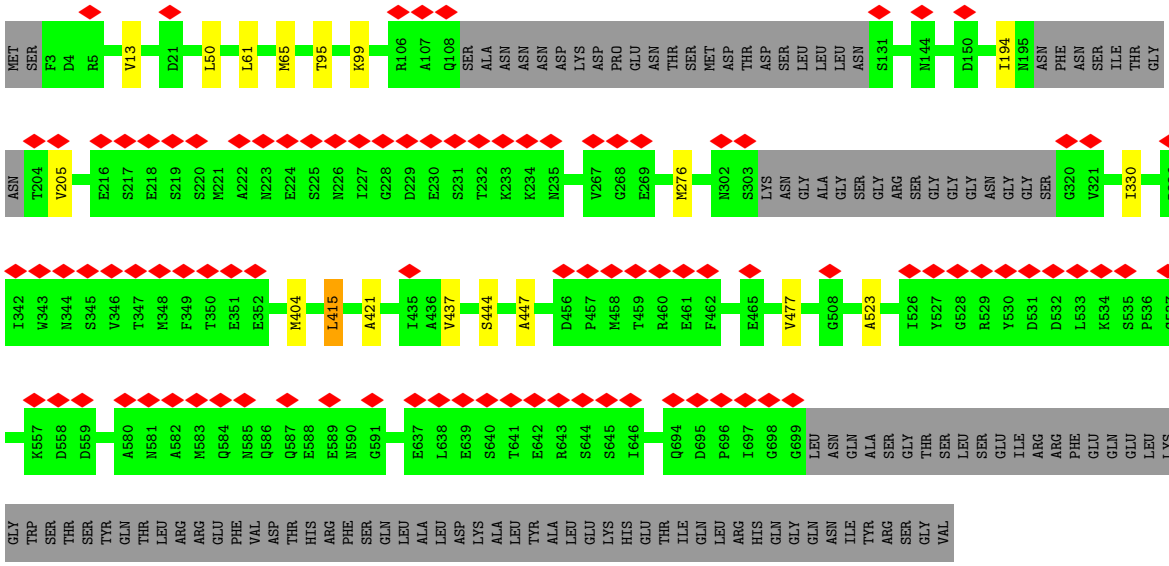
• Molecule 4: Minichromosome maintenance protein 5





• Molecule 4: Minichromosome maintenance protein 5

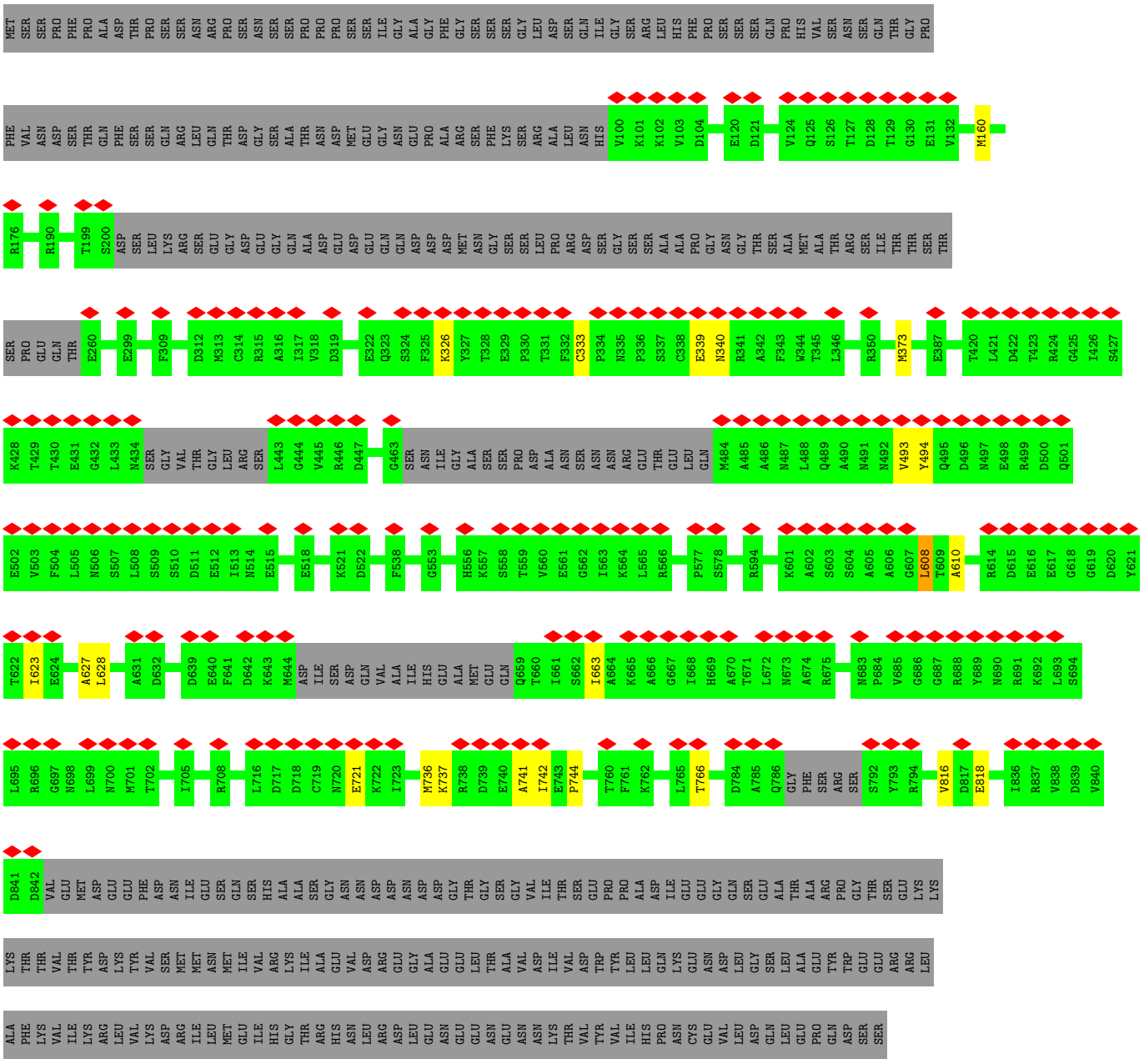




• Molecule 5: DNA replication licensing factor MCM6

Chain 6:

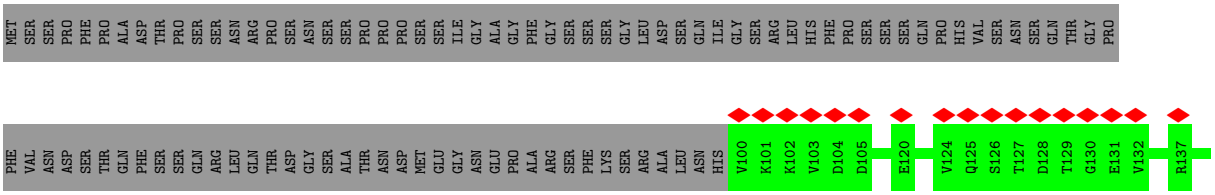


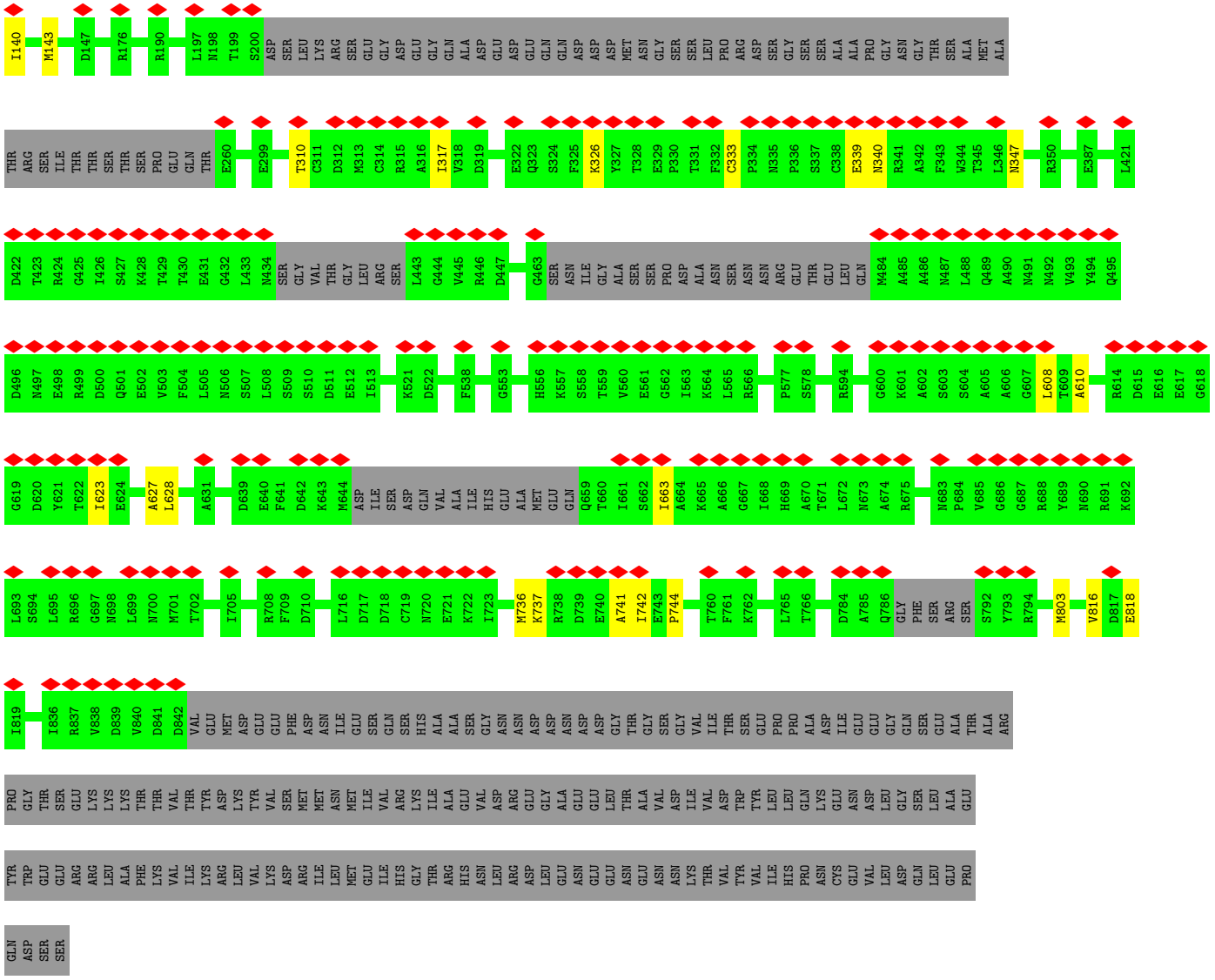


• Molecule 5: DNA replication licensing factor MCM6

Chain e:



