



wwPDB EM Validation Summary Report ⓘ

Jun 30, 2025 – 08:46 AM EDT

PDB ID : 9CGC / pdb_00009cgc
EMDB ID : EMD-45579
Title : Yeast 26S proteasome non-substrate-engaged (S1 state)
Authors : Arkinson, C.; Gee, C.L.; Martin, A.
Deposited on : 2024-06-28
Resolution : 3.61 Å(reported)
Based on initial model : 6j2q

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) : 2.44

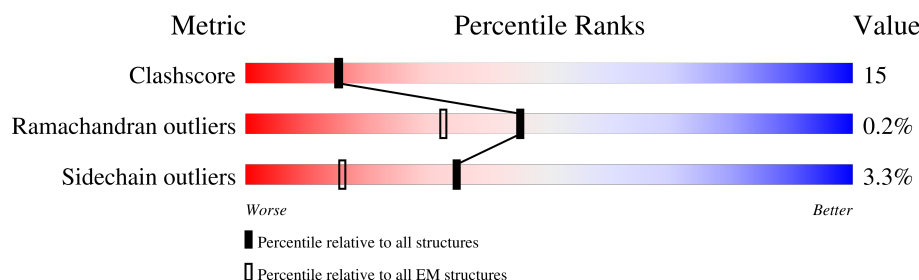
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.61 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	1	215	<div> <div>18%</div> <div>57%</div> <div>37%</div> <div>5%</div> </div>
1	b	215	<div> <div>60%</div> <div>69%</div> <div>26%</div> <div>5%</div> </div>
2	2	261	<div> <div>18%</div> <div>56%</div> <div>28%</div> <div>15%</div> </div>
2	i	261	<div> <div>59%</div> <div>56%</div> <div>29%</div> <div>15%</div> </div>
3	3	205	<div> <div>25%</div> <div>61%</div> <div>37%</div> <div>.</div> </div>
3	h	205	<div> <div>77%</div> <div>58%</div> <div>41%</div> <div>.</div> </div>
4	4	198	<div> <div>23%</div> <div>64%</div> <div>35%</div> <div>.</div> </div>
4	g	198	<div> <div>73%</div> <div>61%</div> <div>38%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
5	5	287	
5	f	287	
6	6	241	
6	e	241	
7	7	266	
7	a	266	
8	A	252	
9	B	250	
10	C	258	
11	D	254	
12	E	260	
13	F	234	
14	G	288	
15	I	437	
16	K	428	
17	L	437	
18	O	393	
19	P	445	
20	R	429	
21	S	523	
22	V	306	
23	W	268	
24	Y	89	
25	J	405	
26	H	467	

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Mol	Chain	Length	Quality of chain
27	M	434	
28	Q	434	
29	U	338	
30	N	945	
31	T	274	
32	o	993	

2 Entry composition [i](#)

There are 36 unique types of molecules in this entry. The entry contains 92952 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 Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	205	Total	C	N	O	S	0	0
			1576	996	261	312	7		
1	b	205	Total	C	N	O	S	0	0
			1576	996	261	312	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	222	Total	C	N	O	S	0	0
			1684	1061	293	323	7		
2	i	222	Total	C	N	O	S	0	0
			1684	1061	293	323	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	204	Total	C	N	O	S	0	0
			1581	1010	258	305	8		
3	h	204	Total	C	N	O	S	0	0
			1581	1010	258	305	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	198	Total	C	N	O	S	0	0
			1585	1005	269	305	6		
4	g	198	Total	C	N	O	S	0	0
			1585	1005	269	305	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	212	Total	C	N	O	S	0	0
			1644	1045	280	312	7		
5	f	212	Total	C	N	O	S	0	0
			1644	1045	280	312	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	222	Total	C	N	O	S	0	0
			1757	1115	303	335	4		
6	e	222	Total	C	N	O	S	0	0
			1757	1115	303	335	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	7	233	Total	C	N	O	S	0	0
			1824	1154	312	351	7		
7	a	233	Total	C	N	O	S	0	0
			1824	1154	312	351	7		

- Molecule 8 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	A	243	Total	C	N	O	S	0	0
			1921	1221	322	370	8		

- Molecule 9 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	B	250	Total	C	N	O	S	0	0
			1915	1219	315	377	4		

- Molecule 10 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	C	244	Total	C	N	O	S	0	0
			1904	1201	321	379	3		

- Molecule 11 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	D	241	Total	C	N	O	S	0	0
			1890	1181	331	374	4		

- Molecule 12 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	E	242	Total	C	N	O	S	0	0
			1861	1162	314	378	7		

- Molecule 13 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	F	233	Total	C	N	O	S	0	0
			1795	1129	312	350	4		

- Molecule 14 is a protein called Probable proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	G	243	Total	C	N	O	S	0	0
			1888	1201	328	355	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	I	392	Total	C	N	O	S	0	0
			3078	1937	516	608	17		

- Molecule 16 is a protein called 26S proteasome regulatory subunit 6B homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	K	383	Total	C	N	O	S	0	0
			3035	1908	532	585	10		

- Molecule 17 is a protein called 26S proteasome subunit RPT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	L	359	Total	C	N	O	S	0	0
			2820	1783	490	535	12		

- Molecule 18 is a protein called 26S proteasome regulatory subunit RPN9.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	O	386	Total	C	N	O	S	0	0
			3169	2040	517	604	8		

- Molecule 19 is a protein called 26S proteasome regulatory subunit RPN5.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	P	436	Total	C	N	O	S	0	0
			3575	2279	597	690	9		

- Molecule 20 is a protein called 26S proteasome regulatory subunit RPN7.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	R	397	Total	C	N	O	S	0	0
			3195	2043	524	618	10		

- Molecule 21 is a protein called 26S proteasome regulatory subunit RPN3.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	S	461	Total	C	N	O	S	0	0
			3770	2412	629	714	15		

- Molecule 22 is a protein called Ubiquitin carboxyl-terminal hydrolase RPN11.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	288	Total	C	N	O	S	0	0
			2267	1421	388	444	14		

- Molecule 23 is a protein called 26S proteasome regulatory subunit RPN10.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	190	Total	C	N	O	S	0	0
			1484	933	262	287	2		

- Molecule 24 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	Y	33	Total	C	N	O	0	0
			281	176	38	67		

- Molecule 25 is a protein called 26S proteasome regulatory subunit 8 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	J	370	Total	C	N	O	S	0	0
			2913	1836	524	536	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	H	385	Total	C	N	O	S	0	0
			3016	1896	540	563	17		

- Molecule 27 is a protein called 26S proteasome regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	M	363	Total	C	N	O	S	0	0
			2827	1771	493	550	13		

- Molecule 28 is a protein called 26S proteasome regulatory subunit RPN6.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Q	411	Total	C	N	O	S	0	0
			3347	2137	552	643	15		

- Molecule 29 is a protein called 26S proteasome regulatory subunit RPN8.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	U	292	Total	C	N	O	S	0	0
			2333	1476	401	449	7		

- Molecule 30 is a protein called 26S proteasome regulatory subunit RPN2.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	N	869	Total	C	N	O	S	0	0
			6725	4275	1130	1292	28		

- Molecule 31 is a protein called 26S proteasome regulatory subunit RPN12.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	T	257	Total	C	N	O	S	0	0
			2106	1357	335	410	4		

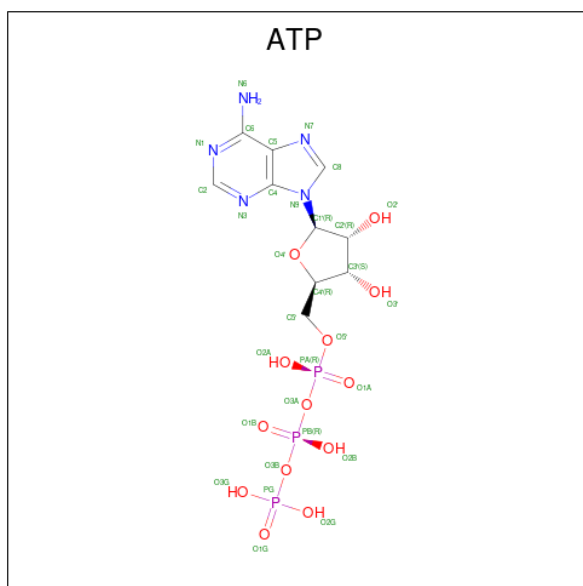
- Molecule 32 is a protein called 26S proteasome regulatory subunit RPN1.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	o	819	Total	C	N	O	S	0	0
			6347	4039	1040	1239	29		

- Molecule 33 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
33	I	1	Total	Mg	0
			1	1	
33	K	1	Total	Mg	0
			1	1	
33	L	1	Total	Mg	0
			1	1	
33	H	1	Total	Mg	0
			1	1	
33	M	1	Total	Mg	0
			1	1	

- Molecule 34 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
34	H	1	Total 31	C 10	N 5	O 13	P 3	0
34	M	1	Total 31	C 10	N 5	O 13	P 3	0

- | Mol | Chain | Residues | Atoms | AltConf |
|-----|-------|----------|-----------------|---------|
| 35 | V | 1 | Total Zn
1 1 | 0 |

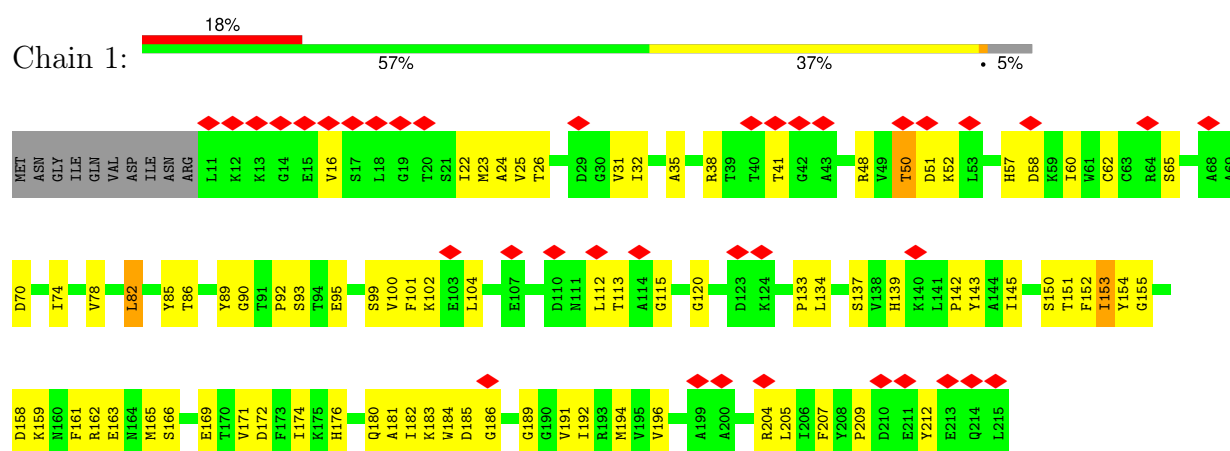
- # ADP

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

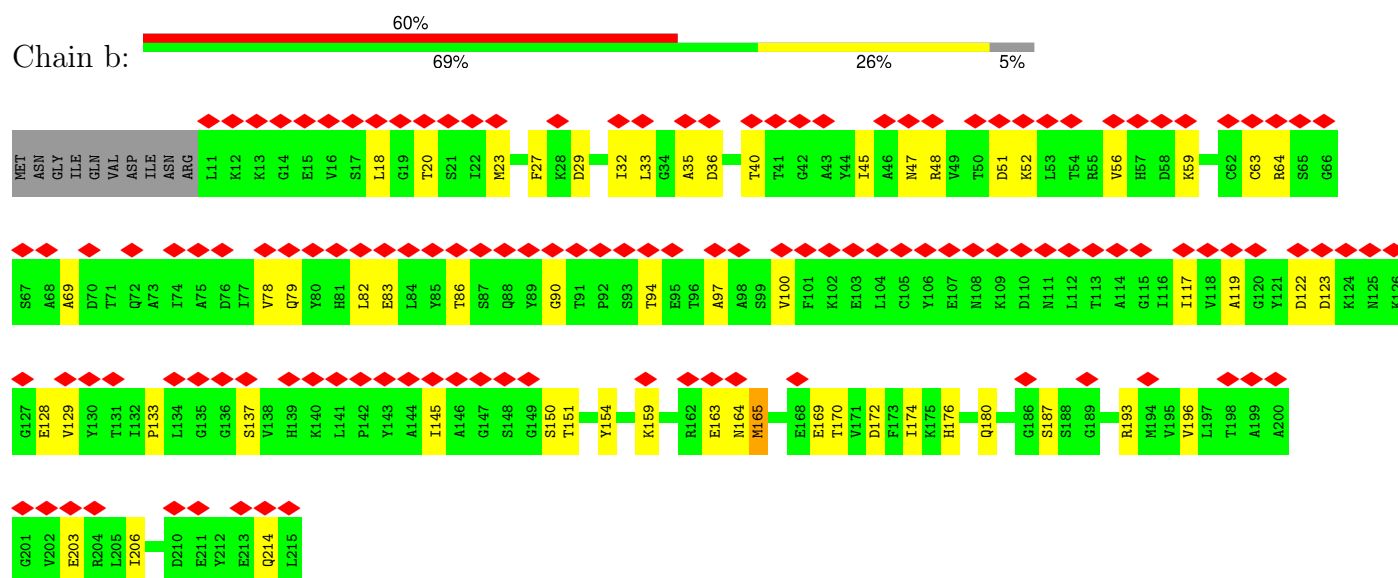
3 Residue-property plots

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: Proteasome subunit beta type-1



