



wwPDB EM Validation Summary Report ⓘ

Nov 2, 2024 – 01:14 PM EDT

PDB ID : 5T0H
EMDB ID : EMD-8335
Title : Structural basis for dynamic regulation of the human 26S proteasome
Authors : Chen, S.; Wu, J.; Lu, Y.; Ma, Y.B.; Lee, B.H.; Yu, Z.; Ouyang, Q.; Finley, D.;
Kirschner, M.W.; Mao, Y.
Deposited on : 2016-08-16
Resolution : 6.80 Å(reported)

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

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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:

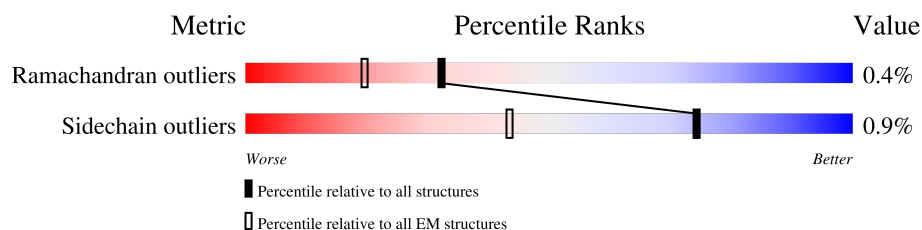
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 6.80 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)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	433	
2	B	440	
3	C	398	
4	D	418	
5	E	403	
6	F	439	
7	G	245	
8	H	233	
9	I	260	

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Mol	Chain	Length	Quality of chain
10	J	247	
11	K	240	
12	L	268	
13	M	254	
14	N	238	
15	O	276	
16	P	204	
17	Q	201	
18	R	262	
19	S	240	
20	T	263	
21	U	953	
22	V	533	
23	W	456	
24	X	422	
25	Y	389	
26	Z	324	
27	a	376	
28	b	377	
29	c	309	
30	d	349	
31	e	70	
32	f	749	

2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 73509 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	361	Total	C	N	O	S	0	0
			2835	1788	501	528	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	341	Total	C	N	O	S	0	0
			2662	1671	453	526	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	384	Total	C	N	O	S	0	0
			3015	1894	540	564	17		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	353	Total	C	N	O	S	0	0
			2790	1755	494	525	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	366	Total	C	N	O	S	0	0
			2863	1802	496	549	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	240	Total	C	N	O	S	0	0
			1826	1160	305	348	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	232	Total	C	N	O	S	0	0
			1708	1081	289	333	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	250	Total	C	N	O	S	0	0
			1912	1204	329	371	8		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	228	Total	C	N	O	S	0	0
			1722	1080	284	348	10		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 20 is a protein called Proteasome subunit beta type-4.

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

- Molecule 21 is a protein called 26S proteasome non-ATPase regulatory subunit 1.

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

- Molecule 22 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	480	Total	C	N	O	S	0	0
			3852	2444	684	710	14		

- Molecule 23 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	236	Total	C	N	O	S	0	0
			1940	1237	331	361	11		

- Molecule 24 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	81	Total	C	N	O	S	0	0
			647	414	107	124	2		

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

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

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

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

- Molecule 27 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

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

- Molecule 28 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

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

- Molecule 29 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

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

- Molecule 30 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

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

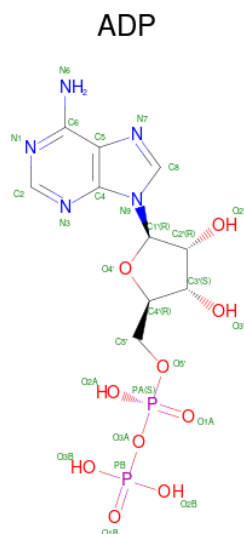
- Molecule 31 is a protein called 26S proteasome complex subunit DSS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	e	24	Total	C	N	O	S	0	0
			197	121	34	40	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
32	f	694	Total	C	N	O	S	0	0
			5331	3364	899	1027	41		

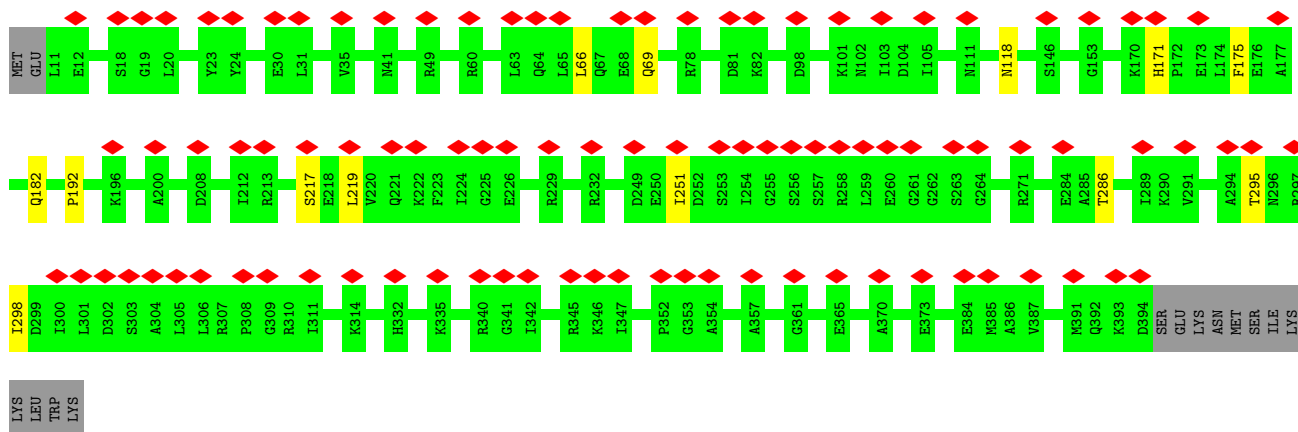
- Molecule 33 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



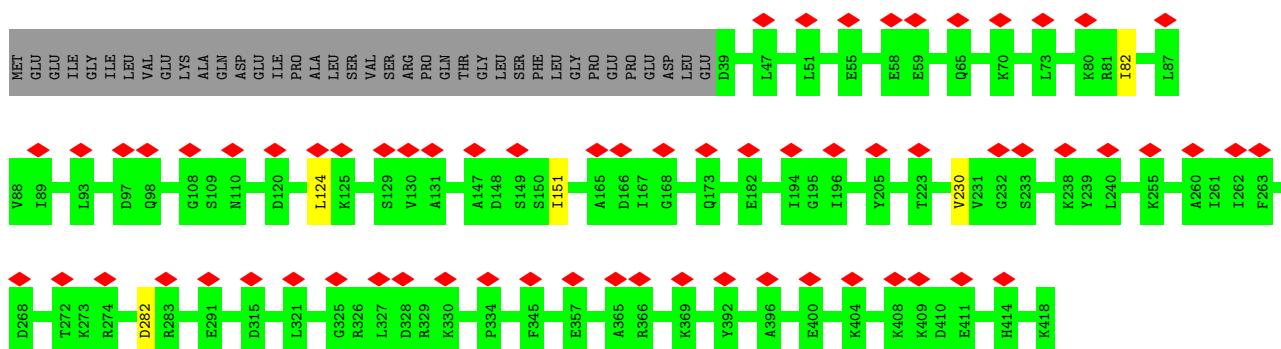
Mol	Chain	Residues	Atoms					AltConf
33	A	1	Total 27	C 10	N 5	O 10	P 2	0
33	B	1	Total 27	C 10	N 5	O 10	P 2	0
33	C	1	Total 27	C 10	N 5	O 10	P 2	0
33	D	1	Total 27	C 10	N 5	O 10	P 2	0
33	E	1	Total 27	C 10	N 5	O 10	P 2	0
33	F	1	Total 27	C 10	N 5	O 10	P 2	0

- Molecule 34 is ZINC ION (three-letter code: ZN) (formula: Zn).

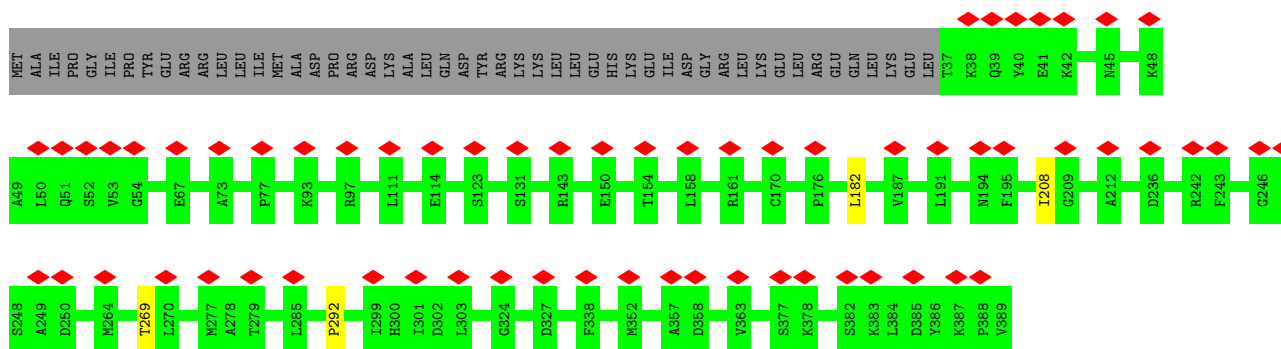
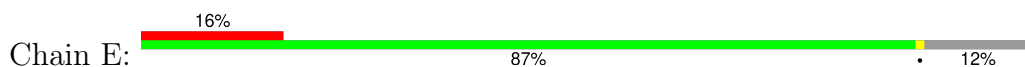
Mol	Chain	Residues	Atoms	AltConf
34	c	1	Total Zn 1 1	0



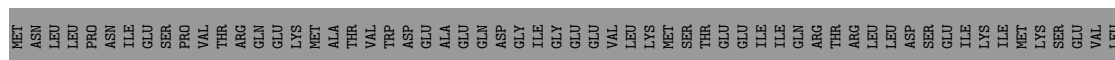
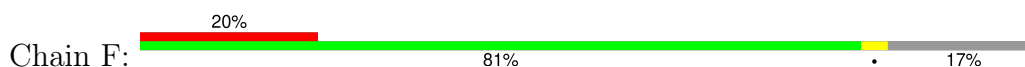
• Molecule 4: 26S protease regulatory subunit 6B

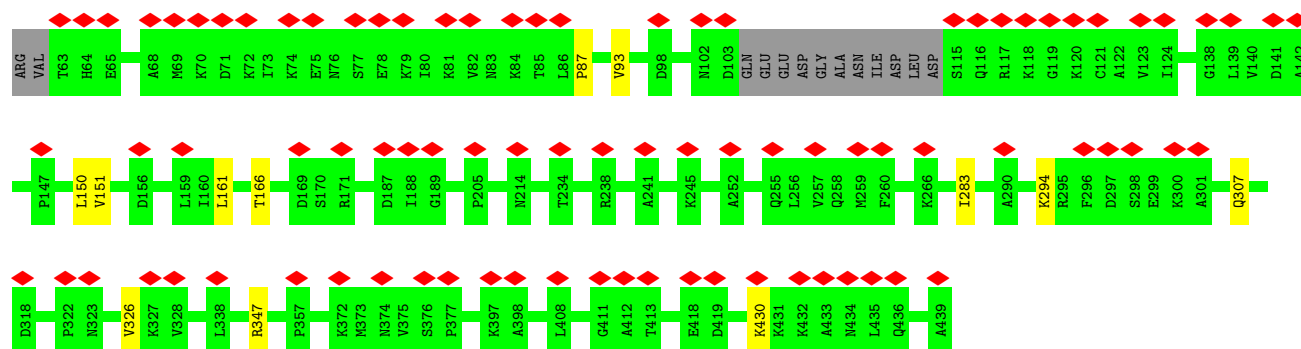


• Molecule 5: 26S protease regulatory subunit 10B

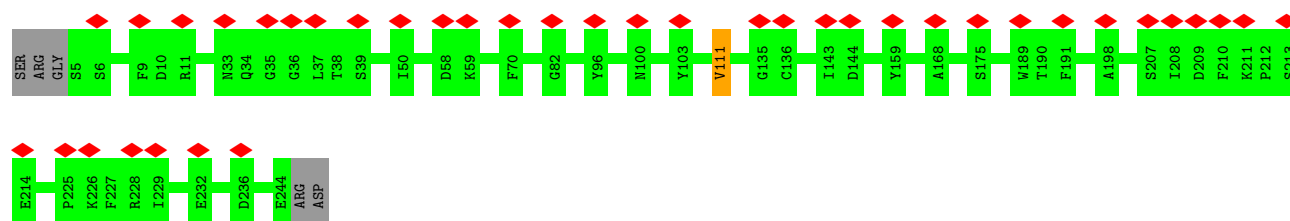


• Molecule 6: 26S protease regulatory subunit 6A

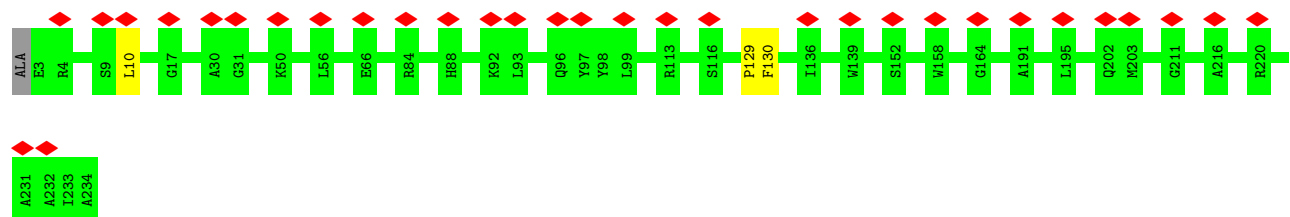




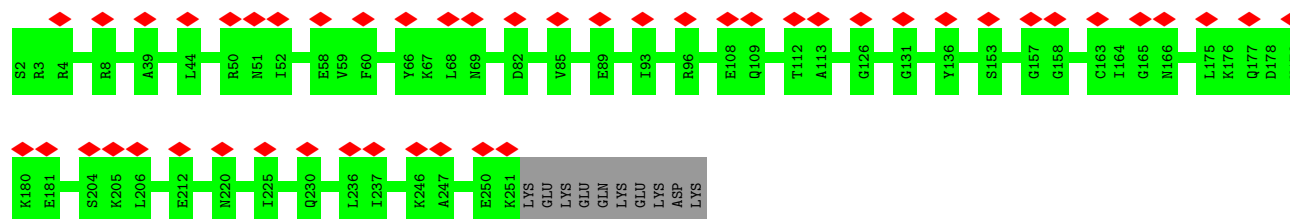
- Molecule 7: Proteasome subunit alpha type-6



