



wwPDB EM Validation Summary Report ⓘ

Mar 24, 2026 – 02:57 AM UTC

PDB ID : 9E8J / pdb_00009e8j
EMDB ID : EMD-47722
Title : Nub1/Fat10-processing human 26S proteasome bound to Txnl1 with Rpt1 at top of spiral staircase
Authors : Arkinson, C.; Gee, C.L.; Martin, A.
Deposited on : 2024-11-05
Resolution : 3.47 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:

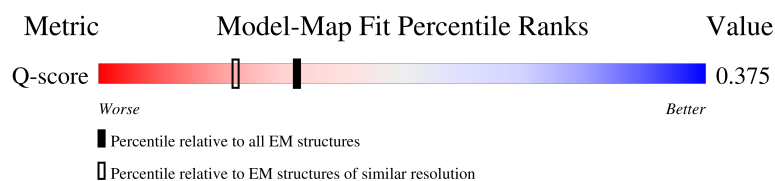
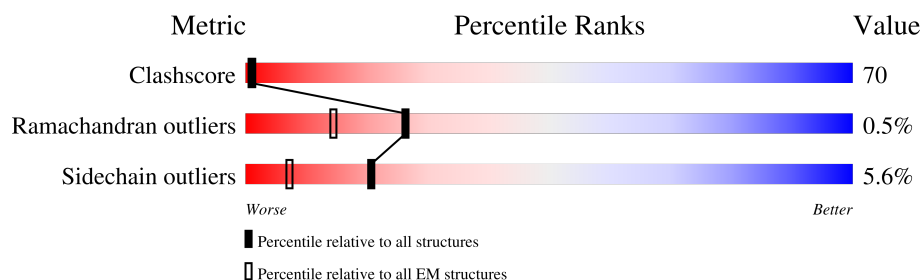
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.47 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.



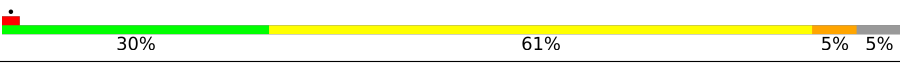
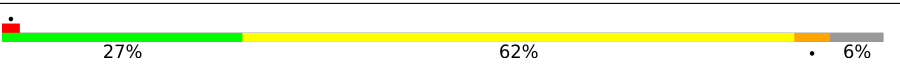
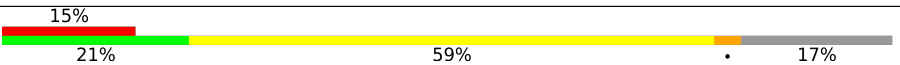
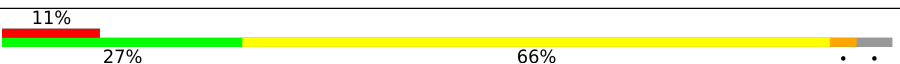
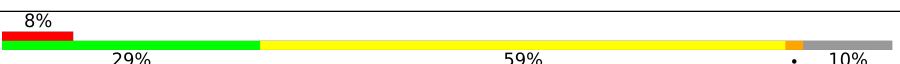
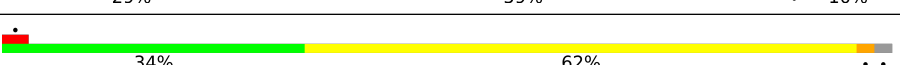
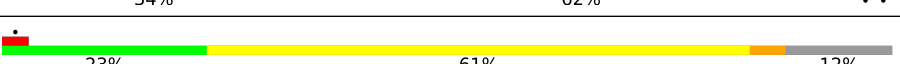
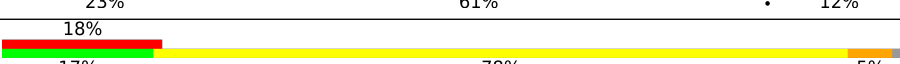
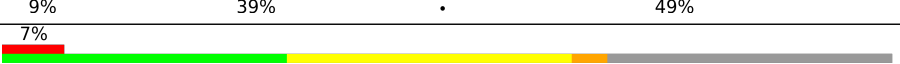
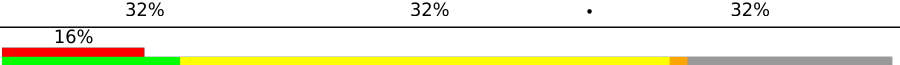
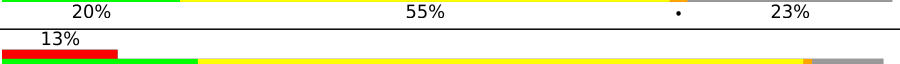
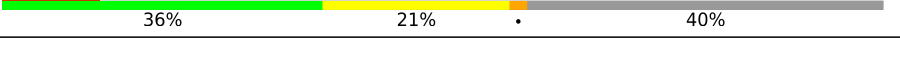
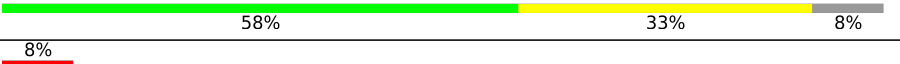
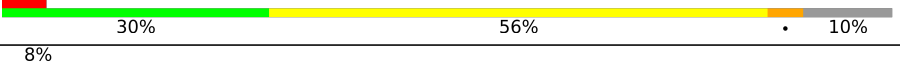
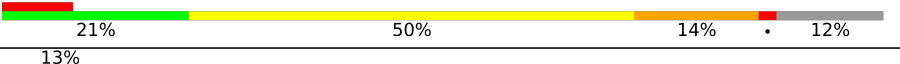
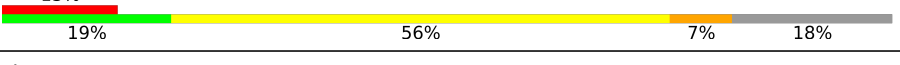
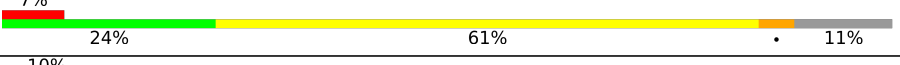
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13733 (2.97 - 3.97)

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	C	406	
2	D	418	
3	G	246	
4	H	234	

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Mol	Chain	Length	Quality of chain
5	I	261	
6	J	248	
7	L	263	
8	M	255	
9	V	534	
10	W	456	
11	X	422	
12	Y	389	
13	Z	324	
14	a	376	
15	b	377	
16	c	424	
17	d	350	
18	f	908	
19	g	601	
20	u	289	
21	v	12	
22	A	433	
23	B	440	
24	E	389	
25	F	439	
26	K	241	
27	U	953	
28	e	70	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	ATP	F	501	-	-	X	-

2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 70858 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 protease regulatory subunit 8.

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

- Molecule 2 is a protein called 26S proteasome regulatory subunit 6B.

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

- Molecule 3 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	239	Total	C	N	O	S	0	0
			1820	1157	304	346	13		

- Molecule 4 is a protein called Proteasome subunit alpha type-2.

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

- Molecule 5 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	248	Total	C	N	O	S	0	0
			1895	1195	324	368	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	239	Total	C	N	O	S	0	0
			1733	1076	315	337	5		

- Molecule 7 is a protein called Proteasome subunit alpha type-1.

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

- Molecule 8 is a protein called Proteasome subunit alpha type-3.

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

- Molecule 9 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	V	443	Total	C	N	O	S	0	0
			3608	2299	644	652	13		

- Molecule 10 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

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

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

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

- Molecule 12 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Y	380	Total	C	N	O	S	0	0
			3127	1995	535	580	17		

- Molecule 13 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

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

- Molecule 14 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

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

- Molecule 15 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

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

- Molecule 16 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	c	289	Total	C	N	O	S	0	0
			2269	1436	391	423	19		

There are 114 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
c	311	LEU	-	expression tag	UNP O00487
c	312	ILE	-	expression tag	UNP O00487
c	313	ASN	-	expression tag	UNP O00487
c	314	HIS	-	expression tag	UNP O00487
c	315	HIS	-	expression tag	UNP O00487
c	316	HIS	-	expression tag	UNP O00487
c	317	HIS	-	expression tag	UNP O00487
c	318	HIS	-	expression tag	UNP O00487
c	319	HIS	-	expression tag	UNP O00487
c	320	ASP	-	expression tag	UNP O00487
c	321	TYR	-	expression tag	UNP O00487
c	322	ASP	-	expression tag	UNP O00487
c	323	ILE	-	expression tag	UNP O00487
c	324	PRO	-	expression tag	UNP O00487
c	325	THR	-	expression tag	UNP O00487
c	326	THR	-	expression tag	UNP O00487
c	327	ALA	-	expression tag	UNP O00487
c	328	SER	-	expression tag	UNP O00487
c	329	GLU	-	expression tag	UNP O00487
c	330	ASN	-	expression tag	UNP O00487
c	331	LEU	-	expression tag	UNP O00487
c	332	TYR	-	expression tag	UNP O00487
c	333	PHE	-	expression tag	UNP O00487
c	334	GLN	-	expression tag	UNP O00487
c	335	GLY	-	expression tag	UNP O00487

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Chain	Residue	Modelled	Actual	Comment	Reference
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c	337	LEU	-	expression tag	UNP O00487
c	338	GLY	-	expression tag	UNP O00487
c	339	MET	-	expression tag	UNP O00487
c	340	ARG	-	expression tag	UNP O00487
c	341	GLY	-	expression tag	UNP O00487
c	342	SER	-	expression tag	UNP O00487
c	343	ALA	-	expression tag	UNP O00487
c	344	GLY	-	expression tag	UNP O00487
c	345	LYS	-	expression tag	UNP O00487
c	346	ALA	-	expression tag	UNP O00487
c	347	GLY	-	expression tag	UNP O00487
c	348	GLU	-	expression tag	UNP O00487
c	349	GLY	-	expression tag	UNP O00487
c	350	GLU	-	expression tag	UNP O00487
c	351	ILE	-	expression tag	UNP O00487
c	352	PRO	-	expression tag	UNP O00487
c	353	ALA	-	expression tag	UNP O00487
c	354	PRO	-	expression tag	UNP O00487
c	355	LEU	-	expression tag	UNP O00487
c	356	ALA	-	expression tag	UNP O00487
c	357	GLY	-	expression tag	UNP O00487
c	358	THR	-	expression tag	UNP O00487
c	359	VAL	-	expression tag	UNP O00487
c	360	SER	-	expression tag	UNP O00487
c	361	LYS	-	expression tag	UNP O00487
c	362	ILE	-	expression tag	UNP O00487
c	363	LEU	-	expression tag	UNP O00487
c	364	VAL	-	expression tag	UNP O00487
c	365	LYS	-	expression tag	UNP O00487
c	366	GLU	-	expression tag	UNP O00487
c	367	GLY	-	expression tag	UNP O00487
c	368	ASP	-	expression tag	UNP O00487
c	369	THR	-	expression tag	UNP O00487
c	370	VAL	-	expression tag	UNP O00487
c	371	LYS	-	expression tag	UNP O00487
c	372	ALA	-	expression tag	UNP O00487
c	373	GLY	-	expression tag	UNP O00487
c	374	GLN	-	expression tag	UNP O00487
c	375	THR	-	expression tag	UNP O00487
c	376	VAL	-	expression tag	UNP O00487
c	377	LEU	-	expression tag	UNP O00487

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Chain	Residue	Modelled	Actual	Comment	Reference
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c	380	GLU	-	expression tag	UNP O00487
c	381	ALA	-	expression tag	UNP O00487
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c	383	LYS	-	expression tag	UNP O00487
c	384	MET	-	expression tag	UNP O00487
c	385	GLU	-	expression tag	UNP O00487
c	386	THR	-	expression tag	UNP O00487
c	387	GLU	-	expression tag	UNP O00487
c	388	ILE	-	expression tag	UNP O00487
c	389	ASN	-	expression tag	UNP O00487
c	390	ALA	-	expression tag	UNP O00487
c	391	PRO	-	expression tag	UNP O00487
c	392	THR	-	expression tag	UNP O00487
c	393	ASP	-	expression tag	UNP O00487
c	394	GLY	-	expression tag	UNP O00487
c	395	LYS	-	expression tag	UNP O00487
c	396	VAL	-	expression tag	UNP O00487
c	397	GLU	-	expression tag	UNP O00487
c	398	LYS	-	expression tag	UNP O00487
c	399	VAL	-	expression tag	UNP O00487
c	400	LEU	-	expression tag	UNP O00487
c	401	VAL	-	expression tag	UNP O00487
c	402	LYS	-	expression tag	UNP O00487
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c	410	GLY	-	expression tag	UNP O00487
c	411	GLN	-	expression tag	UNP O00487
c	412	GLY	-	expression tag	UNP O00487
c	413	LEU	-	expression tag	UNP O00487
c	414	ILE	-	expression tag	UNP O00487
c	415	LYS	-	expression tag	UNP O00487
c	416	ILE	-	expression tag	UNP O00487
c	417	GLY	-	expression tag	UNP O00487
c	418	VAL	-	expression tag	UNP O00487
c	419	HIS	-	expression tag	UNP O00487

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Chain	Residue	Modelled	Actual	Comment	Reference
c	420	HIS	-	expression tag	UNP O00487
c	421	HIS	-	expression tag	UNP O00487
c	422	HIS	-	expression tag	UNP O00487
c	423	HIS	-	expression tag	UNP O00487
c	424	HIS	-	expression tag	UNP O00487

- Molecule 17 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

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

- Molecule 18 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	f	832	Total	C	N	O	S	0	0
			6442	4076	1090	1231	45		

- Molecule 19 is a protein called Isoform 2 of NEDD8 ultimate buster 1.

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

- Molecule 20 is a protein called Thioredoxin-like protein 1.

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

- Molecule 21 is a protein called substrate peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	v	11	Total	C	N	O	0	0
			55	33	11	11		

- Molecule 22 is a protein called 26S proteasome regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	A	407	Total	C	N	O	S	0	0
			3199	2015	561	605	18		

- Molecule 23 is a protein called 26S proteasome regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	B	396	Total	C	N	O	S	0	0
			3107	1957	529	606	15		

- Molecule 24 is a protein called 26S protease regulatory subunit 10B.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	E	343	Total	C	N	O	S	0	0
			2701	1699	477	509	16		

- Molecule 25 is a protein called 26S proteasome regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	F	359	Total	C	N	O	S	0	0
			2801	1768	485	532	16		

- Molecule 26 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	K	228	Total	C	N	O	S	0	0
			1737	1092	286	349	10		

There is a discrepancy between the modelled and reference sequences:

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

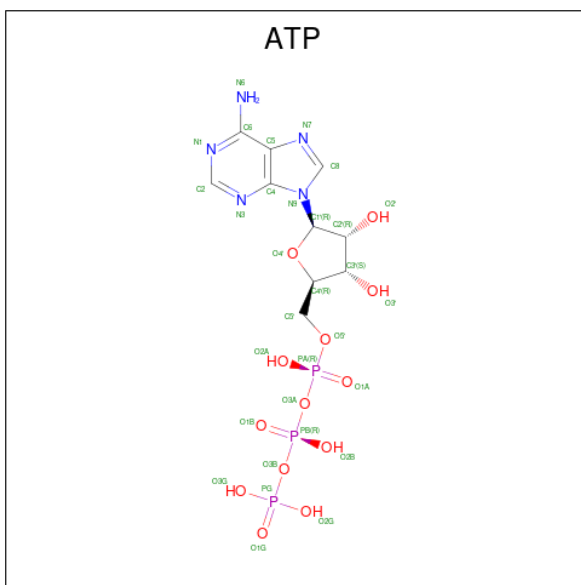
- Molecule 27 is a protein called 26S proteasome non-ATPase regulatory subunit 1.

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

- Molecule 28 is a protein called 26S proteasome complex subunit SEM1.

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

- Molecule 29 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).

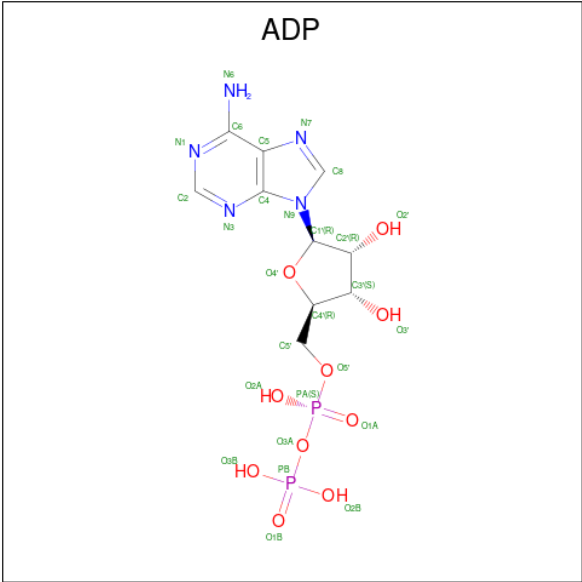


Mol	Chain	Residues	Atoms					AltConf
29	C	1	Total 31	C 10	N 5	O 13	P 3	0
29	A	1	Total 31	C 10	N 5	O 13	P 3	0
29	B	1	Total 31	C 10	N 5	O 13	P 3	0
29	F	1	Total 31	C 10	N 5	O 13	P 3	0

- Molecule 30 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

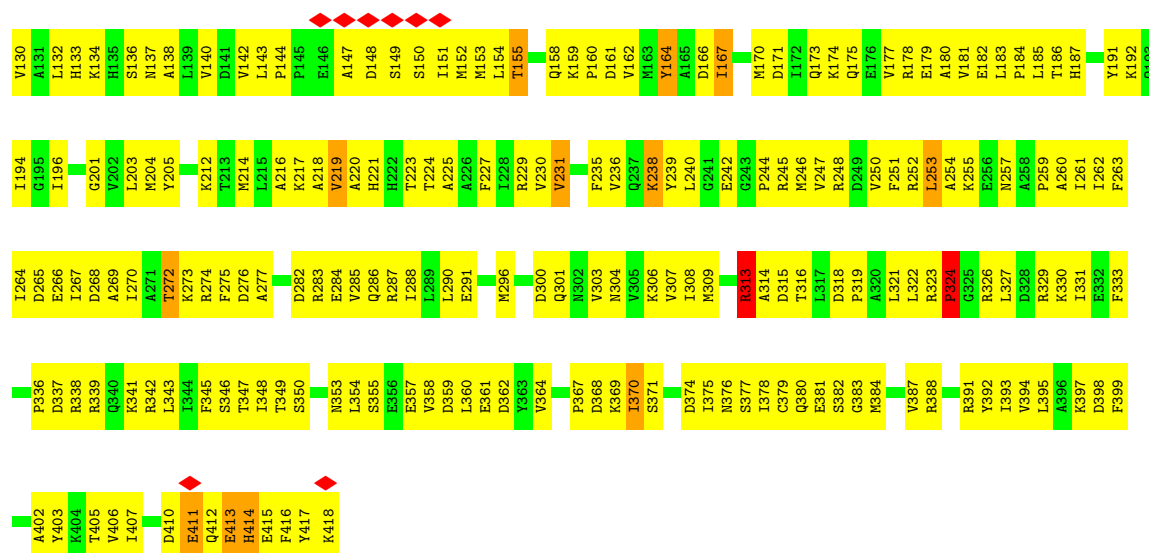
- Molecule 31 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$) (labeled as "Ligand of Interest" by depositor).



