



wwPDB EM Validation Summary Report ⓘ

Mar 6, 2026 – 10:41 AM UTC

PDB ID : 8K0G / pdb_00008k0g
EMDB ID : EMD-36764
Title : Cryo-EM structure of human 26S RP (Ed state) bound to K11/K48-branched ubiquitin (Ub) chain composed of four Ub.
Authors : Hsu, S.T.D.; Draczkowski, P.; Wang, Y.S.
Deposited on : 2023-07-09
Resolution : 3.80 Å(reported)
Based on initial model : 6MSK

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:

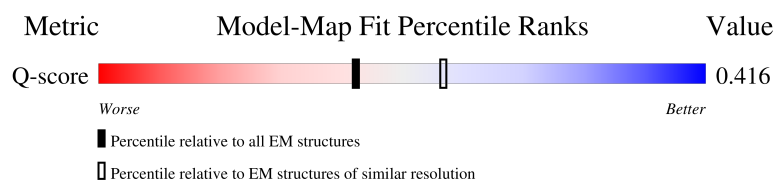
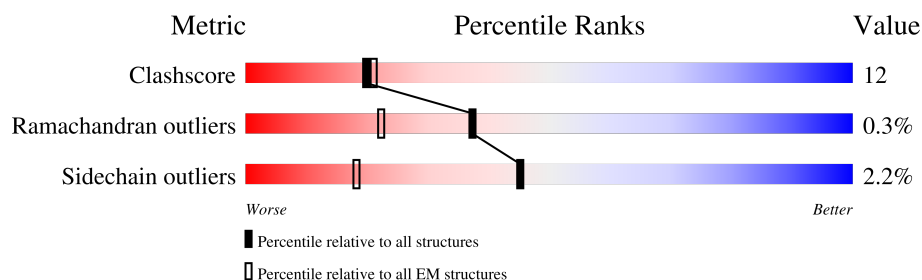
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.80 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.



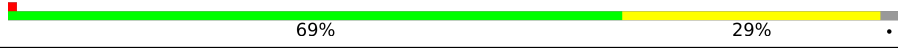
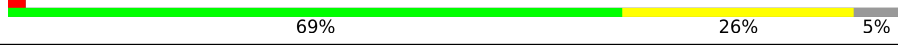
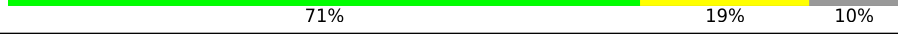
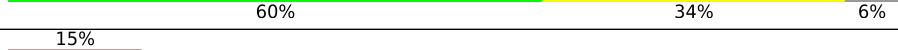
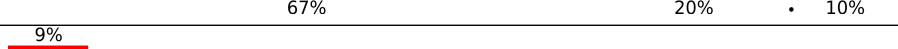
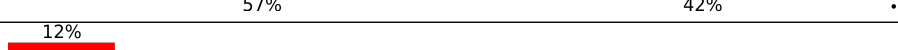
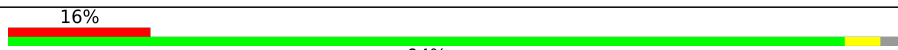
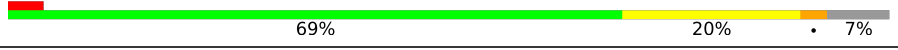
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10198 (3.30 - 4.30)

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	70% 25% 5%
2	B	440	69% 23% 8%
3	D	418	68% 22% 9%
4	F	439	11% 62% 26% 12%

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Mol	Chain	Length	Quality of chain
5	C	406	
6	G	246	
7	H	234	
8	I	261	
9	J	248	
10	K	241	
11	L	263	
12	M	255	
13	V	534	
14	W	456	
15	X	422	
16	Y	389	
17	d	350	
18	e	70	
19	f	908	
20	y	69	
21	E	389	
22	U	953	
23	Z	324	
24	a	376	
25	b	377	
26	c	310	
27	u	81	
27	v	81	
27	w	81	

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Mol	Chain	Length	Quality of chain
27	x	81	19% 74% 20% 6%

2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 68848 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 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	413	Total	C	N	O	S	0	0
			3228	2032	567	611	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	404	Total	C	N	O	S	0	0
			3103	1953	532	604	14		

- Molecule 3 is a protein called 26S protease regulatory subunit 6B.

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

- Molecule 4 is a protein called 26S protease regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	387	Total	C	N	O	S	0	0
			2981	1879	518	567	17		

- Molecule 5 is a protein called 26S protease regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	391	Total	C	N	O	S	0	0
			3080	1937	552	573	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	239	Total	C	N	O	S	0	0
			1865	1186	309	357	13		

- Molecule 7 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	230	Total	C	N	O	S	0	0
			1793	1147	302	338	6		

- Molecule 8 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	248	Total	C	N	O	S	0	0
			1954	1236	334	374	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	239	Total	C	N	O	S	0	0
			1887	1183	334	365	5		

- Molecule 10 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	228	Total	C	N	O	S	0	0
			1753	1103	289	351	10		

- Molecule 11 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	238	Total	C	N	O	S	0	0
			1873	1172	337	353	11		

- Molecule 12 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	240	Total	C	N	O	S	0	0
			1881	1193	321	356	11		

- Molecule 13 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	V	480	Total	C	N	O	S	0	0
			3197	1991	604	596	6		

- Molecule 14 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

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

- Molecule 15 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	X	380	Total	C	N	O	S	0	0
			2815	1779	490	537	9		

- Molecule 16 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	d	257	Total	C	N	O	S	0	0
			1682	1057	304	316	5		

- Molecule 18 is a protein called 26S proteasome complex subunit DSS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	e	37	Total	C	N	O	S	0	0
			282	170	48	63	1		

- Molecule 19 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	f	889	Total	C	N	O	S	0	0
			4380	2602	889	889			

- Molecule 20 is a protein called Protein SIC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	y	26	Total	C	N	O	S	0	0
			188	111	37	39	1		

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
y	-9	MET	-	initiating methionine	UNP P38634
y	-8	GLU	-	expression tag	UNP P38634
y	-7	PHE	-	expression tag	UNP P38634
y	-2	PRO	-	insertion	UNP P38634
y	-1	PRO	-	insertion	UNP P38634
y	2	TYR	ARG	conflict	UNP P38634
y	26	ARG	LYS	conflict	UNP P38634
y	27	ALA	THR	conflict	UNP P38634
y	39	CYS	THR	conflict	UNP P38634
y	43	GLY	-	expression tag	UNP P38634
y	44	GLY	-	expression tag	UNP P38634
y	45	GLY	-	expression tag	UNP P38634
y	46	GLY	-	expression tag	UNP P38634
y	47	SER	-	expression tag	UNP P38634
y	48	LEU	-	expression tag	UNP P38634
y	49	PRO	-	expression tag	UNP P38634
y	50	GLU	-	expression tag	UNP P38634
y	51	THR	-	expression tag	UNP P38634
y	52	GLY	-	expression tag	UNP P38634
y	53	GLY	-	expression tag	UNP P38634
y	54	HIS	-	expression tag	UNP P38634
y	55	HIS	-	expression tag	UNP P38634
y	56	HIS	-	expression tag	UNP P38634
y	57	HIS	-	expression tag	UNP P38634
y	58	HIS	-	expression tag	UNP P38634
y	59	HIS	-	expression tag	UNP P38634

- Molecule 21 is a protein called 26S protease regulatory subunit 10B.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	E	367	Total	C	N	O	S	0	0
			2900	1827	515	542	16		

- Molecule 22 is a protein called 26S proteasome non-ATPase regulatory subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	U	872	Total	C	N	O	S	0	0
			6590	4170	1136	1240	44		

- Molecule 23 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

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

- Molecule 24 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

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

- Molecule 25 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	c	287	Total	C	N	O	S	0	0
			2260	1430	389	422	19		

- Molecule 27 is a protein called Polyubiquitin-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	u	76	Total	C	N	O	S	0	0
			604	378	107	118	1		
27	v	76	Total	C	N	O	S	0	0
			603	378	107	117	1		
27	w	76	Total	C	N	O	S	0	0
			603	378	107	117	1		
27	x	76	Total	C	N	O	S	0	0
			603	378	107	117	1		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
u	-4	GLY	-	linker	UNP P0CG47
u	-3	SER	-	linker	UNP P0CG47
u	-2	GLY	-	linker	UNP P0CG47
u	-1	GLY	-	linker	UNP P0CG47
u	0	SER	-	linker	UNP P0CG47
u	63	ARG	LYS	engineered mutation	UNP P0CG47

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Chain	Residue	Modelled	Actual	Comment	Reference
v	-4	GLY	-	linker	UNP P0CG47
v	-3	SER	-	linker	UNP P0CG47
v	-2	GLY	-	linker	UNP P0CG47
v	-1	GLY	-	linker	UNP P0CG47
v	0	SER	-	linker	UNP P0CG47
v	63	ARG	LYS	engineered mutation	UNP P0CG47
w	-4	GLY	-	linker	UNP P0CG47
w	-3	SER	-	linker	UNP P0CG47
w	-2	GLY	-	linker	UNP P0CG47
w	-1	GLY	-	linker	UNP P0CG47
w	0	SER	-	linker	UNP P0CG47
w	63	ARG	LYS	engineered mutation	UNP P0CG47
x	-4	GLY	-	linker	UNP P0CG47
x	-3	SER	-	linker	UNP P0CG47
x	-2	GLY	-	linker	UNP P0CG47
x	-1	GLY	-	linker	UNP P0CG47
x	0	SER	-	linker	UNP P0CG47
x	63	ARG	LYS	engineered mutation	UNP P0CG47

- # ATP



WORLDWIDE
PDB
PROTEIN DATA BANK

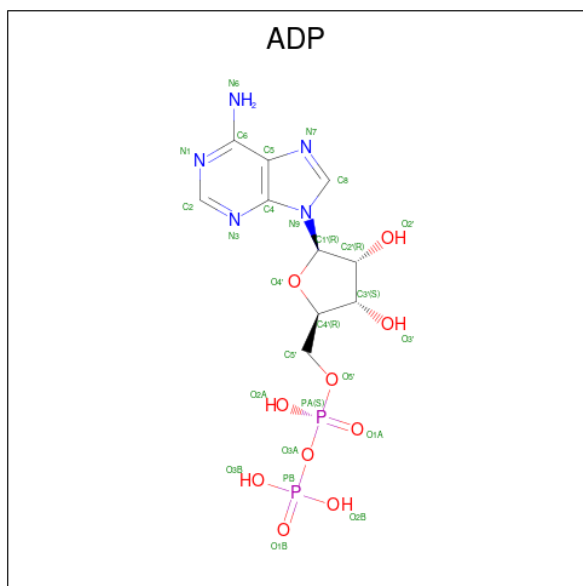
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Mol	Chain	Residues	Atoms					AltConf
28	F	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 29 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 30 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).

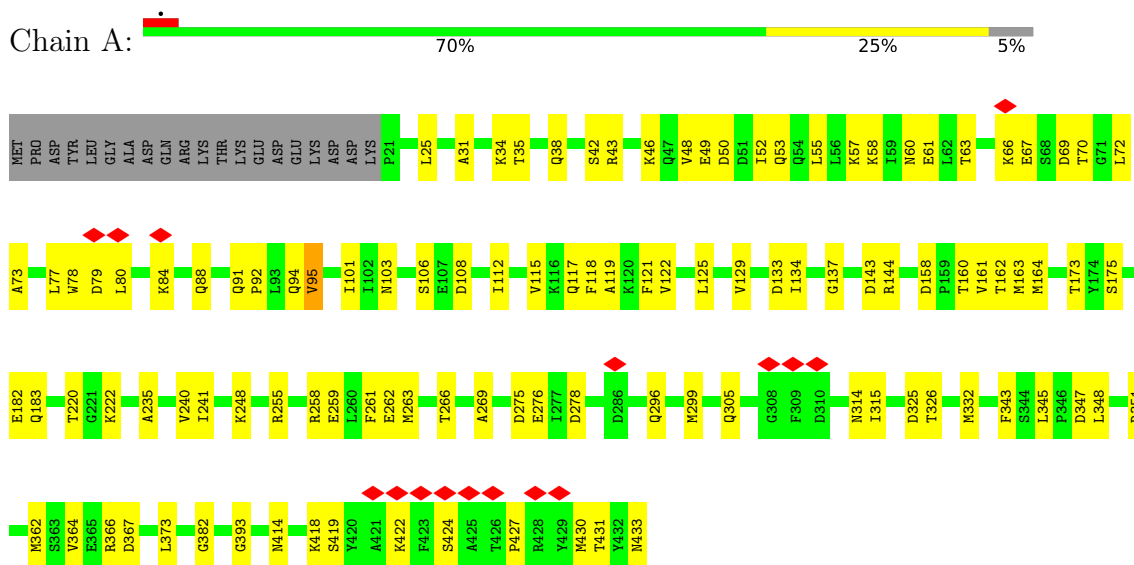


Mol	Chain	Residues	Atoms					AltConf
30	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
30	C	1	Total	C	N	O	P	0
			27	10	5	10	2	

