Full wwPDB EM Validation Report ⓘ

Dec 11, 2022 – 01:56 pm GMT

PDB ID	:	6SKO
EMDB ID	:	EMD-10230
Title	:	Cryo-EM Structure of the Fork Protection Complex Bound to CMG at a Replication Fork - conformation 2 MCM CTD:ssDNA
Authors	:	Yeeles, J.; Baretic, D.; Jenkyn-Bedford, M.
Deposited on	:	2019-08-16
Resolution	:	3.40 Å(reported)
Based on initial model	:	5U8S

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:

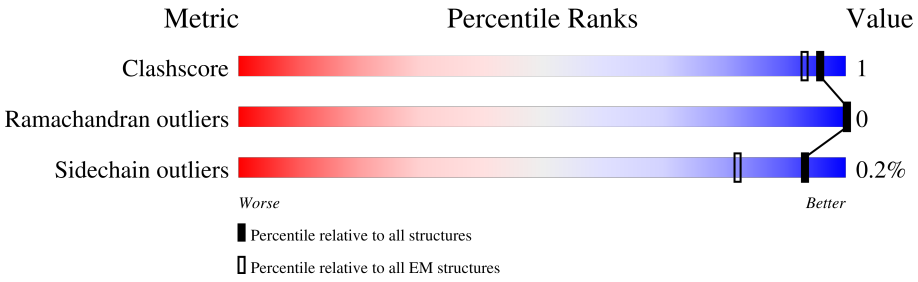
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance

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

The reported resolution of this entry is 3.40 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	6	1017	5% 30% 68%
2	7	845	37% 60%
3	2	868	12% 37% 60%
4	5	775	6% 33% 64%
5	3	971	32% 65%
6	4	933	34% 65%
7	I	85	12% 18% 81%

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 31618 atoms, of which 15903 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 MCM6.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	6	328	5130	1605	2579	443	490	13	0	0

- Molecule 2 is a protein called DNA replication licensing factor MCM7.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	7	335	5242	1624	2652	448	501	17	0	0

- Molecule 3 is a protein called DNA replication licensing factor MCM2.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	2	346	5499	1710	2775	492	512	10	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	5	280	4460	1383	2276	377	412	12	0	0

- Molecule 5 is a protein called DNA replication licensing factor MCM3.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	3	336	5327	1645	2709	473	491	9	0	0

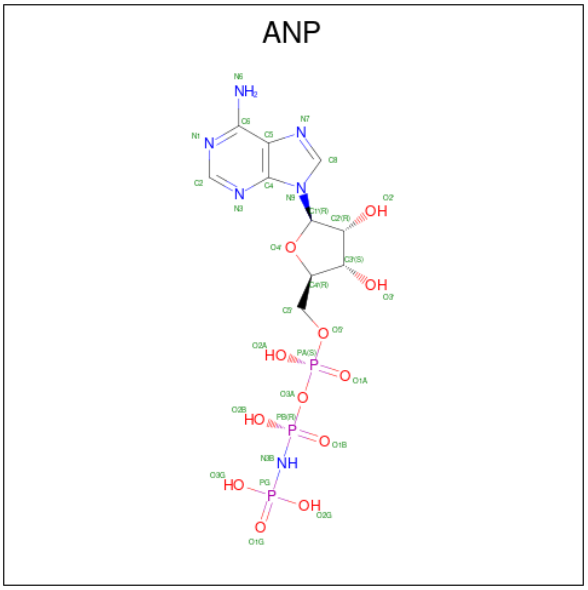
- Molecule 6 is a protein called DNA replication licensing factor MCM4.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
6	4	330	5223	1622	2655	440	495	11	0	0

- Molecule 7 is a DNA chain called ssDNA, leading-strand template.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	I	16	Total	C	H	N	O	P	0	0
			512	160	192	32	112	16		

- Molecule 8 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
8	6	1	Total	C	H	N	O	P	0
			44	10	13	6	12	3	
8	7	1	Total	C	H	N	O	P	0
			44	10	13	6	12	3	
8	2	1	Total	C	H	N	O	P	0
			44	10	13	6	12	3	
8	3	1	Total	C	H	N	O	P	0
			44	10	13	6	12	3	
8	4	1	Total	C	H	N	O	P	0
			44	10	13	6	12	3	

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
9	6	1	Total	Mg	0
			1	1	
9	7	1	Total	Mg	0
			1	1	

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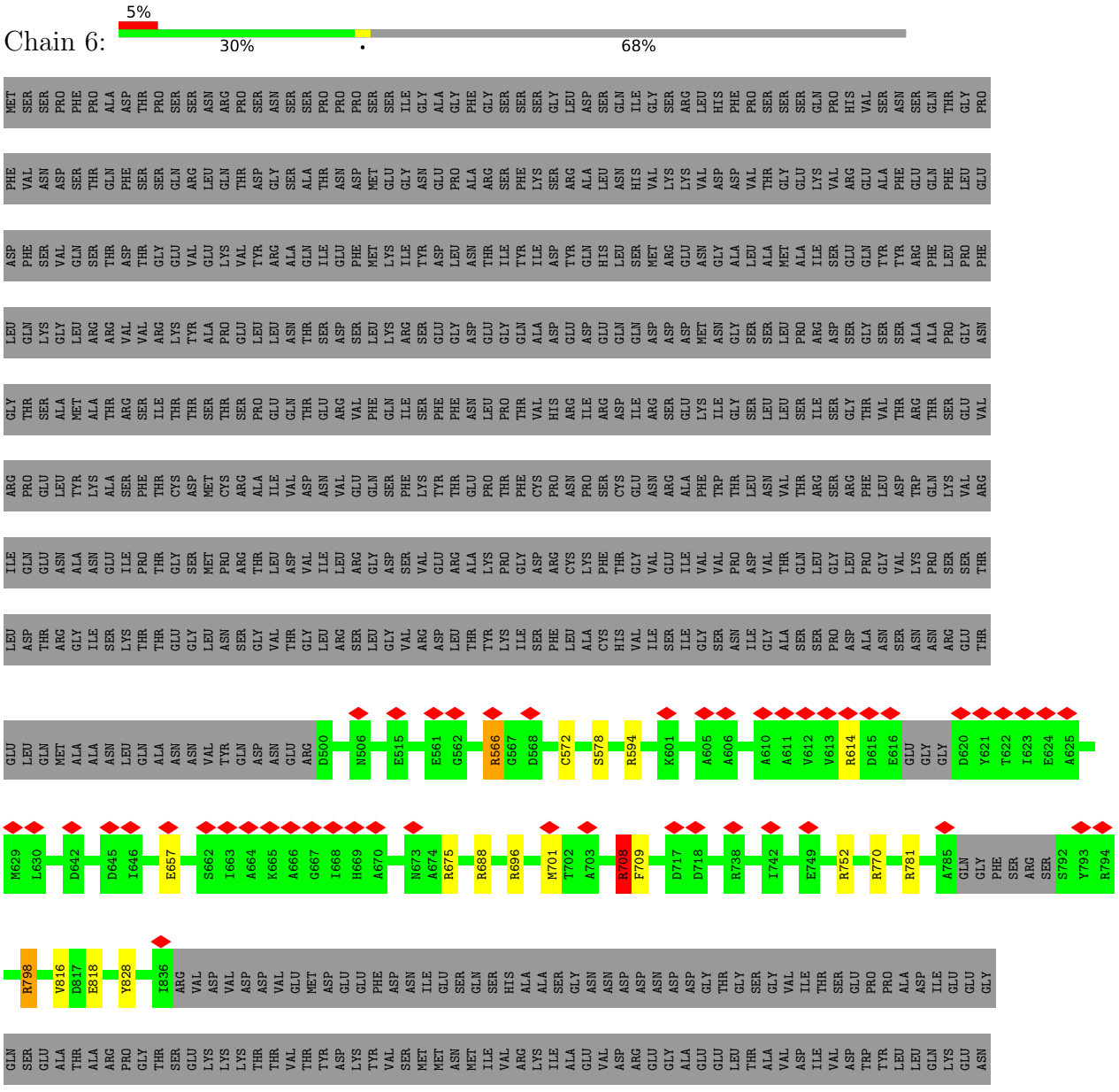
Mol	Chain	Residues	Atoms	AltConf
9	2	1	Total Mg 1 1	0
9	3	1	Total Mg 1 1	0
9	4	1	Total Mg 1 1	0

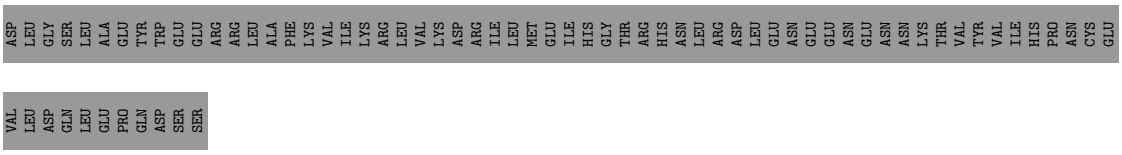
3 Residue-property plots (i)

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

• Molecule 1: DNA replication licensing factor MCM6

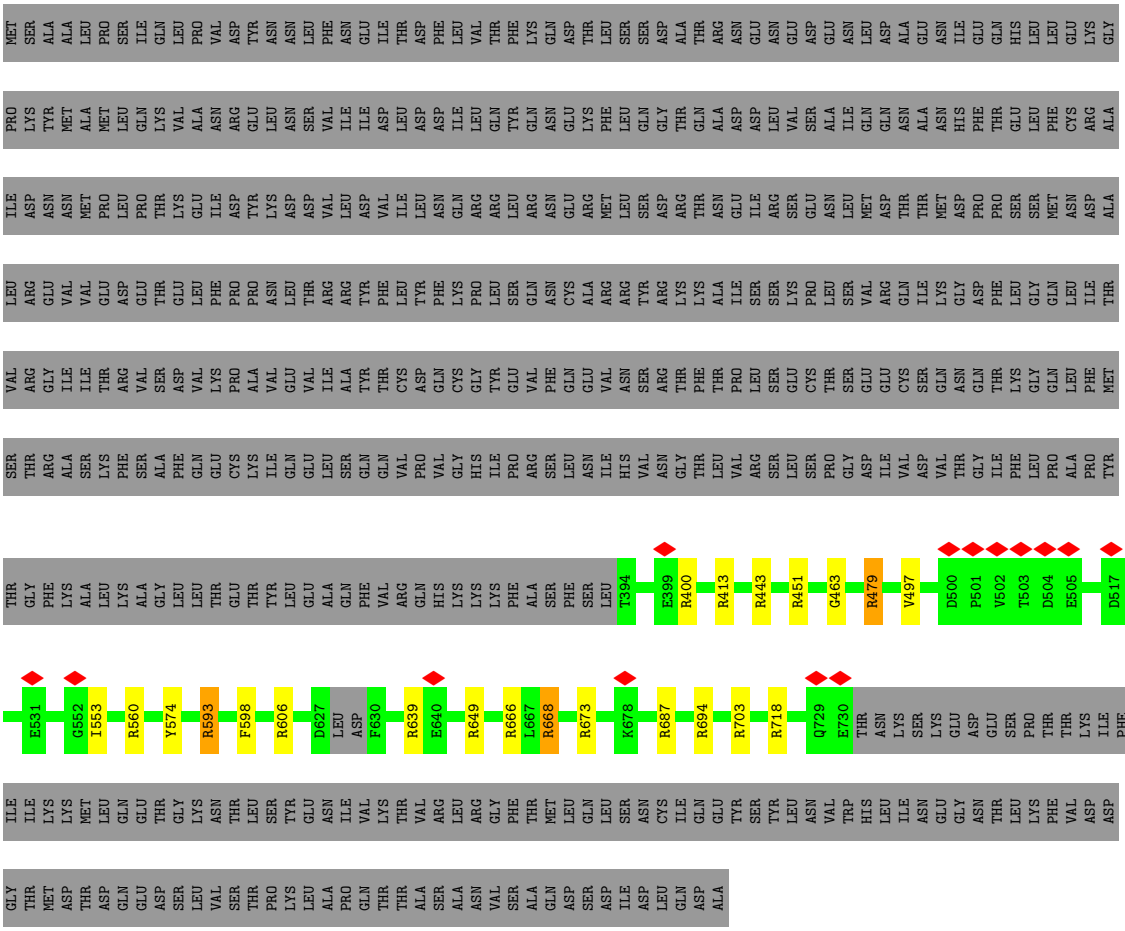
Chain 6:





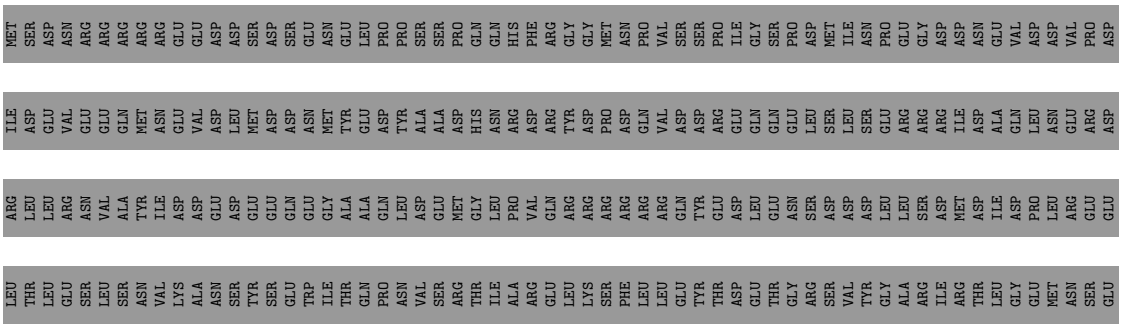
• Molecule 2: DNA replication licensing factor MCM7