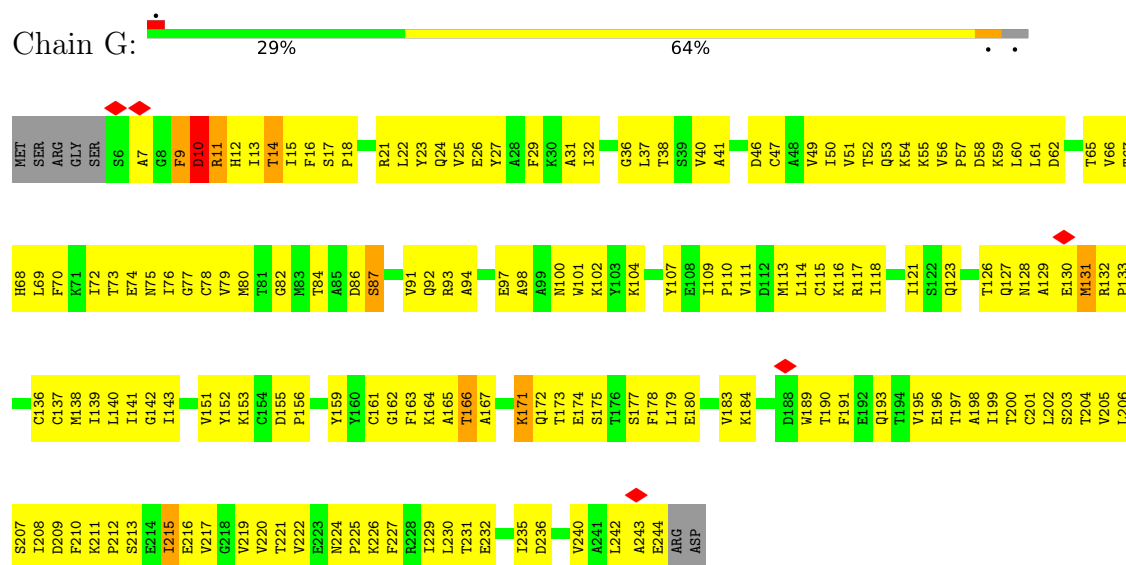
Mol	Chain	Residues	Atoms					AltConf
31	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
31	E	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 32 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

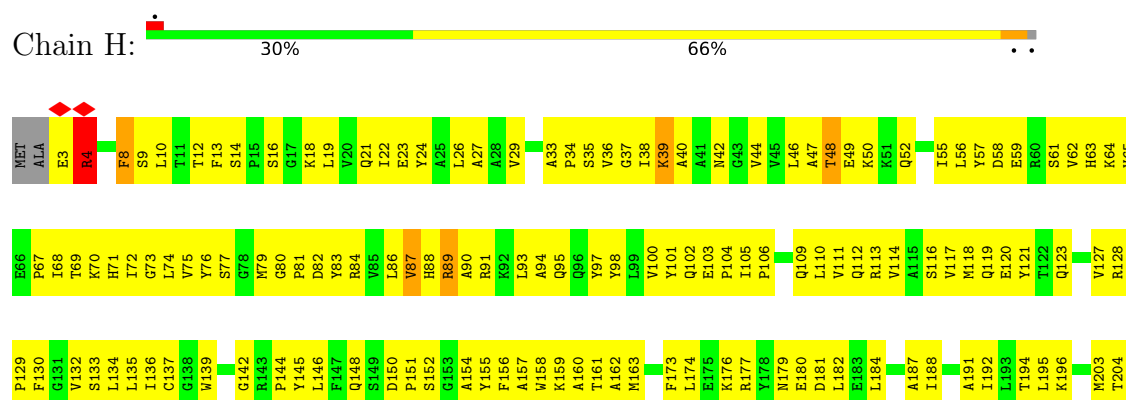
Mol	Chain	Residues	Atoms		AltConf
32	c	1	Total	Zn	0
			1	1	



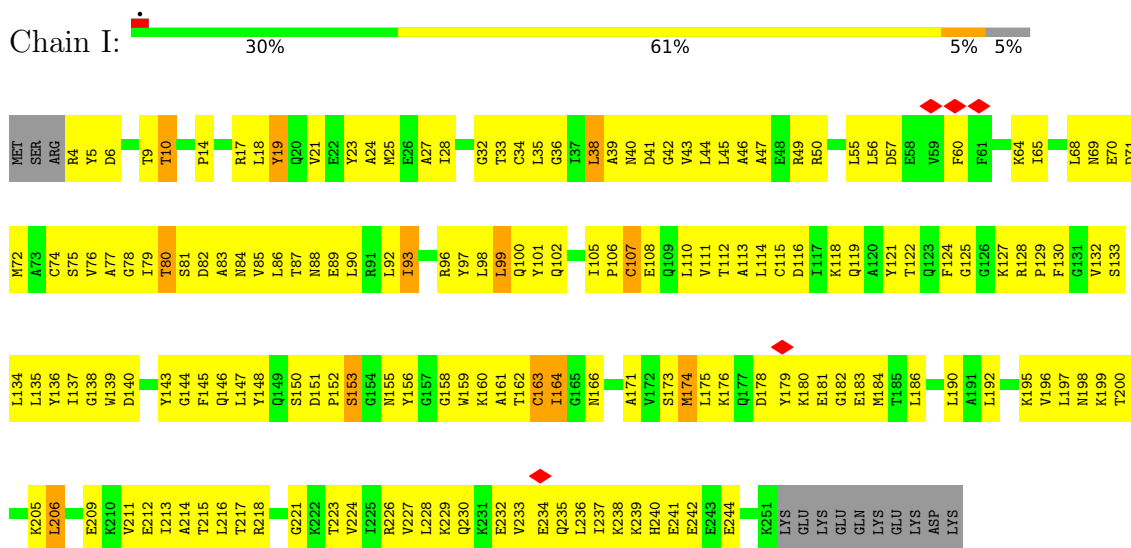
• Molecule 3: Proteasome subunit alpha type-6



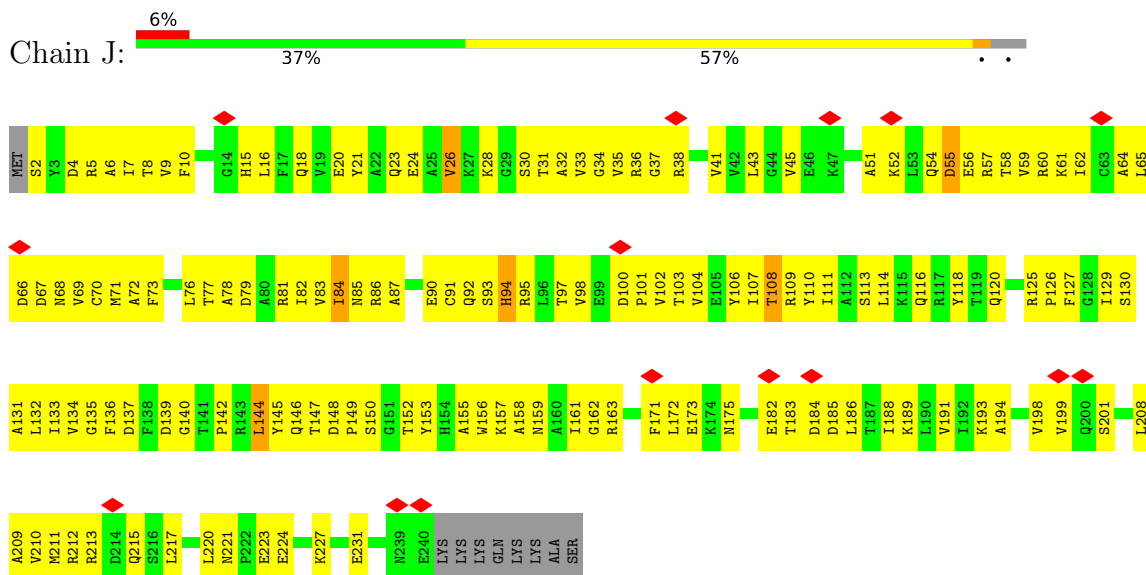
• Molecule 4: Proteasome subunit alpha type-2



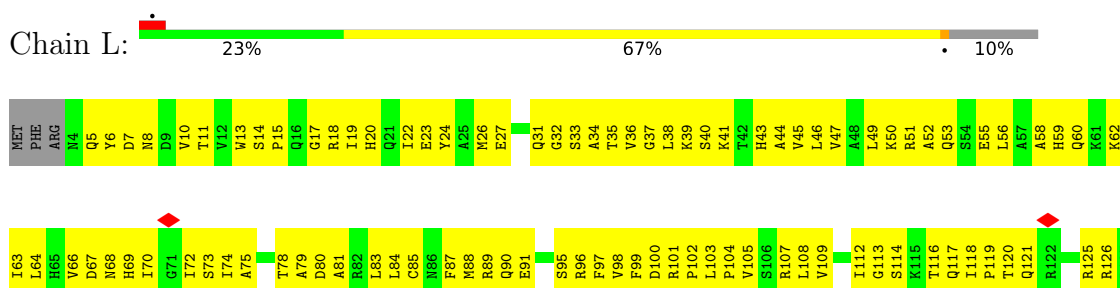
- Molecule 5: Proteasome subunit alpha type-4

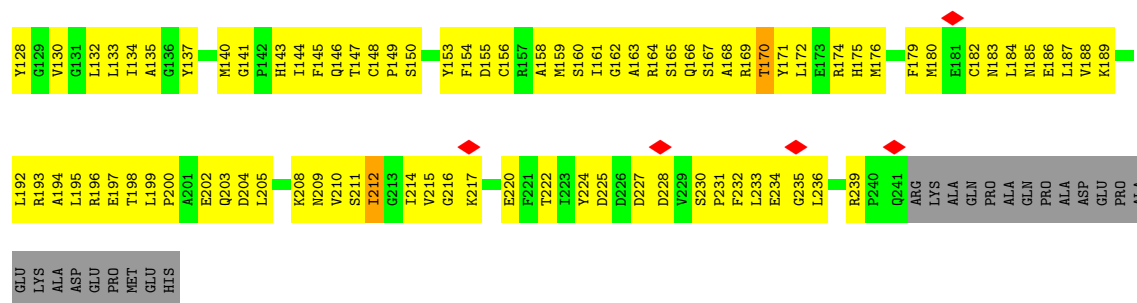


- Molecule 6: Proteasome subunit alpha type-7

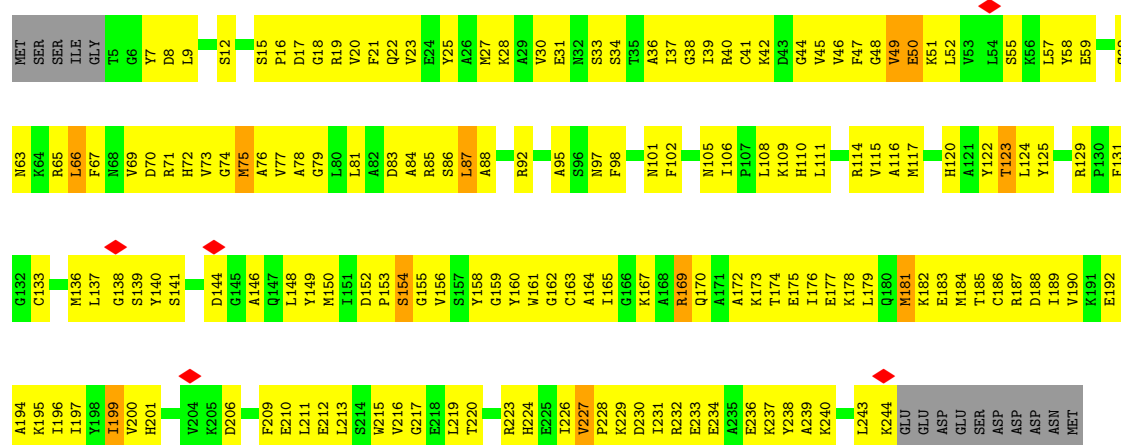


- Molecule 7: Proteasome subunit alpha type-1

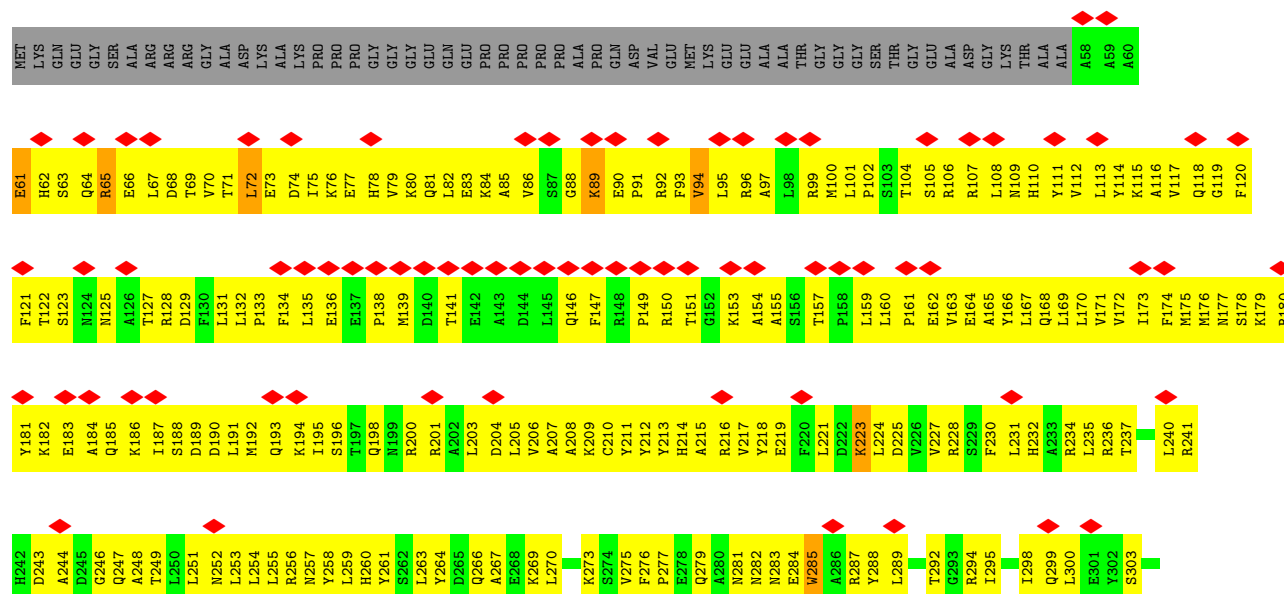




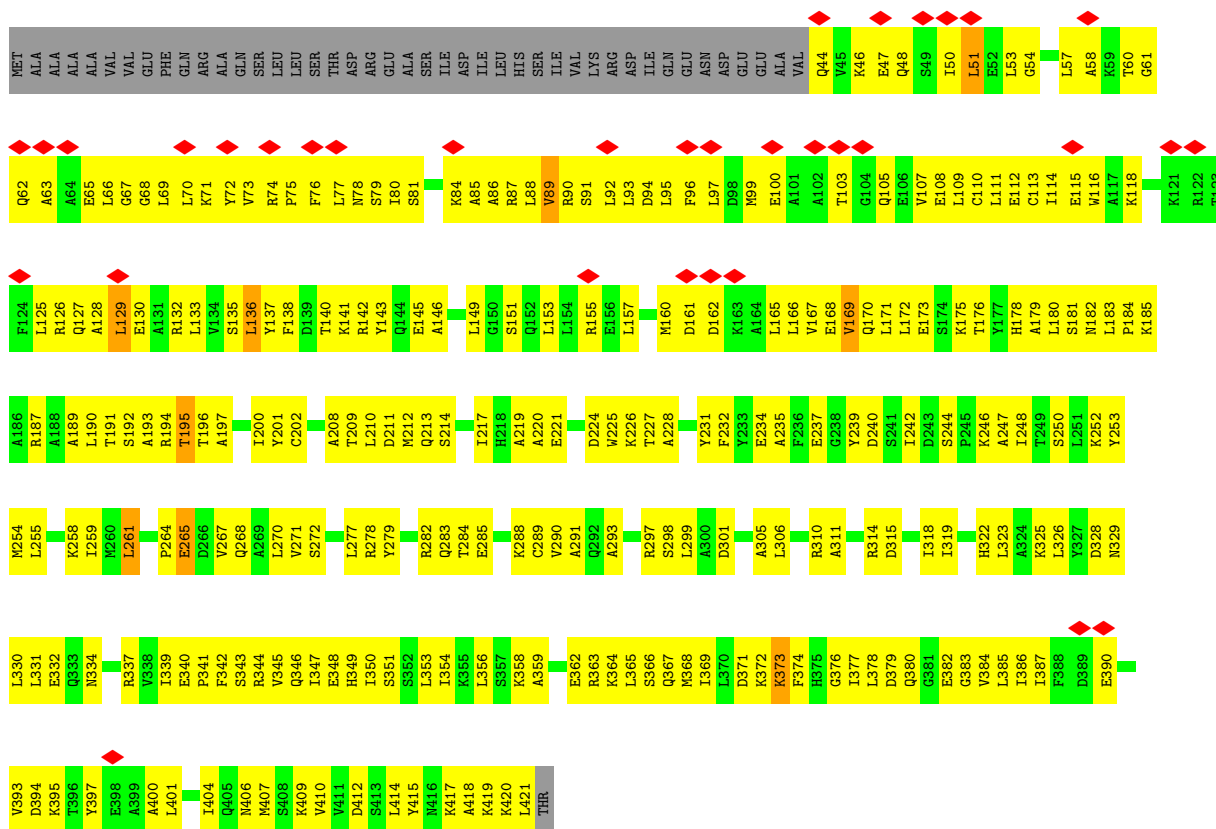
• Molecule 8: Proteasome subunit alpha type-3