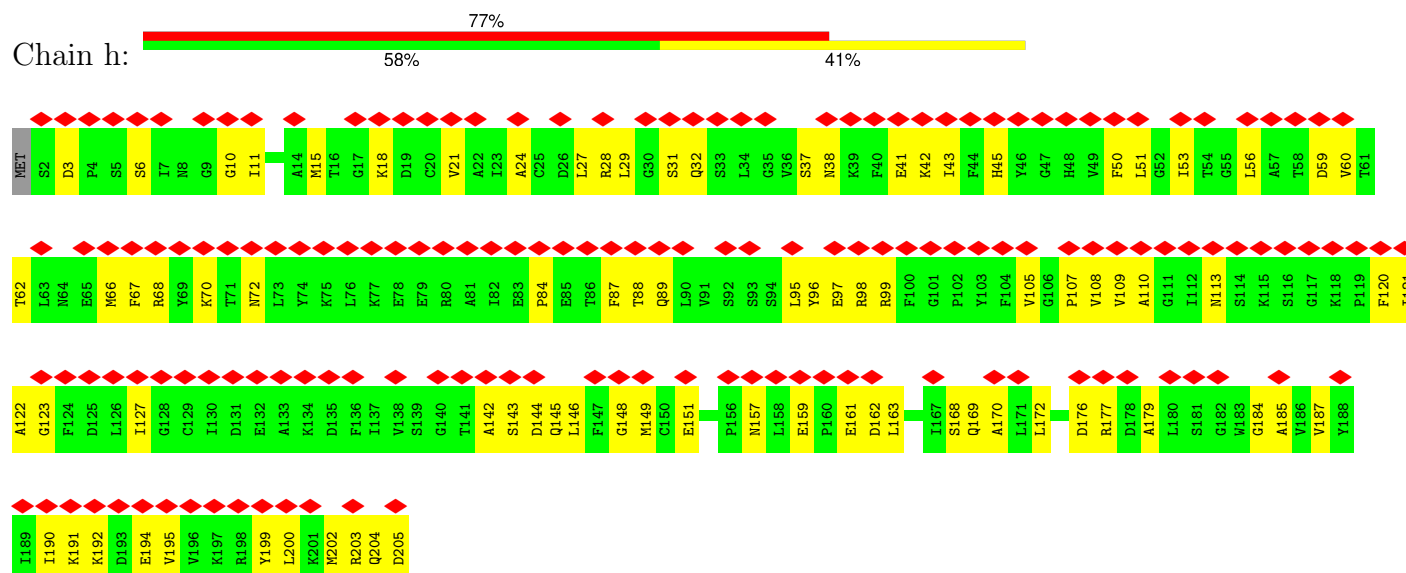
• Molecule 1: Proteasome subunit beta type-1



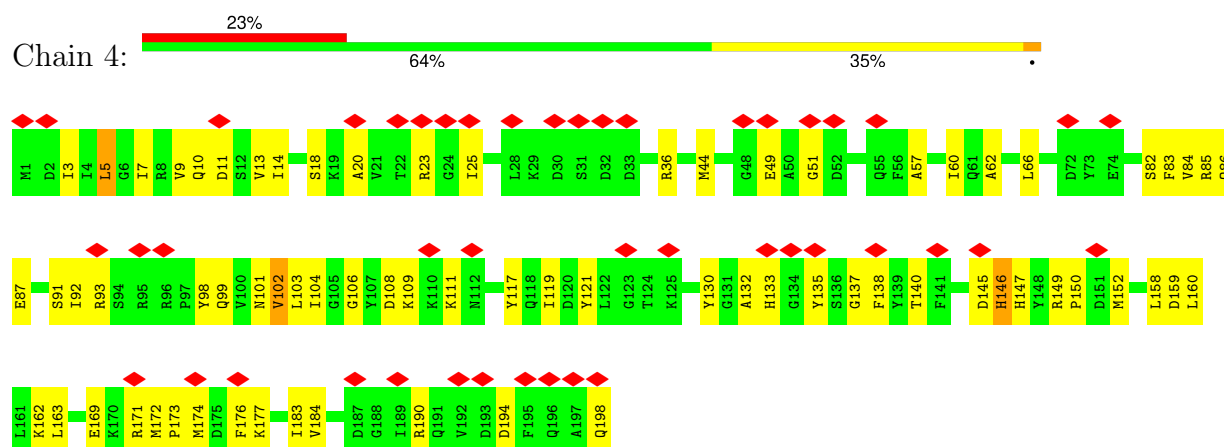
• Molecule 2: Proteasome subunit beta type-2



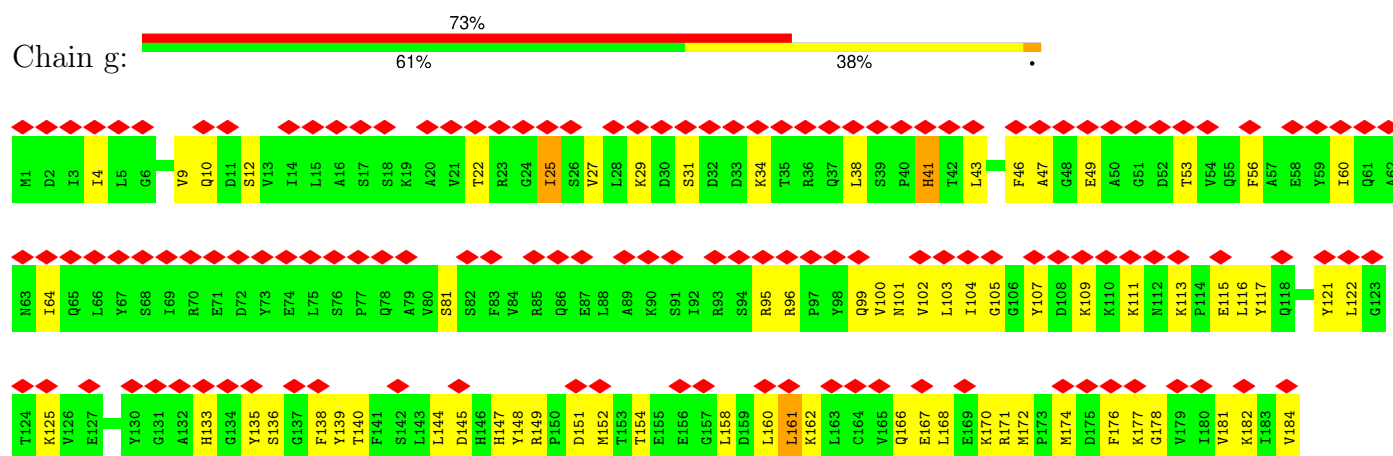
- Molecule 3: Proteasome subunit beta type-3

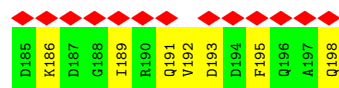


- Molecule 4: Proteasome subunit beta type-4

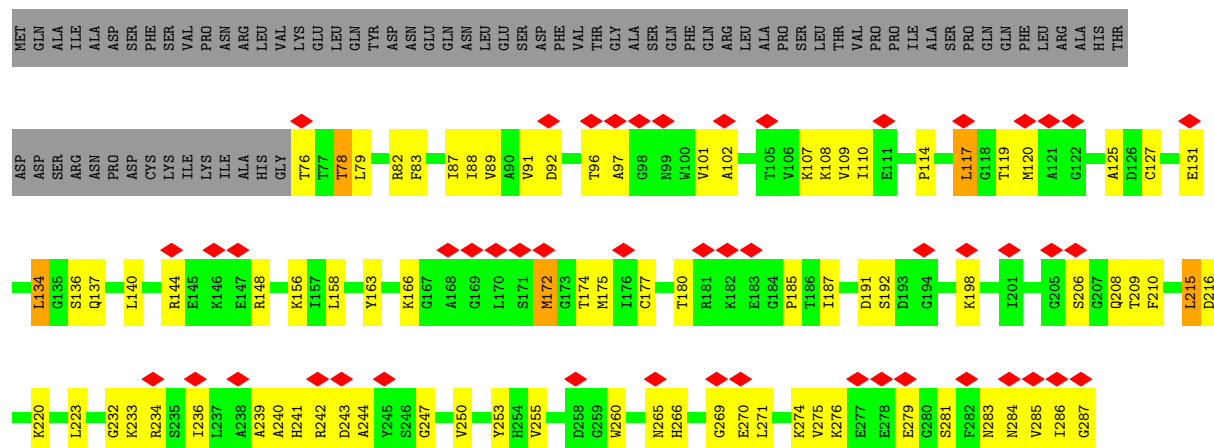
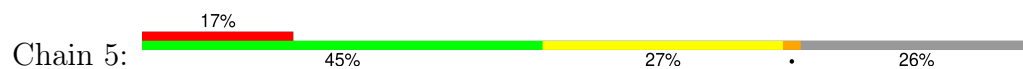