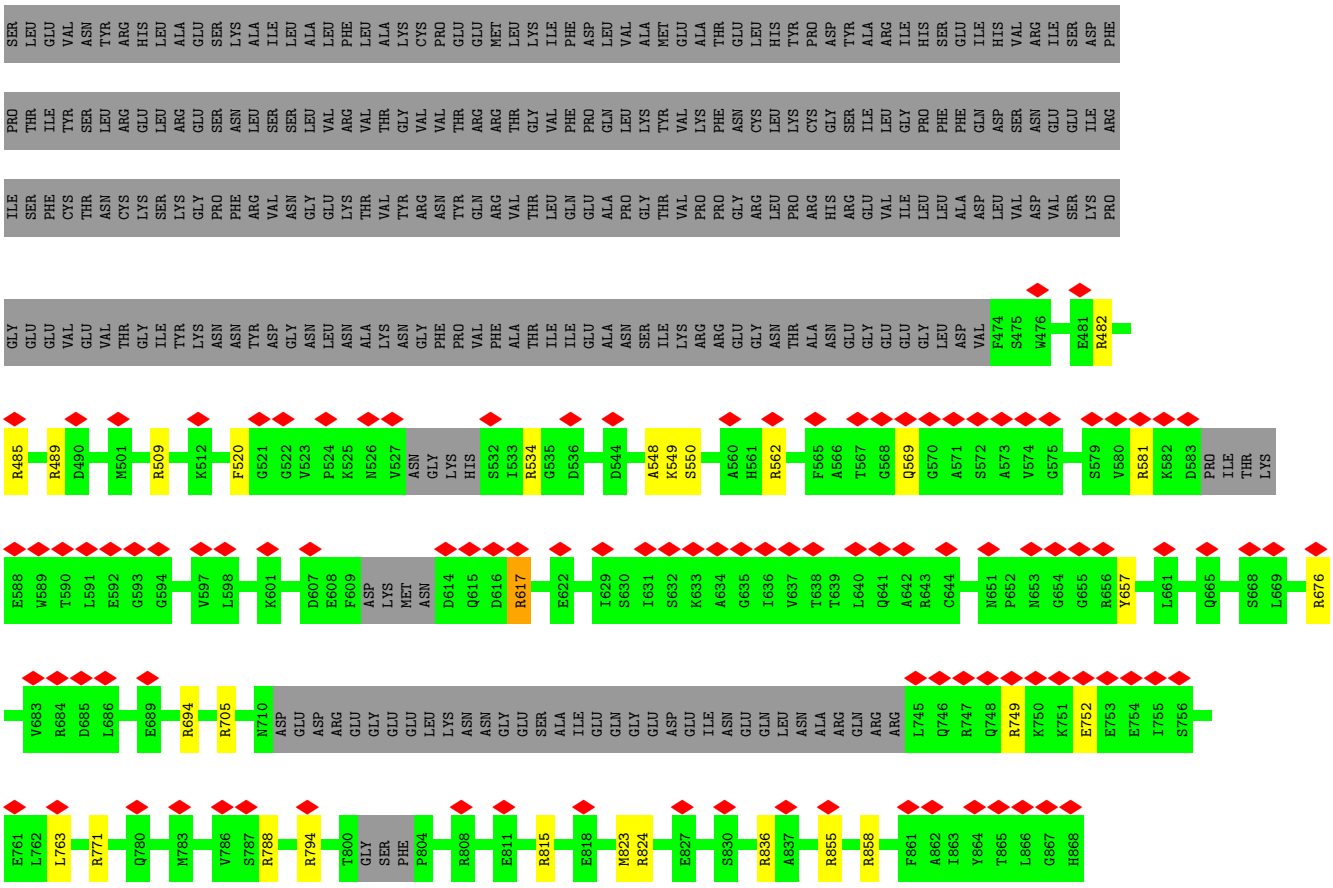
Chain 7:



• Molecule 3: DNA replication licensing factor MCM2

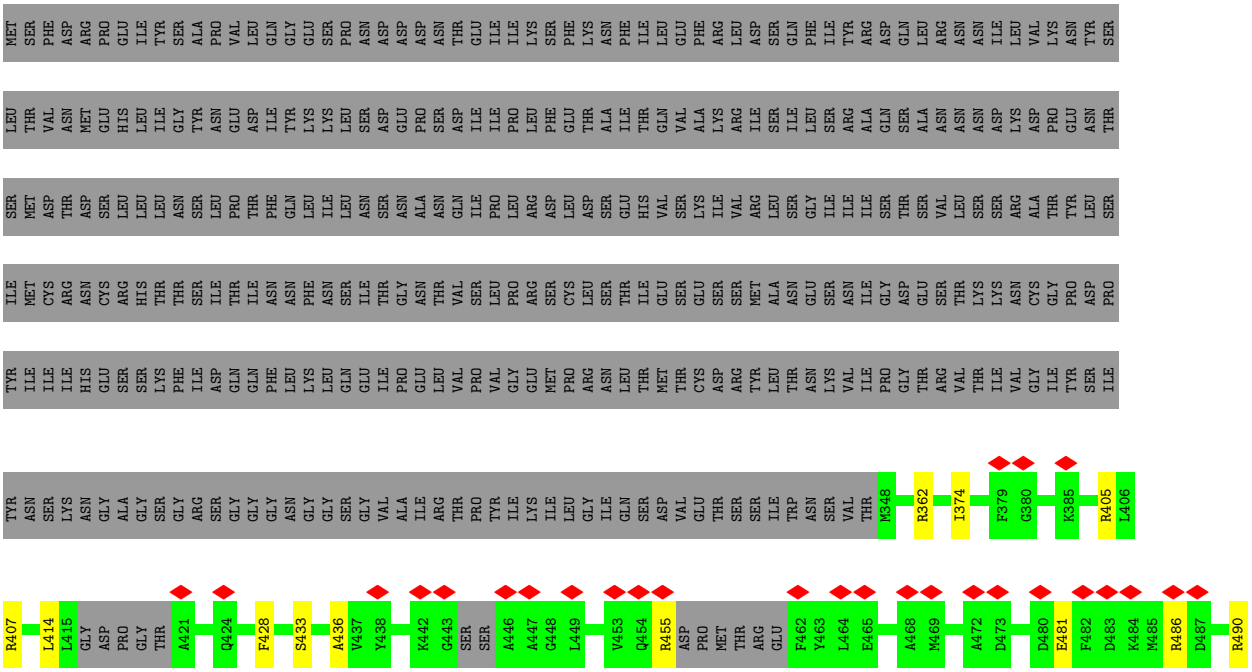
Chain 2:

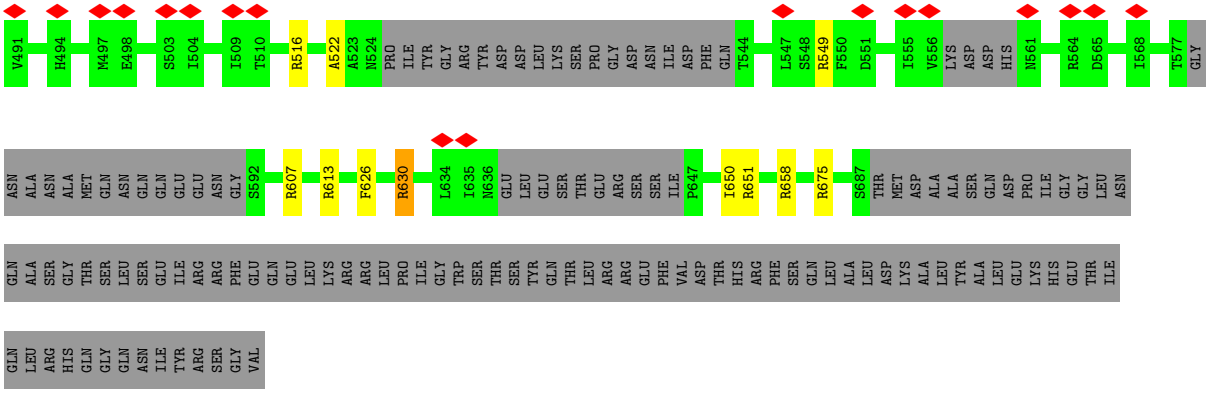




• Molecule 4: Minichromosome maintenance protein 5

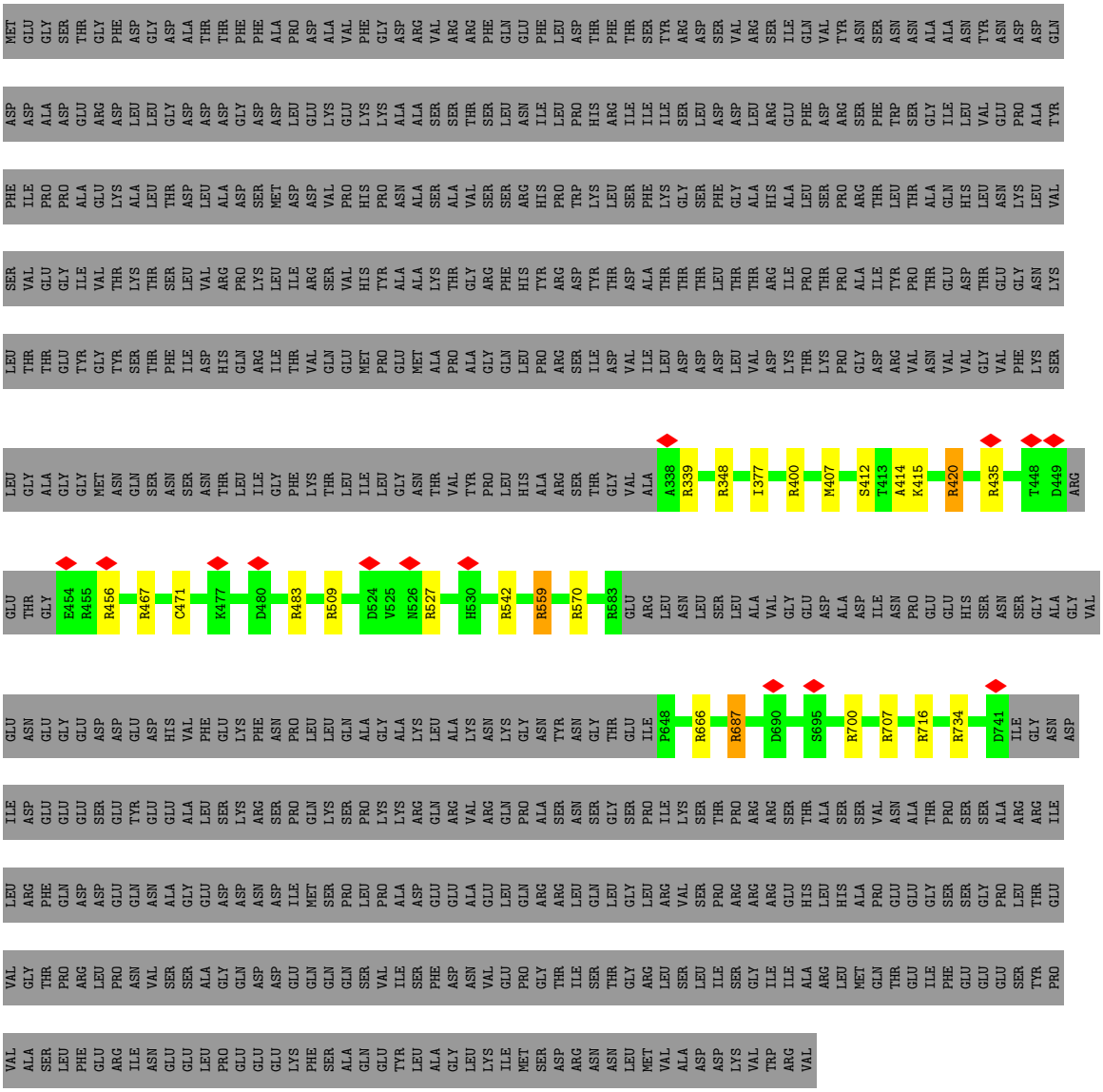
Chain 5:





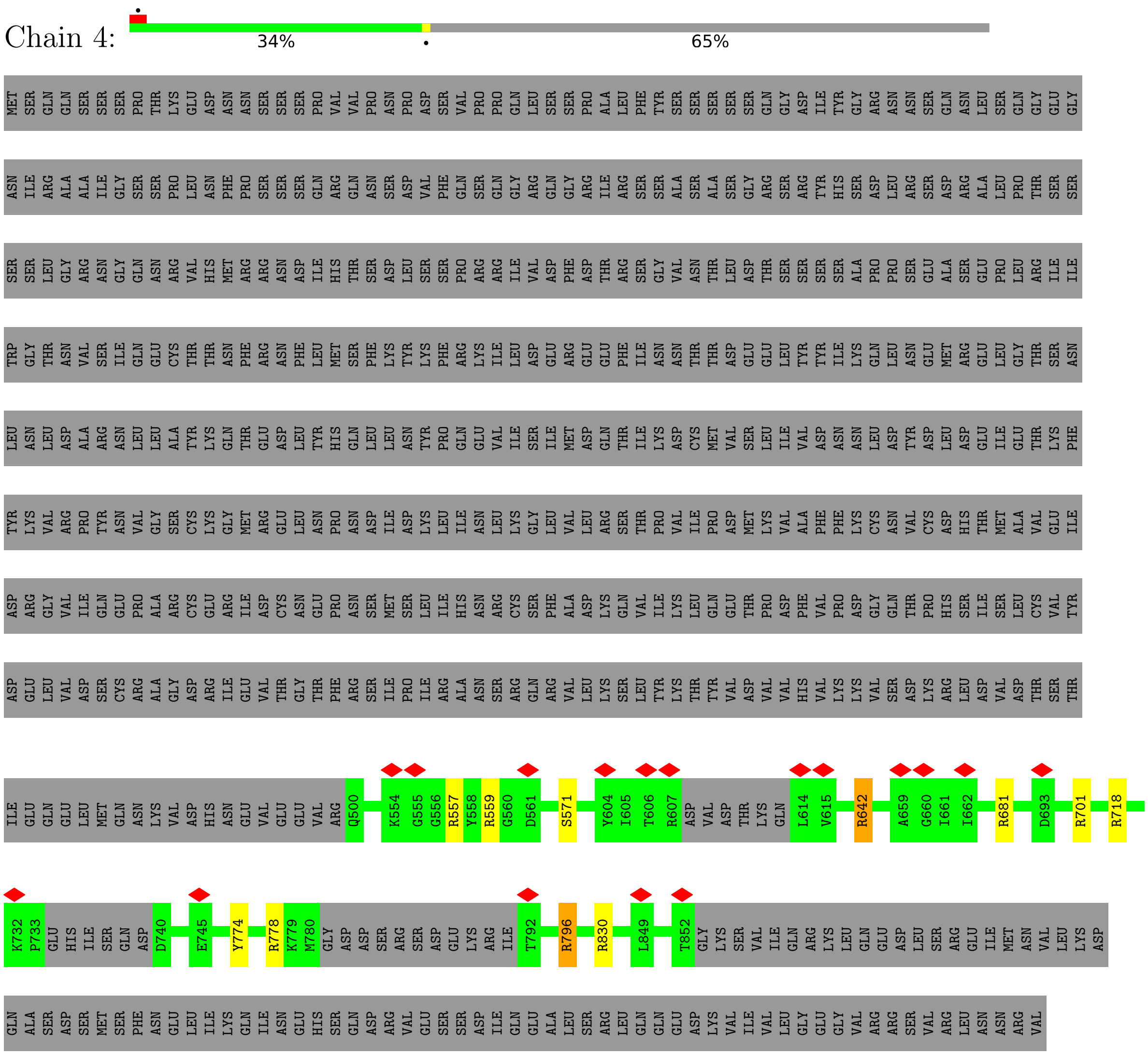
• Molecule 5: DNA replication licensing factor MCM3

Chain 3:



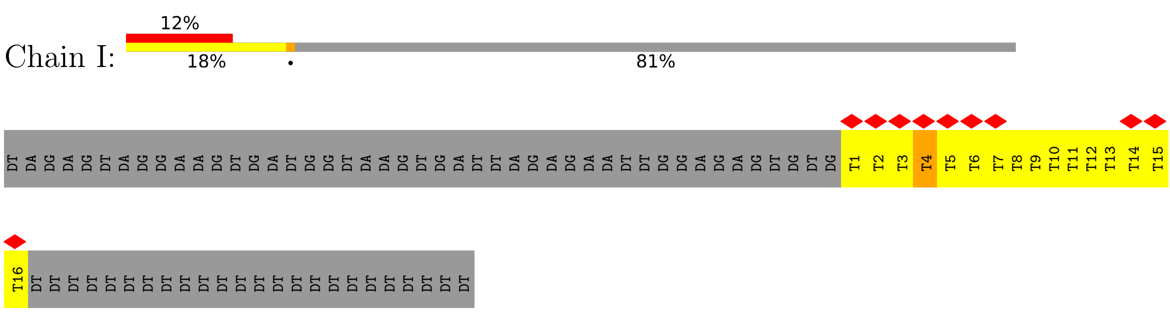
• Molecule 6: DNA replication licensing factor MCM4

Chain 4:



- Molecule 7: ssDNA, leading-strand template

Chain I:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	182000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	37	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.071	Depositor
Minimum map value	-0.026	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.014	Depositor
Map size (Å)	377.64, 377.64, 377.64	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.049, 1.049, 1.049	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ANP, 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	6	0.69	0/2586	1.16	14/3485 (0.4%)
2	7	0.65	1/2623 (0.0%)	1.09	16/3541 (0.5%)
3	2	0.72	0/2762	1.20	19/3718 (0.5%)
4	5	0.65	0/2203	1.13	14/2957 (0.5%)
5	3	0.66	0/2652	1.12	23/3587 (0.6%)
6	4	0.63	0/2601	1.06	10/3515 (0.3%)
7	I	1.59	0/351	2.60	37/540 (6.9%)
All	All	0.70	1/15778 (0.0%)	1.19	133/21343 (0.6%)

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
1	6	0	3
2	7	0	7
3	2	0	4
4	5	0	2
5	3	0	2
6	4	0	2
7	I	0	1
All	All	0	21

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	7	593	ARG	CZ-NH2	-5.39	1.26	1.33

All (133) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	3	700	ARG	NE-CZ-NH2	13.17	126.89	120.30
6	4	796	ARG	NE-CZ-NH1	13.04	126.82	120.30
1	6	798	ARG	NE-CZ-NH2	11.03	125.81	120.30
1	6	708	ARG	NE-CZ-NH1	10.97	125.79	120.30
7	I	16	DT	O4'-C1'-N1	10.19	115.13	108.00
1	6	798	ARG	NE-CZ-NH1	-9.61	115.49	120.30
7	I	3	DT	N3-C2-O2	-9.44	116.64	122.30
7	I	2	DT	N3-C2-O2	-9.19	116.78	122.30
1	6	566	ARG	NE-CZ-NH2	8.93	124.76	120.30
1	6	696	ARG	NE-CZ-NH1	8.44	124.52	120.30
4	5	630	ARG	NE-CZ-NH1	8.26	124.43	120.30
5	3	542	ARG	NE-CZ-NH1	7.83	124.21	120.30
2	7	687	ARG	NE-CZ-NH1	7.78	124.19	120.30
3	2	676	ARG	NE-CZ-NH1	7.77	124.19	120.30
5	3	483	ARG	NE-CZ-NH2	7.77	124.19	120.30
1	6	688	ARG	NE-CZ-NH1	7.75	124.17	120.30
4	5	651	ARG	NE-CZ-NH2	7.72	124.16	120.30
3	2	836	ARG	NE-CZ-NH1	7.62	124.11	120.30
2	7	606	ARG	NE-CZ-NH1	7.52	124.06	120.30
5	3	400	ARG	NE-CZ-NH2	7.51	124.05	120.30
3	2	562	ARG	NE-CZ-NH1	7.49	124.05	120.30
7	I	11	DT	N3-C2-O2	-7.46	117.82	122.30
5	3	456	ARG	NE-CZ-NH1	7.43	124.02	120.30
3	2	489	ARG	NE-CZ-NH1	7.30	123.95	120.30
7	I	11	DT	C6-C5-C7	-7.29	118.53	122.90
7	I	16	DT	C6-C5-C7	-7.26	118.54	122.90
4	5	481	GLU	N-CA-CB	7.25	123.64	110.60
6	4	559	ARG	NE-CZ-NH2	7.23	123.92	120.30
2	7	443	ARG	NE-CZ-NH1	7.20	123.90	120.30
4	5	607	ARG	NE-CZ-NH1	7.17	123.89	120.30
4	5	486	ARG	NE-CZ-NH2	7.12	123.86	120.30
3	2	788	ARG	NE-CZ-NH1	7.09	123.85	120.30
7	I	5	DT	C6-C5-C7	-7.06	118.67	122.90
4	5	407	ARG	NE-CZ-NH2	7.04	123.82	120.30
4	5	549	ARG	NE-CZ-NH2	7.04	123.82	120.30
7	I	1	DT	N3-C2-O2	-7.01	118.09	122.30
7	I	8	DT	C6-C5-C7	-6.88	118.77	122.90
5	3	666	ARG	NE-CZ-NH1	6.85	123.72	120.30
2	7	560	ARG	NE-CZ-NH2	6.84	123.72	120.30
5	3	527	ARG	NE-CZ-NH1	6.83	123.72	120.30
7	I	4	DT	N3-C2-O2	-6.77	118.24	122.30
4	5	405	ARG	NE-CZ-NH1	6.71	123.65	120.30
2	7	718	ARG	NE-CZ-NH2	6.63	123.61	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	5	362	ARG	NE-CZ-NH1	6.62	123.61	120.30
4	5	490	ARG	NE-CZ-NH2	6.60	123.60	120.30
4	5	455	ARG	NE-CZ-NH2	6.53	123.56	120.30
2	7	400	ARG	NE-CZ-NH2	6.44	123.52	120.30
5	3	420	ARG	NE-CZ-NH2	6.44	123.52	120.30
6	4	778	ARG	NE-CZ-NH1	6.43	123.52	120.30
7	I	2	DT	C6-C5-C7	-6.42	119.05	122.90
7	I	2	DT	O4'-C1'-N1	6.42	112.50	108.00
6	4	830	ARG	NE-CZ-NH1	6.41	123.51	120.30
3	2	855	ARG	NE-CZ-NH2	6.39	123.50	120.30
7	I	12	DT	C6-C5-C7	-6.36	119.08	122.90
5	3	707	ARG	NE-CZ-NH1	6.34	123.47	120.30
5	3	559	ARG	NE-CZ-NH1	6.32	123.46	120.30
2	7	694	ARG	NE-CZ-NH2	6.31	123.45	120.30
4	5	613	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	6	594	ARG	NE-CZ-NH1	6.29	123.44	120.30
7	I	9	DT	N3-C2-O2	-6.26	118.54	122.30
2	7	668	ARG	NE-CZ-NH1	6.22	123.41	120.30
7	I	4	DT	C6-C5-C7	-6.20	119.18	122.90
3	2	794	ARG	NE-CZ-NH1	6.12	123.36	120.30
3	2	771	ARG	NE-CZ-NH1	6.10	123.35	120.30
7	I	10	DT	C6-C5-C7	-6.08	119.25	122.90
7	I	7	DT	C6-C5-C7	-6.07	119.26	122.90
5	3	570	ARG	NE-CZ-NH1	6.07	123.33	120.30
5	3	467	ARG	NE-CZ-NH1	6.03	123.31	120.30
7	I	6	DT	N3-C2-O2	-6.03	118.68	122.30
1	6	675	ARG	NE-CZ-NH1	6.01	123.31	120.30
5	3	339	ARG	NE-CZ-NH1	5.91	123.26	120.30
3	2	815	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	6	752	ARG	NE-CZ-NH1	5.89	123.25	120.30
5	3	687	ARG	NE-CZ-NH2	-5.89	117.36	120.30
3	2	509	ARG	NE-CZ-NH2	5.87	123.24	120.30
1	6	566	ARG	NE-CZ-NH1	-5.87	117.37	120.30
7	I	1	DT	C6-C5-C7	-5.86	119.39	122.90
5	3	687	ARG	NE-CZ-NH1	5.83	123.22	120.30
4	5	516	ARG	NE-CZ-NH1	5.80	123.20	120.30
6	4	718	ARG	NE-CZ-NH1	5.79	123.19	120.30
5	3	509	ARG	NE-CZ-NH1	5.72	123.16	120.30
7	I	6	DT	C6-C5-C7	-5.72	119.47	122.90
2	7	649	ARG	NE-CZ-NH1	5.72	123.16	120.30
7	I	4	DT	O4'-C1'-C2'	-5.71	101.33	105.90
3	2	705	ARG	NE-CZ-NH2	5.69	123.15	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	3	716	ARG	NE-CZ-NH1	5.68	123.14	120.30
7	I	14	DT	C6-C5-C7	-5.68	119.49	122.90
3	2	617	ARG	NE-CZ-NH1	5.67	123.14	120.30
7	I	13	DT	N3-C2-O2	-5.66	118.90	122.30
3	2	694	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	6	781	ARG	NE-CZ-NH2	5.62	123.11	120.30
7	I	10	DT	N3-C2-O2	-5.57	118.96	122.30
5	3	400	ARG	NH1-CZ-NH2	-5.56	113.28	119.40
7	I	13	DT	C6-C5-C7	-5.56	119.56	122.90
6	4	557	ARG	NE-CZ-NH2	5.53	123.06	120.30
3	2	858	ARG	NE-CZ-NH1	5.49	123.04	120.30
7	I	3	DT	C6-C5-C7	-5.48	119.61	122.90
6	4	642	ARG	NE-CZ-NH1	5.44	123.02	120.30
6	4	701	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	6	701	MET	CA-CB-CG	5.43	122.52	113.30
2	7	639	ARG	NE-CZ-NH1	5.42	123.01	120.30
7	I	15	DT	C4'-C3'-C2'	-5.40	98.24	103.10
6	4	681	ARG	NE-CZ-NH2	5.36	122.98	120.30
3	2	482	ARG	NE-CZ-NH2	5.36	122.98	120.30
7	I	16	DT	N3-C2-O2	-5.36	119.08	122.30
2	7	703	ARG	NE-CZ-NH2	5.36	122.98	120.30
3	2	749	ARG	NE-CZ-NH2	5.35	122.97	120.30
2	7	479	ARG	NE-CZ-NH2	5.34	122.97	120.30
1	6	614	ARG	NE-CZ-NH2	5.33	122.96	120.30
3	2	815	ARG	NE-CZ-NH1	5.31	122.96	120.30
2	7	413	ARG	NE-CZ-NH1	5.28	122.94	120.30
7	I	3	DT	N1-C2-N3	5.27	117.76	114.60
7	I	4	DT	C5-C6-N1	-5.27	120.54	123.70
5	3	348	ARG	NE-CZ-NH1	5.25	122.93	120.30
6	4	796	ARG	NH1-CZ-NH2	-5.25	113.62	119.40
4	5	675	ARG	NE-CZ-NH1	5.25	122.92	120.30
5	3	435	ARG	NE-CZ-NH2	5.24	122.92	120.30
3	2	485	ARG	NE-CZ-NH2	5.24	122.92	120.30
3	2	581	ARG	NE-CZ-NH1	5.22	122.91	120.30
7	I	8	DT	O4'-C4'-C3'	5.17	109.10	106.00
5	3	734	ARG	NE-CZ-NH2	5.15	122.88	120.30
5	3	471	CYS	CA-CB-SG	-5.11	104.80	114.00
2	7	666	ARG	NE-CZ-NH1	5.11	122.86	120.30
2	7	673	ARG	NE-CZ-NH1	5.11	122.85	120.30
1	6	770	ARG	NE-CZ-NH1	5.10	122.85	120.30
7	I	15	DT	C6-C5-C7	-5.08	119.85	122.90
7	I	1	DT	N1-C2-N3	5.05	117.63	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	I	2	DT	C4-C5-C6	5.05	121.03	118.00
7	I	1	DT	C4-C5-C6	5.05	121.03	118.00
5	3	700	ARG	NH1-CZ-NH2	-5.04	113.85	119.40
7	I	2	DT	N1-C2-N3	5.04	117.62	114.60
7	I	8	DT	C5-C6-N1	-5.02	120.69	123.70
2	7	593	ARG	NE-CZ-NH1	5.01	122.80	120.30