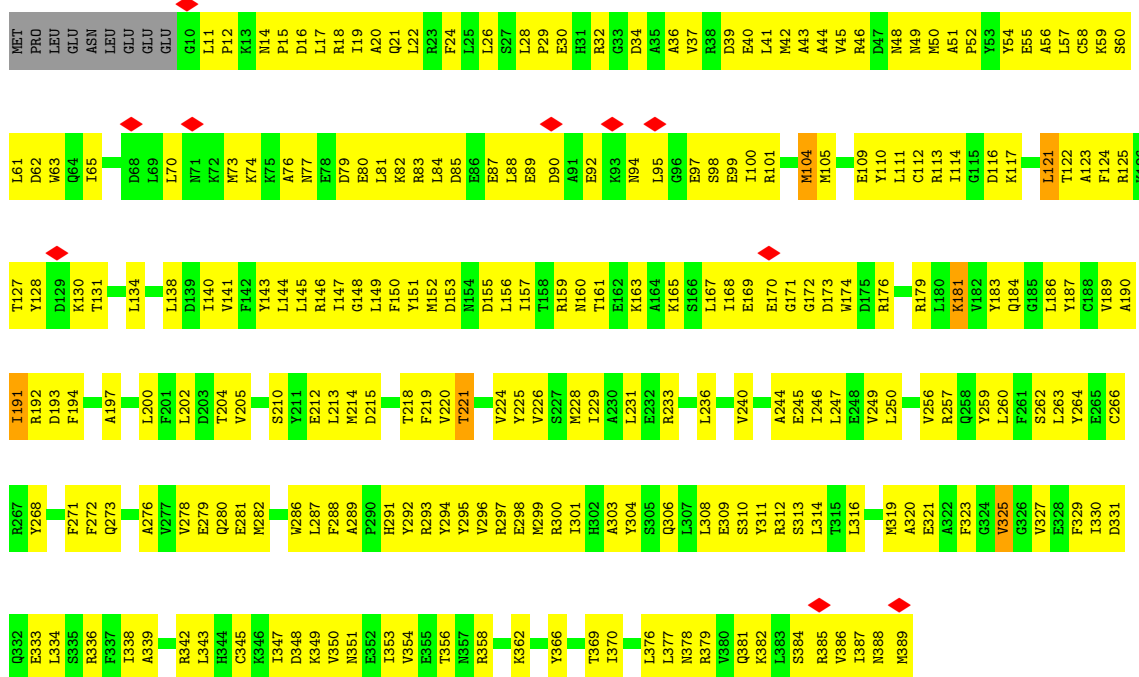
• Molecule 9: 26S proteasome non-ATPase regulatory subunit 3



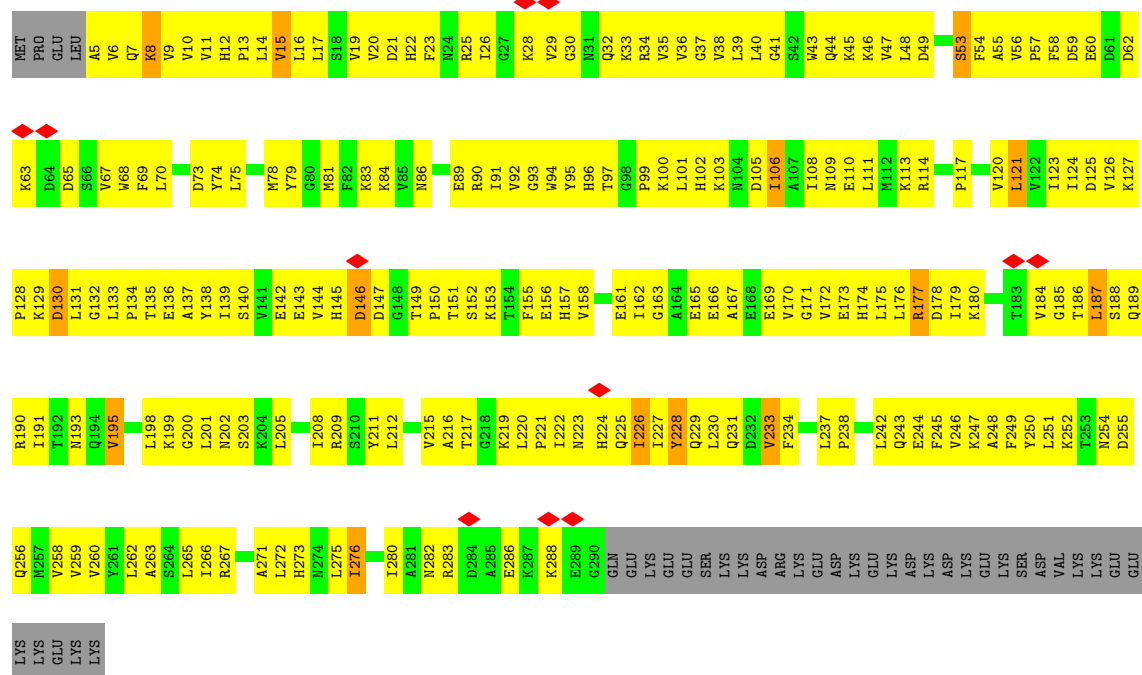




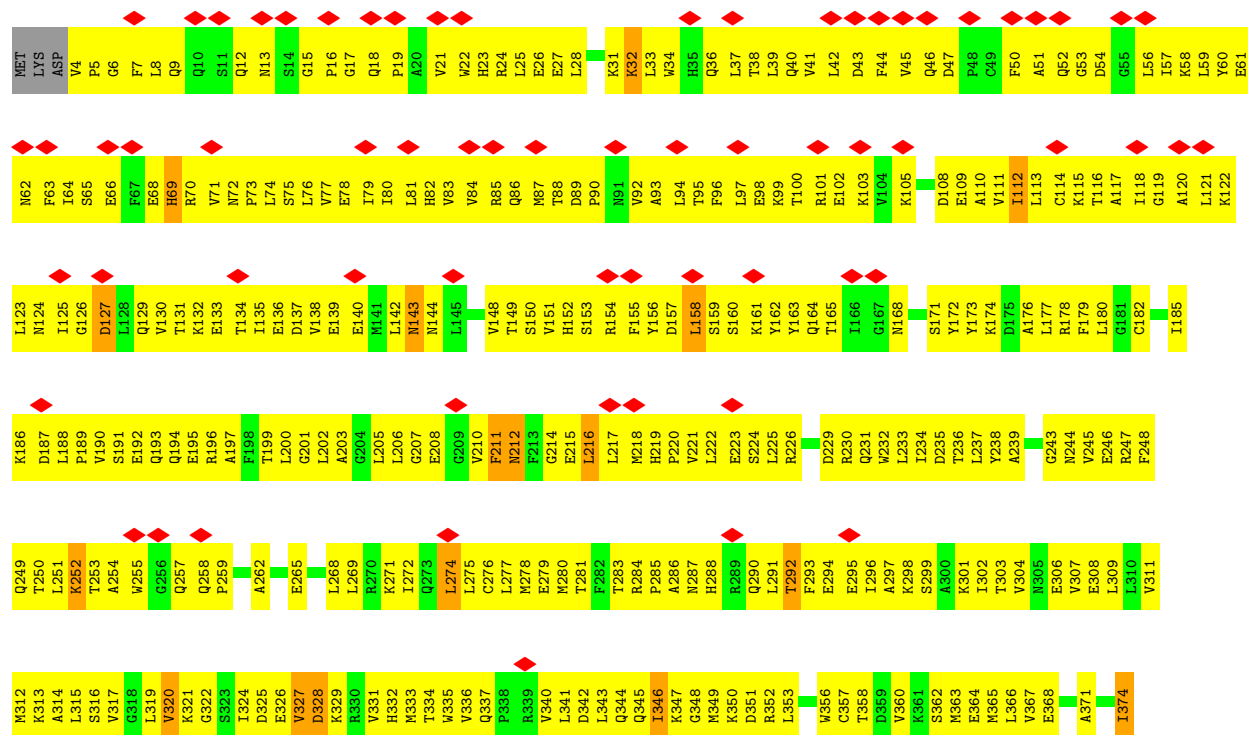
• Molecule 12: 26S proteasome non-ATPase regulatory subunit 6



• Molecule 13: 26S proteasome non-ATPase regulatory subunit 7



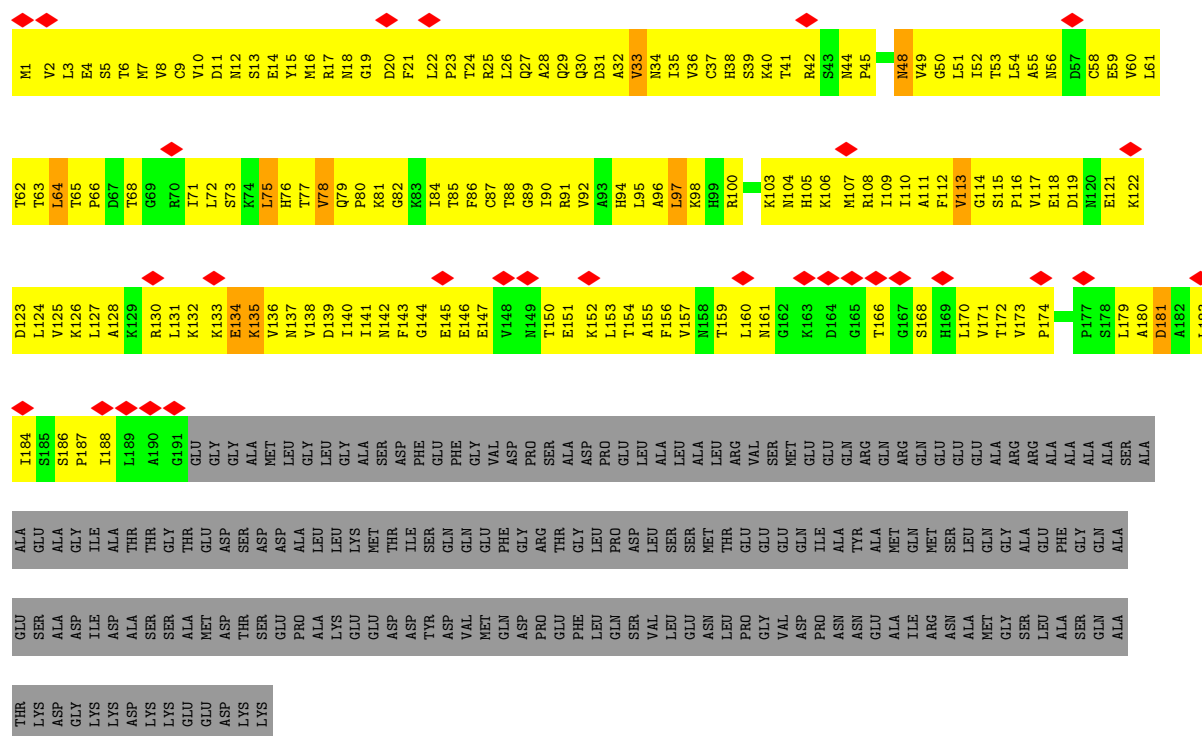
Chain a:



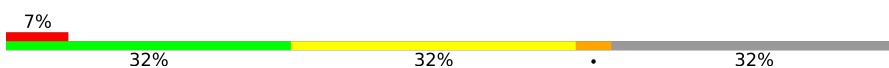
L375
T376

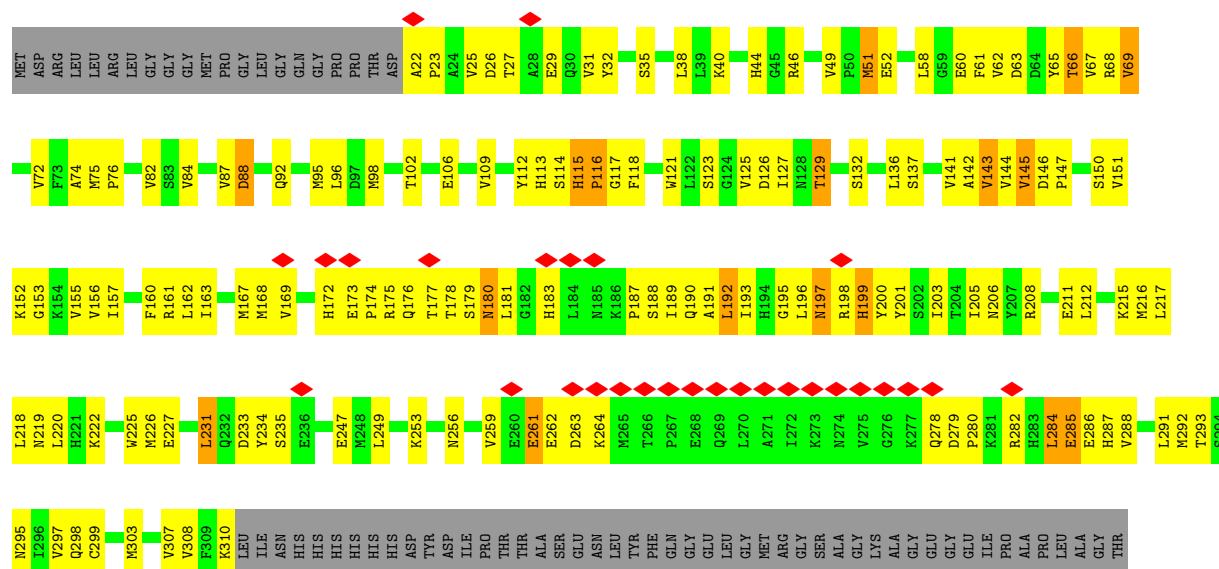
• Molecule 15: 26S proteasome non-ATPase regulatory subunit 4

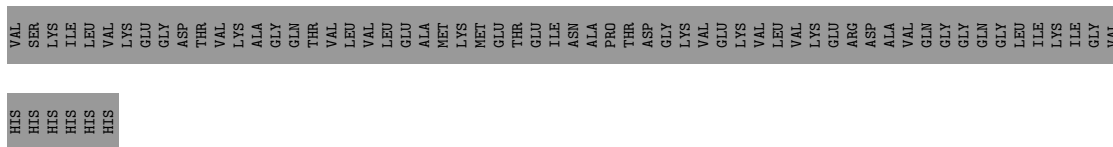
Chain b: 



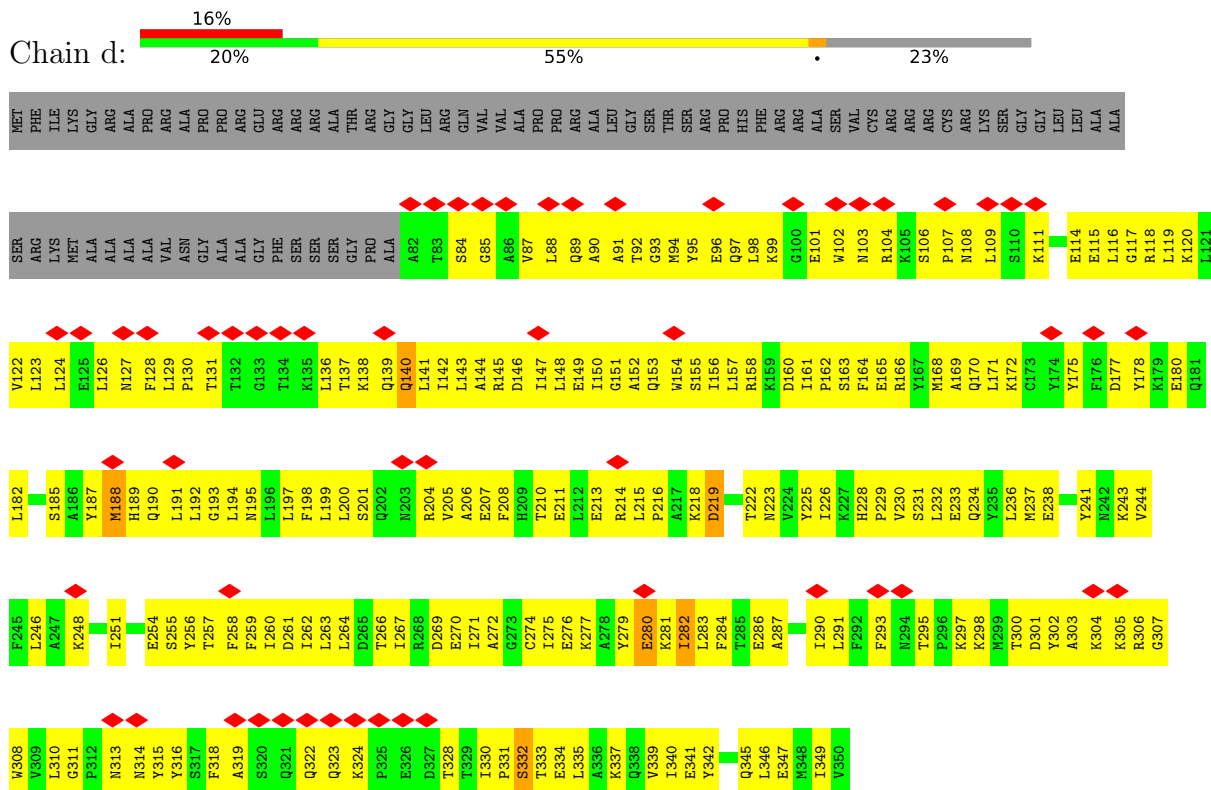
• Molecule 16: 26S proteasome non-ATPase regulatory subunit 14

Chain c: 