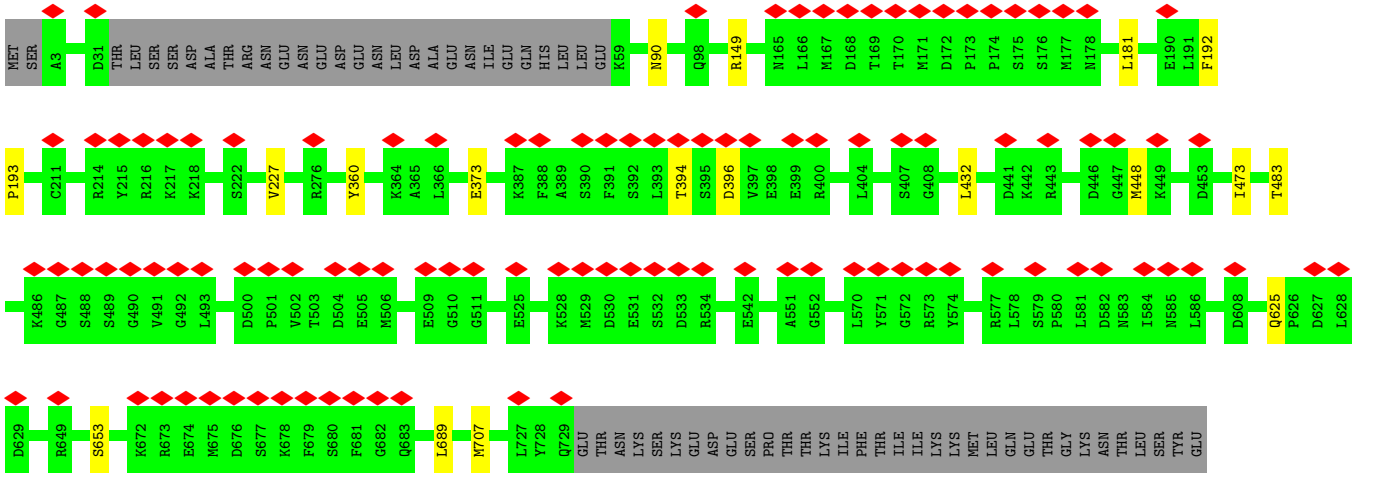


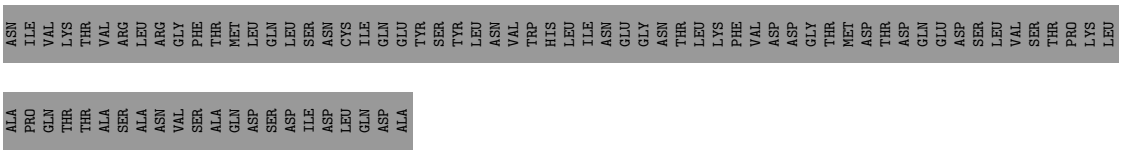


• Molecule 6: DNA replication licensing factor MCM7

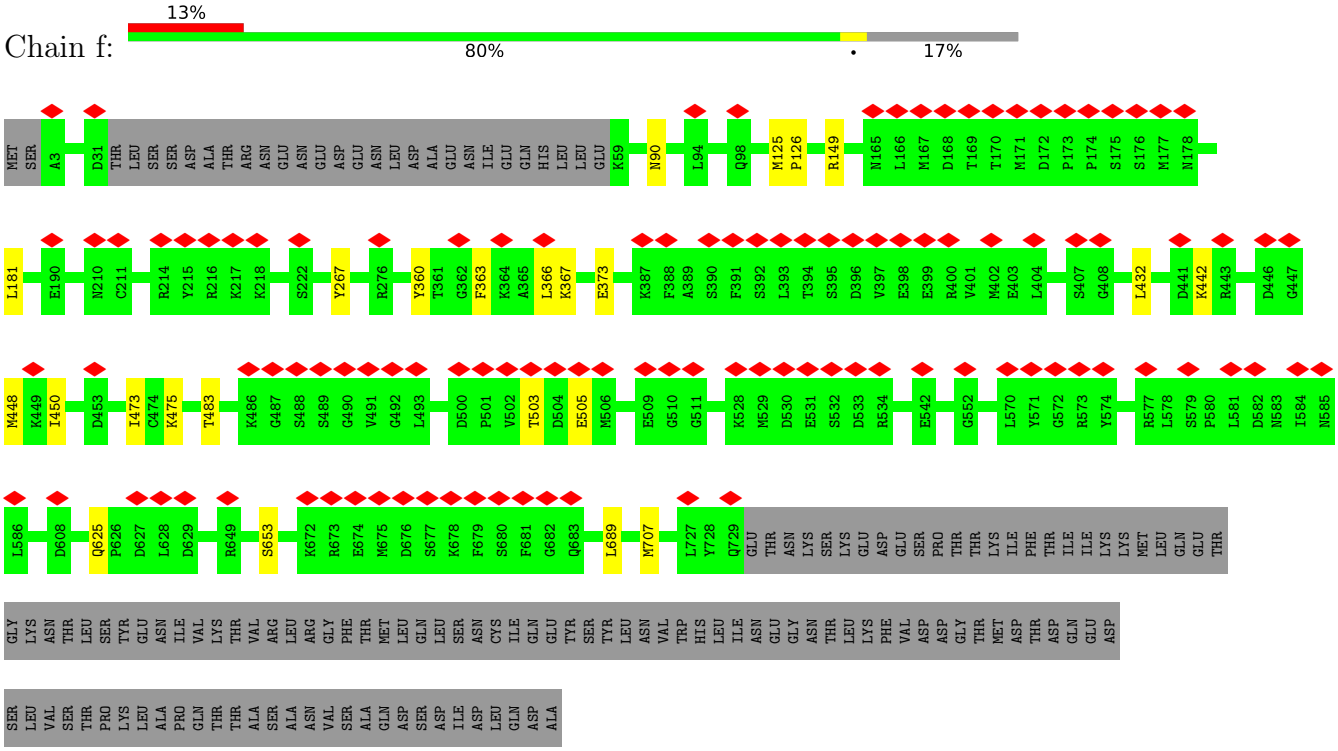
Chain 7:



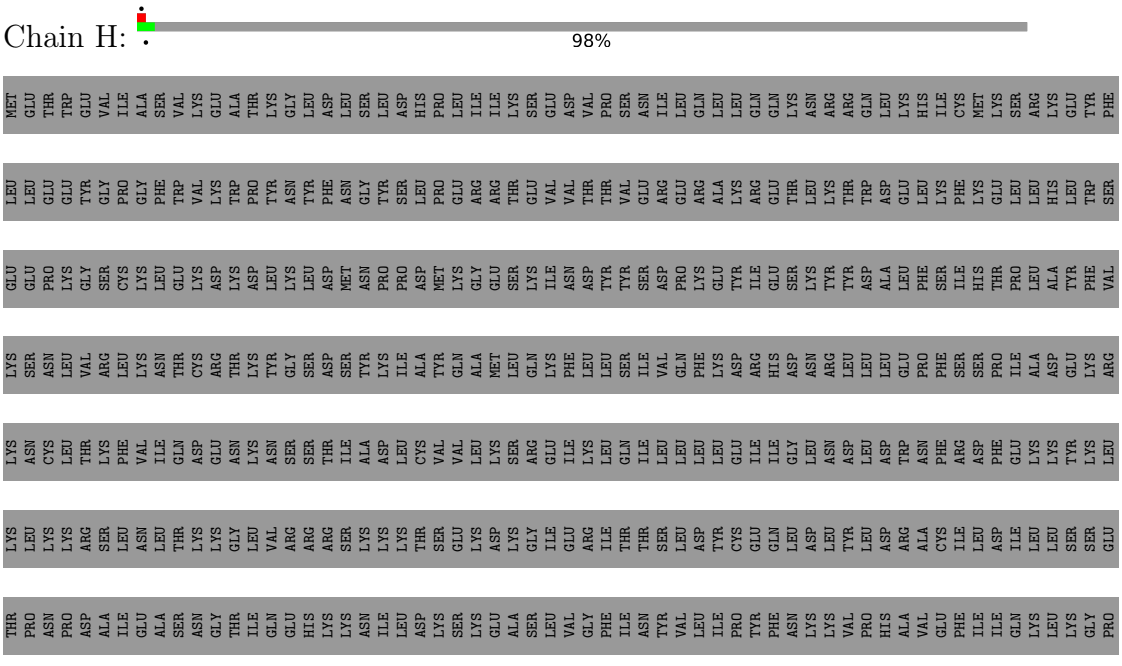


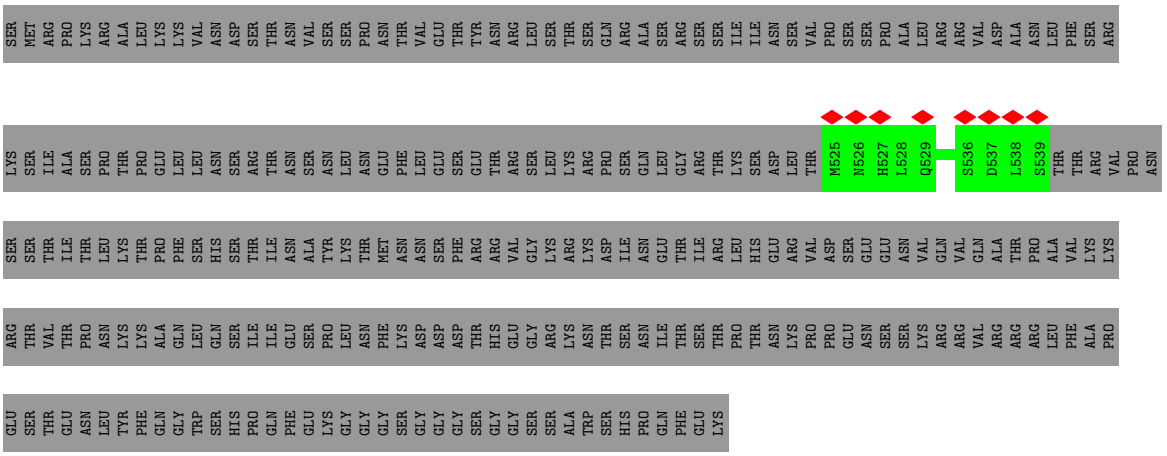


• Molecule 6: DNA replication licensing factor MCM7



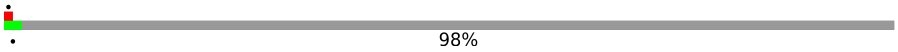
• Molecule 7: DNA replication regulator SLD3

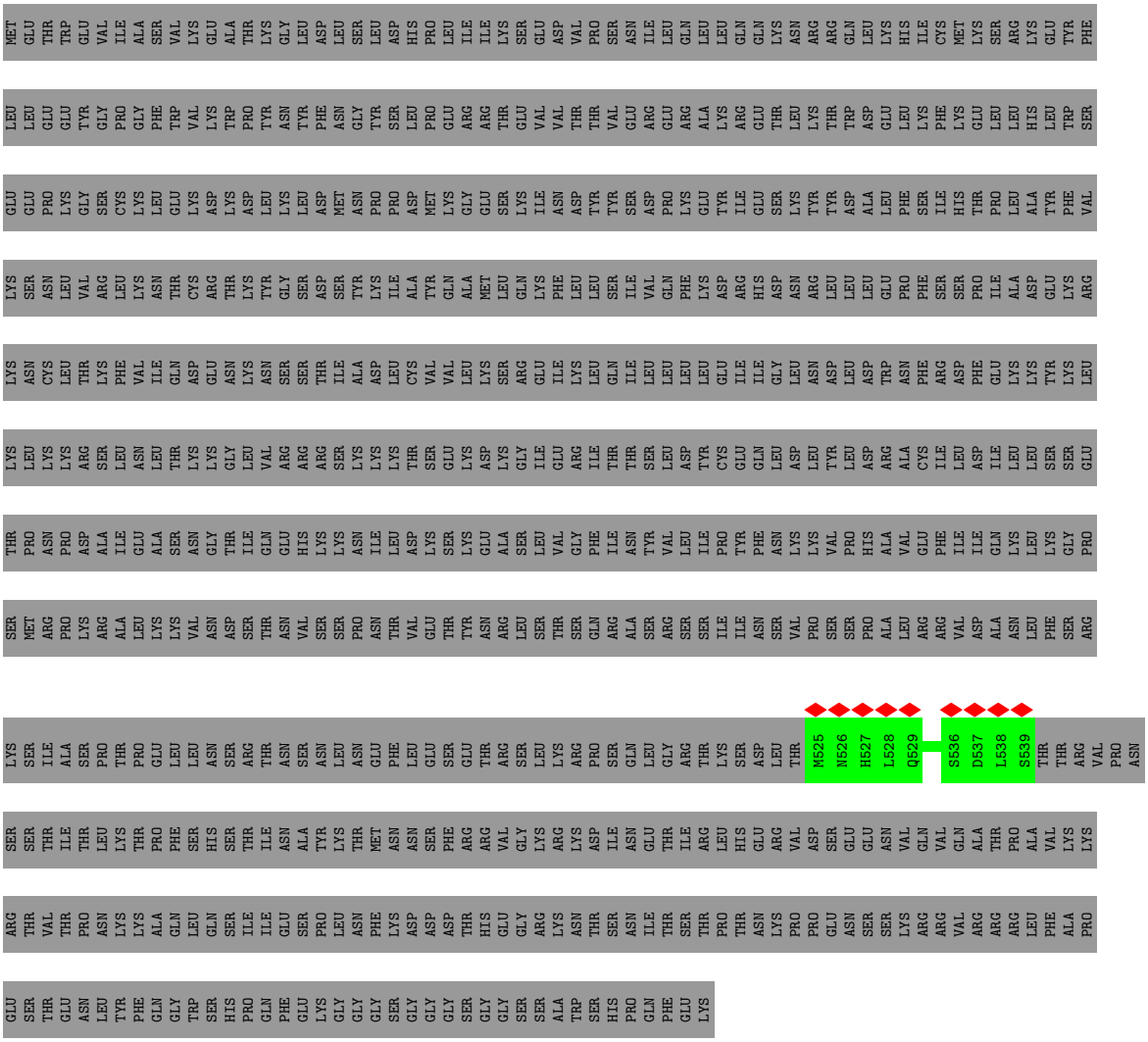




• Molecule 7: DNA replication regulator SLD3

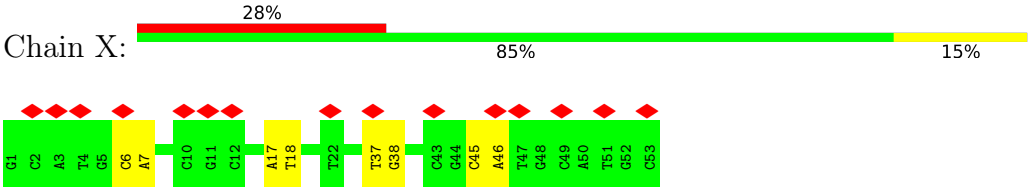
Chain I:





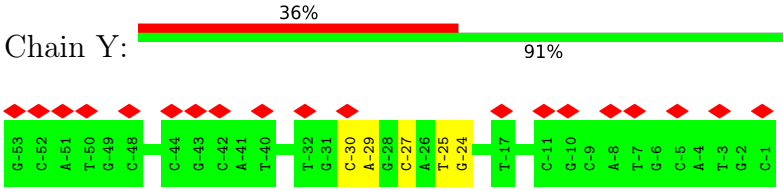
• Molecule 8: DNA (53-MER)

Chain X:



• Molecule 9: DNA (53-MER)

