



wwPDB EM Validation Summary Report ⓘ

Oct 5, 2024 – 10:59 PM EDT

PDB ID : 6PTO
EMDB ID : EMD-20473
Title : Structure of Ctf4 trimer in complex with three CMG helicases
Authors : Yuan, Z.; Georgescu, R.; Bai, L.; Santos, R.; Donnell, M.; Li, H.
Deposited on : 2019-07-16
Resolution : 7.00 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

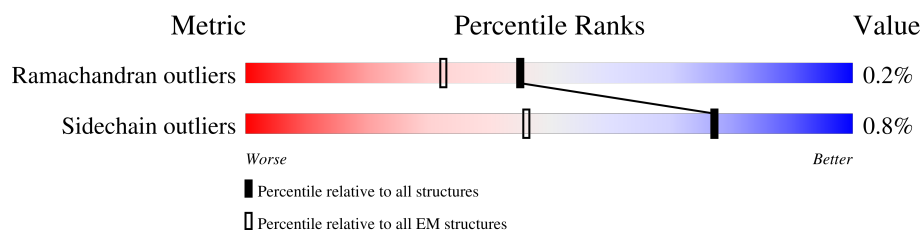
EMDB validation analysis : 0.0.1.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

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 7.00 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)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	X	927	
1	Y	927	
1	Z	927	
2	A	208	
2	a	208	
2	n	208	
3	B	213	
3	b	213	
3	o	213	

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Mol	Chain	Length	Quality of chain
4	C	194	
4	c	194	
4	p	194	
5	D	294	
5	d	294	
5	q	294	
6	E	650	
6	e	650	
6	r	650	
7	2	868	
7	F	868	
7	h	868	
8	3	971	
8	G	971	
8	i	971	
9	4	933	
9	H	933	
9	j	933	
10	5	775	
10	I	775	
10	k	775	
11	6	1017	
11	J	1017	
11	l	1017	
12	7	845	

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Mol	Chain	Length	Quality of chain
12	K	845	<div><div><div>64%</div><div>78%</div><div>22%</div></div></div>
12	m	845	<div><div><div>46%</div><div>78%</div><div>22%</div></div></div>

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 132192 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 polymerase alpha-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	X	424	Total	C	N	O	S	1	0
			3416	2193	566	642	15		
1	Y	431	Total	C	N	O	S	0	0
			3464	2223	574	651	16		
1	Z	424	Total	C	N	O	S	1	0
			3416	2193	566	642	15		

- Molecule 2 is a protein called DNA replication complex GINS protein PSF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	n	208	Total	C	N	O	S	0	0
			1696	1065	290	331	10		
2	A	208	Total	C	N	O	S	0	0
			1696	1065	290	331	10		
2	a	208	Total	C	N	O	S	0	0
			1696	1065	290	331	10		

- Molecule 3 is a protein called DNA replication complex GINS protein PSF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	o	181	Total	C	N	O	S	0	0
			1513	978	261	270	4		
3	B	181	Total	C	N	O	S	0	0
			1513	978	261	270	4		
3	b	181	Total	C	N	O	S	0	0
			1513	978	261	270	4		

- Molecule 4 is a protein called DNA replication complex GINS protein PSF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	p	159	Total	C	N	O	S	0	0
			1288	843	207	232	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	159	Total	C	N	O	S	0	0
			1288	843	207	232	6		
4	c	159	Total	C	N	O	S	0	0
			1288	843	207	232	6		

- Molecule 5 is a protein called DNA replication complex GINS protein SLD5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	q	234	Total	C	N	O	S	0	0
			1924	1224	315	372	13		
5	D	234	Total	C	N	O	S	0	0
			1924	1224	315	372	13		
5	d	234	Total	C	N	O	S	0	0
			1924	1224	315	372	13		

- Molecule 6 is a protein called Cell division control protein 45.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	e	553	Total	C	N	O	S	0	0
			4482	2862	763	844	13		
6	E	553	Total	C	N	O	S	0	0
			4482	2862	763	844	13		
6	r	553	Total	C	N	O	S	0	0
			4482	2862	763	844	13		

- Molecule 7 is a protein called DNA replication licensing factor MCM2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	h	634	Total	C	N	O	S	0	0
			4970	3122	897	934	17		
7	2	634	Total	C	N	O	S	0	0
			4970	3122	897	934	17		
7	F	634	Total	C	N	O	S	0	0
			4970	3122	897	934	17		

- Molecule 8 is a protein called DNA replication licensing factor MCM3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	i	594	Total	C	N	O	S	0	0
			4659	2936	832	878	13		
8	3	594	Total	C	N	O	S	0	0
			4659	2936	832	878	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	594	Total	C	N	O	S	0	0
			4659	2936	832	878	13		

- Molecule 9 is a protein called DNA replication licensing factor MCM4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	j	682	Total	C	N	O	S	0	0
			5410	3397	946	1039	28		
9	4	682	Total	C	N	O	S	0	0
			5410	3397	946	1039	28		
9	H	682	Total	C	N	O	S	0	0
			5410	3397	946	1039	28		

- Molecule 10 is a protein called Minichromosome maintenance protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	k	597	Total	C	N	O	S	0	0
			4688	2946	808	910	24		
10	5	597	Total	C	N	O	S	0	0
			4688	2946	808	910	24		
10	I	597	Total	C	N	O	S	0	0
			4688	2946	808	910	24		

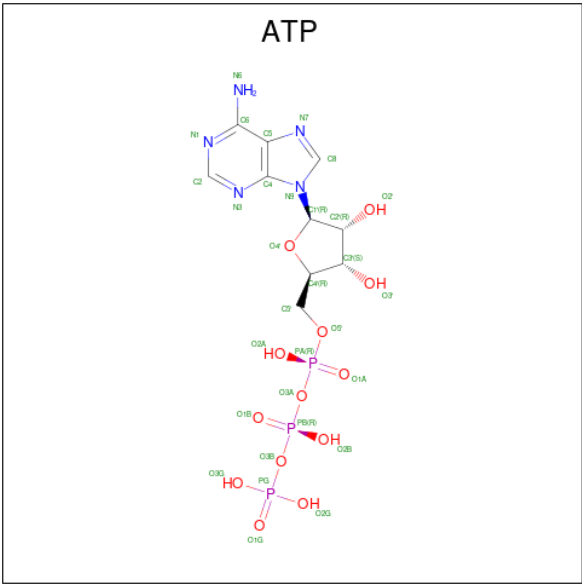
- Molecule 11 is a protein called DNA replication licensing factor MCM6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	l	614	Total	C	N	O	S	0	0
			4720	2971	836	893	20		
11	6	614	Total	C	N	O	S	0	0
			4720	2971	836	893	20		
11	J	614	Total	C	N	O	S	0	0
			4720	2971	836	893	20		

- Molecule 12 is a protein called DNA replication licensing factor MCM7.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	m	663	Total	C	N	O	S	0	0
			5220	3290	904	996	30		
12	7	663	Total	C	N	O	S	0	0
			5220	3290	904	996	30		
12	K	663	Total	C	N	O	S	0	0
			5220	3290	904	996	30		

- Molecule 13 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).

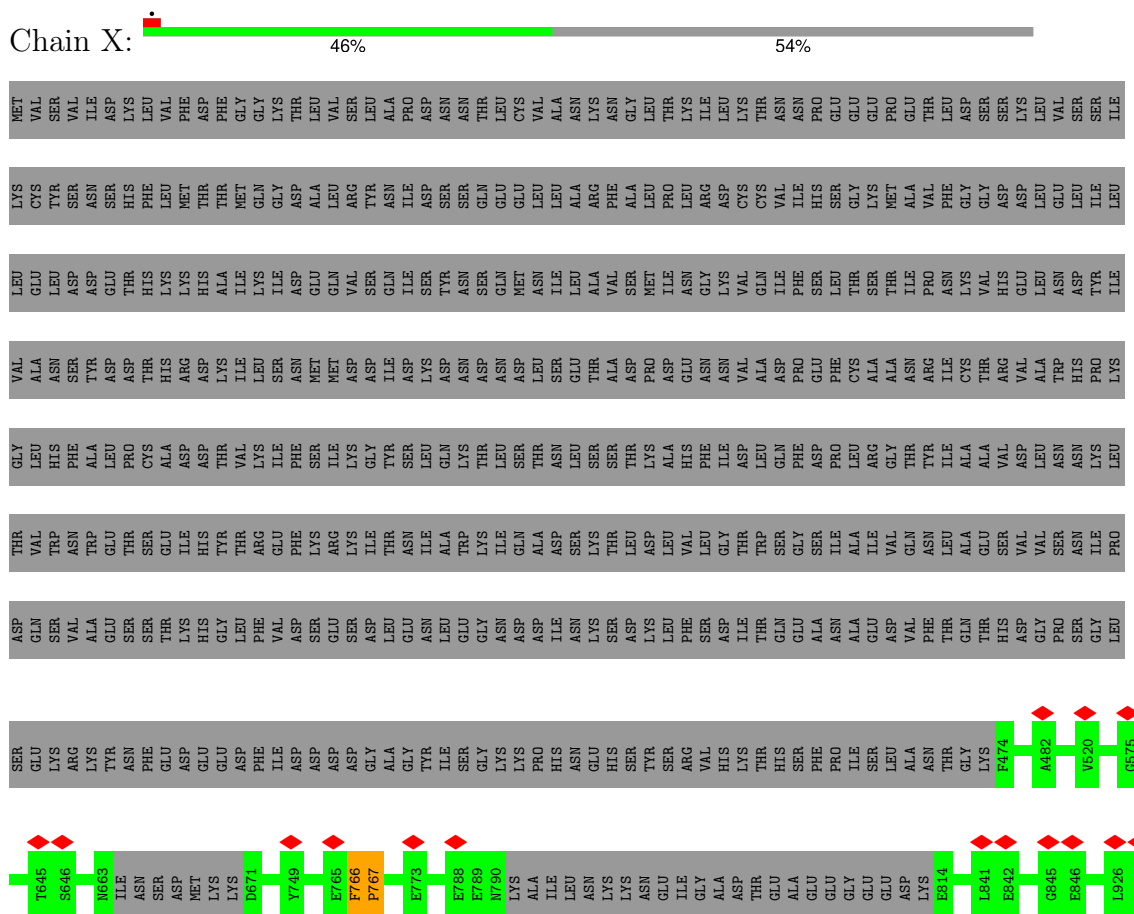


Mol	Chain	Residues	Atoms					AltConf
13	h	1	Total	C	N	O	P	0
			31	10	5	13	3	
13	i	1	Total	C	N	O	P	0
			31	10	5	13	3	
13	k	1	Total	C	N	O	P	0
			31	10	5	13	3	
13	2	1	Total	C	N	O	P	0
			31	10	5	13	3	
13	3	1	Total	C	N	O	P	0
			31	10	5	13	3	
13	5	1	Total	C	N	O	P	0
			31	10	5	13	3	

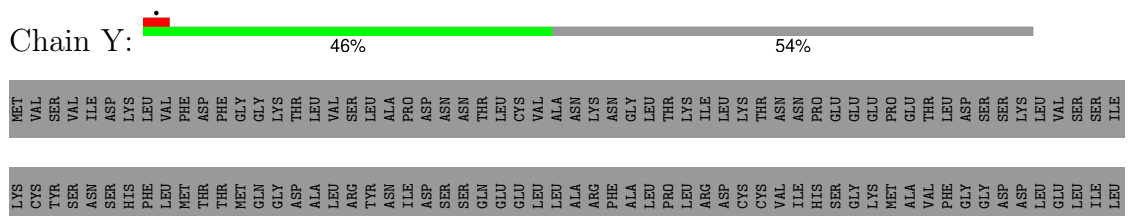
3 Residue-property plots

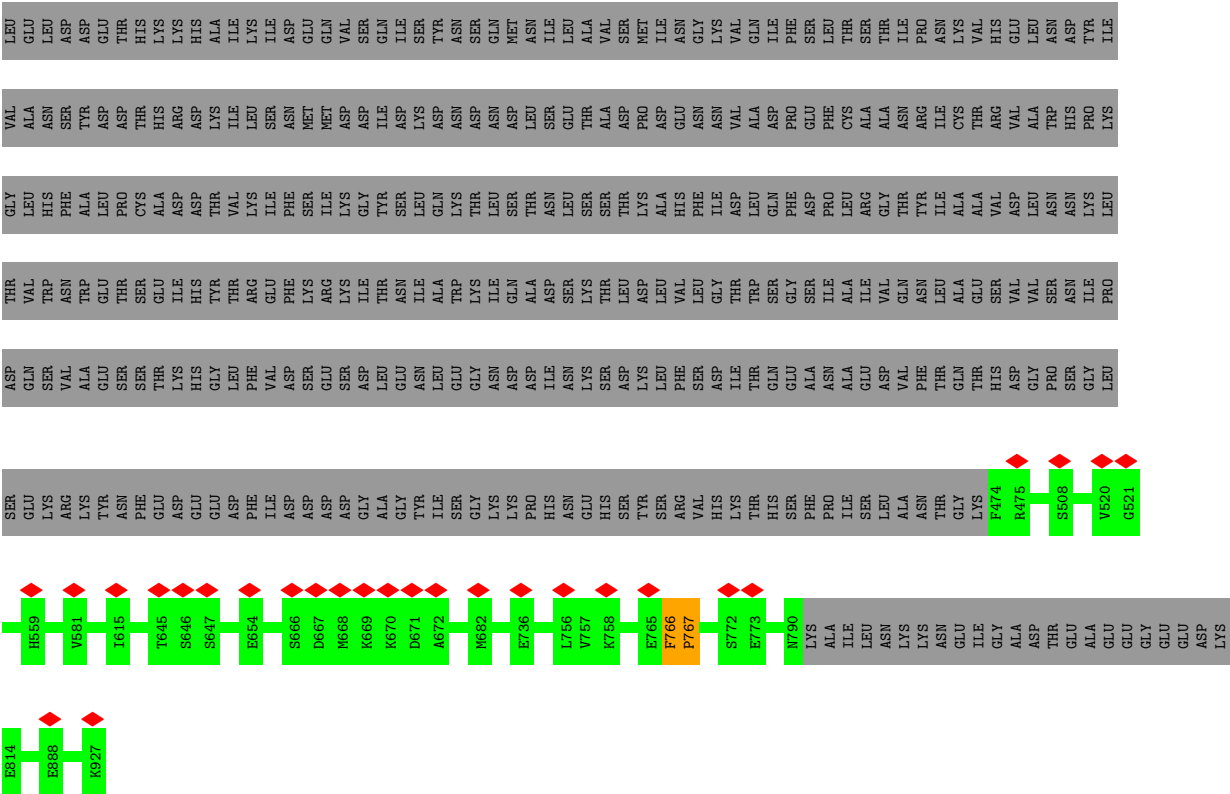
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: DNA polymerase alpha-binding protein

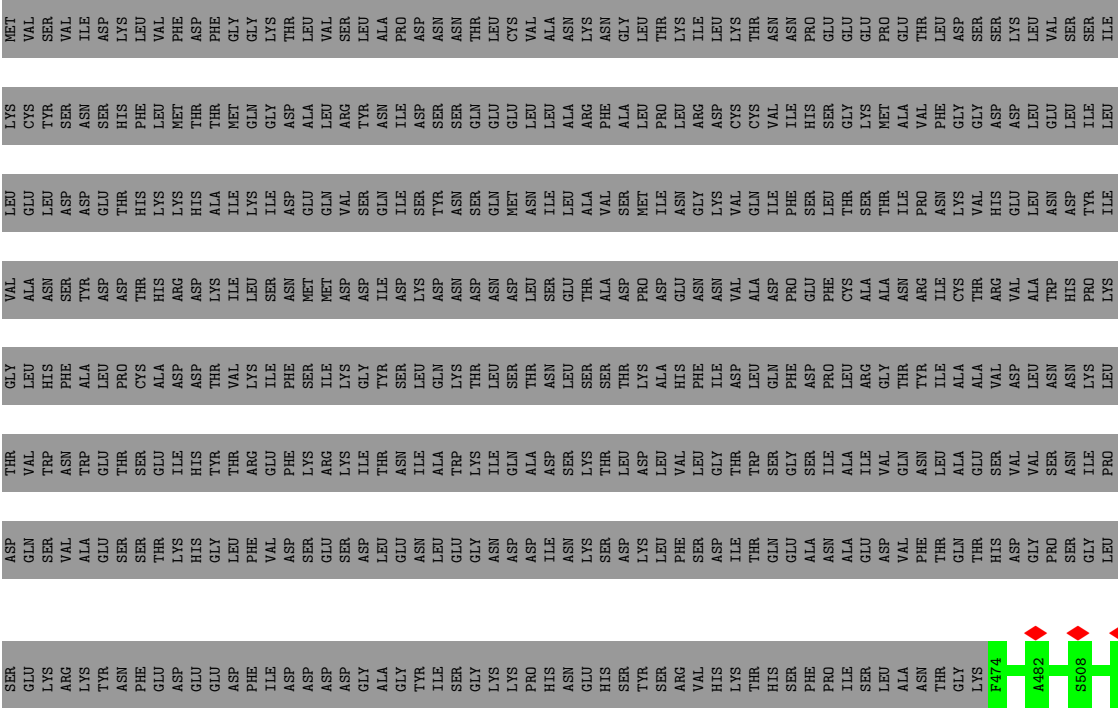


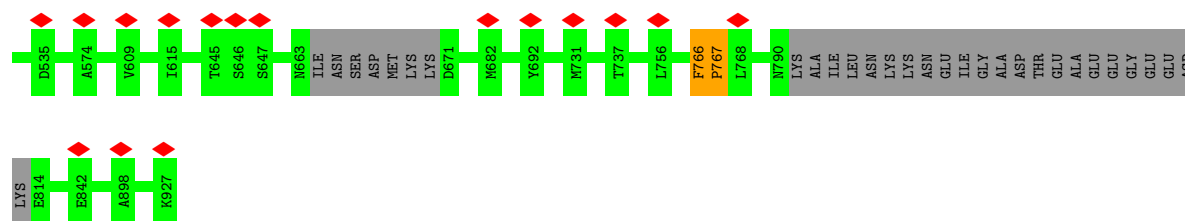
- Molecule 1: DNA polymerase alpha-binding protein