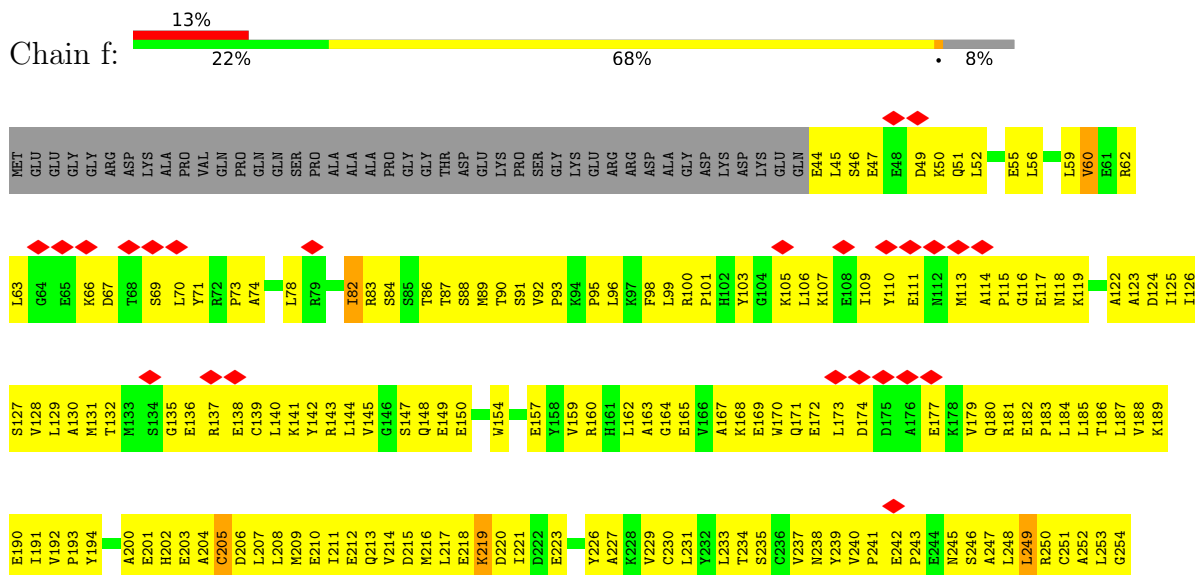


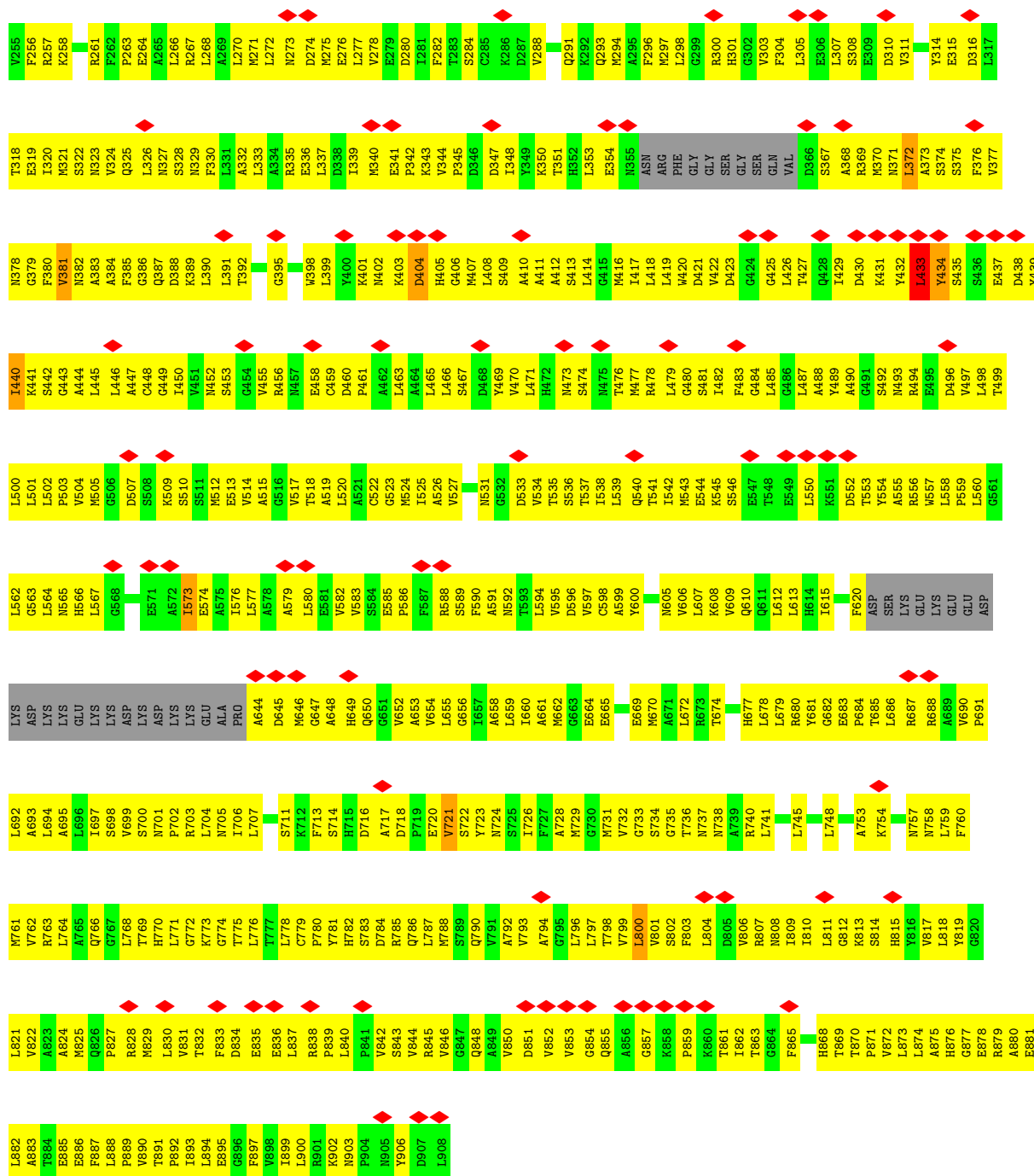


- Molecule 17: 26S proteasome non-ATPase regulatory subunit 8

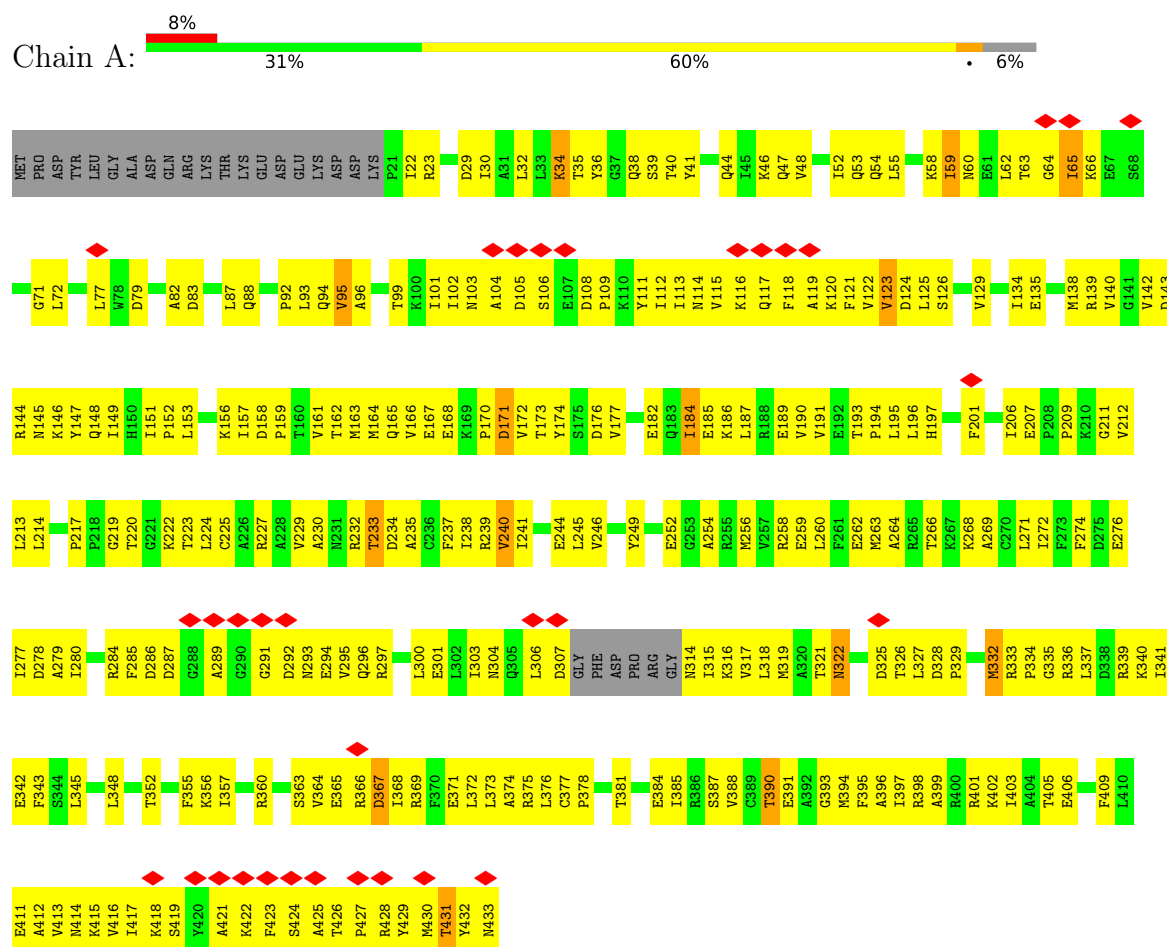


- Molecule 18: 26S proteasome non-ATPase regulatory subunit 2

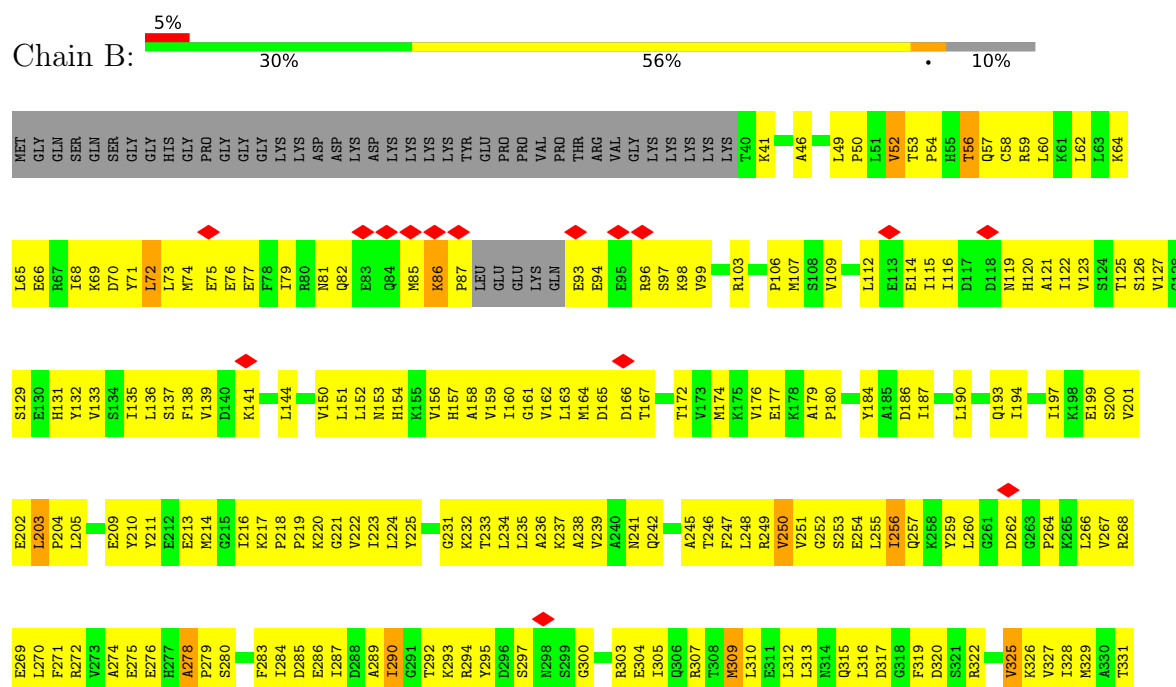


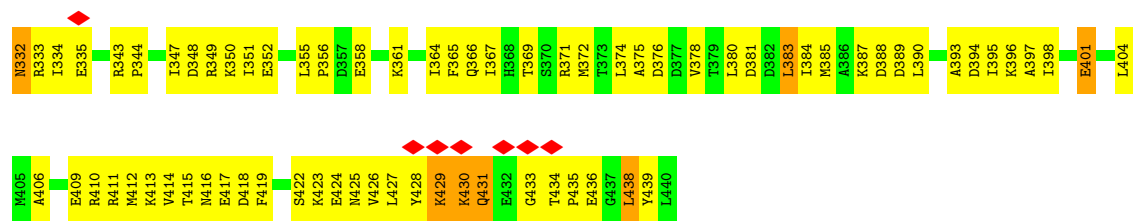


• Molecule 22: 26S proteasome regulatory subunit 7

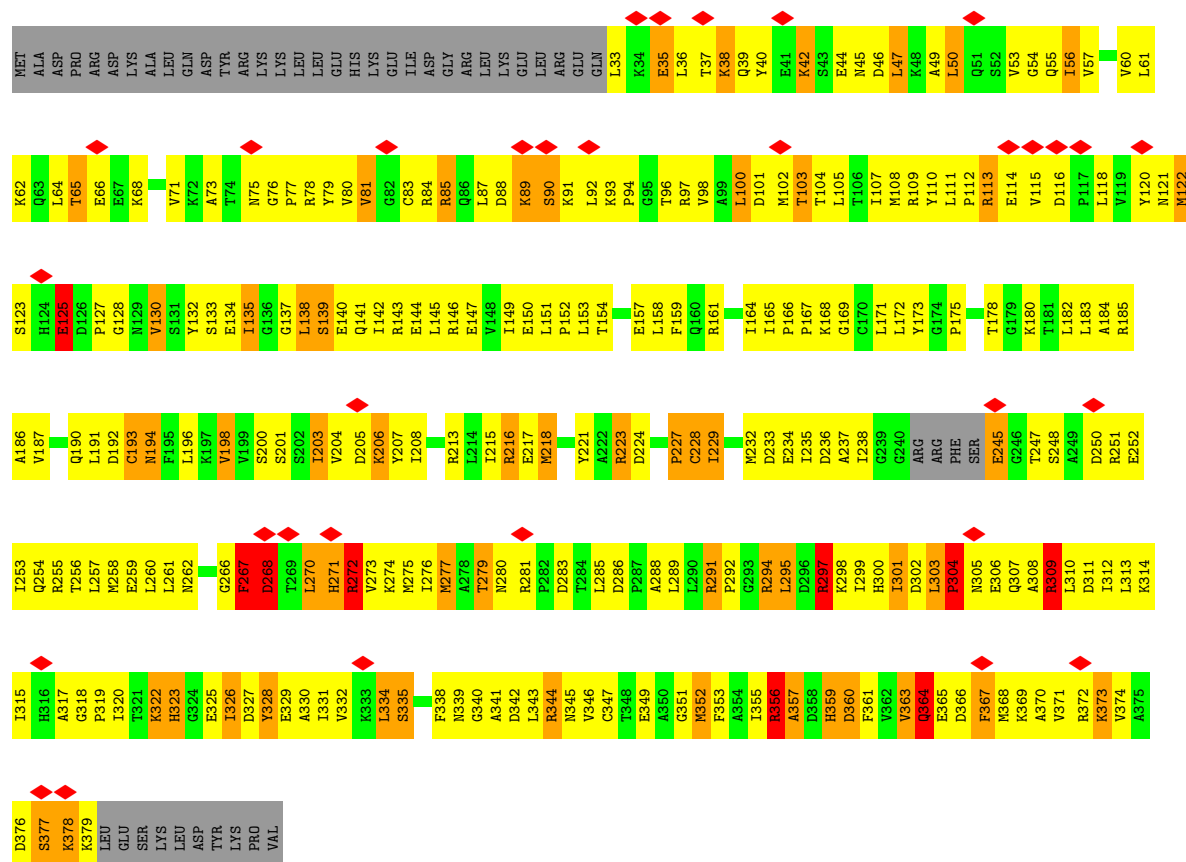
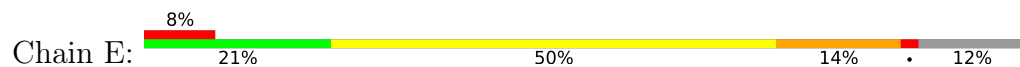


• Molecule 23: 26S proteasome regulatory subunit 4



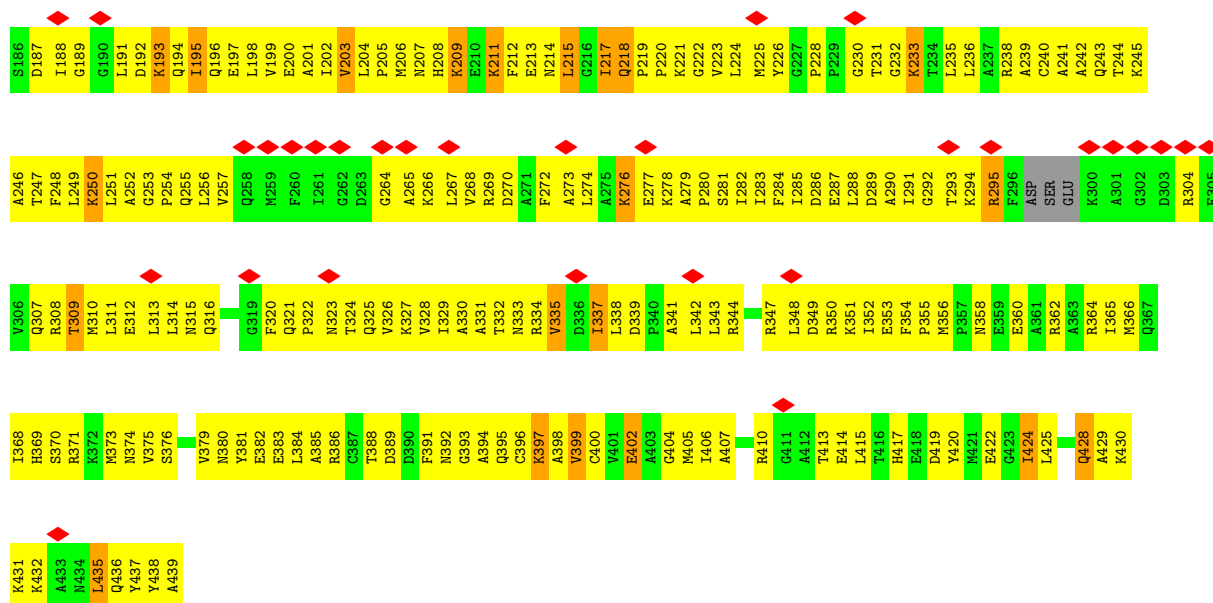


• Molecule 24: 26S protease regulatory subunit 10B

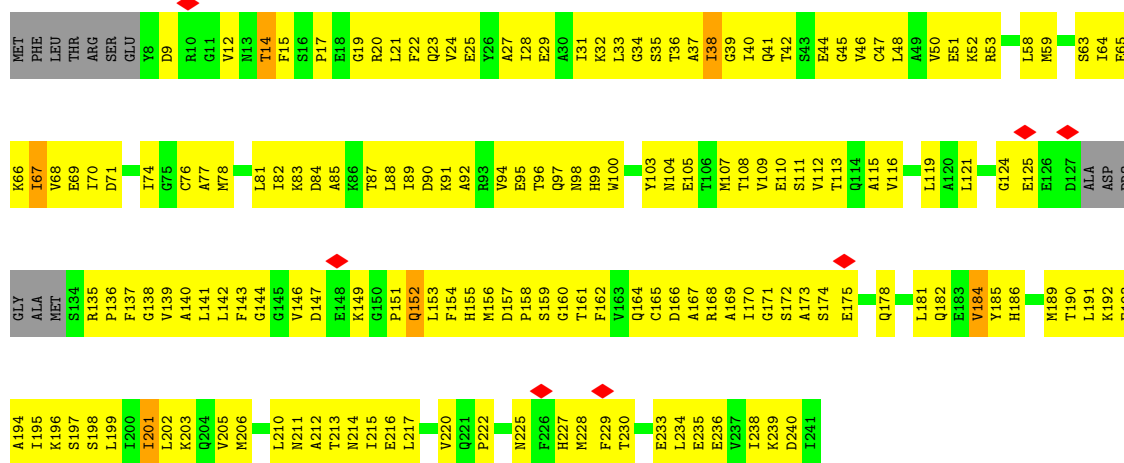


• Molecule 25: 26S proteasome regulatory subunit 6A

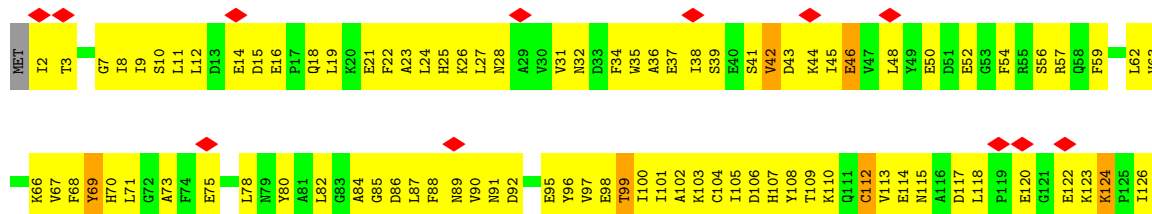




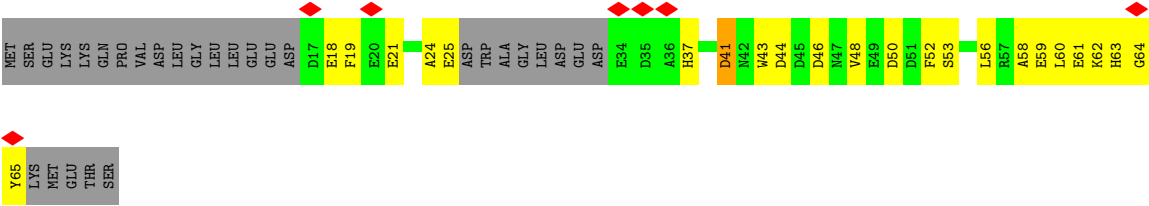
• Molecule 26: Proteasome subunit alpha type-5



