



Full wwPDB EM Validation Report ⓘ

Nov 5, 2022 – 09:02 AM EDT

PDB ID : 5VFQ
EMDB ID : EMD-8664
Title : Nucleotide-driven Triple-state Remodeling of the AAA-ATPase Channel in the Activated Human 26S Proteasome
Authors : Zhu, Y.; Wang, W.L.; Yu, D.; Ouyang, Q.; Lu, Y.; Mao, Y.
Deposited on : 2017-04-09
Resolution : 4.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

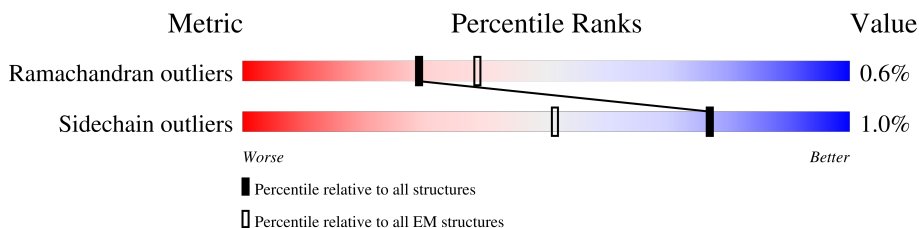
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (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 4.20 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 ≥ 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	G	240	16% (red), 99% (green)
1	g	240	12% (red), 100% (green)
2	H	232	9% (red), 99% (green), 1% (grey), 1% (yellow)
2	h	232	11% (red), 100% (green)
3	I	250	20% (red), 98% (green), 1% (grey), 1% (yellow)
3	i	250	18% (red), 99% (green), 1% (grey), 1% (yellow)
4	J	243	15% (red), 96% (green), 1% (grey), 1% (yellow)
4	j	243	19% (red), 95% (green), 1% (grey), 1% (yellow)
5	K	234	9% (red), 94% (green), 1% (grey), 1% (yellow)

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Mol	Chain	Length	Quality of chain
5	k	234	15% 97%
6	L	238	7% 100%
6	l	238	6% 100%
7	M	245	9% 98%
7	m	245	13% 98%
8	N	191	• 99%
8	n	191	• 98%
9	O	220	5% 100%
9	o	220	5% 100%
10	P	204	• 100%
10	p	204	5% 100%
11	Q	199	• 97%
11	q	199	5% 97%
12	R	201	• 100%
12	r	201	• 100%
13	S	213	• 100%
13	s	213	• 100%
14	T	215	• 100%
14	t	215	• 100%
15	U	911	27% 87% 12%
16	V	480	43% 88% 5% 7%
17	W	456	55% 98%
18	X	380	62% 98%
19	Y	378	24% 97%
20	Z	286	33% 96%

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Mol	Chain	Length	Quality of chain
21	a	373	
22	b	191	
23	c	287	
24	d	257	
25	e	70	
26	A	399	
27	B	389	
28	C	392	
29	D	380	
30	E	375	
31	F	396	
32	f	908	

2 Entry composition [i](#)

There are 34 unique types of molecules in this entry. The entry contains 101134 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 type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	G	239	Total	C	N	O	S	0	0
			1820	1157	304	346	13		
1	g	240	Total	C	N	O	S	0	0
			1826	1160	305	348	13		

- Molecule 2 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	H	230	Total	C	N	O	S	0	0
			1688	1070	284	329	5		
2	h	232	Total	C	N	O	S	0	0
			1708	1081	289	333	5		

- Molecule 3 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	I	248	Total	C	N	O	S	0	0
			1895	1195	324	368	8		
3	i	250	Total	C	N	O	S	0	0
			1912	1204	329	371	8		

- Molecule 4 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	J	239	Total	C	N	O	S	0	0
			1704	1056	308	335	5		
4	j	239	Total	C	N	O	S	0	0
			1704	1056	308	335	5		

- Molecule 5 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	K	228	1729	1086	284	349	10	0	0
5	k	228	1722	1080	284	348	10	0	0

- Molecule 6 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	L	238	1850	1159	334	346	11	0	0
6	l	238	1850	1159	334	346	11	0	0

- Molecule 7 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	M	240	1856	1178	314	353	11	0	0
7	m	240	1856	1178	314	353	11	0	0

- Molecule 8 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	N	191	1430	893	245	280	12	0	0
8	n	191	1430	893	245	280	12	0	0

- Molecule 9 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	O	220	1643	1033	280	318	12	0	0
9	o	220	1643	1033	280	318	12	0	0

- Molecule 10 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	P	204	1585	1010	262	294	19	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	p	204	Total	C	N	O	S	0	0
			1585	1010	262	294	19		

- Molecule 11 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	Q	199	Total	C	N	O	S	0	0
			1570	1006	265	290	9		
11	q	199	Total	C	N	O	S	0	0
			1570	1006	265	290	9		

- Molecule 12 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	R	201	Total	C	N	O	S	0	0
			1548	974	273	292	9		
12	r	201	Total	C	N	O	S	0	0
			1548	974	273	292	9		

- Molecule 13 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	S	213	Total	C	N	O	S	0	0
			1641	1036	282	313	10		
13	s	213	Total	C	N	O	S	0	0
			1641	1036	282	313	10		

- Molecule 14 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	T	215	Total	C	N	O	S	0	0
			1667	1052	285	318	12		
14	t	215	Total	C	N	O	S	0	0
			1667	1052	285	318	12		

- Molecule 15 is a protein called 26S proteasome non-ATPase regulatory subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	U	806	Total	C	N	O	S	0	0
			6287	3990	1075	1178	44		

- Molecule 16 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	V	447	3600	2287	639	660	14	0	0

- Molecule 17 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	W	456	3703	2339	635	704	25	0	0

- Molecule 18 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	X	380	3009	1918	509	570	12	0	0

- Molecule 19 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	Y	378	3115	1987	533	578	17	0	0

- Molecule 20 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	Z	286	2281	1457	392	427	5	0	0

- Molecule 21 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	a	373	2995	1911	510	559	15	0	0

- Molecule 22 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	b	191	1458	910	261	279	8	0	0

- Molecule 23 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	c	278	2187	1389	374	406	18	0	0

- Molecule 24 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	d	257	2116	1371	346	390	9	0	0

- Molecule 25 is a protein called Sem1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	e	40	334	200	55	77	2	0	0

- Molecule 26 is a protein called 26S proteasome regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	A	380	2893	1817	515	543	18	0	0

- Molecule 27 is a protein called 26S proteasome regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	B	370	2806	1763	478	553	12	0	0

- Molecule 28 is a protein called 26S proteasome regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	C	363	2859	1804	513	525	17	0	0

- Molecule 29 is a protein called 26S proteasome regulatory subunit 6B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	D	380	3040	1923	524	580	13	0	0

- Molecule 30 is a protein called 26S proteasome regulatory subunit 10B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	E	375	2860	1796	512	536	16	0	0

- Molecule 31 is a protein called 26S proteasome regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	F	376	2859	1802	496	546	15	0	0

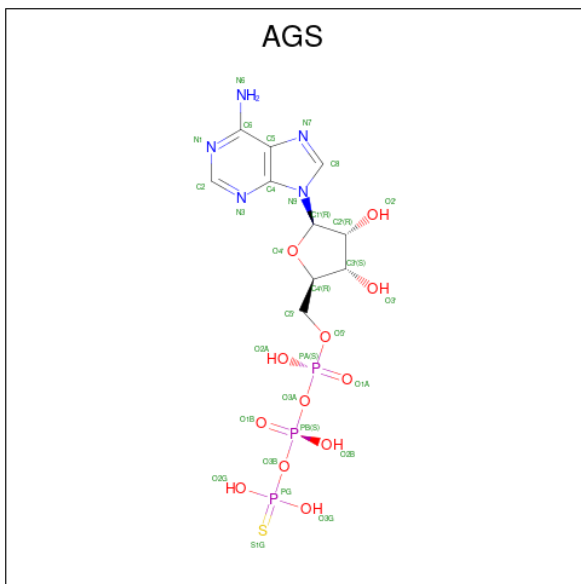
- Molecule 32 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	f	689	5319	3343	904	1037	35	0	0

- Molecule 33 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
33	c	1	1	1	0

- Molecule 34 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S).



Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
34	A	1	31	10	5	12	3	1	0

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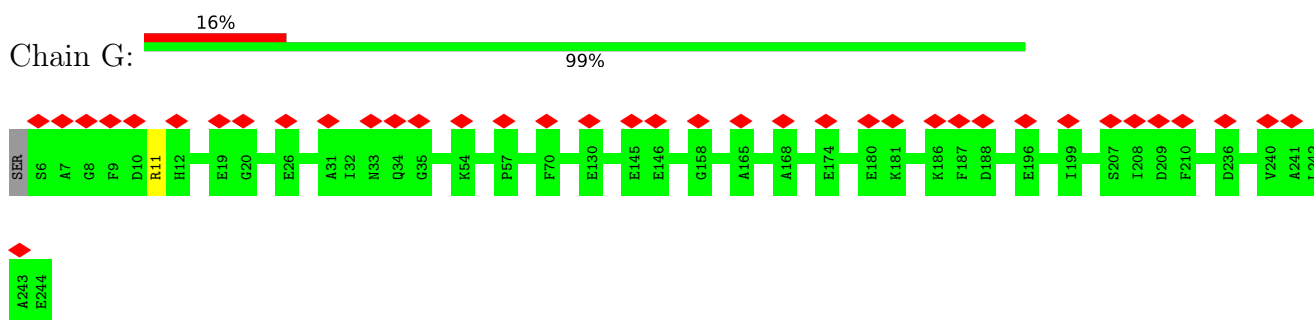
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Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
34	C	1	Total 31	10	5	12	3	1	0
34	D	1	Total 31	10	5	12	3	1	0
34	F	1	Total 31	10	5	12	3	1	0

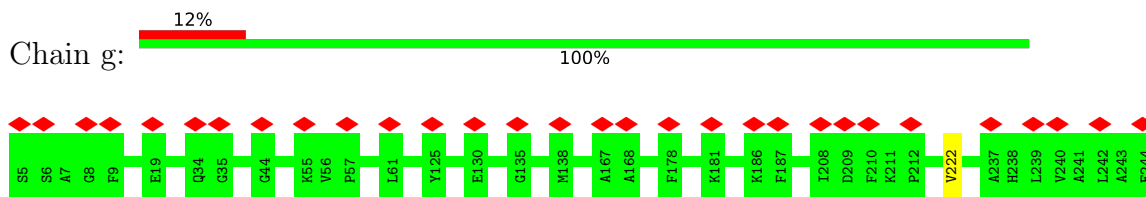
3 Residue-property plots [i](#)

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

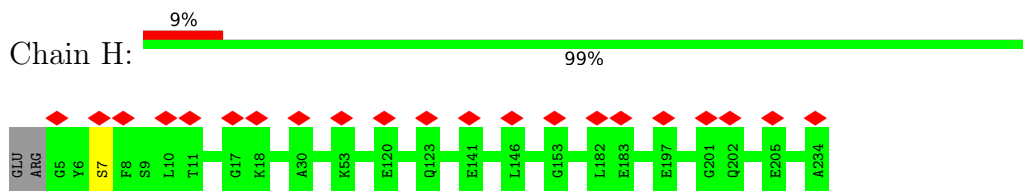
- Molecule 1: Proteasome subunit alpha type-6



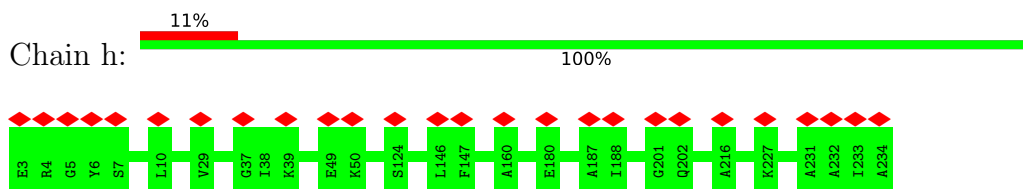
- Molecule 1: Proteasome subunit alpha type-6



- Molecule 2: Proteasome subunit alpha type-2

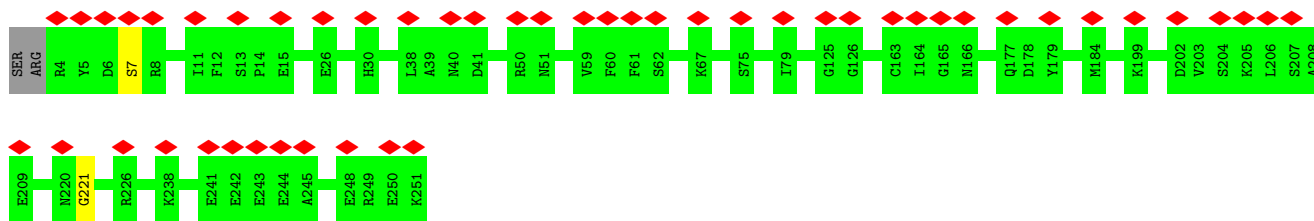


- Molecule 2: Proteasome subunit alpha type-2

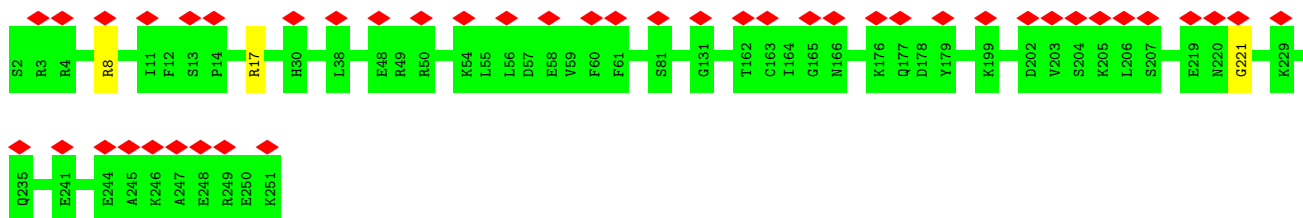


- Molecule 3: Proteasome subunit alpha type-4

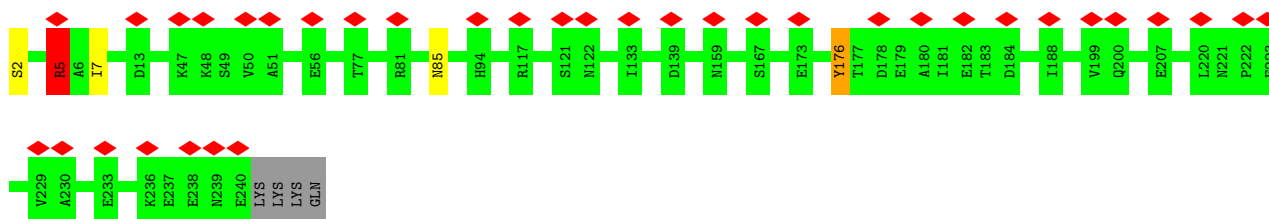




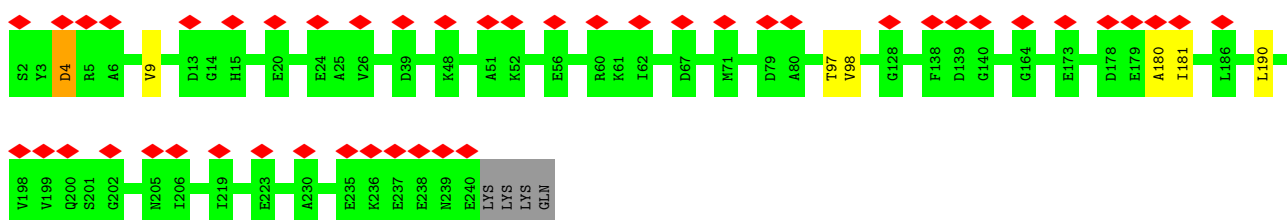
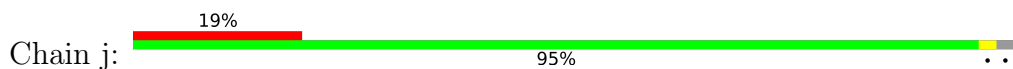
- Molecule 3: Proteasome subunit alpha type-4



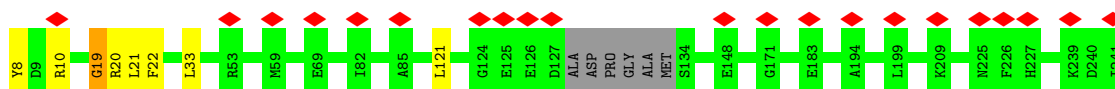
- Molecule 4: Proteasome subunit alpha type-7