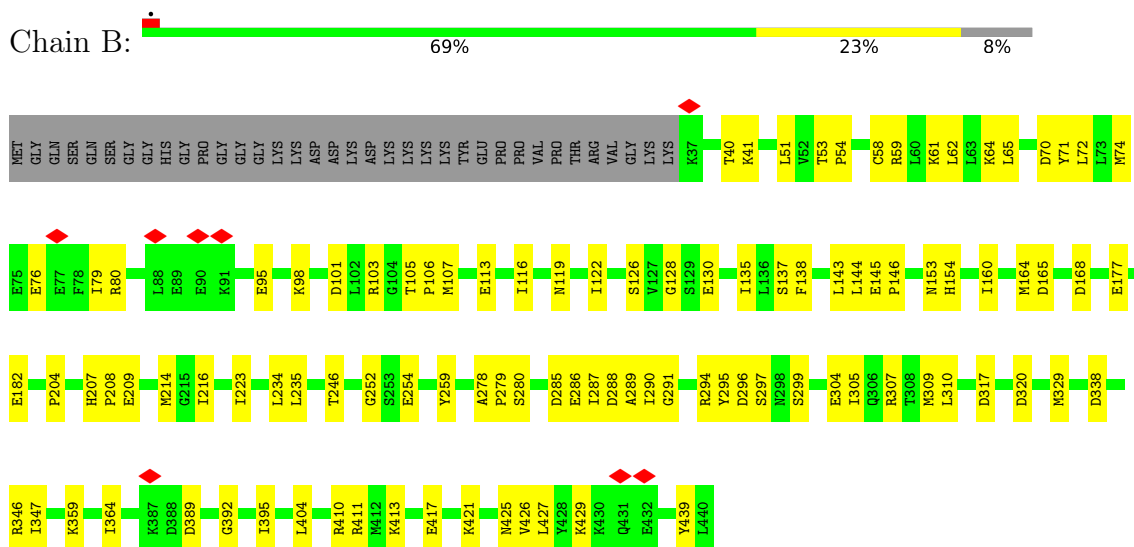
3 Residue-property plots

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 protease regulatory subunit 7



- Molecule 2: 26S protease regulatory subunit 4



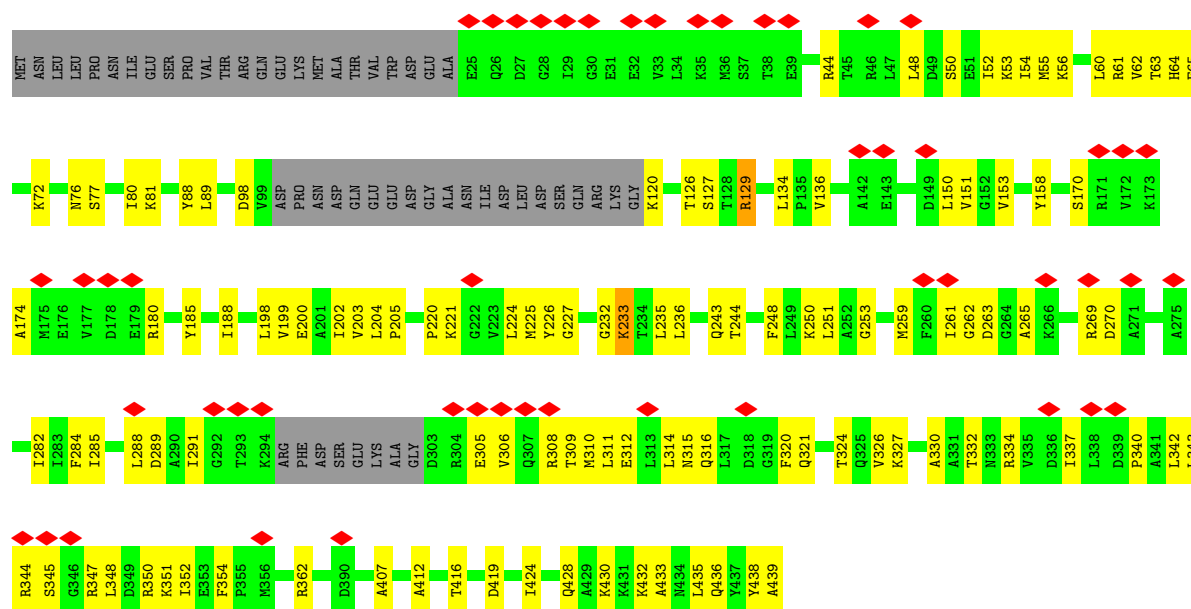
- Molecule 3: 26S protease regulatory subunit 6B

Chain D:  68% 22% 9%



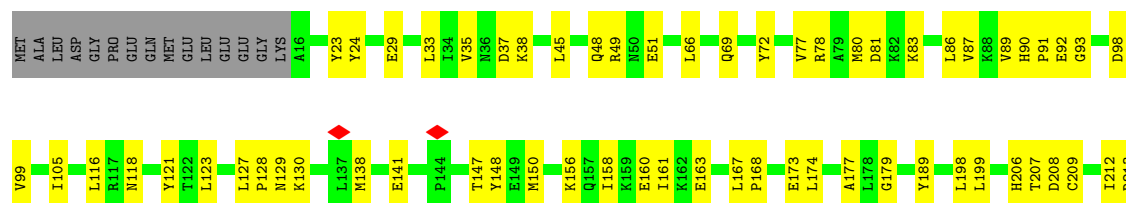
• Molecule 4: 26S protease regulatory subunit 6A

Chain F:  11% 62% 26% 12%



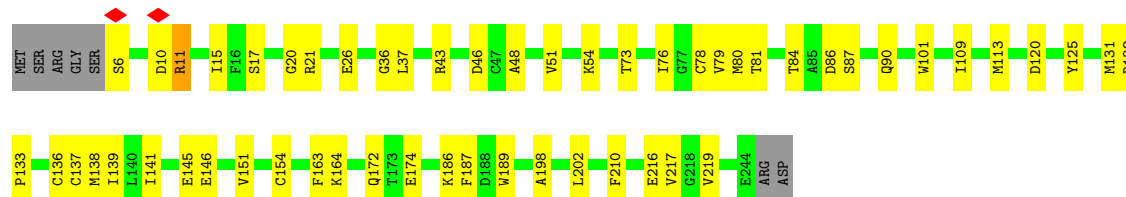
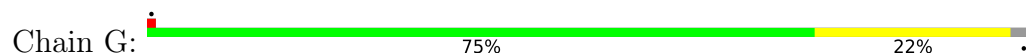
• Molecule 5: 26S protease regulatory subunit 8

Chain C:  73% 23% 4%

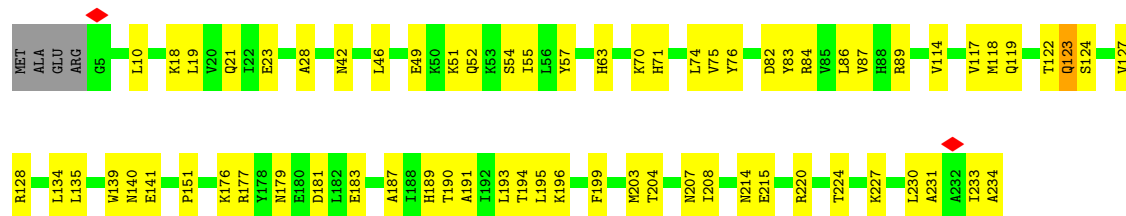




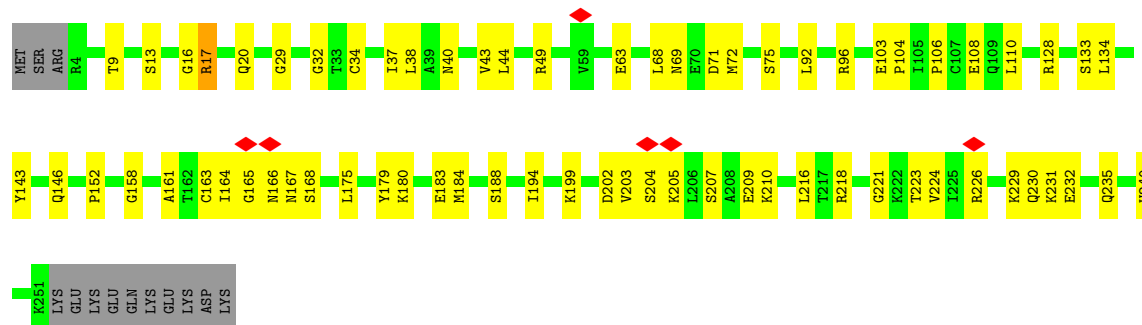
• Molecule 6: Proteasome subunit alpha type-6



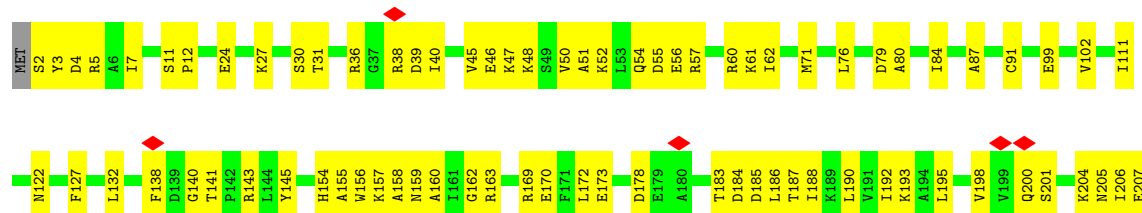
• Molecule 7: Proteasome subunit alpha type-2



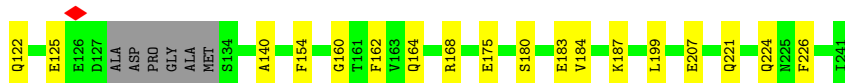
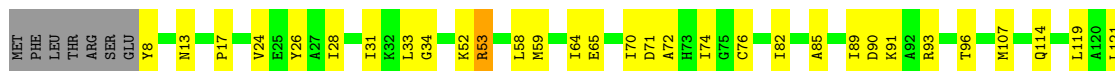
• Molecule 8: Proteasome subunit alpha type-4



• Molecule 9: Proteasome subunit alpha type-7



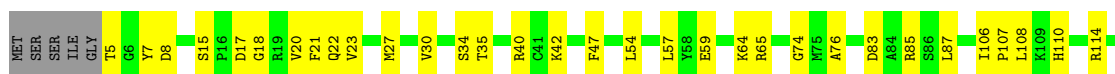
- Molecule 10: Proteasome subunit alpha type-5



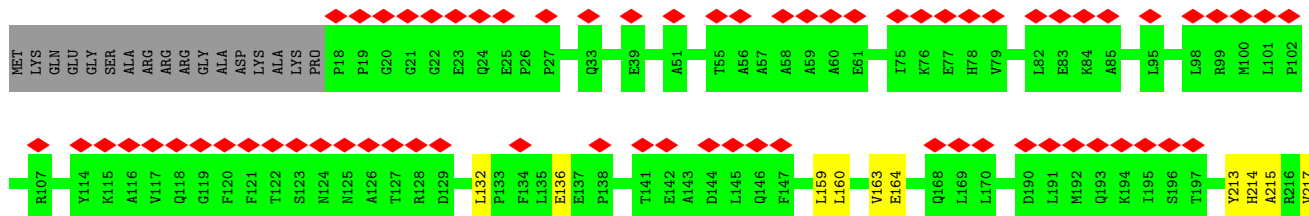
- Molecule 11: Proteasome subunit alpha type-1