Chain Y:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	359025	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 ($e^-/Å^2$)	49.8	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.737	Depositor
Minimum map value	-0.273	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.17	Depositor
Map size (Å)	483.84003, 483.84003, 483.84003	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, 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	0.30	0/5019	0.66	0/6781
1	a	0.29	0/5019	0.65	0/6781
2	3	0.27	0/5081	0.58	0/6889
2	b	0.27	0/5081	0.59	0/6889
3	4	0.27	0/5434	0.62	2/7345 (0.0%)
3	c	0.28	0/5434	0.63	2/7345 (0.0%)
4	5	0.29	0/5170	0.64	1/6992 (0.0%)
4	d	0.29	0/5170	0.63	0/6992
5	6	0.28	0/5119	0.62	2/6906 (0.0%)
5	e	0.29	0/5119	0.63	2/6906 (0.0%)
6	7	0.27	0/5599	0.61	1/7569 (0.0%)
6	f	0.27	0/5599	0.60	1/7569 (0.0%)
7	H	0.27	0/125	0.72	0/165
7	I	0.26	0/125	0.71	0/165
8	X	0.21	0/1217	0.46	0/1876
9	Y	0.23	0/1219	0.48	0/1879
All	All	0.28	0/65530	0.62	11/89049 (0.0%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	e	339	GLU	CA-CB-CG	7.32	128.74	114.10
5	6	339	GLU	CA-CB-CG	6.61	127.32	114.10
5	6	339	GLU	CB-CA-C	6.41	121.56	112.07
5	e	339	GLU	CB-CA-C	6.02	120.98	112.07
3	4	312	LYS	CB-CG-CD	5.23	123.33	111.30
3	c	421	ASP	CB-CA-C	-5.23	110.12	117.23
3	c	312	LYS	CB-CG-CD	5.22	123.31	111.30
3	4	421	ASP	CB-CA-C	-5.19	110.17	117.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	7	625	GLN	CA-CB-CG	5.14	124.37	114.10
6	f	625	GLN	CA-CB-CG	5.08	124.27	114.10
4	5	355	GLU	CA-CB-CG	5.06	124.22	114.10

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	4932	0	4985	10	0
1	a	4932	0	4985	11	0
2	3	4994	0	5059	8	0
2	b	4994	0	5059	6	0
3	4	5356	0	5410	11	0
3	c	5356	0	5410	8	0
4	5	5097	0	5143	15	0
4	d	5097	0	5143	10	0
5	6	5041	0	5065	15	0
5	e	5041	0	5065	13	0
6	7	5513	0	5575	7	0
6	f	5513	0	5575	12	0
7	H	124	0	122	0	0
7	I	124	0	122	0	0
8	X	1086	0	596	4	0
9	Y	1087	0	595	3	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	a	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	3	27	0	12	0	0
11	5	27	0	12	1	0
11	b	27	0	12	0	0
11	d	27	0	12	1	0
12	3	1	0	0	0	0
12	5	1	0	0	0	0
12	b	1	0	0	0	0
12	d	1	0	0	0	0
All	All	64409	0	63957	118	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 1.

All (118) 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)
3:4:616:LEU:HB3	5:6:373:MET:HE3	1.77	0.64
4:5:209:ARG:HH22	9:Y:-27:DC:H4'	1.62	0.63
4:d:194:ILE:HG12	4:d:205:VAL:HG21	1.84	0.59
5:e:608:LEU:HD13	5:e:627:ALA:HB3	1.85	0.59
4:5:194:ILE:HG12	4:5:205:VAL:HG21	1.84	0.58
5:e:816:VAL:HG12	5:e:818:GLU:H	1.68	0.58
5:6:816:VAL:HG12	5:6:818:GLU:H	1.68	0.58
1:2:442:ASN:HA	5:6:326:LYS:HE2	1.85	0.58
5:6:608:LEU:HD13	5:6:627:ALA:HB3	1.86	0.58
4:d:444:SER:HB2	4:d:447:ALA:HB3	1.87	0.57
4:5:444:SER:HB2	4:5:447:ALA:HB3	1.87	0.57
1:a:789:VAL:HG21	1:a:838:ILE:HD13	1.87	0.56
5:6:608:LEU:HD12	5:6:628:LEU:HG	1.88	0.56
1:2:789:VAL:HG21	1:2:838:ILE:HD13	1.88	0.56
2:3:417:GLN:HB3	4:5:404:MET:HE1	1.90	0.54
2:3:486:ILE:HG22	2:3:490:MET:HE2	1.90	0.54
6:7:653:SER:HB3	6:7:707:MET:HE1	1.88	0.54
2:b:417:GLN:HB3	4:d:404:MET:HE1	1.91	0.53
4:5:182:MET:HE3	4:5:244:ILE:HD11	1.90	0.53
6:7:149:ARG:HE	4:d:13:VAL:HA	1.72	0.53
5:e:608:LEU:HD12	5:e:628:LEU:HG	1.91	0.53
6:f:653:SER:HB3	6:f:707:MET:HE1	1.91	0.52
1:a:442:ASN:HA	5:e:326:LYS:HE2	1.92	0.52
5:6:737:LYS:HB2	5:6:741:ALA:HB2	1.92	0.52
1:a:402:LEU:HD23	5:e:623:ILE:HG13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:402:LEU:HD23	5:6:623:ILE:HG13	1.92	0.51
3:4:692:ILE:HG21	3:4:699:LEU:HD21	1.93	0.51
3:c:692:ILE:HG21	3:c:699:LEU:HD21	1.93	0.51
2:b:486:ILE:HG22	2:b:490:MET:HE2	1.93	0.51
5:e:737:LYS:HB2	5:e:741:ALA:HB2	1.92	0.50
5:6:736:MET:HG2	5:6:737:LYS:HG3	1.93	0.50
6:f:360:TYR:HA	6:f:373:GLU:HG2	1.93	0.50
6:7:360:TYR:HA	6:7:373:GLU:HG2	1.93	0.50
5:e:736:MET:HG2	5:e:737:LYS:HG3	1.93	0.50
6:f:125:MET:HE3	6:f:126:PRO:HD2	1.94	0.49
8:X:6:DC:H2"	8:X:7:DA:C8	2.48	0.49
5:e:333:CYS:HB2	5:e:340:ASN:HB3	1.95	0.49
5:6:333:CYS:HB2	5:6:340:ASN:HB3	1.95	0.48
2:b:444:ALA:HB1	2:b:463:VAL:HG12	1.95	0.48
3:c:593:GLY:HA2	3:c:637:MET:HE3	1.95	0.48
3:4:593:GLY:HA2	3:4:637:MET:HE3	1.95	0.48
6:f:503:THR:HG22	6:f:505:GLU:HG2	1.95	0.48
8:X:37:DT:H2"	8:X:38:DG:C8	2.49	0.47
6:f:363:PHE:HB2	6:f:366:LEU:HD23	1.96	0.47
3:c:621:LEU:HD13	3:c:648:VAL:HG21	1.97	0.47
1:a:780:GLN:O	1:a:783:MET:HB3	2.14	0.47
4:d:415:LEU:HD12	4:d:523:ALA:HB3	1.95	0.47
2:b:384:MET:HE1	2:b:513:ILE:HB	1.97	0.47
1:2:343:LYS:HE3	1:2:369:SER:HB3	1.97	0.46
4:d:437:VAL:HG23	4:d:477:VAL:HG23	1.97	0.46
2:3:384:MET:HE1	2:3:513:ILE:HB	1.97	0.46
3:4:611:THR:HG22	3:4:613:GLN:H	1.80	0.46
3:4:752:SER:O	3:4:756:GLU:HG2	2.16	0.46
2:b:442:LEU:HD23	2:b:442:LEU:HA	1.86	0.46
2:3:263:GLU:HG3	2:3:586:LEU:HD11	1.97	0.45
3:c:611:THR:HG22	3:c:613:GLN:H	1.81	0.45
1:2:191:ALA:HB3	1:2:197:TRP:HB2	1.98	0.45
3:c:752:SER:O	3:c:756:GLU:HG2	2.16	0.45
1:a:633:LYS:HB3	1:a:633:LYS:HE2	1.73	0.45
1:2:233:THR:HA	1:2:236:GLU:HG2	1.98	0.45
5:e:803:MET:HE3	5:e:803:MET:HB2	1.86	0.45
3:4:779:LYS:HD3	3:4:779:LYS:HA	1.81	0.45
1:2:271:PHE:HD1	1:2:295:VAL:HG21	1.81	0.45
1:2:325:THR:HB	1:2:389:THR:HG23	1.99	0.45
3:c:724:LEU:HD12	6:f:689:LEU:HD23	1.99	0.44
9:Y:-25:DT:H2"	9:Y:-24:DG:C8	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:191:ALA:HB3	1:a:197:TRP:HB2	1.99	0.44
6:f:432:LEU:HB3	6:f:473:ILE:HD11	1.98	0.44
1:2:781:MET:H	1:2:781:MET:HG2	1.61	0.44
3:4:327:ASN:HA	3:4:435:VAL:O	2.18	0.44
6:7:432:LEU:HB3	6:7:473:ILE:HD11	1.99	0.44
3:c:637:MET:HG3	3:c:641:THR:HB	2.00	0.44
5:e:742:ILE:HG23	5:e:744:PRO:HD3	2.00	0.44
1:a:612:MET:HE3	1:a:617:ARG:HG2	2.00	0.44
9:Y:-30:DC:H2"	9:Y:-29:DA:C8	2.52	0.44
4:5:437:VAL:HG23	4:5:477:VAL:HG23	1.99	0.43
1:a:325:THR:HB	1:a:389:THR:HG23	2.00	0.43
3:4:779:LYS:HE2	5:6:721:GLU:HB3	2.01	0.43
3:4:724:LEU:HD12	6:7:689:LEU:HD23	1.99	0.43
1:a:358:GLU:HB3	1:a:360:ARG:HH12	1.83	0.43
8:X:45:DC:H2"	8:X:46:DA:C8	2.54	0.43
3:4:637:MET:HG3	3:4:641:THR:HB	2.01	0.43
5:e:610:ALA:HB3	5:e:663:ILE:HD11	2.01	0.43
5:6:160:MET:HE3	5:6:160:MET:HB3	1.93	0.43
5:6:742:ILE:HG23	5:6:744:PRO:HD3	2.00	0.43
6:7:394:THR:HG22	6:7:396:ASP:H	1.84	0.43
1:2:843:ASP:HA	1:2:846:VAL:HG12	2.02	0.42
4:5:103:ILE:HD13	4:5:106:ARG:HH21	1.84	0.42
4:d:95:THR:O	4:d:99:LYS:HG2	2.19	0.42
1:a:779:HIS:HB3	1:a:781:MET:HE3	2.01	0.42
1:a:843:ASP:HA	1:a:846:VAL:HG12	2.01	0.42
2:b:487:HIS:O	2:b:491:GLU:HG2	2.19	0.42
5:e:310:THR:HG22	5:e:317:ILE:HG12	2.01	0.42
5:6:326:LYS:HA	5:6:326:LYS:HD2	1.88	0.42
4:d:276:MET:HE3	4:d:330:ILE:HD11	2.02	0.42
6:f:442:LYS:HB3	6:f:450:ILE:HB	2.02	0.42
3:c:449:ARG:H	3:c:449:ARG:HG2	1.76	0.42
4:d:50:LEU:HD13	4:d:61:LEU:HD12	2.01	0.42
4:5:421:ALA:HB2	11:5:801:ADP:C8	2.55	0.42
2:3:435:ARG:HD2	2:3:435:ARG:HA	1.83	0.42
4:5:276:MET:HE3	4:5:330:ILE:HD11	2.02	0.42
5:6:610:ALA:HB3	5:6:663:ILE:HD11	2.01	0.41
4:5:50:LEU:HD13	4:5:61:LEU:HD12	2.03	0.41
4:d:421:ALA:HB2	11:d:801:ADP:C8	2.55	0.41
2:3:97:ILE:HG12	2:3:156:SER:HB2	2.02	0.41
2:3:487:HIS:O	2:3:491:GLU:HG2	2.20	0.41
5:6:493:VAL:HG23	5:6:494:TYR:HD2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:e:140:ILE:HA	5:e:143:MET:HG3	2.01	0.41
4:5:415:LEU:HD12	4:5:523:ALA:HB3	2.02	0.41
4:5:12:PRO:HB3	6:f:267:TYR:CZ	2.56	0.41
4:5:13:VAL:HA	6:f:149:ARG:HE	1.85	0.41
6:f:475:LYS:HE3	6:f:475:LYS:HB2	1.95	0.40
8:X:17:DA:H2"	8:X:18:DT:H5"	2.03	0.40
4:5:31:PHE:O	4:5:35:ILE:HG13	2.21	0.40
2:3:442:LEU:HD23	2:3:442:LEU:HA	1.87	0.40
3:4:536:VAL:O	3:4:540:ILE:HG12	2.22	0.40
4:5:227:ILE:HD11	6:f:367:LYS:HE2	2.03	0.40
6:7:192:PHE:HA	6:7:193:PRO:HD3	1.97	0.40