- Molecule 4: Proteasome subunit beta type-4

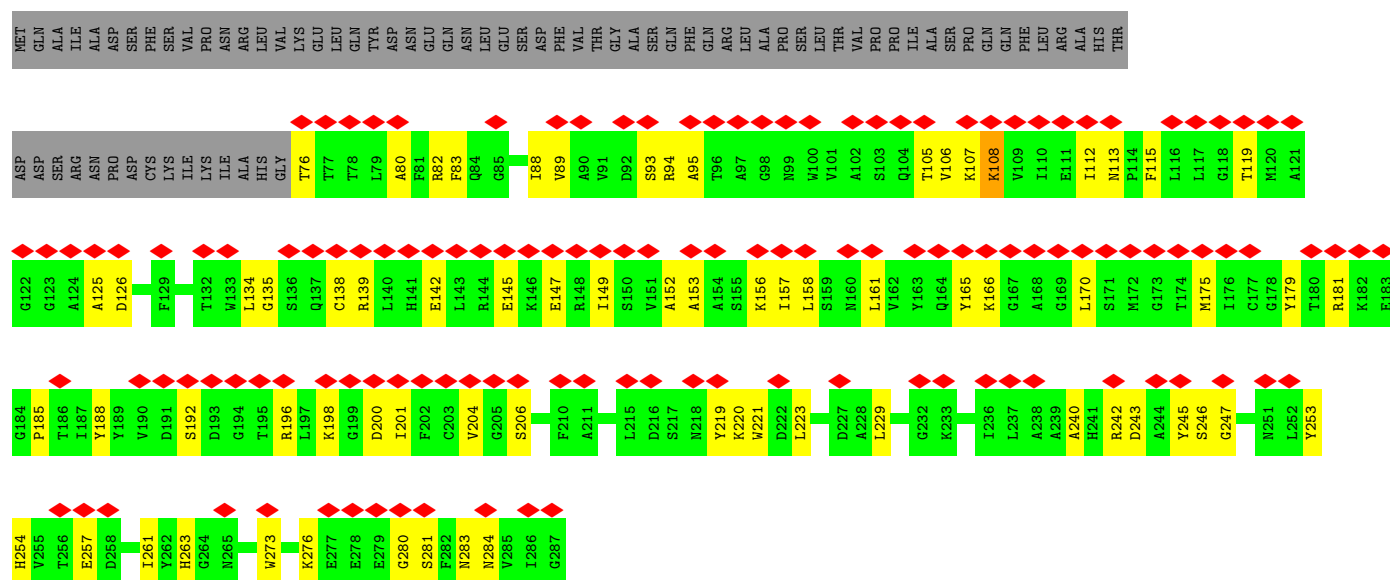




• Molecule 5: Proteasome subunit beta type-5

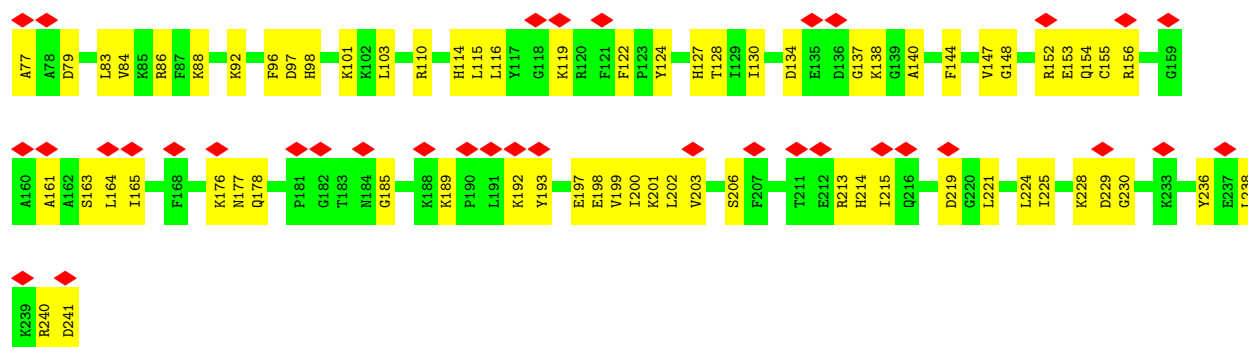


• Molecule 5: Proteasome subunit beta type-5

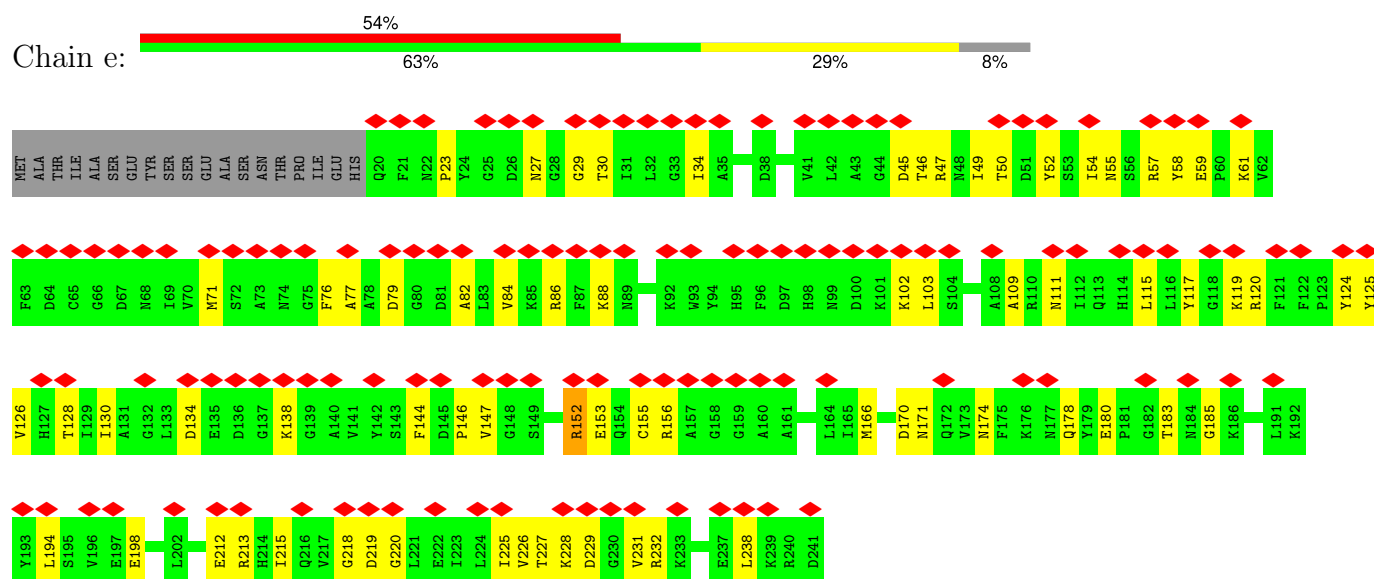


• Molecule 6: Proteasome subunit beta type-6

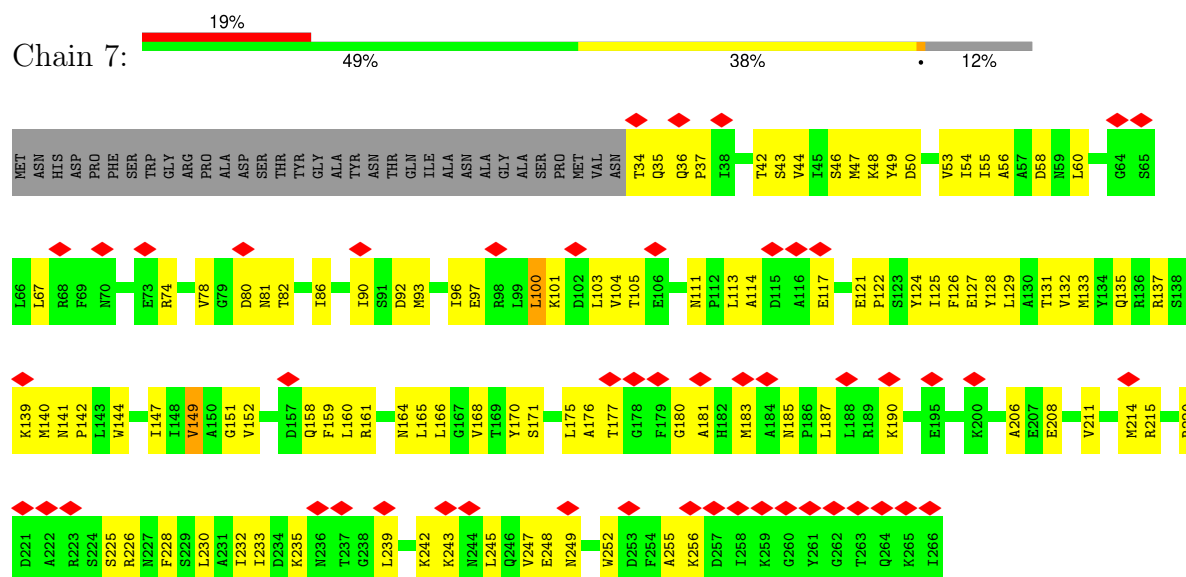




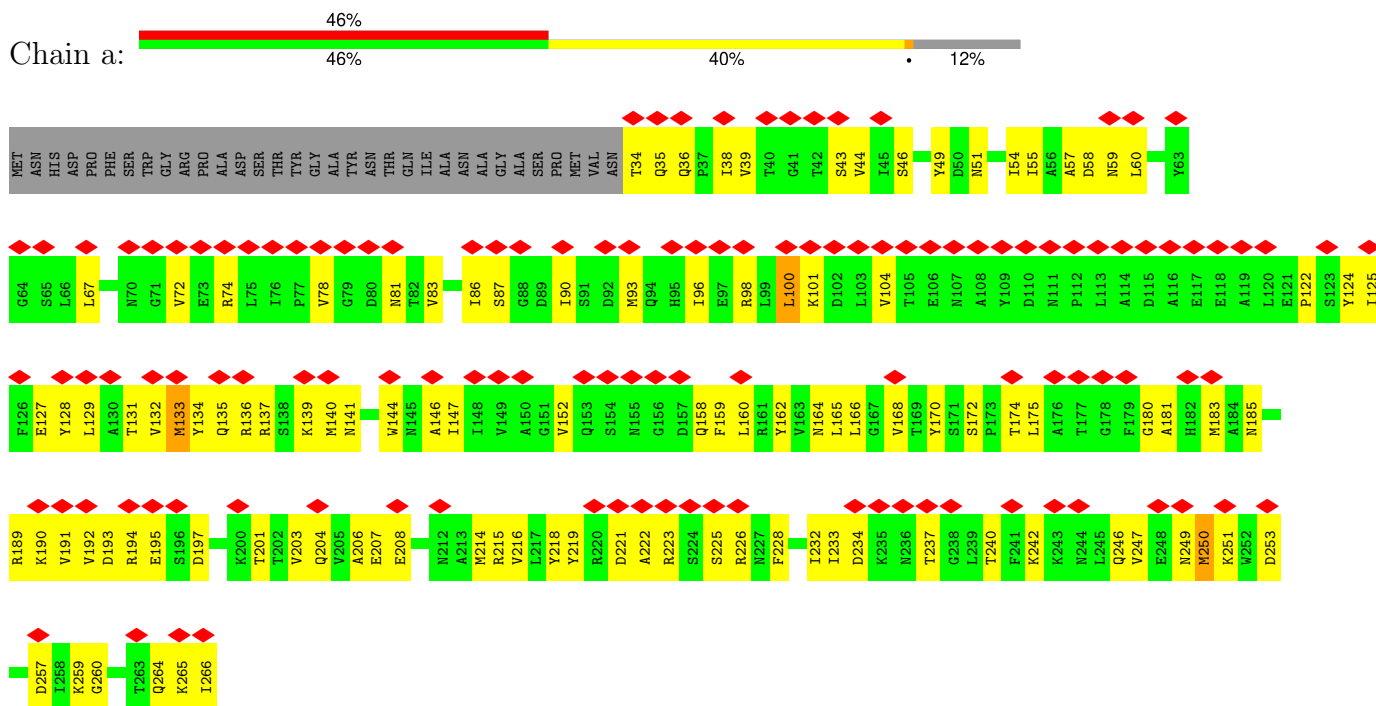
• Molecule 6: Proteasome subunit beta type-6



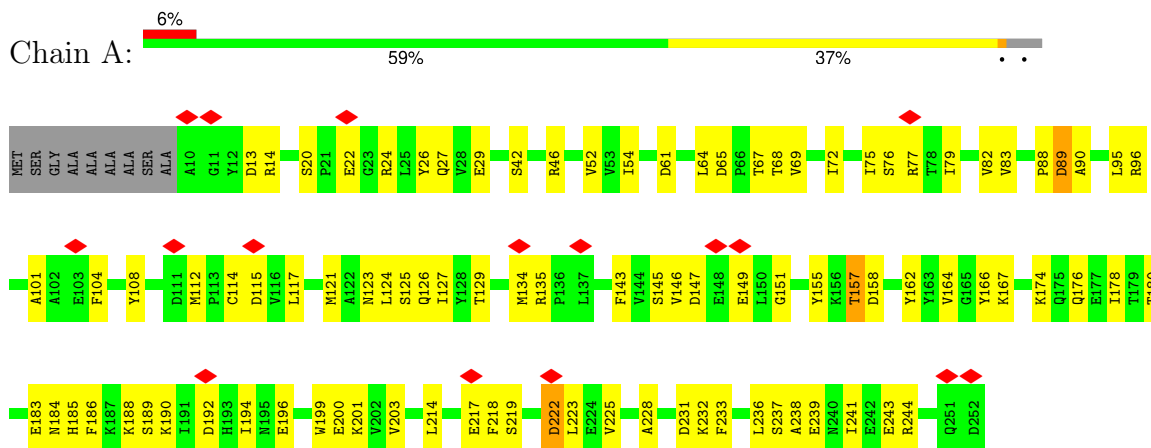
• Molecule 7: Proteasome subunit beta type-7



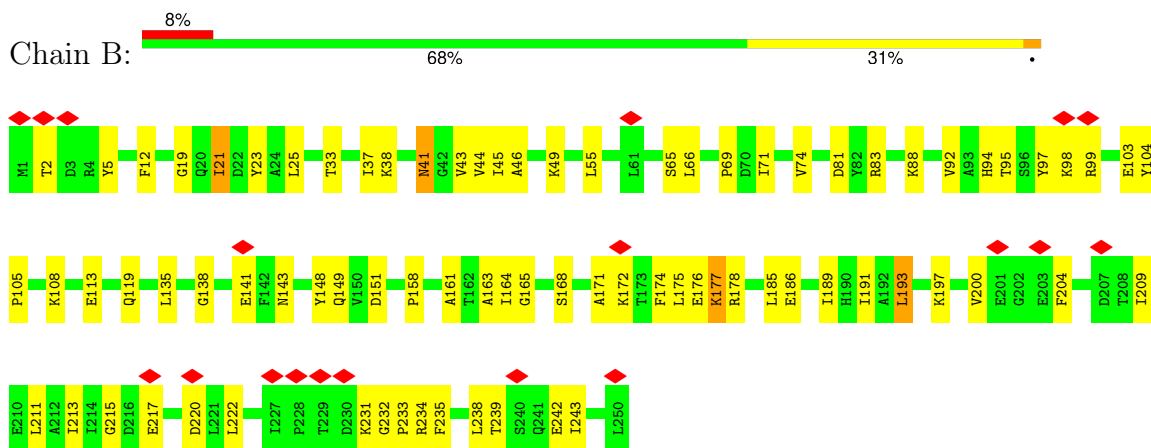
• Molecule 7: Proteasome subunit beta type-7



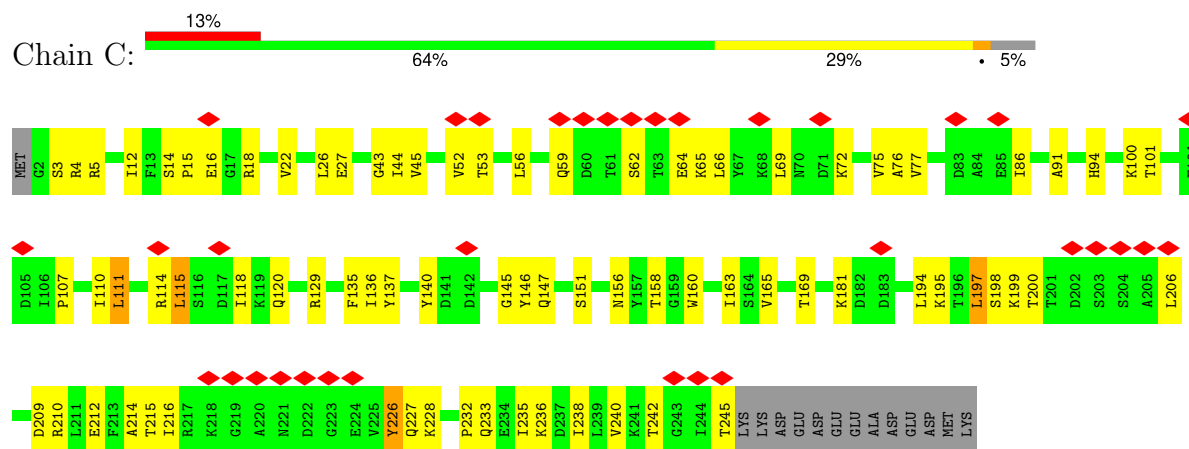
• Molecule 8: Proteasome subunit alpha type-1



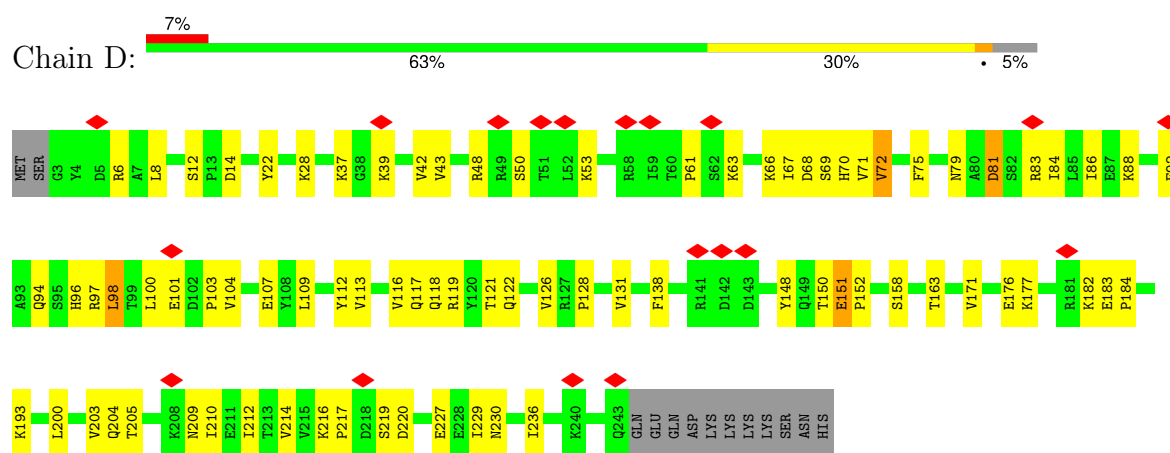
• Molecule 9: Proteasome subunit alpha type-2