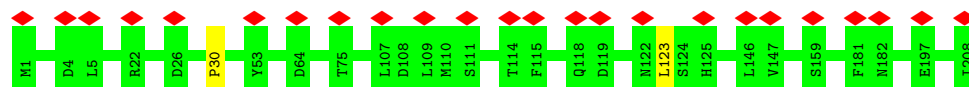


● Molecule 1: DNA polymerase alpha-binding protein

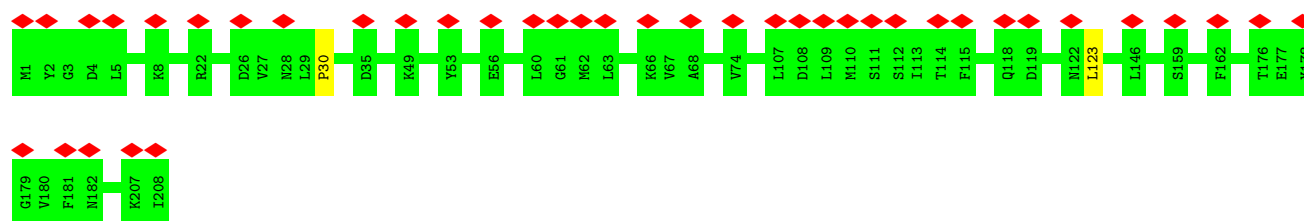




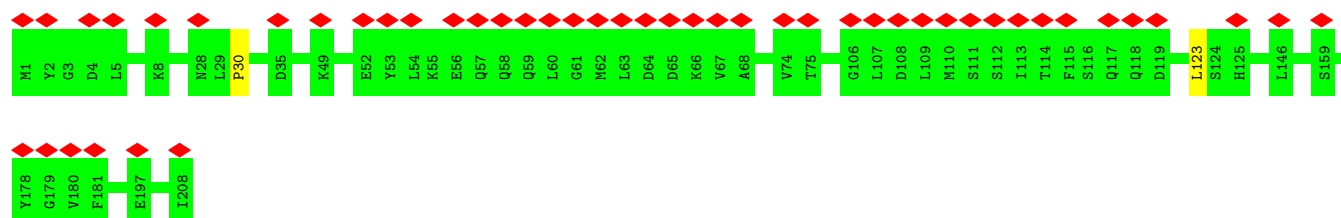
- Molecule 2: DNA replication complex GINS protein PSF1



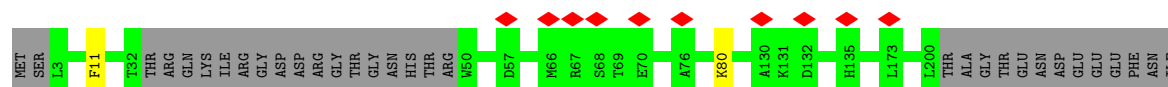
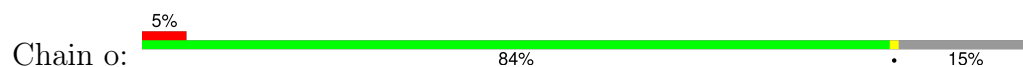
- Molecule 2: DNA replication complex GINS protein PSF1



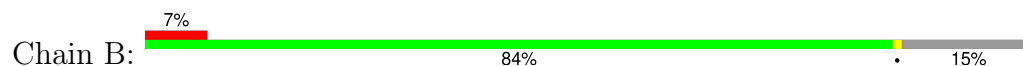
- Molecule 2: DNA replication complex GINS protein PSF1

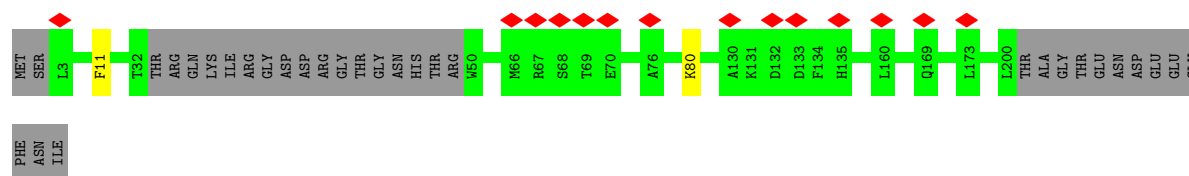


- Molecule 3: DNA replication complex GINS protein PSF2

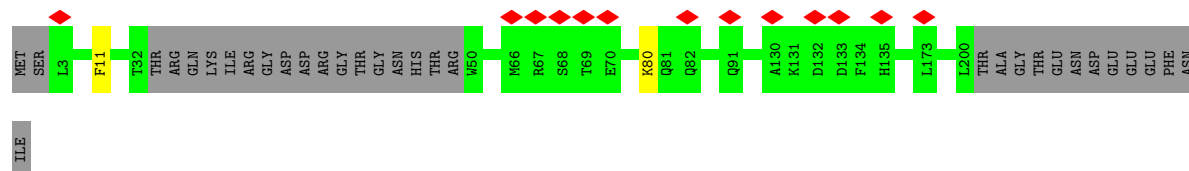
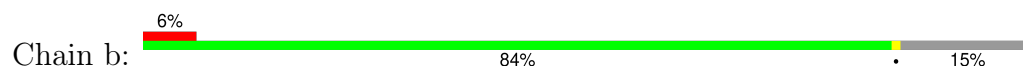


- Molecule 3: DNA replication complex GINS protein PSF2

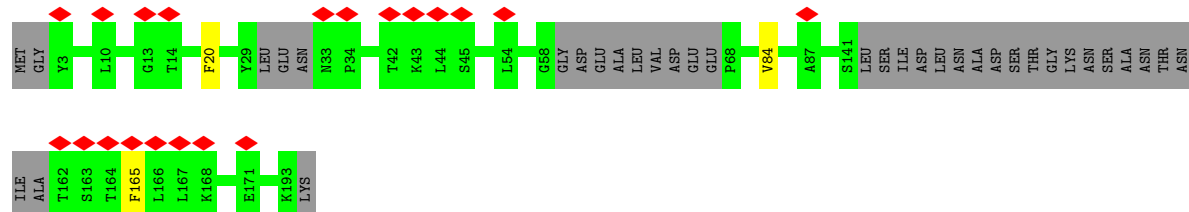
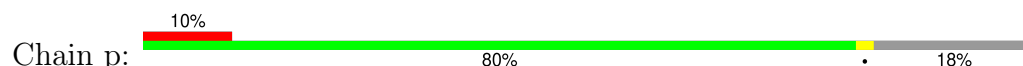




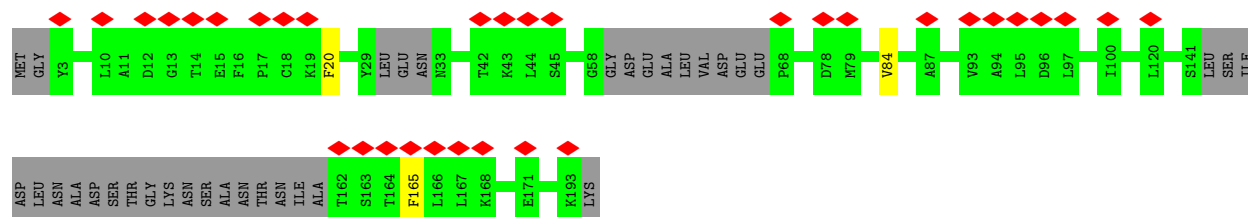
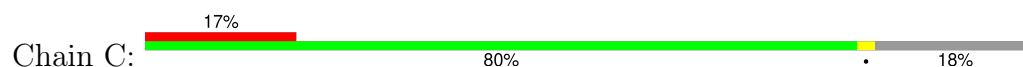
- Molecule 3: DNA replication complex GINS protein PSF2



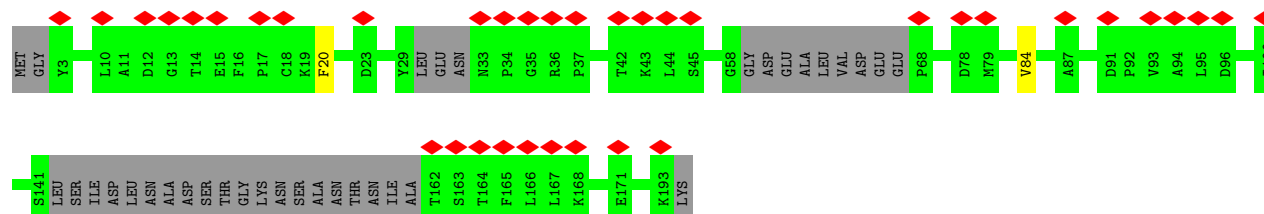
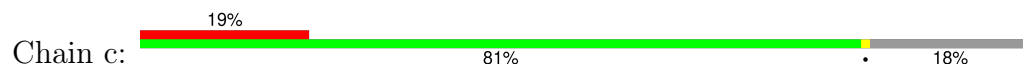
- Molecule 4: DNA replication complex GINS protein PSF3



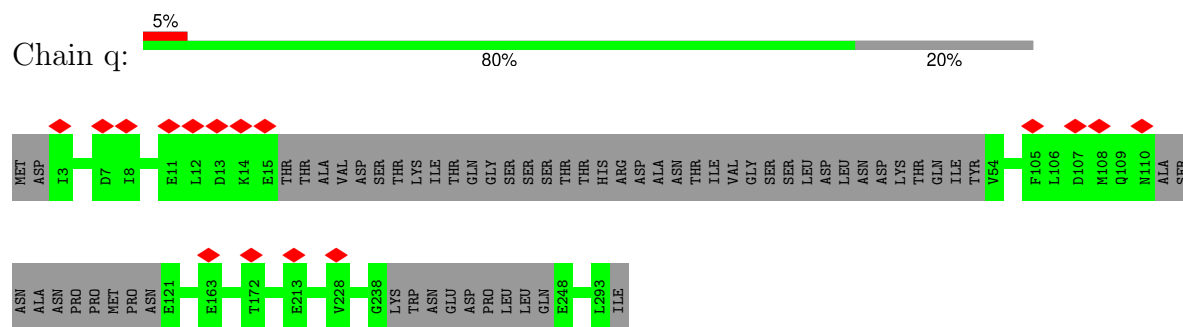
- Molecule 4: DNA replication complex GINS protein PSF3



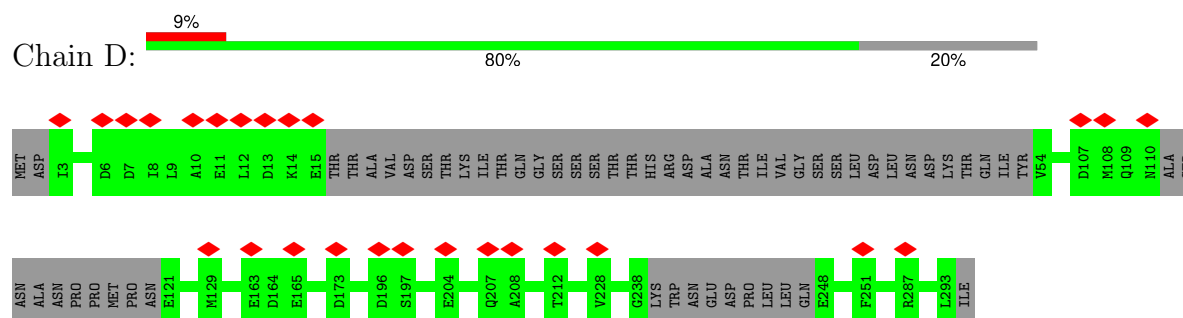
- Molecule 4: DNA replication complex GINS protein PSF3



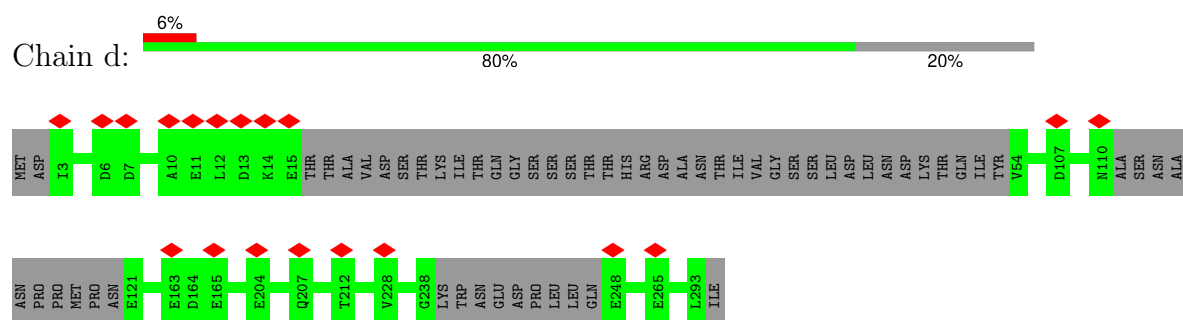
- Molecule 5: DNA replication complex GINS protein SLD5



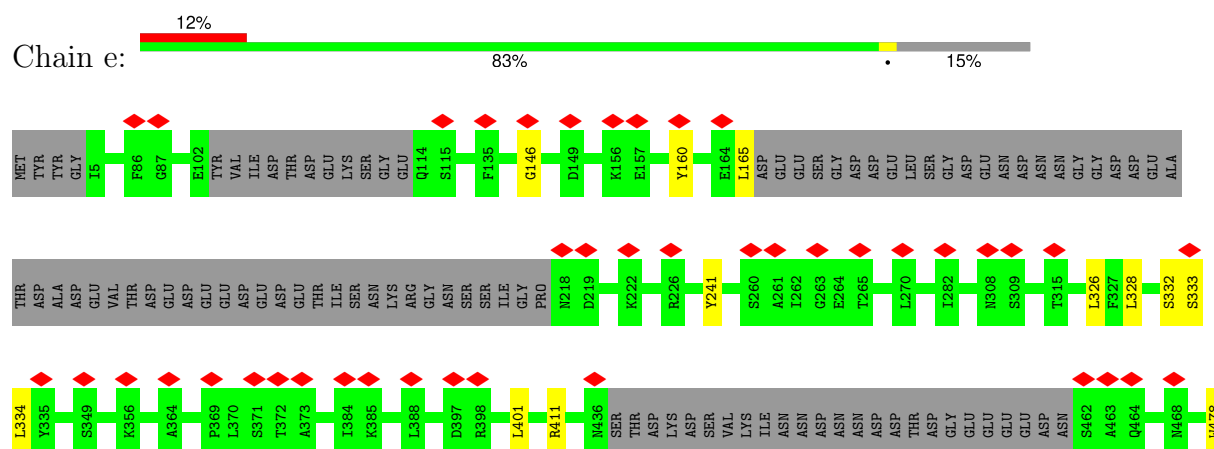
- Molecule 5: DNA replication complex GINS protein SLD5

