



wwPDB EM Validation Summary Report ⓘ

Jul 10, 2026 – 01:27 PM JST

PDB ID : 9XRL / pdb_00009xrl
EMDB ID : EMD-67147
Title : Structure of mouse cytoplasmic lattice (CPL) repeating unit
Authors : Chi, P.L.; Wang, X.; Li, J.L.; Deng, D.
Deposited on : 2025-11-19
Resolution : 3.74 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.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

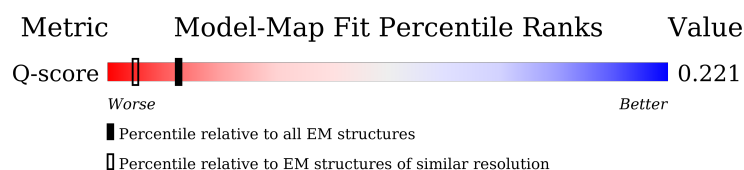
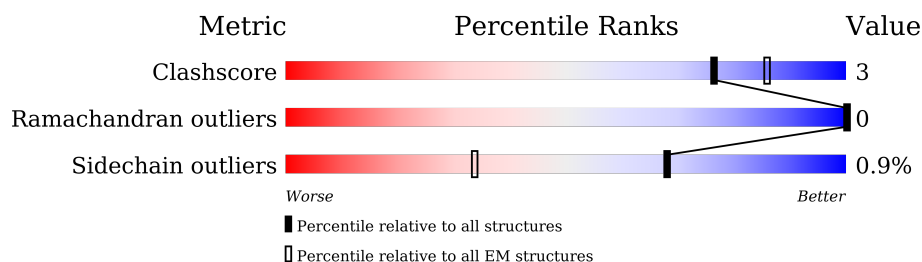
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.74 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



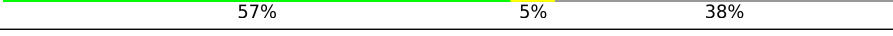
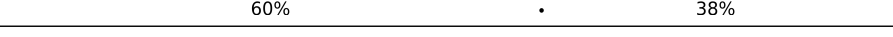
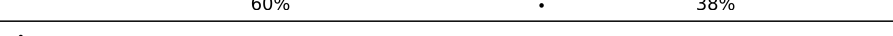
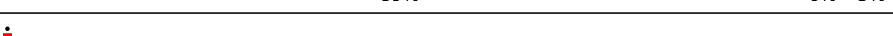
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10346 (3.24 - 4.24)

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	1	228	
1	3	228	
1	9	228	
2	4	440	

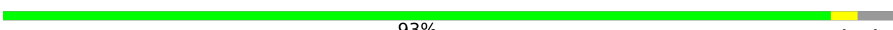
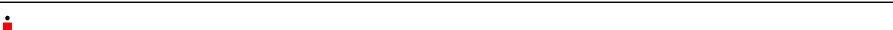
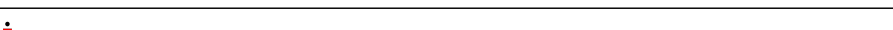
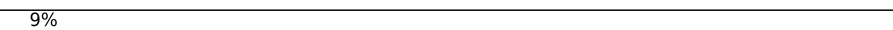
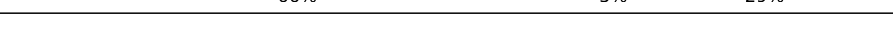
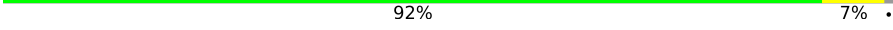
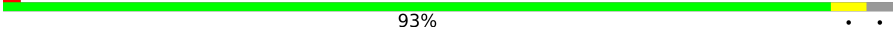
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Mol	Chain	Length	Quality of chain
2	6	440	
2	AA	440	
3	A	468	
4	D	163	
4	F	163	
4	O	163	
4	p	163	
4	q	163	
5	8	581	
5	AC	581	
5	E	581	
5	I	581	
5	P	581	
5	z	581	
6	H	937	
6	Q	937	
6	h	937	
6	i	937	
7	B	682	
7	K	682	
7	S	682	
7	T	682	
7	U	682	
7	V	682	
7	W	682	

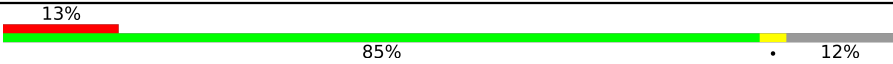
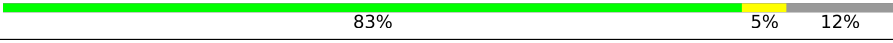
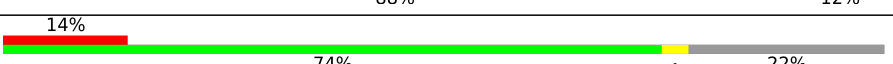
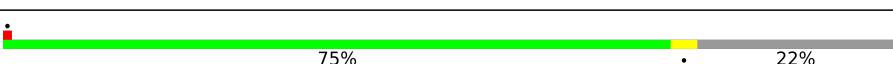
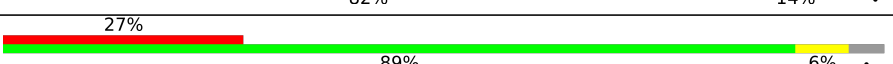
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Mol	Chain	Length	Quality of chain
7	X	682	 90% 6%
7	Y	682	 94%
7	Z	682	 93%
7	b	682	 90% 6%
7	c	682	 83% 12%
7	d	682	 89% 7%
7	f	682	 87% 9%
7	j	682	 85% 11%
7	m	682	 87% 9%
7	n	682	 88% 9%
7	o	682	 87% 9%
7	r	682	 89% 6% 5%
7	s	682	 88% 8%
8	AH	164	 9% 66% 5% 29%
8	AI	164	 60% 10% 29%
8	AJ	164	 58% 12% 29%
8	AT	164	 6% 66% 11% 22%
8	e	164	 10% 64% 14% 22%
8	g	164	 64% 14% 22%
9	k	469	 84% 15%
9	l	469	 92% 7%
10	AE	445	 32% 89% 8%
10	AN	445	 91% 6%
10	t	445	 93%
11	0	1059	 86% 12%

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Mol	Chain	Length	Quality of chain
11	2	1059	
11	5	1059	
11	7	1059	
11	AB	1059	
11	y	1059	
12	AF	451	
12	AO	451	
12	u	451	
13	AK	993	
13	AQ	993	
13	w	993	
14	AD	147	
14	AM	147	
14	AS	147	
15	AL	782	
15	AR	782	
15	x	782	
16	C	466	
16	L	466	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	GTP	AF	501	-	-	X	-

2 Entry composition [i](#)

There are 20 unique types of molecules in this entry. The entry contains 281032 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 Zinc finger BED domain-containing protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	56	Total	C	N	O	S	0	0
			427	268	80	74	5		
1	3	56	Total	C	N	O	S	0	0
			453	288	84	75	6		
1	9	56	Total	C	N	O	S	0	0
			453	288	84	75	6		

- Molecule 2 is a protein called KH domain-containing protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	4	124	Total	C	N	O	S	0	0
			977	633	167	171	6		
2	6	124	Total	C	N	O	S	0	0
			1028	667	178	175	8		
2	AA	124	Total	C	N	O	S	0	0
			1028	667	178	175	8		

- Molecule 3 is a protein called F-box and WD-40 domain protein 21.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	450	Total	C	N	O	S	0	0
			3650	2372	604	651	23		

- Molecule 4 is a protein called S-phase kinase-associated protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	148	Total	C	N	O	S	0	0
			1195	756	196	237	6		
4	p	148	Total	C	N	O	S	0	0
			1190	750	195	239	6		
4	O	148	Total	C	N	O	S	0	0
			1199	758	196	239	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	q	148	Total	C	N	O	S	0	0
			1190	750	195	239	6		
4	F	148	Total	C	N	O	S	0	0
			1199	758	196	239	6		

- Molecule 5 is a protein called Transducin-like enhancer protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	358	Total	C	N	O	S	0	0
			2799	1771	493	515	20		
5	I	358	Total	C	N	O	S	0	0
			2817	1786	495	516	20		
5	z	358	Total	C	N	O	S	0	0
			2813	1785	494	514	20		
5	P	358	Total	C	N	O	S	0	0
			2817	1786	495	516	20		
5	AC	358	Total	C	N	O	S	0	0
			2817	1786	495	516	20		
5	8	358	Total	C	N	O	S	0	0
			2817	1786	495	516	20		

- Molecule 6 is a protein called NLR family, pyrin domain containing 4F.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	723	Total	C	N	O	S	0	0
			5803	3706	973	1070	54		
6	Q	636	Total	C	N	O	S	0	0
			5099	3248	850	948	53		
6	i	721	Total	C	N	O	S	0	0
			5738	3657	961	1064	56		
6	h	721	Total	C	N	O	S	0	0
			5781	3684	971	1071	55		

- Molecule 7 is a protein called Inactive protein-arginine deiminase type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	S	647	Total	C	N	O	S	0	0
			5102	3271	836	958	37		
7	T	654	Total	C	N	O	S	0	0
			5162	3310	849	965	38		
7	Y	658	Total	C	N	O	S	0	0
			5099	3279	836	949	35		

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Mol	Chain	Residues	Atoms					AltConf	Trace
7	b	656	Total	C	N	O	S	0	0
			5149	3304	845	962	38		
7	X	652	Total	C	N	O	S	0	0
			5161	3308	851	964	38		
7	Z	652	Total	C	N	O	S	0	0
			5133	3291	846	958	38		
7	V	652	Total	C	N	O	S	0	0
			5139	3297	845	959	38		
7	W	654	Total	C	N	O	S	0	0
			5151	3302	848	963	38		
7	n	658	Total	C	N	O	S	0	0
			5105	3282	839	949	35		
7	f	654	Total	C	N	O	S	0	0
			5168	3312	850	968	38		
7	s	656	Total	C	N	O	S	0	0
			5146	3303	845	960	38		
7	m	652	Total	C	N	O	S	0	0
			5161	3308	851	964	38		
7	o	652	Total	C	N	O	S	0	0
			5138	3294	845	961	38		
7	d	652	Total	C	N	O	S	0	0
			5130	3293	841	958	38		
7	j	654	Total	C	N	O	S	0	0
			5155	3305	849	963	38		
7	r	650	Total	C	N	O	S	0	0
			5144	3298	849	960	37		
7	B	651	Total	C	N	O	S	0	0
			5141	3293	849	962	37		
7	K	652	Total	C	N	O	S	0	0
			5145	3294	850	964	37		
7	U	655	Total	C	N	O	S	0	0
			5163	3304	853	968	38		
7	c	655	Total	C	N	O	S	0	0
			5167	3308	853	968	38		

- Molecule 8 is a protein called Oocyte-expressed protein homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	e	128	Total	C	N	O	S	0	0
			928	590	164	169	5		
8	g	128	Total	C	N	O	S	0	0
			928	590	164	169	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
8	AH	116	Total	C	N	O	S	0	0
			875	560	152	162	1		
8	AJ	116	Total	C	N	O	S	0	0
			938	600	162	171	5		
8	AI	116	Total	C	N	O	S	0	0
			935	597	162	171	5		
8	AT	128	Total	C	N	O	S	0	0
			928	590	164	169	5		

- Molecule 9 is a protein called Expressed sequence C85627.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	k	463	Total	C	N	O	S	0	0
			3729	2406	616	678	29		
9	l	463	Total	C	N	O	S	0	0
			3732	2409	616	678	29		

- Molecule 10 is a protein called Tubulin beta-4B chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	t	430	Total	C	N	O	S	0	0
			3373	2119	578	650	26		
10	AE	430	Total	C	N	O	S	0	0
			3358	2110	572	650	26		
10	AN	430	Total	C	N	O	S	0	0
			3373	2119	578	650	26		

- Molecule 11 is a protein called NACHT, LRR and PYD domains-containing protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	y	936	Total	C	N	O	S	0	0
			7262	4624	1230	1343	65		
11	AB	936	Total	C	N	O	S	0	0
			7322	4663	1239	1354	66		
11	0	935	Total	C	N	O	S	0	0
			7316	4658	1238	1354	66		
11	7	936	Total	C	N	O	S	0	0
			7319	4660	1239	1354	66		
11	5	935	Total	C	N	O	S	0	0
			7312	4655	1238	1353	66		
11	2	934	Total	C	N	O	S	0	0
			7221	4600	1222	1334	65		

- Molecule 12 is a protein called Tubulin alpha-1A chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	u	430	Total	C	N	O	S	0	0
			3368	2136	573	637	22		
12	AF	430	Total	C	N	O	S	0	0
			3365	2135	573	635	22		
12	AO	430	Total	C	N	O	S	0	0
			3368	2136	573	637	22		

- Molecule 13 is a protein called NACHT, LRR and PYD domains-containing protein 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	w	948	Total	C	N	O	S	0	0
			7473	4754	1292	1366	61		
13	AK	948	Total	C	N	O	S	0	0
			7417	4719	1284	1354	60		
13	AQ	948	Total	C	N	O	S	0	0
			7472	4754	1292	1365	61		

- Molecule 14 is a protein called Ubiquitin-conjugating enzyme E2 D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AM	147	Total	C	N	O	S	0	0
			1167	748	197	215	7		
14	AS	147	Total	C	N	O	S	0	0
			1168	748	197	215	8		
14	AD	147	Total	C	N	O	S	0	0
			1168	748	197	215	8		

- Molecule 15 is a protein called E3 ubiquitin-protein ligase UHRF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AL	608	Total	C	N	O	S	0	0
			4872	3059	886	895	32		
15	AR	608	Total	C	N	O	S	0	0
			4872	3059	886	895	32		
15	x	608	Total	C	N	O	S	0	0
			4854	3050	881	891	32		

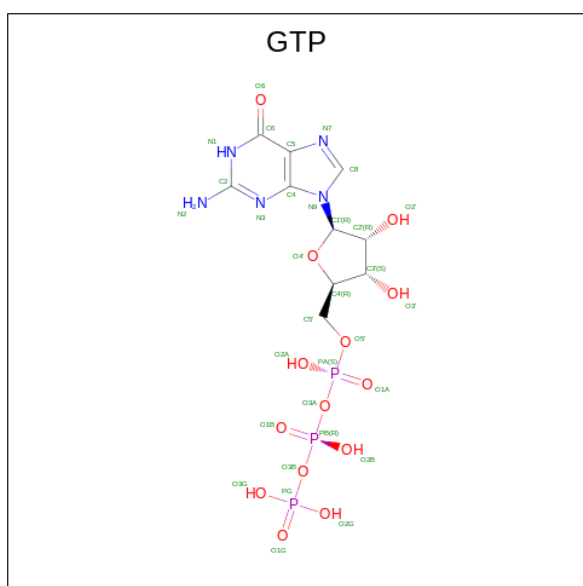
- Molecule 16 is a protein called F-box and WD-40 domain protein 19.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	449	Total	C	N	O	S	0	0
			3611	2322	617	643	29		
16	C	449	Total	C	N	O	S	0	0
			3601	2317	614	641	29		

- Molecule 17 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
17	1	1	Total	Zn	0
			1	1	
17	3	1	Total	Zn	0
			1	1	
17	9	1	Total	Zn	0
			1	1	
17	AL	2	Total	Zn	0
			2	2	
17	AR	4	Total	Zn	0
			4	4	
17	x	4	Total	Zn	0
			4	4	

- Molecule 18 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



Mol	Chain	Residues	Atoms					AltConf
18	t	1	Total	C	N	O	P	0
			32	10	5	14	3	
18	u	1	Total	C	N	O	P	0
			32	10	5	14	3	

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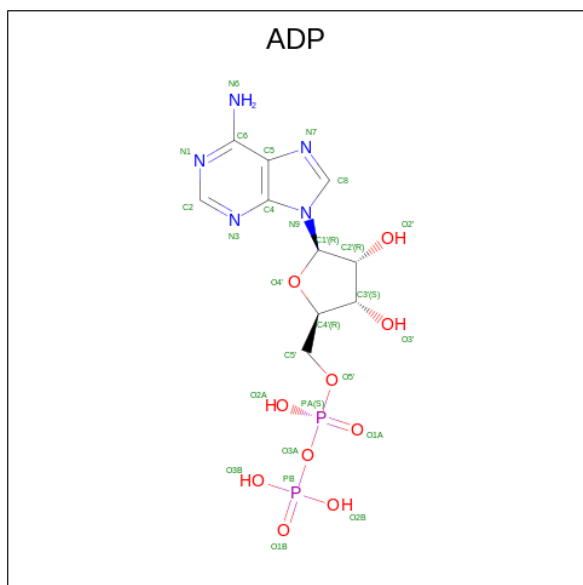
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Mol	Chain	Residues	Atoms					AltConf
18	AF	1	Total	C	N	O	P	0
			32	10	5	14	3	
18	AO	1	Total	C	N	O	P	0
			32	10	5	14	3	
18	AN	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 19 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
19	t	1	Total	Mg	0
			1	1	
19	u	1	Total	Mg	0
			1	1	
19	AO	1	Total	Mg	0
			1	1	
19	AN	1	Total	Mg	0
			1	1	

- Molecule 20 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					AltConf
20	w	1	Total	C	N	O	P	0
			27	10	5	10	2	
20	AK	1	Total	C	N	O	P	0
			27	10	5	10	2	

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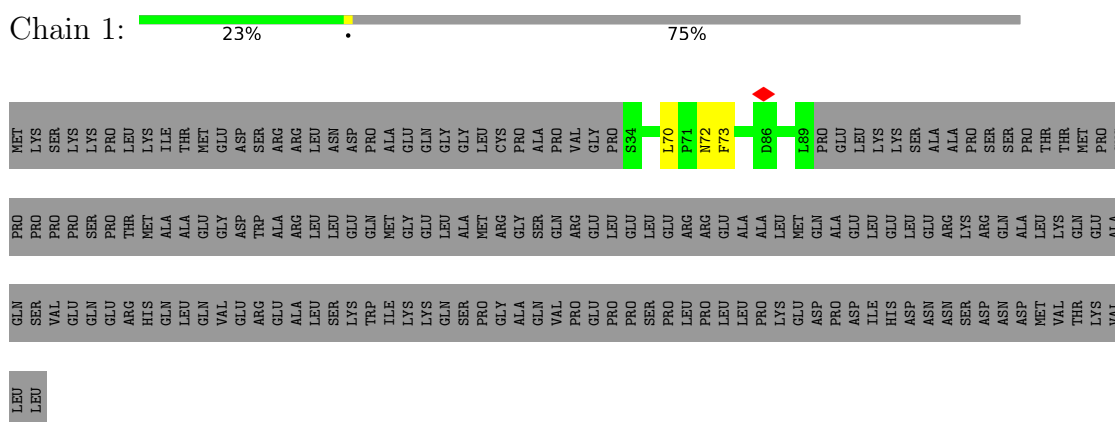
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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
20	AQ	1	27	10	5	10	2	0

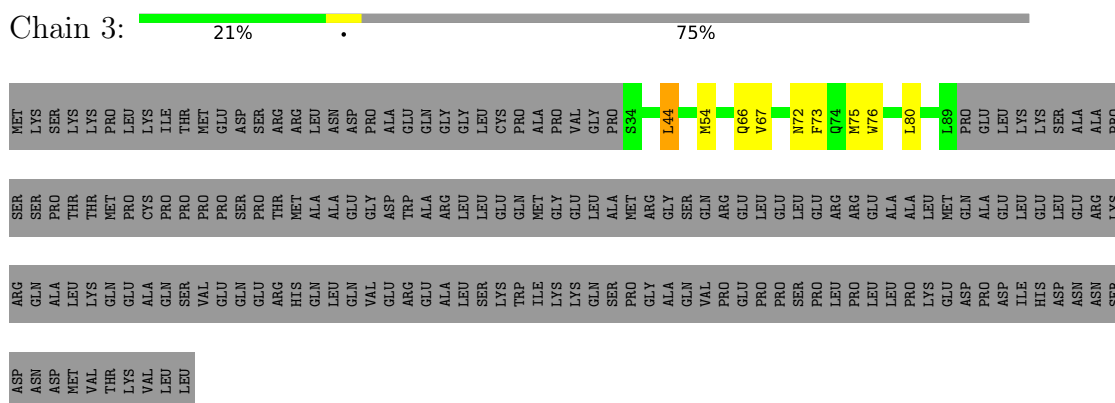
3 Residue-property plots

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.

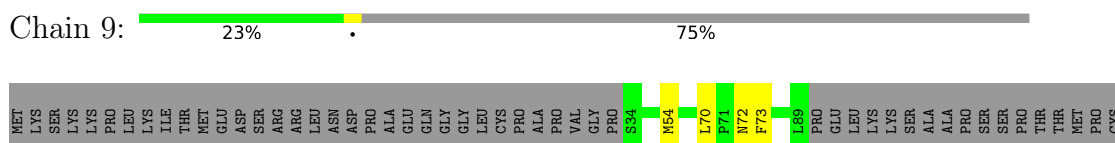
- Molecule 1: Zinc finger BED domain-containing protein 3



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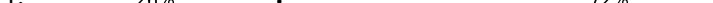


- Molecule 1: Zinc finger BED domain-containing protein 3



[illegible]

- Molecule 2: KH domain-containing protein 3

Chain 4:  26% 72%

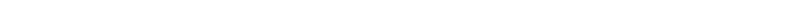
[illegible]

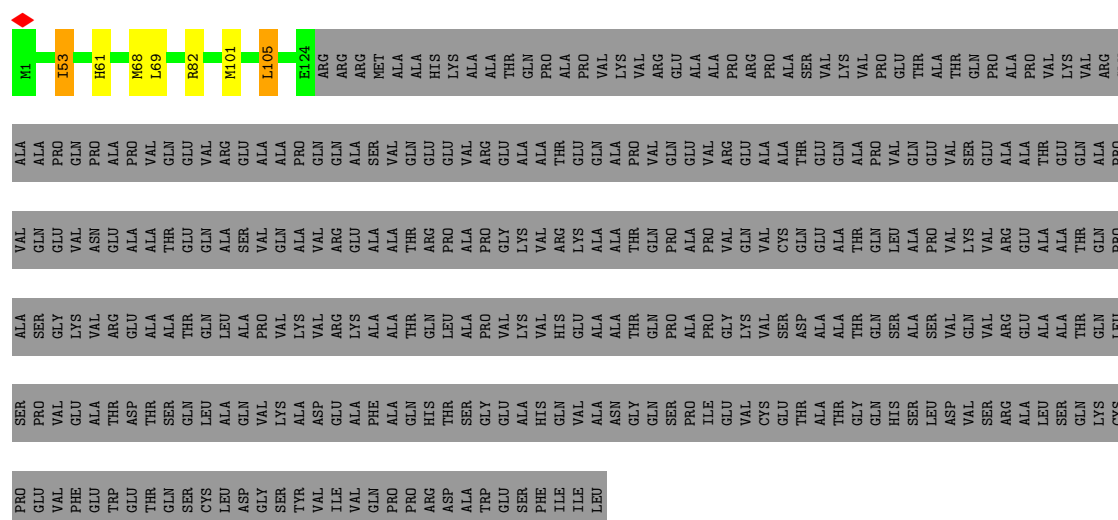
- Molecule 2: KH domain-containing protein 3

Chain 6: 26% . 72%

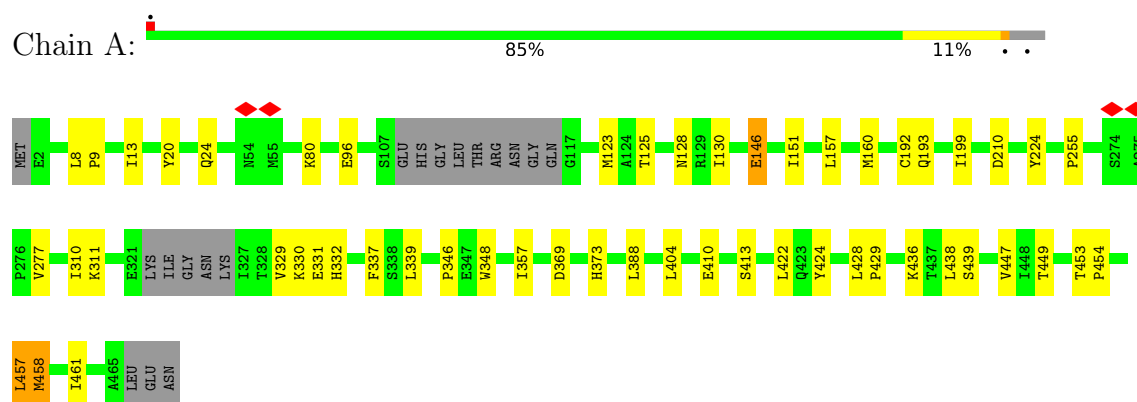
[illegible]

