



wwPDB EM Validation Summary Report ⓘ

Jun 3, 2025 – 03:39 PM EDT

PDB ID : 9BW4 / pdb_00009bw4
EMDB ID : EMD-44952
Title : TXNL1-bound proteasome
Authors : Gao, J.; Yip, M.C.J.; Shao, S.
Deposited on : 2024-05-20
Resolution : 3.30 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.dev118
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0rc1
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) : 2.43.1

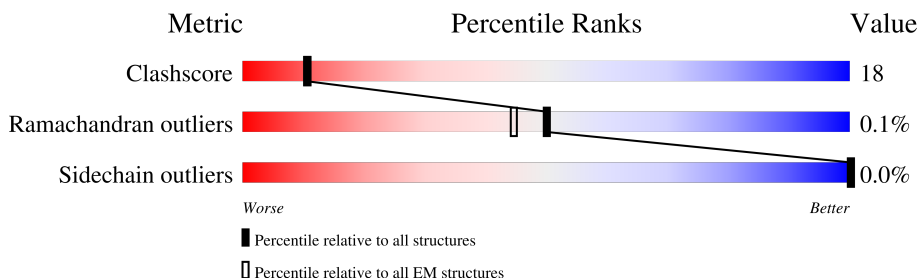
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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.





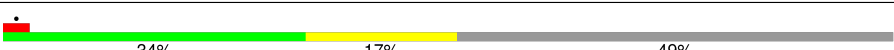
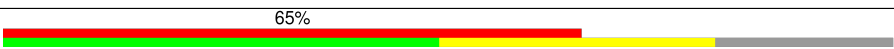
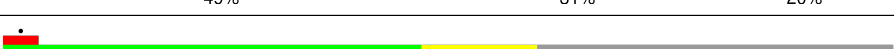
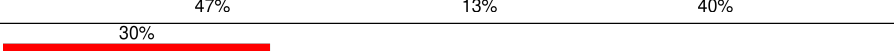
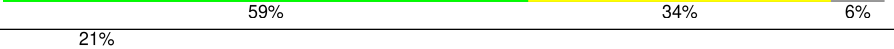





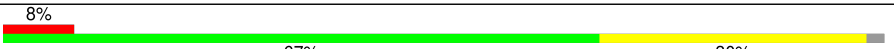


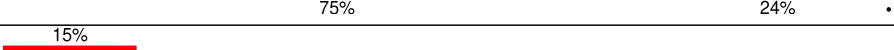






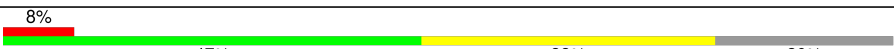

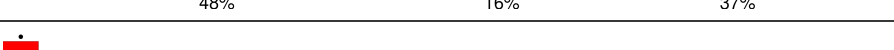
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	U	953	
2	V	534	
3	W	456	
4	X	422	
5	Y	389	
6	Z	324	
7	a	376	
8	b	377	

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Mol	Chain	Length	Quality of chain
9	c	310	
10	d	350	
11	e	70	
12	f	908	
13	x	289	
14	A	433	
15	B	440	
16	C	406	
17	D	418	
18	E	389	
19	F	439	
20	G	246	
21	H	234	
22	I	261	
23	J	248	
24	K	241	
25	L	263	
26	M	255	
27	N	239	
27	n	239	
28	O	277	
28	o	277	
29	P	205	
29	p	205	
30	Q	201	

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Mol	Chain	Length	Quality of chain
30	q	201	
31	R	263	
31	r	263	
32	S	241	
32	s	241	
33	T	264	
33	t	264	

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 90418 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	U	857	Total	C	N	O	S	0	0
			6685	4243	1136	1261	45		

- Molecule 2 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	V	421	Total	C	N	O	S	0	0
			3434	2192	613	617	12		

- Molecule 3 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	W	424	Total	C	N	O	S	0	0
			3465	2194	595	653	23		

- Molecule 4 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	X	421	Total	C	N	O	S	0	0
			3327	2111	566	638	12		

- Molecule 5 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

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

- Molecule 6 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Z	287	Total	C	N	O	S	0	0
			2290	1462	394	429	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	a	375	Total	C	N	O	S	0	0
			3012	1921	513	563	15		

- Molecule 8 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	b	191	Total	C	N	O	S	0	0
			1459	910	261	281	7		

- Molecule 9 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	c	277	Total	C	N	O	S	0	0
			2184	1382	375	408	19		

- Molecule 10 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	d	258	Total	C	N	O	S	0	0
			2099	1362	341	387	9		

- Molecule 11 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	e	36	Total	C	N	O	0	0
			314	193	50	71		

- Molecule 12 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	f	727	Total	C	N	O	S	0	0
			5633	3561	958	1069	45		

- Molecule 13 is a protein called Thioredoxin-like protein 1.

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

- Molecule 14 is a protein called 26S proteasome regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	A	405	Total	C	N	O	S	0	0
			3183	2002	561	602	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	B	390	Total	C	N	O	S	0	0
			3065	1931	521	598	15		

- Molecule 16 is a protein called 26S protease regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	C	389	Total	C	N	O	S	0	0
			3071	1932	550	571	18		

- Molecule 17 is a protein called 26S proteasome regulatory subunit 6B.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	D	373	Total	C	N	O	S	0	0
			2990	1894	517	567	12		

- Molecule 18 is a protein called 26S protease regulatory subunit 10B.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	E	296	Total	C	N	O	S	0	0
			2353	1481	414	442	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	F	368	Total	C	N	O	S	0	0
			2881	1821	496	547	17		

- Molecule 20 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	G	241	Total	C	N	O	S	0	0
			1885	1196	314	362	13		

- Molecule 21 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	H	233	Total	C	N	O	S	0	0
			1818	1161	308	343	6		

- Molecule 22 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	I	258	Total	C	N	O	S	0	0
			2044	1290	350	394	10		

- Molecule 23 is a protein called Proteasome subunit alpha type-7.

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

- Molecule 24 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	K	232	Total	C	N	O	S	0	0
			1778	1116	295	356	11		

- Molecule 25 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	L	236	Total	C	N	O	S	0	0
			1857	1162	334	350	11		

- Molecule 26 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	M	245	Total	C	N	O	S	0	0
			1920	1214	326	369	11		

- Molecule 27 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	N	198	Total	C	N	O	S	0	0
			1487	931	254	290	12		
27	n	179	Total	C	N	O	S	0	0
			1336	836	230	258	12		

- Molecule 28 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	O	221	Total	C	N	O	S	0	0
			1667	1050	284	321	12		
28	o	175	Total	C	N	O	S	0	0
			1307	817	227	252	11		

- Molecule 29 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	P	204	Total	C	N	O	S	0	0
			1591	1013	265	294	19		
29	p	164	Total	C	N	O	S	0	0
			1264	802	210	235	17		

- Molecule 30 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Q	197	Total	C	N	O	S	0	0
			1578	1011	268	290	9		
30	q	173	Total	C	N	O	S	0	0
			1380	890	234	248	8		

- Molecule 31 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	R	199	Total	C	N	O	S	0	0
			1549	977	272	291	9		
31	r	187	Total	C	N	O	S	0	0
			1432	904	248	271	9		

- Molecule 32 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	S	212	Total	C	N	O	S	0	0
			1643	1041	280	312	10		
32	s	206	Total	C	N	O	S	0	0
			1597	1015	269	303	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
33	T	213	Total	C	N	O	S	0	0
			1665	1050	288	316	11		

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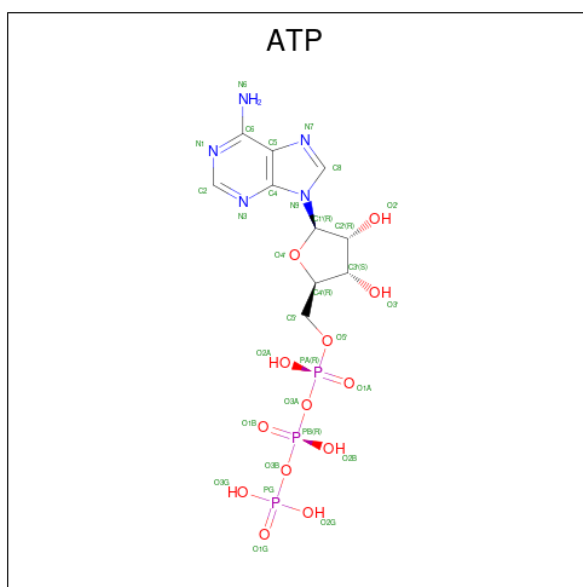
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Mol	Chain	Residues	Atoms					AltConf	Trace
33	t	206	Total	C	N	O	S	0	0
			1609	1016	279	302	12		

- Molecule 34 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 35 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

- Molecule 36 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

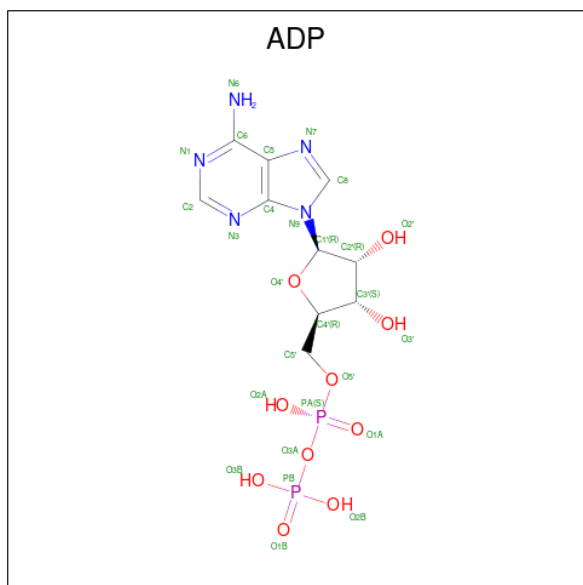
Mol	Chain	Residues	Atoms		AltConf
36	A	1	Total	Mg	0
			1	1	
36	B	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
36	C	1	Total	Mg	0
			1	1	
36	D	1	Total	Mg	0
			1	1	
36	E	1	Total	Mg	0
			1	1	

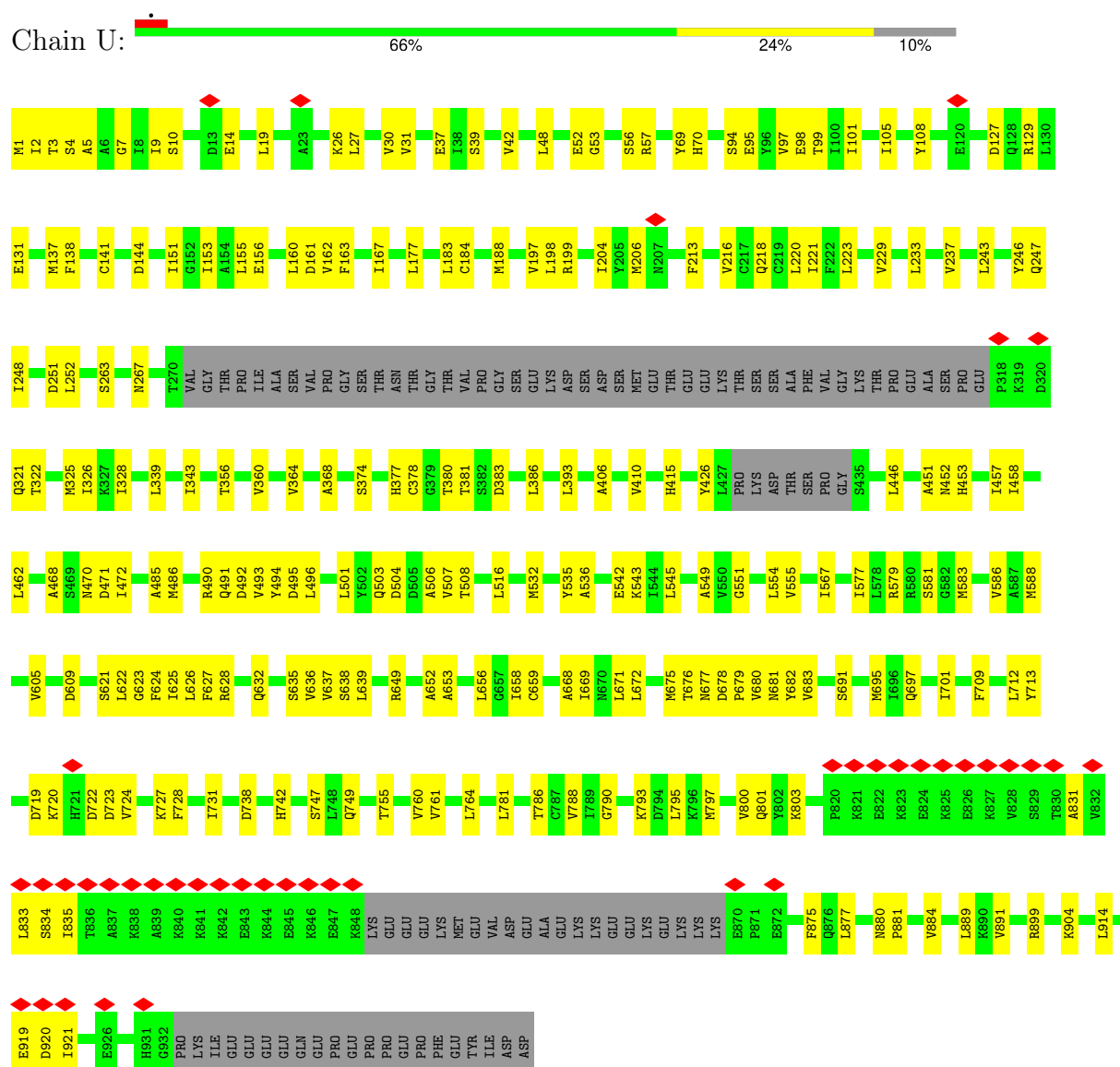
- Molecule 37 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



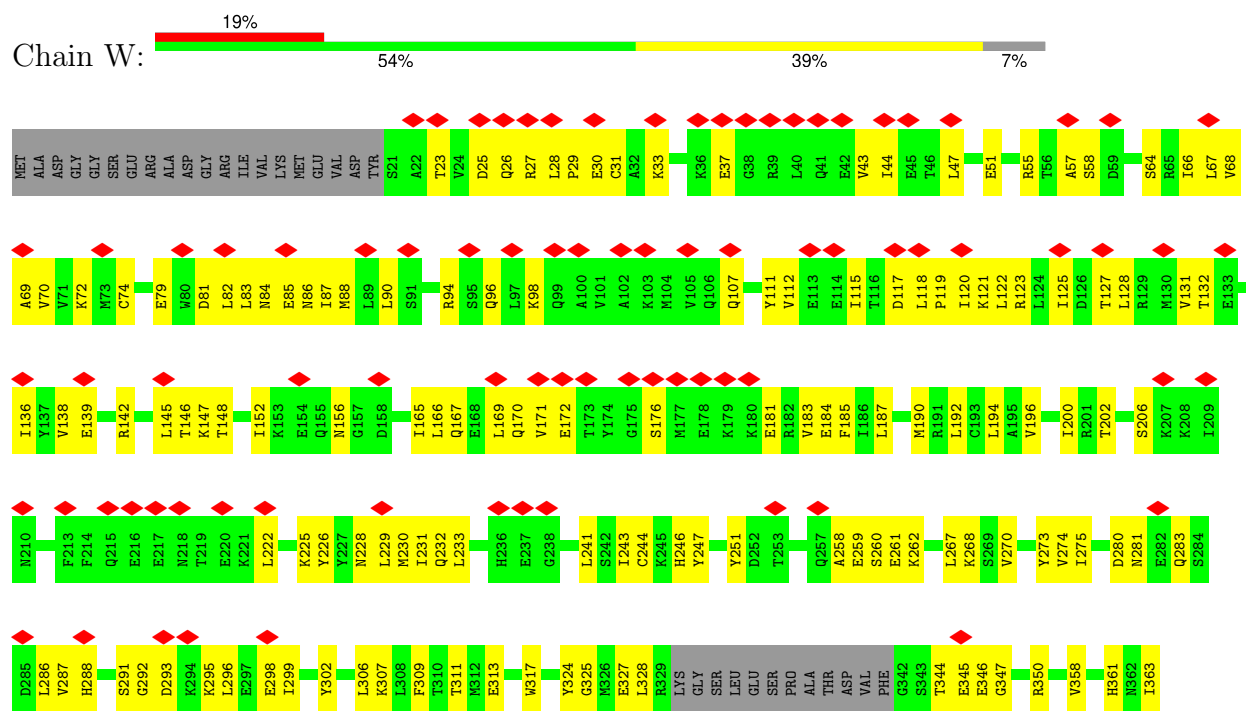
3 Residue-property plots

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 proteasome non-ATPase regulatory subunit 1

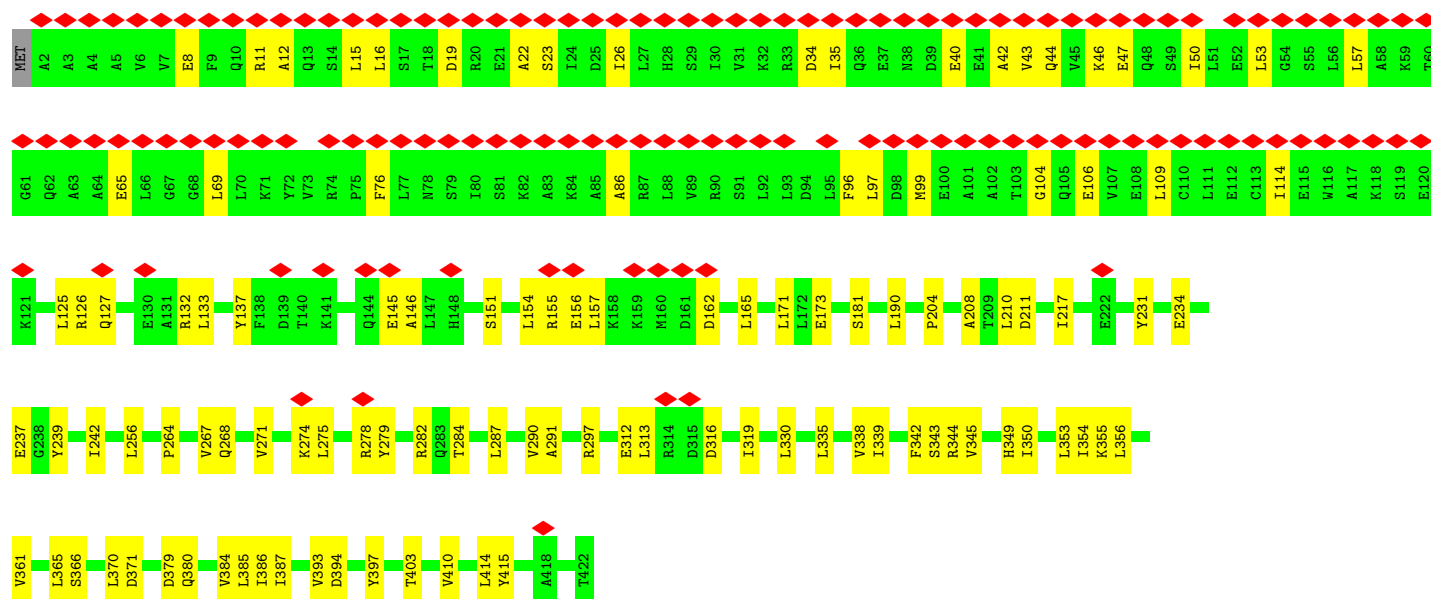
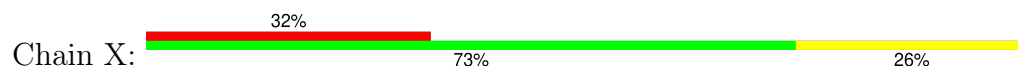