• Molecule 27: 26S proteasome non-ATPase regulatory subunit 1







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	19309	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	0.618	Depositor
Minimum map value	-0.230	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.034	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	356.32, 356.32, 356.32	wwPDB
Map dimensions	340, 340, 340	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.048, 1.048, 1.048	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	C	0.29	0/3092	0.45	0/4154
2	D	0.44	0/3090	0.65	0/4168
3	G	0.28	0/1853	0.45	2/2515 (0.1%)
4	H	0.29	0/1852	0.52	1/2507 (0.0%)
5	I	0.23	0/1925	0.39	0/2606
6	J	0.22	0/1758	0.37	0/2394
7	L	0.24	0/1885	0.36	0/2552
8	M	0.25	0/1891	0.40	0/2552
9	V	0.20	0/3678	0.40	0/4965
10	W	0.19	0/3618	0.32	0/4868
11	X	0.24	0/3038	0.38	0/4095
12	Y	0.24	0/3185	0.31	0/4290
13	Z	0.28	0/2324	0.40	0/3150
14	a	0.20	0/3053	0.43	0/4133
15	b	0.21	0/1478	0.42	0/2001
16	c	0.38	0/2311	0.60	2/3124 (0.1%)
17	d	0.16	0/2234	0.34	0/3018
18	f	0.19	0/6550	0.34	0/8865
19	g	0.31	0/778	0.93	4/1041 (0.4%)
20	u	0.20	0/1403	0.36	0/1892
21	v	0.80	0/4	1.05	0/4
22	A	0.26	0/3250	0.45	0/4386
23	B	0.32	0/3153	0.49	0/4255
24	E	0.77	1/2742 (0.0%)	1.23	21/3696 (0.6%)
25	F	0.37	0/2838	0.63	1/3825 (0.0%)
26	K	0.26	0/1763	0.43	0/2383
27	U	0.23	0/6696	0.38	2/9052 (0.0%)
28	e	0.20	0/362	0.32	0/490
All	All	0.30	1/71804 (0.0%)	0.49	33/96981 (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
2	D	0	2
4	H	0	1
23	B	0	1
24	E	0	16
25	F	0	1
27	U	0	1
All	All	0	22

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	E	89	LYS	CA-C	5.07	1.59	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	g	166	ARG	N-CA-C	-14.71	95.40	113.20
24	E	90	SER	N-CA-C	9.07	122.09	111.02
19	g	171	LEU	N-CA-C	-8.62	100.90	111.33
19	g	165	ALA	N-CA-C	-8.33	101.11	113.61
27	U	644	TYR	CA-C-N	-8.05	109.27	121.83

There are no chirality outliers.

5 of 22 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
23	B	53	THR	Peptide
2	D	313	ARG	Sidechain
2	D	85	ILE	Peptide
24	E	84	ARG	Sidechain
4	H	4	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	C	3051	0	3165	449	0
2	D	3040	0	3075	400	0
3	G	1820	0	1789	275	0
4	H	1813	0	1802	246	0
5	I	1895	0	1833	271	0
6	J	1733	0	1570	205	0
7	L	1850	0	1822	306	0
8	M	1856	0	1814	281	0
9	V	3608	0	3677	642	0
10	W	3570	0	3685	526	0
11	X	2994	0	3097	412	0
12	Y	3127	0	3133	330	0
13	Z	2281	0	2312	375	0
14	a	2995	0	3012	752	0
15	b	1458	0	1505	334	0
16	c	2269	0	2282	190	0
17	d	2188	0	2216	354	0
18	f	6442	0	6463	1089	0
19	g	771	0	815	380	0
20	u	1376	0	1324	64	0
21	v	55	0	17	3	0
22	A	3199	0	3258	409	0
23	B	3107	0	3169	408	0
24	E	2701	0	2758	391	0
25	F	2801	0	2877	494	0
26	K	1737	0	1699	277	0
27	U	6584	0	6626	1014	0
28	e	353	0	276	34	0
29	A	31	0	12	2	0
29	B	31	0	12	5	0
29	C	31	0	12	2	0
29	F	31	0	12	9	0
30	A	1	0	0	0	0
30	B	1	0	0	0	0
30	C	1	0	0	0	0
30	D	1	0	0	0	0
30	F	1	0	0	0	0
31	D	27	0	12	1	0
31	E	27	0	12	0	0
32	c	1	0	0	0	0
All	All	70858	0	71143	9936	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 70.

The worst 5 of 9936 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)
24:E:352:MET:SD	24:E:355:ILE:HD12	1.44	1.58
24:E:235:ILE:CD1	24:E:277:MET:HB3	1.29	1.55
24:E:235:ILE:CD1	24:E:277:MET:CB	1.80	1.55
24:E:277:MET:CE	24:E:295:LEU:HD13	1.37	1.54
24:E:235:ILE:HD11	24:E:277:MET:CB	1.36	1.43

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	384/406 (95%)	349 (91%)	32 (8%)	3 (1%)	16	49
2	D	378/418 (90%)	330 (87%)	44 (12%)	4 (1%)	11	42
3	G	237/246 (96%)	217 (92%)	17 (7%)	3 (1%)	9	39
4	H	230/234 (98%)	212 (92%)	18 (8%)	0	100	100
5	I	246/261 (94%)	232 (94%)	13 (5%)	1 (0%)	30	62
6	J	237/248 (96%)	213 (90%)	24 (10%)	0	100	100
7	L	236/263 (90%)	227 (96%)	9 (4%)	0	100	100
8	M	238/255 (93%)	219 (92%)	19 (8%)	0	100	100
9	V	441/534 (83%)	415 (94%)	24 (5%)	2 (0%)	24	58
10	W	436/456 (96%)	415 (95%)	20 (5%)	1 (0%)	43	74
11	X	376/422 (89%)	354 (94%)	22 (6%)	0	100	100
12	Y	378/389 (97%)	362 (96%)	16 (4%)	0	100	100
13	Z	284/324 (88%)	252 (89%)	29 (10%)	3 (1%)	11	42
14	a	371/376 (99%)	331 (89%)	40 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	b	189/377 (50%)	158 (84%)	31 (16%)	0	100	100
16	c	287/424 (68%)	239 (83%)	45 (16%)	3 (1%)	12	44
17	d	267/350 (76%)	246 (92%)	20 (8%)	1 (0%)	30	62
18	f	824/908 (91%)	757 (92%)	66 (8%)	1 (0%)	48	79
19	g	93/601 (16%)	68 (73%)	25 (27%)	0	100	100
20	u	170/289 (59%)	162 (95%)	6 (4%)	2 (1%)	10	41
22	A	403/433 (93%)	373 (93%)	28 (7%)	2 (0%)	24	58
23	B	392/440 (89%)	351 (90%)	40 (10%)	1 (0%)	36	67
24	E	339/389 (87%)	297 (88%)	33 (10%)	9 (3%)	4	27
25	F	353/439 (80%)	307 (87%)	45 (13%)	1 (0%)	36	67
26	K	224/241 (93%)	209 (93%)	15 (7%)	0	100	100
27	U	834/953 (88%)	731 (88%)	98 (12%)	5 (1%)	21	53
28	e	37/70 (53%)	34 (92%)	3 (8%)	0	100	100
All	All	8884/10746 (83%)	8060 (91%)	782 (9%)	42 (0%)	26	58

5 of 42 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	82	LYS
2	D	413	GLU
3	G	10	ASP
3	G	11	ARG
3	G	184	LYS

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	C	338/352 (96%)	322 (95%)	16 (5%)	23	50
2	D	333/366 (91%)	309 (93%)	24 (7%)	13	38
3	G	192/210 (91%)	184 (96%)	8 (4%)	26	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	H	190/191 (100%)	182 (96%)	8 (4%)	26	52
5	I	191/221 (86%)	179 (94%)	12 (6%)	16	43
6	J	158/211 (75%)	151 (96%)	7 (4%)	25	51
7	L	198/224 (88%)	193 (98%)	5 (2%)	42	63
8	M	192/212 (91%)	179 (93%)	13 (7%)	14	41
9	V	391/460 (85%)	376 (96%)	15 (4%)	29	56
10	W	403/416 (97%)	386 (96%)	17 (4%)	26	52
11	X	325/362 (90%)	313 (96%)	12 (4%)	30	56
12	Y	335/344 (97%)	324 (97%)	11 (3%)	33	58
13	Z	257/295 (87%)	246 (96%)	11 (4%)	26	52
14	a	333/336 (99%)	314 (94%)	19 (6%)	18	45
15	b	167/312 (54%)	154 (92%)	13 (8%)	11	37
16	c	252/359 (70%)	238 (94%)	14 (6%)	19	46
17	d	237/294 (81%)	232 (98%)	5 (2%)	47	66
18	f	702/763 (92%)	685 (98%)	17 (2%)	43	64
19	g	85/527 (16%)	82 (96%)	3 (4%)	32	57
20	u	156/253 (62%)	146 (94%)	10 (6%)	16	43
22	A	350/372 (94%)	329 (94%)	21 (6%)	17	44
23	B	348/385 (90%)	328 (94%)	20 (6%)	18	45
24	E	298/341 (87%)	226 (76%)	72 (24%)	1	4
25	F	304/379 (80%)	269 (88%)	35 (12%)	5	24
26	K	189/204 (93%)	182 (96%)	7 (4%)	30	56
27	U	718/816 (88%)	684 (95%)	34 (5%)	23	50
28	e	37/63 (59%)	35 (95%)	2 (5%)	20	47
All	All	7679/9268 (83%)	7248 (94%)	431 (6%)	21	46

5 of 431 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
20	u	165	LEU
24	E	53	VAL
27	U	124	LYS
20	u	268	THR
22	A	431	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 108 such sidechains are listed below:

Mol	Chain	Res	Type
18	f	198	HIS
20	u	183	GLN
27	U	373	ASN
18	f	329	ASN
18	f	766	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	$\# Z > 2$
31	ADP	E	501	-	28,29,29	0.42	0	43,45,45	0.54	0
29	ATP	A	501	30	32,33,33	0.55	0	48,52,52	0.60	0
29	ATP	B	501	30	32,33,33	0.59	1 (3%)	48,52,52	0.39	0
31	ADP	D	501	30	28,29,29	0.46	0	43,45,45	0.52	0
29	ATP	F	501	30	32,33,33	0.57	0	48,52,52	0.63	0
29	ATP	C	501	30	32,33,33	0.60	0	48,52,52	0.63	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
31	ADP	E	501	-	-	5/16/32/32	0/3/3/3
29	ATP	A	501	30	-	2/22/38/38	0/3/3/3
29	ATP	B	501	30	-	6/22/38/38	0/3/3/3
31	ADP	D	501	30	-	6/16/32/32	0/3/3/3
29	ATP	F	501	30	-	6/22/38/38	0/3/3/3
29	ATP	C	501	30	-	8/22/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	B	501	ATP	PB-O3B	-2.06	1.57	1.59

There are no bond angle outliers.

There are no chirality outliers.

5 of 33 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
29	C	501	ATP	C5'-O5'-PA-O2A
29	C	501	ATP	C5'-O5'-PA-O3A
29	B	501	ATP	C5'-O5'-PA-O1A
29	B	501	ATP	C5'-O5'-PA-O2A
29	B	501	ATP	C5'-O5'-PA-O3A

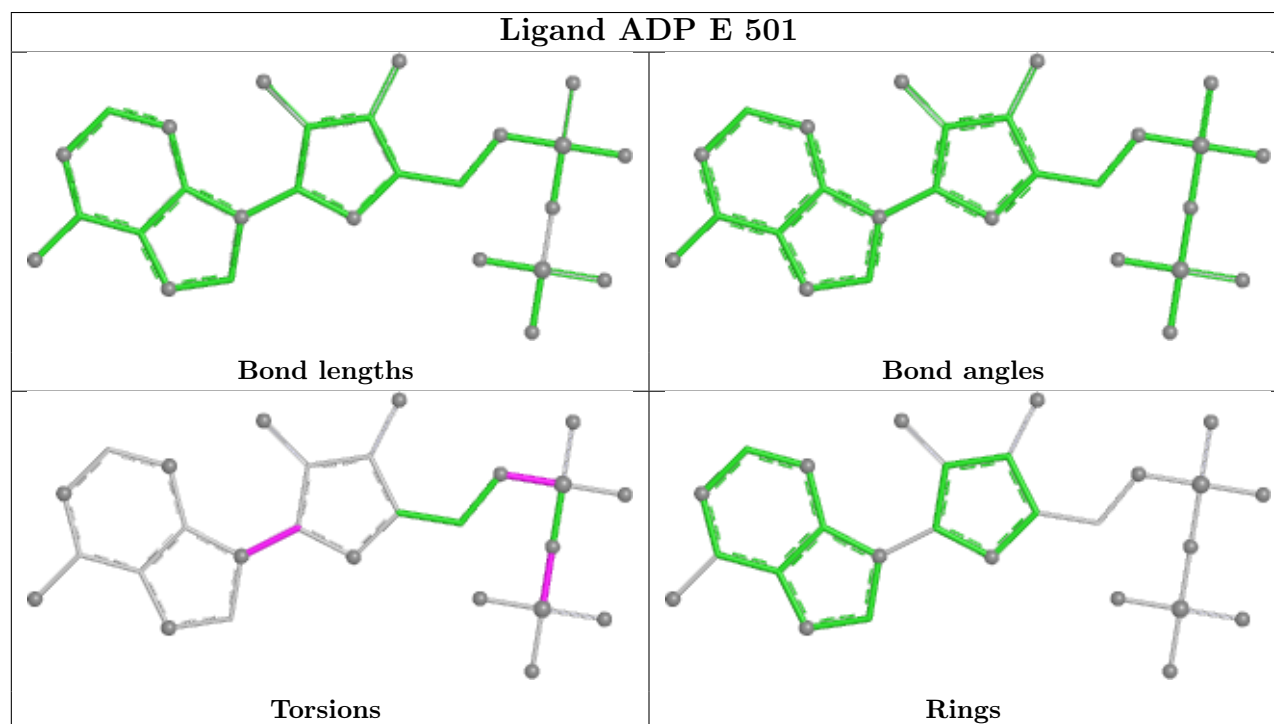
There are no ring outliers.

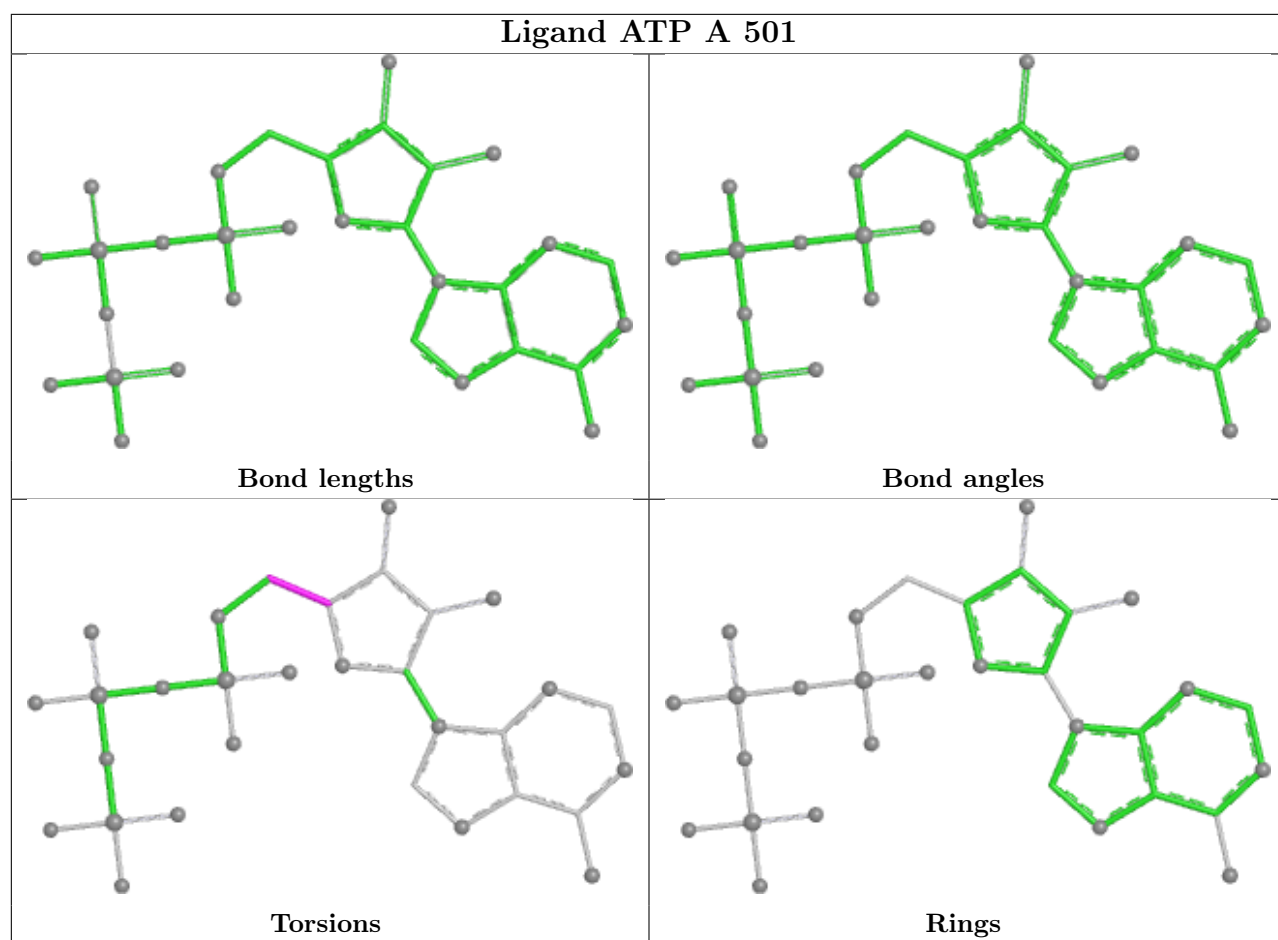
5 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	A	501	ATP	2	0
29	B	501	ATP	5	0
31	D	501	ADP	1	0
29	F	501	ATP	9	0
29	C	501	ATP	2	0