- Molecule 2: KH domain-containing protein 3

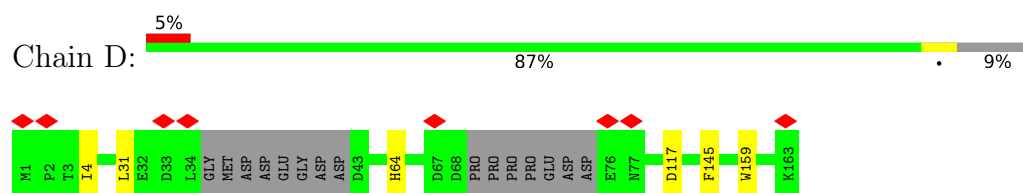
Chain AA:  27% : 72%



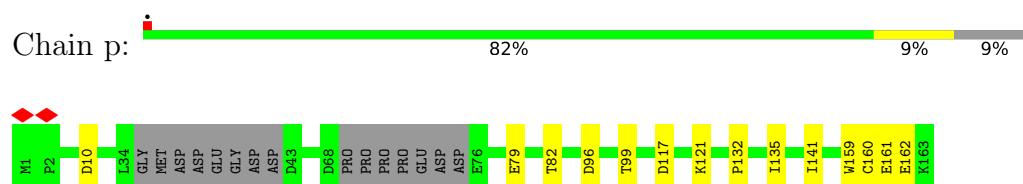
• Molecule 3: F-box and WD-40 domain protein 21



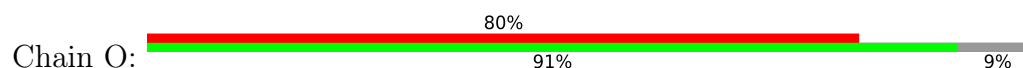
• Molecule 4: S-phase kinase-associated protein 1

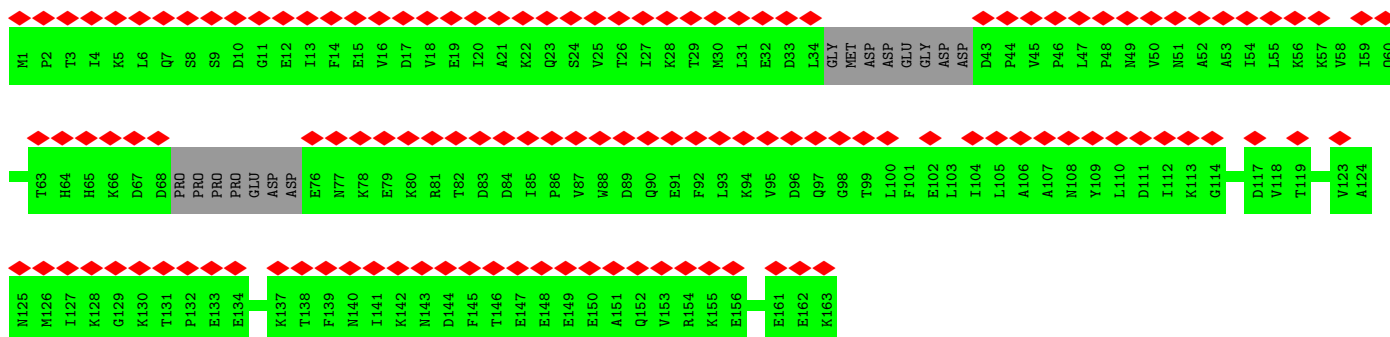


• Molecule 4: S-phase kinase-associated protein 1

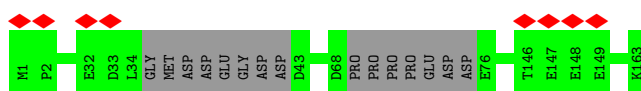
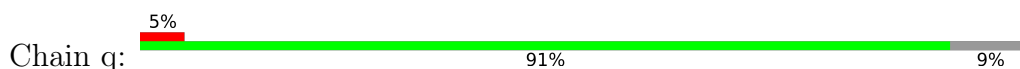


• Molecule 4: S-phase kinase-associated protein 1

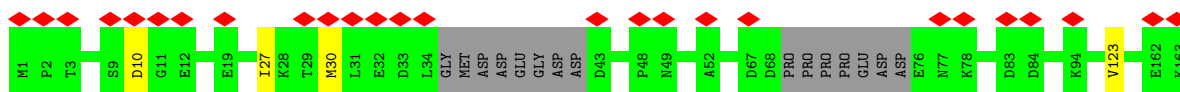
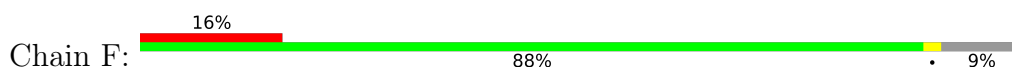




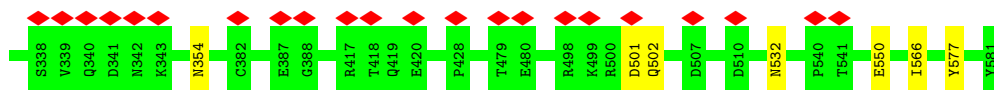
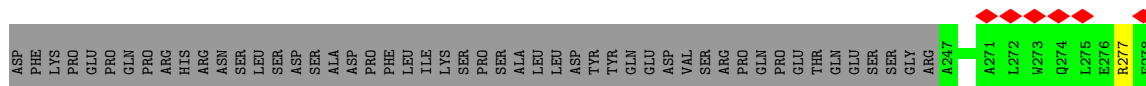
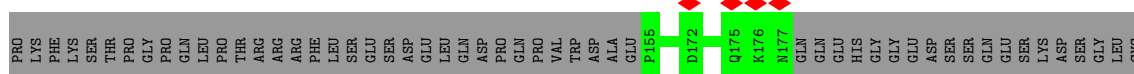
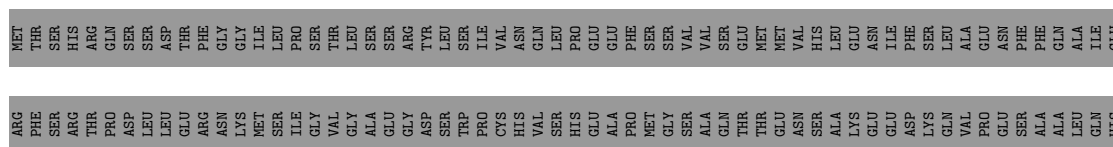
- Molecule 4: S-phase kinase-associated protein 1



- Molecule 4: S-phase kinase-associated protein 1

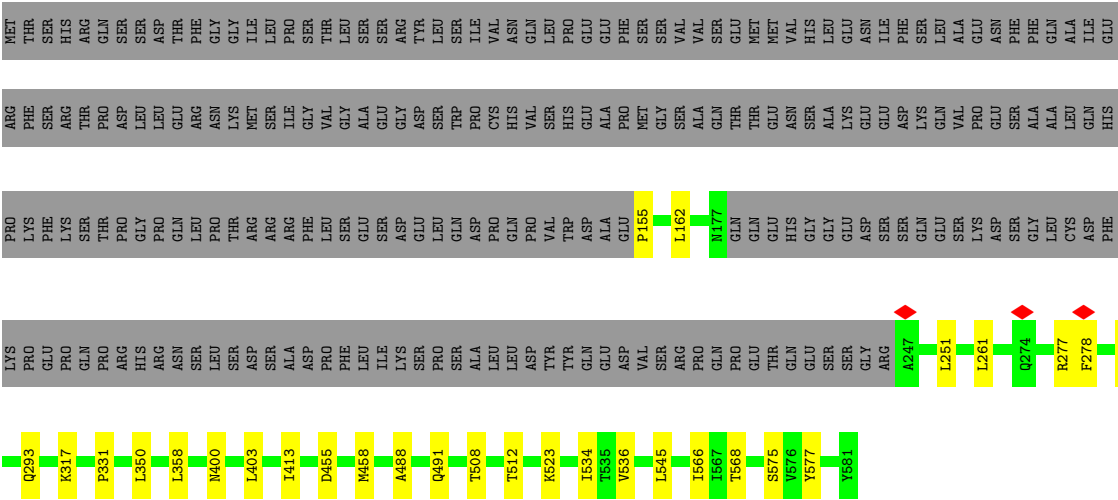


- Molecule 5: Transducin-like enhancer protein 6

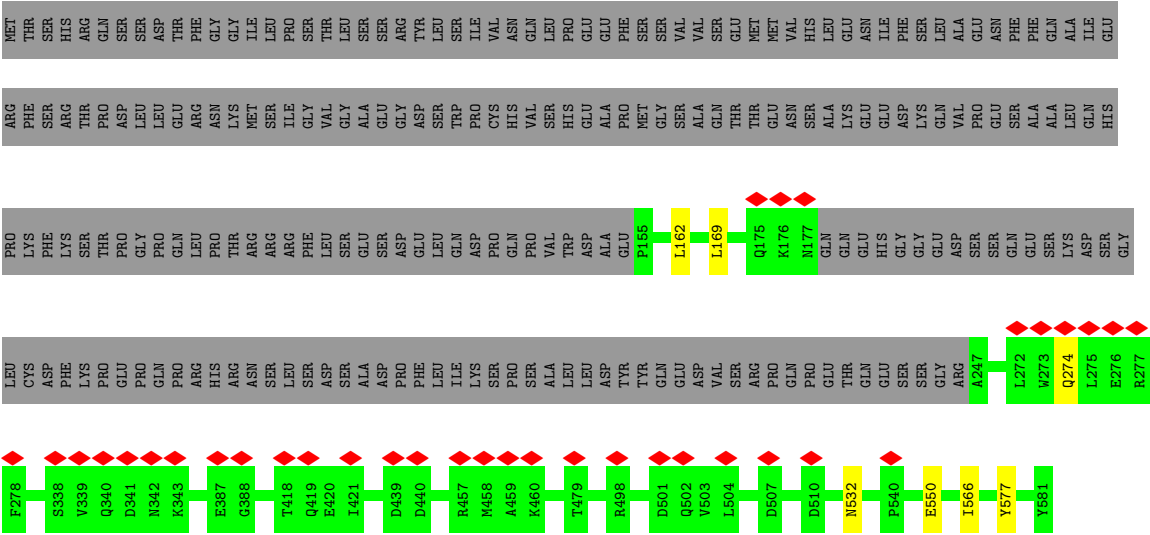


- Molecule 5: Transducin-like enhancer protein 6

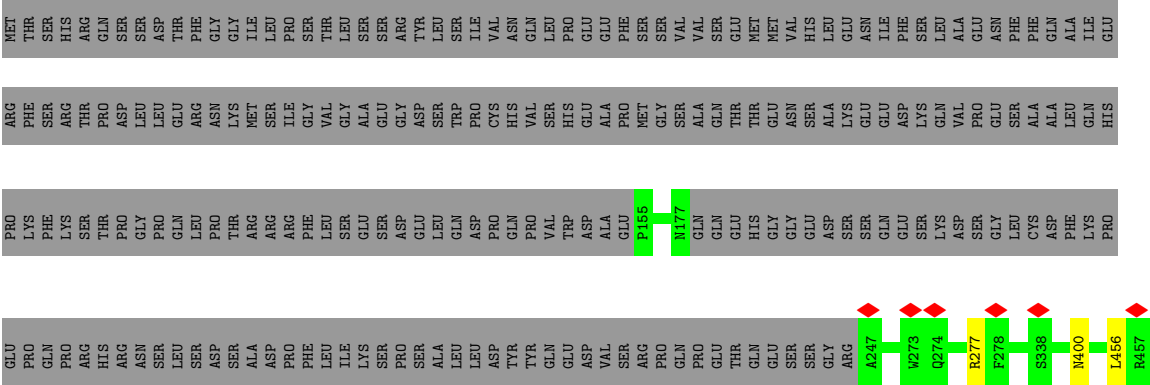


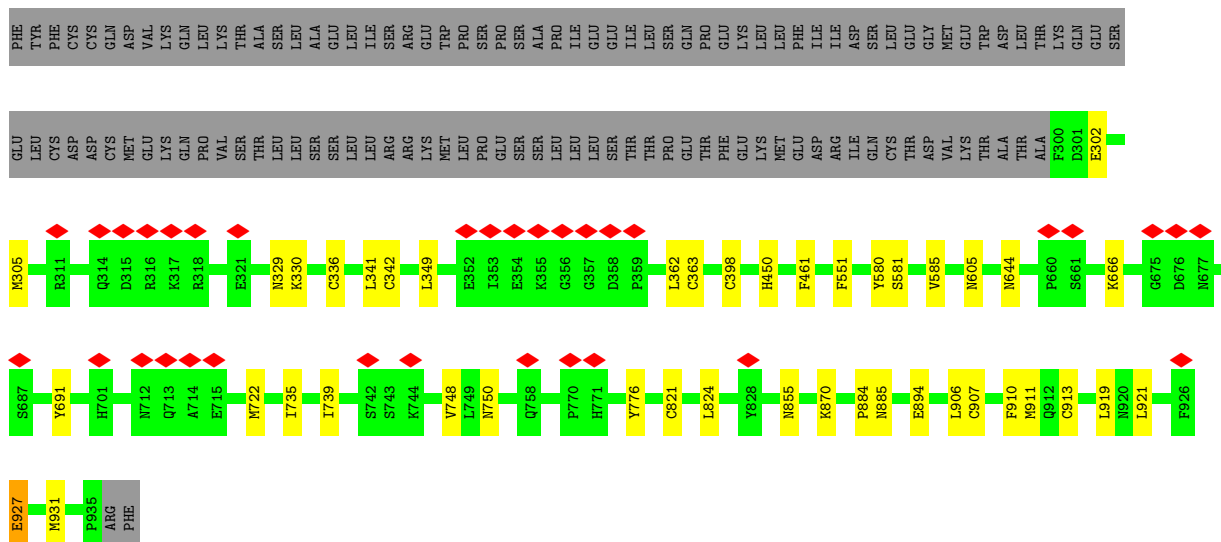


• Molecule 5: Transducin-like enhancer protein 6

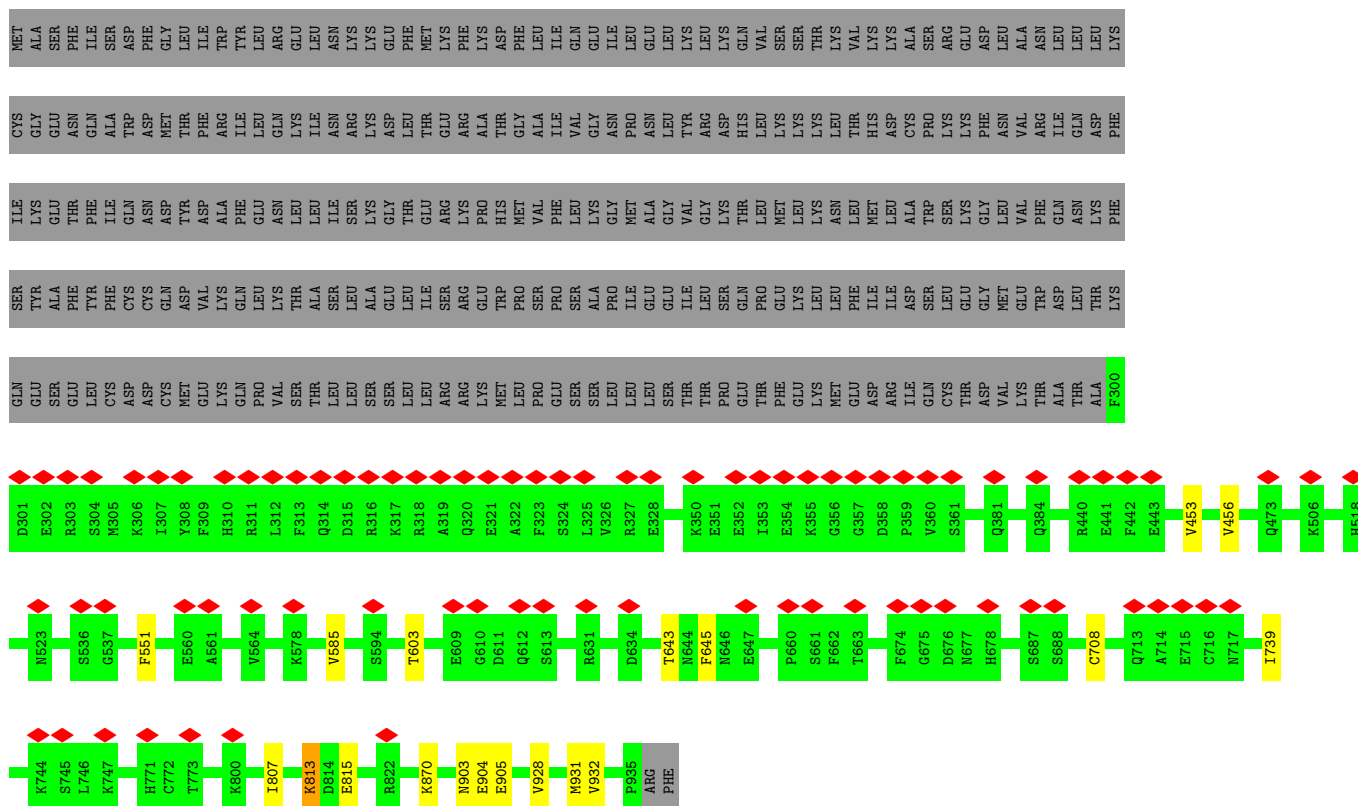


• Molecule 5: Transducin-like enhancer protein 6





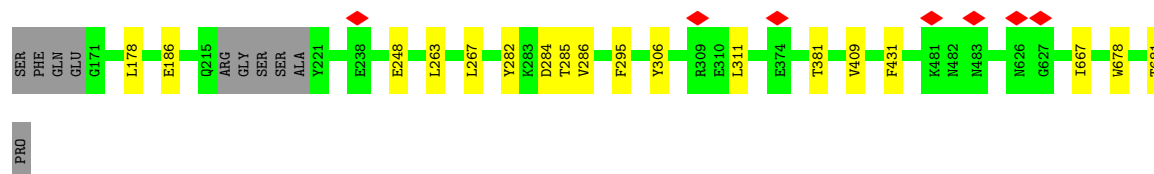
- Molecule 6: NLR family, pyrin domain containing 4F



- Molecule 6: NLR family, pyrin domain containing 4F

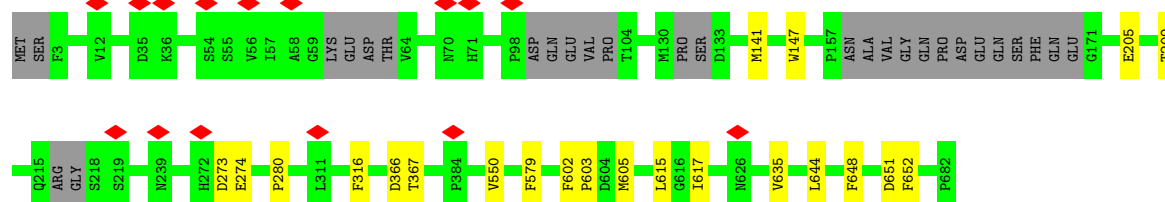






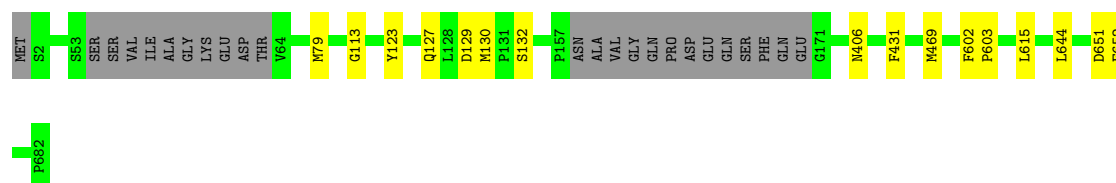
- Molecule 7: Inactive protein-arginine deiminase type-6

Chain T: 93%



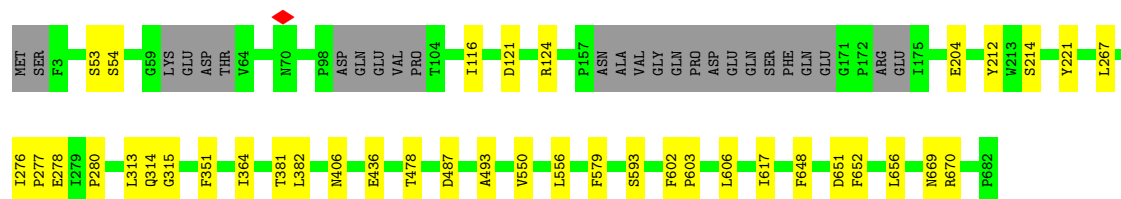
- Molecule 7: Inactive protein-arginine deiminase type-6

Chain Y: 94%



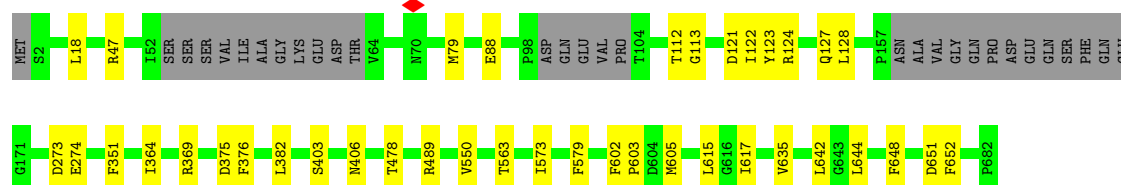
- Molecule 7: Inactive protein-arginine deiminase type-6

Chain b: 90% 6%

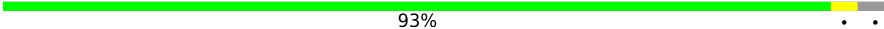


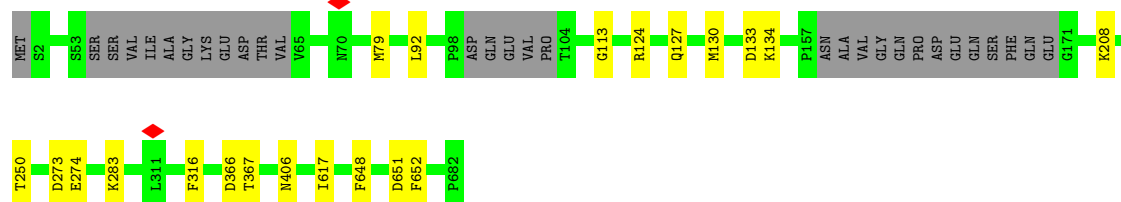
- Molecule 7: Inactive protein-arginine deiminase type-6

Chain X: 90% 6%



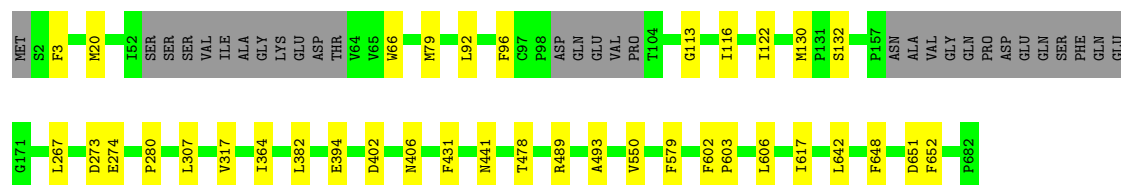
- Molecule 7: Inactive protein-arginine deiminase type-6

Chain Z:  93%

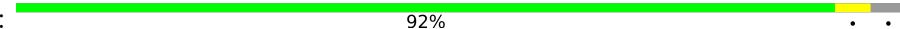


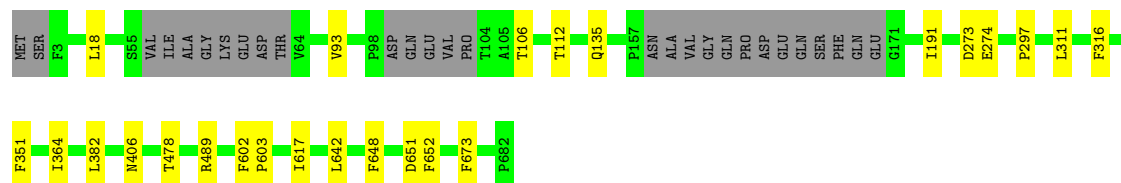
- Molecule 7: Inactive protein-arginine deiminase type-6