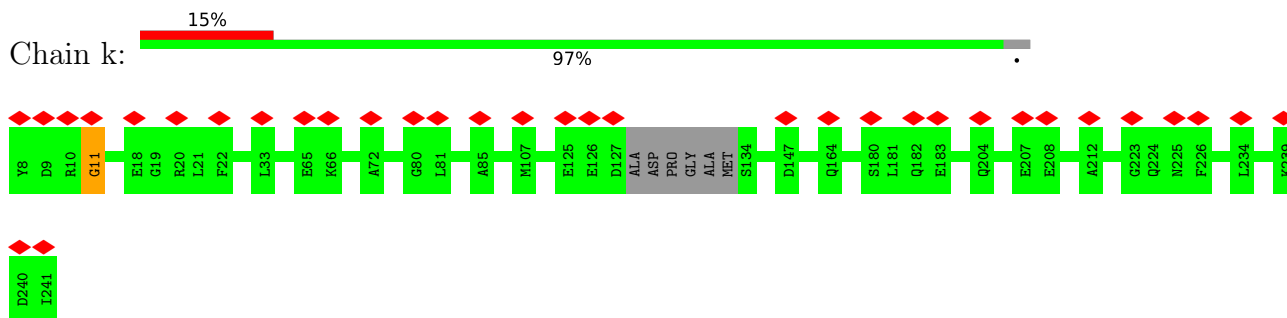
- Molecule 4: Proteasome subunit alpha type-7



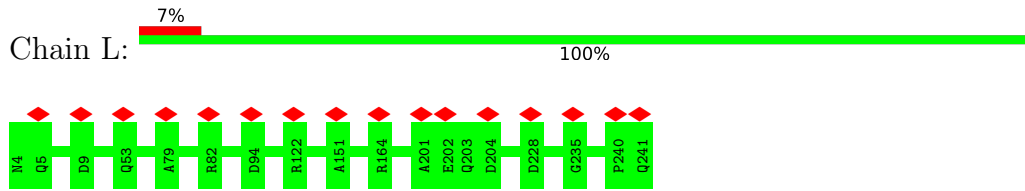
- Molecule 5: Proteasome subunit alpha type-5



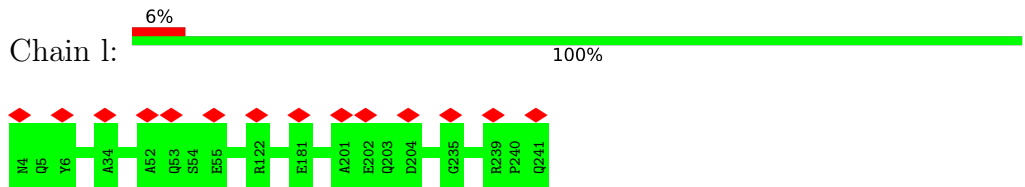
- Molecule 5: Proteasome subunit alpha type-5



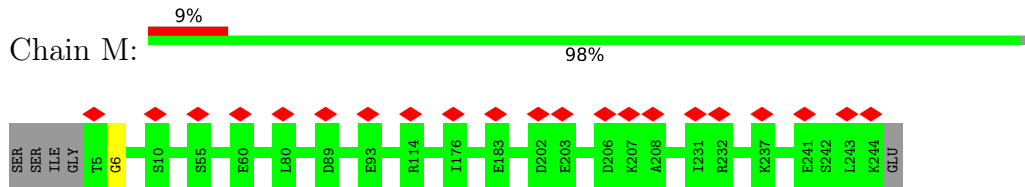
• Molecule 6: Proteasome subunit alpha type-1



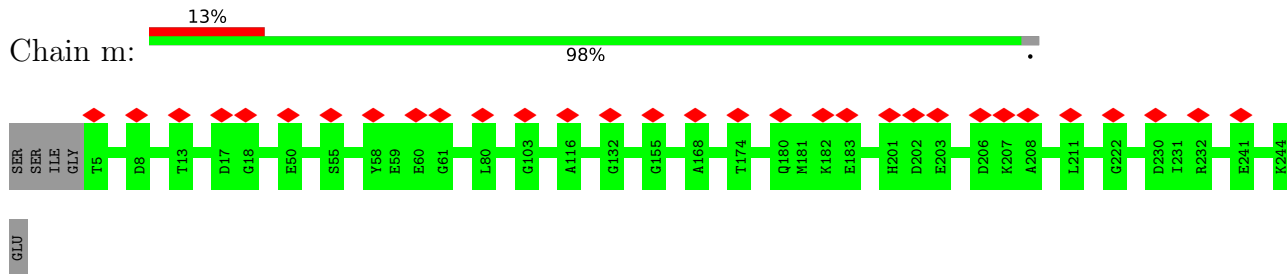
• Molecule 6: Proteasome subunit alpha type-1



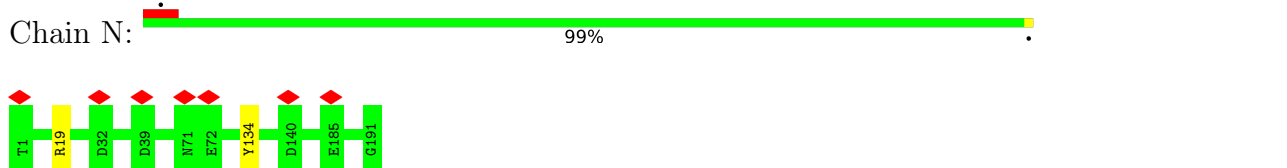
• Molecule 7: Proteasome subunit alpha type-3



• Molecule 7: Proteasome subunit alpha type-3

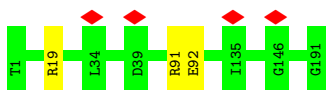


• Molecule 8: Proteasome subunit beta type-6



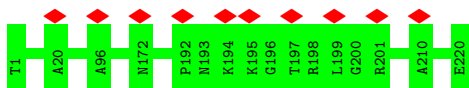
• Molecule 8: Proteasome subunit beta type-6

Chain n:  98%



- Molecule 9: Proteasome subunit beta type-7

Chain O:  5% 100%



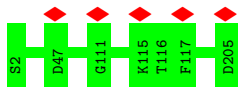
- Molecule 9: Proteasome subunit beta type-7

Chain o:  5% 100%



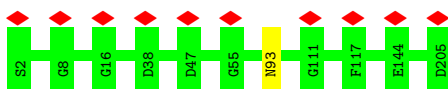
- Molecule 10: Proteasome subunit beta type-3

Chain P:  100%



- Molecule 10: Proteasome subunit beta type-3

Chain p:  5% 100%



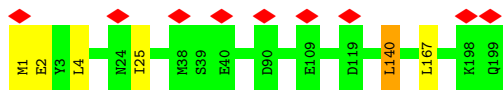
- Molecule 11: Proteasome subunit beta type-2

Chain Q:  97%



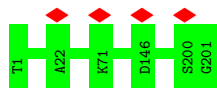
- Molecule 11: Proteasome subunit beta type-2

Chain q:  5% 97%



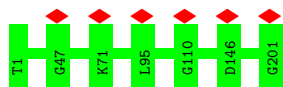
- Molecule 12: Proteasome subunit beta type-5

Chain R: 100%



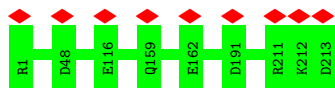
- Molecule 12: Proteasome subunit beta type-5

Chain r: 100%



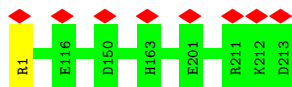
- Molecule 13: Proteasome subunit beta type-1

Chain S: 100%



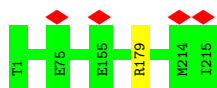
- Molecule 13: Proteasome subunit beta type-1

Chain s: 100%



- Molecule 14: Proteasome subunit beta type-4

Chain T: 100%

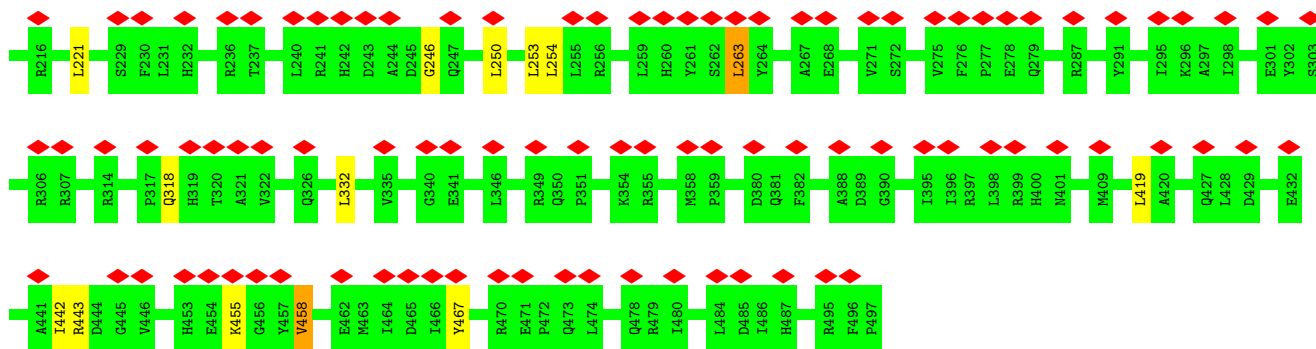


- Molecule 14: Proteasome subunit beta type-4

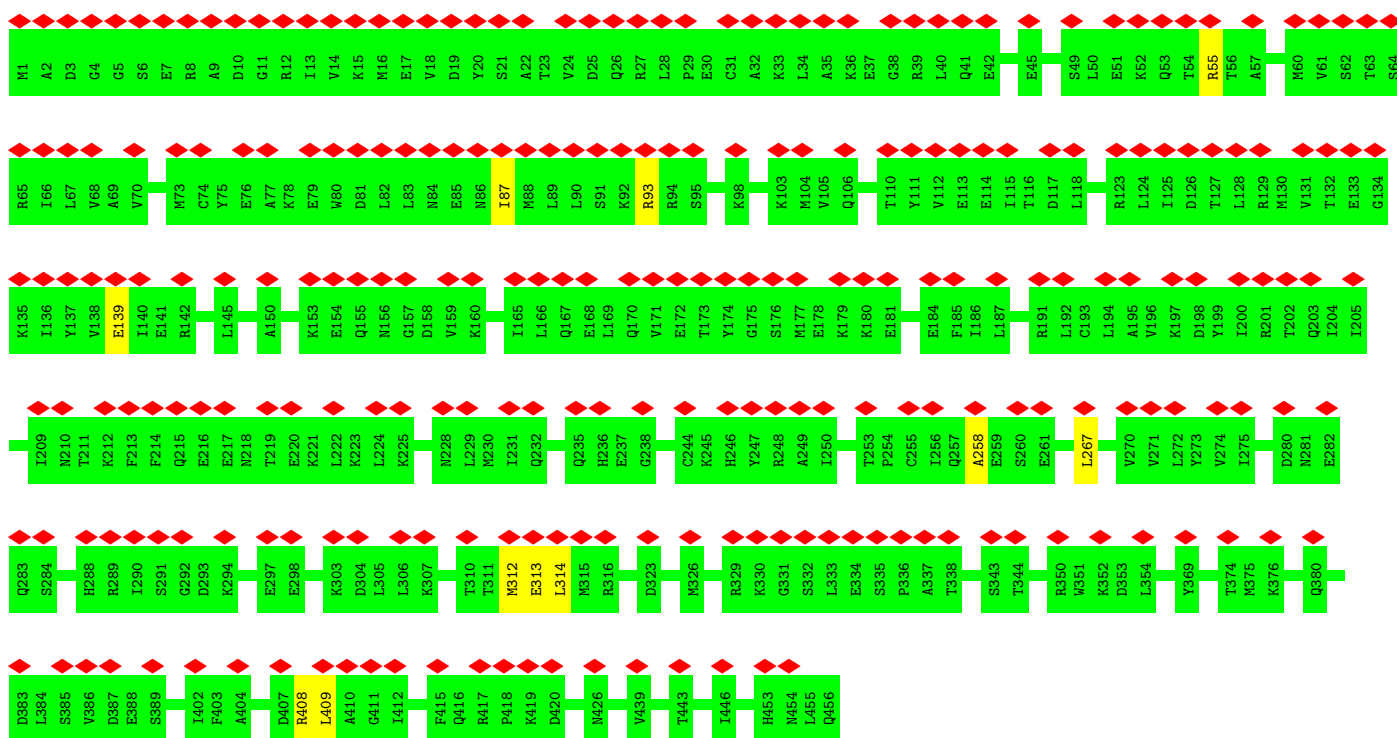
Chain t: 100%



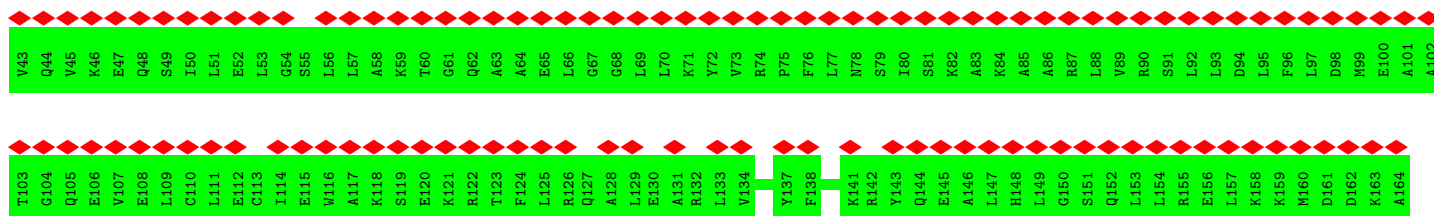
- Molecule 15: 26S proteasome non-ATPase regulatory subunit 1

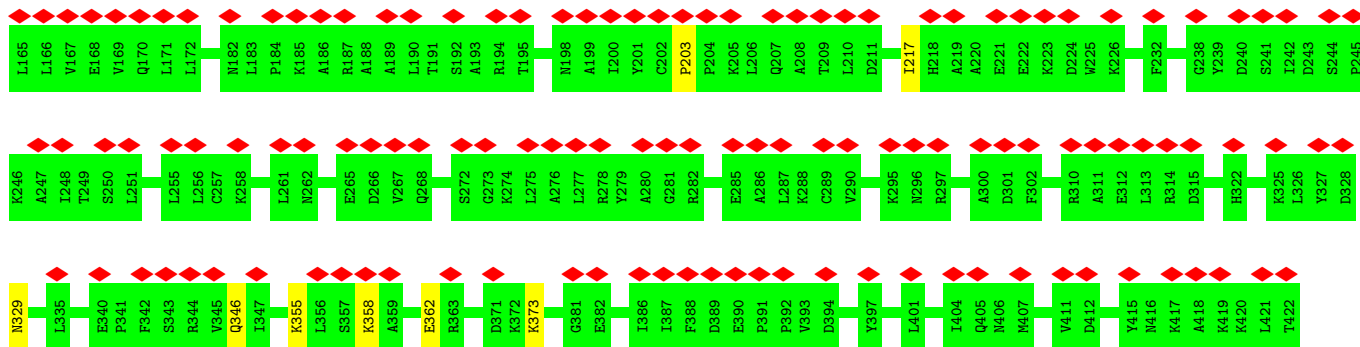


• Molecule 17: 26S proteasome non-ATPase regulatory subunit 12

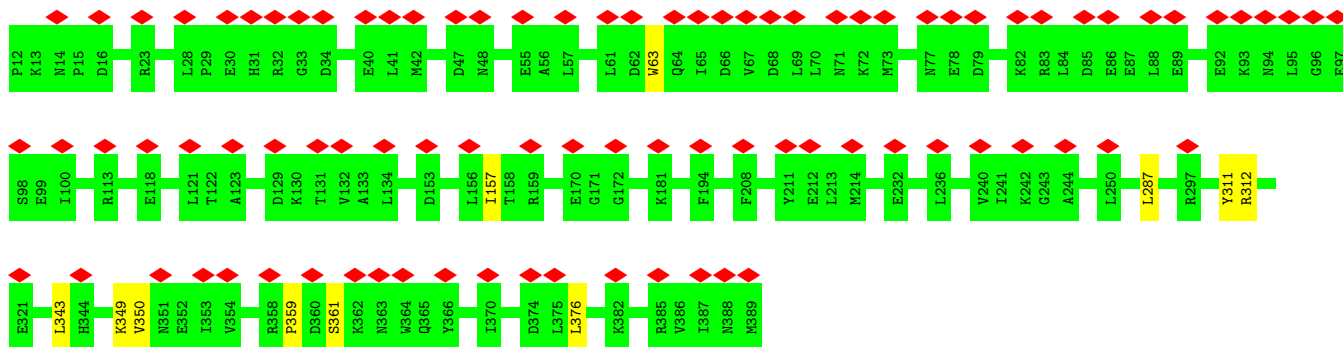


• Molecule 18: 26S proteasome non-ATPase regulatory subunit 11

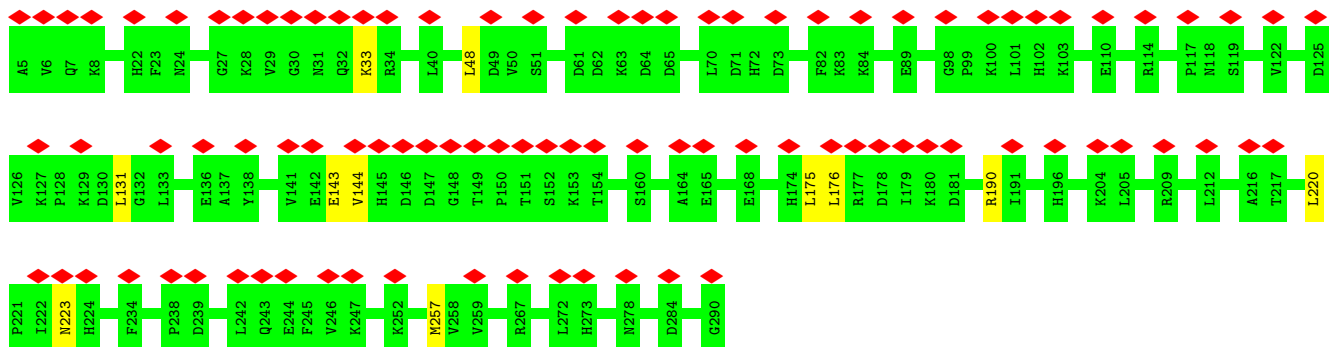




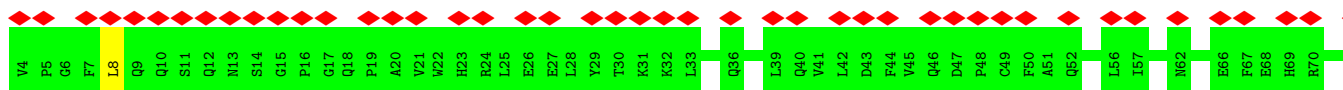
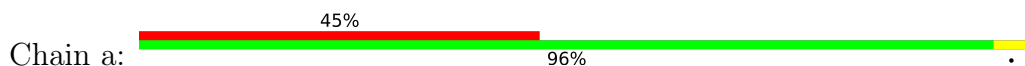
• Molecule 19: 26S proteasome non-ATPase regulatory subunit 6