There are no chirality outliers.

All (21) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	2	534	ARG	Sidechain
3	2	617	ARG	Sidechain
3	2	657	TYR	Sidechain
3	2	824	ARG	Sidechain
5	3	559	ARG	Sidechain
5	3	687	ARG	Sidechain
6	4	642	ARG	Sidechain
6	4	774	TYR	Sidechain
4	5	630	ARG	Sidechain
4	5	658	ARG	Sidechain
1	6	566	ARG	Sidechain
1	6	708	ARG	Sidechain
1	6	828	TYR	Sidechain
2	7	451	ARG	Sidechain
2	7	479	ARG	Sidechain
2	7	526	PHE	Sidechain
2	7	574	TYR	Sidechain
2	7	593	ARG	Sidechain
2	7	598	PHE	Sidechain
2	7	668	ARG	Sidechain
7	I	4	DT	Sidechain

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	6	2551	2579	2573	6	0
2	7	2590	2652	2649	3	0
3	2	2724	2775	2764	8	0
4	5	2184	2276	2269	4	0
5	3	2618	2709	2705	5	0
6	4	2568	2655	2651	3	0
7	I	320	192	193	0	0
8	2	31	13	13	8	0
8	3	31	13	13	4	0
8	4	31	13	13	2	0
8	6	31	13	13	2	0
8	7	31	13	13	2	0
9	2	1	0	0	0	0
9	3	1	0	0	0	0
9	4	1	0	0	0	0
9	6	1	0	0	0	0
9	7	1	0	0	0	0
All	All	15715	15903	15869	29	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 (29) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:3:412:SER:H	8:3:1500:ANP:HNB1	1.14	0.96
2:7:463:GLY:H	8:7:1500:ANP:HNB1	1.19	0.86
1:6:578:SER:H	8:6:1500:ANP:HNB1	1.31	0.78
6:4:571:SER:H	8:4:1500:ANP:HNB1	1.33	0.75
5:3:377:ILE:HD13	5:3:407:MET:HE3	1.82	0.61
8:6:1500:ANP:PG	6:4:796:ARG:HH22	2.28	0.56
4:5:374:ILE:HA	4:5:428:PHE:CZ	2.45	0.51
2:7:463:GLY:N	8:7:1500:ANP:HNB1	1.98	0.51
4:5:626:PHE:CZ	4:5:650:ILE:HD13	2.47	0.50
5:3:414:ALA:H	8:3:1500:ANP:C5'	2.25	0.50
3:2:549:LYS:HZ2	8:2:1500:ANP:PB	2.34	0.50
5:3:415:LYS:HZ3	8:3:1500:ANP:PB	2.34	0.49
1:6:708:ARG:HH22	8:2:1500:ANP:PG	2.36	0.49
6:4:571:SER:N	8:4:1500:ANP:HNB1	2.06	0.48
3:2:520:PHE:CD2	3:2:823:MET:HG2	2.48	0.48
3:2:548:ALA:HA	8:2:1500:ANP:O1A	2.16	0.46
1:6:816:VAL:HG12	1:6:818:GLU:H	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:3:412:SER:N	8:3:1500:ANP:HNB1	1.96	0.45
1:6:798:ARG:HH12	8:2:1500:ANP:HNB1	1.62	0.44
4:5:433:SER:HB3	4:5:436:ALA:HB2	1.99	0.43
3:2:550:SER:HB3	8:2:1500:ANP:PA	2.59	0.43
1:6:572:CYS:HB2	1:6:709:PHE:CE1	2.54	0.43
4:5:414:LEU:O	4:5:522:ALA:HA	2.19	0.42
1:6:657:GLU:HG2	1:6:708:ARG:HB2	2.02	0.42
3:2:549:LYS:NZ	8:2:1500:ANP:O2B	2.53	0.41
3:2:550:SER:HB3	8:2:1500:ANP:O2A	2.20	0.41
2:7:497:VAL:HG13	2:7:553:ILE:HD12	2.02	0.41
3:2:550:SER:HB3	8:2:1500:ANP:O1A	2.21	0.41
3:2:763:LEU:HD23	3:2:763:LEU:HA	1.96	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	6	322/1017 (32%)	299 (93%)	23 (7%)	0	100	100
2	7	331/845 (39%)	315 (95%)	16 (5%)	0	100	100
3	2	334/868 (38%)	303 (91%)	31 (9%)	0	100	100
4	5	264/775 (34%)	251 (95%)	13 (5%)	0	100	100
5	3	330/971 (34%)	315 (96%)	15 (4%)	0	100	100
6	4	322/933 (34%)	306 (95%)	16 (5%)	0	100	100
All	All	1903/5409 (35%)	1789 (94%)	114 (6%)	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	6	276/886 (31%)	276 (100%)	0	100 100
2	7	287/753 (38%)	287 (100%)	0	100 100
3	2	298/770 (39%)	296 (99%)	2 (1%)	84 92
4	5	242/688 (35%)	242 (100%)	0	100 100
5	3	289/835 (35%)	288 (100%)	1 (0%)	92 97
6	4	287/848 (34%)	287 (100%)	0	100 100
All	All	1679/4780 (35%)	1676 (100%)	3 (0%)	93 98

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	2	569	GLN
3	2	752	GLU
5	3	420	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	6	658	GLN
3	2	551	GLN
3	2	561	HIS
3	2	768	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 5 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	ANP	7	1500	9	29,33,33	1.52	7 (24%)	31,52,52	1.67	6 (19%)
8	ANP	3	1500	9	29,33,33	1.75	4 (13%)	31,52,52	2.64	9 (29%)
8	ANP	6	1500	9	29,33,33	1.47	5 (17%)	31,52,52	2.36	10 (32%)
8	ANP	4	1500	9	29,33,33	1.80	9 (31%)	31,52,52	2.08	7 (22%)
8	ANP	2	1500	9	29,33,33	2.89	9 (31%)	31,52,52	2.29	6 (19%)

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	ANP	7	1500	9	-	4/14/38/38	0/3/3/3
8	ANP	3	1500	9	-	7/14/38/38	0/3/3/3
8	ANP	6	1500	9	-	6/14/38/38	0/3/3/3
8	ANP	4	1500	9	-	5/14/38/38	0/3/3/3
8	ANP	2	1500	9	-	4/14/38/38	0/3/3/3

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	2	1500	ANP	PB-O3A	-12.82	1.42	1.59
8	3	1500	ANP	PB-O3A	-5.52	1.52	1.59
8	4	1500	ANP	PB-O3A	-4.04	1.54	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	4	1500	ANP	PB-O1B	3.96	1.52	1.46
8	3	1500	ANP	PG-O1G	3.82	1.52	1.46
8	2	1500	ANP	PB-O2B	-3.77	1.46	1.56
8	6	1500	ANP	PB-O1B	3.54	1.51	1.46
8	7	1500	ANP	PB-O1B	3.49	1.51	1.46
8	2	1500	ANP	PG-N3B	-3.41	1.54	1.63
8	6	1500	ANP	O4'-C1'	3.01	1.45	1.41
8	6	1500	ANP	PG-O1G	2.99	1.50	1.46
8	4	1500	ANP	PG-O1G	2.89	1.50	1.46
8	2	1500	ANP	PB-N3B	-2.84	1.55	1.63
8	4	1500	ANP	PG-N3B	-2.76	1.56	1.63
8	4	1500	ANP	PG-O2G	-2.73	1.49	1.56
8	2	1500	ANP	PG-O1G	2.70	1.50	1.46
8	7	1500	ANP	PG-O3G	-2.57	1.49	1.56
8	7	1500	ANP	PG-O1G	2.55	1.50	1.46
8	3	1500	ANP	PG-N3B	-2.54	1.56	1.63
8	7	1500	ANP	PB-O2B	-2.54	1.49	1.56
8	4	1500	ANP	PB-O2B	-2.51	1.50	1.56
8	7	1500	ANP	C5-C4	-2.48	1.34	1.40
8	4	1500	ANP	O4'-C1'	2.41	1.44	1.41
8	3	1500	ANP	PB-N3B	-2.37	1.57	1.63
8	7	1500	ANP	PG-O2G	-2.26	1.50	1.56
8	4	1500	ANP	PB-N3B	-2.22	1.57	1.63
8	7	1500	ANP	PG-N3B	-2.21	1.57	1.63
8	2	1500	ANP	C5-C4	-2.17	1.35	1.40
8	2	1500	ANP	O4'-C1'	2.15	1.44	1.41
8	2	1500	ANP	PG-O3G	-2.11	1.51	1.56
8	2	1500	ANP	PG-O2G	-2.09	1.51	1.56
8	6	1500	ANP	C5-C4	-2.05	1.35	1.40
8	4	1500	ANP	C5-C4	-2.04	1.35	1.40
8	6	1500	ANP	PG-O2G	-2.03	1.51	1.56

