



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 07:32 AM UTC

PDB ID : 9E8G / pdb_00009e8g
EMDB ID : EMD-47719
Title : Nub1/Fat10-processing human 26S proteasome bound to Txnl1 with Rpt5 at top of spiral staircase
Authors : Arkinson, C.; Gee, C.L.; Martin, A.
Deposited on : 2024-11-05
Resolution : 3.01 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

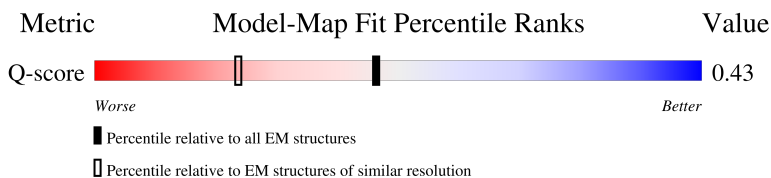
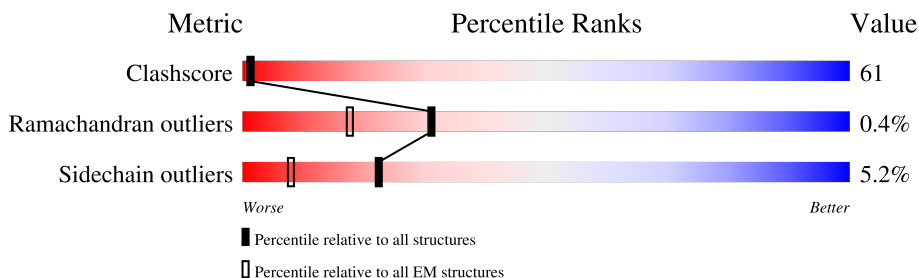
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.01 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13882 (2.51 - 3.51)

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	A	433	
2	B	440	
3	C	406	
4	D	418	

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Mol	Chain	Length	Quality of chain
5	E	389	
6	F	439	
7	G	246	
8	H	234	
9	I	261	
10	J	248	
11	K	241	
12	L	263	
13	M	255	
14	N	239	
15	P	277	
16	Q	205	
17	R	201	
18	S	263	
19	T	241	
20	U	953	
21	V	534	
22	W	456	
23	X	422	
24	Y	389	
25	Z	324	
26	a	376	
27	b	377	
28	c	424	
29	d	350	

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Mol	Chain	Length	Quality of chain
30	e	70	
31	f	908	
32	g	601	
33	h	264	
34	u	289	
35	v	12	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
38	ADP	C	501	-	-	X	-
38	ADP	D	501	-	-	X	-

2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 82193 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 26S proteasome regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	401	Total	C	N	O	S	0	0
			3163	1995	557	593	18		

- Molecule 2 is a protein called 26S proteasome regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	398	Total	C	N	O	S	0	0
			3126	1968	532	611	15		

- Molecule 3 is a protein called 26S protease regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	386	Total	C	N	O	S	0	0
			3051	1919	547	567	18		

- Molecule 4 is a protein called 26S proteasome regulatory subunit 6B.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	377	Total	C	N	O	S	0	0
			3018	1911	521	573	13		

- Molecule 5 is a protein called 26S protease regulatory subunit 10B.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	347	Total	C	N	O	S	0	0
			2750	1736	487	511	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	364	Total	C	N	O	S	0	0
			2850	1803	492	538	17		

- Molecule 7 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	239	Total	C	N	O	S	0	0
			1831	1164	306	348	13		

- Molecule 8 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	232	Total	C	N	O	S	0	0
			1813	1158	307	342	6		

- Molecule 9 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	248	Total	C	N	O	S	0	0
			1908	1205	325	369	9		

- Molecule 10 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	239	Total	C	N	O	S	0	0
			1813	1136	320	352	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	230	VAL	ALA	conflict	UNP O14818

- Molecule 11 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	231	Total	C	N	O	S	0	0
			1763	1106	292	355	10		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	83	LYS	ALA	conflict	UNP P28066

- Molecule 12 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	237	Total	C	N	O	S	0	0
			1845	1156	333	345	11		

- Molecule 13 is a protein called Proteasome subunit alpha type-3.

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

- Molecule 14 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	197	Total	C	N	O	S	0	0
			1482	928	253	289	12		

- Molecule 15 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	220	Total	C	N	O	S	0	0
			1645	1035	278	320	12		

- Molecule 16 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	204	Total	C	N	O	S	0	0
			1587	1010	264	294	19		

- Molecule 17 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	199	Total	C	N	O	S	0	0
			1588	1017	270	292	9		

- Molecule 18 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	201	Total	C	N	O	S	0	0
			1559	982	274	294	9		

- Molecule 19 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	213	Total	C	N	O	S	0	0
			1641	1041	281	309	10		

- Molecule 20 is a protein called 26S proteasome non-ATPase regulatory subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	U	844	Total	C	N	O	S	0	0
			6584	4178	1119	1243	44		

- Molecule 21 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	442	Total	C	N	O	S	0	0
			3602	2296	643	650	13		

- Molecule 22 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	438	Total	C	N	O	S	0	0
			3570	2261	609	677	23		

- Molecule 23 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	378	Total	C	N	O	S	0	0
			2994	1909	507	566	12		

- Molecule 24 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	379	Total	C	N	O	S	0	0
			3123	1993	534	579	17		

- Molecule 25 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	a	372	Total	C	N	O	S	0	0
			2991	1909	509	558	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	190	Total	C	N	O	S	0	0
			1454	908	260	278	8		

- Molecule 28 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	c	288	Total	C	N	O	S	0	0
			2264	1433	390	422	19		

- Molecule 29 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	d	269	Total	C	N	O	S	0	0
			2188	1414	359	406	9		

- Molecule 30 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	e	41	Total	C	N	O	0	0
			353	217	55	81		

- Molecule 31 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	f	842	Total	C	N	O	S	0	0
			6512	4117	1105	1245	45		

- Molecule 32 is a protein called Isoform 2 of NEDD8 ultimate buster 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	g	95	Total	C	N	O	S	0	0
			771	487	139	144	1		

- Molecule 33 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	h	206	Total	C	N	O	S	0	0
			1601	1010	277	303	11		

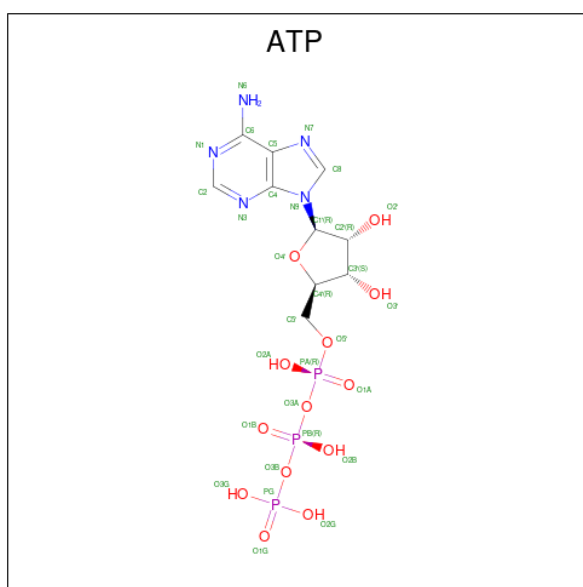
- Molecule 34 is a protein called Thioredoxin-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	u	172	Total	C	N	O	S	0	0
			1376	865	226	276	9		

- Molecule 35 is a protein called substrate peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	v	12	Total	C	N	O	0	0
			60	36	12	12		

- Molecule 36 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



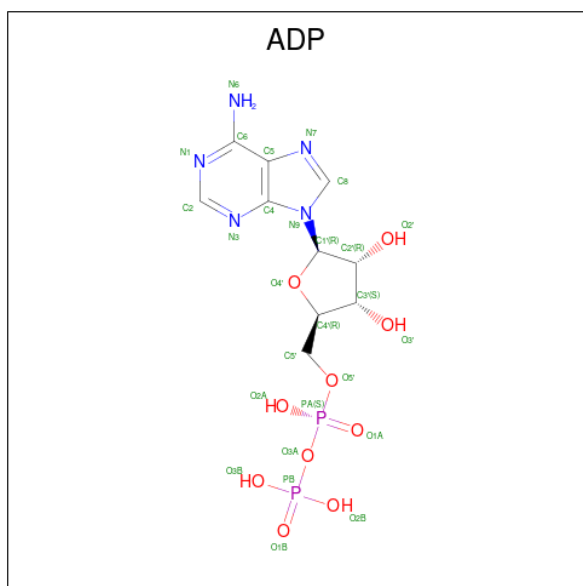
Mol	Chain	Residues	Atoms					AltConf
36	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
36	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
36	F	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 37 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of

Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
37	A	1	Total	Mg	0
			1	1	
37	B	1	Total	Mg	0
			1	1	
37	C	1	Total	Mg	0
			1	1	
37	D	1	Total	Mg	0
			1	1	
37	F	1	Total	Mg	0
			1	1	

- Molecule 38 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
38	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
38	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
38	E	1	Total	C	N	O	P	0
			27	10	5	10	2	

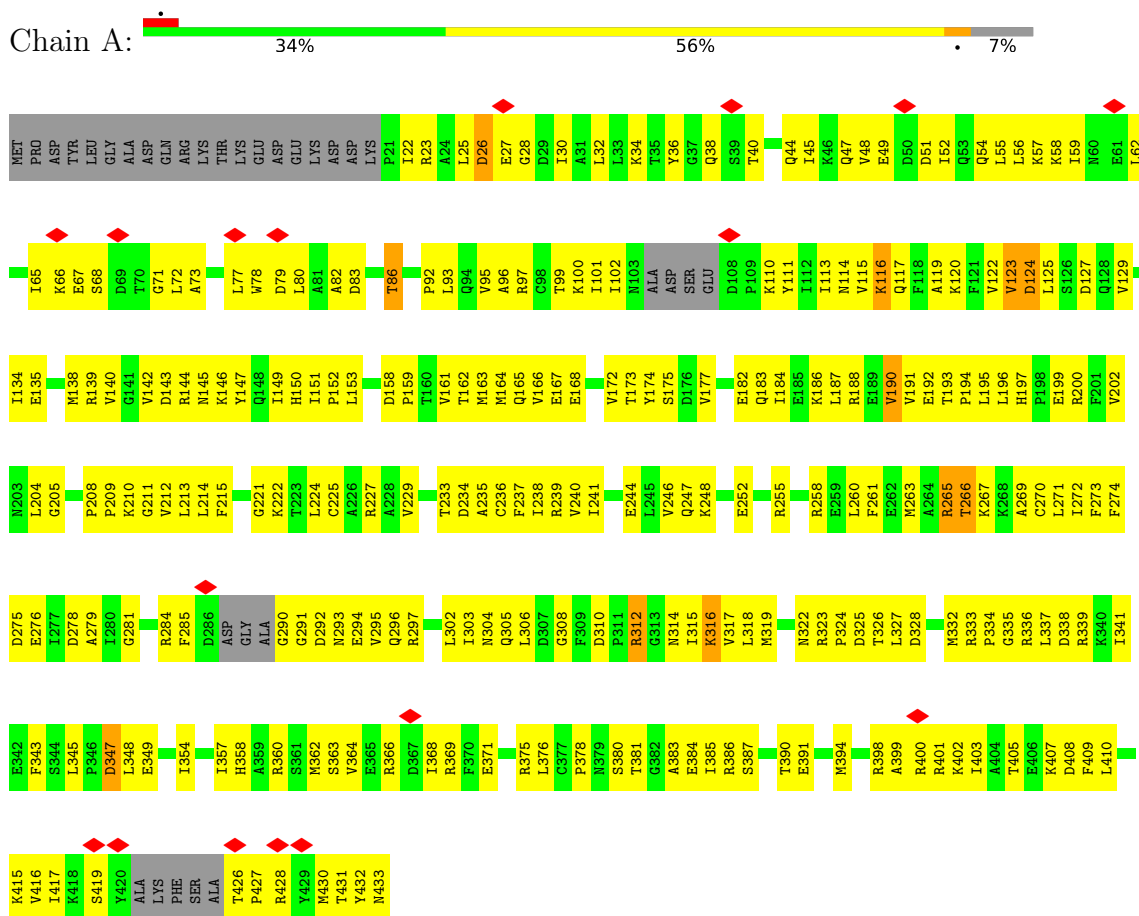
- Molecule 39 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
39	u	1	Total	Zn	0
			1	1	

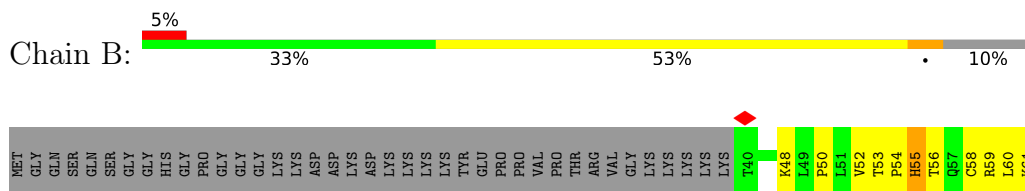
3 Residue-property plots

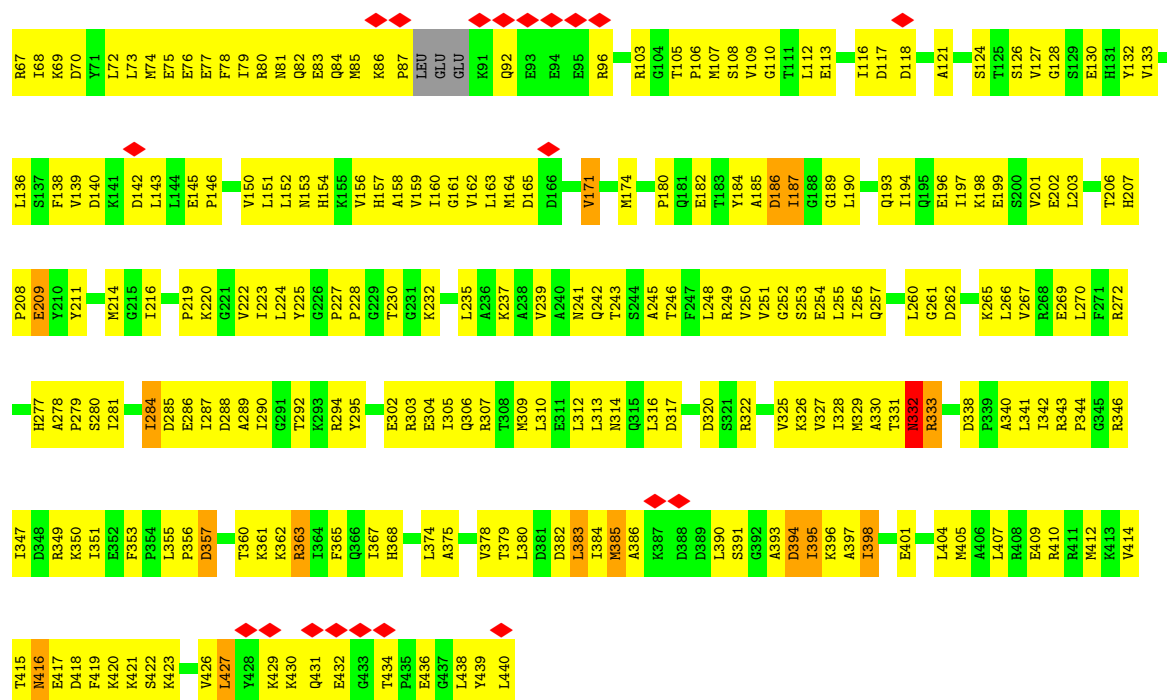
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: 26S proteasome regulatory subunit 7



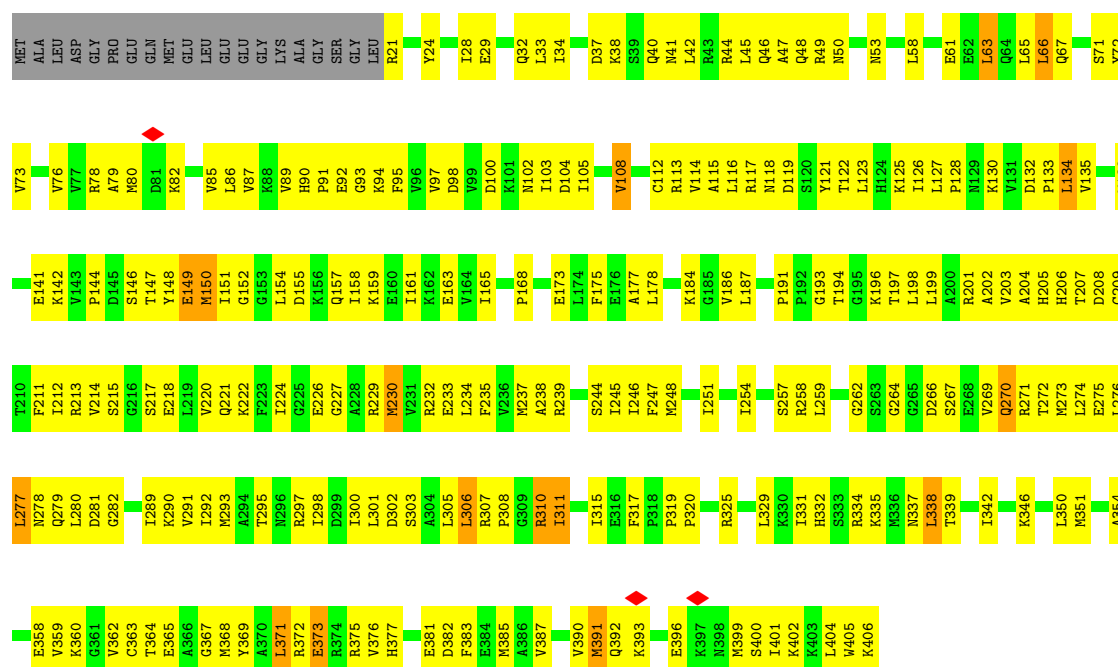
• Molecule 2: 26S proteasome regulatory subunit 4