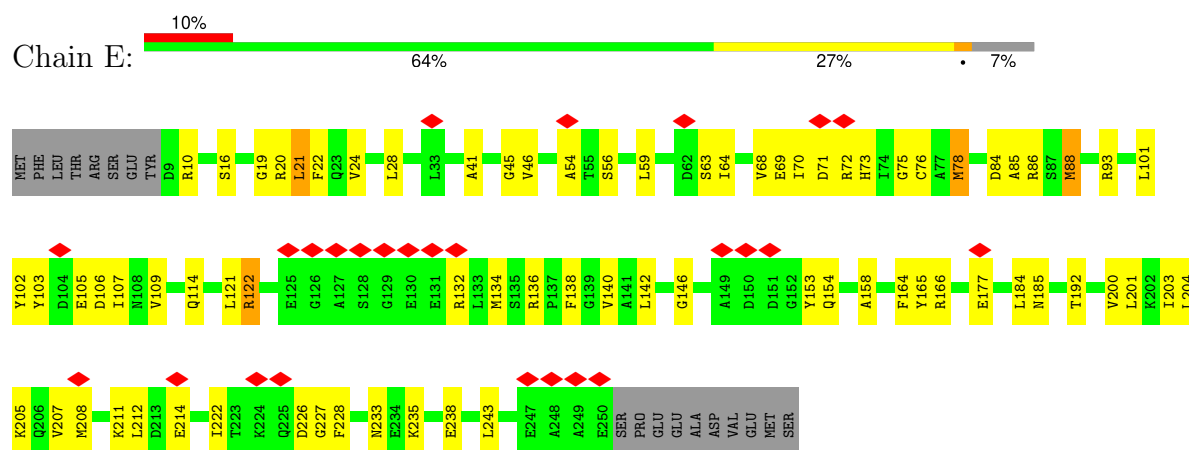
- Molecule 10: Proteasome subunit alpha type-3



- Molecule 11: Proteasome subunit alpha type-4



- Molecule 12: Proteasome subunit alpha type-5



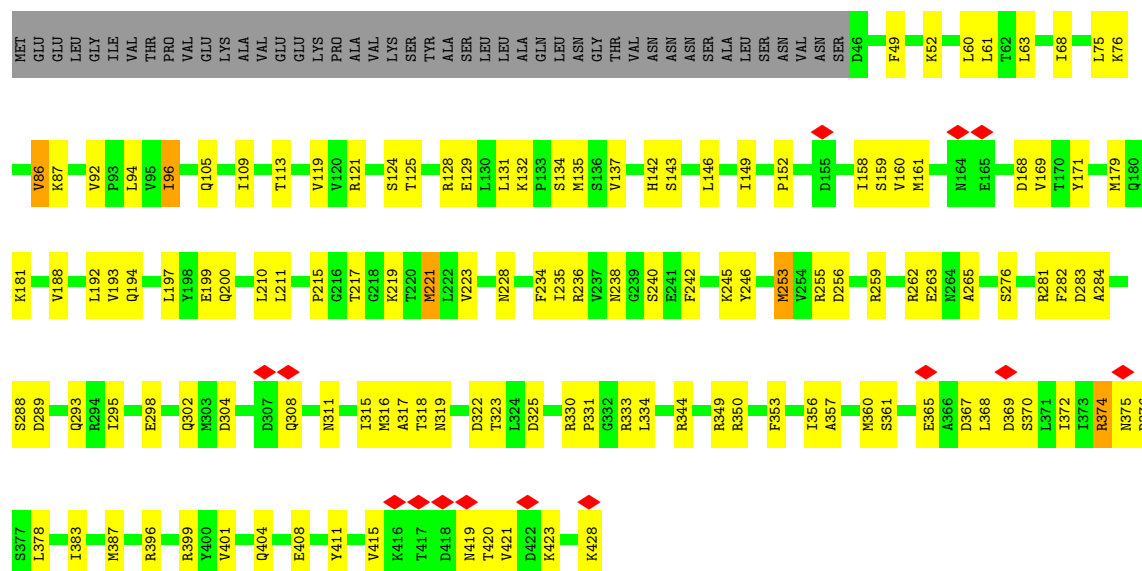
- Molecule 13: Proteasome subunit alpha type-6





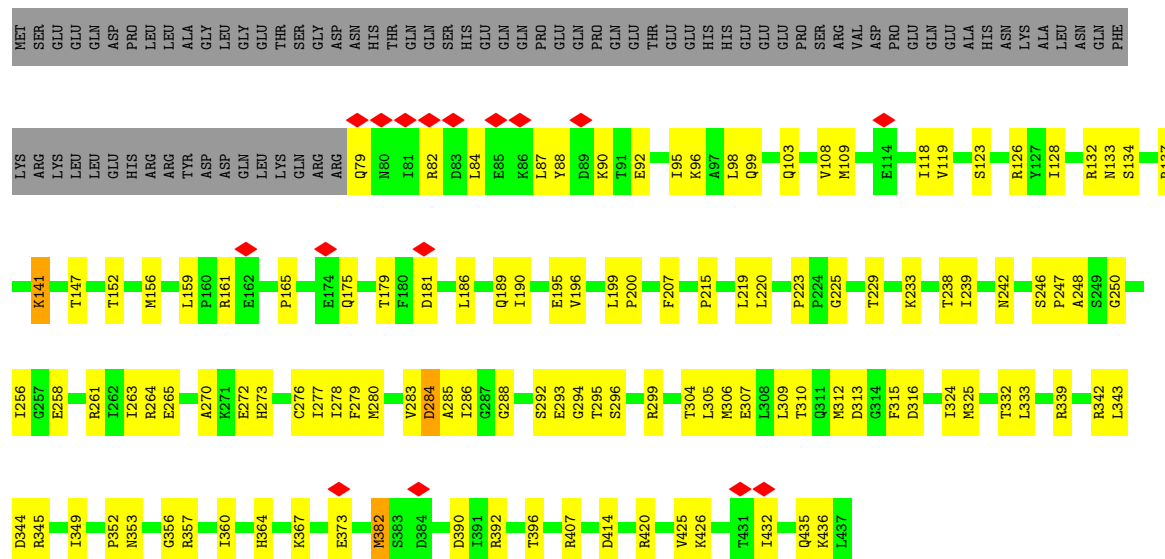
- Molecule 16: 26S proteasome regulatory subunit 6B homolog

Chain K: 59% 29% 11%



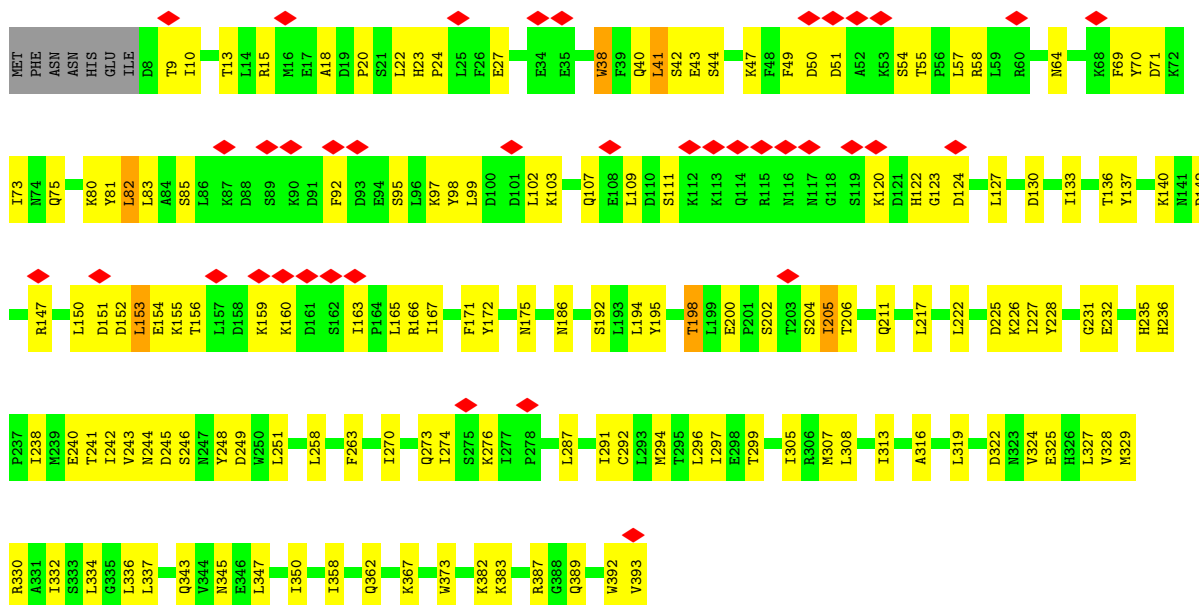
- Molecule 17: 26S proteasome subunit RPT4

Chain L: 55% 27% 18%



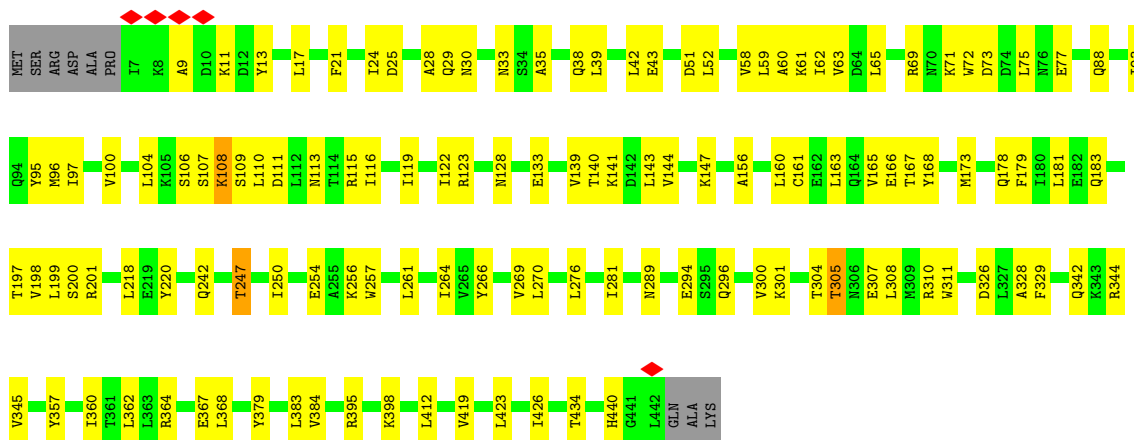
- Molecule 18: 26S proteasome regulatory subunit RPN9

Chain O: 10% 60% 36%



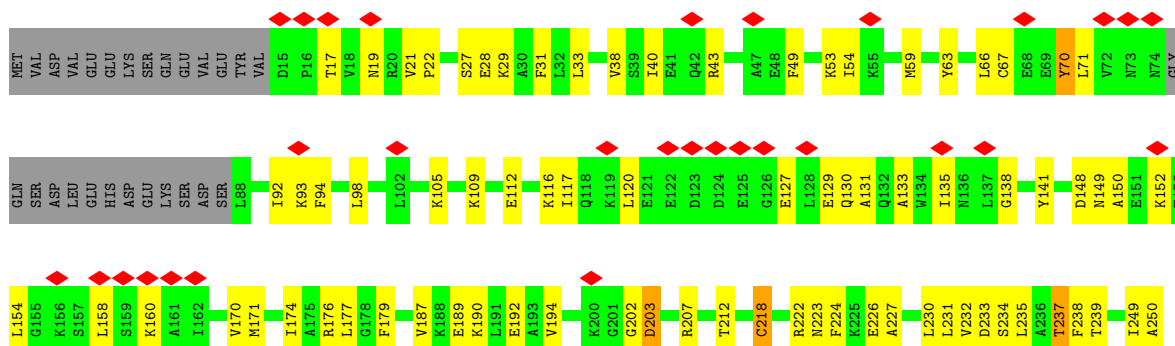
- Molecule 19: 26S proteasome regulatory subunit RPN5