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	3	1500	ANP	O1B-PB-N3B	-7.90	100.13	111.77
8	2	1500	ANP	PB-O3A-PA	-6.90	108.31	132.62
8	2	1500	ANP	O1B-PB-N3B	6.63	121.53	111.77
8	6	1500	ANP	O1G-PG-N3B	-6.62	102.03	111.77
8	3	1500	ANP	PB-O3A-PA	-6.19	110.81	132.62
8	6	1500	ANP	O3G-PG-O1G	-5.77	98.95	113.45
8	3	1500	ANP	O2B-PB-O3A	5.24	122.11	104.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	4	1500	ANP	O2B-PB-O3A	4.87	120.89	104.64
8	4	1500	ANP	C4-C5-N7	4.67	114.27	109.40
8	2	1500	ANP	C4-C5-N7	4.59	114.18	109.40
8	4	1500	ANP	O3A-PB-N3B	-4.59	93.87	106.59
8	7	1500	ANP	C4-C5-N7	4.40	113.99	109.40
8	6	1500	ANP	C4-C5-N7	4.35	113.94	109.40
8	3	1500	ANP	O3A-PB-N3B	-4.30	94.65	106.59
8	7	1500	ANP	PB-O3A-PA	-4.10	118.17	132.62
8	3	1500	ANP	C4-C5-N7	4.03	113.60	109.40
8	7	1500	ANP	O1B-PB-N3B	3.89	117.49	111.77
8	6	1500	ANP	O3A-PB-N3B	-3.67	96.40	106.59
8	6	1500	ANP	O2B-PB-O3A	3.66	116.85	104.64
8	6	1500	ANP	PB-O3A-PA	-3.60	119.92	132.62
8	4	1500	ANP	O1B-PB-N3B	3.43	116.83	111.77
8	3	1500	ANP	O4'-C1'-C2'	-3.43	101.91	106.93
8	4	1500	ANP	O2G-PG-O1G	-3.38	104.95	113.45
8	4	1500	ANP	PB-O3A-PA	-3.30	121.00	132.62
8	6	1500	ANP	O1B-PB-N3B	-3.25	106.99	111.77
8	2	1500	ANP	O3G-PG-O1G	-3.11	105.64	113.45
8	7	1500	ANP	O3G-PG-O1G	-2.76	106.51	113.45
8	3	1500	ANP	C3'-C2'-C1'	2.65	104.96	100.98
8	3	1500	ANP	C2-N1-C6	-2.56	114.37	118.75
8	6	1500	ANP	N6-C6-N1	-2.46	113.46	118.57
8	2	1500	ANP	O5'-C5'-C4'	-2.40	100.74	108.99
8	7	1500	ANP	O4'-C1'-C2'	-2.25	103.64	106.93
8	2	1500	ANP	O3A-PB-N3B	-2.25	100.36	106.59
8	4	1500	ANP	C3'-C2'-C1'	2.18	104.27	100.98
8	6	1500	ANP	O2G-PG-O3G	2.14	113.34	107.64
8	3	1500	ANP	N6-C6-N1	-2.13	114.15	118.57
8	6	1500	ANP	C5-C6-N6	2.09	123.53	120.35
8	7	1500	ANP	O3A-PB-N3B	-2.04	100.92	106.59

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	6	1500	ANP	PG-N3B-PB-O1B
8	6	1500	ANP	PA-O3A-PB-O1B
8	6	1500	ANP	PA-O3A-PB-O2B
8	6	1500	ANP	C5'-O5'-PA-O1A
8	6	1500	ANP	C5'-O5'-PA-O2A
8	7	1500	ANP	PB-N3B-PG-O1G

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Mol	Chain	Res	Type	Atoms
8	7	1500	ANP	PA-O3A-PB-O1B
8	7	1500	ANP	PA-O3A-PB-O2B
8	2	1500	ANP	PB-N3B-PG-O1G
8	2	1500	ANP	PG-N3B-PB-O1B
8	2	1500	ANP	PG-N3B-PB-O3A
8	3	1500	ANP	PB-N3B-PG-O1G
8	3	1500	ANP	PG-N3B-PB-O1B
8	3	1500	ANP	C5'-O5'-PA-O1A
8	3	1500	ANP	C5'-O5'-PA-O3A
8	3	1500	ANP	O4'-C4'-C5'-O5'
8	3	1500	ANP	C3'-C4'-C5'-O5'
8	4	1500	ANP	PB-N3B-PG-O1G
8	4	1500	ANP	C4'-C5'-O5'-PA
8	4	1500	ANP	O4'-C4'-C5'-O5'
8	4	1500	ANP	C3'-C4'-C5'-O5'
8	6	1500	ANP	C5'-O5'-PA-O3A
8	3	1500	ANP	C4'-C5'-O5'-PA
8	7	1500	ANP	C5'-O5'-PA-O1A
8	2	1500	ANP	O4'-C4'-C5'-O5'
8	4	1500	ANP	C5'-O5'-PA-O1A

There are no ring outliers.

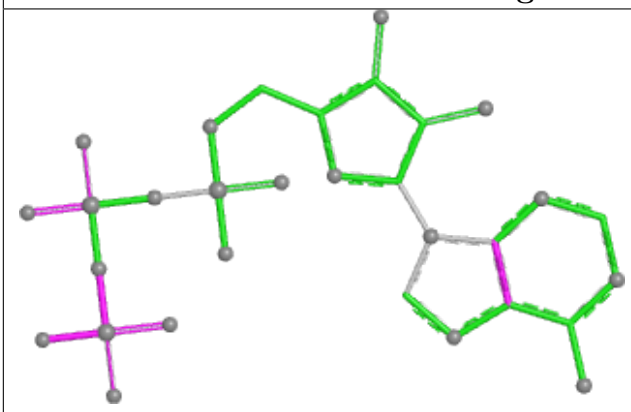
5 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	7	1500	ANP	2	0
8	3	1500	ANP	4	0
8	6	1500	ANP	2	0
8	4	1500	ANP	2	0
8	2	1500	ANP	8	0

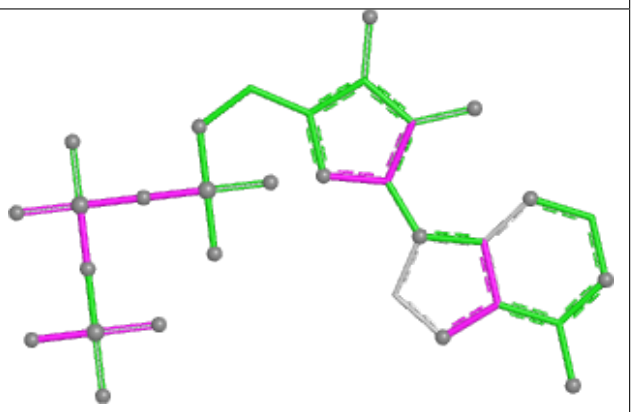
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

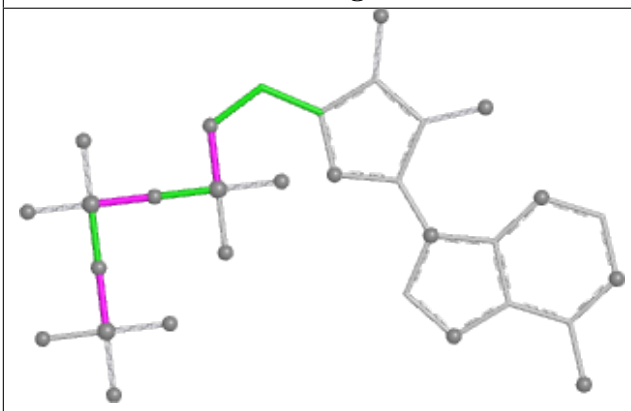
Ligand ANP 7 1500



Bond lengths



Bond angles



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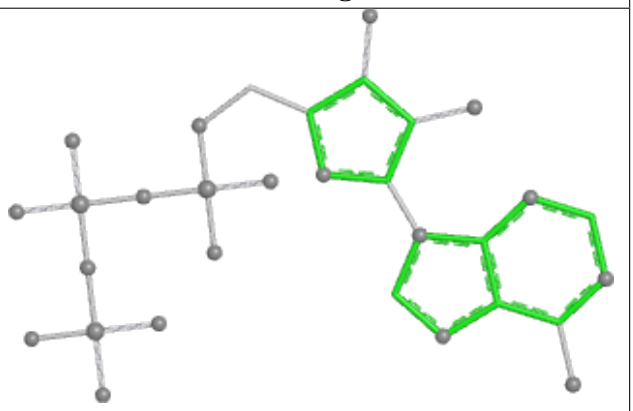

Rings

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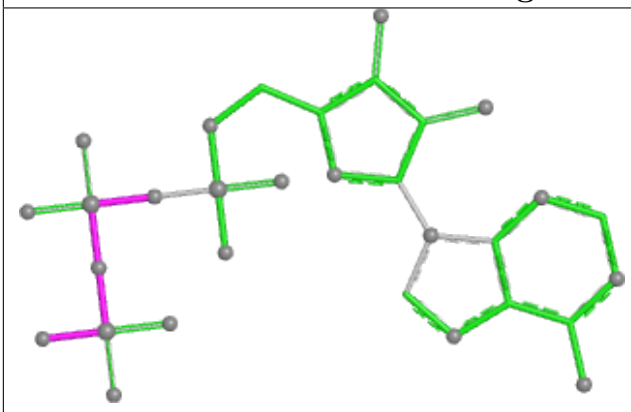
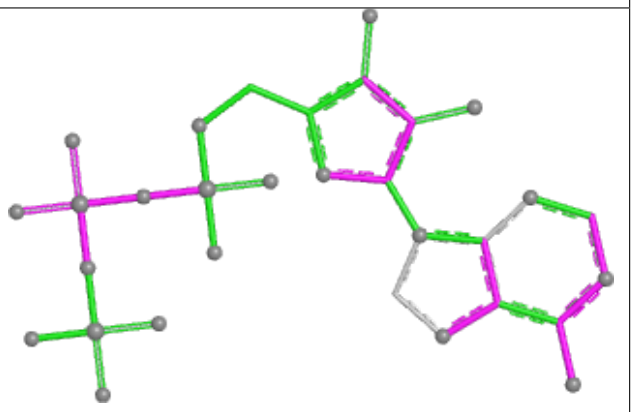
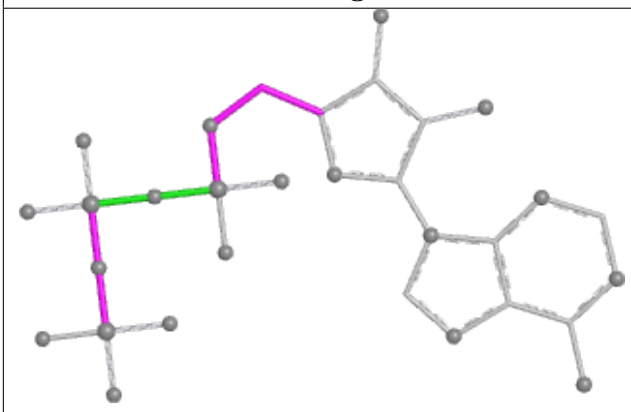