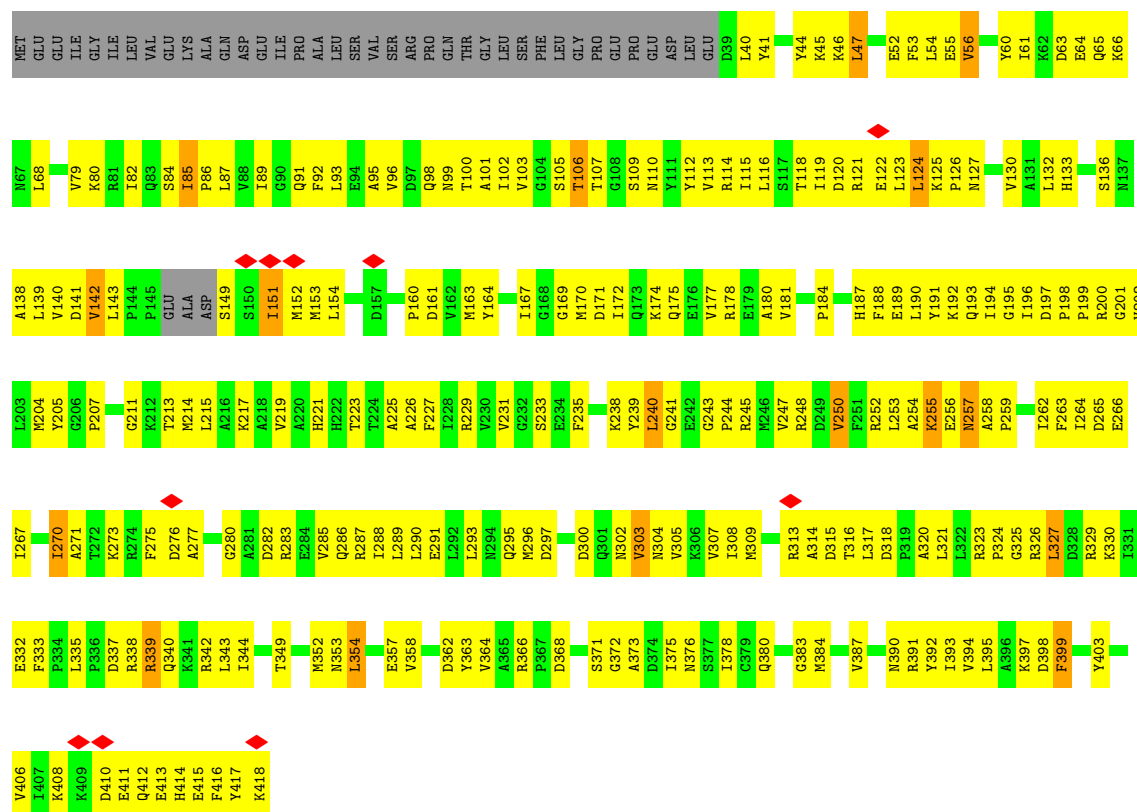
• Molecule 3: 26S protease regulatory subunit 8

Chain C: 37% 54% 5%

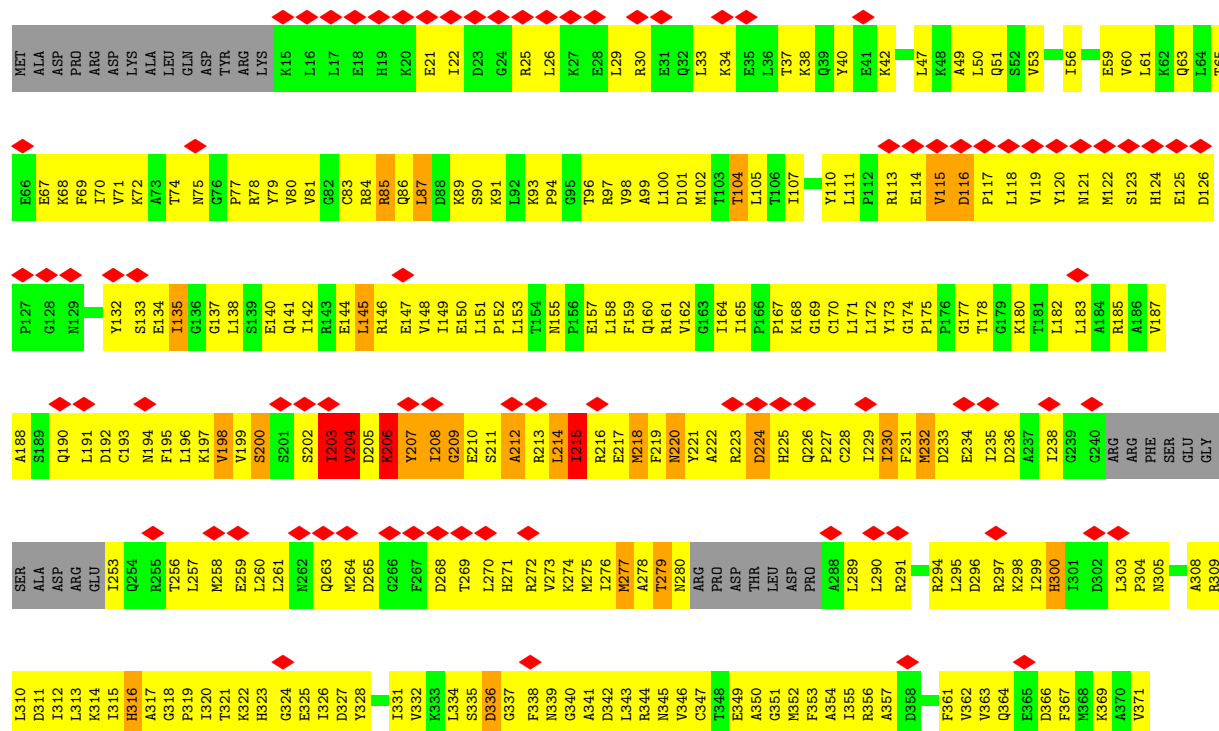


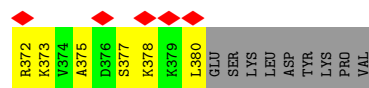
• Molecule 4: 26S proteasome regulatory subunit 6B

Chain D: 33% 54% 10%

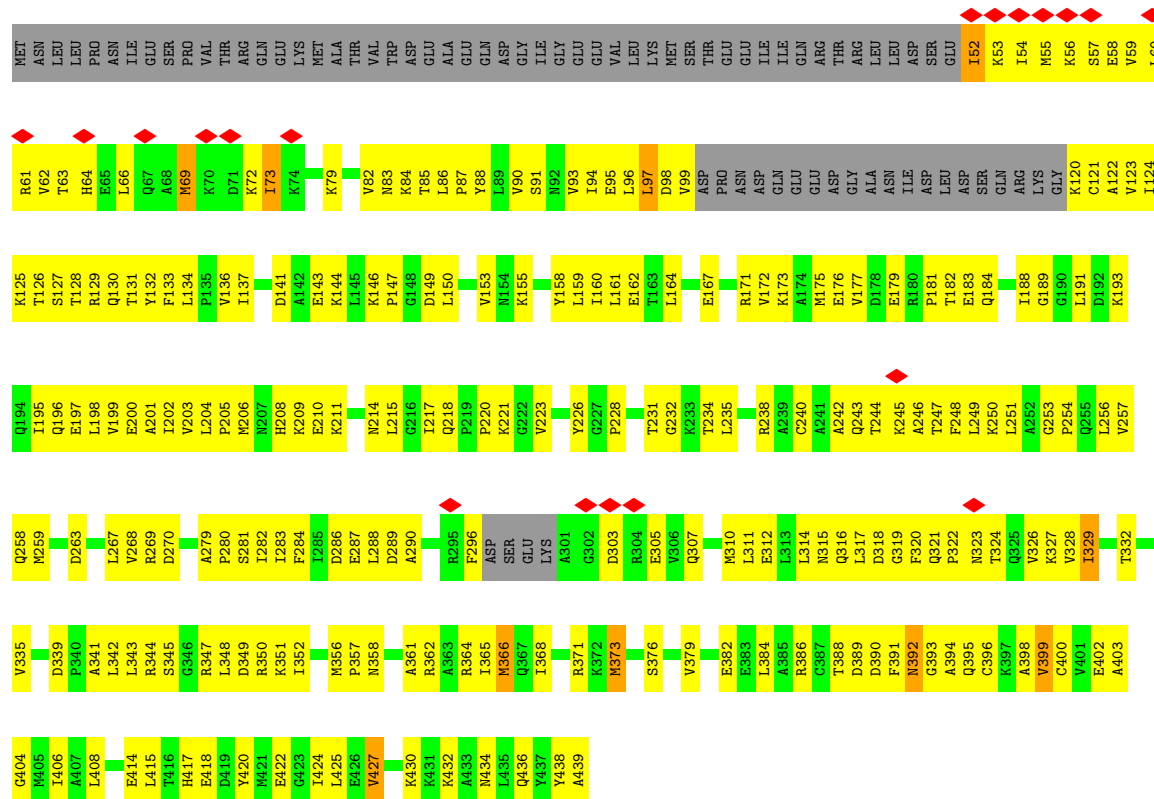
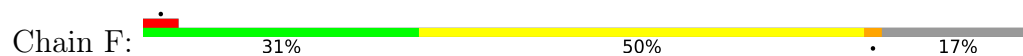


• Molecule 5: 26S protease regulatory subunit 10B

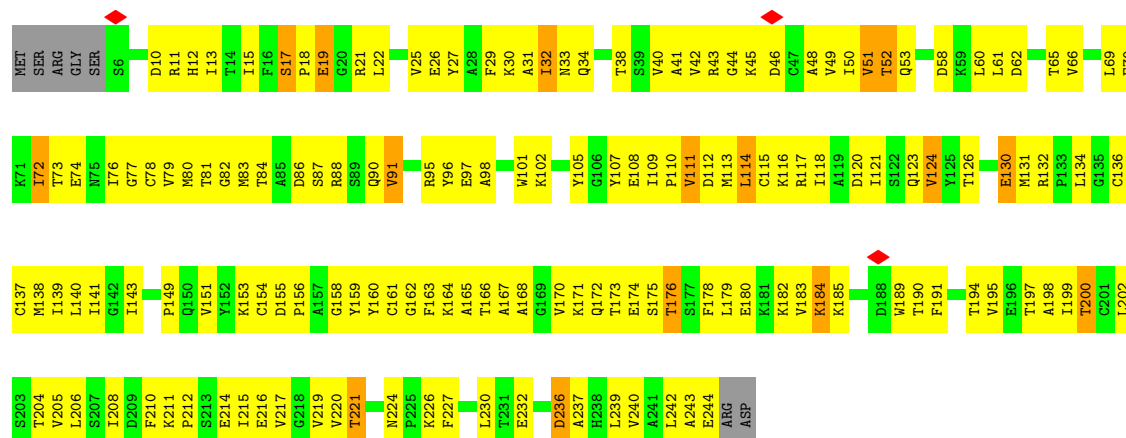




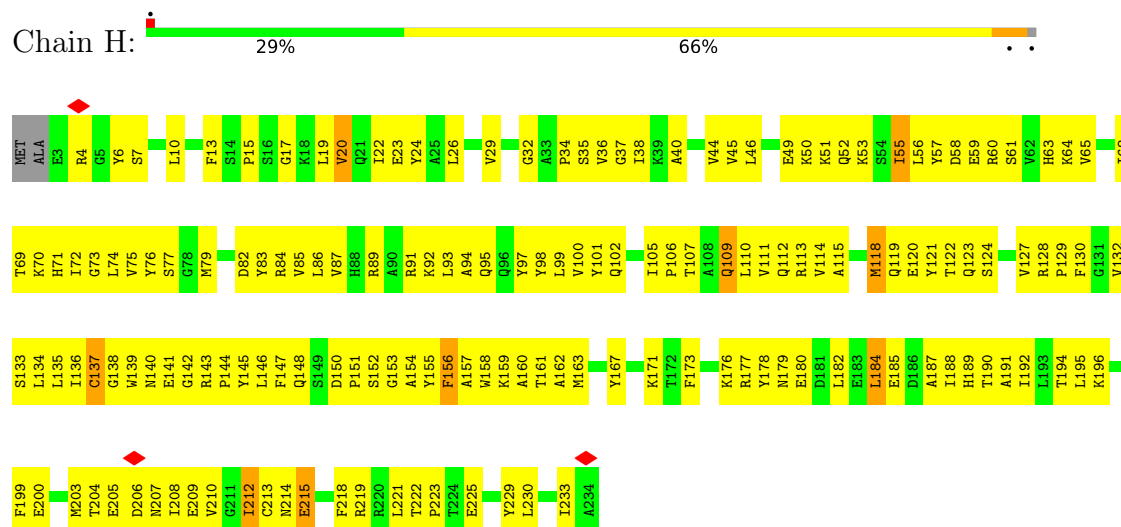
• Molecule 6: 26S proteasome regulatory subunit 6A



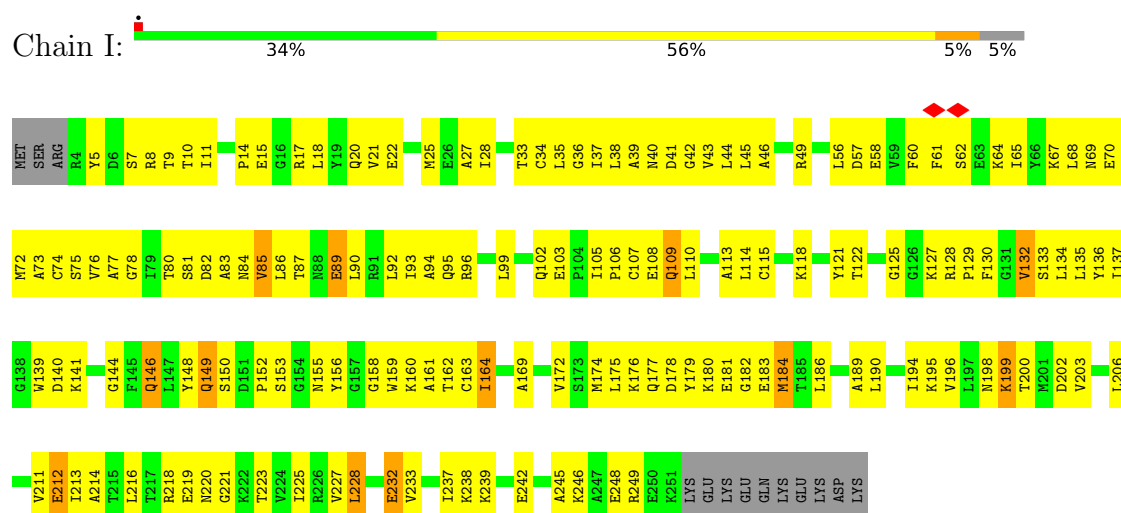
• Molecule 7: Proteasome subunit alpha type-6



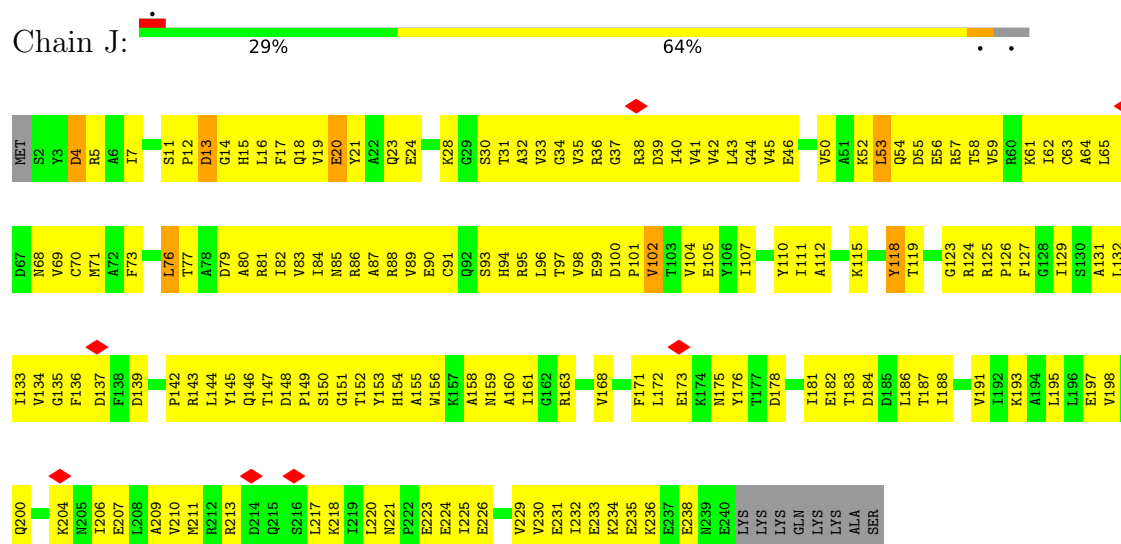
• Molecule 8: Proteasome subunit alpha type-2



• Molecule 9: Proteasome subunit alpha type-4

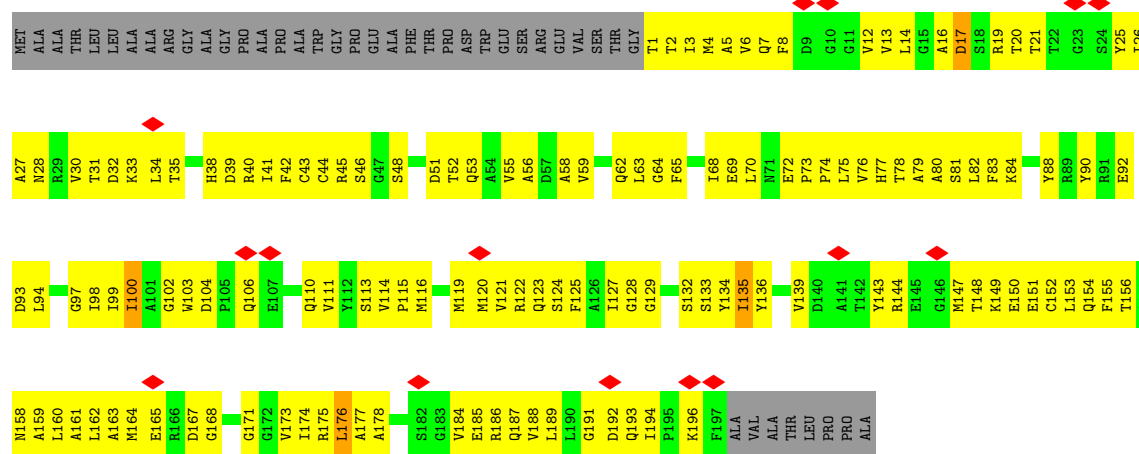


• Molecule 10: Proteasome subunit alpha type-7

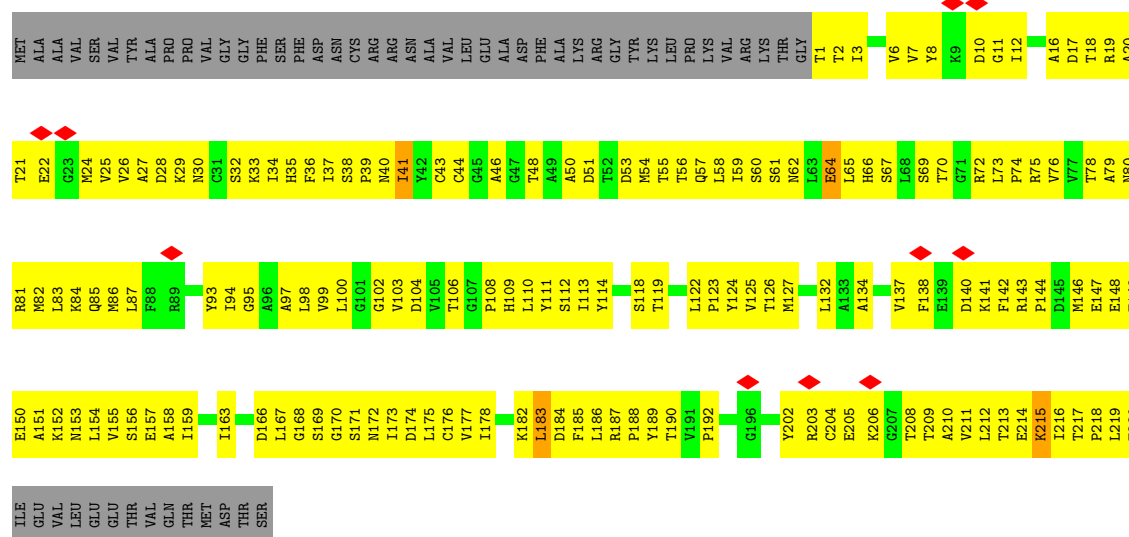




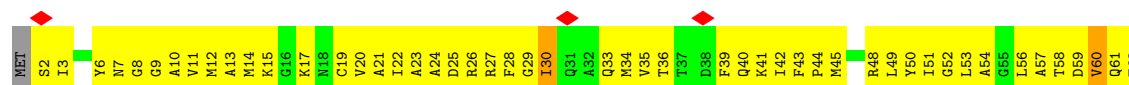
• Molecule 14: Proteasome subunit beta type-6