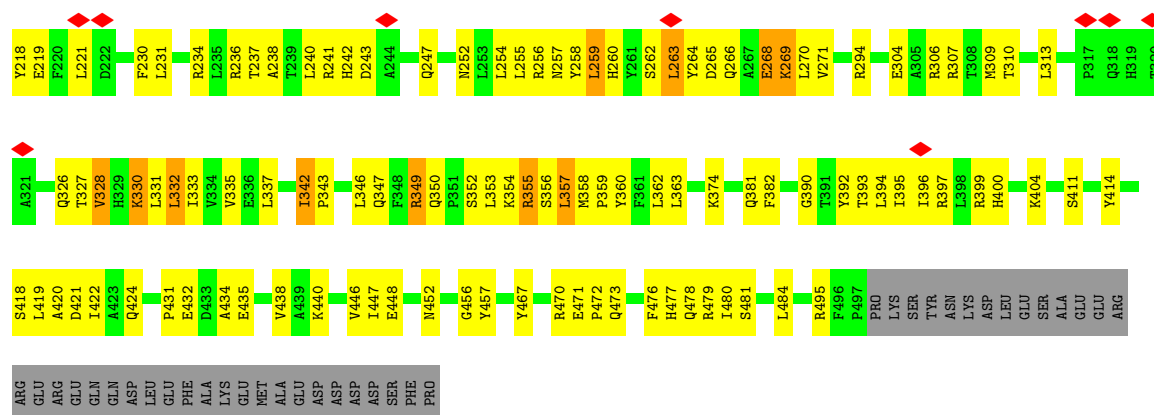


- Molecule 12: Proteasome subunit alpha type-3

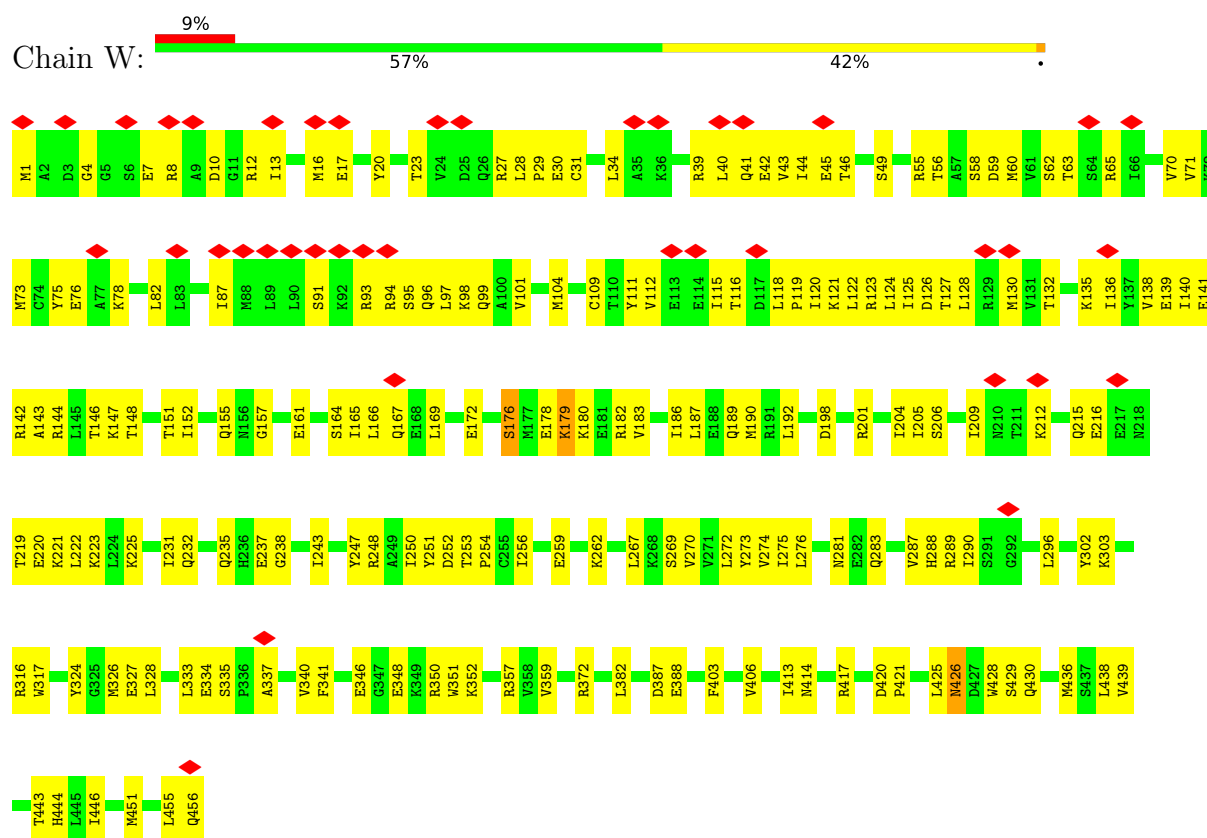


- Molecule 13: 26S proteasome non-ATPase regulatory subunit 3

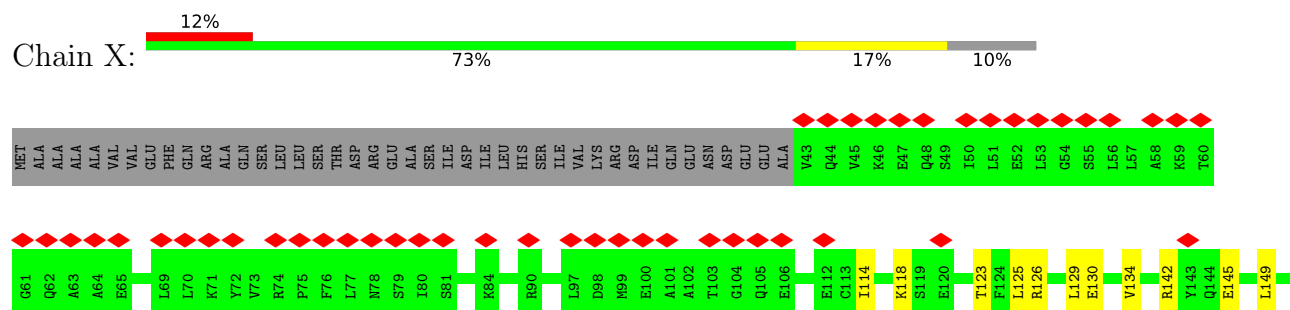


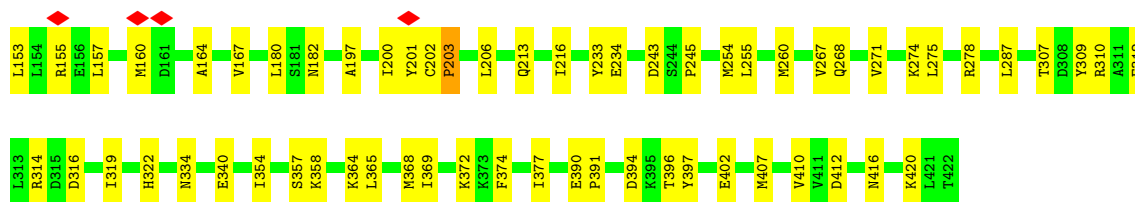


• Molecule 14: 26S proteasome non-ATPase regulatory subunit 12

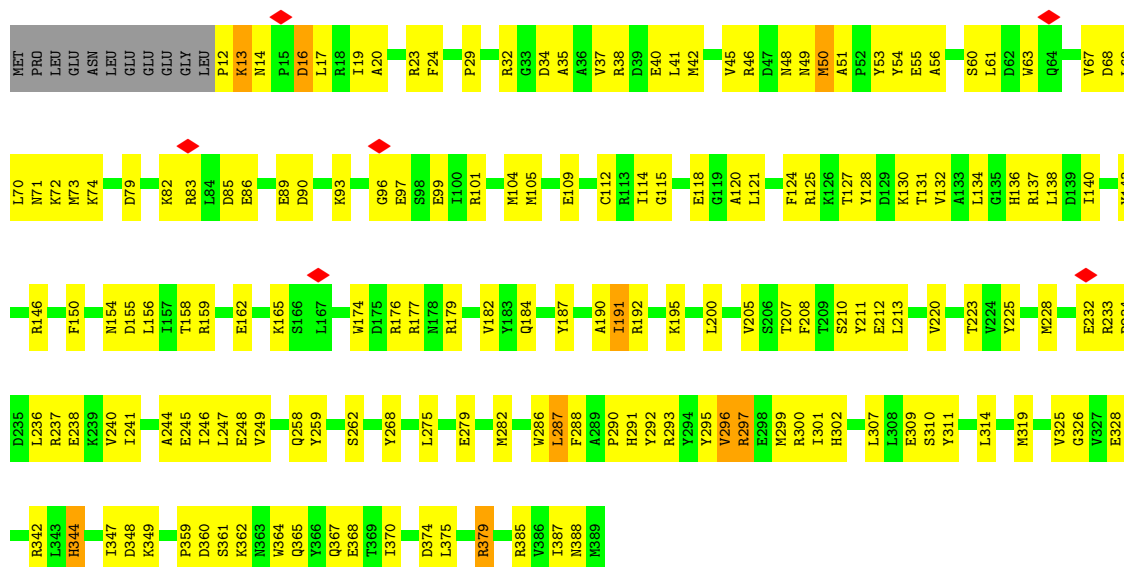


• Molecule 15: 26S proteasome non-ATPase regulatory subunit 11

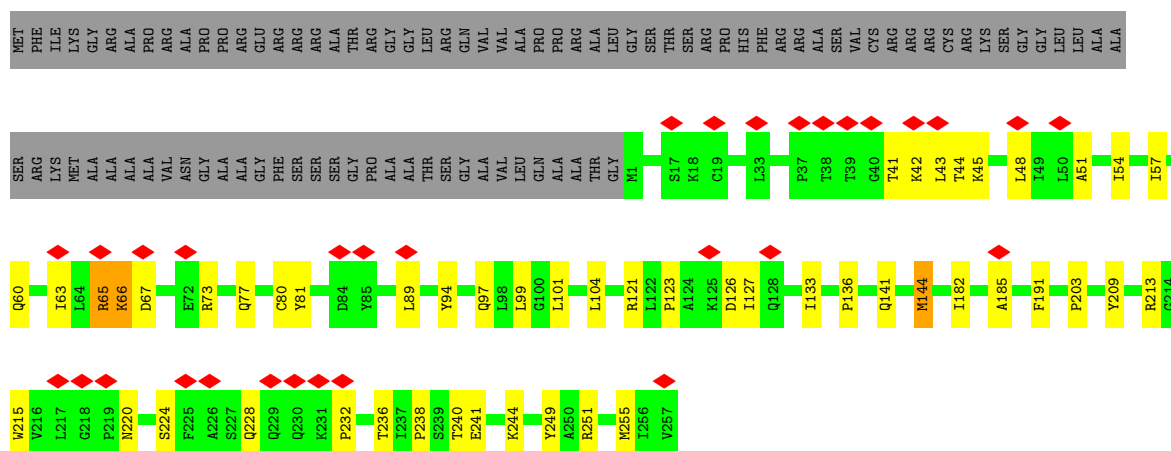




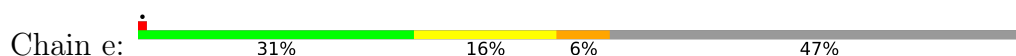
- Molecule 16: 26S proteasome non-ATPase regulatory subunit 6

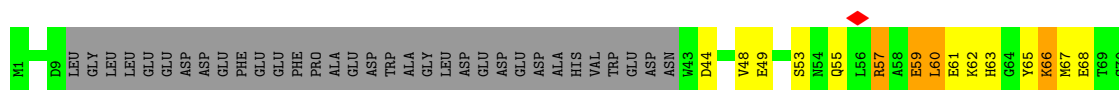


- Molecule 17: 26S proteasome non-ATPase regulatory subunit 8



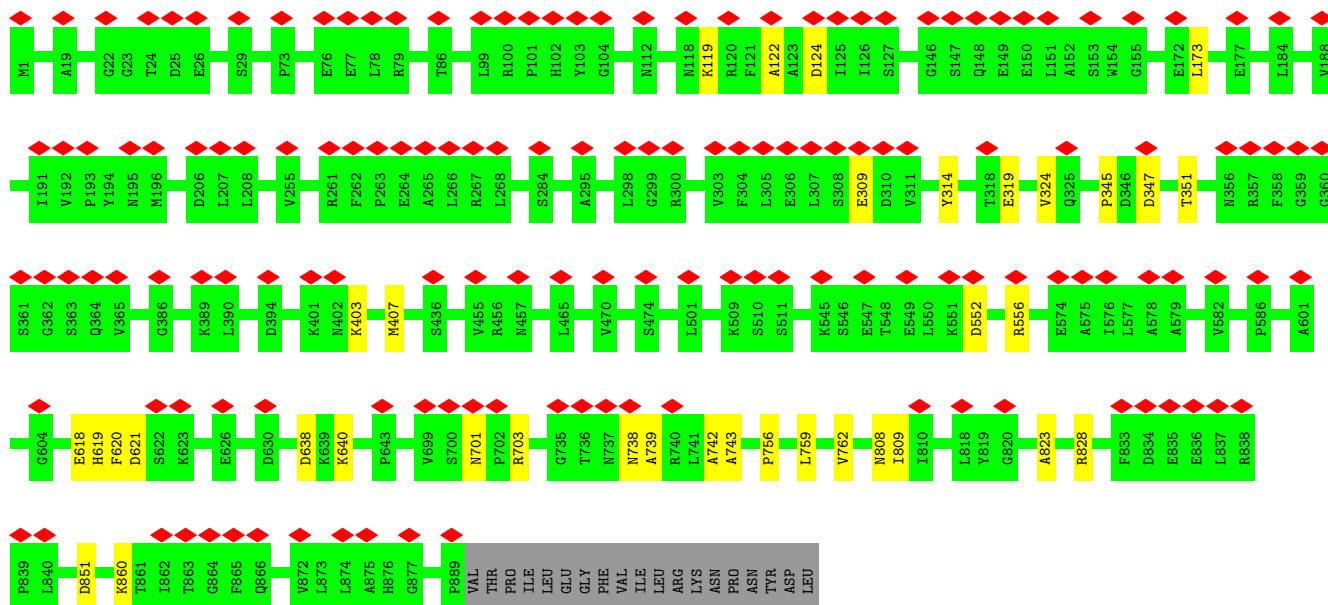
- Molecule 18: 26S proteasome complex subunit DSS1





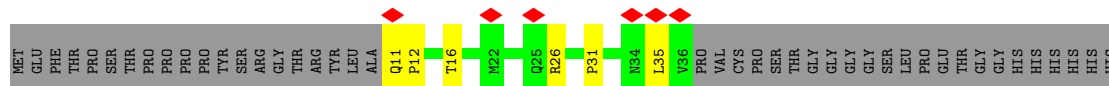
- Molecule 19: 26S proteasome non-ATPase regulatory subunit 2

