



wwPDB EM Validation Summary Report ⓘ

Jun 3, 2025 – 04:14 PM EDT

PDB ID : 9BV2 / pdb_00009bv2
EMDB ID : EMD-44929
Title : M2B Midnolin-Proteasome (translocating)
Authors : Gao, J.; Yip, M.C.J.; Shao, S.
Deposited on : 2024-05-19
Resolution : 3.40 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

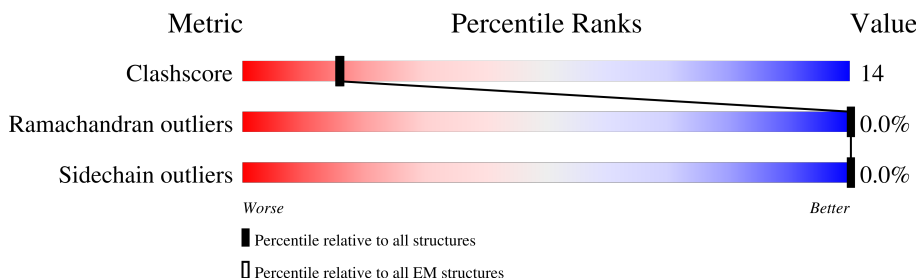
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY









The reported resolution of this entry is 3.40 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.





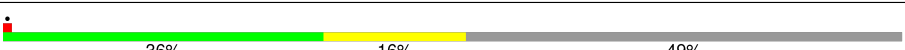
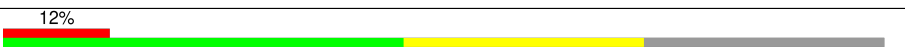

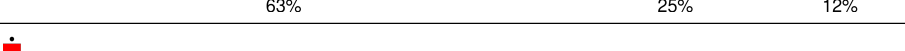
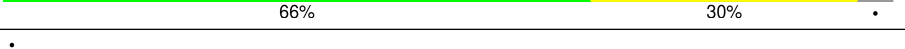





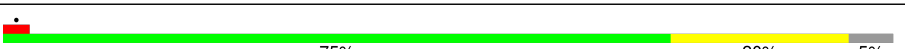


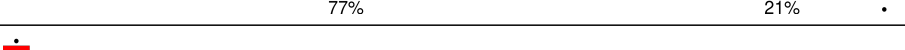





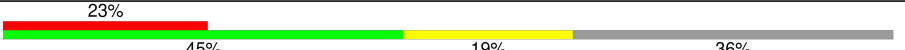


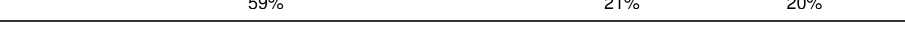
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	A	433	
13	B	440	
14	C	406	
15	D	418	
16	E	389	
17	F	439	
18	G	246	
19	H	234	
20	I	261	
21	J	248	
22	K	241	
23	L	263	
24	M	255	
25	N	239	
25	n	239	
26	O	277	
26	o	277	
27	P	205	
27	p	205	
28	Q	201	
28	q	201	
29	R	263	

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Mol	Chain	Length	Quality of chain
29	r	263	
30	S	241	
30	s	241	
31	T	264	
31	t	264	
32	f	908	
33	y	505	

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 88606 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	852	Total	C	N	O	S	0	0
			6640	4215	1128	1252	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	430	Total	C	N	O	S	0	0
			3510	2224	601	662	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 regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	A	316	Total	C	N	O	S	0	0
			2518	1598	440	467	13		

- Molecule 13 is a protein called 26S proteasome regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	B	386	Total	C	N	O	S	0	0
			3037	1916	514	592	15		

- Molecule 14 is a protein called 26S protease regulatory subunit 8.

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

- Molecule 15 is a protein called 26S proteasome regulatory subunit 6B.

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

- Molecule 16 is a protein called 26S protease regulatory subunit 10B.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	E	341	Total	C	N	O	S	0	0
			2706	1699	484	507	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	F	231	Total	C	N	O	S	0	0
			1812	1152	311	337	12		

- Molecule 18 is a protein called Proteasome subunit alpha type-6.

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

- Molecule 19 is a protein called Proteasome subunit alpha type-2.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	I	249	Total	C	N	O	S	0	0
			1963	1242	336	375	10		

- Molecule 21 is a protein called Proteasome subunit alpha type-7.

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

- Molecule 22 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	K	235	Total	C	N	O	S	0	0
			1804	1132	299	362	11		

- Molecule 23 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	L	237	Total	C	N	O	S	0	0
			1868	1168	338	351	11		

- Molecule 24 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	M	244	Total	C	N	O	S	0	0
			1916	1212	325	368	11		

- Molecule 25 is a protein called Proteasome subunit beta type-6.

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

- Molecule 26 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	O	221	Total	C	N	O	S	0	0
			1667	1050	284	321	12		
26	o	176	Total	C	N	O	S	0	0
			1315	823	228	253	11		

- Molecule 27 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	P	204	Total	C	N	O	S	0	0
			1591	1013	265	294	19		

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Mol	Chain	Residues	Atoms					AltConf	Trace
27	p	164	Total	C	N	O	S	0	0
			1264	802	210	235	17		

- Molecule 28 is a protein called Proteasome subunit beta type-2.

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

- Molecule 29 is a protein called Proteasome subunit beta type-5.

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

- Molecule 30 is a protein called Proteasome subunit beta type-1.

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

- Molecule 31 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	T	213	Total	C	N	O	S	0	0
			1665	1050	288	316	11		
31	t	206	Total	C	N	O	S	0	0
			1609	1016	279	302	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
32	f	819	Total	C	N	O	S	0	0
			6351	4019	1073	1215	44		

- Molecule 33 is a protein called Midnolin.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	y	31	Total	C	N	O	S	0	0
			273	164	66	42	1		

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
y	-36	MET	-	initiating methionine	UNP Q504T8
y	-35	ASP	-	expression tag	UNP Q504T8
y	-34	TYR	-	expression tag	UNP Q504T8
y	-33	LYS	-	expression tag	UNP Q504T8
y	-32	ASP	-	expression tag	UNP Q504T8
y	-31	ASP	-	expression tag	UNP Q504T8
y	-30	ASP	-	expression tag	UNP Q504T8
y	-29	ASP	-	expression tag	UNP Q504T8
y	-28	LYS	-	expression tag	UNP Q504T8
y	-27	ASP	-	expression tag	UNP Q504T8
y	-26	TYR	-	expression tag	UNP Q504T8
y	-25	LYS	-	expression tag	UNP Q504T8
y	-24	ASP	-	expression tag	UNP Q504T8
y	-23	ASP	-	expression tag	UNP Q504T8
y	-22	ASP	-	expression tag	UNP Q504T8
y	-21	ASP	-	expression tag	UNP Q504T8
y	-20	LYS	-	expression tag	UNP Q504T8
y	-19	GLY	-	expression tag	UNP Q504T8
y	-18	GLY	-	expression tag	UNP Q504T8
y	-17	GLY	-	expression tag	UNP Q504T8
y	-16	GLY	-	expression tag	UNP Q504T8
y	-15	SER	-	expression tag	UNP Q504T8
y	-14	GLY	-	expression tag	UNP Q504T8
y	-13	GLY	-	expression tag	UNP Q504T8
y	-12	GLY	-	expression tag	UNP Q504T8
y	-11	GLY	-	expression tag	UNP Q504T8
y	-10	PHE	-	expression tag	UNP Q504T8
y	-9	GLU	-	expression tag	UNP Q504T8
y	-8	THR	-	expression tag	UNP Q504T8
y	-7	SER	-	expression tag	UNP Q504T8
y	-6	LEU	-	expression tag	UNP Q504T8
y	-5	TYR	-	expression tag	UNP Q504T8
y	-4	LYS	-	expression tag	UNP Q504T8
y	-3	LYS	-	expression tag	UNP Q504T8
y	-2	ALA	-	expression tag	UNP Q504T8
y	-1	GLY	-	expression tag	UNP Q504T8
y	0	THR	-	expression tag	UNP Q504T8

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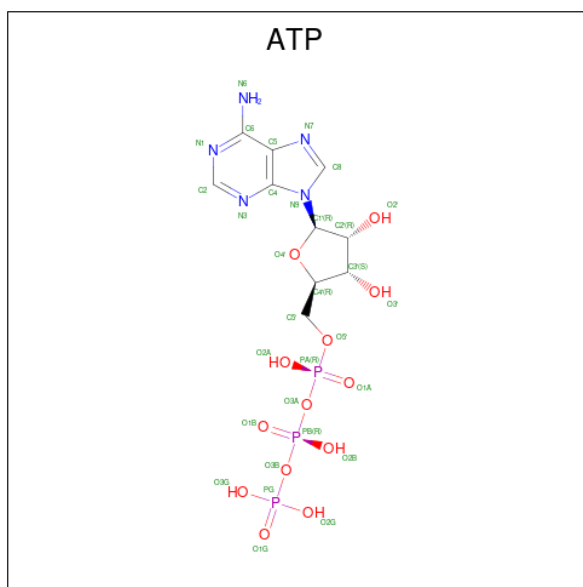
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Chain	Residue	Modelled	Actual	Comment	Reference
y	457	ALA	VAL	conflict	UNP Q504T8

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

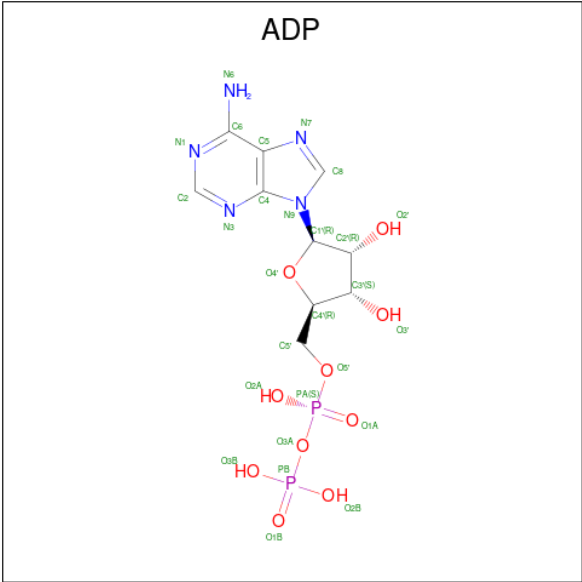
Mol	Chain	Residues	Atoms		AltConf
34	c	1	Total	Zn	0
			1	1	

- 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	
35	D	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 36 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).

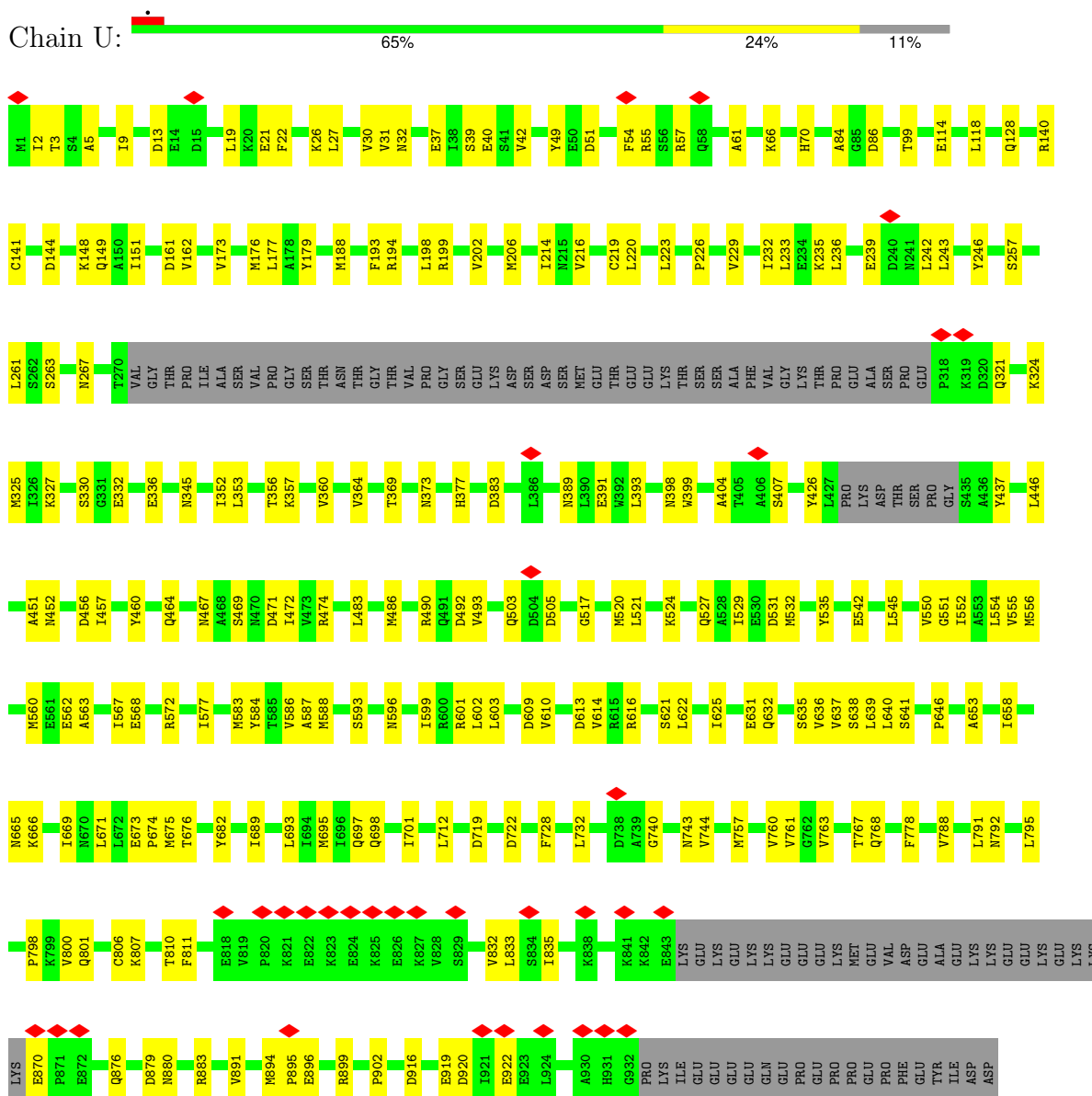


Mol	Chain	Residues	Atoms					AltConf
36	E	1	Total	C	N	O	P	0
			27	10	5	10	2	

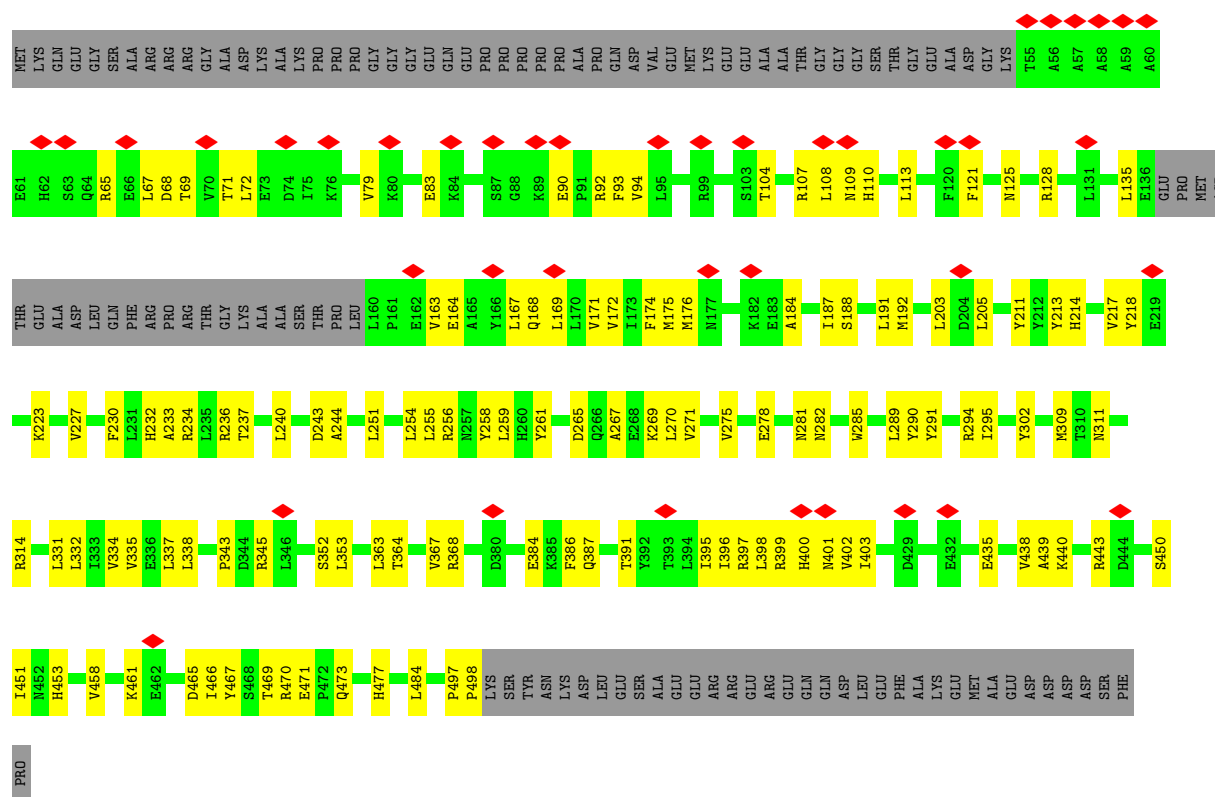
3 Residue-property plots

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

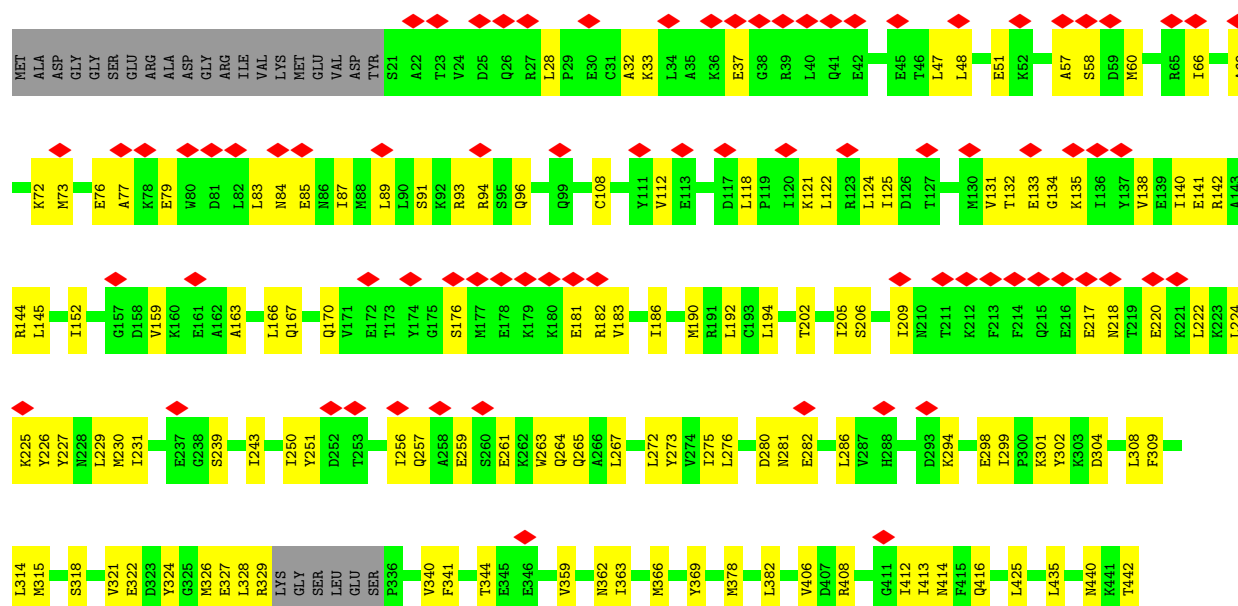
- Molecule 1: 26S proteasome non-ATPase regulatory subunit 1