- Molecule 2: 26S proteasome non-ATPase regulatory subunit 3

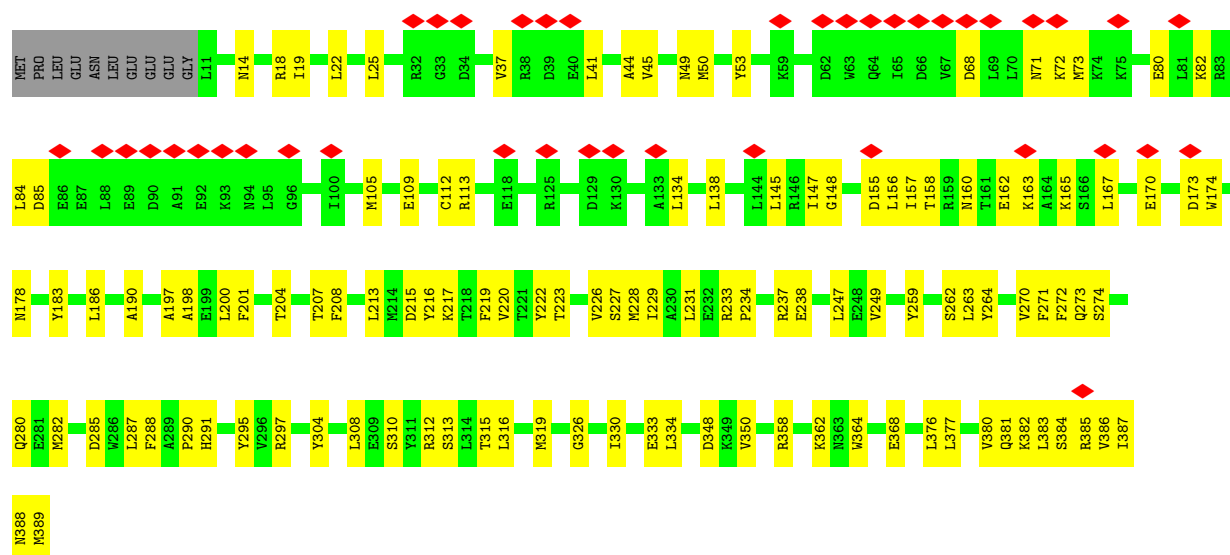




- Molecule 4: 26S proteasome non-ATPase regulatory subunit 11

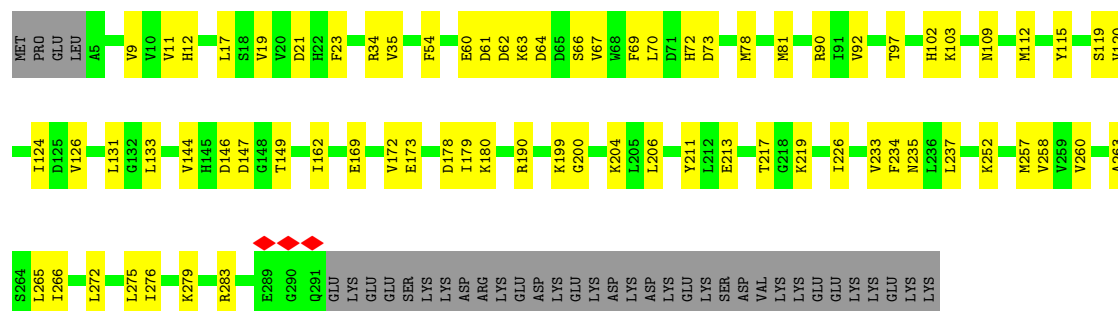


- Molecule 5: 26S proteasome non-ATPase regulatory subunit 6

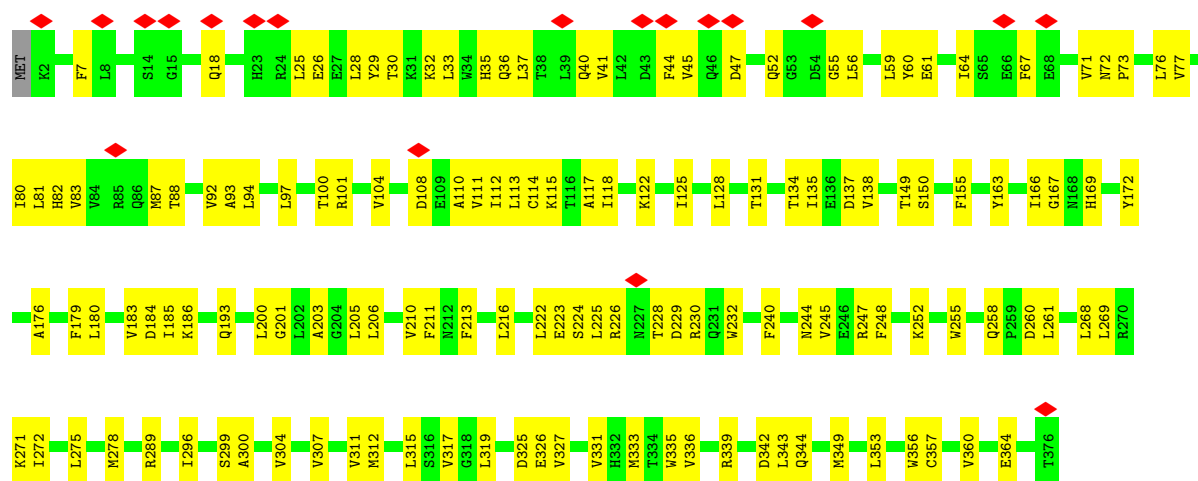


- Molecule 6: 26S proteasome non-ATPase regulatory subunit 7

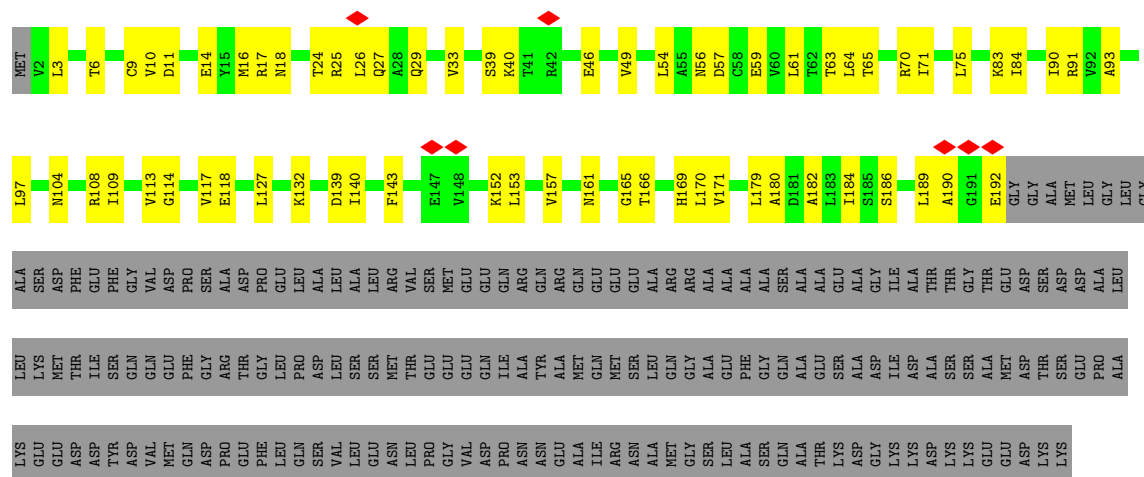
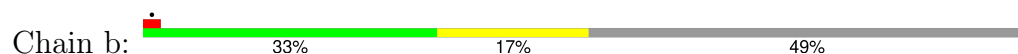




• Molecule 7: 26S proteasome non-ATPase regulatory subunit 13

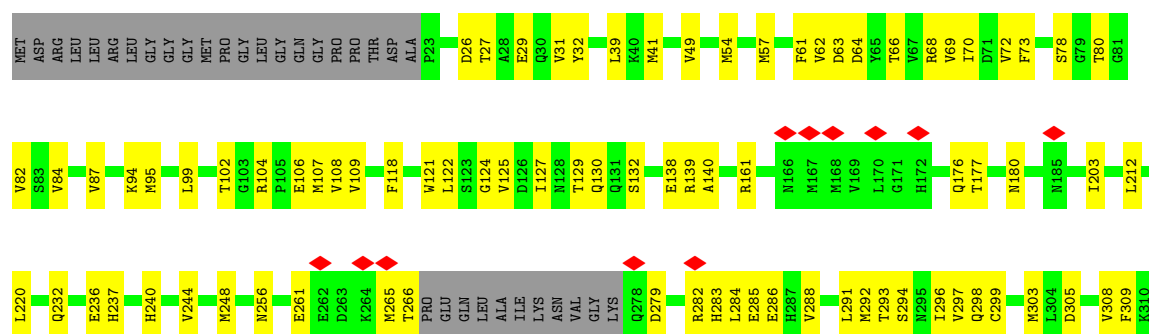


• Molecule 8: 26S proteasome non-ATPase regulatory subunit 4

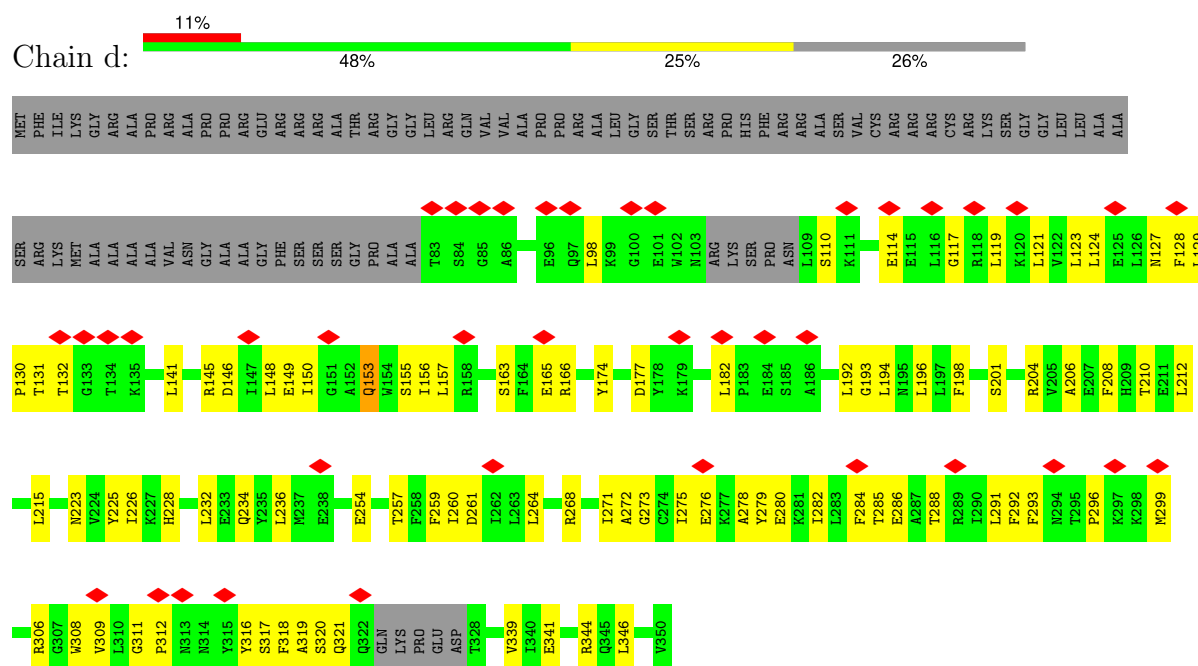


• Molecule 9: 26S proteasome non-ATPase regulatory subunit 14

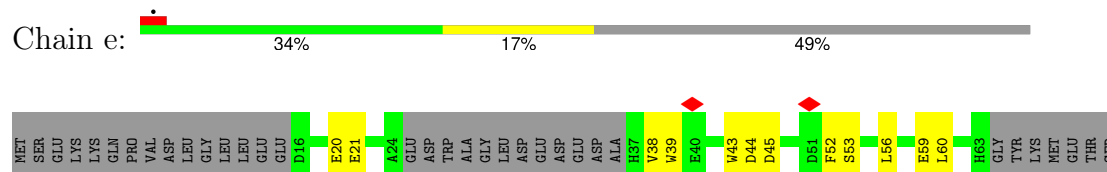




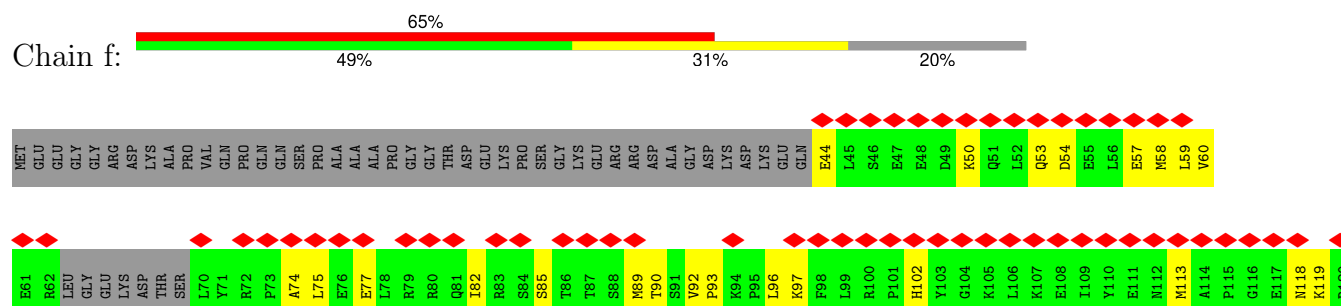
• Molecule 10: 26S proteasome non-ATPase regulatory subunit 8



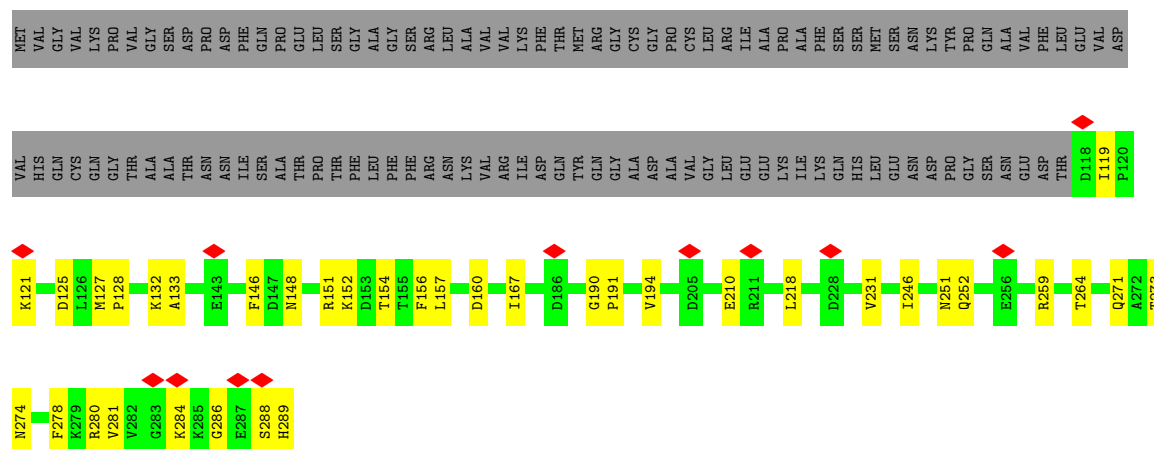
• Molecule 11: 26S proteasome complex subunit SEM1



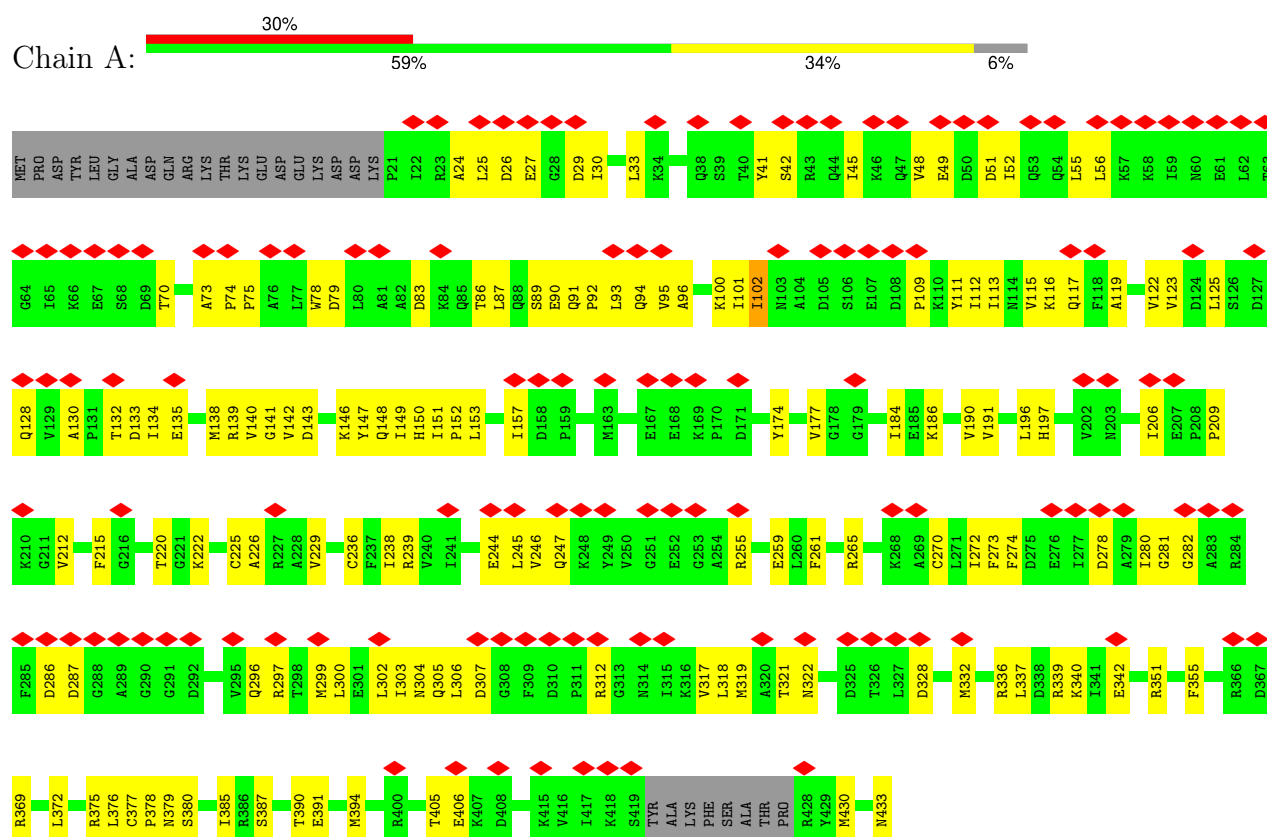
• Molecule 12: 26S proteasome non-ATPase regulatory subunit 2