Chain f: 16% 94%



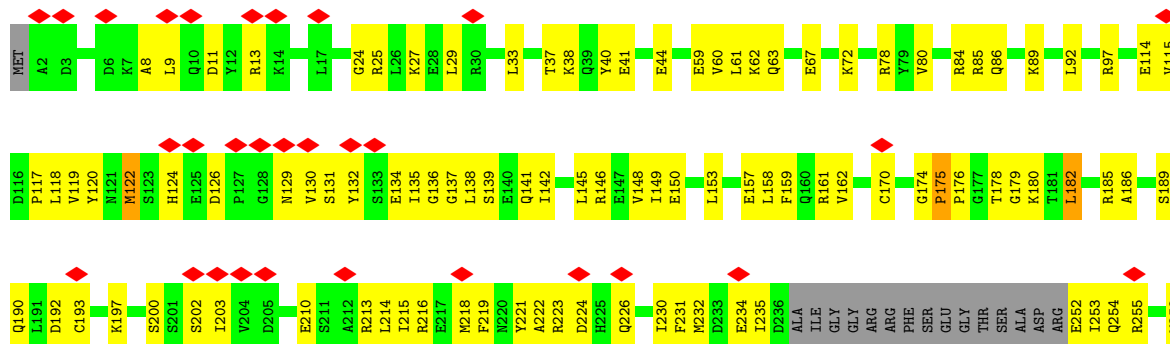
- Molecule 20: Protein SIC1

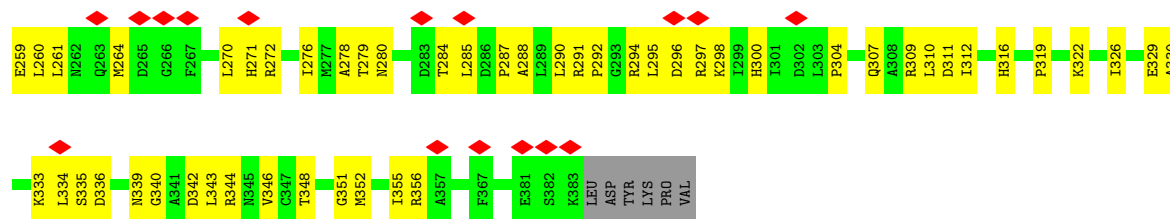
Chain y: 9% 29% 9% 62%



- Molecule 21: 26S protease regulatory subunit 10B

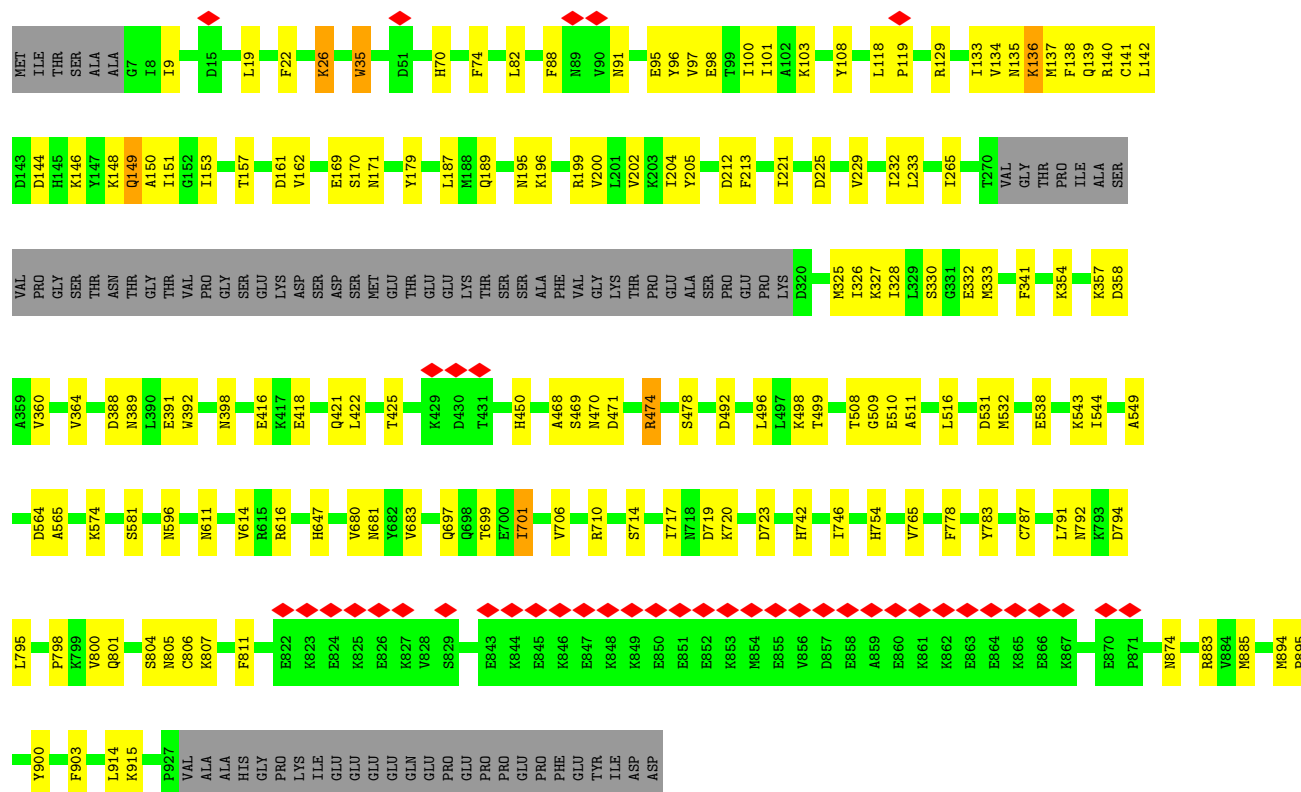
Chain E: 12% 55% 38% 6%





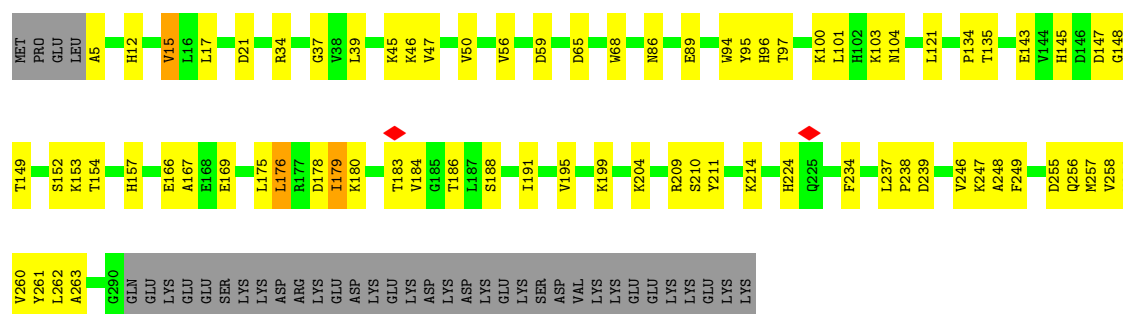
• Molecule 22: 26S proteasome non-ATPase regulatory subunit 1

Chain U: 75% 16% 8%



• Molecule 23: 26S proteasome non-ATPase regulatory subunit 7

Chain Z: 65% 23% 12%

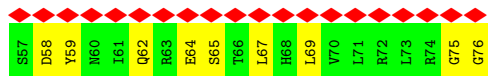
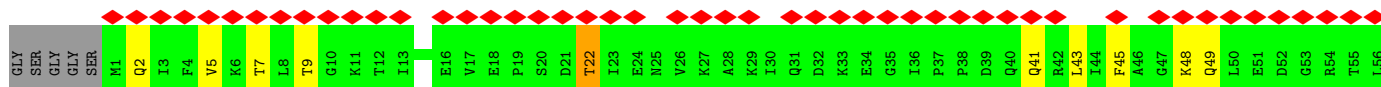
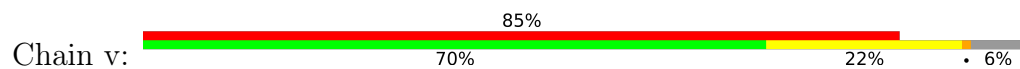


• Molecule 24: 26S proteasome non-ATPase regulatory subunit 13

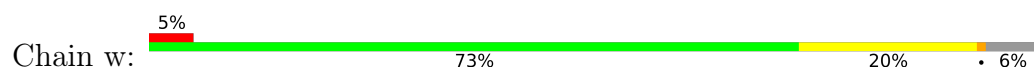
Chain u: 67% 25% 6%



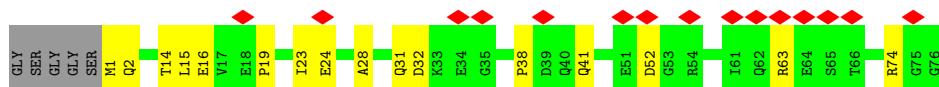
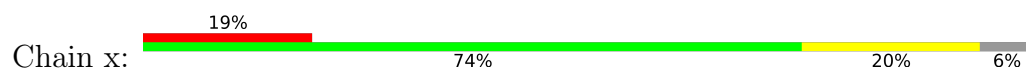
- Molecule 27: Polyubiquitin-B



- Molecule 27: Polyubiquitin-B



- Molecule 27: Polyubiquitin-B



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	84476	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	49	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	70000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	57.124	Depositor
Minimum map value	-28.796	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	5.5	Depositor
Map size (Å)	560.0, 560.0, 560.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4, 1.4, 1.4	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.41	0/3281	0.55	0/4431
2	B	0.47	0/3148	0.58	0/4257
3	D	0.41	0/3090	0.54	0/4168
4	F	0.23	0/3018	0.46	0/4069
5	C	0.49	0/3121	0.58	0/4194
6	G	0.28	0/1899	0.46	0/2568
7	H	0.30	0/1832	0.47	0/2481
8	I	0.27	0/1984	0.47	0/2672
9	J	0.29	0/1913	0.47	0/2581
10	K	0.34	0/1779	0.45	0/2400
11	L	0.28	0/1908	0.43	0/2579
12	M	0.26	0/1916	0.45	0/2580
13	V	0.30	0/3237	0.55	0/4419
14	W	0.28	0/3751	0.50	0/5042
15	X	0.29	0/2855	0.43	0/3865
16	Y	0.38	0/3173	0.59	0/4273
17	d	0.24	0/1702	0.52	0/2325
18	e	0.36	0/285	0.69	0/382
19	f	0.14	0/4379	0.39	0/6090
20	y	0.20	0/190	0.44	0/256
21	E	0.22	0/2943	0.49	0/3963
22	U	0.39	0/6700	0.53	0/9082
23	Z	0.44	0/2324	0.60	1/3150 (0.0%)
24	a	0.32	0/3053	0.52	0/4133
25	b	0.33	0/1478	0.52	0/2001
26	c	0.43	0/2302	0.66	1/3110 (0.0%)
27	u	0.37	0/610	0.54	0/819
27	v	0.12	0/609	0.33	0/819
27	w	0.25	0/609	0.42	0/819
27	x	0.18	0/609	0.40	0/819
All	All	0.34	0/69698	0.51	2/94347 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
23	Z	237	LEU	N-CA-C	5.44	121.83	109.81
26	c	179	SER	N-CA-C	5.11	119.00	112.87

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3228	0	3263	82	0
2	B	3103	0	3096	82	0
3	D	3040	0	3076	79	0
4	F	2981	0	3029	96	0
5	C	3080	0	3201	75	0
6	G	1865	0	1872	46	0
7	H	1793	0	1787	60	0
8	I	1954	0	1974	52	0
9	J	1887	0	1905	82	0
10	K	1753	0	1739	42	0
11	L	1873	0	1860	39	0
12	M	1881	0	1866	67	0
13	V	3197	0	2654	85	0
14	W	3703	0	3822	168	0
15	X	2815	0	2699	63	0
16	Y	3115	0	3120	144	0
17	d	1682	0	1340	35	0
18	e	282	0	221	6	0
19	f	4380	0	2048	17	0
20	y	188	0	186	9	0
21	E	2900	0	2954	115	0
22	U	6590	0	6408	109	0
23	Z	2281	0	2312	66	0
24	a	2995	0	3012	65	0
25	b	1458	0	1505	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	c	2260	0	2276	55	0
27	u	604	0	629	18	0
27	v	603	0	629	15	0
27	w	603	0	629	12	0
27	x	603	0	629	12	0
28	A	31	0	12	2	0
28	B	31	0	12	2	0
28	F	31	0	12	4	0
29	A	1	0	0	0	0
29	B	1	0	0	0	0
29	C	1	0	0	0	0
29	D	1	0	0	0	0
30	C	27	0	12	0	0
30	D	27	0	12	0	0
All	All	68848	0	65801	1664	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 12.

The worst 5 of 1664 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:287:ILE:HD11	2:B:329:MET:HB3	1.50	0.94
23:Z:209:ARG:HH21	24:a:354:GLU:HA	1.32	0.93
1:A:69:ASP:HB3	2:B:164:MET:HB2	1.56	0.87
13:V:477:HIS:HD1	17:d:249:TYR:HH	1.22	0.87
13:V:476:PHE:HB3	23:Z:260:VAL:HG21	1.56	0.87

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	A	411/433 (95%)	369 (90%)	42 (10%)	0	100	100
2	B	402/440 (91%)	343 (85%)	57 (14%)	2 (0%)	24	57
3	D	378/418 (90%)	341 (90%)	35 (9%)	2 (0%)	24	57
4	F	381/439 (87%)	352 (92%)	29 (8%)	0	100	100
5	C	389/406 (96%)	355 (91%)	33 (8%)	1 (0%)	36	67
6	G	237/246 (96%)	230 (97%)	7 (3%)	0	100	100
7	H	228/234 (97%)	214 (94%)	14 (6%)	0	100	100
8	I	246/261 (94%)	222 (90%)	24 (10%)	0	100	100
9	J	237/248 (96%)	213 (90%)	24 (10%)	0	100	100
10	K	224/241 (93%)	208 (93%)	16 (7%)	0	100	100
11	L	236/263 (90%)	224 (95%)	12 (5%)	0	100	100
12	M	238/255 (93%)	229 (96%)	9 (4%)	0	100	100
13	V	478/534 (90%)	419 (88%)	56 (12%)	3 (1%)	21	54
14	W	454/456 (100%)	423 (93%)	31 (7%)	0	100	100
15	X	378/422 (90%)	353 (93%)	24 (6%)	1 (0%)	36	67
16	Y	376/389 (97%)	336 (89%)	38 (10%)	2 (0%)	24	57
17	d	255/350 (73%)	224 (88%)	26 (10%)	5 (2%)	6	32
18	e	33/70 (47%)	29 (88%)	4 (12%)	0	100	100
19	f	887/908 (98%)	749 (84%)	135 (15%)	3 (0%)	36	67
20	y	24/69 (35%)	21 (88%)	3 (12%)	0	100	100
21	E	363/389 (93%)	337 (93%)	23 (6%)	3 (1%)	16	48
22	U	868/953 (91%)	799 (92%)	69 (8%)	0	100	100
23	Z	284/324 (88%)	258 (91%)	26 (9%)	0	100	100
24	a	371/376 (99%)	335 (90%)	34 (9%)	2 (0%)	24	57
25	b	189/377 (50%)	171 (90%)	17 (9%)	1 (0%)	24	57
26	c	285/310 (92%)	245 (86%)	38 (13%)	2 (1%)	18	51
27	u	74/81 (91%)	68 (92%)	6 (8%)	0	100	100
27	v	74/81 (91%)	70 (95%)	4 (5%)	0	100	100
27	w	74/81 (91%)	72 (97%)	2 (3%)	0	100	100
27	x	74/81 (91%)	72 (97%)	2 (3%)	0	100	100
All	All	9148/10135 (90%)	8281 (90%)	840 (9%)	27 (0%)	37	67

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	V	269	LYS
17	d	203	PRO
17	d	232	PRO
19	f	756	PRO
21	E	175	PRO