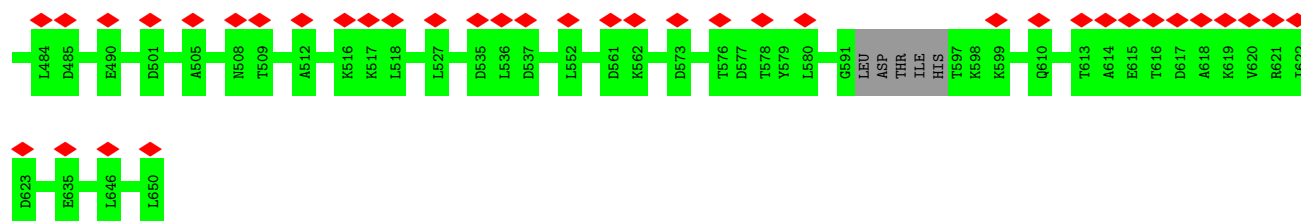


- Molecule 5: DNA replication complex GINS protein SLD5



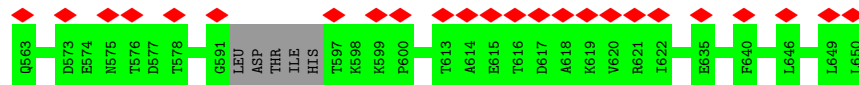
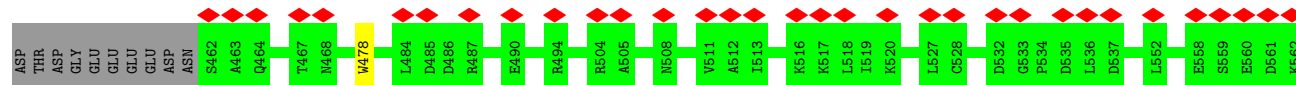
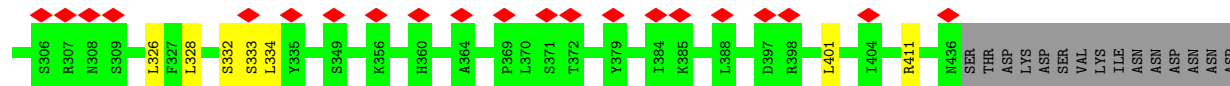
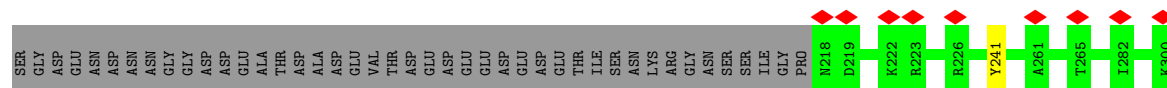
- Molecule 6: Cell division control protein 45





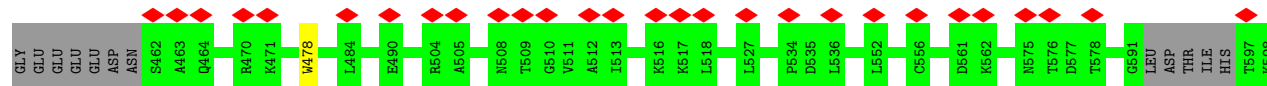
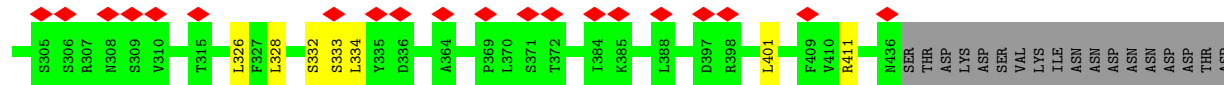
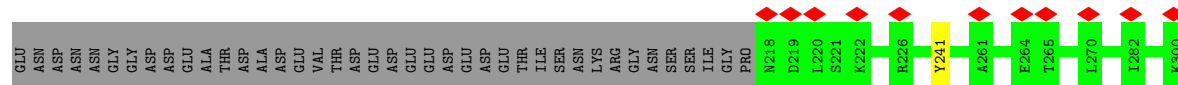
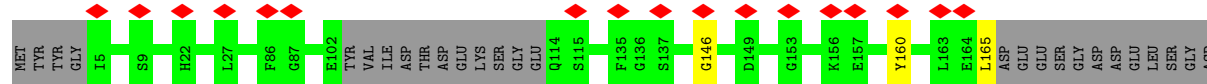
• Molecule 6: Cell division control protein 45

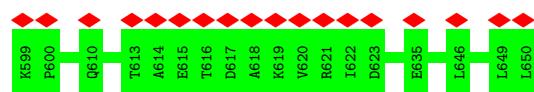
Chain E: 16% 83% 15%



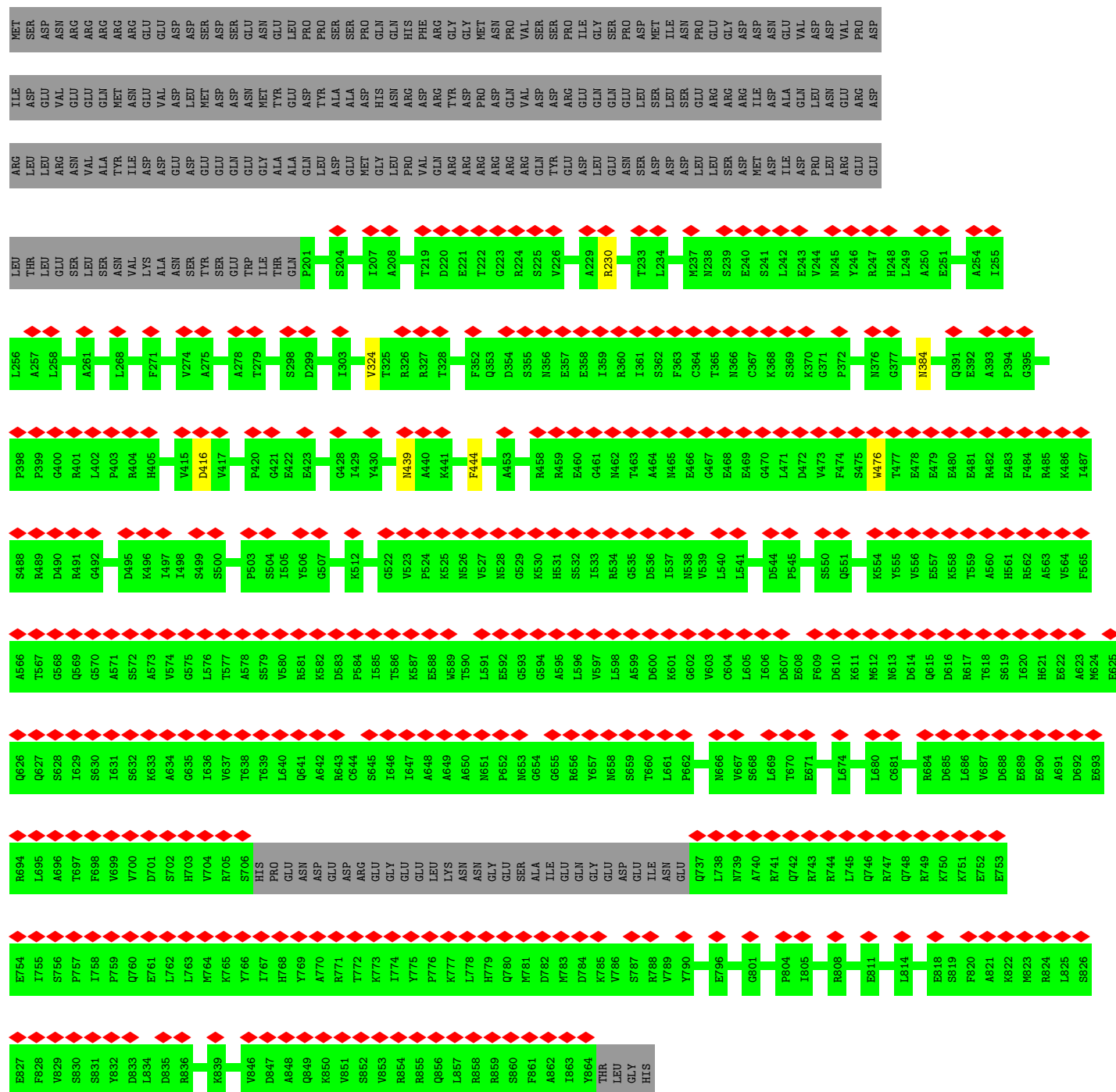
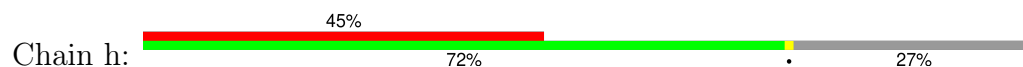
• Molecule 6: Cell division control protein 45

Chain r: 14% 83% 15%



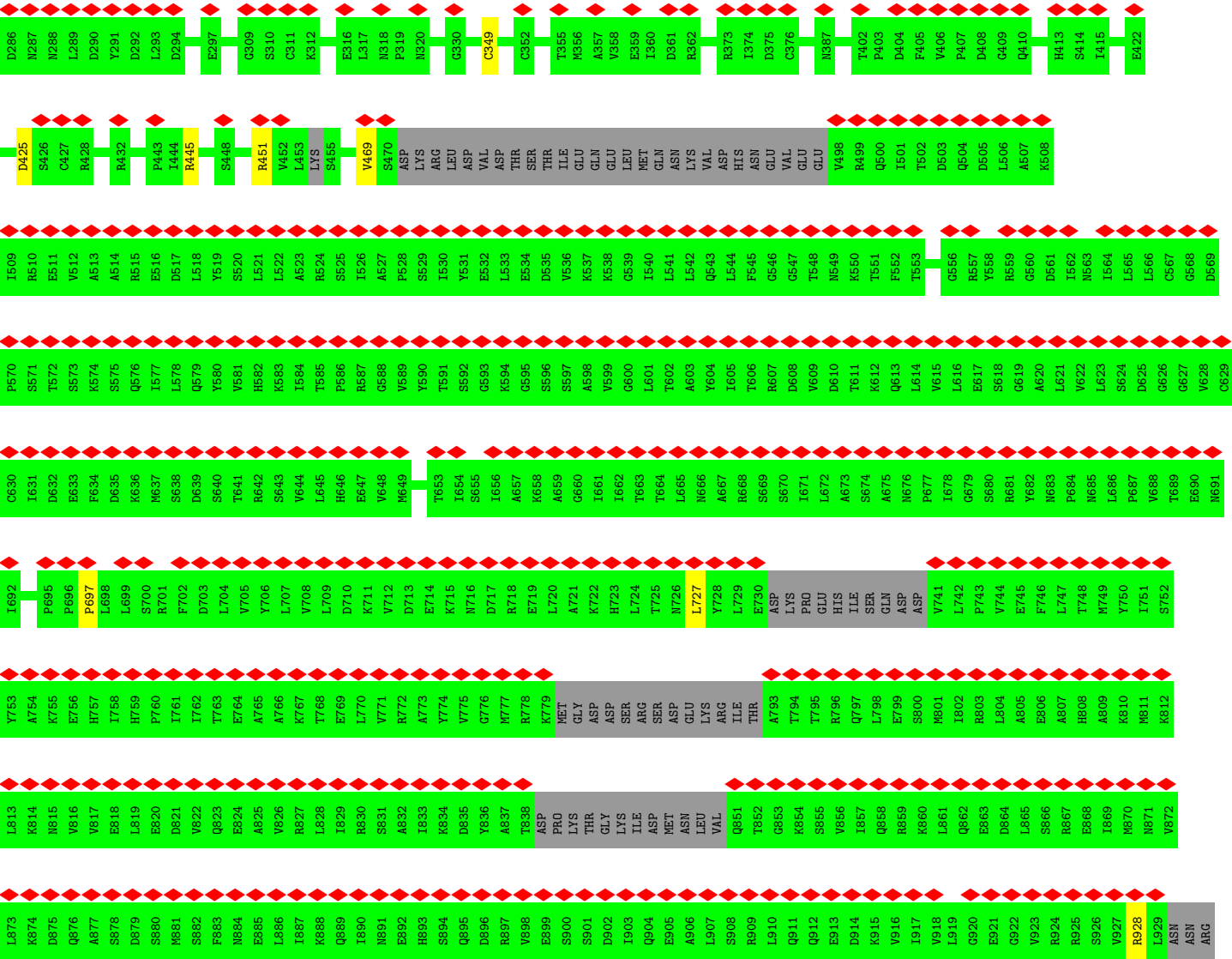


• Molecule 7: DNA replication licensing factor MCM2



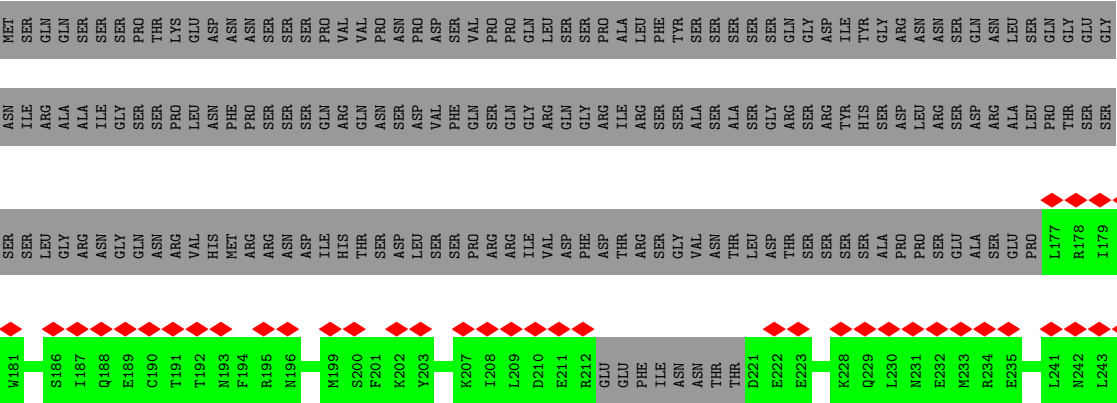
• Molecule 7: DNA replication licensing factor MCM2