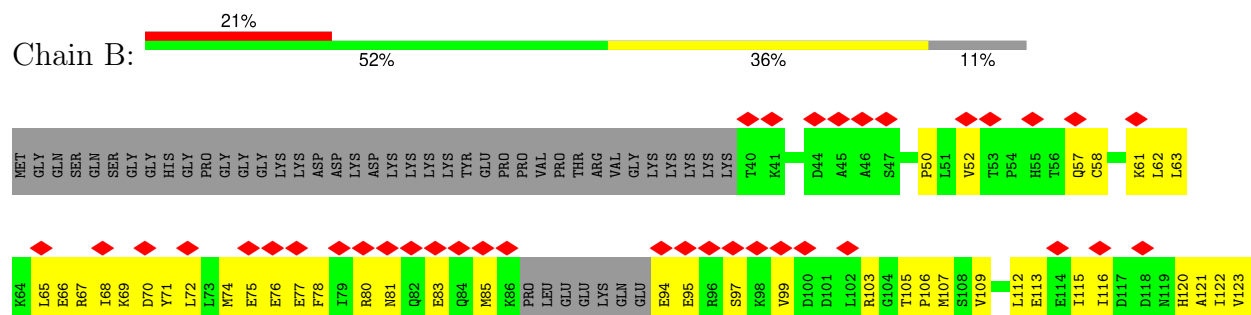


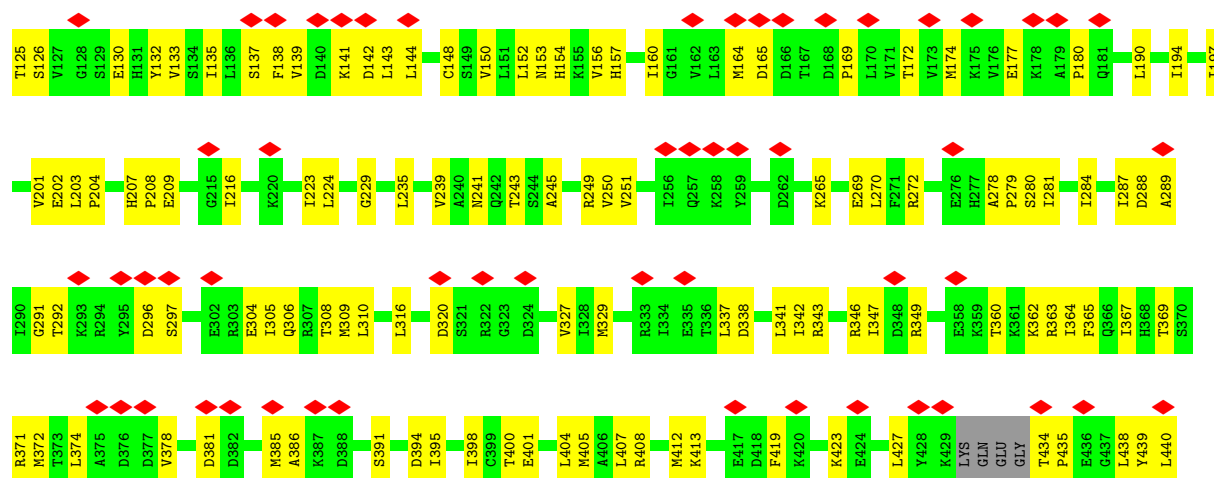


• Molecule 14: 26S proteasome regulatory subunit 7

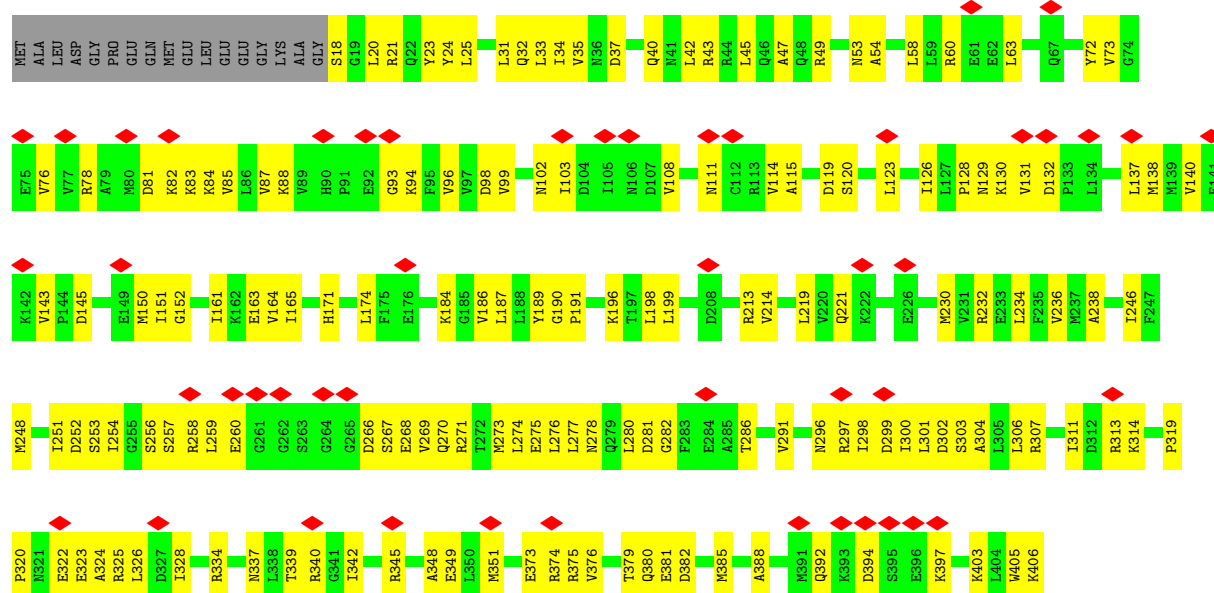


• Molecule 15: 26S proteasome regulatory subunit 4

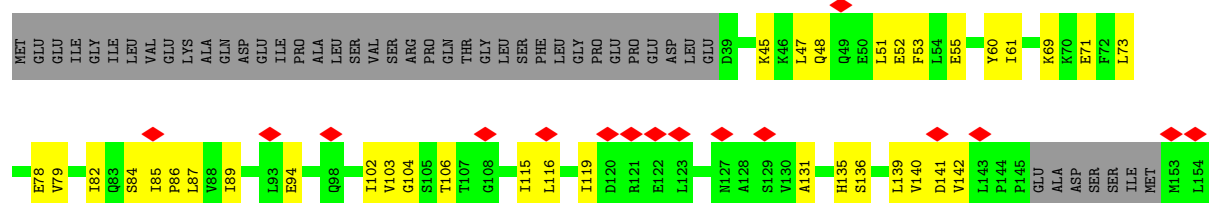


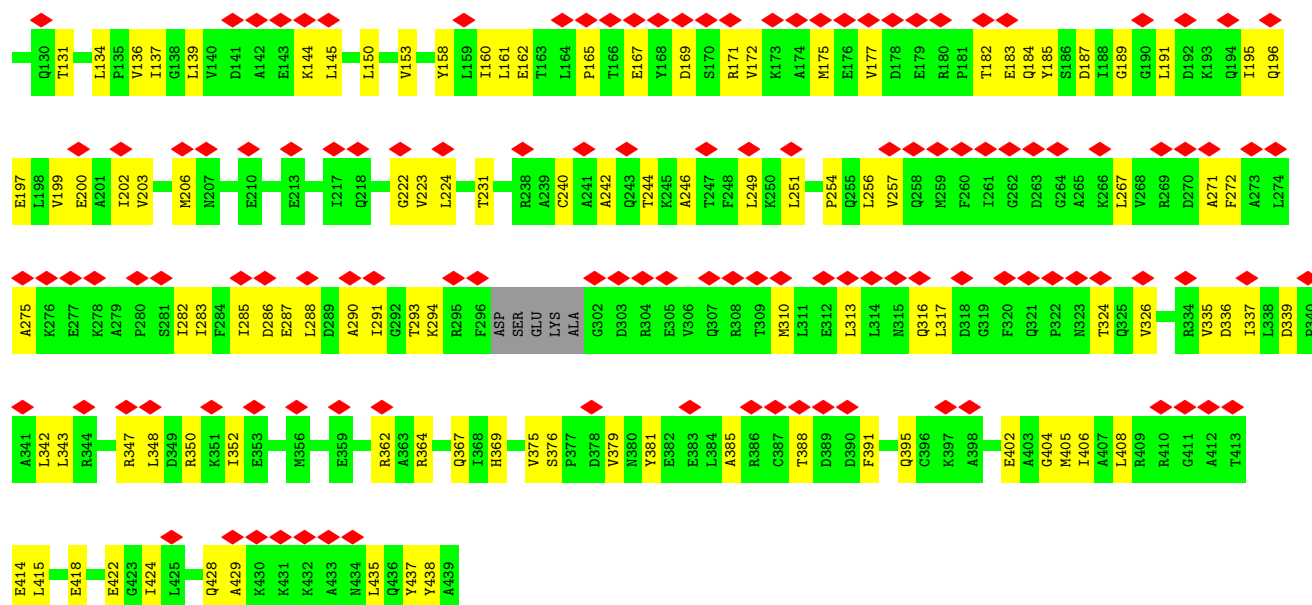


• Molecule 16: 26S protease regulatory subunit 8

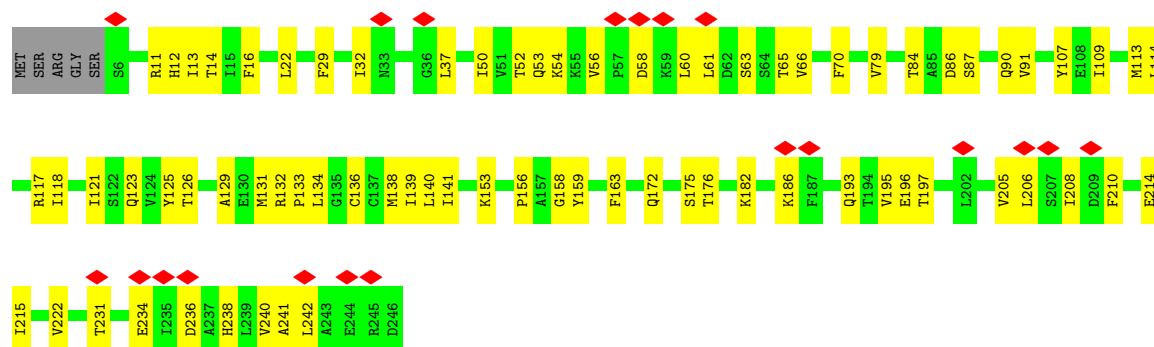


• Molecule 17: 26S proteasome regulatory subunit 6B

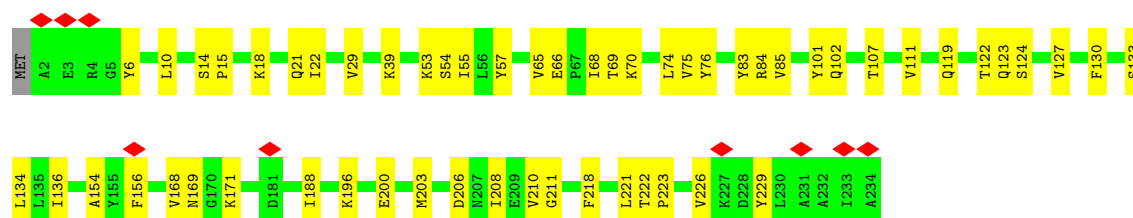
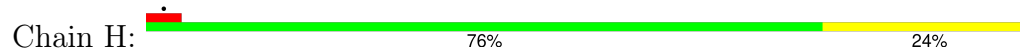




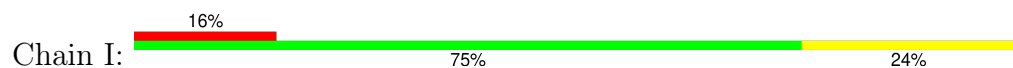
• Molecule 20: Proteasome subunit alpha type-6

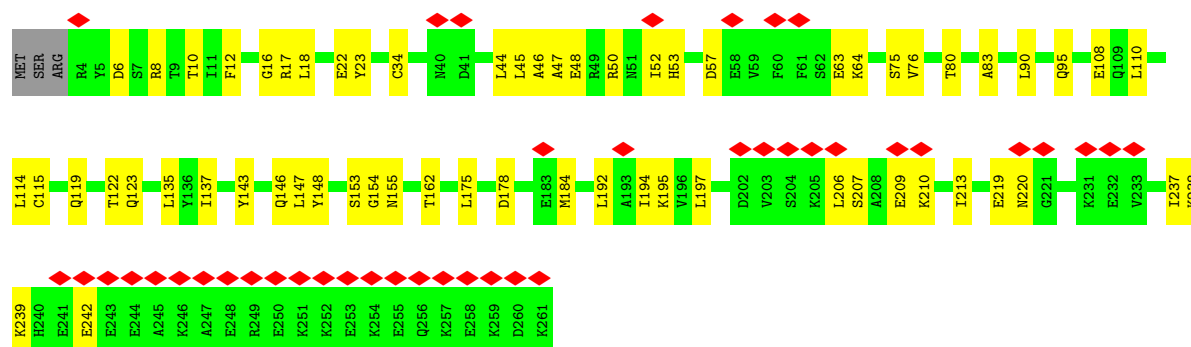


• Molecule 21: Proteasome subunit alpha type-2

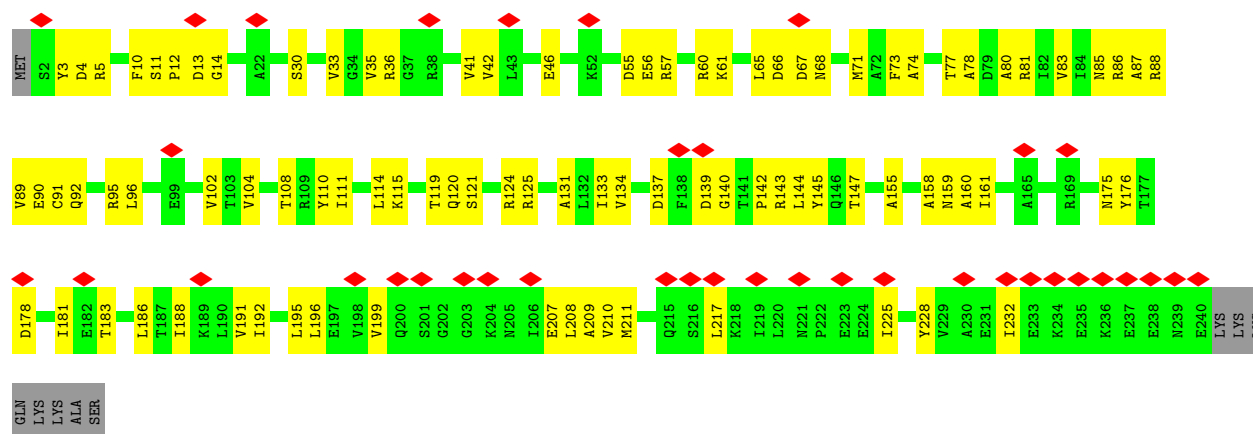


• Molecule 22: Proteasome subunit alpha type-4

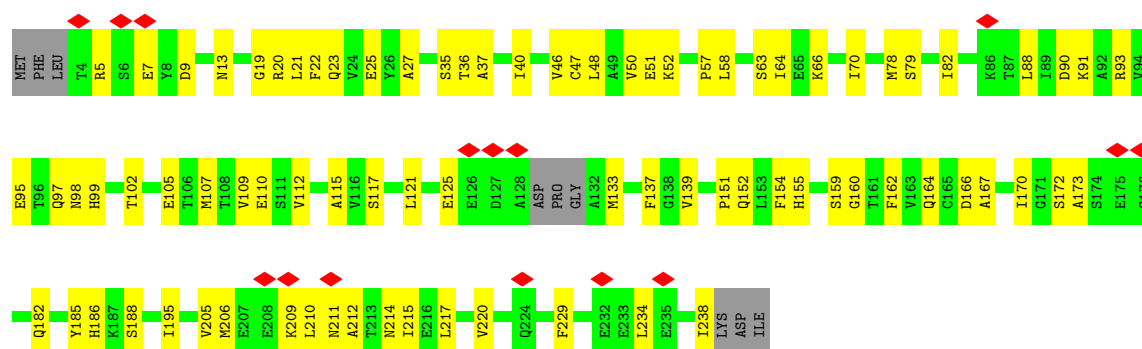




• Molecule 23: Proteasome subunit alpha type-7

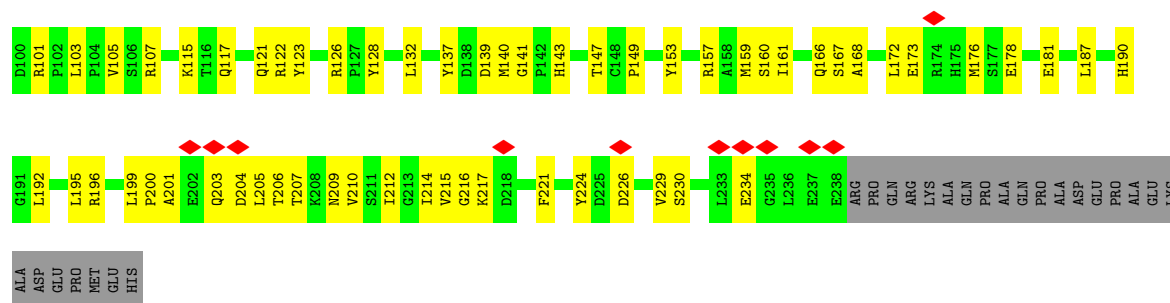


• Molecule 24: Proteasome subunit alpha type-5

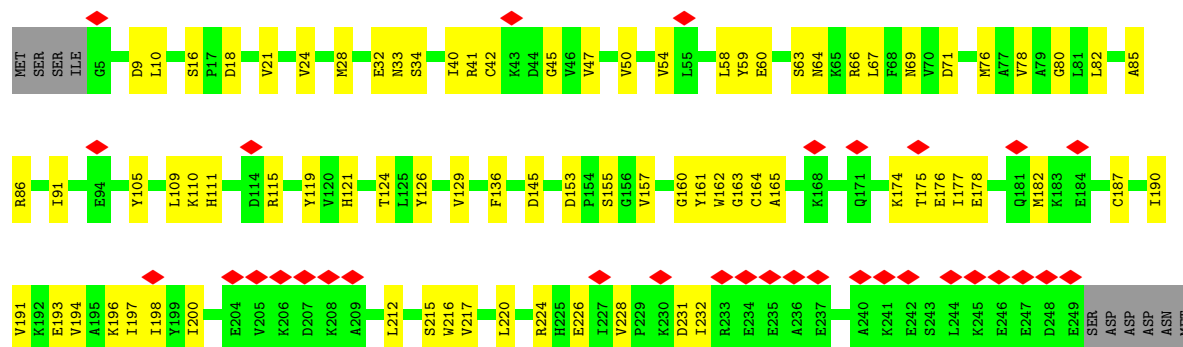


• Molecule 25: Proteasome subunit alpha type-1

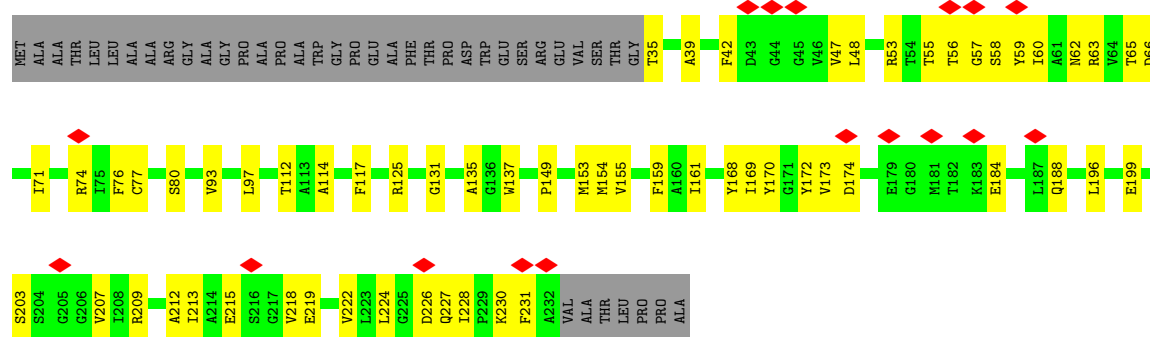




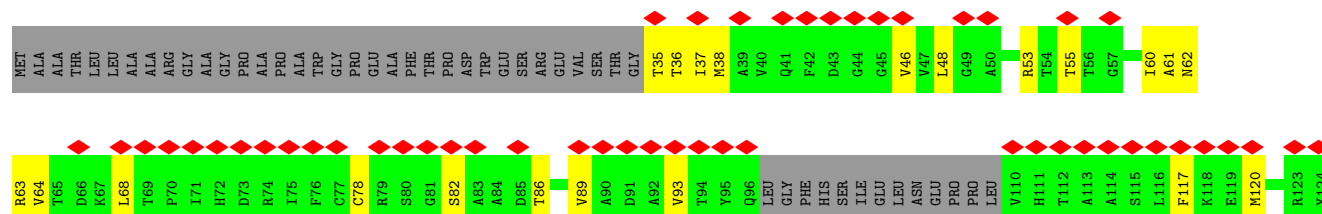
• Molecule 26: Proteasome subunit alpha type-3