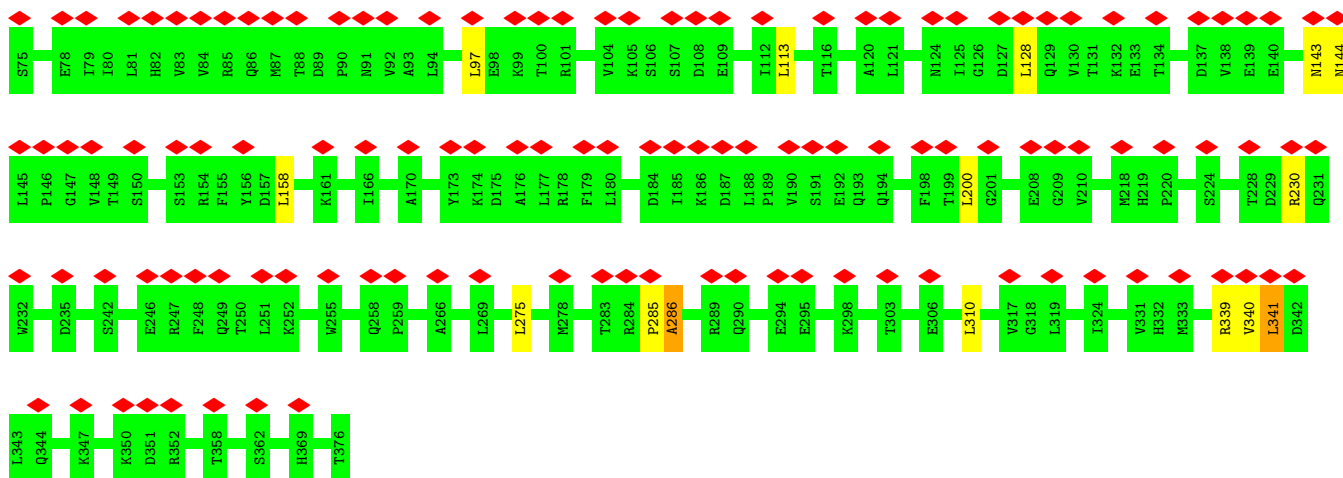


• Molecule 20: 26S proteasome non-ATPase regulatory subunit 7

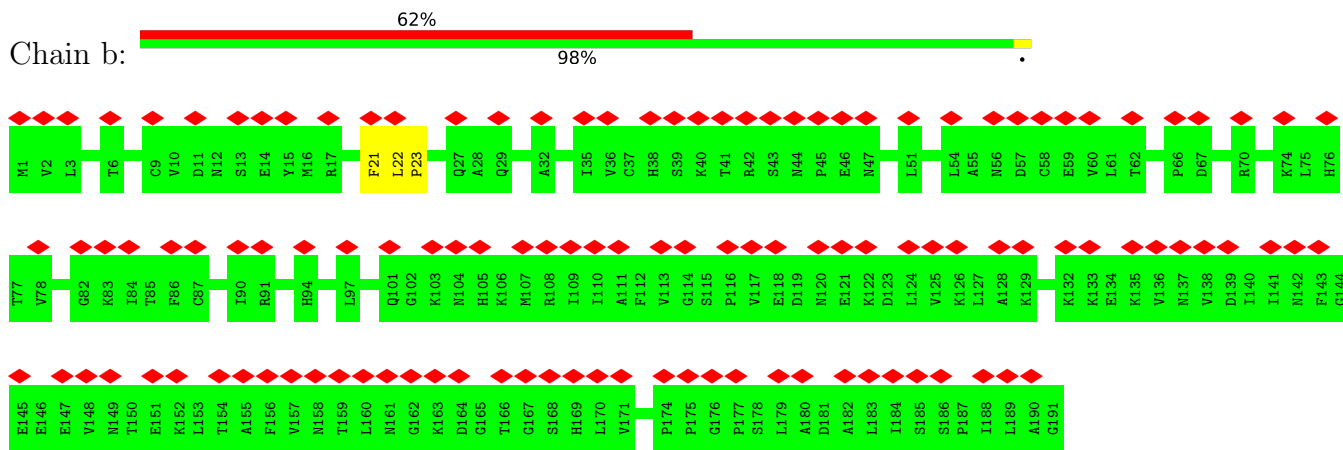


• Molecule 21: 26S proteasome non-ATPase regulatory subunit 13

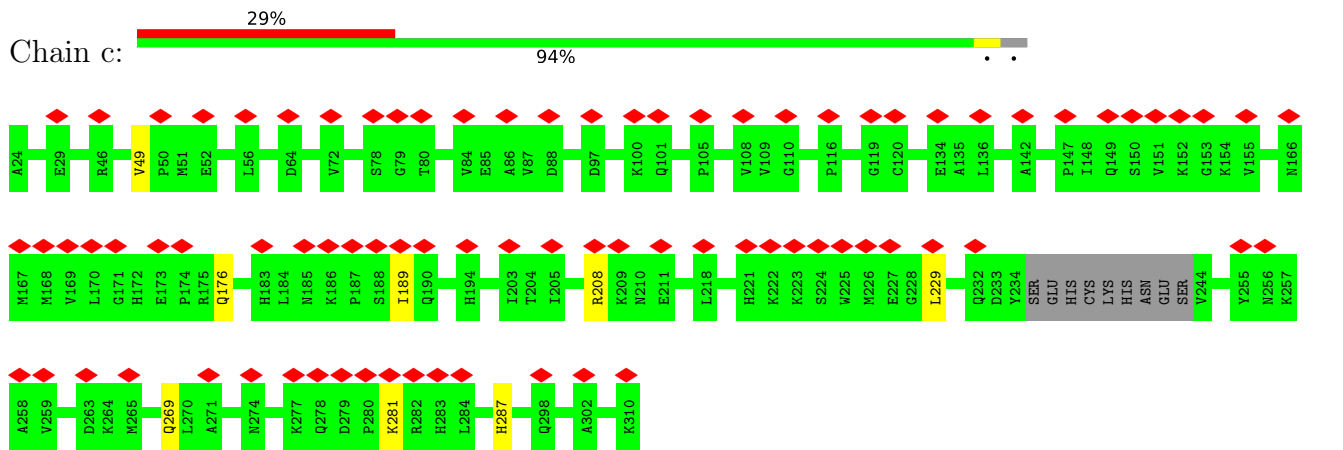




• Molecule 22: 26S proteasome non-ATPase regulatory subunit 4

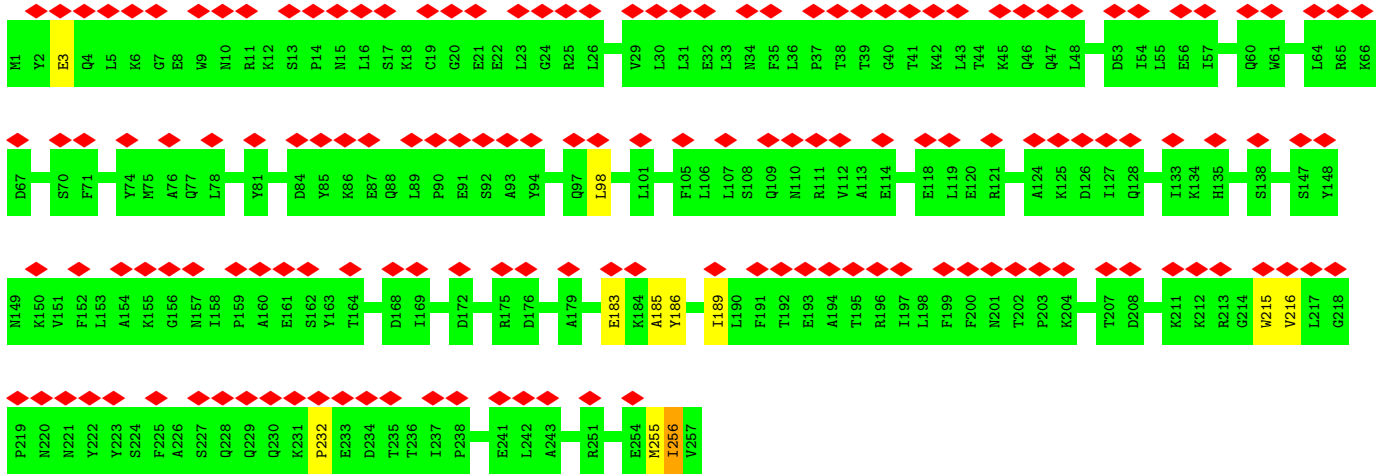


• Molecule 23: 26S proteasome non-ATPase regulatory subunit 14

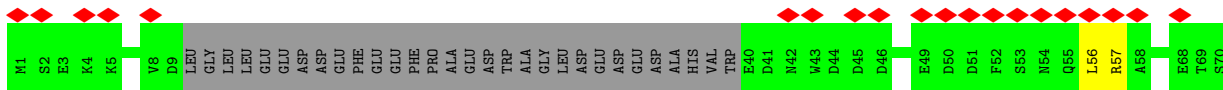


• Molecule 24: 26S proteasome non-ATPase regulatory subunit 8

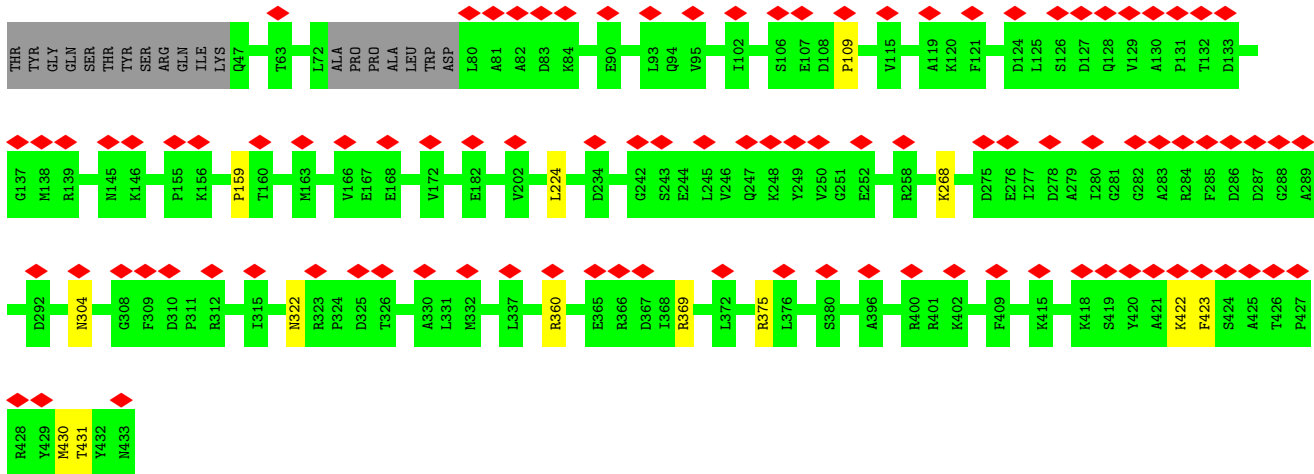
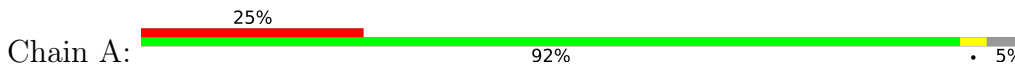




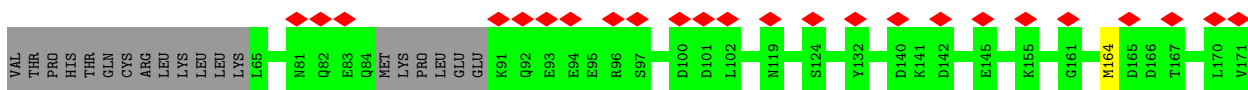
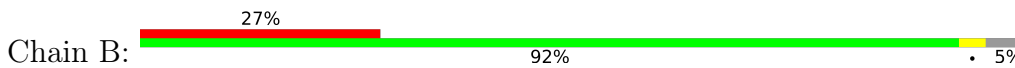
• Molecule 25: Sem1

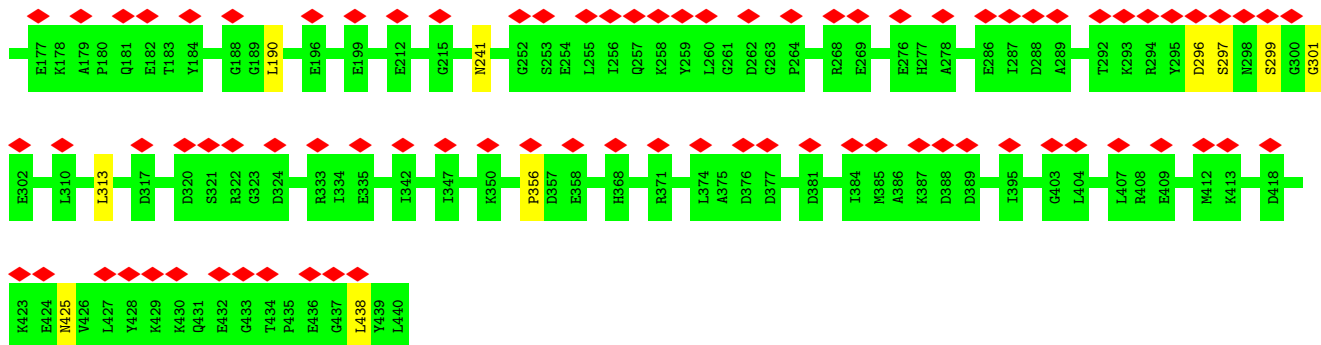


• Molecule 26: 26S proteasome regulatory subunit 7

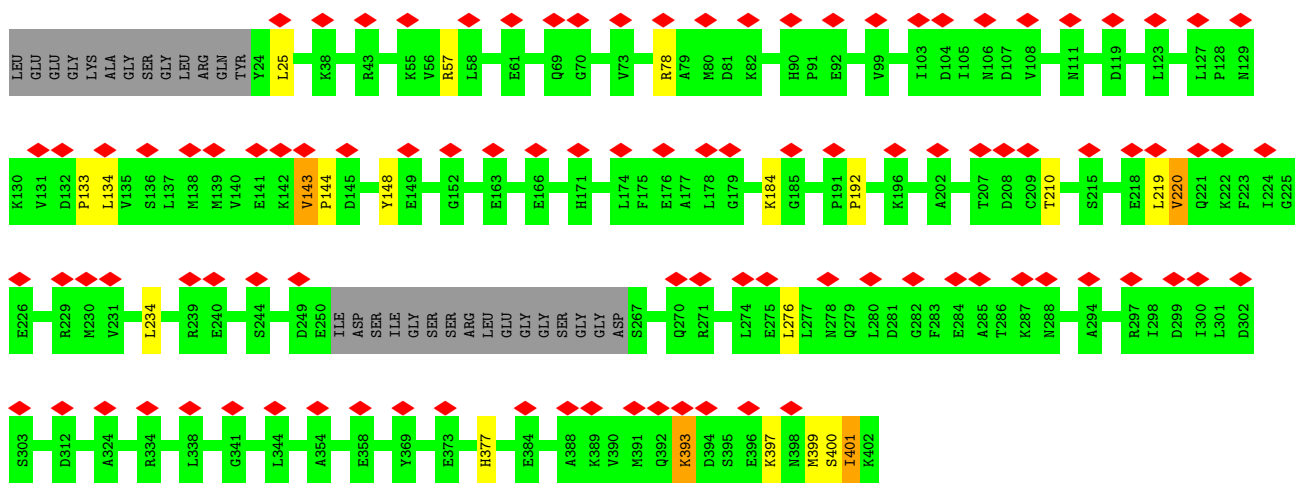
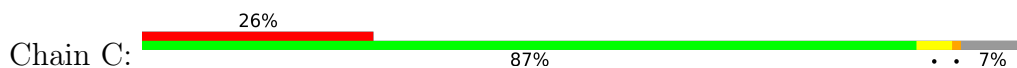