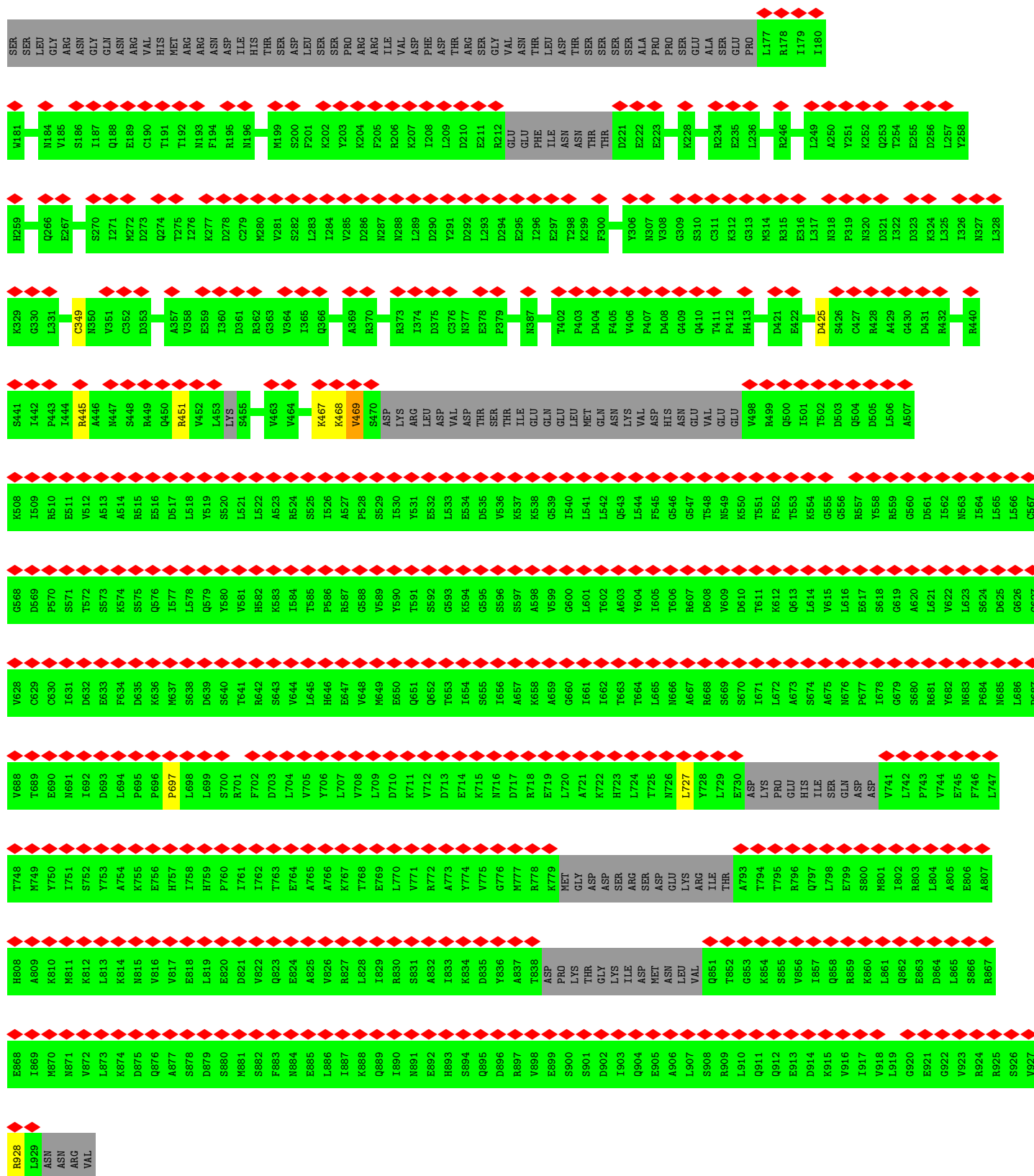




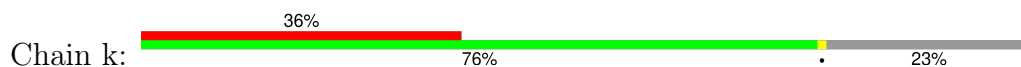
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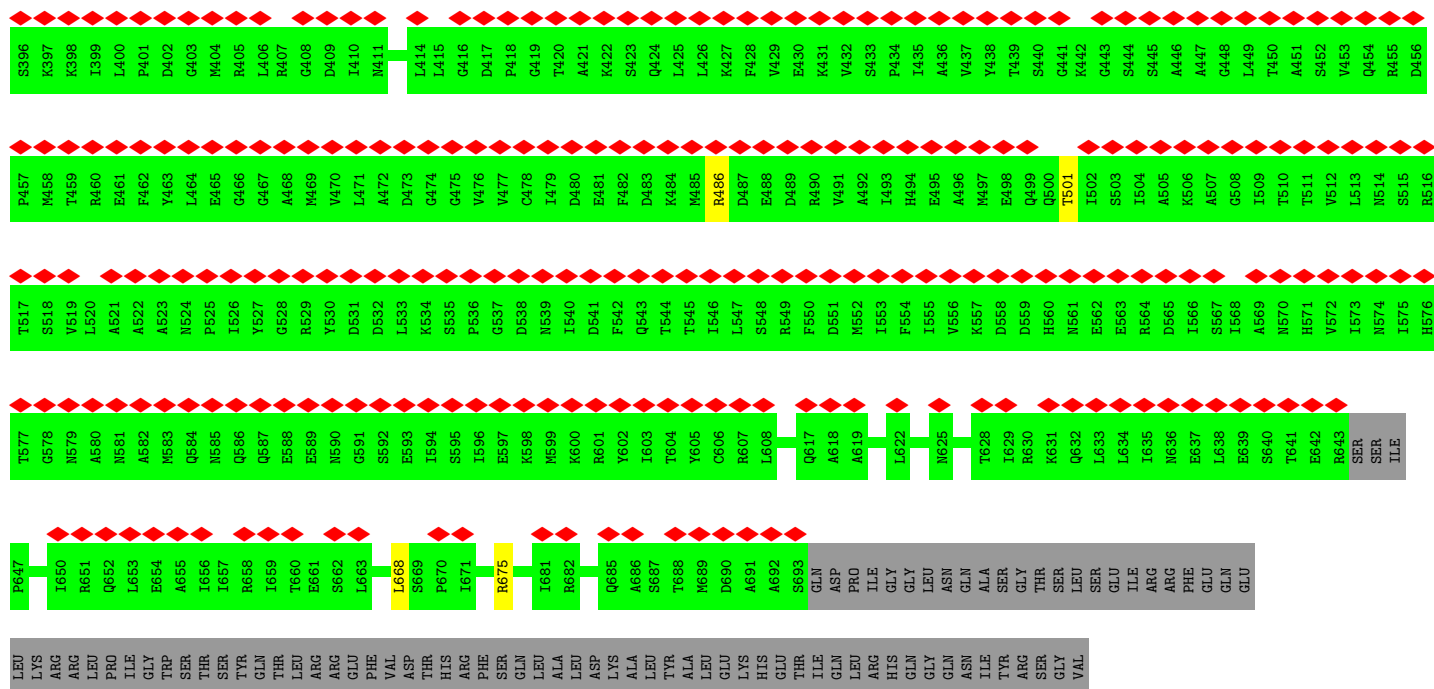
• Molecule 9: DNA replication licensing factor MCM4



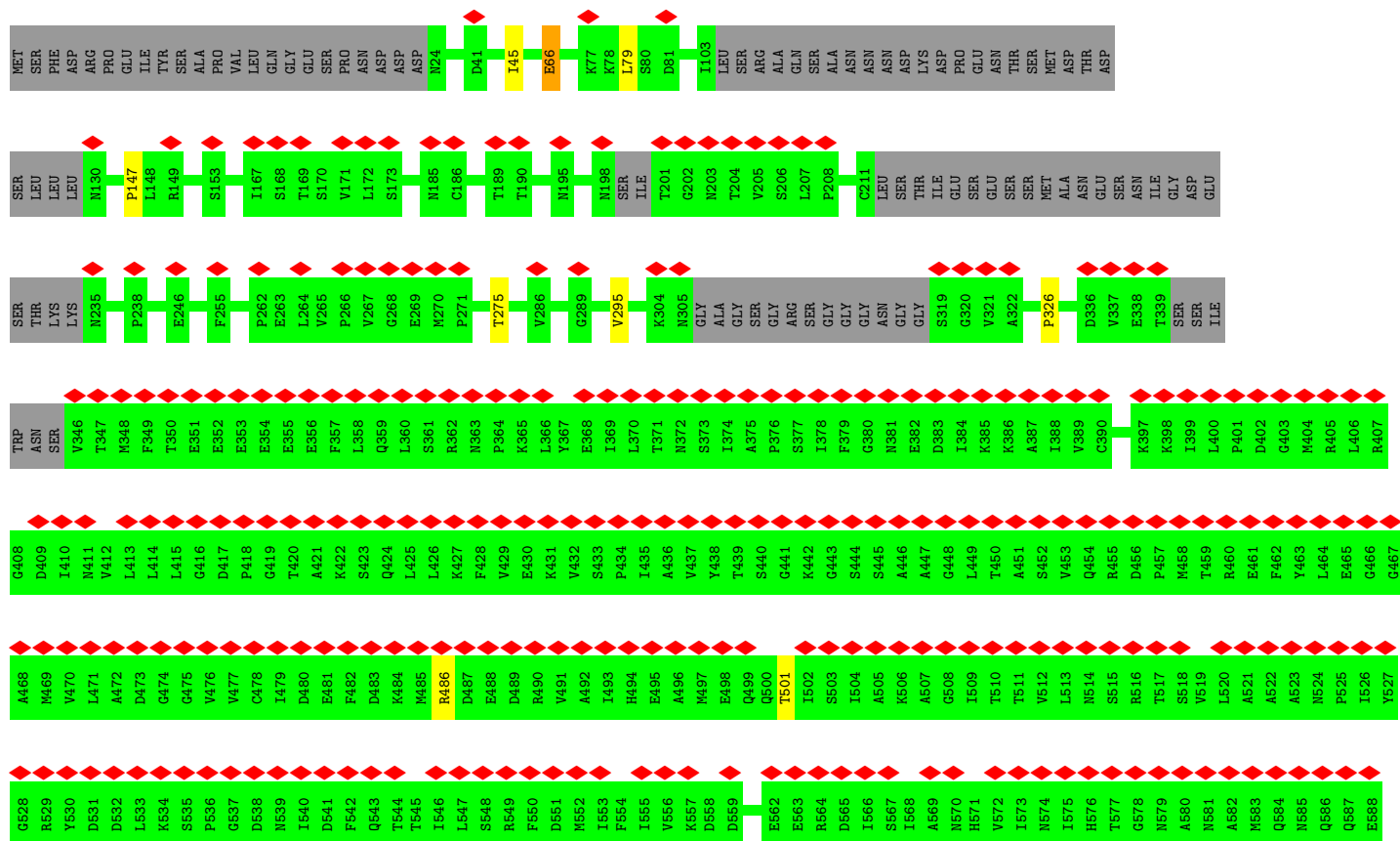
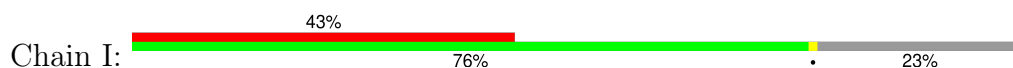


• Molecule 10: Minichromosome maintenance protein 5





• Molecule 10: Minichromosome maintenance protein 5





I548	D608	R668	Y728	THR
S649	D609	Q669	Q729	LEU
K550	E610	Q670	GLU	ASN
A651	K611	S671	THR	VAL
G552	L612	S672	TRP	HIS
I553	A613	R673	LEU	LEU
N554	E614	E674	ILE	ASN
T555	H615	M675	GLY	GLY
L556	V616	D676	GLU	ASP
T557	T617	S677	GLU	ASN
N558	Y618	K678	THR	THR
A559	V619	F679	THR	LYS
R560	H620	S680	THR	LYS
T561	M621	F681	VAL	ASP
S562	H622	G682	THR	ASP
I563	N623	Q683	GLY	GLY
L564	K624	A684	THR	THR
A565	Q625	T685	ILE	ASP
A566	P626	P686	LYS	ASP
A567	D627	R687	LEU	THR
N568	L628	T688	GLN	GLN
P569	D629	L689	GLU	GLU
L570	F630	L690	THR	ASP
Y571	T631	G691	LEU	SER
G572	P632	I692	VAL	SER
R573	V633	I693	THR	THR
Y574	E634	R694	LEU	PRO
N575	P635	L695	LYS	LYS
P576	S636	S696	LEU	LEU
S577	K637	Q697	ALA	ALA
L578	M638	A698	PRO	GLN
S579	R639	L699	THR	THR
P580	E640	A700	THR	ALA
L581	Y641	K701	SER	SER
D582	I642	L702	ASP	ASP
N583	A643	R703	THR	ALA
I584	Y644	L704	VAL	VAL
N585	A645	A705	ARG	ARG
L586	K646	D706	GLY	GLY
P587	T647	M707	THR	THR
A588	K648	V708	LEU	LEU
A589	R649	D709	GLU	GLU
L590	P650	I710	ASP	ASP
L591	V651	D711	ASN	ASN
S592	M652	D712	ILE	ILE
R593	S653	V713	GLN	GLN
F594	E654	E714	GLU	GLU
D595	A655	E715	TTR	SER
I596	V656	A716		
L597	N657	L717		
F598	D658	R718		
L599	Y659	L719		
M600	V660	V720		
L601	V661	R721		
D602	Q662	V722		
I603	A663	S723		
P604	Y664	K724		
S605	I665	E725		
R606	R666	S726		
D607	L667	L727		

● Molecule 12: DNA replication licensing factor MCM7



M1	P61	Y134	P194	S286	V381	D441	P501
S2	K62	K135	N195	E287	R382	K442	V502
A3	Y63	D136	L196	E288	Q383	K443	T503
A4	M64	D137	T197	C289	H384	V444	D504
L5	A65	V138	R198	S290	K385	G445	E505
P6	M66	L139	R199	Q291	K386	D446	M506
S7	L67	D140	F204	N292	LYS	G447	I507
I8	Q68	V141	K205	Q293	PHE	M448	L508
L10	K69	I142	ALA	T294	ALA	L509	E509
P11	N72	L143	P206	R303	SER	K449	G510
V12	R73	Q144	L207	A304	PHE	I450	G511
D13	E74	Q145	S208	F310	SER	R451	A512
Y14	L75	R146	Q209	Q320	L393	G452	L513
N15	I80	R147	N210	Q321	T394	D453	V514
N16	F18	L148	C211	V322	S395	N455	L515
L17	D83	N150	A212	P323	D396	V456	A516
F18	I85	E151	R213	Y215	V397	C457	D517
N19	L86	R152	R214	R216	E398	L458	N518
E20	Q87	M153	Y215	G325	R400	M459	G519
I21	Y88	L154	LYS	H326	V401	G460	I520
T22	Q89	S155	ALA	R329	M402	D461	C521
D23	R90	D156	I220	N336	E403	G463	C522
F24	L25	I157	L225	G337	L404	V464	I523
V26	V26	T158	S226	T338	L405	A465	D524
T27	K92	ASN	V227	L339	T406	S467	E525
F28	F93	ILE	I230	V340	S407	Q468	F526
K29	L94	ARG	K231	R341	G408	L469	D527
Q30	Q95	SER	G232	R342	D409	M529	K528
D31	G96	GLU	D233	L343	V410	L470	M529
THR	T97	ASN	I245	S344	Y411	K471	D530
LEU	Q98	LEU	T246	P345	M412	I472	E531
SER	A99	THR	T247	G346	R413	C473	S532
SER	D100	THR	R247	D347	L414	K475	D533
ASP	D101	THR	D263	I354	A415	I476	R534
ALA	L102	THR	Q264	F355	K416	S477	T535
ARG	V103	THR	C265	L356	S417	I477	A536
ASN	S104	THR	G266	P357	I418	S478	I537
GLY	A105	THR	Y267	A358	A419	P478	H538
ASN	E115	THR	E268	P359	P420	R479	E539
GLY	I116	THR	V269	E269	E421	G480	V540
ASP	F117	THR	F270	Q271	I422	Y481	M541
ALA	R119	THR	Q272	V273	Y423	Y482	E542
GLU	A120	THR	V273	N274	G424	T483	Q543
ASP	L121	THR	V274	S275	M425	T484	Q544
ASP	D122	THR	S275	F278	D427	G485	T545
ALA	N123	THR	E190	T279	V428	K486	I546
HIS	M124	THR	L191	P280	K429	G487	S547
LEU	P126	THR	F192	L281	K430	S488	I548
LEU	I127	THR	P193	T285	A431	S489	S549
GLU	K59	THR			L432	K490	K550
G60	G60	THR			L433	V491	A551
		THR			L434	G492	G552
		THR			L435	L493	I553
		THR			L436	T494	N554
		THR			L437	A495	T555
		THR			L438	A496	T556
		THR			L439	V497	L557
		THR			L440	N498	N558
		THR			L441	K499	A559
		THR			L442	D500	R560

LEU	LYS	THR	F681	M621	T561
LYS	THR	LYS	G682	H622	S562
PHE	LYS	PHE	Q683	N623	I563
VAL	ILE	VAL	A684	K624	L564
ASP	THR	THR	T685	Q625	A565
GLY	ILE	ILE	P686	P626	A566
THR	THR	THR	R687	D627	A567
MET	LYS	LYS	T688	L628	N568
ASP	THR	THR	L689	D629	P569
THR	THR	LEU	G690	F630	L570
GLN	GLN	GLN	G691	T631	Y571
GLU	GLU	GLU	G692	P632	G572
ASP	THR	THR	I693	V633	R573
LYS	GLY	LYS	I694	E634	Y574
LEU	LEU	ASN	R695	P635	N575
VAL	THR	THR	S696	S636	F576
SER	THR	LEU	Q697	K637	R577
PRO	PRO	SER	T698	M638	L578
LYS	LYS	GLU	A699	R639	S579
LEU	LEU	ASN	L699	E640	P580
ALA	ALA	ILE	A700	Y641	L581
ALA	THR	VAL	K701	I642	D582
ALA	THR	VAL	L702	I643	N583
ALA	THR	ARG	R703	Y644	I584
ALA	LEU	LEU	L704	A645	N585
ASN	ARG	ARG	A705	K646	L586
ASN	GLY	GLY	D706	T647	P587
VAL	PHE	THR	M707	K648	A588
ALA	ALA	MET	V708	R649	A589
GLN	GLN	LEU	D709	P650	L590
ASP	GLN	LEU	I710	V651	L591
ASP	LEU	LEU	D711	M652	S592
ILE	ILE	SER	D712	S653	R593
ASN	ASN	ASN	V713	E654	F594
LEU	CYS	CYS	V714	A655	D595
GLN	ILE	ILE	E715	V656	I596
ASP	GLN	GLU	T716	N657	L597
ALA	GLU	SER	A717	D658	F598
	SER	THR	L718	V659	L599
	LEU	LEU	R719	M660	M600
	ASN	VAL	V720	V661	L601
	ASN	VAL	V721	Q662	D602
	TRP	TRP	R722	A663	I603
	HIS	HIS	V723	Y664	P604
	LEU	LEU	K724	I665	S605
	ILE	ILE	S725	R666	R606
	ASN	ASN	T726	L667	D607
	GLY	GLY	L727	R668	D608
	GLU	GLU	Q728	Q669	D609
	ASN	ASN	D729	D670	E610
	THR	THR	S710	S671	K611
	ASN	ASN	L711	K672	L612
	LYS	LYS	R673	E674	A613
	SER	SER	R674	M675	E614
	LYS	LYS	E675	D676	V615
	GLU	GLU	P676	S677	V616
	ASP	ASP	K678	V679	T617
	GLU	GLU	S680		Y618
	SER	SER			V619
	THR	THR			H620