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

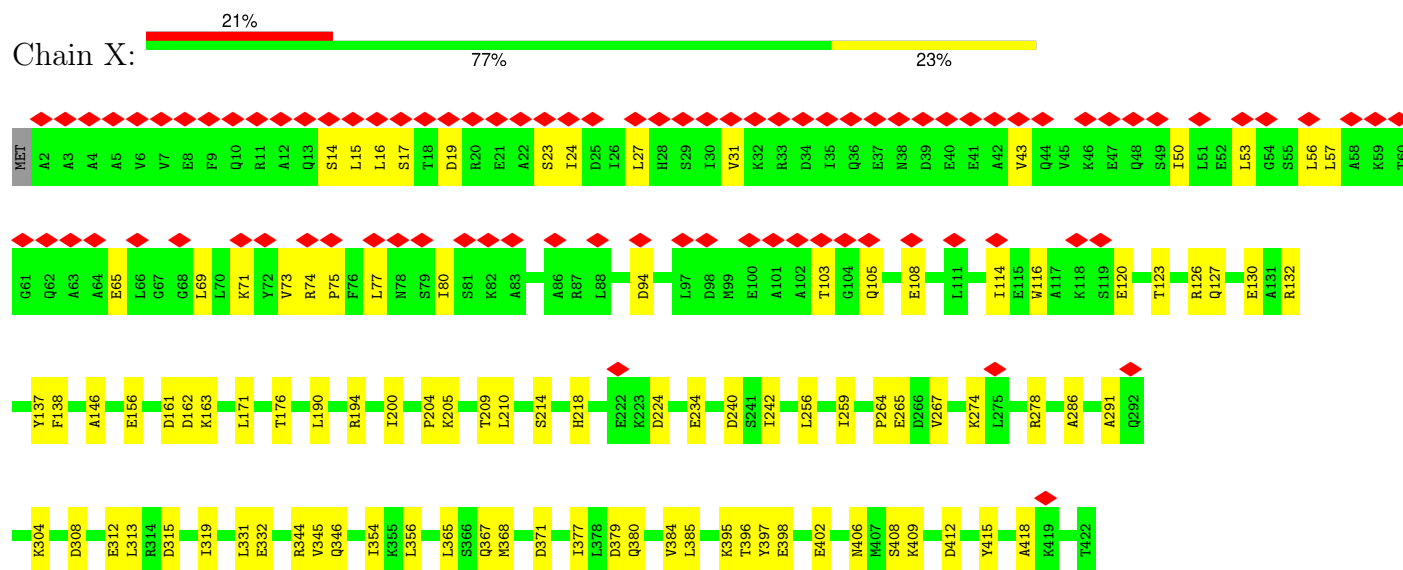


- Molecule 3: 26S proteasome non-ATPase regulatory subunit 12

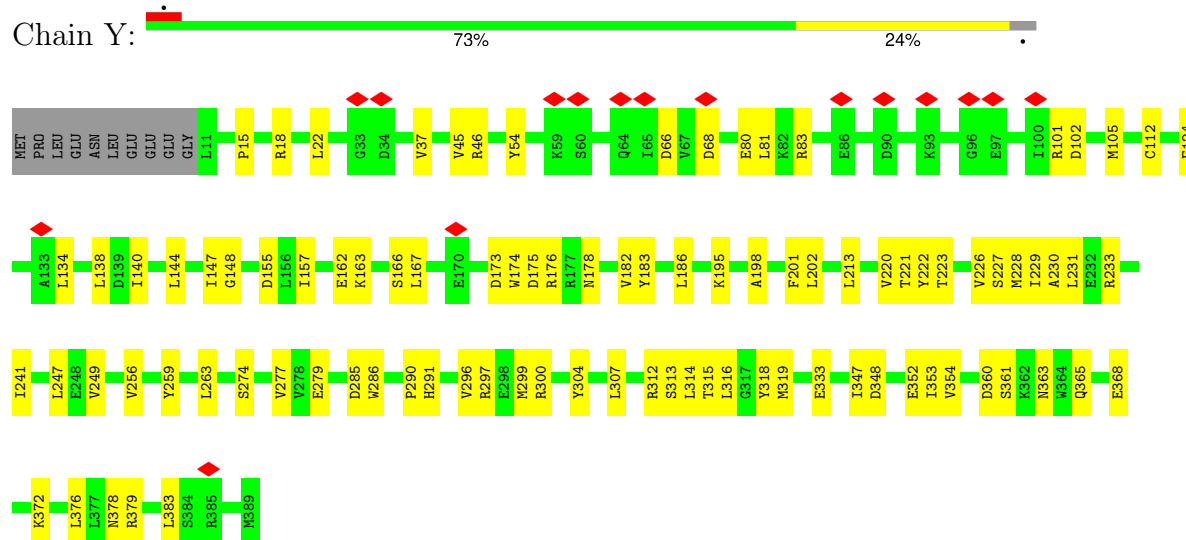




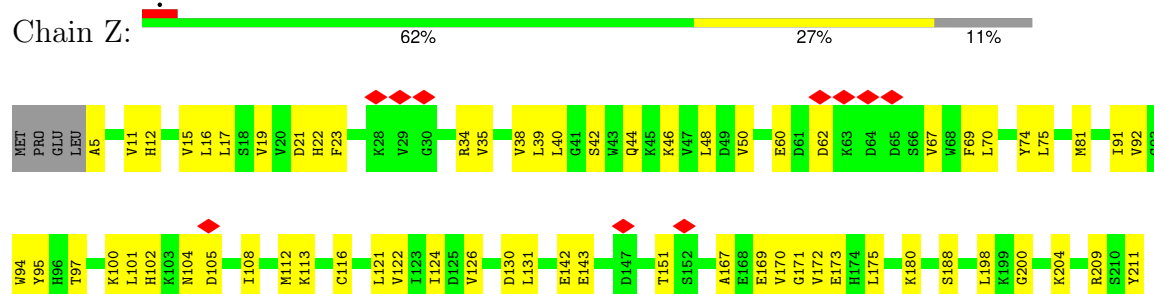
- Molecule 4: 26S proteasome non-ATPase regulatory subunit 11

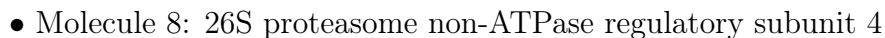


- Molecule 5: 26S proteasome non-ATPase regulatory subunit 6

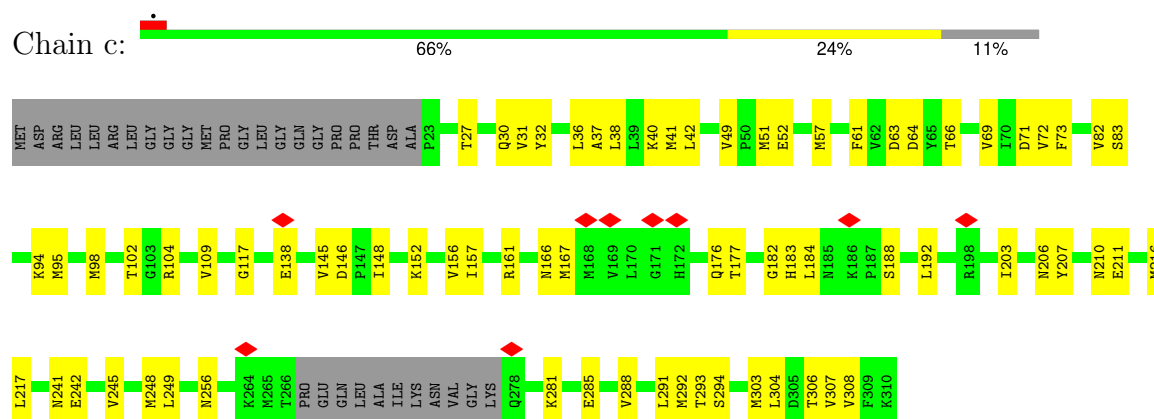


- Molecule 6: 26S proteasome non-ATPase regulatory subunit 7

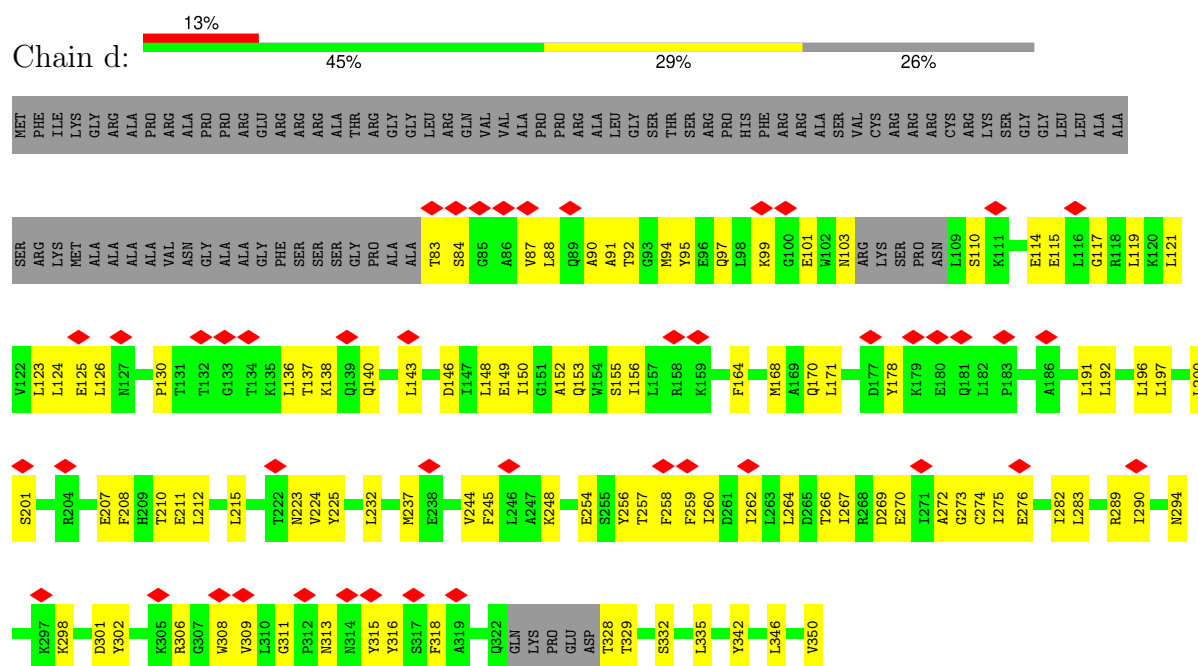




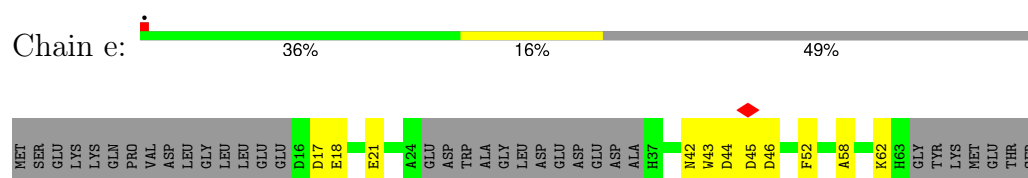
- Molecule 9: 26S proteasome non-ATPase regulatory subunit 14



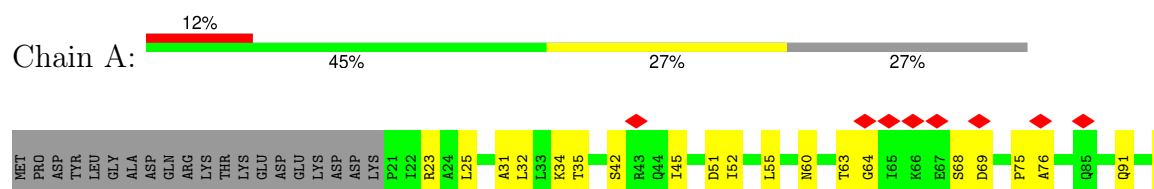
- Molecule 10: 26S proteasome non-ATPase regulatory subunit 8