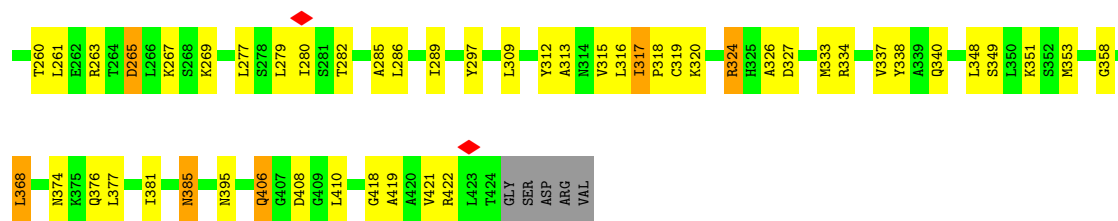
Chain P: 70% 27%

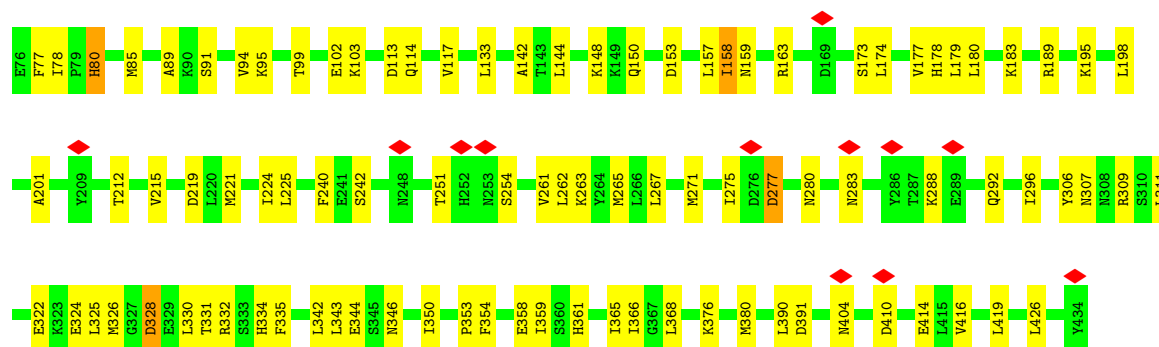


- Molecule 20: 26S proteasome regulatory subunit RPN7

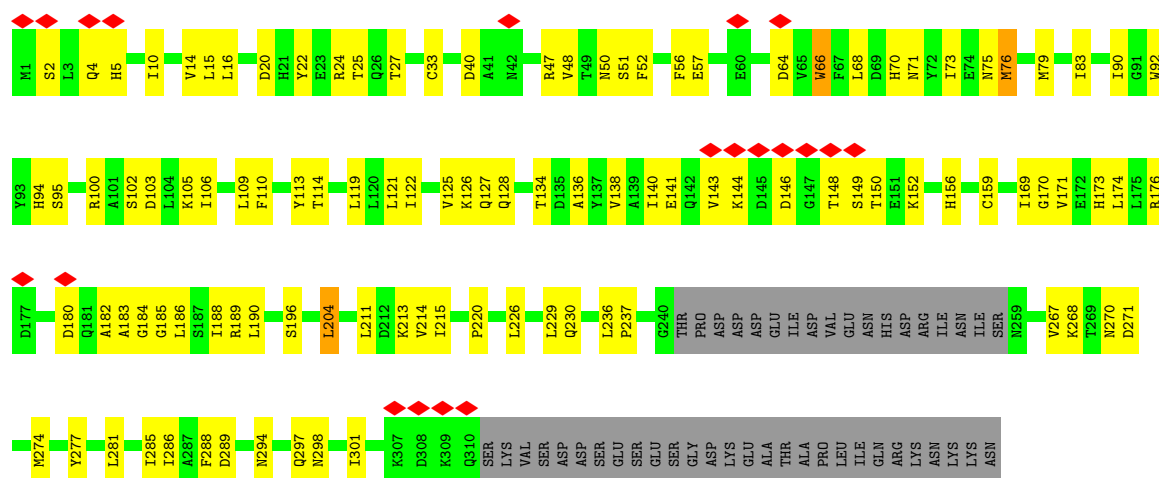
Chain R: 7% 63% 28% 7%



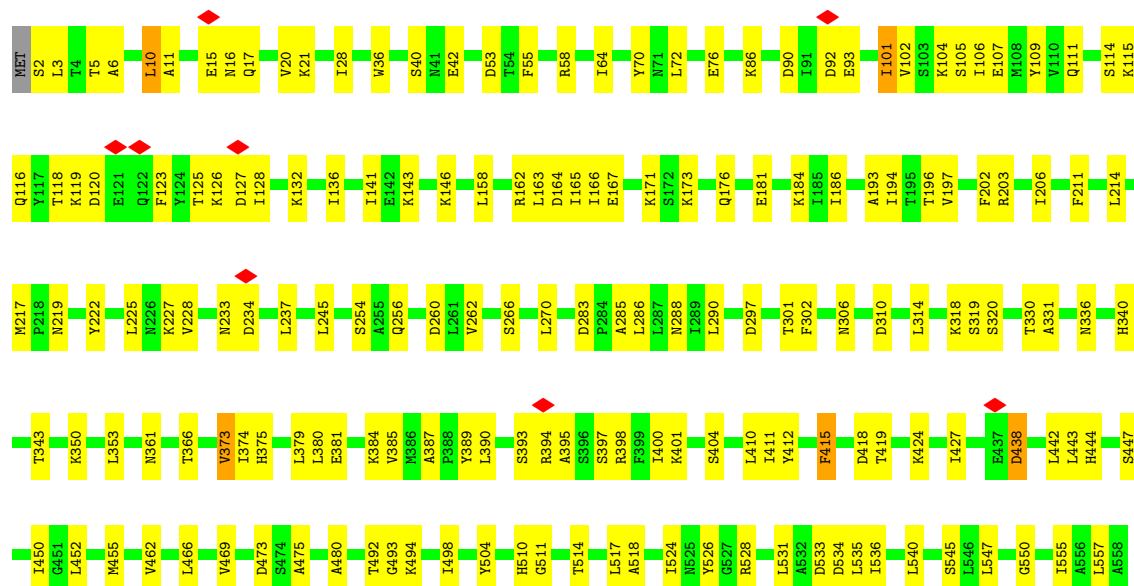


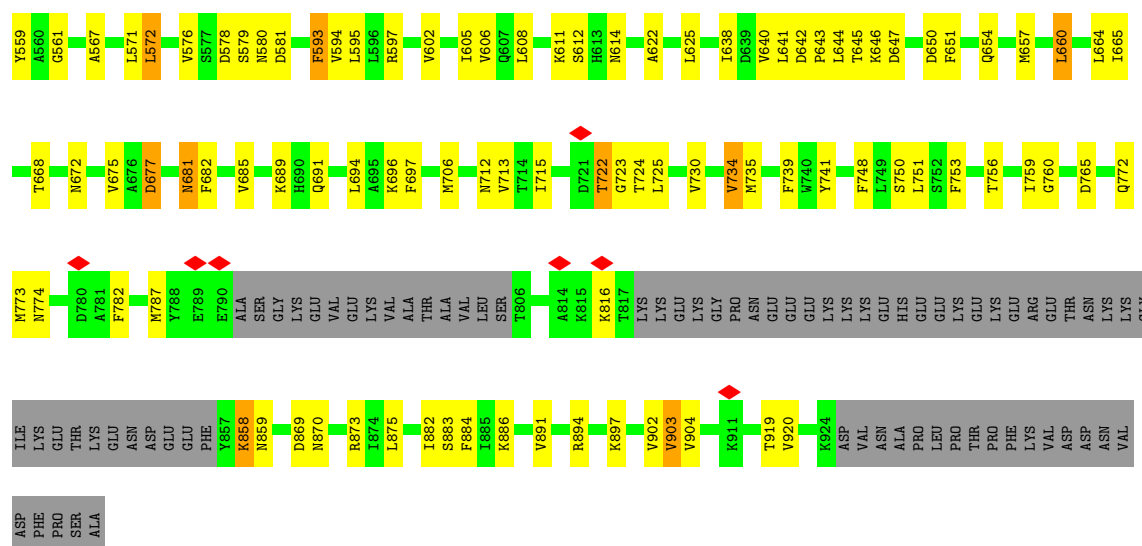


• Molecule 29: 26S proteasome regulatory subunit RPN8



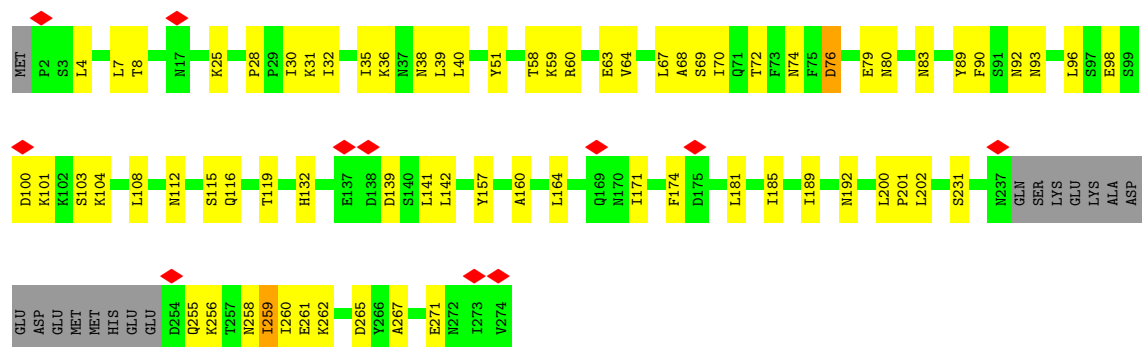
• Molecule 30: 26S proteasome regulatory subunit RPN2





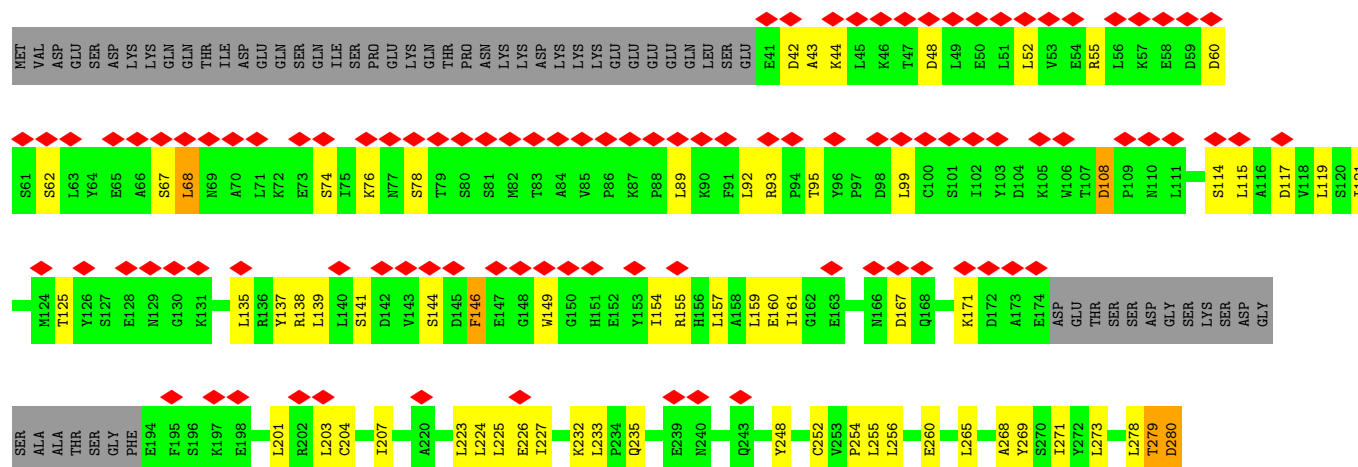
• Molecule 31: 26S proteasome regulatory subunit RPN12

Chain T: 68% 25% 6%



• Molecule 32: 26S proteasome regulatory subunit RPN1

Chain o: 55% 26% 18%





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	110527	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.926	Depositor
Minimum map value	-0.797	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.072	Depositor
Recommended contour level	0.33	Depositor
Map size (Å)	379.1, 379.1, 379.1	wwPDB
Map dimensions	340, 340, 340	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.115, 1.115, 1.115	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, ZN, MG, 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	1	0.11	0/1605	0.30	0/2171
1	b	0.11	0/1605	0.28	0/2171
2	2	0.11	0/1715	0.31	0/2326
2	i	0.09	0/1715	0.27	0/2326
3	3	0.11	0/1611	0.29	0/2174
3	h	0.11	0/1611	0.28	0/2174
4	4	0.11	0/1613	0.34	0/2173
4	g	0.11	0/1613	0.32	0/2173
5	5	0.10	0/1681	0.30	0/2274
5	f	0.09	0/1681	0.29	0/2274
6	6	0.10	0/1795	0.29	0/2420
6	e	0.09	0/1795	0.24	0/2420
7	7	0.12	0/1855	0.36	0/2514
7	a	0.12	0/1855	0.36	0/2514
8	A	0.13	0/1959	0.33	0/2652
9	B	0.13	0/1952	0.37	1/2642 (0.0%)
10	C	0.11	0/1934	0.31	0/2618
11	D	0.12	0/1919	0.31	0/2598
12	E	0.11	0/1886	0.29	0/2541
13	F	0.16	0/1823	0.34	0/2463
14	G	0.14	0/1928	0.37	0/2603
15	I	0.14	0/3120	0.42	1/4204 (0.0%)
16	K	0.14	0/3078	0.35	0/4154
17	L	0.14	0/2862	0.35	0/3851
18	O	0.11	0/3230	0.33	0/4357
19	P	0.11	0/3629	0.31	0/4894
20	R	0.12	0/3249	0.33	0/4385
21	S	0.11	0/3839	0.31	0/5186
22	V	0.15	0/2302	0.39	0/3105
23	W	0.11	0/1507	0.29	0/2045
24	Y	0.15	0/287	0.40	0/391
25	J	0.13	0/2950	0.35	0/3960

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
26	H	0.14	0/3063	0.37	0/4120
27	M	0.13	0/2863	0.36	0/3855
28	Q	0.12	0/3402	0.31	0/4577
29	U	0.14	0/2364	0.37	0/3190
30	N	0.12	0/6835	0.32	1/9243 (0.0%)
31	T	0.12	0/2147	0.32	0/2900
32	o	0.12	0/6462	0.32	0/8771
All	All	0.12	0/94340	0.33	3/127409 (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
16	K	0	1
32	o	0	1
All	All	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	I	381	VAL	N-CA-C	-6.17	107.27	113.20
30	N	86	LYS	CB-CA-C	-5.48	109.78	117.23
9	B	2	THR	CB-CA-C	-5.32	109.46	115.79

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	K	92	VAL	Peptide
32	o	953	THR	Peptide

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	1	1576	0	1552	62	0
1	b	1576	0	1552	51	0
2	2	1684	0	1685	62	0
2	i	1684	0	1685	54	0
3	3	1581	0	1571	62	0
3	h	1581	0	1571	62	0
4	4	1585	0	1590	58	0
4	g	1585	0	1590	61	0
5	5	1644	0	1592	66	0
5	f	1644	0	1592	55	0
6	6	1757	0	1708	66	0
6	e	1757	0	1708	55	0
7	7	1824	0	1829	79	0
7	a	1824	0	1829	81	0
8	A	1921	0	1910	73	0
9	B	1915	0	1929	59	0
10	C	1904	0	1901	57	0
11	D	1890	0	1900	59	0
12	E	1861	0	1836	60	0
13	F	1795	0	1797	61	0
14	G	1888	0	1880	71	0
15	I	3078	0	3147	131	0
16	K	3035	0	3099	102	0
17	L	2820	0	2895	99	0
18	O	3169	0	3196	105	0
19	P	3575	0	3662	99	0
20	R	3195	0	3214	94	0
21	S	3770	0	3819	101	0
22	V	2267	0	2266	77	0
23	W	1484	0	1494	47	0
24	Y	281	0	224	15	0
25	J	2913	0	3050	89	0
26	H	3016	0	3086	111	0
27	M	2827	0	2887	89	0
28	Q	3347	0	3380	75	0
29	U	2333	0	2396	83	0
30	N	6725	0	6796	189	0
31	T	2106	0	2099	50	0
32	o	6347	0	6319	192	0
33	H	1	0	0	0	0
33	I	1	0	0	0	0
33	K	1	0	0	0	0
33	L	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	M	1	0	0	0	0
34	H	31	0	12	3	0
34	J	31	0	12	3	0
34	K	31	0	12	6	0
34	L	31	0	12	0	0
34	M	31	0	12	4	0
35	V	1	0	0	0	0
36	J	27	0	12	4	0
All	All	92952	0	93308	2720	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 15.