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	53117	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.076	Depositor
Minimum map value	-0.035	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0234	Depositor
Map size (Å)	429.6, 429.6, 429.6	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.074, 1.074, 1.074	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	X	0.41	0/3501	0.60	3/4741 (0.1%)
1	Y	0.40	0/3550	0.61	3/4806 (0.1%)
1	Z	0.41	0/3500	0.62	3/4738 (0.1%)
2	A	0.42	0/1718	0.66	2/2314 (0.1%)
2	a	0.42	0/1718	0.66	2/2314 (0.1%)
2	n	0.43	0/1718	0.66	2/2314 (0.1%)
3	B	0.46	1/1545 (0.1%)	0.65	0/2092
3	b	0.46	1/1545 (0.1%)	0.65	0/2092
3	o	0.46	1/1545 (0.1%)	0.65	0/2092
4	C	0.47	0/1320	0.63	1/1784 (0.1%)
4	c	0.47	0/1320	0.63	0/1784
4	p	0.47	0/1320	0.63	1/1784 (0.1%)
5	D	0.43	0/1956	0.58	0/2638
5	d	0.43	0/1956	0.58	0/2638
5	q	0.43	0/1956	0.58	0/2638
6	E	0.46	1/4563 (0.0%)	0.67	5/6173 (0.1%)
6	e	0.46	1/4563 (0.0%)	0.67	5/6173 (0.1%)
6	r	0.46	1/4563 (0.0%)	0.67	5/6173 (0.1%)
7	2	0.45	0/5051	0.64	1/6821 (0.0%)
7	F	0.45	0/5051	0.64	1/6821 (0.0%)
7	h	0.45	0/5051	0.64	1/6821 (0.0%)
8	3	0.44	0/4739	0.78	3/6425 (0.0%)
8	G	0.44	0/4739	0.78	3/6425 (0.0%)
8	i	0.44	0/4739	0.78	3/6425 (0.0%)
9	4	0.37	0/5479	0.61	2/7392 (0.0%)
9	H	0.38	1/5479 (0.0%)	0.65	5/7392 (0.1%)
9	j	0.37	0/5479	0.61	2/7392 (0.0%)
10	5	0.47	0/4750	0.69	4/6412 (0.1%)
10	I	0.47	0/4750	0.69	4/6412 (0.1%)
10	k	0.47	0/4750	0.69	4/6412 (0.1%)
11	6	0.43	0/4789	0.65	3/6466 (0.0%)
11	J	0.43	0/4789	0.65	3/6466 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
11	l	0.43	0/4789	0.65	3/6466 (0.0%)
12	7	0.37	0/5299	0.61	3/7160 (0.0%)
12	K	0.37	0/5299	0.61	3/7160 (0.0%)
12	m	0.37	0/5299	0.61	3/7160 (0.0%)
All	All	0.43	7/134178 (0.0%)	0.66	83/181316 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	X	0	1
1	Y	0	1
1	Z	0	1
8	3	0	1
8	G	0	1
8	i	0	1
All	All	0	6

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	478	TRP	CB-CG	-6.10	1.39	1.50
6	e	478	TRP	CB-CG	-6.08	1.39	1.50
6	r	478	TRP	CB-CG	-6.07	1.39	1.50
3	o	11	PHE	C-N	-5.28	1.22	1.34
3	B	11	PHE	C-N	-5.27	1.22	1.34

The worst 5 of 83 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	3	17	PRO	CA-C-O	-29.20	50.11	120.20
8	i	17	PRO	CA-C-O	-29.18	50.16	120.20
8	G	17	PRO	CA-C-O	-29.18	50.17	120.20
8	G	17	PRO	CA-C-N	15.27	150.79	117.20
8	3	17	PRO	CA-C-N	15.26	150.76	117.20

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	3	17	PRO	Mainchain
1	X	766	PHE	Peptide
1	Y	766	PHE	Peptide
1	Z	766	PHE	Peptide
8	i	17	PRO	Mainchain

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	X	419/927 (45%)	408 (97%)	10 (2%)	1 (0%)	44	78
1	Y	427/927 (46%)	414 (97%)	12 (3%)	1 (0%)	44	78
1	Z	417/927 (45%)	407 (98%)	9 (2%)	1 (0%)	44	78
2	A	206/208 (99%)	179 (87%)	26 (13%)	1 (0%)	25	64
2	a	206/208 (99%)	180 (87%)	25 (12%)	1 (0%)	25	64
2	n	206/208 (99%)	180 (87%)	25 (12%)	1 (0%)	25	64
3	B	177/213 (83%)	150 (85%)	27 (15%)	0	100	100
3	b	177/213 (83%)	150 (85%)	27 (15%)	0	100	100
3	o	177/213 (83%)	150 (85%)	27 (15%)	0	100	100
4	C	151/194 (78%)	140 (93%)	11 (7%)	0	100	100
4	c	151/194 (78%)	139 (92%)	12 (8%)	0	100	100
4	p	151/194 (78%)	139 (92%)	12 (8%)	0	100	100
5	D	226/294 (77%)	202 (89%)	24 (11%)	0	100	100
5	d	226/294 (77%)	202 (89%)	24 (11%)	0	100	100
5	q	226/294 (77%)	202 (89%)	24 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	E	543/650 (84%)	476 (88%)	64 (12%)	3 (1%)	22	60
6	e	543/650 (84%)	476 (88%)	64 (12%)	3 (1%)	22	60
6	r	543/650 (84%)	476 (88%)	64 (12%)	3 (1%)	22	60
7	2	630/868 (73%)	538 (85%)	92 (15%)	0	100	100
7	F	630/868 (73%)	538 (85%)	92 (15%)	0	100	100
7	h	630/868 (73%)	537 (85%)	93 (15%)	0	100	100
8	3	584/971 (60%)	506 (87%)	77 (13%)	1 (0%)	44	78
8	G	584/971 (60%)	506 (87%)	76 (13%)	2 (0%)	37	73
8	i	584/971 (60%)	505 (86%)	77 (13%)	2 (0%)	37	73
9	4	668/933 (72%)	579 (87%)	88 (13%)	1 (0%)	48	83
9	H	668/933 (72%)	578 (86%)	88 (13%)	2 (0%)	37	73
9	j	668/933 (72%)	579 (87%)	88 (13%)	1 (0%)	48	83
10	5	583/775 (75%)	493 (85%)	89 (15%)	1 (0%)	44	78
10	I	583/775 (75%)	493 (85%)	89 (15%)	1 (0%)	44	78
10	k	583/775 (75%)	493 (85%)	89 (15%)	1 (0%)	44	78
11	6	606/1017 (60%)	506 (84%)	99 (16%)	1 (0%)	44	78
11	J	606/1017 (60%)	506 (84%)	99 (16%)	1 (0%)	44	78
11	l	606/1017 (60%)	507 (84%)	98 (16%)	1 (0%)	44	78
12	7	653/845 (77%)	556 (85%)	97 (15%)	0	100	100
12	K	653/845 (77%)	555 (85%)	98 (15%)	0	100	100
12	m	653/845 (77%)	555 (85%)	98 (15%)	0	100	100
All	All	16344/23685 (69%)	14200 (87%)	2114 (13%)	30 (0%)	45	78

5 of 30 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	j	469	VAL
9	H	469	VAL
6	e	334	LEU
6	E	334	LEU
6	r	334	LEU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	X	377/825 (46%)	377 (100%)	0	100	100
1	Y	383/825 (46%)	383 (100%)	0	100	100
1	Z	377/825 (46%)	377 (100%)	0	100	100
2	A	193/193 (100%)	193 (100%)	0	100	100
2	a	193/193 (100%)	193 (100%)	0	100	100
2	n	193/193 (100%)	193 (100%)	0	100	100
3	B	171/198 (86%)	170 (99%)	1 (1%)	84	88
3	b	171/198 (86%)	170 (99%)	1 (1%)	84	88
3	o	171/198 (86%)	170 (99%)	1 (1%)	84	88
4	C	144/173 (83%)	142 (99%)	2 (1%)	62	75
4	c	144/173 (83%)	142 (99%)	2 (1%)	62	75
4	p	144/173 (83%)	142 (99%)	2 (1%)	62	75
5	D	225/279 (81%)	225 (100%)	0	100	100
5	d	225/279 (81%)	225 (100%)	0	100	100
5	q	225/279 (81%)	225 (100%)	0	100	100
6	E	499/586 (85%)	496 (99%)	3 (1%)	84	88
6	e	499/586 (85%)	496 (99%)	3 (1%)	84	88
6	r	499/586 (85%)	496 (99%)	3 (1%)	84	88
7	2	535/770 (70%)	529 (99%)	6 (1%)	70	80
7	F	535/770 (70%)	529 (99%)	6 (1%)	70	80
7	h	535/770 (70%)	529 (99%)	6 (1%)	70	80
8	3	515/835 (62%)	512 (99%)	3 (1%)	84	88
8	G	515/835 (62%)	512 (99%)	3 (1%)	84	88
8	i	515/835 (62%)	512 (99%)	3 (1%)	84	88
9	4	610/848 (72%)	605 (99%)	5 (1%)	79	85
9	H	610/848 (72%)	604 (99%)	6 (1%)	73	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	j	610/848 (72%)	605 (99%)	5 (1%)	79	85
10	5	534/688 (78%)	527 (99%)	7 (1%)	65	77
10	I	534/688 (78%)	527 (99%)	7 (1%)	65	77
10	k	534/688 (78%)	527 (99%)	7 (1%)	65	77
11	6	493/886 (56%)	487 (99%)	6 (1%)	67	78
11	J	493/886 (56%)	487 (99%)	6 (1%)	67	78
11	l	493/886 (56%)	487 (99%)	6 (1%)	67	78
12	7	585/753 (78%)	581 (99%)	4 (1%)	81	87
12	K	585/753 (78%)	581 (99%)	4 (1%)	81	87
12	m	585/753 (78%)	581 (99%)	4 (1%)	81	87
All	All	14649/21102 (69%)	14537 (99%)	112 (1%)	77	85

5 of 112 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	5	66	GLU
12	K	479	ARG
12	7	329	ARG
12	K	329	ARG
10	I	486	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 241 such sidechains are listed below:

Mol	Chain	Res	Type
7	2	238	ASN
10	I	561	ASN
10	5	254	GLN
10	I	254	GLN
12	K	326	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
13	ATP	5	801	-	28,33,33	0.74	0	34,52,52	1.69	5 (14%)
13	ATP	h	901	-	28,33,33	0.81	0	34,52,52	1.21	3 (8%)
13	ATP	3	1001	-	28,33,33	0.90	0	34,52,52	1.27	3 (8%)
13	ATP	2	901	-	28,33,33	0.82	0	34,52,52	1.21	3 (8%)
13	ATP	i	1001	-	28,33,33	0.89	0	34,52,52	1.27	3 (8%)
13	ATP	k	801	-	28,33,33	0.74	0	34,52,52	1.68	5 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	ATP	5	801	-	-	4/18/38/38	0/3/3/3
13	ATP	h	901	-	-	6/18/38/38	0/3/3/3
13	ATP	3	1001	-	-	5/18/38/38	0/3/3/3
13	ATP	2	901	-	-	6/18/38/38	0/3/3/3
13	ATP	i	1001	-	-	5/18/38/38	0/3/3/3
13	ATP	k	801	-	-	4/18/38/38	0/3/3/3

There are no bond length outliers.

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	5	801	ATP	C4'-O4'-C1'	-5.00	105.34	109.92
13	k	801	ATP	C4'-O4'-C1'	-4.88	105.46	109.92
13	k	801	ATP	N3-C2-N1	-4.29	122.85	128.67
13	5	801	ATP	N3-C2-N1	-4.28	122.87	128.67
13	k	801	ATP	O4'-C1'-N9	3.92	113.94	108.75

There are no chirality outliers.

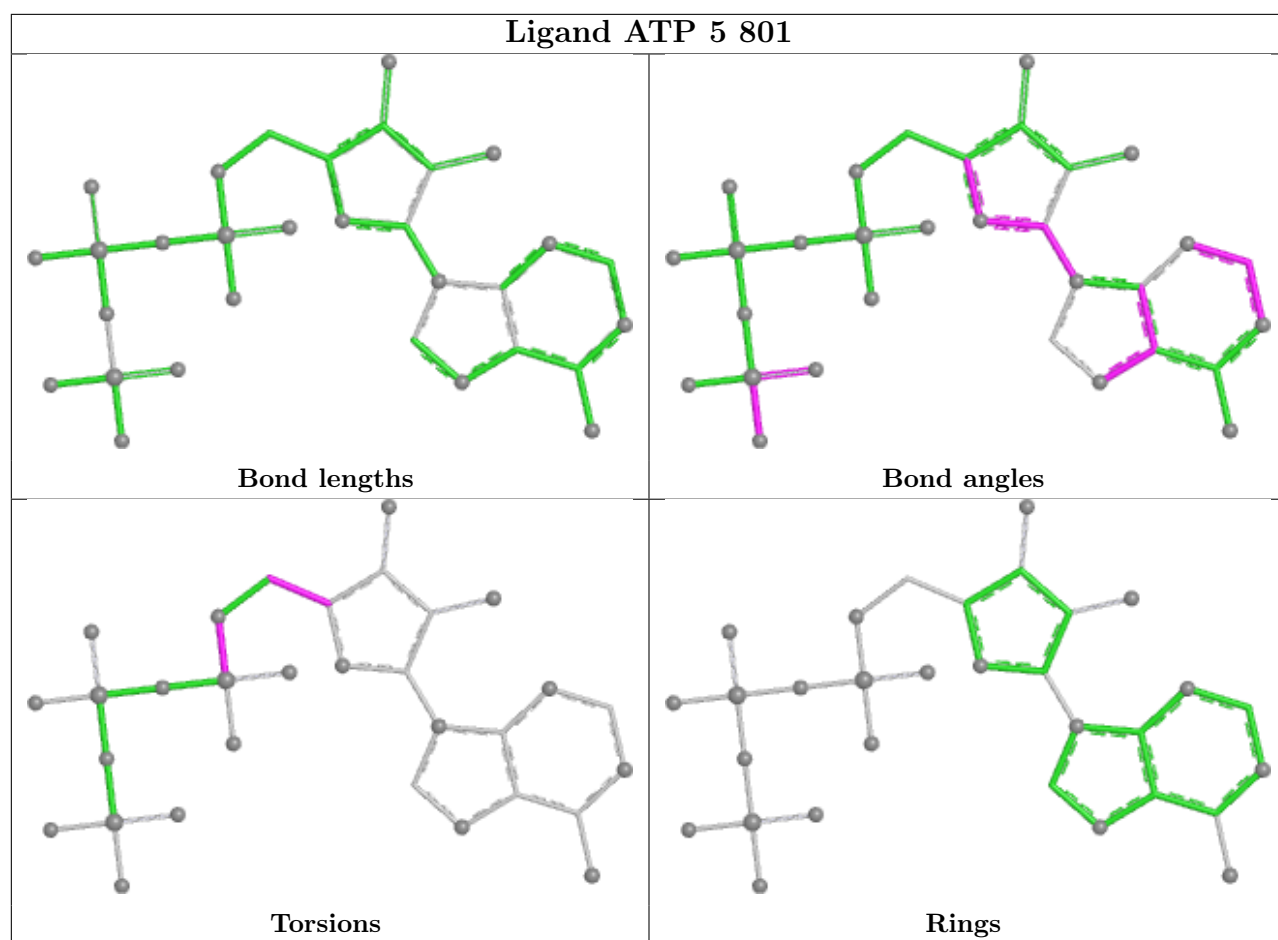
5 of 30 torsion outliers are listed below:

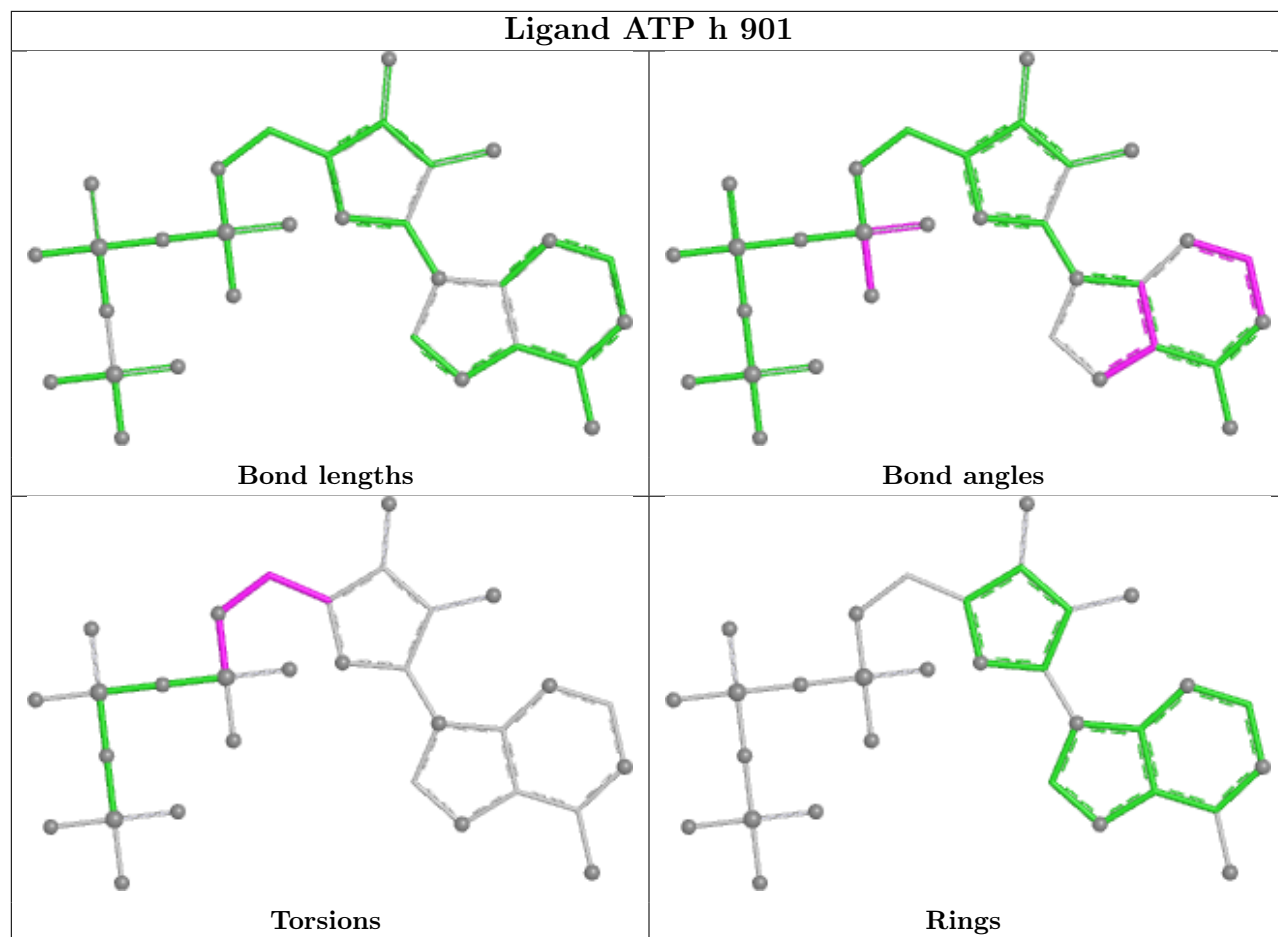
Mol	Chain	Res	Type	Atoms
13	h	901	ATP	C5'-O5'-PA-O1A
13	h	901	ATP	C5'-O5'-PA-O2A
13	h	901	ATP	C5'-O5'-PA-O3A
13	i	1001	ATP	C5'-O5'-PA-O2A
13	i	1001	ATP	C5'-O5'-PA-O3A

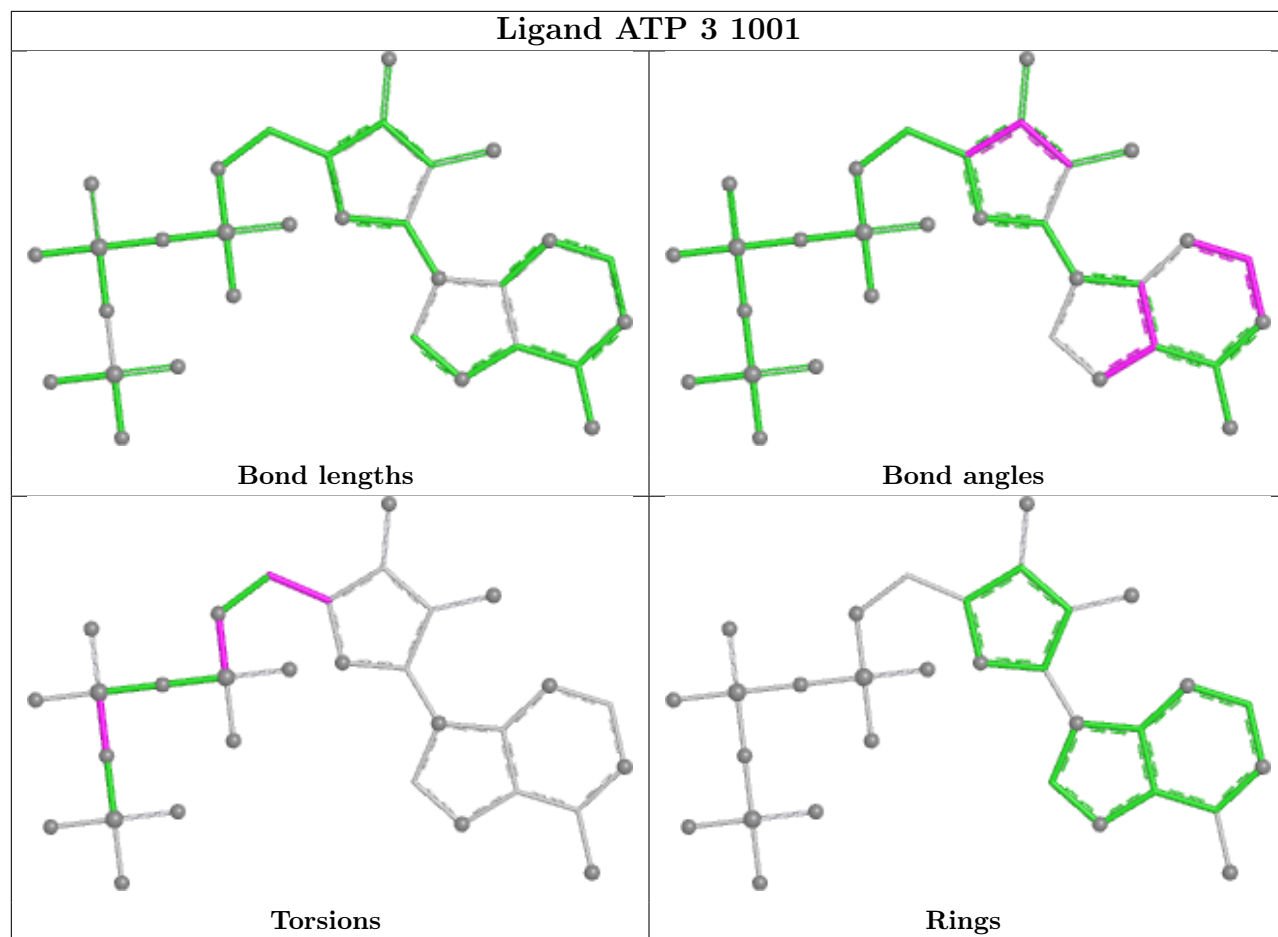
There are no ring outliers.

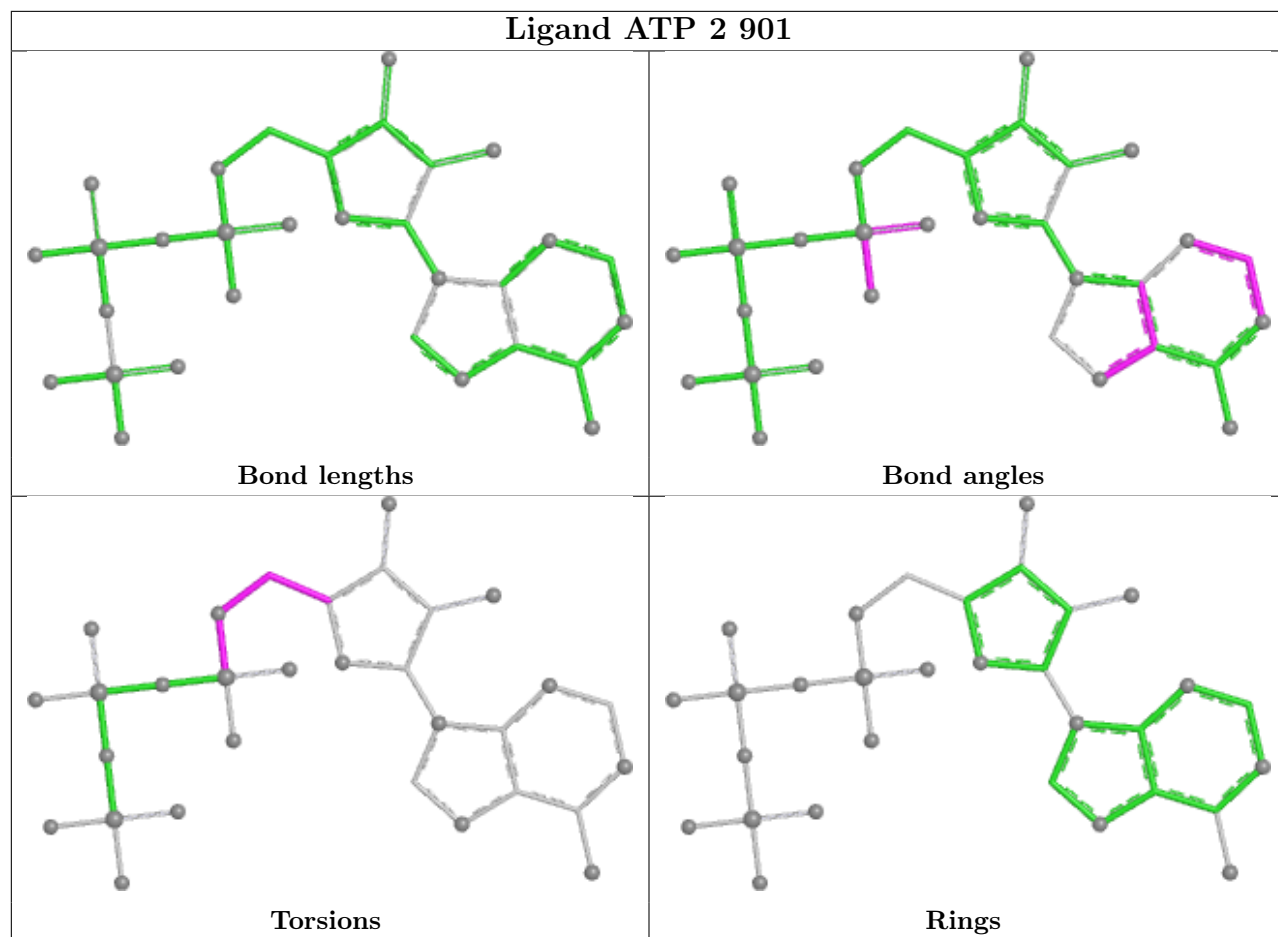
No monomer is involved in short contacts.

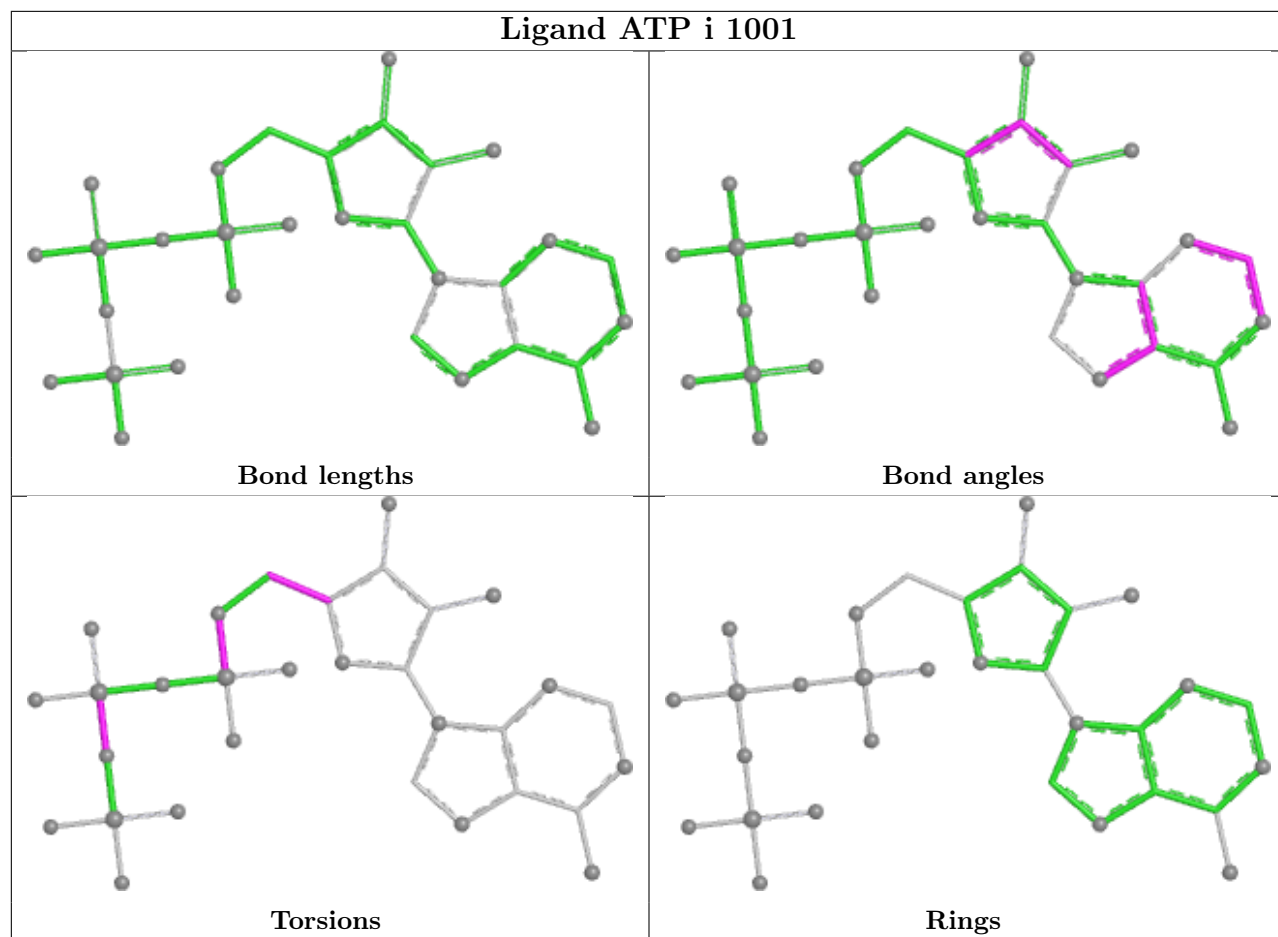
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