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	617/868 (71%)	610 (99%)	7 (1%)	0	100	100
1	a	617/868 (71%)	610 (99%)	7 (1%)	0	100	100
2	3	628/1006 (62%)	621 (99%)	7 (1%)	0	100	100
2	b	628/1006 (62%)	619 (99%)	9 (1%)	0	100	100
3	4	668/933 (72%)	657 (98%)	11 (2%)	0	100	100
3	c	668/933 (72%)	658 (98%)	10 (2%)	0	100	100
4	5	643/775 (83%)	632 (98%)	11 (2%)	0	100	100
4	d	643/775 (83%)	632 (98%)	11 (2%)	0	100	100
5	6	625/1017 (62%)	614 (98%)	11 (2%)	0	100	100
5	e	625/1017 (62%)	613 (98%)	12 (2%)	0	100	100
6	7	696/845 (82%)	688 (99%)	8 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	f	696/845 (82%)	688 (99%)	8 (1%)	0	100	100
7	H	13/704 (2%)	13 (100%)	0	0	100	100
7	I	13/704 (2%)	13 (100%)	0	0	100	100
All	All	7780/12296 (63%)	7668 (99%)	112 (1%)	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	547/770 (71%)	545 (100%)	2 (0%)	84	86
1	a	547/770 (71%)	542 (99%)	5 (1%)	70	80
2	3	550/864 (64%)	548 (100%)	2 (0%)	84	86
2	b	550/864 (64%)	548 (100%)	2 (0%)	84	86
3	4	611/848 (72%)	610 (100%)	1 (0%)	87	89
3	c	611/848 (72%)	611 (100%)	0	100	100
4	5	583/688 (85%)	582 (100%)	1 (0%)	87	89
4	d	583/688 (85%)	580 (100%)	3 (0%)	81	85
5	6	557/886 (63%)	555 (100%)	2 (0%)	84	86
5	e	557/886 (63%)	556 (100%)	1 (0%)	87	89
6	7	619/753 (82%)	614 (99%)	5 (1%)	73	81
6	f	619/753 (82%)	615 (99%)	4 (1%)	78	83
7	H	15/654 (2%)	15 (100%)	0	100	100
7	I	15/654 (2%)	15 (100%)	0	100	100
All	All	6964/10926 (64%)	6936 (100%)	28 (0%)	81	86

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	2	437	ASN
1	2	585	ILE
2	3	105	GLU
2	3	251	ILE
3	4	252	LYS
4	5	480	ASP
5	6	608	LEU
5	6	766	THR
6	7	90	ASN
6	7	181	LEU
6	7	227	VAL
6	7	448	MET
6	7	483	THR
1	a	231	ILE
1	a	271	PHE
1	a	437	ASN
1	a	585	ILE
1	a	783	MET
2	b	105	GLU
2	b	251	ILE
4	d	65	MET
4	d	338	GLU
4	d	415	LEU
5	e	347	ASN
6	f	90	ASN
6	f	181	LEU
6	f	448	MET
6	f	483	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (72) such sidechains are listed below:

Mol	Chain	Res	Type
1	2	384	ASN
1	2	528	ASN
1	2	531	HIS
1	2	569	GLN
1	2	768	HIS
1	2	849	GLN
2	3	259	GLN
2	3	307	ASN
2	3	308	GLN
2	3	507	ASN
2	3	522	GLN

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Mol	Chain	Res	Type
2	3	691	ASN
3	4	196	ASN
3	4	253	GLN
3	4	726	ASN
4	5	223	ASN
4	5	245	HIS
4	5	273	ASN
4	5	334	GLN
4	5	424	GLN
4	5	581	ASN
4	5	585	ASN
4	5	632	GLN
5	6	156	GLN
5	6	157	HIS
5	6	269	ASN
5	6	323	GLN
5	6	550	GLN
5	6	799	GLN
5	6	814	ASN
6	7	178	ASN
6	7	326	HIS
6	7	334	HIS
6	7	336	ASN
6	7	412	ASN
6	7	518	ASN
6	7	554	ASN
7	H	532	GLN
1	a	384	ASN
1	a	528	ASN
1	a	531	HIS
1	a	569	GLN
1	a	849	GLN
2	b	253	HIS
2	b	307	ASN
2	b	308	GLN
2	b	507	ASN
2	b	522	GLN
2	b	691	ASN
2	b	731	ASN
3	c	320	ASN
3	c	726	ASN
3	c	757	HIS

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Mol	Chain	Res	Type
4	d	223	ASN
4	d	245	HIS
4	d	273	ASN
4	d	334	GLN
4	d	424	GLN
4	d	581	ASN
4	d	585	ASN
4	d	632	GLN
5	e	156	GLN
5	e	157	HIS
5	e	269	ASN
5	e	550	GLN
5	e	799	GLN
5	e	814	ASN
6	f	326	HIS
6	f	334	HIS
6	f	412	ASN
6	f	518	ASN
6	f	554	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 18 ligands modelled in this entry, 14 are monoatomic - leaving 4 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	ADP	5	801	12	27,29,29	1.41	4 (14%)	42,45,45	2.01	10 (23%)
11	ADP	b	1001	12	27,29,29	1.38	4 (14%)	42,45,45	1.98	10 (23%)
11	ADP	3	1001	12	27,29,29	1.38	4 (14%)	42,45,45	1.98	10 (23%)
11	ADP	d	801	12	27,29,29	1.41	4 (14%)	42,45,45	2.01	10 (23%)

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	ADP	5	801	12	-	6/16/32/32	0/3/3/3
11	ADP	b	1001	12	-	6/16/32/32	0/3/3/3
11	ADP	3	1001	12	-	6/16/32/32	0/3/3/3
11	ADP	d	801	12	-	6/16/32/32	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	5	801	ADP	C5-C4	4.75	1.47	1.39
11	d	801	ADP	C5-C4	4.75	1.47	1.39
11	3	1001	ADP	C5-C4	4.68	1.47	1.39
11	b	1001	ADP	C5-C4	4.68	1.47	1.39
11	d	801	ADP	C5-C6	2.79	1.48	1.41
11	5	801	ADP	C5-C6	2.79	1.48	1.41
11	b	1001	ADP	C5-C6	2.69	1.48	1.41
11	3	1001	ADP	C5-C6	2.69	1.48	1.41
11	3	1001	ADP	C8-N7	2.39	1.36	1.31
11	b	1001	ADP	C8-N7	2.39	1.36	1.31
11	5	801	ADP	C8-N7	2.29	1.35	1.31
11	d	801	ADP	C5-N7	-2.29	1.34	1.39
11	d	801	ADP	C8-N7	2.28	1.35	1.31
11	5	801	ADP	C5-N7	-2.28	1.34	1.39
11	b	1001	ADP	C5-N7	-2.22	1.34	1.39
11	3	1001	ADP	C5-N7	-2.22	1.34	1.39

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	5	801	ADP	C5-C4-N3	-6.57	118.17	126.75
11	d	801	ADP	C5-C4-N3	-6.57	118.18	126.75
11	3	1001	ADP	C5-C4-N3	-6.18	118.69	126.75
11	b	1001	ADP	C5-C4-N3	-6.17	118.70	126.75
11	d	801	ADP	N3-C4-N9	5.12	135.52	127.08
11	5	801	ADP	N3-C4-N9	5.12	135.51	127.08
11	3	1001	ADP	N3-C4-N9	4.95	135.23	127.08
11	b	1001	ADP	N3-C4-N9	4.94	135.23	127.08
11	5	801	ADP	C2-N3-C4	3.92	121.00	111.75
11	d	801	ADP	C2-N3-C4	3.91	121.00	111.75
11	3	1001	ADP	C2-N3-C4	3.86	120.86	111.75
11	b	1001	ADP	C2-N3-C4	3.86	120.86	111.75
11	b	1001	ADP	PA-O3A-PB	-3.50	120.83	132.83
11	3	1001	ADP	PA-O3A-PB	-3.49	120.85	132.83
11	5	801	ADP	C4-C5-N7	-3.47	106.39	110.62
11	d	801	ADP	C4-C5-N7	-3.46	106.40	110.62
11	b	1001	ADP	N3-C2-N1	-3.16	123.66	128.60
11	3	1001	ADP	N3-C2-N1	-3.16	123.66	128.60
11	3	1001	ADP	C4-C5-N7	-3.09	106.86	110.62
11	b	1001	ADP	C4-C5-N7	-3.09	106.86	110.62
11	5	801	ADP	PA-O3A-PB	-2.97	122.64	132.83
11	d	801	ADP	PA-O3A-PB	-2.96	122.66	132.83
11	d	801	ADP	N3-C2-N1	-2.87	124.11	128.60
11	5	801	ADP	N3-C2-N1	-2.87	124.11	128.60
11	5	801	ADP	C5-N7-C8	2.82	107.52	103.51
11	d	801	ADP	C5-N7-C8	2.82	107.51	103.51
11	b	1001	ADP	C5-N7-C8	2.61	107.22	103.51
11	3	1001	ADP	C5-N7-C8	2.61	107.21	103.51
11	3	1001	ADP	C4-N9-C8	2.60	108.55	105.73
11	b	1001	ADP	C4-N9-C8	2.60	108.54	105.73
11	b	1001	ADP	C3'-C2'-C1'	2.56	106.30	101.43
11	3	1001	ADP	C3'-C2'-C1'	2.56	106.30	101.43
11	d	801	ADP	C3'-C2'-C1'	2.39	105.97	101.43
11	d	801	ADP	C4-N9-C8	2.39	108.32	105.73
11	5	801	ADP	C3'-C2'-C1'	2.39	105.96	101.43
11	5	801	ADP	C4-N9-C8	2.39	108.31	105.73
11	b	1001	ADP	C6-C5-N7	2.11	135.95	132.02
11	3	1001	ADP	C6-C5-N7	2.11	135.95	132.02
11	5	801	ADP	C6-C5-N7	2.05	135.84	132.02
11	d	801	ADP	C6-C5-N7	2.05	135.83	132.02

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	3	1001	ADP	PA-O3A-PB-O2B
11	3	1001	ADP	C5'-O5'-PA-O1A
11	3	1001	ADP	C5'-O5'-PA-O3A
11	5	801	ADP	PA-O3A-PB-O2B
11	5	801	ADP	C5'-O5'-PA-O3A
11	b	1001	ADP	PA-O3A-PB-O2B
11	b	1001	ADP	C5'-O5'-PA-O1A
11	b	1001	ADP	C5'-O5'-PA-O3A
11	d	801	ADP	PA-O3A-PB-O2B
11	d	801	ADP	C5'-O5'-PA-O3A
11	5	801	ADP	C3'-C4'-C5'-O5'
11	d	801	ADP	C3'-C4'-C5'-O5'
11	5	801	ADP	O4'-C4'-C5'-O5'
11	d	801	ADP	O4'-C4'-C5'-O5'
11	3	1001	ADP	C5'-O5'-PA-O2A
11	5	801	ADP	C5'-O5'-PA-O2A
11	b	1001	ADP	C5'-O5'-PA-O2A
11	d	801	ADP	C5'-O5'-PA-O2A
11	3	1001	ADP	PA-O3A-PB-O1B
11	b	1001	ADP	PA-O3A-PB-O1B
11	d	801	ADP	PA-O3A-PB-O1B
11	5	801	ADP	PA-O3A-PB-O1B
11	3	1001	ADP	O4'-C4'-C5'-O5'
11	b	1001	ADP	O4'-C4'-C5'-O5'

There are no ring outliers.