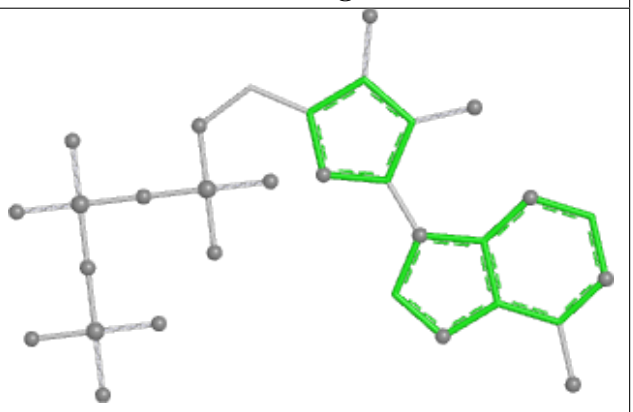
Bond lengths



Bond angles

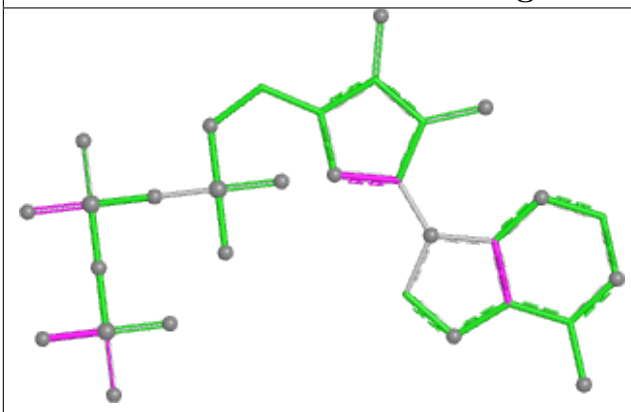


Torsions

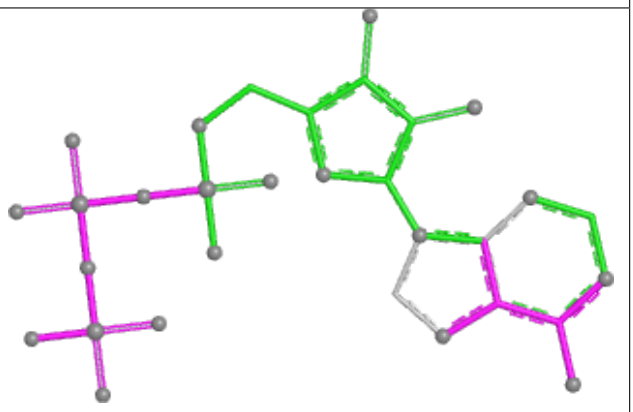


Rings

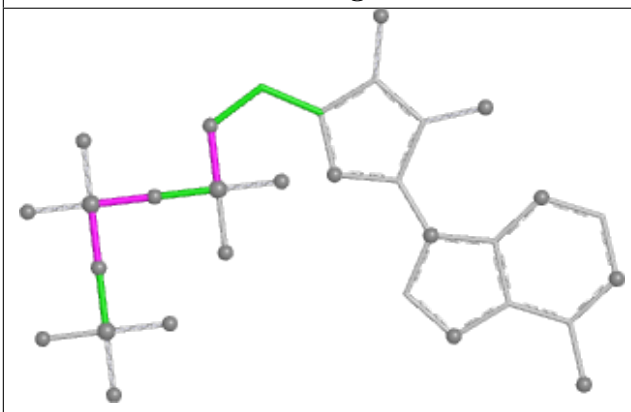
Ligand ANP 6 1500



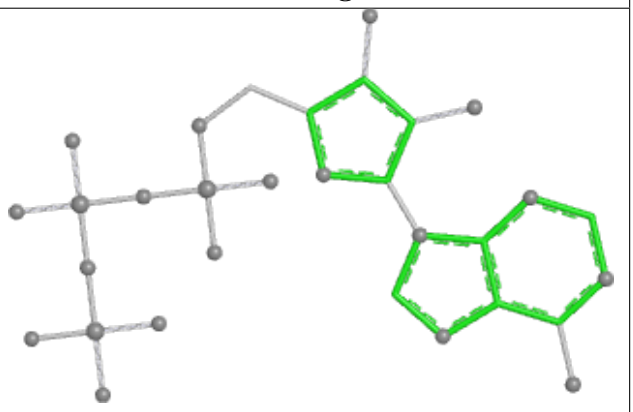
Bond lengths



Bond angles

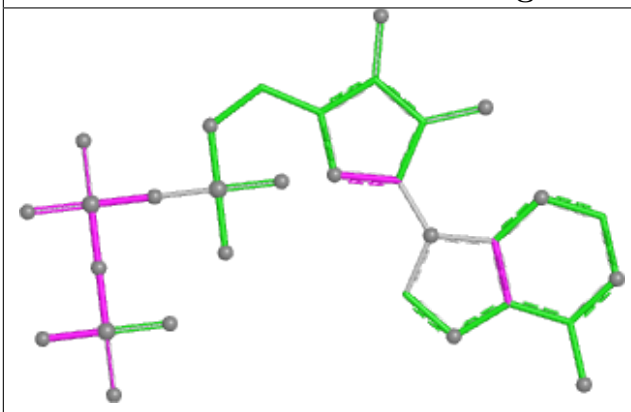


Torsions

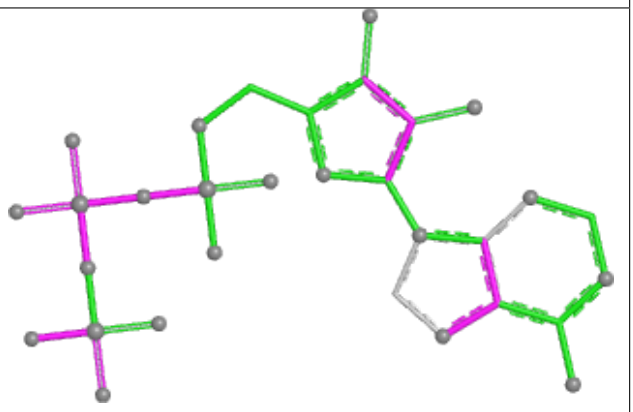


Rings

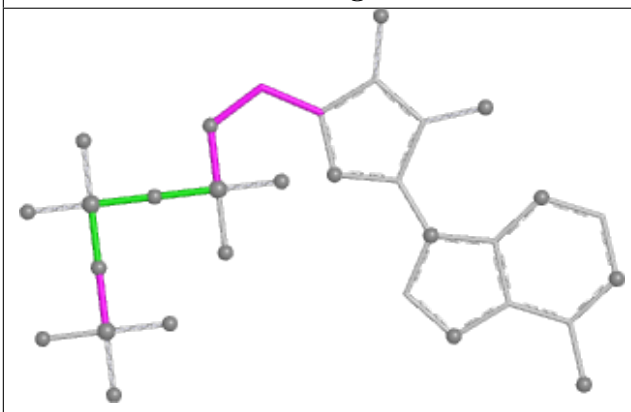
Ligand ANP 4 1500



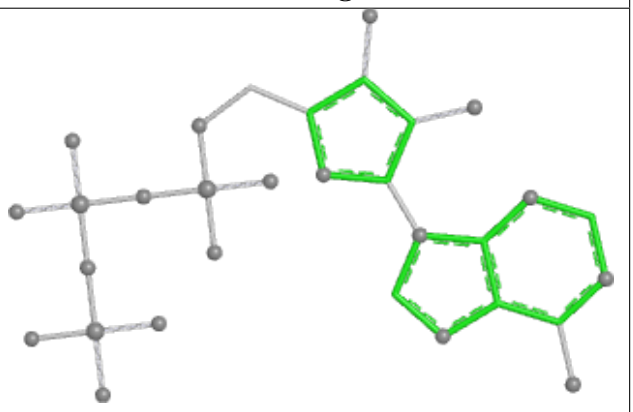
Bond lengths



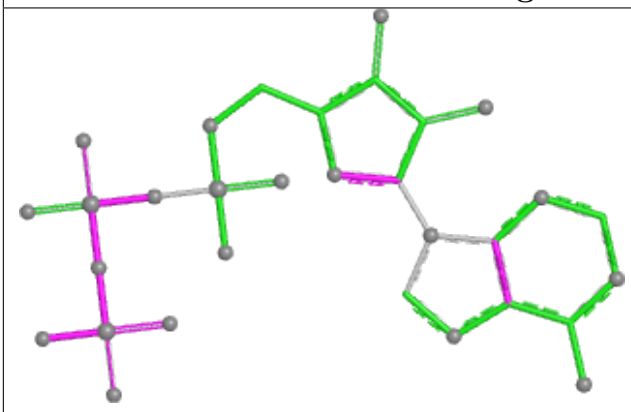
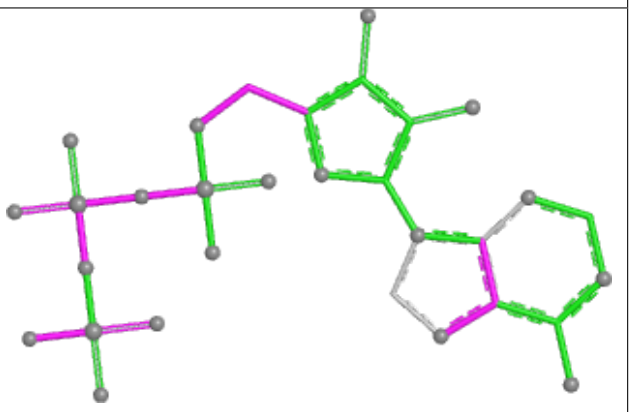
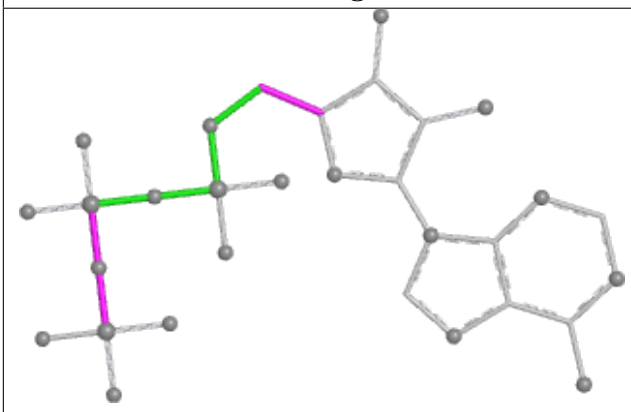
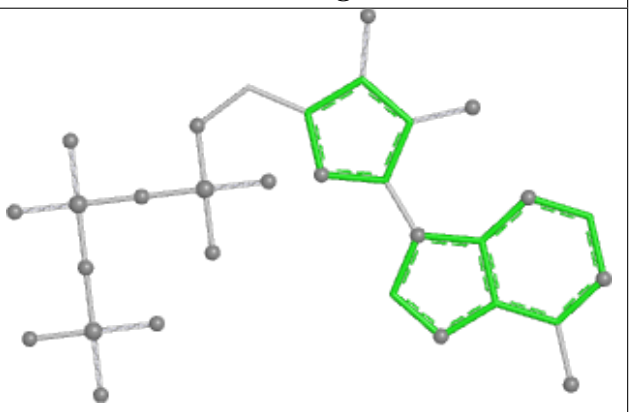
Bond angles



Torsions



Rings

Ligand ANP 2 1500	
 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.

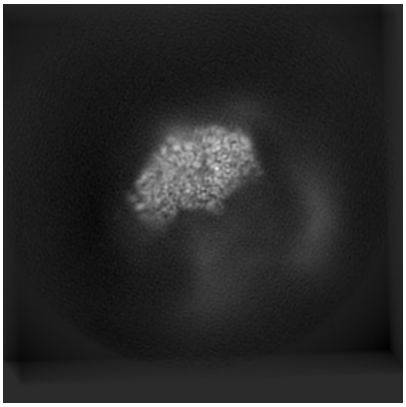
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-10230. These allow visual inspection of the internal detail of the map and identification of artifacts.

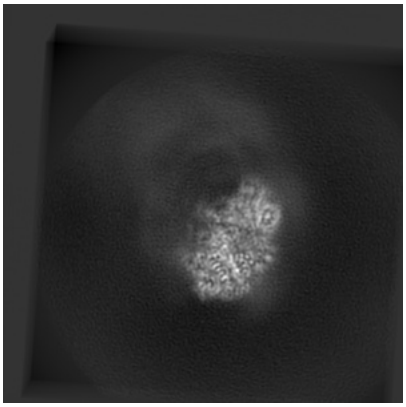
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

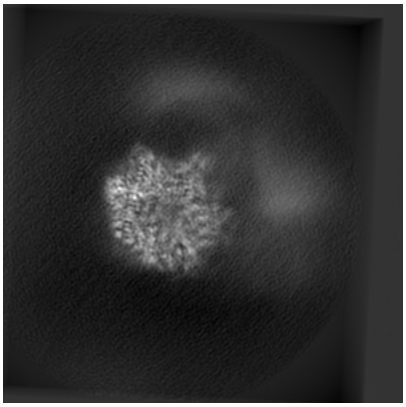
6.1.1 Primary map



X



Y

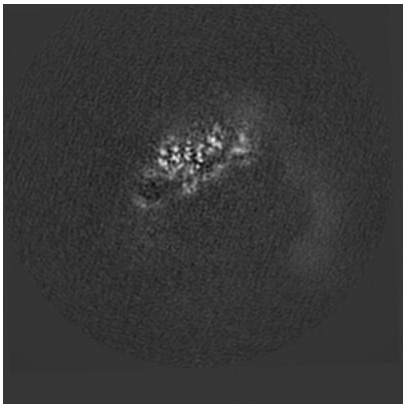


Z

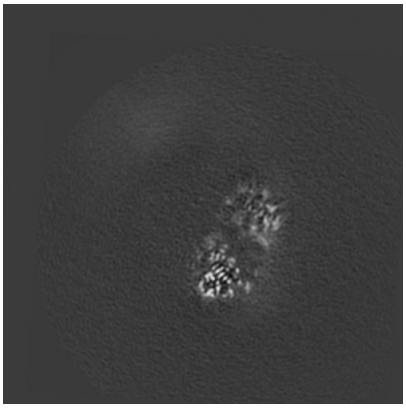
The images above show the map projected in three orthogonal directions.