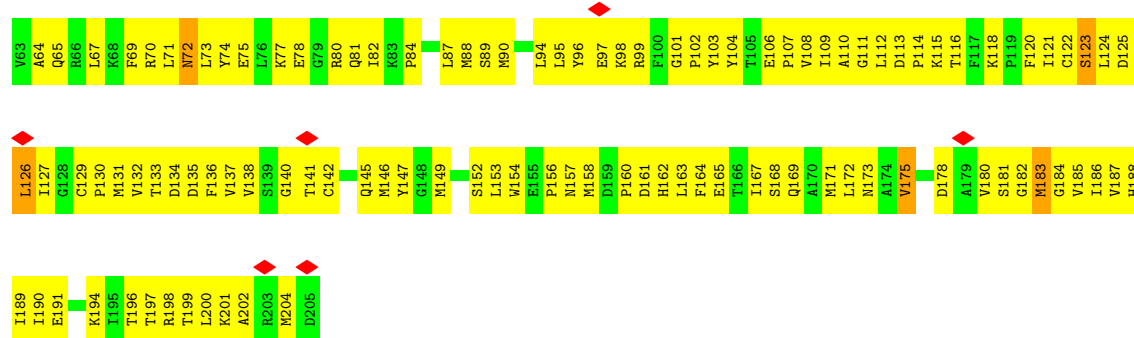


• Molecule 15: Proteasome subunit beta type-7

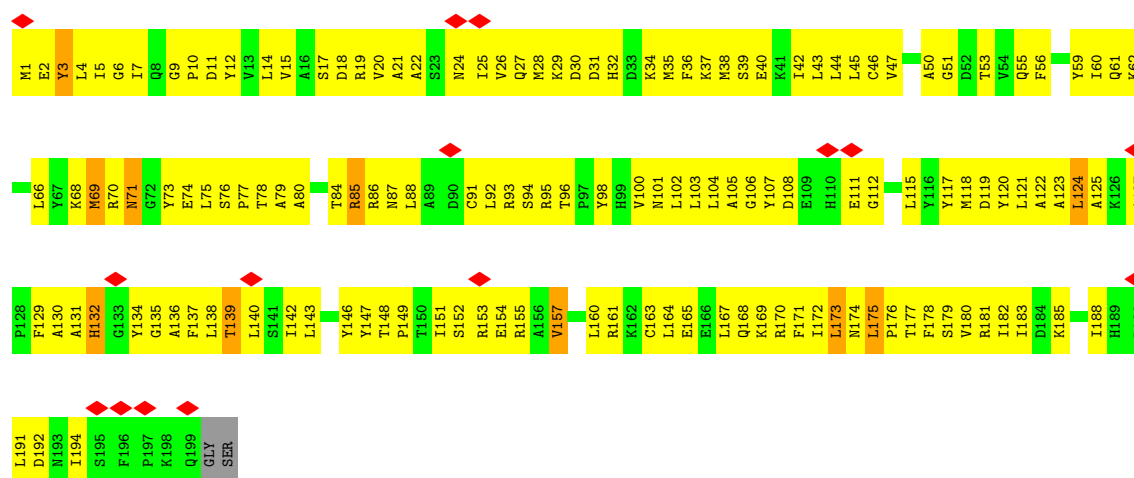


• Molecule 16: Proteasome subunit beta type-3

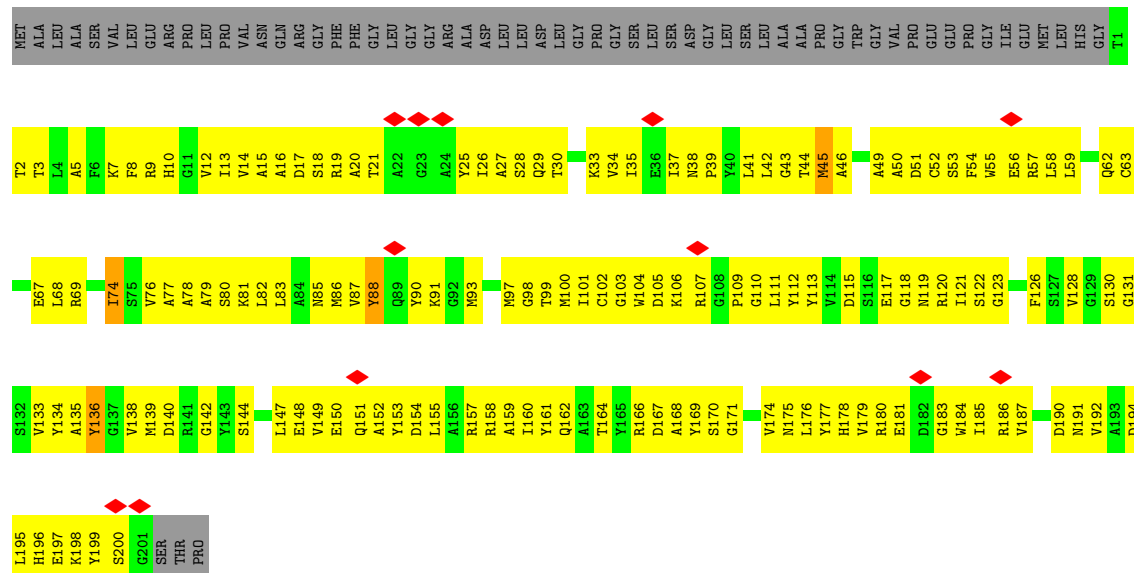
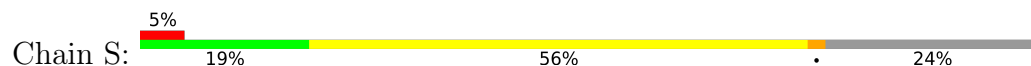




• Molecule 17: Proteasome subunit beta type-2



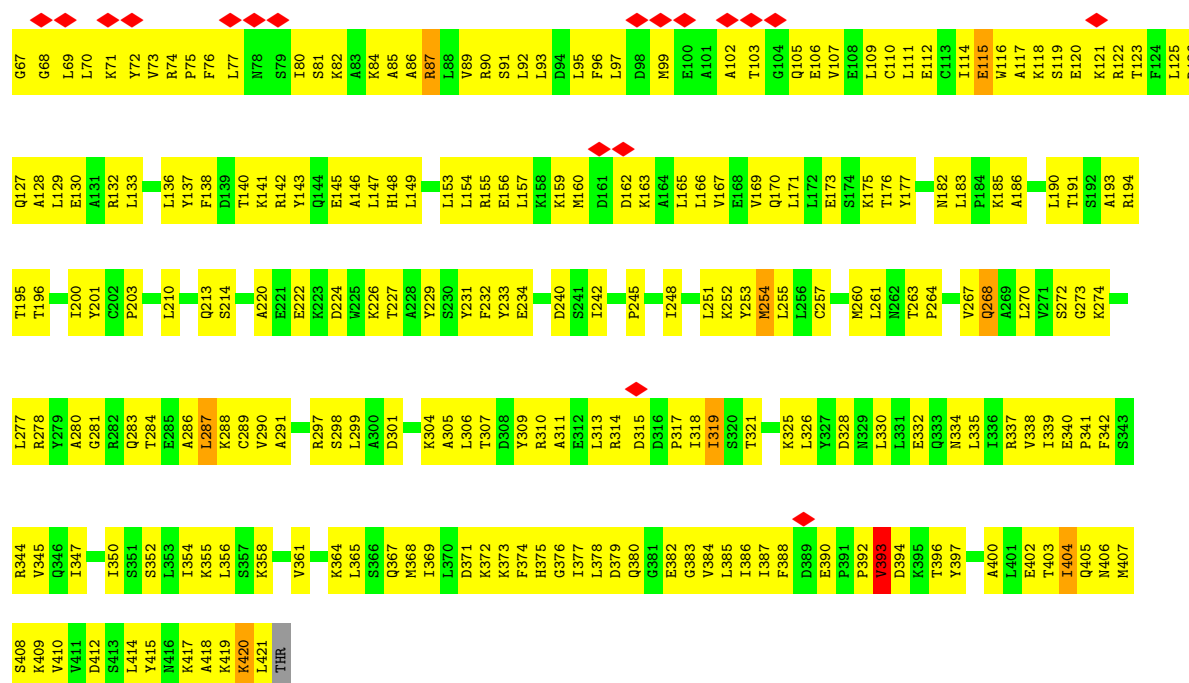
• Molecule 18: Proteasome subunit beta type-5



Chain T:

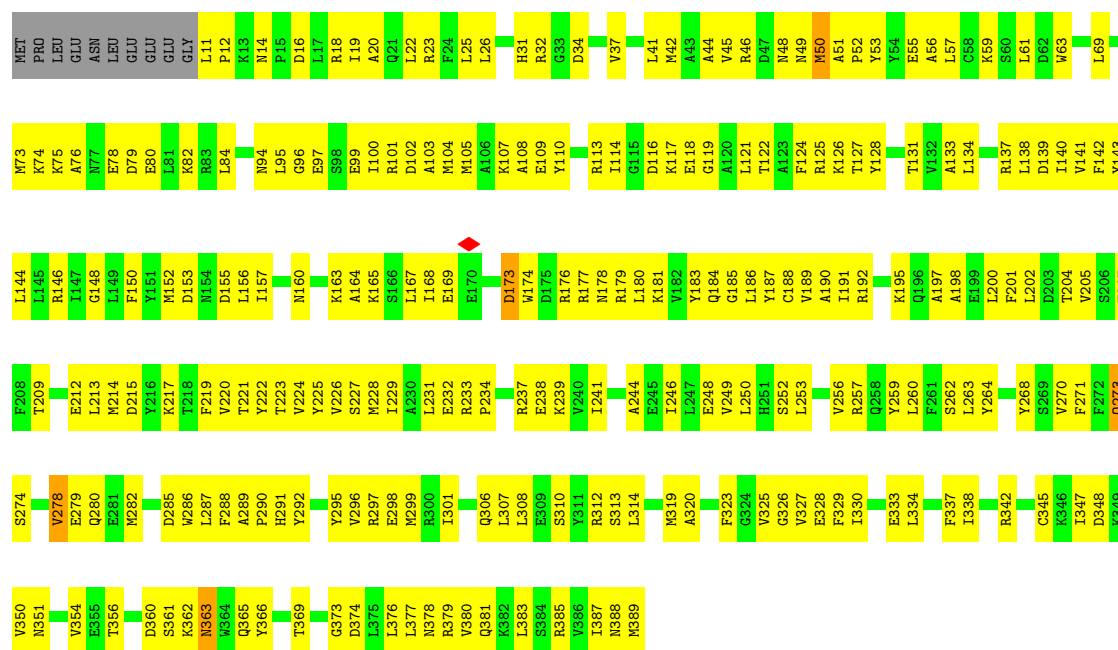
Chain U:





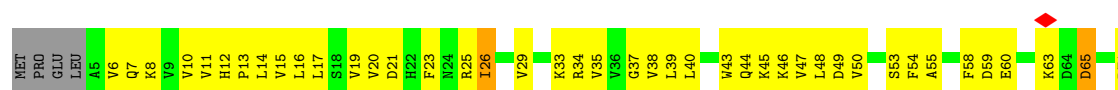
• Molecule 24: 26S proteasome non-ATPase regulatory subunit 6

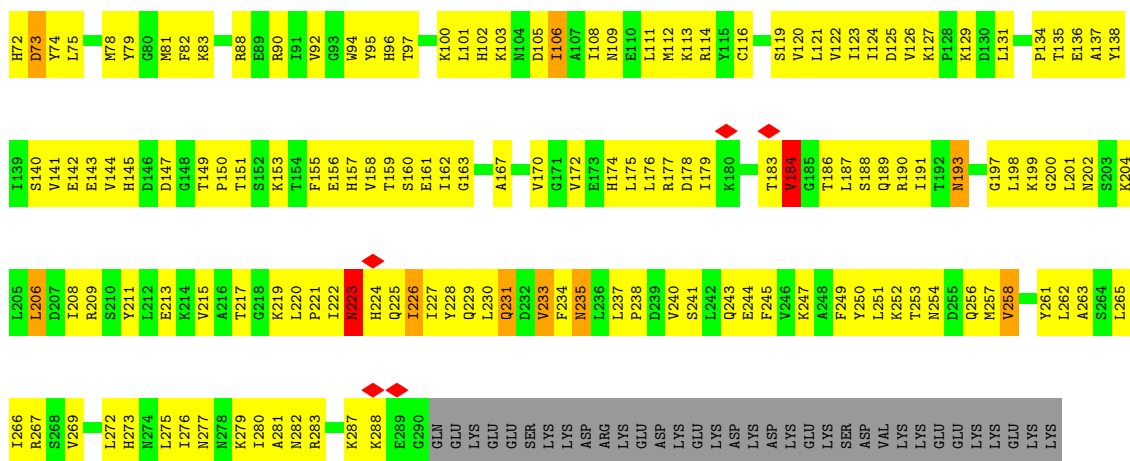
Chain Y: 38% 59%



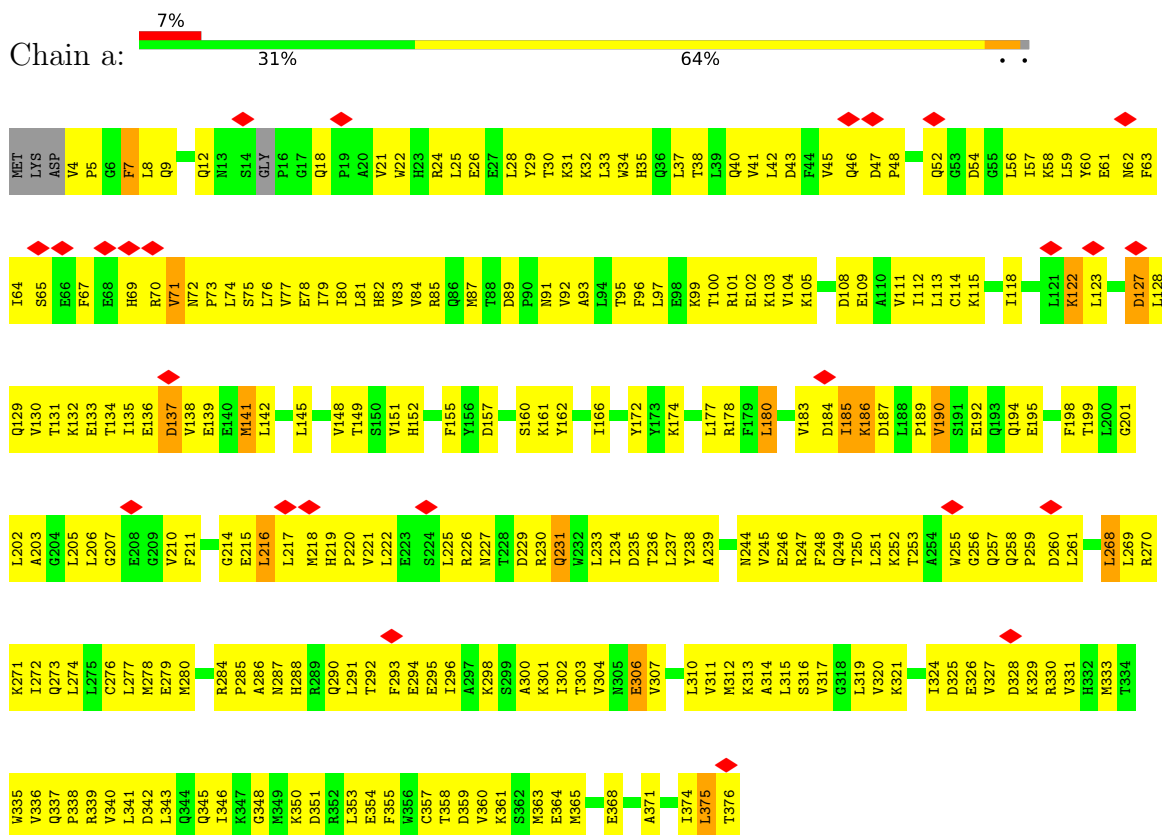
• Molecule 25: 26S proteasome non-ATPase regulatory subunit 7