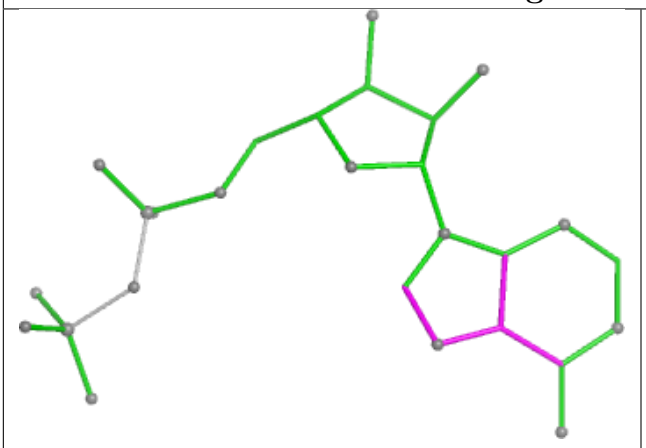
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	5	801	ADP	1	0
11	d	801	ADP	1	0

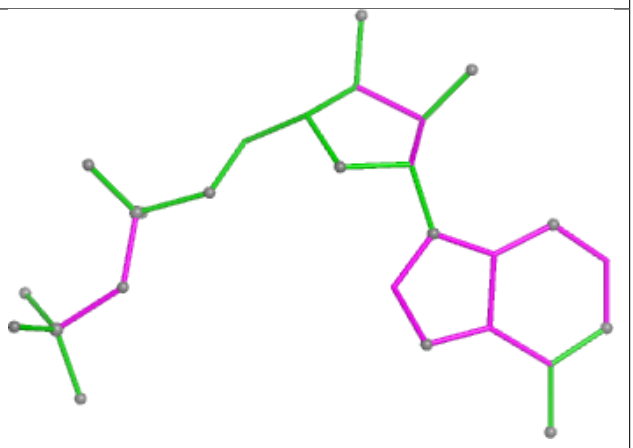
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

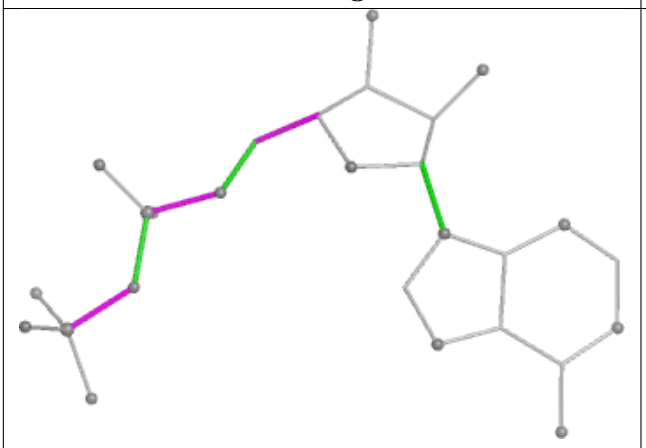
Ligand ADP 5 801



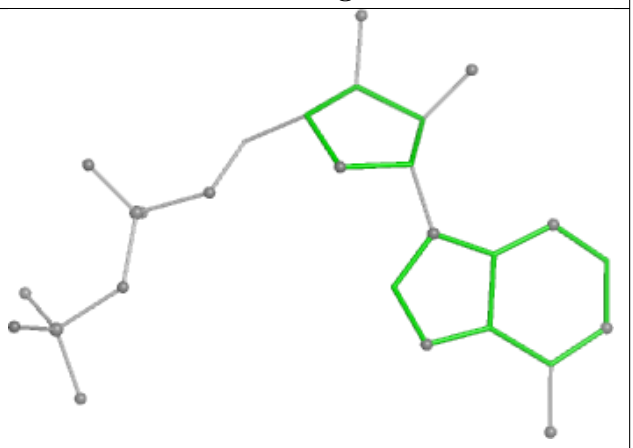
Bond lengths



Bond angles

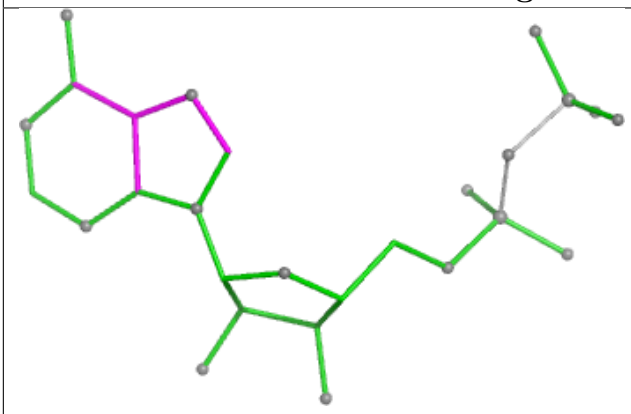


Torsions



Rings

Ligand ADP b 1001



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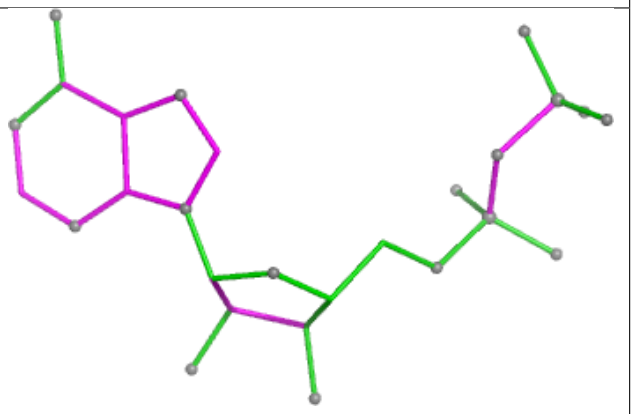
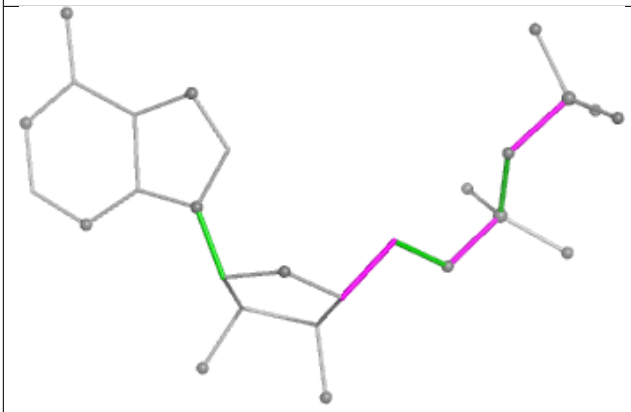
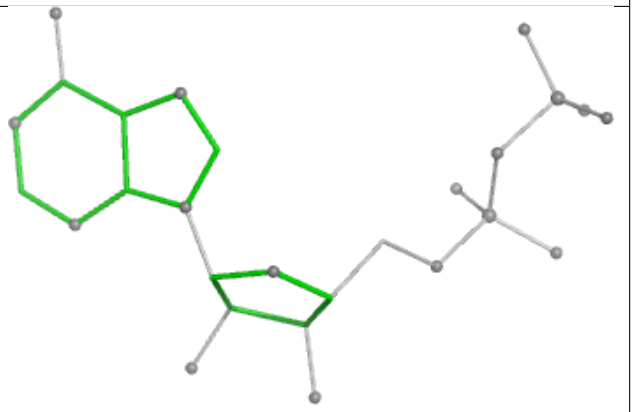


Bond angles

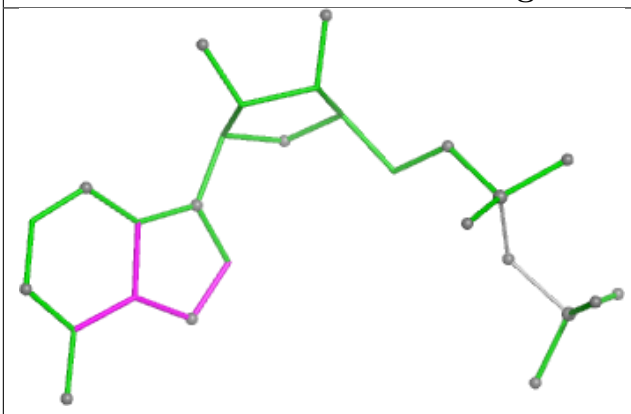


Torsions

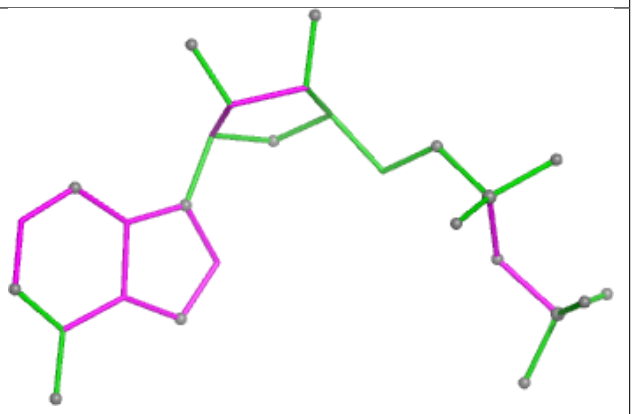


Rings

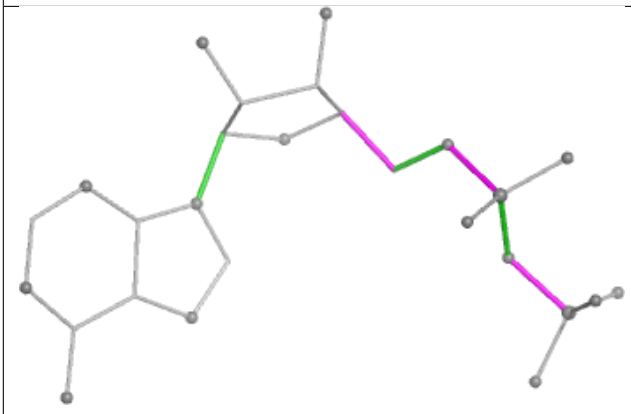
Ligand ADP 3 1001



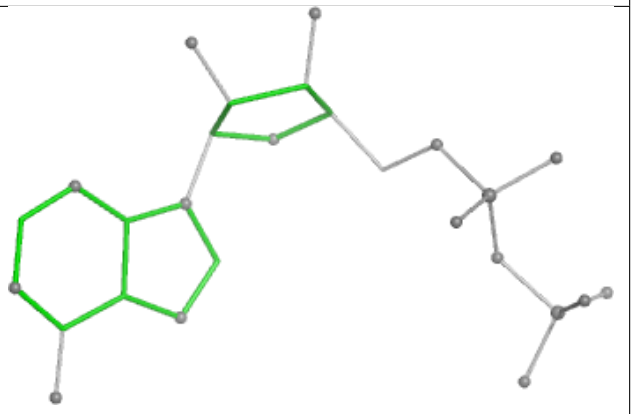
Bond lengths



Bond angles

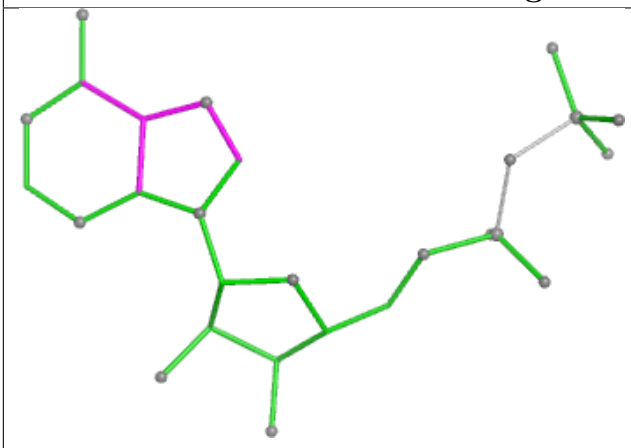


Torsions

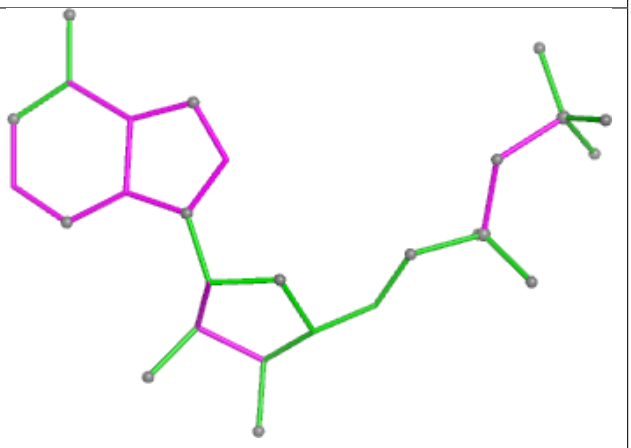


Rings

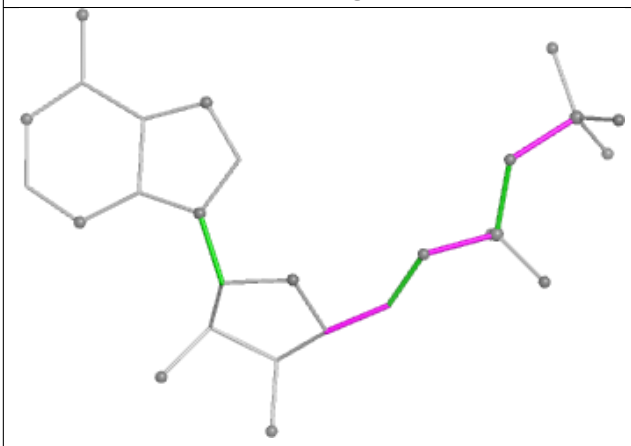
Ligand ADP d 801



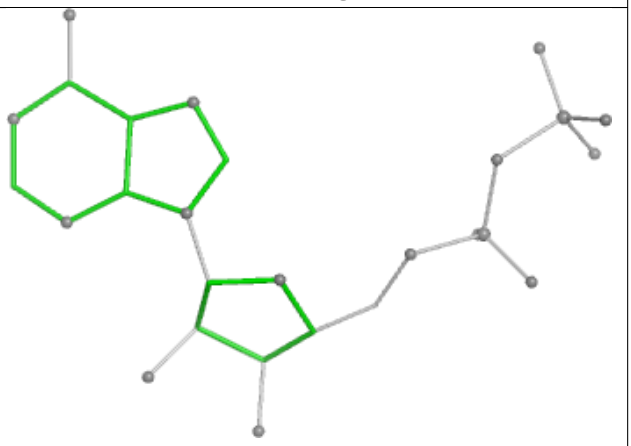
Bond lengths



Bond angles



Torsions



Rings

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.

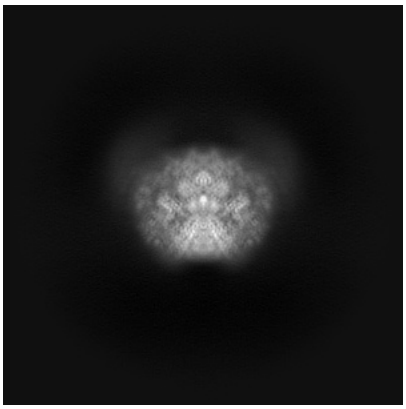
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-53972. These allow visual inspection of the internal detail of the map and identification of artifacts.

