



## wwPDB EM Validation Summary Report ⓘ

Nov 20, 2022 – 07:24 am GMT

PDB ID : 6HEA  
EMDB ID : EMD-0214  
Title : PAN-proteasome in state 3  
Authors : Majumder, P.; Rudack, T.; Beck, F.; Baumeister, W.  
Deposited on : 2018-08-20  
Resolution : 7.04 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

---

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

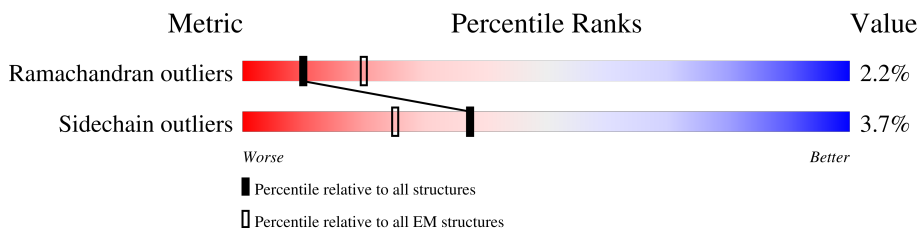
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 7.04 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	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	A	242	
1	B	242	
1	C	242	
1	D	242	
1	E	242	
1	F	242	
1	G	242	
1	a	242	
1	b	242	

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	c	242	12% 74% 19% . . .
1	d	242	12% 69% 26% . .
1	e	242	11% 76% 20% . .
1	f	242	11% 75% 21% . .
1	g	242	11% 73% 20% 5% .
2	1	202	24% 76% 21% .
2	2	202	20% 71% 22% 6% .
2	3	202	21% 76% 22% .
2	4	202	19% 73% 25% .
2	5	202	17% 74% 22% .
2	6	202	21% 72% 25% .
2	7	202	16% 76% 21% .
2	h	202	20% 78% 19% .
2	i	202	23% 75% 22% .
2	j	202	25% 79% 18% .
2	k	202	20% 71% 23% 6% .
2	l	202	22% 76% 20% .
2	m	202	24% 77% 20% .
2	n	202	22% 73% 22% .
3	H	390	25% 72% 24% . .
3	I	390	22% 73% 21% 5% .
3	J	390	19% 78% 18% .
3	K	390	19% 75% 22% .
3	L	390	26% 73% 22% 5% .
3	M	390	29% 74% 20% 5% .

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 66909 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 Proteasome subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	242	1907	1211	321	368	7	0	0
1	a	237	1866	1186	315	359	6	0	0
1	B	242	1907	1211	321	368	7	0	0
1	b	237	1866	1186	315	359	6	0	0
1	C	242	1907	1211	321	368	7	0	0
1	c	237	1866	1186	315	359	6	0	0
1	D	242	1907	1211	321	368	7	0	0
1	d	237	1866	1186	315	359	6	0	0
1	E	242	1907	1211	321	368	7	0	0
1	e	237	1866	1186	315	359	6	0	0
1	F	242	1907	1211	321	368	7	0	0
1	f	237	1866	1186	315	359	6	0	0
1	G	242	1907	1211	321	368	7	0	0
1	g	237	1866	1186	315	359	6	0	0

- Molecule 2 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	1	202	1553	982	260	305	6	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	h	202	1553	982	260	305	6	0	0
2	2	202	1553	982	260	305	6	0	0
2	i	202	1553	982	260	305	6	0	0
2	3	202	1553	982	260	305	6	0	0
2	j	202	1553	982	260	305	6	0	0
2	4	202	1553	982	260	305	6	0	0
2	k	202	1553	982	260	305	6	0	0
2	5	202	1553	982	260	305	6	0	0
2	l	202	1553	982	260	305	6	0	0
2	6	202	1553	982	260	305	6	0	0
2	m	202	1553	982	260	305	6	0	0
2	7	202	1553	982	260	305	6	0	0
2	n	202	1553	982	260	305	6	0	0

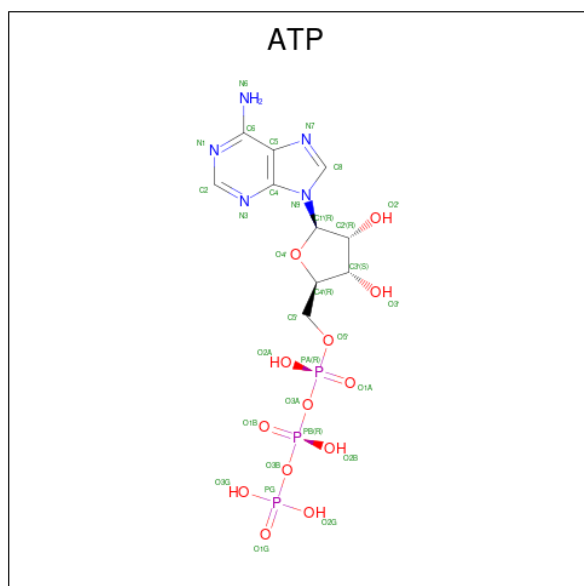
- Molecule 3 is a protein called Proteasome-activating nucleotidase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	H	390	3100	1974	535	583	8	0	0
3	I	390	3100	1974	535	583	8	0	0
3	K	390	3100	1974	535	583	8	0	0
3	L	390	3100	1974	535	583	8	0	0
3	M	390	3100	1974	535	583	8	0	0
3	J	390	3100	1974	535	583	8	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
4	H	1	Total	Mg	0
			1	1	
4	I	1	Total	Mg	0
			1	1	
4	K	1	Total	Mg	0
			1	1	
4	M	1	Total	Mg	0
			1	1	
4	J	1	Total	Mg	0
			1	1	

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



Mol	Chain	Residues	Atoms					AltConf
5	I	1	Total	C	N	O	P	0
			62	20	10	26	6	
5	I	1	Total	C	N	O	P	0
			62	20	10	26	6	
5	M	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	J	1	Total	C	N	O	P	0
			31	10	5	13	3	

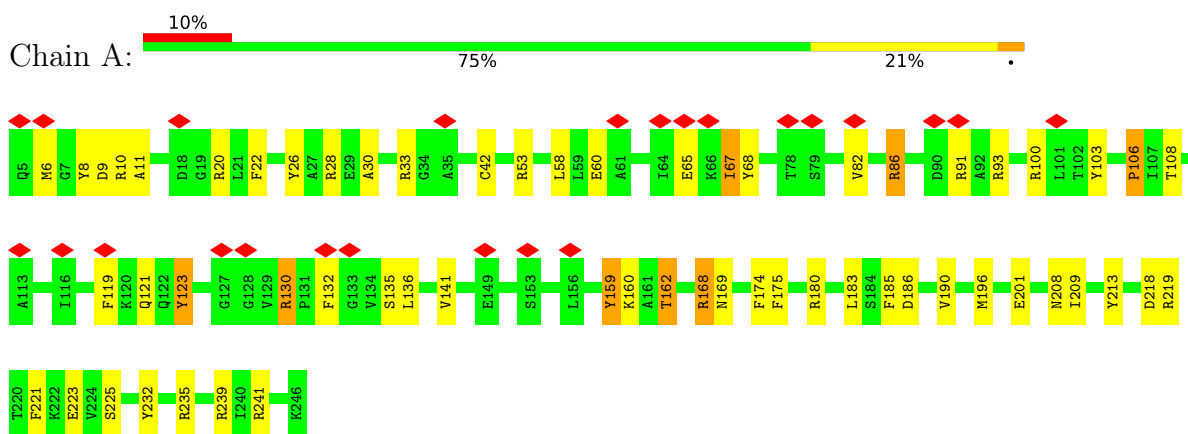
- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



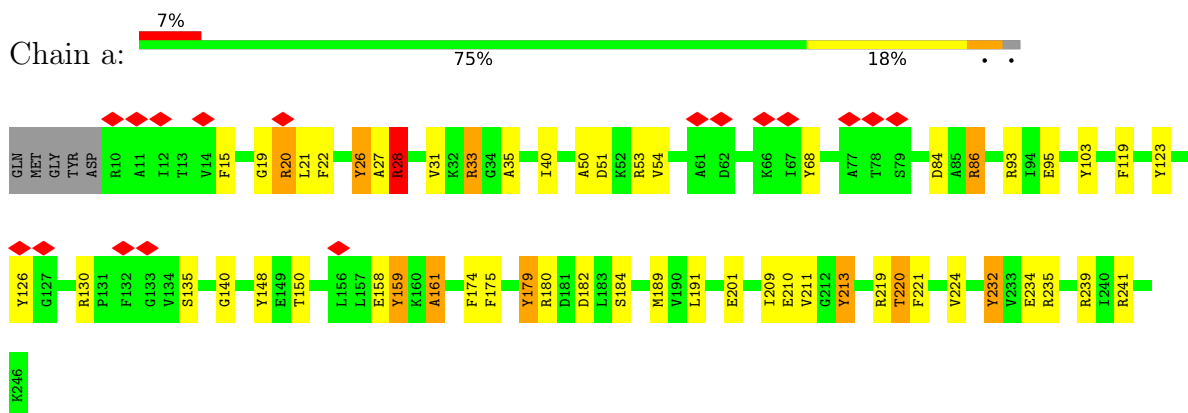
### 3 Residue-property plots [i](#)

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

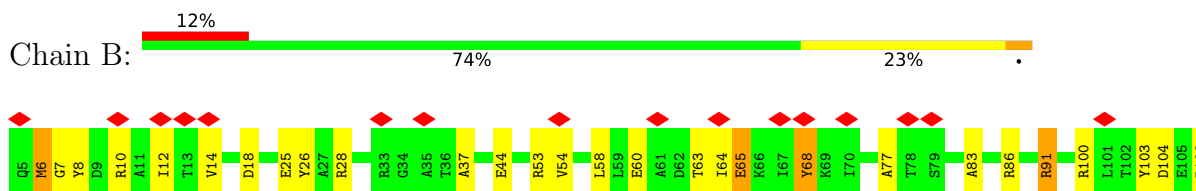
- Molecule 1: Proteasome subunit alpha



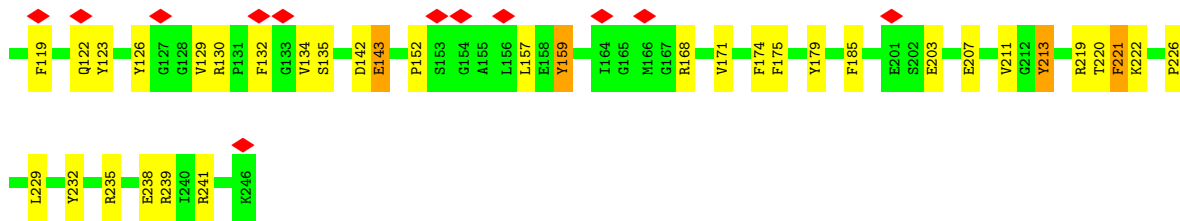
- Molecule 1: Proteasome subunit alpha



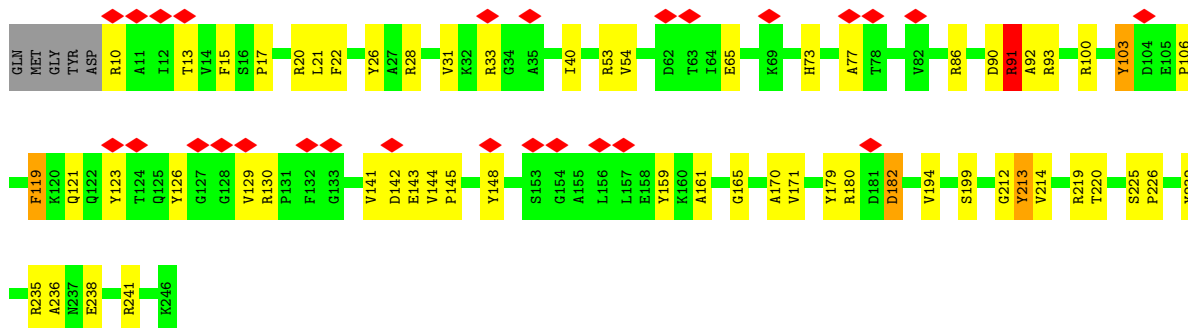
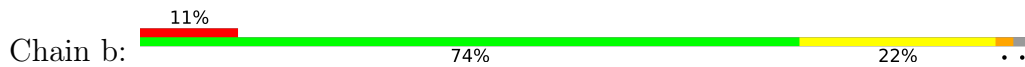
- Molecule 1: Proteasome subunit alpha



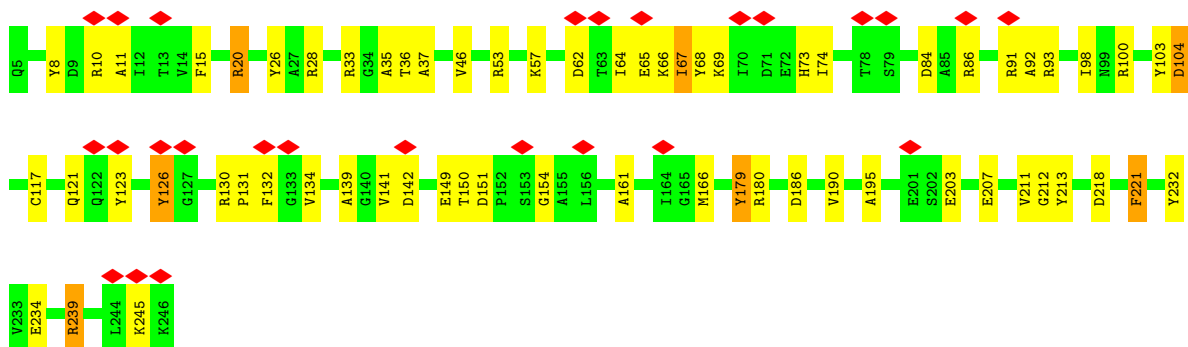
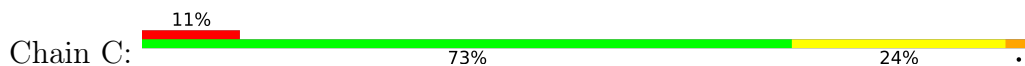