The worst 5 of 2720 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)
16:K:61:LEU:HD21	25:J:37:LYS:HB3	1.49	0.94
28:Q:419:LEU:HD23	29:U:285:ILE:HD12	1.48	0.93
29:U:126:LYS:HB2	29:U:128:GLN:HE22	1.36	0.90
15:I:67:ASP:HB3	32:o:614:VAL:HG11	1.58	0.85
12:E:166:ARG:HG2	13:F:58:SER:HB3	1.59	0.82

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	1	203/215 (94%)	195 (96%)	8 (4%)	0	100	100
1	b	203/215 (94%)	197 (97%)	6 (3%)	0	100	100
2	2	220/261 (84%)	217 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	i	220/261 (84%)	217 (99%)	3 (1%)	0	100	100
3	3	202/205 (98%)	192 (95%)	10 (5%)	0	100	100
3	h	202/205 (98%)	196 (97%)	6 (3%)	0	100	100
4	4	196/198 (99%)	191 (97%)	5 (3%)	0	100	100
4	g	196/198 (99%)	192 (98%)	4 (2%)	0	100	100
5	5	210/287 (73%)	207 (99%)	3 (1%)	0	100	100
5	f	210/287 (73%)	206 (98%)	4 (2%)	0	100	100
6	6	220/241 (91%)	214 (97%)	5 (2%)	1 (0%)	25	59
6	e	220/241 (91%)	217 (99%)	3 (1%)	0	100	100
7	7	231/266 (87%)	223 (96%)	8 (4%)	0	100	100
7	a	231/266 (87%)	224 (97%)	7 (3%)	0	100	100
8	A	241/252 (96%)	236 (98%)	5 (2%)	0	100	100
9	B	248/250 (99%)	242 (98%)	6 (2%)	0	100	100
10	C	242/258 (94%)	234 (97%)	7 (3%)	1 (0%)	30	62
11	D	239/254 (94%)	231 (97%)	8 (3%)	0	100	100
12	E	240/260 (92%)	232 (97%)	8 (3%)	0	100	100
13	F	231/234 (99%)	223 (96%)	8 (4%)	0	100	100
14	G	241/288 (84%)	233 (97%)	8 (3%)	0	100	100
15	I	390/437 (89%)	345 (88%)	43 (11%)	2 (0%)	25	59
16	K	381/428 (89%)	336 (88%)	43 (11%)	2 (0%)	25	59
17	L	357/437 (82%)	320 (90%)	36 (10%)	1 (0%)	37	67
18	O	384/393 (98%)	356 (93%)	25 (6%)	3 (1%)	16	50
19	P	434/445 (98%)	415 (96%)	18 (4%)	1 (0%)	44	73
20	R	393/429 (92%)	373 (95%)	19 (5%)	1 (0%)	37	67
21	S	459/523 (88%)	430 (94%)	28 (6%)	1 (0%)	44	73
22	V	286/306 (94%)	265 (93%)	20 (7%)	1 (0%)	37	67
23	W	188/268 (70%)	172 (92%)	16 (8%)	0	100	100
24	Y	29/89 (33%)	26 (90%)	2 (7%)	1 (3%)	3	24
25	J	364/405 (90%)	345 (95%)	19 (5%)	0	100	100
26	H	379/467 (81%)	333 (88%)	46 (12%)	0	100	100
27	M	359/434 (83%)	330 (92%)	28 (8%)	1 (0%)	37	67

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	Q	407/434 (94%)	385 (95%)	22 (5%)	0	100	100
29	U	288/338 (85%)	270 (94%)	17 (6%)	1 (0%)	37	67
30	N	863/945 (91%)	816 (95%)	47 (5%)	0	100	100
31	T	253/274 (92%)	237 (94%)	15 (6%)	1 (0%)	30	62
32	o	811/993 (82%)	756 (93%)	55 (7%)	0	100	100
All	All	11671/13187 (88%)	11029 (94%)	624 (5%)	18 (0%)	45	73

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	K	143	SER
18	O	205	ILE
22	V	161	THR
15	I	178	THR
17	L	175	GLN

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	1	169/178 (95%)	162 (96%)	7 (4%)	26	54
1	b	169/178 (95%)	168 (99%)	1 (1%)	84	91
2	2	181/214 (85%)	177 (98%)	4 (2%)	47	69
2	i	181/214 (85%)	178 (98%)	3 (2%)	56	75
3	3	172/173 (99%)	167 (97%)	5 (3%)	37	63
3	h	172/173 (99%)	170 (99%)	2 (1%)	67	82
4	4	175/175 (100%)	172 (98%)	3 (2%)	56	75
4	g	175/175 (100%)	172 (98%)	3 (2%)	56	75
5	5	169/235 (72%)	164 (97%)	5 (3%)	36	62
5	f	169/235 (72%)	164 (97%)	5 (3%)	36	62
6	6	185/201 (92%)	185 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	e	185/201 (92%)	183 (99%)	2 (1%)	70	83
7	7	199/224 (89%)	196 (98%)	3 (2%)	60	77
7	a	199/224 (89%)	193 (97%)	6 (3%)	36	62
8	A	207/210 (99%)	200 (97%)	7 (3%)	32	59
9	B	209/209 (100%)	204 (98%)	5 (2%)	44	67
10	C	203/216 (94%)	195 (96%)	8 (4%)	27	56
11	D	213/226 (94%)	205 (96%)	8 (4%)	28	57
12	E	198/215 (92%)	189 (96%)	9 (4%)	23	52
13	F	192/193 (100%)	184 (96%)	8 (4%)	25	54
14	G	200/239 (84%)	191 (96%)	9 (4%)	23	52
15	I	349/385 (91%)	333 (95%)	16 (5%)	23	51
16	K	336/374 (90%)	319 (95%)	17 (5%)	20	48
17	L	305/377 (81%)	296 (97%)	9 (3%)	36	62
18	O	361/368 (98%)	348 (96%)	13 (4%)	30	58
19	P	408/415 (98%)	399 (98%)	9 (2%)	47	69
20	R	349/379 (92%)	332 (95%)	17 (5%)	21	49
21	S	433/489 (88%)	414 (96%)	19 (4%)	24	53
22	V	252/268 (94%)	237 (94%)	15 (6%)	16	44
23	W	165/230 (72%)	161 (98%)	4 (2%)	44	67
24	Y	31/82 (38%)	31 (100%)	0	100	100
25	J	322/352 (92%)	310 (96%)	12 (4%)	29	57
26	H	326/399 (82%)	318 (98%)	8 (2%)	42	66
27	M	311/375 (83%)	294 (94%)	17 (6%)	18	47
28	Q	374/391 (96%)	363 (97%)	11 (3%)	37	63
29	U	265/308 (86%)	255 (96%)	10 (4%)	28	57
30	N	729/797 (92%)	701 (96%)	28 (4%)	28	57
31	T	240/256 (94%)	237 (99%)	3 (1%)	65	80
32	o	697/850 (82%)	677 (97%)	20 (3%)	37	63
All	All	10175/11403 (89%)	9844 (97%)	331 (3%)	35	60

5 of 331 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
25	J	248	ASP
30	N	260	ASP
26	H	200	VAL
28	Q	80	HIS
30	N	724	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 116 such sidechains are listed below:

Mol	Chain	Res	Type
21	S	205	ASN
32	o	403	ASN
7	a	185	ASN
32	o	391	ASN
30	N	361	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 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
34	ATP	M	501	33	28,33,33	0.66	0	34,52,52	0.66	1 (2%)
36	ADP	J	502	-	24,29,29	0.89	0	29,45,45	1.28	3 (10%)
34	ATP	J	501	33	28,33,33	0.65	0	34,52,52	0.75	2 (5%)
34	ATP	H	501	33	28,33,33	0.67	0	34,52,52	0.65	1 (2%)
34	ATP	K	501	33	28,33,33	0.68	0	34,52,52	0.68	1 (2%)
34	ATP	L	501	33	28,33,33	0.71	0	34,52,52	0.64	1 (2%)

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
34	ATP	M	501	33	-	3/18/38/38	0/3/3/3
36	ADP	J	502	-	-	2/12/32/32	0/3/3/3
34	ATP	J	501	33	-	4/18/38/38	0/3/3/3
34	ATP	H	501	33	-	4/18/38/38	0/3/3/3
34	ATP	K	501	33	-	1/18/38/38	0/3/3/3
34	ATP	L	501	33	-	3/18/38/38	0/3/3/3

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	J	502	ADP	N3-C2-N1	-3.57	123.82	128.67
34	J	501	ATP	C4'-O4'-C1'	-2.68	107.47	109.92
36	J	502	ADP	C4'-O4'-C1'	2.41	112.13	109.92
36	J	502	ADP	C4-C5-N7	-2.32	106.89	109.34
34	M	501	ATP	C5-C6-N6	2.32	123.84	120.31