6.2 Central slices

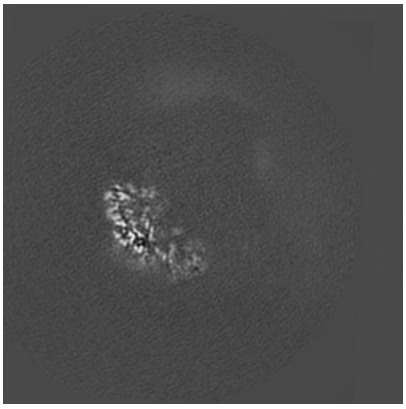
6.2.1 Primary map



X Index: 180



Y Index: 180

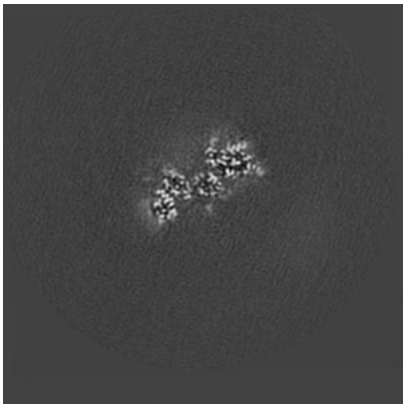


Z Index: 180

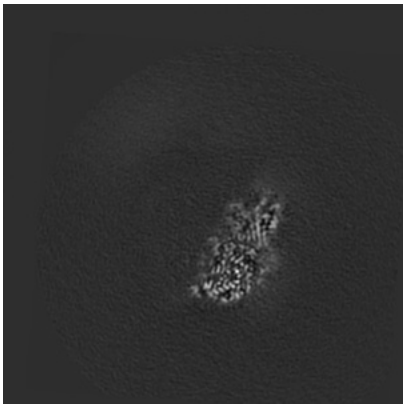
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

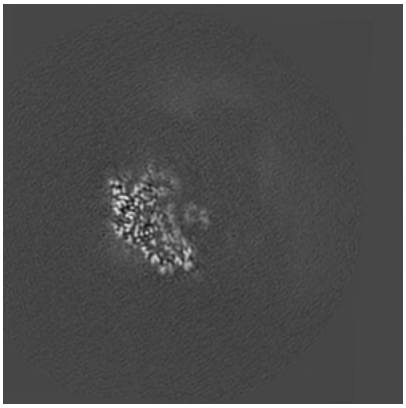
6.3.1 Primary map



X Index: 123



Y Index: 193

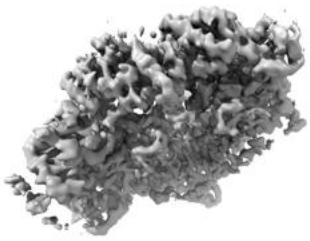


Z Index: 193

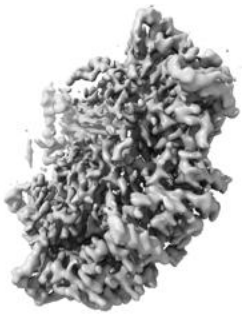
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

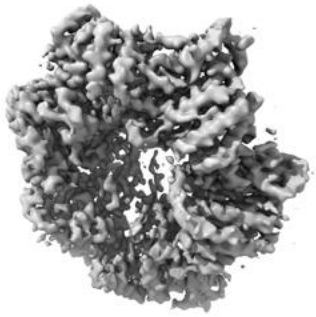
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.014. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

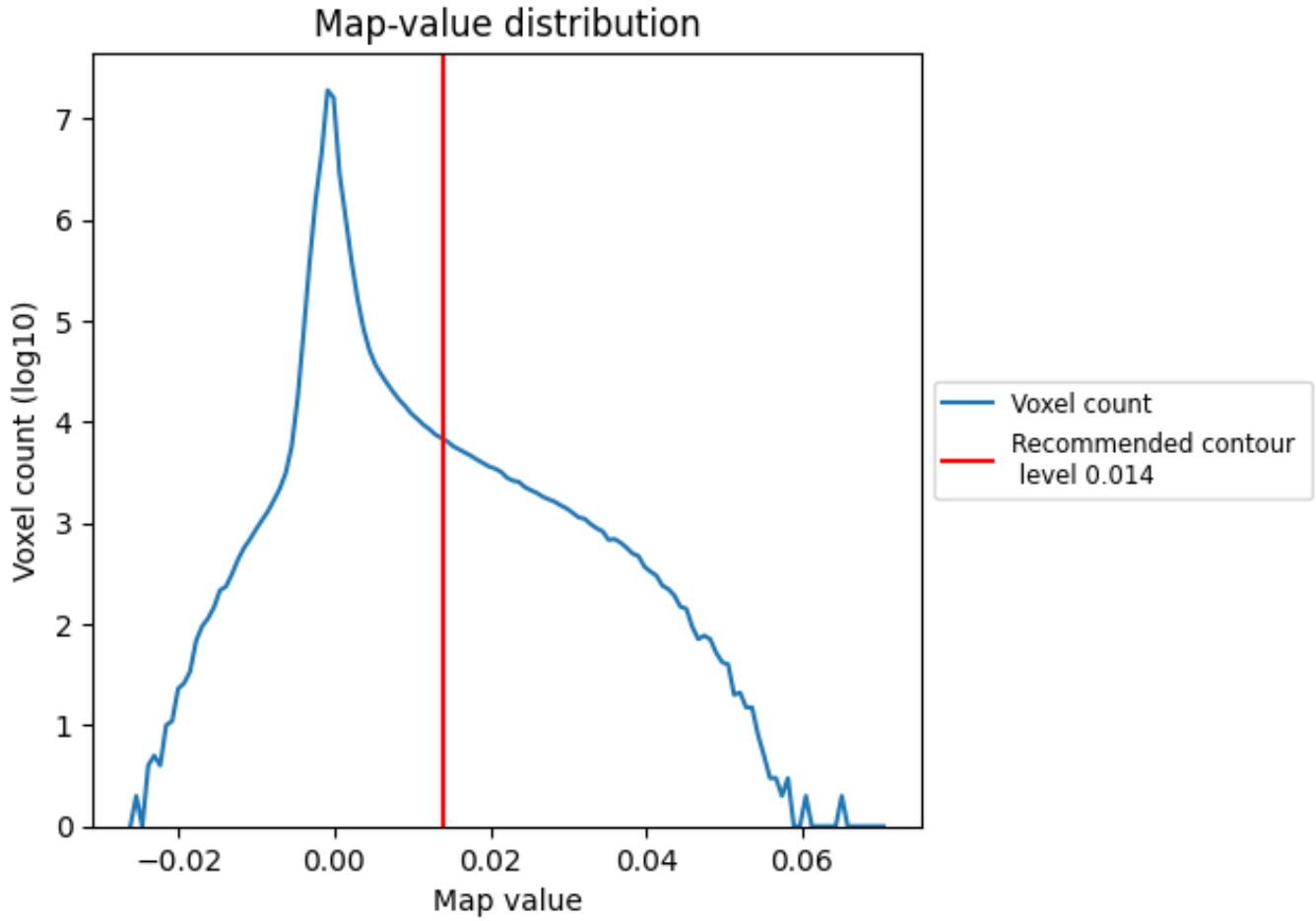
6.5 Mask visualisation (i)

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

7 Map analysis

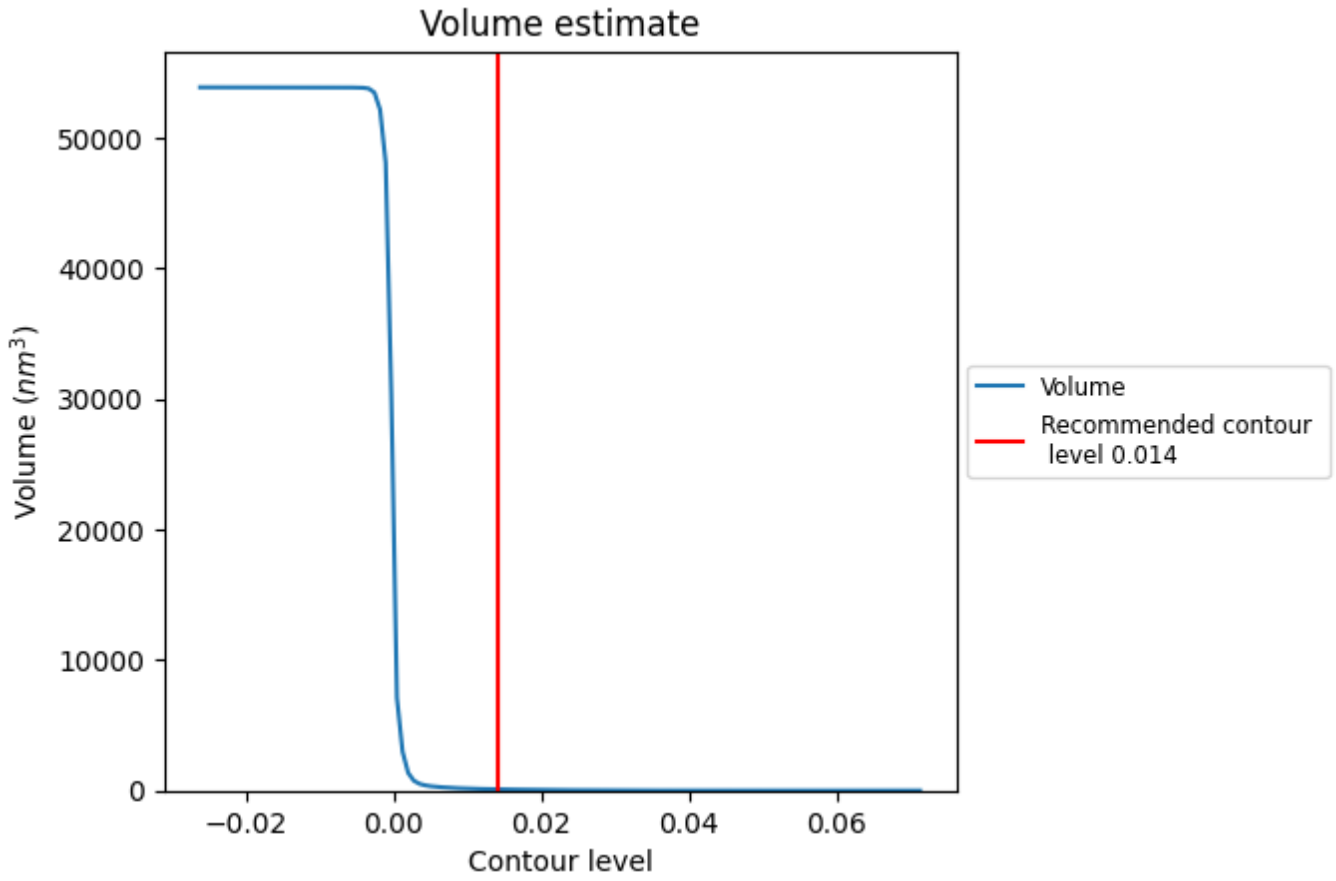
This section contains the results of statistical analysis of the map.

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.

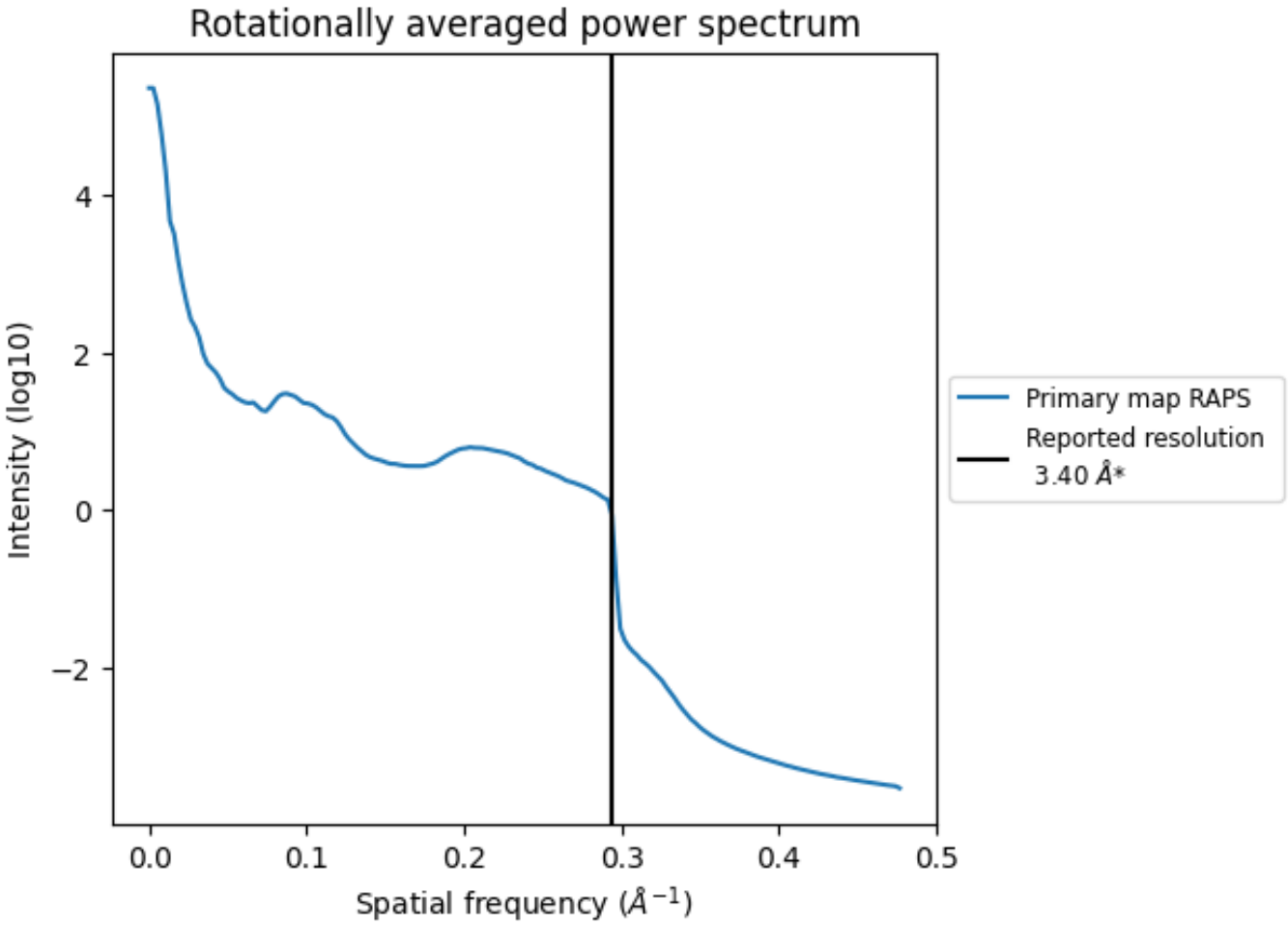
7.2 Volume estimate (i)



The volume at the recommended contour level is 97 nm^3; this corresponds to an approximate mass of 88 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)