• Molecule 27: 26S proteasome regulatory subunit 4

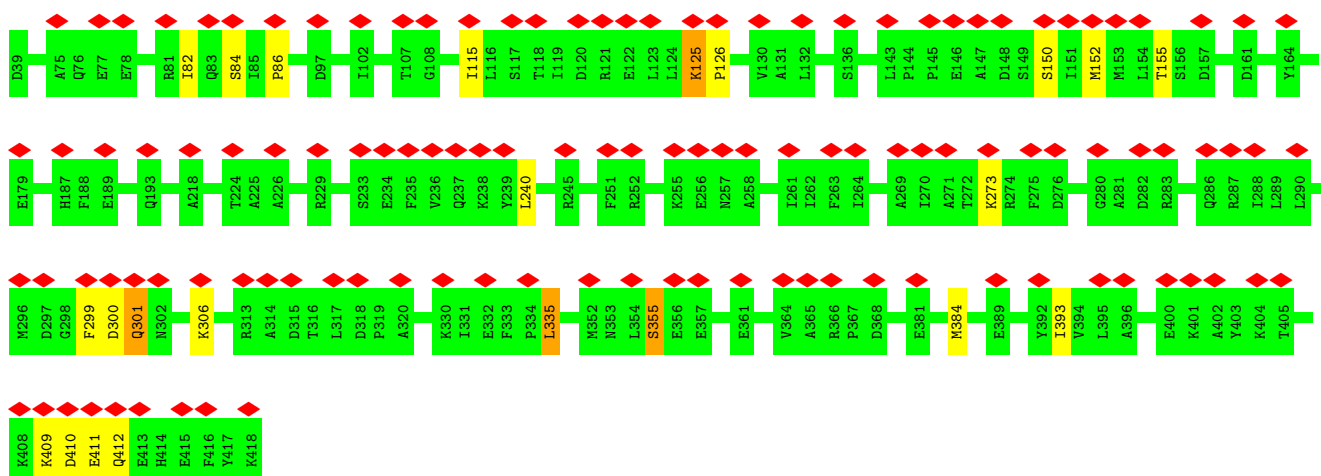




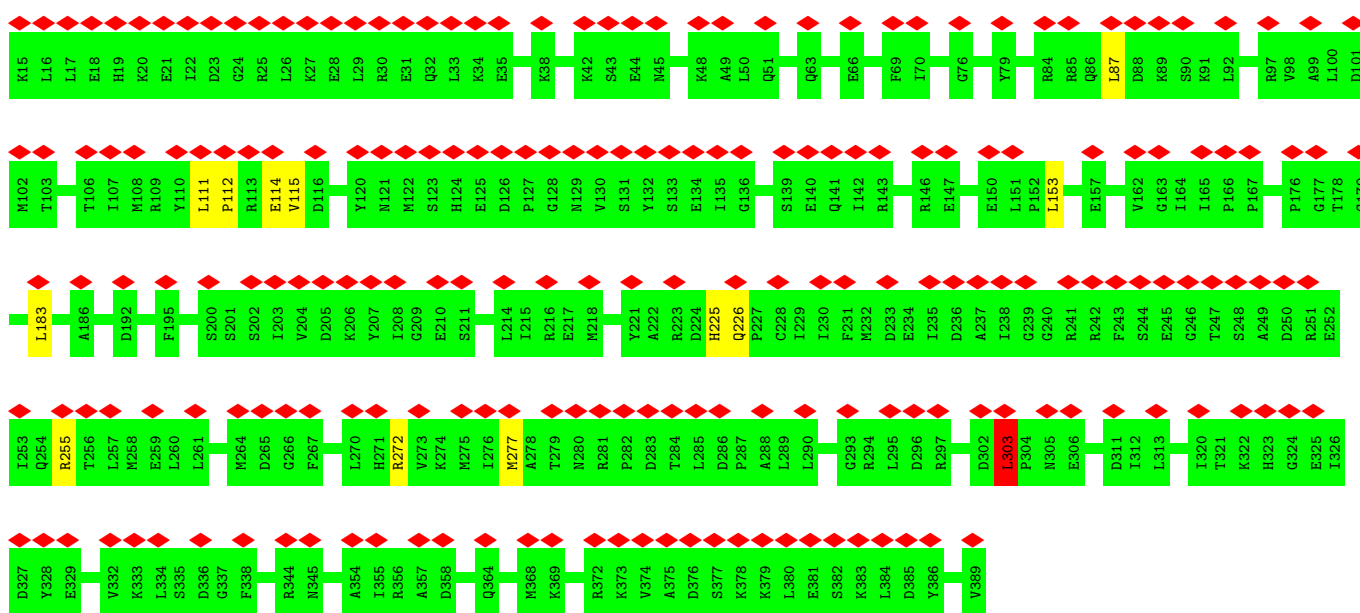
• Molecule 28: 26S proteasome regulatory subunit 8



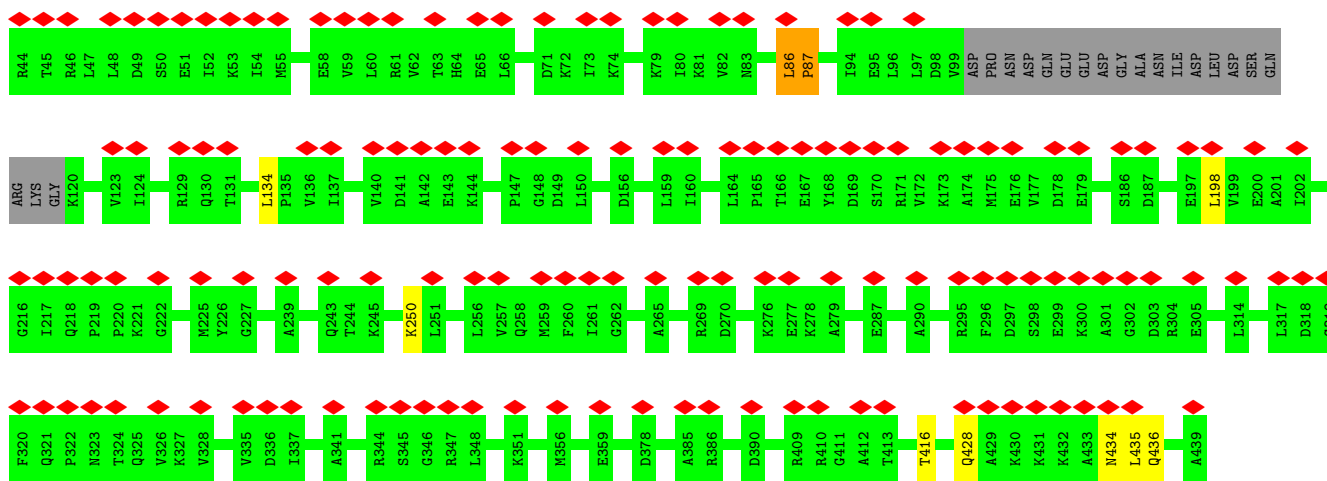
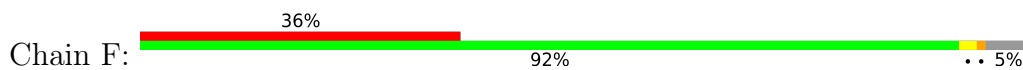
• Molecule 29: 26S proteasome regulatory subunit 6B



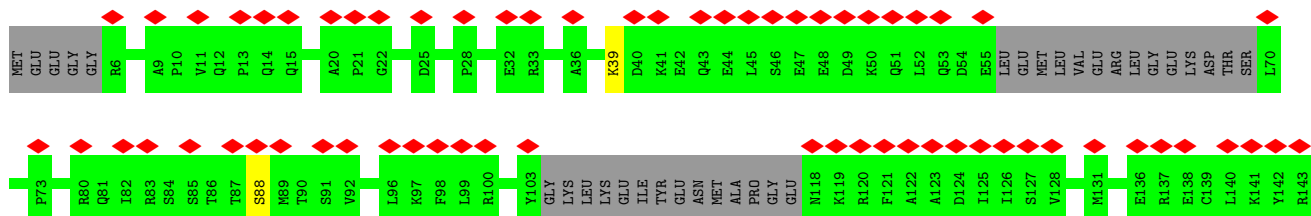
• Molecule 30: 26S proteasome regulatory subunit 10B

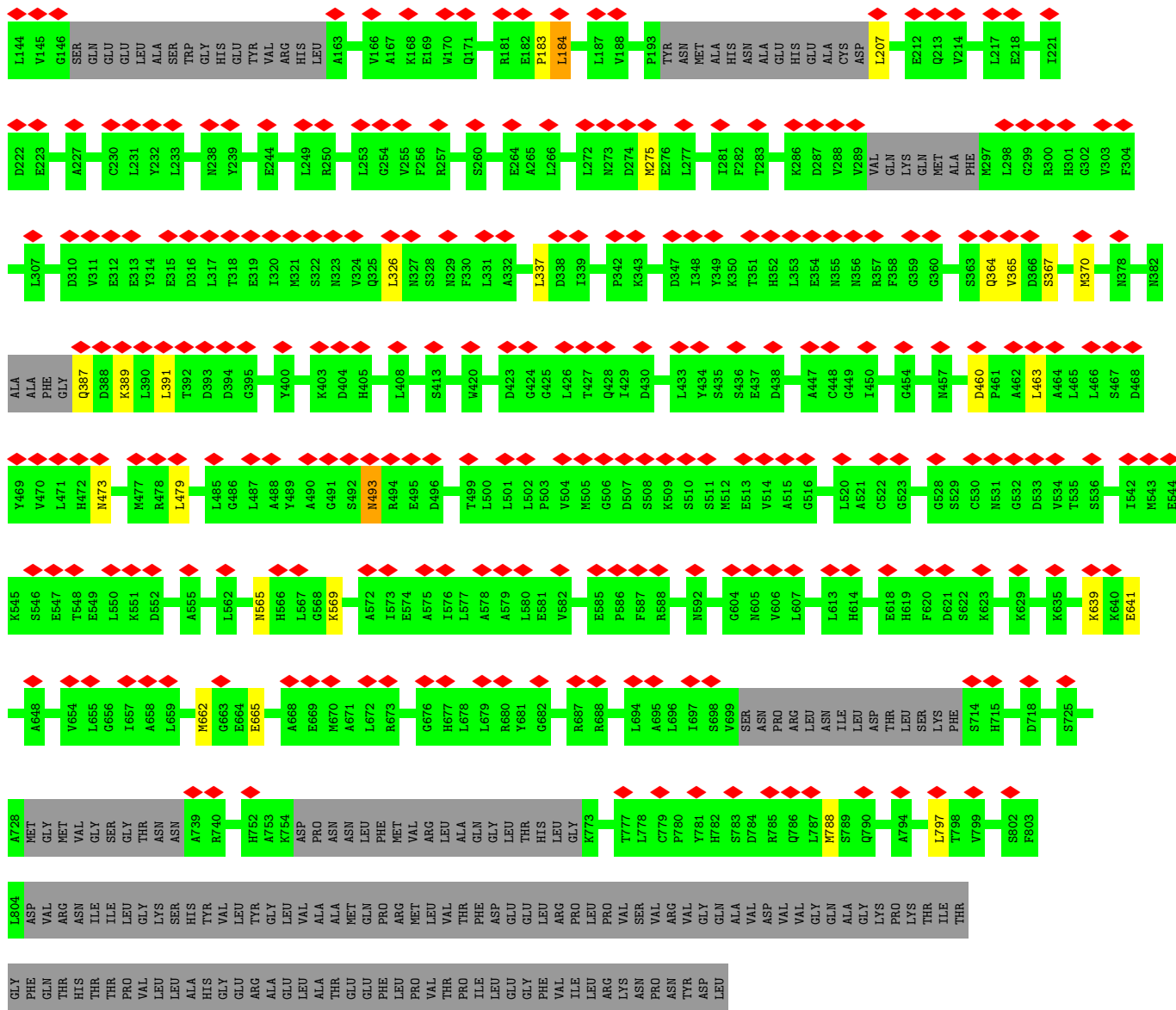


• Molecule 31: 26S proteasome regulatory subunit 6A



• Molecule 32: 26S proteasome non-ATPase regulatory subunit 2





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	66246	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	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	0.020	Depositor
Minimum map value	-0.009	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.00577	Depositor
Map size (Å)	420.0, 420.0, 420.0	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.75, 0.75, 0.75	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: ZN, AGS

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	G	0.42	0/1853	0.68	0/2515
1	g	0.41	0/1859	0.63	0/2523
2	H	0.42	0/1723	0.66	1/2346 (0.0%)
2	h	0.41	0/1743	0.61	0/2372
3	I	0.42	0/1925	0.74	0/2606
3	i	0.41	0/1942	0.72	0/2628
4	J	0.50	0/1728	0.80	2/2358 (0.1%)
4	j	0.47	0/1728	0.77	2/2358 (0.1%)
5	K	0.42	0/1755	0.75	5/2375 (0.2%)
5	k	0.37	0/1747	0.64	0/2364
6	L	0.43	0/1885	0.65	0/2552
6	l	0.42	0/1885	0.65	0/2552
7	M	0.45	0/1891	0.65	1/2552 (0.0%)
7	m	0.46	0/1891	0.63	0/2552
8	N	0.47	0/1454	0.67	1/1967 (0.1%)
8	n	0.45	0/1454	0.67	0/1967
9	O	0.44	0/1670	0.65	0/2265
9	o	0.44	0/1670	0.70	1/2265 (0.0%)
10	P	0.41	0/1614	0.60	0/2177
10	p	0.44	0/1614	0.61	0/2177
11	Q	0.50	0/1603	0.73	1/2174 (0.0%)
11	q	0.49	0/1603	0.78	4/2174 (0.2%)
12	R	0.44	0/1579	0.60	0/2134
12	r	0.46	0/1579	0.61	0/2134
13	S	0.45	0/1671	0.64	0/2253
13	s	0.44	0/1671	0.64	0/2253
14	T	0.44	0/1700	0.61	0/2305
14	t	0.44	0/1700	0.62	0/2305
15	U	0.36	0/6396	0.66	4/8646 (0.0%)
16	V	0.39	0/3668	0.79	10/4952 (0.2%)
17	W	0.37	0/3751	0.74	3/5042 (0.1%)
18	X	0.38	0/3053	0.68	0/4115

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
19	Y	0.39	0/3173	0.71	4/4273 (0.1%)
20	Z	0.40	0/2324	0.77	5/3150 (0.2%)
21	a	0.37	0/3053	0.79	10/4133 (0.2%)
22	b	0.34	0/1478	0.64	0/2001
23	c	0.39	0/2226	0.71	1/3007 (0.0%)
24	d	0.36	0/2162	0.74	2/2919 (0.1%)
25	e	0.34	0/338	0.73	1/450 (0.2%)
26	A	0.36	0/2939	0.66	1/3970 (0.0%)
27	B	0.36	0/2844	0.68	1/3846 (0.0%)
28	C	0.40	0/2896	0.77	6/3895 (0.2%)
29	D	0.40	0/3090	0.76	2/4168 (0.0%)
30	E	0.35	0/2904	0.71	3/3924 (0.1%)
31	F	0.37	0/2897	0.71	3/3912 (0.1%)
32	f	0.32	0/5393	0.68	1/7271 (0.0%)
All	All	0.40	0/102722	0.70	75/138877 (0.1%)

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	g	0	1
3	i	0	1
4	J	0	1
4	j	0	2
5	K	0	3
5	k	0	1
9	o	0	1
11	q	0	1
16	V	0	3
17	W	0	1
18	X	0	3
19	Y	0	5
20	Z	0	3
21	a	0	4
22	b	0	2
23	c	0	1
24	d	0	3
26	A	0	2
27	B	0	3
28	C	0	5

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Mol	Chain	#Chirality outliers	#Planarity outliers
29	D	0	11
30	E	0	6
31	F	0	3
All	All	0	66

There are no bond length outliers.