Chain Z: 29% 55% 12%

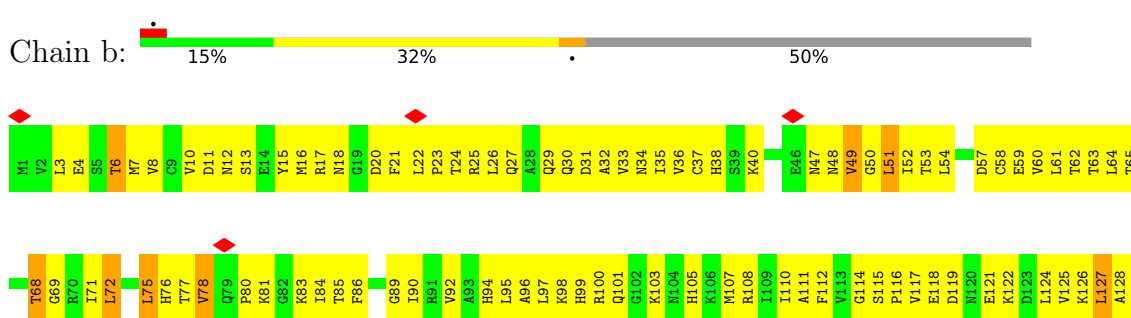




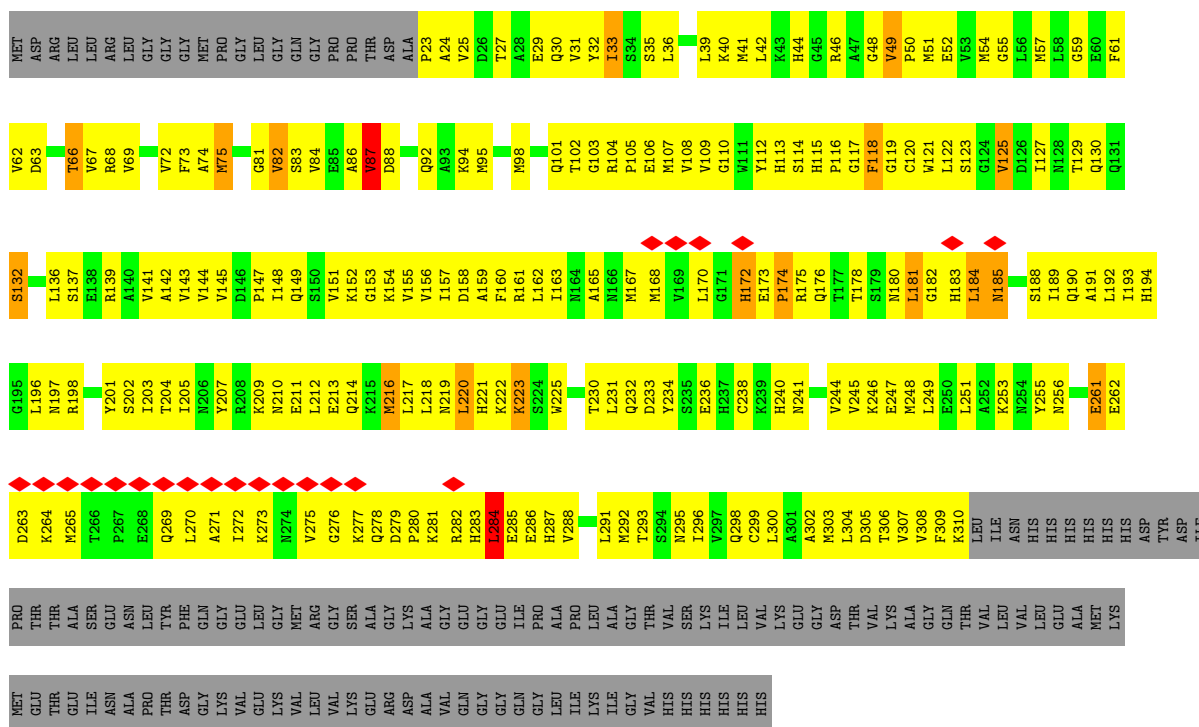
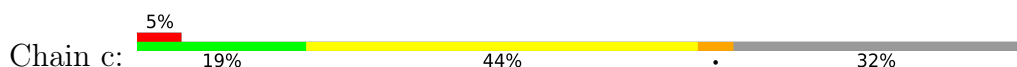
• Molecule 26: 26S proteasome non-ATPase regulatory subunit 13



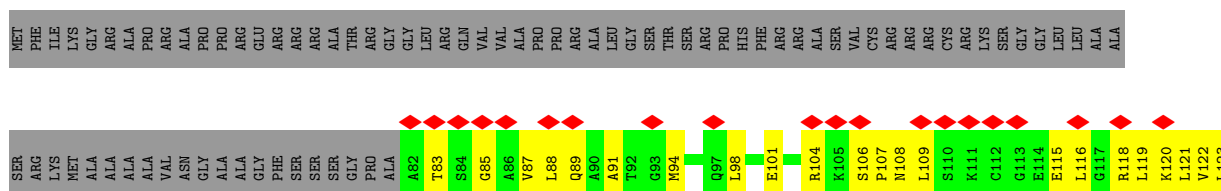
• Molecule 27: 26S proteasome non-ATPase regulatory subunit 4

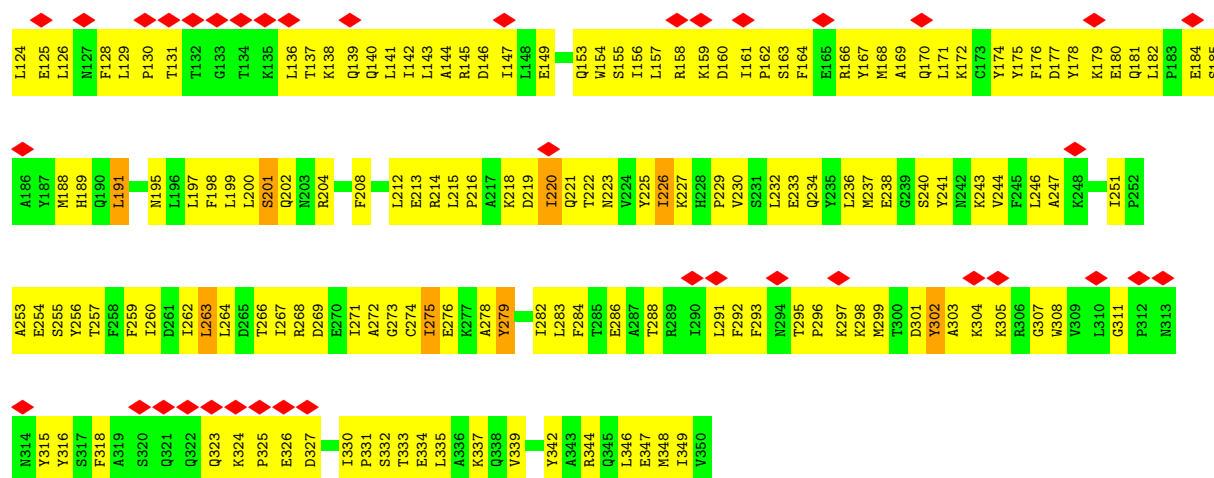


- Molecule 28: 26S proteasome non-ATPase regulatory subunit 14

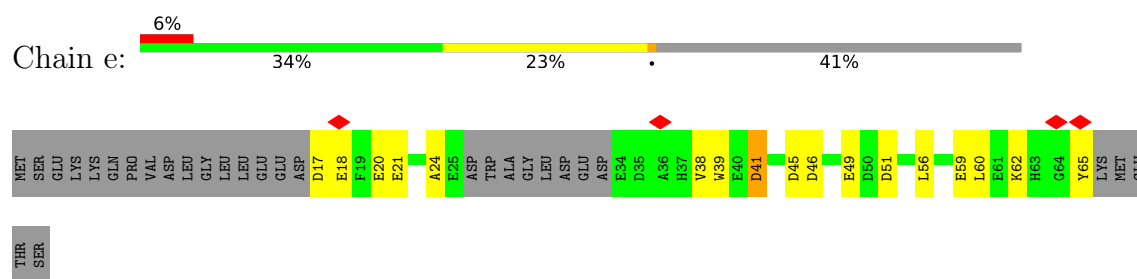


- Molecule 29: 26S proteasome non-ATPase regulatory subunit 8

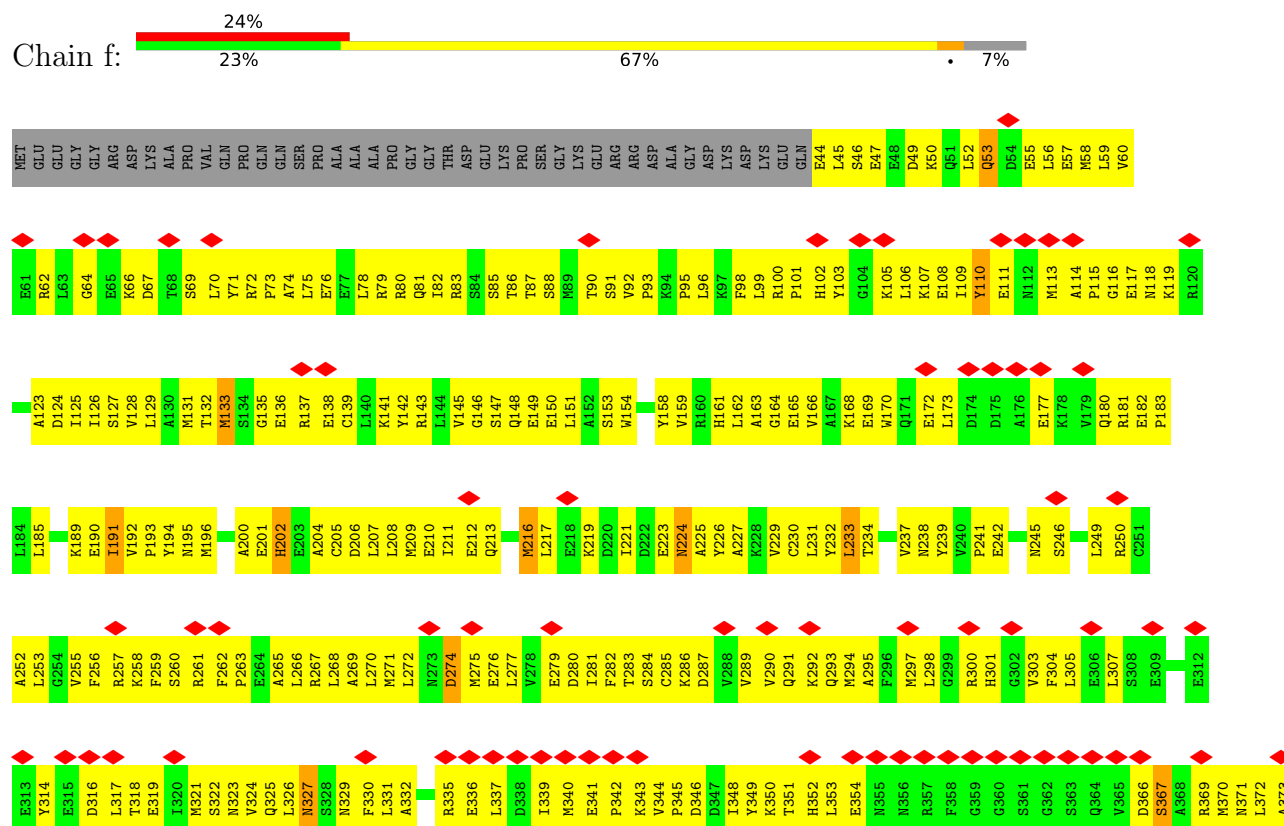


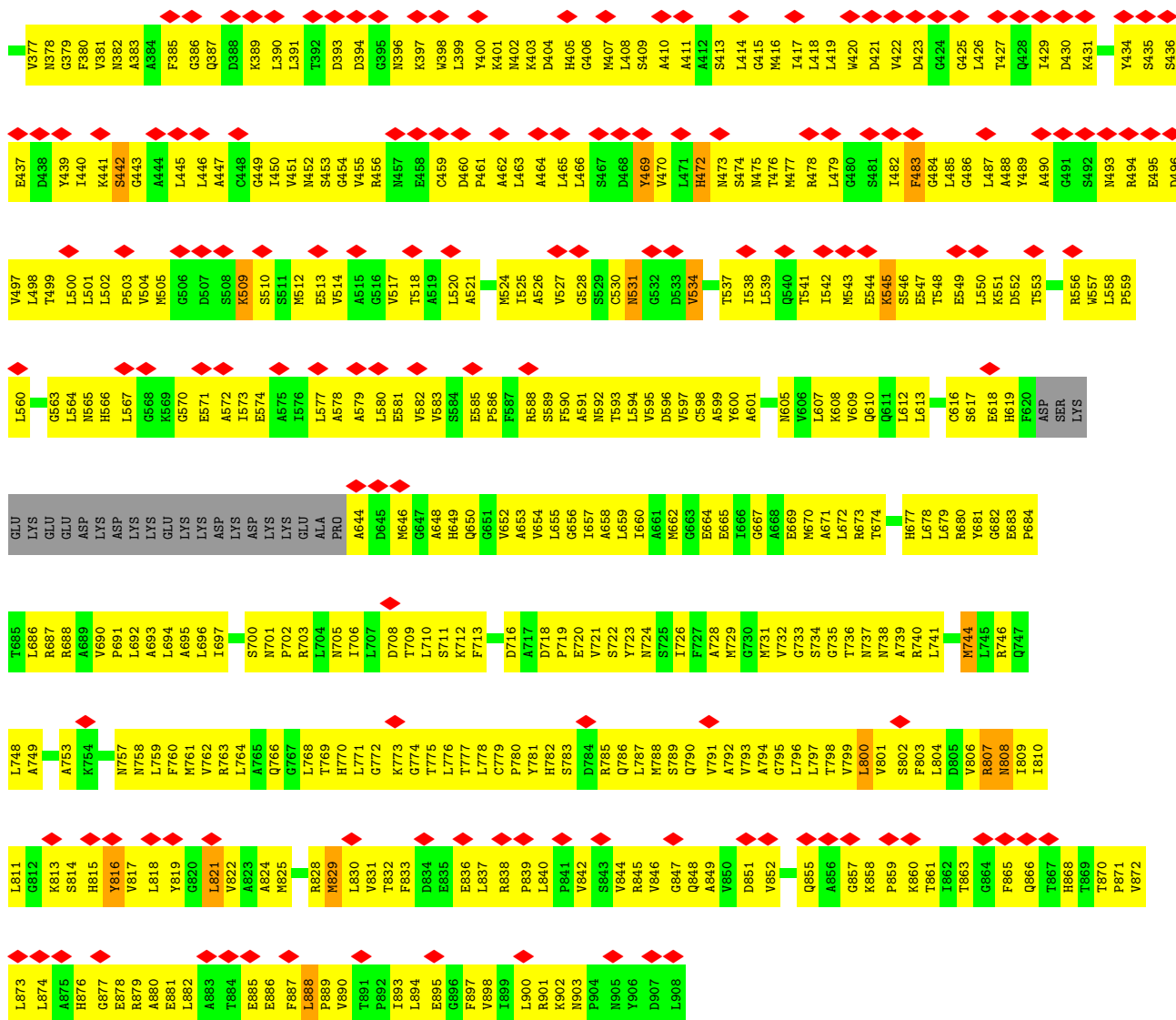


• Molecule 30: 26S proteasome complex subunit SEM1

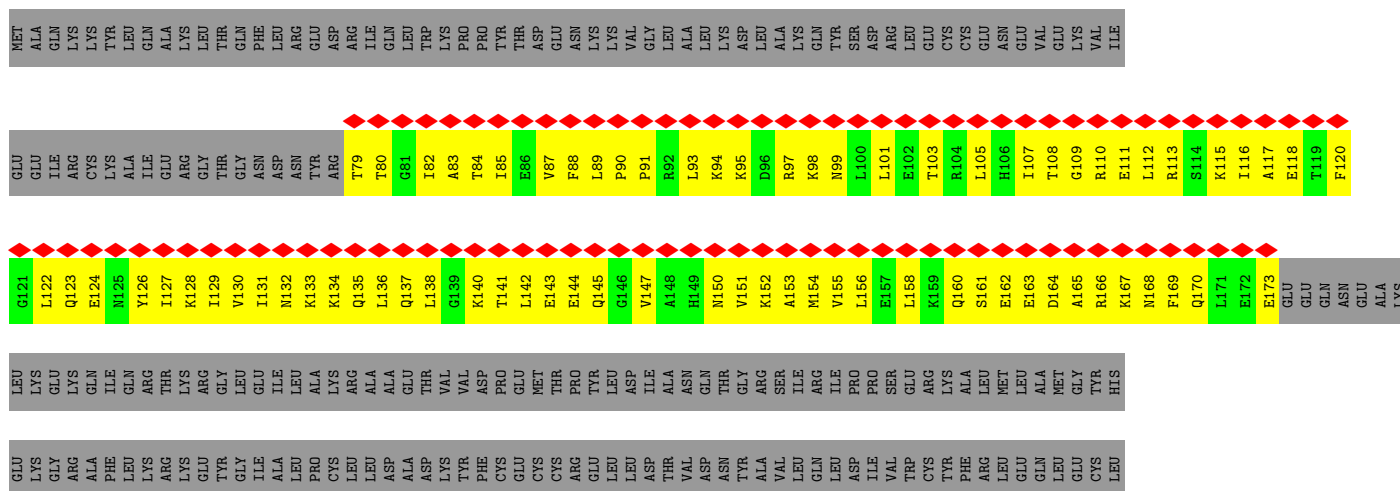


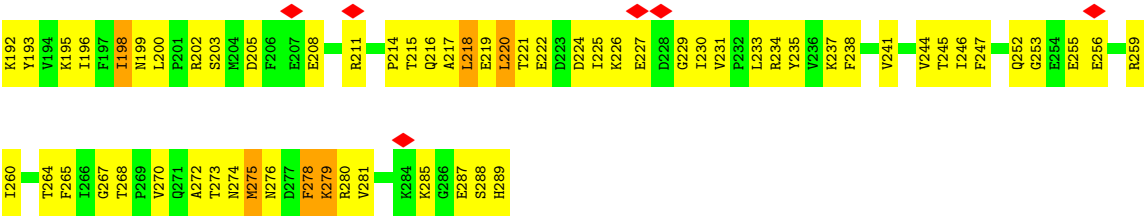
• Molecule 31: 26S proteasome non-ATPase regulatory subunit 2