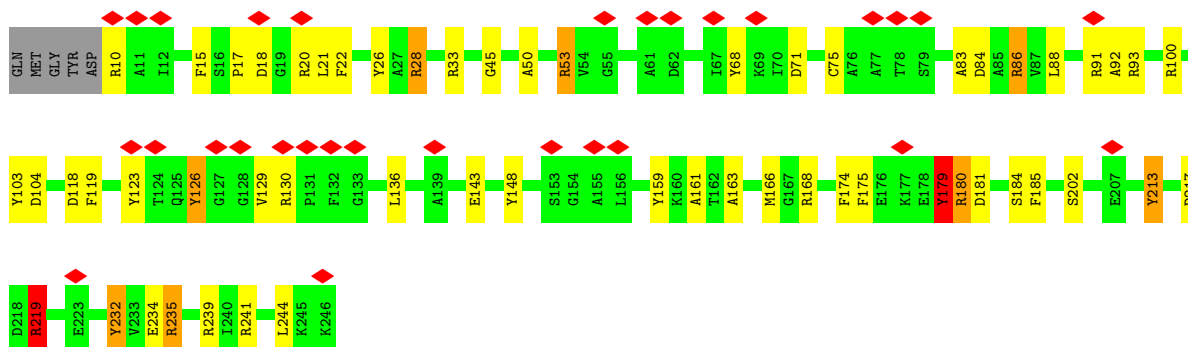
• Molecule 1: Proteasome subunit alpha



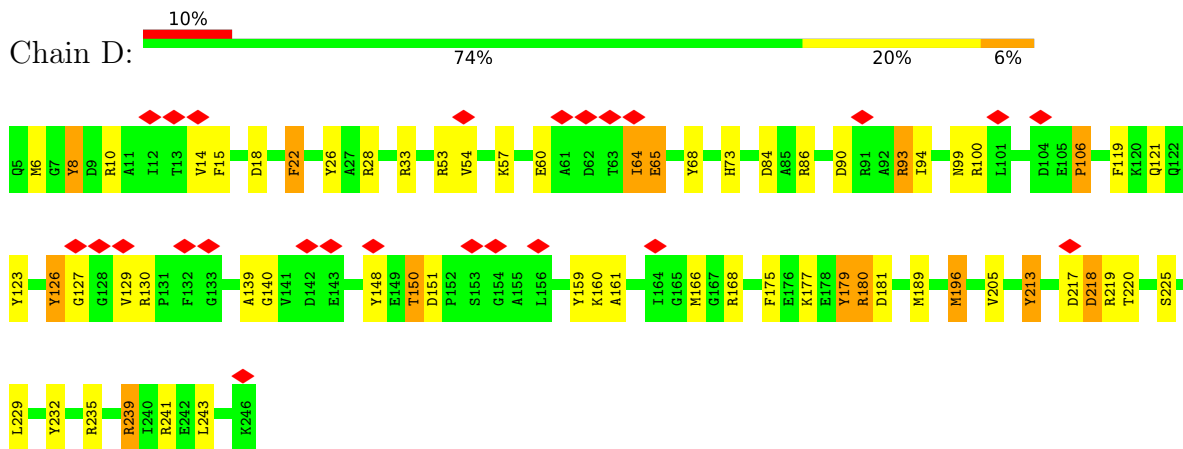
• Molecule 1: Proteasome subunit alpha



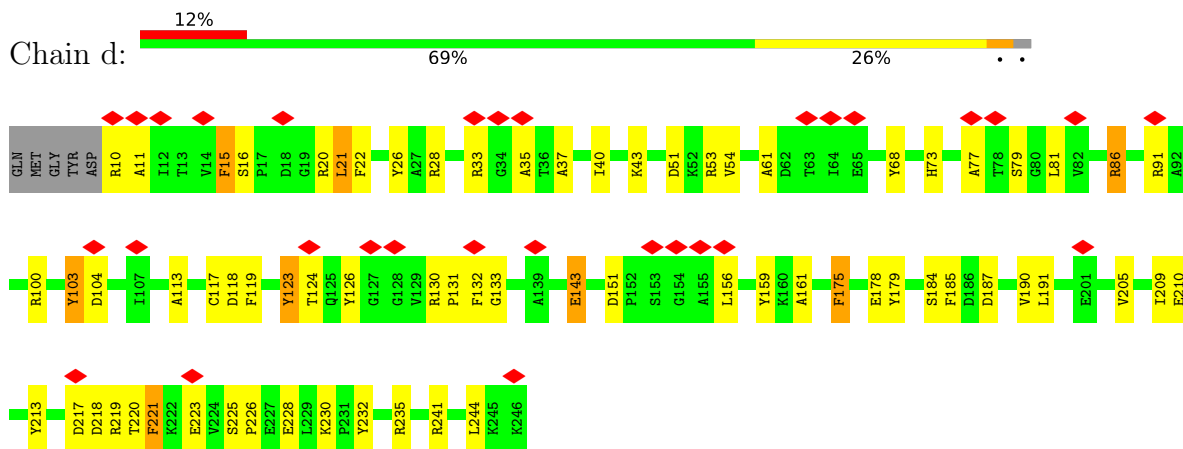
• Molecule 1: Proteasome subunit alpha



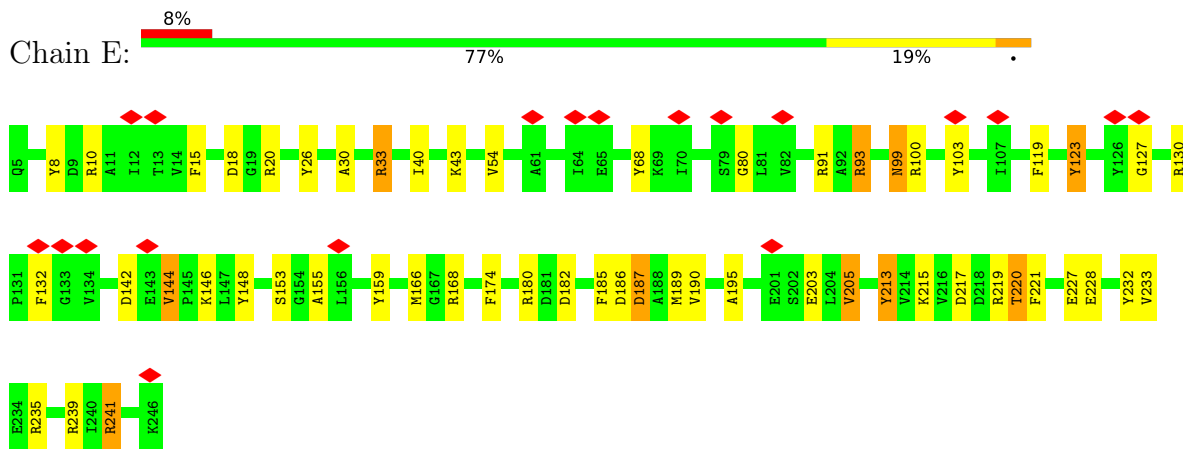
• Molecule 1: Proteasome subunit alpha



• Molecule 1: Proteasome subunit alpha

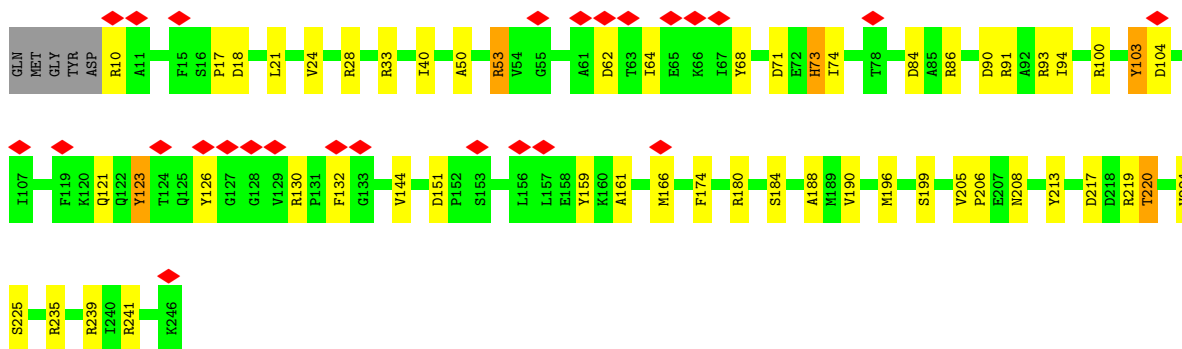


• Molecule 1: Proteasome subunit alpha

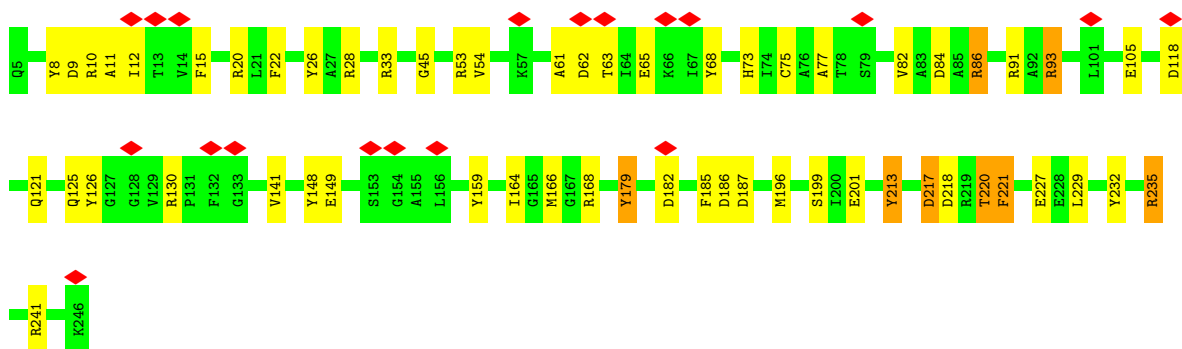
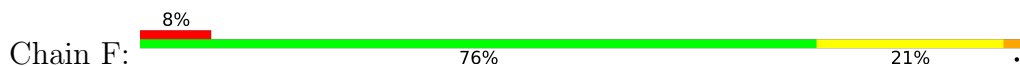


• Molecule 1: Proteasome subunit alpha

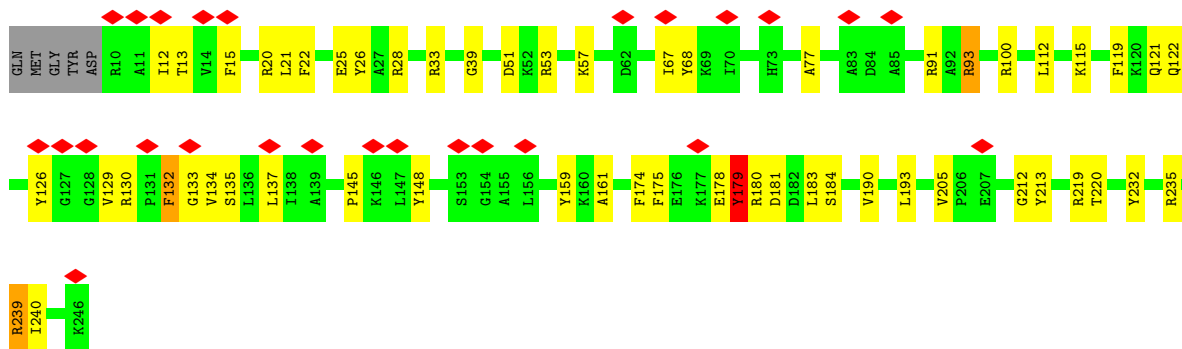
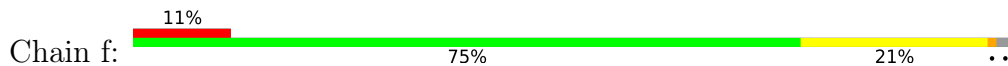




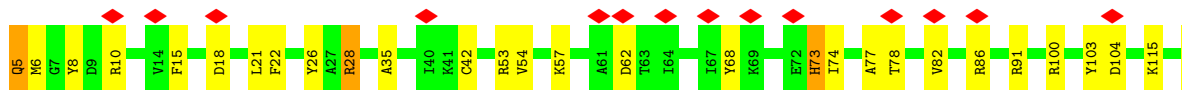
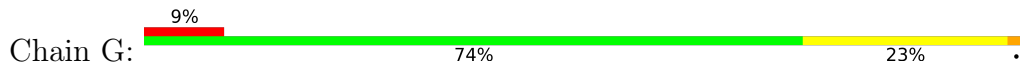
• Molecule 1: Proteasome subunit alpha

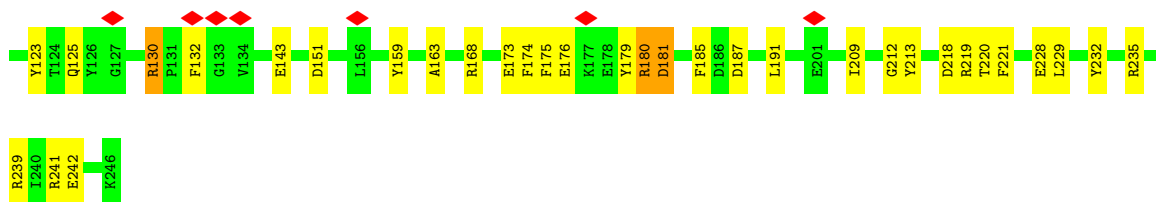


• Molecule 1: Proteasome subunit alpha

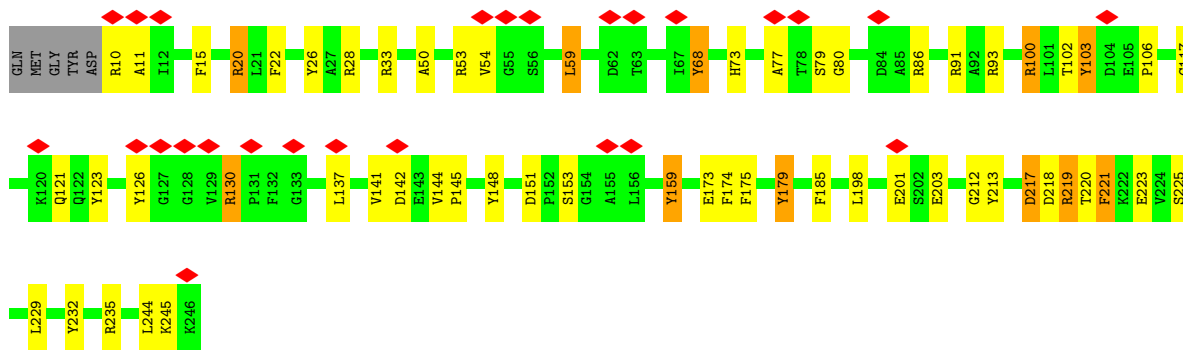
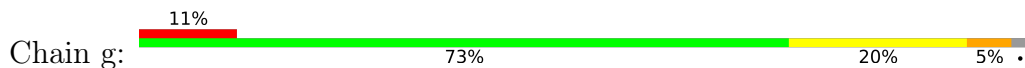