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	F	86	LEU	CA-CB-CG	12.76	144.64	115.30
21	a	341	LEU	CA-CB-CG	8.83	135.61	115.30
16	V	101	LEU	CA-CB-CG	8.31	134.42	115.30
21	a	275	LEU	CB-CG-CD2	-8.09	97.24	111.00
21	a	275	LEU	CA-CB-CG	7.78	133.20	115.30
11	q	140	LEU	CA-CB-CG	7.78	133.20	115.30
11	q	1	MET	CG-SD-CE	7.77	112.63	100.20
5	K	21	LEU	C-N-CA	7.49	140.42	121.70
4	J	5	ARG	NE-CZ-NH2	-7.34	116.63	120.30
30	E	183	LEU	CA-CB-CG	7.14	131.72	115.30
25	e	56	LEU	CA-CB-CG	7.13	131.69	115.30
4	J	2	SER	C-N-CA	6.91	138.98	121.70
5	K	33	LEU	CB-CG-CD1	6.86	122.66	111.00
19	Y	359	PRO	C-N-CA	6.83	138.77	121.70
21	a	128	LEU	CA-CB-CG	6.73	130.78	115.30
16	V	419	LEU	CA-CB-CG	6.67	130.65	115.30
5	K	8	TYR	C-N-CA	6.65	138.33	121.70
21	a	200	LEU	CA-CB-CG	6.45	130.13	115.30
19	Y	287	LEU	CA-CB-CG	6.41	130.05	115.30
30	E	153	LEU	CA-CB-CG	6.39	129.99	115.30
16	V	253	LEU	CB-CG-CD1	-6.38	100.15	111.00
21	a	310	LEU	CA-CB-CG	6.37	129.95	115.30
28	C	234	LEU	CA-CB-CG	6.36	129.93	115.30
29	D	412	GLN	C-N-CA	6.31	137.47	121.70
28	C	276	LEU	CA-CB-CG	-6.25	100.93	115.30
16	V	263	LEU	CB-CG-CD1	-6.07	100.67	111.00
7	M	6	GLY	C-N-CA	6.04	136.79	121.70
16	V	332	LEU	CA-CB-CG	5.95	128.99	115.30
16	V	145	LEU	CA-CB-CG	5.82	128.69	115.30
20	Z	176	LEU	CA-CB-CG	5.77	128.57	115.30
21	a	97	LEU	CA-CB-CG	5.74	128.50	115.30
21	a	113	LEU	CA-CB-CG	5.67	128.33	115.30
15	U	168	LEU	CA-CB-CG	5.63	128.25	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	f	493	ASN	N-CA-C	-5.58	95.93	111.00
21	a	8	LEU	CA-CB-CG	5.58	128.13	115.30
2	H	7	SER	C-N-CA	5.55	135.58	121.70
20	Z	257	MET	CA-CB-CG	5.54	122.72	113.30
16	V	170	LEU	CA-CB-CG	5.53	128.02	115.30
28	C	393	LYS	C-N-CA	5.53	135.51	121.70
30	E	303	LEU	C-N-CD	-5.52	108.45	120.60
21	a	158	LEU	CA-CB-CG	5.49	127.93	115.30
20	Z	48	LEU	CA-CB-CG	5.48	127.90	115.30
19	Y	343	LEU	CA-CB-CG	5.46	127.86	115.30
11	Q	4	LEU	CB-CG-CD2	5.45	120.27	111.00
15	U	337	LEU	CA-CB-CG	5.39	127.69	115.30
24	d	98	LEU	CA-CB-CG	5.38	127.68	115.30
31	F	198	LEU	CA-CB-CG	5.38	127.67	115.30
16	V	250	LEU	CA-CB-CG	5.37	127.64	115.30
28	C	134	LEU	CA-CB-CG	5.33	127.57	115.30
20	Z	131	LEU	CA-CB-CG	5.31	127.52	115.30
28	C	25	LEU	CA-CB-CG	5.30	127.49	115.30
8	N	134	TYR	CB-CG-CD2	-5.28	117.83	121.00
26	A	224	LEU	CA-CB-CG	5.26	127.41	115.30
16	V	221	LEU	CA-CB-CG	5.26	127.39	115.30
28	C	401	ILE	N-CA-C	5.22	125.09	111.00
5	K	19	GLY	C-N-CA	5.21	134.72	121.70
17	W	312	MET	CA-CB-CG	5.20	122.14	113.30
29	D	393	ILE	CG1-CB-CG2	-5.20	99.97	111.40
5	K	20	ARG	N-CA-CB	5.17	119.91	110.60
9	o	200	GLY	N-CA-C	5.17	126.01	113.10
11	q	1	MET	CA-CB-CG	5.14	122.04	113.30
17	W	409	LEU	CA-CB-CG	5.14	127.12	115.30
16	V	254	LEU	CA-CB-CG	5.13	127.11	115.30
4	j	4	ASP	CB-CG-OD2	5.12	122.90	118.30
24	d	256	ILE	C-N-CA	5.10	134.46	121.70
19	Y	376	LEU	CA-CB-CG	5.10	127.03	115.30
4	j	190	LEU	CA-CB-CG	5.10	127.04	115.30
11	q	140	LEU	CB-CG-CD2	5.07	119.62	111.00
23	c	229	LEU	CA-CB-CG	5.07	126.96	115.30
15	U	224	ASP	CB-CG-OD1	5.07	122.86	118.30
17	W	267	LEU	CA-CB-CG	5.06	126.93	115.30
31	F	434	ASN	C-N-CA	5.06	134.34	121.70
27	B	313	LEU	CA-CB-CG	5.04	126.90	115.30
15	U	764	LEU	CA-CB-CG	5.04	126.89	115.30
20	Z	175	LEU	CA-CB-CG	5.03	126.86	115.30

There are no chirality outliers.

All (66) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	A	159	PRO	Peptide
26	A	422	LYS	Peptide
27	B	296	ASP	Peptide
27	B	297	SER	Peptide
27	B	301	GLY	Peptide
28	C	143	VAL	Peptide
28	C	220	VAL	Peptide
28	C	397	LYS	Peptide
28	C	399	MET	Peptide
28	C	400	SER	Peptide
29	D	125	LYS	Peptide
29	D	150	SER	Peptide
29	D	155	THR	Peptide
29	D	240	LEU	Peptide
29	D	299	PHE	Peptide
29	D	300	ASP	Peptide
29	D	301	GLN	Mainchain
29	D	335	LEU	Peptide
29	D	355	SER	Peptide
29	D	410	ASP	Peptide
29	D	84	SER	Peptide
30	E	111	LEU	Peptide
30	E	112	PRO	Peptide
30	E	114	GLU	Peptide
30	E	115	VAL	Peptide
30	E	225	HIS	Peptide
30	E	303	LEU	Peptide
31	F	435	LEU	Peptide
31	F	86	LEU	Peptide
31	F	87	PRO	Peptide
4	J	5	ARG	Peptide
5	K	121	LEU	Peptide
5	K	19	GLY	Peptide
5	K	22	PHE	Peptide
16	V	100	MET	Peptide
16	V	56	ALA	Peptide
16	V	64	GLN	Peptide
17	W	258	ALA	Peptide
18	X	203	PRO	Peptide
18	X	346	GLN	Peptide

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Mol	Chain	Res	Type	Group
18	X	362	GLU	Peptide
19	Y	157	ILE	Peptide
19	Y	311	TYR	Peptide
19	Y	349	LYS	Peptide
19	Y	361	SER	Peptide
19	Y	63	TRP	Peptide
20	Z	143	GLU	Peptide
20	Z	220	LEU	Peptide
20	Z	223	ASN	Peptide
21	a	285	PRO	Peptide
21	a	286	ALA	Mainchain
21	a	339	ARG	Peptide
21	a	341	LEU	Peptide
22	b	21	PHE	Peptide
22	b	22	LEU	Peptide
23	c	189	ILE	Peptide
24	d	185	ALA	Peptide
24	d	186	TYR	Peptide
24	d	215	TRP	Peptide
1	g	222	VAL	Peptide
3	i	8	ARG	Peptide
4	j	180	ALA	Peptide
4	j	4	ASP	Mainchain
5	k	11	GLY	Peptide
9	o	200	GLY	Peptide
11	q	2	GLU	Mainchain

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	237/240 (99%)	214 (90%)	23 (10%)	0	100	100
1	g	238/240 (99%)	219 (92%)	19 (8%)	0	100	100
2	H	228/232 (98%)	210 (92%)	18 (8%)	0	100	100
2	h	230/232 (99%)	219 (95%)	11 (5%)	0	100	100
3	I	246/250 (98%)	222 (90%)	22 (9%)	2 (1%)	19	60
3	i	248/250 (99%)	218 (88%)	29 (12%)	1 (0%)	34	72
4	J	237/243 (98%)	221 (93%)	15 (6%)	1 (0%)	34	72
4	j	237/243 (98%)	218 (92%)	15 (6%)	4 (2%)	9	44
5	K	224/234 (96%)	204 (91%)	19 (8%)	1 (0%)	34	72
5	k	224/234 (96%)	204 (91%)	19 (8%)	1 (0%)	34	72
6	L	236/238 (99%)	221 (94%)	15 (6%)	0	100	100
6	l	236/238 (99%)	220 (93%)	16 (7%)	0	100	100
7	M	238/245 (97%)	218 (92%)	20 (8%)	0	100	100
7	m	238/245 (97%)	219 (92%)	19 (8%)	0	100	100
8	N	189/191 (99%)	178 (94%)	10 (5%)	1 (0%)	29	68
8	n	189/191 (99%)	178 (94%)	8 (4%)	3 (2%)	9	45
9	O	218/220 (99%)	206 (94%)	12 (6%)	0	100	100
9	o	218/220 (99%)	208 (95%)	10 (5%)	0	100	100
10	P	202/204 (99%)	190 (94%)	12 (6%)	0	100	100
10	p	202/204 (99%)	190 (94%)	12 (6%)	0	100	100
11	Q	197/199 (99%)	180 (91%)	16 (8%)	1 (0%)	29	68
11	q	197/199 (99%)	183 (93%)	14 (7%)	0	100	100
12	R	199/201 (99%)	190 (96%)	9 (4%)	0	100	100
12	r	199/201 (99%)	190 (96%)	9 (4%)	0	100	100
13	S	211/213 (99%)	198 (94%)	13 (6%)	0	100	100
13	s	211/213 (99%)	198 (94%)	13 (6%)	0	100	100
14	T	213/215 (99%)	202 (95%)	11 (5%)	0	100	100
14	t	213/215 (99%)	203 (95%)	10 (5%)	0	100	100
15	U	798/911 (88%)	737 (92%)	61 (8%)	0	100	100
16	V	441/480 (92%)	371 (84%)	62 (14%)	8 (2%)	8	42
17	W	454/456 (100%)	396 (87%)	54 (12%)	4 (1%)	17	56
18	X	378/380 (100%)	339 (90%)	38 (10%)	1 (0%)	41	76

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	Y	376/378 (100%)	328 (87%)	47 (12%)	1 (0%)	41	76
20	Z	284/286 (99%)	243 (86%)	40 (14%)	1 (0%)	34	72
21	a	371/373 (100%)	314 (85%)	53 (14%)	4 (1%)	14	52
22	b	189/191 (99%)	167 (88%)	21 (11%)	1 (0%)	29	68
23	c	274/287 (96%)	239 (87%)	34 (12%)	1 (0%)	34	72
24	d	255/257 (99%)	206 (81%)	44 (17%)	5 (2%)	7	40
25	e	36/70 (51%)	28 (78%)	8 (22%)	0	100	100
26	A	376/399 (94%)	320 (85%)	53 (14%)	3 (1%)	19	60
27	B	366/389 (94%)	299 (82%)	65 (18%)	2 (0%)	29	68
28	C	359/392 (92%)	304 (85%)	48 (13%)	7 (2%)	8	41
29	D	378/380 (100%)	307 (81%)	63 (17%)	8 (2%)	7	39
30	E	373/375 (100%)	317 (85%)	54 (14%)	2 (0%)	29	68
31	F	372/396 (94%)	329 (88%)	40 (11%)	3 (1%)	19	60
32	f	669/908 (74%)	579 (86%)	82 (12%)	8 (1%)	13	50
All	All	12904/13558 (95%)	11544 (90%)	1286 (10%)	74 (1%)	29	64

All (74) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	V	196	SER
16	V	198	GLN
17	W	314	LEU
21	a	286	ALA
21	a	340	VAL
24	d	189	ILE
8	n	91	ARG
8	n	92	GLU
27	B	299	SER
28	C	220	VAL
29	D	411	GLU
30	E	303	LEU
31	F	436	GLN
32	f	337	LEU
32	f	364	GLN
32	f	367	SER
32	f	665	GLU
4	J	176	TYR

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Mol	Chain	Res	Type
5	K	10	ARG
16	V	246	GLY
21	a	144	ASN
23	c	287	HIS
24	d	216	VAL
4	j	181	ILE
28	C	219	LEU
32	f	183	PRO
32	f	365	VAL
16	V	443	ARG
16	V	458	VAL
18	X	355	LYS
19	Y	350	VAL
24	d	232	PRO
5	k	11	GLY
26	A	431	THR
32	f	184	LEU
32	f	326	LEU
3	I	7	SER
8	N	19	ARG
11	Q	72	GLY
16	V	467	TYR
17	W	87	ILE
8	n	19	ARG
26	A	423	PHE
28	C	143	VAL
29	D	409	LYS
31	F	428	GLN
17	W	139	GLU
17	W	313	GLU
21	a	143	ASN
24	d	3	GLU
24	d	183	GLU
4	j	9	VAL
4	j	97	THR
27	B	356	PRO
29	D	301	GLN
29	D	335	LEU
29	D	355	SER
22	b	23	PRO
4	j	98	VAL
26	A	109	PRO

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Mol	Chain	Res	Type
29	D	82	ILE
29	D	86	PRO
28	C	133	PRO
28	C	144	PRO
28	C	192	PRO
28	C	401	ILE
16	V	101	LEU
3	i	221	GLY
29	D	126	PRO
3	I	221	GLY
16	V	442	ILE
31	F	87	PRO
20	Z	144	VAL
30	E	226	GLN

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	G	192/205 (94%)	191 (100%)	1 (0%)	88	93
1	g	193/205 (94%)	193 (100%)	0	100	100
2	H	162/190 (85%)	162 (100%)	0	100	100
2	h	164/190 (86%)	164 (100%)	0	100	100
3	I	191/210 (91%)	191 (100%)	0	100	100
3	i	193/210 (92%)	192 (100%)	1 (0%)	88	93
4	J	152/207 (73%)	148 (97%)	4 (3%)	46	67
4	j	152/207 (73%)	152 (100%)	0	100	100
5	K	187/196 (95%)	187 (100%)	0	100	100
5	k	186/196 (95%)	186 (100%)	0	100	100
6	L	198/204 (97%)	198 (100%)	0	100	100
6	l	198/204 (97%)	198 (100%)	0	100	100
7	M	192/202 (95%)	192 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	m	192/202 (95%)	192 (100%)	0	100	100
8	N	148/148 (100%)	148 (100%)	0	100	100
8	n	148/148 (100%)	148 (100%)	0	100	100
9	O	177/181 (98%)	177 (100%)	0	100	100
9	o	177/181 (98%)	177 (100%)	0	100	100
10	P	172/173 (99%)	172 (100%)	0	100	100
10	p	172/173 (99%)	171 (99%)	1 (1%)	86	92
11	Q	164/170 (96%)	161 (98%)	3 (2%)	59	76
11	q	164/170 (96%)	160 (98%)	4 (2%)	49	69
12	R	153/156 (98%)	153 (100%)	0	100	100
12	r	153/156 (98%)	153 (100%)	0	100	100
13	S	174/178 (98%)	174 (100%)	0	100	100
13	s	174/178 (98%)	173 (99%)	1 (1%)	86	92
14	T	175/178 (98%)	174 (99%)	1 (1%)	86	92
14	t	175/178 (98%)	174 (99%)	1 (1%)	86	92
15	U	685/779 (88%)	679 (99%)	6 (1%)	78	87
16	V	387/414 (94%)	380 (98%)	7 (2%)	59	76
17	W	416/416 (100%)	413 (99%)	3 (1%)	84	90
18	X	327/327 (100%)	323 (99%)	4 (1%)	71	83
19	Y	334/334 (100%)	333 (100%)	1 (0%)	92	95
20	Z	257/257 (100%)	255 (99%)	2 (1%)	81	89
21	a	333/333 (100%)	332 (100%)	1 (0%)	92	95
22	b	167/167 (100%)	167 (100%)	0	100	100
23	c	243/252 (96%)	238 (98%)	5 (2%)	53	71
24	d	231/231 (100%)	229 (99%)	2 (1%)	78	87
25	e	38/63 (60%)	37 (97%)	1 (3%)	46	67
26	A	297/343 (87%)	290 (98%)	7 (2%)	49	69
27	B	300/345 (87%)	295 (98%)	5 (2%)	60	78
28	C	315/340 (93%)	308 (98%)	7 (2%)	52	70
29	D	333/333 (100%)	327 (98%)	6 (2%)	59	76
30	E	298/329 (91%)	294 (99%)	4 (1%)	69	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	F	296/340 (87%)	293 (99%)	3 (1%)	76	86
32	f	580/763 (76%)	559 (96%)	21 (4%)	35	60
All	All	10715/11562 (93%)	10613 (99%)	102 (1%)	77	86