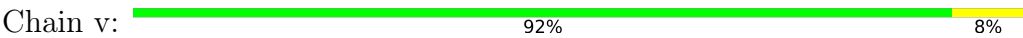


● Molecule 32: Isoform 2 of NEDD8 ultimate buster 1





• Molecule 35: substrate peptide



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	95437	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1700	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.771	Depositor
Minimum map value	-0.285	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.034	Depositor
Recommended contour level	0.15	Depositor
Map size ($\text{\AA}$)	356.32, 356.32, 356.32	wwPDB
Map dimensions	340, 340, 340	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.048, 1.048, 1.048	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.21	0/3213	0.39	1/4333 (0.0%)
2	B	0.31	0/3171	0.54	2/4276 (0.0%)
3	C	0.19	0/3092	0.35	1/4154 (0.0%)
4	D	0.16	0/3067	0.33	0/4135
5	E	0.27	0/2789	0.41	0/3751
6	F	0.26	0/2888	0.45	0/3889
7	G	0.16	0/1864	0.32	2/2527 (0.1%)
8	H	0.15	0/1852	0.31	0/2507
9	I	0.16	0/1938	0.33	0/2622
10	J	0.15	0/1838	0.28	0/2493
11	K	0.19	0/1789	0.34	0/2417
12	L	0.14	0/1880	0.27	0/2545
13	M	0.15	0/1891	0.28	0/2552
14	N	0.14	0/1508	0.28	0/2040
15	P	0.13	0/1672	0.31	0/2267
16	Q	0.18	0/1616	0.33	0/2180
17	R	0.35	0/1621	0.68	2/2194 (0.1%)
18	S	0.24	2/1590 (0.1%)	0.31	0/2147
19	T	0.13	0/1671	0.30	0/2252
20	U	0.33	4/6696 (0.1%)	0.65	12/9052 (0.1%)
21	V	0.18	0/3672	0.31	0/4957
22	W	0.13	0/3618	0.26	0/4868
23	X	0.13	0/3038	0.25	0/4095
24	Y	0.14	0/3181	0.24	0/4285
25	Z	0.24	0/2324	0.54	4/3150 (0.1%)
26	a	0.14	0/3048	0.31	0/4124
27	b	0.19	0/1474	0.41	1/1996 (0.1%)
28	c	0.46	0/2306	0.79	5/3117 (0.2%)
29	d	0.14	0/2234	0.31	0/3018
30	e	0.14	0/362	0.25	0/490
31	f	0.13	0/6623	0.31	0/8965
32	g	0.12	0/778	0.23	0/1041

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	h	0.14	0/1631	0.33	0/2206
34	u	0.42	0/1403	0.62	3/1892 (0.2%)
All	All	0.22	6/83338 (0.0%)	0.41	33/112537 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
17	R	0	2
20	U	0	1
21	V	0	1
25	Z	0	1
28	c	0	1
All	All	0	9

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	U	697	GLN	CD-OE1	-8.47	1.07	1.23
20	U	697	GLN	CG-CD	7.67	1.71	1.52
20	U	697	GLN	CD-NE2	7.56	1.49	1.33
20	U	697	GLN	C-N	5.74	1.41	1.33
18	S	88	TYR	CE2-CZ	-5.23	1.25	1.38

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	U	697	GLN	OE1-CD-NE2	-21.59	101.01	122.60
20	U	697	GLN	CG-CD-NE2	-21.22	84.56	116.40
20	U	697	GLN	CB-CA-C	18.23	136.43	111.63
25	Z	223	ASN	CB-CG-ND2	-14.85	94.13	116.40
20	U	697	GLN	CG-CD-OE1	12.84	146.47	120.80

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	258	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	265	ARG	Sidechain
1	A	312	ARG	Sidechain
17	R	85	ARG	Sidechain
17	R	86	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3163	0	3226	338	0
2	B	3126	0	3188	385	0
3	C	3051	0	3165	363	0
4	D	3018	0	3060	347	0
5	E	2750	0	2832	466	0
6	F	2850	0	2944	304	0
7	G	1831	0	1813	255	0
8	H	1813	0	1804	246	0
9	I	1908	0	1864	243	0
10	J	1813	0	1751	246	0
11	K	1763	0	1723	236	0
12	L	1845	0	1820	227	0
13	M	1856	0	1814	234	0
14	N	1482	0	1450	203	0
15	P	1645	0	1648	259	0
16	Q	1587	0	1598	332	0
17	R	1588	0	1584	266	0
18	S	1559	0	1522	223	0
19	T	1641	0	1639	296	0
20	U	6584	0	6624	869	0
21	V	3602	0	3672	518	0
22	W	3570	0	3685	472	0
23	X	2994	0	3097	321	0
24	Y	3123	0	3130	302	0
25	Z	2281	0	2312	305	0
26	a	2991	0	3009	410	0
27	b	1454	0	1502	209	0
28	c	2264	0	2278	280	0
29	d	2188	0	2216	348	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	e	353	0	276	25	0
31	f	6512	0	6529	1085	0
32	g	771	0	815	145	0
33	h	1601	0	1587	295	0
34	u	1376	0	1324	141	0
35	v	60	0	16	1	0
36	A	31	0	12	2	0
36	B	31	0	12	2	0
36	F	31	0	12	8	0
37	A	1	0	0	0	0
37	B	1	0	0	0	0
37	C	1	0	0	0	0
37	D	1	0	0	0	0
37	F	1	0	0	0	0
38	C	27	0	12	9	0
38	D	27	0	12	9	0
38	E	27	0	12	5	0
39	u	1	0	0	0	0
All	All	82193	0	82589	10100	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 61.

The worst 5 of 10100 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:U:353:LEU:HD22	20:U:385:PHE:CE2	1.52	1.45
31:f:208:LEU:HD13	31:f:217:LEU:CD2	1.65	1.26
20:U:353:LEU:HD22	20:U:385:PHE:CD2	1.70	1.25
21:V:443:ARG:HH22	29:d:273:GLY:C	1.46	1.21
16:Q:61:GLN:OE1	17:R:124:LEU:HD21	1.41	1.19

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	393/433 (91%)	363 (92%)	28 (7%)	2 (0%)	24	59
2	B	394/440 (90%)	361 (92%)	32 (8%)	1 (0%)	36	68
3	C	384/406 (95%)	352 (92%)	31 (8%)	1 (0%)	36	68
4	D	373/418 (89%)	335 (90%)	35 (9%)	3 (1%)	16	48
5	E	341/389 (88%)	290 (85%)	37 (11%)	14 (4%)	2	12
6	F	358/439 (82%)	340 (95%)	17 (5%)	1 (0%)	36	68
7	G	237/246 (96%)	230 (97%)	6 (2%)	1 (0%)	30	63
8	H	230/234 (98%)	226 (98%)	4 (2%)	0	100	100
9	I	246/261 (94%)	239 (97%)	7 (3%)	0	100	100
10	J	237/248 (96%)	231 (98%)	6 (2%)	0	100	100
11	K	227/241 (94%)	219 (96%)	8 (4%)	0	100	100
12	L	235/263 (89%)	227 (97%)	8 (3%)	0	100	100
13	M	238/255 (93%)	228 (96%)	10 (4%)	0	100	100
14	N	195/239 (82%)	190 (97%)	5 (3%)	0	100	100
15	P	218/277 (79%)	213 (98%)	5 (2%)	0	100	100
16	Q	202/205 (98%)	196 (97%)	6 (3%)	0	100	100
17	R	197/201 (98%)	191 (97%)	6 (3%)	0	100	100
18	S	199/263 (76%)	195 (98%)	4 (2%)	0	100	100
19	T	211/241 (88%)	196 (93%)	15 (7%)	0	100	100
20	U	834/953 (88%)	771 (92%)	59 (7%)	4 (0%)	24	59
21	V	440/534 (82%)	416 (94%)	23 (5%)	1 (0%)	43	75
22	W	436/456 (96%)	416 (95%)	19 (4%)	1 (0%)	43	75
23	X	376/422 (89%)	358 (95%)	17 (4%)	1 (0%)	36	68
24	Y	377/389 (97%)	371 (98%)	6 (2%)	0	100	100
25	Z	284/324 (88%)	269 (95%)	13 (5%)	2 (1%)	18	51
26	a	368/376 (98%)	344 (94%)	21 (6%)	3 (1%)	16	48
27	b	188/377 (50%)	161 (86%)	26 (14%)	1 (0%)	24	59
28	c	286/424 (68%)	248 (87%)	34 (12%)	4 (1%)	9	34
29	d	267/350 (76%)	255 (96%)	12 (4%)	0	100	100
30	e	37/70 (53%)	37 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	f	838/908 (92%)	789 (94%)	49 (6%)	0	100	100
32	g	93/601 (16%)	90 (97%)	3 (3%)	0	100	100
33	h	204/264 (77%)	197 (97%)	7 (3%)	0	100	100
34	u	170/289 (59%)	160 (94%)	7 (4%)	3 (2%)	6	29
All	All	10313/12436 (83%)	9704 (94%)	566 (6%)	43 (0%)	31	63

5 of 43 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	85	ILE
4	D	339	ARG
5	E	85	ARG
5	E	116	ASP
5	E	203	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	347/372 (93%)	335 (96%)	12 (4%)	32	64
2	B	351/385 (91%)	332 (95%)	19 (5%)	20	52
3	C	338/352 (96%)	320 (95%)	18 (5%)	20	52
4	D	331/366 (90%)	314 (95%)	17 (5%)	21	54
5	E	303/341 (89%)	283 (93%)	20 (7%)	15	44
6	F	311/379 (82%)	298 (96%)	13 (4%)	26	59
7	G	195/210 (93%)	178 (91%)	17 (9%)	9	34
8	H	190/191 (100%)	180 (95%)	10 (5%)	20	52
9	I	195/221 (88%)	180 (92%)	15 (8%)	12	38
10	J	183/212 (86%)	175 (96%)	8 (4%)	25	58
11	K	192/204 (94%)	180 (94%)	12 (6%)	16	46
12	L	198/224 (88%)	189 (96%)	9 (4%)	24	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	M	192/212 (91%)	181 (94%)	11 (6%)	18	50
14	N	154/181 (85%)	150 (97%)	4 (3%)	40	71
15	P	178/228 (78%)	172 (97%)	6 (3%)	32	64
16	Q	172/174 (99%)	163 (95%)	9 (5%)	21	53
17	R	168/171 (98%)	153 (91%)	15 (9%)	9	33
18	S	156/202 (77%)	150 (96%)	6 (4%)	29	62
19	T	175/199 (88%)	165 (94%)	10 (6%)	18	50
20	U	718/816 (88%)	668 (93%)	50 (7%)	14	42
21	V	390/460 (85%)	375 (96%)	15 (4%)	29	62
22	W	403/416 (97%)	385 (96%)	18 (4%)	24	57
23	X	325/362 (90%)	308 (95%)	17 (5%)	21	53
24	Y	335/344 (97%)	326 (97%)	9 (3%)	39	70
25	Z	257/295 (87%)	245 (95%)	12 (5%)	23	56
26	a	333/336 (99%)	315 (95%)	18 (5%)	20	52
27	b	167/312 (54%)	155 (93%)	12 (7%)	13	41
28	c	252/359 (70%)	233 (92%)	19 (8%)	12	39
29	d	237/294 (81%)	226 (95%)	11 (5%)	24	57
30	e	37/63 (59%)	35 (95%)	2 (5%)	20	52
31	f	709/763 (93%)	678 (96%)	31 (4%)	25	58
32	g	85/527 (16%)	85 (100%)	0	100	100
33	h	169/215 (79%)	161 (95%)	8 (5%)	23	56
34	u	156/253 (62%)	149 (96%)	7 (4%)	24	57
All	All	8902/10639 (84%)	8442 (95%)	460 (5%)	22	53

5 of 460 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
20	U	25	HIS
31	f	829	MET
21	V	222	ASP
31	f	800	LEU
28	c	261	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
29	d	338	GLN
31	f	472	HIS
34	u	276	ASN
17	R	61	GLN
17	R	55	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 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	$\# Z > 2$
38	ADP	C	501	37	28,29,29	1.37	4 (14%)	43,45,45	1.84	8 (18%)
38	ADP	D	501	37	28,29,29	0.48	0	43,45,45	0.60	0
36	ATP	F	501	37	32,33,33	0.51	0	48,52,52	0.64	0
36	ATP	B	501	37	32,33,33	0.50	0	48,52,52	0.55	0
38	ADP	E	501	-	28,29,29	1.37	4 (14%)	43,45,45	1.90	11 (25%)
36	ATP	A	501	37	32,33,33	0.53	0	48,52,52	0.60	0

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
38	ADP	C	501	37	-	4/16/32/32	0/3/3/3
38	ADP	D	501	37	-	3/16/32/32	0/3/3/3
36	ATP	F	501	37	-	7/22/38/38	0/3/3/3
36	ATP	B	501	37	-	7/22/38/38	0/3/3/3
38	ADP	E	501	-	-	5/16/32/32	0/3/3/3
36	ATP	A	501	37	-	4/22/38/38	0/3/3/3

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	E	501	ADP	C5-C4	4.42	1.47	1.39
38	C	501	ADP	C5-C4	4.42	1.47	1.39
38	C	501	ADP	C5-C6	2.61	1.48	1.41
38	E	501	ADP	C5-C6	2.57	1.48	1.41
38	E	501	ADP	C5-N7	-2.49	1.34	1.39

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	E	501	ADP	C5-C4-N3	-5.93	118.55	126.72
38	C	501	ADP	C5-C4-N3	-5.83	118.69	126.72
38	E	501	ADP	N3-C4-N9	4.59	134.97	127.17
38	C	501	ADP	N3-C4-N9	4.54	134.89	127.17
38	E	501	ADP	C2-N3-C4	4.00	121.59	111.83

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

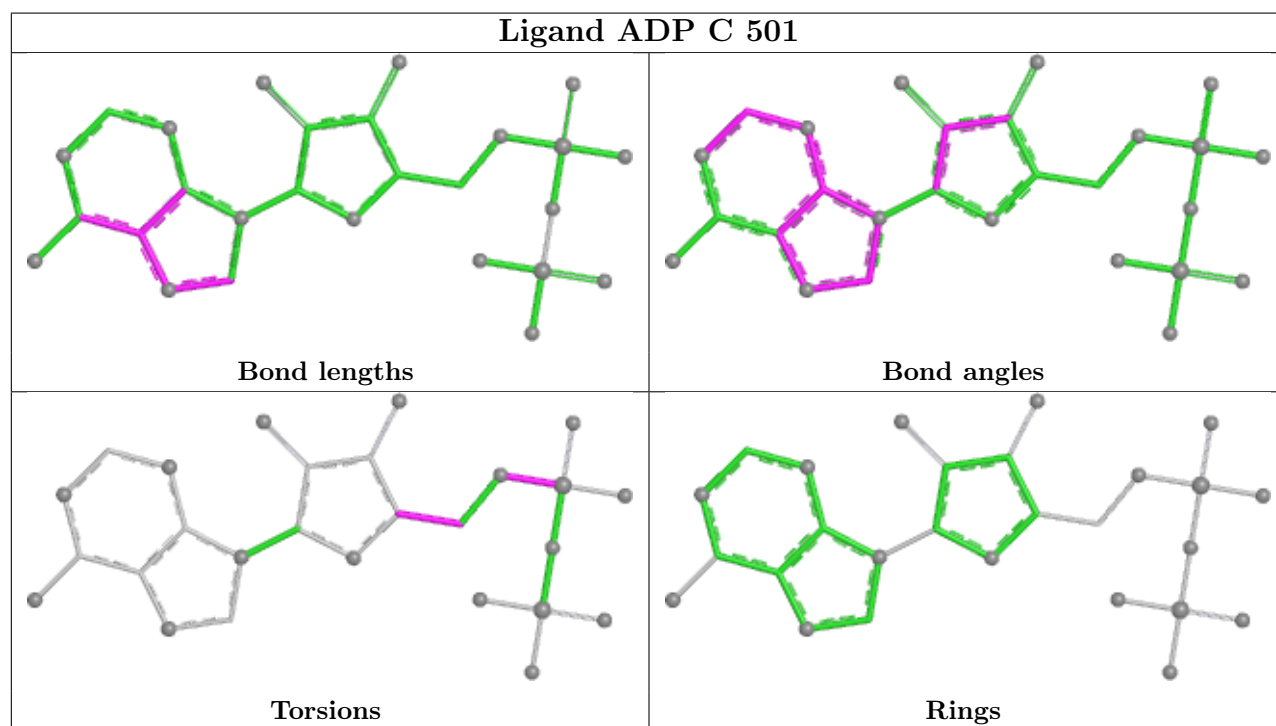
Mol	Chain	Res	Type	Atoms
36	A	501	ATP	C5'-O5'-PA-O1A
36	A	501	ATP	C5'-O5'-PA-O2A
36	A	501	ATP	C5'-O5'-PA-O3A
36	B	501	ATP	PB-O3B-PG-O2G
36	B	501	ATP	PB-O3B-PG-O3G