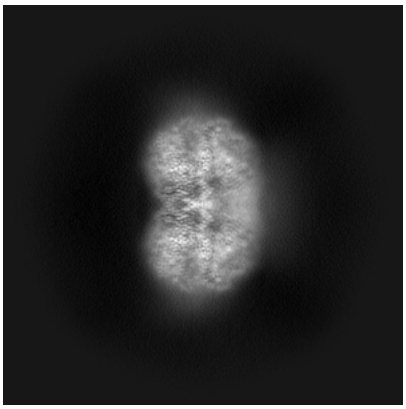
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

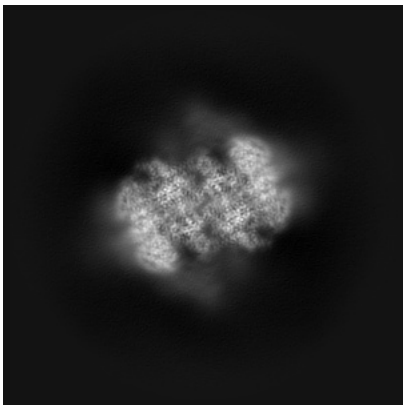
6.1.1 Primary map



X

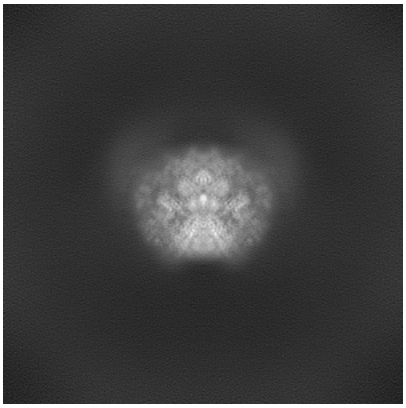


Y

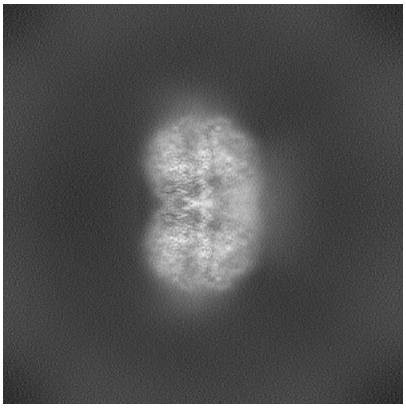


Z

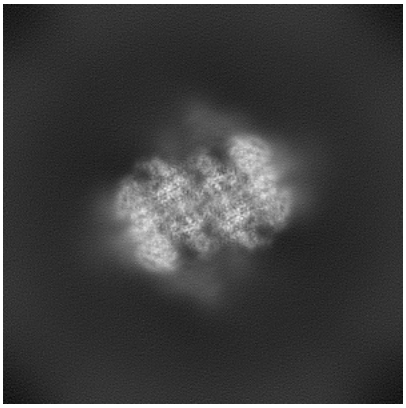
6.1.2 Raw map



X



Y

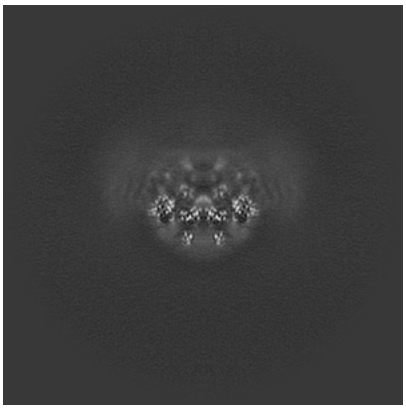


Z

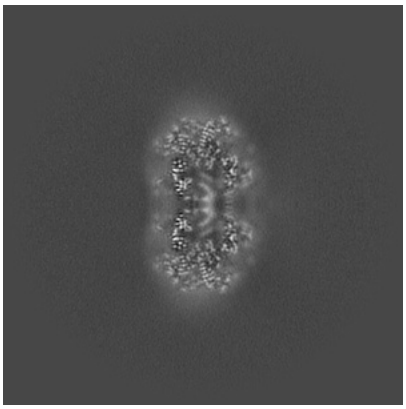
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

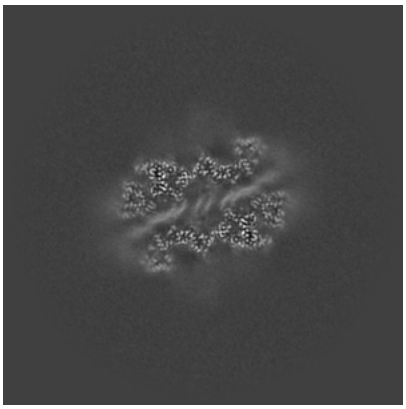
6.2.1 Primary map



X Index: 224

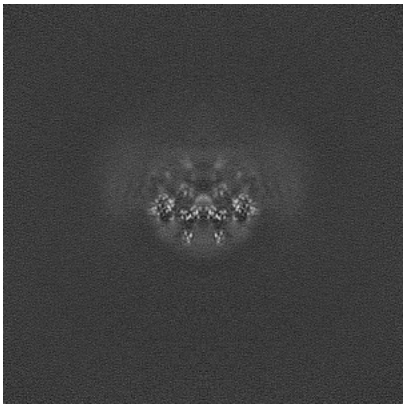


Y Index: 224

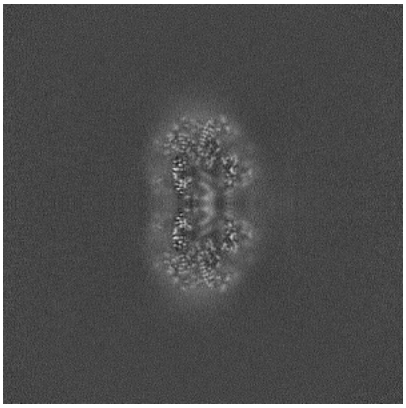


Z Index: 224

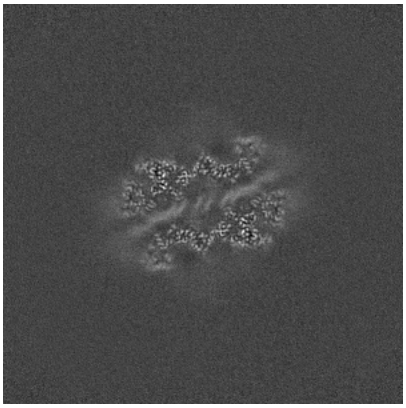
6.2.2 Raw map



X Index: 224



Y Index: 224

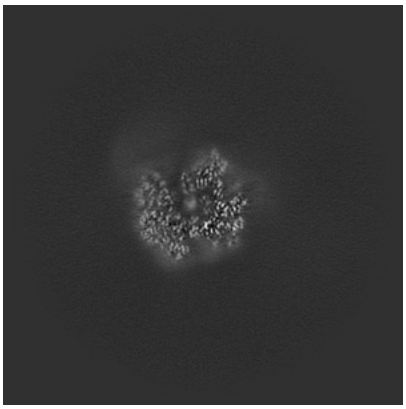


Z Index: 224

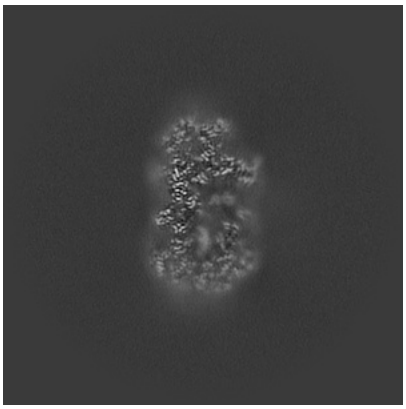
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

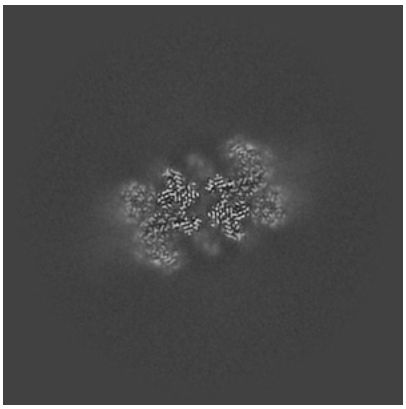
6.3.1 Primary map



X Index: 182

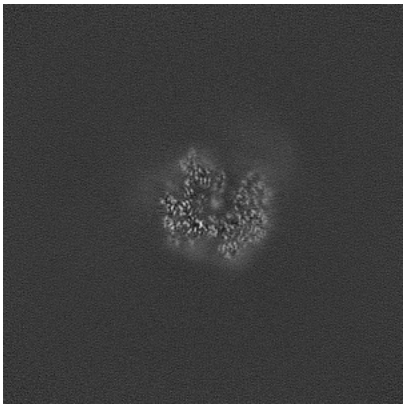


Y Index: 213

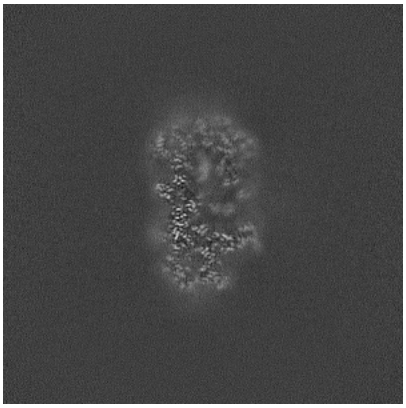


Z Index: 195

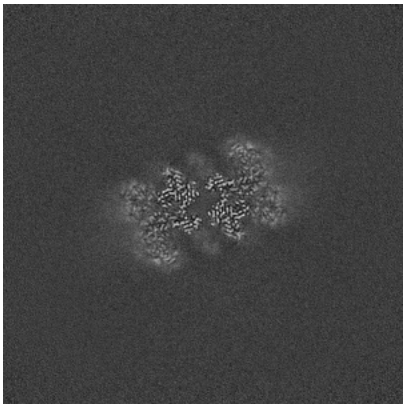
6.3.2 Raw map



X Index: 266



Y Index: 235

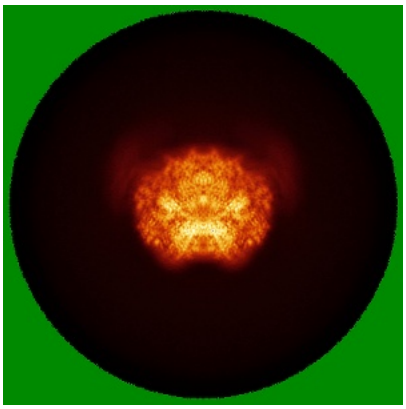


Z Index: 195

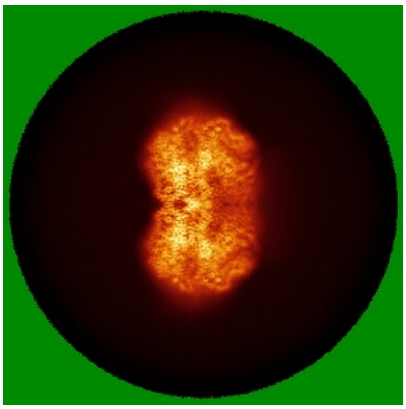
The images above show the largest variance slices of the map in three orthogonal directions.

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

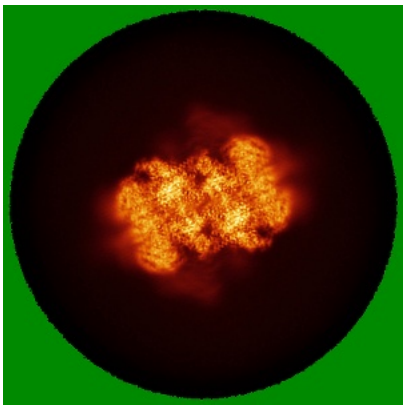
6.4.1 Primary map



X

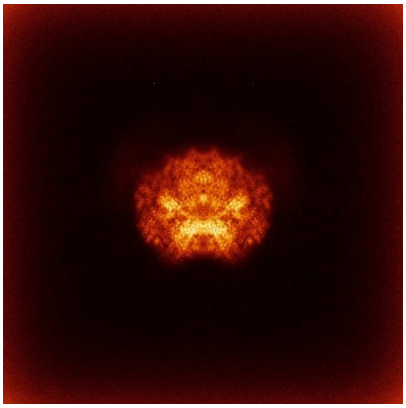


Y

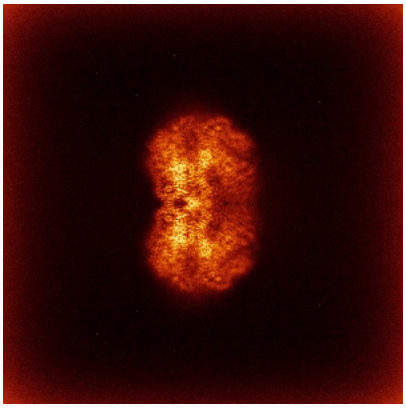


Z

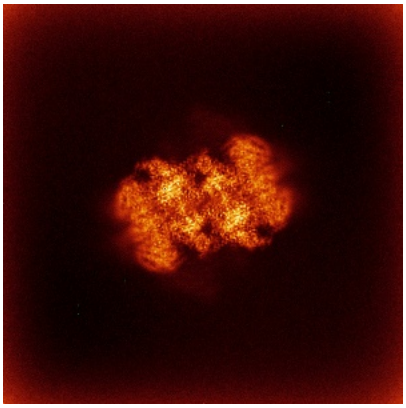
6.4.2 Raw map



X



Y

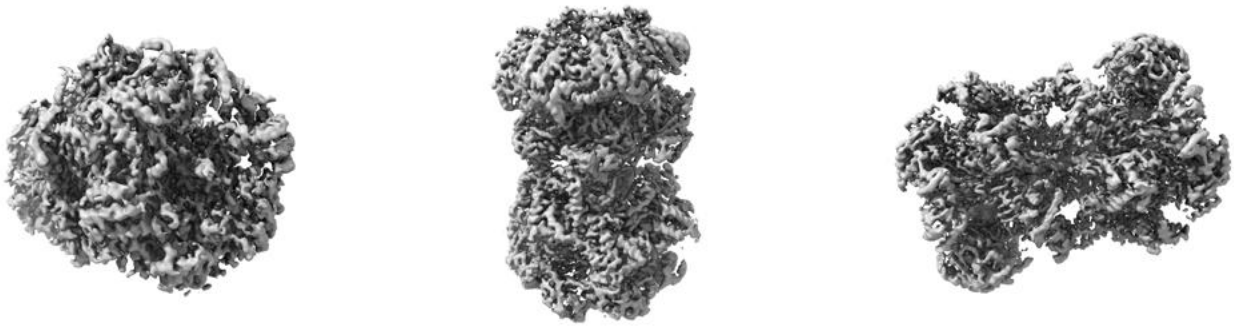


Z

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 0.17. 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.