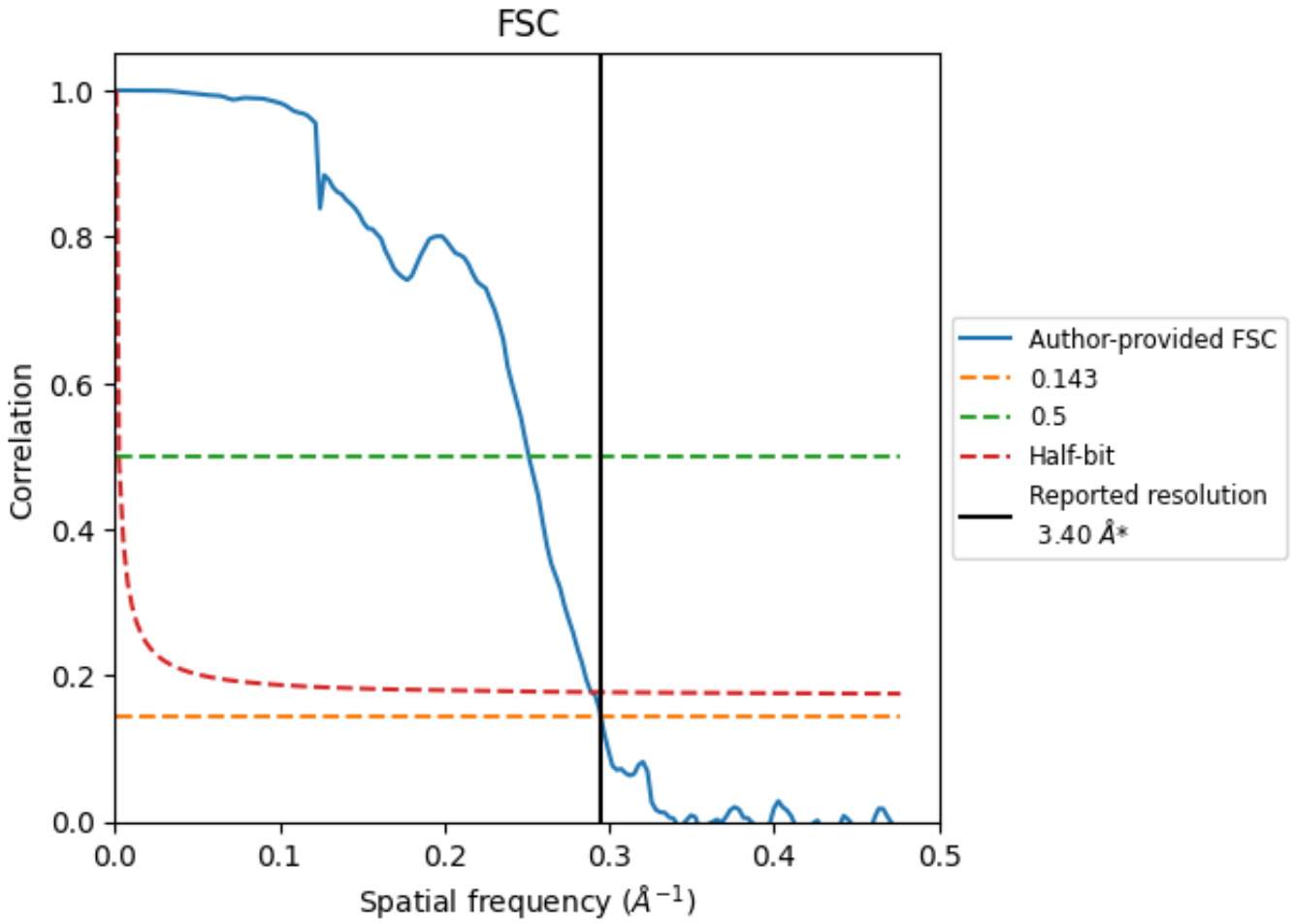


*Reported resolution corresponds to spatial frequency of 0.294 $Å^{-1}$

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 0.294 Å^{-1}

8.2 Resolution estimates (i)

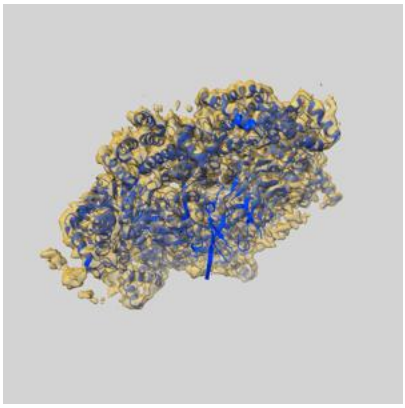
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.39	3.98	3.46
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

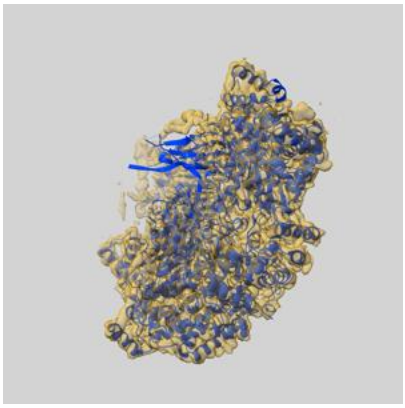
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-10230 and PDB model 6SKO. Per-residue inclusion information can be found in section 3 on page 6.

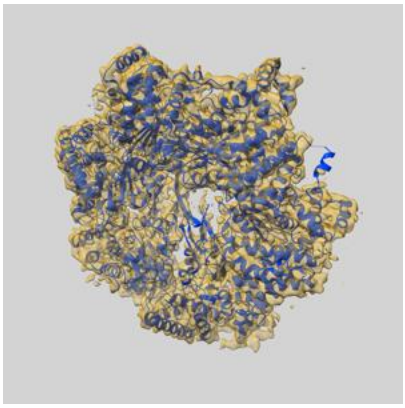
9.1 Map-model overlay



X



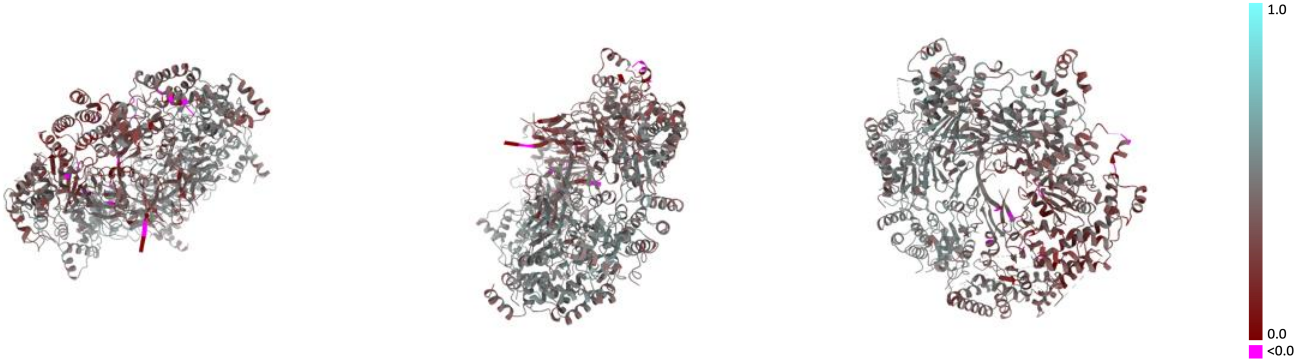
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.014 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.

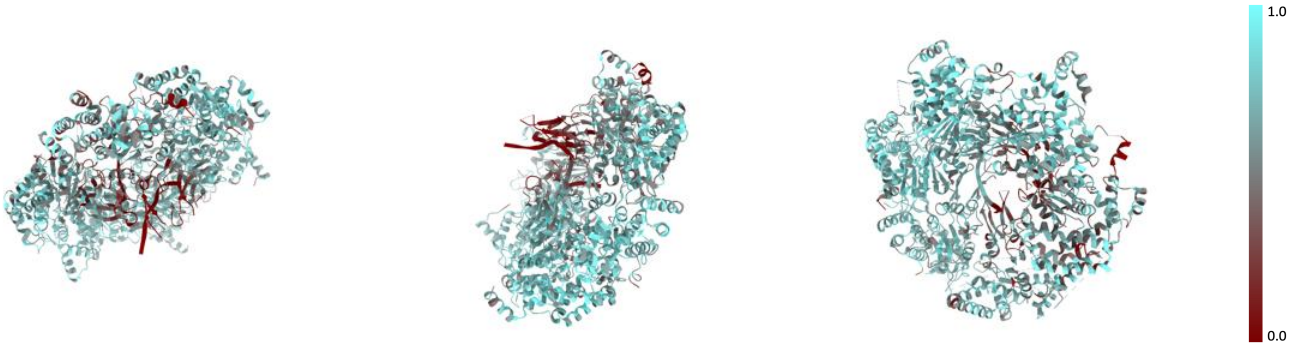
9.2 Q-score mapped to coordinate model



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.

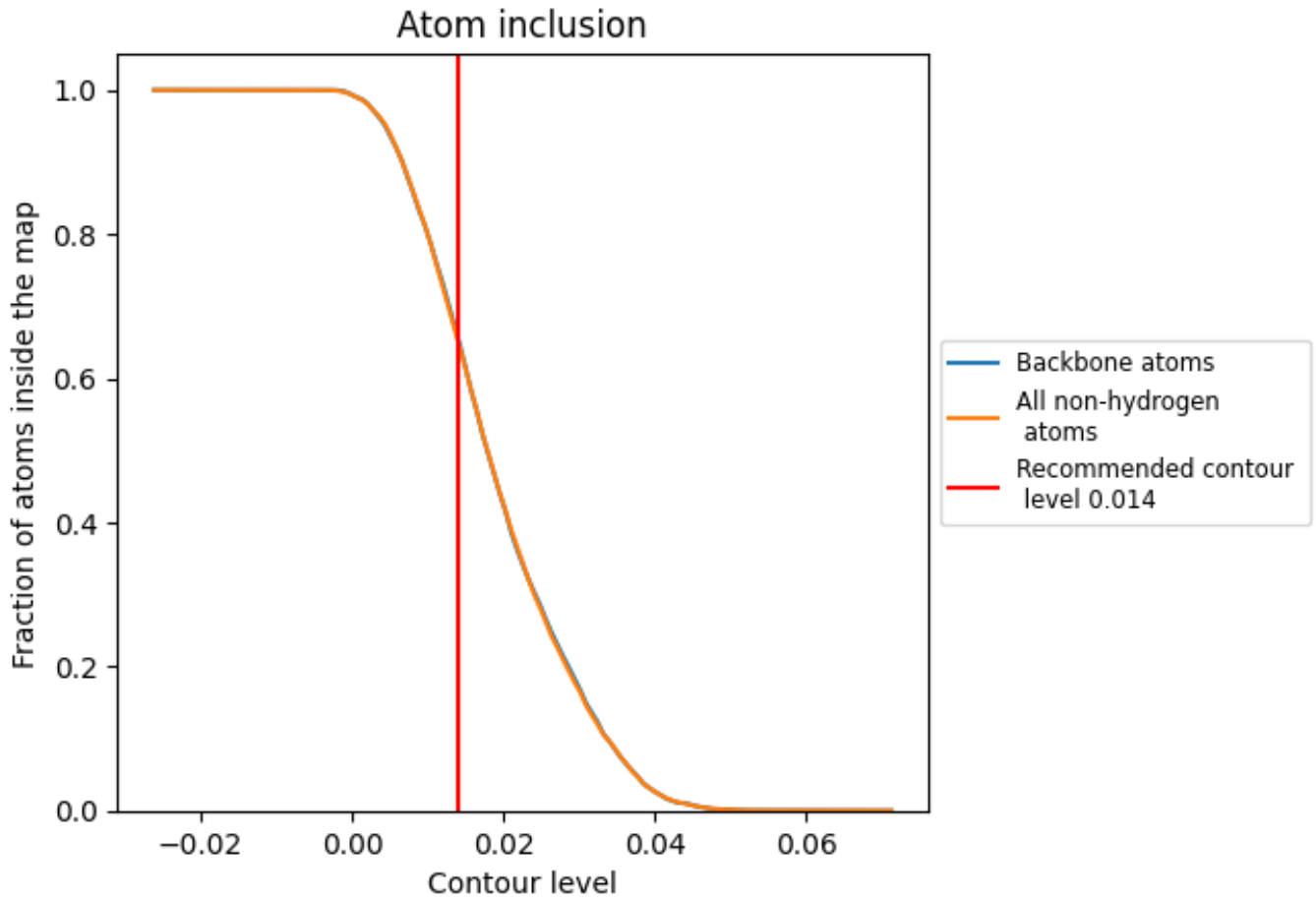
9.3 Atom inclusion mapped to coordinate model



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 (0.014).

9.4 Atom inclusion (i)



At the recommended contour level, 66% of all backbone atoms, 65% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.014) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6510	0.4110
2	0.5318	0.3080
3	0.7380	0.4690
4	0.7346	0.4670
5	0.6149	0.3570
6	0.6410	0.4100
7	0.7606	0.4640
I	0.2844	0.3080