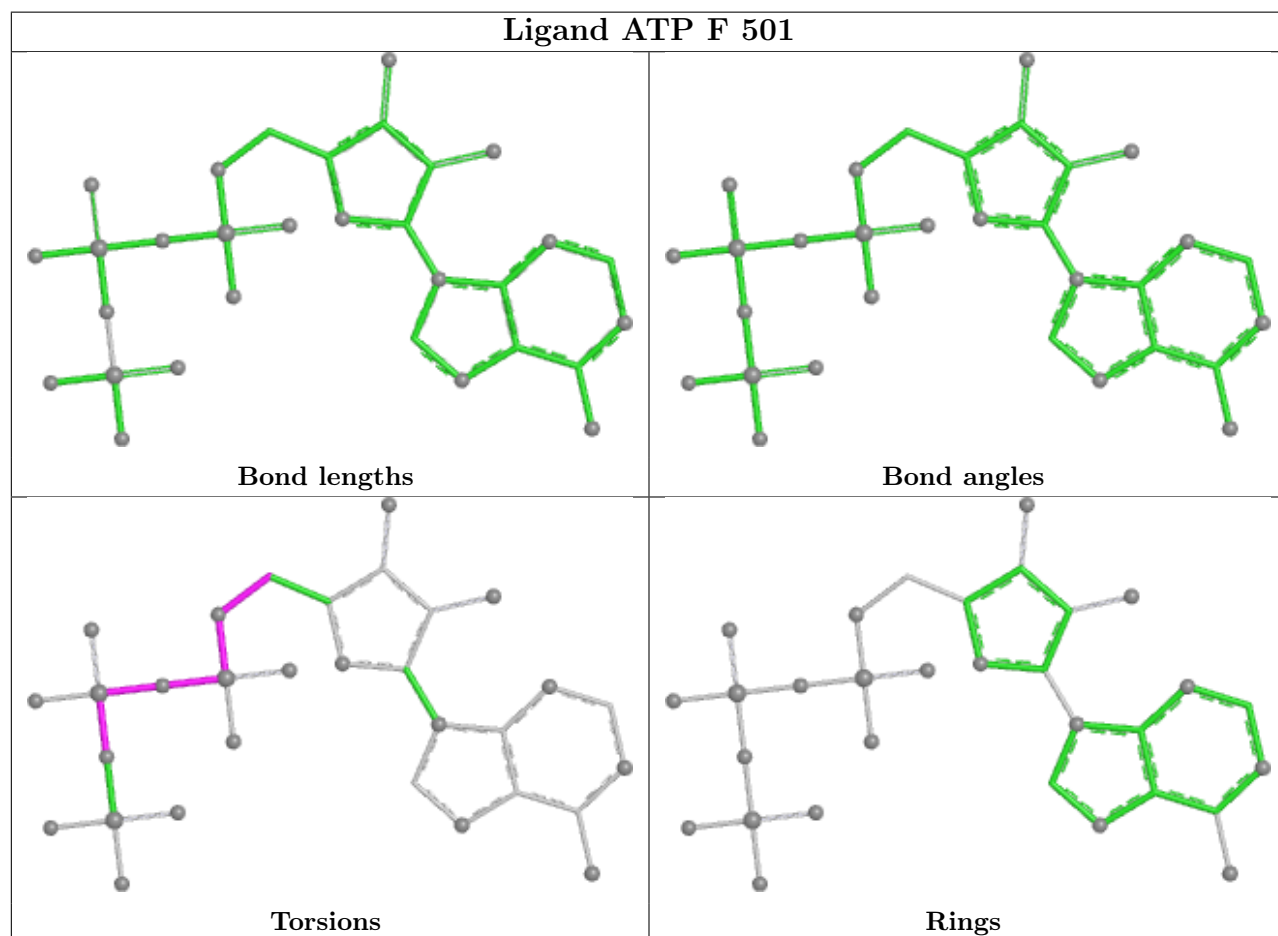
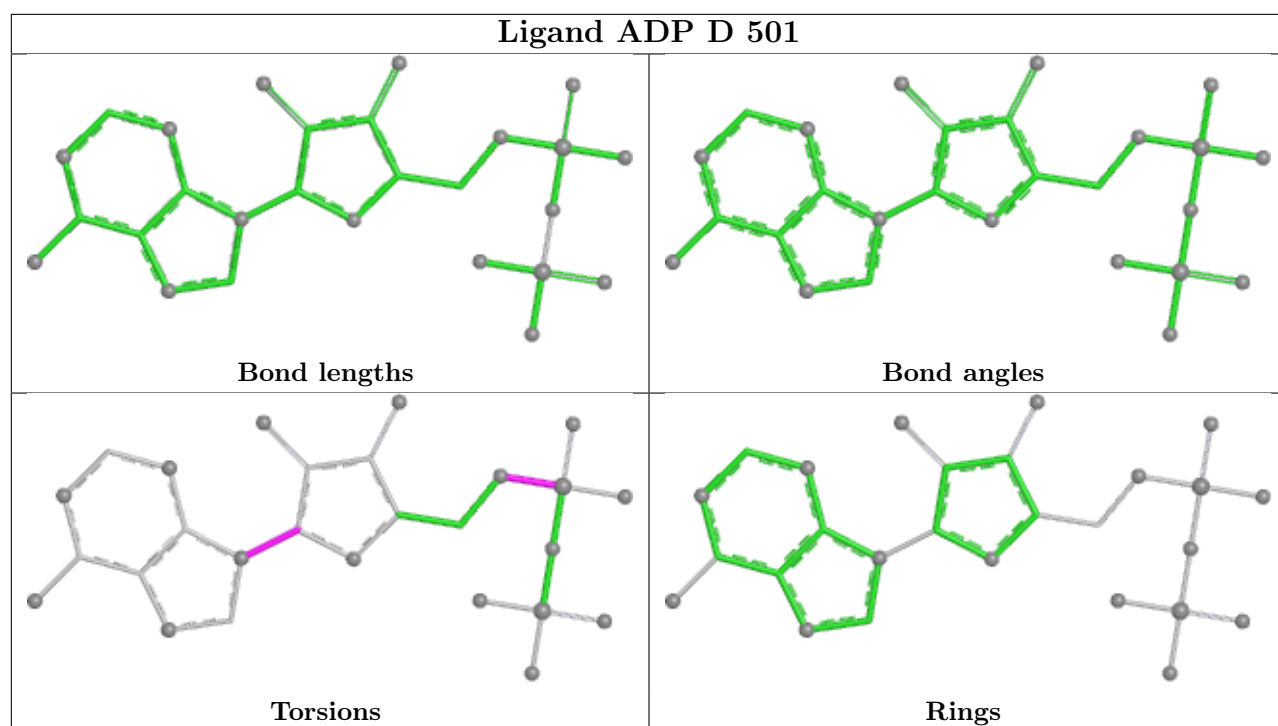
There are no ring outliers.

6 monomers are involved in 35 short contacts:

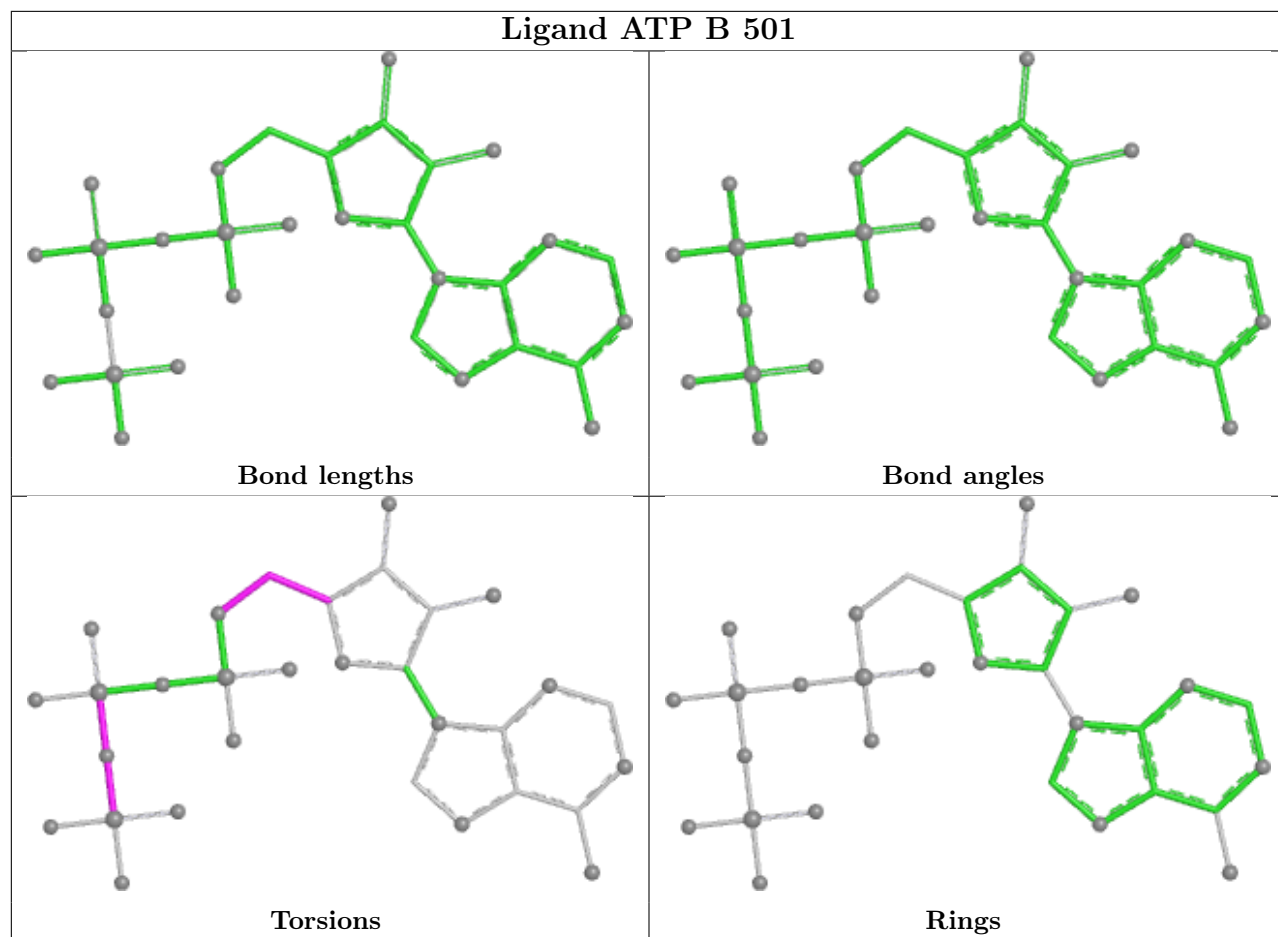
Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	C	501	ADP	9	0
38	D	501	ADP	9	0
36	F	501	ATP	8	0
36	B	501	ATP	2	0
38	E	501	ADP	5	0
36	A	501	ATP	2	0

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

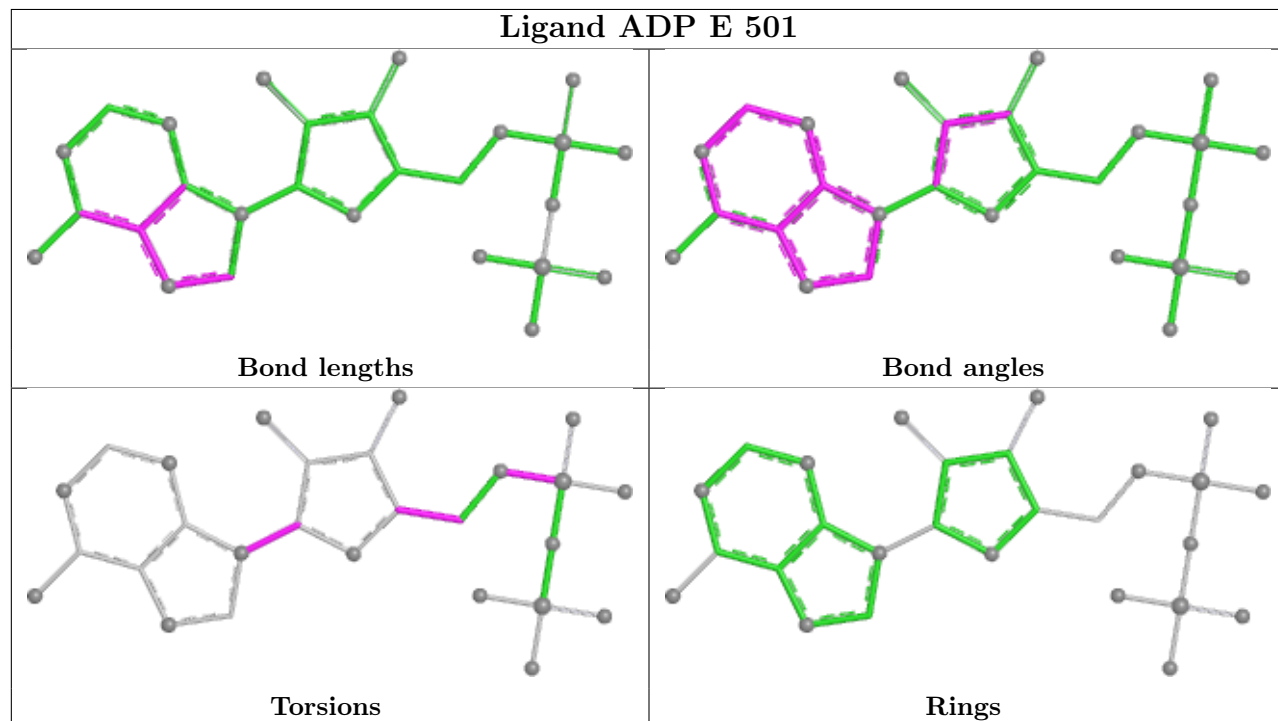


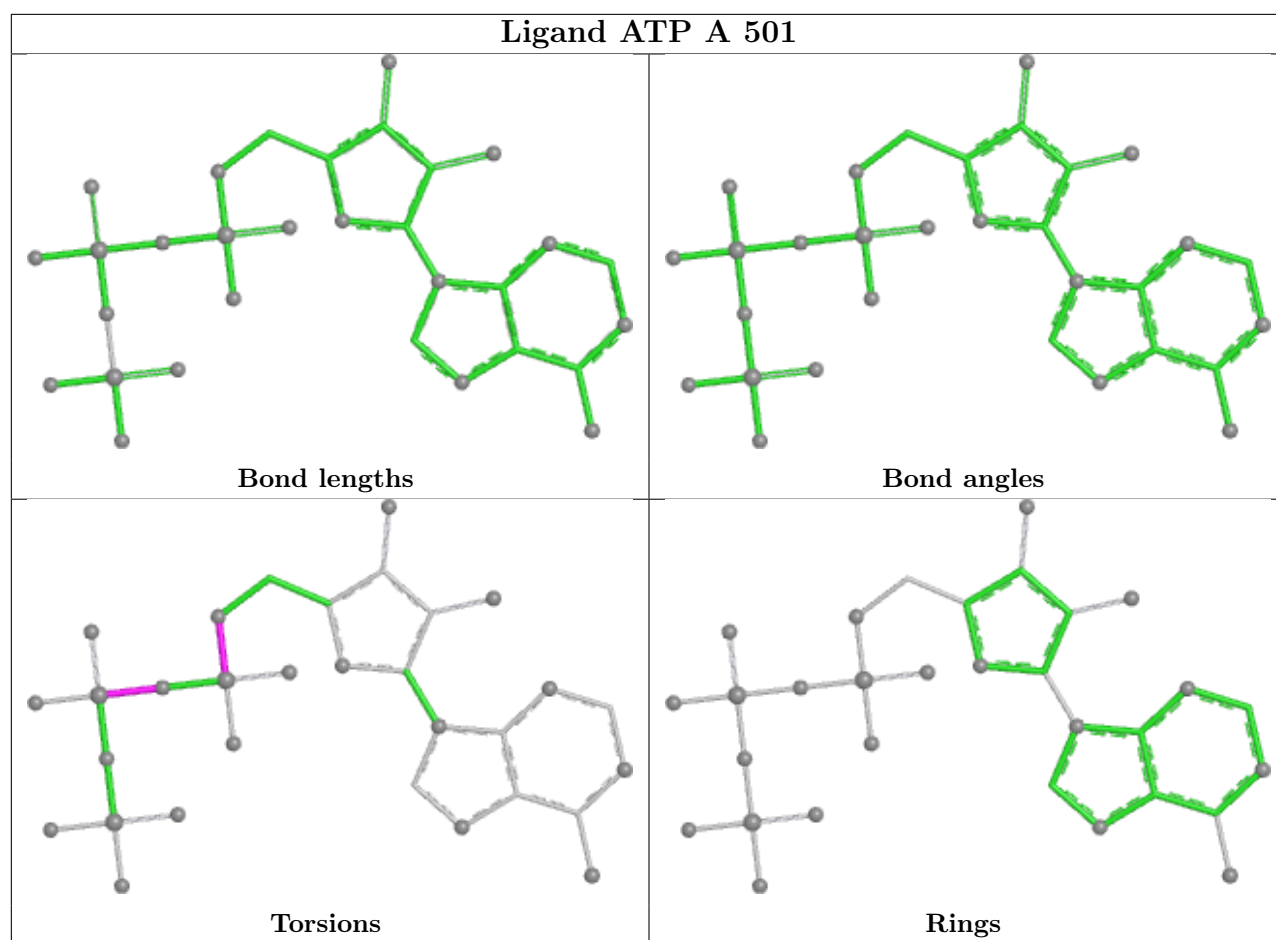


Ligand ATP B 501



Ligand ADP E 501





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

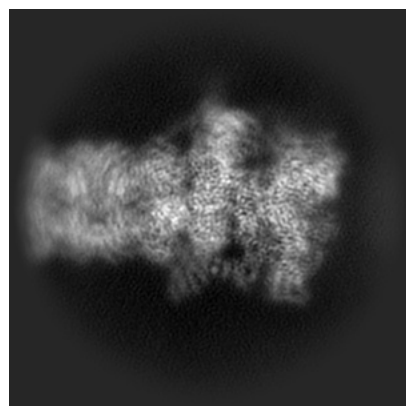
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47719. These allow visual inspection of the internal detail of the map and identification of artifacts.

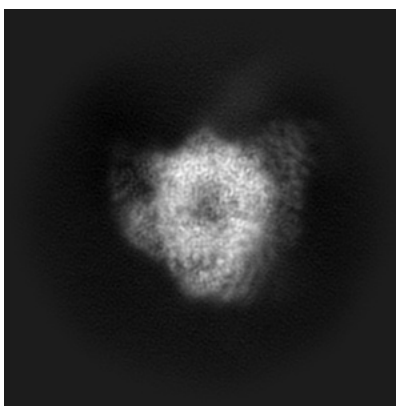
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

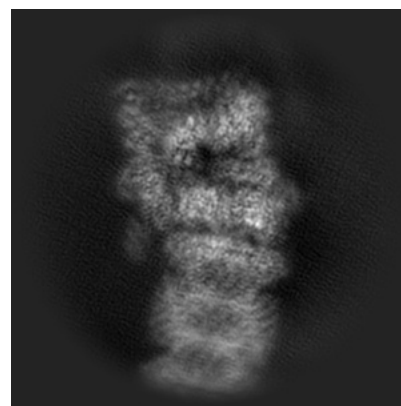
6.1.1 Primary map



X

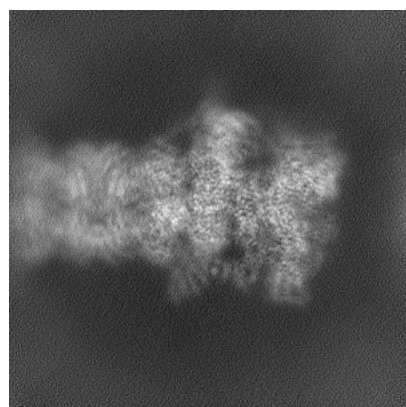


Y

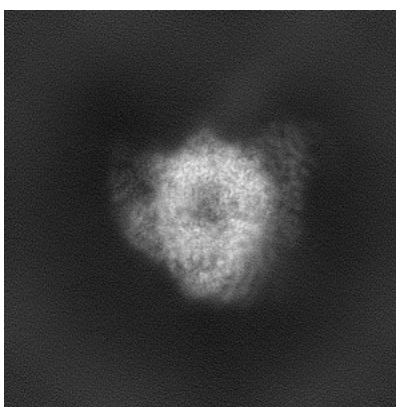


Z

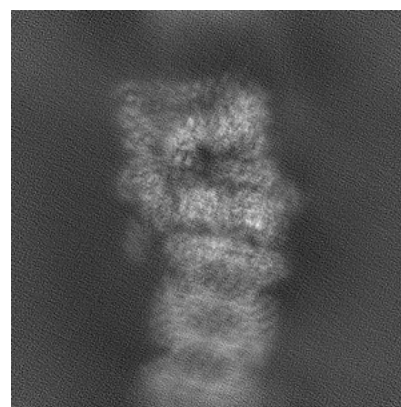
6.1.2 Raw map



X



Y

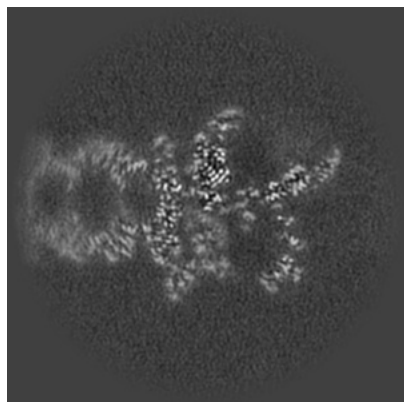


Z

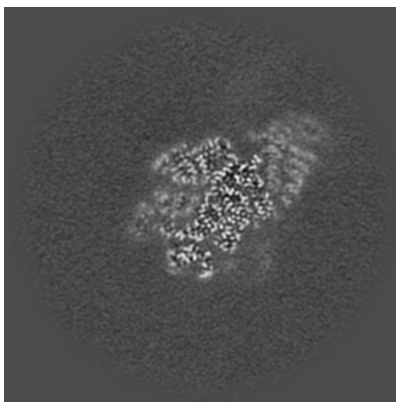
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