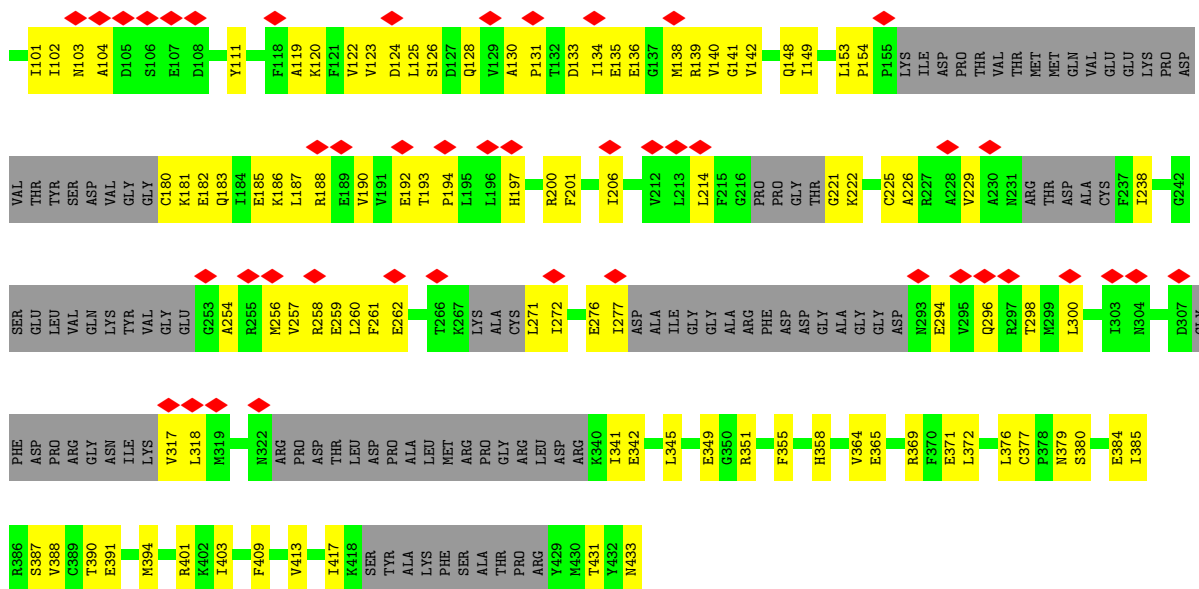


- Molecule 11: 26S proteasome complex subunit SEM1

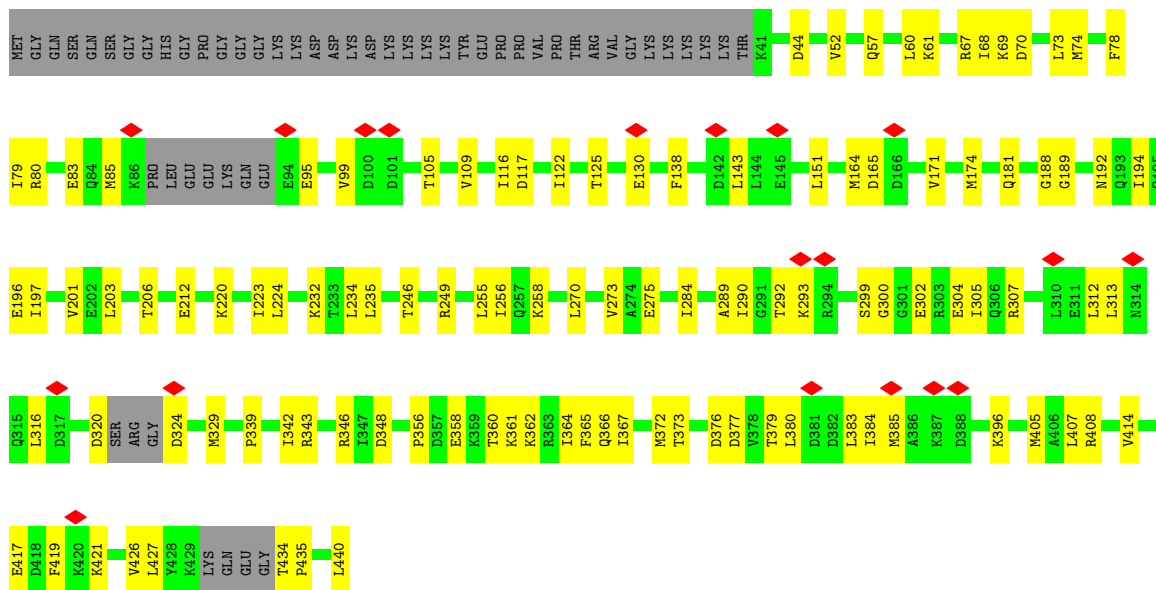


- Molecule 12: 26S proteasome regulatory subunit 7

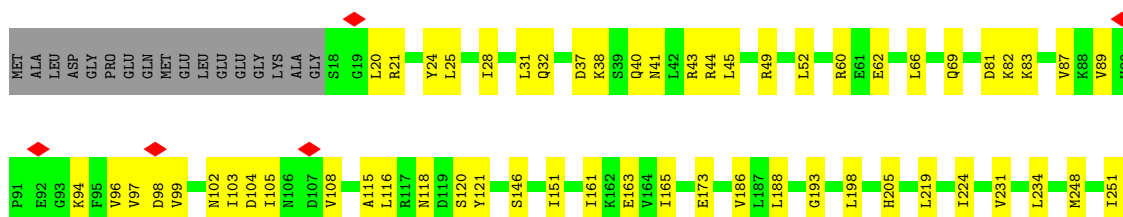


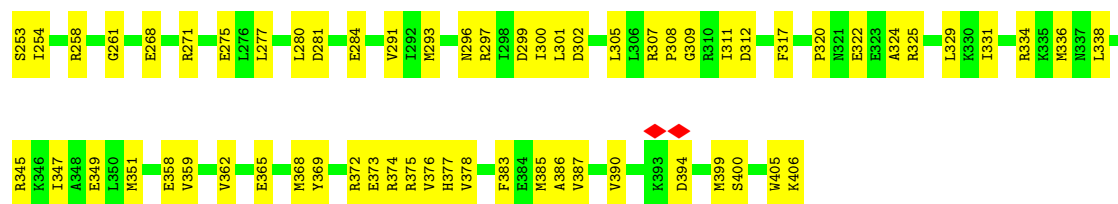


• Molecule 13: 26S proteasome regulatory subunit 4

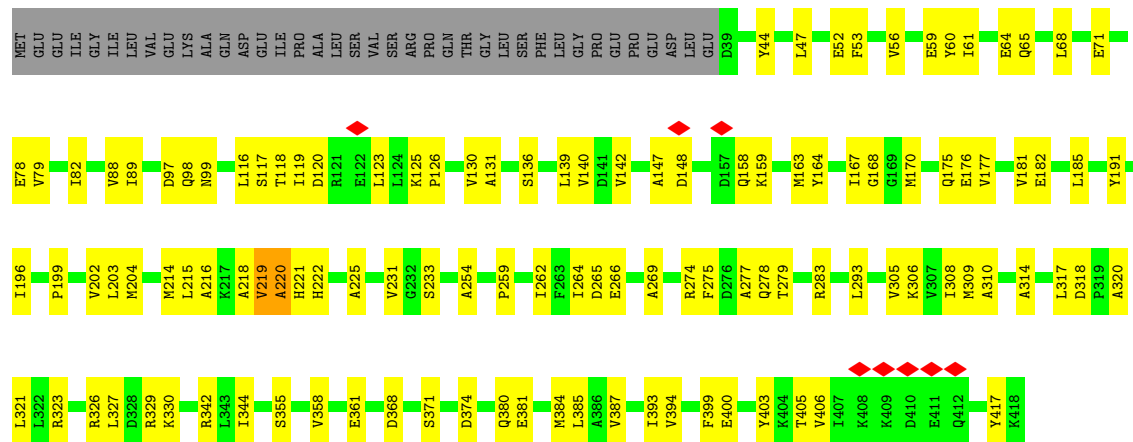


• Molecule 14: 26S protease regulatory subunit 8

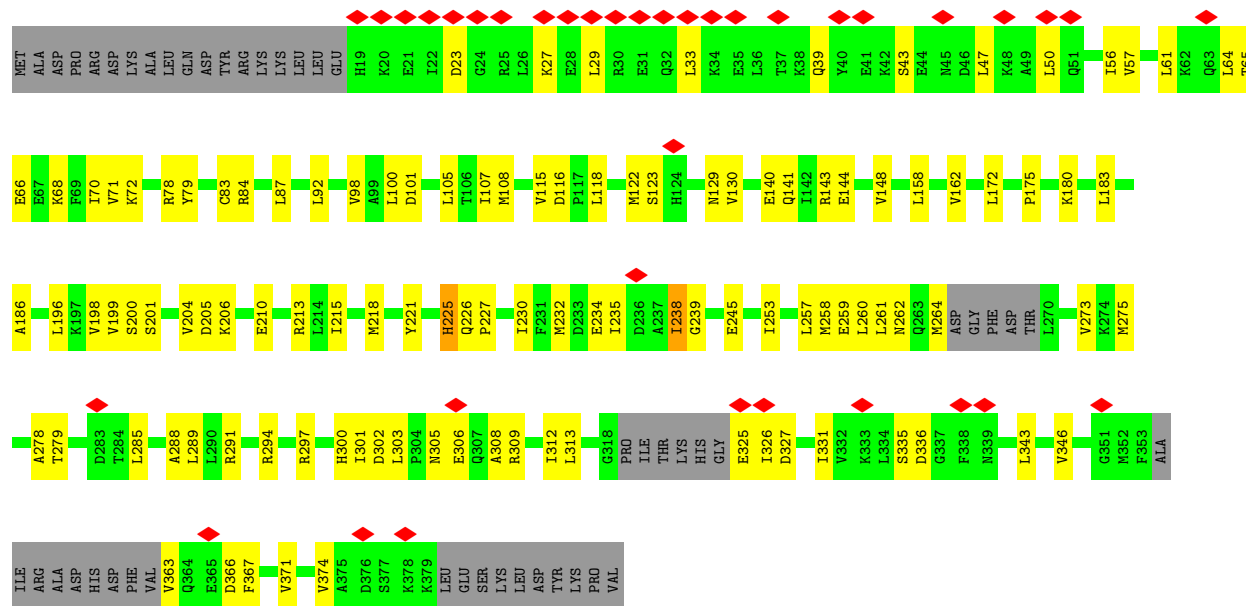




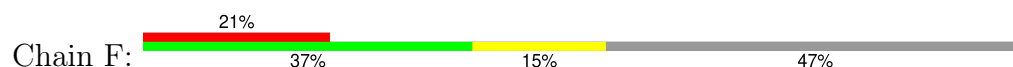
• Molecule 15: 26S proteasome regulatory subunit 6B

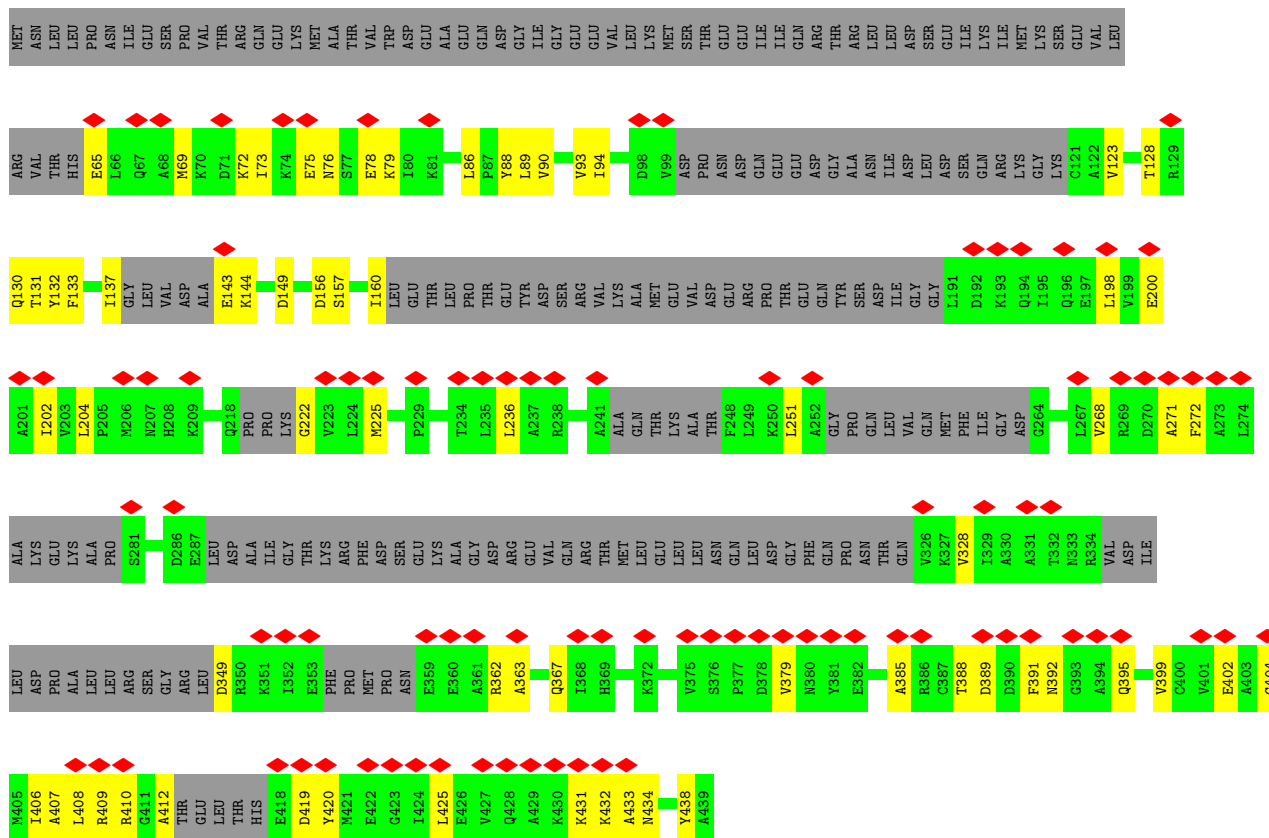


• Molecule 16: 26S protease regulatory subunit 10B

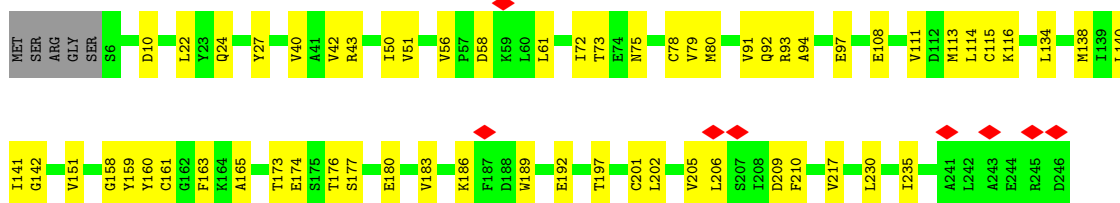


• Molecule 17: 26S proteasome regulatory subunit 6A

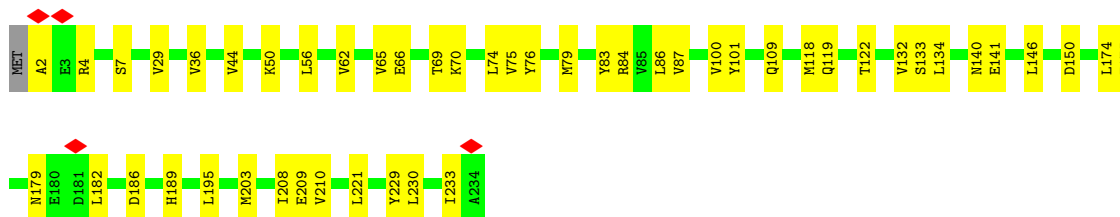
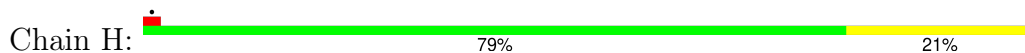




- Molecule 18: Proteasome subunit alpha type-6

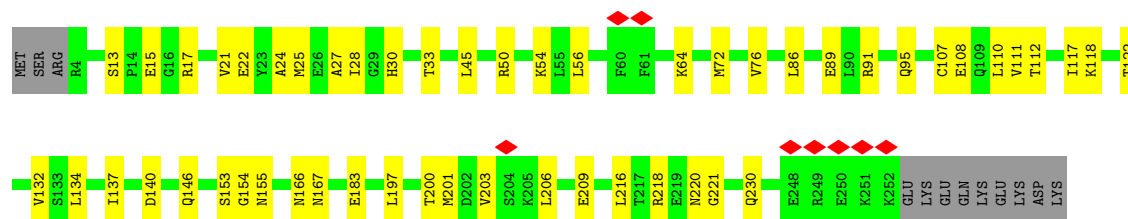


- Molecule 19: Proteasome subunit alpha type-2

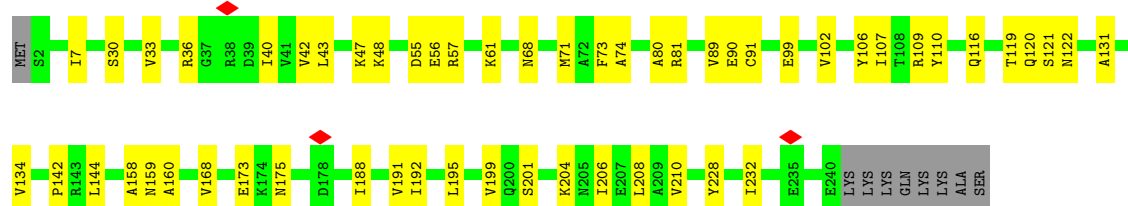


- Molecule 20: Proteasome subunit alpha type-4

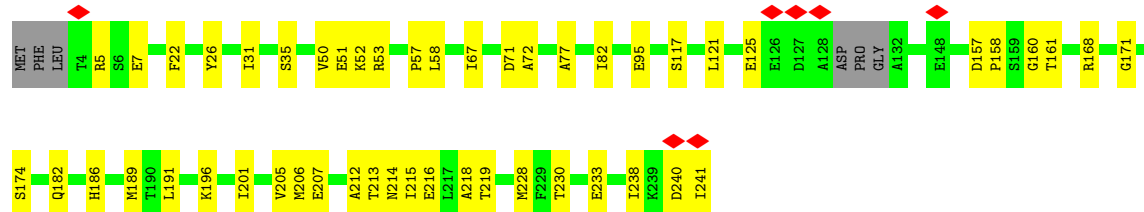
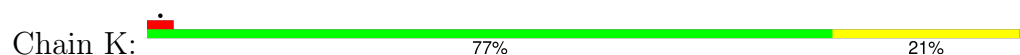




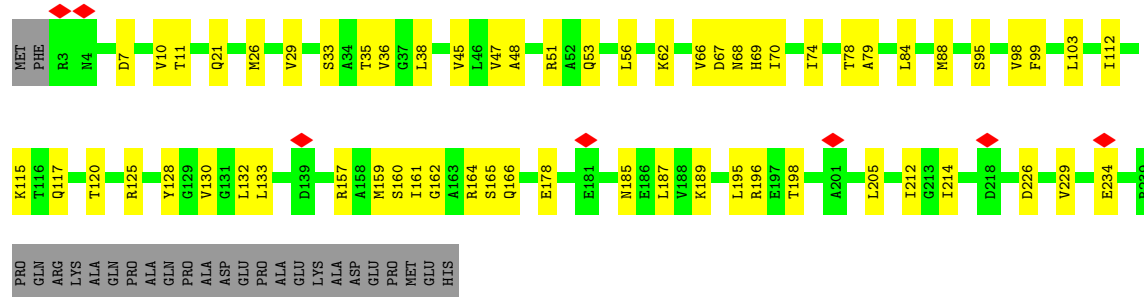
• Molecule 21: Proteasome subunit alpha type-7



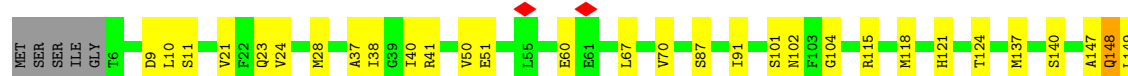
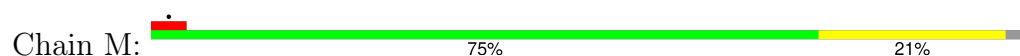
• Molecule 22: Proteasome subunit alpha type-5

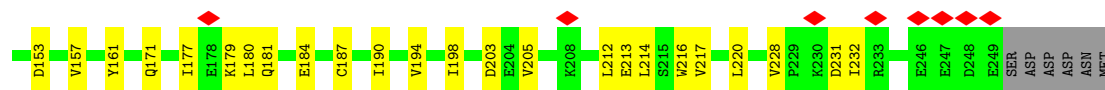


• Molecule 23: Proteasome subunit alpha type-1

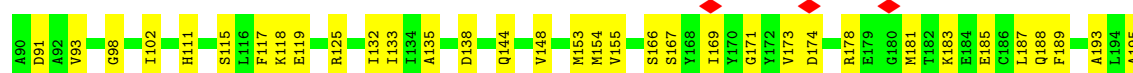
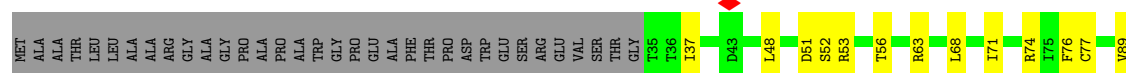


• Molecule 24: Proteasome subunit alpha type-3

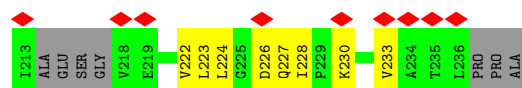
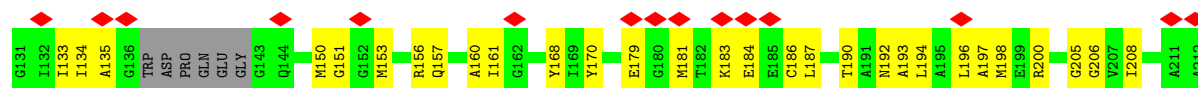
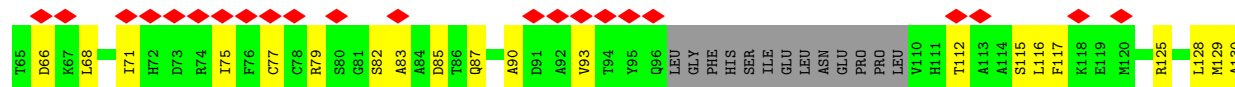
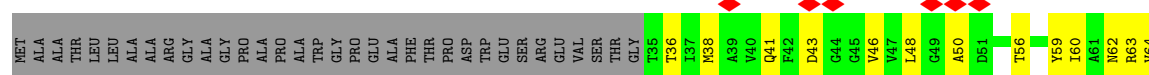




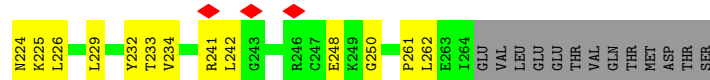
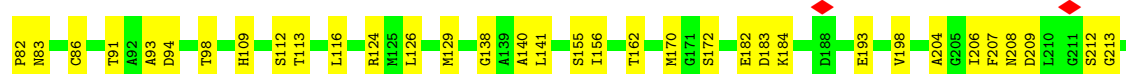
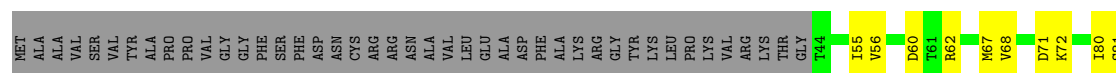
• Molecule 25: Proteasome subunit beta type-6



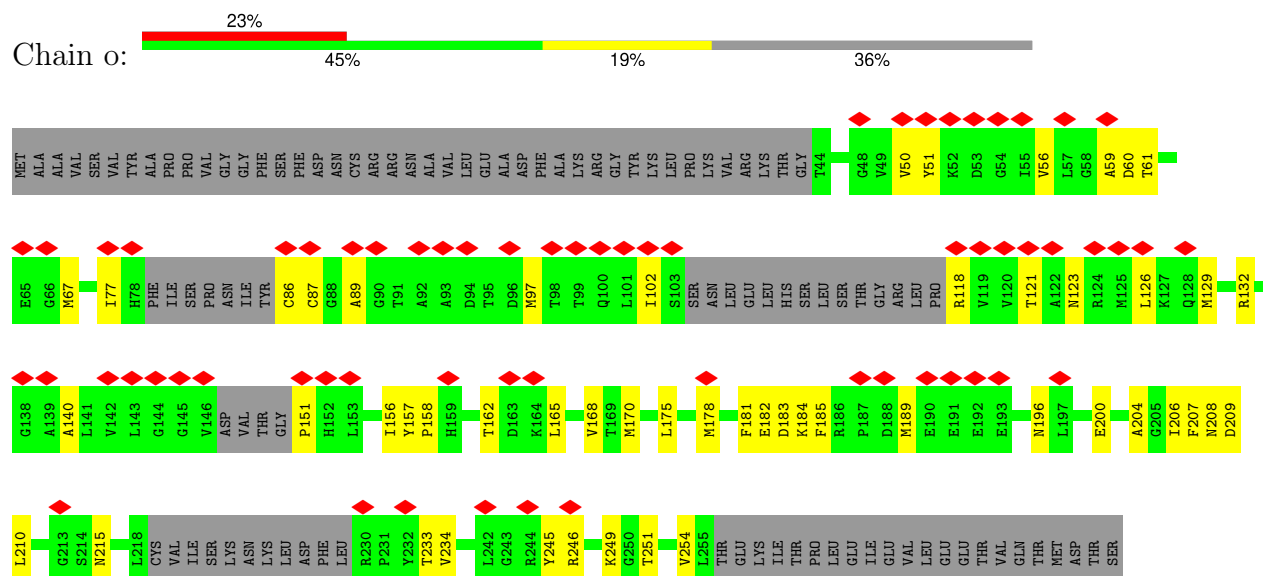
• Molecule 25: Proteasome subunit beta type-6