- Molecule 8: Proteasome subunit alpha type-2

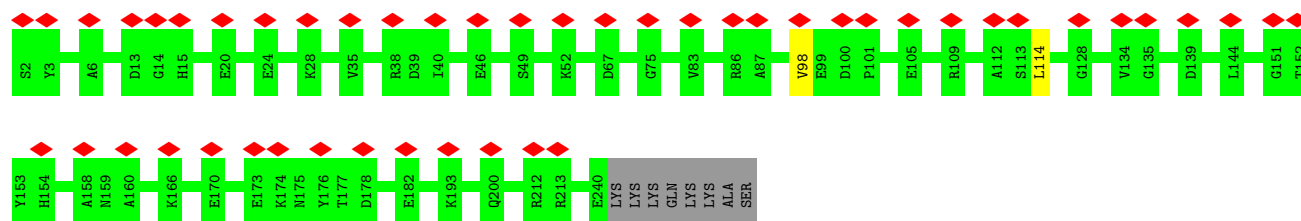


- Molecule 9: Proteasome subunit alpha type-4



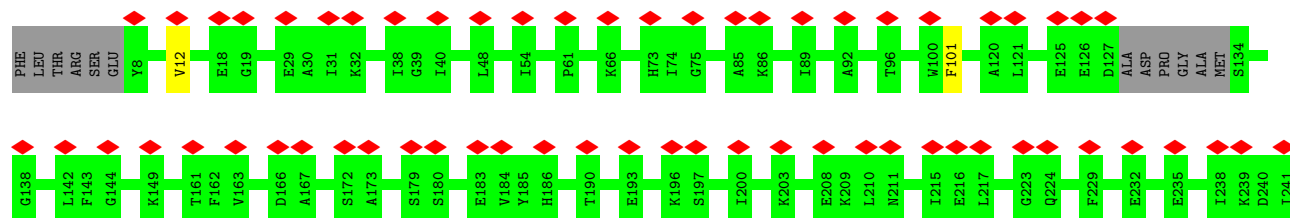
- Molecule 10: Proteasome subunit alpha type-7





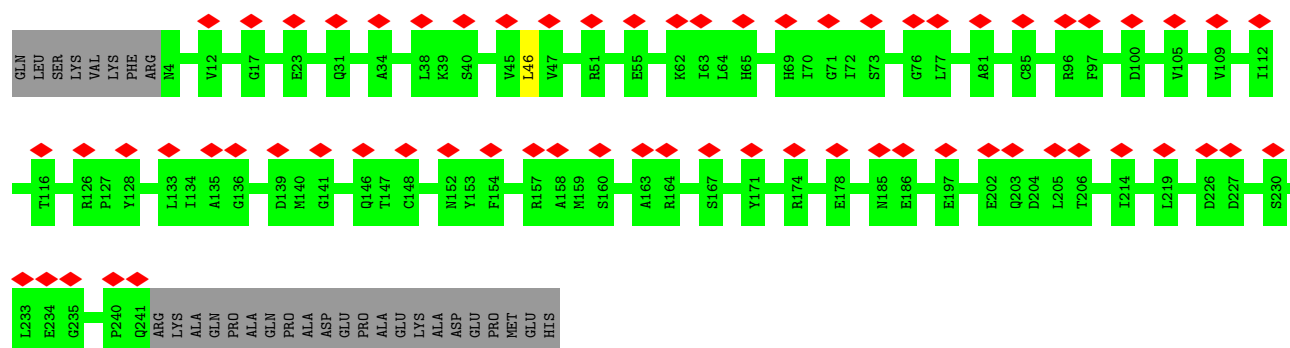
• Molecule 11: Proteasome subunit alpha type-5

Chain K: 25% 94% 5%



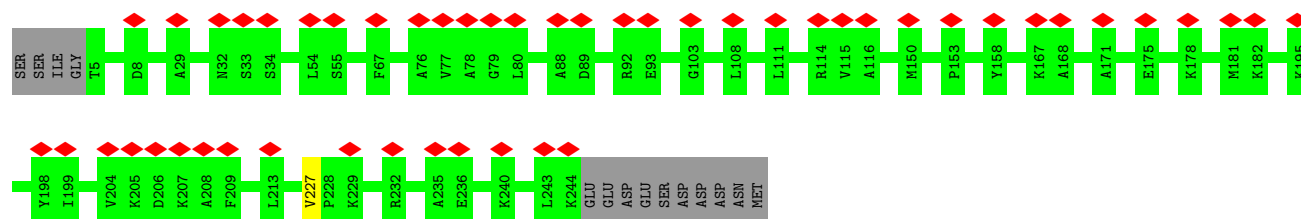
• Molecule 12: Proteasome subunit alpha type-1

Chain L: 24% 88% 11%



• Molecule 13: Proteasome subunit alpha type-3

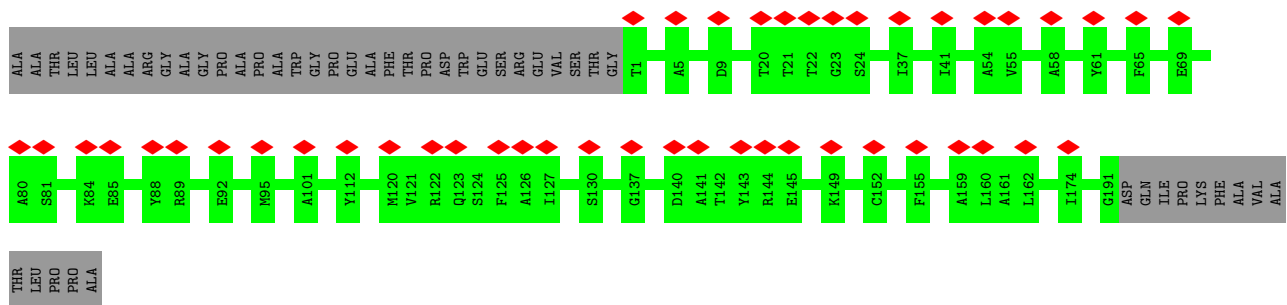
Chain M: 20% 94% 6%



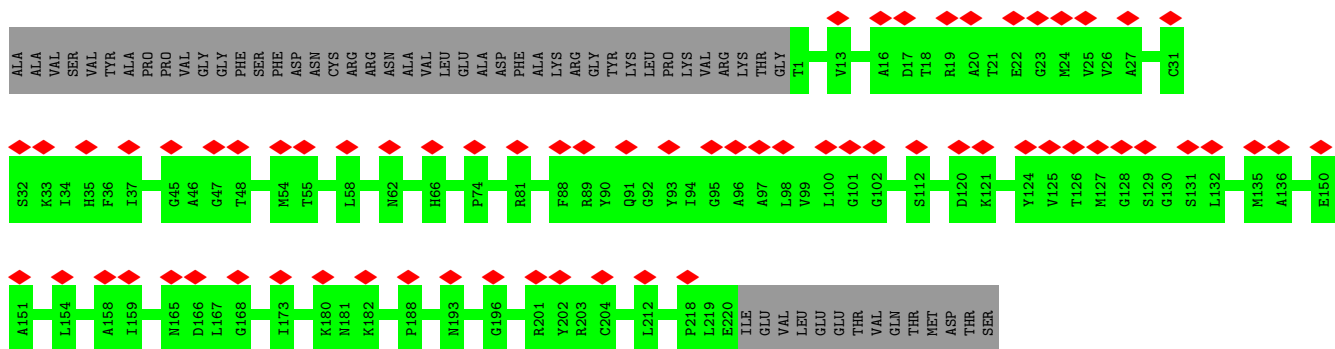
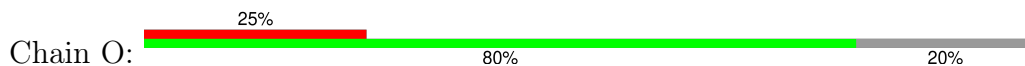
• Molecule 14: Proteasome subunit beta type-6

Chain N: 19% 80% 20%

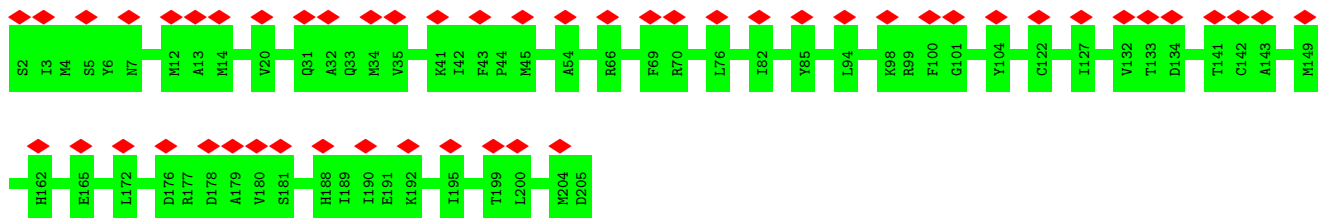




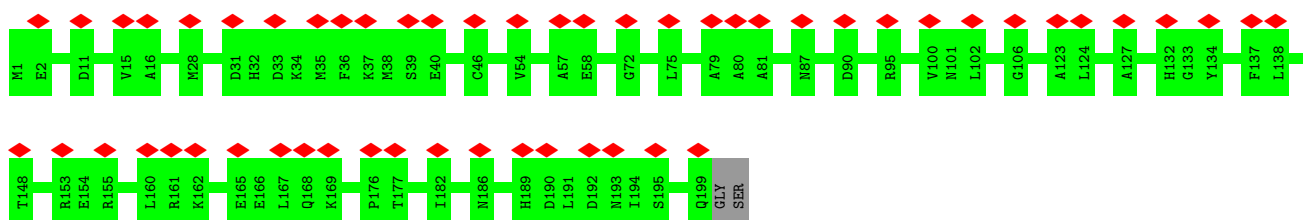
- Molecule 15: Proteasome subunit beta type-7



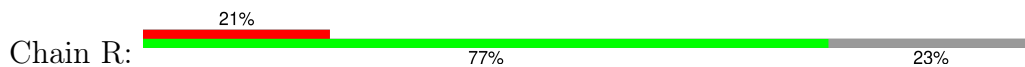
- Molecule 16: Proteasome subunit beta type-3