Chain V:  90%



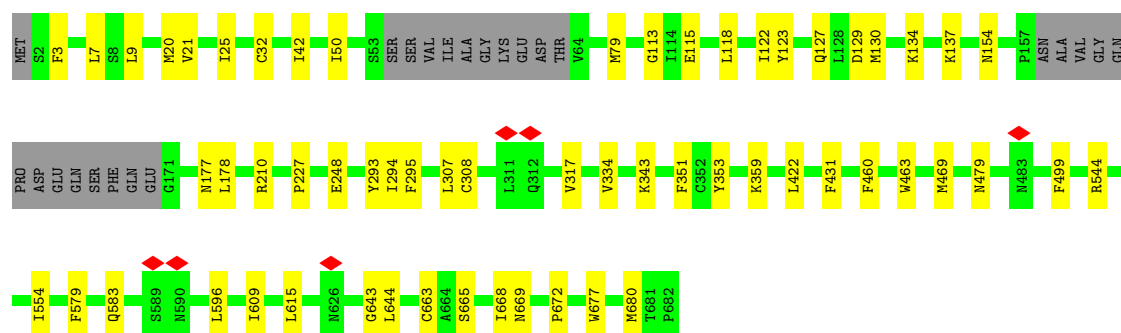
- Molecule 7: Inactive protein-arginine deiminase type-6

Chain W:  92%



- Molecule 7: Inactive protein-arginine deiminase type-6

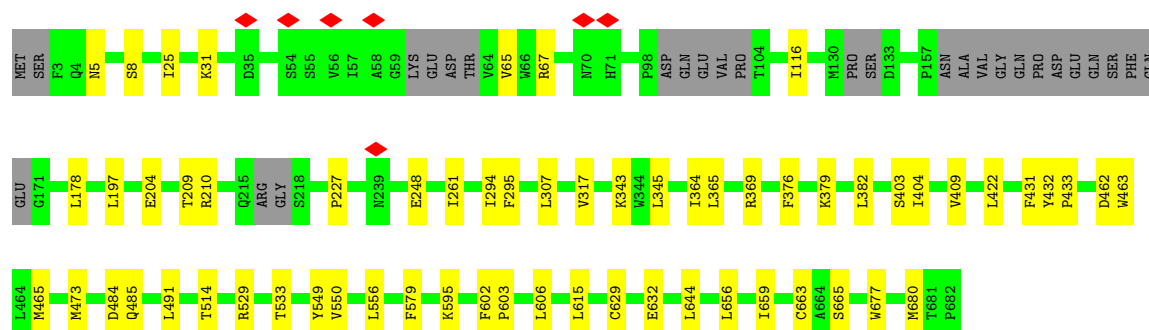
Chain n:  88%



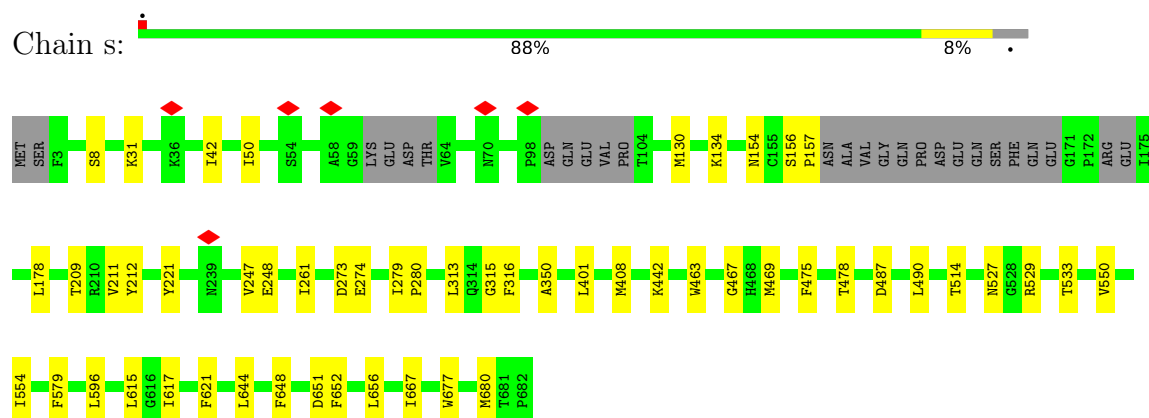
- Molecule 7: Inactive protein-arginine deiminase type-6

Chain f:  87%

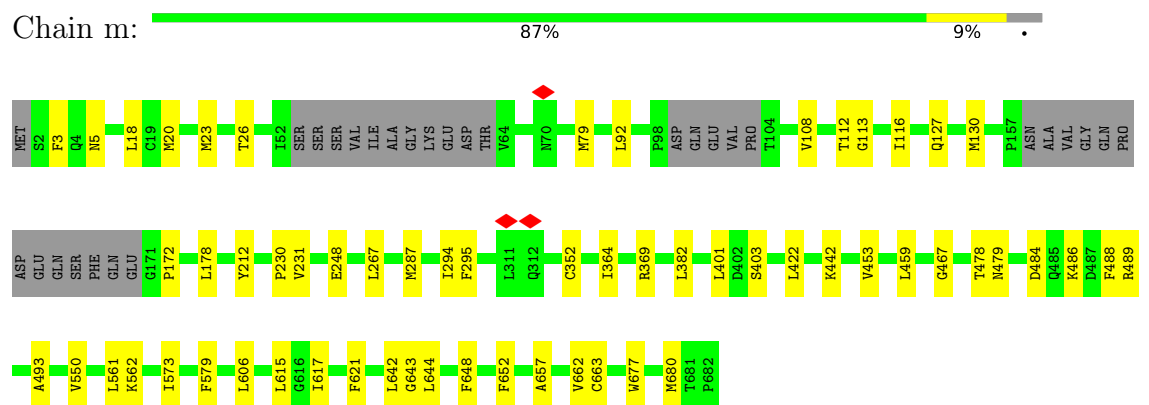




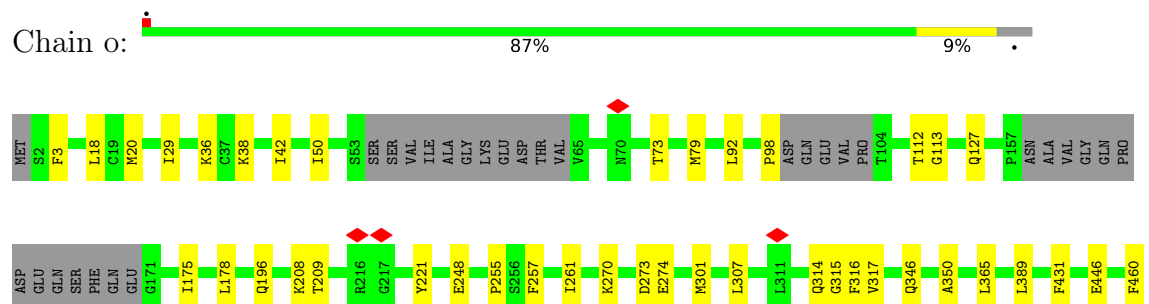
• Molecule 7: Inactive protein-arginine deiminase type-6



• Molecule 7: Inactive protein-arginine deiminase type-6



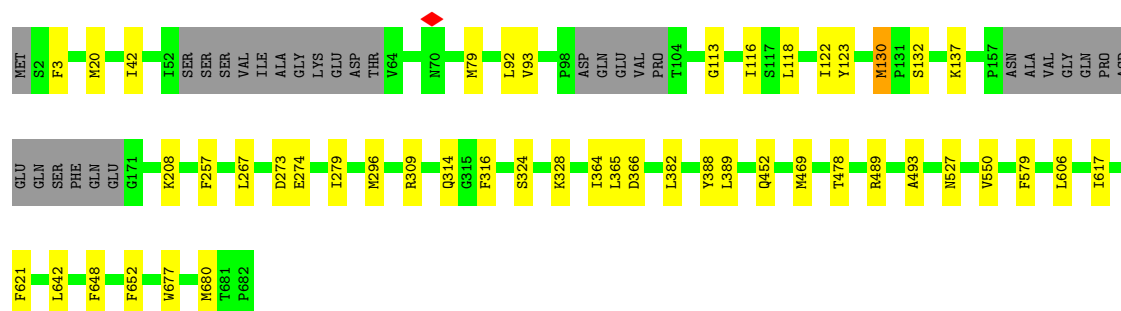
• Molecule 7: Inactive protein-arginine deiminase type-6





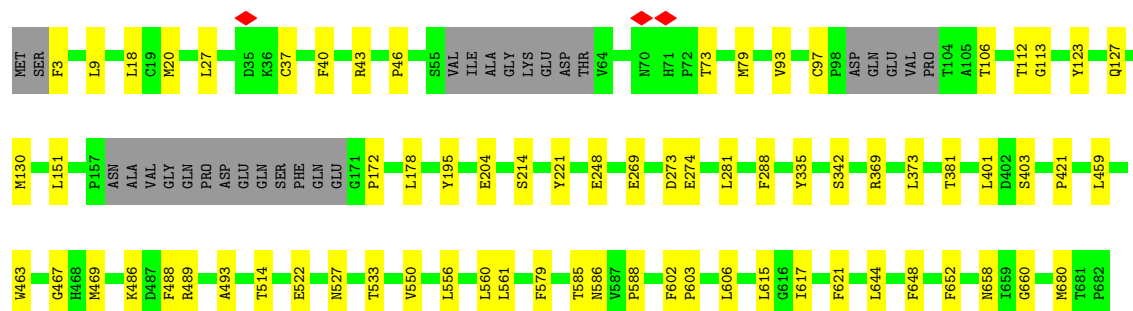
- Molecule 7: Inactive protein-arginine deiminase type-6

Chain d: 89% 7% .



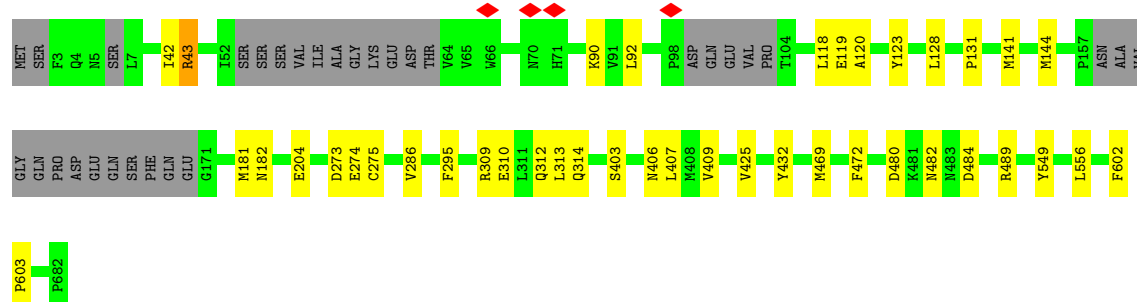
- Molecule 7: Inactive protein-arginine deiminase type-6

Chain j: 85% 11% .



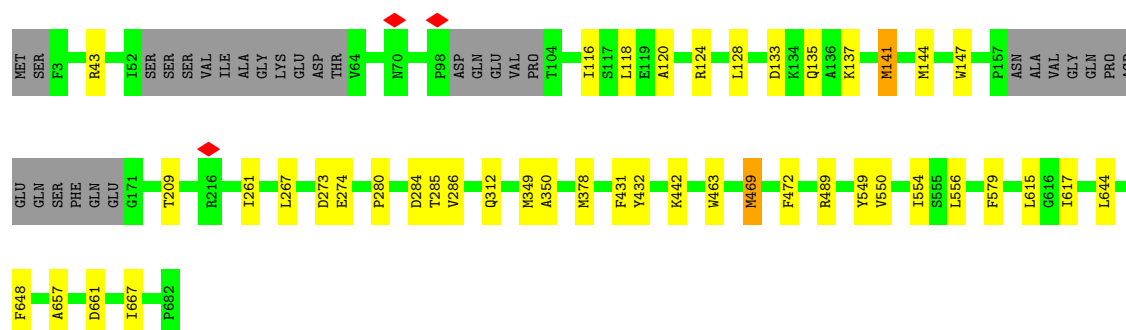
- Molecule 7: Inactive protein-arginine deiminase type-6

Chain r: 89% 6% 5%



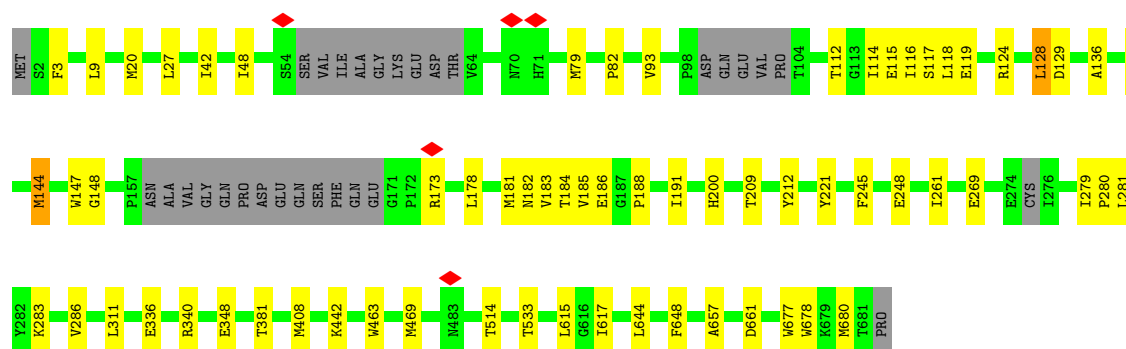
- Molecule 7: Inactive protein-arginine deiminase type-6

Chain B: 89% 6% 5%



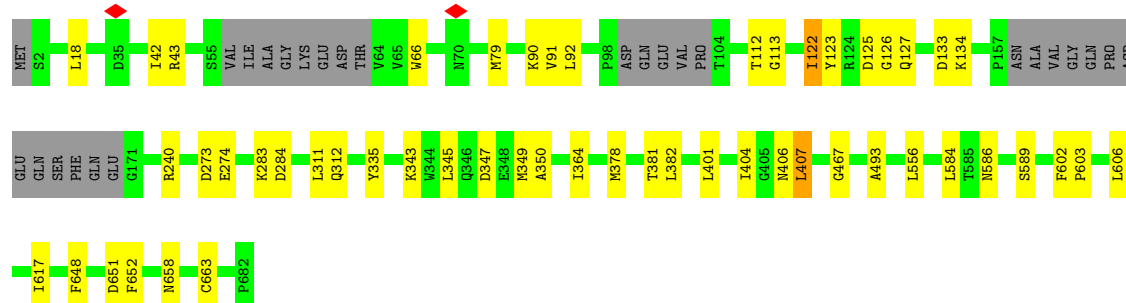
- Molecule 7: Inactive protein-arginine deiminase type-6

Chain K: 86% 10% .



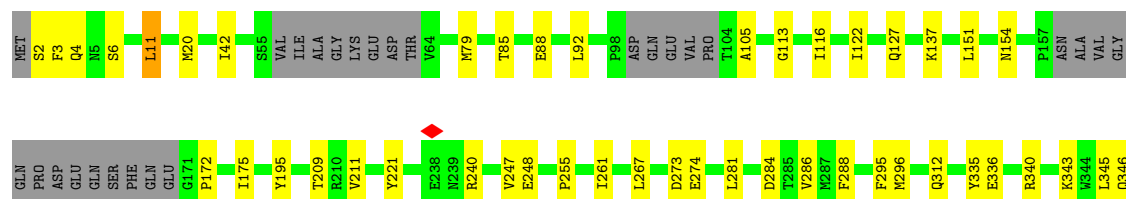
- Molecule 7: Inactive protein-arginine deiminase type-6

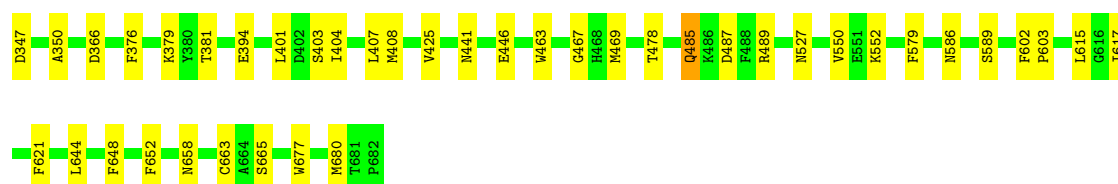
Chain U: 88% 7% .



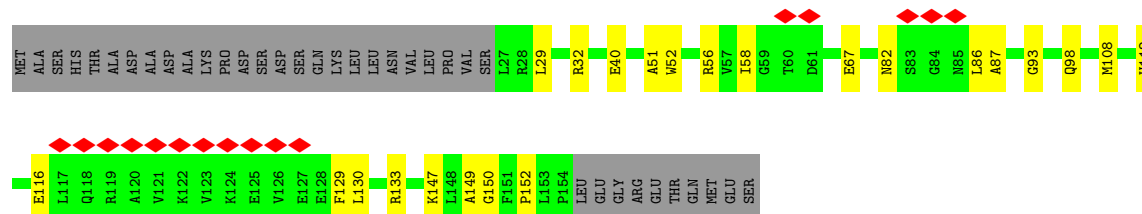
- Molecule 7: Inactive protein-arginine deiminase type-6

Chain c: 83% 12% .

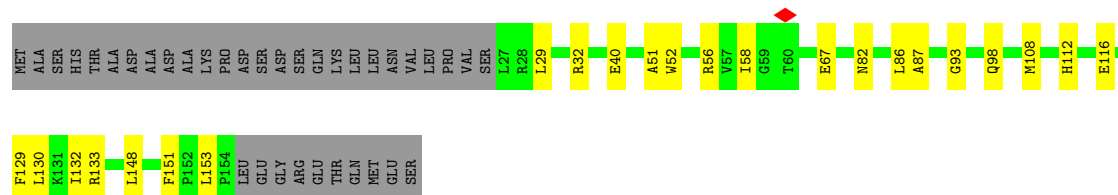




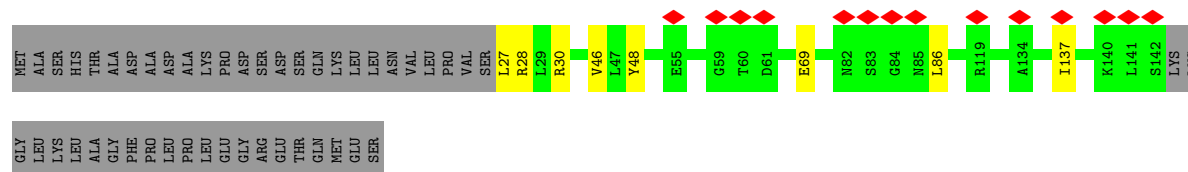
• Molecule 8: Oocyte-expressed protein homolog



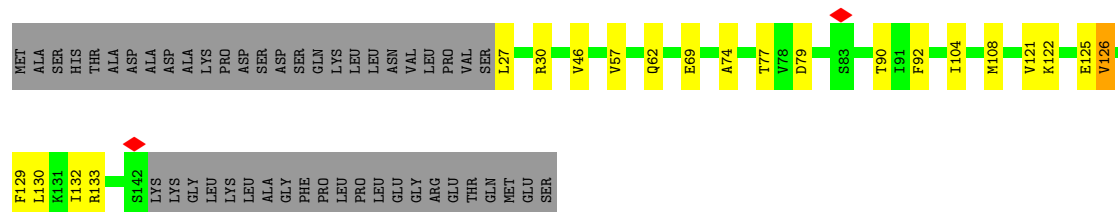
• Molecule 8: Oocyte-expressed protein homolog



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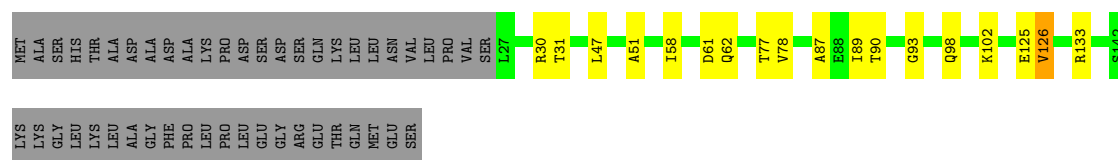


• Molecule 8: Oocyte-expressed protein homolog



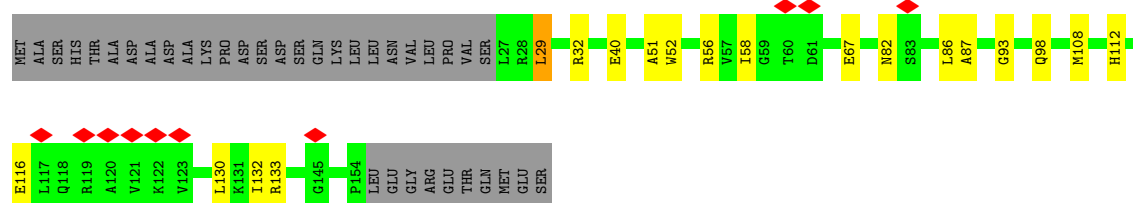
• Molecule 8: Oocyte-expressed protein homolog

Chain AI:  60% 10% 29%



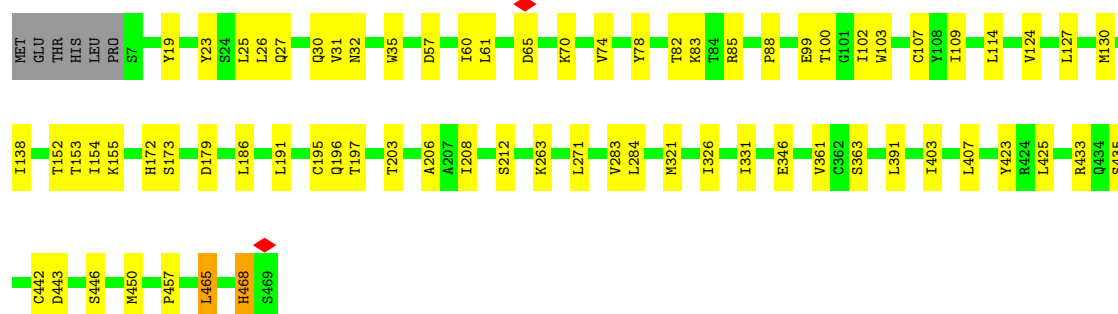
- Molecule 8: Oocyte-expressed protein homolog

Chain AT:  6% 66% 11% 22%

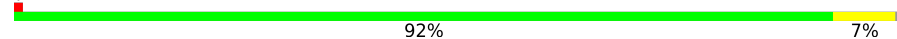


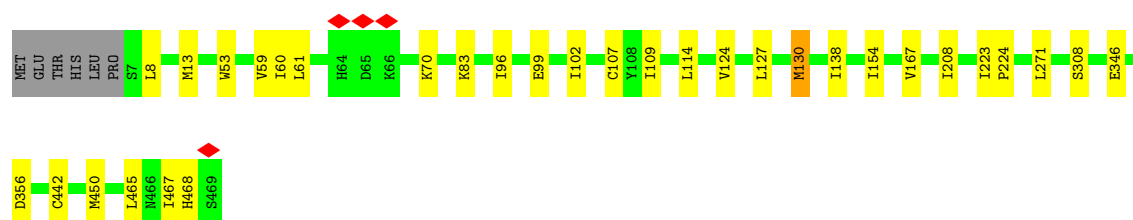
- Molecule 9: Expressed sequence C85627

Chain k:  84% 15%

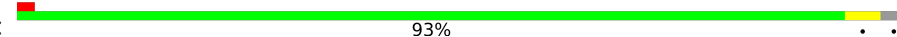


- Molecule 9: Expressed sequence C85627

Chain l:  92% 7%

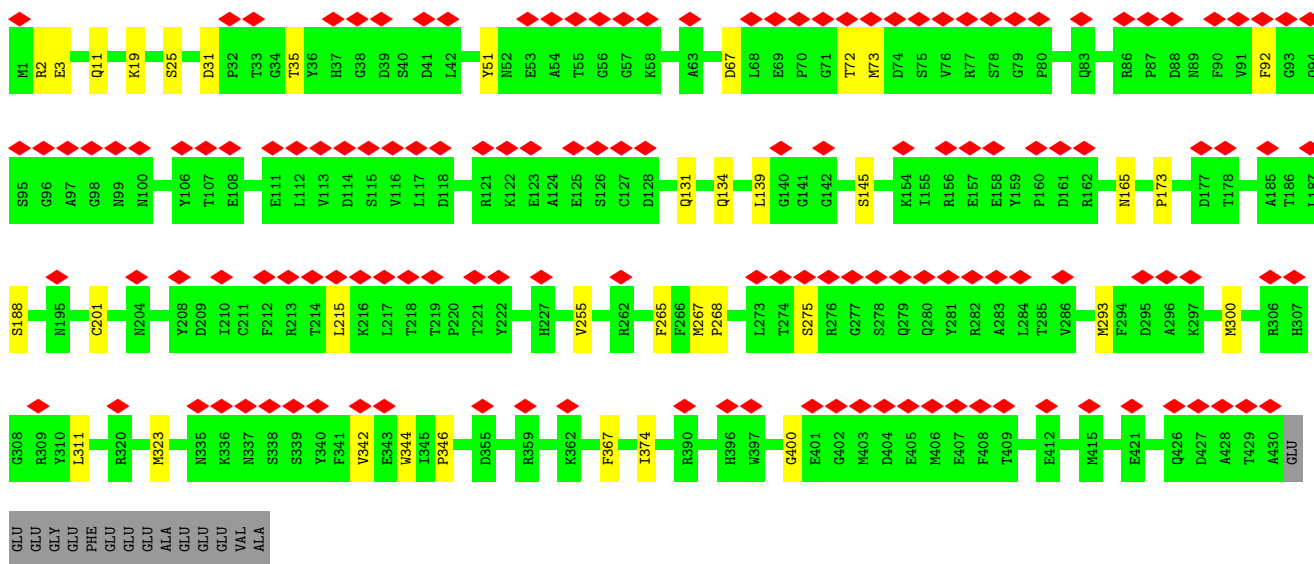


- Molecule 10: Tubulin beta-4B chain

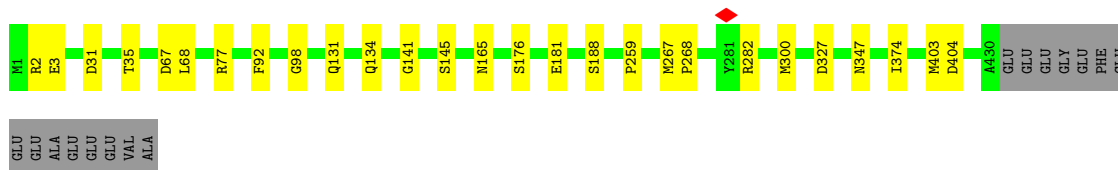
Chain t:  93%



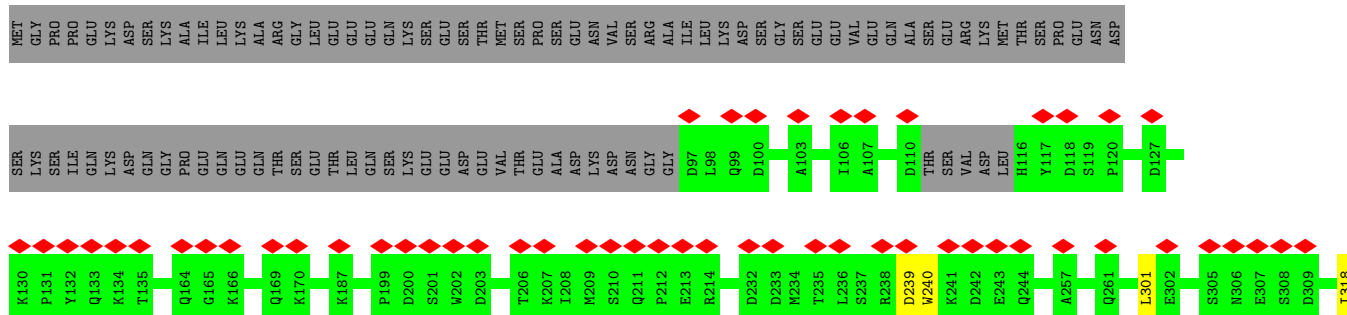
Chain AE:

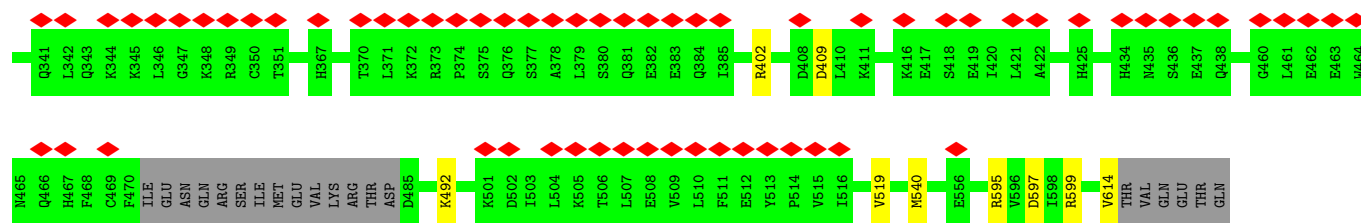


Chain AN: 91% 6%

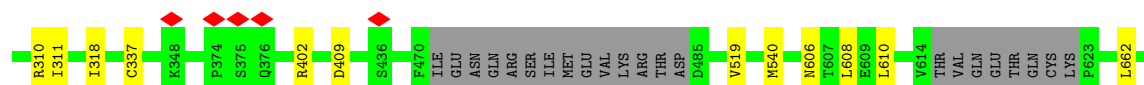
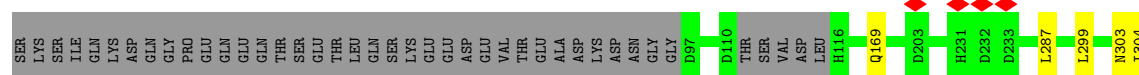
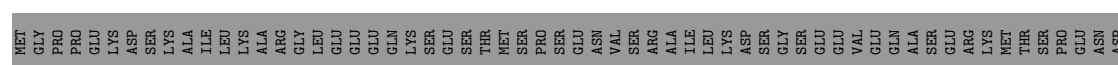


Chain y:

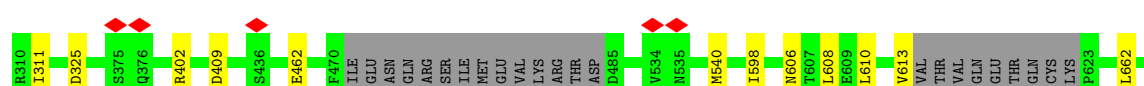
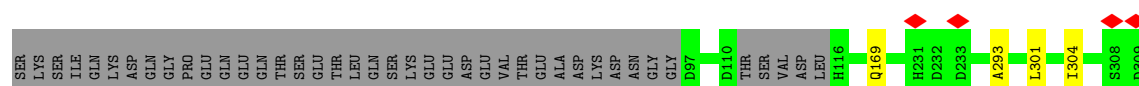
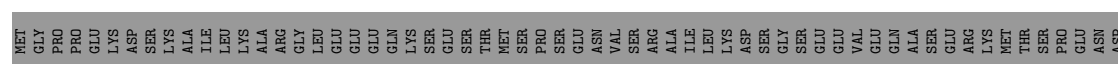
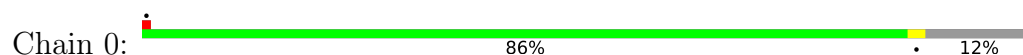




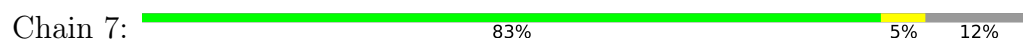
• Molecule 11: NACHT, LRR and PYD domains-containing protein 5

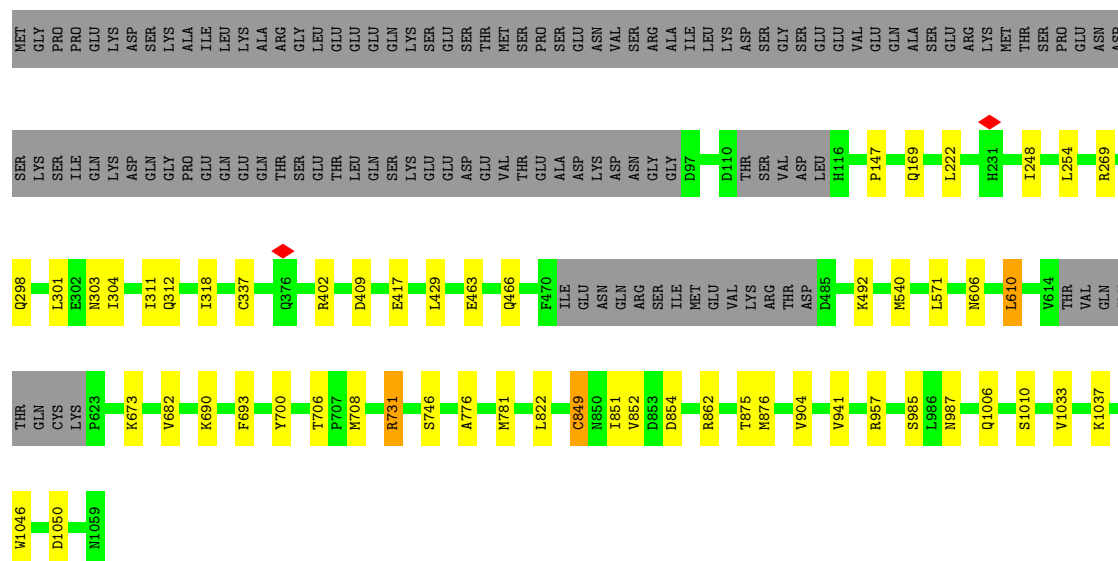


• Molecule 11: NACHT, LRR and PYD domains-containing protein 5



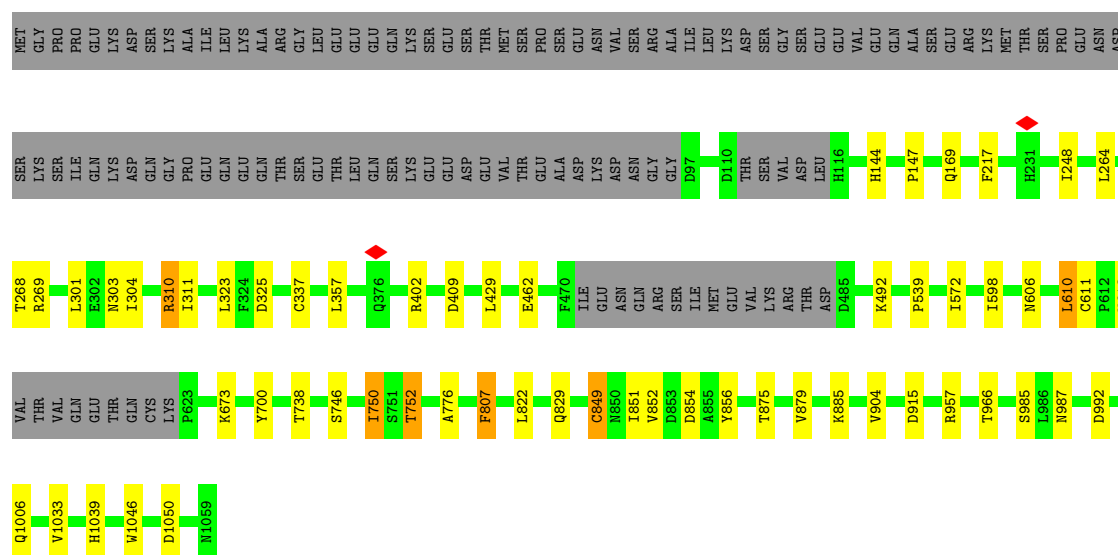
• Molecule 11: NACHT, LRR and PYD domains-containing protein 5





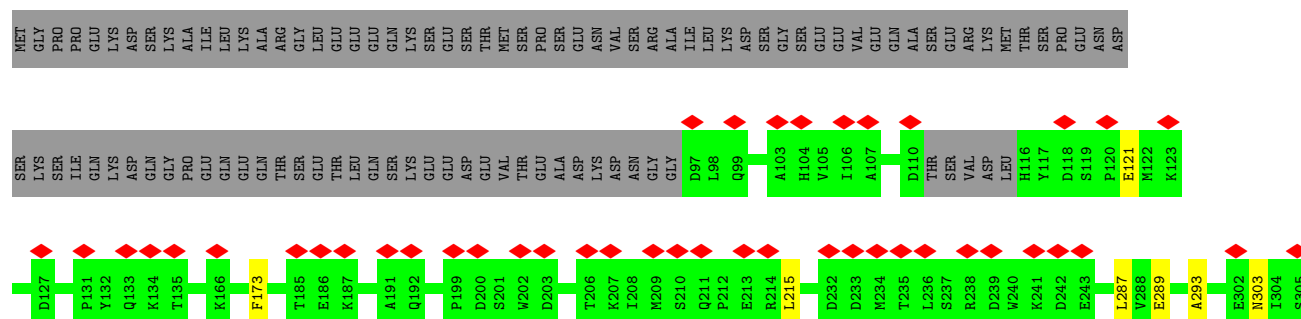
- Molecule 11: NACHT, LRR and PYD domains-containing protein 5

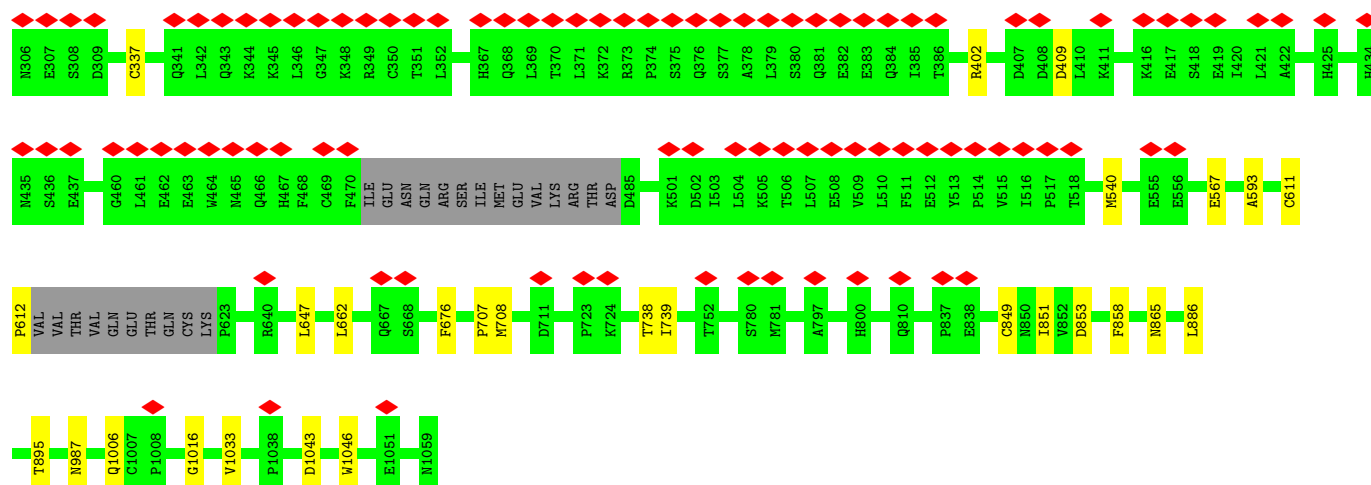
Chain 5: 83% 5% 12%



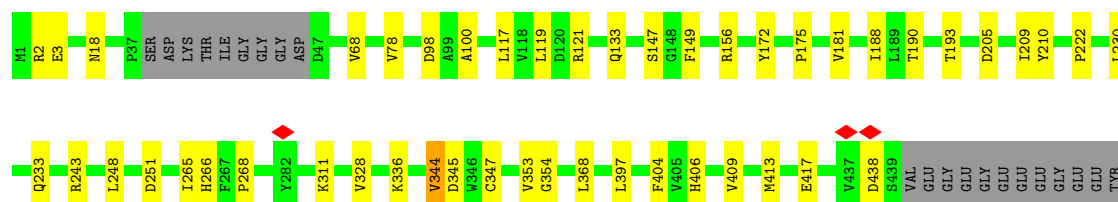
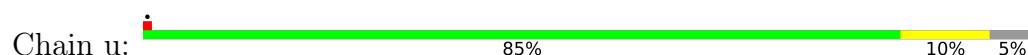
- Molecule 11: NACHT, LRR and PYD domains-containing protein 5

Chain 2: 13% 85% 12%

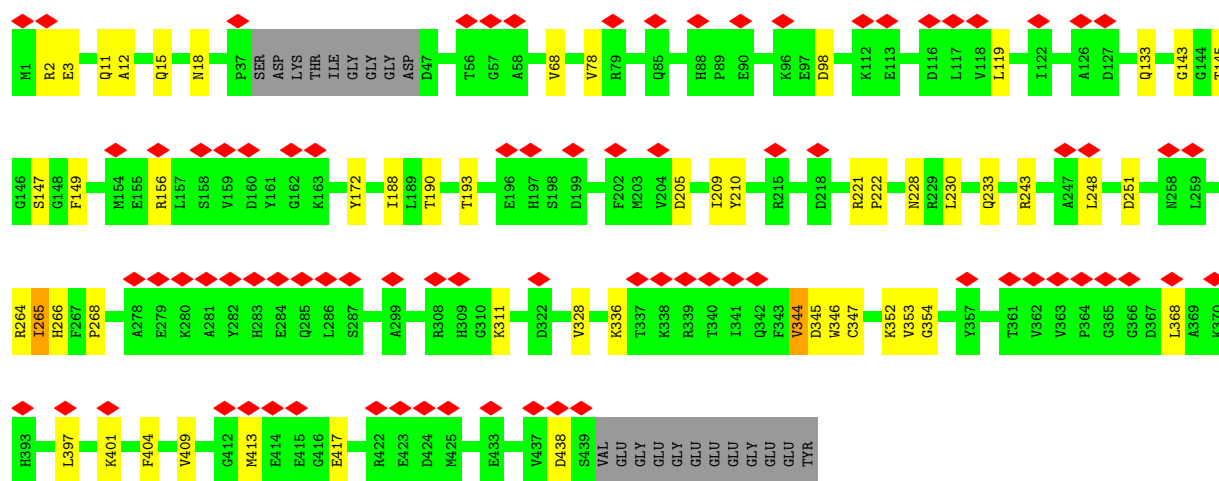
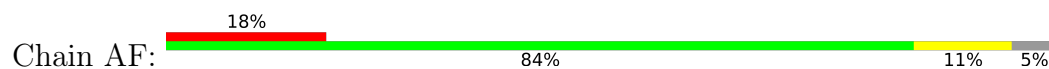




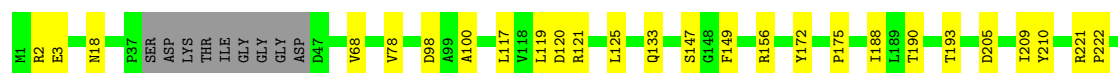
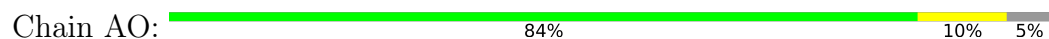
• Molecule 12: Tubulin alpha-1A chain



• Molecule 12: Tubulin alpha-1A chain

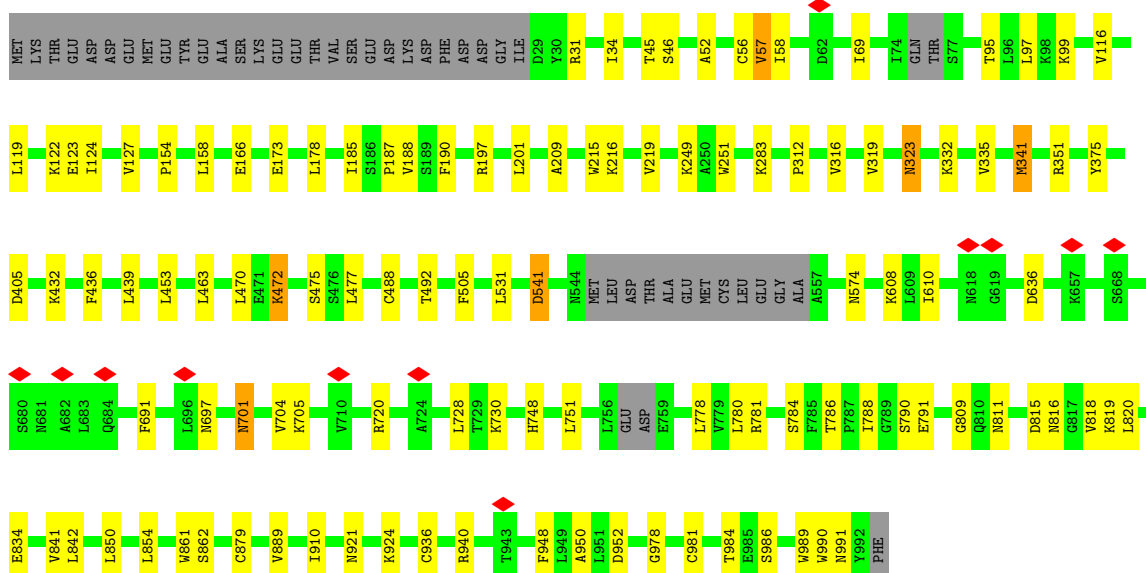
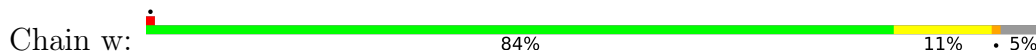


• Molecule 12: Tubulin alpha-1A chain

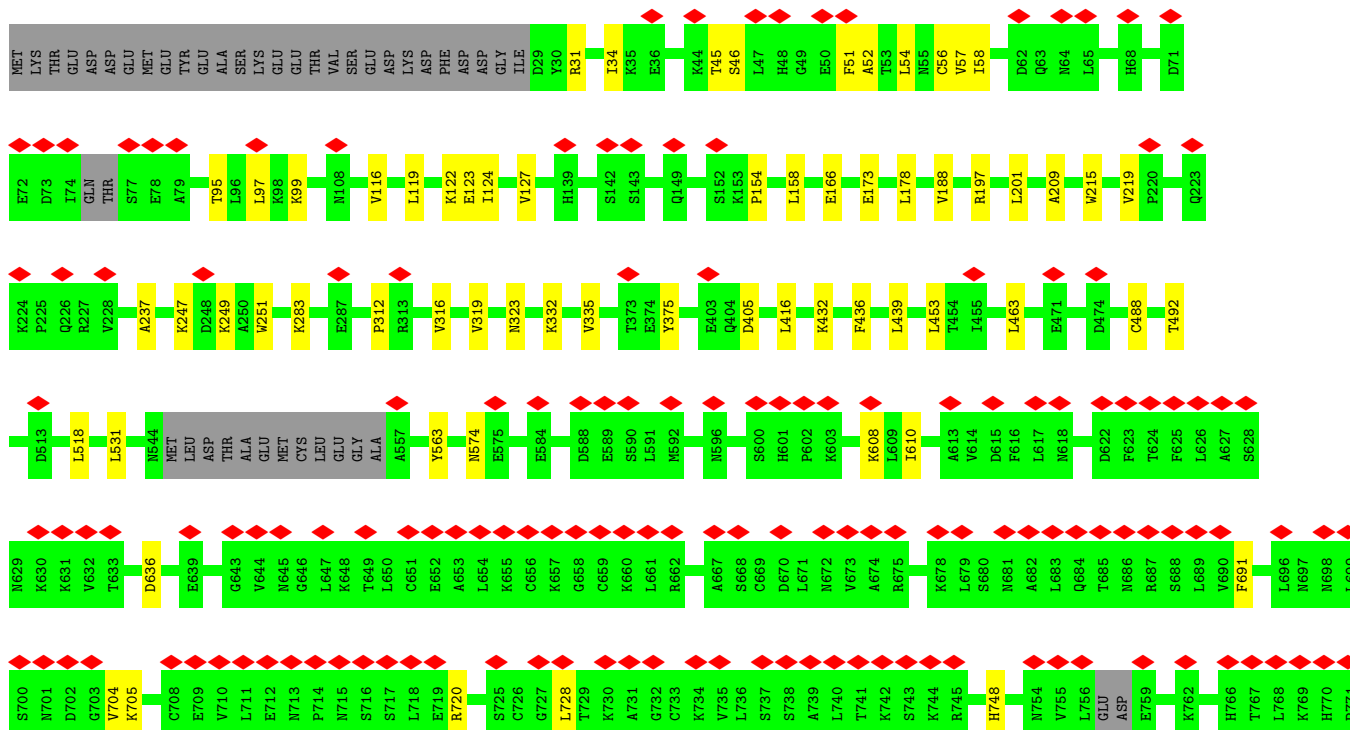
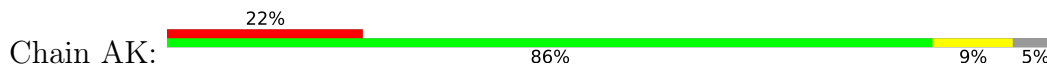