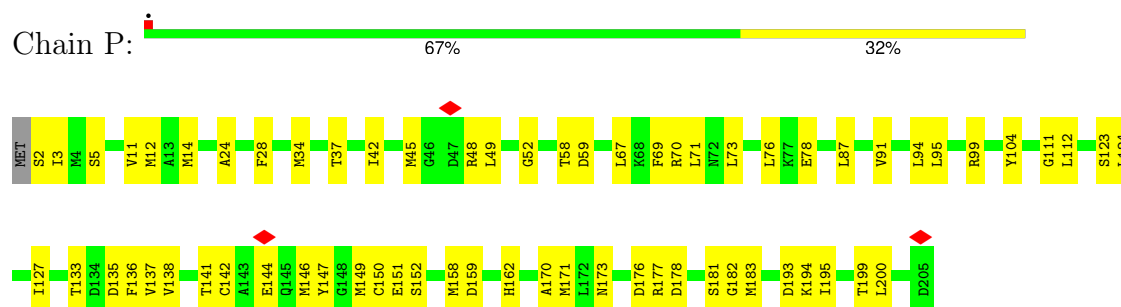
• Molecule 26: Proteasome subunit beta type-7



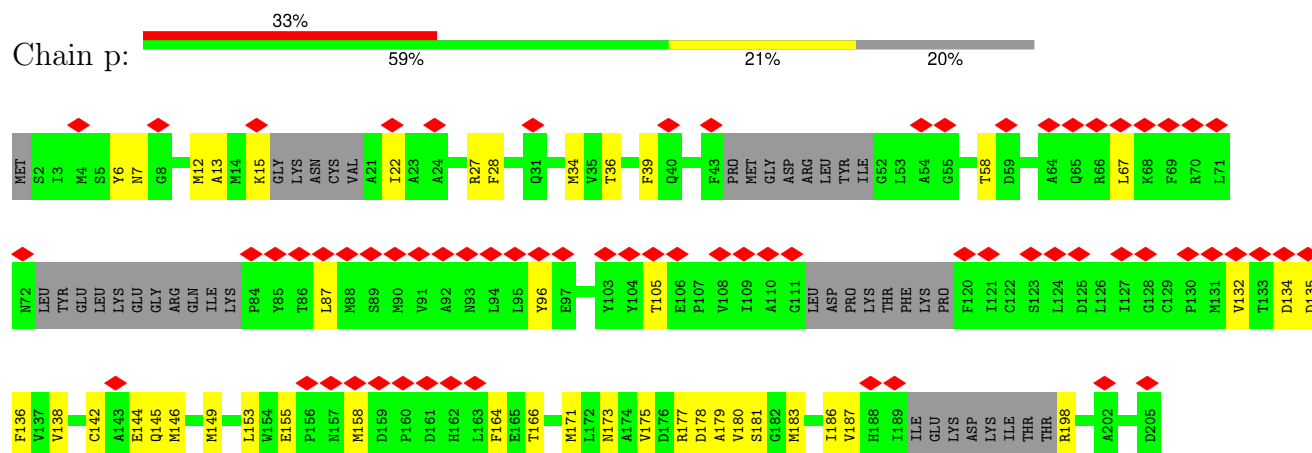
- Molecule 26: Proteasome subunit beta type-7



- Molecule 27: Proteasome subunit beta type-3

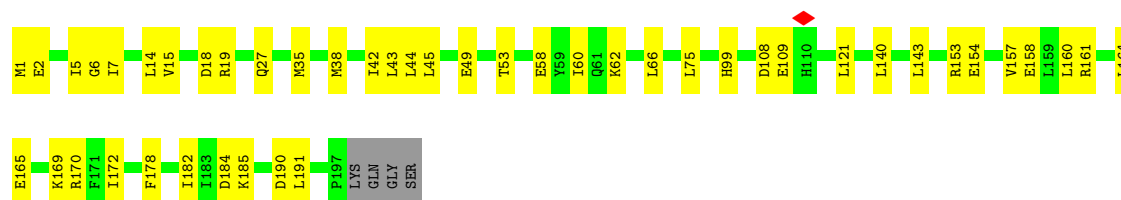


- Molecule 27: Proteasome subunit beta type-3

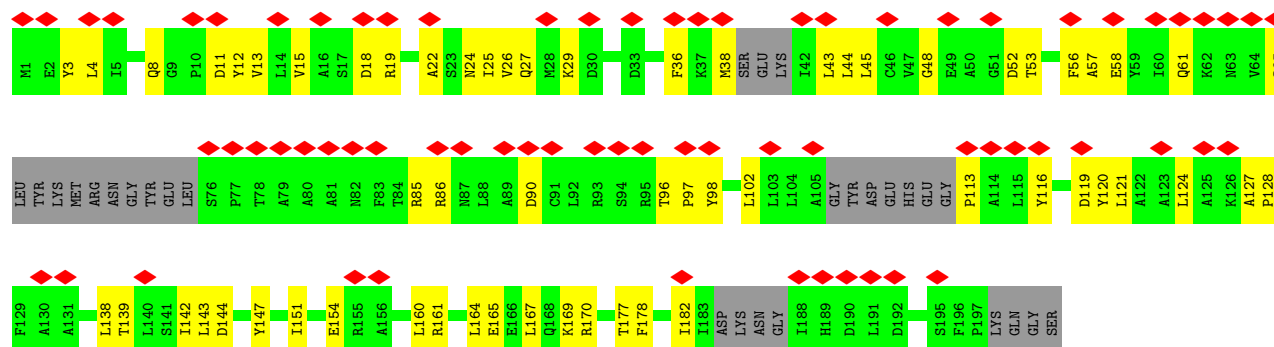


- Molecule 28: Proteasome subunit beta type-2

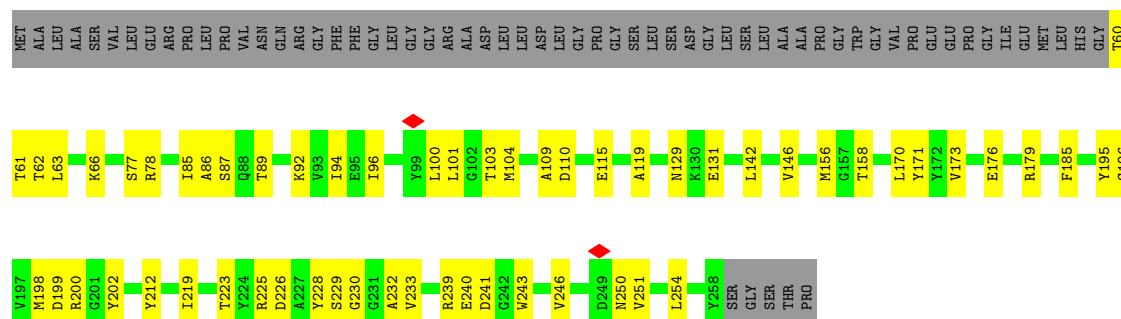




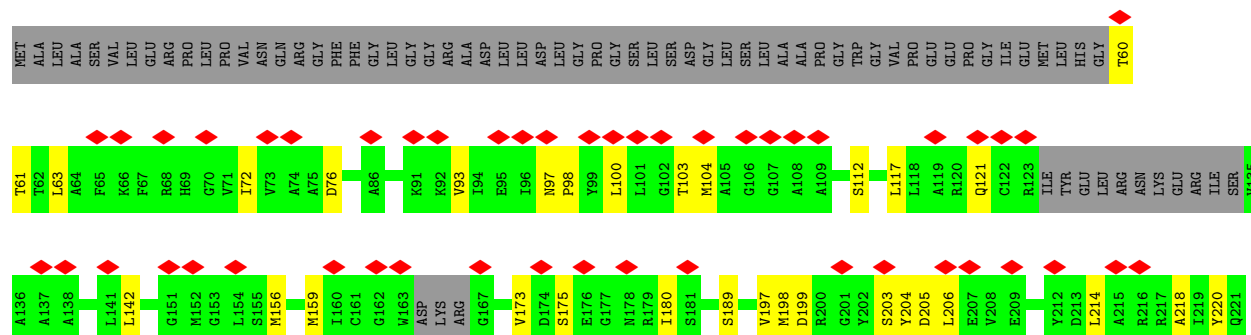
• Molecule 28: Proteasome subunit beta type-2

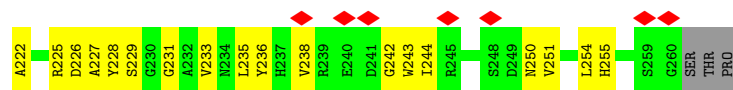


• Molecule 29: Proteasome subunit beta type-5



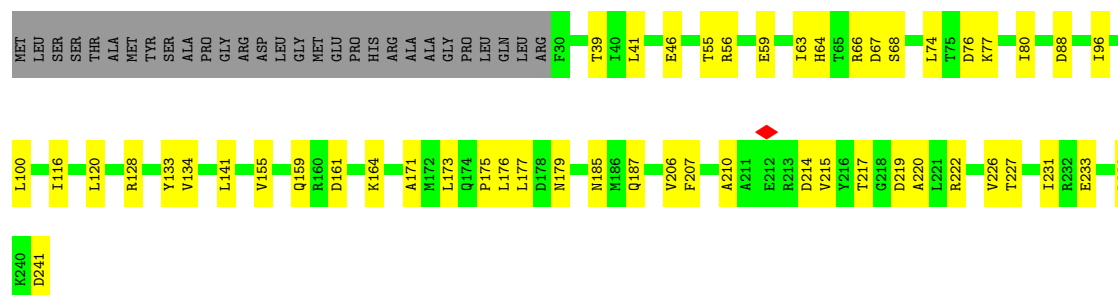
• Molecule 29: Proteasome subunit beta type-5





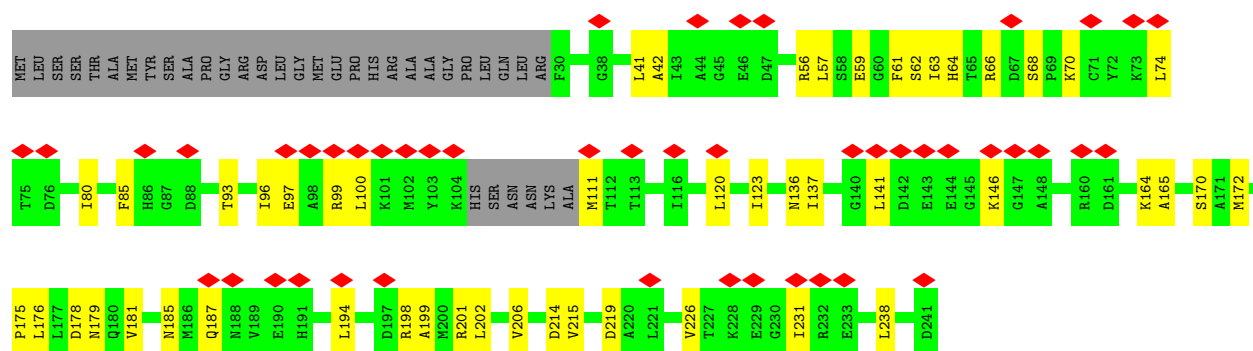
• Molecule 30: Proteasome subunit beta type-1

Chain S: 67% 21% 12%



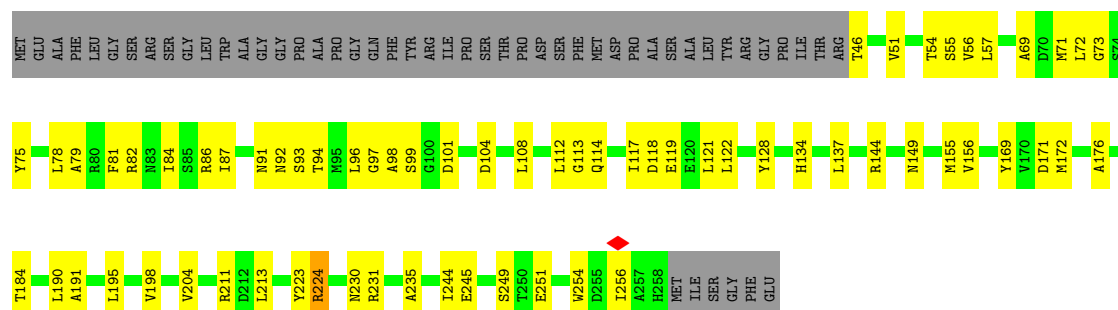
• Molecule 30: Proteasome subunit beta type-1

Chain s: 20% 65% 21% 15%



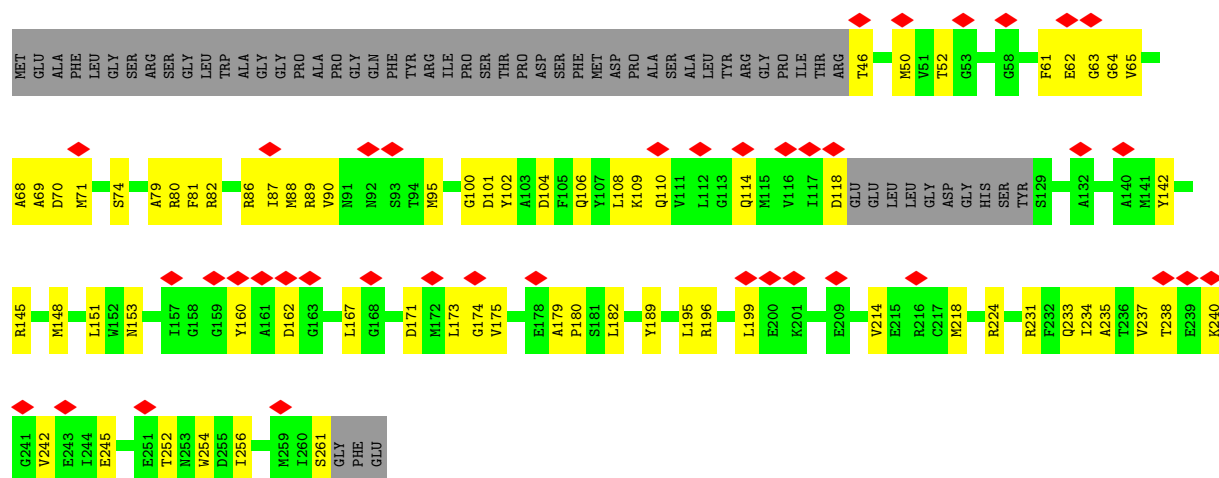
• Molecule 31: Proteasome subunit beta type-4