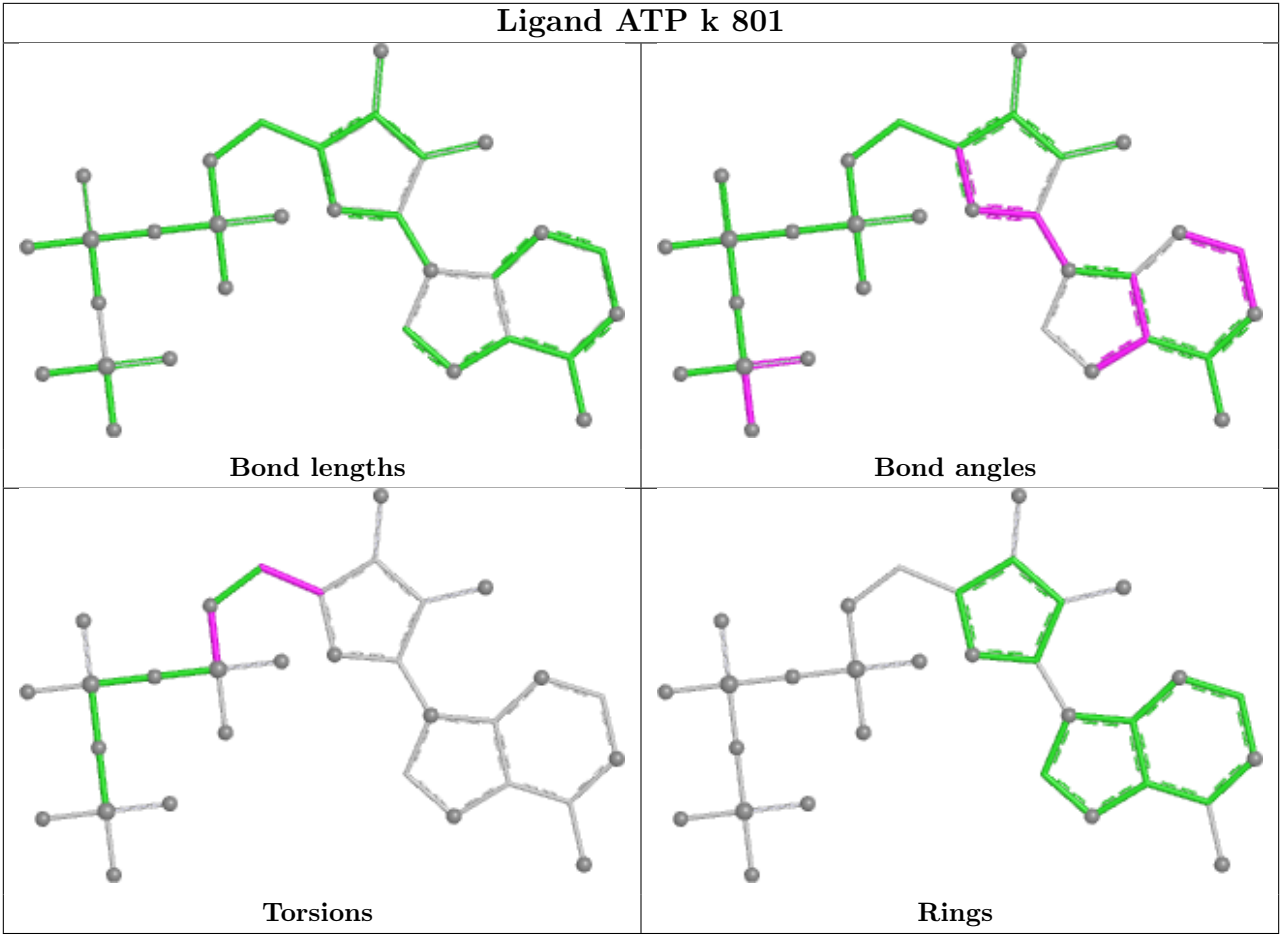












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	Z	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Z	776:ILE	C	777:ARG	N	2.04

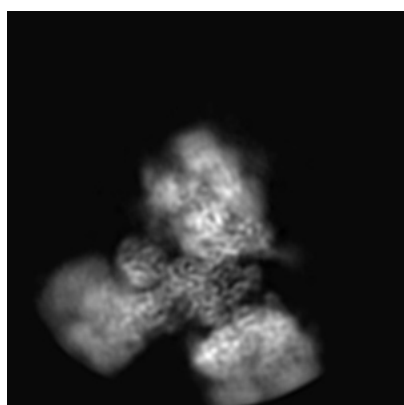
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20473. These allow visual inspection of the internal detail of the map and identification of artifacts.

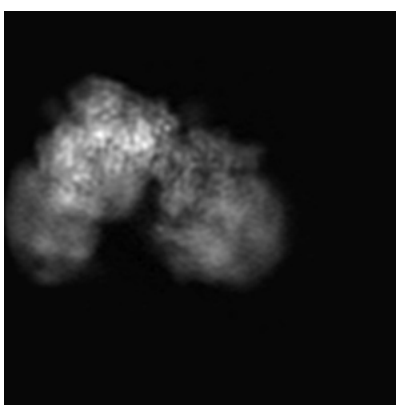
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

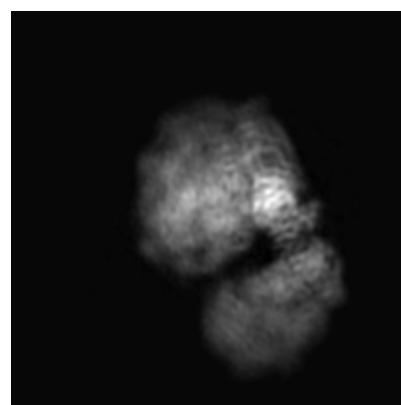
6.1.1 Primary map



X



Y

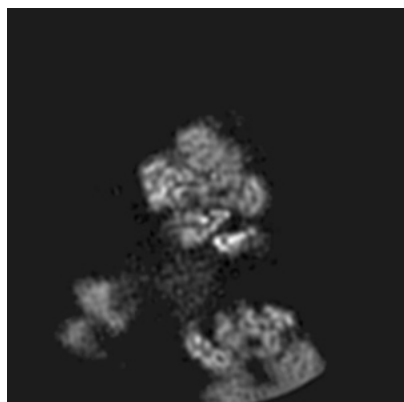


Z

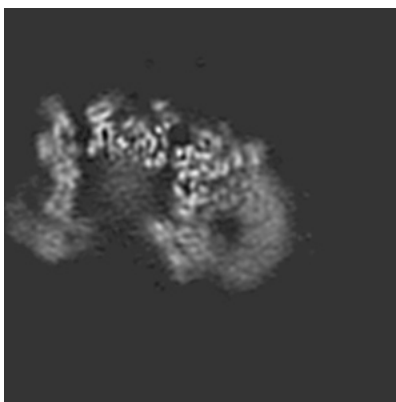
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

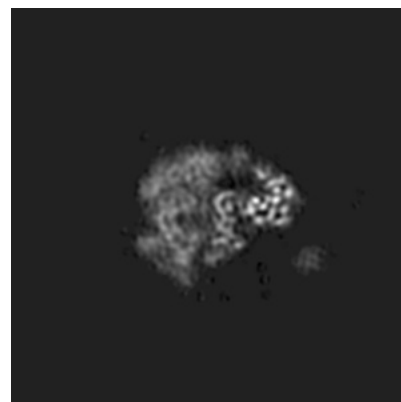
6.2.1 Primary map



X Index: 200



Y Index: 200

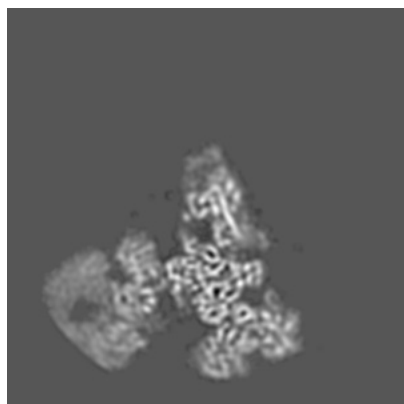


Z Index: 200

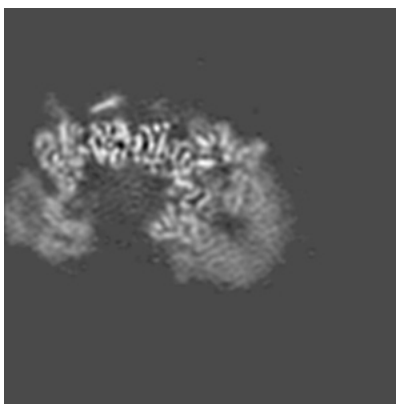
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

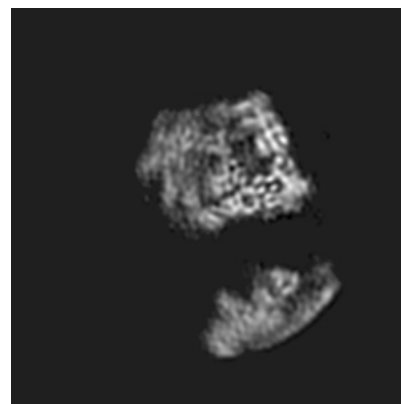
6.3.1 Primary map



X Index: 265



Y Index: 207



Z Index: 66

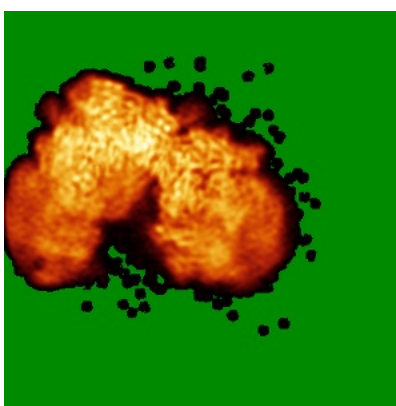
The images above show the largest variance slices of the map in three orthogonal directions.

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

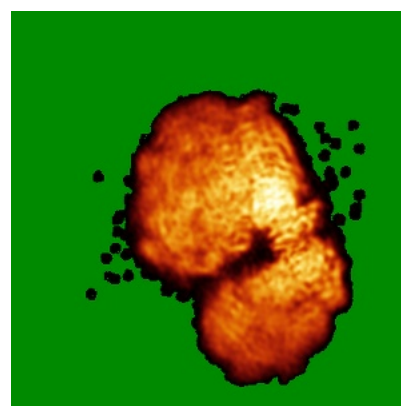
6.4.1 Primary map



X



Y

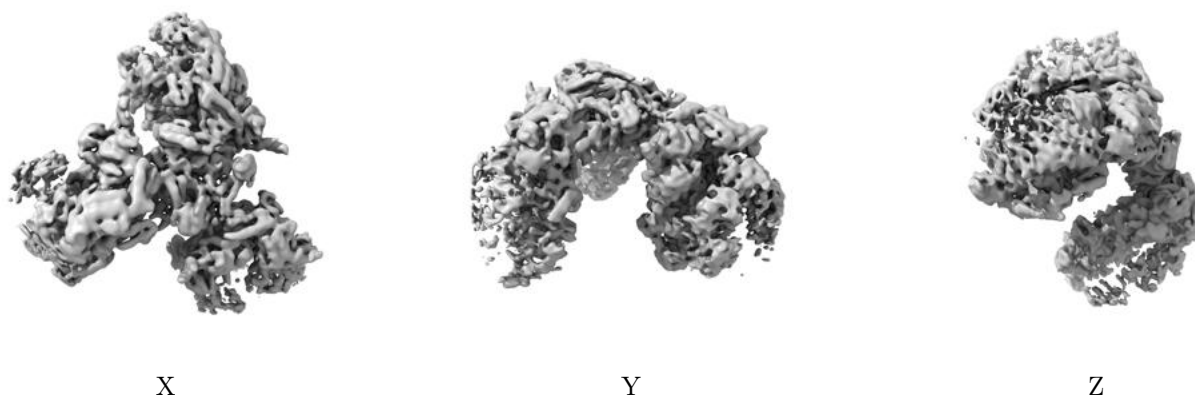


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0234. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

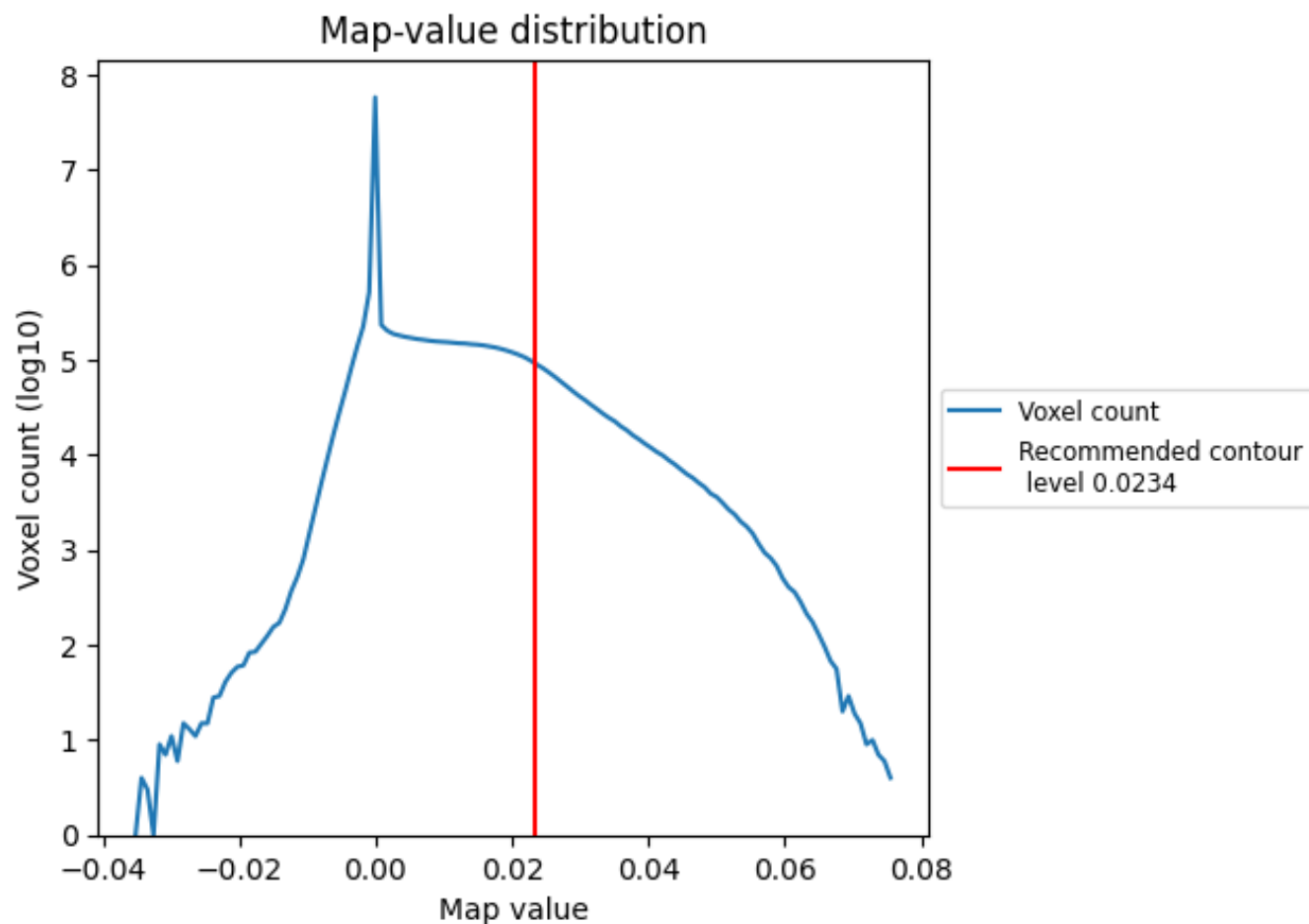
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