- Molecule 13: NACHT, LRR and PYD domains-containing protein 14

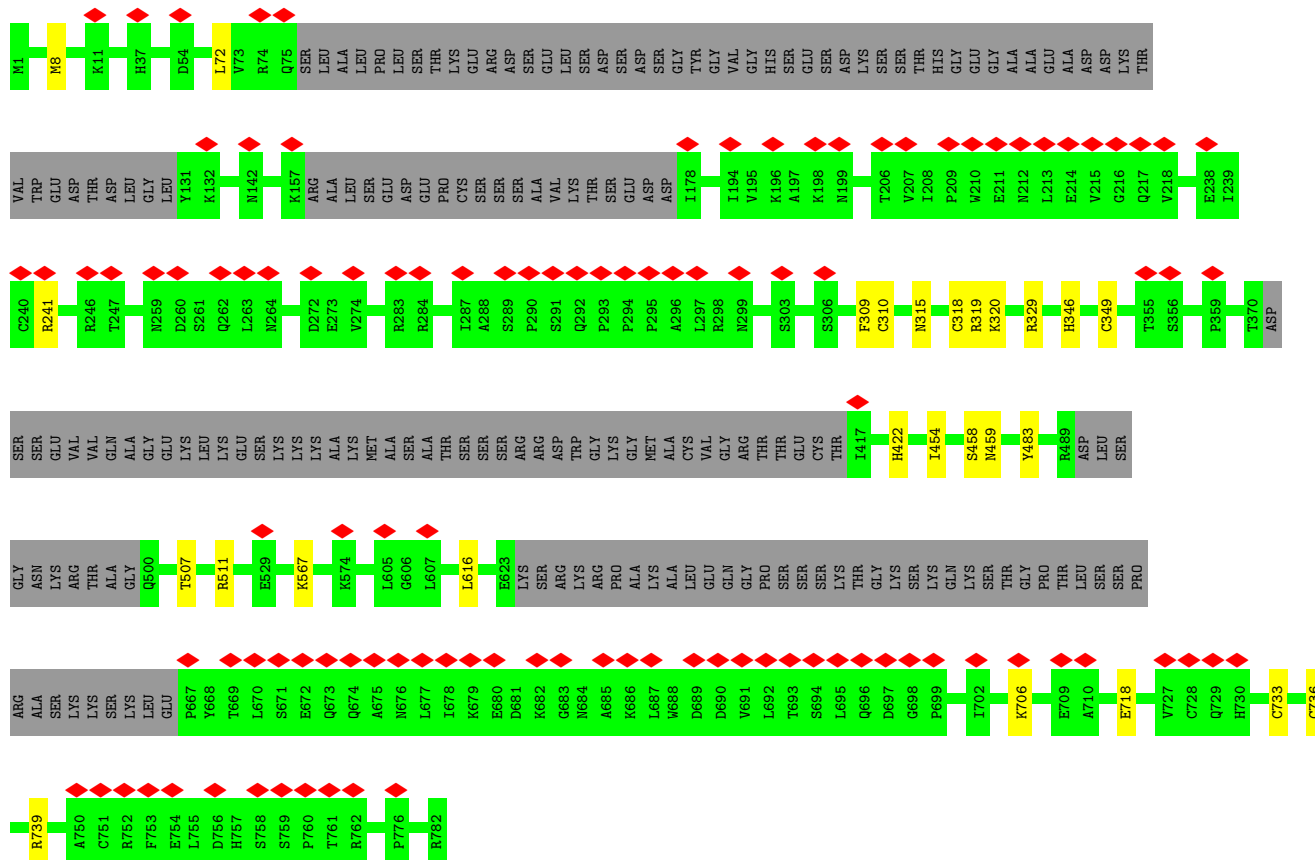
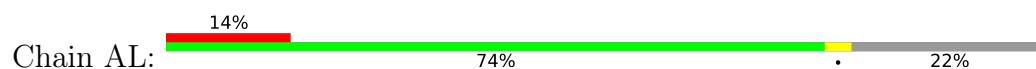


- Molecule 13: NACHT, LRR and PYD domains-containing protein 14

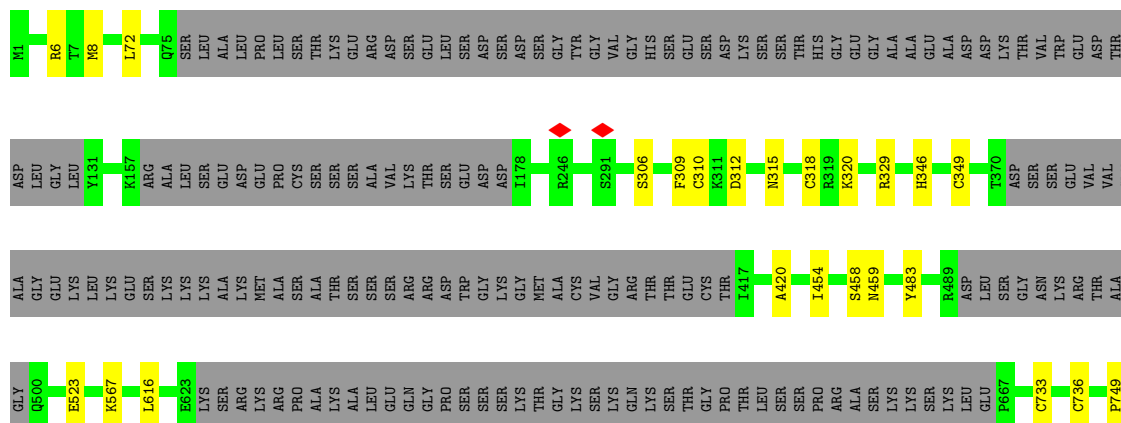
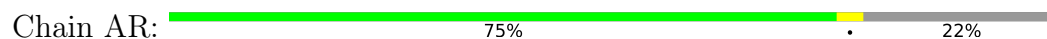




• Molecule 15: E3 ubiquitin-protein ligase UHRF1



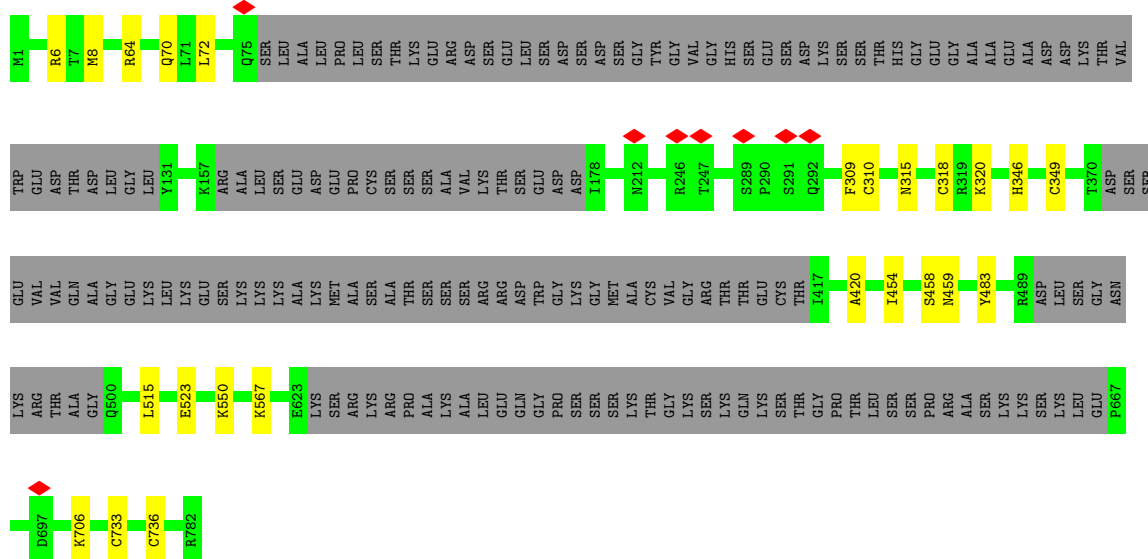
• Molecule 15: E3 ubiquitin-protein ligase UHRF1





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Chain x: 75% 22%



V164	T165	D167	M168	I172	R180	L188	T200	S203	G213	F218	V229	F232	G235	I236	D237	L249	I250	I251	Q254	R255	Y263	F283	K289	I299	S303	D309	I323	I329	L367	F368	D369	L373	Q376	E384
H394	L404	E410	S413	G426	TYR	LEU	PRO	LEU	SER	G432	K436	T437	L438	E441	L446	S450	SER	PRO	I453	M458	V464	CYS	SER											

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	349408	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.165	Depositor
Minimum map value	-0.062	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.02	Depositor
Map size ($\text{\AA}$)	611.328, 611.328, 611.328	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.194, 1.194, 1.194	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	1	0.16	0/440	0.34	0/598
1	3	0.13	0/469	0.32	0/637
1	9	0.18	0/469	0.35	0/637
2	4	0.18	0/1006	0.38	0/1367
2	6	0.14	0/1058	0.31	0/1431
2	AA	0.15	0/1058	0.34	0/1431
3	A	0.12	0/3749	0.29	0/5094
4	D	0.13	0/1212	0.29	0/1634
4	F	0.10	0/1216	0.25	0/1639
4	O	0.12	0/1216	0.25	0/1639
4	p	0.16	0/1205	0.32	0/1623
4	q	0.12	0/1205	0.28	0/1623
5	8	0.13	0/2879	0.28	0/3904
5	AC	0.17	0/2879	0.30	0/3904
5	E	0.16	0/2858	0.34	0/3875
5	I	0.12	0/2879	0.28	0/3904
5	P	0.15	0/2879	0.30	0/3904
5	z	0.17	0/2875	0.34	0/3899
6	H	0.11	0/5908	0.27	0/7956
6	Q	0.12	0/5195	0.30	0/7004
6	h	0.13	0/5883	0.34	2/7920 (0.0%)
6	i	0.11	0/5839	0.28	0/7868
7	B	0.15	0/5256	0.31	0/7126
7	K	0.13	0/5258	0.30	0/7126
7	S	0.33	0/5216	0.63	0/7073
7	T	0.14	0/5276	0.31	0/7150
7	U	0.30	0/5280	0.37	1/7157 (0.0%)
7	V	0.26	0/5255	0.33	0/7125
7	W	0.22	0/5268	0.33	0/7144
7	X	0.22	0/5278	0.33	0/7154
7	Y	0.19	0/5218	0.32	0/7091
7	Z	0.18	0/5250	0.32	0/7119

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
7	b	0.24	0/5265	0.33	0/7139
7	c	0.27	0/5284	0.36	0/7162
7	d	0.23	0/5246	0.34	0/7114
7	f	0.15	0/5282	0.31	0/7158
7	j	0.22	0/5272	0.33	0/7148
7	m	0.21	0/5278	0.33	0/7154
7	n	0.17	0/5224	0.32	0/7098
7	o	0.16	0/5254	0.32	0/7124
7	r	0.32	0/5260	0.60	2/7131 (0.0%)
7	s	0.18	0/5262	0.31	0/7135
8	AH	0.19	0/892	0.38	0/1218
8	AI	0.11	0/953	0.27	0/1292
8	AJ	0.18	0/956	0.35	0/1296
8	AT	0.28	0/946	0.38	0/1294
8	e	0.28	0/946	0.38	0/1294
8	g	0.28	0/946	0.38	0/1294
9	k	0.14	0/3822	0.30	0/5197
9	l	0.17	0/3825	0.33	0/5201
10	AE	0.18	0/3433	0.31	0/4655
10	AN	0.11	0/3448	0.24	0/4673
10	t	0.13	0/3448	0.29	0/4673
11	0	0.16	0/7443	0.28	0/10068
11	2	0.16	0/7347	0.33	0/9945
11	5	0.12	0/7439	0.26	0/10063
11	7	0.13	0/7446	0.27	0/10073
11	AB	0.17	0/7449	0.30	0/10077
11	y	0.17	0/7389	0.32	0/10000
12	AF	0.18	0/3442	0.32	0/4673
12	AO	0.18	0/3445	0.32	0/4677
12	u	0.18	0/3445	0.32	0/4677
13	AK	0.16	0/7554	0.32	0/10222
13	AQ	0.16	0/7609	0.32	0/10291
13	w	0.16	0/7610	0.32	0/10292
14	AD	0.15	0/1203	0.31	0/1640
14	AM	0.15	0/1202	0.31	0/1639
14	AS	0.15	0/1203	0.31	0/1640
15	AL	0.16	0/4988	0.30	0/6753
15	AR	0.15	0/4988	0.30	0/6753
15	x	0.16	0/4970	0.30	0/6732
16	C	0.13	0/3687	0.31	0/5006
16	L	0.12	0/3697	0.32	0/5018
All	All	0.18	0/286730	0.33	5/388445 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	r	43	ARG	N-CA-C	6.83	120.03	108.90
7	U	311	LEU	CB-CA-C	-5.44	109.83	117.23
6	h	426	ASP	CA-C-N	5.33	123.60	120.24
6	h	426	ASP	C-N-CA	5.33	123.60	120.24
7	r	42	ILE	CB-CA-C	5.10	117.77	110.33

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	427	0	382	4	0
1	3	453	0	424	14	0
1	9	453	0	424	6	0
2	4	977	0	933	30	0
2	6	1028	0	1036	7	0
2	AA	1028	0	1036	13	0
3	A	3650	0	3613	23	0
4	D	1195	0	1198	8	0
4	F	1199	0	1202	3	0
4	O	1199	0	1202	0	0
4	p	1190	0	1194	25	0
4	q	1190	0	1194	0	0
5	8	2817	0	2801	15	0
5	AC	2817	0	2801	4	0
5	E	2799	0	2782	5	0
5	I	2817	0	2801	15	0
5	P	2817	0	2801	2	0
5	z	2813	0	2794	6	0
6	H	5803	0	5835	42	0
6	Q	5099	0	5098	12	0
6	h	5781	0	5793	14	0
6	i	5738	0	5726	55	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	5141	0	5149	42	0
7	K	5145	0	5157	54	0
7	S	5102	0	5087	44	0
7	T	5162	0	5174	13	0
7	U	5163	0	5151	50	0
7	V	5139	0	5151	32	0
7	W	5151	0	5153	22	0
7	X	5161	0	5179	29	0
7	Y	5099	0	5034	17	0
7	Z	5133	0	5130	12	0
7	b	5149	0	5151	34	0
7	c	5167	0	5162	72	0
7	d	5130	0	5136	49	0
7	f	5168	0	5180	45	0
7	j	5155	0	5164	78	0
7	m	5161	0	5179	50	0
7	n	5105	0	5045	43	0
7	o	5138	0	5142	35	0
7	r	5144	0	5151	33	0
7	s	5146	0	5149	36	0
8	AH	875	0	840	11	0
8	AI	935	0	947	13	0
8	AJ	938	0	956	18	0
8	AT	928	0	857	20	0
8	e	928	0	857	34	0
8	g	928	0	857	22	0
9	k	3729	0	3716	52	0
9	l	3732	0	3725	10	0
10	AE	3358	0	3226	28	0
10	AN	3373	0	3257	27	0
10	t	3373	0	3257	27	0
11	0	7316	0	7369	10	0
11	2	7221	0	7205	34	0
11	5	7312	0	7357	28	0
11	7	7319	0	7366	35	0
11	AB	7322	0	7375	17	0
11	y	7262	0	7254	44	0
12	AF	3365	0	3282	45	0
12	AO	3368	0	3284	35	0
12	u	3368	0	3284	38	0
13	AK	7417	0	7398	63	0
13	AQ	7472	0	7522	77	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	w	7473	0	7525	59	0
14	AD	1168	0	1150	10	0
14	AM	1167	0	1147	22	0
14	AS	1168	0	1150	9	0
15	AL	4872	0	4707	42	0
15	AR	4872	0	4701	26	0
15	x	4854	0	4666	26	0
16	C	3601	0	3620	40	0
16	L	3611	0	3635	13	0
17	1	1	0	0	0	0
17	3	1	0	0	0	0
17	9	1	0	0	0	0
17	AL	2	0	0	0	0
17	AR	4	0	0	0	0
17	x	4	0	0	0	0
18	AF	32	0	12	9	0
18	AN	32	0	12	7	0
18	AO	32	0	12	2	0
18	t	32	0	12	8	0
18	u	32	0	12	2	0
19	AN	1	0	0	0	0
19	AO	1	0	0	0	0
19	t	1	0	0	0	0
19	u	1	0	0	0	0
20	AK	27	0	12	0	0
20	AQ	27	0	12	0	0
20	w	27	0	12	0	0
All	All	281032	0	279482	1653	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 3.

The worst 5 of 1653 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)
2:4:82:ARG:HA	6:i:424:ASP:CB	1.50	1.42
2:4:81:GLU:O	6:i:425:SER:N	1.63	1.30
6:H:913:CYS:O	8:e:147:LYS:NZ	1.67	1.27
7:j:586:ASN:HB2	15:AL:511:ARG:CD	1.70	1.21
15:AR:458:SER:HB2	7:U:586:ASN:OD1	1.37	1.21

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	1	54/228 (24%)	54 (100%)	0	0	100	100
1	3	54/228 (24%)	53 (98%)	1 (2%)	0	100	100
1	9	54/228 (24%)	52 (96%)	2 (4%)	0	100	100
2	4	122/440 (28%)	119 (98%)	3 (2%)	0	100	100
2	6	122/440 (28%)	121 (99%)	1 (1%)	0	100	100
2	AA	122/440 (28%)	120 (98%)	2 (2%)	0	100	100
3	A	444/468 (95%)	432 (97%)	12 (3%)	0	100	100
4	D	142/163 (87%)	142 (100%)	0	0	100	100
4	F	142/163 (87%)	142 (100%)	0	0	100	100
4	O	142/163 (87%)	142 (100%)	0	0	100	100
4	p	142/163 (87%)	142 (100%)	0	0	100	100
4	q	142/163 (87%)	142 (100%)	0	0	100	100
5	8	354/581 (61%)	345 (98%)	9 (2%)	0	100	100
5	AC	354/581 (61%)	344 (97%)	10 (3%)	0	100	100
5	E	354/581 (61%)	343 (97%)	11 (3%)	0	100	100
5	I	354/581 (61%)	342 (97%)	12 (3%)	0	100	100
5	P	354/581 (61%)	345 (98%)	9 (2%)	0	100	100
5	z	354/581 (61%)	343 (97%)	11 (3%)	0	100	100
6	H	719/937 (77%)	703 (98%)	16 (2%)	0	100	100
6	Q	634/937 (68%)	625 (99%)	9 (1%)	0	100	100
6	h	715/937 (76%)	708 (99%)	7 (1%)	0	100	100
6	i	717/937 (76%)	707 (99%)	10 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	B	643/682 (94%)	639 (99%)	4 (1%)	0	100	100
7	K	642/682 (94%)	631 (98%)	11 (2%)	0	100	100
7	S	635/682 (93%)	626 (99%)	9 (1%)	0	100	100
7	T	642/682 (94%)	635 (99%)	7 (1%)	0	100	100
7	U	647/682 (95%)	628 (97%)	19 (3%)	0	100	100
7	V	644/682 (94%)	632 (98%)	12 (2%)	0	100	100
7	W	646/682 (95%)	638 (99%)	8 (1%)	0	100	100
7	X	644/682 (94%)	633 (98%)	11 (2%)	0	100	100
7	Y	652/682 (96%)	644 (99%)	8 (1%)	0	100	100
7	Z	644/682 (94%)	636 (99%)	8 (1%)	0	100	100
7	b	646/682 (95%)	635 (98%)	11 (2%)	0	100	100
7	c	647/682 (95%)	636 (98%)	11 (2%)	0	100	100
7	d	644/682 (94%)	638 (99%)	6 (1%)	0	100	100
7	f	642/682 (94%)	637 (99%)	5 (1%)	0	100	100
7	j	646/682 (95%)	639 (99%)	7 (1%)	0	100	100
7	m	644/682 (94%)	637 (99%)	7 (1%)	0	100	100
7	n	652/682 (96%)	644 (99%)	8 (1%)	0	100	100
7	o	644/682 (94%)	640 (99%)	4 (1%)	0	100	100
7	r	640/682 (94%)	632 (99%)	8 (1%)	0	100	100
7	s	646/682 (95%)	635 (98%)	11 (2%)	0	100	100
8	AH	114/164 (70%)	112 (98%)	2 (2%)	0	100	100
8	AI	114/164 (70%)	113 (99%)	1 (1%)	0	100	100
8	AJ	114/164 (70%)	112 (98%)	2 (2%)	0	100	100
8	AT	126/164 (77%)	123 (98%)	3 (2%)	0	100	100
8	e	126/164 (77%)	123 (98%)	3 (2%)	0	100	100
8	g	126/164 (77%)	123 (98%)	3 (2%)	0	100	100
9	k	461/469 (98%)	456 (99%)	5 (1%)	0	100	100
9	l	461/469 (98%)	452 (98%)	9 (2%)	0	100	100
10	AE	428/445 (96%)	426 (100%)	2 (0%)	0	100	100
10	AN	428/445 (96%)	425 (99%)	3 (1%)	0	100	100
10	t	428/445 (96%)	422 (99%)	6 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	0	927/1059 (88%)	910 (98%)	17 (2%)	0	100	100
11	2	926/1059 (87%)	910 (98%)	16 (2%)	0	100	100
11	5	927/1059 (88%)	910 (98%)	17 (2%)	0	100	100
11	7	928/1059 (88%)	915 (99%)	13 (1%)	0	100	100
11	AB	928/1059 (88%)	910 (98%)	18 (2%)	0	100	100
11	y	928/1059 (88%)	913 (98%)	15 (2%)	0	100	100
12	AF	426/451 (94%)	422 (99%)	4 (1%)	0	100	100
12	AO	426/451 (94%)	422 (99%)	4 (1%)	0	100	100
12	u	426/451 (94%)	422 (99%)	4 (1%)	0	100	100
13	AK	940/993 (95%)	933 (99%)	7 (1%)	0	100	100
13	AQ	940/993 (95%)	932 (99%)	8 (1%)	0	100	100
13	w	940/993 (95%)	932 (99%)	8 (1%)	0	100	100
14	AD	145/147 (99%)	145 (100%)	0	0	100	100
14	AM	145/147 (99%)	145 (100%)	0	0	100	100
14	AS	145/147 (99%)	145 (100%)	0	0	100	100
15	AL	596/782 (76%)	591 (99%)	5 (1%)	0	100	100
15	AR	596/782 (76%)	591 (99%)	5 (1%)	0	100	100
15	x	596/782 (76%)	592 (99%)	4 (1%)	0	100	100
16	C	441/466 (95%)	435 (99%)	6 (1%)	0	100	100
16	L	441/466 (95%)	432 (98%)	9 (2%)	0	100	100
All	All	35174/41823 (84%)	34675 (99%)	499 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	1	41/197 (21%)	41 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	3	47/197 (24%)	46 (98%)	1 (2%)	47	64
1	9	47/197 (24%)	47 (100%)	0	100	100
2	4	99/357 (28%)	99 (100%)	0	100	100
2	6	112/357 (31%)	110 (98%)	2 (2%)	51	66
2	AA	112/357 (31%)	110 (98%)	2 (2%)	51	66
3	A	404/431 (94%)	390 (96%)	14 (4%)	32	54
4	D	136/150 (91%)	136 (100%)	0	100	100
4	F	137/150 (91%)	137 (100%)	0	100	100
4	O	137/150 (91%)	137 (100%)	0	100	100
4	p	136/150 (91%)	136 (100%)	0	100	100
4	q	136/150 (91%)	136 (100%)	0	100	100
5	8	313/516 (61%)	312 (100%)	1 (0%)	86	83
5	AC	313/516 (61%)	311 (99%)	2 (1%)	78	79
5	E	310/516 (60%)	310 (100%)	0	100	100
5	I	313/516 (61%)	311 (99%)	2 (1%)	78	79
5	P	313/516 (61%)	308 (98%)	5 (2%)	55	68
5	z	311/516 (60%)	311 (100%)	0	100	100
6	H	659/862 (76%)	653 (99%)	6 (1%)	70	74
6	Q	586/862 (68%)	581 (99%)	5 (1%)	70	74
6	h	656/862 (76%)	654 (100%)	2 (0%)	86	83
6	i	646/862 (75%)	646 (100%)	0	100	100
7	B	582/613 (95%)	575 (99%)	7 (1%)	63	71
7	K	584/613 (95%)	579 (99%)	5 (1%)	70	74
7	S	578/613 (94%)	578 (100%)	0	100	100
7	T	585/613 (95%)	585 (100%)	0	100	100
7	U	583/613 (95%)	577 (99%)	6 (1%)	68	74
7	V	581/613 (95%)	580 (100%)	1 (0%)	87	86
7	W	583/613 (95%)	583 (100%)	0	100	100
7	X	586/613 (96%)	586 (100%)	0	100	100
7	Y	561/613 (92%)	561 (100%)	0	100	100
7	Z	579/613 (94%)	578 (100%)	1 (0%)	87	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	b	581/613 (95%)	581 (100%)	0	100	100
7	c	584/613 (95%)	580 (99%)	4 (1%)	76	77
7	d	579/613 (94%)	577 (100%)	2 (0%)	86	83
7	f	587/613 (96%)	587 (100%)	0	100	100
7	j	584/613 (95%)	582 (100%)	2 (0%)	86	83
7	m	586/613 (96%)	585 (100%)	1 (0%)	87	86
7	n	562/613 (92%)	562 (100%)	0	100	100
7	o	581/613 (95%)	581 (100%)	0	100	100
7	r	582/613 (95%)	567 (97%)	15 (3%)	40	60
7	s	580/613 (95%)	580 (100%)	0	100	100
8	AH	86/143 (60%)	86 (100%)	0	100	100
8	AI	102/143 (71%)	100 (98%)	2 (2%)	48	64
8	AJ	103/143 (72%)	98 (95%)	5 (5%)	22	48
8	AT	85/143 (59%)	80 (94%)	5 (6%)	18	44
8	e	85/143 (59%)	80 (94%)	5 (6%)	18	44
8	g	85/143 (59%)	80 (94%)	5 (6%)	18	44
9	k	423/435 (97%)	408 (96%)	15 (4%)	32	54
9	l	424/435 (98%)	407 (96%)	17 (4%)	28	52
10	AE	365/380 (96%)	365 (100%)	0	100	100
10	AN	368/380 (97%)	368 (100%)	0	100	100
10	t	368/380 (97%)	368 (100%)	0	100	100
11	0	823/960 (86%)	807 (98%)	16 (2%)	50	65
11	2	797/960 (83%)	795 (100%)	2 (0%)	86	83
11	5	821/960 (86%)	803 (98%)	18 (2%)	45	63
11	7	822/960 (86%)	810 (98%)	12 (2%)	57	68
11	AB	823/960 (86%)	809 (98%)	14 (2%)	53	67
11	y	805/960 (84%)	805 (100%)	0	100	100
12	AF	361/378 (96%)	354 (98%)	7 (2%)	50	65
12	AO	362/378 (96%)	354 (98%)	8 (2%)	45	63
12	u	362/378 (96%)	355 (98%)	7 (2%)	50	65
13	AK	820/909 (90%)	818 (100%)	2 (0%)	87	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	AQ	839/909 (92%)	836 (100%)	3 (0%)	84	81
13	w	840/909 (92%)	815 (97%)	25 (3%)	36	57
14	AD	131/132 (99%)	129 (98%)	2 (2%)	57	68
14	AM	130/132 (98%)	130 (100%)	0	100	100
14	AS	131/132 (99%)	129 (98%)	2 (2%)	57	68
15	AL	524/682 (77%)	523 (100%)	1 (0%)	87	86
15	AR	524/682 (77%)	523 (100%)	1 (0%)	87	86
15	x	519/682 (76%)	519 (100%)	0	100	100
16	C	407/430 (95%)	395 (97%)	12 (3%)	37	57
16	L	409/430 (95%)	393 (96%)	16 (4%)	28	52
All	All	31316/37438 (84%)	31028 (99%)	288 (1%)	68	74