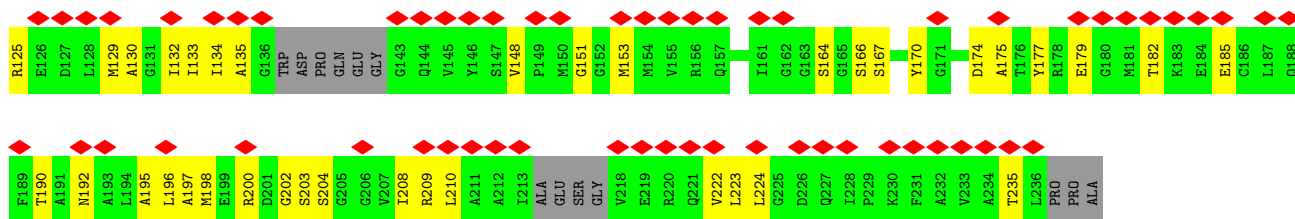


• Molecule 27: Proteasome subunit beta type-6

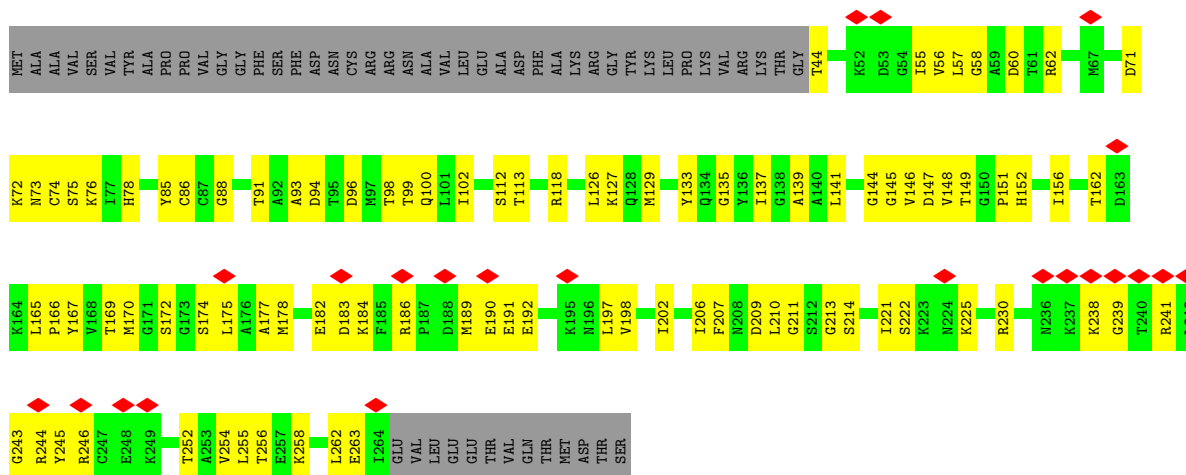


• Molecule 27: Proteasome subunit beta type-6

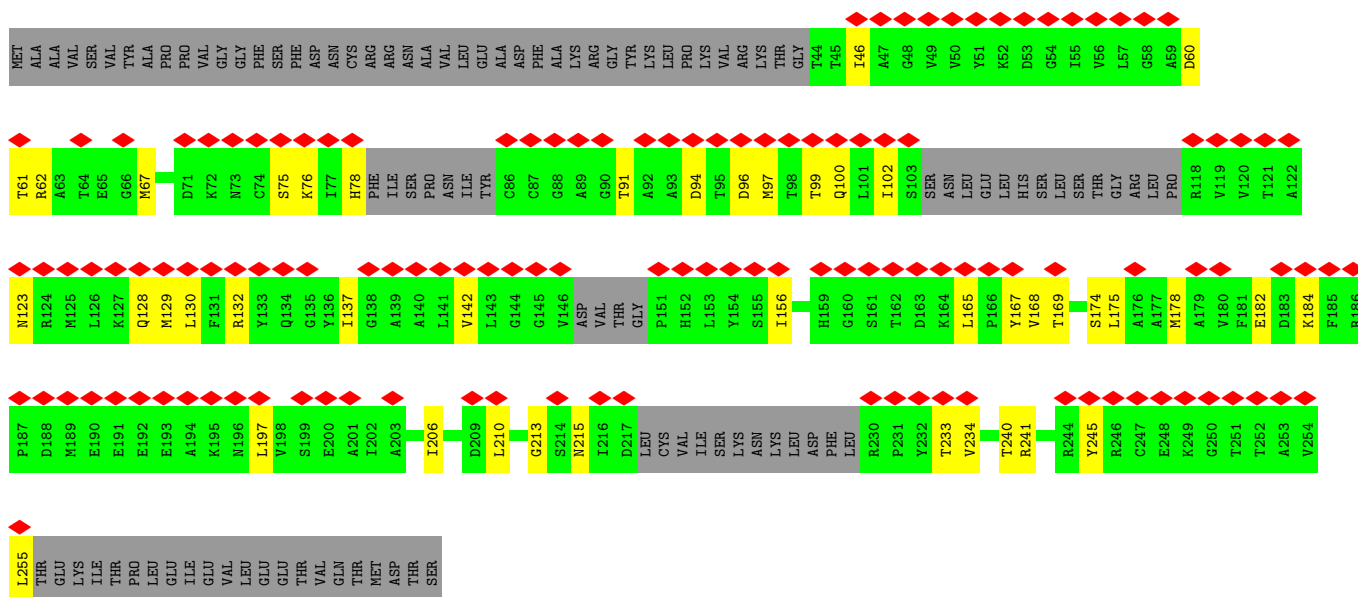




• Molecule 28: Proteasome subunit beta type-7

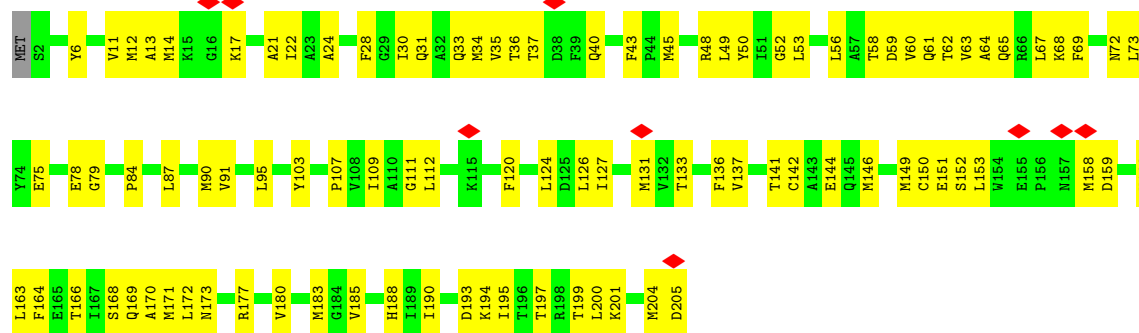


• Molecule 28: Proteasome subunit beta type-7



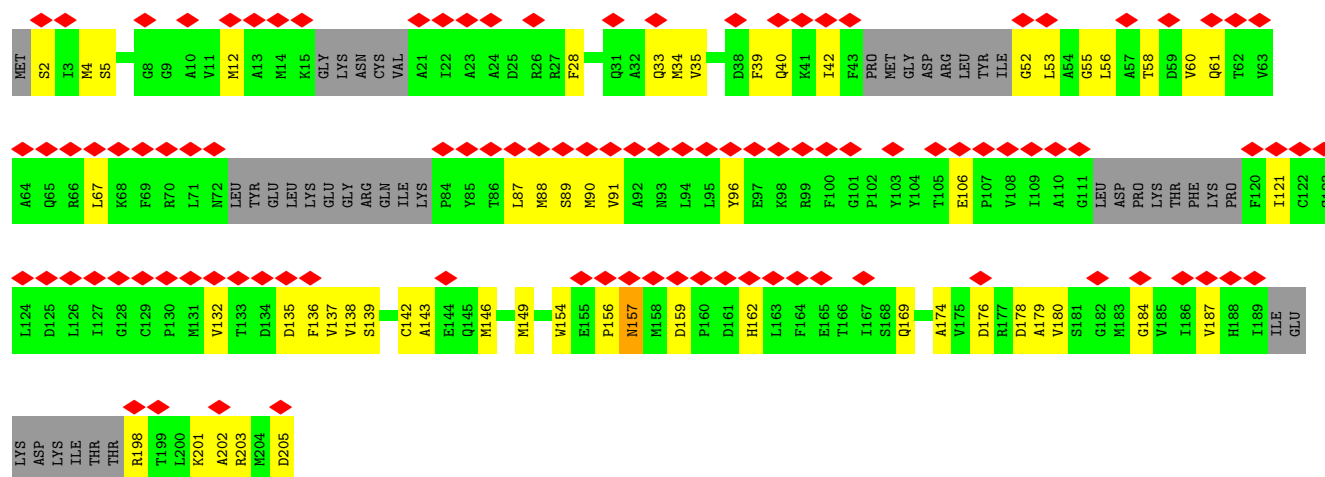
• Molecule 29: Proteasome subunit beta type-3

Chain P: 



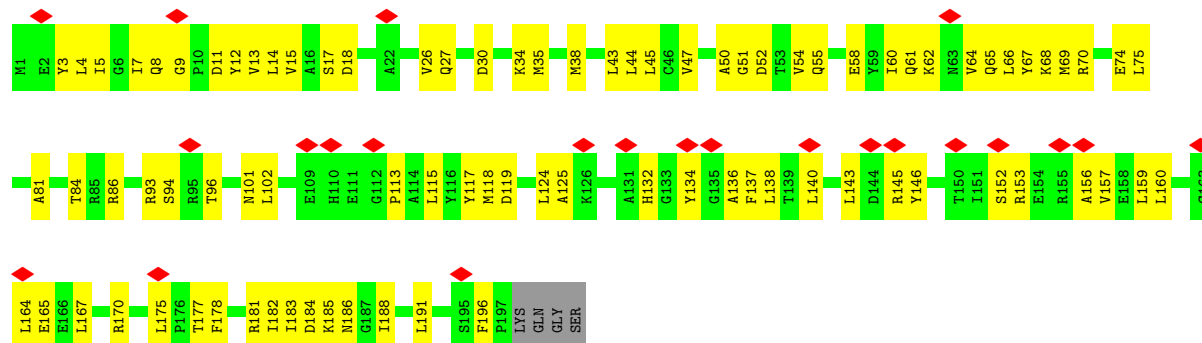
• Molecule 29: Proteasome subunit beta type-3

Chain p: 



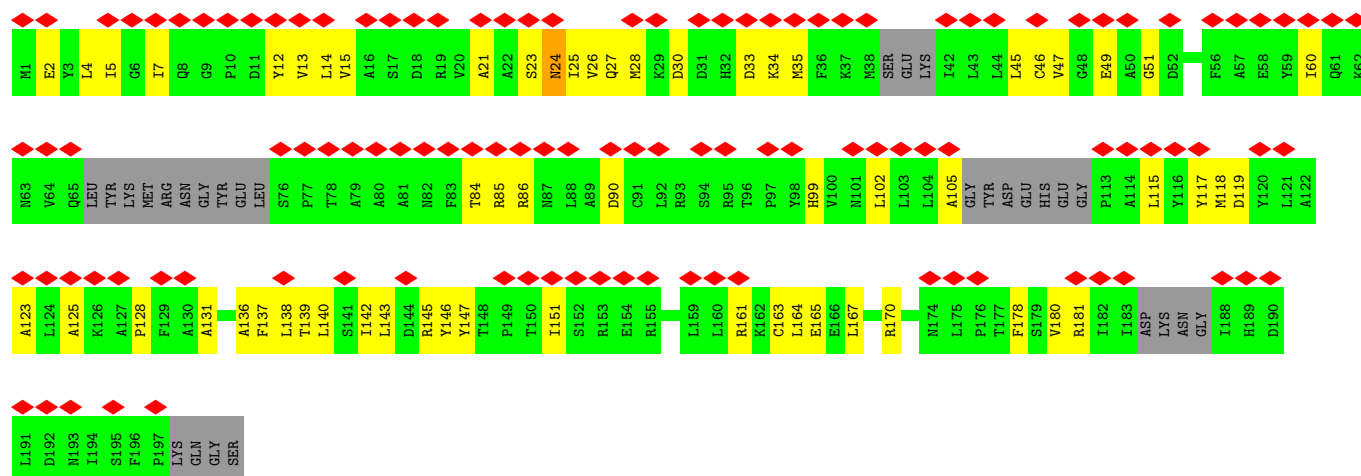
• Molecule 30: Proteasome subunit beta type-2

Chain Q: 



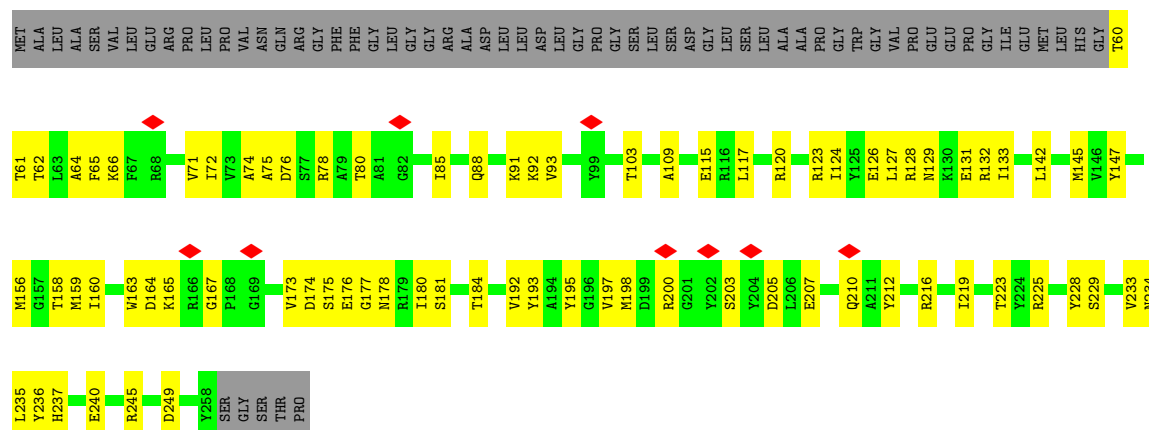
• Molecule 30: Proteasome subunit beta type-2

Chain q: 



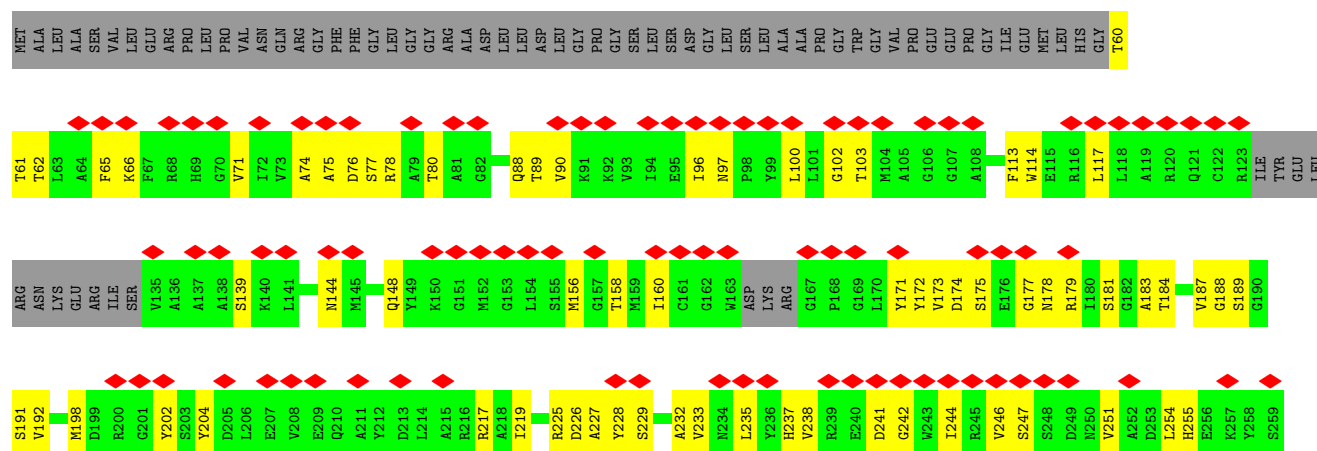
• Molecule 31: Proteasome subunit beta type-5

Chain R: 46% 29% 24%



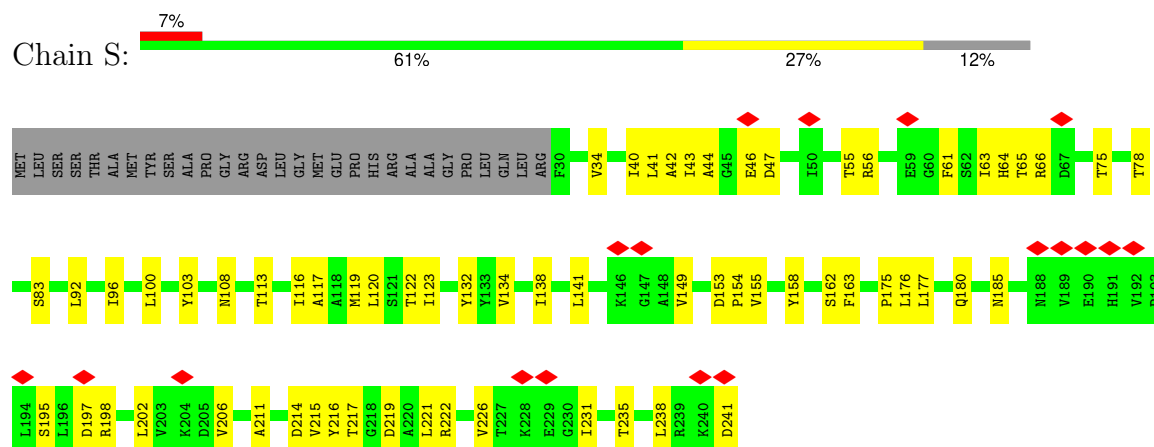
• Molecule 31: Proteasome subunit beta type-5