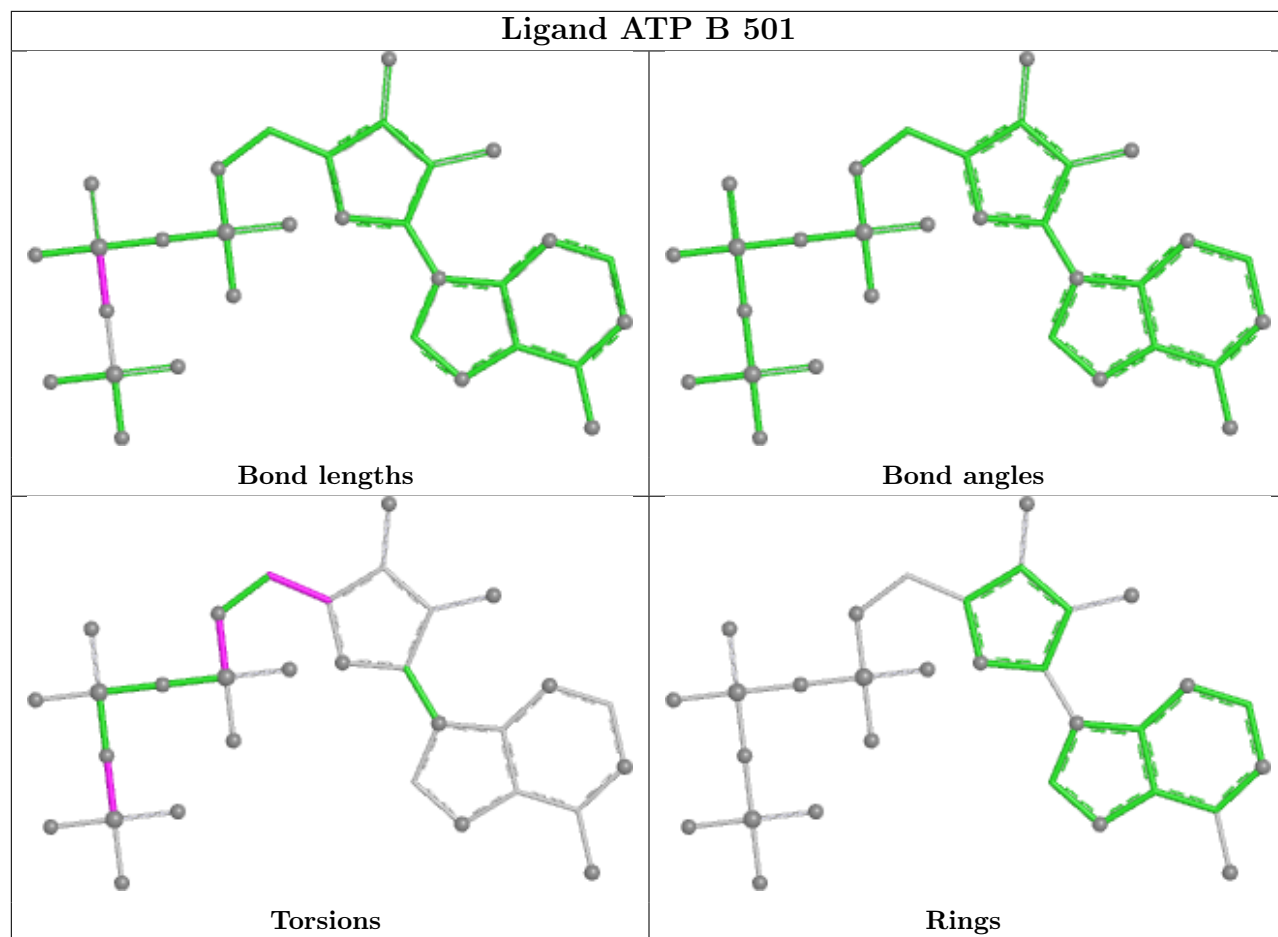
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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.

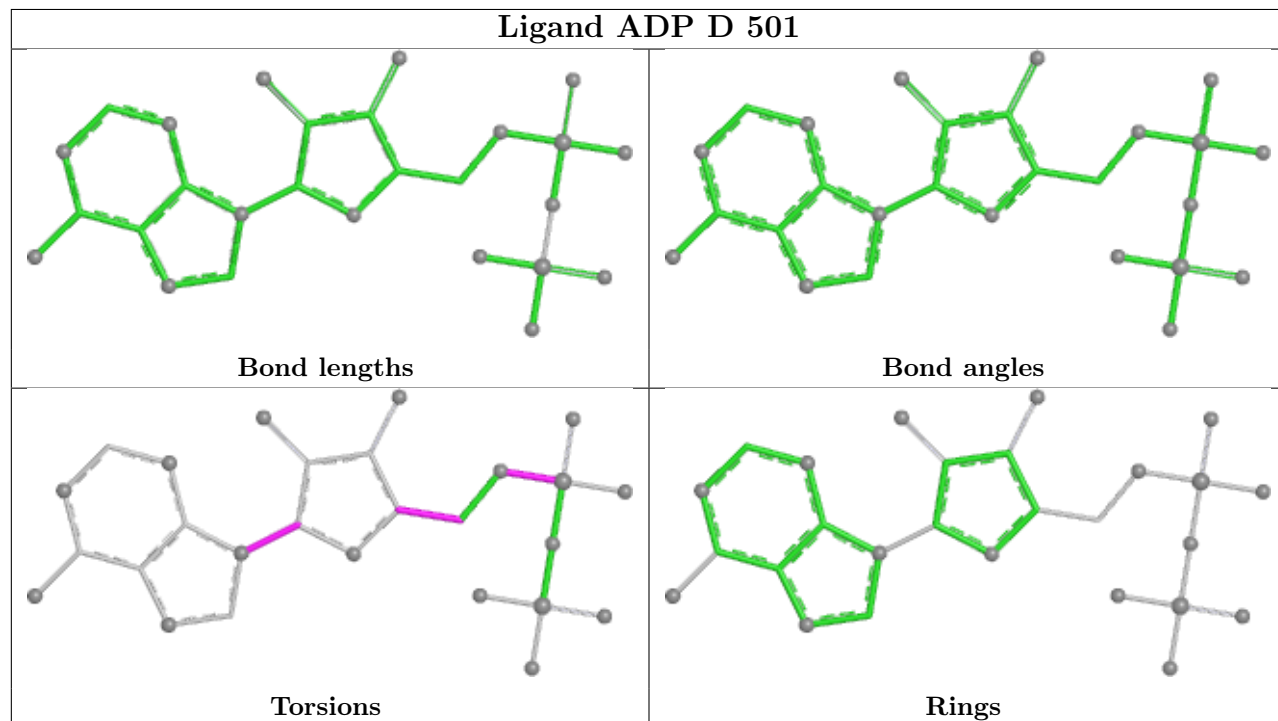


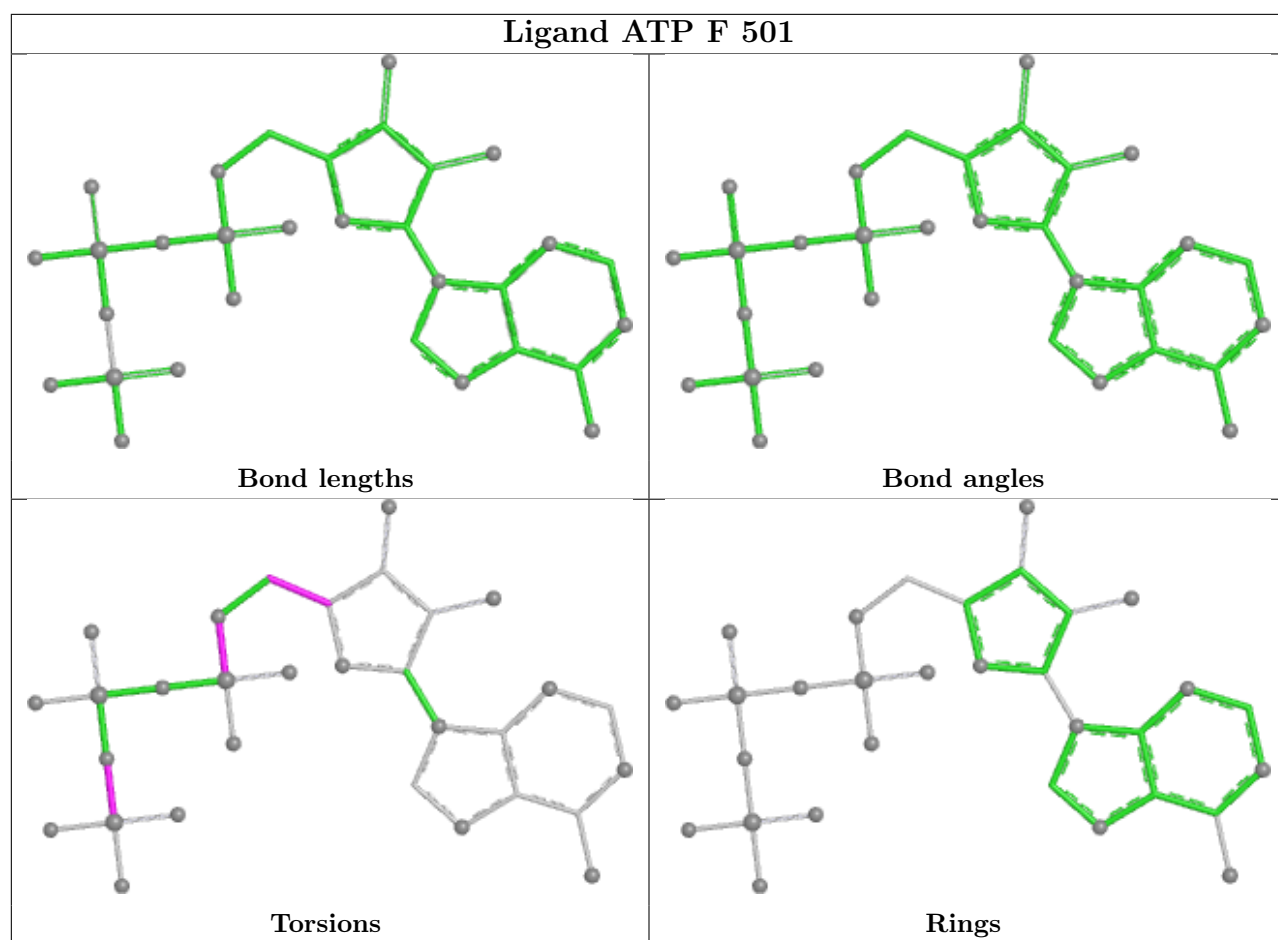


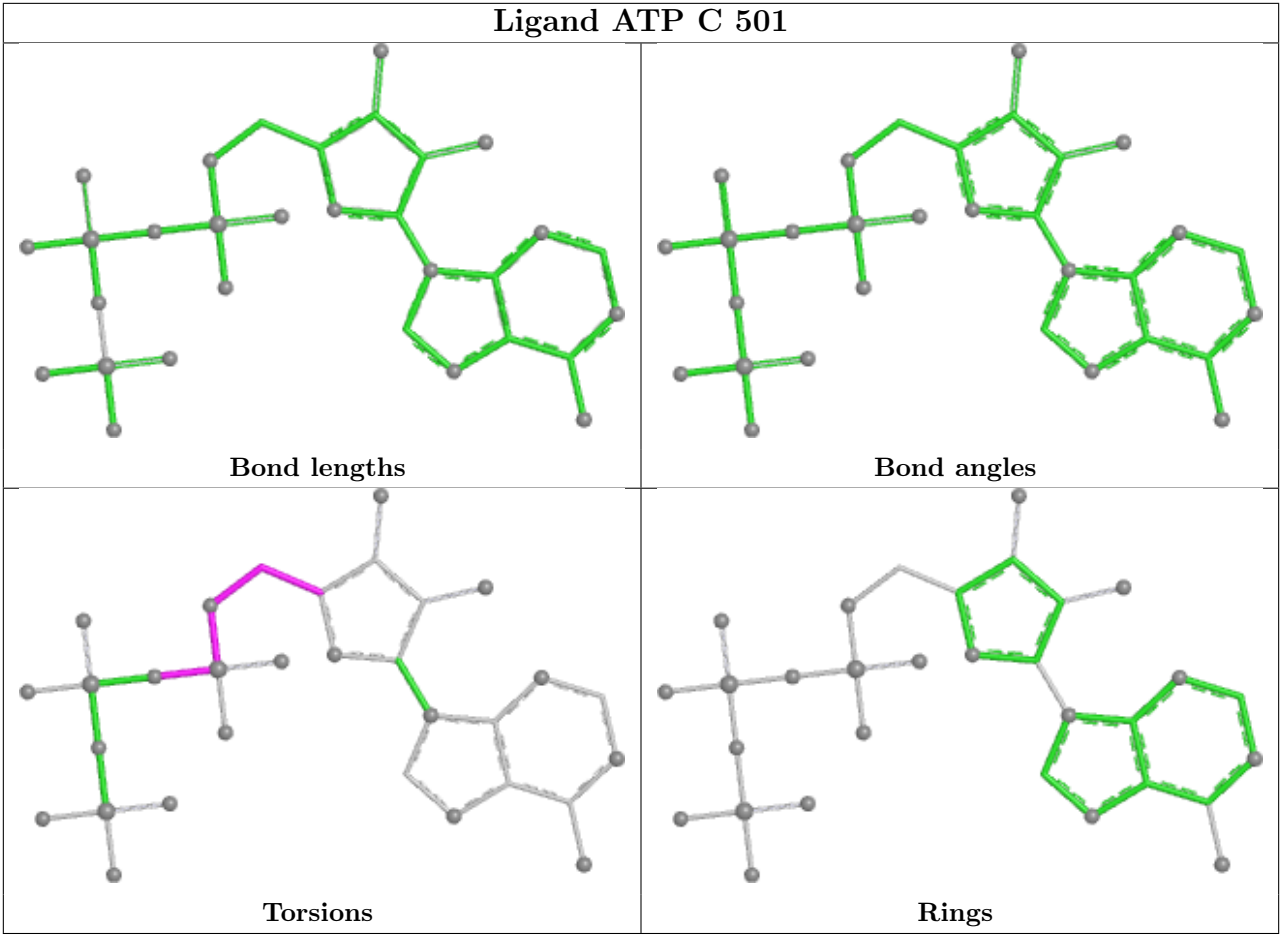
Ligand ATP B 501



Ligand ADP D 501







5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
18	f	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	f	646:MET	C	647:GLY	N	3.77

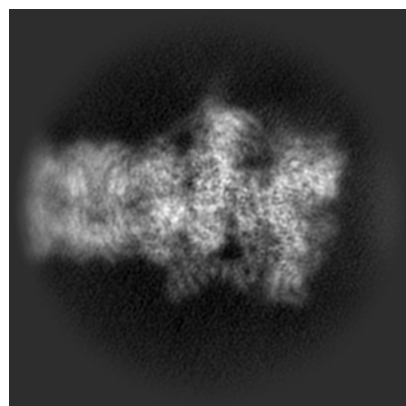
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47722. These allow visual inspection of the internal detail of the map and identification of artifacts.

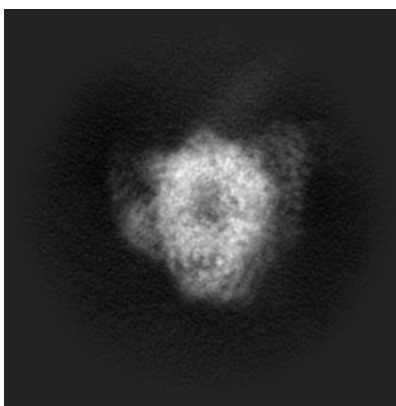
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

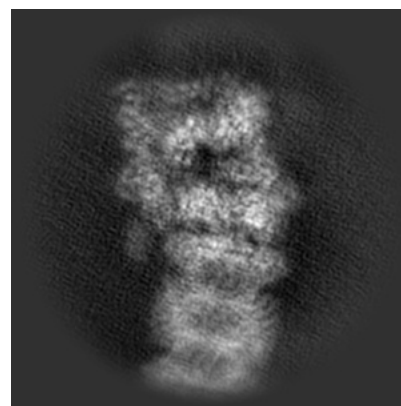
6.1.1 Primary map



X

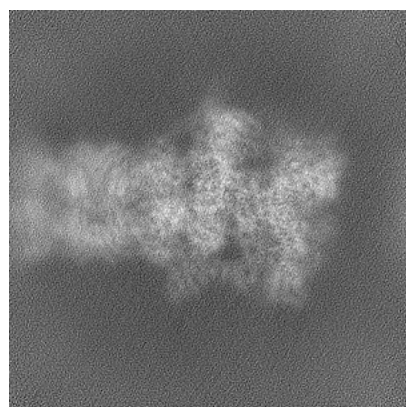


Y

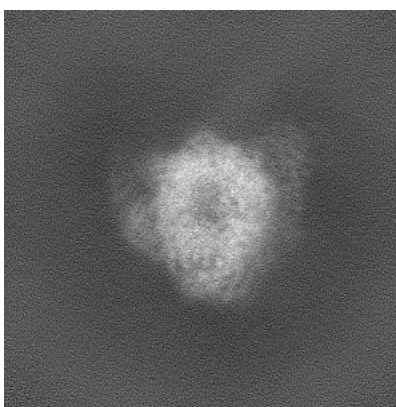


Z

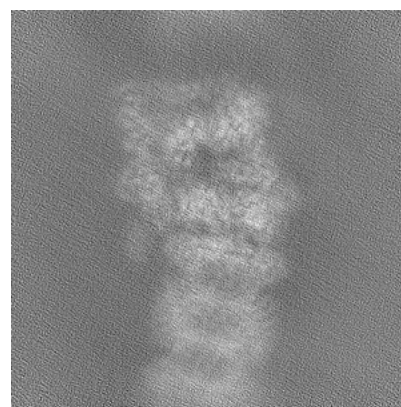
6.1.2 Raw map



X



Y

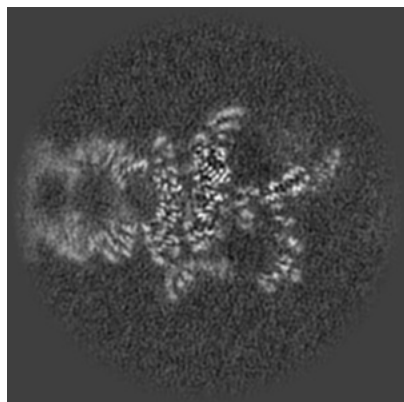


Z

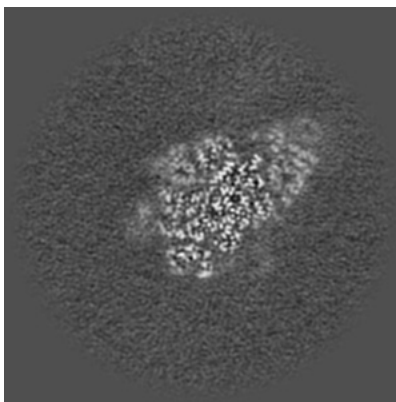
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