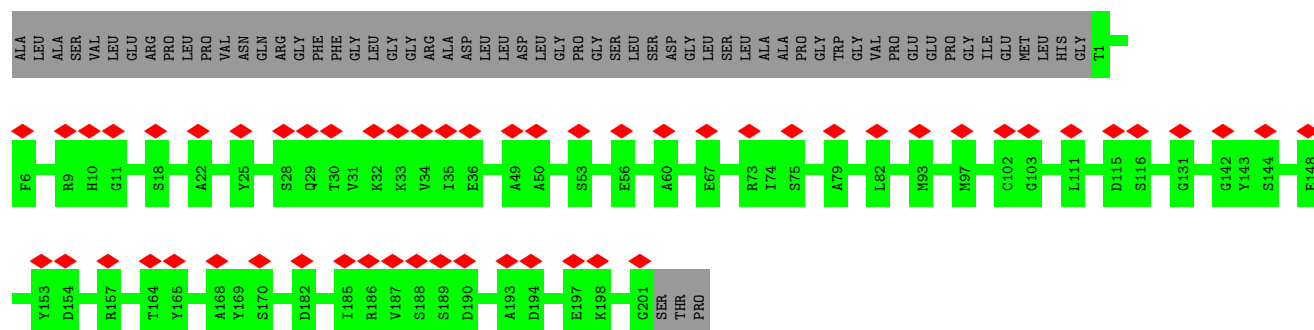


- Molecule 17: Proteasome subunit beta type-2



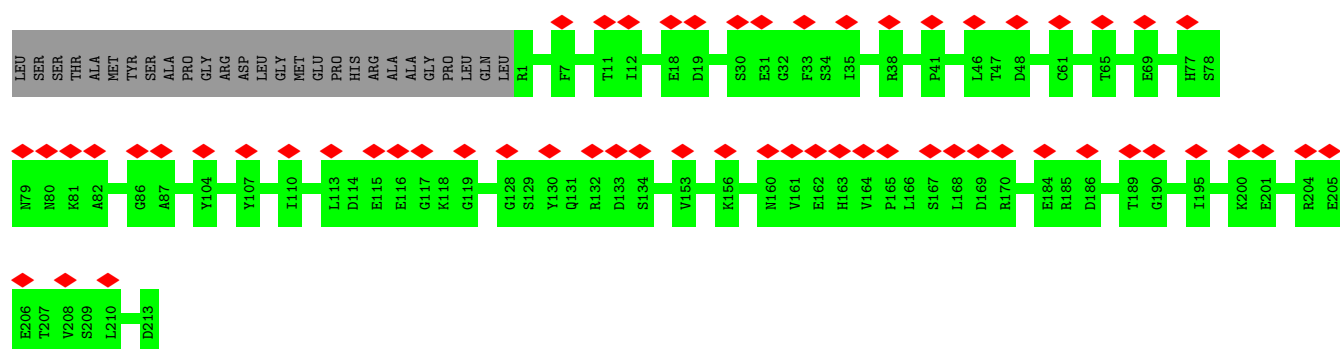
- Molecule 18: Proteasome subunit beta type-5





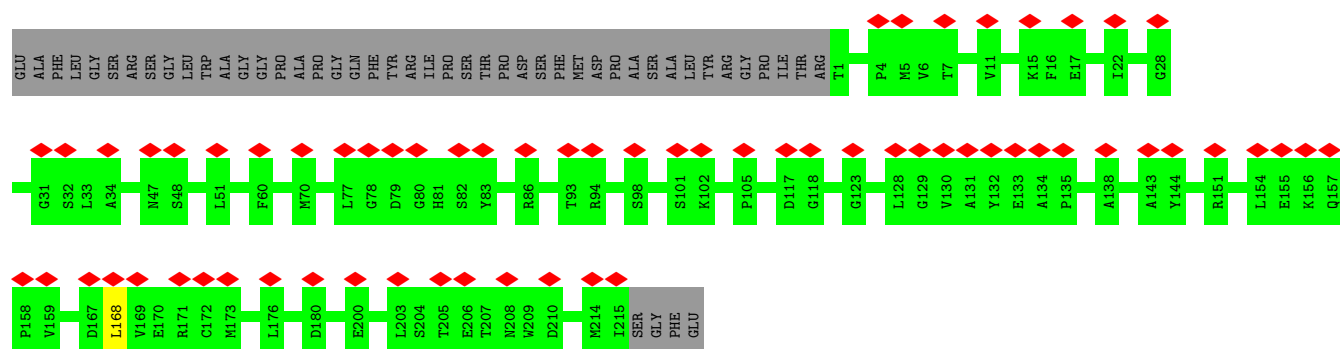
• Molecule 19: Proteasome subunit beta type-1

Chain S: 25% 89% 11%



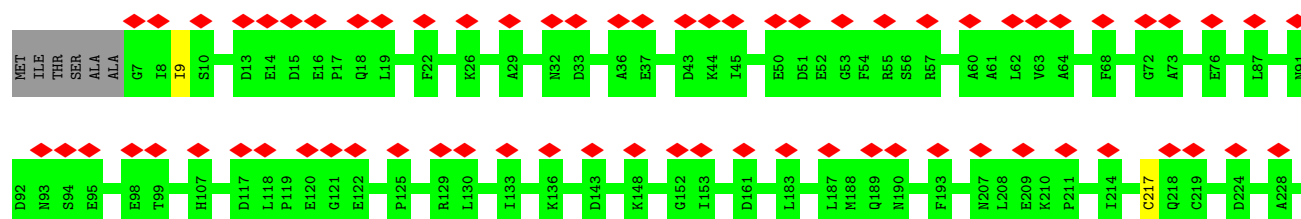
• Molecule 20: Proteasome subunit beta type-4

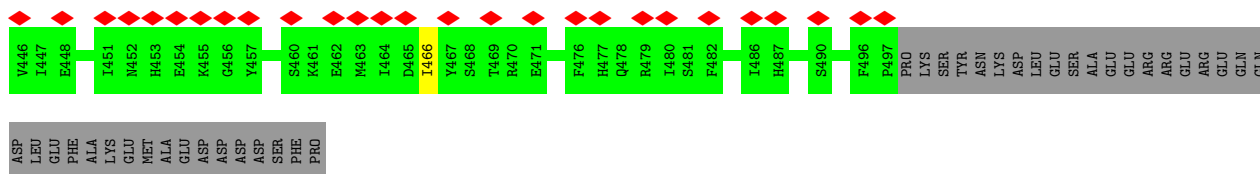
Chain T: 25% 81% 18%



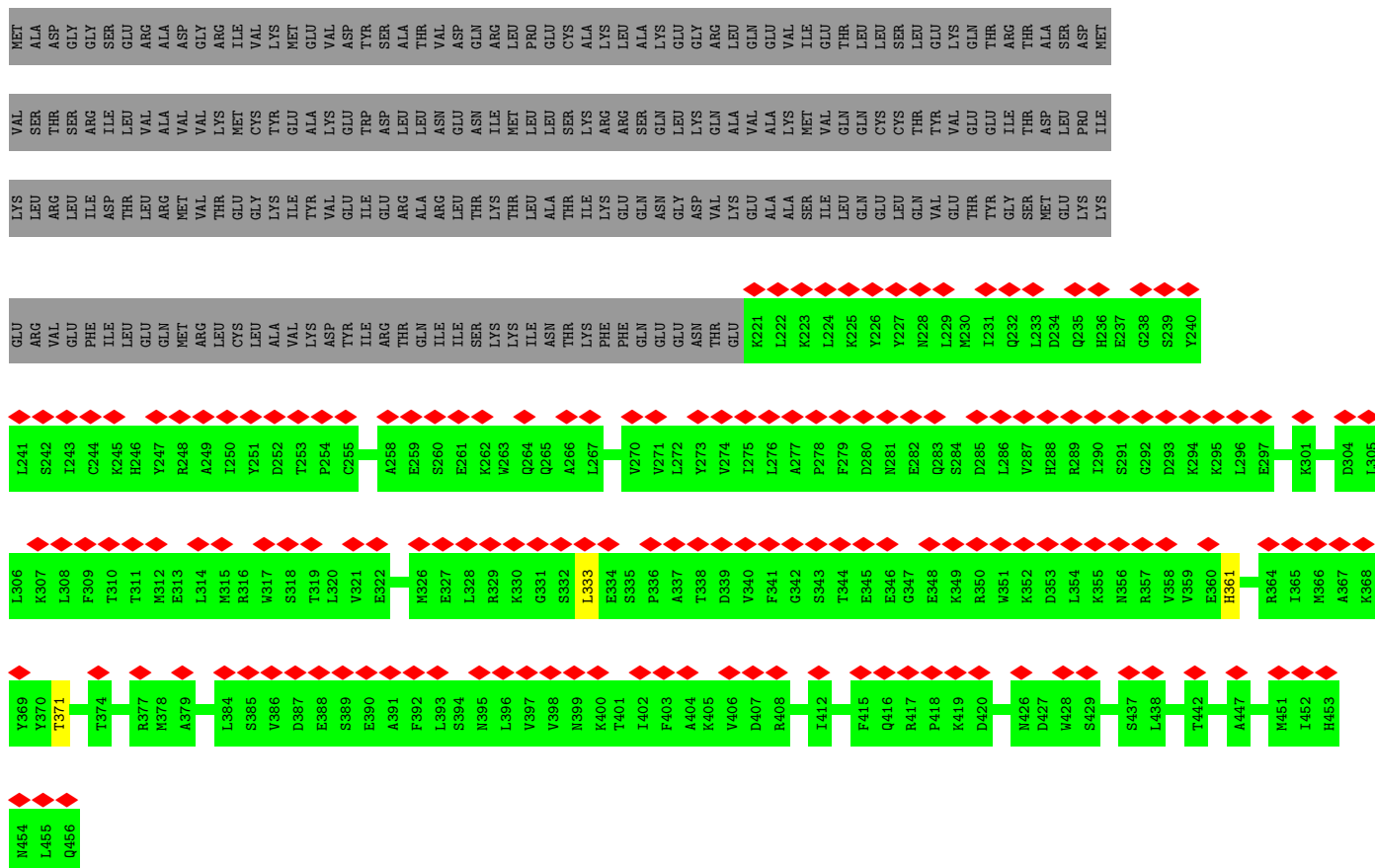
• Molecule 21: 26S proteasome non-ATPase regulatory subunit 1

Chain U: 23% 84% 15%

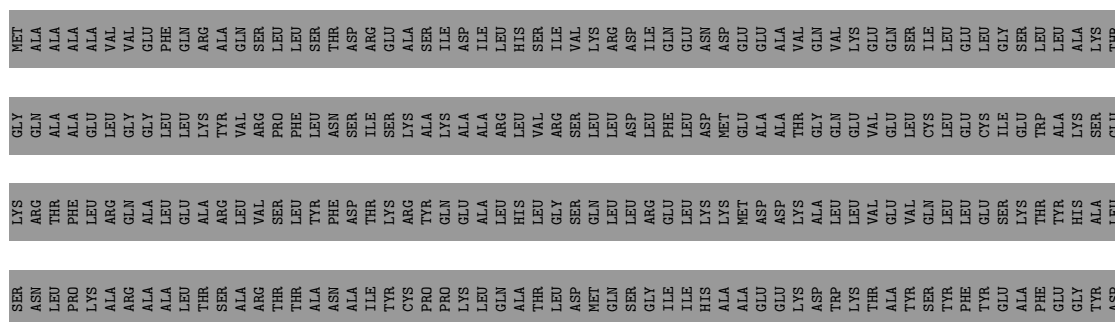


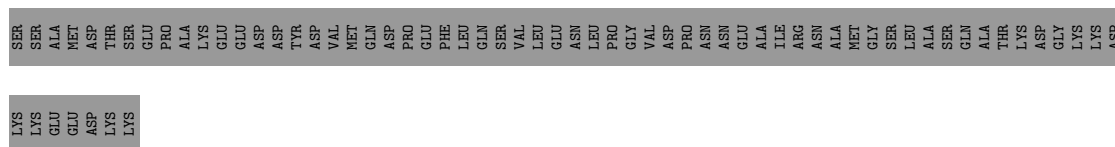


• Molecule 23: 26S proteasome non-ATPase regulatory subunit 12

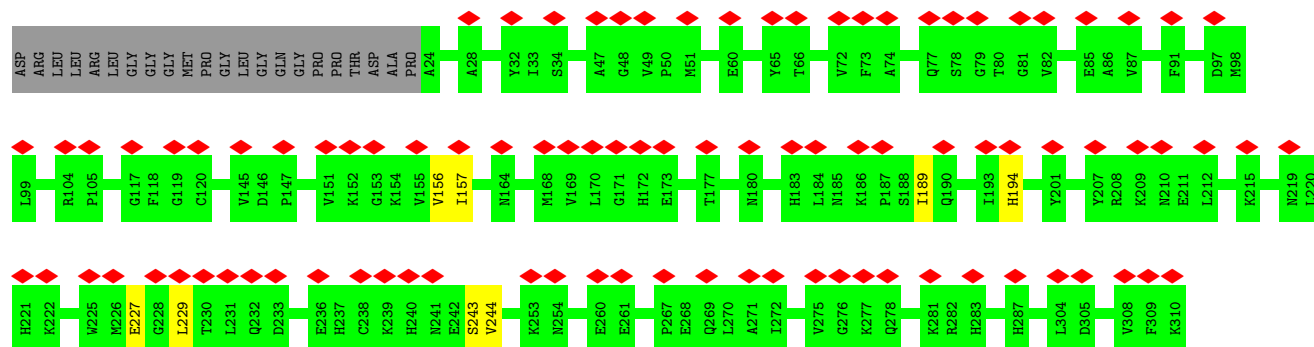
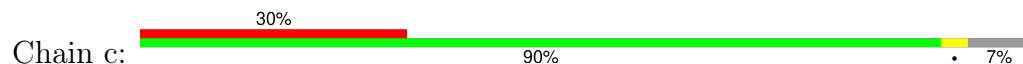