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	349/372 (94%)	339 (97%)	10 (3%)	37	58
2	B	334/385 (87%)	333 (100%)	1 (0%)	86	84
3	D	333/366 (91%)	333 (100%)	0	100	100
4	F	317/379 (84%)	314 (99%)	3 (1%)	70	74
5	C	340/352 (97%)	336 (99%)	4 (1%)	63	72
6	G	204/210 (97%)	202 (99%)	2 (1%)	68	74
7	H	188/191 (98%)	186 (99%)	2 (1%)	65	73
8	I	208/221 (94%)	206 (99%)	2 (1%)	68	74
9	J	203/211 (96%)	203 (100%)	0	100	100
10	K	193/203 (95%)	192 (100%)	1 (0%)	81	81
11	L	204/224 (91%)	204 (100%)	0	100	100
12	M	198/212 (93%)	197 (100%)	1 (0%)	81	81
13	V	226/460 (49%)	207 (92%)	19 (8%)	10	34
14	W	416/416 (100%)	409 (98%)	7 (2%)	53	67
15	X	267/362 (74%)	267 (100%)	0	100	100
16	Y	334/344 (97%)	323 (97%)	11 (3%)	33	56
17	d	111/294 (38%)	105 (95%)	6 (5%)	20	45
18	e	26/63 (41%)	14 (54%)	12 (46%)	0	0
20	y	22/57 (39%)	22 (100%)	0	100	100
21	E	316/341 (93%)	313 (99%)	3 (1%)	70	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	U	677/816 (83%)	663 (98%)	14 (2%)	47	64
23	Z	257/295 (87%)	243 (95%)	14 (5%)	20	45
24	a	333/336 (99%)	321 (96%)	12 (4%)	31	54
25	b	167/312 (54%)	161 (96%)	6 (4%)	31	54
26	c	252/268 (94%)	237 (94%)	15 (6%)	17	43
27	u	68/70 (97%)	66 (97%)	2 (3%)	37	58
27	v	68/70 (97%)	67 (98%)	1 (2%)	57	69
27	w	68/70 (97%)	66 (97%)	2 (3%)	37	58
27	x	68/70 (97%)	68 (100%)	0	100	100
All	All	6747/7970 (85%)	6597 (98%)	150 (2%)	45	63

5 of 150 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
24	a	145	LEU
26	c	275	VAL
24	a	225	LEU
26	c	25	VAL
14	W	179	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 58 such sidechains are listed below:

Mol	Chain	Res	Type
16	Y	178	ASN
27	u	41	GLN
21	E	280	ASN
26	c	241	ASN
25	b	161	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	ATP	F	501	-	32,33,33	0.61	1 (3%)	48,52,52	0.31	0
30	ADP	D	501	29	28,29,29	1.39	6 (21%)	43,45,45	1.78	10 (23%)
30	ADP	C	501	29	28,29,29	1.40	4 (14%)	43,45,45	1.89	11 (25%)
28	ATP	A	501	29	32,33,33	1.75	2 (6%)	48,52,52	0.52	0
28	ATP	B	501	29	32,33,33	1.29	2 (6%)	48,52,52	0.48	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
28	ATP	F	501	-	-	7/22/38/38	0/3/3/3
30	ADP	D	501	29	-	5/16/32/32	0/3/3/3
30	ADP	C	501	29	-	3/16/32/32	0/3/3/3
28	ATP	A	501	29	-	6/22/38/38	0/3/3/3
28	ATP	B	501	29	-	4/22/38/38	0/3/3/3

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	A	501	ATP	PB-O3B	-7.95	1.50	1.59
28	B	501	ATP	PA-O3A	-5.40	1.53	1.59
28	A	501	ATP	PA-O3A	-4.94	1.54	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	B	501	ATP	PB-O3B	-4.23	1.54	1.59
30	D	501	ADP	C5-C4	3.98	1.46	1.39

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	C	501	ADP	C5-C4-N3	-6.01	118.44	126.72
30	D	501	ADP	C5-C4-N3	-5.42	119.26	126.72
30	C	501	ADP	N3-C4-N9	5.01	135.69	127.17
30	D	501	ADP	N3-C4-N9	4.22	134.34	127.17
30	C	501	ADP	C2-N3-C4	3.61	120.65	111.83

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
28	A	501	ATP	C5'-O5'-PA-O1A
28	A	501	ATP	C5'-O5'-PA-O3A
28	A	501	ATP	O4'-C4'-C5'-O5'
28	F	501	ATP	PB-O3B-PG-O2G
28	F	501	ATP	PB-O3B-PG-O3G

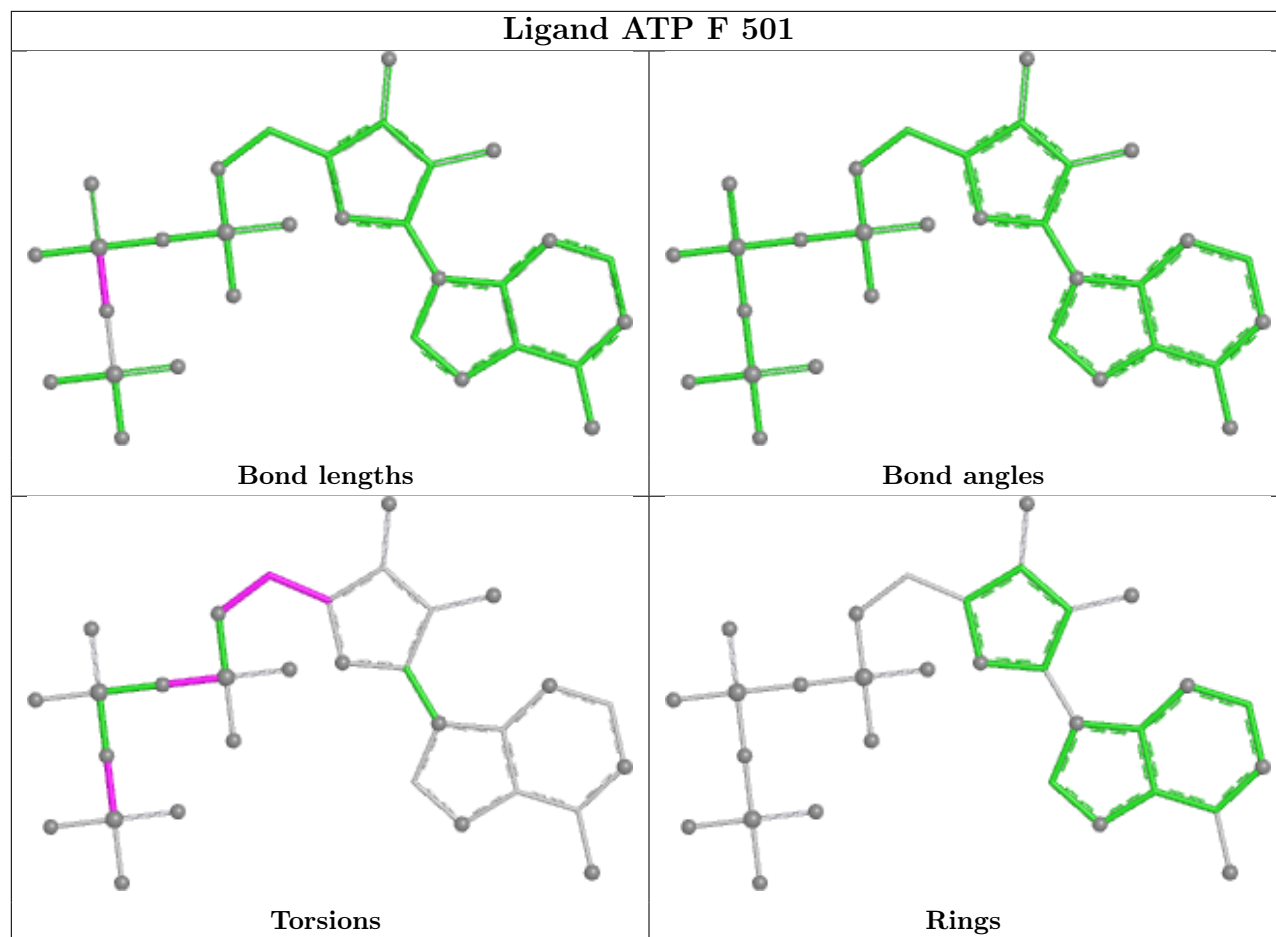
There are no ring outliers.

3 monomers are involved in 8 short contacts:

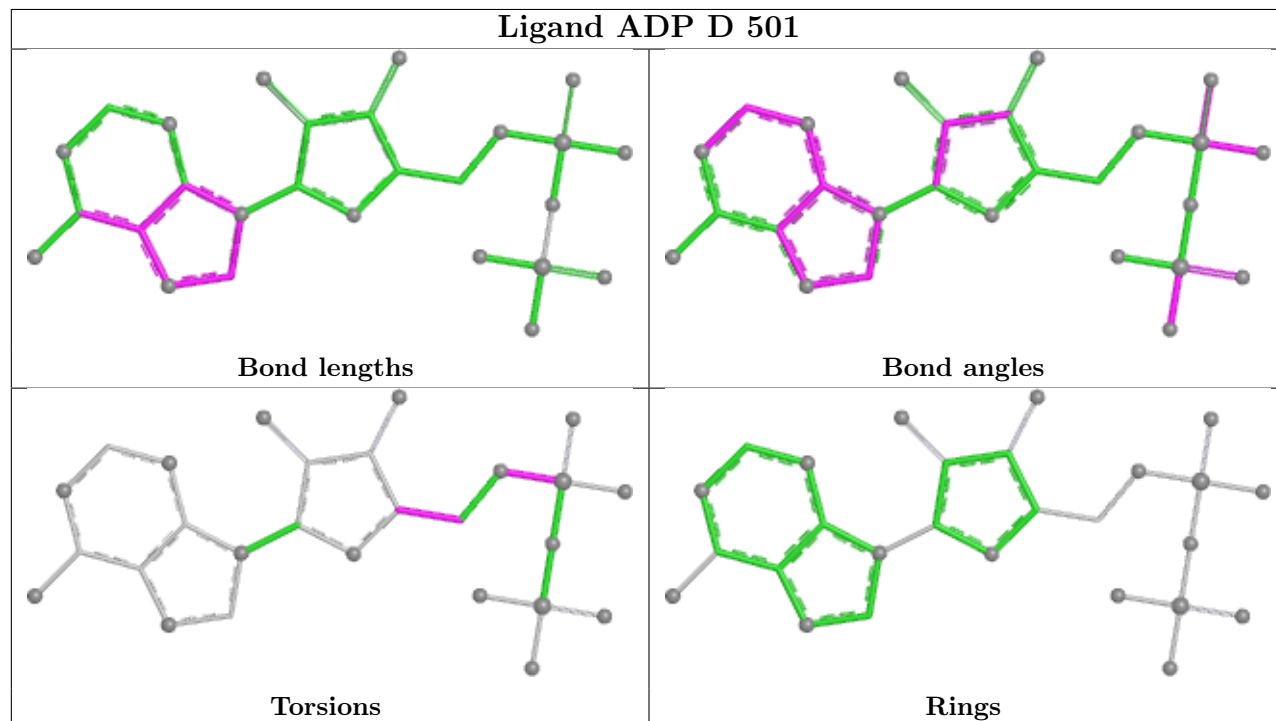
Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	F	501	ATP	4	0
28	A	501	ATP	2	0
28	B	501	ATP	2	0