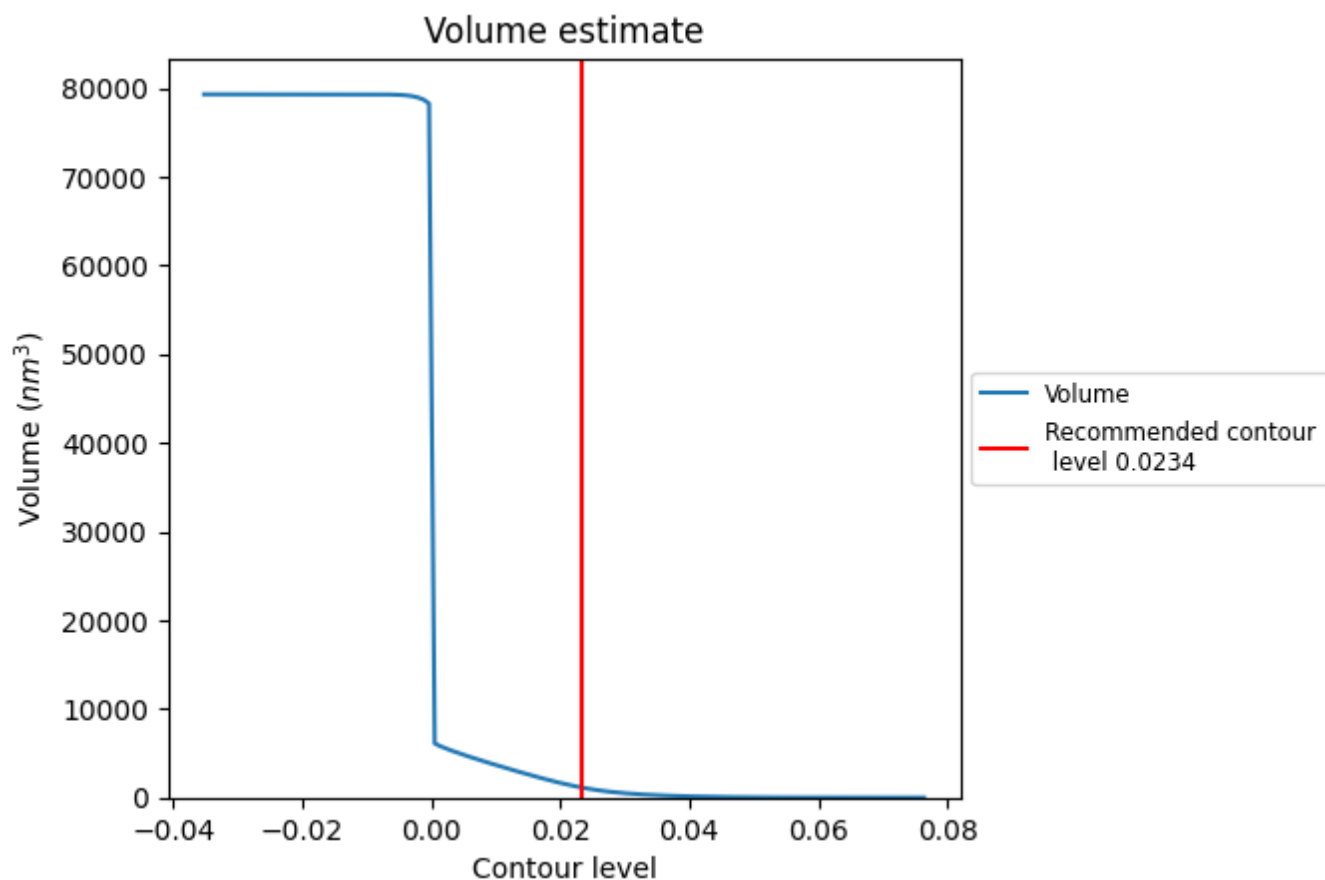
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

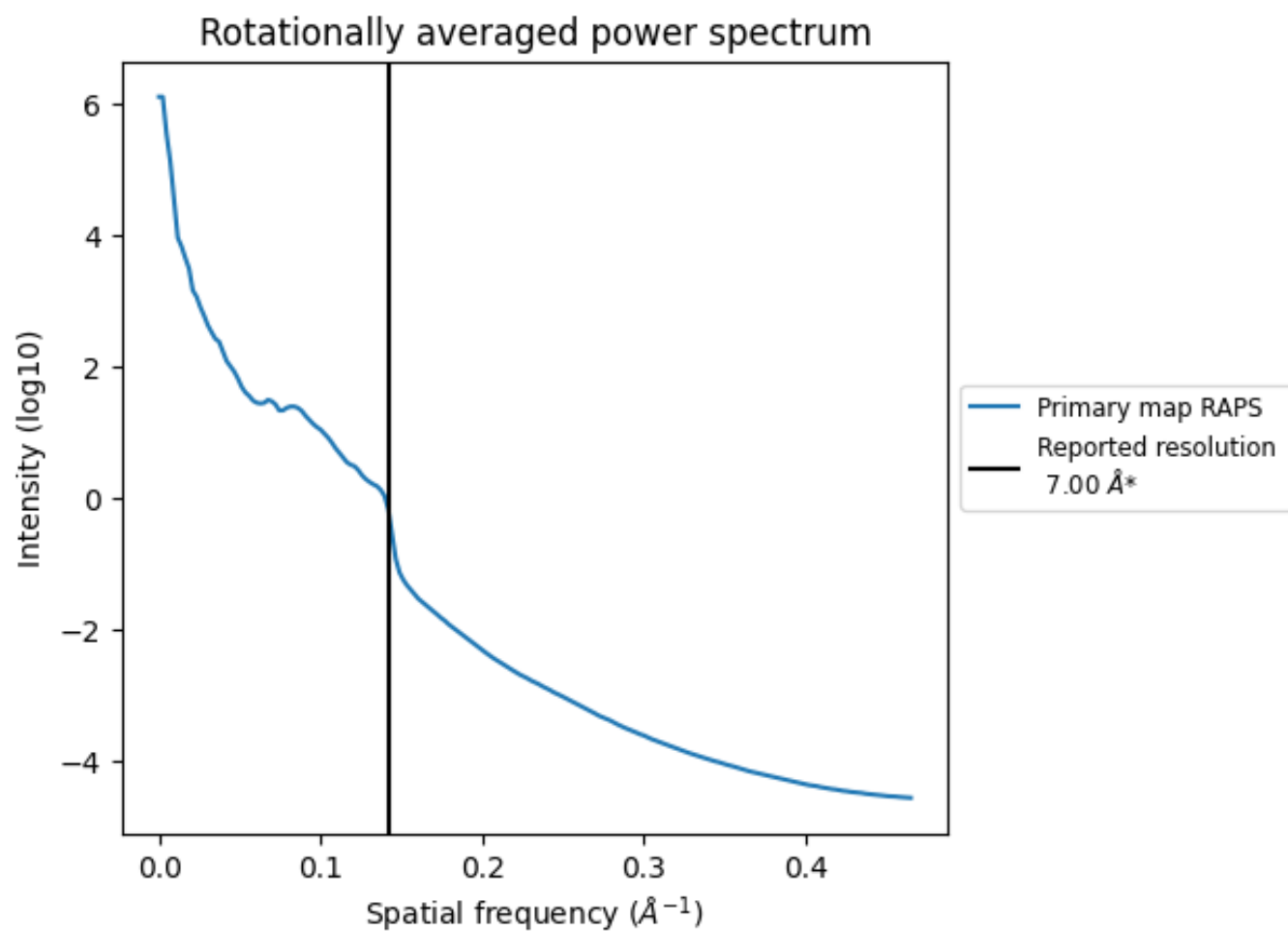
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1122 nm³; this corresponds to an approximate mass of 1014 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.143 Å⁻¹

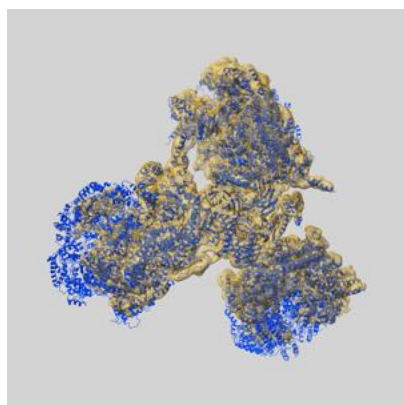
8 Fourier-Shell correlation

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

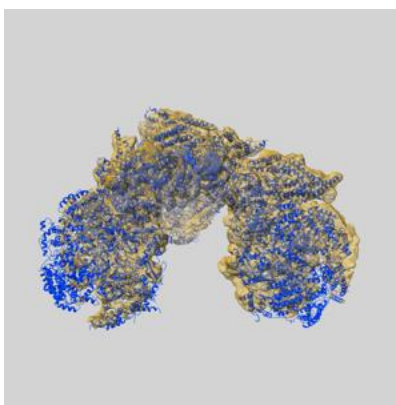
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-20473 and PDB model 6PTO. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

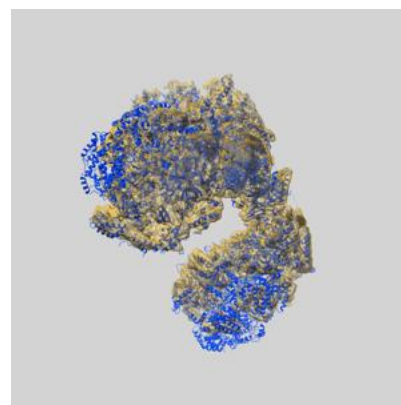
9.1 Map-model overlay [i](#)



X



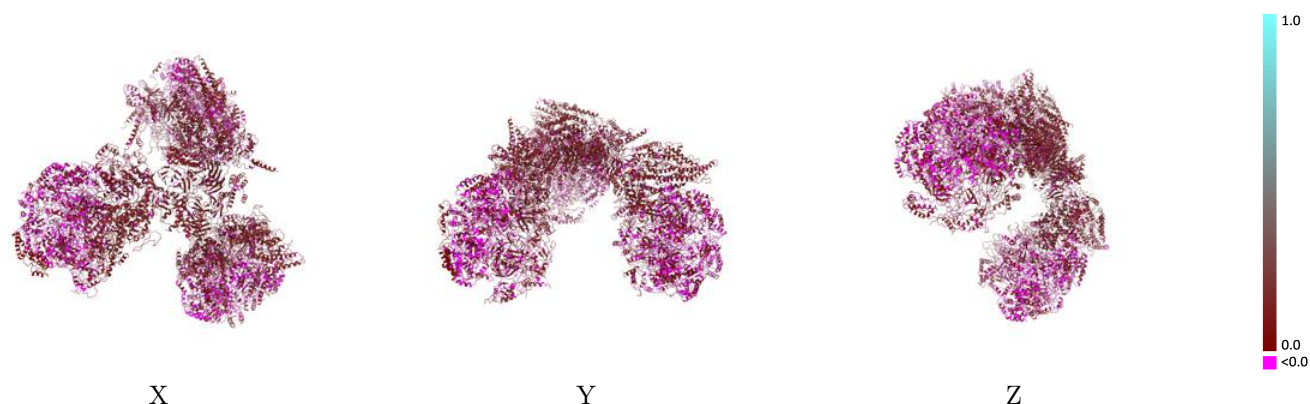
Y



Z

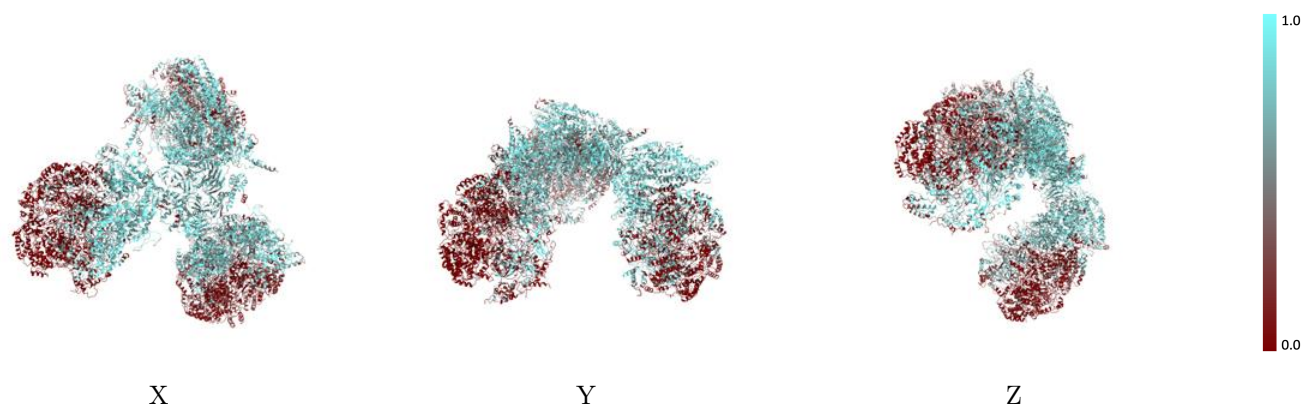
The images above show the 3D surface view of the map at the recommended contour level 0.0234 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



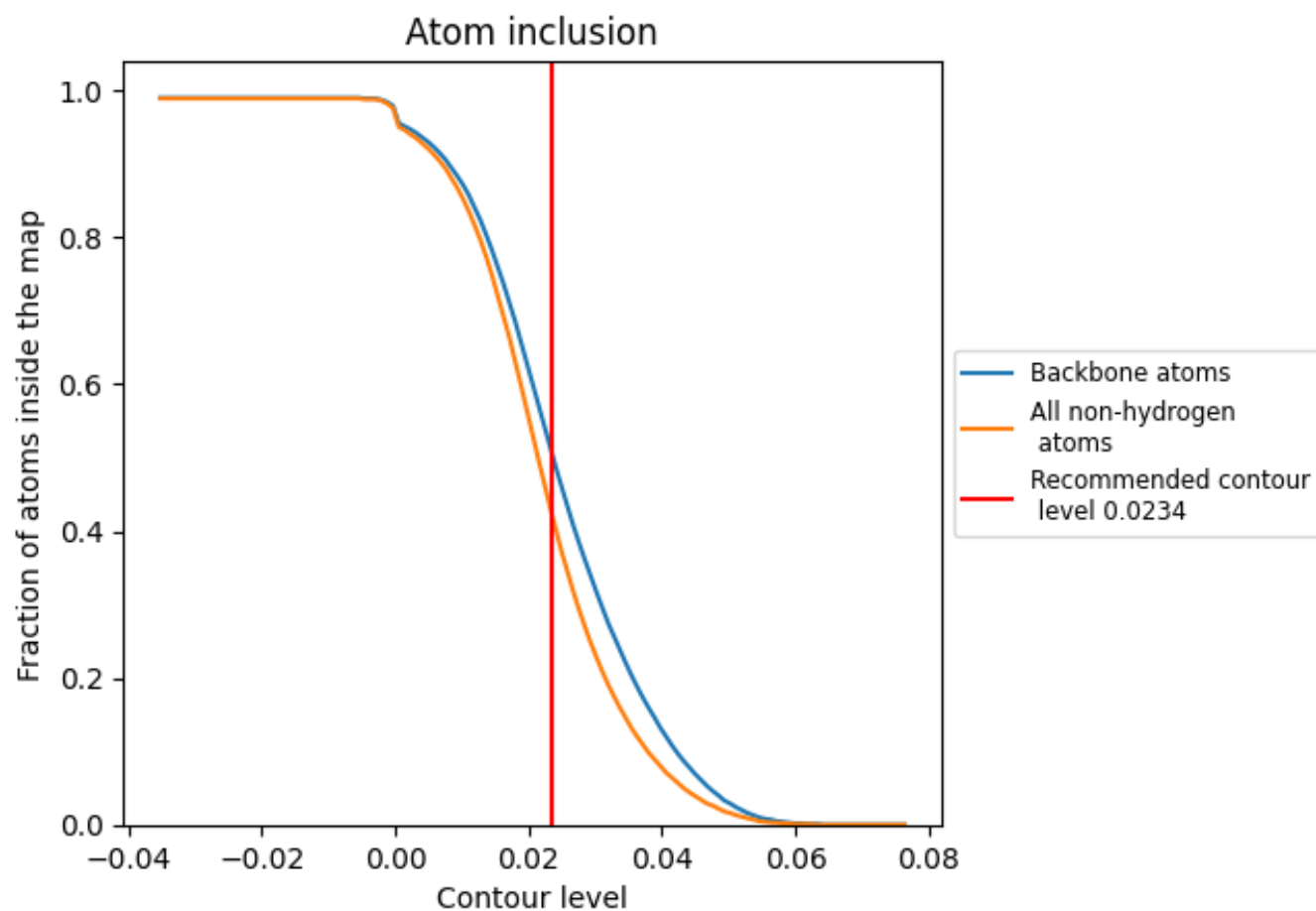
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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 (0.0234).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 51% of all backbone atoms, 43% 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 (0.0234) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4260	 0.0870
2	 0.2190	 0.0410
3	 0.2970	 0.0790
4	 0.1310	 0.0410
5	 0.3340	 0.0720
6	 0.1700	 0.0510
7	 0.1560	 0.0520
A	 0.6580	 0.1510
B	 0.7130	 0.1650
C	 0.6750	 0.1510
D	 0.7320	 0.1650
E	 0.6710	 0.1370
F	 0.2620	 0.0490
G	 0.3150	 0.0730
H	 0.1730	 0.0370
I	 0.3690	 0.0780
J	 0.2410	 0.0570
K	 0.1670	 0.0350
X	 0.7230	 0.1610
Y	 0.7180	 0.1510
Z	 0.7200	 0.1520
a	 0.6520	 0.1330
b	 0.7170	 0.1590
c	 0.6720	 0.1470
d	 0.7660	 0.1680
e	 0.7240	 0.1340
h	 0.3570	 0.0330
i	 0.5370	 0.0840
j	 0.2780	 0.0500
k	 0.4550	 0.0760
l	 0.3830	 0.0590
m	 0.3770	 0.0560
n	 0.7410	 0.1570
o	 0.7400	 0.1680
p	 0.7610	 0.1550



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Chain	Atom inclusion	Q-score
q	 0.7800	 0.1700
r	 0.7000	 0.1360