• Molecule 24: 26S proteasome non-ATPase regulatory subunit 11

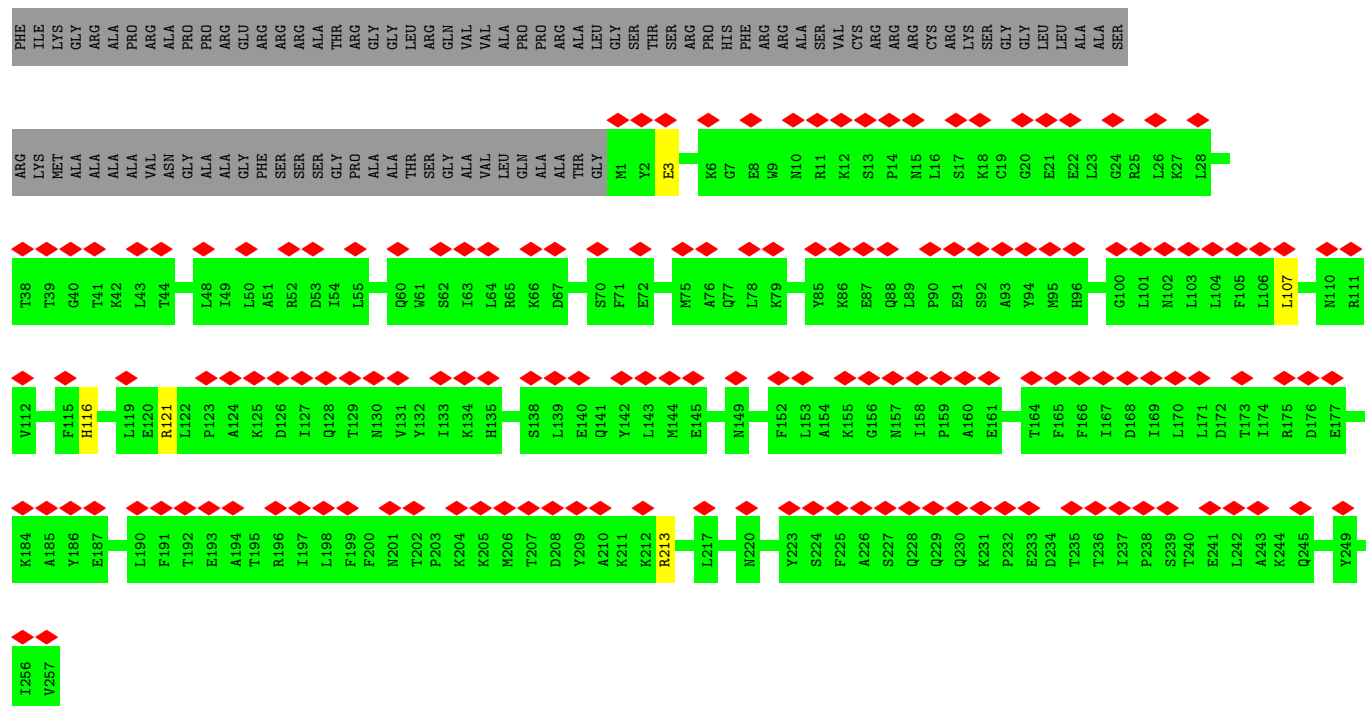




• Molecule 29: 26S proteasome non-ATPase regulatory subunit 14



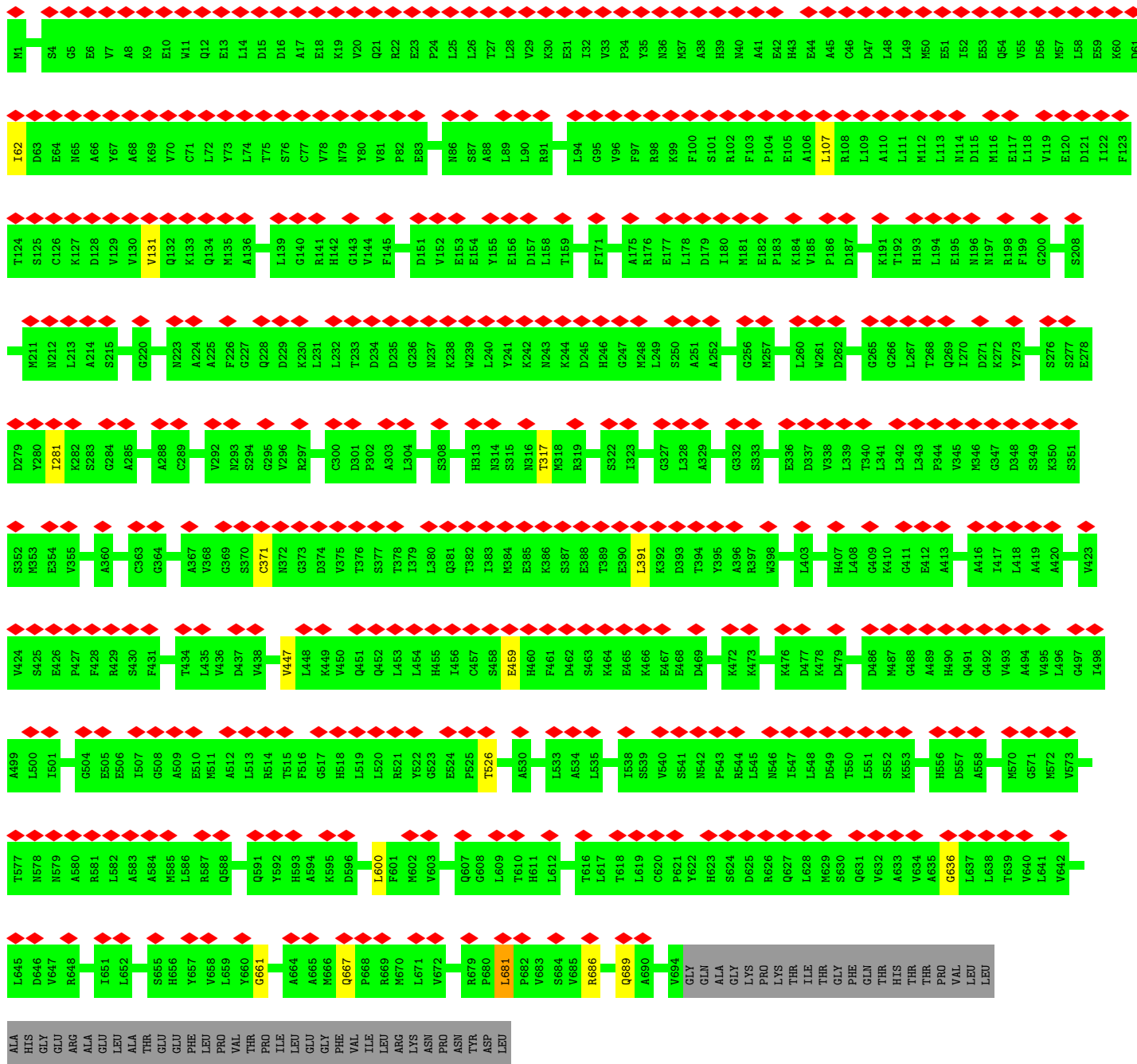
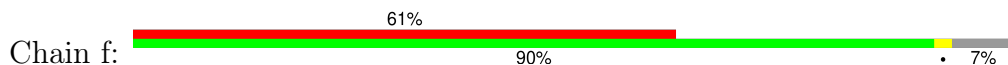
• Molecule 30: 26S proteasome non-ATPase regulatory subunit 8



• Molecule 31: 26S proteasome complex subunit DSS1



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	18443	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.005	Depositor
Minimum map value	-0.002	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0015	Depositor
Map size (Å)	309.6, 309.6, 309.6	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.86, 0.86, 0.86	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.27	0/2886	0.54	0/3899
2	B	0.27	0/2700	0.55	0/3645
3	C	0.25	0/3054	0.52	1/4107 (0.0%)
4	D	0.26	0/3090	0.53	0/4168
5	E	0.25	0/2835	0.48	0/3821
6	F	0.26	0/2903	0.54	0/3912
7	G	0.23	0/1859	0.45	0/2523
8	H	0.25	0/1743	0.46	0/2372
9	I	0.23	0/1942	0.45	0/2628
10	J	0.23	0/1728	0.44	0/2358
11	K	0.24	0/1747	0.44	0/2364
12	L	0.24	0/1885	0.44	0/2552
13	M	0.23	0/1891	0.42	0/2552
14	N	0.24	0/1454	0.42	0/1967
15	O	0.23	0/1670	0.43	0/2265
16	P	0.24	0/1614	0.41	0/2177
17	Q	0.23	0/1603	0.41	0/2174
18	R	0.23	0/1579	0.39	0/2134
19	S	0.24	0/1671	0.41	0/2253
20	T	0.25	0/1700	0.41	0/2305
21	U	0.23	0/6396	0.42	0/8646
22	V	0.25	0/3929	0.52	2/5309 (0.0%)
23	W	0.24	0/1975	0.46	0/2659
24	X	0.22	0/655	0.40	0/877
25	Y	0.24	0/3173	0.47	2/4273 (0.0%)
26	Z	1.86	6/2324 (0.3%)	0.53	0/3150
27	a	1.52	2/3052 (0.1%)	0.55	4/4130 (0.1%)
28	b	0.25	0/1478	0.43	0/2001
29	c	0.25	0/2302	0.53	2/3110 (0.1%)
30	d	0.25	0/2162	0.51	0/2919
31	e	0.24	0/198	0.53	0/258
32	f	0.27	1/5413 (0.0%)	0.53	3/7317 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.51	9/74611 (0.0%)	0.48	14/100825 (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	B	0	2
3	C	0	1
5	E	0	1
6	F	0	2
21	U	0	3
22	V	0	2
25	Y	0	1
30	d	0	1
32	f	0	2
All	All	0	15

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	a	215	GLU	CG-CD	82.57	2.75	1.51
26	Z	228	TYR	CD2-CE2	46.09	2.08	1.39
26	Z	228	TYR	CD1-CE1	45.24	2.07	1.39
26	Z	228	TYR	CE1-CZ	34.72	1.83	1.38
26	Z	228	TYR	CE2-CZ	33.47	1.82	1.38

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	a	215	GLU	OE1-CD-OE2	-19.13	100.35	123.30
27	a	215	GLU	CG-CD-OE1	6.35	131.00	118.30
29	c	243	SER	C-N-CA	6.19	137.17	121.70
27	a	215	GLU	CB-CG-CD	6.17	130.86	114.20
32	f	459	GLU	N-CA-C	6.13	127.56	111.00

There are no chirality outliers.

5 of 15 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	133	VAL	Peptide
2	B	264	PRO	Peptide
3	C	171	HIS	Peptide
5	E	292	PRO	Peptide
6	F	87	PRO	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	359/433 (83%)	304 (85%)	53 (15%)	2 (1%)	22	60
2	B	339/440 (77%)	298 (88%)	38 (11%)	3 (1%)	14	52
3	C	382/398 (96%)	317 (83%)	62 (16%)	3 (1%)	16	55
4	D	378/418 (90%)	328 (87%)	49 (13%)	1 (0%)	37	73
5	E	351/403 (87%)	299 (85%)	51 (14%)	1 (0%)	37	73
6	F	362/439 (82%)	316 (87%)	45 (12%)	1 (0%)	37	73
7	G	238/245 (97%)	221 (93%)	16 (7%)	1 (0%)	30	68
8	H	230/233 (99%)	210 (91%)	19 (8%)	1 (0%)	30	68
9	I	248/260 (95%)	230 (93%)	18 (7%)	0	100	100
10	J	237/247 (96%)	221 (93%)	15 (6%)	1 (0%)	30	68
11	K	224/240 (93%)	203 (91%)	20 (9%)	1 (0%)	30	68
12	L	236/268 (88%)	222 (94%)	14 (6%)	0	100	100
13	M	238/254 (94%)	218 (92%)	20 (8%)	0	100	100
14	N	189/238 (79%)	175 (93%)	14 (7%)	0	100	100
15	O	218/276 (79%)	209 (96%)	9 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	P	202/204 (99%)	188 (93%)	14 (7%)	0	100	100
17	Q	197/201 (98%)	183 (93%)	14 (7%)	0	100	100
18	R	199/262 (76%)	190 (96%)	9 (4%)	0	100	100
19	S	211/240 (88%)	199 (94%)	12 (6%)	0	100	100
20	T	213/263 (81%)	204 (96%)	9 (4%)	0	100	100
21	U	798/953 (84%)	729 (91%)	67 (8%)	2 (0%)	37	73
22	V	478/533 (90%)	416 (87%)	60 (13%)	2 (0%)	30	68
23	W	234/456 (51%)	213 (91%)	21 (9%)	0	100	100
24	X	79/422 (19%)	75 (95%)	4 (5%)	0	100	100
25	Y	376/389 (97%)	336 (89%)	38 (10%)	2 (0%)	25	64
26	Z	284/324 (88%)	251 (88%)	32 (11%)	1 (0%)	30	68
27	a	369/376 (98%)	340 (92%)	27 (7%)	2 (0%)	25	64
28	b	189/377 (50%)	178 (94%)	11 (6%)	0	100	100
29	c	285/309 (92%)	242 (85%)	39 (14%)	4 (1%)	9	41
30	d	255/349 (73%)	219 (86%)	34 (13%)	2 (1%)	16	55
31	e	20/70 (29%)	16 (80%)	4 (20%)	0	100	100
32	f	686/749 (92%)	574 (84%)	108 (16%)	4 (1%)	22	60
All	All	9304/11269 (83%)	8324 (90%)	946 (10%)	34 (0%)	32	68