• Molecule 1: Proteasome subunit alpha

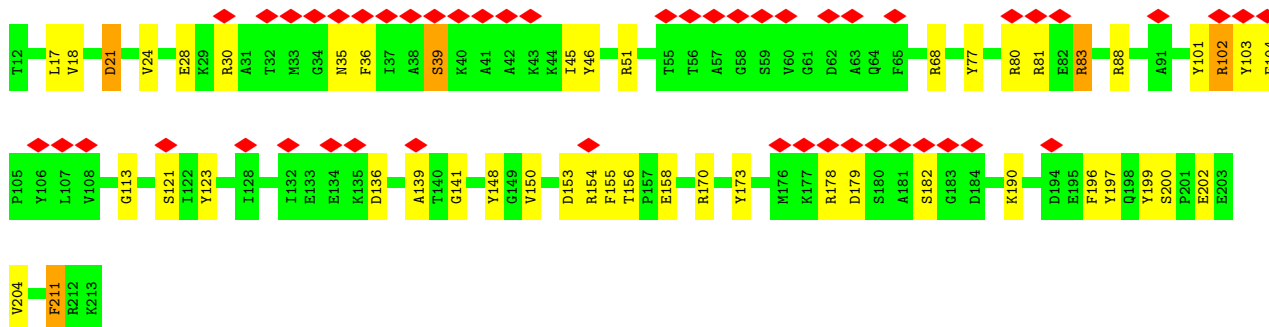
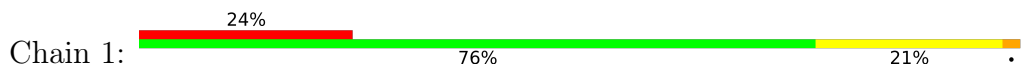




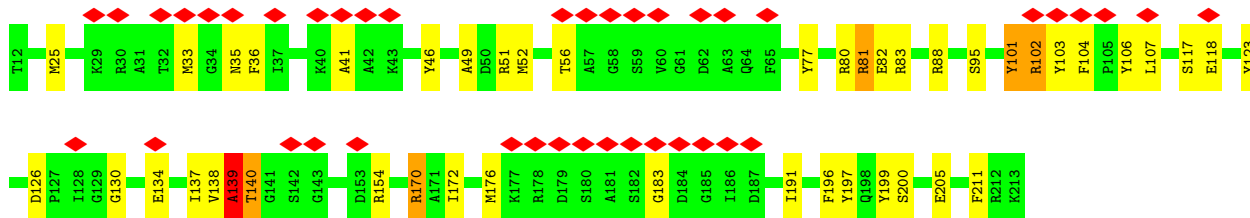
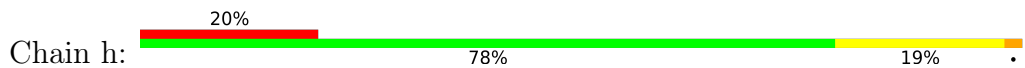
• Molecule 1: Proteasome subunit alpha



• Molecule 2: Proteasome subunit beta

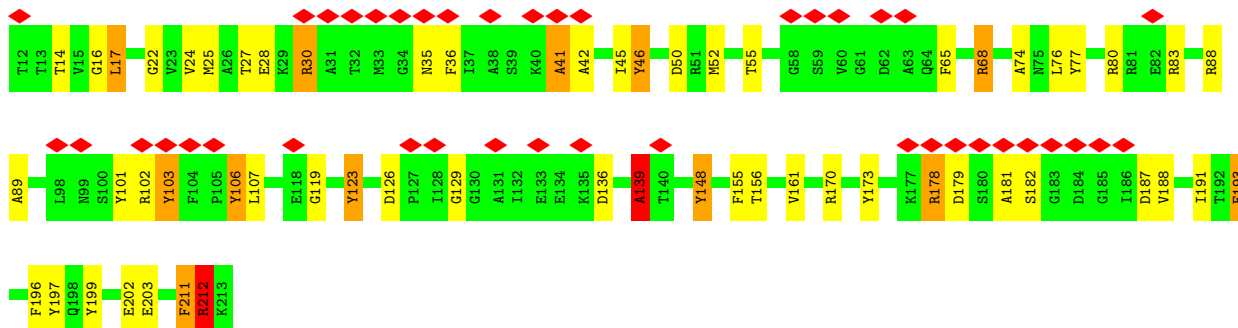


• Molecule 2: Proteasome subunit beta

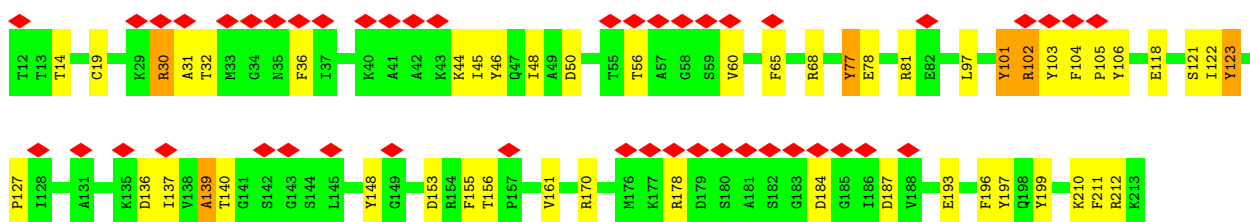
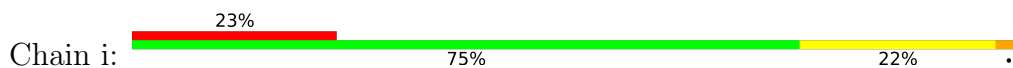


• Molecule 2: Proteasome subunit beta

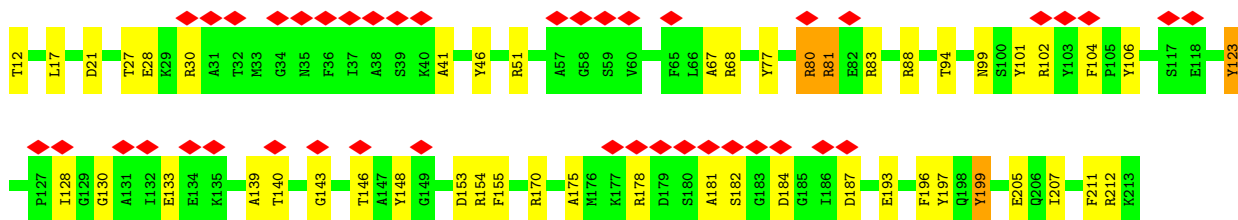
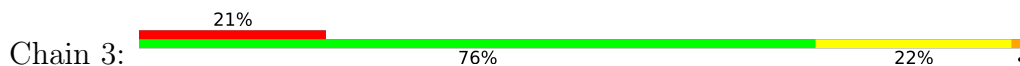




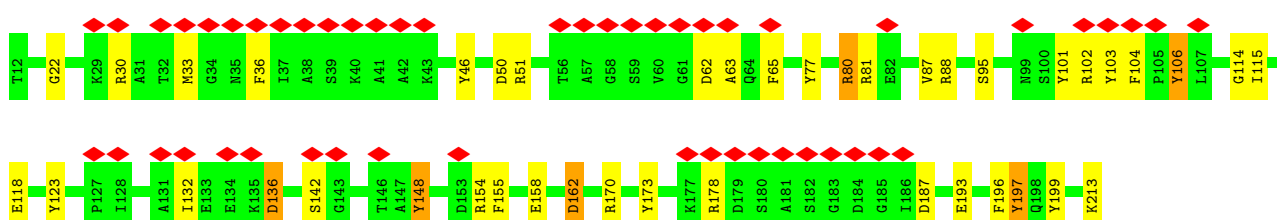
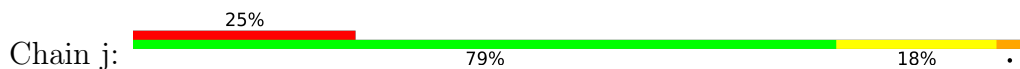
• Molecule 2: Proteasome subunit beta



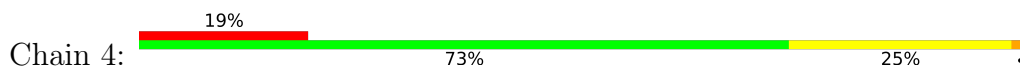
• Molecule 2: Proteasome subunit beta

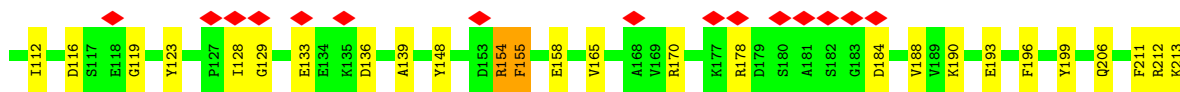


• Molecule 2: Proteasome subunit beta

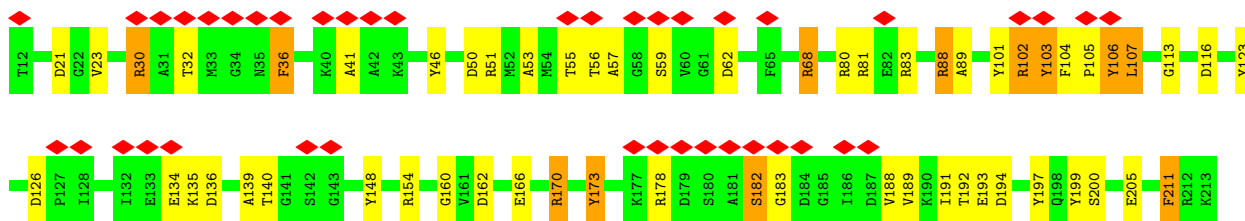


• Molecule 2: Proteasome subunit beta

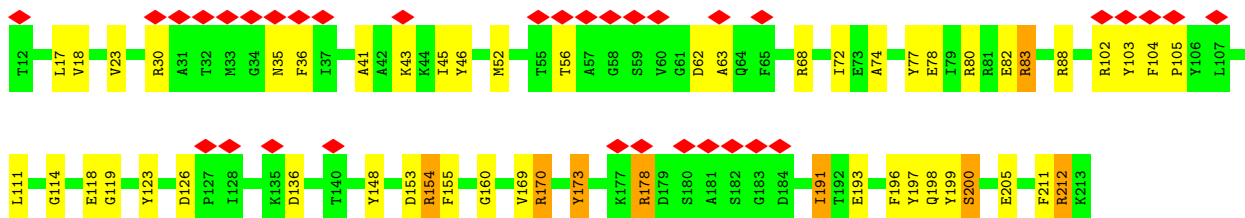
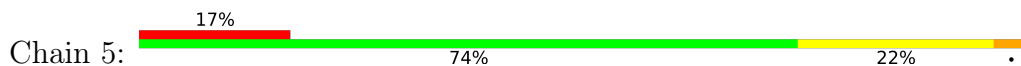




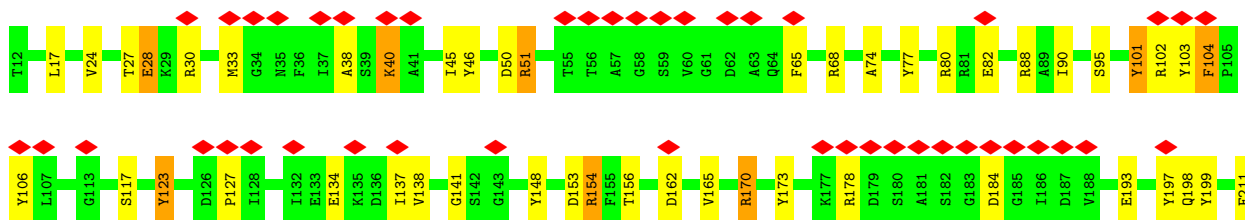
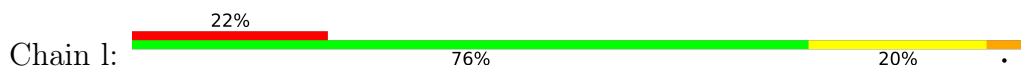
• Molecule 2: Proteasome subunit beta



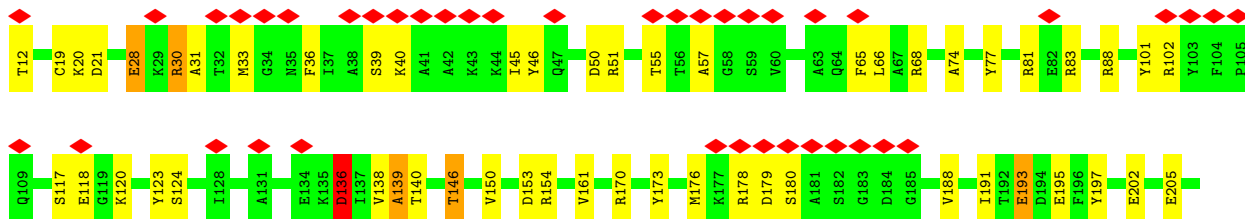
• Molecule 2: Proteasome subunit beta



• Molecule 2: Proteasome subunit beta

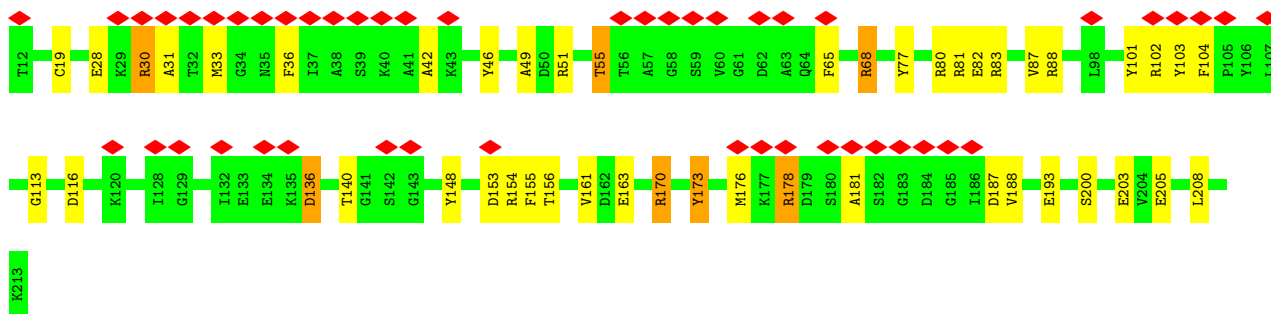
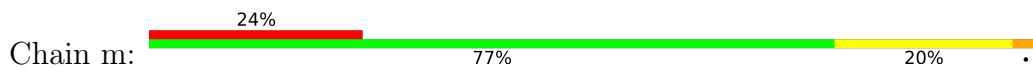