Chain r: 35% 45% 26% 29%





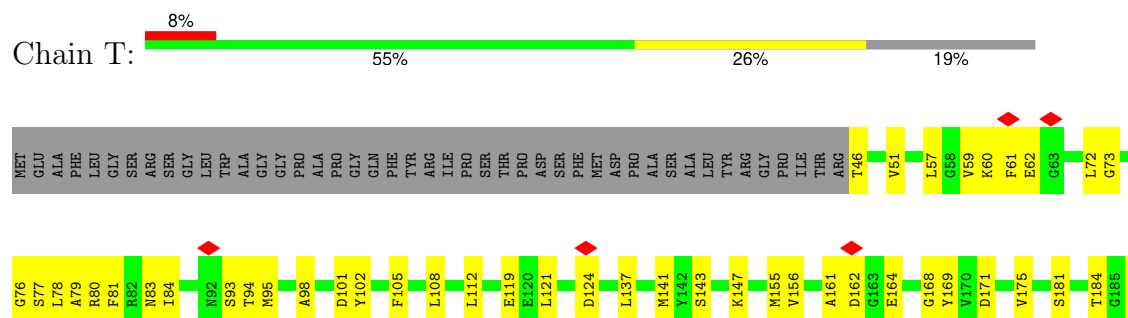
- Molecule 32: Proteasome subunit beta type-1



- Molecule 32: Proteasome subunit beta type-1

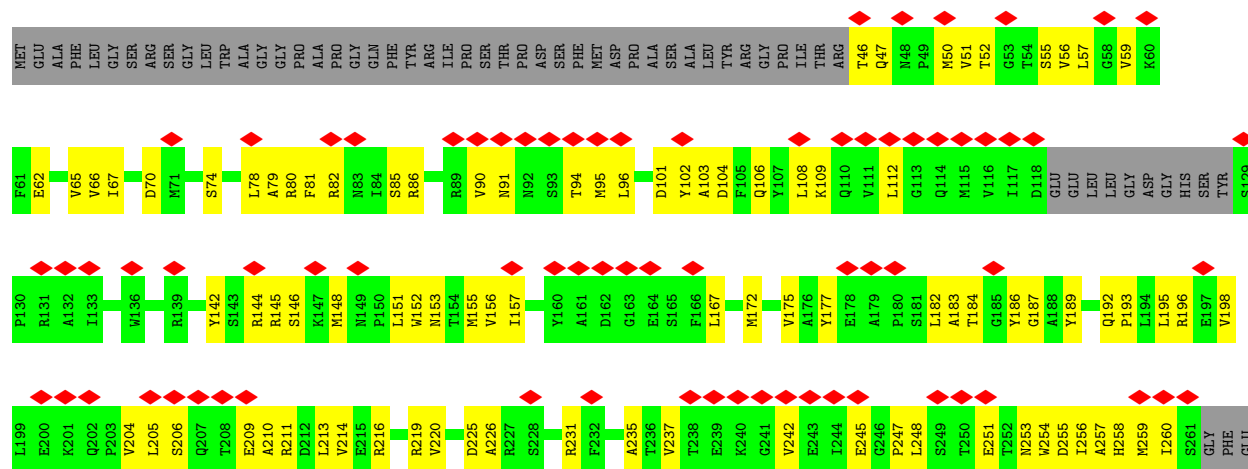
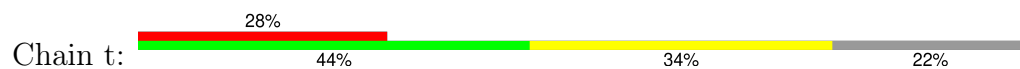


- Molecule 33: Proteasome subunit beta type-4





• Molecule 33: Proteasome subunit beta type-4



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	103163	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 ($e^-/\text{\AA}^2$)	53	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.642	Depositor
Minimum map value	-0.340	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	363.0, 363.0, 363.0	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.825, 0.825, 0.825	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: ATP, MG, 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	U	0.27	0/6800	0.36	0/9192
2	V	0.27	0/3499	0.43	0/4722
3	W	0.21	0/3509	0.37	0/4716
4	X	0.21	0/3373	0.34	0/4548
5	Y	0.26	0/3181	0.38	0/4285
6	Z	0.30	0/2333	0.38	0/3162
7	a	0.23	0/3070	0.39	0/4155
8	b	0.21	0/1479	0.34	0/2003
9	c	0.30	0/2225	0.40	0/3005
10	d	0.22	0/2141	0.42	0/2891
11	e	0.22	0/322	0.40	0/436
12	f	0.16	0/5724	0.39	0/7735
13	x	0.20	0/1403	0.30	0/1892
14	A	0.23	0/3233	0.41	1/4362 (0.0%)
15	B	0.23	0/3109	0.39	0/4193
16	C	0.25	0/3112	0.41	0/4182
17	D	0.24	0/3039	0.42	0/4098
18	E	0.17	0/2380	0.38	0/3192
19	F	0.20	0/2919	0.39	0/3931
20	G	0.26	0/1919	0.42	0/2593
21	H	0.31	0/1857	0.38	0/2514
22	I	0.26	0/2074	0.34	0/2786
23	J	0.26	0/1913	0.38	0/2581
24	K	0.32	0/1804	0.46	0/2435
25	L	0.27	0/1891	0.39	0/2555
26	M	0.26	0/1955	0.39	0/2632
27	N	0.26	0/1513	0.41	0/2047
27	n	0.19	0/1352	0.35	0/1822
28	O	0.27	0/1694	0.40	0/2293
28	o	0.17	0/1323	0.37	0/1780
29	P	0.28	0/1620	0.42	0/2184
29	p	0.15	0/1282	0.37	0/1722

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
30	Q	0.28	0/1611	0.43	0/2180
30	q	0.18	0/1405	0.34	0/1899
31	R	0.25	0/1580	0.36	0/2134
31	r	0.26	0/1460	0.44	0/1972
32	S	0.25	0/1673	0.37	0/2254
32	s	0.18	0/1625	0.35	0/2188
33	T	0.25	0/1698	0.39	0/2299
33	t	0.18	0/1639	0.34	0/2217
All	All	0.24	0/91739	0.39	1/123787 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	75	PRO	CA-N-CD	-5.33	104.55	112.00

There are no chirality outliers.

There are no planarity outliers.

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	U	6685	0	6748	180	0
2	V	3434	0	3503	134	0
3	W	3465	0	3591	153	0
4	X	3327	0	3423	103	0
5	Y	3123	0	3130	102	0
6	Z	2290	0	2320	76	0
7	a	3012	0	3029	119	0
8	b	1459	0	1499	53	0
9	c	2184	0	2191	85	0
10	d	2099	0	2127	77	0
11	e	314	0	247	14	0
12	f	5633	0	5648	262	0
13	x	1376	0	1324	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	A	3183	0	3242	163	0
15	B	3065	0	3130	165	0
16	C	3071	0	3193	156	0
17	D	2990	0	3029	152	0
18	E	2353	0	2404	135	0
19	F	2881	0	2973	116	0
20	G	1885	0	1889	76	0
21	H	1818	0	1811	51	0
22	I	2044	0	2069	62	0
23	J	1887	0	1905	93	0
24	K	1778	0	1761	78	0
25	L	1857	0	1845	81	0
26	M	1920	0	1893	79	0
27	N	1487	0	1452	66	0
27	n	1336	0	1324	62	0
28	O	1667	0	1689	100	0
28	o	1307	0	1310	39	0
29	P	1591	0	1609	100	0
29	p	1264	0	1255	44	0
30	Q	1578	0	1580	92	0
30	q	1380	0	1399	61	0
31	R	1549	0	1512	66	0
31	r	1432	0	1384	75	0
32	S	1643	0	1640	62	0
32	s	1597	0	1597	82	0
33	T	1665	0	1638	66	0
33	t	1609	0	1597	91	0
34	c	1	0	0	0	0
35	A	31	0	12	3	0
35	B	31	0	12	1	0
35	C	31	0	12	3	0
36	A	1	0	0	0	0
36	B	1	0	0	0	0
36	C	1	0	0	0	0
36	D	1	0	0	0	0
36	E	1	0	0	0	0
37	D	27	0	12	6	0
37	E	27	0	12	2	0
37	F	27	0	12	2	0
All	All	90418	0	90982	3336	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 18.

The worst 5 of 3336 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)
14:A:339:ARG:NH2	19:F:405:MET:SD	2.27	1.07
29:P:67:LEU:HD11	29:P:91:VAL:HG22	1.37	1.06
24:K:91:LYS:NZ	24:K:95:GLU:OE2	1.87	1.06
12:f:171:GLN:NE2	12:f:210:GLU:OE2	1.93	1.02
19:F:251:LEU:HD22	19:F:285:ILE:HG23	1.41	1.02

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	U	849/953 (89%)	775 (91%)	74 (9%)	0	100	100
2	V	417/534 (78%)	364 (87%)	53 (13%)	0	100	100
3	W	420/456 (92%)	376 (90%)	44 (10%)	0	100	100
4	X	419/422 (99%)	388 (93%)	31 (7%)	0	100	100
5	Y	377/389 (97%)	357 (95%)	20 (5%)	0	100	100
6	Z	285/324 (88%)	271 (95%)	14 (5%)	0	100	100
7	a	373/376 (99%)	333 (89%)	40 (11%)	0	100	100
8	b	189/377 (50%)	173 (92%)	16 (8%)	0	100	100
9	c	273/310 (88%)	243 (89%)	30 (11%)	0	100	100
10	d	252/350 (72%)	212 (84%)	40 (16%)	0	100	100
11	e	32/70 (46%)	23 (72%)	8 (25%)	1 (3%)	3	21
12	f	715/908 (79%)	611 (86%)	102 (14%)	2 (0%)	37	66
13	x	170/289 (59%)	154 (91%)	16 (9%)	0	100	100
14	A	401/433 (93%)	329 (82%)	71 (18%)	1 (0%)	44	71

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	B	384/440 (87%)	335 (87%)	49 (13%)	0	100	100
16	C	387/406 (95%)	347 (90%)	40 (10%)	0	100	100
17	D	369/418 (88%)	317 (86%)	51 (14%)	1 (0%)	37	66
18	E	280/389 (72%)	224 (80%)	55 (20%)	1 (0%)	30	61
19	F	362/439 (82%)	290 (80%)	72 (20%)	0	100	100
20	G	239/246 (97%)	213 (89%)	26 (11%)	0	100	100
21	H	231/234 (99%)	216 (94%)	15 (6%)	0	100	100
22	I	256/261 (98%)	243 (95%)	13 (5%)	0	100	100
23	J	237/248 (96%)	223 (94%)	14 (6%)	0	100	100
24	K	228/241 (95%)	205 (90%)	23 (10%)	0	100	100
25	L	234/263 (89%)	200 (86%)	33 (14%)	1 (0%)	30	61
26	M	243/255 (95%)	225 (93%)	18 (7%)	0	100	100
27	N	196/239 (82%)	170 (87%)	26 (13%)	0	100	100
27	n	171/239 (72%)	162 (95%)	9 (5%)	0	100	100
28	O	219/277 (79%)	198 (90%)	21 (10%)	0	100	100
28	o	165/277 (60%)	152 (92%)	13 (8%)	0	100	100
29	P	202/205 (98%)	175 (87%)	27 (13%)	0	100	100
29	p	152/205 (74%)	127 (84%)	24 (16%)	1 (1%)	19	50
30	Q	195/201 (97%)	173 (89%)	22 (11%)	0	100	100
30	q	163/201 (81%)	149 (91%)	13 (8%)	1 (1%)	22	53
31	R	197/263 (75%)	180 (91%)	17 (9%)	0	100	100
31	r	181/263 (69%)	160 (88%)	21 (12%)	0	100	100
32	S	210/241 (87%)	195 (93%)	15 (7%)	0	100	100
32	s	202/241 (84%)	181 (90%)	21 (10%)	0	100	100
33	T	211/264 (80%)	184 (87%)	27 (13%)	0	100	100
33	t	202/264 (76%)	178 (88%)	24 (12%)	0	100	100
All	All	11288/13411 (84%)	10031 (89%)	1248 (11%)	9 (0%)	50	76

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	f	211	ILE
17	D	239	TYR

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Mol	Chain	Res	Type
11	e	43	TRP
30	q	24	ASN
18	E	273	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	U	730/816 (90%)	730 (100%)	0	100	100
2	V	371/460 (81%)	371 (100%)	0	100	100
3	W	391/416 (94%)	391 (100%)	0	100	100
4	X	361/362 (100%)	361 (100%)	0	100	100
5	Y	335/344 (97%)	335 (100%)	0	100	100
6	Z	258/295 (88%)	258 (100%)	0	100	100
7	a	335/336 (100%)	335 (100%)	0	100	100
8	b	167/312 (54%)	167 (100%)	0	100	100
9	c	244/268 (91%)	244 (100%)	0	100	100
10	d	227/294 (77%)	226 (100%)	1 (0%)	89	93
11	e	34/63 (54%)	34 (100%)	0	100	100
12	f	611/763 (80%)	611 (100%)	0	100	100
13	x	156/253 (62%)	156 (100%)	0	100	100
14	A	348/372 (94%)	348 (100%)	0	100	100
15	B	344/385 (89%)	344 (100%)	0	100	100
16	C	340/352 (97%)	340 (100%)	0	100	100
17	D	327/366 (89%)	327 (100%)	0	100	100
18	E	261/341 (76%)	261 (100%)	0	100	100
19	F	315/379 (83%)	315 (100%)	0	100	100
20	G	206/210 (98%)	206 (100%)	0	100	100
21	H	190/191 (100%)	189 (100%)	1 (0%)	86	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	I	218/221 (99%)	218 (100%)	0	100	100
23	J	203/211 (96%)	203 (100%)	0	100	100
24	K	195/203 (96%)	194 (100%)	1 (0%)	86	91
25	L	202/224 (90%)	202 (100%)	0	100	100
26	M	202/212 (95%)	202 (100%)	0	100	100
27	N	154/181 (85%)	154 (100%)	0	100	100
27	n	138/181 (76%)	138 (100%)	0	100	100
28	O	182/228 (80%)	182 (100%)	0	100	100
28	o	138/228 (60%)	138 (100%)	0	100	100
29	P	173/174 (99%)	173 (100%)	0	100	100
29	p	136/174 (78%)	136 (100%)	0	100	100
30	Q	168/171 (98%)	168 (100%)	0	100	100
30	q	148/171 (86%)	148 (100%)	0	100	100
31	R	155/202 (77%)	155 (100%)	0	100	100
31	r	142/202 (70%)	142 (100%)	0	100	100
32	S	177/199 (89%)	177 (100%)	0	100	100
32	s	172/199 (86%)	172 (100%)	0	100	100
33	T	176/215 (82%)	176 (100%)	0	100	100
33	t	171/215 (80%)	171 (100%)	0	100	100
All	All	9801/11389 (86%)	9798 (100%)	3 (0%)	100	100

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	d	153	GLN
21	H	102	GLN
24	K	214	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 66 such sidechains are listed below:

Mol	Chain	Res	Type
32	S	188	ASN
27	n	41	GLN
33	t	153	ASN

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Mol	Chain	Res	Type
12	f	396	ASN
12	f	327	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
35	ATP	B	501	36	28,33,33	0.71	0	34,52,52	1.20	5 (14%)
35	ATP	C	501	36	28,33,33	0.86	1 (3%)	34,52,52	0.94	2 (5%)
35	ATP	A	501	36	28,33,33	1.04	2 (7%)	34,52,52	0.95	3 (8%)
37	ADP	E	401	36	24,29,29	0.88	0	29,45,45	1.26	2 (6%)
37	ADP	D	501	36	24,29,29	0.82	0	29,45,45	1.30	2 (6%)
37	ADP	F	501	-	24,29,29	0.80	1 (4%)	29,45,45	0.94	2 (6%)

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
35	ATP	B	501	36	-	4/18/38/38	0/3/3/3
35	ATP	C	501	36	-	5/18/38/38	0/3/3/3
35	ATP	A	501	36	-	6/18/38/38	0/3/3/3
37	ADP	E	401	36	-	3/12/32/32	0/3/3/3
37	ADP	D	501	36	-	2/12/32/32	0/3/3/3
37	ADP	F	501	-	-	2/12/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	A	501	ATP	PA-O3A	-2.96	1.56	1.59
35	A	501	ATP	PB-O3B	-2.79	1.56	1.59
35	C	501	ATP	PA-O3A	-2.10	1.57	1.59
37	F	501	ADP	C8-N7	-2.02	1.31	1.34

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	D	501	ADP	N3-C2-N1	-4.44	122.65	128.67
37	E	401	ADP	N3-C2-N1	-4.18	123.00	128.67
35	B	501	ATP	C4'-O4'-C1'	-3.85	106.40	109.92
37	E	401	ADP	C4-C5-N7	-2.58	106.61	109.34
35	B	501	ATP	O4'-C1'-N9	-2.37	105.60	108.75

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

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

There are no ring outliers.

6 monomers are involved in 17 short contacts:

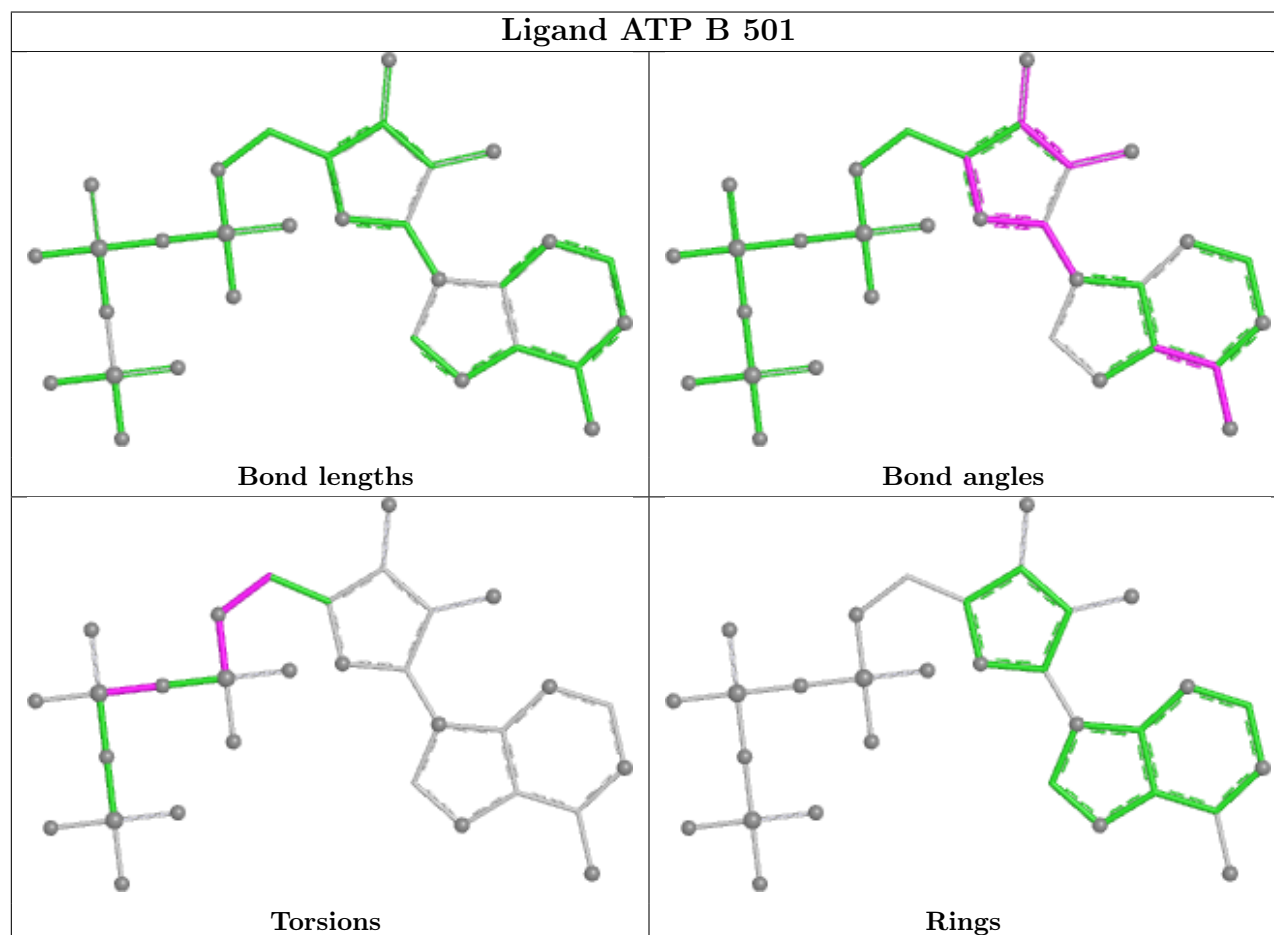
Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	B	501	ATP	1	0