5 of 34 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	G	111	VAL
11	K	12	VAL
21	U	364	VAL
25	Y	350	VAL
29	c	244	VAL

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	308/372 (83%)	305 (99%)	3 (1%)	73	82
2	B	298/385 (77%)	294 (99%)	4 (1%)	65	77
3	C	332/346 (96%)	324 (98%)	8 (2%)	44	62
4	D	333/366 (91%)	329 (99%)	4 (1%)	67	79
5	E	308/353 (87%)	306 (99%)	2 (1%)	84	88
6	F	312/379 (82%)	303 (97%)	9 (3%)	37	56
7	G	193/209 (92%)	192 (100%)	1 (0%)	86	89
8	H	164/190 (86%)	162 (99%)	2 (1%)	67	79
9	I	193/220 (88%)	193 (100%)	0	100	100
10	J	152/210 (72%)	151 (99%)	1 (1%)	81	87
11	K	186/202 (92%)	185 (100%)	1 (0%)	86	89
12	L	198/229 (86%)	197 (100%)	1 (0%)	86	89
13	M	192/211 (91%)	191 (100%)	1 (0%)	86	89
14	N	148/180 (82%)	148 (100%)	0	100	100
15	O	177/227 (78%)	177 (100%)	0	100	100
16	P	172/173 (99%)	172 (100%)	0	100	100
17	Q	164/171 (96%)	164 (100%)	0	100	100
18	R	153/201 (76%)	153 (100%)	0	100	100
19	S	174/198 (88%)	174 (100%)	0	100	100
20	T	175/214 (82%)	174 (99%)	1 (1%)	84	88
21	U	685/816 (84%)	679 (99%)	6 (1%)	75	83
22	V	414/459 (90%)	408 (99%)	6 (1%)	62	75
23	W	218/416 (52%)	215 (99%)	3 (1%)	62	75
24	X	74/362 (20%)	74 (100%)	0	100	100
25	Y	334/344 (97%)	330 (99%)	4 (1%)	67	79
26	Z	257/295 (87%)	254 (99%)	3 (1%)	67	79
27	a	333/336 (99%)	333 (100%)	0	100	100
28	b	167/312 (54%)	166 (99%)	1 (1%)	84	88
29	c	252/267 (94%)	249 (99%)	3 (1%)	67	79
30	d	231/293 (79%)	229 (99%)	2 (1%)	75	83
31	e	22/63 (35%)	22 (100%)	0	100	100
32	f	582/628 (93%)	574 (99%)	8 (1%)	62	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	7901/9627 (82%)	7827 (99%)	74 (1%)	74 83

5 of 74 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
26	Z	133	LEU
32	f	600	LEU
26	Z	191	ILE
30	d	116	HIS
6	F	161	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 61 such sidechains are listed below:

Mol	Chain	Res	Type
7	G	123	GLN
29	c	287	HIS
21	U	685	GLN
29	c	241	ASN
32	f	269	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 7 ligands modelled in this entry, 1 is 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
33	ADP	D	501	-	24,29,29	0.91	1 (4%)	29,45,45	1.18	2 (6%)
33	ADP	B	501	-	24,29,29	0.97	1 (4%)	29,45,45	1.35	4 (13%)
33	ADP	E	401	-	24,29,29	0.94	1 (4%)	29,45,45	1.65	4 (13%)
33	ADP	A	501	-	24,29,29	0.93	1 (4%)	29,45,45	1.17	2 (6%)
33	ADP	C	501	-	24,29,29	0.93	1 (4%)	29,45,45	1.20	2 (6%)
33	ADP	F	501	-	24,29,29	1.00	2 (8%)	29,45,45	1.34	4 (13%)

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
33	ADP	D	501	-	-	2/12/32/32	0/3/3/3
33	ADP	B	501	-	-	5/12/32/32	0/3/3/3
33	ADP	E	401	-	-	6/12/32/32	0/3/3/3
33	ADP	A	501	-	-	3/12/32/32	0/3/3/3
33	ADP	C	501	-	-	4/12/32/32	0/3/3/3
33	ADP	F	501	-	-	7/12/32/32	0/3/3/3

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	E	401	ADP	O4'-C1'	2.42	1.44	1.40
33	B	501	ADP	PA-O3A	2.41	1.62	1.59
33	F	501	ADP	O4'-C1'	2.37	1.44	1.40
33	F	501	ADP	PA-O3A	2.24	1.61	1.59
33	A	501	ADP	O4'-C1'	2.22	1.43	1.40

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	E	401	ADP	O4'-C1'-N9	5.03	115.42	108.75
33	E	401	ADP	N3-C2-N1	-3.75	123.59	128.67
33	B	501	ADP	N3-C2-N1	-3.73	123.61	128.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	D	501	ADP	N3-C2-N1	-3.66	123.71	128.67
33	F	501	ADP	N3-C2-N1	-3.65	123.72	128.67

There are no chirality outliers.

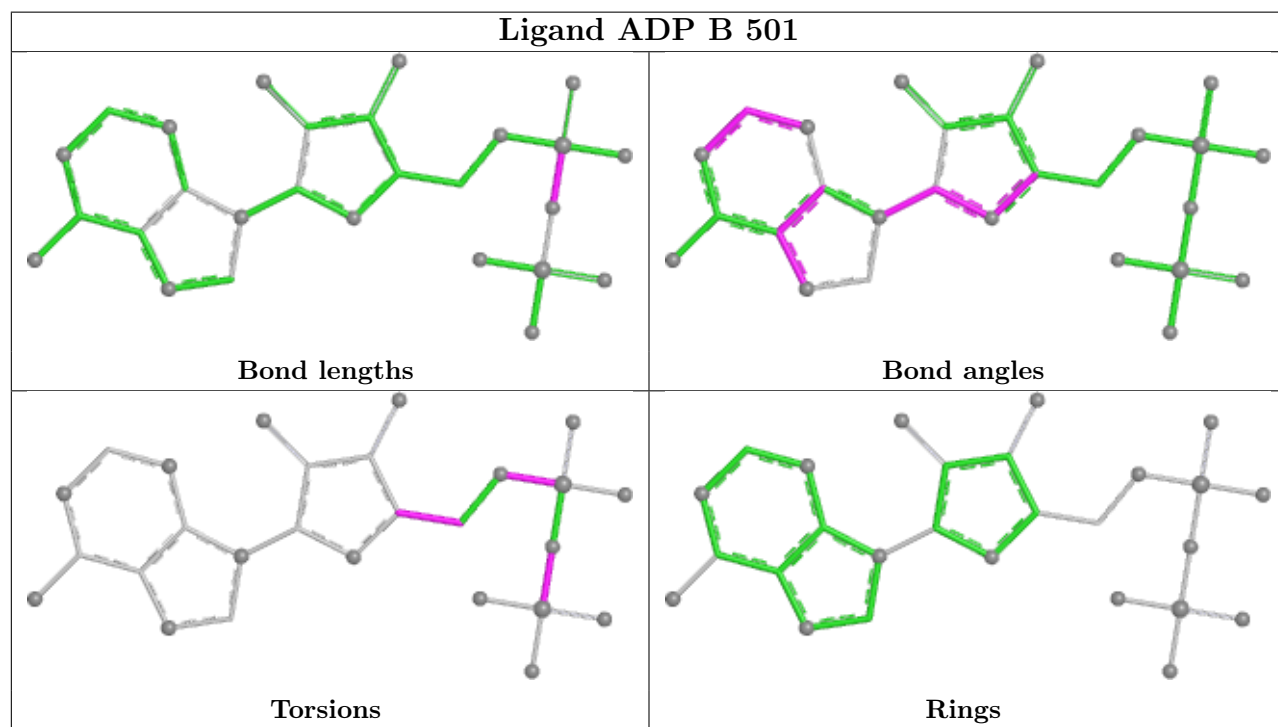
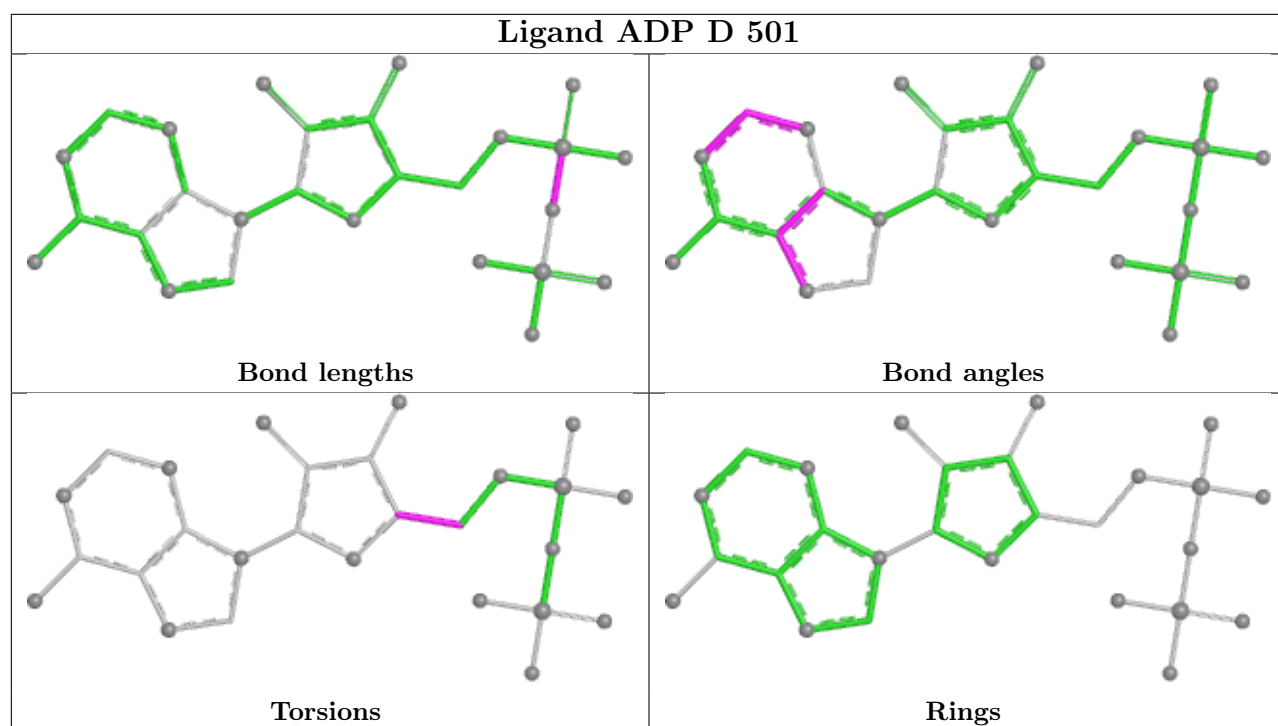
5 of 27 torsion outliers are listed below:

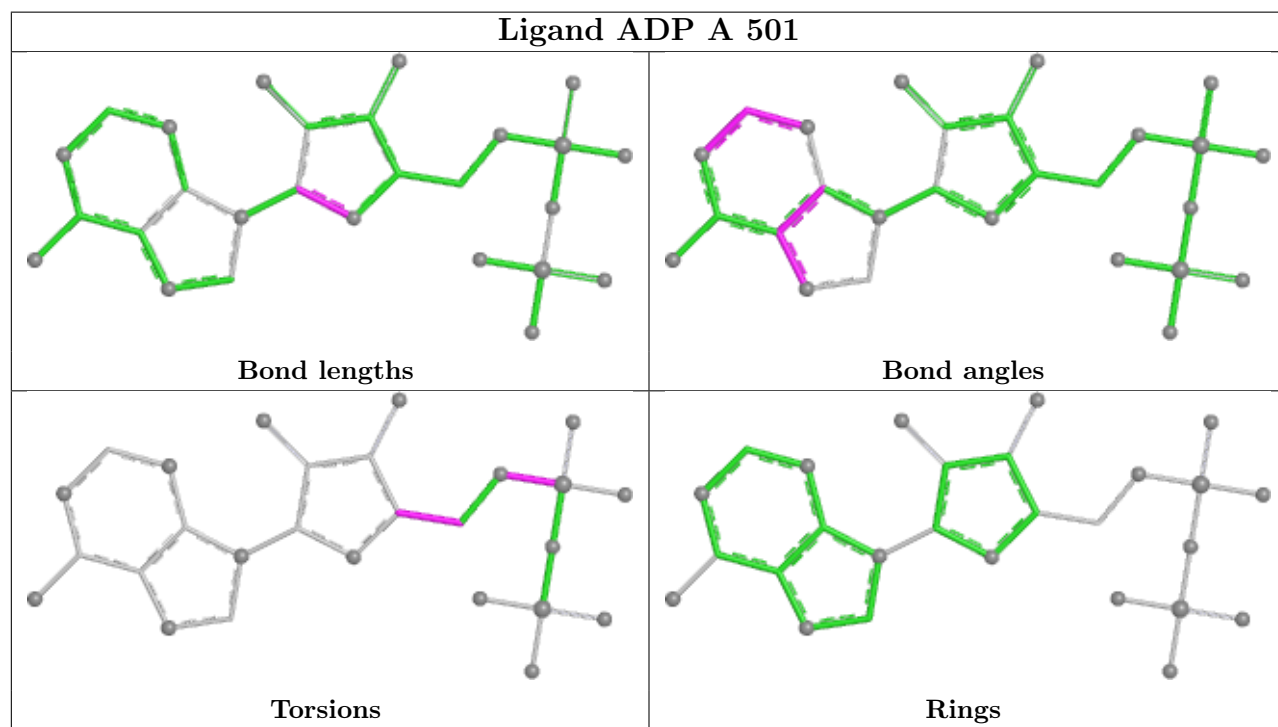
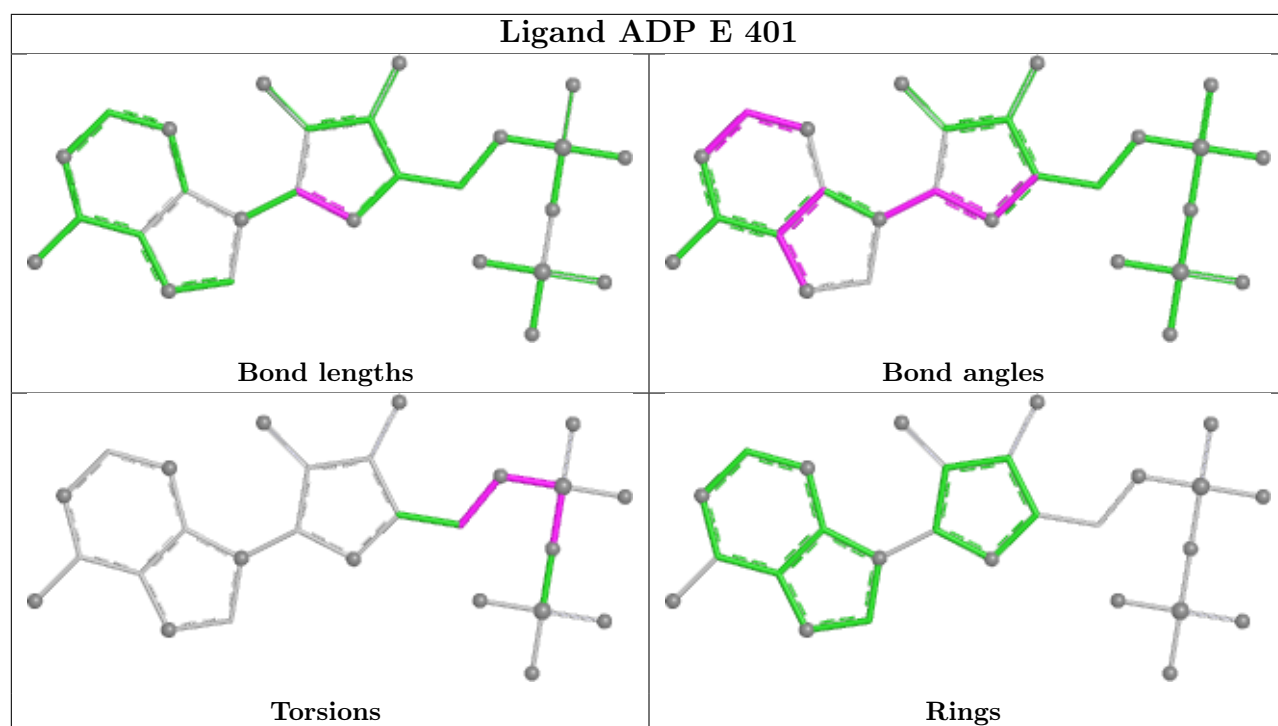
Mol	Chain	Res	Type	Atoms
33	B	501	ADP	PA-O3A-PB-O3B
33	B	501	ADP	C5'-O5'-PA-O3A
33	C	501	ADP	C5'-O5'-PA-O1A
33	E	401	ADP	C5'-O5'-PA-O1A
33	E	401	ADP	C5'-O5'-PA-O3A

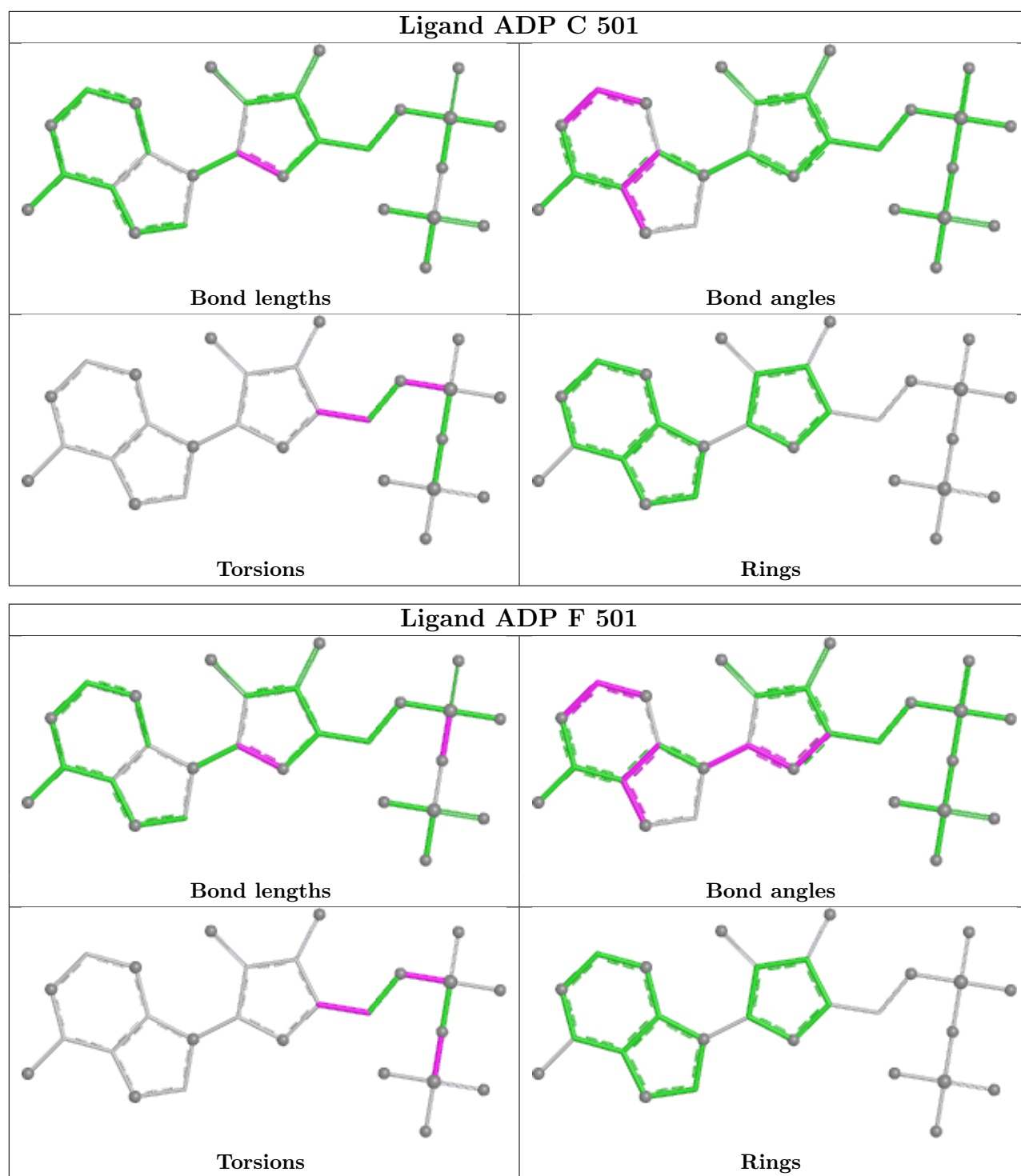
There are no ring outliers.

No monomer is involved in short contacts.

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







5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
32	f	3
27	a	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	f	110:ALA	C	111:LEU	N	8.67
1	f	79:ASN	C	80:TYR	N	7.26
1	f	348:ASP	C	349:SER	N	6.44
1	a	341:LEU	C	342:ASP	N	5.77

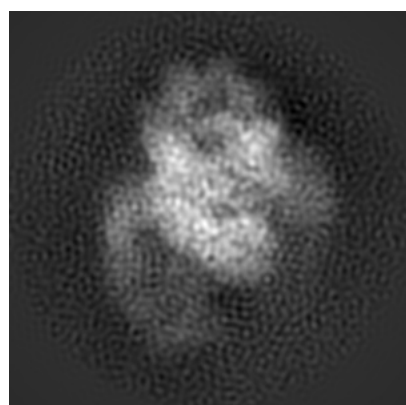
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8335. These allow visual inspection of the internal detail of the map and identification of artifacts.

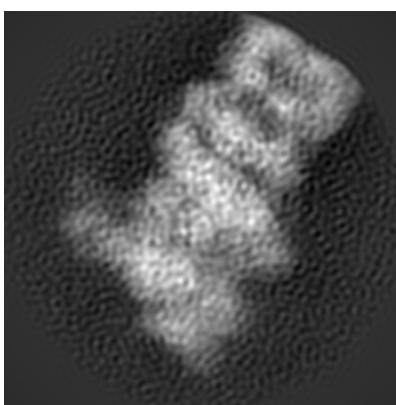
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

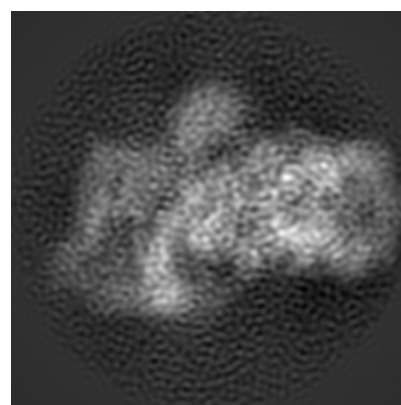
6.1.1 Primary map



X



Y

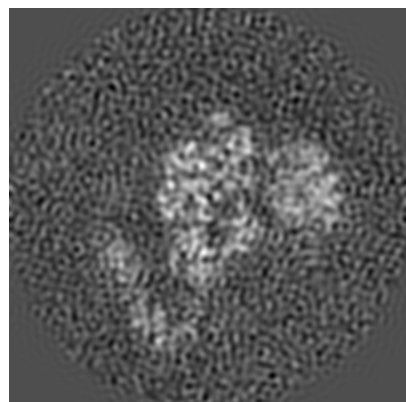


Z

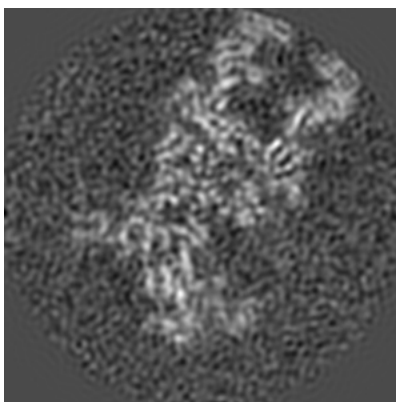
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

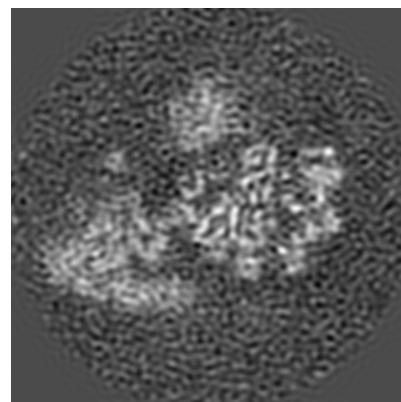
6.2.1 Primary map



X Index: 180



Y Index: 180

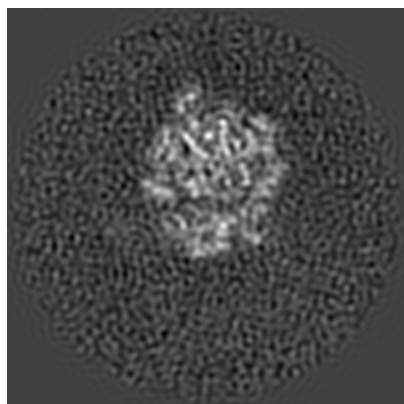


Z Index: 180

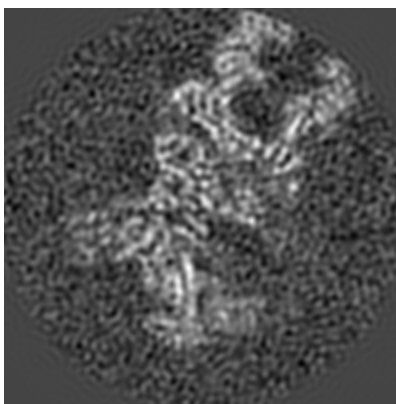
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

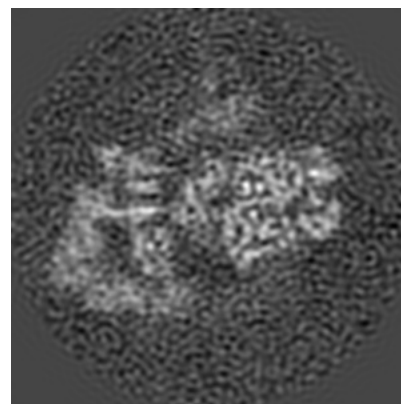
6.3.1 Primary map



X Index: 237



Y Index: 177

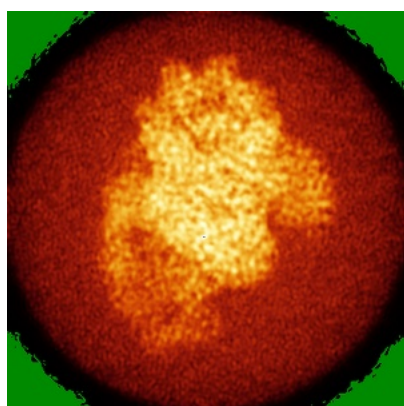


Z Index: 167

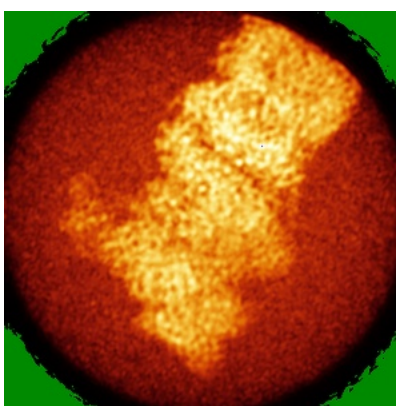
The images above show the largest variance slices of the map in three orthogonal directions.