• Molecule 2: Proteasome subunit beta

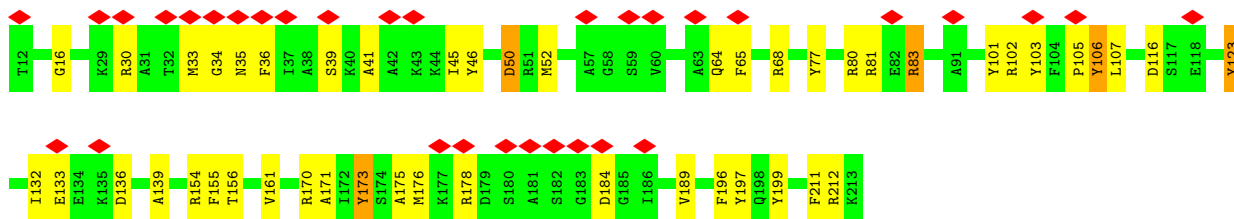
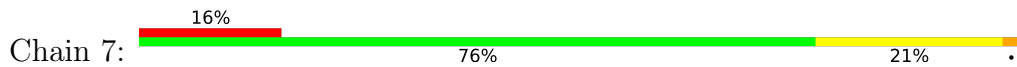




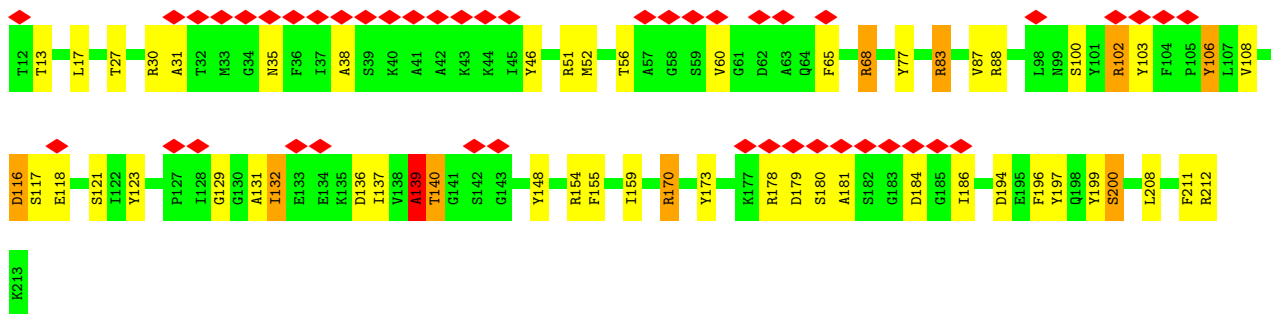
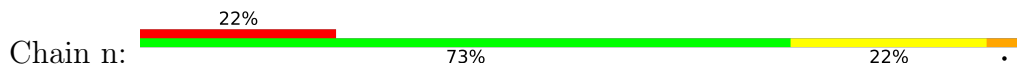
• Molecule 2: Proteasome subunit beta



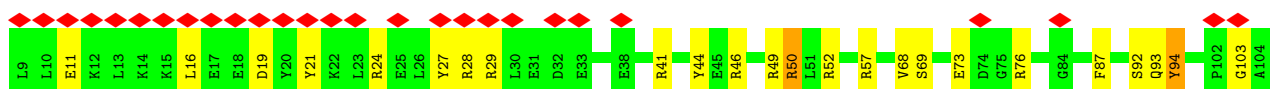
• Molecule 2: Proteasome subunit beta

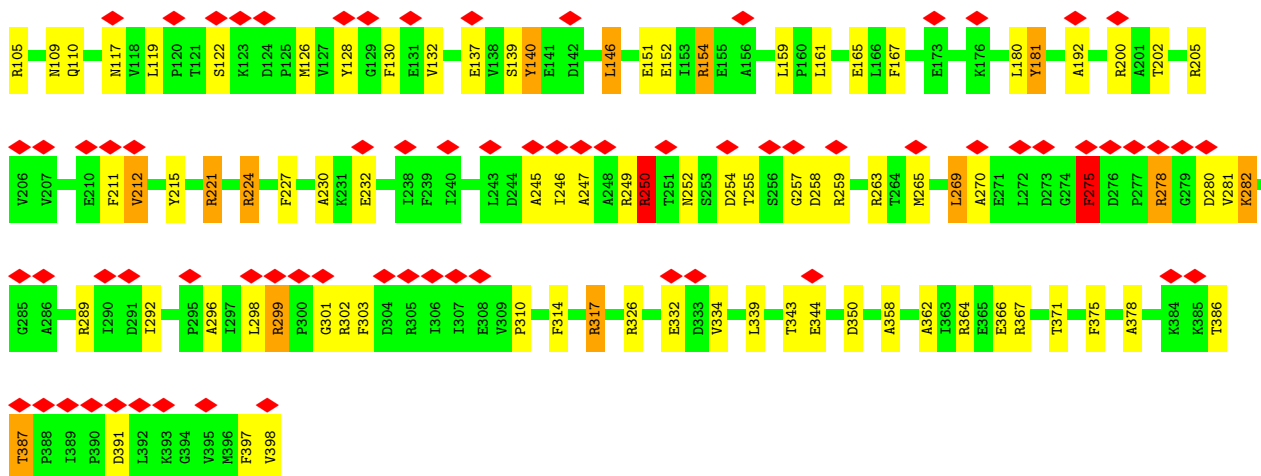


• Molecule 2: Proteasome subunit beta

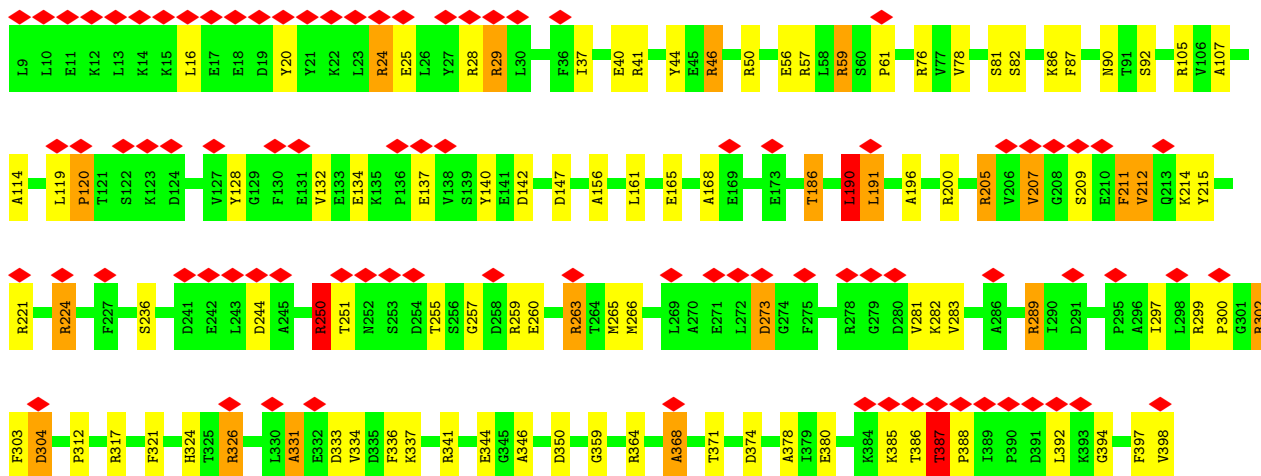


• Molecule 3: Proteasome-activating nucleotidase

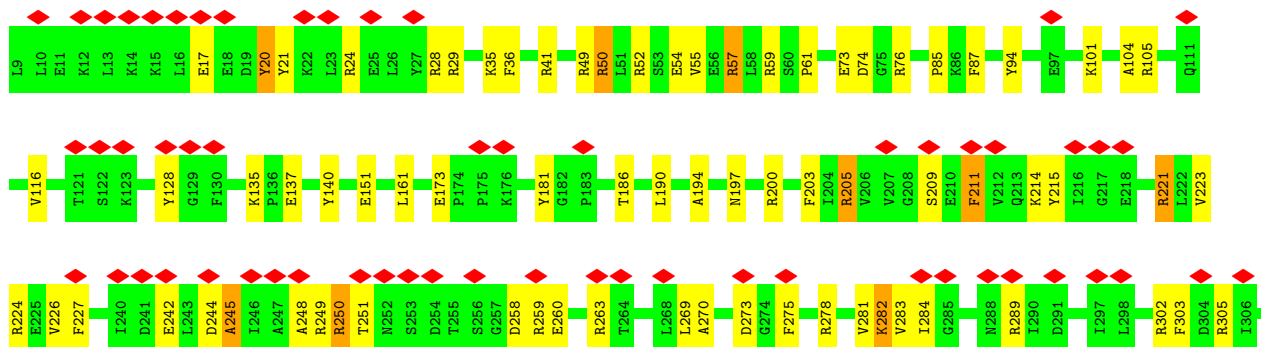
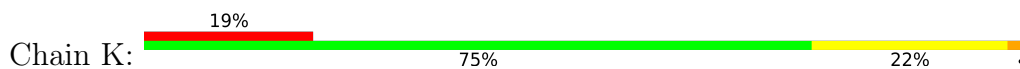




• Molecule 3: Proteasome-activating nucleotidase



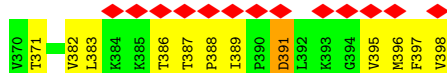
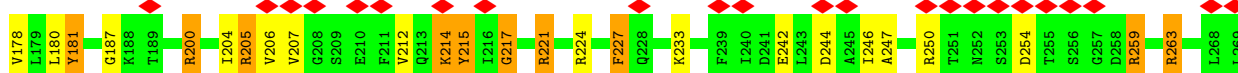
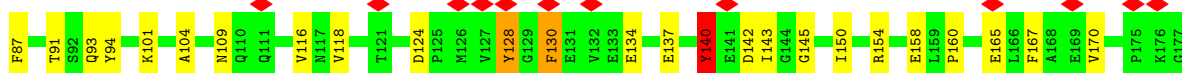
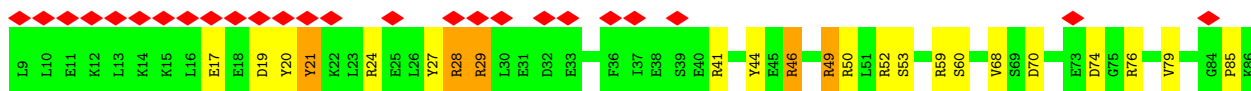
• Molecule 3: Proteasome-activating nucleotidase



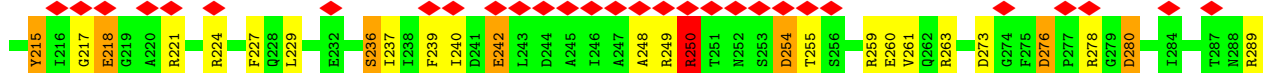
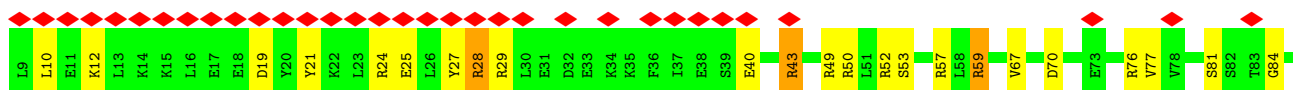
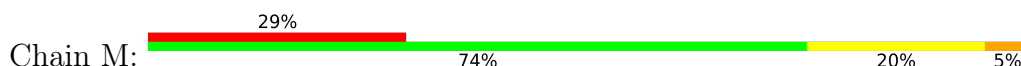




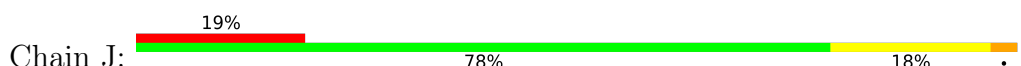
• Molecule 3: Proteasome-activating nucleotidase

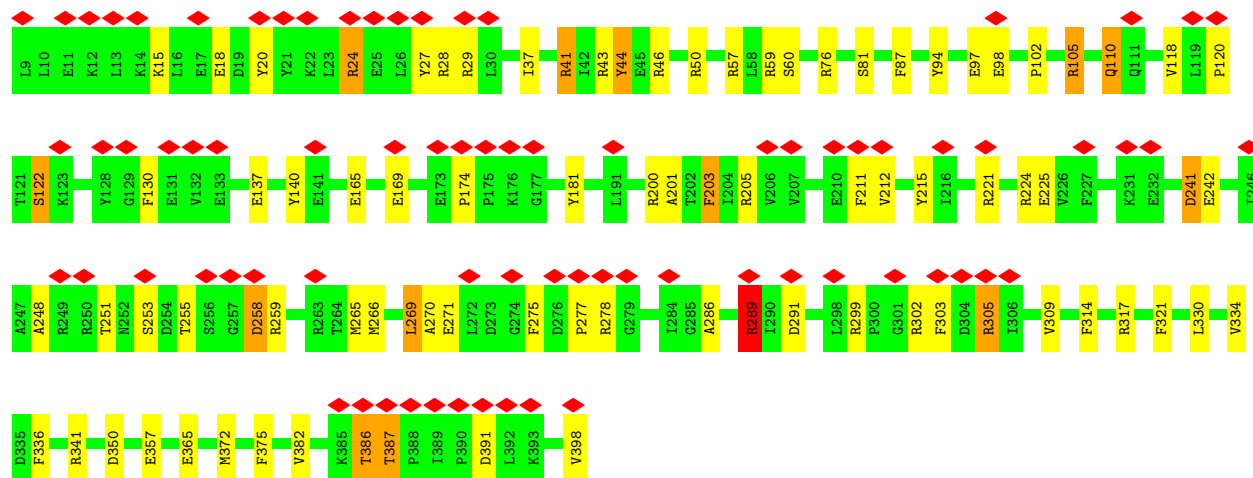


• Molecule 3: Proteasome-activating nucleotidase



• Molecule 3: Proteasome-activating nucleotidase





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	31471	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 ( $e^-/\text{\AA}^2$ )	30	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	0.054	Depositor
Minimum map value	-0.040	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0072	Depositor
Map size (Å)	514.56, 514.56, 514.56	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.34, 1.34, 1.34	Depositor