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

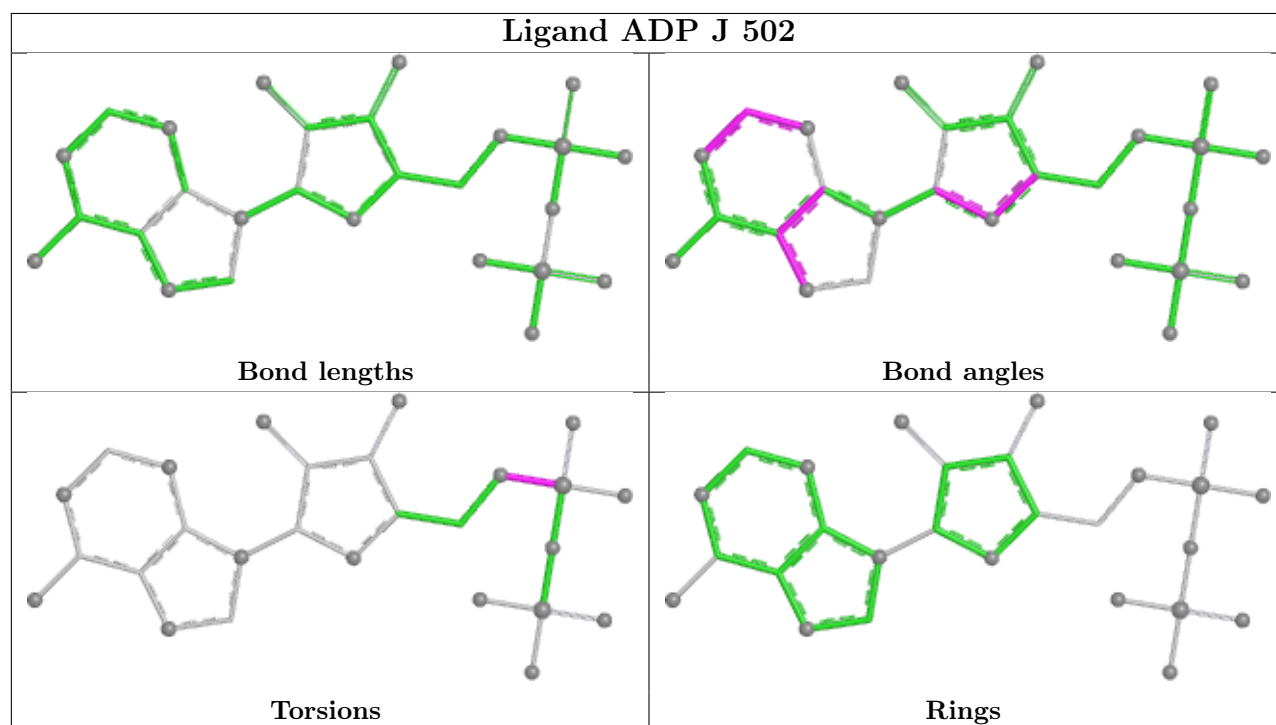
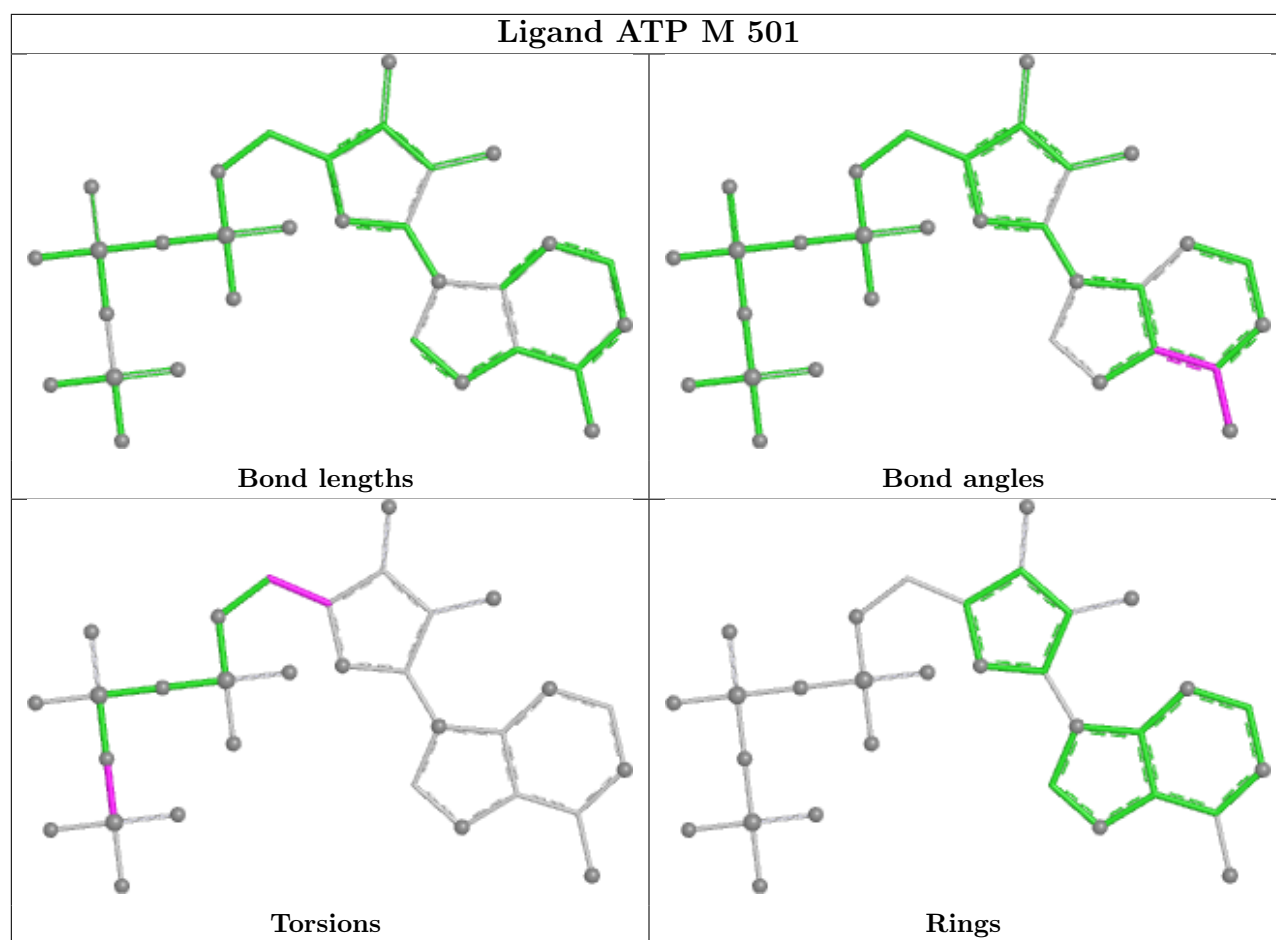
Mol	Chain	Res	Type	Atoms
34	L	501	ATP	C5'-O5'-PA-O2A
34	L	501	ATP	C5'-O5'-PA-O3A
34	J	501	ATP	C5'-O5'-PA-O2A
34	J	501	ATP	C5'-O5'-PA-O3A
34	H	501	ATP	O4'-C4'-C5'-O5'

There are no ring outliers.

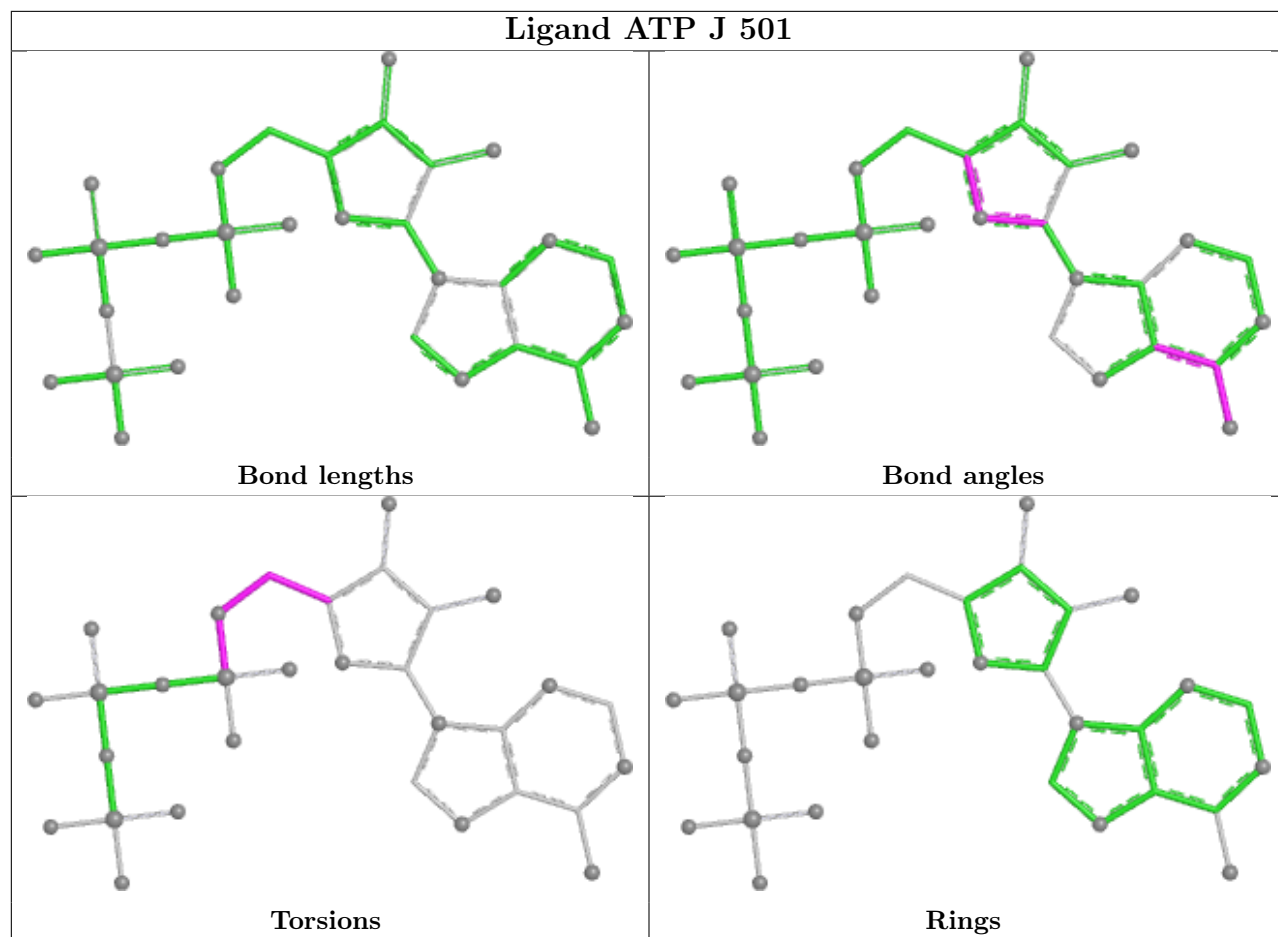
5 monomers are involved in 20 short contacts:

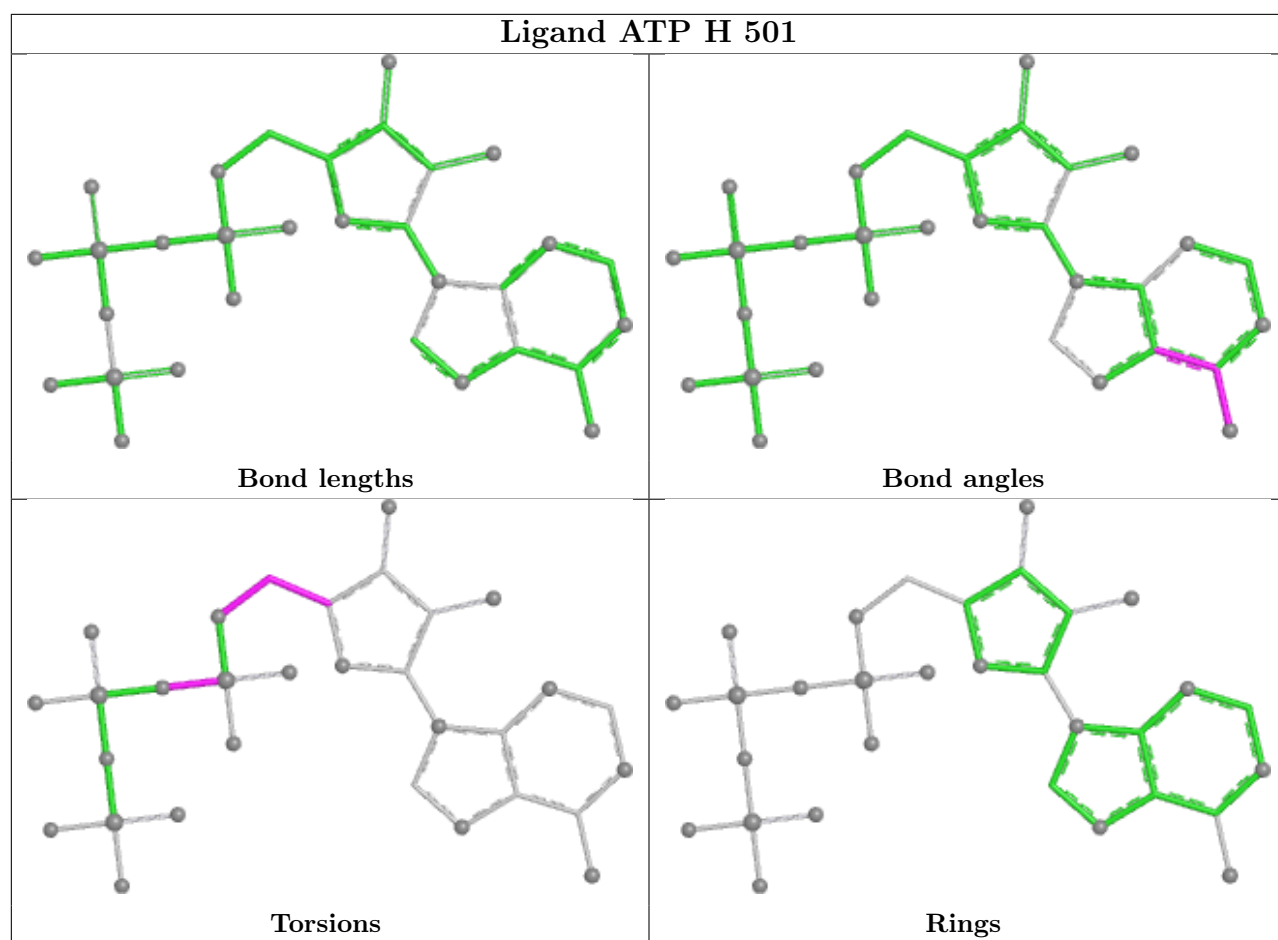
Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	M	501	ATP	4	0
36	J	502	ADP	4	0
34	J	501	ATP	3	0
34	H	501	ATP	3	0
34	K	501	ATP	6	0