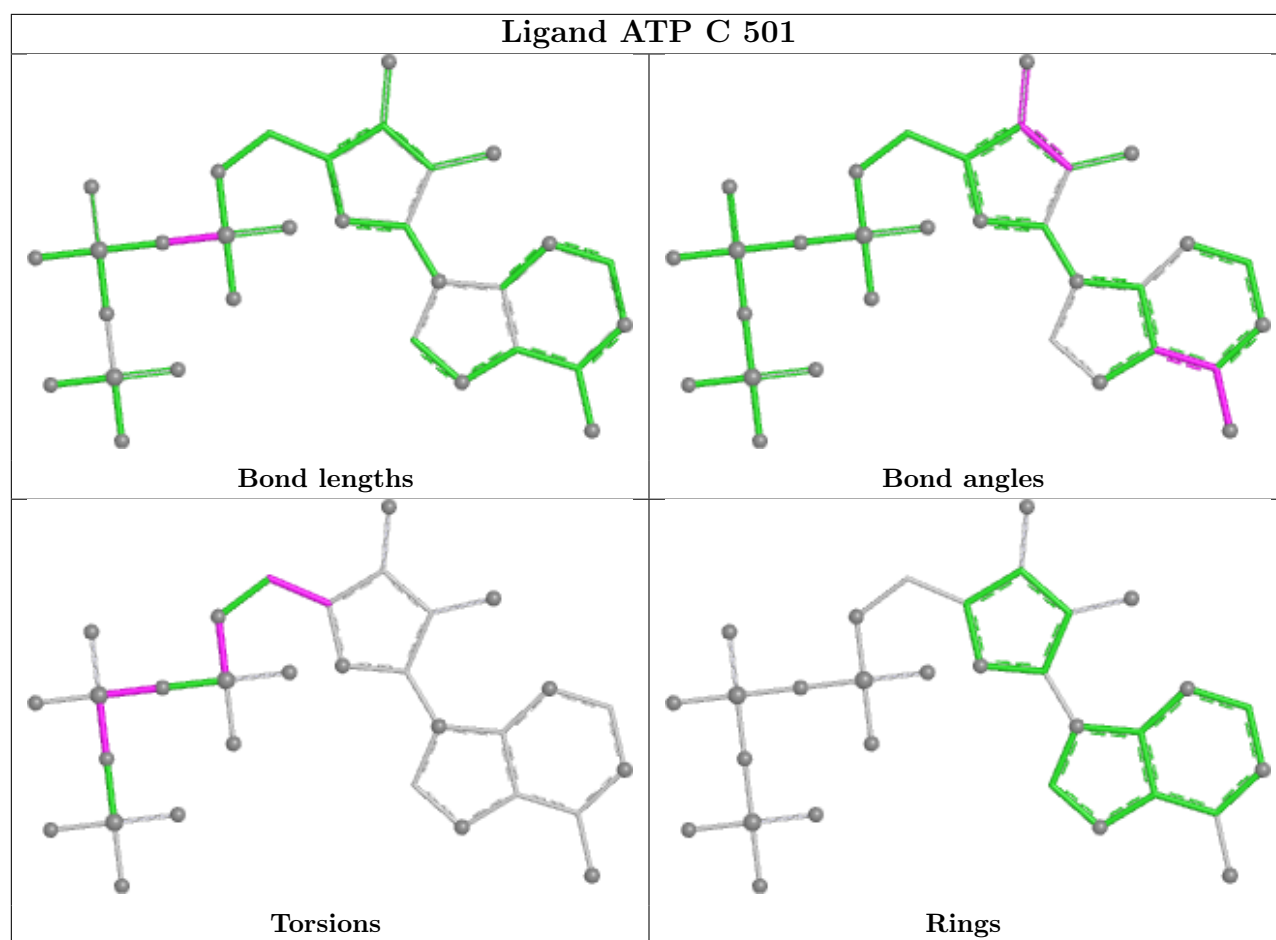
Continued on next page...

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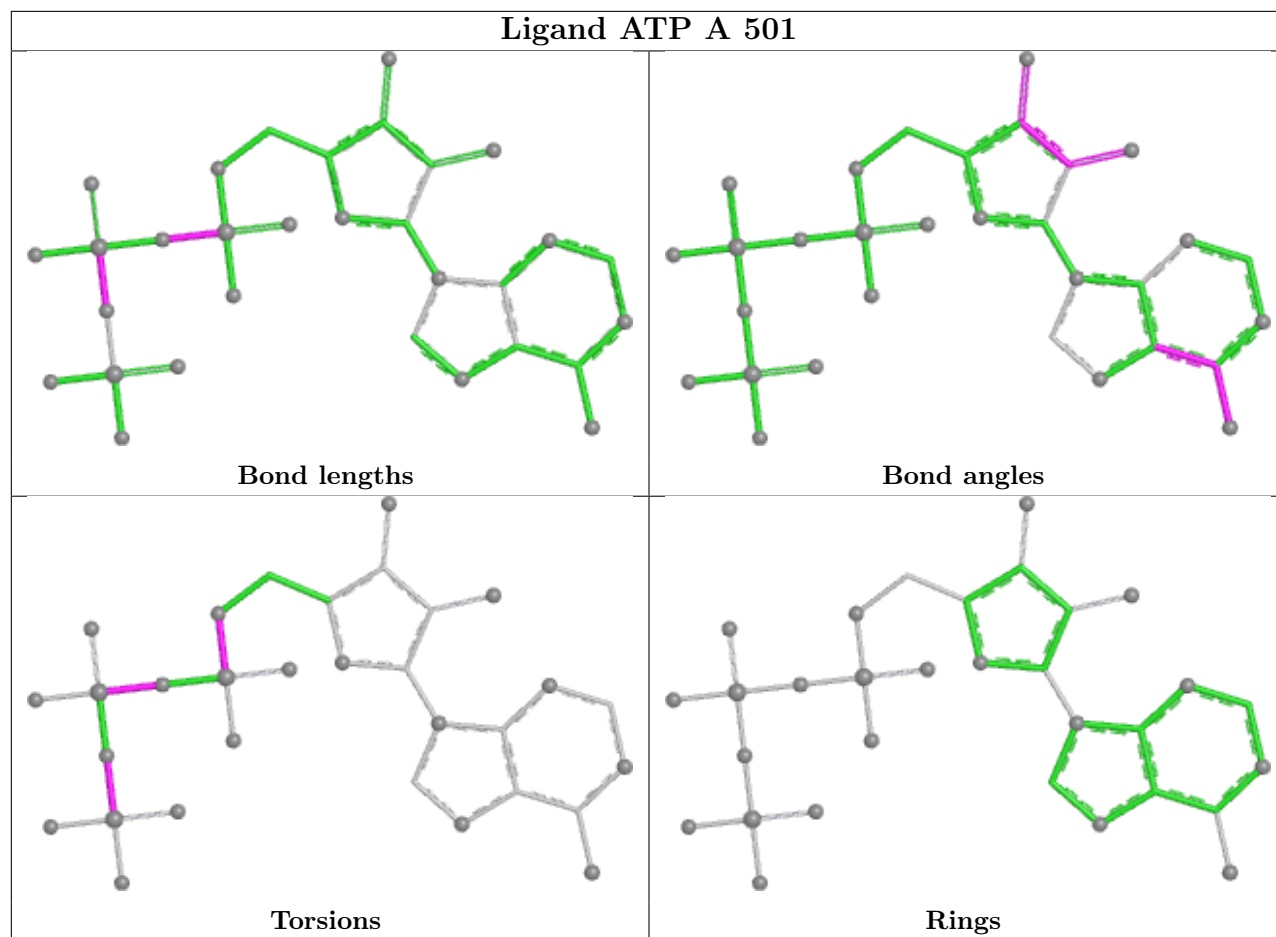
Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	C	501	ATP	3	0
35	A	501	ATP	3	0
37	E	401	ADP	2	0
37	D	501	ADP	6	0
37	F	501	ADP	2	0

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.

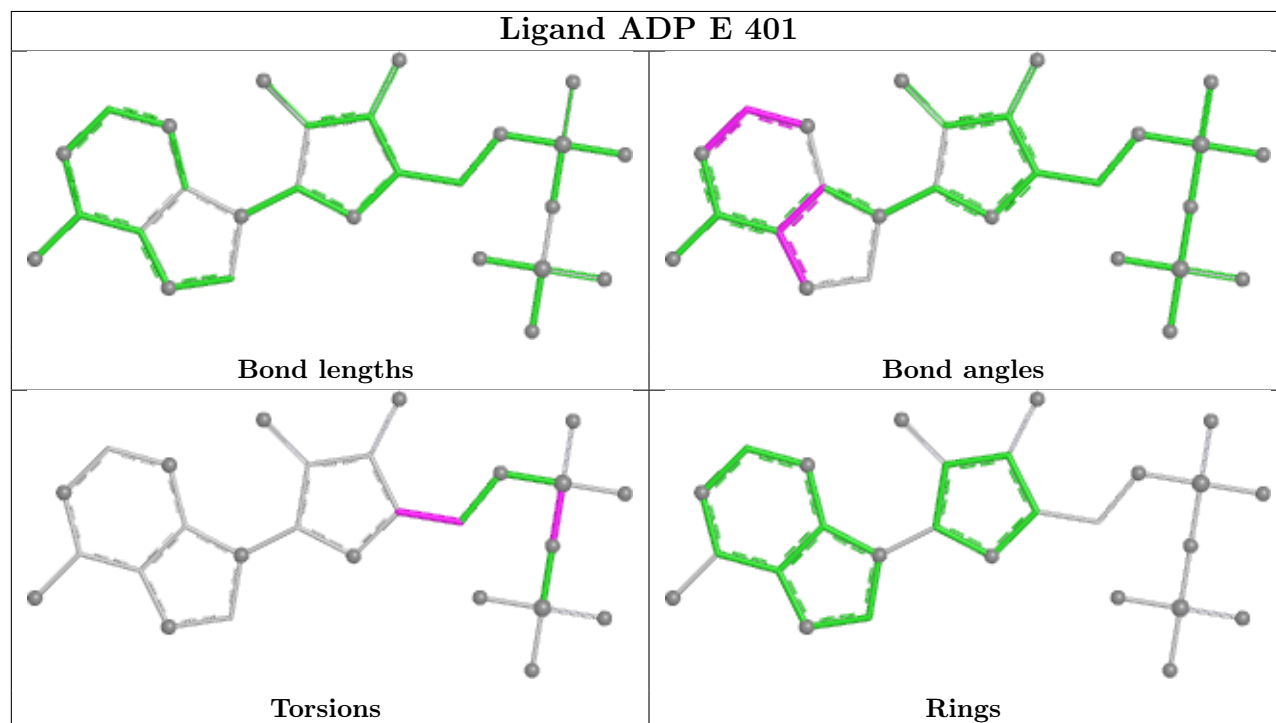


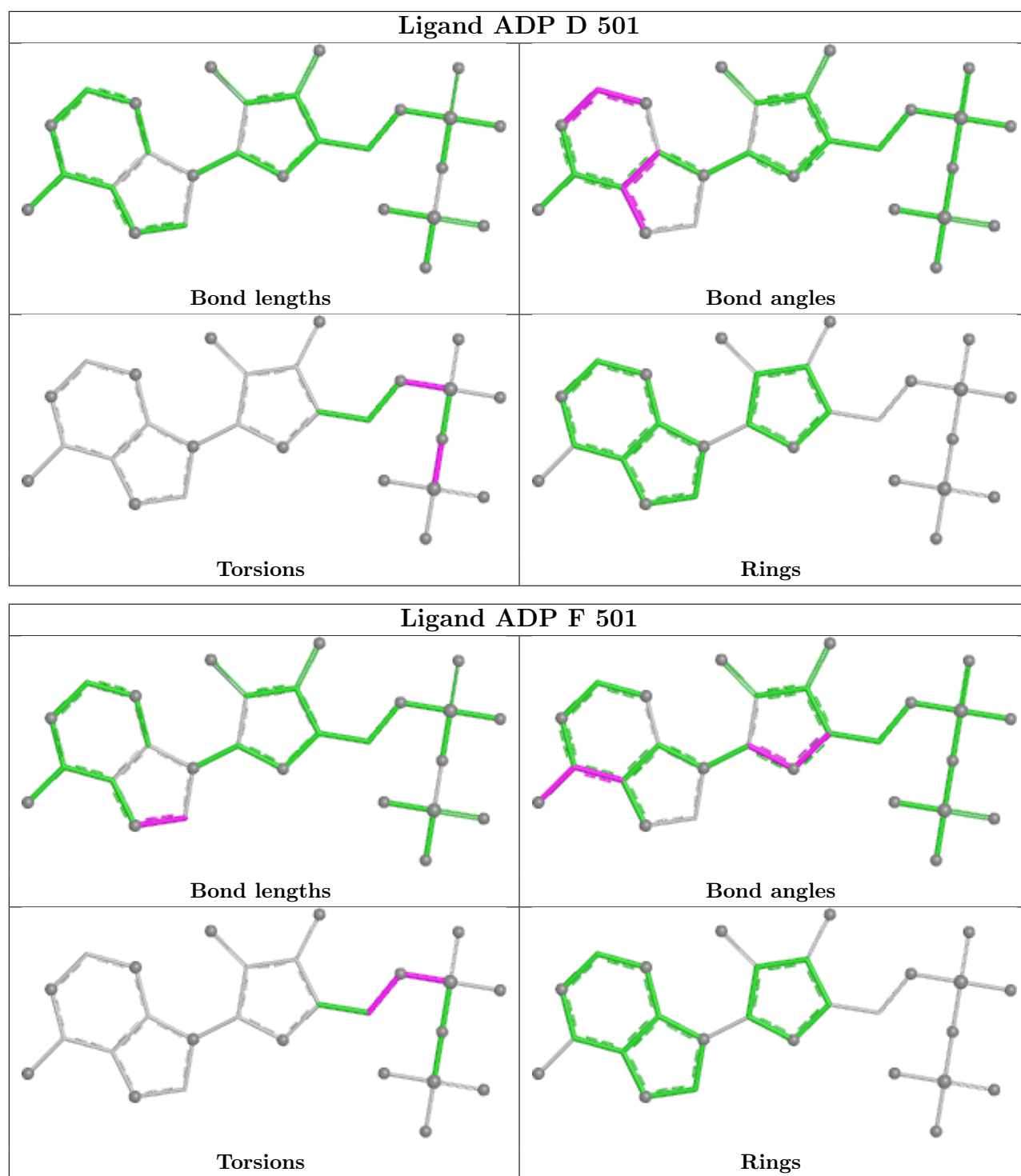


Ligand ATP A 501



Ligand ADP E 401





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

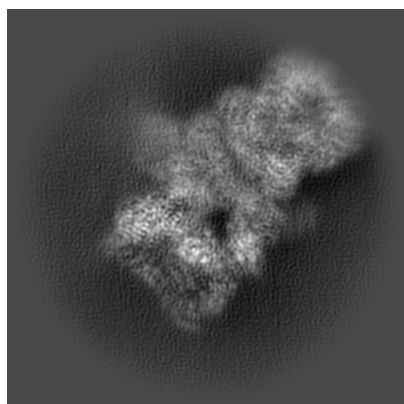
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44952. These allow visual inspection of the internal detail of the map and identification of artifacts.

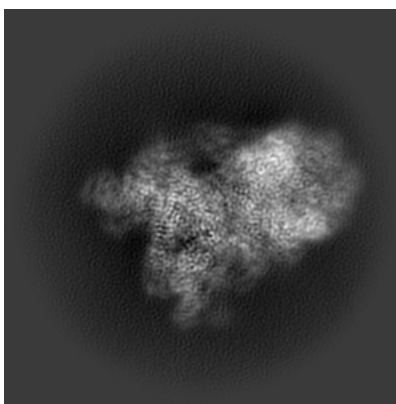
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

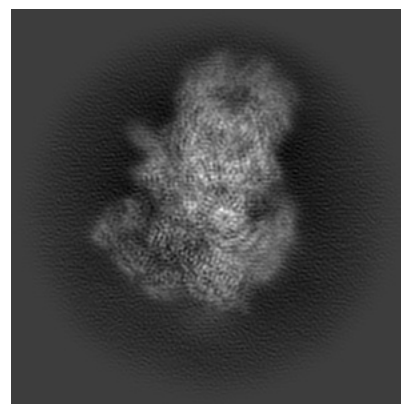
6.1.1 Primary map



X

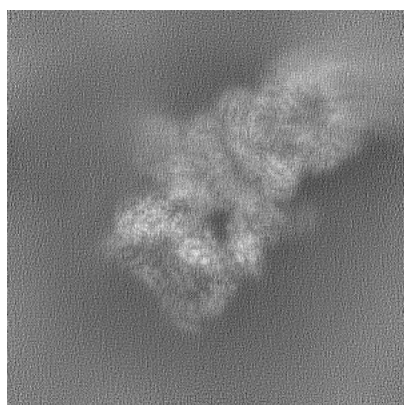


Y

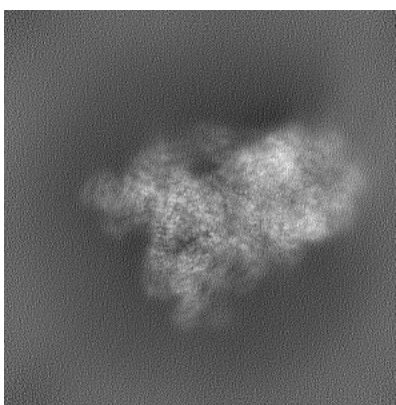


Z

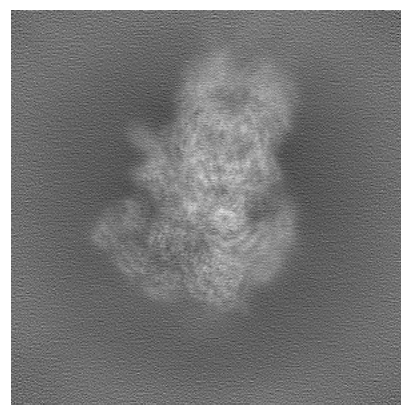
6.1.2 Raw map



X



Y

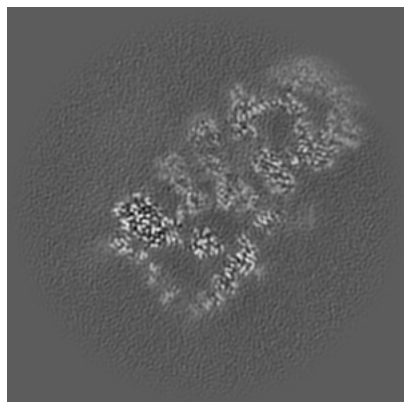


Z

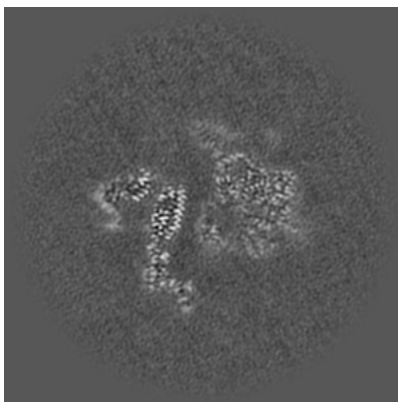
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