## 5 Model quality i

### 5.1 Standard geometry i

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	1.77	19/1934 (1.0%)	2.04	60/2605 (2.3%)
1	B	1.82	27/1934 (1.4%)	1.96	53/2605 (2.0%)
1	C	1.76	16/1934 (0.8%)	2.00	53/2605 (2.0%)
1	D	1.73	22/1934 (1.1%)	2.13	69/2605 (2.6%)
1	E	1.75	19/1934 (1.0%)	2.04	54/2605 (2.1%)
1	F	1.78	15/1934 (0.8%)	2.03	55/2605 (2.1%)
1	G	1.79	19/1934 (1.0%)	1.92	49/2605 (1.9%)
1	a	1.78	22/1892 (1.2%)	2.00	52/2549 (2.0%)
1	b	1.79	27/1892 (1.4%)	1.96	49/2549 (1.9%)
1	c	1.78	24/1892 (1.3%)	2.04	58/2549 (2.3%)
1	d	1.70	20/1892 (1.1%)	2.04	54/2549 (2.1%)
1	e	1.75	17/1892 (0.9%)	1.94	44/2549 (1.7%)
1	f	1.73	16/1892 (0.8%)	2.01	53/2549 (2.1%)
1	g	1.75	23/1892 (1.2%)	2.03	51/2549 (2.0%)
2	1	1.76	16/1573 (1.0%)	2.02	44/2121 (2.1%)
2	2	1.78	18/1573 (1.1%)	2.09	58/2121 (2.7%)
2	3	1.70	18/1573 (1.1%)	1.98	47/2121 (2.2%)
2	4	1.74	27/1573 (1.7%)	2.01	38/2121 (1.8%)
2	5	3.30	25/1573 (1.6%)	2.22	41/2121 (1.9%)
2	6	1.75	11/1573 (0.7%)	2.06	56/2121 (2.6%)
2	7	1.75	14/1573 (0.9%)	2.04	44/2121 (2.1%)
2	h	1.76	16/1573 (1.0%)	1.88	29/2121 (1.4%)
2	i	1.71	13/1573 (0.8%)	1.98	36/2121 (1.7%)
2	j	1.78	14/1573 (0.9%)	1.97	40/2121 (1.9%)
2	k	1.75	18/1573 (1.1%)	2.14	64/2121 (3.0%)
2	l	3.30	23/1573 (1.5%)	2.21	41/2121 (1.9%)
2	m	1.73	17/1573 (1.1%)	1.90	39/2121 (1.8%)
2	n	1.75	17/1573 (1.1%)	2.07	58/2121 (2.7%)
3	H	1.80	35/3146 (1.1%)	1.95	83/4240 (2.0%)
3	I	1.73	33/3146 (1.0%)	1.97	90/4240 (2.1%)
3	J	1.77	33/3146 (1.0%)	1.83	56/4240 (1.3%)
3	K	1.72	31/3146 (1.0%)	1.95	79/4240 (1.9%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
3	L	1.76	38/3146 (1.2%)	1.96	88/4240 (2.1%)
3	M	1.76	34/3146 (1.1%)	1.95	82/4240 (1.9%)
All	All	1.86	737/67680 (1.1%)	2.00	1867/91212 (2.0%)

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	A	0	7
1	B	0	9
1	C	0	4
1	D	0	11
1	E	0	5
1	F	0	8
1	G	0	9
1	a	0	9
1	b	0	6
1	c	0	8
1	d	0	10
1	e	0	7
1	f	0	7
1	g	0	8
2	1	0	4
2	2	0	8
2	3	0	6
2	4	0	7
2	5	0	9
2	6	0	3
2	7	0	8
2	h	0	7
2	i	0	6
2	j	0	4
2	k	0	10
2	l	0	8
2	m	0	6
2	n	0	6
3	H	0	22
3	I	0	19
3	J	0	14
3	K	0	11

*Continued on next page...*

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
3	L	0	21
3	M	0	19
All	All	0	306

The worst 5 of 737 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1	170	ARG	CZ-NH1	60.89	2.12	1.33
2	5	170	ARG	CZ-NH1	60.38	2.11	1.33
2	5	211	PHE	CG-CD2	49.71	2.13	1.38
2	1	211	PHE	CG-CD2	47.70	2.10	1.38
2	1	211	PHE	CG-CD1	45.23	2.06	1.38

The worst 5 of 1867 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	170	ARG	NE-CZ-NH2	-42.88	98.86	120.30
2	1	170	ARG	NE-CZ-NH2	-41.57	99.51	120.30
2	5	170	ARG	NE-CZ-NH1	18.88	129.74	120.30
2	1	170	ARG	NE-CZ-NH1	18.38	129.49	120.30
1	F	28	ARG	NE-CZ-NH2	-18.01	111.29	120.30

There are no chirality outliers.

5 of 306 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	123	TYR	Sidechain
1	A	130	ARG	Sidechain
1	A	159	TYR	Sidechain
1	A	160	LYS	Peptide
1	A	65	GLU	Peptide

## 5.2 Too-close contacts

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	A	240/242 (99%)	228 (95%)	10 (4%)	2 (1%)	19	60
1	B	240/242 (99%)	225 (94%)	10 (4%)	5 (2%)	7	36
1	C	240/242 (99%)	222 (92%)	12 (5%)	6 (2%)	5	32
1	D	240/242 (99%)	222 (92%)	11 (5%)	7 (3%)	4	29
1	E	240/242 (99%)	228 (95%)	11 (5%)	1 (0%)	34	72
1	F	240/242 (99%)	228 (95%)	9 (4%)	3 (1%)	12	48
1	G	240/242 (99%)	227 (95%)	9 (4%)	4 (2%)	9	42
1	a	235/242 (97%)	220 (94%)	10 (4%)	5 (2%)	7	36
1	b	235/242 (97%)	219 (93%)	14 (6%)	2 (1%)	17	57
1	c	235/242 (97%)	220 (94%)	12 (5%)	3 (1%)	12	48
1	d	235/242 (97%)	223 (95%)	7 (3%)	5 (2%)	7	36
1	e	235/242 (97%)	218 (93%)	15 (6%)	2 (1%)	17	57
1	f	235/242 (97%)	222 (94%)	10 (4%)	3 (1%)	12	48
1	g	235/242 (97%)	221 (94%)	8 (3%)	6 (3%)	5	31
2	1	200/202 (99%)	189 (94%)	8 (4%)	3 (2%)	10	46
2	2	200/202 (99%)	181 (90%)	13 (6%)	6 (3%)	4	28
2	3	200/202 (99%)	180 (90%)	18 (9%)	2 (1%)	15	54
2	4	200/202 (99%)	182 (91%)	16 (8%)	2 (1%)	15	54
2	5	200/202 (99%)	182 (91%)	13 (6%)	5 (2%)	5	32
2	6	200/202 (99%)	181 (90%)	13 (6%)	6 (3%)	4	28
2	7	200/202 (99%)	179 (90%)	15 (8%)	6 (3%)	4	28
2	h	200/202 (99%)	180 (90%)	14 (7%)	6 (3%)	4	28
2	i	200/202 (99%)	188 (94%)	10 (5%)	2 (1%)	15	54
2	j	200/202 (99%)	186 (93%)	13 (6%)	1 (0%)	29	69
2	k	200/202 (99%)	183 (92%)	13 (6%)	4 (2%)	7	38

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	l	200/202 (99%)	184 (92%)	13 (6%)	3 (2%)	10	46
2	m	200/202 (99%)	190 (95%)	8 (4%)	2 (1%)	15	54
2	n	200/202 (99%)	181 (90%)	9 (4%)	10 (5%)	2	20
3	H	388/390 (100%)	342 (88%)	27 (7%)	19 (5%)	2	20
3	I	388/390 (100%)	346 (89%)	27 (7%)	15 (4%)	3	23
3	J	388/390 (100%)	353 (91%)	28 (7%)	7 (2%)	8	40
3	K	388/390 (100%)	355 (92%)	22 (6%)	11 (3%)	5	30
3	L	388/390 (100%)	349 (90%)	26 (7%)	13 (3%)	3	26
3	M	388/390 (100%)	351 (90%)	24 (6%)	13 (3%)	3	26
All	All	8453/8556 (99%)	7785 (92%)	478 (6%)	190 (2%)	10	35

5 of 190 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	67	ILE
1	a	35	ALA
1	B	64	ILE
1	C	67	ILE
1	D	65	GLU

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	203/203 (100%)	195 (96%)	8 (4%)	32	56
1	B	203/203 (100%)	198 (98%)	5 (2%)	47	68
1	C	203/203 (100%)	192 (95%)	11 (5%)	22	47
1	D	203/203 (100%)	194 (96%)	9 (4%)	28	53
1	E	203/203 (100%)	192 (95%)	11 (5%)	22	47
1	F	203/203 (100%)	199 (98%)	4 (2%)	55	74
1	G	203/203 (100%)	194 (96%)	9 (4%)	28	53

Continued on next page...



Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	a	199/203 (98%)	193 (97%)	6 (3%)	41	63
1	b	199/203 (98%)	192 (96%)	7 (4%)	36	59
1	c	199/203 (98%)	195 (98%)	4 (2%)	55	74
1	d	199/203 (98%)	193 (97%)	6 (3%)	41	63
1	e	199/203 (98%)	188 (94%)	11 (6%)	21	47
1	f	199/203 (98%)	190 (96%)	9 (4%)	27	52
1	g	199/203 (98%)	191 (96%)	8 (4%)	31	55
2	1	164/164 (100%)	157 (96%)	7 (4%)	29	53
2	2	164/164 (100%)	153 (93%)	11 (7%)	16	41
2	3	164/164 (100%)	163 (99%)	1 (1%)	86	92
2	4	164/164 (100%)	161 (98%)	3 (2%)	59	77
2	5	164/164 (100%)	159 (97%)	5 (3%)	41	63
2	6	164/164 (100%)	155 (94%)	9 (6%)	21	47
2	7	164/164 (100%)	160 (98%)	4 (2%)	49	69
2	h	164/164 (100%)	158 (96%)	6 (4%)	34	58
2	i	164/164 (100%)	155 (94%)	9 (6%)	21	47
2	j	164/164 (100%)	160 (98%)	4 (2%)	49	69
2	k	164/164 (100%)	160 (98%)	4 (2%)	49	69
2	l	164/164 (100%)	157 (96%)	7 (4%)	29	53
2	m	164/164 (100%)	159 (97%)	5 (3%)	41	63
2	n	164/164 (100%)	154 (94%)	10 (6%)	18	44
3	H	338/338 (100%)	330 (98%)	8 (2%)	49	69
3	I	338/338 (100%)	324 (96%)	14 (4%)	30	55
3	J	338/338 (100%)	322 (95%)	16 (5%)	26	51
3	K	338/338 (100%)	329 (97%)	9 (3%)	44	65
3	L	338/338 (100%)	326 (96%)	12 (4%)	35	59
3	M	338/338 (100%)	325 (96%)	13 (4%)	33	57
All	All	7138/7166 (100%)	6873 (96%)	265 (4%)	37	58

5 of 265 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	L	206	VAL

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type
3	M	102	PRO
3	J	255	THR
1	G	181	ASP
1	G	57	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
2	7	99	ASN
3	K	111	GLN
3	M	93	GLN
1	d	122	GLN
1	d	97	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	ADP	K	401	4	24,29,29	1.65	2 (8%)	29,45,45	2.33	8 (27%)
5	ATP	J	401	4	26,33,33	1.32	3 (11%)	31,52,52	2.73	5 (16%)
5	ATP	M	401	4	26,33,33	1.35	3 (11%)	31,52,52	2.09	7 (22%)
5	ATP	I	401	4	26,33,33	1.31	4 (15%)	31,52,52	3.18	9 (29%)
5	ATP	I	402	4	26,33,33	1.09	2 (7%)	31,52,52	2.46	10 (32%)

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
6	ADP	K	401	4	-	1/12/32/32	0/3/3/3
5	ATP	J	401	4	-	4/18/38/38	0/3/3/3
5	ATP	M	401	4	-	4/18/38/38	0/3/3/3
5	ATP	I	401	4	-	7/18/38/38	0/3/3/3
5	ATP	I	402	4	-	1/18/38/38	0/3/3/3

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	K	401	ADP	O4'-C1'	6.26	1.49	1.41
5	J	401	ATP	C8-N7	-4.10	1.27	1.34
5	I	401	ATP	C8-N7	-3.58	1.28	1.34
5	M	401	ATP	C4-N3	-3.54	1.30	1.35
5	J	401	ATP	C2'-C1'	-3.30	1.48	1.53

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	401	ATP	PB-O3B-PG	11.12	170.97	132.83
5	J	401	ATP	PB-O3B-PG	10.79	169.84	132.83
5	I	401	ATP	PA-O3A-PB	10.22	167.89	132.83
5	I	402	ATP	PB-O3B-PG	8.78	162.94	132.83
5	J	401	ATP	PA-O3A-PB	8.18	160.90	132.83

There are no chirality outliers.