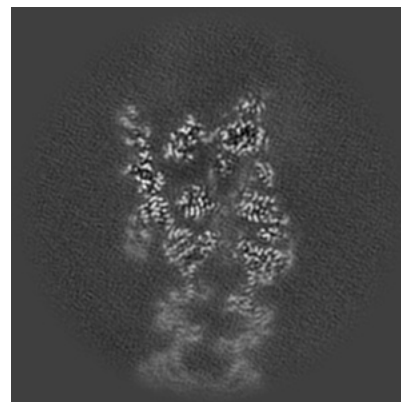
6.2.1 Primary map



X Index: 170

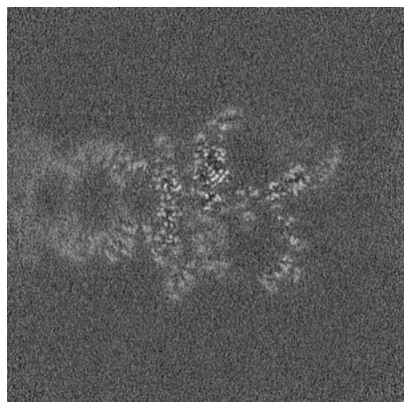


Y Index: 170

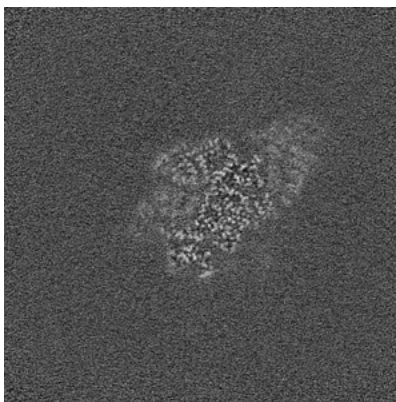


Z Index: 170

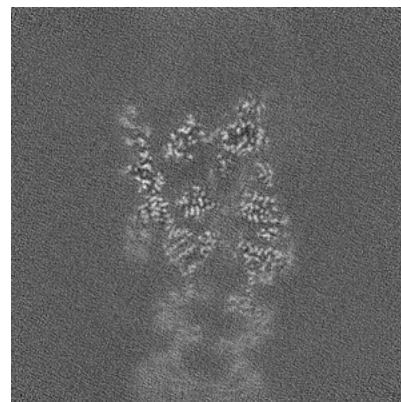
6.2.2 Raw map



X Index: 170



Y Index: 170

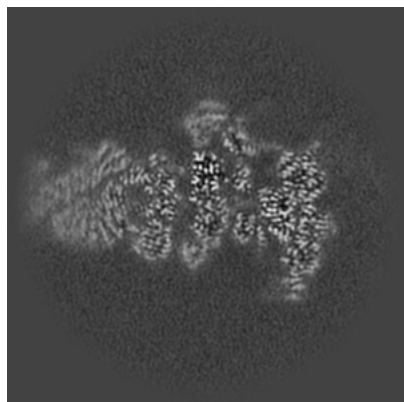


Z Index: 170

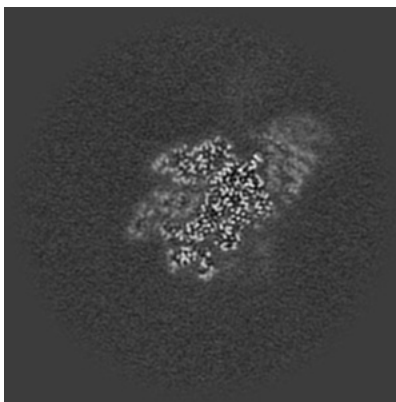
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

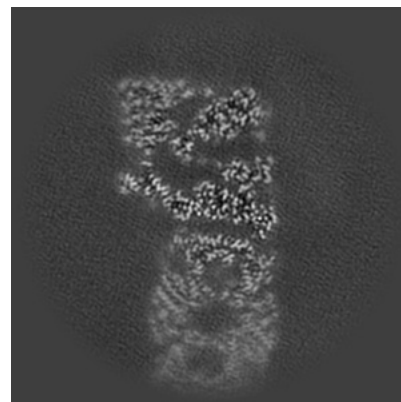
6.3.1 Primary map



X Index: 200

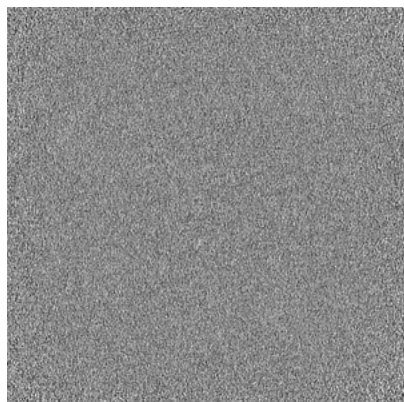


Y Index: 169

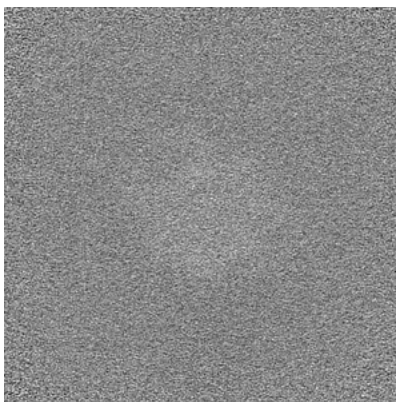


Z Index: 192

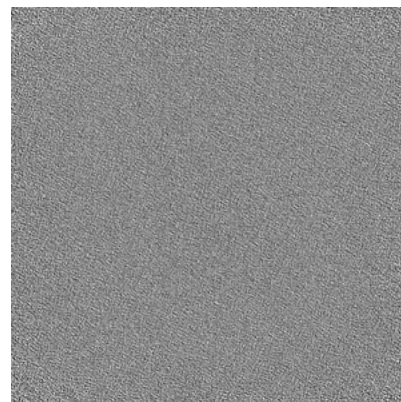
6.3.2 Raw map



X Index: 0



Y Index: 0

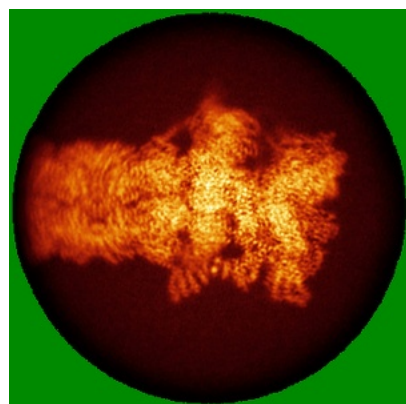


Z Index: 0

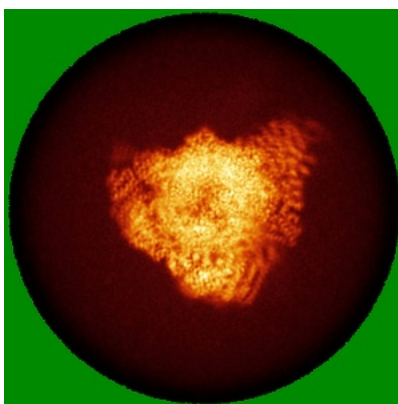
The images above show the largest variance slices of the map in three orthogonal directions.

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

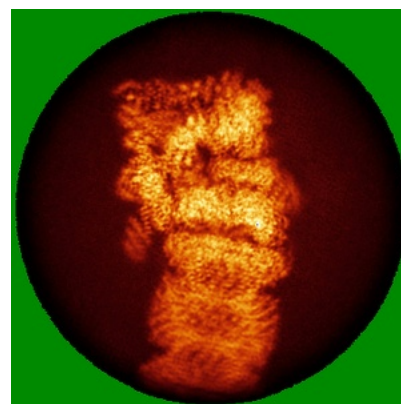
6.4.1 Primary map



X

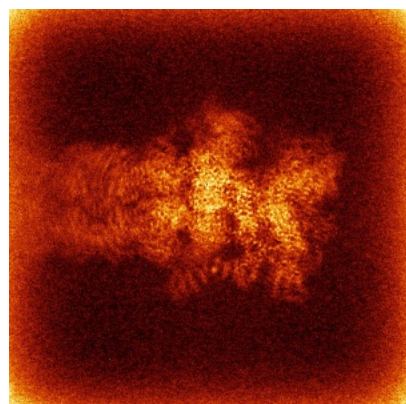


Y

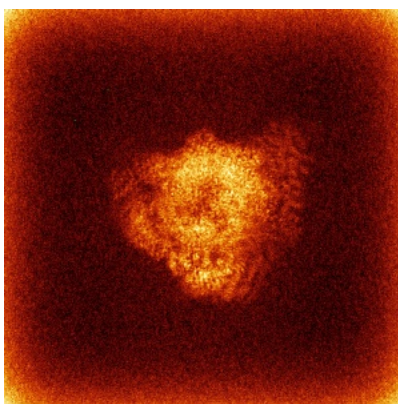


Z

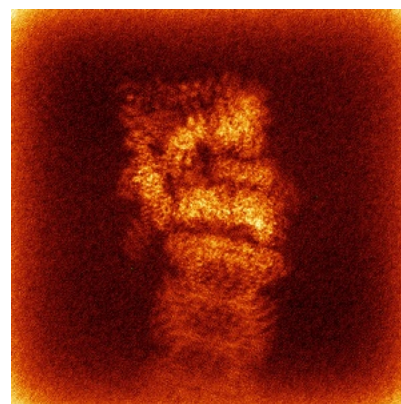
6.4.2 Raw map



X



Y

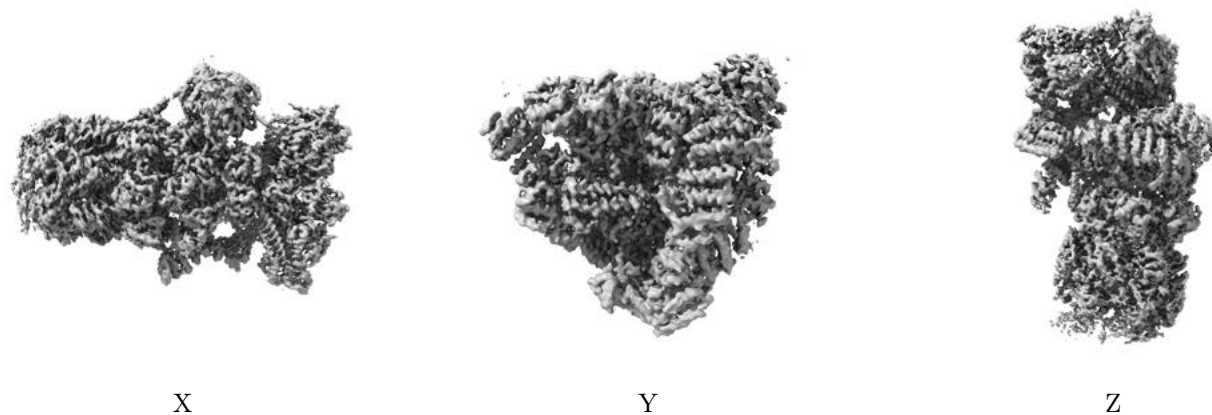


Z

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

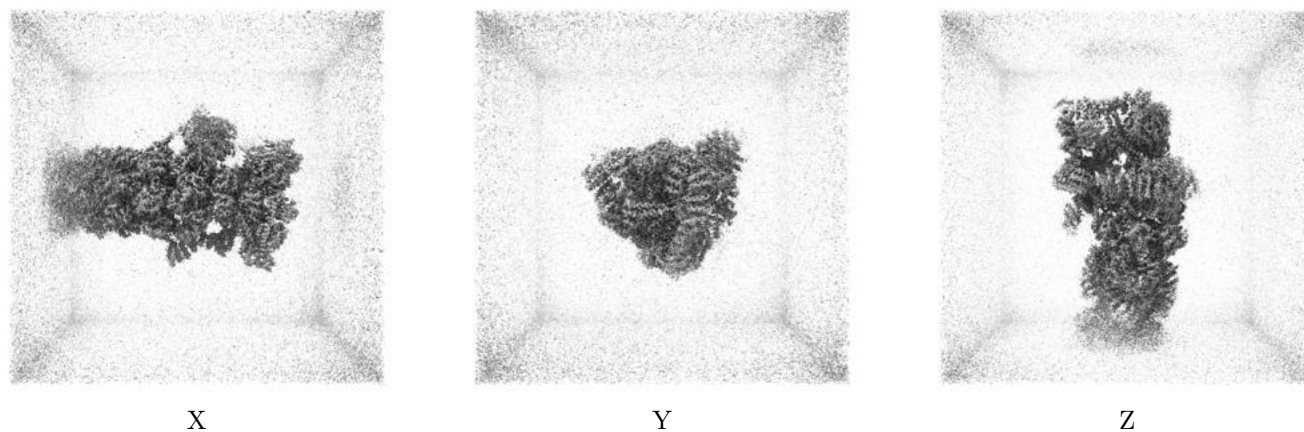
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

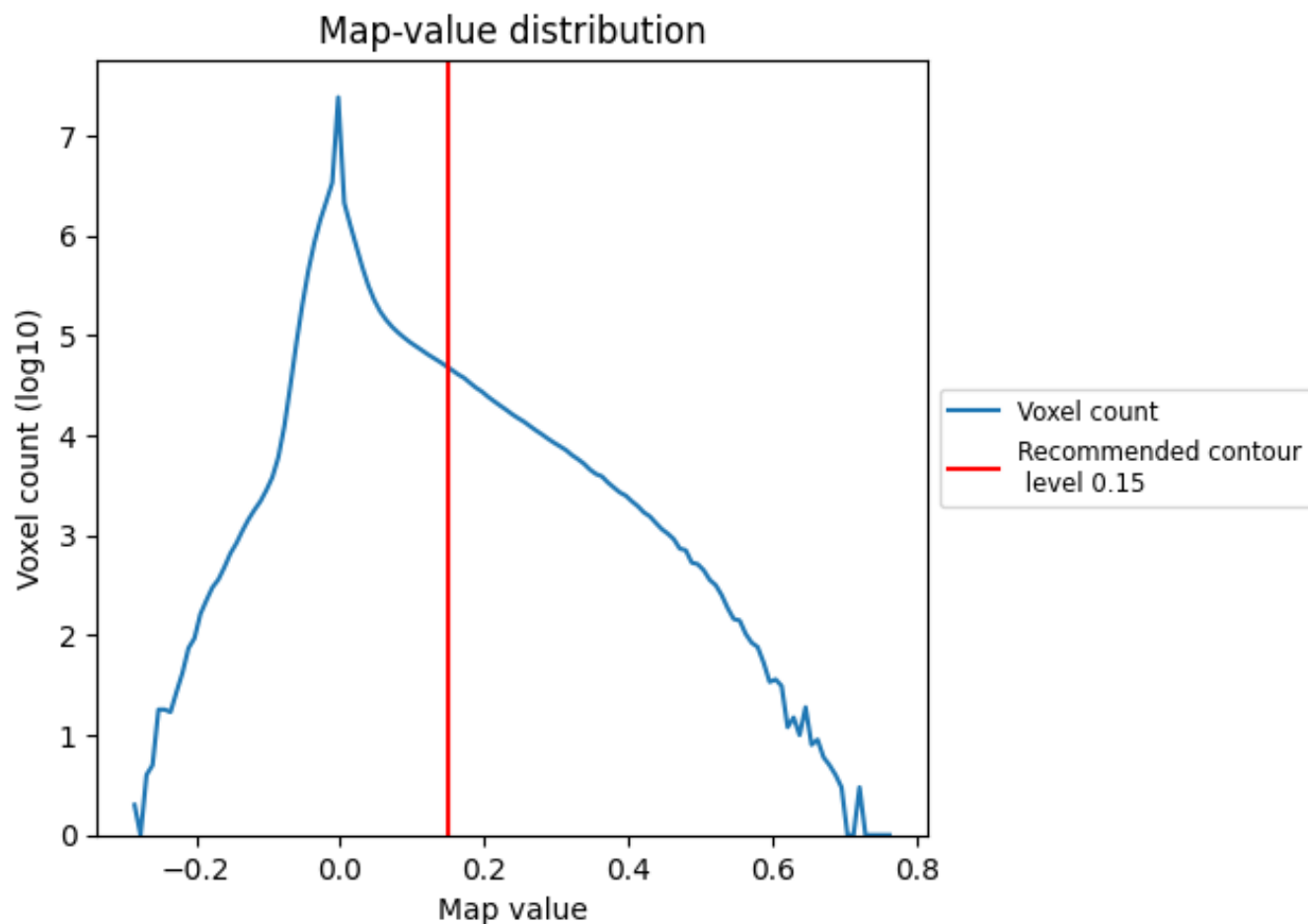
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