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

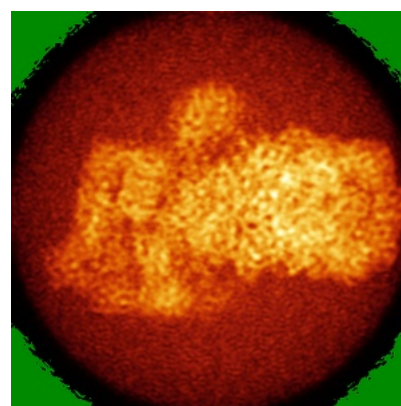
6.4.1 Primary map



X



Y

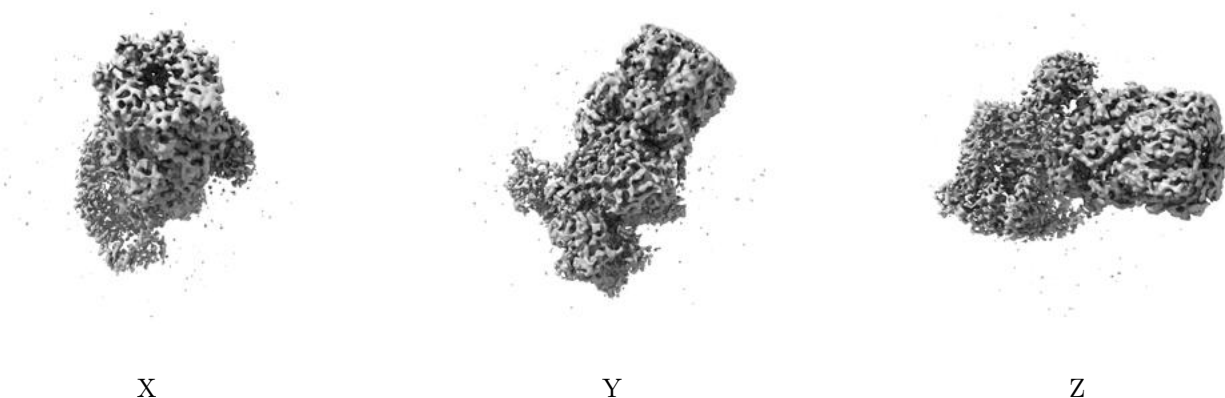


Z

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 0.0015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

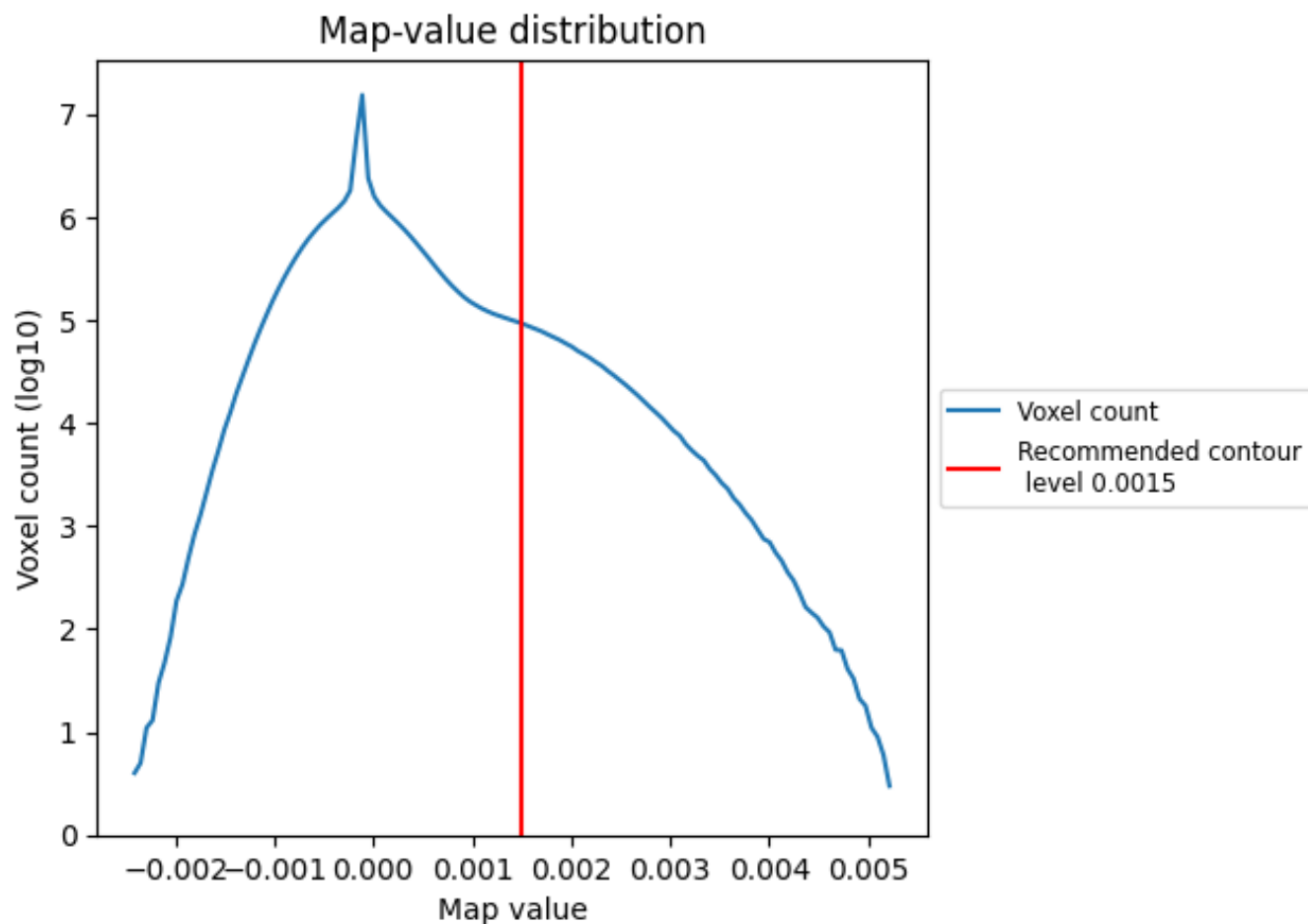
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

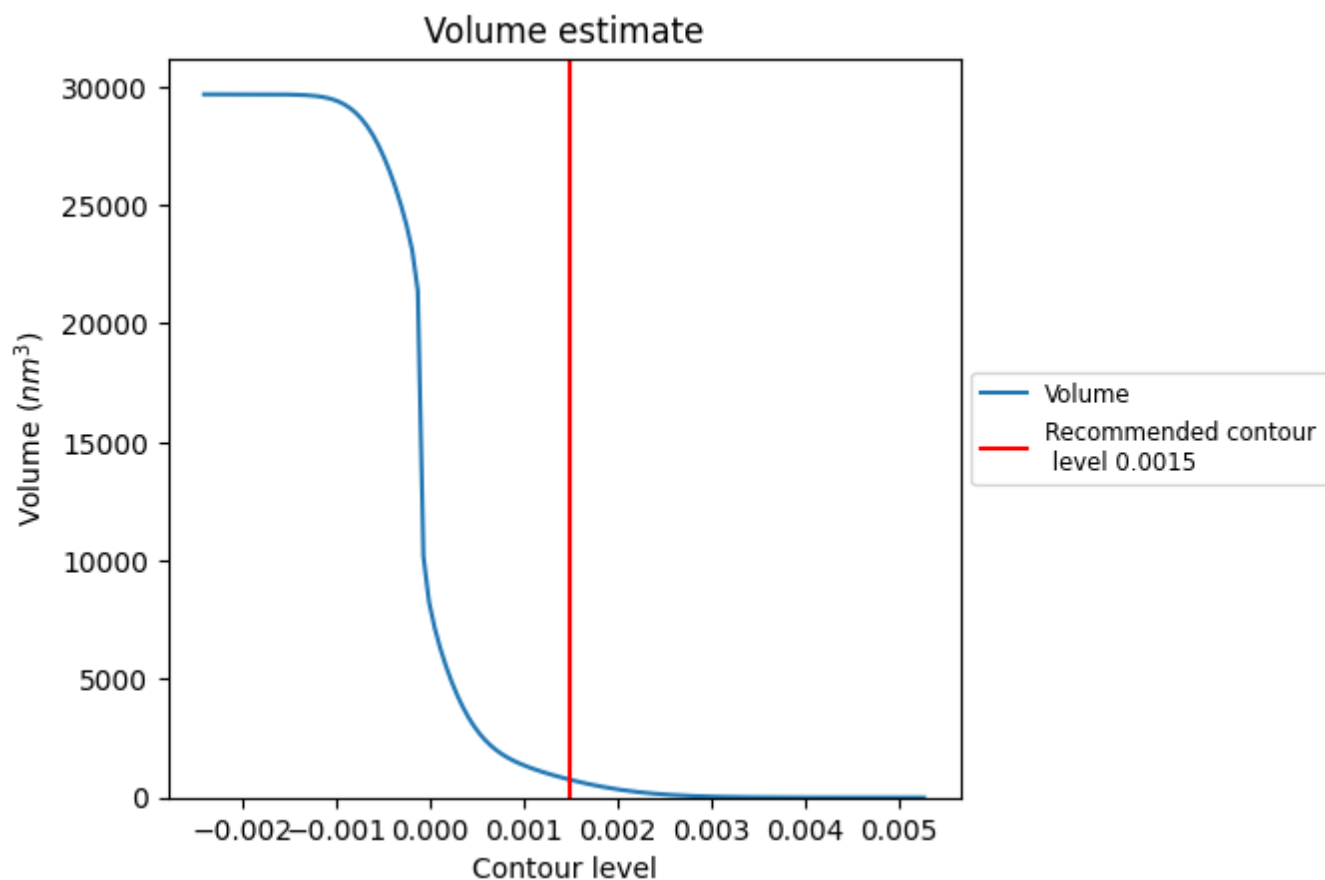
This section contains the results of statistical analysis of the map.

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.