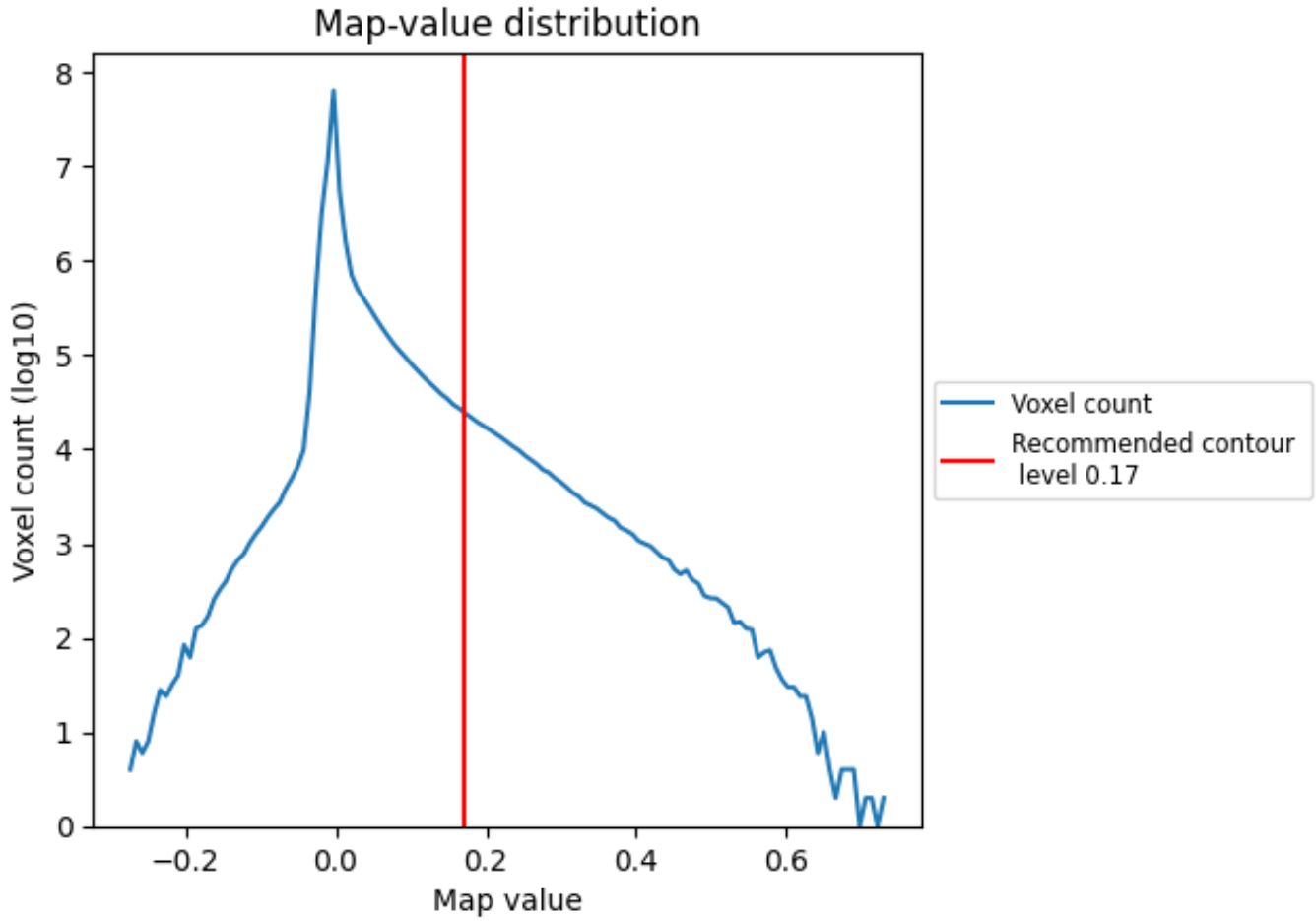
6.6 Mask visualisation (i)

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

7 Map analysis

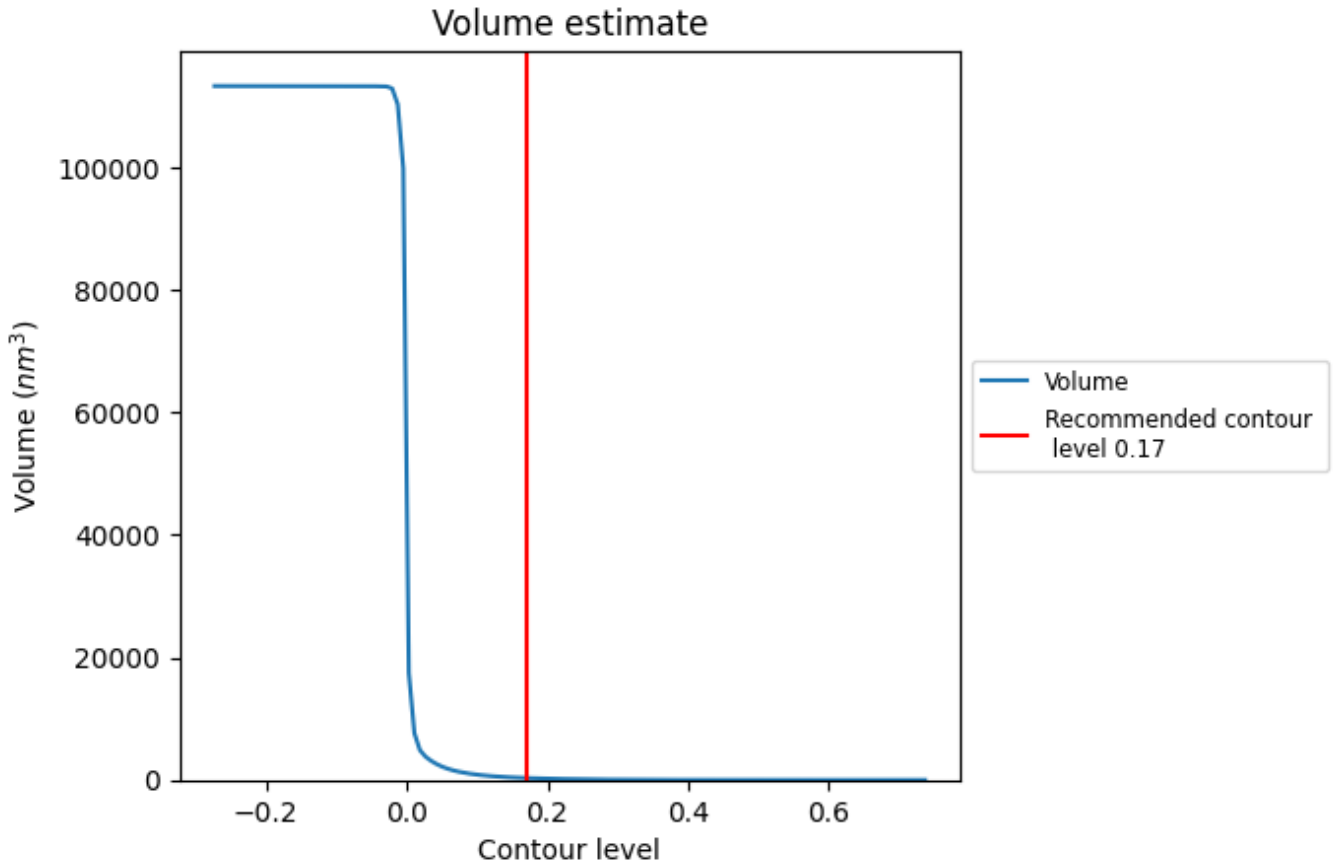
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

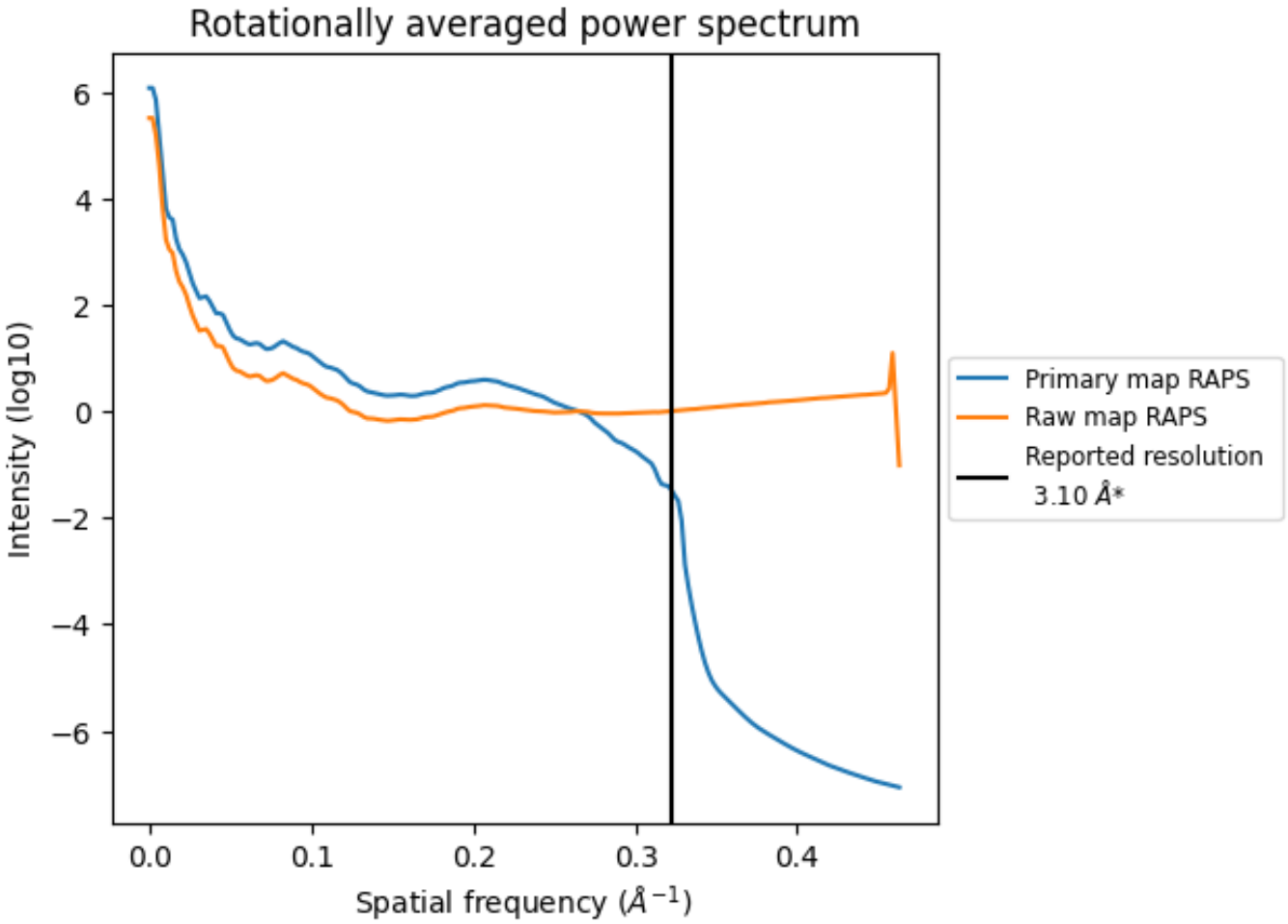
7.2 Volume estimate



The volume at the recommended contour level is 315 nm^3; this corresponds to an approximate mass of 284 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)