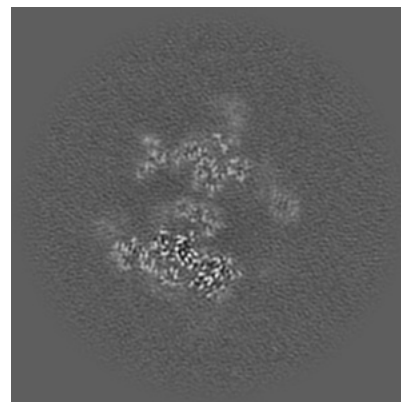
6.2.1 Primary map



X Index: 220

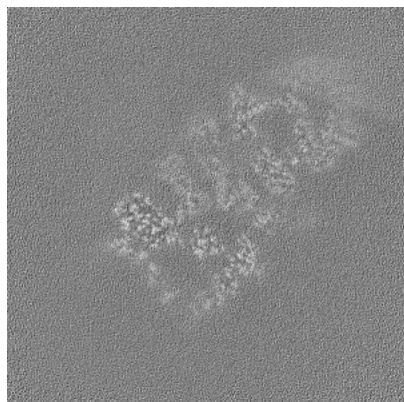


Y Index: 220

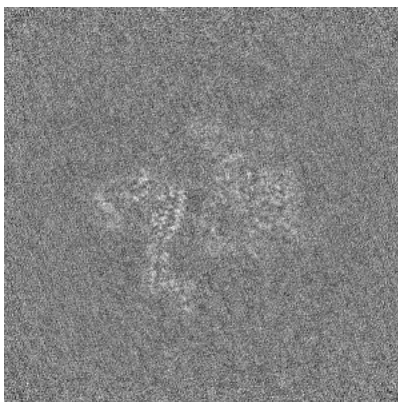


Z Index: 220

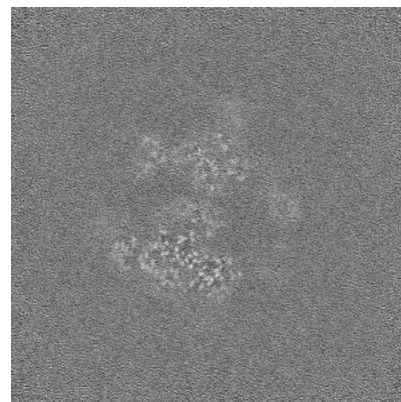
6.2.2 Raw map



X Index: 220



Y Index: 220

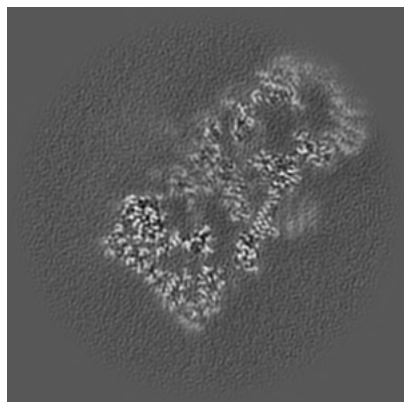


Z Index: 220

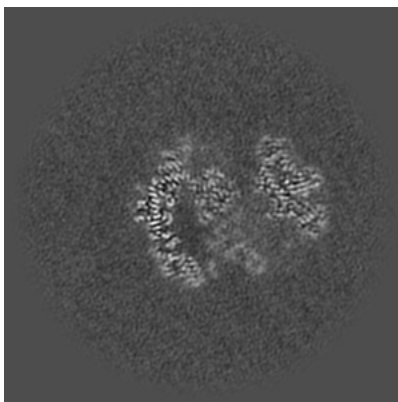
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

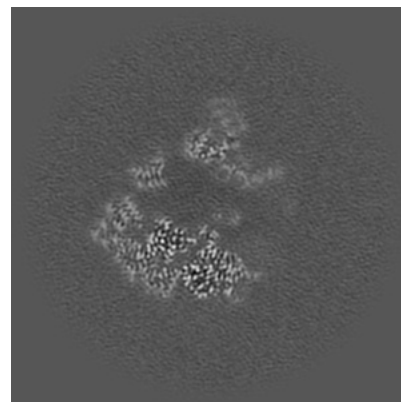
6.3.1 Primary map



X Index: 232

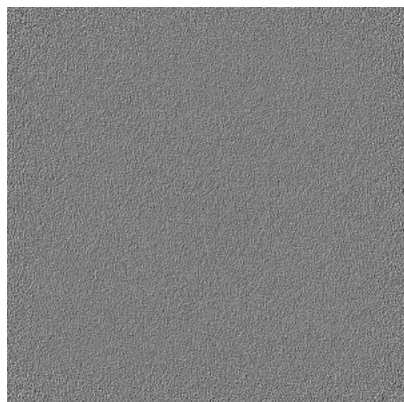


Y Index: 256

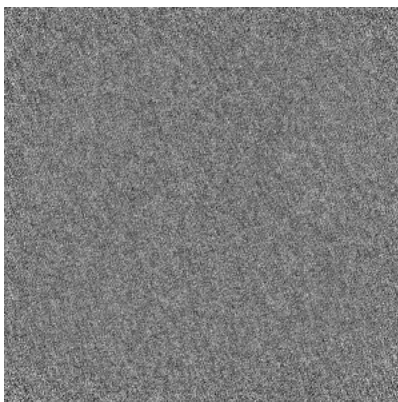


Z Index: 203

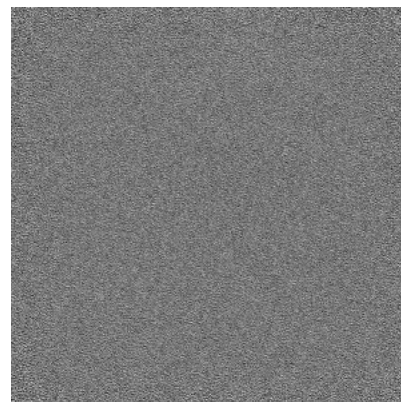
6.3.2 Raw map



X Index: 0



Y Index: 0

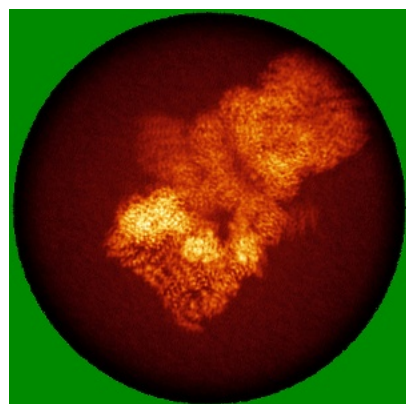


Z Index: 0

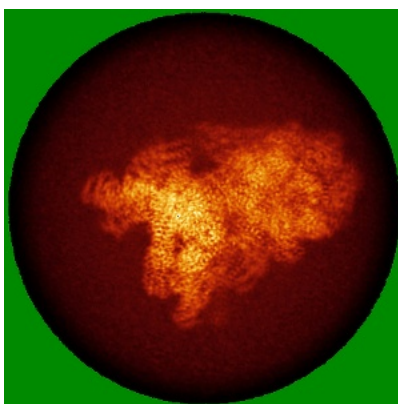
The images above show the largest variance slices of the map in three orthogonal directions.

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

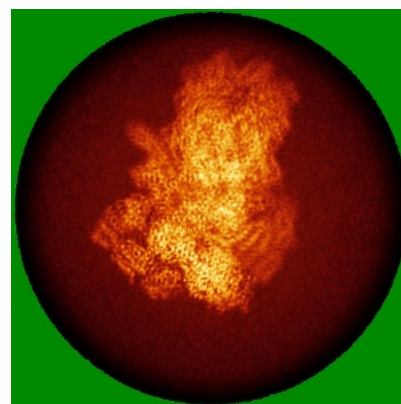
6.4.1 Primary map



X

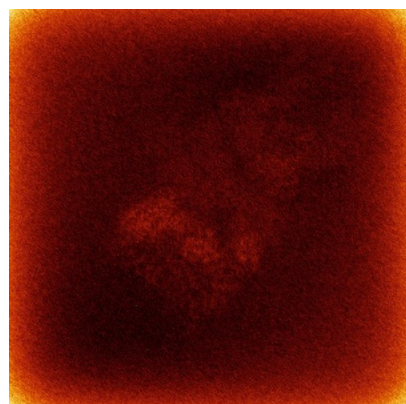


Y

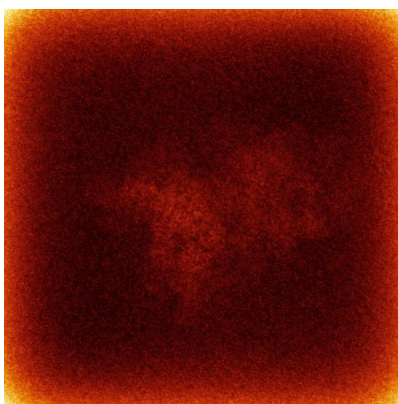


Z

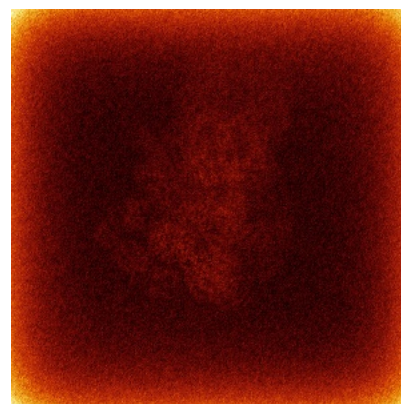
6.4.2 Raw map



X



Y

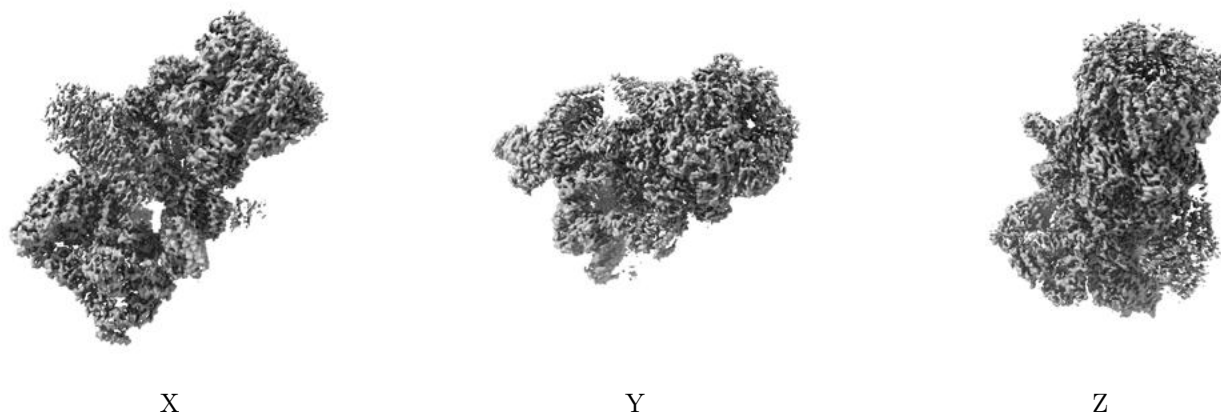


Z

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.

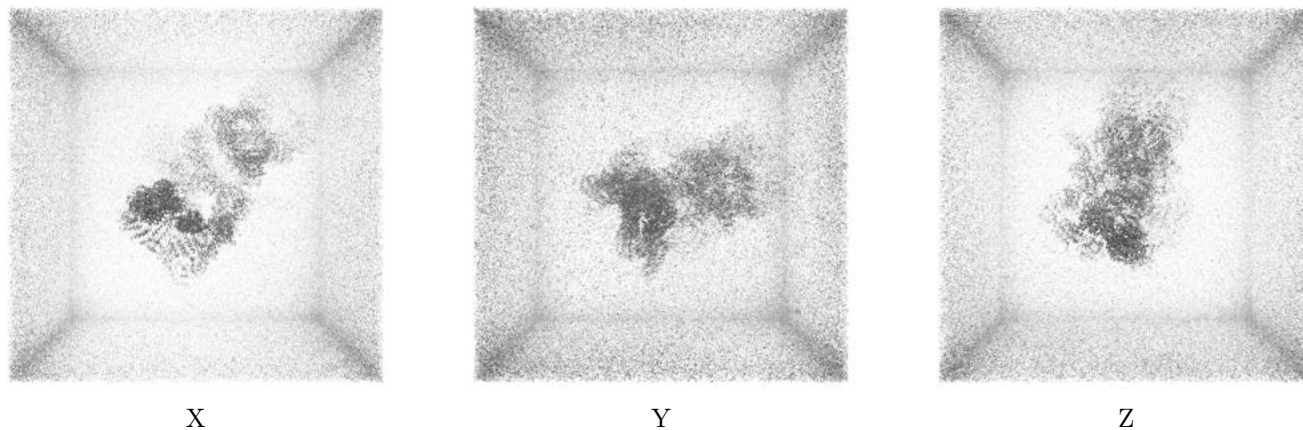
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. 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.

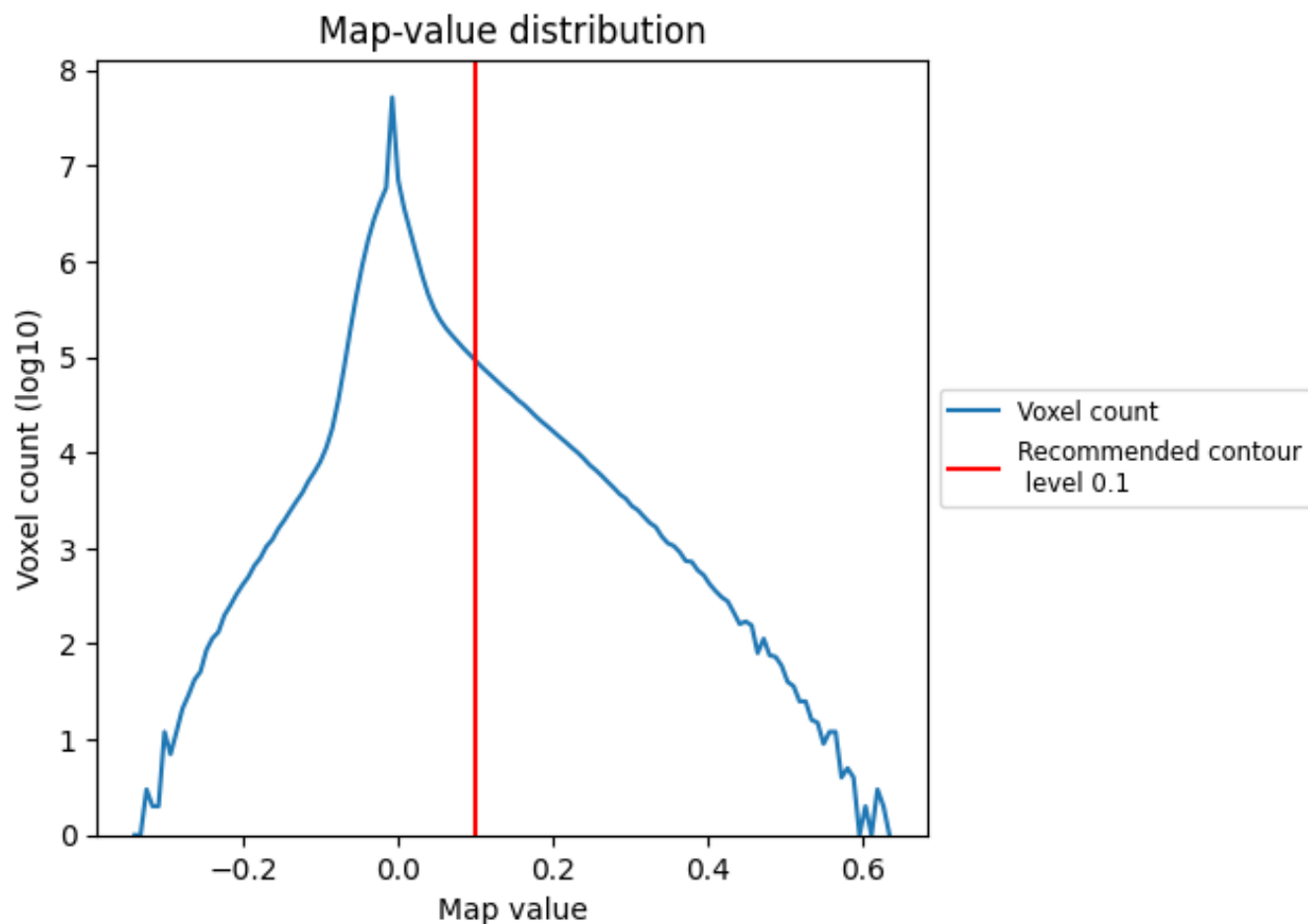
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

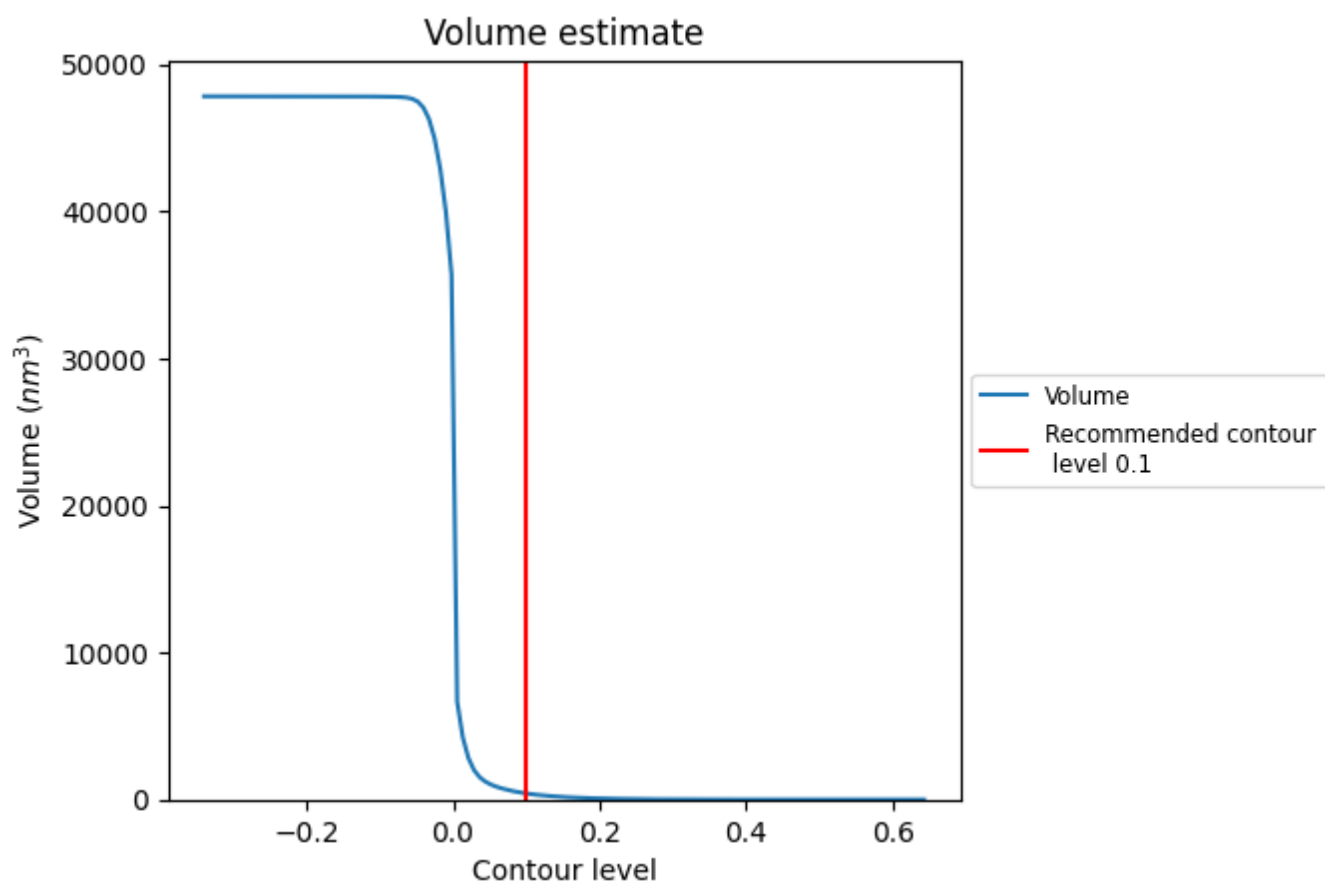
This section contains the results of statistical analysis of the map.