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	11	ARG
4	J	5	ARG
4	J	7	ILE
4	J	85	ASN
4	J	176	TYR
11	Q	25	ILE
11	Q	63	ASN
11	Q	171	PHE
14	T	179	ARG
15	U	194	ARG
15	U	345	ASN
15	U	472	ILE
15	U	496	LEU
15	U	554	LEU
15	U	611	ASN
16	V	99	ARG
16	V	104	THR
16	V	167	LEU
16	V	263	LEU
16	V	318	GLN
16	V	455	LYS
16	V	458	VAL
17	W	55	ARG
17	W	93	ARG
17	W	408	ARG
18	X	217	ILE
18	X	329	ASN
18	X	358	LYS
18	X	373	LYS
19	Y	312	ARG
20	Z	33	LYS
20	Z	190	ARG
21	a	230	ARG
23	c	49	VAL

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Mol	Chain	Res	Type
23	c	176	GLN
23	c	208	ARG
23	c	269	GLN
23	c	281	LYS
24	d	255	MET
24	d	256	ILE
25	e	57	ARG
3	i	17	ARG
10	p	93	ASN
11	q	4	LEU
11	q	25	ILE
11	q	140	LEU
11	q	167	LEU
13	s	1	ARG
14	t	179	ARG
26	A	268	LYS
26	A	304	ASN
26	A	322	ASN
26	A	360	ARG
26	A	369	ARG
26	A	375	ARG
26	A	430	MET
27	B	164	MET
27	B	190	LEU
27	B	241	ASN
27	B	425	ASN
27	B	438	LEU
28	C	57	ARG
28	C	78	ARG
28	C	148	TYR
28	C	184	LYS
28	C	210	THR
28	C	377	HIS
28	C	393	LYS
29	D	115	ILE
29	D	125	LYS
29	D	152	MET
29	D	273	LYS
29	D	306	LYS
29	D	384	MET
30	E	87	LEU
30	E	255	ARG

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Mol	Chain	Res	Type
30	E	272	ARG
30	E	277	MET
31	F	134	LEU
31	F	250	LYS
31	F	416	THR
32	f	39	LYS
32	f	88	SER
32	f	184	LEU
32	f	207	LEU
32	f	275	MET
32	f	370	MET
32	f	387	GLN
32	f	389	LYS
32	f	391	LEU
32	f	460	ASP
32	f	463	LEU
32	f	473	ASN
32	f	479	LEU
32	f	493	ASN
32	f	565	ASN
32	f	569	LYS
32	f	639	LYS
32	f	641	GLU
32	f	662	MET
32	f	788	MET
32	f	797	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	123	GLN
2	H	119	GLN
2	H	123	GLN
2	H	148	GLN
3	I	20	GLN
3	I	119	GLN
3	I	146	GLN
3	I	149	GLN
4	J	54	GLN
4	J	85	ASN
4	J	122	ASN
4	J	154	HIS

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Mol	Chain	Res	Type
5	K	214	ASN
6	L	53	GLN
8	N	28	ASN
8	N	154	GLN
9	O	62	ASN
11	Q	63	ASN
11	Q	132	HIS
12	R	38	ASN
12	R	85	ASN
15	U	18	GLN
15	U	89	ASN
15	U	345	ASN
15	U	503	GLN
15	U	632	GLN
16	V	109	ASN
16	V	193	GLN
16	V	318	GLN
17	W	444	HIS
18	X	178	HIS
18	X	296	ASN
18	X	406	ASN
19	Y	136	HIS
19	Y	306	GLN
20	Z	102	HIS
20	Z	104	ASN
20	Z	225	GLN
21	a	86	GLN
21	a	273	GLN
22	b	34	ASN
23	c	194	HIS
23	c	221	HIS
24	d	109	GLN
3	i	20	GLN
3	i	119	GLN
3	i	146	GLN
5	k	214	ASN
8	n	154	GLN
9	o	62	ASN
11	q	101	ASN
11	q	132	HIS
12	r	85	ASN
14	t	69	GLN

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Mol	Chain	Res	Type
28	C	36	ASN
28	C	182	GLN
28	C	205	HIS
28	C	332	HIS
28	C	398	ASN
29	D	137	ASN
29	D	237	GLN
29	D	304	ASN
30	E	63	GLN
32	f	387	GLN
32	f	452	ASN
32	f	473	ASN
32	f	493	ASN
32	f	540	GLN
32	f	752	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	AGS	D	501	-	26,33,33	0.86	2 (7%)	26,52,52	1.32	3 (11%)
34	AGS	A	501	-	26,33,33	0.89	1 (3%)	26,52,52	1.86	4 (15%)
34	AGS	C	501	-	26,33,33	0.77	0	26,52,52	1.43	3 (11%)
34	AGS	F	501	-	26,33,33	0.85	1 (3%)	26,52,52	1.52	3 (11%)

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
34	AGS	D	501	-	-	8/17/38/38	0/3/3/3
34	AGS	A	501	-	-	4/17/38/38	0/3/3/3
34	AGS	C	501	-	-	8/17/38/38	0/3/3/3
34	AGS	F	501	-	-	4/17/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	D	501	AGS	C8-N7	-2.30	1.30	1.34
34	F	501	AGS	PG-S1G	2.02	1.95	1.90
34	A	501	AGS	PA-O2A	-2.02	1.45	1.55
34	D	501	AGS	PG-S1G	2.01	1.95	1.90

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	A	501	AGS	PA-O3A-PB	-7.41	107.39	132.83
34	F	501	AGS	PA-O3A-PB	-6.51	110.48	132.83
34	C	501	AGS	PA-O3A-PB	-5.11	115.28	132.83
34	D	501	AGS	PA-O3A-PB	-5.09	115.34	132.83
34	A	501	AGS	C1'-N9-C4	3.87	133.43	126.64
34	C	501	AGS	C3'-C2'-C1'	2.89	105.34	100.98
34	A	501	AGS	C5-C6-N6	2.77	124.56	120.35
34	D	501	AGS	C5-C6-N6	2.68	124.42	120.35
34	D	501	AGS	O2G-PG-O3B	2.25	112.16	104.64
34	A	501	AGS	C4-C5-N7	2.20	111.70	109.40
34	F	501	AGS	C5-C6-N6	2.19	123.68	120.35
34	F	501	AGS	C4-C5-N7	2.12	111.61	109.40
34	C	501	AGS	C4-C5-N7	2.04	111.52	109.40

There are no chirality outliers.

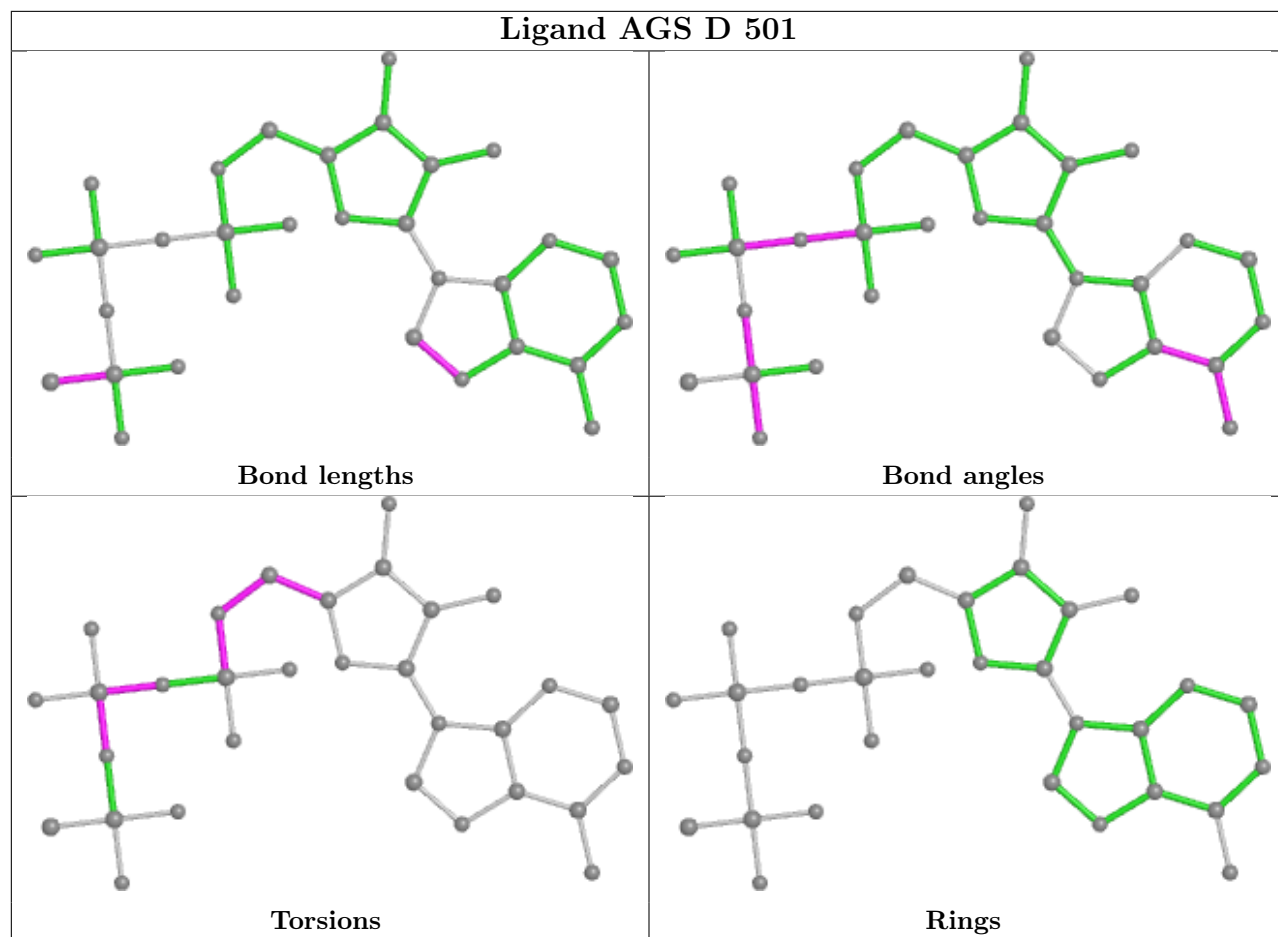
All (24) torsion outliers are listed below:

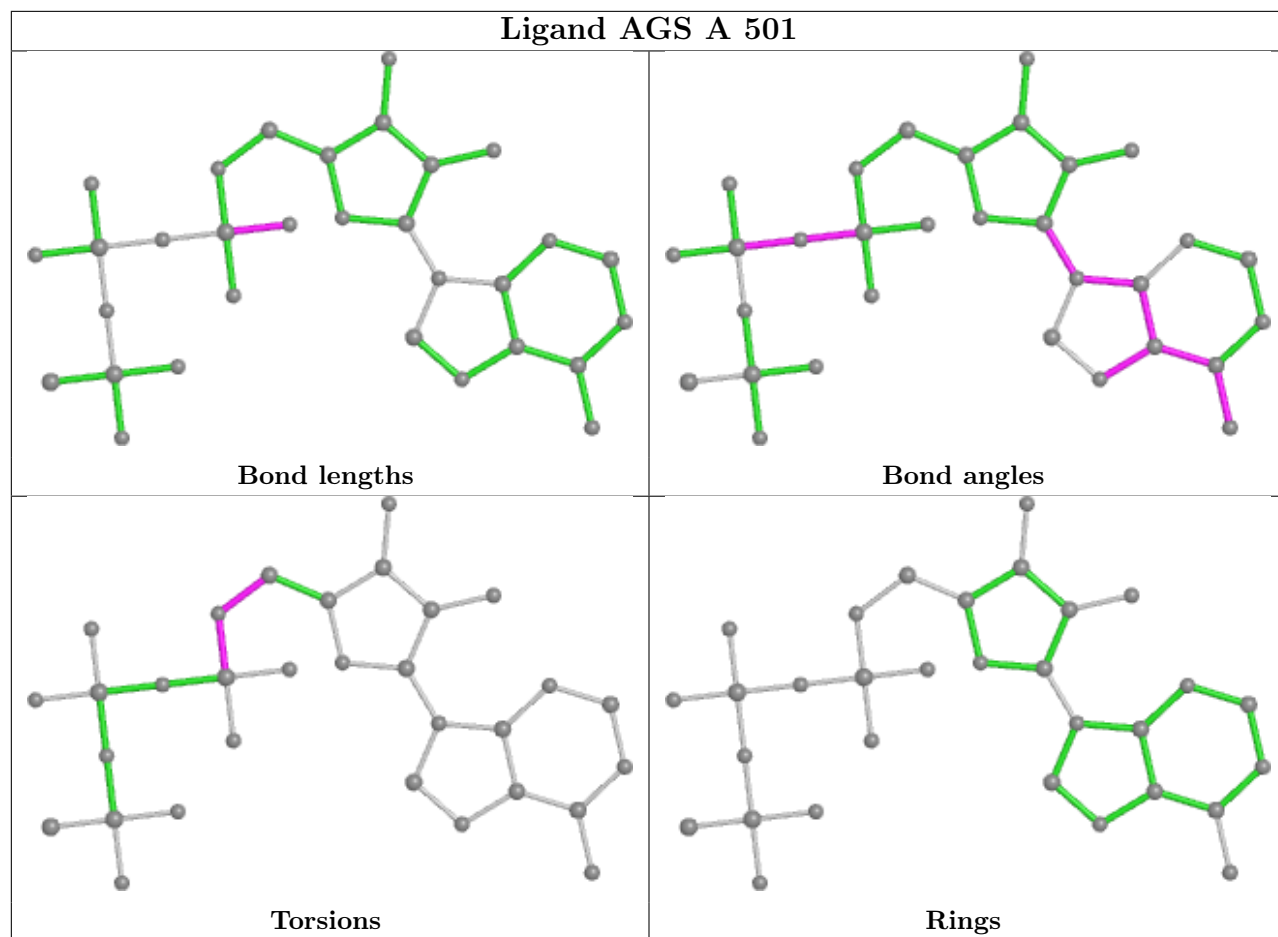
Mol	Chain	Res	Type	Atoms
34	A	501	AGS	C5'-O5'-PA-O1A
34	C	501	AGS	PB-O3B-PG-O2G
34	C	501	AGS	PB-O3B-PG-O3G
34	C	501	AGS	C5'-O5'-PA-O1A
34	C	501	AGS	C5'-O5'-PA-O2A
34	C	501	AGS	C5'-O5'-PA-O3A
34	D	501	AGS	C5'-O5'-PA-O1A
34	F	501	AGS	C5'-O5'-PA-O1A
34	F	501	AGS	C5'-O5'-PA-O2A
34	C	501	AGS	O4'-C4'-C5'-O5'
34	C	501	AGS	C3'-C4'-C5'-O5'
34	A	501	AGS	C4'-C5'-O5'-PA
34	D	501	AGS	PG-O3B-PB-O1B
34	D	501	AGS	C4'-C5'-O5'-PA
34	A	501	AGS	C5'-O5'-PA-O3A
34	D	501	AGS	C5'-O5'-PA-O3A
34	F	501	AGS	C5'-O5'-PA-O3A
34	C	501	AGS	PB-O3A-PA-O1A
34	A	501	AGS	C5'-O5'-PA-O2A
34	D	501	AGS	C5'-O5'-PA-O2A
34	F	501	AGS	C4'-C5'-O5'-PA
34	D	501	AGS	PA-O3A-PB-O2B
34	D	501	AGS	PA-O3A-PB-O1B
34	D	501	AGS	O4'-C4'-C5'-O5'

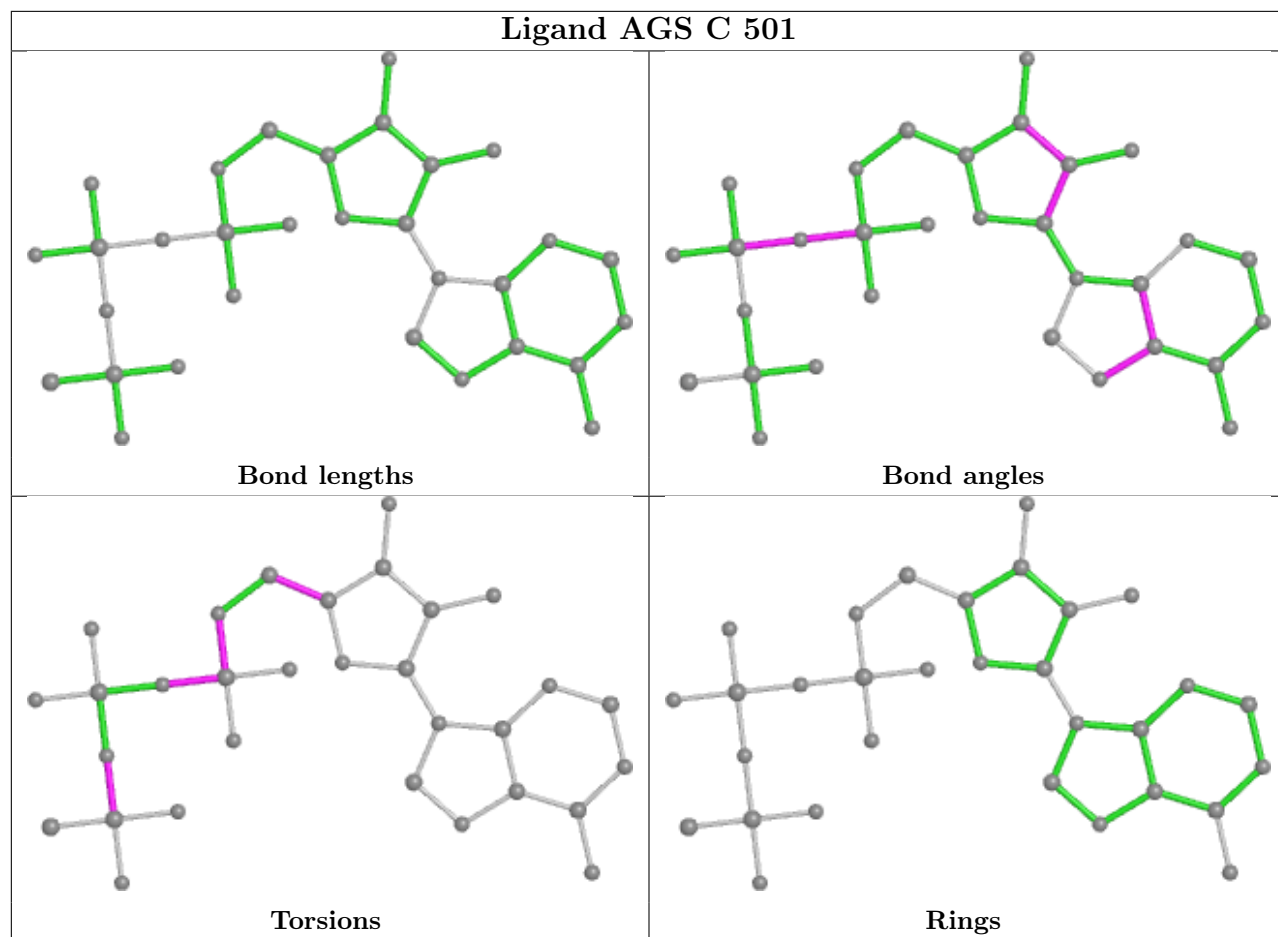
There are no ring outliers.