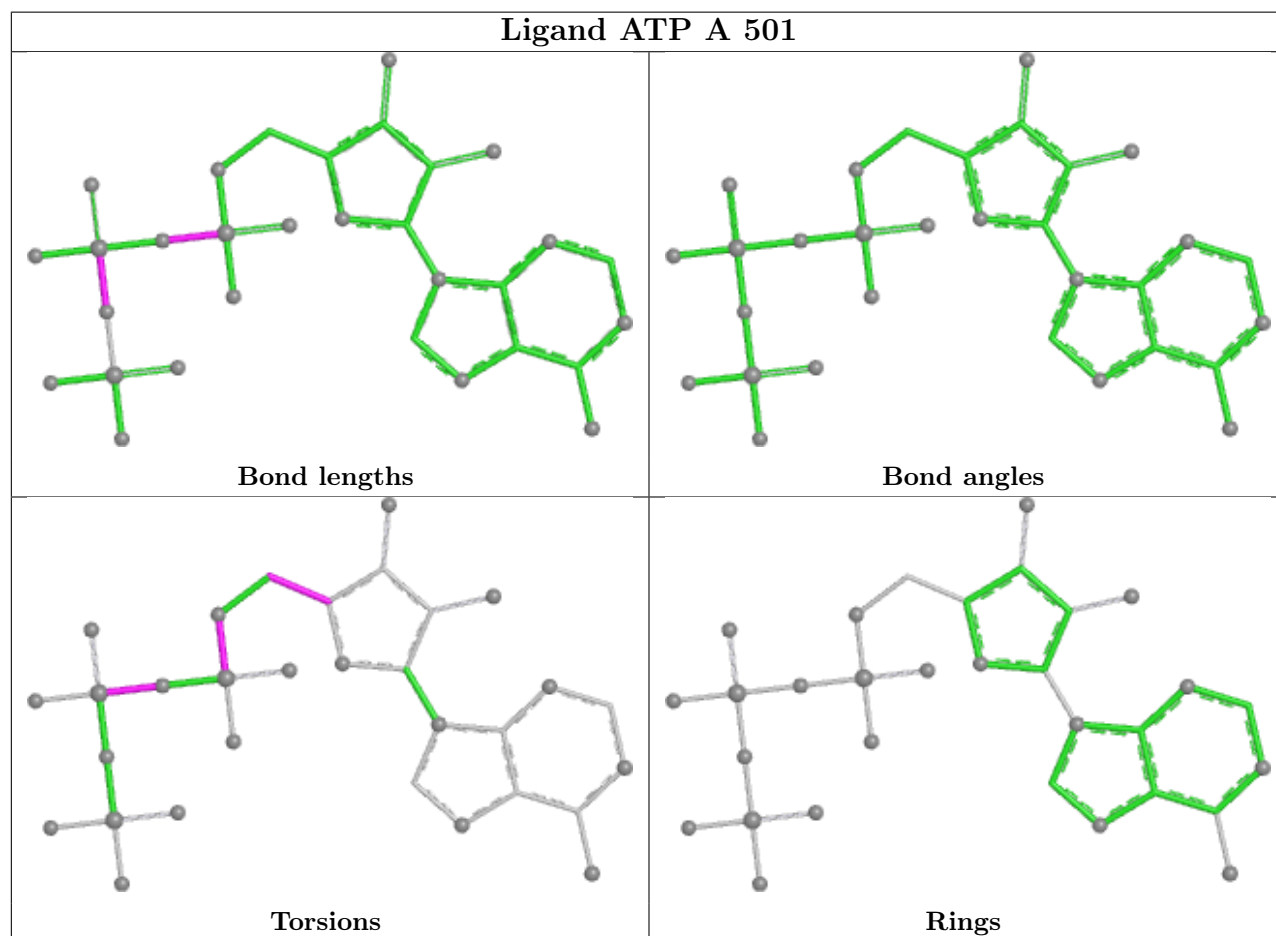
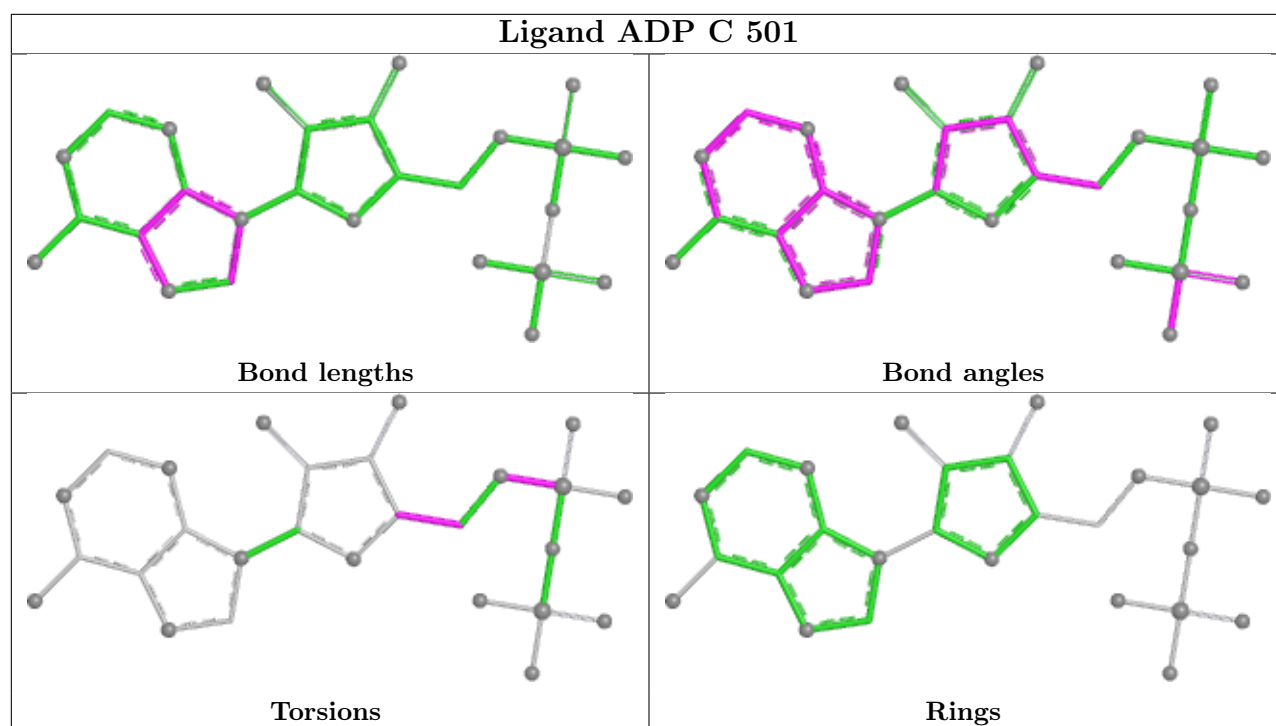
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

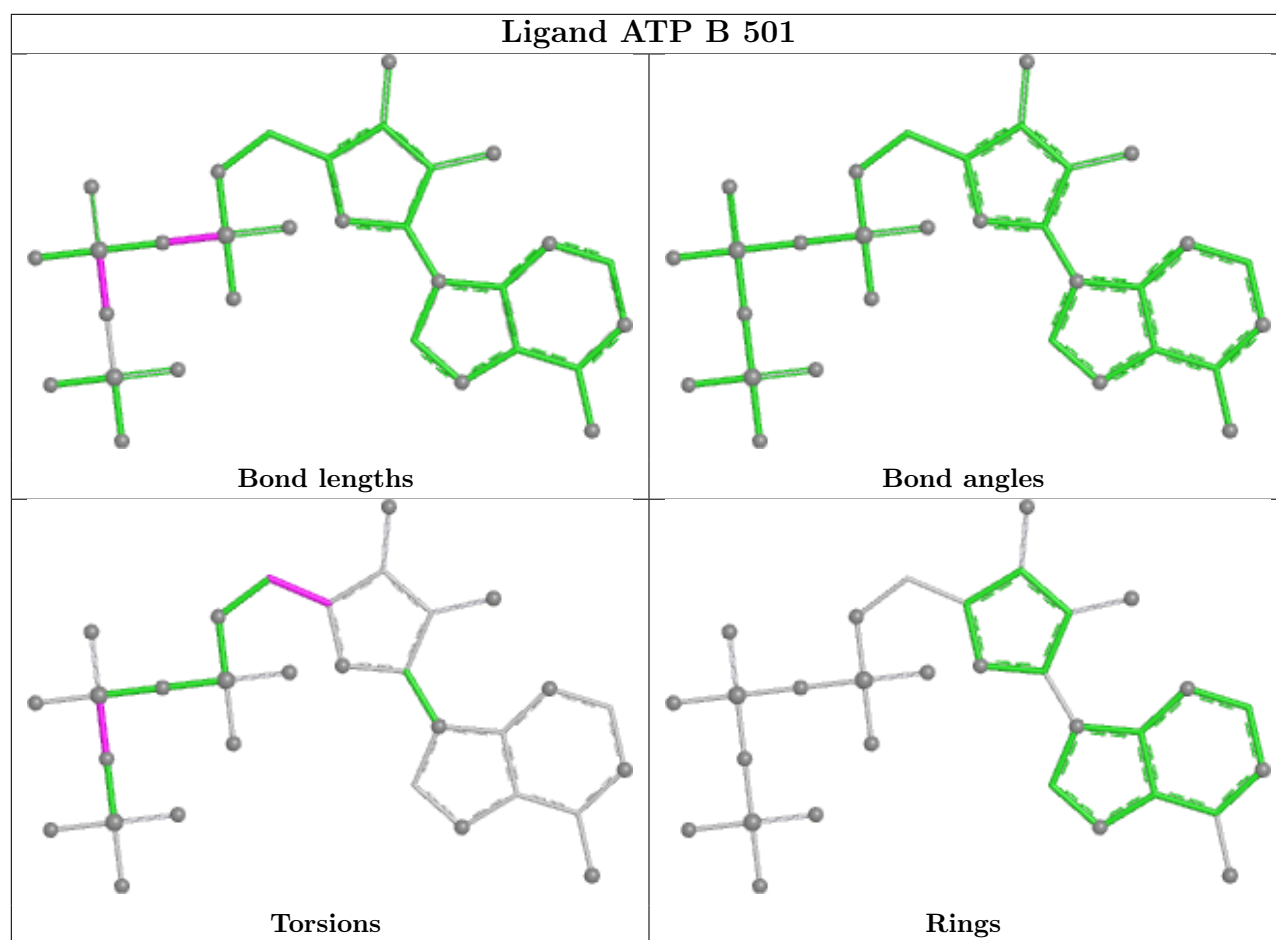
Ligand ATP F 501



Ligand ADP D 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.

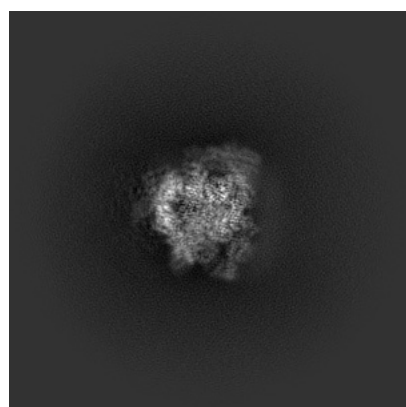
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36764. These allow visual inspection of the internal detail of the map and identification of artifacts.

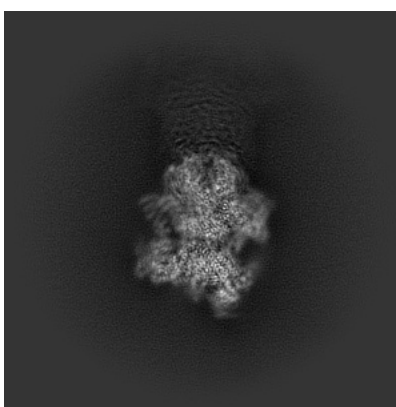
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

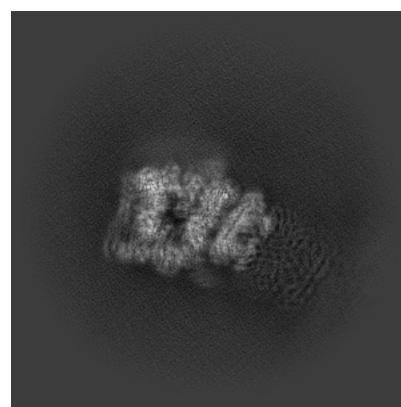
6.1.1 Primary map



X



Y

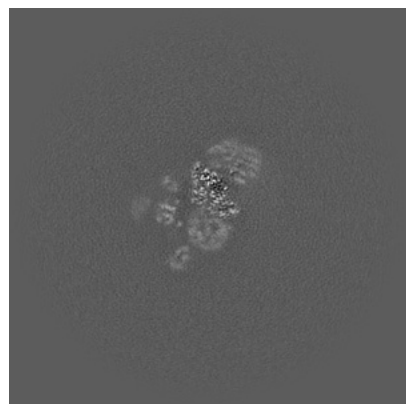


Z

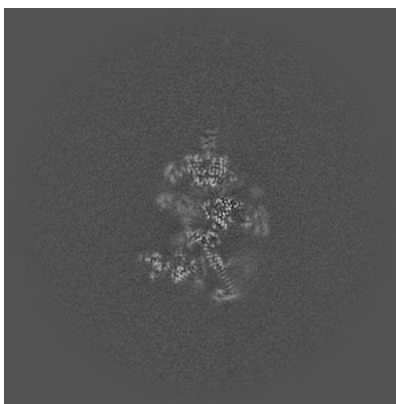
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

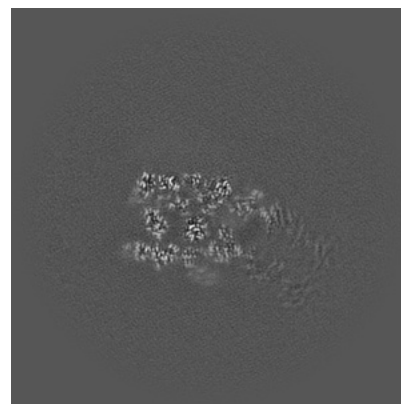
6.2.1 Primary map



X Index: 200



Y Index: 200

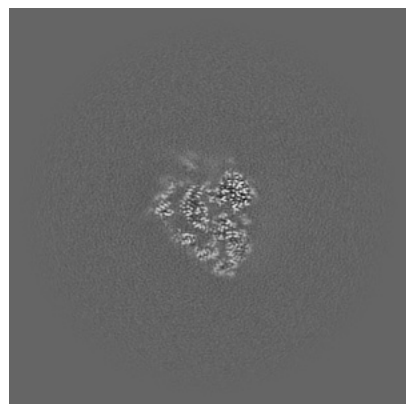


Z Index: 200

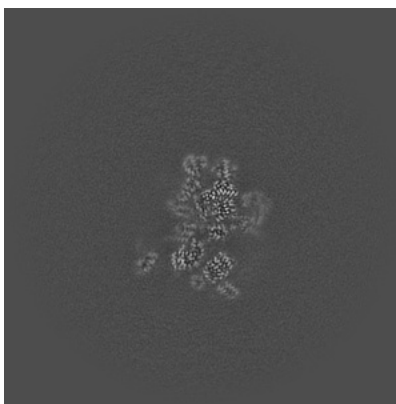
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

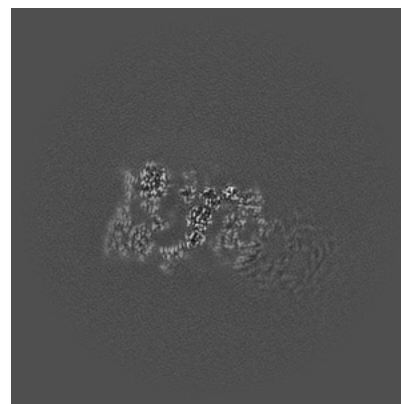
6.3.1 Primary map



X Index: 143



Y Index: 213

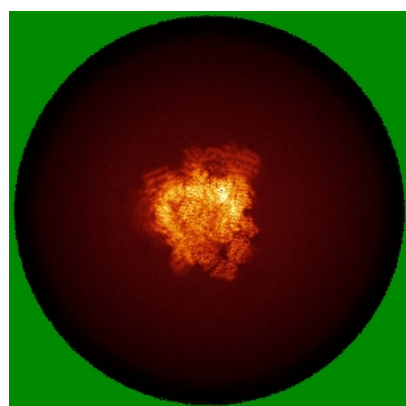


Z Index: 217

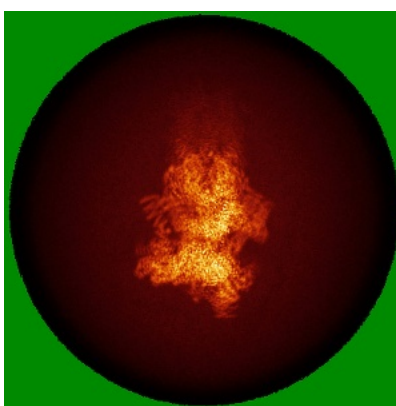
The images above show the largest variance slices of the map in three orthogonal directions.