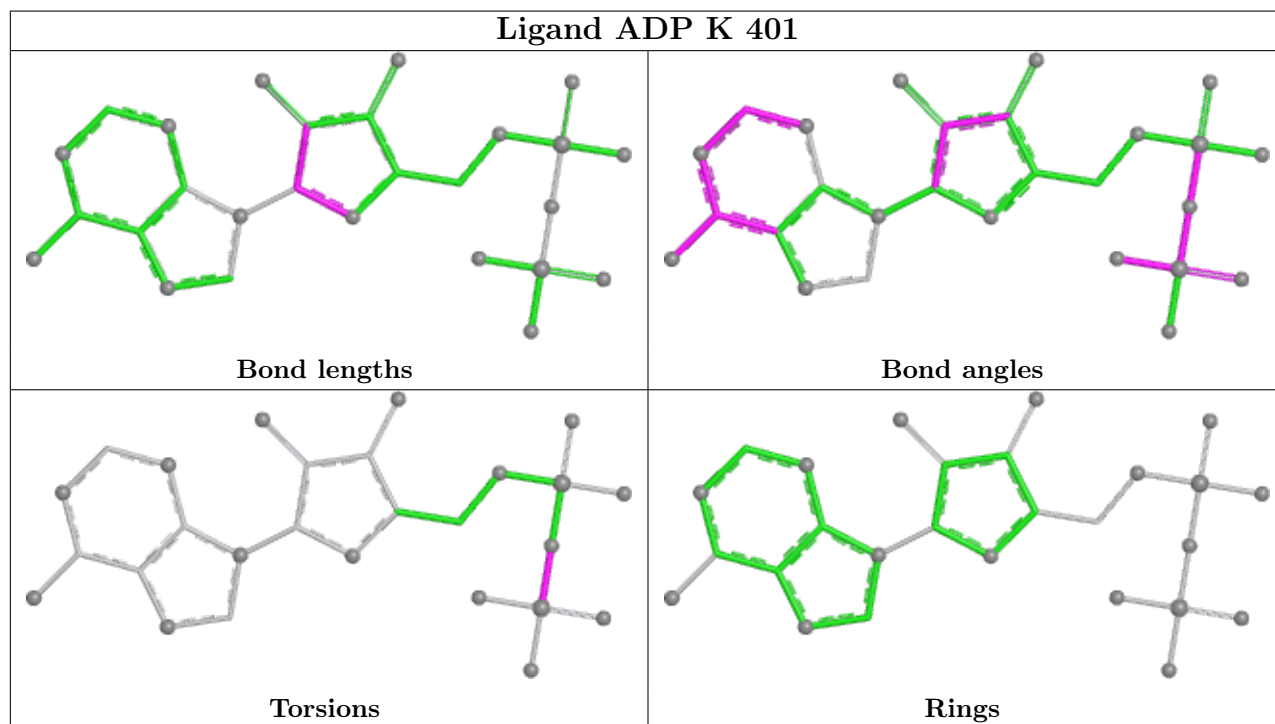
5 of 17 torsion outliers are listed below:

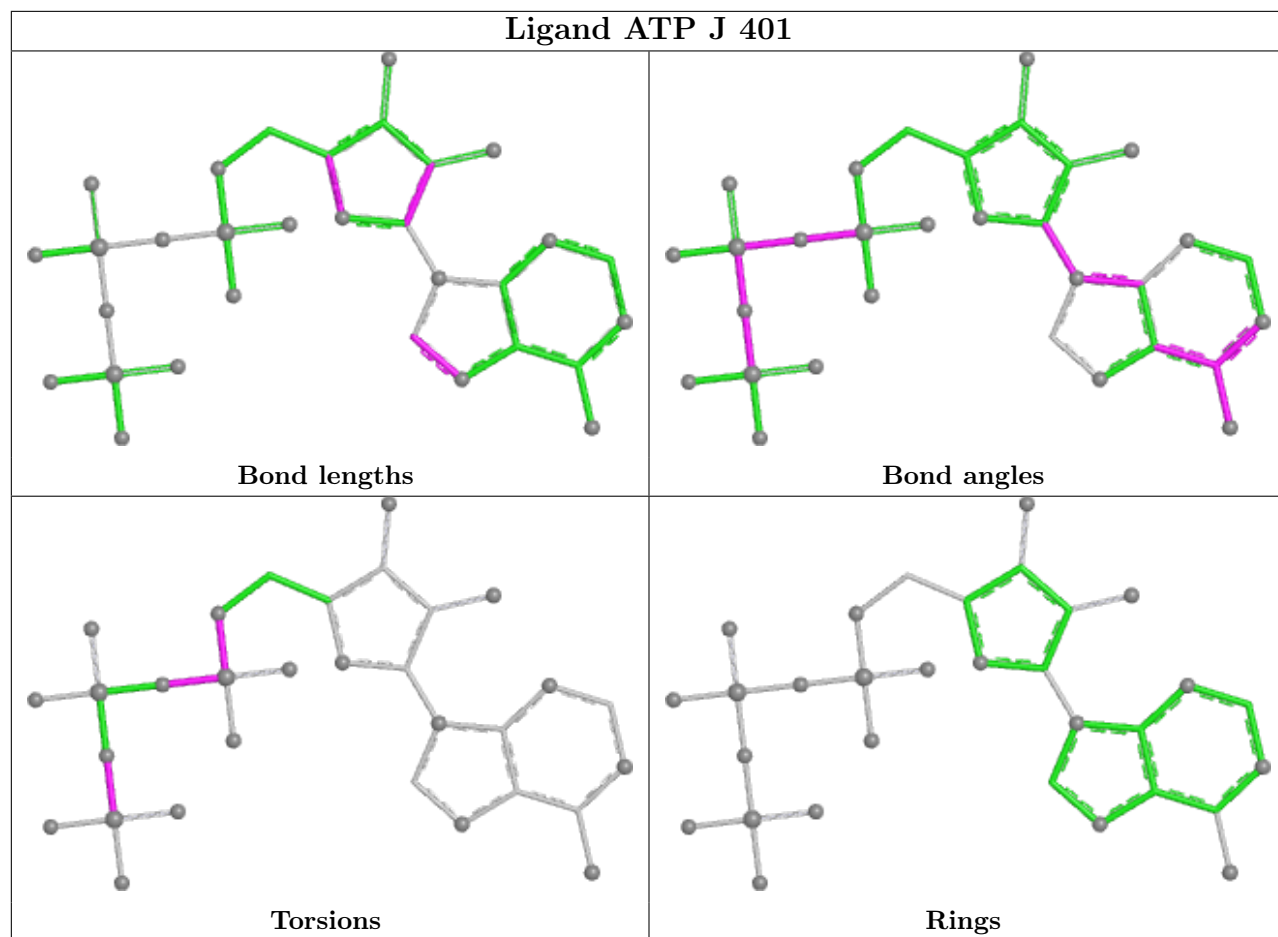
Mol	Chain	Res	Type	Atoms
5	I	401	ATP	PB-O3B-PG-O2G
5	I	401	ATP	C5'-O5'-PA-O1A
6	K	401	ADP	PA-O3A-PB-O2B
5	I	402	ATP	C4'-C5'-O5'-PA
5	M	401	ATP	C3'-C4'-C5'-O5'

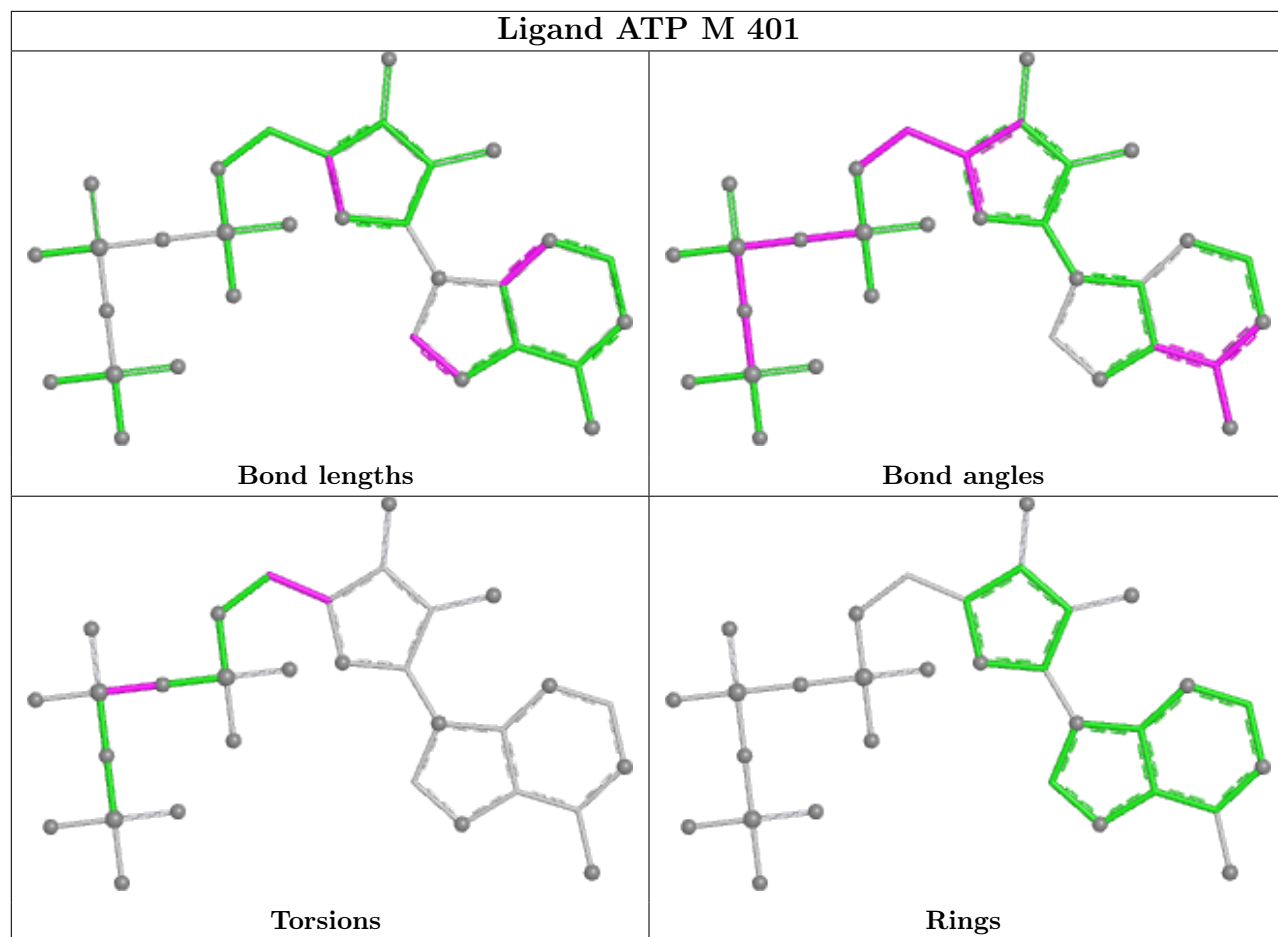
There are no ring outliers.

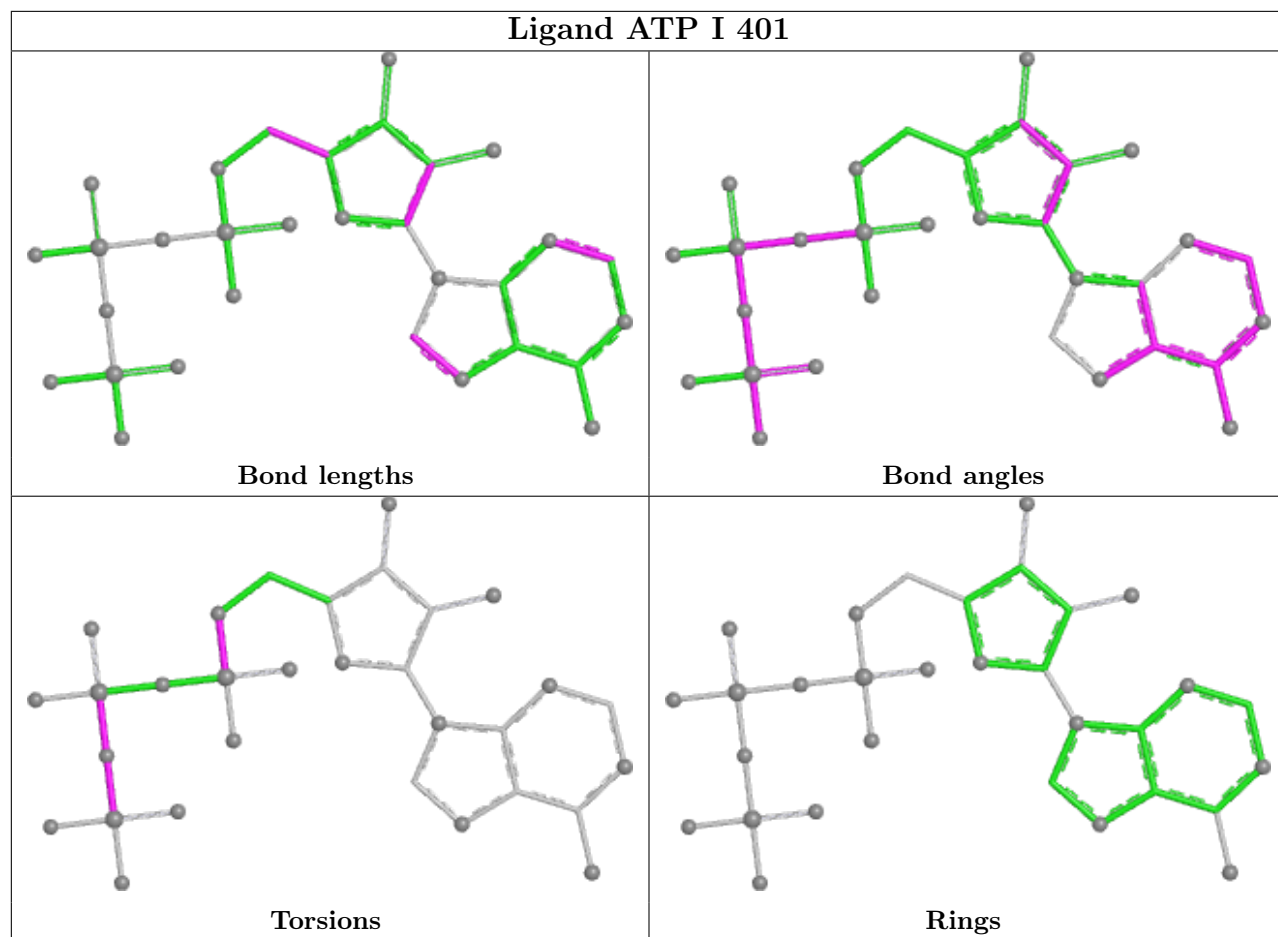
No monomer is involved in short contacts.