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.

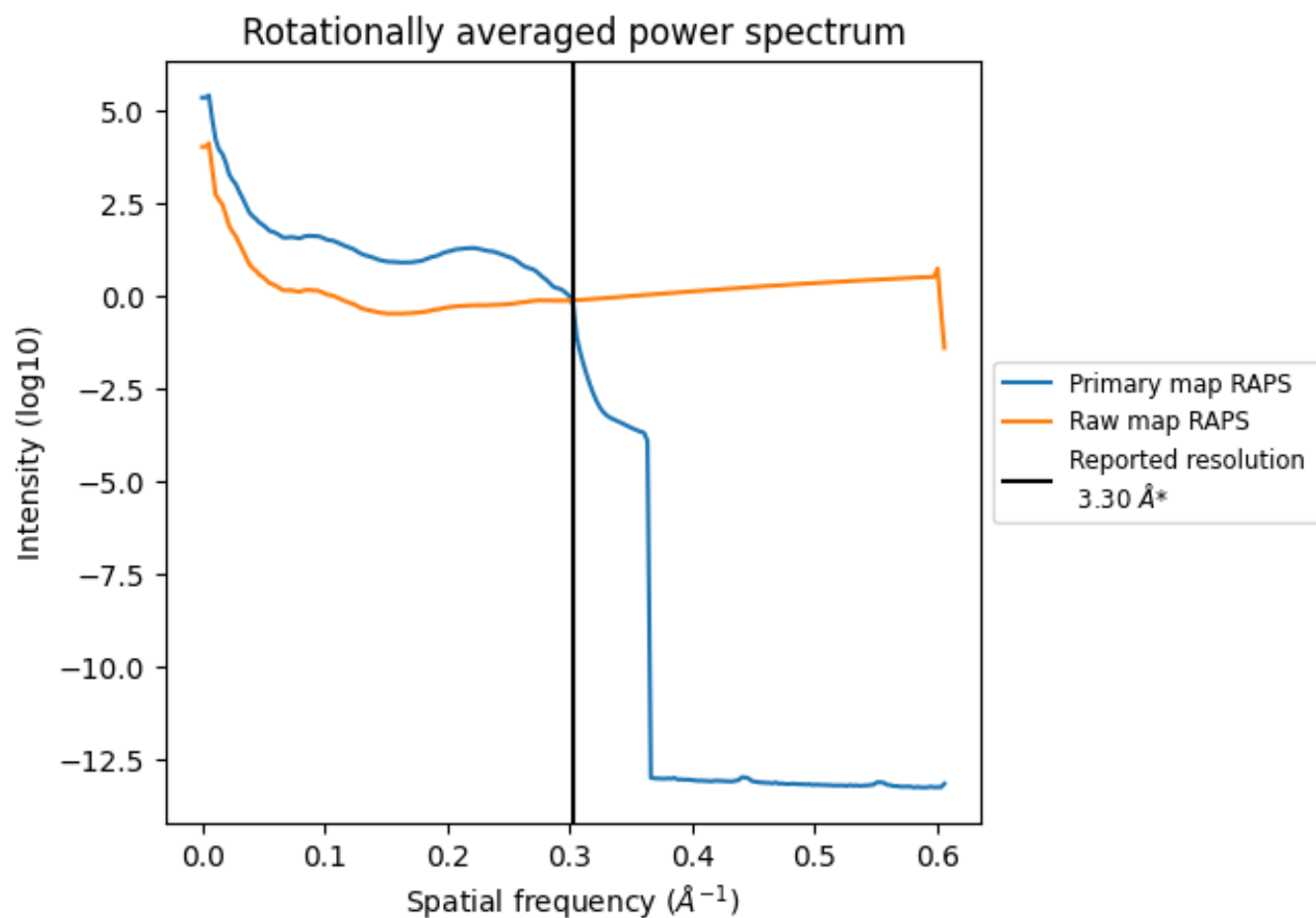
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 415 nm³; this corresponds to an approximate mass of 375 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 ⓘ

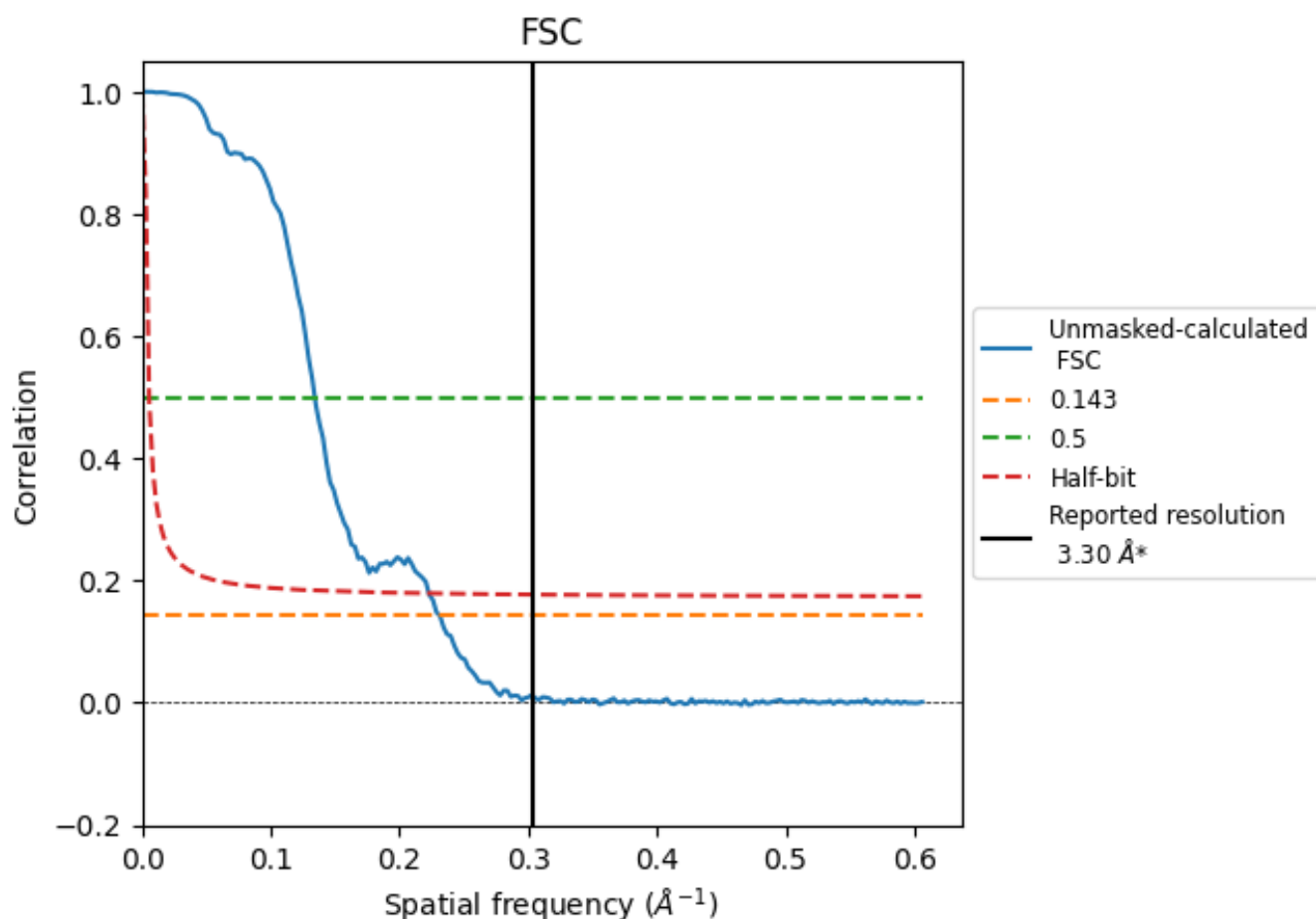


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

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 0.303 Å⁻¹

8.2 Resolution estimates [i](#)

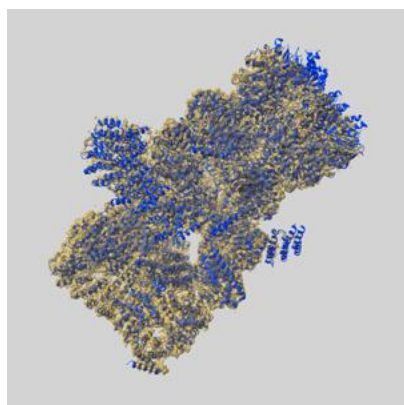
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.33	7.46	4.49

*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 4.33 differs from the reported value 3.3 by more than 10 %

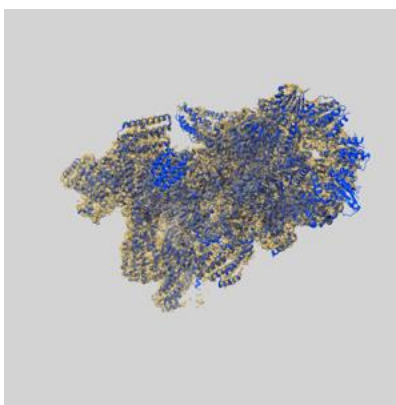
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-44952 and PDB model 9BW4. Per-residue inclusion information can be found in [section 3](#) on [page 12](#).

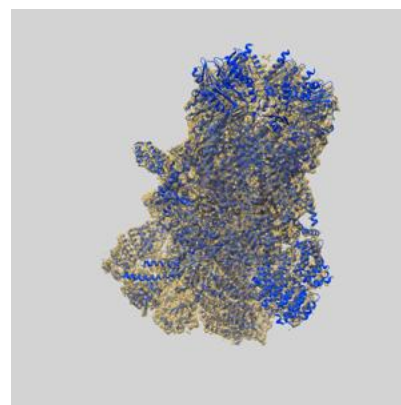
9.1 Map-model overlay [i](#)



X



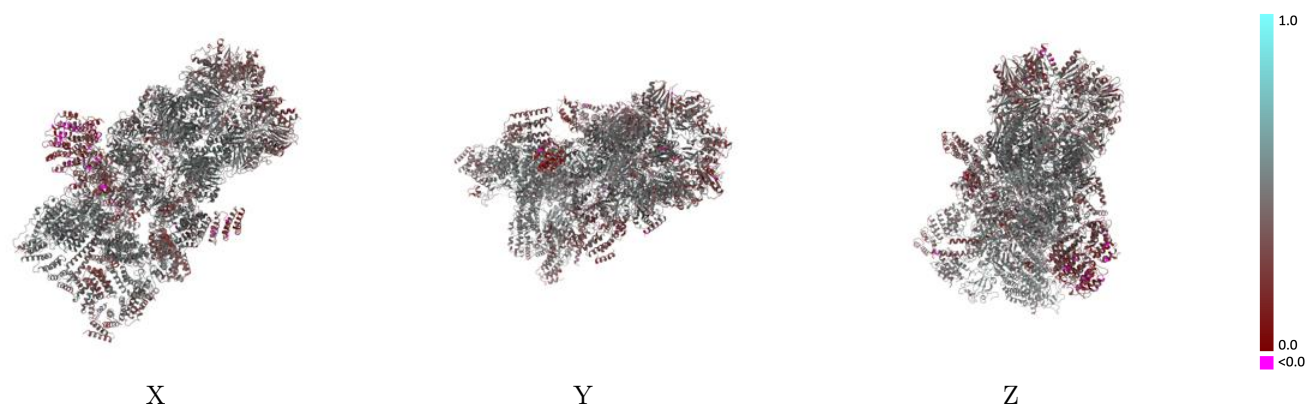
Y



Z

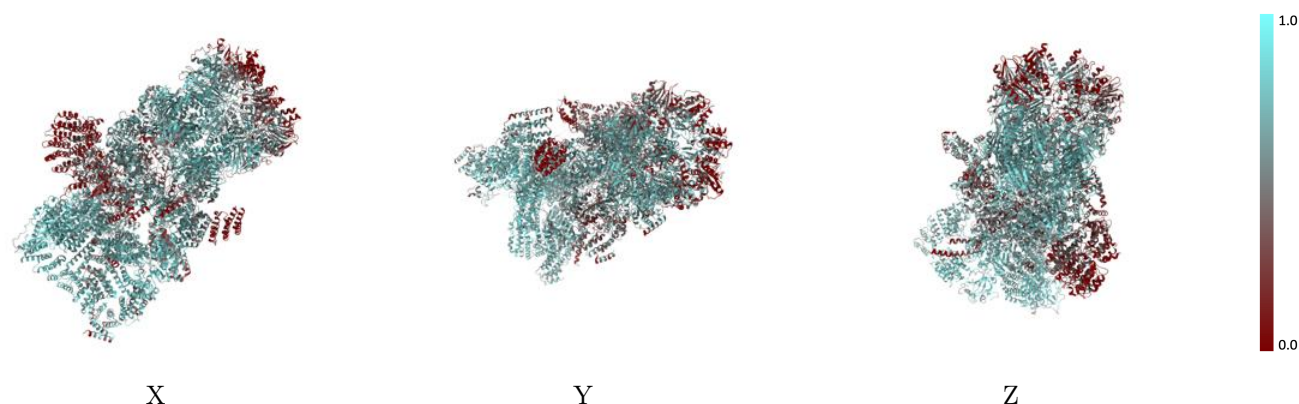
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



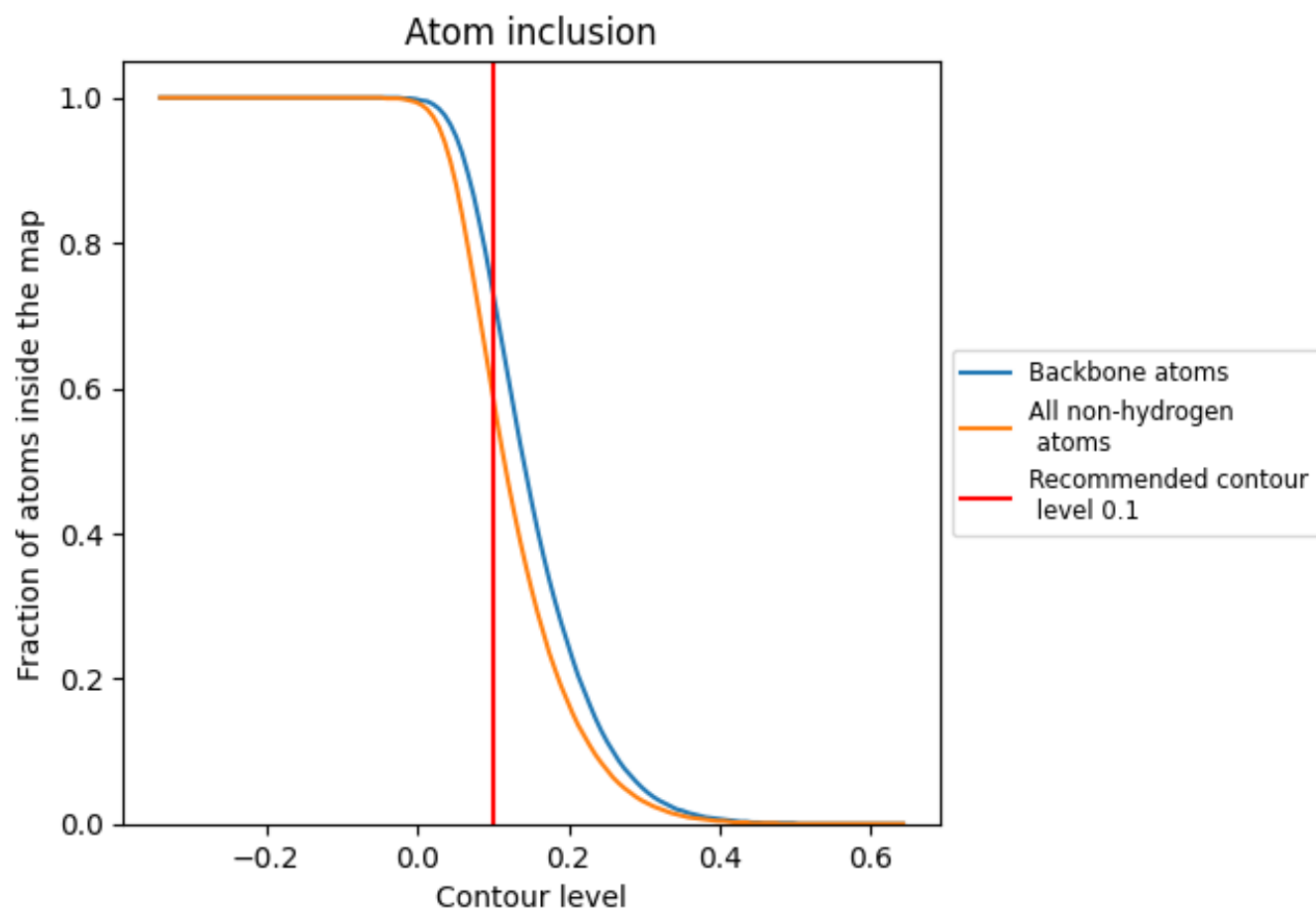
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 59% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5890	 0.4290
A	 0.5130	 0.4200
B	 0.5430	 0.4470
C	 0.6400	 0.4670
D	 0.6060	 0.4520
E	 0.4040	 0.3570
F	 0.4630	 0.4150
G	 0.6670	 0.4630
H	 0.7210	 0.5060
I	 0.6300	 0.4600
J	 0.6450	 0.4600
K	 0.6790	 0.4660
L	 0.7270	 0.4890
M	 0.6620	 0.4510
N	 0.6380	 0.4560
O	 0.6570	 0.4670
P	 0.6940	 0.4850
Q	 0.6460	 0.4490
R	 0.7010	 0.4520
S	 0.6720	 0.4510
T	 0.6810	 0.4590
U	 0.7520	 0.4760
V	 0.6870	 0.4250
W	 0.6170	 0.4120
X	 0.5200	 0.3950
Y	 0.7030	 0.4430
Z	 0.7690	 0.5030
a	 0.7140	 0.4270
b	 0.7540	 0.4510
c	 0.7740	 0.4980
d	 0.6320	 0.3910
e	 0.6810	 0.4530
f	 0.2170	 0.2630
n	 0.3040	 0.3700
o	 0.2210	 0.3400



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Chain	Atom inclusion	Q-score
p	 0.2800	 0.3700
q	 0.3150	 0.3850
r	 0.3980	 0.3970
s	 0.4530	 0.4100
t	 0.4620	 0.3980
x	 0.7180	 0.4650