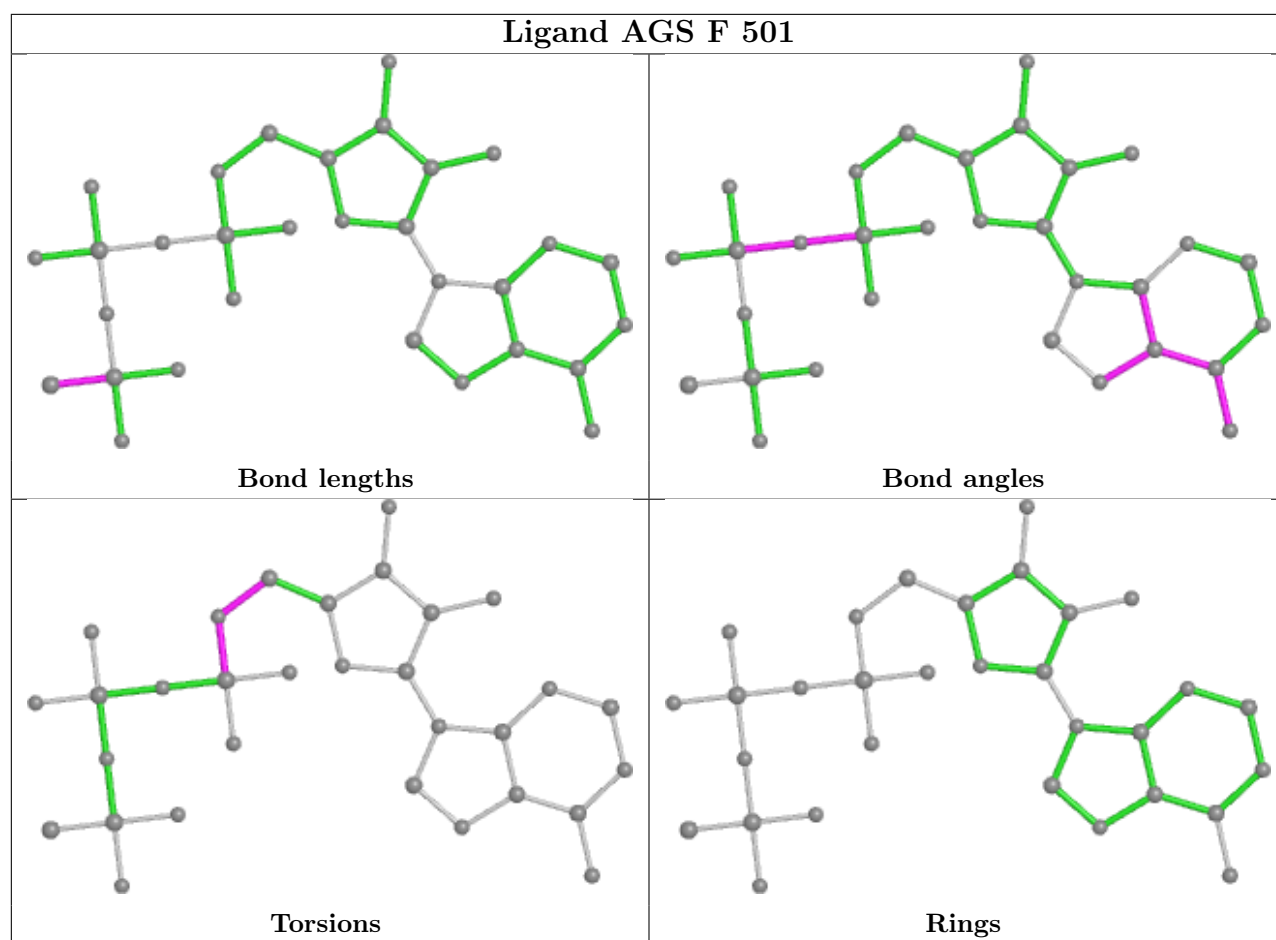
No monomer is involved in short contacts.

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.

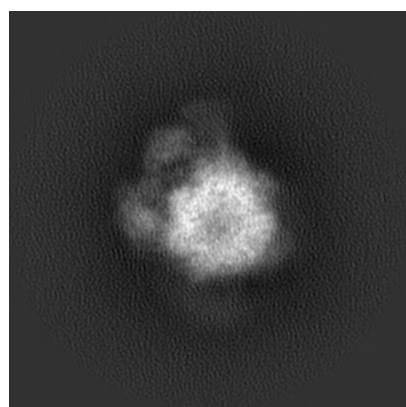
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8664. These allow visual inspection of the internal detail of the map and identification of artifacts.

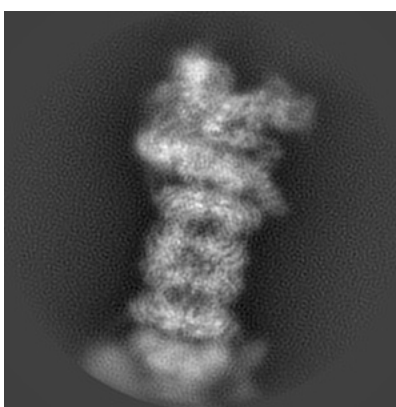
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

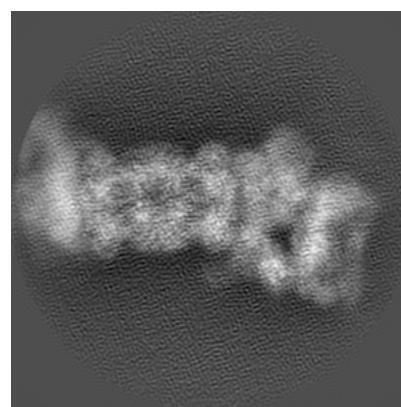
6.1.1 Primary map



X



Y

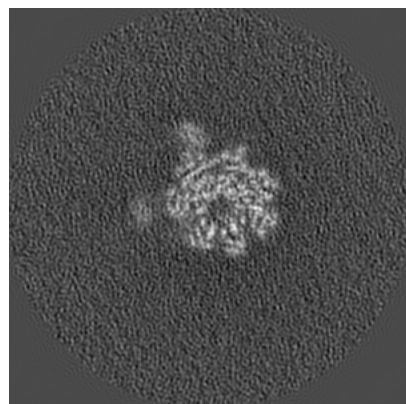


Z

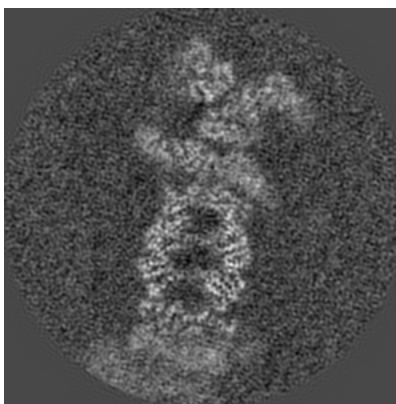
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

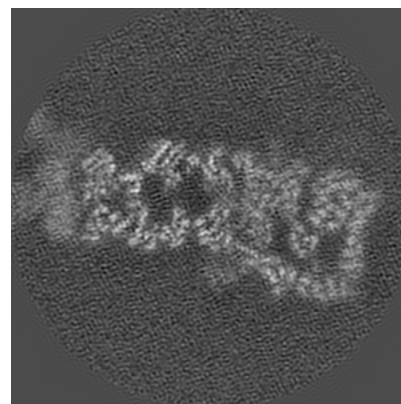
6.2.1 Primary map



X Index: 280



Y Index: 280

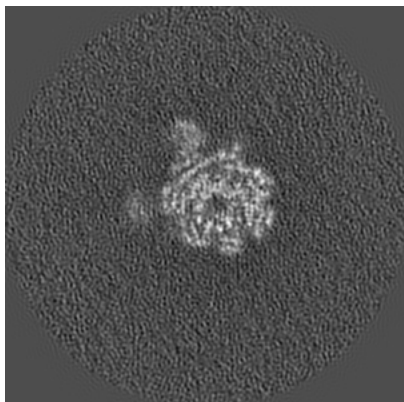


Z Index: 280

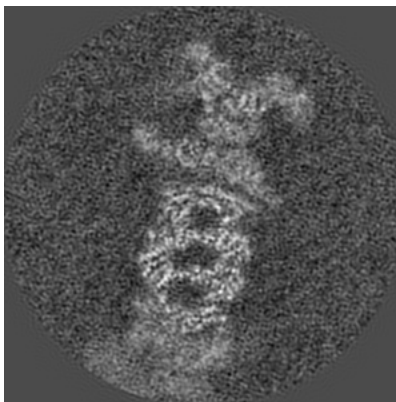
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

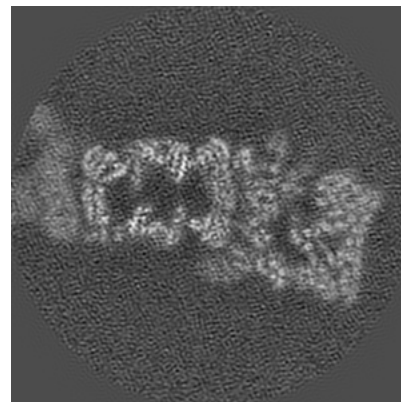
6.3.1 Primary map



X Index: 282



Y Index: 274

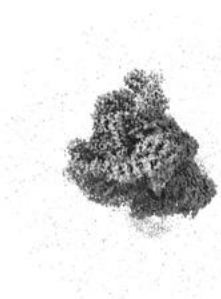


Z Index: 271

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

6.4 Orthogonal surface views [i](#)

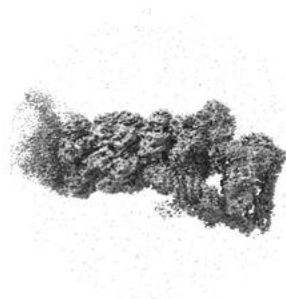
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.00577. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

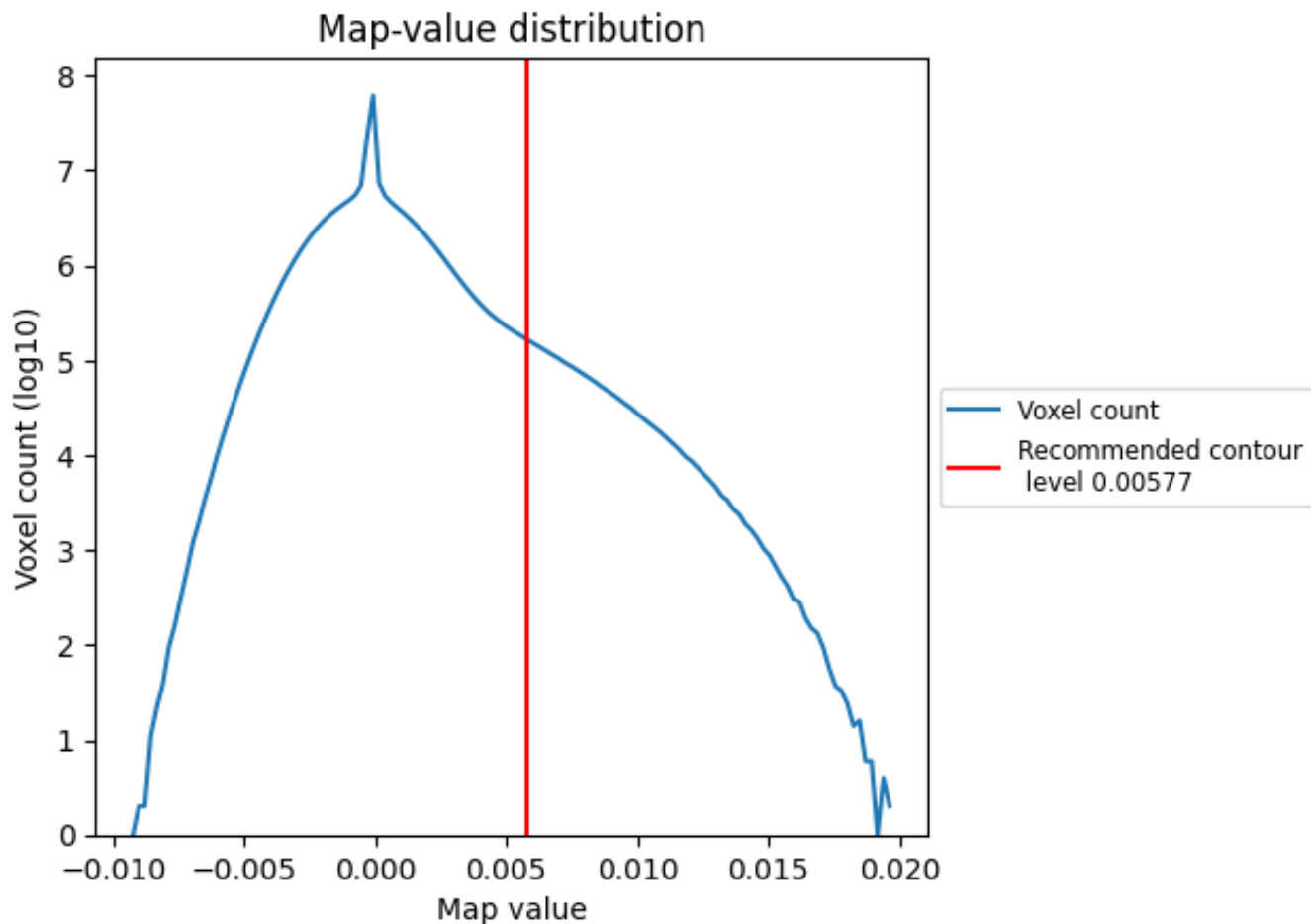
6.5 Mask visualisation

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

7 Map analysis [i](#)

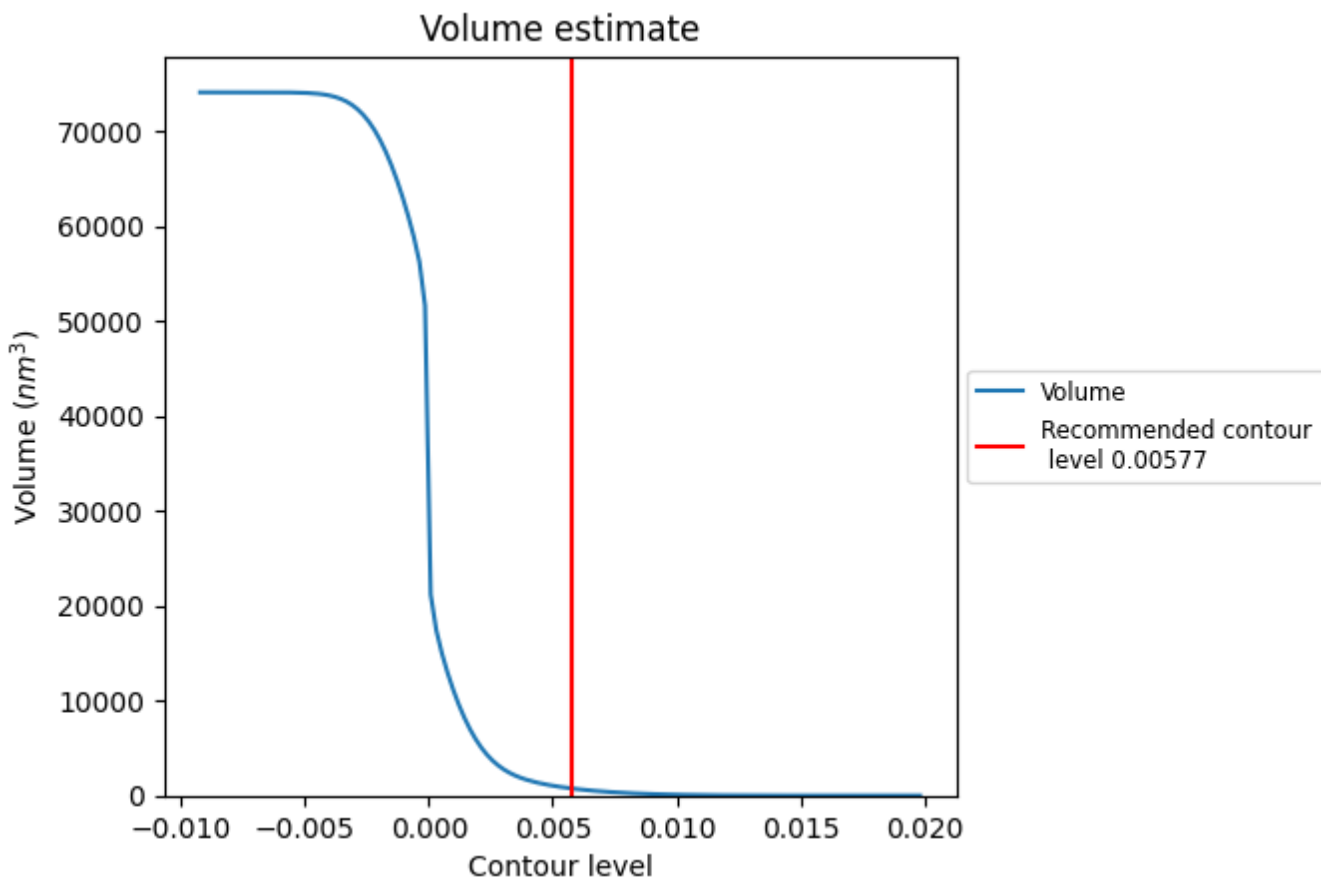
This section contains the results of statistical analysis of the map.