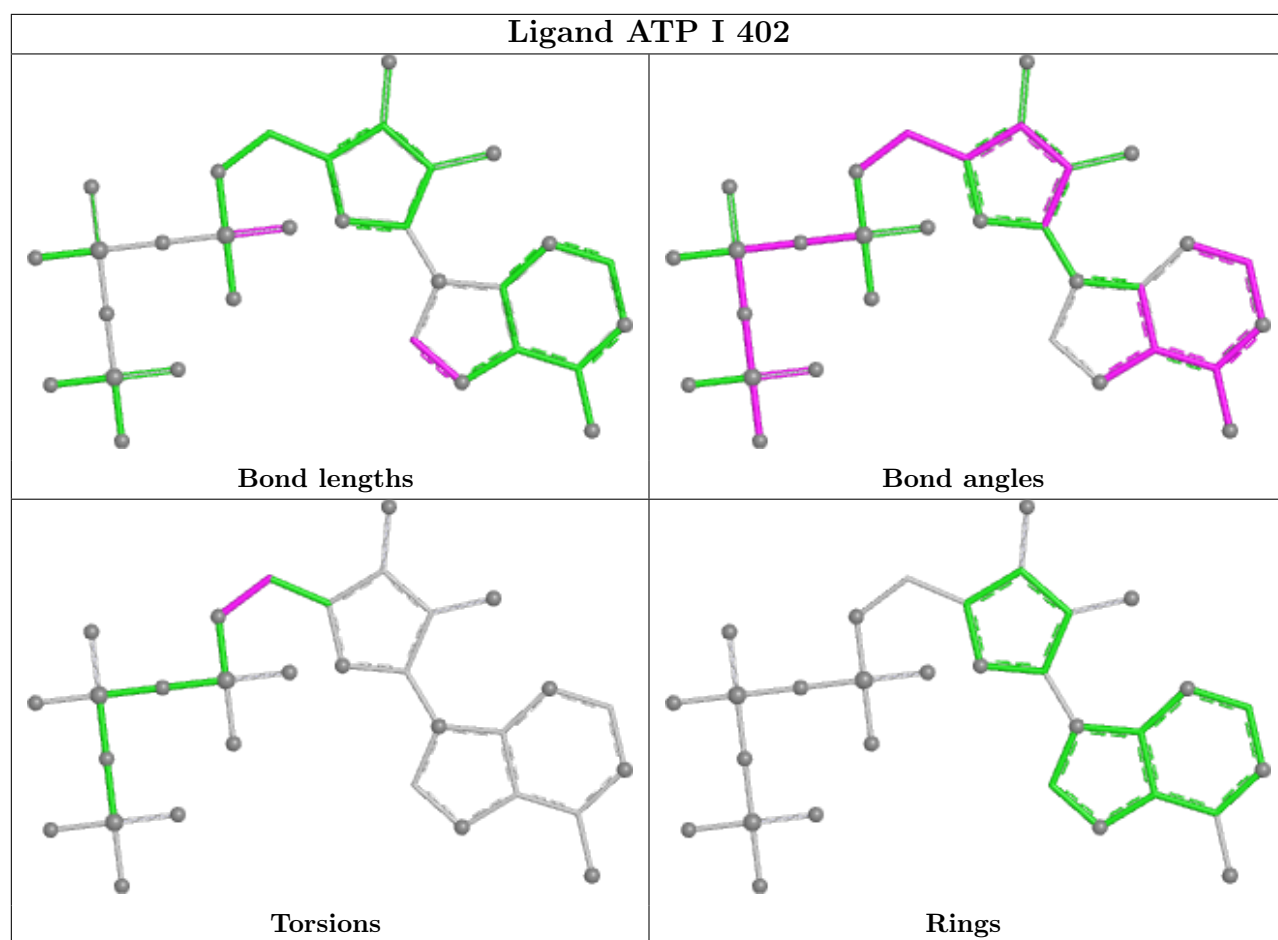
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



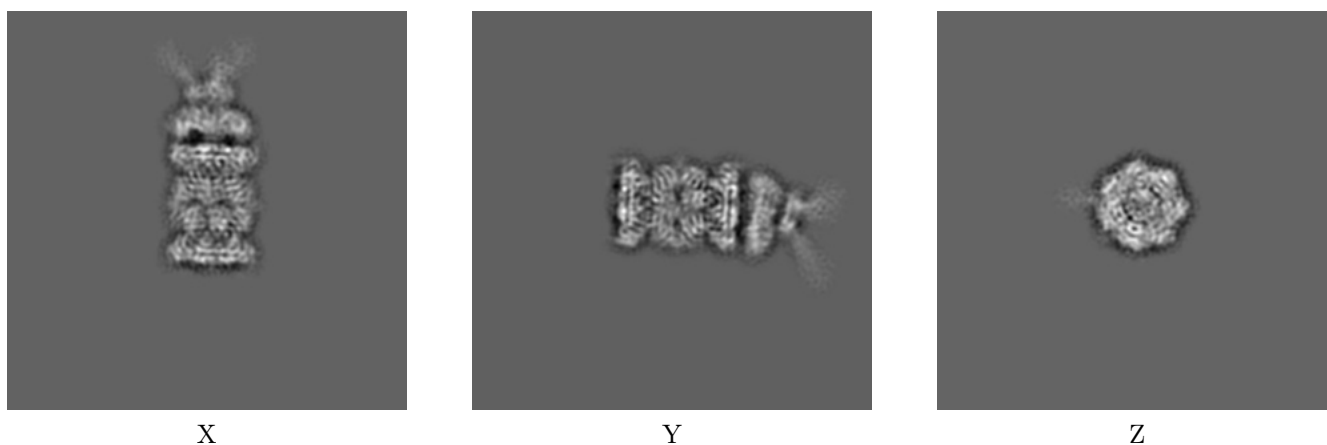
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0214. 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](#)

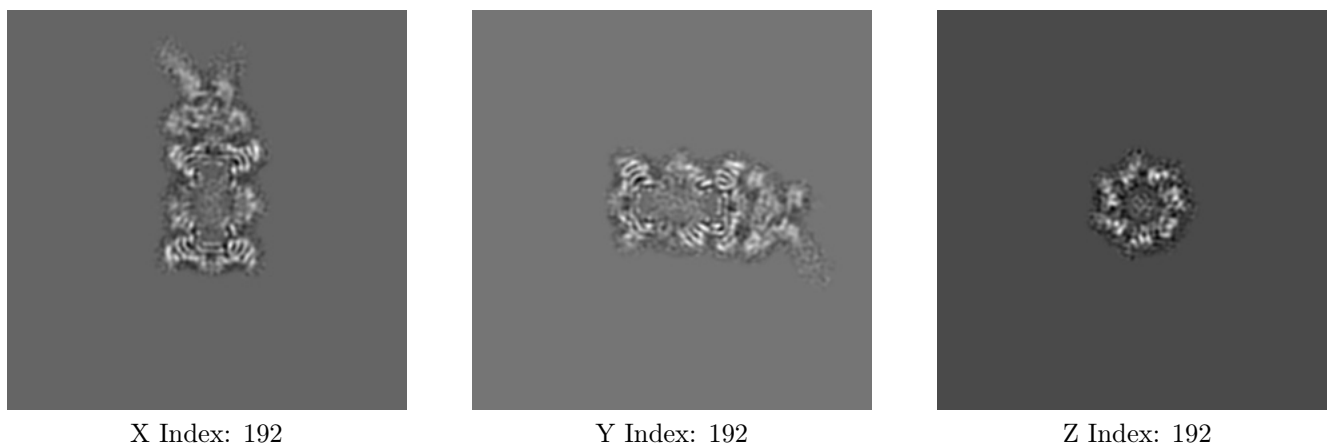
#### 6.1.1 Primary map



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

### 6.2 Central slices [i](#)

#### 6.2.1 Primary map



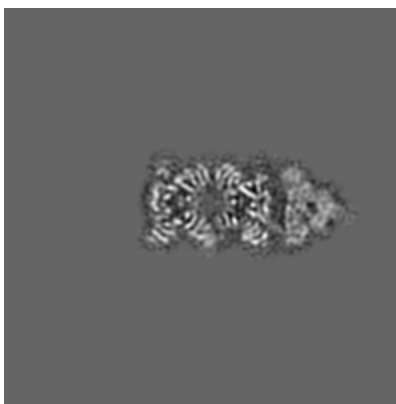
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

### 6.3.1 Primary map



X Index: 179



Y Index: 181



Z Index: 250

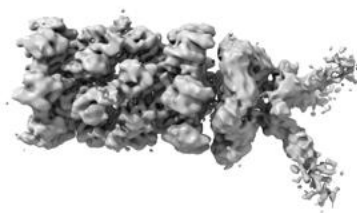
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0072. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

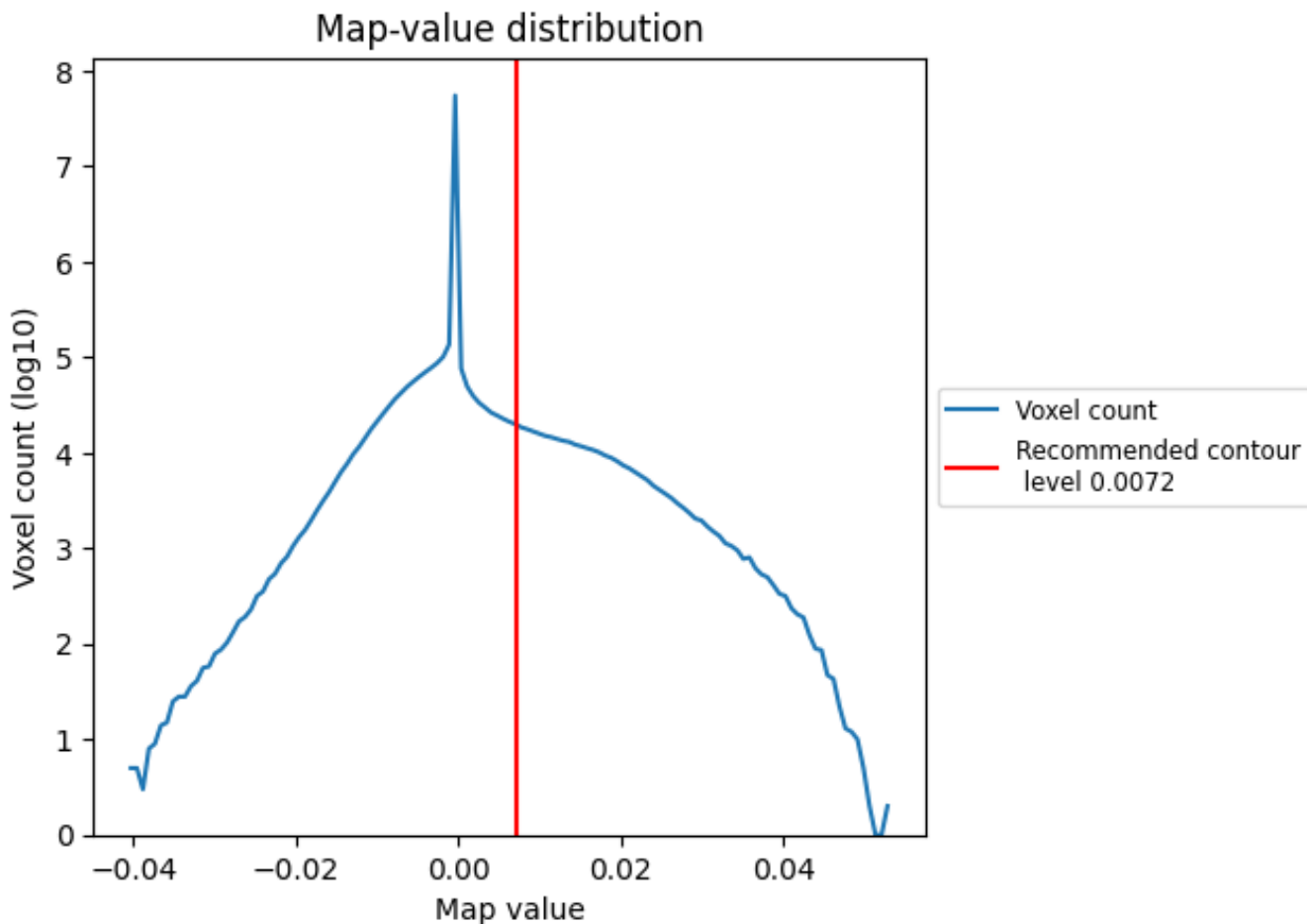
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

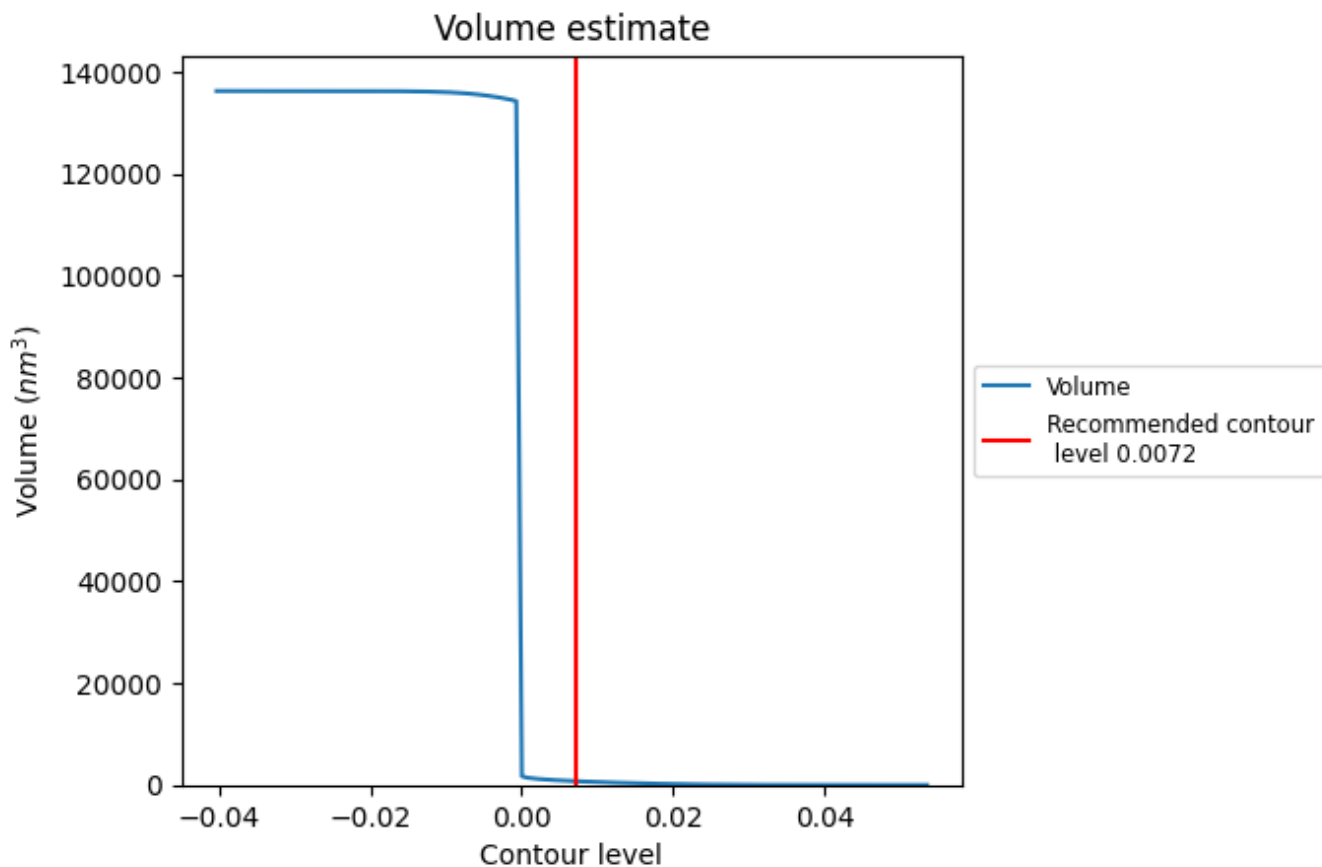
This section contains the results of statistical analysis of the map.