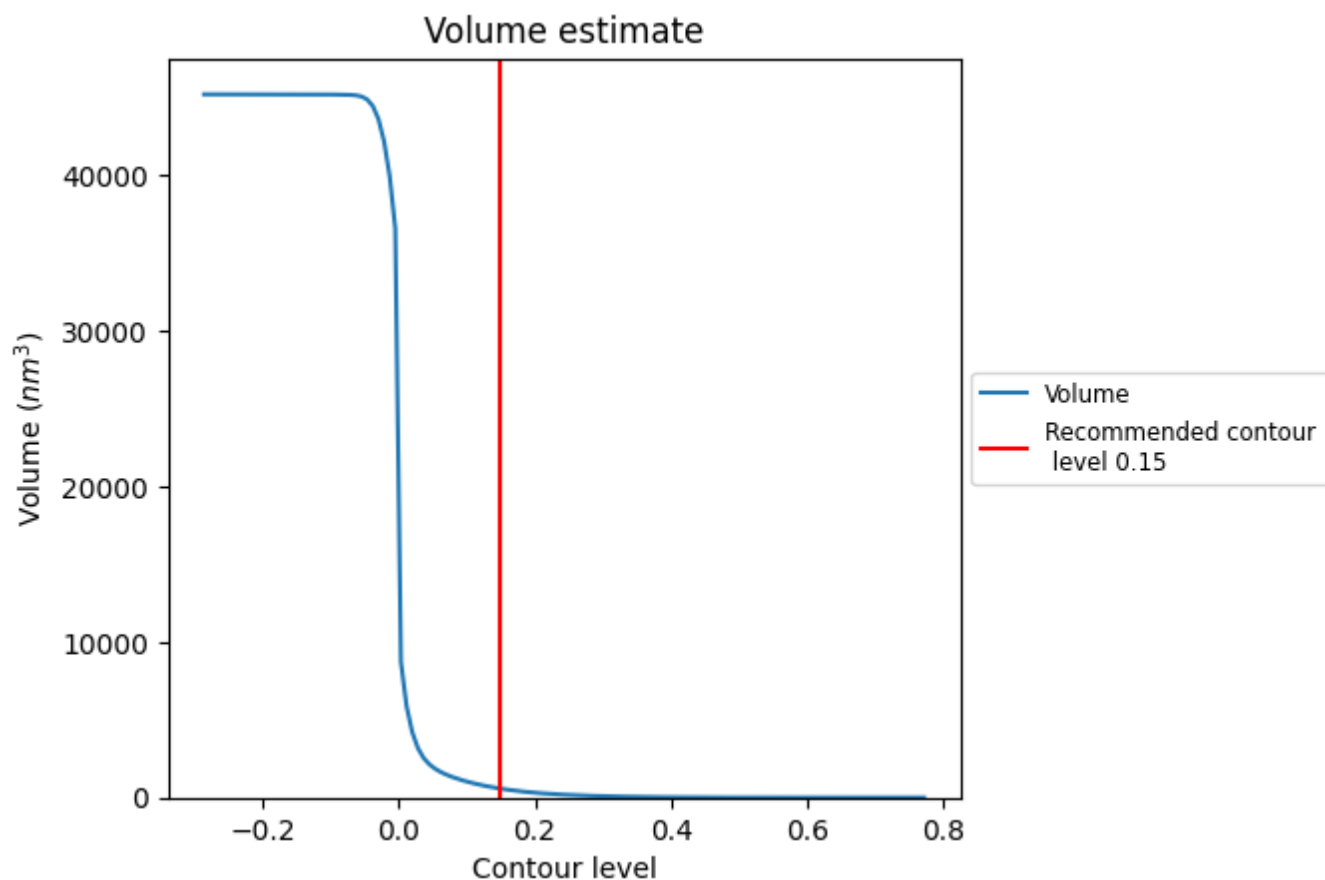
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

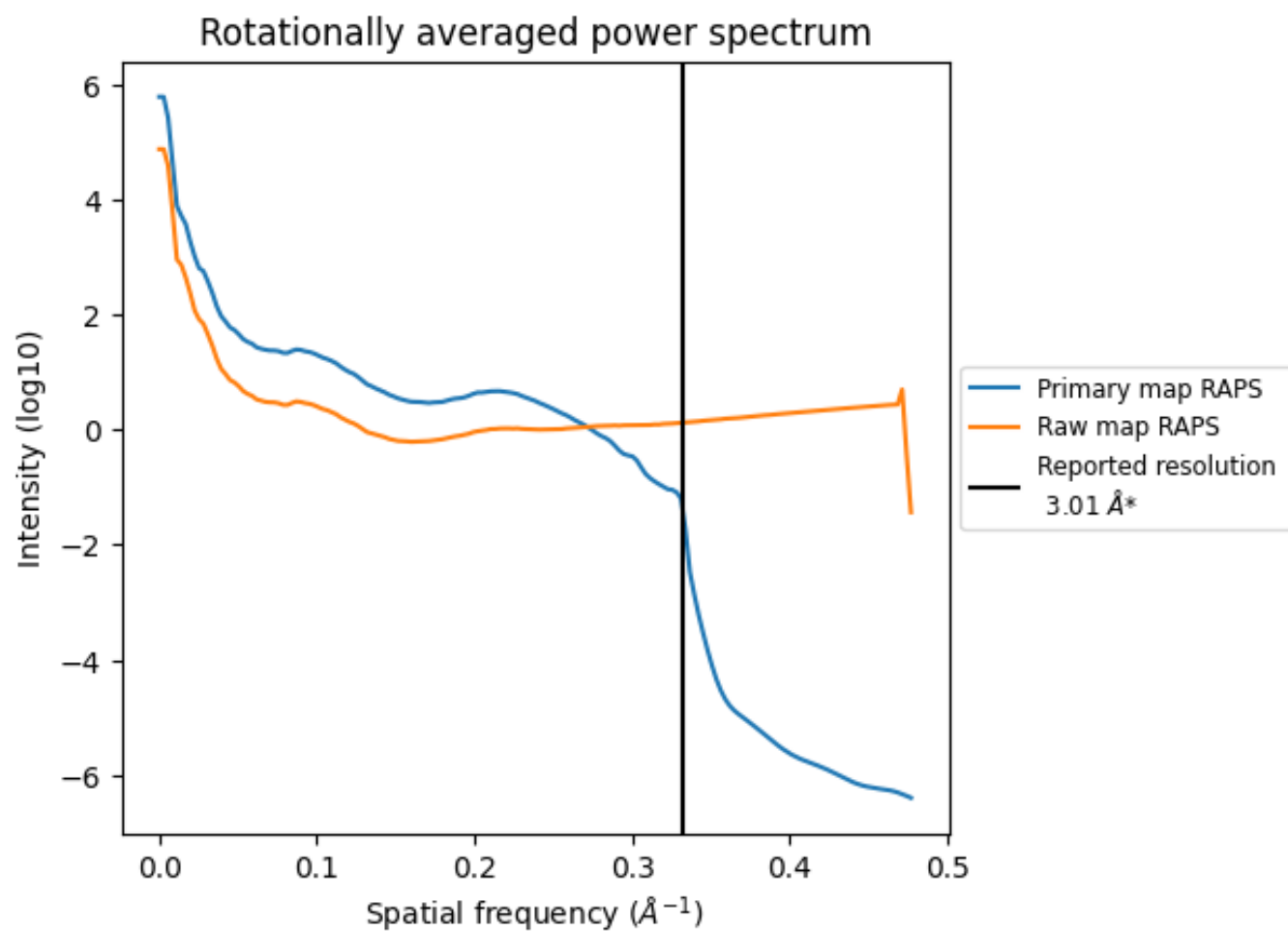
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 574 nm³; this corresponds to an approximate mass of 518 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

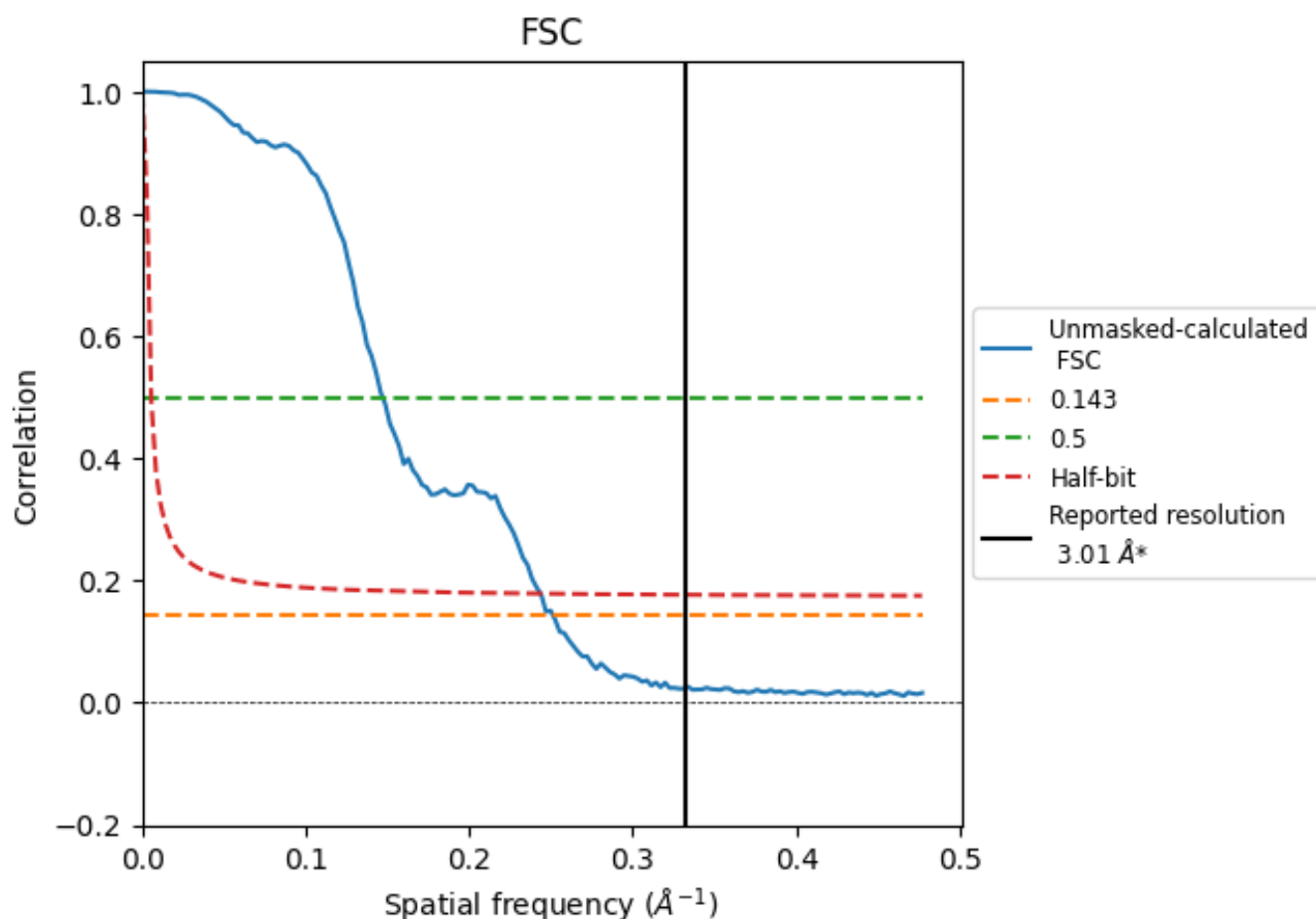


*Reported resolution corresponds to spatial frequency of 0.332 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.332 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.01	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.98	6.80	4.11

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.98 differs from the reported value 3.01 by more than 10 %

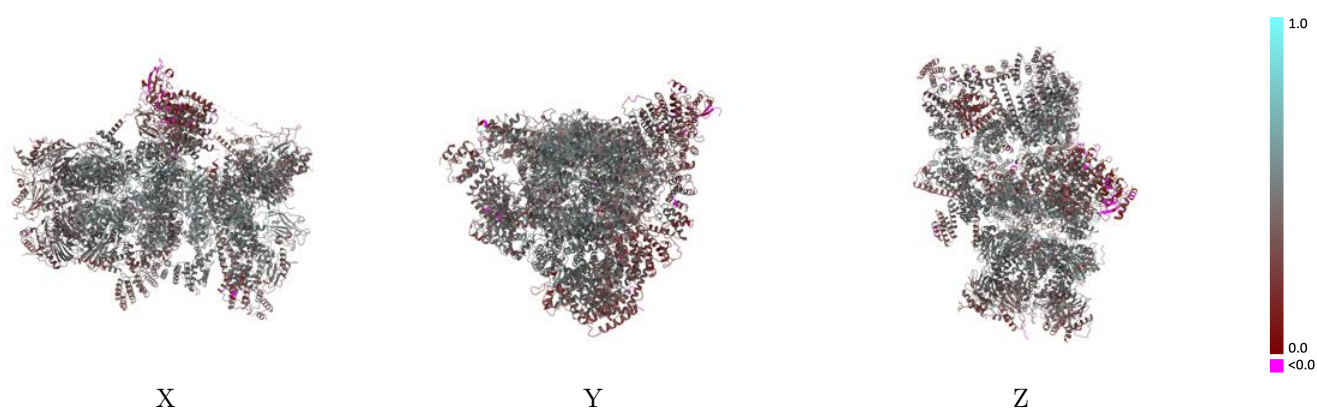
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-47719 and PDB model 9E8G. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay [i](#)

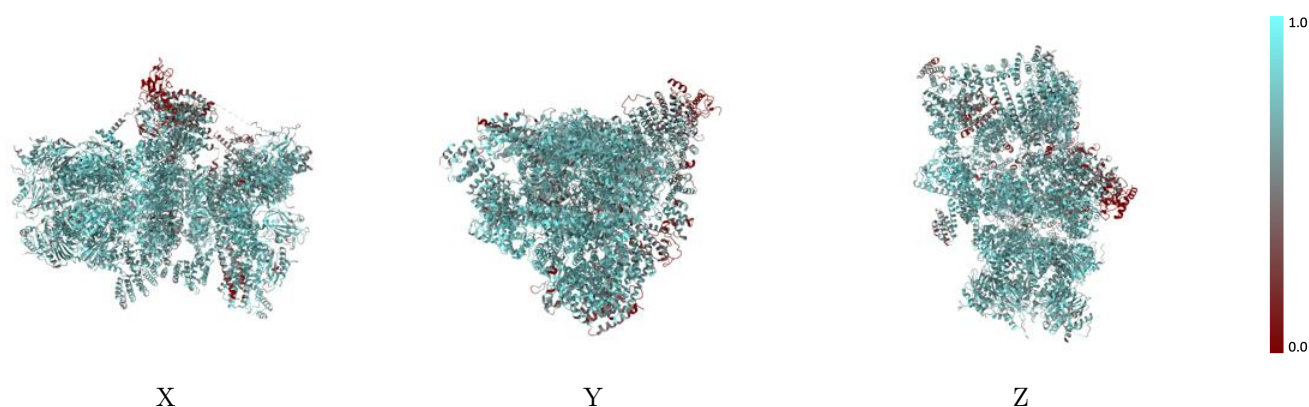
This section was not generated.

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



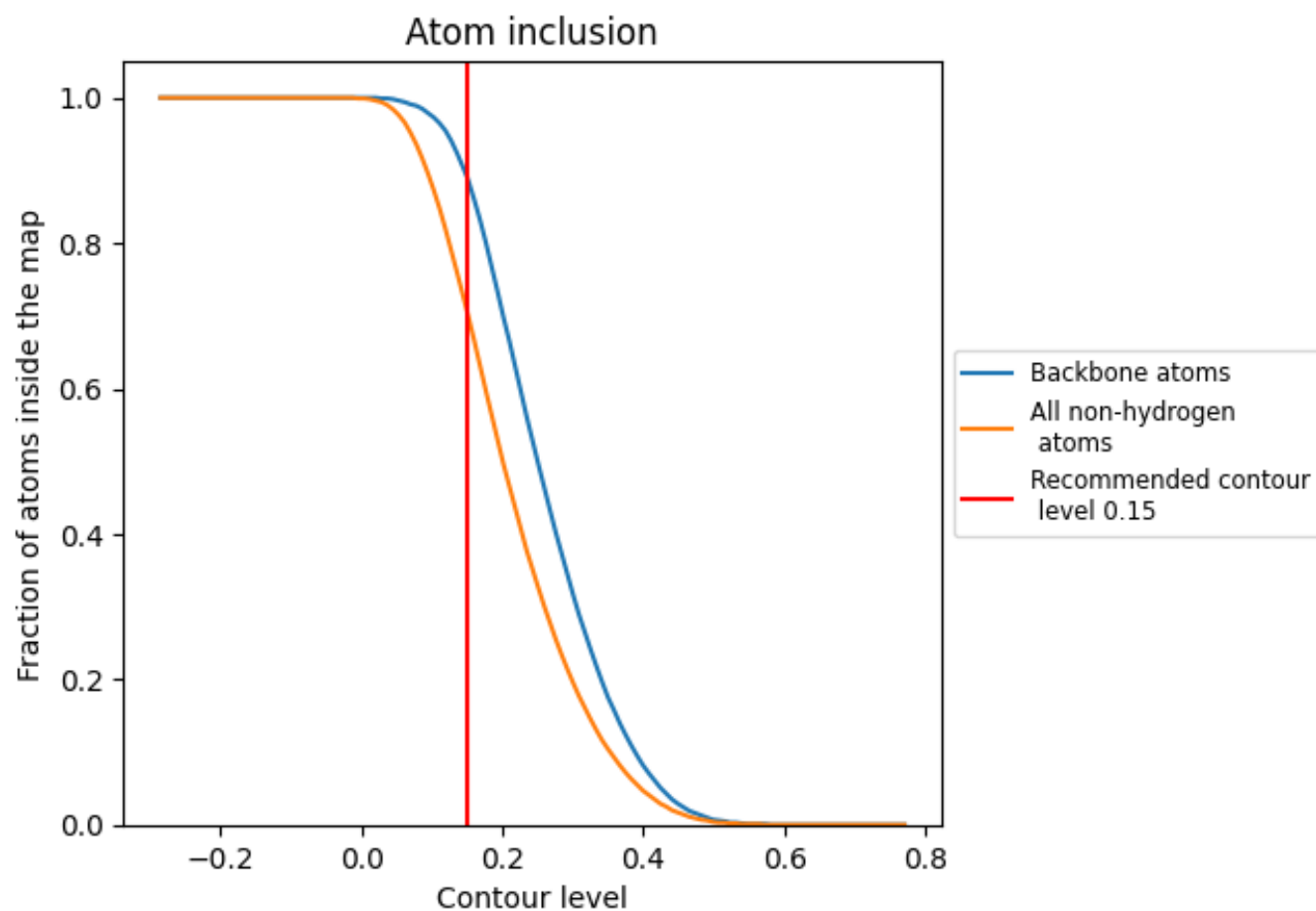
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 71% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7060	 0.4300
A	 0.7700	 0.4910
B	 0.7550	 0.4890
C	 0.7820	 0.5010
D	 0.7700	 0.4930
E	 0.5510	 0.3450
F	 0.7250	 0.4710
G	 0.7730	 0.4720
H	 0.7890	 0.4830
I	 0.7840	 0.4720
J	 0.7720	 0.4640
K	 0.7760	 0.4810
L	 0.7920	 0.4860
M	 0.7620	 0.4580
N	 0.6900	 0.3960
P	 0.7120	 0.4070
Q	 0.7090	 0.4020
R	 0.6830	 0.3810
S	 0.7120	 0.3920
T	 0.7030	 0.3860
U	 0.6980	 0.4290
V	 0.6310	 0.3820
W	 0.7340	 0.4360
X	 0.7550	 0.4440
Y	 0.8320	 0.4690
Z	 0.7730	 0.4870
a	 0.7110	 0.4070
b	 0.6950	 0.4420
c	 0.7280	 0.4740
d	 0.5840	 0.3570
e	 0.7560	 0.4460
f	 0.5580	 0.3320
g	 0.0030	 0.1250
h	 0.6930	 0.3790
u	 0.6680	 0.4660
v	 0.8830	 0.5600