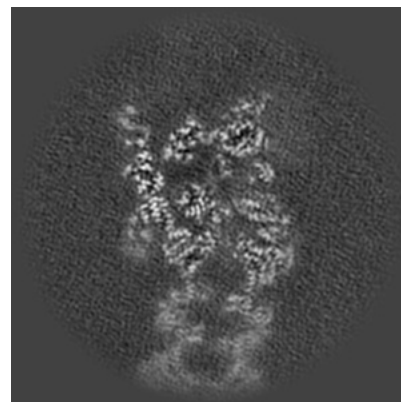
6.2.1 Primary map



X Index: 170

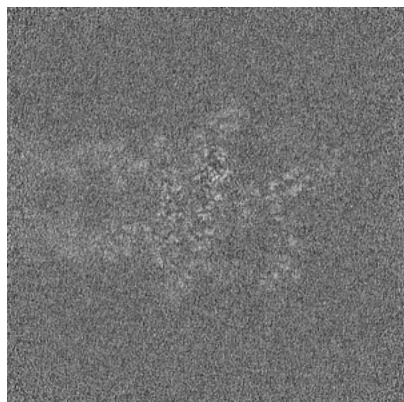


Y Index: 170

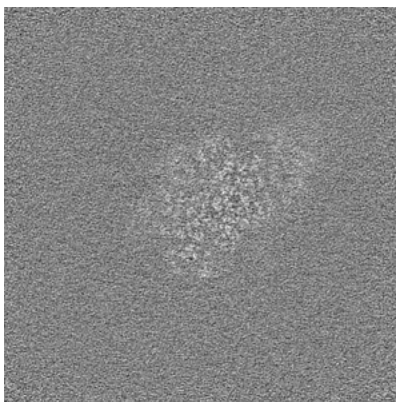


Z Index: 170

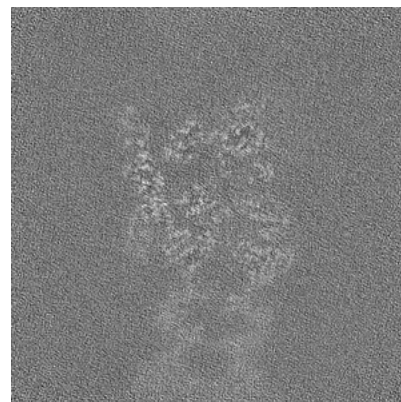
6.2.2 Raw map



X Index: 170



Y Index: 170

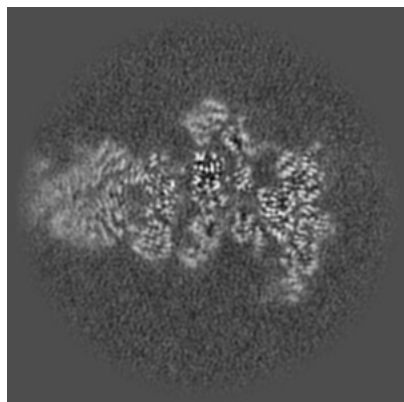


Z Index: 170

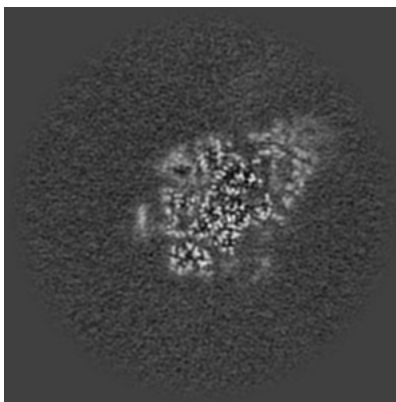
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

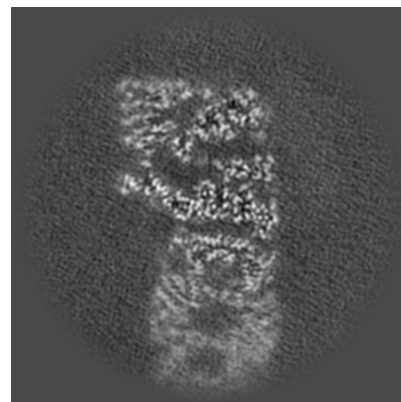
6.3.1 Primary map



X Index: 200

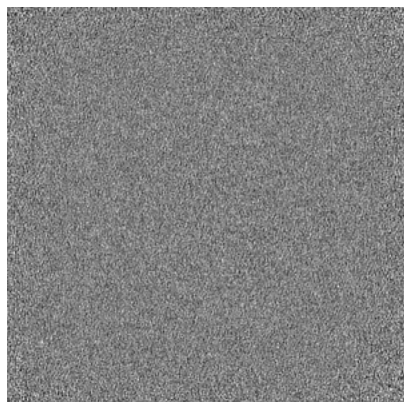


Y Index: 172

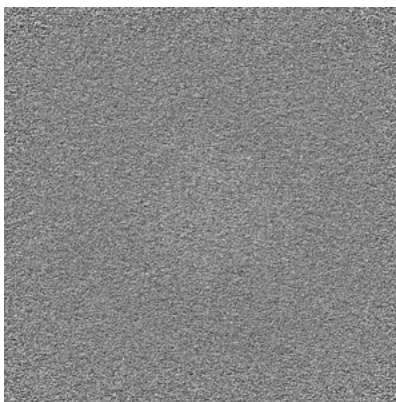


Z Index: 192

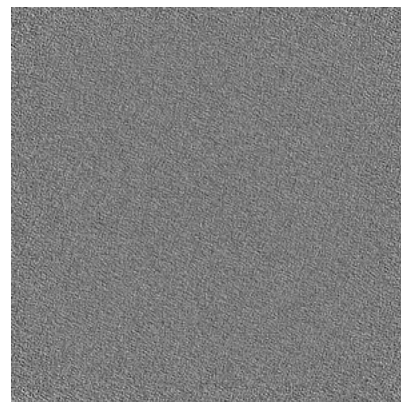
6.3.2 Raw map



X Index: 0



Y Index: 0

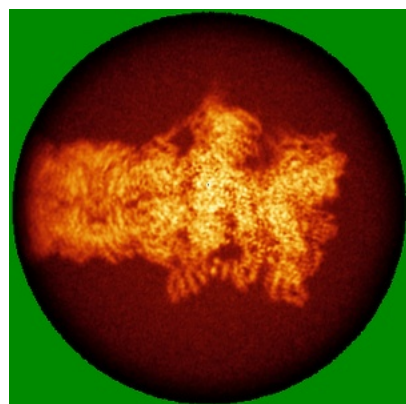


Z Index: 0

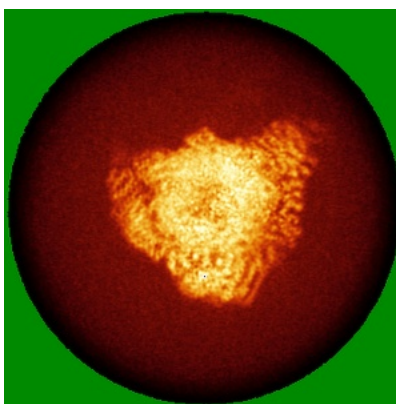
The images above show the largest variance slices of the map in three orthogonal directions.

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

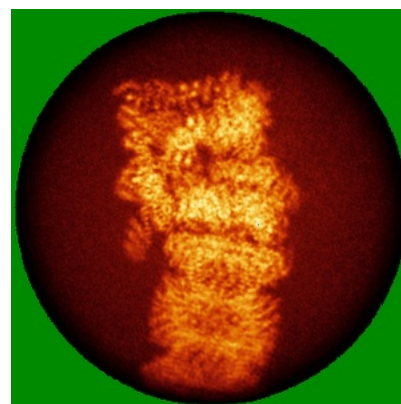
6.4.1 Primary map



X

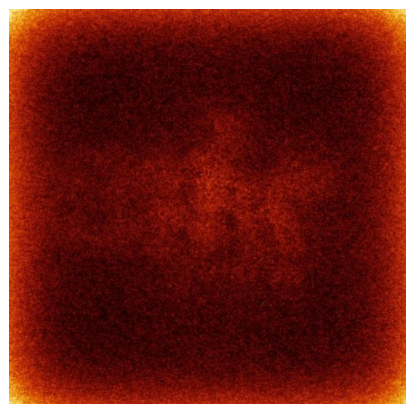


Y

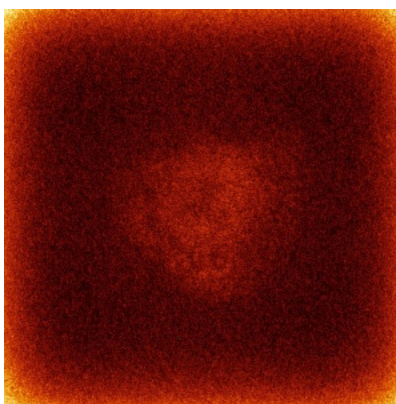


Z

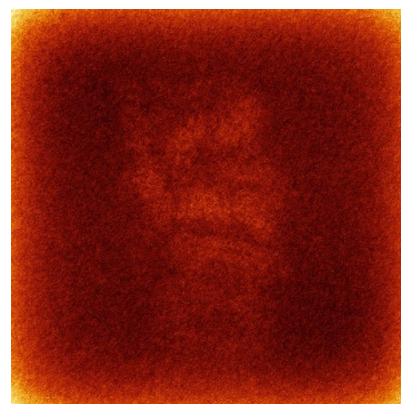
6.4.2 Raw map



X



Y

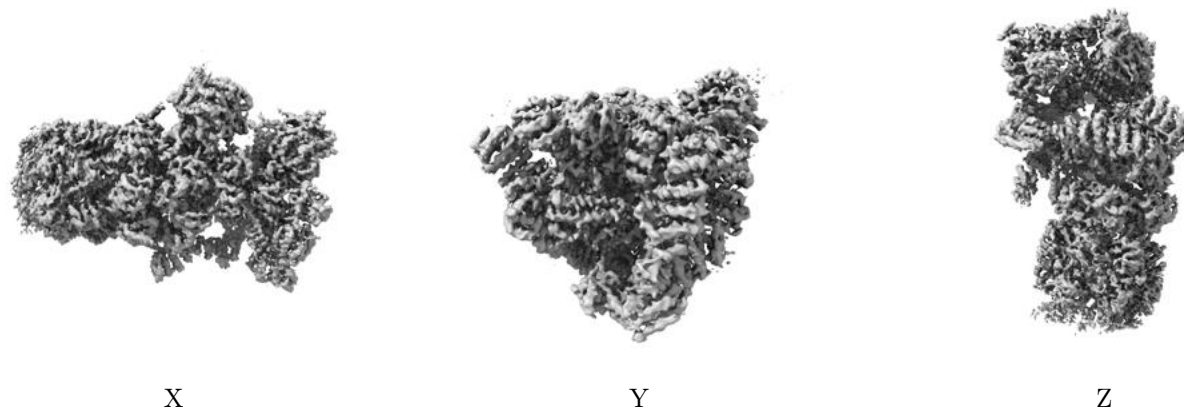


Z

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.

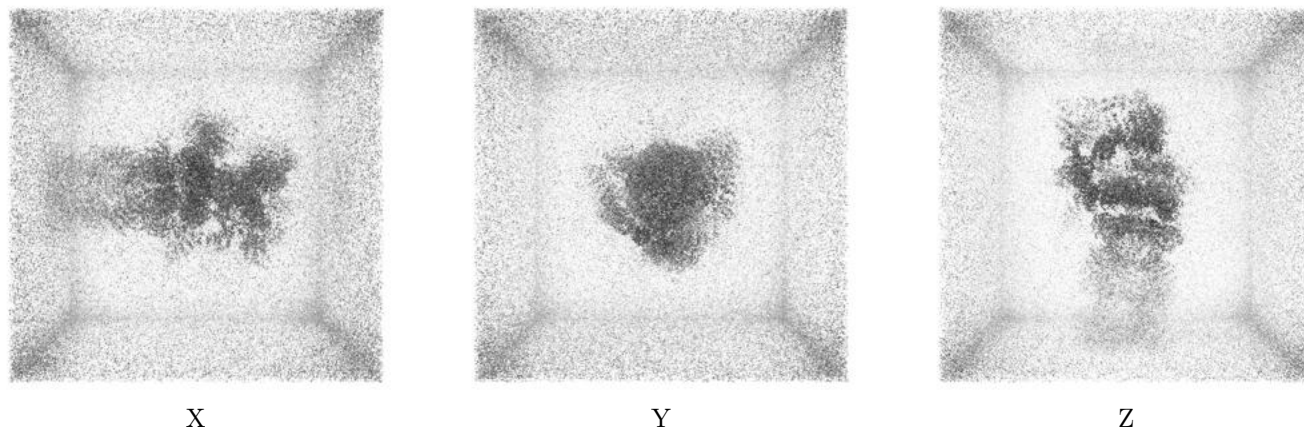
6.5 Orthogonal surface views [i](#)

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.

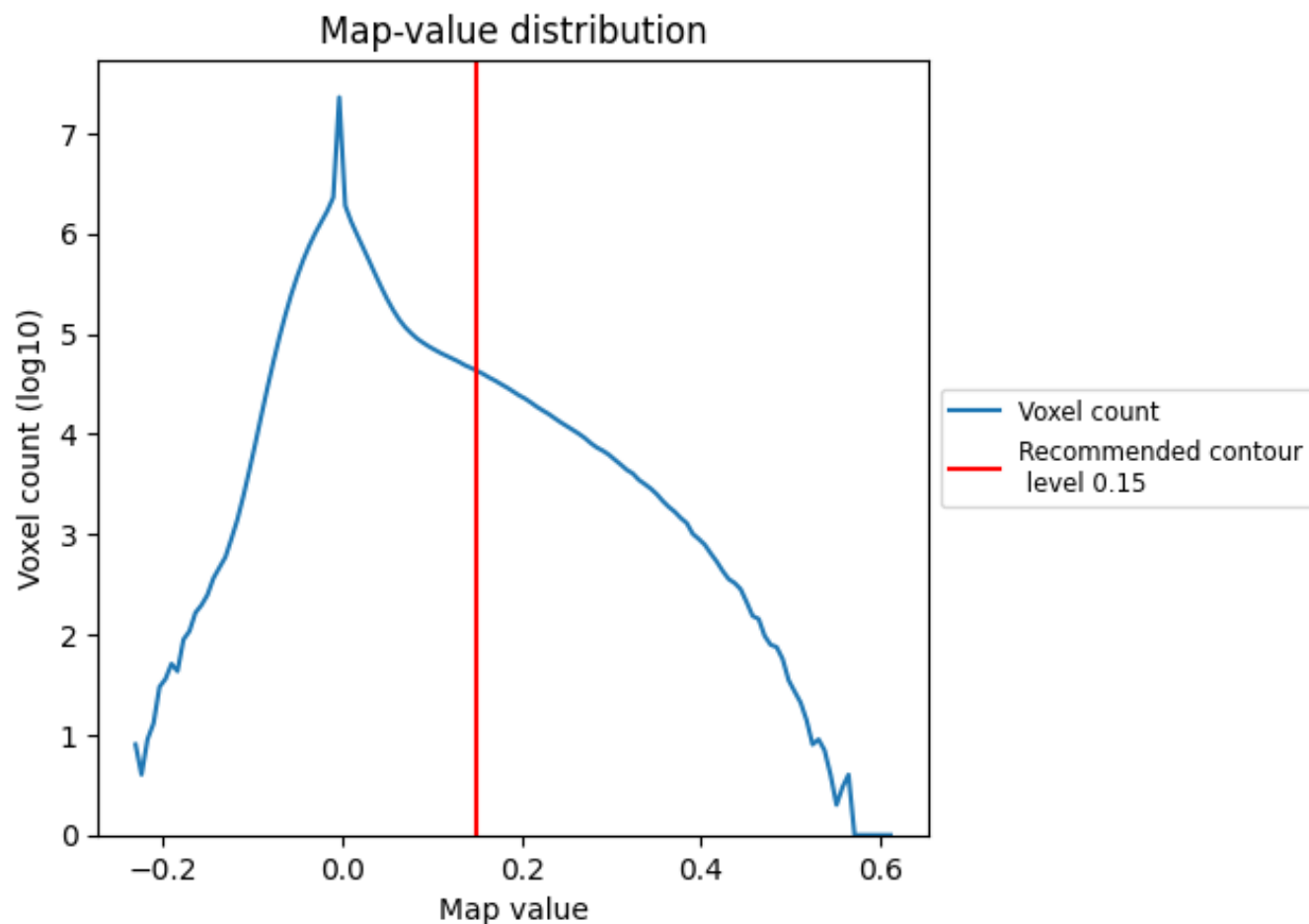
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

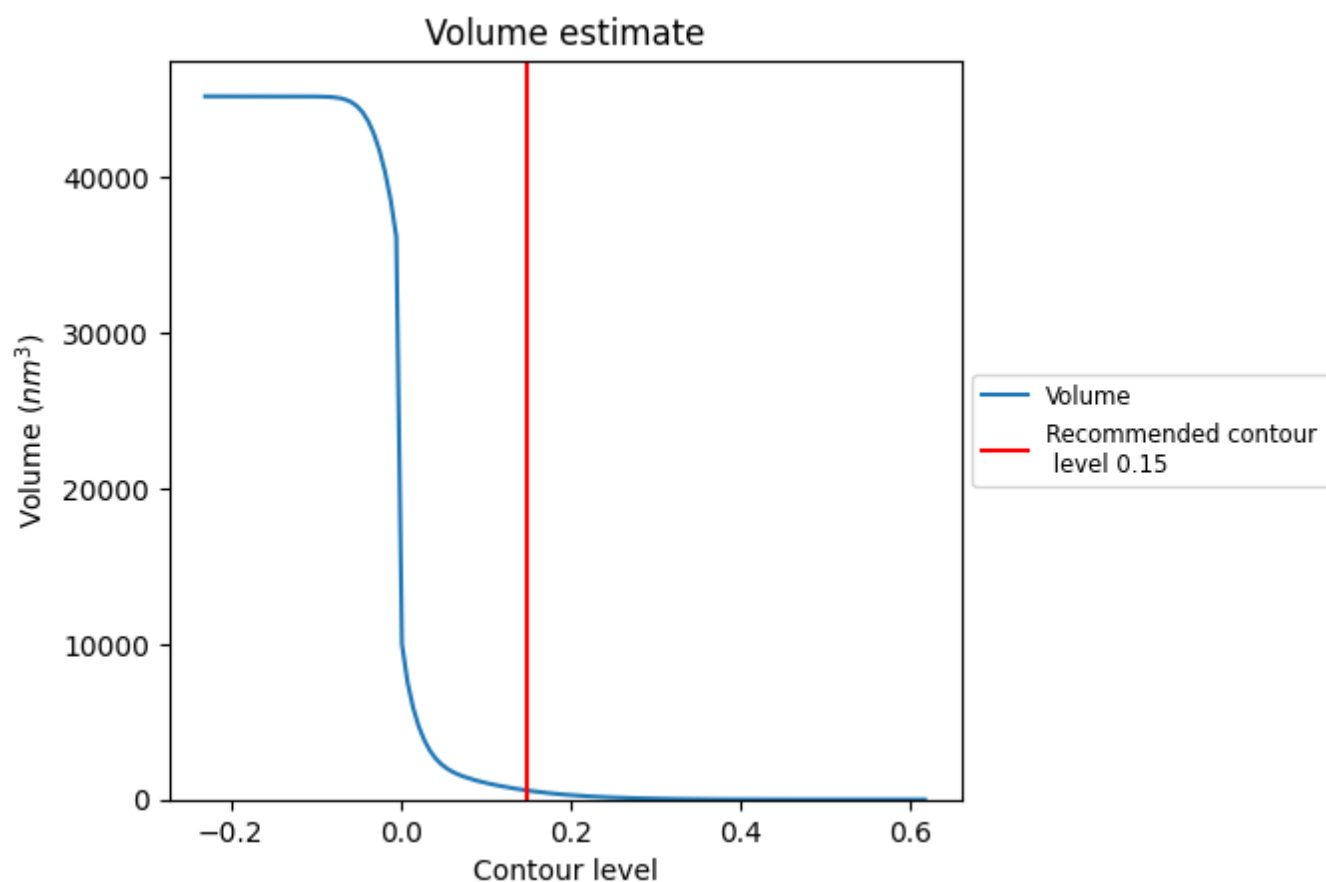
This section contains the results of statistical analysis of the map.