### 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.

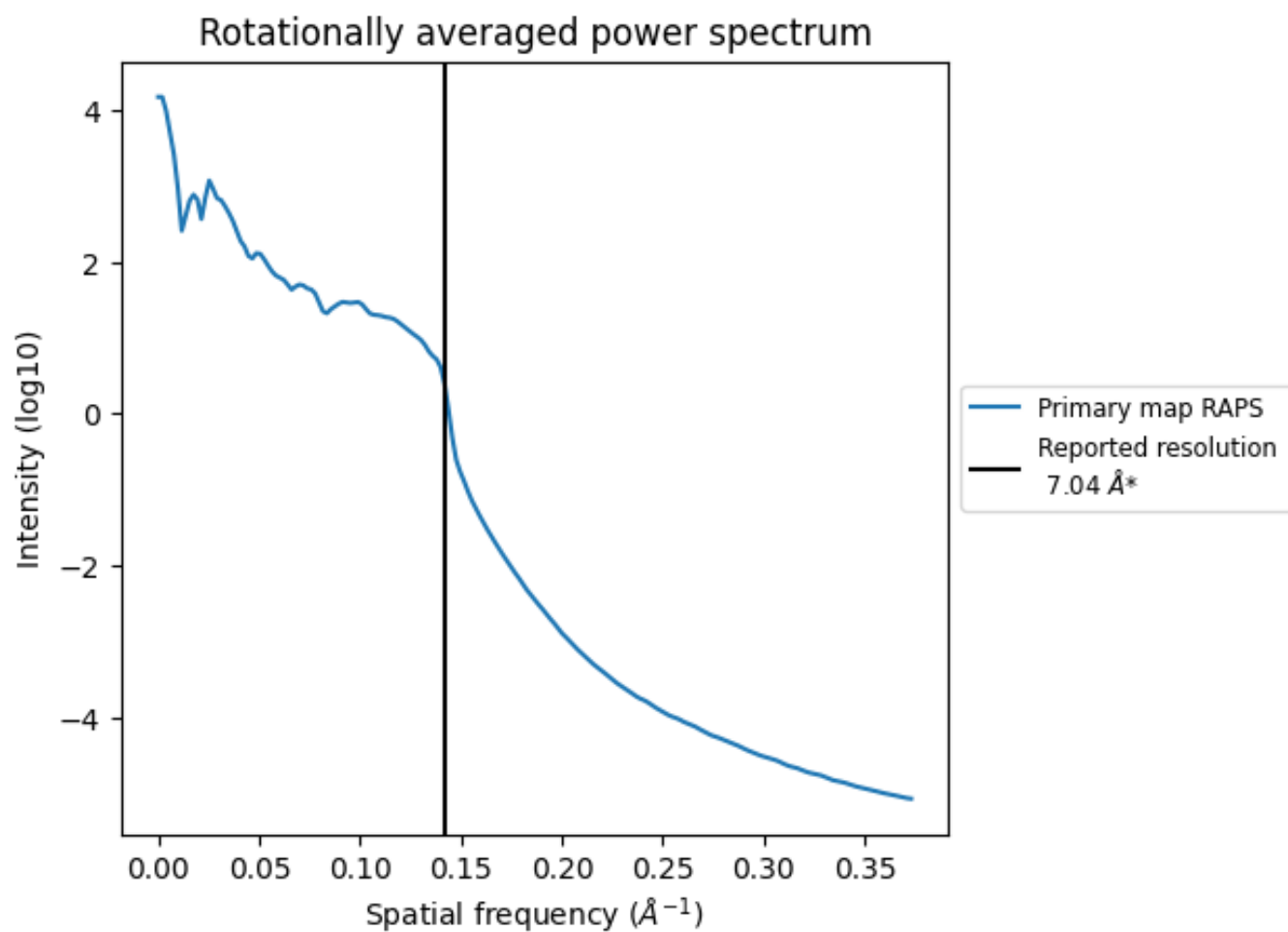
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 742 nm<sup>3</sup>; this corresponds to an approximate mass of 670 kDa.

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

### 7.3 Rotationally averaged power spectrum [i](#)



\*Reported resolution corresponds to spatial frequency of  $0.142 \text{\AA}^{-1}$

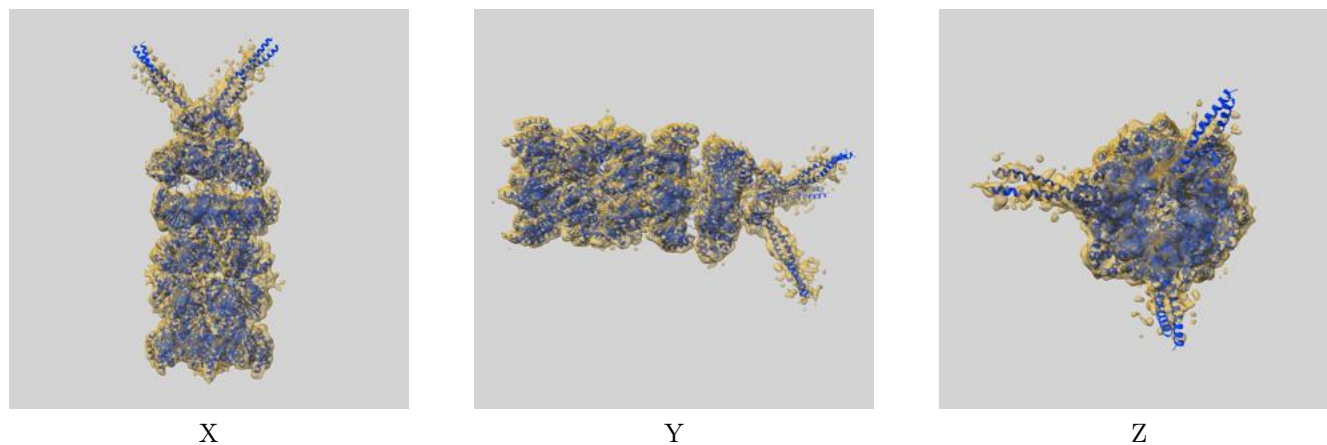
## 8 Fourier-Shell correlation

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-0214 and PDB model 6HEA. Per-residue inclusion information can be found in section 3 on page 8.

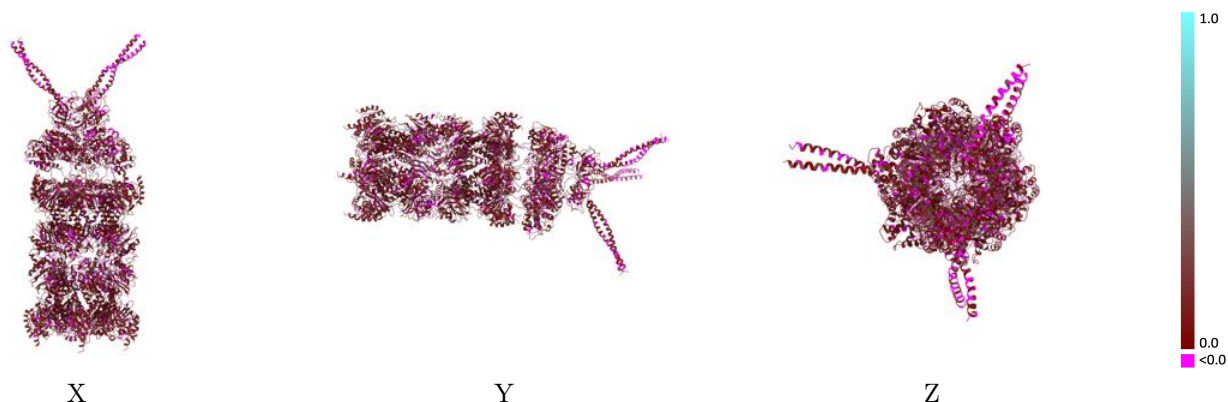
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.0072 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.

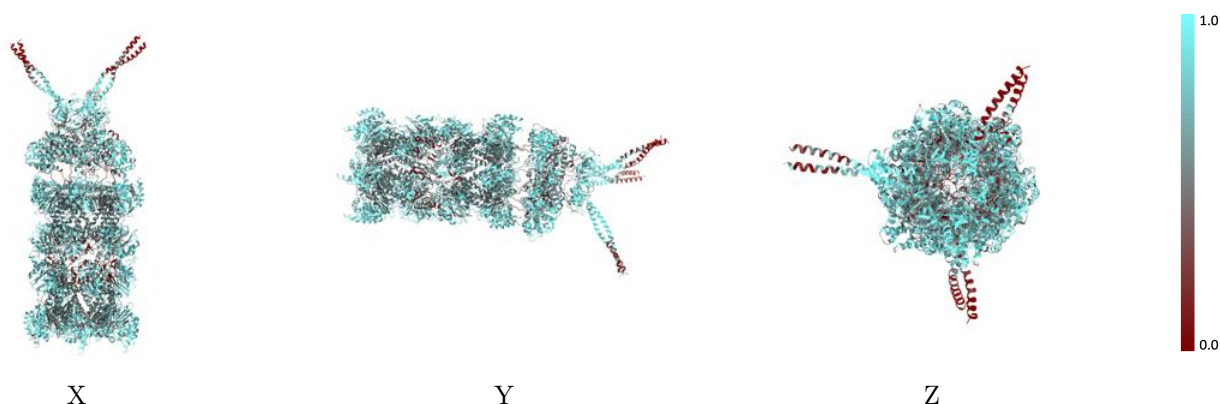


## 9.2 Q-score mapped to coordinate model [i](#)



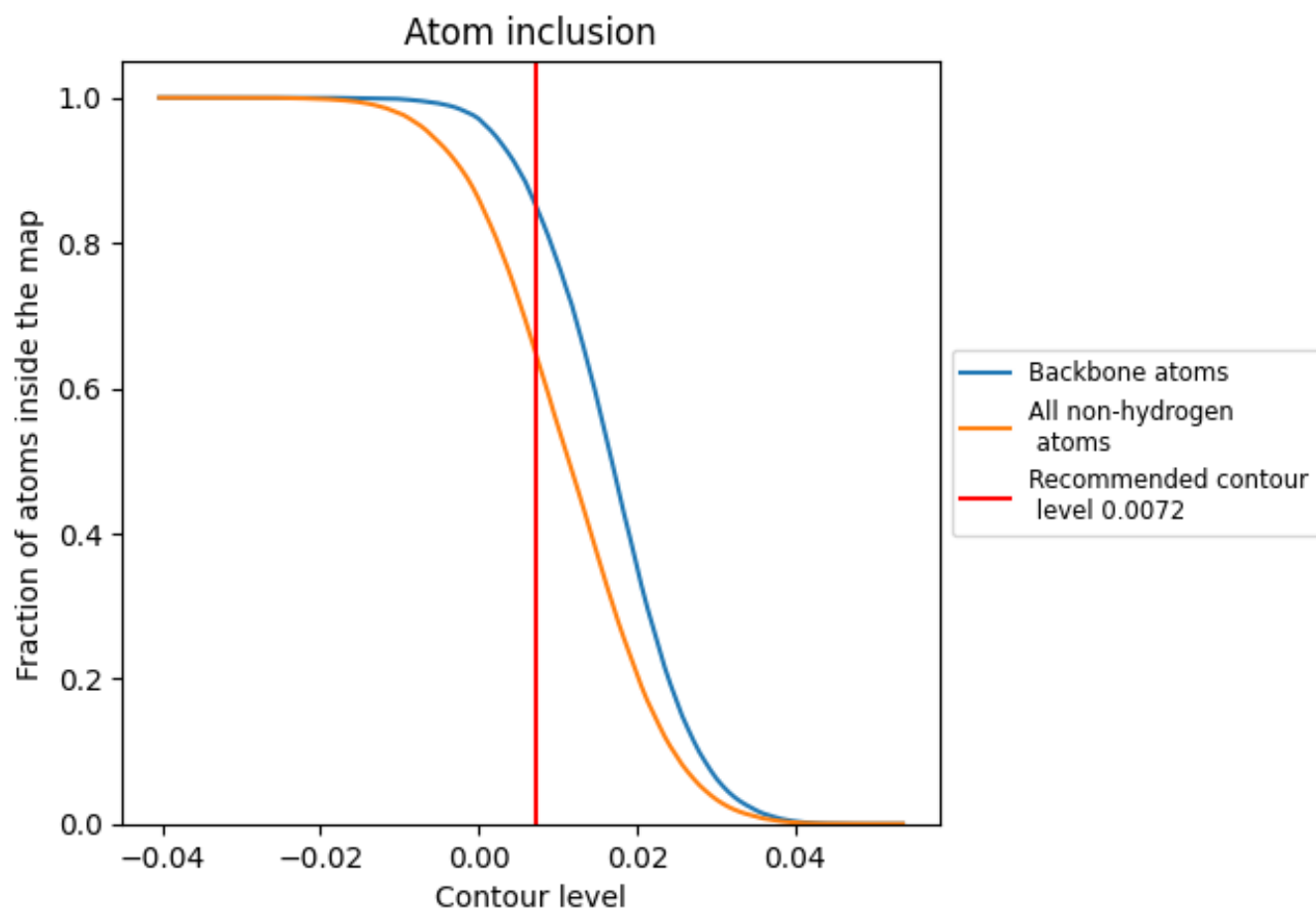
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0072).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 65% 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 (0.0072) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6487	 0.1140
1	 0.6149	 0.1140
2	 0.6215	 0.1250
3	 0.6136	 0.1170
4	 0.6208	 0.1240
5	 0.6182	 0.1200
6	 0.6228	 0.1150
7	 0.6406	 0.1110
A	 0.6770	 0.1260
B	 0.6765	 0.1320
C	 0.6803	 0.1260
D	 0.6776	 0.1340
E	 0.6840	 0.1250
F	 0.6845	 0.1240
G	 0.6845	 0.1240
H	 0.6314	 0.1010
I	 0.6498	 0.1000
J	 0.6705	 0.1110
K	 0.6697	 0.1060
L	 0.6224	 0.0890
M	 0.6077	 0.0880
a	 0.6941	 0.1220
b	 0.6875	 0.1260
c	 0.6711	 0.1180
d	 0.6678	 0.1180
e	 0.6820	 0.1220
f	 0.6727	 0.1140
g	 0.6743	 0.1220
h	 0.6149	 0.1160
i	 0.6201	 0.1120
j	 0.6149	 0.1180
k	 0.6142	 0.1170
l	 0.6116	 0.1130
m	 0.6063	 0.1020
n	 0.6050	 0.1090