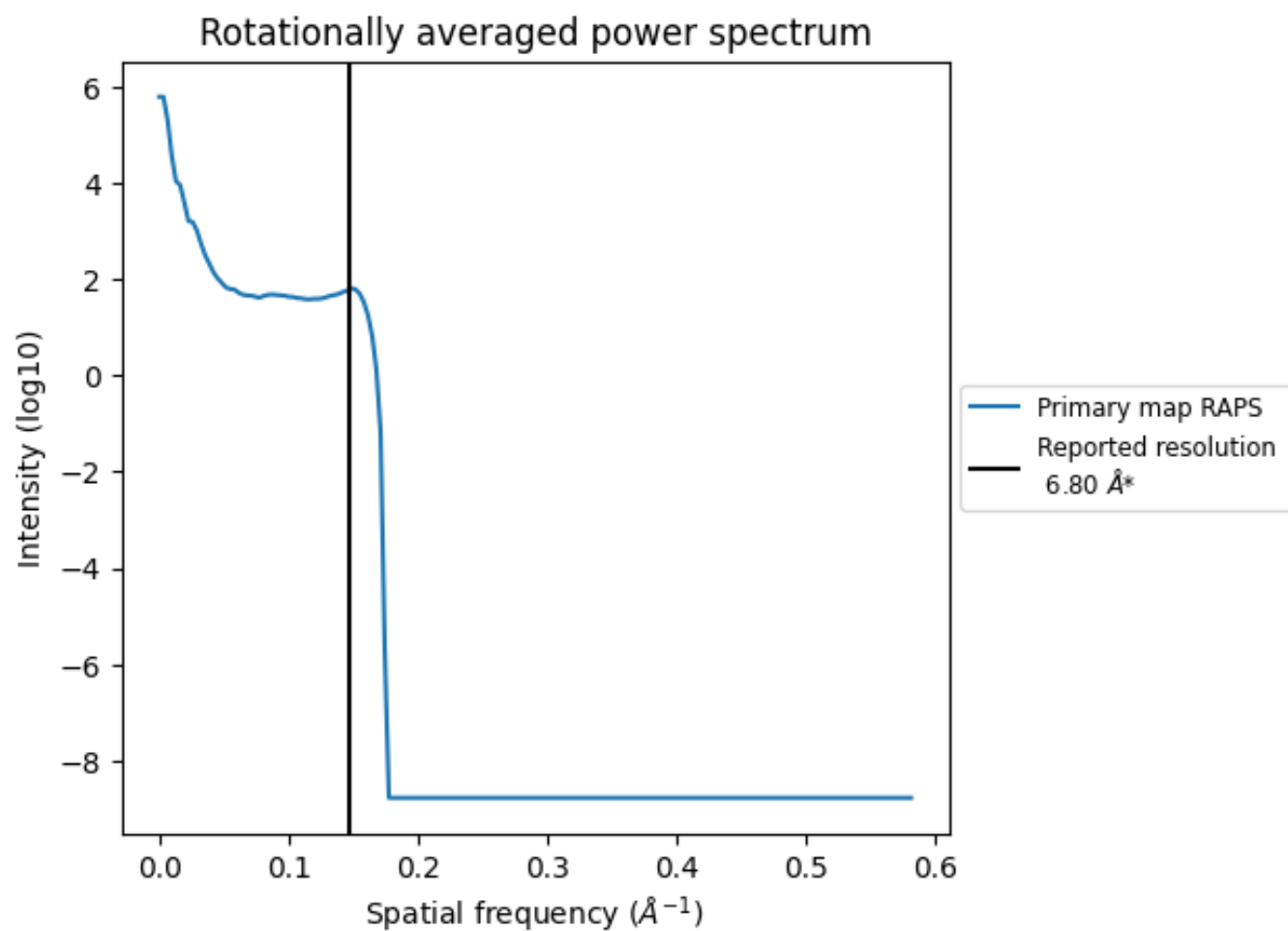
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 749 nm³; this corresponds to an approximate mass of 677 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 0.147 Å⁻¹

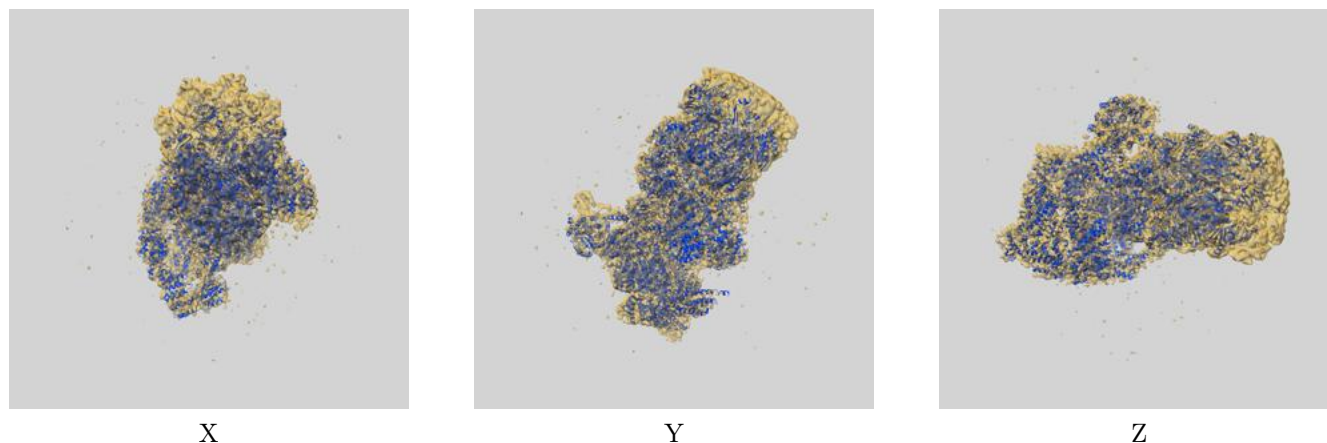
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

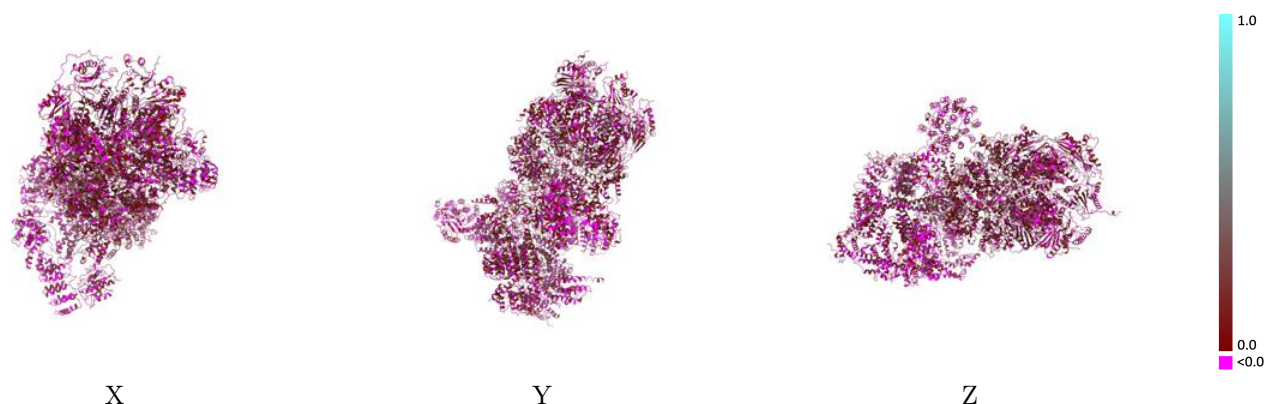
This section contains information regarding the fit between EMDB map EMD-8335 and PDB model 5T0H. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

9.1 Map-model overlay [i](#)



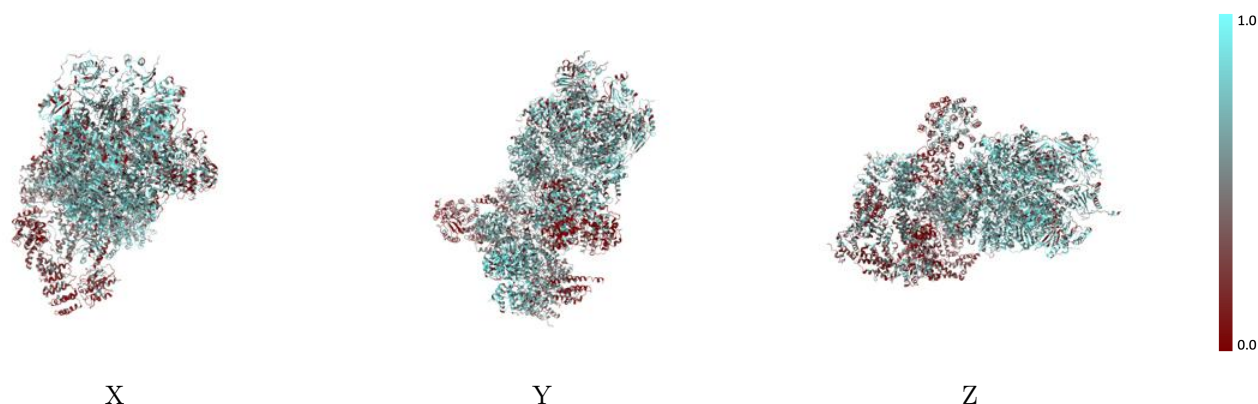
The images above show the 3D surface view of the map at the recommended contour level 0.0015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



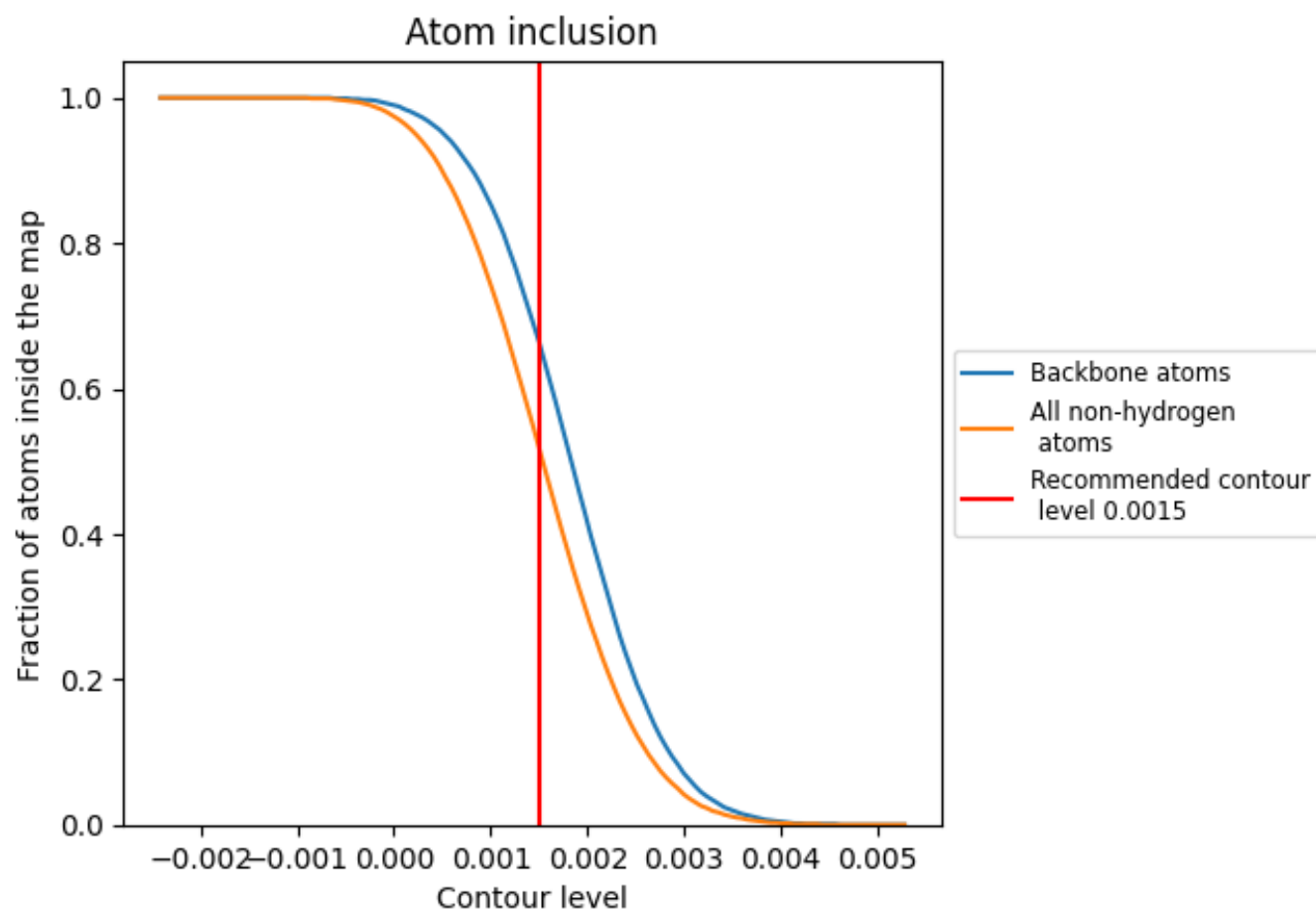
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0015).



































































9.4 Atom inclusion [i](#)



At the recommended contour level, 66% of all backbone atoms, 52% 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 (0.0015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5180	 0.0940
A	 0.6000	 0.1350
B	 0.5950	 0.1460
C	 0.5700	 0.1290
D	 0.6380	 0.1430
E	 0.6230	 0.1420
F	 0.5990	 0.1360
G	 0.6700	 0.1350
H	 0.6730	 0.1420
I	 0.6320	 0.1350
J	 0.6450	 0.1320
K	 0.5930	 0.1010
L	 0.6170	 0.0950
M	 0.6510	 0.1320
N	 0.6170	 0.0820
O	 0.5860	 0.0800
P	 0.6040	 0.0920
Q	 0.6100	 0.1010
R	 0.6060	 0.1100
S	 0.5770	 0.1030
T	 0.5710	 0.0900
U	 0.6110	 0.1040
V	 0.3610	 0.0500
W	 0.2710	 0.0440
X	 0.3850	 0.0340
Y	 0.3140	 0.0350
Z	 0.5040	 0.0940
a	 0.2540	 0.0280
b	 0.1900	 0.0580
c	 0.5310	 0.0940
d	 0.3390	 0.0440
e	 0.5310	 0.0880
f	 0.3230	 0.0270