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.

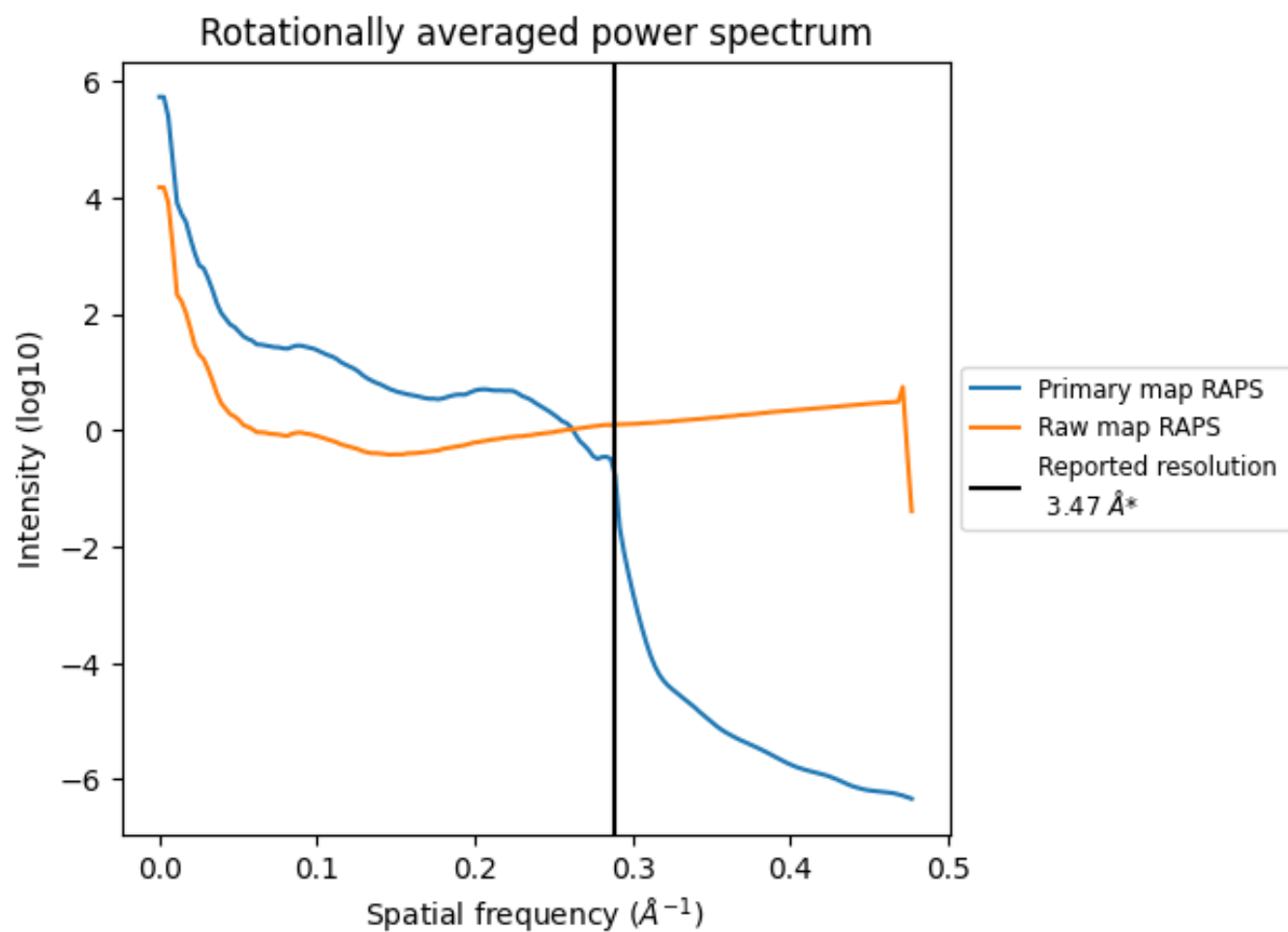
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 582 nm³; this corresponds to an approximate mass of 526 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 ⓘ

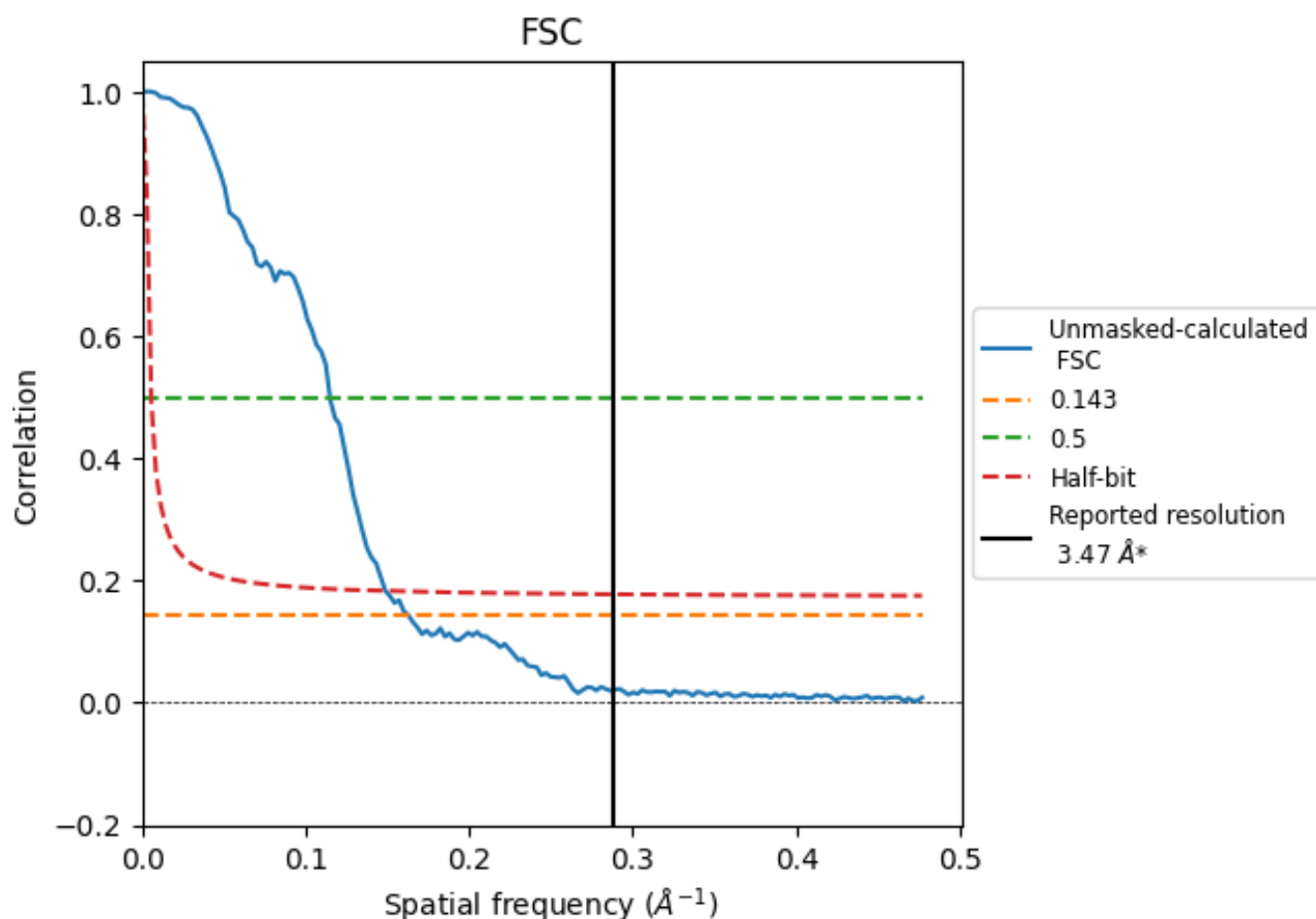


*Reported resolution corresponds to spatial frequency of 0.288 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.288 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

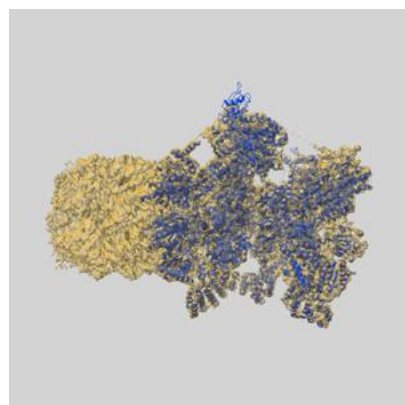
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.47	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.14	8.71	6.71

*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 6.14 differs from the reported value 3.47 by more than 10 %

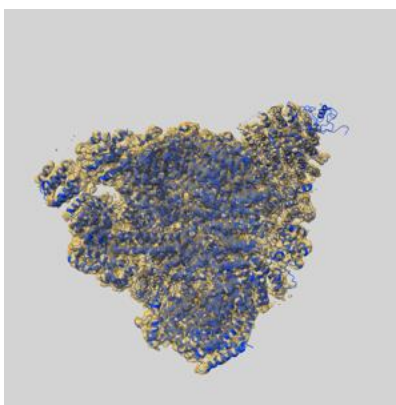
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-47722 and PDB model 9E8J. Per-residue inclusion information can be found in section 3 on page 14.

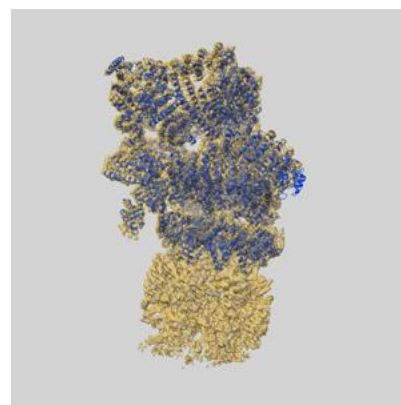
9.1 Map-model overlay [i](#)



X



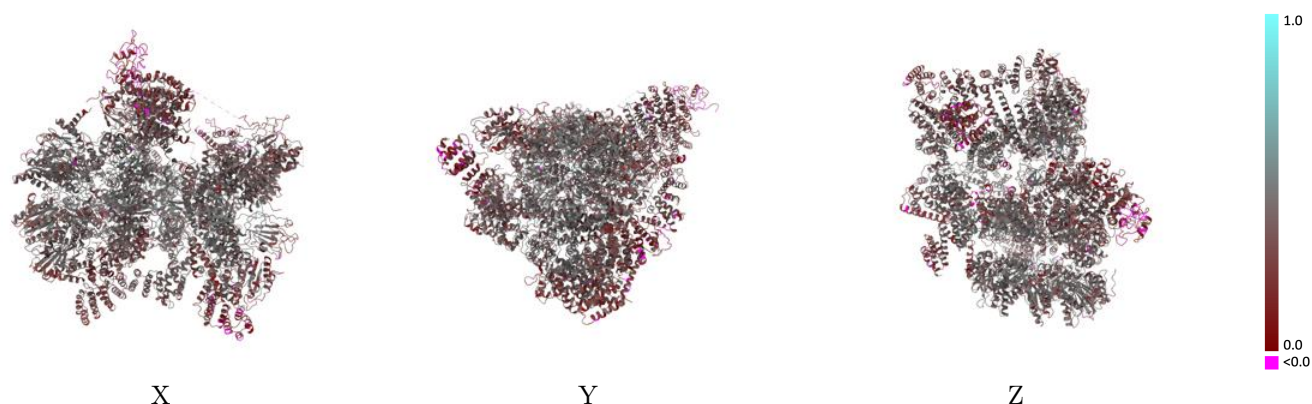
Y



Z

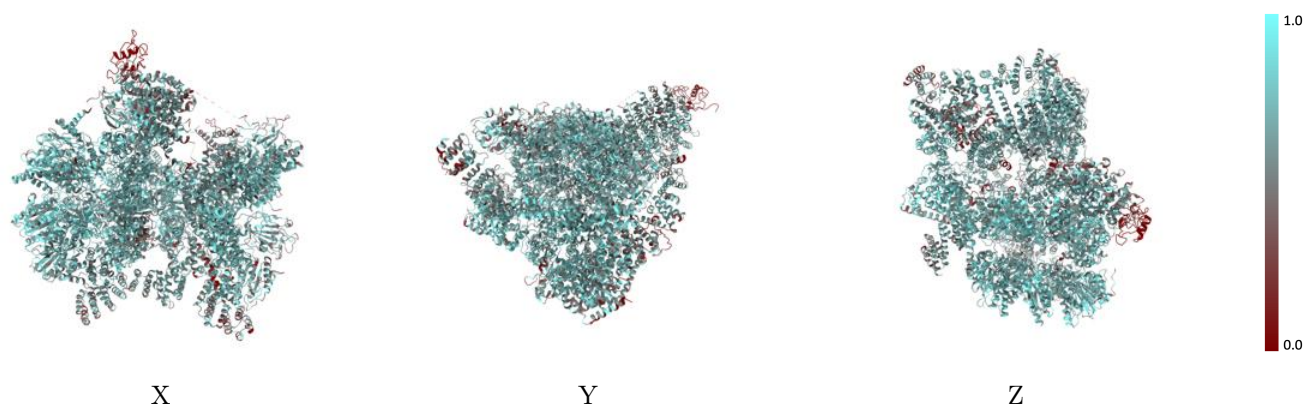
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



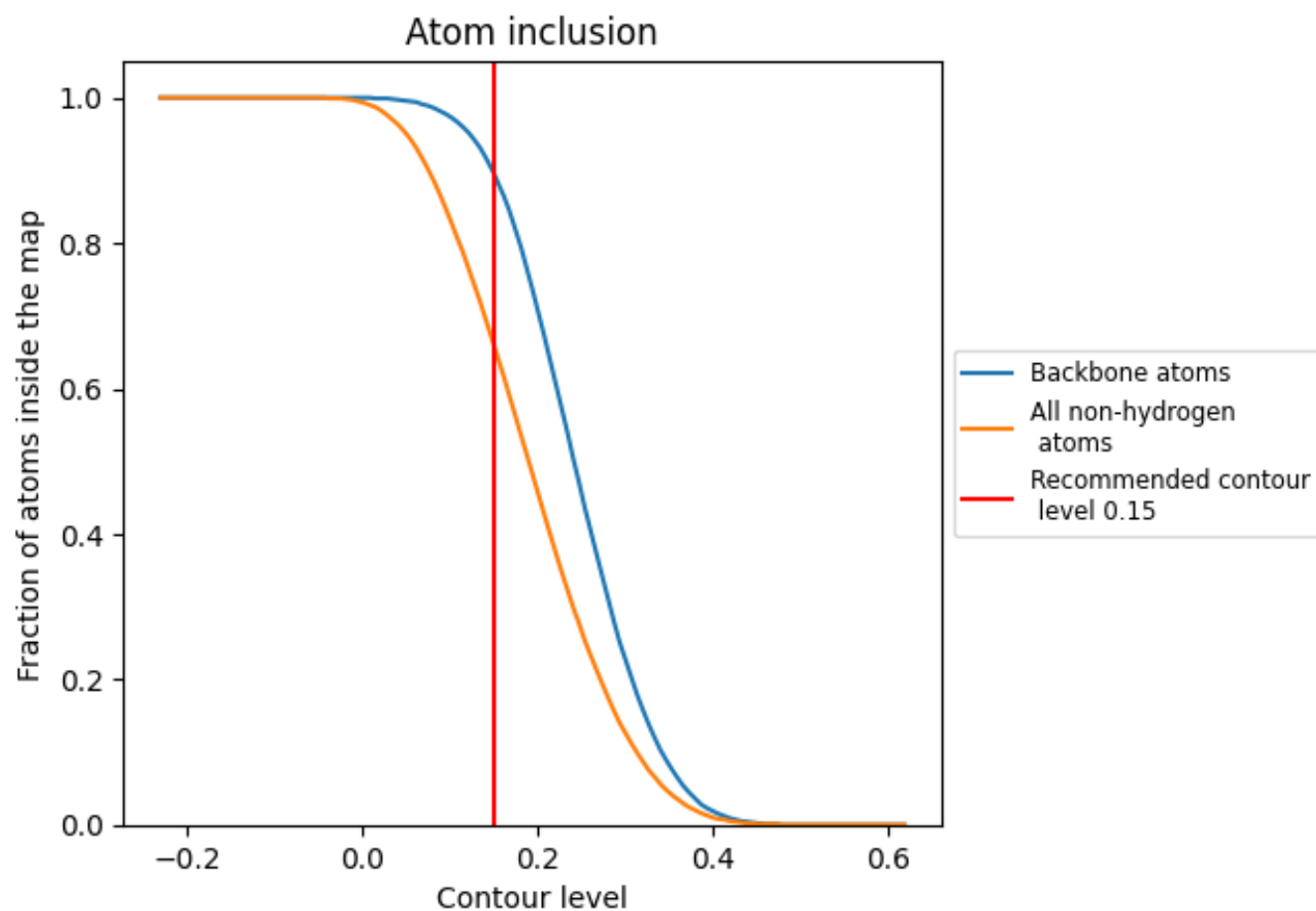
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 66% 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	 0.6600	 0.3750
A	 0.6760	 0.4140
B	 0.6950	 0.4400
C	 0.7280	 0.4500
D	 0.7200	 0.4410
E	 0.6320	 0.3570
F	 0.6100	 0.3610
G	 0.7180	 0.4170
H	 0.7320	 0.4250
I	 0.7260	 0.4060
J	 0.7320	 0.4070
K	 0.7160	 0.4060
L	 0.7280	 0.4090
M	 0.6940	 0.3900
U	 0.6620	 0.3720
V	 0.6050	 0.3250
W	 0.6270	 0.3530
X	 0.6910	 0.3810
Y	 0.7620	 0.4110
Z	 0.7200	 0.4240
a	 0.6000	 0.2920
b	 0.6070	 0.3340
c	 0.6740	 0.4080
d	 0.5530	 0.2890
e	 0.6670	 0.3560
f	 0.6100	 0.3150
g	 0.0200	 0.0650
u	 0.5690	 0.3850
v	 0.9270	 0.5470