5 of 288 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	5	248	ILE
8	AT	58	ILE
11	5	613	VAL
8	AI	125	GLU
13	w	477	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 280 such sidechains are listed below:

Mol	Chain	Res	Type
11	2	848	HIS
7	U	658	ASN
13	AK	754	ASN
7	d	523	GLN
7	d	314	GLN

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](#)

Of 25 ligands modelled in this entry, 17 are monoatomic - leaving 8 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$
20	ADP	AK	1001	-	27,29,29	2.93	13 (48%)	42,45,45	1.87	12 (28%)
20	ADP	w	1001	-	27,29,29	2.93	13 (48%)	42,45,45	1.87	12 (28%)
20	ADP	AQ	1001	-	27,29,29	2.93	13 (48%)	42,45,45	1.87	12 (28%)
18	GTP	AO	501	19	30,34,34	2.17	7 (23%)	46,54,54	1.64	10 (21%)
18	GTP	AF	501	-	30,34,34	2.14	8 (26%)	46,54,54	1.57	9 (19%)
18	GTP	u	502	19	30,34,34	2.17	7 (23%)	46,54,54	1.64	10 (21%)
18	GTP	t	501	19	30,34,34	2.31	8 (26%)	46,54,54	1.63	12 (26%)
18	GTP	AN	501	19	30,34,34	2.31	8 (26%)	46,54,54	1.64	12 (26%)

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
20	ADP	AK	1001	-	-	8/16/32/32	0/3/3/3
20	ADP	w	1001	-	-	8/16/32/32	0/3/3/3
20	ADP	AQ	1001	-	-	8/16/32/32	0/3/3/3
18	GTP	AO	501	19	-	9/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	GTP	AF	501	-	-	6/22/38/38	0/3/3/3
18	GTP	u	502	19	-	9/22/38/38	0/3/3/3
18	GTP	t	501	19	-	4/22/38/38	0/3/3/3
18	GTP	AN	501	19	-	4/22/38/38	0/3/3/3

The worst 5 of 77 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	AK	1001	ADP	PA-O5'	7.95	1.91	1.59
20	w	1001	ADP	PA-O5'	7.94	1.91	1.59
20	AQ	1001	ADP	PA-O5'	7.93	1.91	1.59
18	t	501	GTP	PA-O5'	7.78	1.90	1.59
18	AN	501	GTP	PA-O5'	7.78	1.90	1.59

The worst 5 of 89 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	AN	501	GTP	O5'-PA-O1A	-4.54	91.32	109.07
18	t	501	GTP	O5'-PA-O1A	-4.54	91.33	109.07
20	w	1001	ADP	O5'-PA-O1A	-4.36	92.01	109.07
20	AQ	1001	ADP	O5'-PA-O1A	-4.36	92.04	109.07
18	u	502	GTP	O5'-PA-O1A	-4.31	92.23	109.07

There are no chirality outliers.

5 of 56 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	t	501	GTP	C5'-O5'-PA-O3A
18	t	501	GTP	C5'-O5'-PA-O1A
18	u	502	GTP	C5'-O5'-PA-O3A
18	u	502	GTP	C5'-O5'-PA-O2A
18	u	502	GTP	O4'-C4'-C5'-O5'

There are no ring outliers.

5 monomers are involved in 28 short contacts:

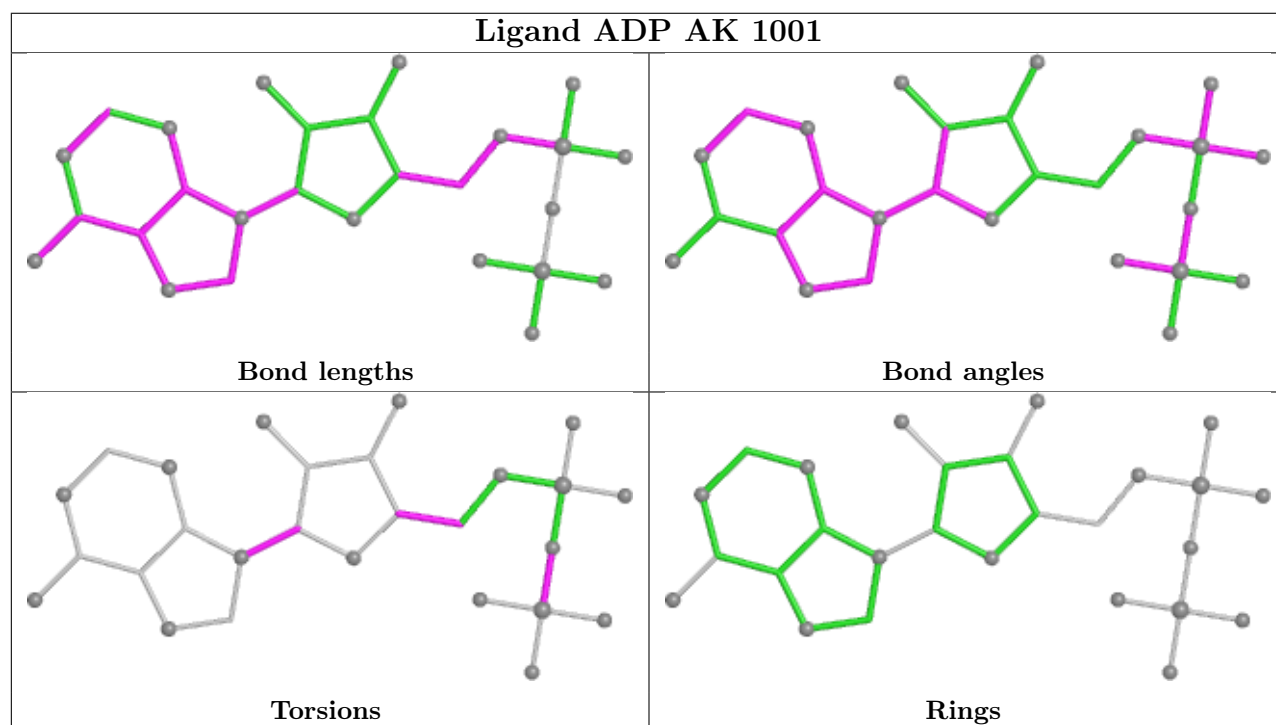
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	AO	501	GTP	2	0
18	AF	501	GTP	9	0
18	u	502	GTP	2	0

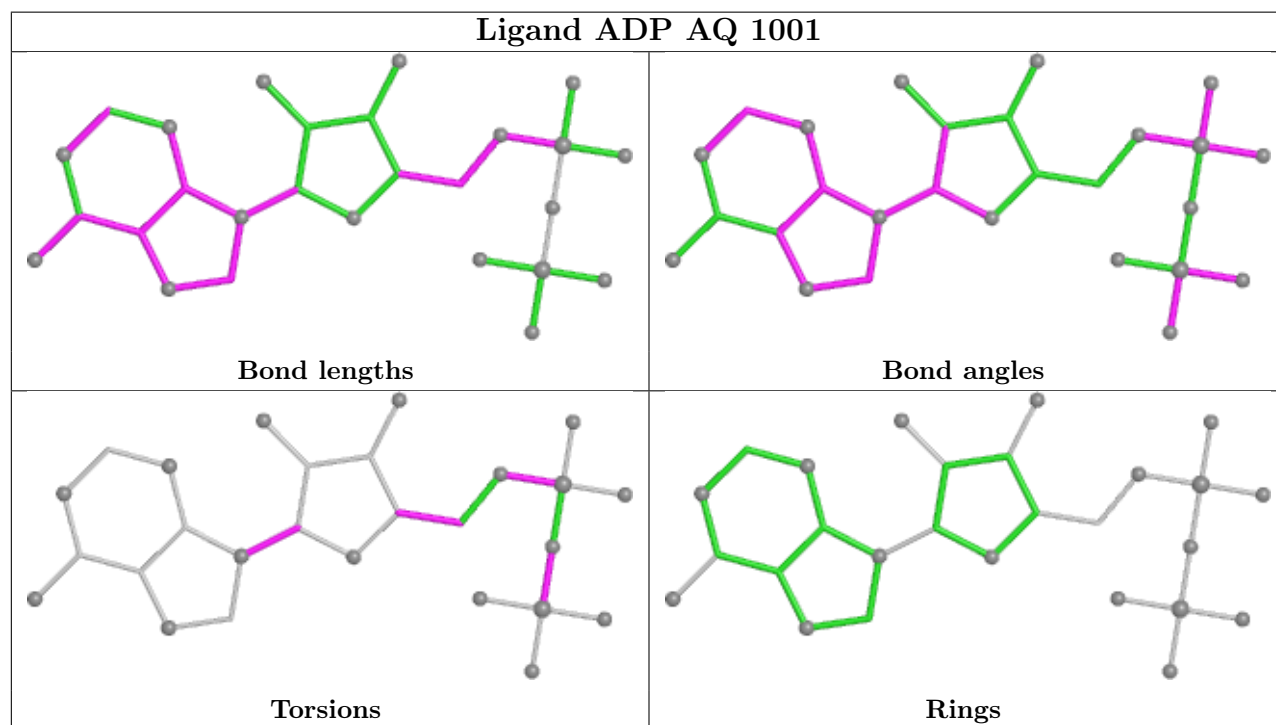
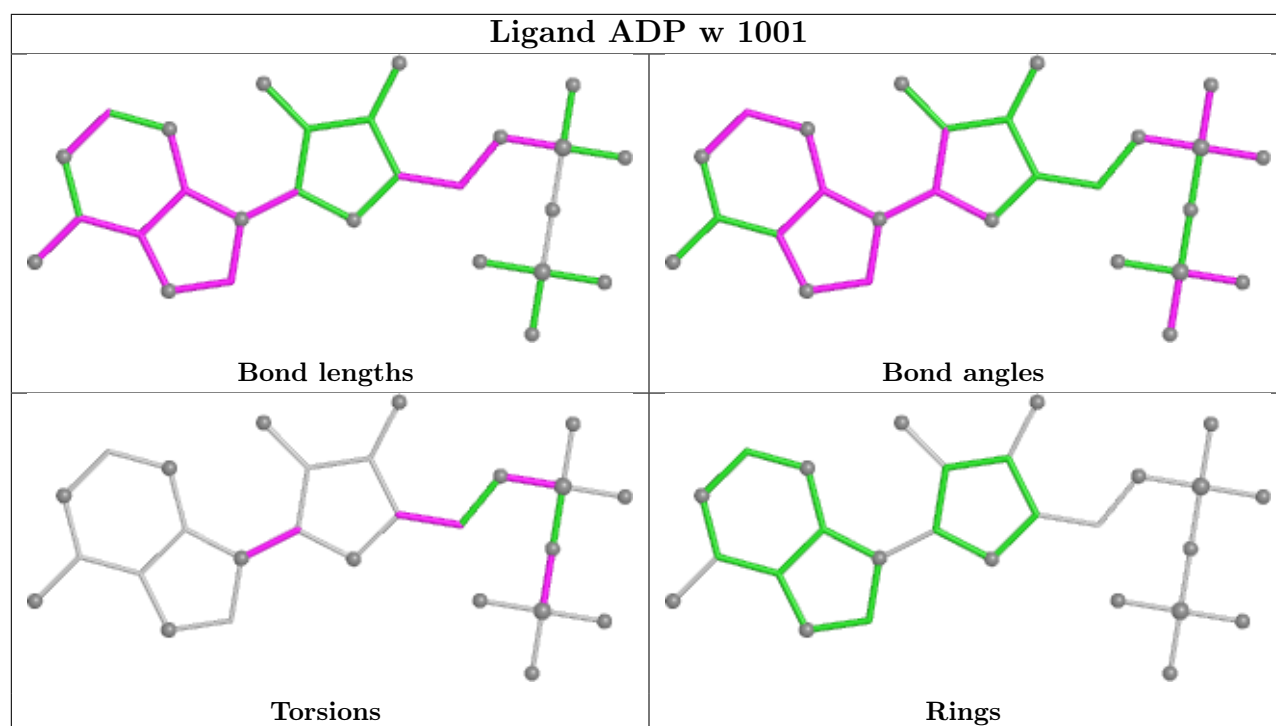
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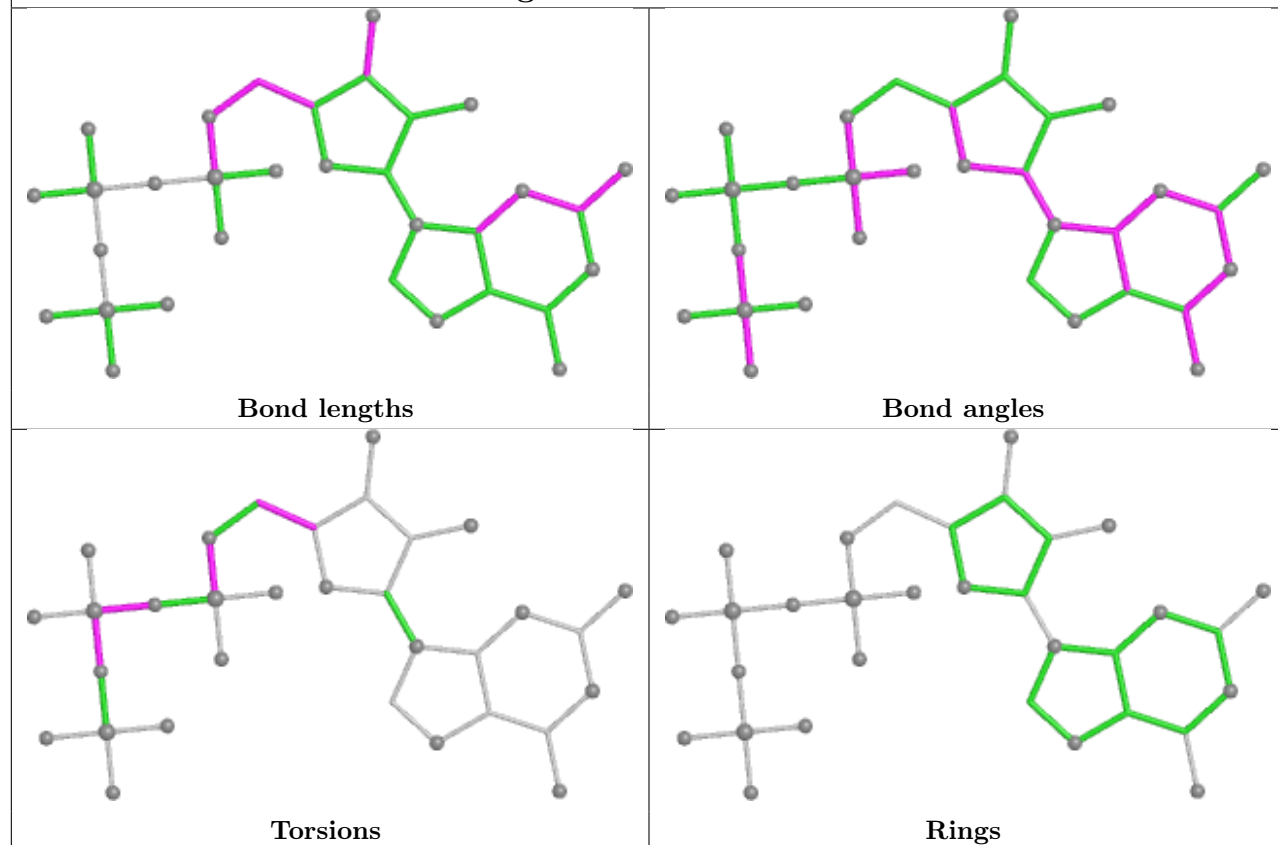
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	t	501	GTP	8	0
18	AN	501	GTP	7	0