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

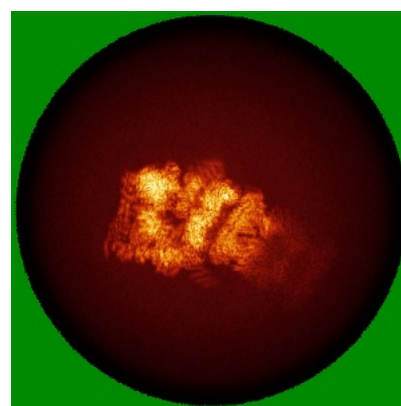
6.4.1 Primary map



X



Y

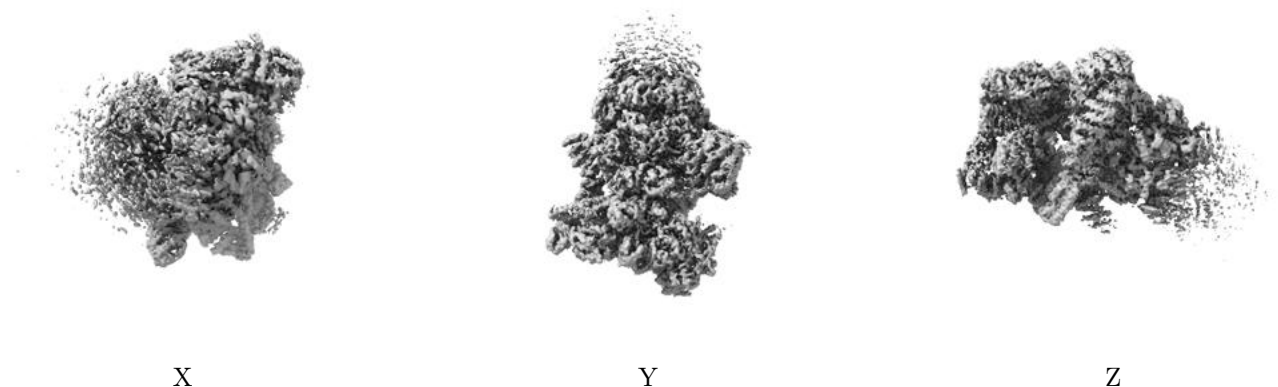


Z

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 5.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

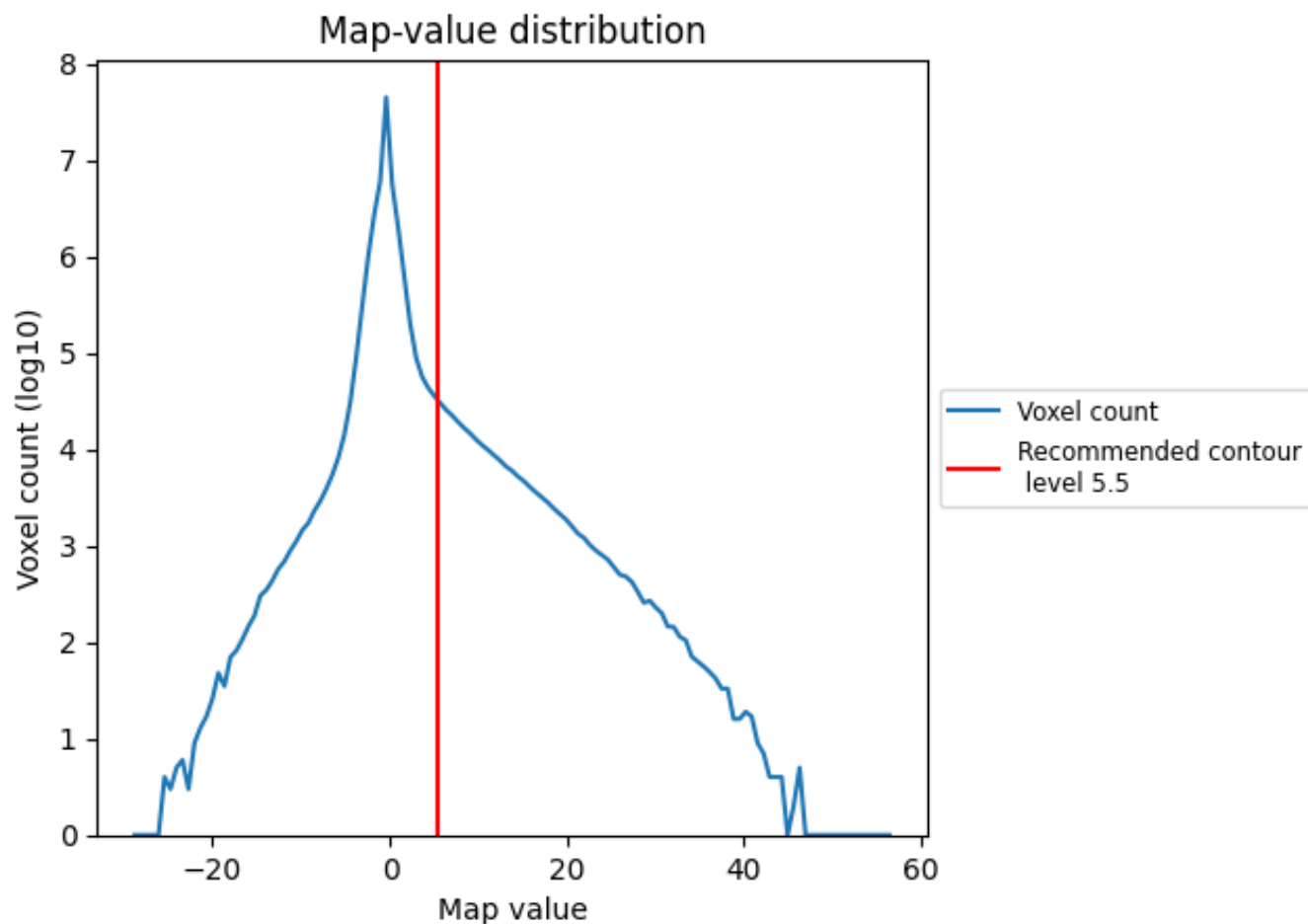
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

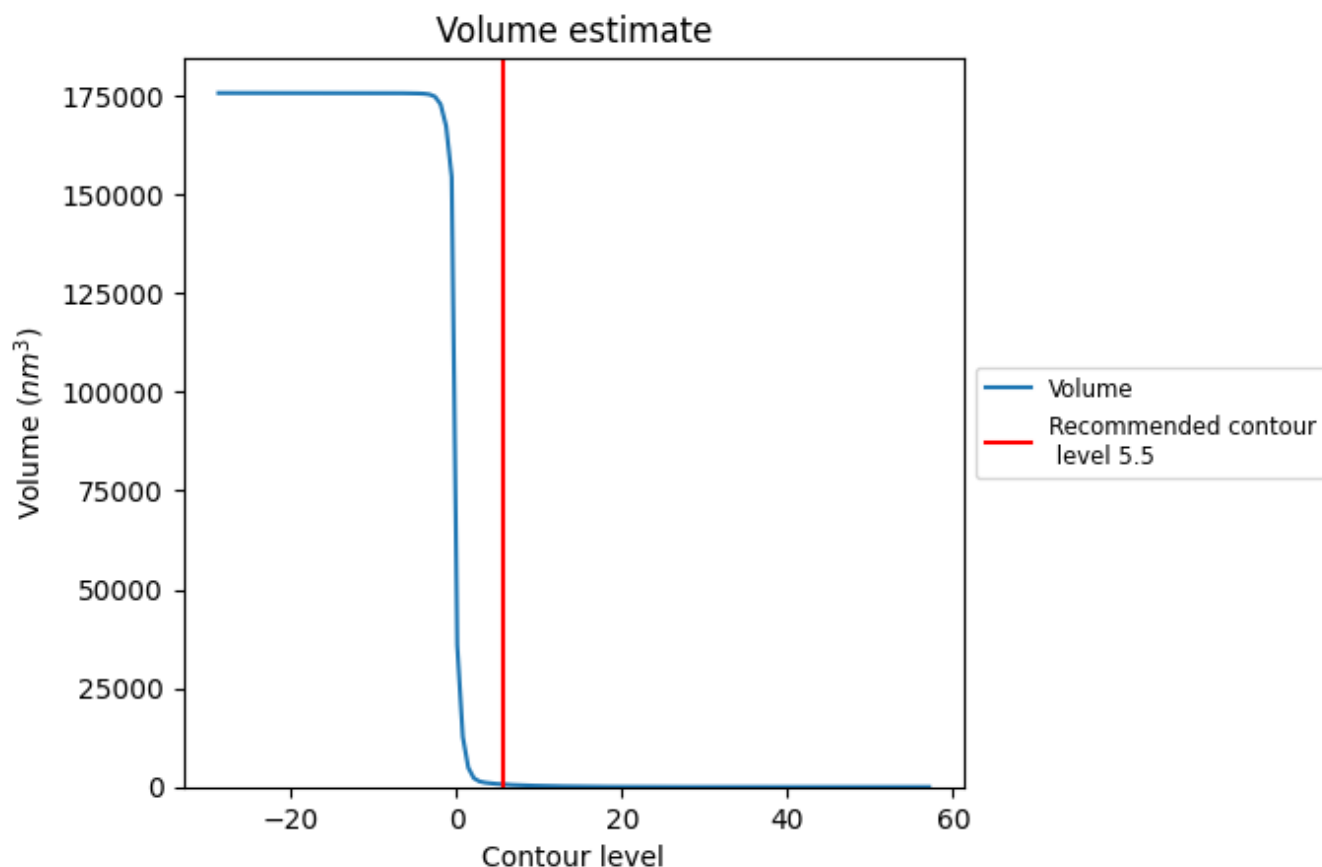
This section contains the results of statistical analysis of the map.

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.

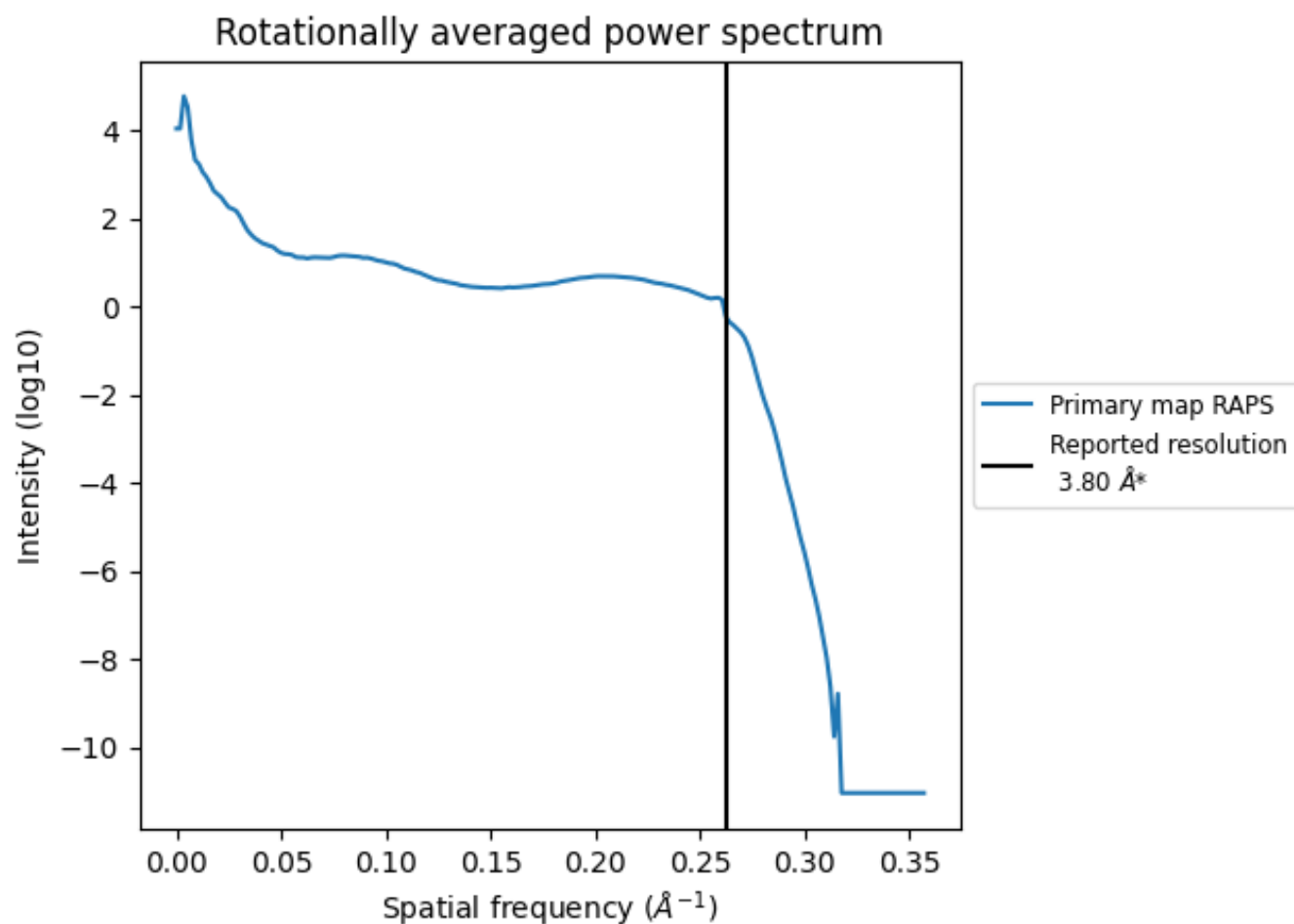
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 670 nm^3 ; this corresponds to an approximate mass of 605 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 ⓘ