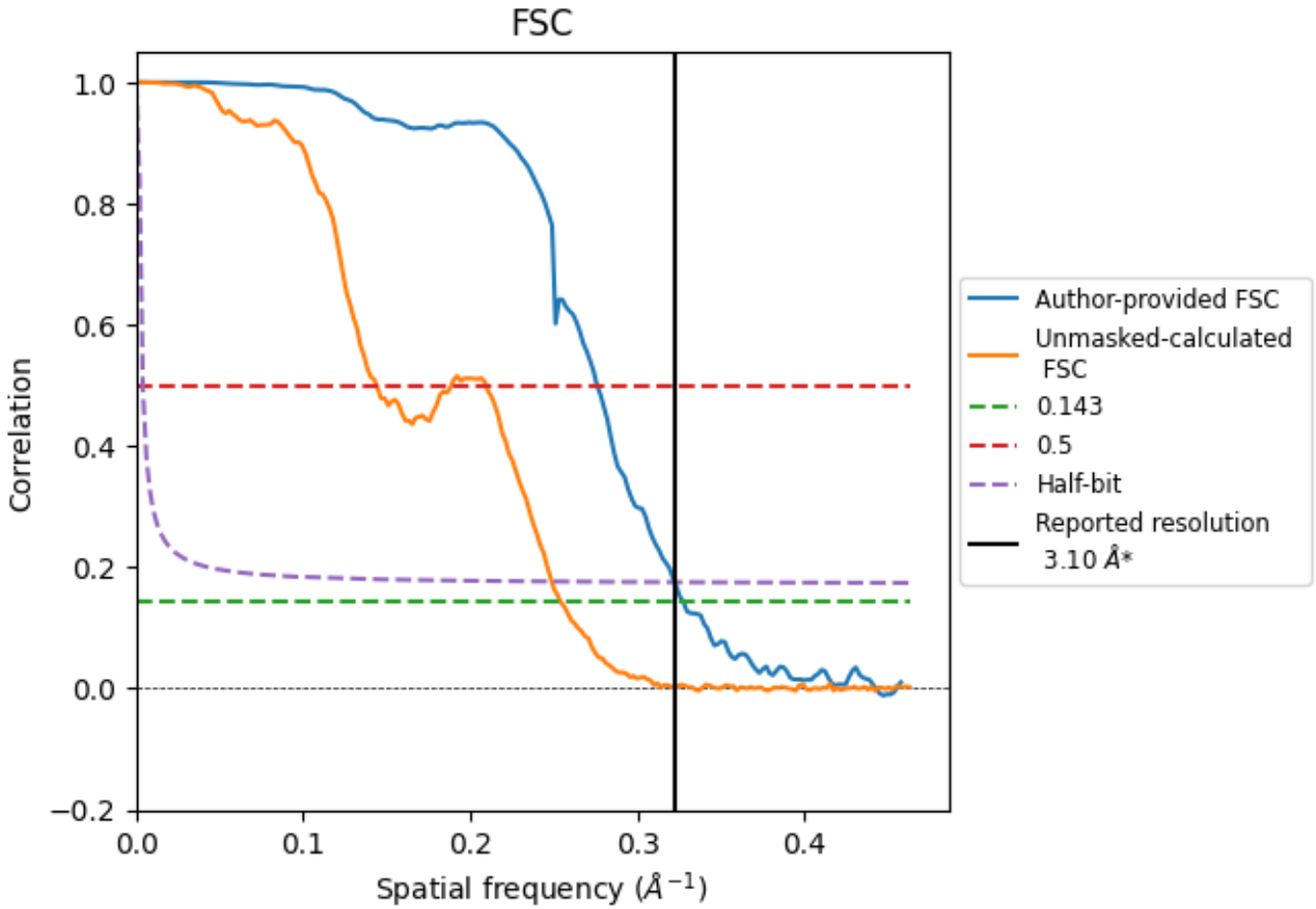


*Reported resolution corresponds to spatial frequency of 0.323 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

8.2 Resolution estimates (i)

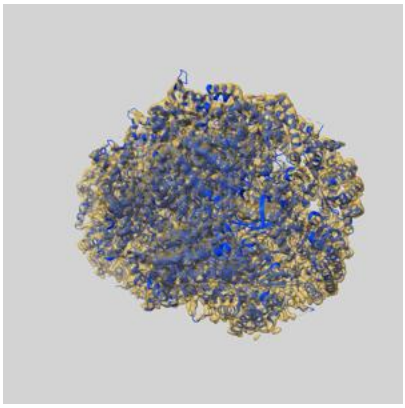
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.05	3.62	3.10
Unmasked-calculated*	3.94	6.95	4.02

*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 3.94 differs from the reported value 3.1 by more than 10 %

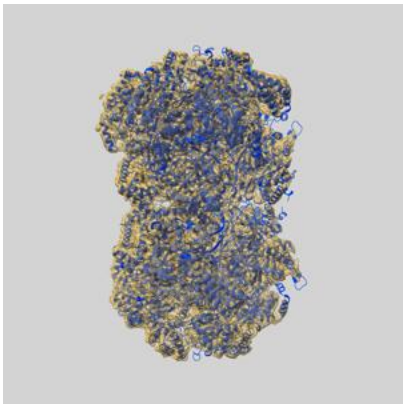
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-53972 and PDB model 9RHL. Per-residue inclusion information can be found in section 3 on page 11.

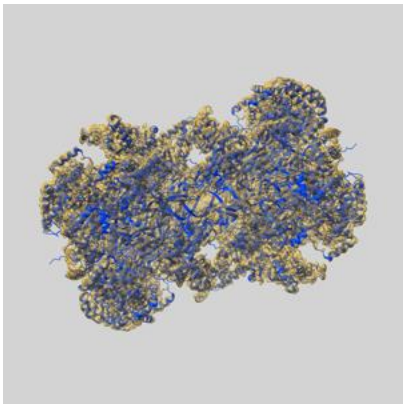
9.1 Map-model overlay



X



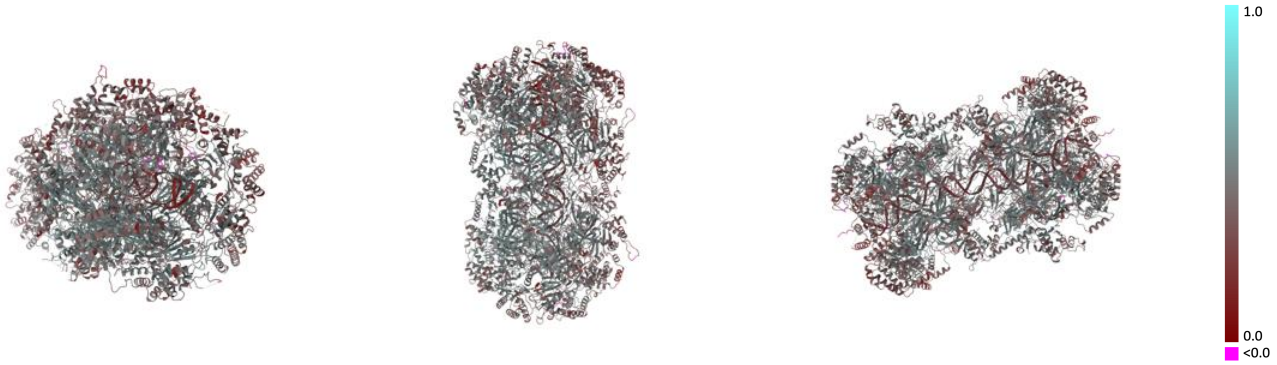
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.17 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.

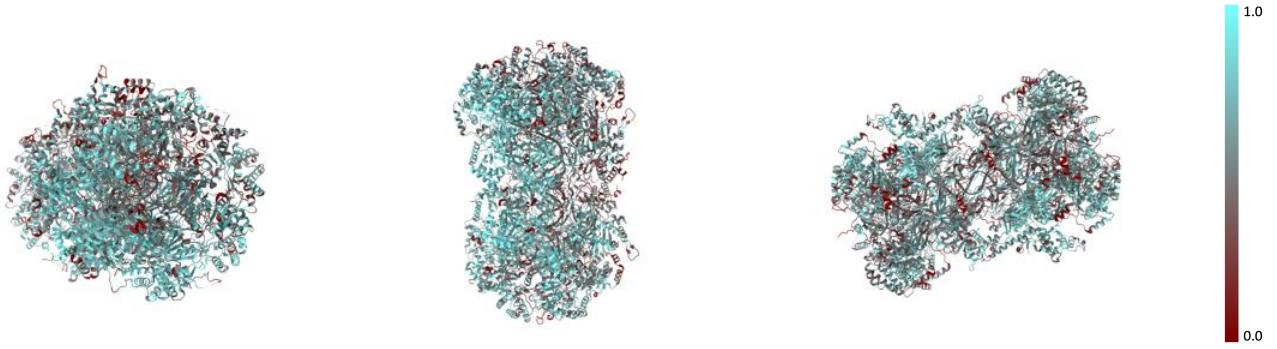
9.2 Q-score mapped to coordinate model (i)



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.

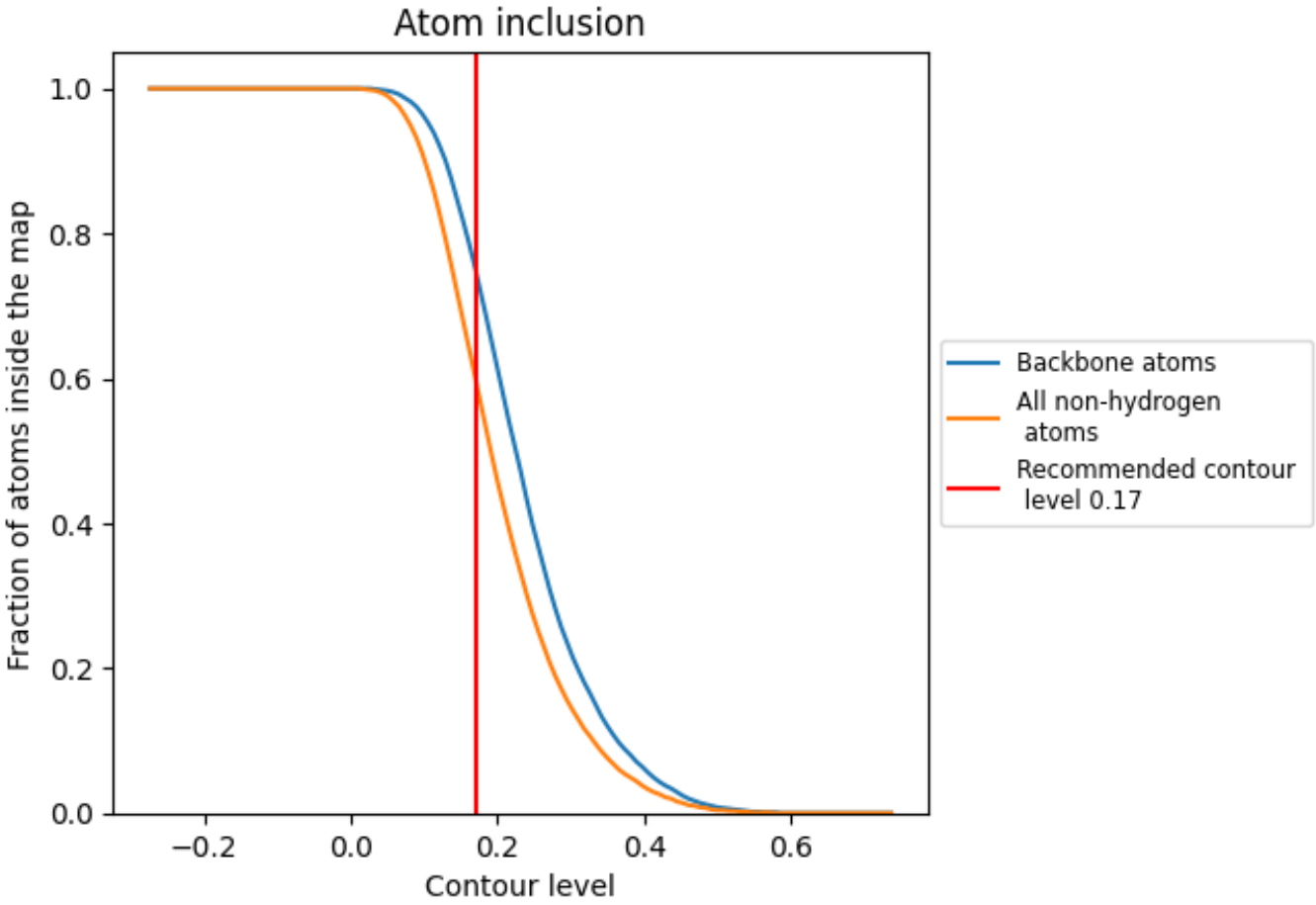
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.17).

9.4 Atom inclusion (i)



At the recommended contour level, 75% of all backbone atoms, 60% 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 (0.17) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6010	0.4410
2	0.4870	0.4150
3	0.7250	0.4920
4	0.6150	0.4480
5	0.6380	0.4560
6	0.5020	0.4050
7	0.6680	0.4740
H	0.3770	0.4040
I	0.3610	0.4020
X	0.4640	0.2630
Y	0.4600	0.2590
a	0.4800	0.4100
b	0.7250	0.4890
c	0.6160	0.4490
d	0.6360	0.4500
e	0.4990	0.4040
f	0.6680	0.4750