Chain T: 55% 25% 19%

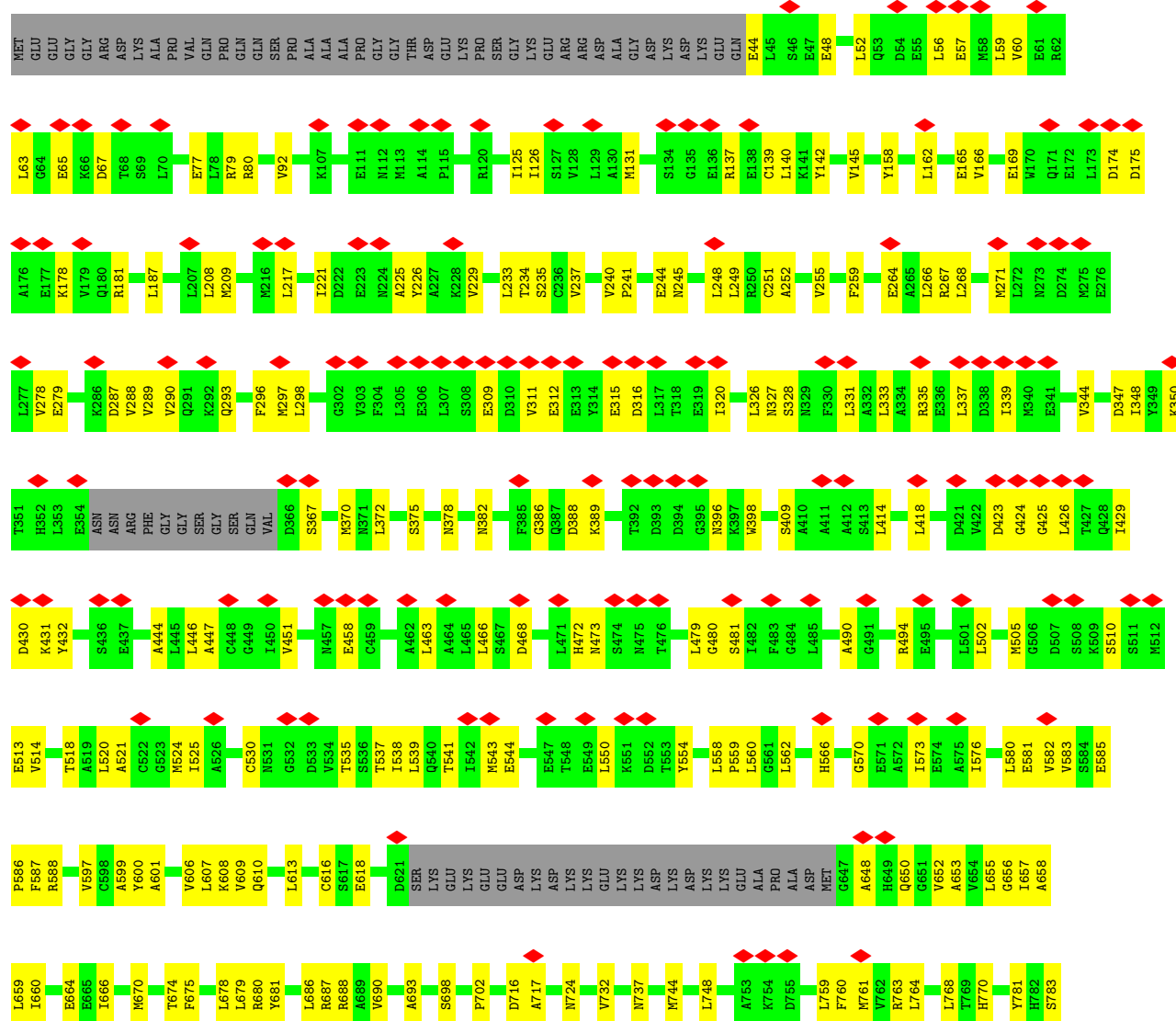


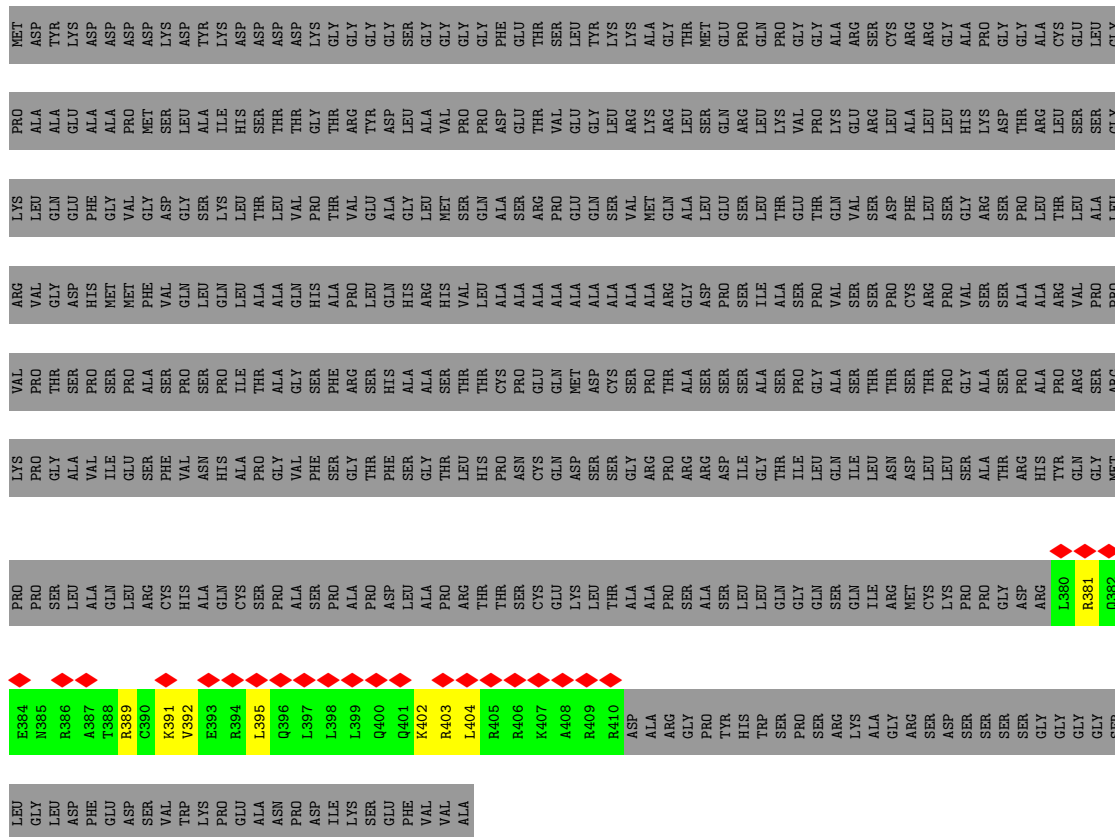
• Molecule 31: Proteasome subunit beta type-4

Chain t: 15% 52% 26% 22%



• 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	87326	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	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	1.528	Depositor
Minimum map value	-0.907	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.063	Depositor
Recommended contour level	0.25	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 ⓘ

5.1 Standard geometry ⓘ

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

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	0.13	0/6755	0.29	0/9135
2	V	0.14	0/3499	0.33	0/4722
3	W	0.17	0/3556	0.38	0/4781
4	X	0.11	0/3373	0.27	0/4548
5	Y	0.13	0/3181	0.29	0/4285
6	Z	0.13	0/2333	0.30	0/3162
7	a	0.14	0/3070	0.34	0/4155
8	b	0.11	0/1479	0.30	0/2003
9	c	0.14	0/2225	0.33	0/3005
10	d	0.17	0/2141	0.40	0/2891
11	e	0.10	0/322	0.25	0/436
12	A	0.12	0/2548	0.33	0/3423
13	B	0.13	0/3080	0.32	0/4153
14	C	0.14	0/3112	0.32	0/4182
15	D	0.20	0/3090	0.42	1/4168 (0.0%)
16	E	0.17	0/2742	0.37	0/3685
17	F	0.12	0/1823	0.34	0/2433
18	G	0.13	0/1919	0.29	0/2593
19	H	0.14	0/1857	0.27	0/2514
20	I	0.13	0/1993	0.29	0/2683
21	J	0.14	0/1913	0.29	0/2581
22	K	0.12	0/1830	0.30	0/2468
23	L	0.12	0/1902	0.29	0/2569
24	M	0.12	0/1951	0.29	0/2627
25	N	0.14	0/1513	0.32	0/2047
25	n	0.13	0/1352	0.31	0/1822
26	O	0.13	0/1694	0.30	0/2293
26	o	0.14	0/1331	0.35	0/1791
27	P	0.14	0/1620	0.32	0/2184
27	p	0.15	0/1282	0.37	0/1722
28	Q	0.14	0/1611	0.29	0/2180
28	q	0.16	0/1405	0.36	1/1899 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
29	R	0.12	0/1580	0.29	0/2134
29	r	0.12	0/1460	0.32	0/1972
30	S	0.11	0/1673	0.27	0/2254
30	s	0.12	0/1625	0.31	0/2188
31	T	0.12	0/1698	0.31	0/2299
31	t	0.13	0/1639	0.34	0/2217
32	f	0.13	0/6458	0.30	0/8743
33	y	0.11	0/272	0.28	0/357
All	All	0.14	0/89907	0.32	2/121304 (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
31	T	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	q	97	PRO	CA-N-CD	-5.77	103.93	112.00
15	D	219	VAL	N-CA-C	-5.76	101.27	109.51

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
31	T	224	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	U	6640	0	6697	184	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	V	3434	0	3503	114	0
3	W	3510	0	3633	131	0
4	X	3327	0	3423	79	0
5	Y	3123	0	3130	72	0
6	Z	2290	0	2320	92	0
7	a	3012	0	3029	98	0
8	b	1459	0	1499	39	0
9	c	2184	0	2191	88	0
10	d	2099	0	2127	91	0
11	e	314	0	247	10	0
12	A	2518	0	2588	107	0
13	B	3037	0	3101	102	0
14	C	3071	0	3193	105	0
15	D	3040	0	3076	118	0
16	E	2706	0	2779	106	0
17	F	1812	0	1882	67	0
18	G	1885	0	1889	55	0
19	H	1818	0	1811	38	0
20	I	1963	0	1987	41	0
21	J	1887	0	1905	50	0
22	K	1804	0	1789	43	0
23	L	1868	0	1858	58	0
24	M	1916	0	1890	49	0
25	N	1487	0	1452	55	0
25	n	1336	0	1324	64	0
26	O	1667	0	1689	56	0
26	o	1315	0	1321	39	0
27	P	1591	0	1609	61	0
27	p	1264	0	1255	42	0
28	Q	1578	0	1580	43	0
28	q	1380	0	1399	50	0
29	R	1549	0	1512	51	0
29	r	1432	0	1384	45	0
30	S	1643	0	1640	49	0
30	s	1597	0	1597	47	0
31	T	1665	0	1638	63	0
31	t	1609	0	1597	70	0
32	f	6351	0	6362	196	0
33	y	273	0	309	8	0
34	c	1	0	0	0	0
35	A	31	0	12	4	0
35	B	31	0	12	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	C	31	0	12	1	0
35	D	31	0	12	2	0
36	E	27	0	12	1	0
All	All	88606	0	89275	2529	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 14.

The worst 5 of 2529 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)
28:Q:5:ILE:HD11	28:Q:143:LEU:HD11	1.44	0.98
12:A:63:THR:O	32:f:681:TYR:OH	1.82	0.98
17:F:438:TYR:OH	23:L:62:LYS:NZ	1.98	0.97
6:Z:39:LEU:HD11	6:Z:95:TYR:HB3	1.50	0.94
27:p:58:THR:OG1	28:q:121:LEU:O	1.88	0.91

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	844/953 (89%)	781 (92%)	63 (8%)	0	100	100
2	V	417/534 (78%)	389 (93%)	28 (7%)	0	100	100
3	W	426/456 (93%)	392 (92%)	34 (8%)	0	100	100
4	X	419/422 (99%)	391 (93%)	28 (7%)	0	100	100
5	Y	377/389 (97%)	361 (96%)	16 (4%)	0	100	100
6	Z	285/324 (88%)	274 (96%)	11 (4%)	0	100	100
7	a	373/376 (99%)	343 (92%)	30 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	b	189/377 (50%)	172 (91%)	17 (9%)	0	100	100
9	c	273/310 (88%)	253 (93%)	20 (7%)	0	100	100
10	d	252/350 (72%)	215 (85%)	37 (15%)	0	100	100
11	e	32/70 (46%)	31 (97%)	1 (3%)	0	100	100
12	A	296/433 (68%)	258 (87%)	38 (13%)	0	100	100
13	B	378/440 (86%)	346 (92%)	32 (8%)	0	100	100
14	C	387/406 (95%)	354 (92%)	33 (8%)	0	100	100
15	D	378/418 (90%)	336 (89%)	41 (11%)	1 (0%)	37	66
16	E	333/389 (86%)	303 (91%)	29 (9%)	1 (0%)	37	66
17	F	207/439 (47%)	183 (88%)	24 (12%)	0	100	100
18	G	239/246 (97%)	226 (95%)	13 (5%)	0	100	100
19	H	231/234 (99%)	218 (94%)	13 (6%)	0	100	100
20	I	247/261 (95%)	240 (97%)	7 (3%)	0	100	100
21	J	237/248 (96%)	223 (94%)	14 (6%)	0	100	100
22	K	231/241 (96%)	213 (92%)	18 (8%)	0	100	100
23	L	235/263 (89%)	220 (94%)	15 (6%)	0	100	100
24	M	242/255 (95%)	234 (97%)	8 (3%)	0	100	100
25	N	196/239 (82%)	180 (92%)	16 (8%)	0	100	100
25	n	171/239 (72%)	164 (96%)	7 (4%)	0	100	100
26	O	219/277 (79%)	210 (96%)	9 (4%)	0	100	100
26	o	166/277 (60%)	155 (93%)	11 (7%)	0	100	100
27	P	202/205 (98%)	186 (92%)	16 (8%)	0	100	100
27	p	152/205 (74%)	139 (91%)	13 (9%)	0	100	100
28	Q	195/201 (97%)	186 (95%)	9 (5%)	0	100	100
28	q	163/201 (81%)	152 (93%)	11 (7%)	0	100	100
29	R	197/263 (75%)	187 (95%)	10 (5%)	0	100	100
29	r	181/263 (69%)	165 (91%)	16 (9%)	0	100	100
30	S	210/241 (87%)	198 (94%)	12 (6%)	0	100	100
30	s	202/241 (84%)	191 (95%)	11 (5%)	0	100	100
31	T	211/264 (80%)	200 (95%)	11 (5%)	0	100	100
31	t	202/264 (76%)	183 (91%)	19 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	f	811/908 (89%)	746 (92%)	65 (8%)	0	100	100
33	y	29/505 (6%)	29 (100%)	0	0	100	100
All	All	11035/13627 (81%)	10227 (93%)	806 (7%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	D	220	ALA
16	E	238	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	U	725/816 (89%)	725 (100%)	0	100	100
2	V	371/460 (81%)	371 (100%)	0	100	100
3	W	396/416 (95%)	396 (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%)	227 (100%)	0	100	100
11	e	34/63 (54%)	34 (100%)	0	100	100
12	A	277/372 (74%)	277 (100%)	0	100	100
13	B	341/385 (89%)	341 (100%)	0	100	100
14	C	340/352 (97%)	340 (100%)	0	100	100
15	D	333/366 (91%)	333 (100%)	0	100	100
16	E	299/341 (88%)	298 (100%)	1 (0%)	91	95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	F	196/379 (52%)	196 (100%)	0	100	100
18	G	206/210 (98%)	206 (100%)	0	100	100
19	H	190/191 (100%)	190 (100%)	0	100	100
20	I	209/221 (95%)	209 (100%)	0	100	100
21	J	203/211 (96%)	203 (100%)	0	100	100
22	K	198/203 (98%)	198 (100%)	0	100	100
23	L	203/224 (91%)	203 (100%)	0	100	100
24	M	202/212 (95%)	201 (100%)	1 (0%)	86	91
25	N	154/181 (85%)	154 (100%)	0	100	100
25	n	138/181 (76%)	138 (100%)	0	100	100
26	O	182/228 (80%)	182 (100%)	0	100	100
26	o	139/228 (61%)	139 (100%)	0	100	100
27	P	173/174 (99%)	173 (100%)	0	100	100
27	p	136/174 (78%)	136 (100%)	0	100	100
28	Q	168/171 (98%)	168 (100%)	0	100	100
28	q	148/171 (86%)	148 (100%)	0	100	100
29	R	155/202 (77%)	155 (100%)	0	100	100
29	r	142/202 (70%)	142 (100%)	0	100	100
30	S	177/199 (89%)	177 (100%)	0	100	100
30	s	172/199 (86%)	172 (100%)	0	100	100
31	T	176/215 (82%)	176 (100%)	0	100	100
31	t	171/215 (80%)	171 (100%)	0	100	100
32	f	693/763 (91%)	693 (100%)	0	100	100
33	y	29/403 (7%)	29 (100%)	0	100	100
All	All	9603/11539 (83%)	9601 (100%)	2 (0%)	100	100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
16	E	225	HIS
24	M	148	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 56 such sidechains are listed below:

Mol	Chain	Res	Type
15	D	294	ASN
32	f	876	HIS
18	G	12	HIS
32	f	291	GLN
26	o	123	ASN

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 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
35	ATP	B	501	-	28,33,33	0.73	0	34,52,52	0.96	1 (2%)
35	ATP	C	501	-	28,33,33	0.71	0	34,52,52	0.95	1 (2%)
36	ADP	E	401	-	24,29,29	0.89	0	29,45,45	1.26	2 (6%)
35	ATP	D	501	-	28,33,33	0.69	0	34,52,52	0.94	1 (2%)
35	ATP	A	501	-	28,33,33	0.63	0	34,52,52	0.92	2 (5%)

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	-	-	1/18/38/38	0/3/3/3
35	ATP	C	501	-	-	7/18/38/38	0/3/3/3
36	ADP	E	401	-	-	2/12/32/32	0/3/3/3
35	ATP	D	501	-	-	5/18/38/38	0/3/3/3
35	ATP	A	501	-	-	4/18/38/38	0/3/3/3

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	E	401	ADP	N3-C2-N1	-4.10	123.10	128.67
36	E	401	ADP	C4-C5-N7	-2.59	106.60	109.34
35	D	501	ATP	C5-C6-N6	2.33	123.86	120.31
35	C	501	ATP	C5-C6-N6	2.31	123.83	120.31
35	A	501	ATP	C5-C6-N6	2.31	123.83	120.31

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

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

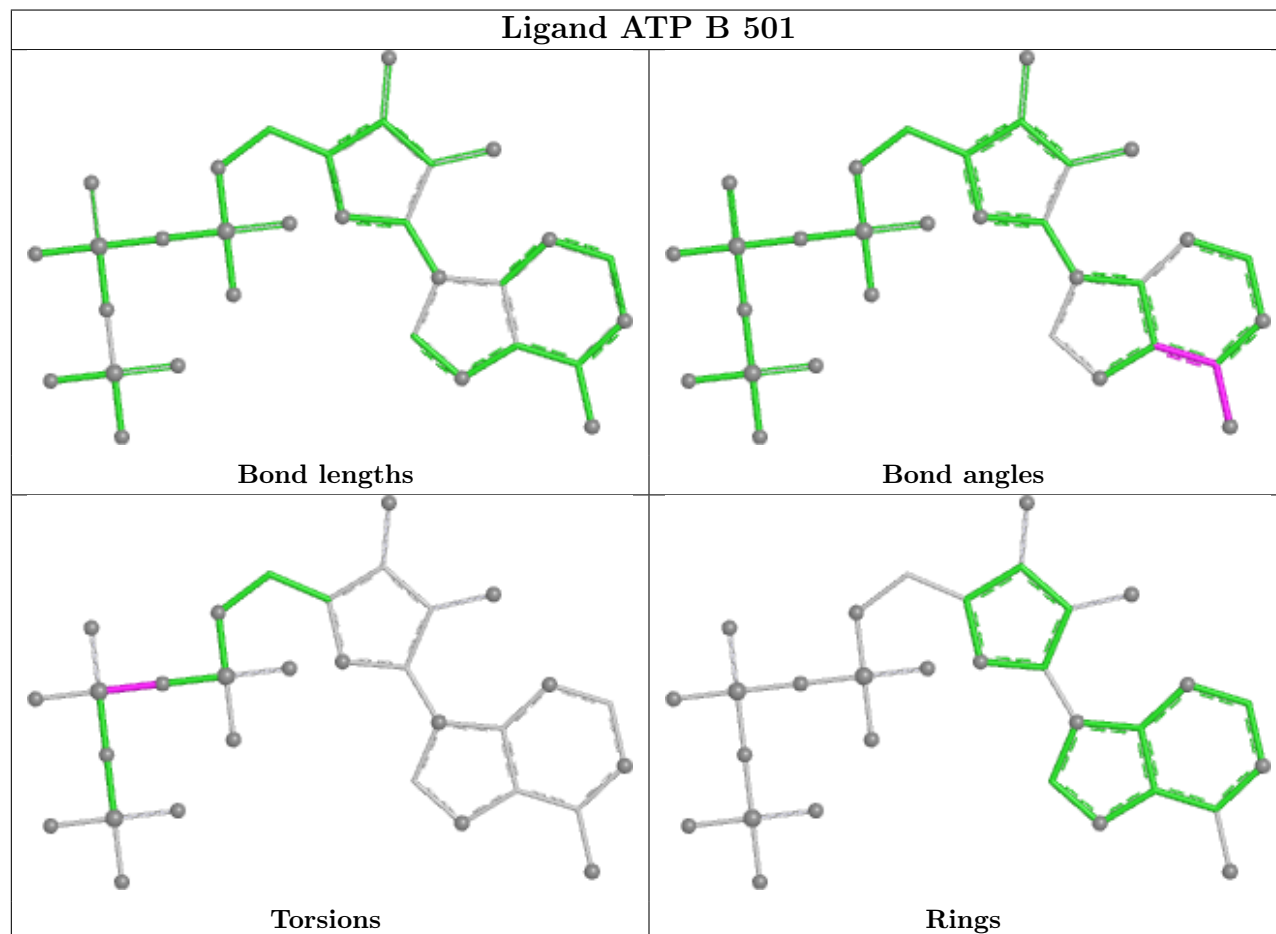
There are no ring outliers.