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.

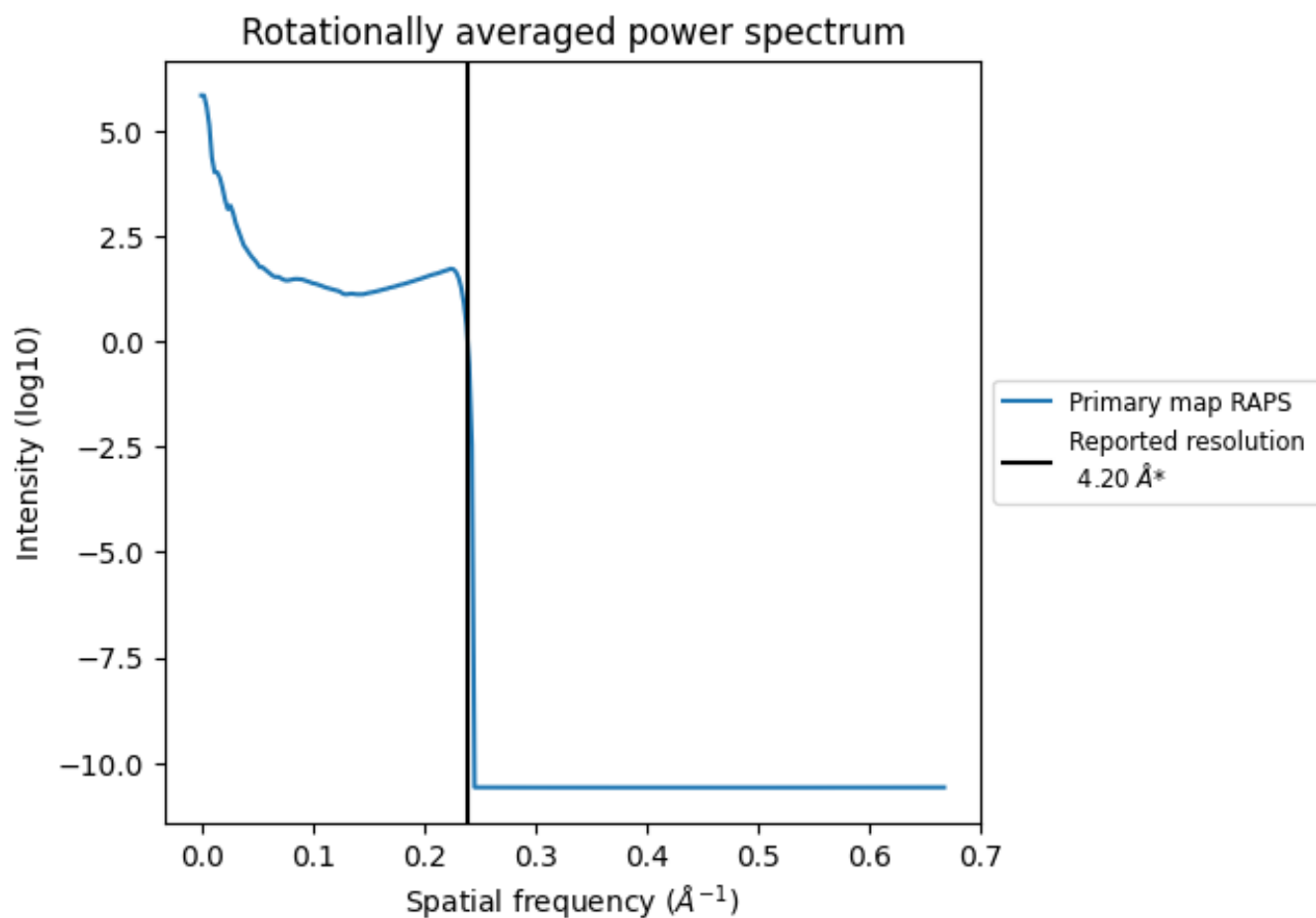
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 747 nm³; this corresponds to an approximate mass of 675 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 0.238 Å⁻¹

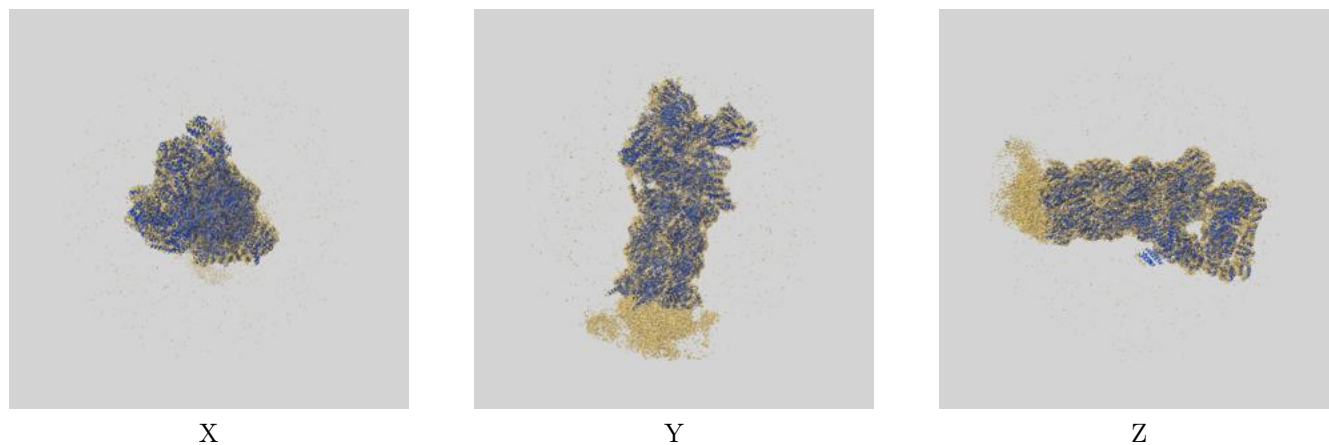
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

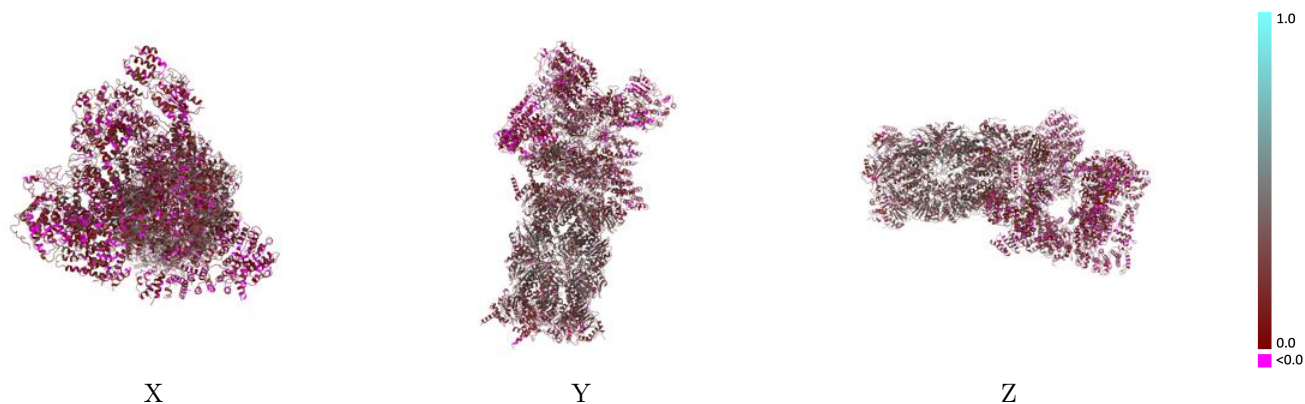
This section contains information regarding the fit between EMDB map EMD-8664 and PDB model 5VFQ. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay [i](#)



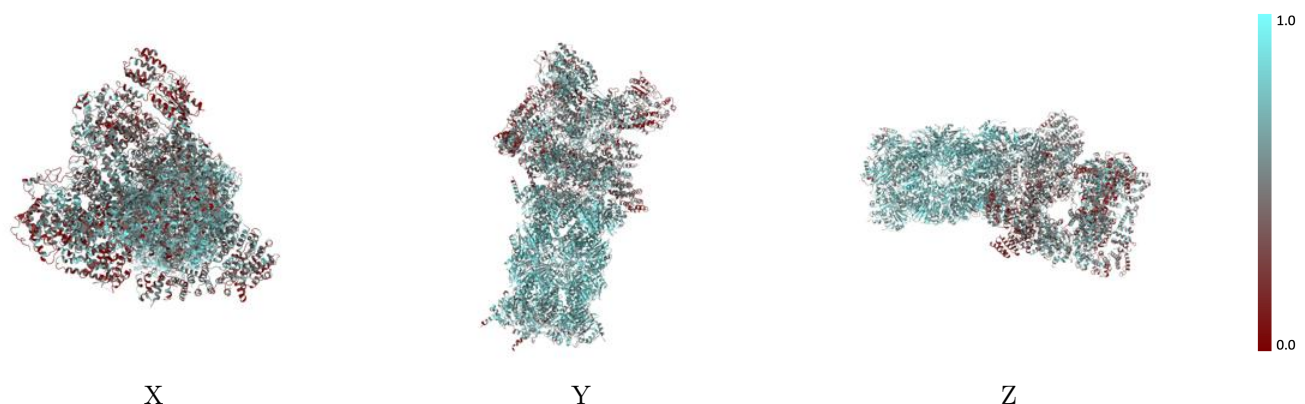
The images above show the 3D surface view of the map at the recommended contour level 0.00577 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



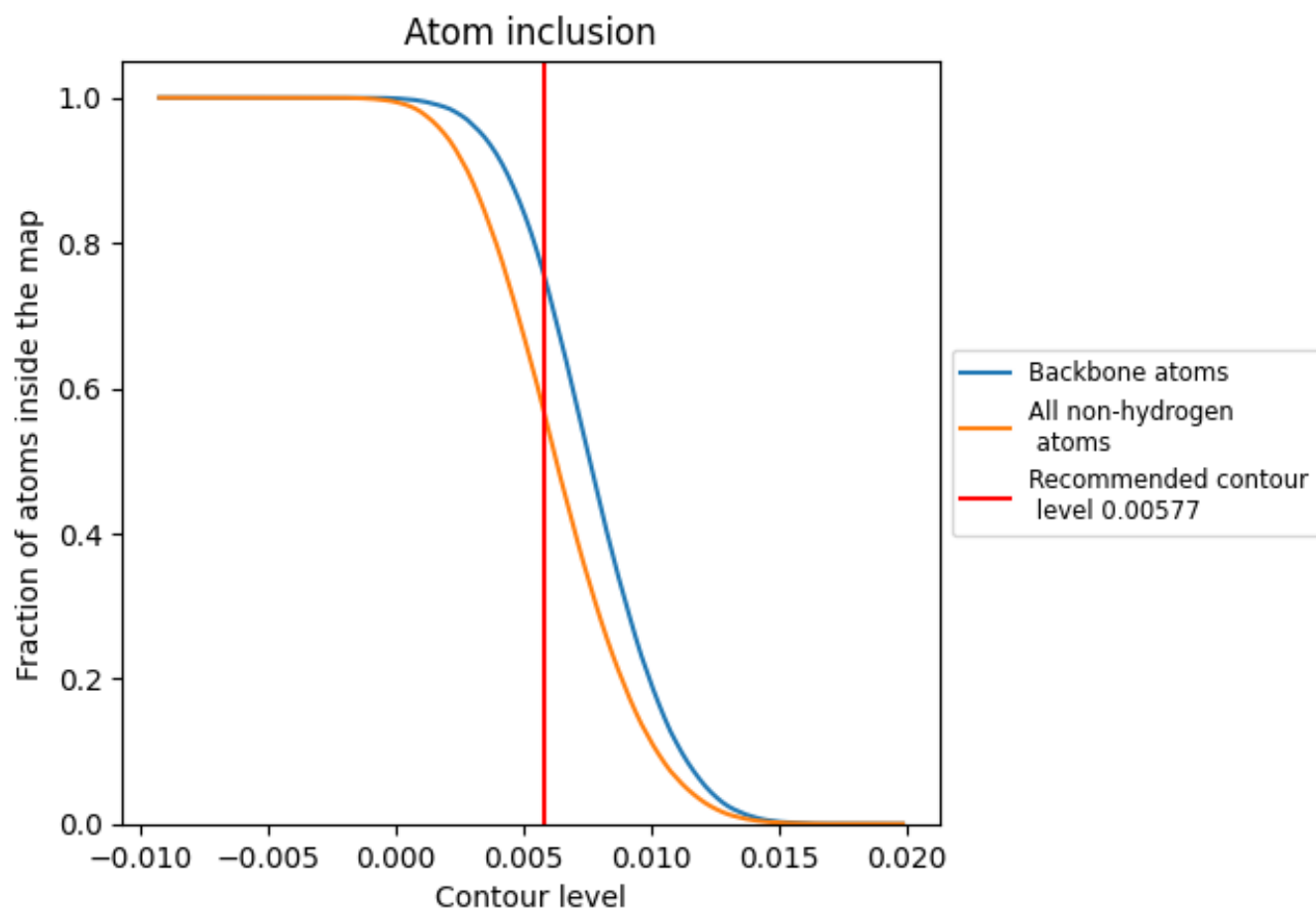
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00577).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 57% 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 (0.00577) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5713	 0.2320
A	 0.5554	 0.2440
B	 0.5407	 0.2530
C	 0.5406	 0.2550
D	 0.5100	 0.2380
E	 0.3741	 0.1640
F	 0.4877	 0.2180
G	 0.6257	 0.2550
H	 0.6825	 0.2870
I	 0.6036	 0.2560
J	 0.6471	 0.2710
K	 0.6431	 0.2680
L	 0.7178	 0.3020
M	 0.6720	 0.2740
N	 0.7411	 0.3140
O	 0.7299	 0.3220
P	 0.7304	 0.3280
Q	 0.7199	 0.3070
R	 0.7730	 0.3440
S	 0.7259	 0.3400
T	 0.7566	 0.3390
U	 0.5266	 0.1670
V	 0.4318	 0.1550
W	 0.3887	 0.1540
X	 0.3427	 0.1720
Y	 0.5734	 0.1910
Z	 0.4953	 0.1860
a	 0.4364	 0.1550
b	 0.3213	 0.1270
c	 0.5354	 0.1960
d	 0.3574	 0.1420
e	 0.4000	 0.1480
f	 0.4213	 0.0820
g	 0.6297	 0.2490
h	 0.6496	 0.2730



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Chain	Atom inclusion	Q-score
i	 0.5993	 0.2280
j	 0.6291	 0.2470
k	 0.6465	 0.2620
l	 0.6945	 0.2700
m	 0.6434	 0.2620
n	 0.7525	 0.3240
o	 0.7230	 0.3260
p	 0.7105	 0.3170
q	 0.7505	 0.3390
r	 0.7830	 0.3330
s	 0.7184	 0.3250
t	 0.7609	 0.3290