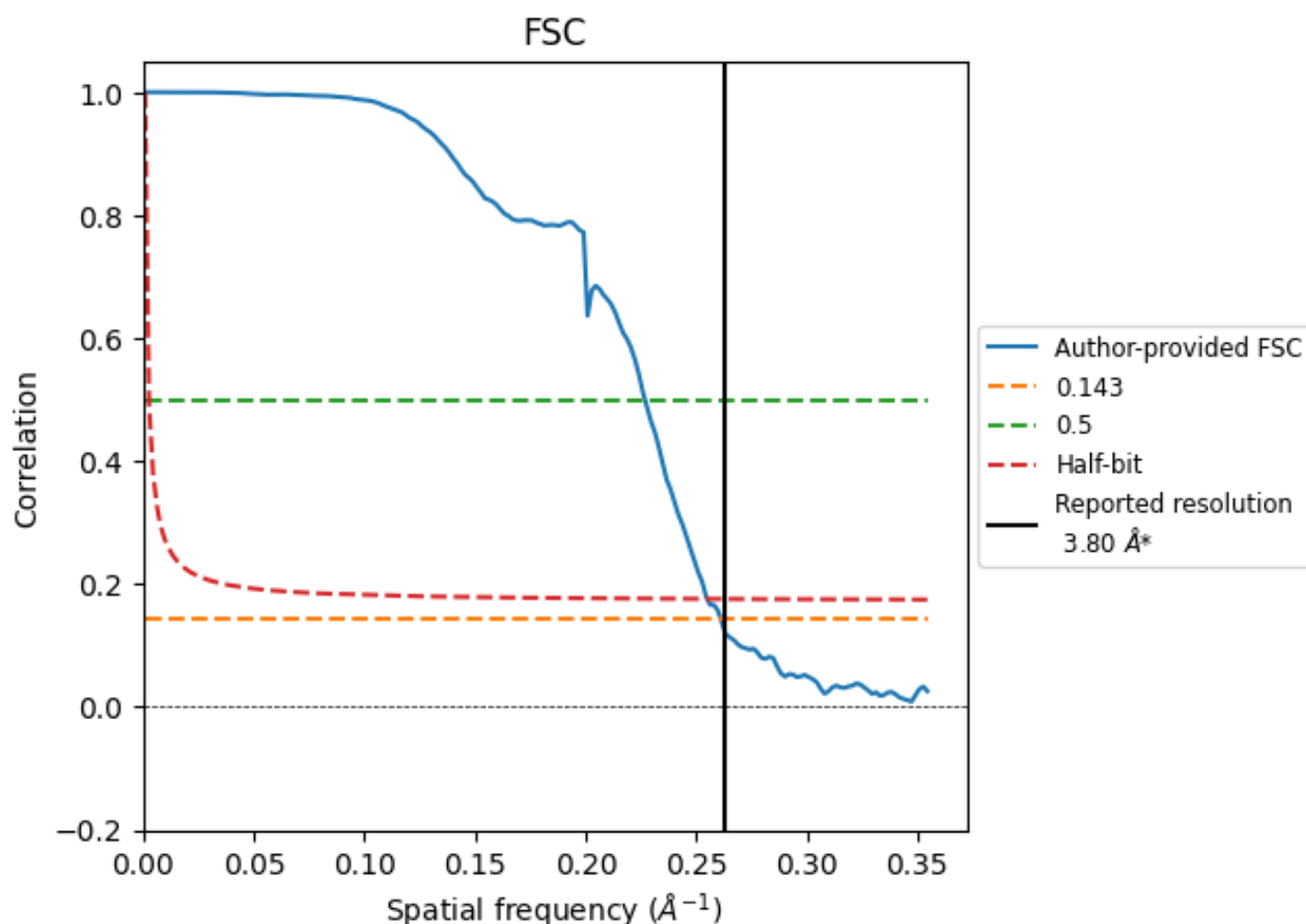


*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

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 0.263 Å⁻¹

8.2 Resolution estimates [i](#)

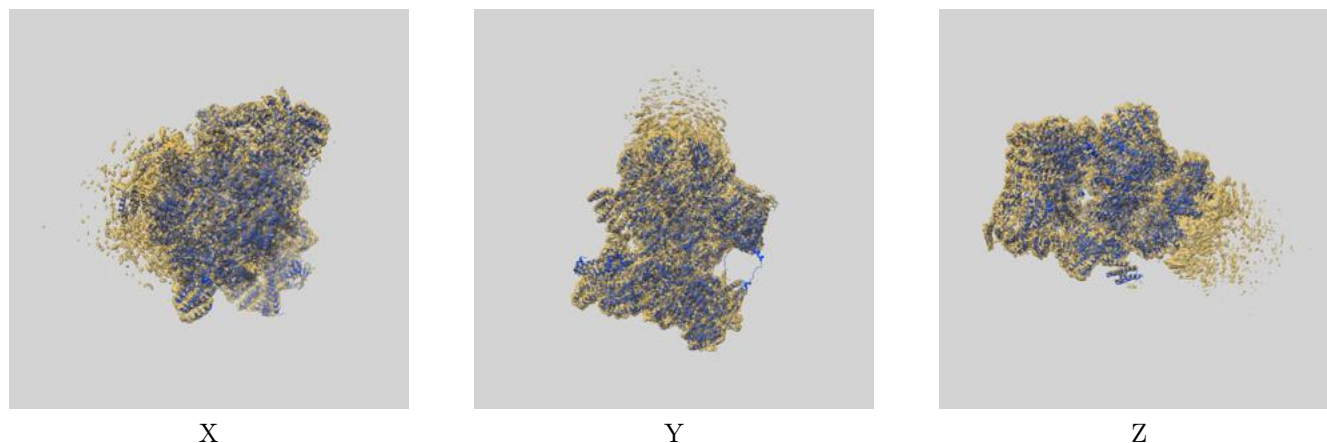
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.83	4.41	3.92
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

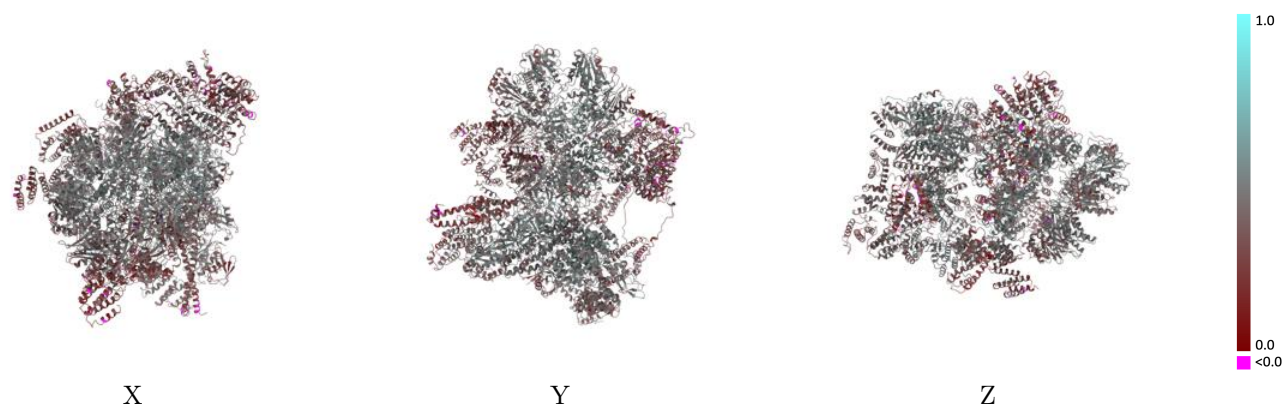
This section contains information regarding the fit between EMDB map EMD-36764 and PDB model 8K0G. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay [i](#)



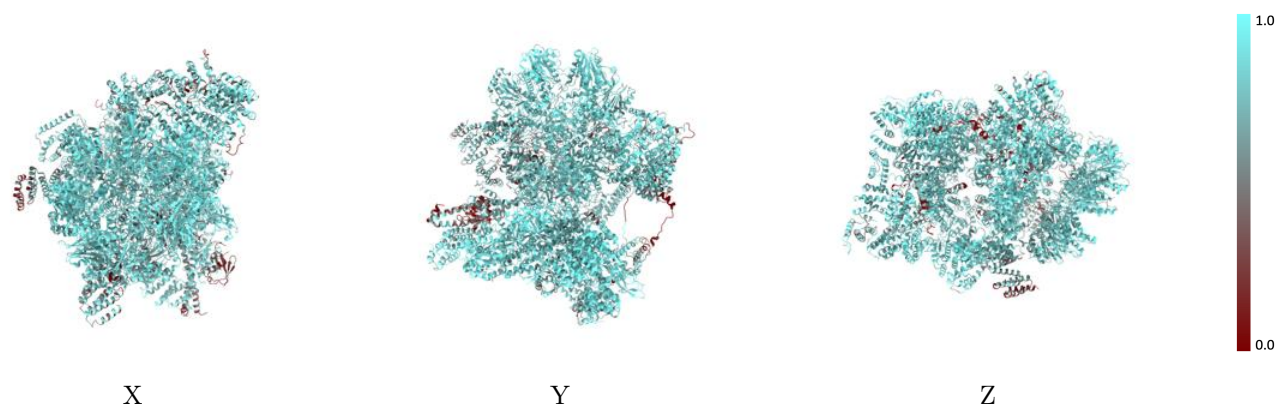
The images above show the 3D surface view of the map at the recommended contour level 5.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



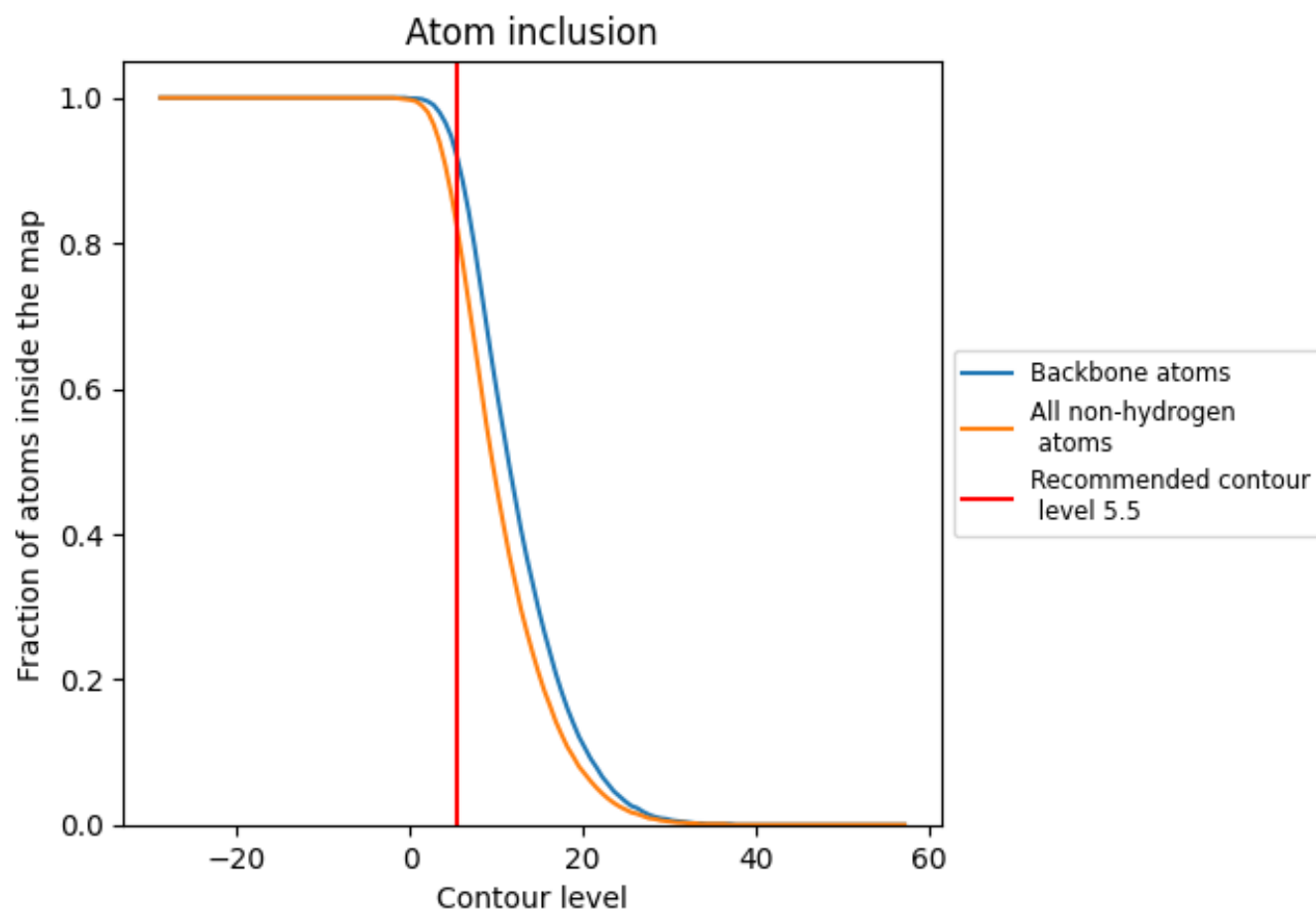
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (5.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 82% 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 (5.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8180	 0.4160
A	 0.8490	 0.4590
B	 0.8820	 0.4830
C	 0.8910	 0.4930
D	 0.8680	 0.4670
E	 0.6750	 0.3270
F	 0.7160	 0.3580
G	 0.8490	 0.4190
H	 0.8660	 0.4540
I	 0.8090	 0.4230
J	 0.8340	 0.4270
K	 0.8840	 0.4580
L	 0.8860	 0.4540
M	 0.8420	 0.4180
U	 0.8690	 0.4540
V	 0.7750	 0.3730
W	 0.7510	 0.3360
X	 0.7520	 0.3910
Y	 0.8660	 0.3930
Z	 0.8670	 0.4730
a	 0.8720	 0.4230
b	 0.8750	 0.4370
c	 0.8560	 0.4720
d	 0.7650	 0.3710
e	 0.8530	 0.4130
f	 0.7680	 0.3280
u	 0.9270	 0.4620
v	 0.1640	 0.2850
w	 0.8330	 0.4070
x	 0.6180	 0.3940
y	 0.6290	 0.4220