5 monomers are involved in 11 short contacts:

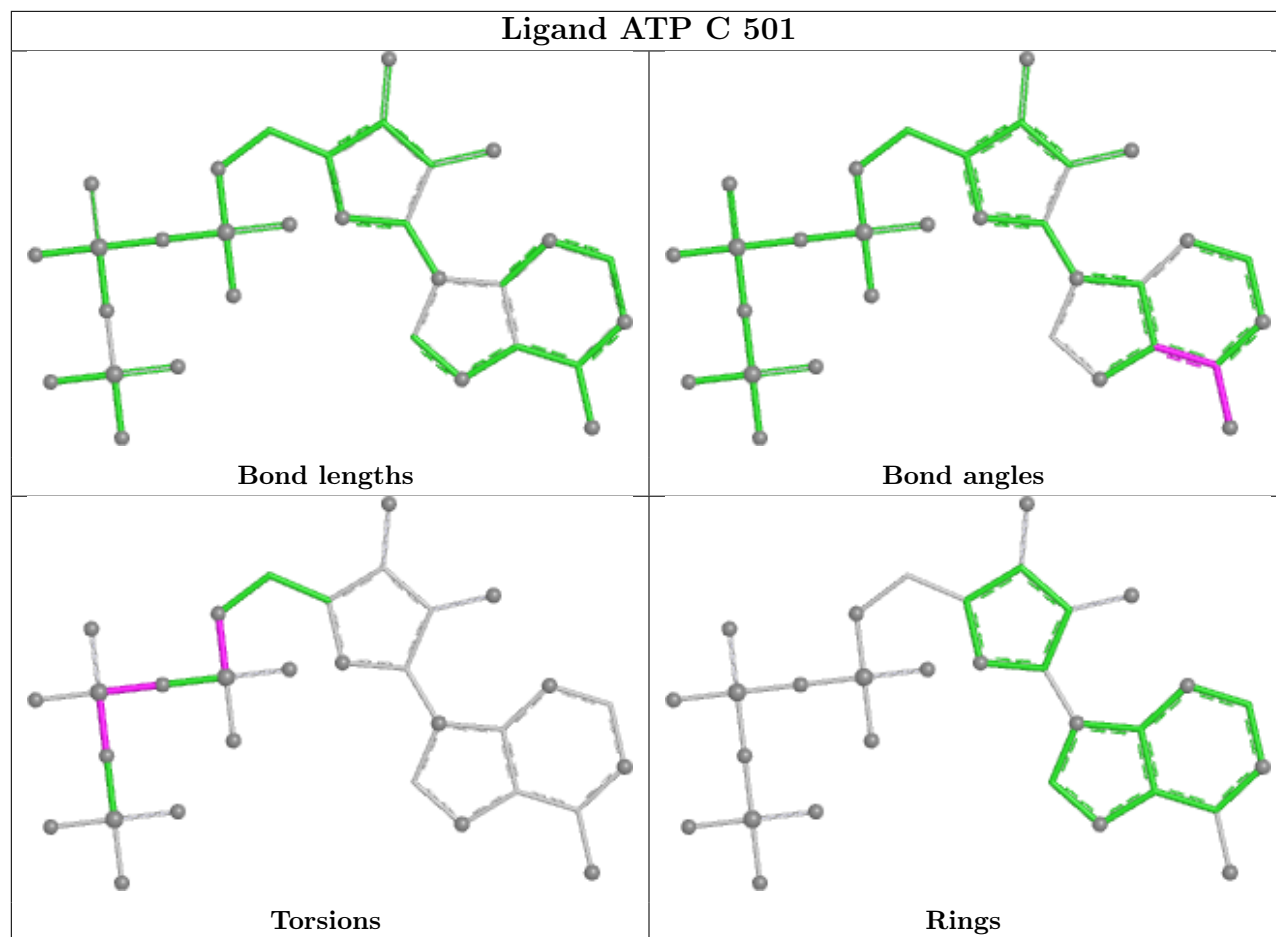
Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	B	501	ATP	3	0
35	C	501	ATP	1	0
36	E	401	ADP	1	0
35	D	501	ATP	2	0
35	A	501	ATP	4	0

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

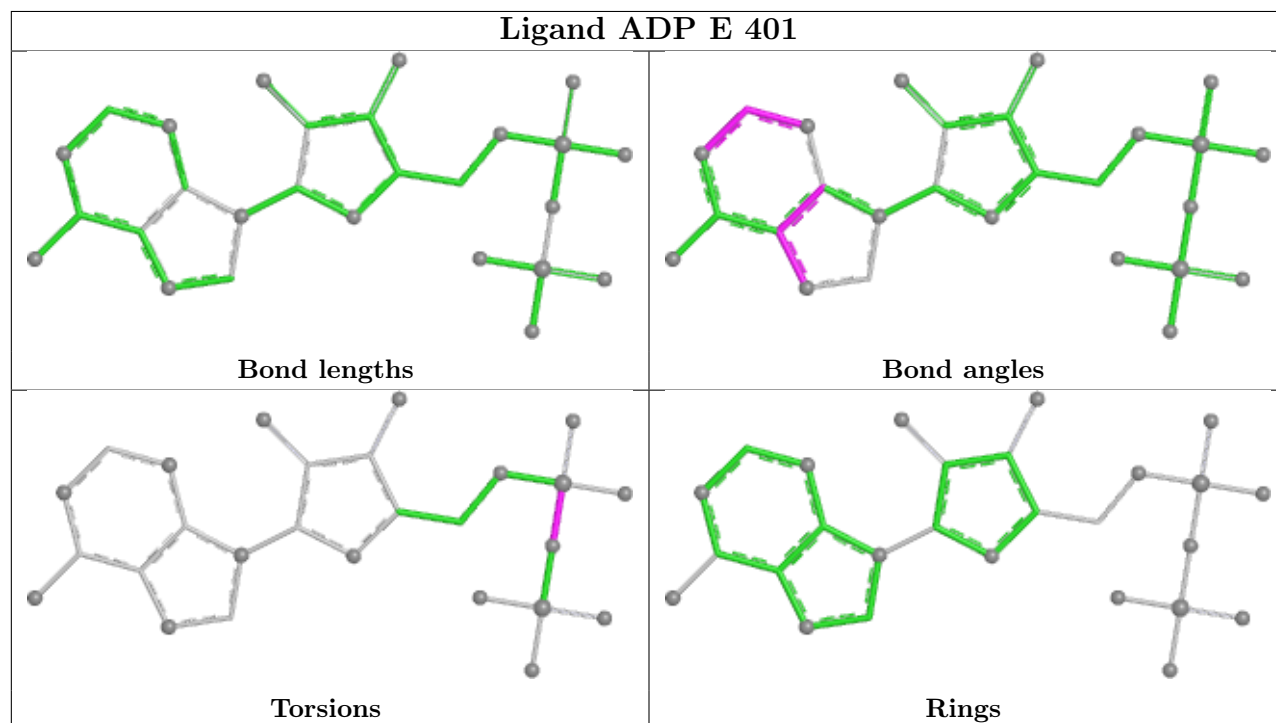
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.

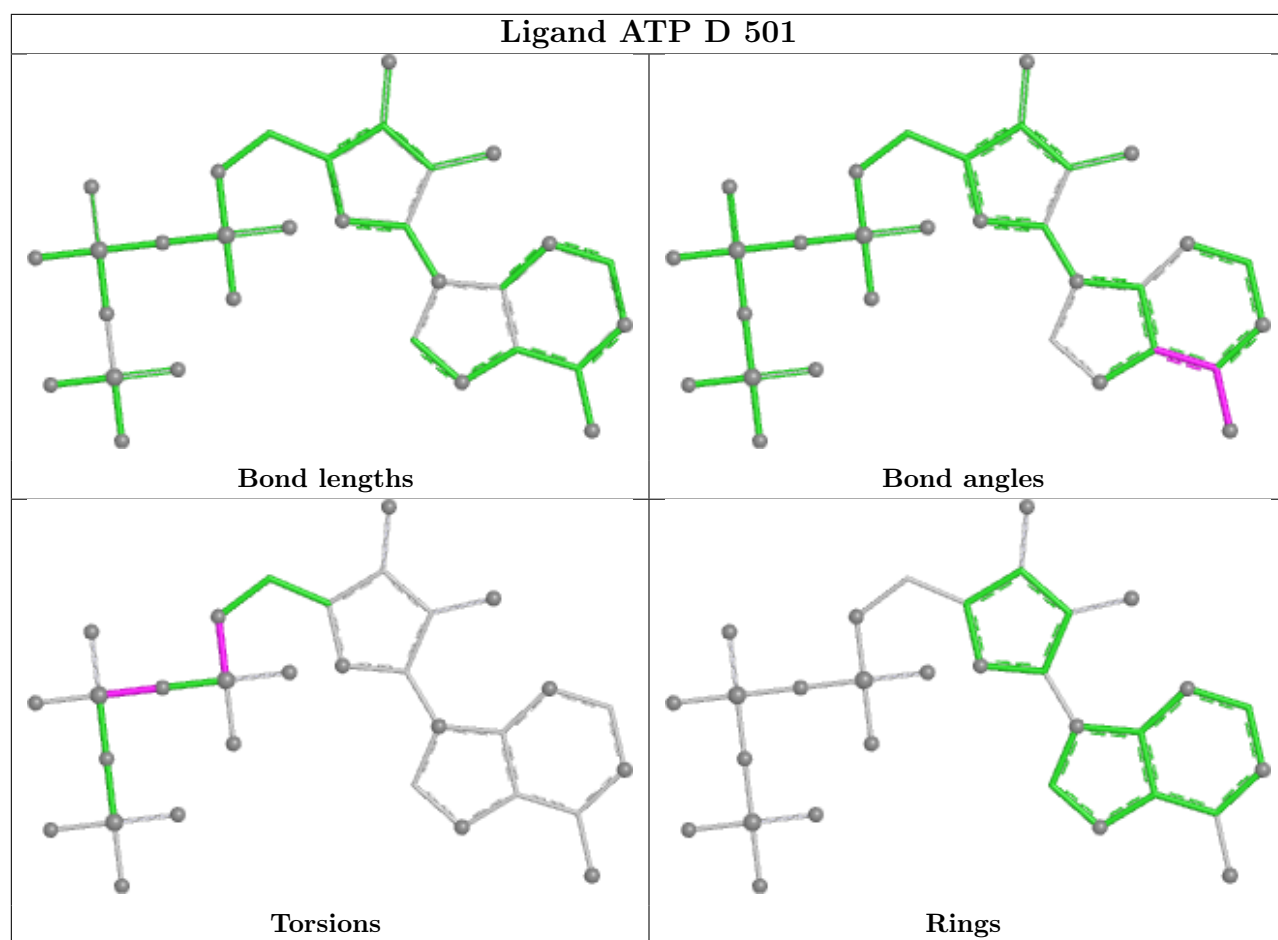


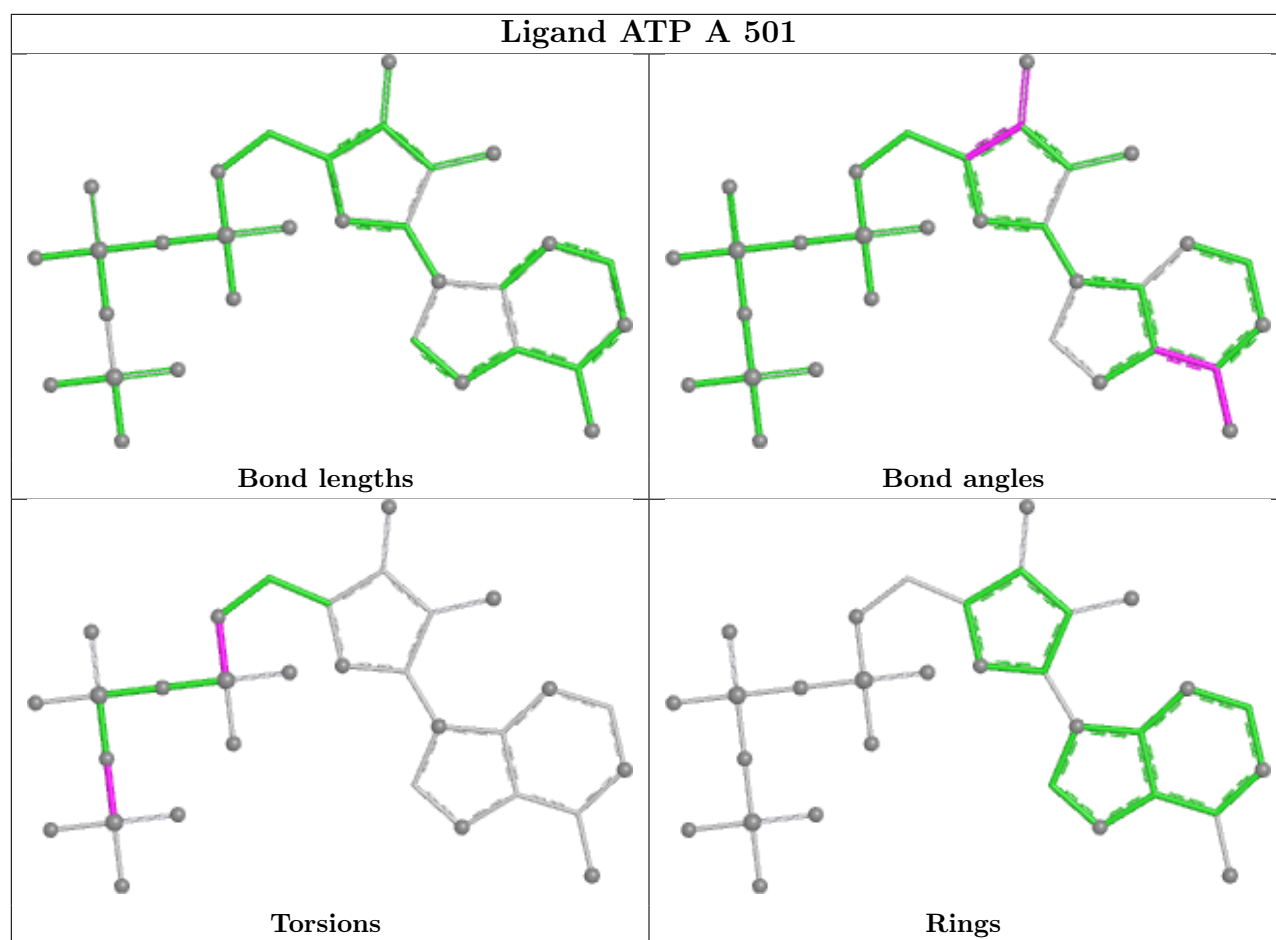
Ligand ATP C 501



Ligand ADP E 401







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

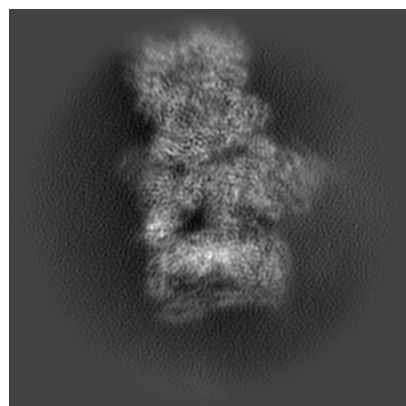
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44929. These allow visual inspection of the internal detail of the map and identification of artifacts.

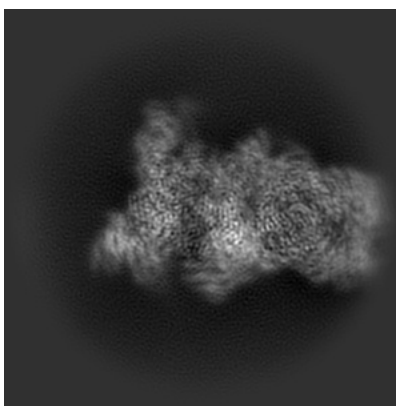
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

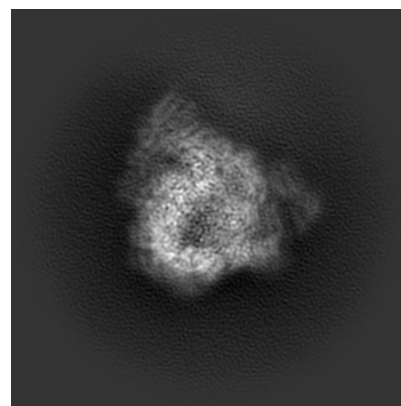
6.1.1 Primary map



X

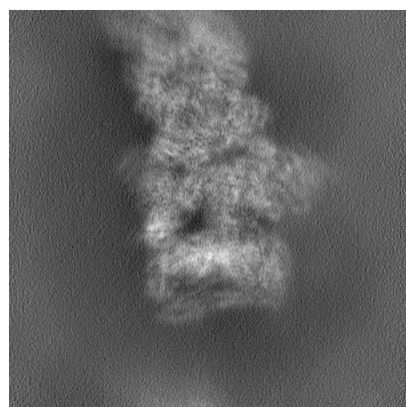


Y

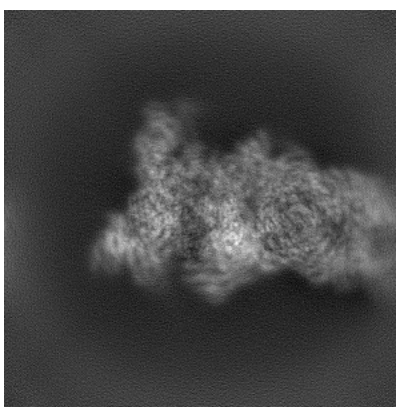


Z

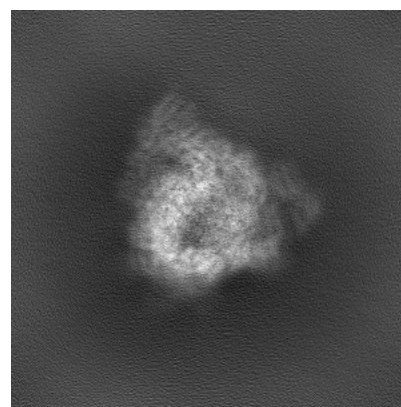
6.1.2 Raw map



X



Y

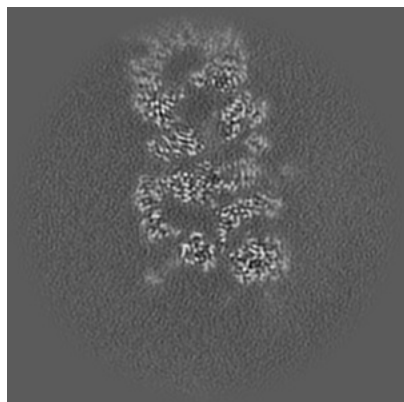


Z

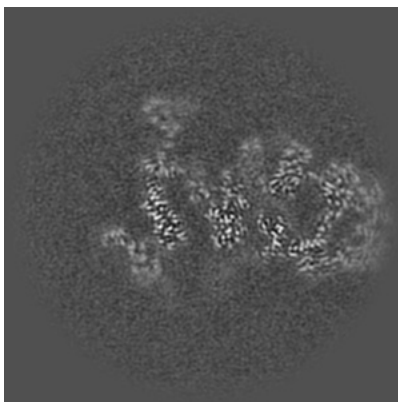
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