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

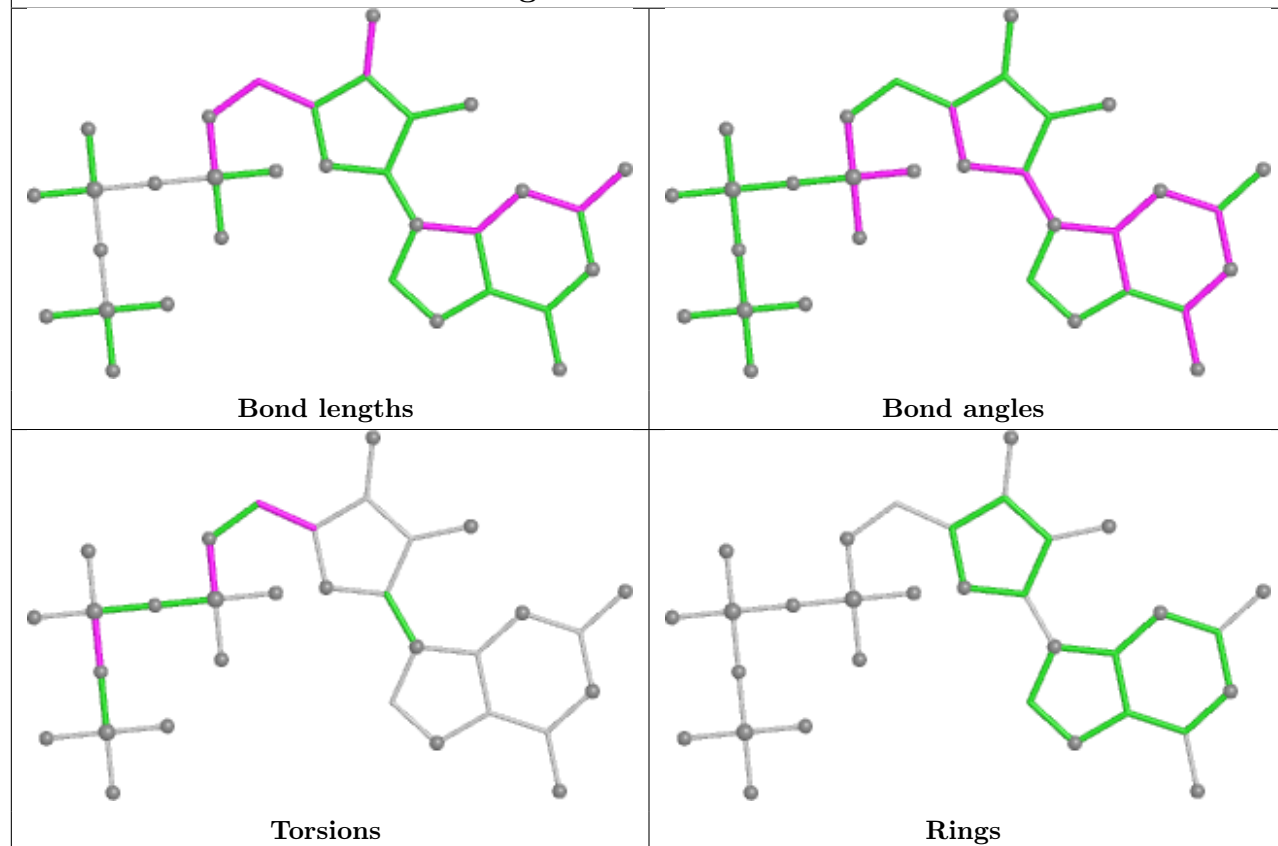




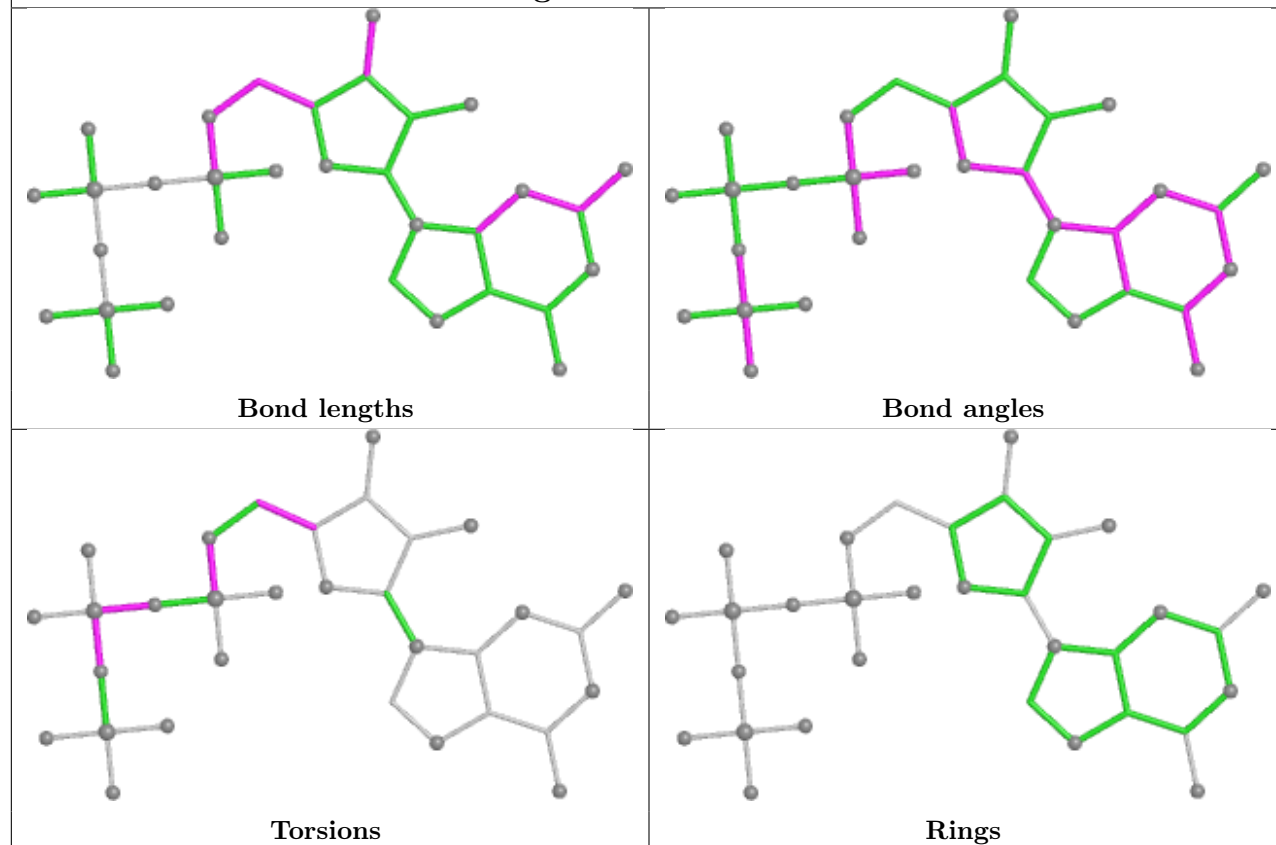
Ligand GTP AO 501



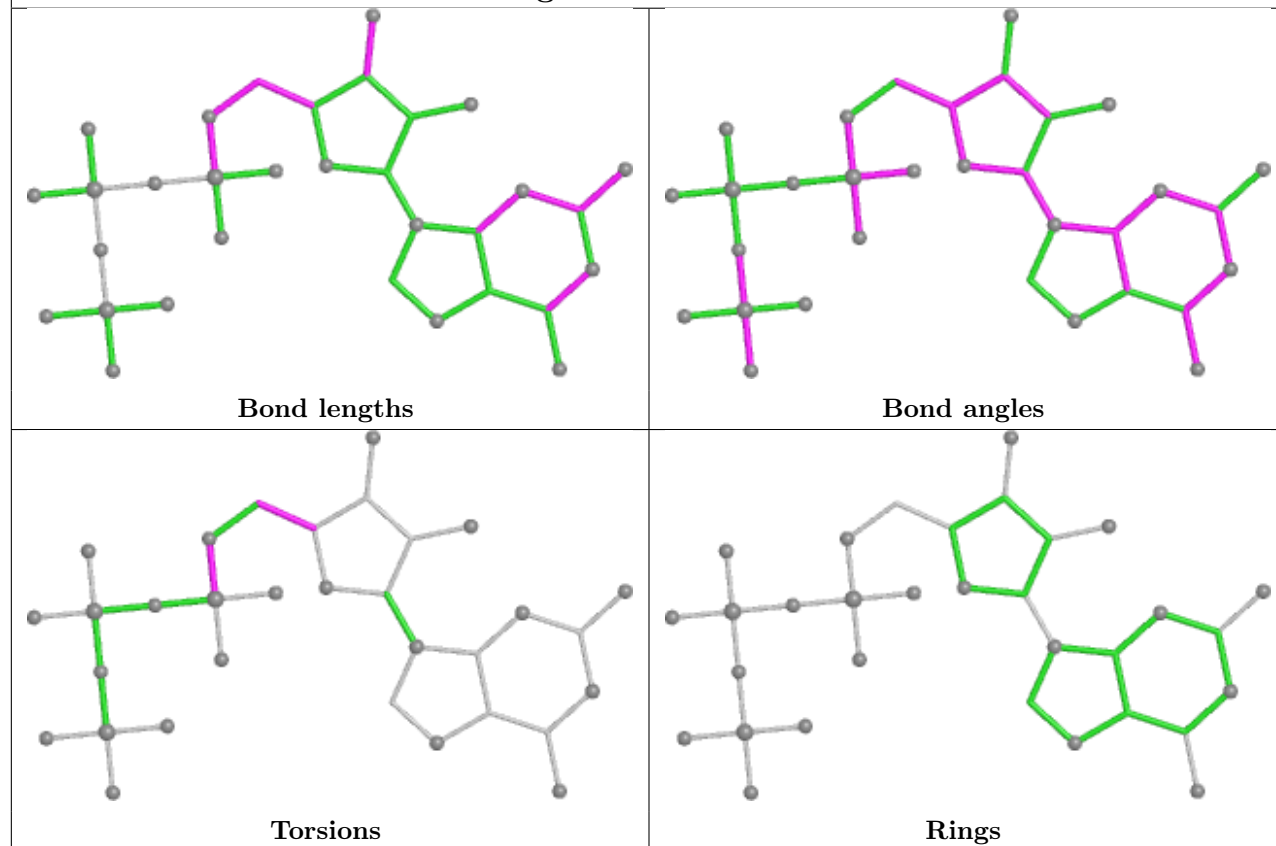
Ligand GTP AF 501

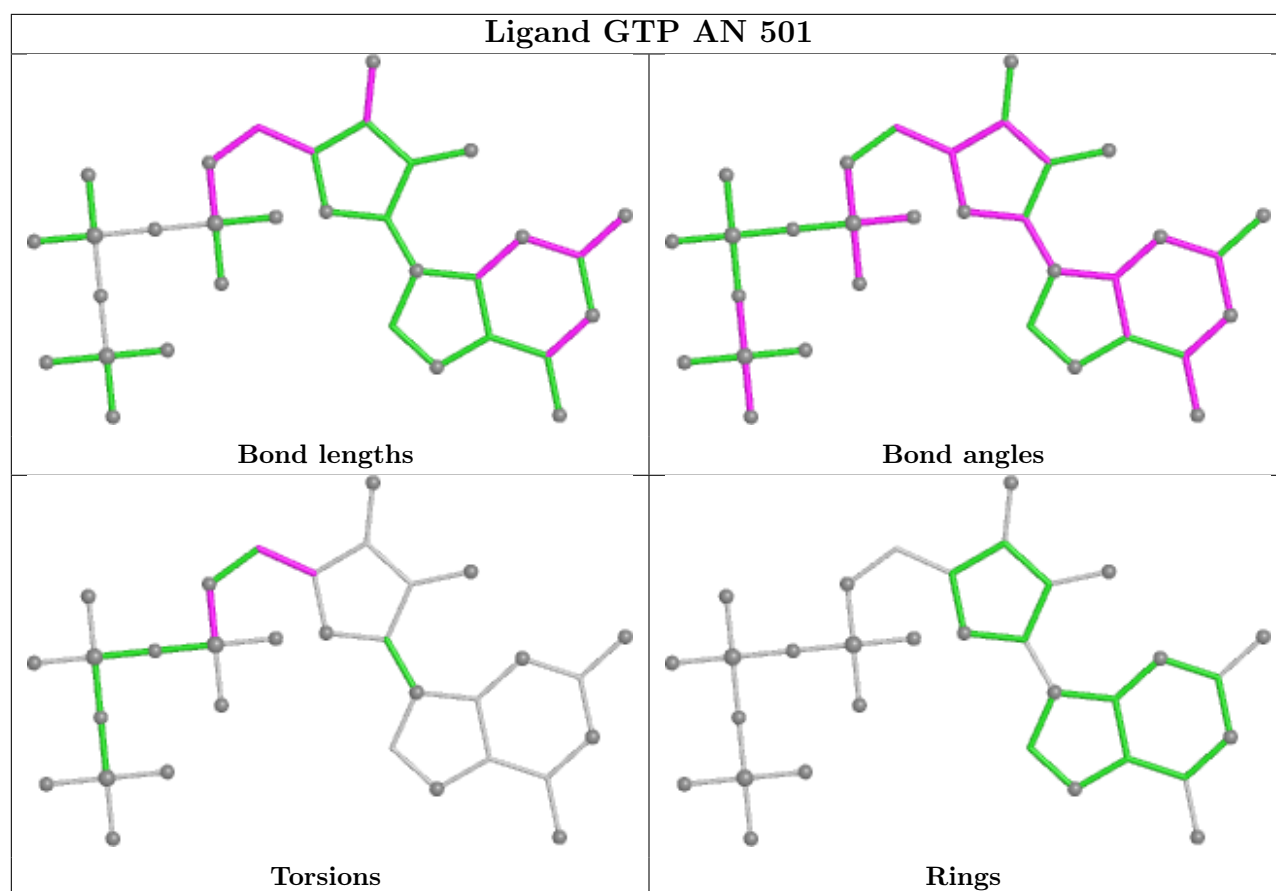


Ligand GTP u 502



Ligand GTP t 501





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

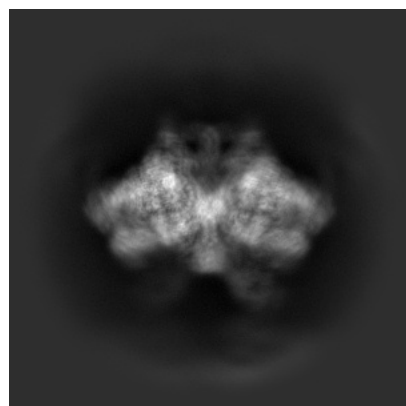
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-67147. These allow visual inspection of the internal detail of the map and identification of artifacts.

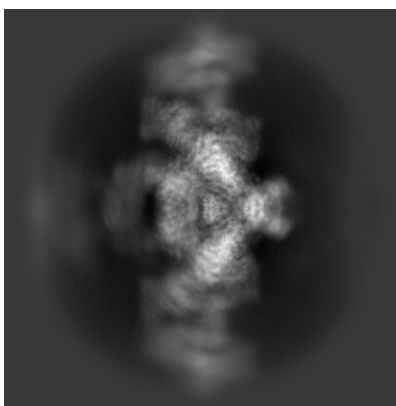
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

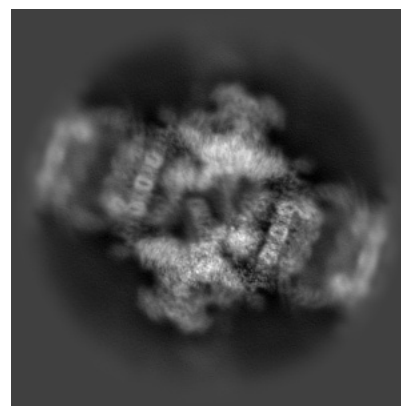
6.1.1 Primary map



X

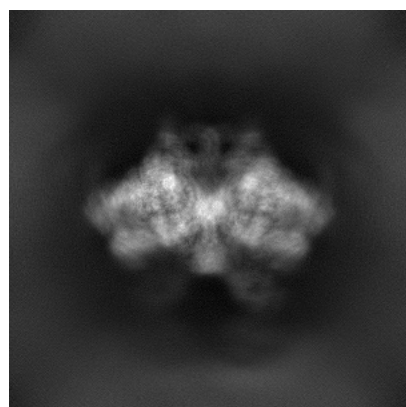


Y

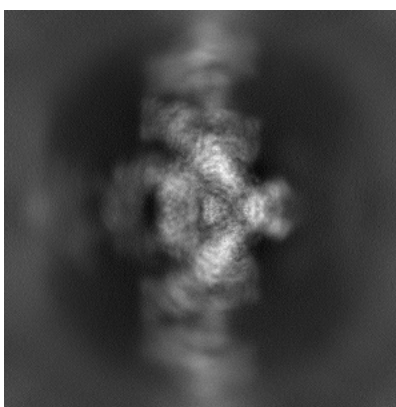


Z

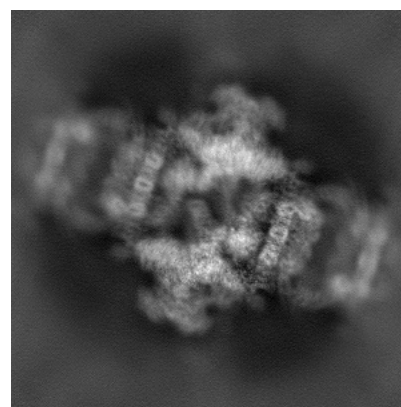
6.1.2 Raw map



X



Y

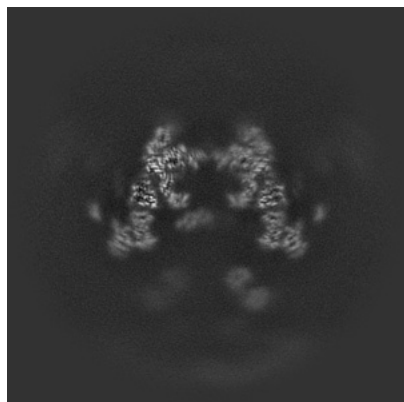


Z

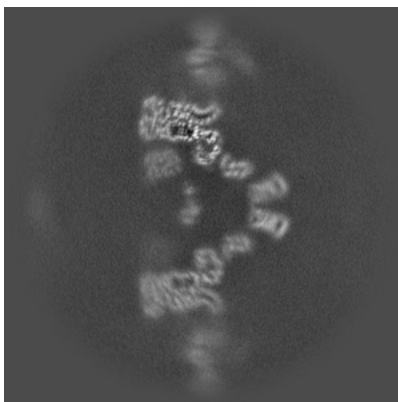
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

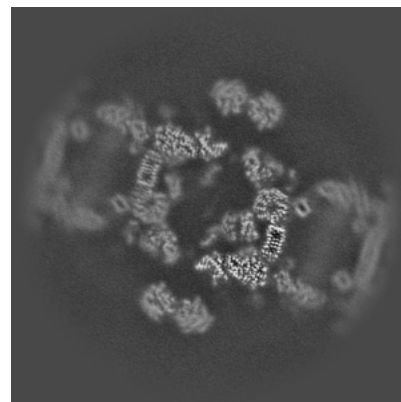
6.2.1 Primary map



X Index: 256

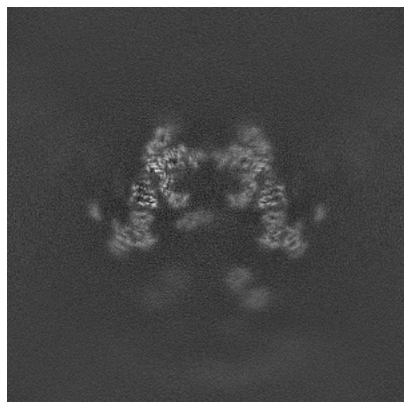


Y Index: 256

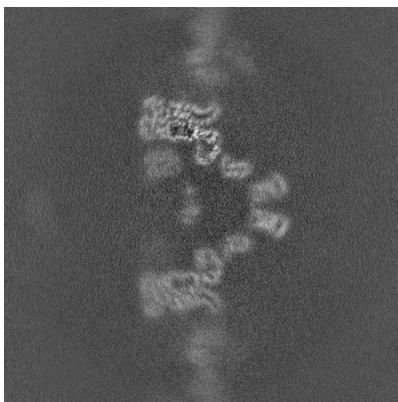


Z Index: 256

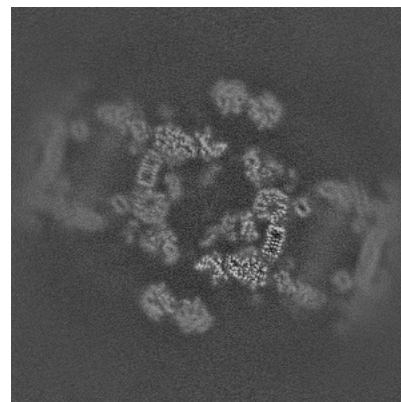
6.2.2 Raw map



X Index: 256



Y Index: 256

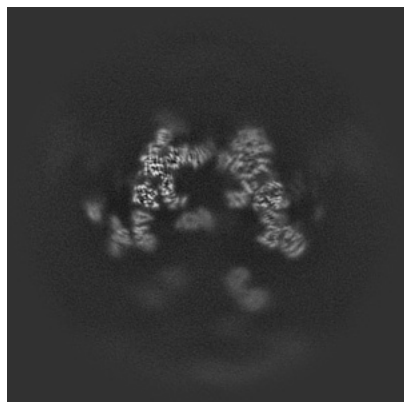


Z Index: 256

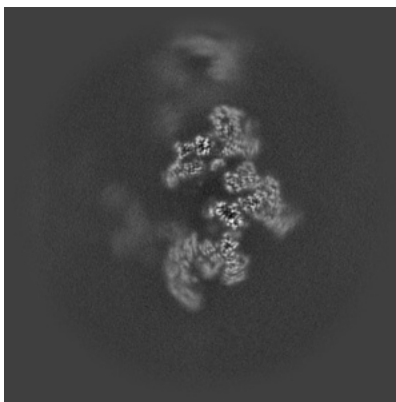
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

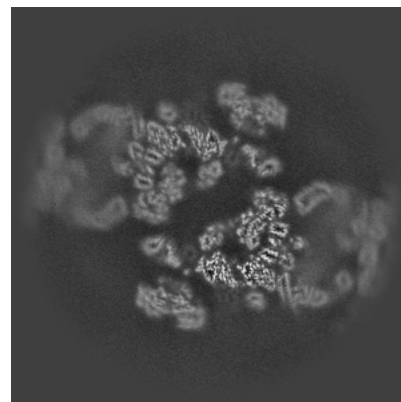
6.3.1 Primary map



X Index: 252

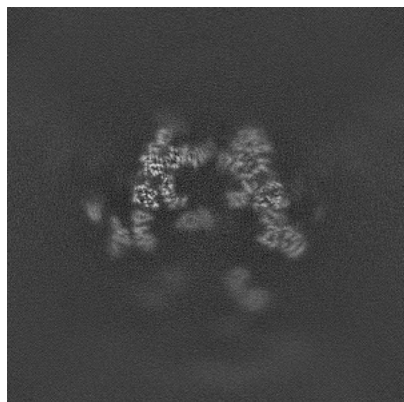


Y Index: 205

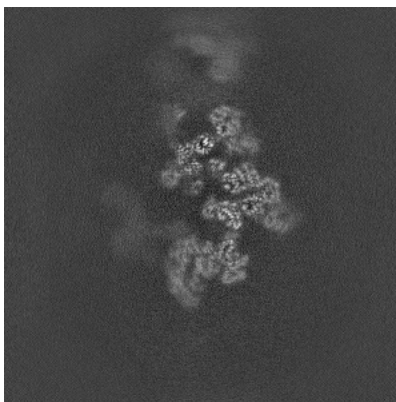


Z Index: 267

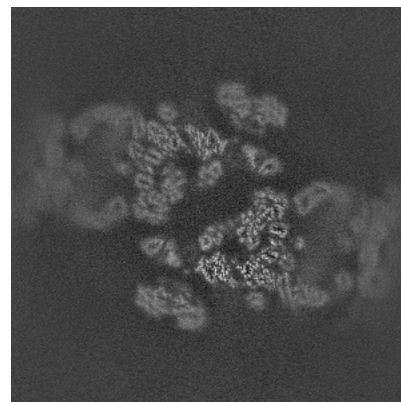
6.3.2 Raw map



X Index: 252



Y Index: 209

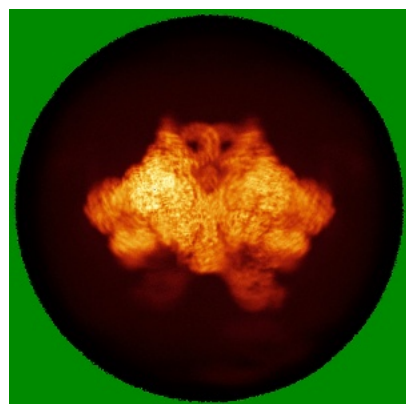


Z Index: 266

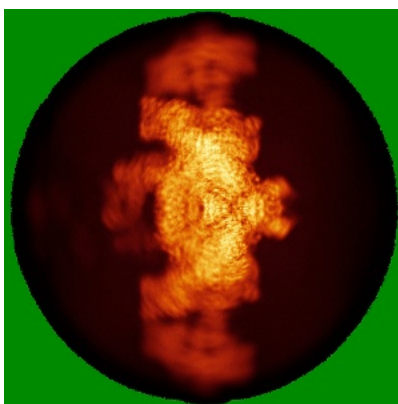
The images above show the largest variance slices of the map in three orthogonal directions.

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

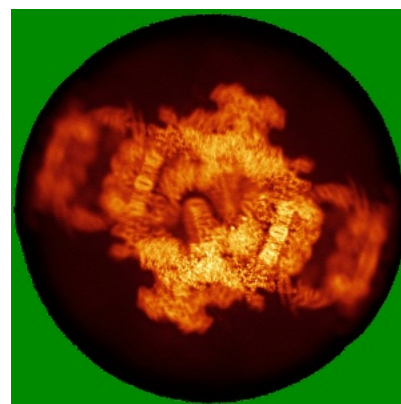
6.4.1 Primary map



X

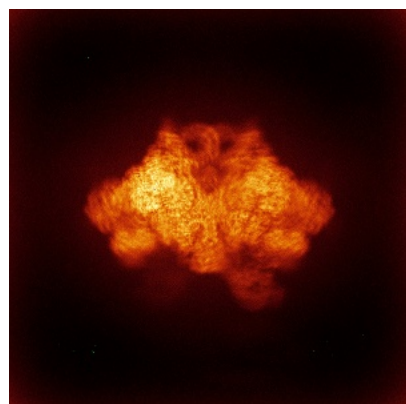


Y

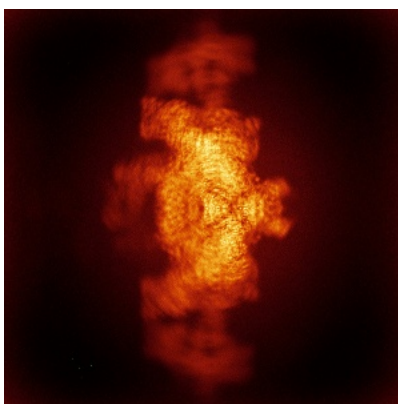


Z

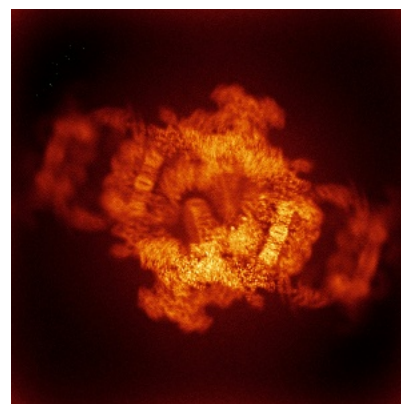
6.4.2 Raw map



X



Y



Z

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

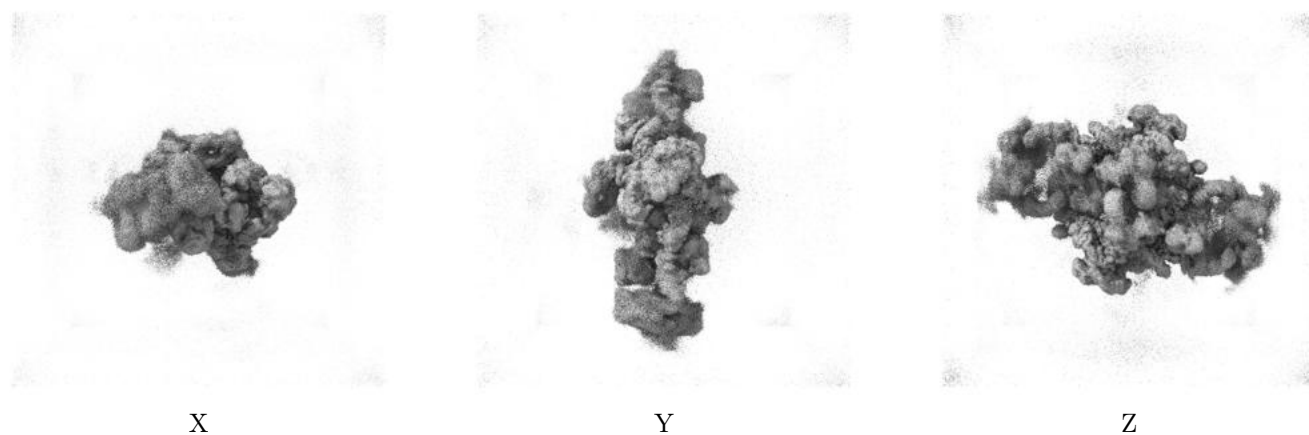
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

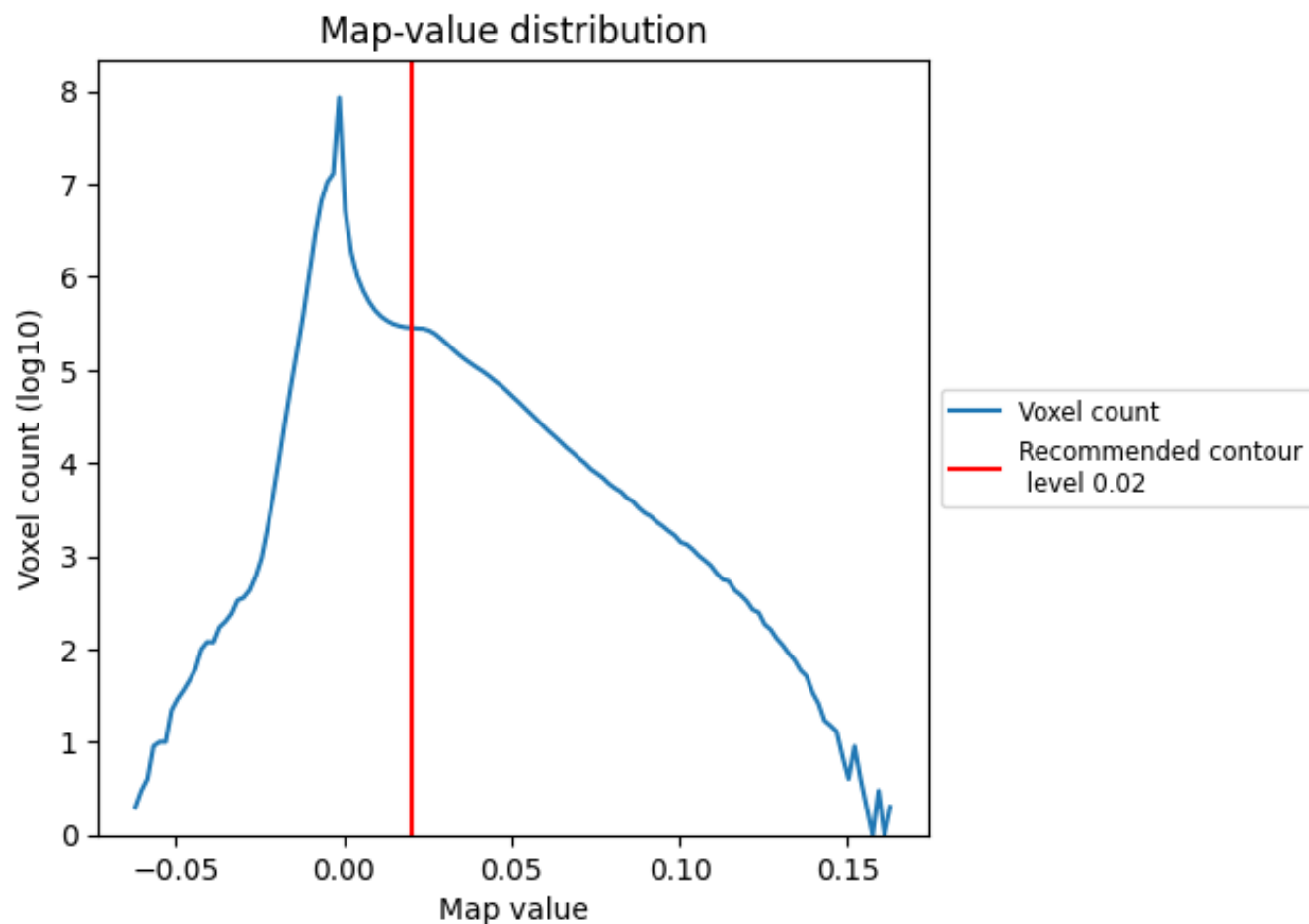
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