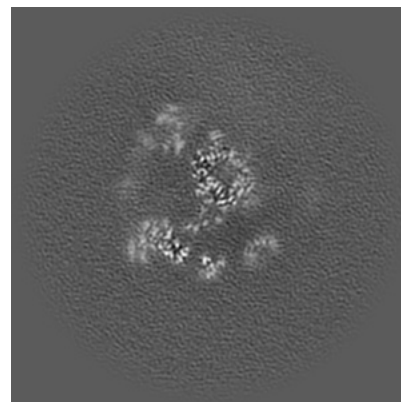
6.2.1 Primary map



X Index: 220

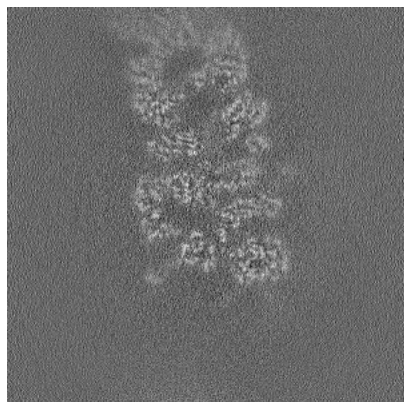


Y Index: 220

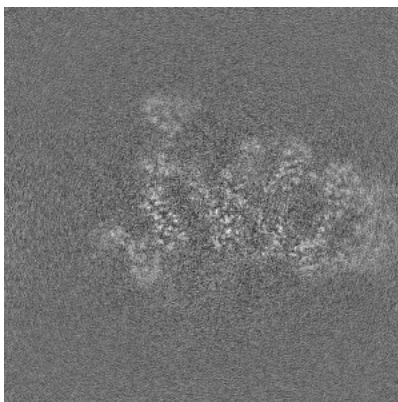


Z Index: 220

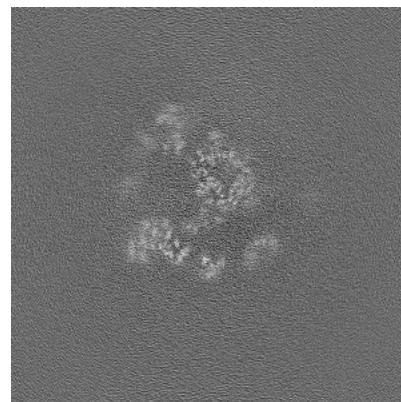
6.2.2 Raw map



X Index: 220



Y Index: 220

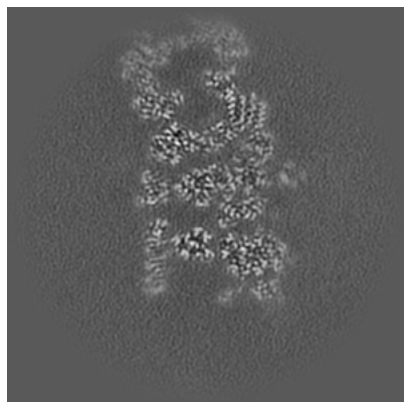


Z Index: 220

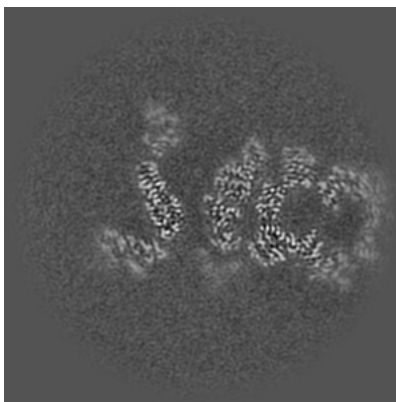
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

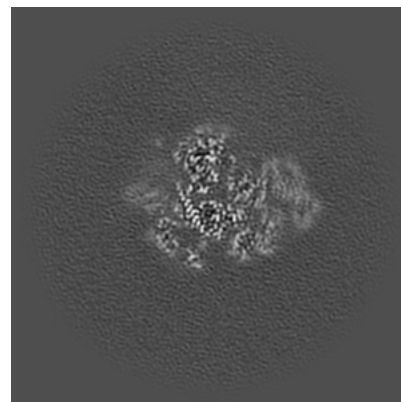
6.3.1 Primary map



X Index: 209

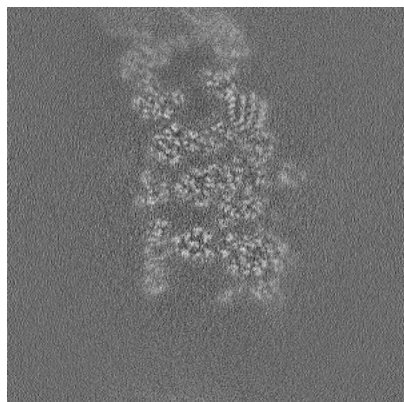


Y Index: 205

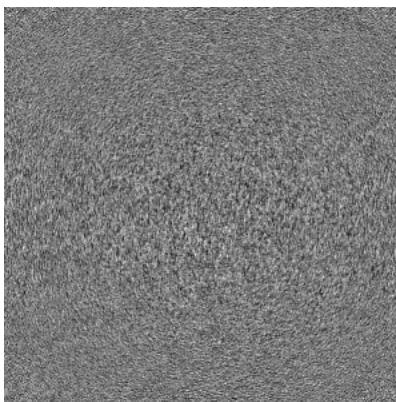


Z Index: 170

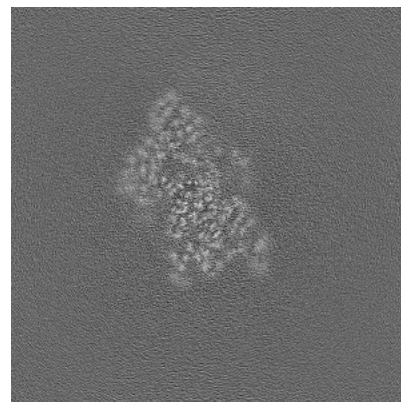
6.3.2 Raw map



X Index: 209



Y Index: 0

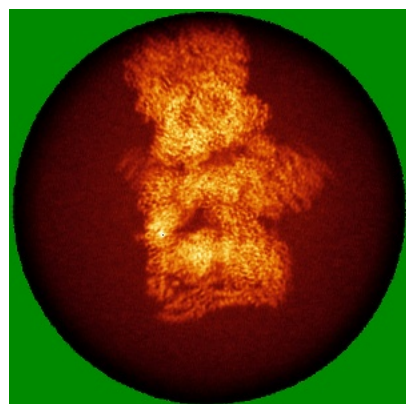


Z Index: 243

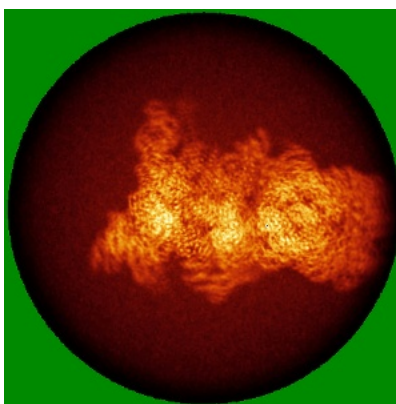
The images above show the largest variance slices of the map in three orthogonal directions.

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

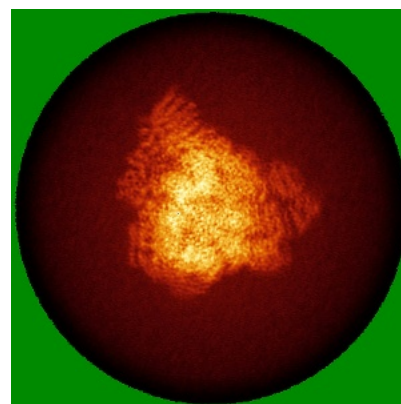
6.4.1 Primary map



X

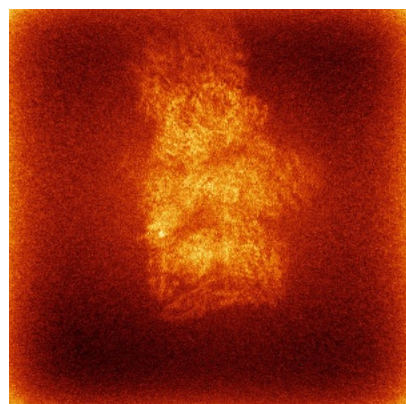


Y

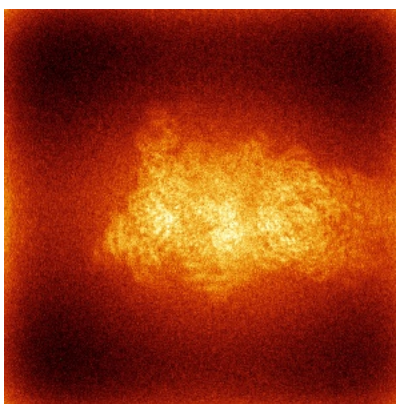


Z

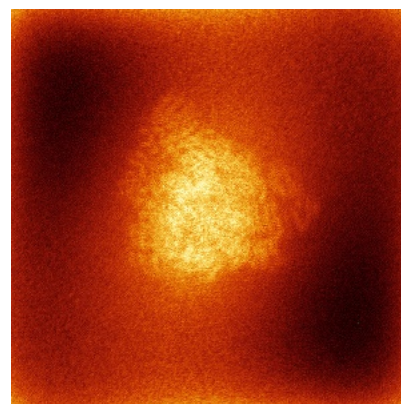
6.4.2 Raw map



X



Y

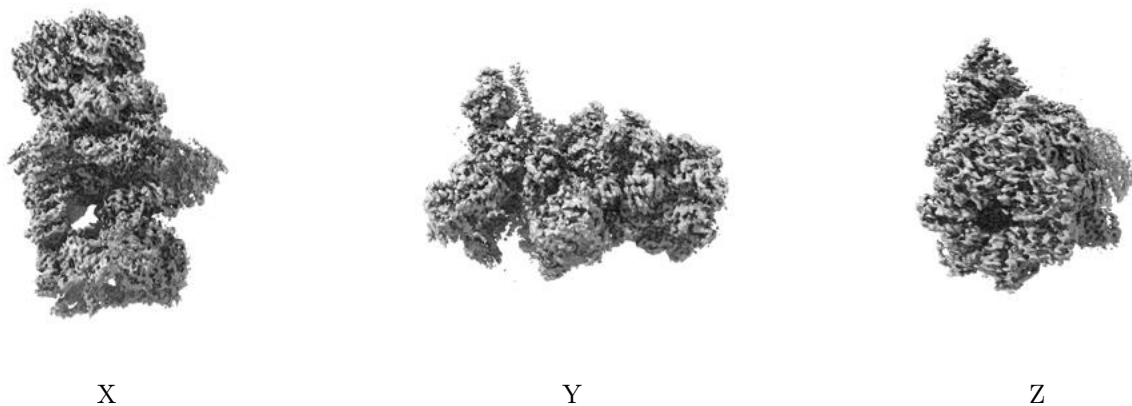


Z

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.

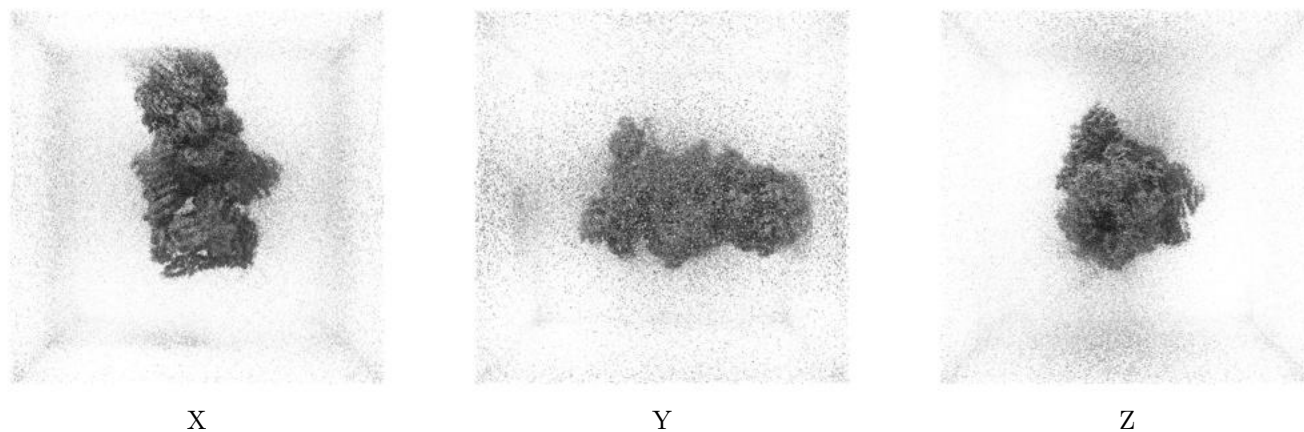
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.25. 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.

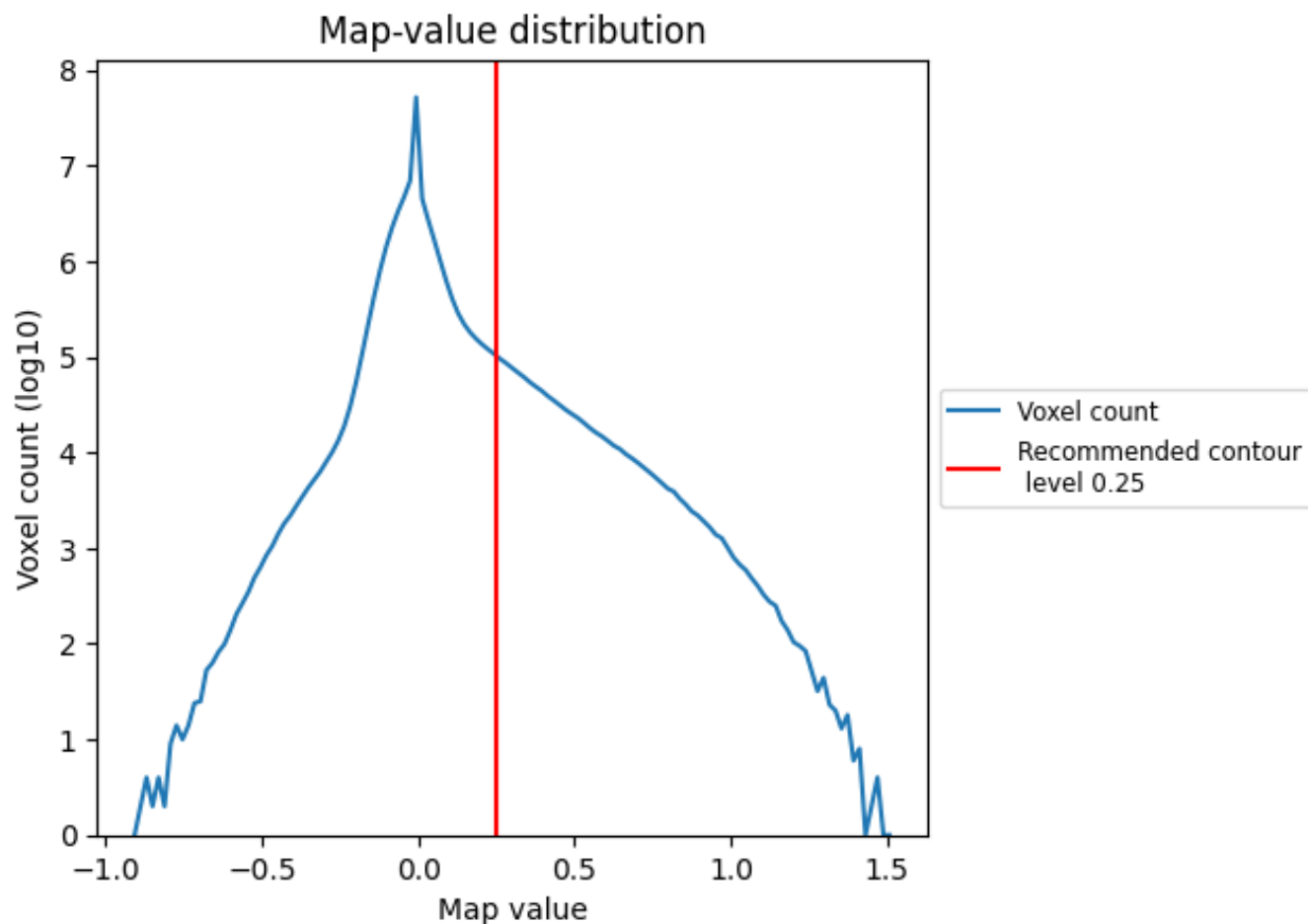
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

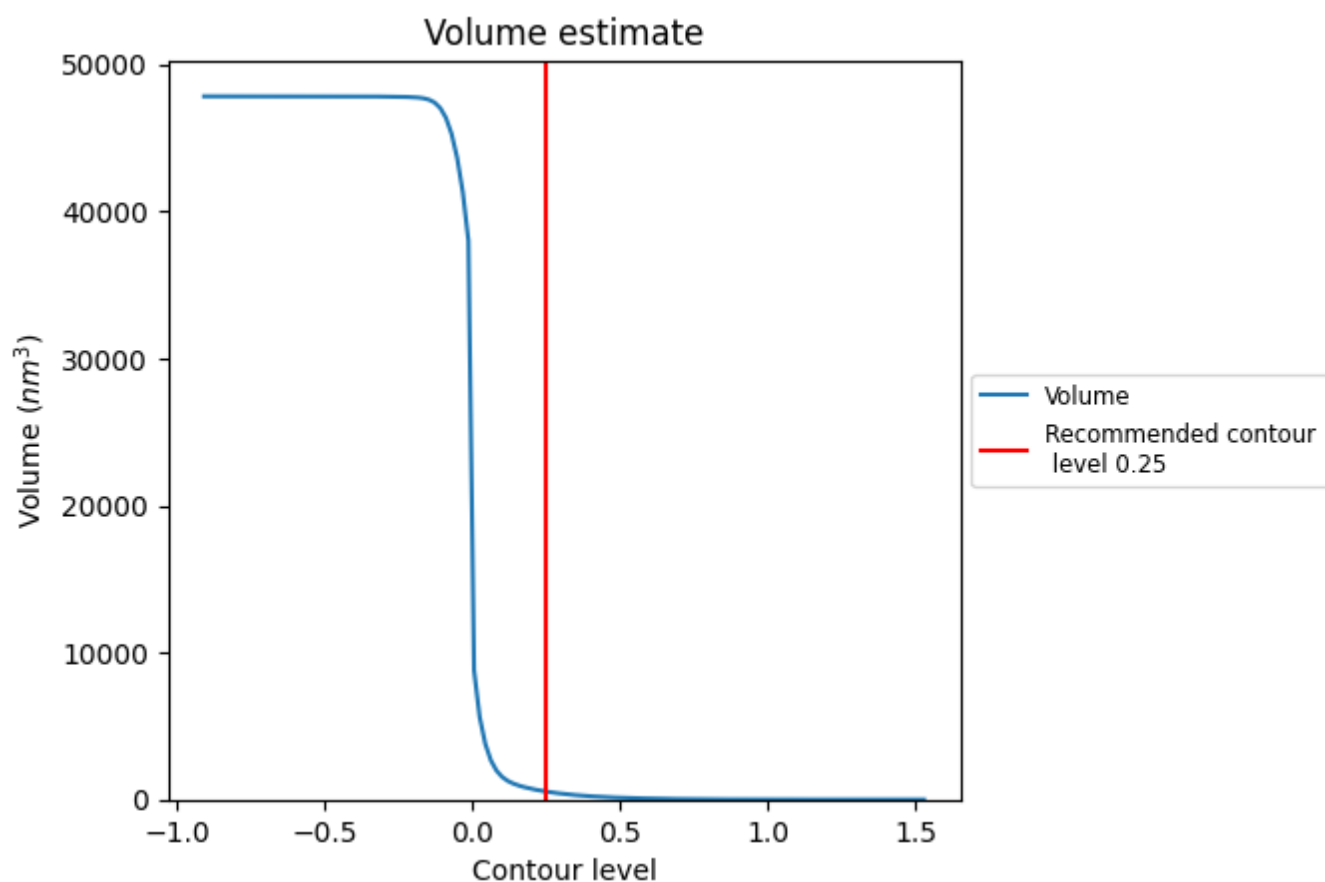
This section contains the results of statistical analysis of the map.

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.

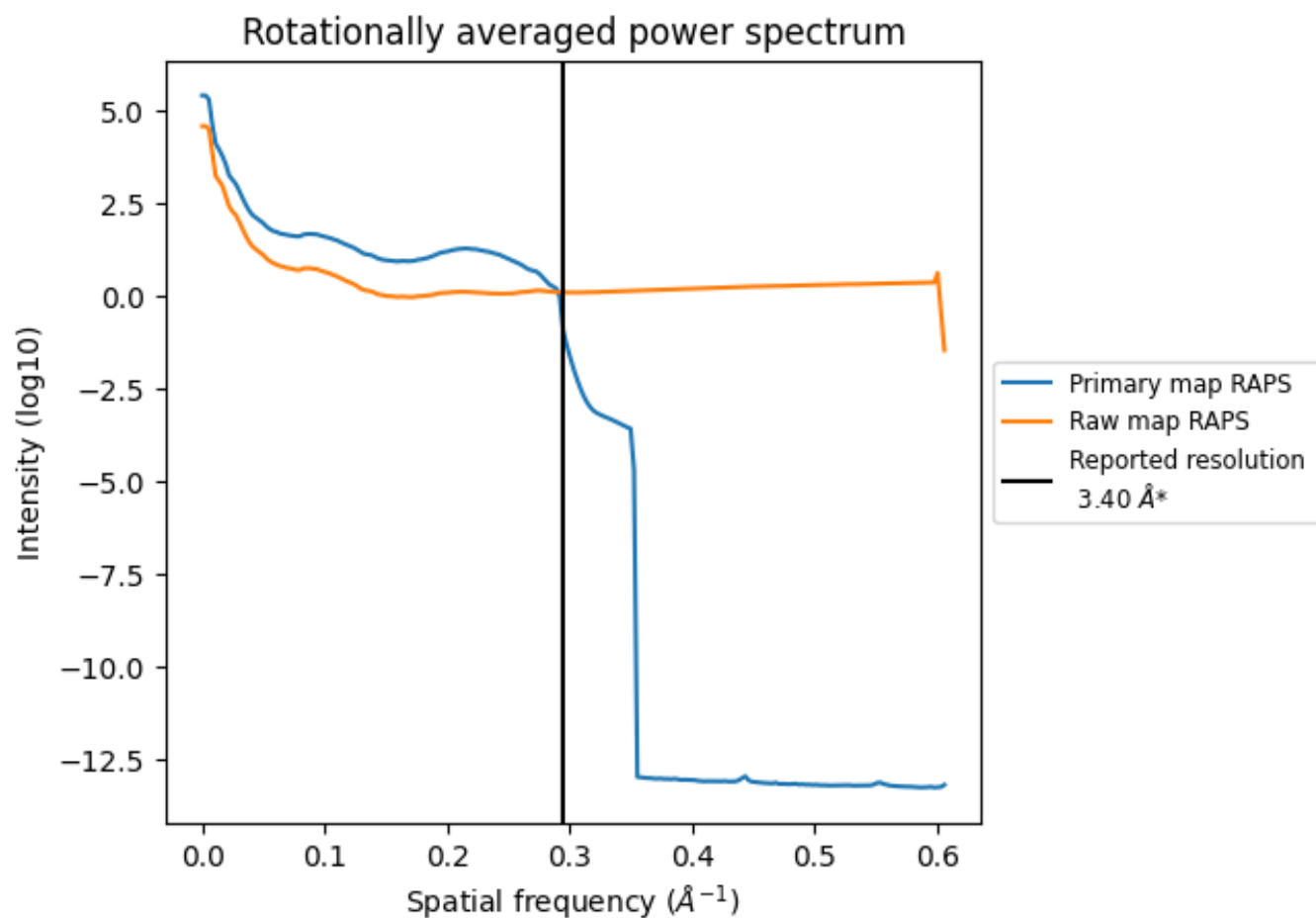
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 545 nm³; this corresponds to an approximate mass of 492 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 ⓘ

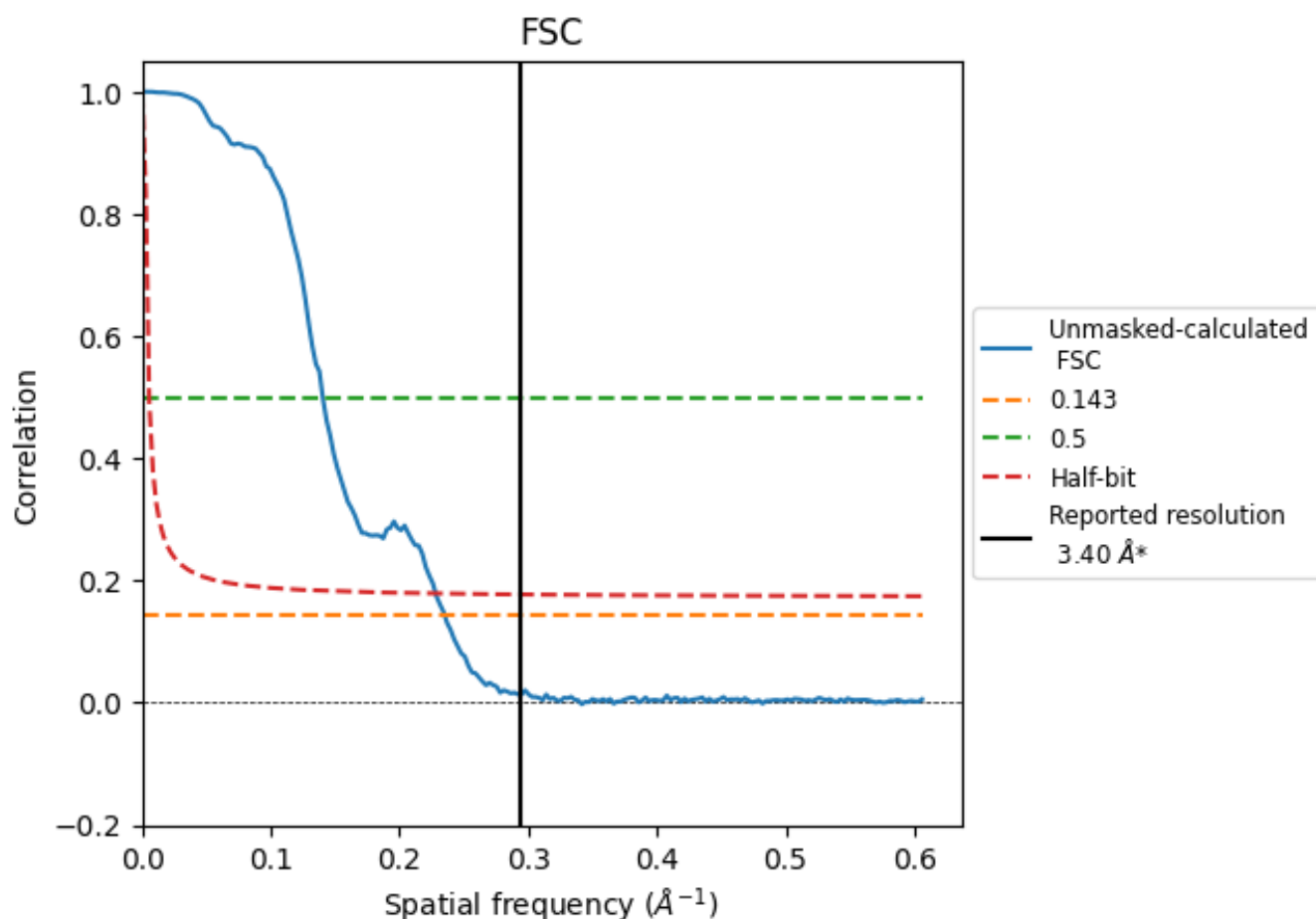


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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 0.294 Å⁻¹

8.2 Resolution estimates [i](#)

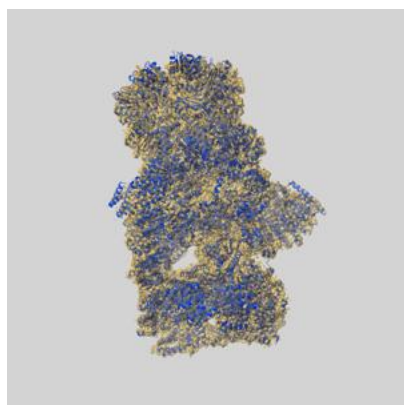
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.26	7.13	4.39

*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 4.26 differs from the reported value 3.4 by more than 10 %

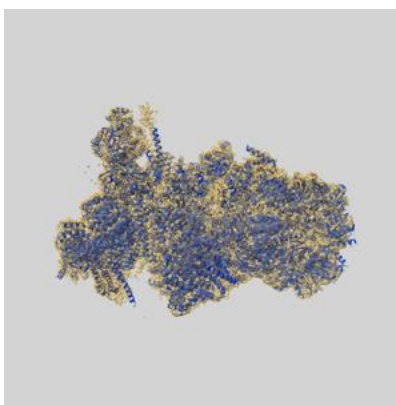
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-44929 and PDB model 9BV2. Per-residue inclusion information can be found in section [3](#) on page [13](#).

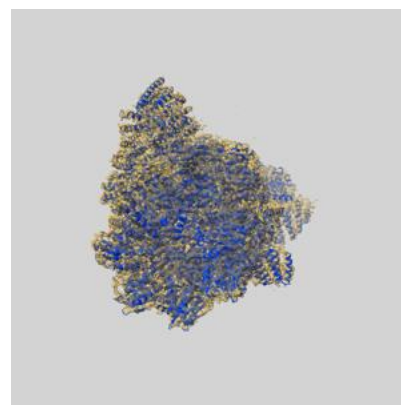
9.1 Map-model overlay [i](#)



X



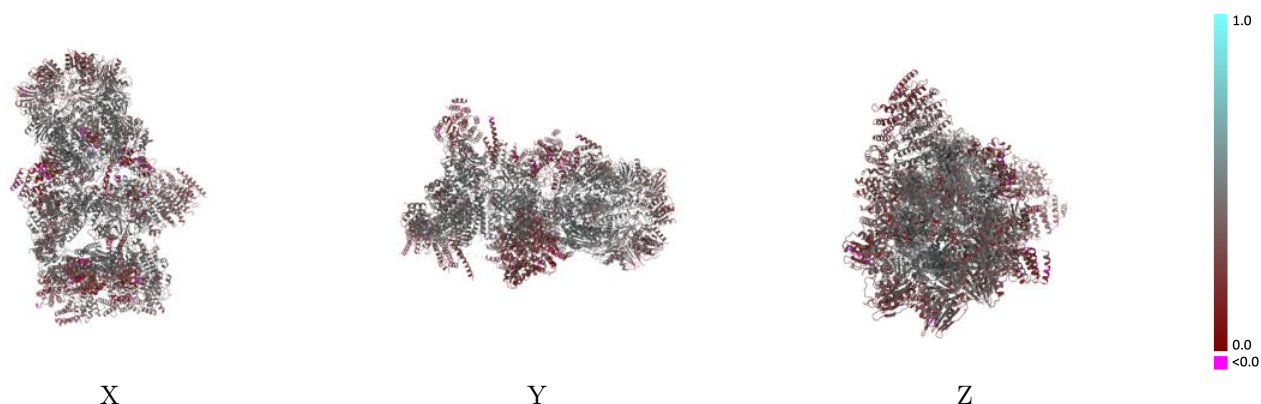
Y



Z

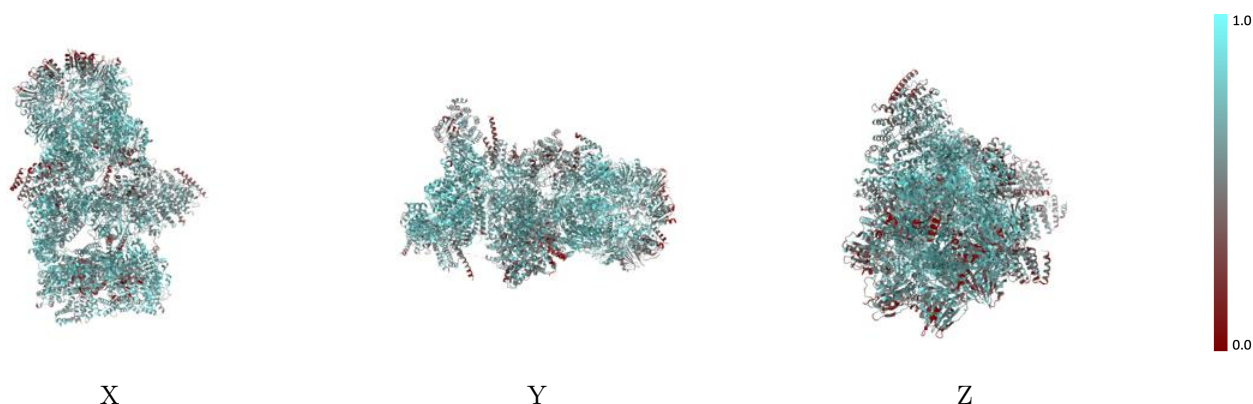
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



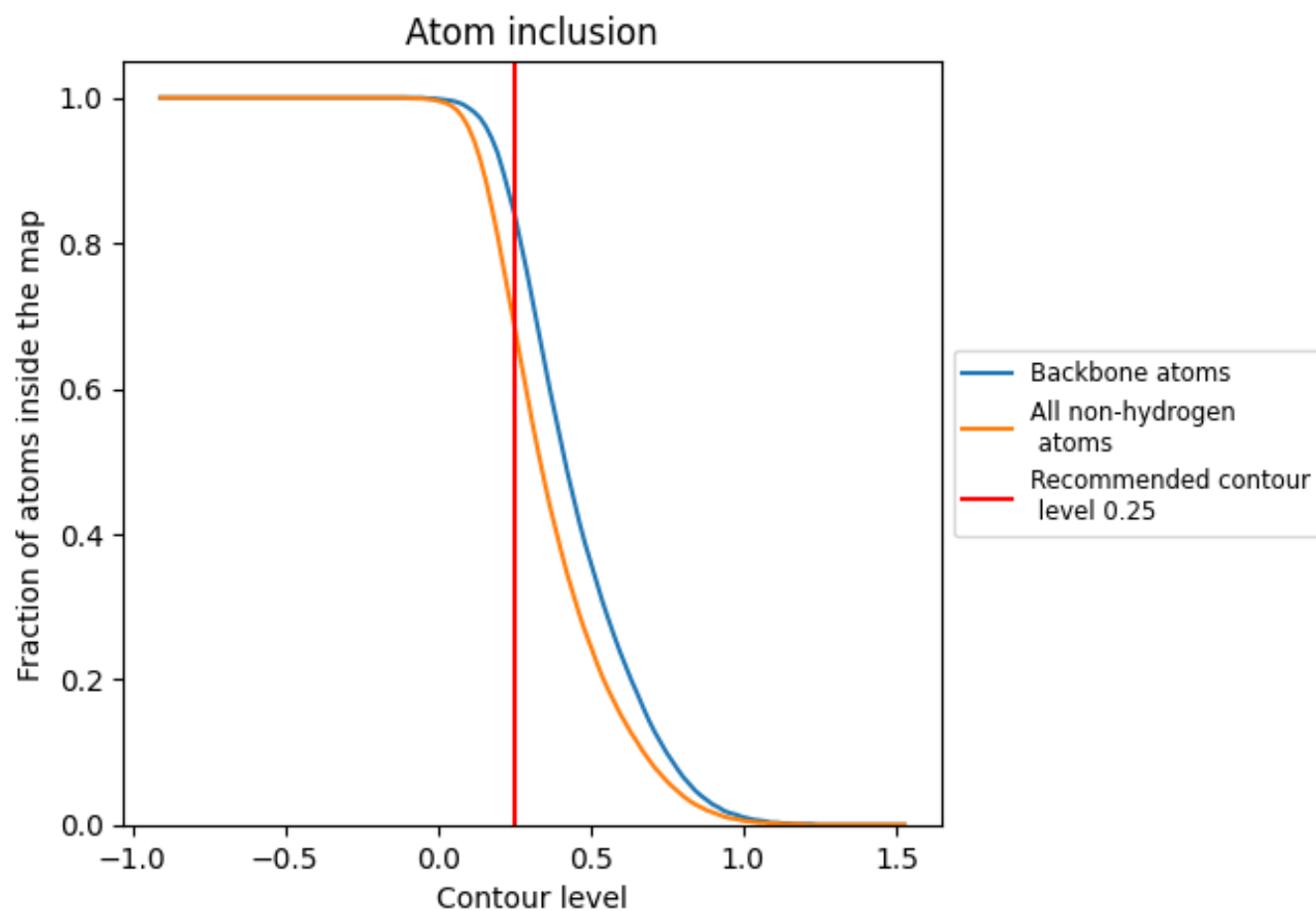
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.25).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 69% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6890	 0.4080
A	 0.6130	 0.3640
B	 0.7170	 0.4540
C	 0.7870	 0.4860
D	 0.7800	 0.4890
E	 0.6910	 0.4240
F	 0.4740	 0.2760
G	 0.7480	 0.4510
H	 0.8170	 0.5000
I	 0.7880	 0.4940
J	 0.7860	 0.4840
K	 0.7720	 0.4780
L	 0.7890	 0.4490
M	 0.7300	 0.4230
N	 0.7700	 0.4530
O	 0.7620	 0.4740
P	 0.7850	 0.4750
Q	 0.7670	 0.4670
R	 0.8100	 0.4590
S	 0.7790	 0.4550
T	 0.7730	 0.4340
U	 0.7630	 0.4310
V	 0.7040	 0.3890
W	 0.6160	 0.3470
X	 0.6430	 0.3880
Y	 0.7790	 0.4300
Z	 0.7620	 0.4550
a	 0.6470	 0.3340
b	 0.5130	 0.2890
c	 0.7530	 0.4680
d	 0.6200	 0.3010
e	 0.7610	 0.4480
f	 0.5860	 0.3090
n	 0.5370	 0.3750
o	 0.4950	 0.3490



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
p	 0.4610	 0.3570
q	 0.4730	 0.3400
r	 0.5150	 0.3360
s	 0.5570	 0.3610
t	 0.5790	 0.3830
y	 0.2470	 0.2550