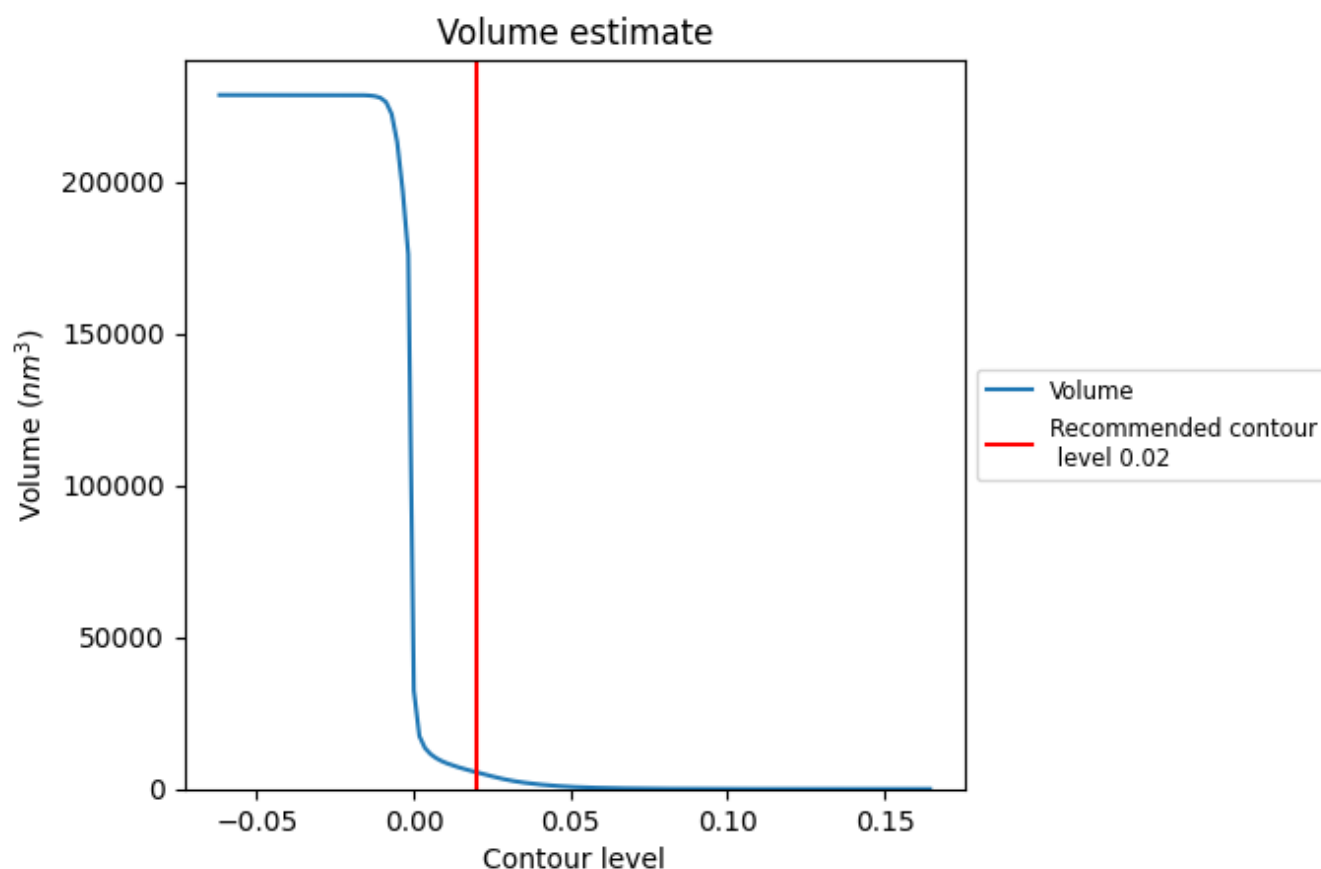
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

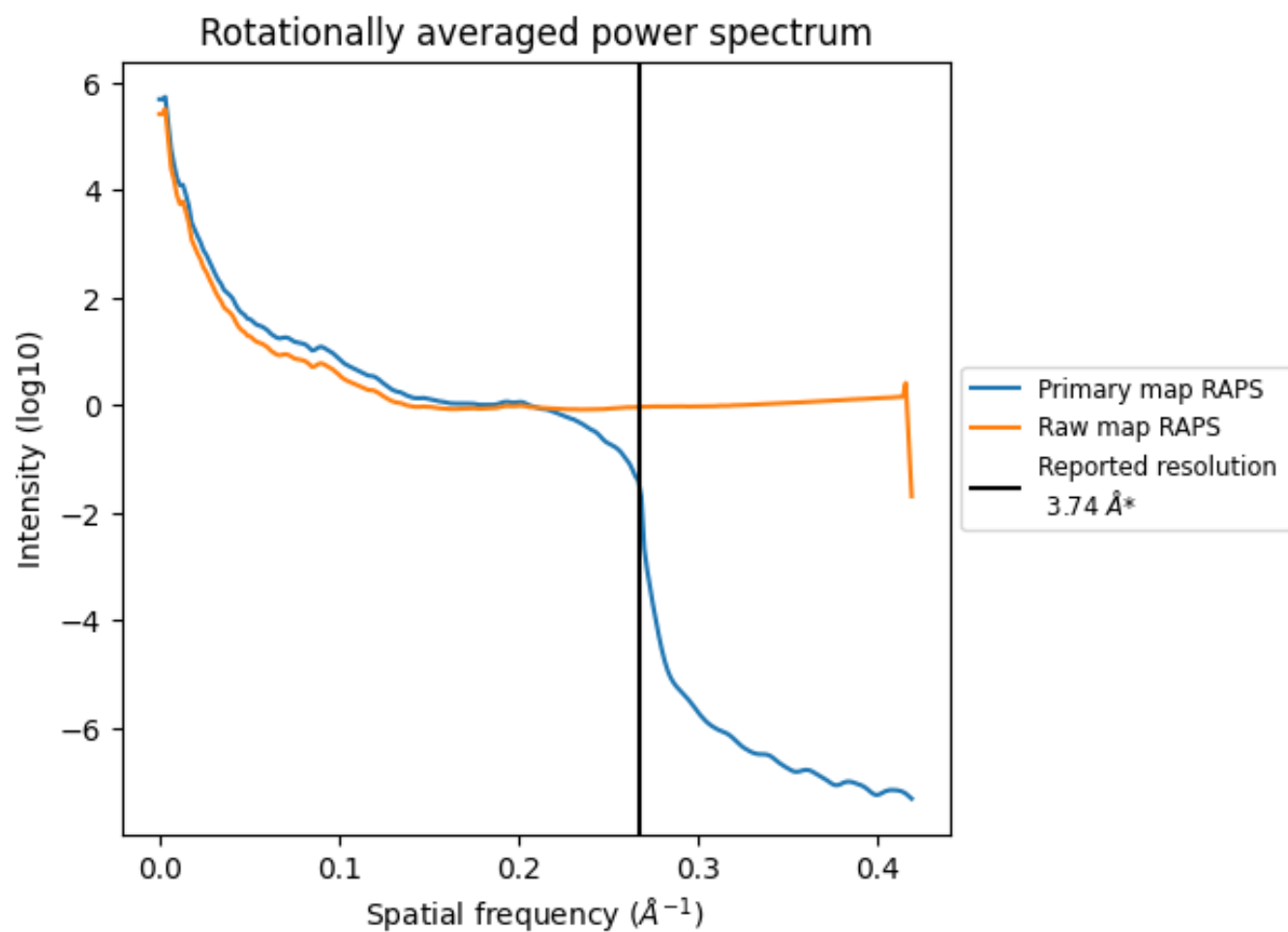
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 5490 nm³; this corresponds to an approximate mass of 4959 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 ⓘ

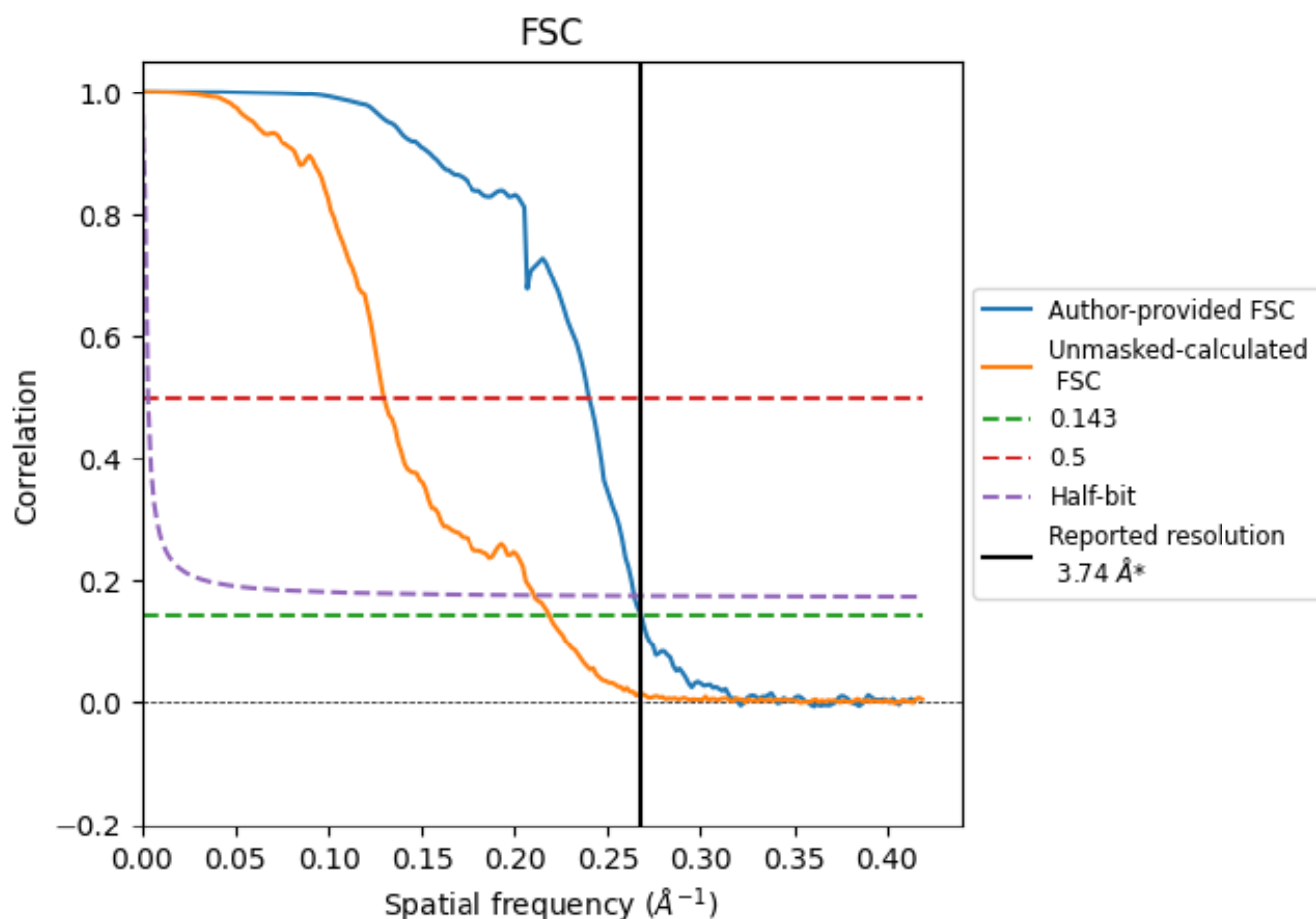


*Reported resolution corresponds to spatial frequency of 0.267 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.267 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

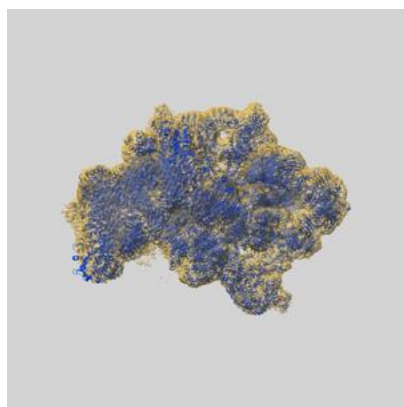
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.74	-	-
Author-provided FSC curve	3.74	4.17	3.79
Unmasked-calculated*	4.57	7.70	4.75

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.57 differs from the reported value 3.74 by more than 10 %

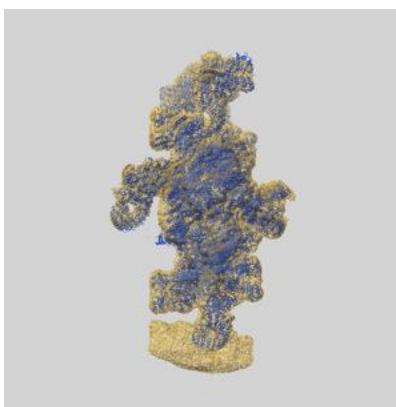
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-67147 and PDB model 9XRL. Per-residue inclusion information can be found in section 3 on page 14.

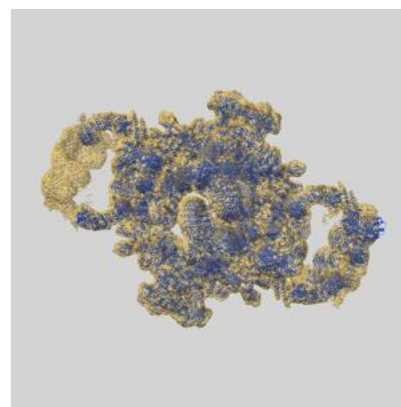
9.1 Map-model overlay [i](#)



X



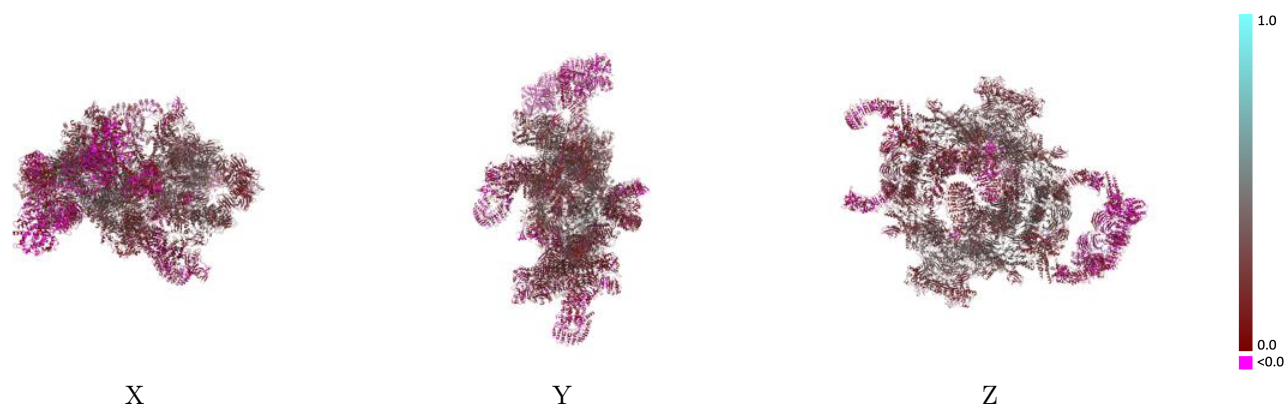
Y



Z

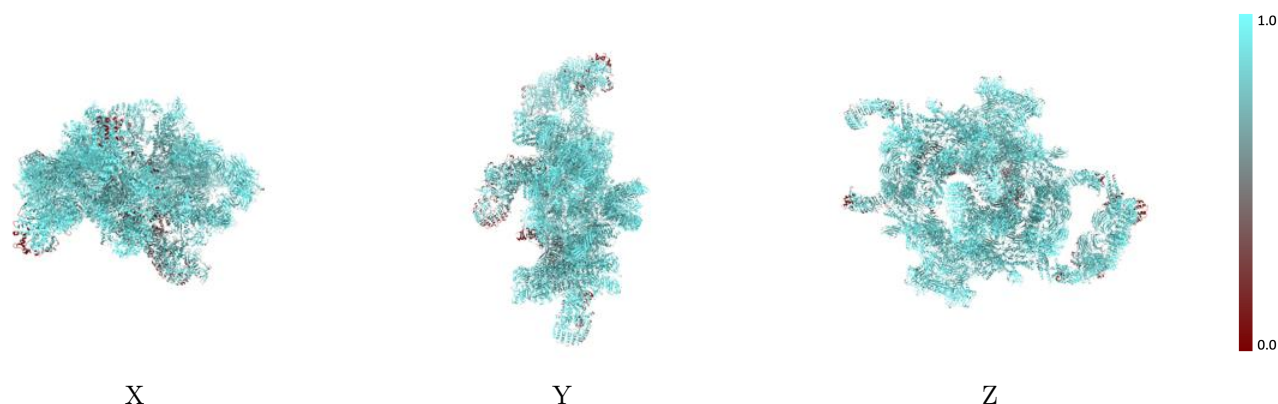
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



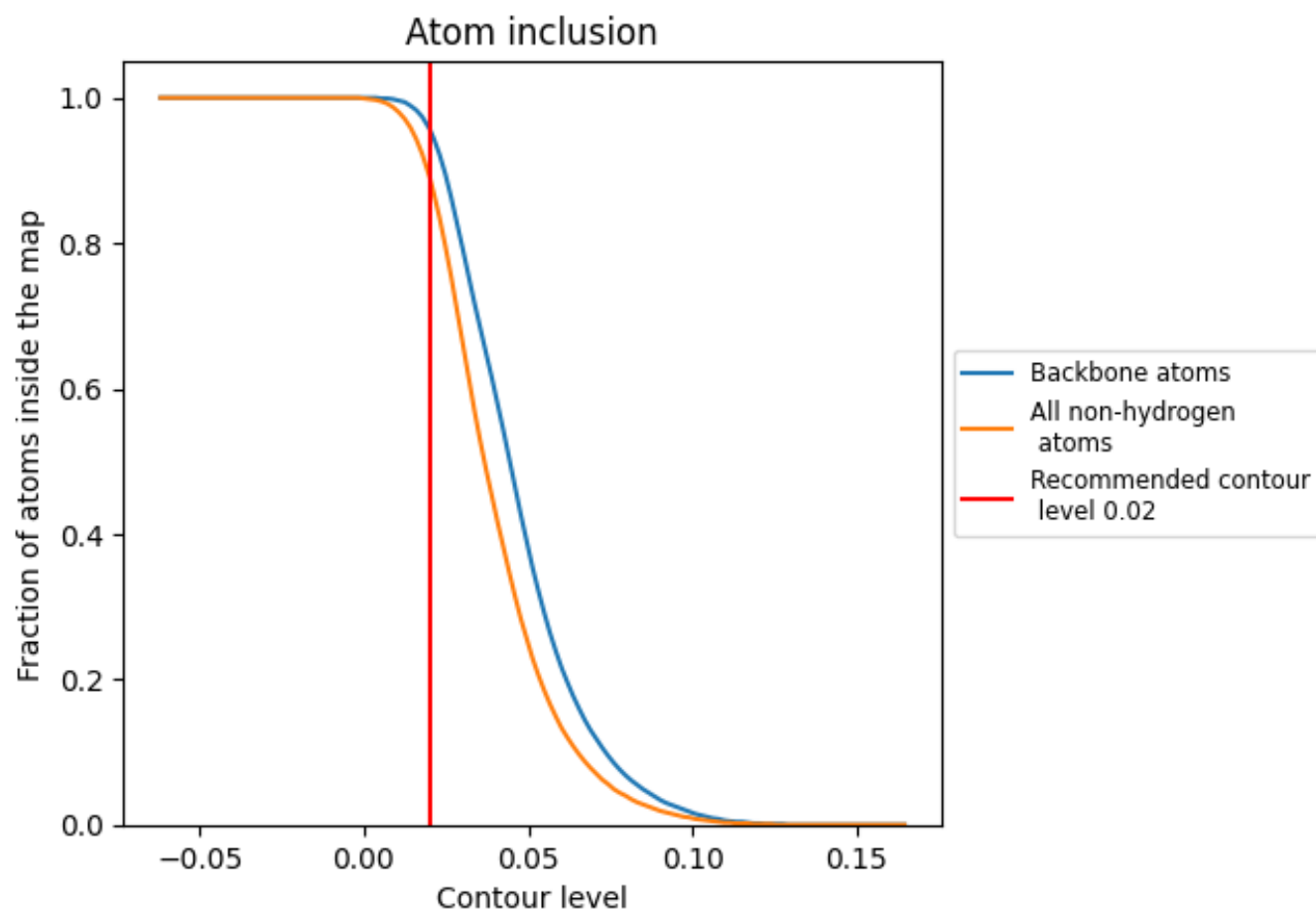
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 89% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8910	 0.2210
0	 0.9230	 0.1970
1	 0.9500	 0.0520
2	 0.8070	 0.0420
3	 0.9770	 0.3130
4	 0.7940	 0.0550
5	 0.9350	 0.3000
6	 0.8910	 0.2380
7	 0.9360	 0.2900
8	 0.9500	 0.3220
9	 0.9750	 0.2030
A	 0.8610	 0.3070
AA	 0.8810	 0.1810
AB	 0.9250	 0.1700
AC	 0.9380	 0.1690
AD	 0.9340	 0.3040
AE	 0.5320	 0.1740
AF	 0.6800	 0.1420
AH	 0.8430	 0.0440
AI	 0.9180	 0.2630
AJ	 0.9170	 0.1740
AK	 0.6820	 0.1000
AL	 0.7360	 0.1370
AM	 0.8510	 0.2130
AN	 0.9240	 0.3320
AO	 0.9440	 0.3190
AQ	 0.9510	 0.2420
AR	 0.9550	 0.2810
AS	 0.9500	 0.3830
AT	 0.9150	 0.1490
B	 0.9260	 0.3630
C	 0.9340	 0.3720
D	 0.8730	 0.2040
E	 0.8630	 0.0410
F	 0.6860	 0.1460



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Chain	Atom inclusion	Q-score
H	 0.8650	 0.1240
I	 0.9440	 0.3000
K	 0.9180	 0.3270
L	 0.5670	 0.1310
O	 0.1290	 0.0530
P	 0.9370	 0.1550
Q	 0.7620	 0.0900
S	 0.9200	 0.2420
T	 0.9210	 0.1710
U	 0.9430	 0.3870
V	 0.9590	 0.3570
W	 0.9510	 0.2410
X	 0.9560	 0.2240
Y	 0.9650	 0.2340
Z	 0.9580	 0.2110
b	 0.9460	 0.3760
c	 0.9360	 0.3450
d	 0.9510	 0.3090
e	 0.8650	 0.0460
f	 0.9330	 0.2860
g	 0.9500	 0.2860
h	 0.8300	 0.0970
i	 0.8730	 0.1480
j	 0.9390	 0.2940
k	 0.9430	 0.3340
l	 0.9330	 0.1990
m	 0.9470	 0.2570
n	 0.9600	 0.2210
o	 0.9520	 0.2020
p	 0.8820	 0.1770
q	 0.8210	 0.1170
r	 0.9250	 0.3170
s	 0.9370	 0.3240
t	 0.9220	 0.1800
u	 0.9340	 0.1900
w	 0.9210	 0.1480
x	 0.9290	 0.2020
y	 0.8270	 0.0440
z	 0.8600	 0.0320