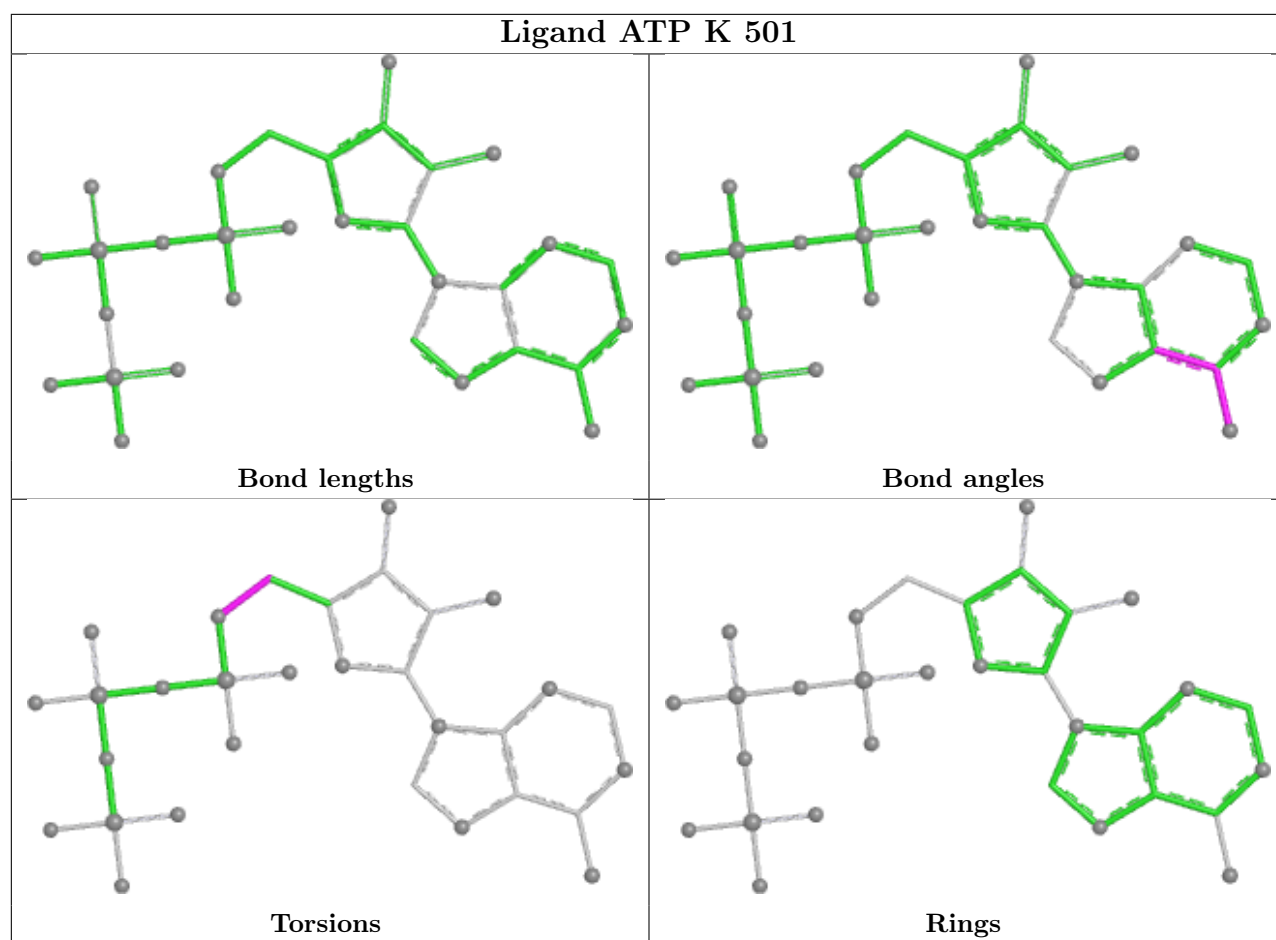
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

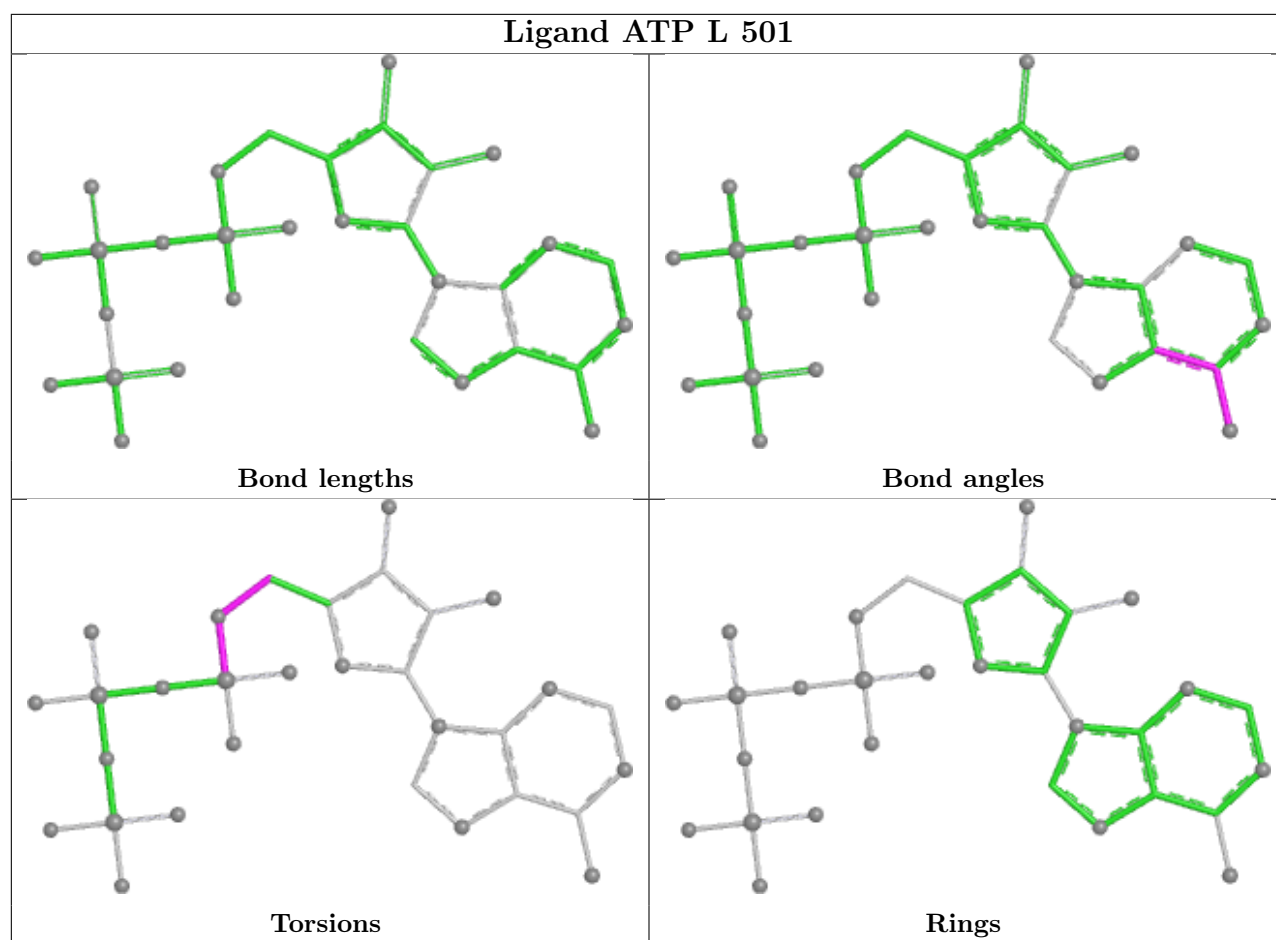


Ligand ATP J 501









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

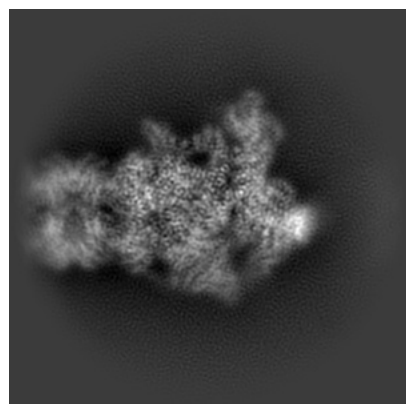
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45579. These allow visual inspection of the internal detail of the map and identification of artifacts.

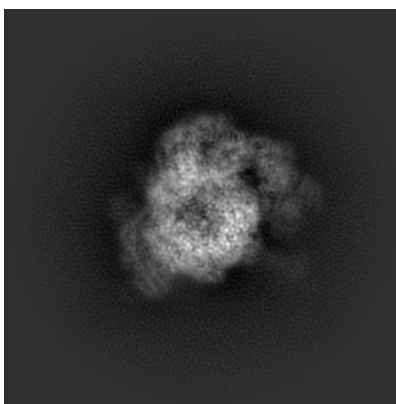
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

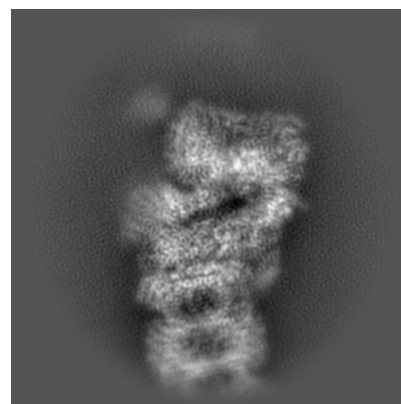
6.1.1 Primary map



X

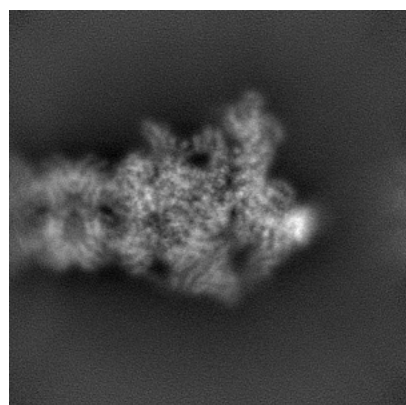


Y

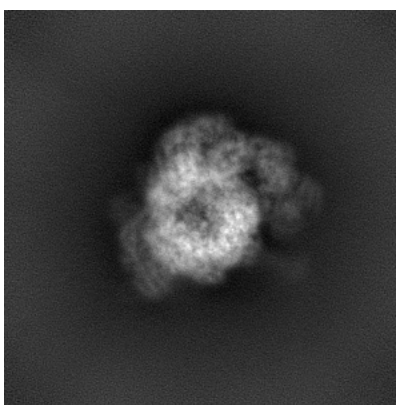


Z

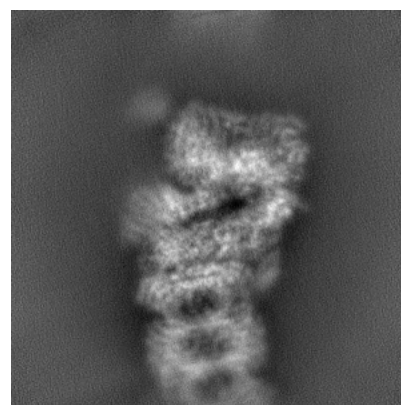
6.1.2 Raw map



X



Y

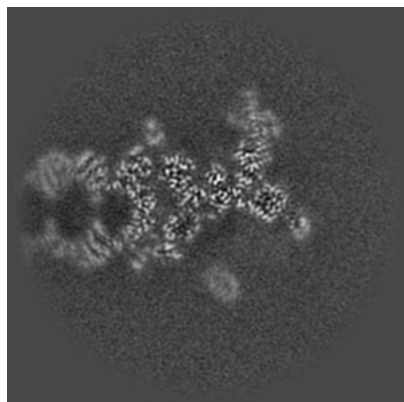


Z

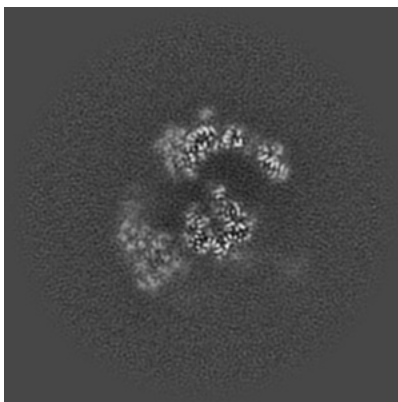
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

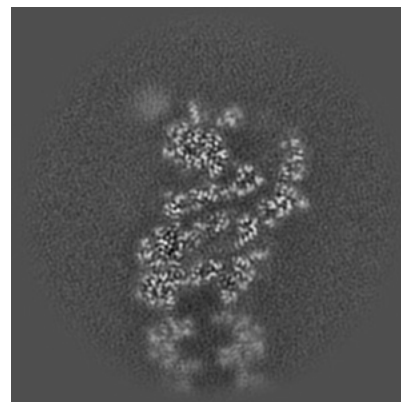
6.2.1 Primary map



X Index: 170

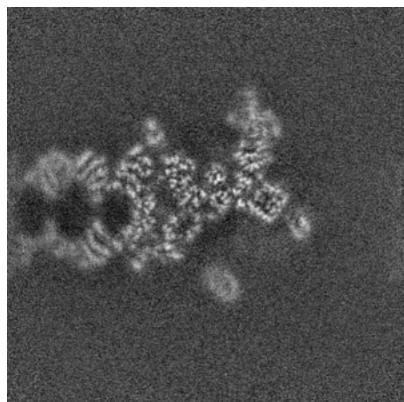


Y Index: 170

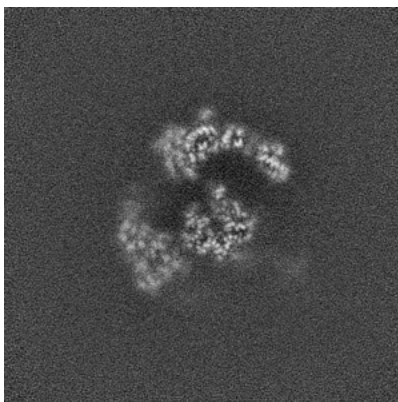


Z Index: 170

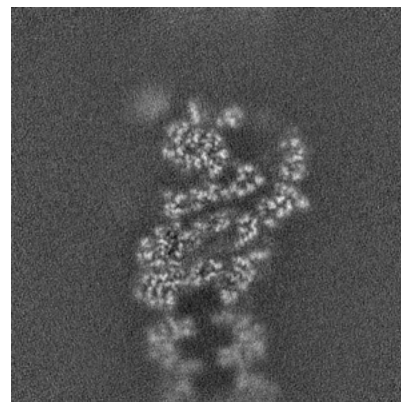
6.2.2 Raw map



X Index: 170



Y Index: 170

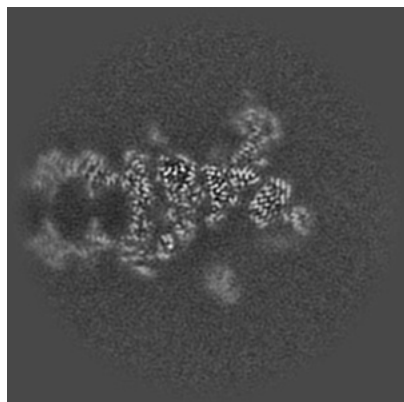


Z Index: 170

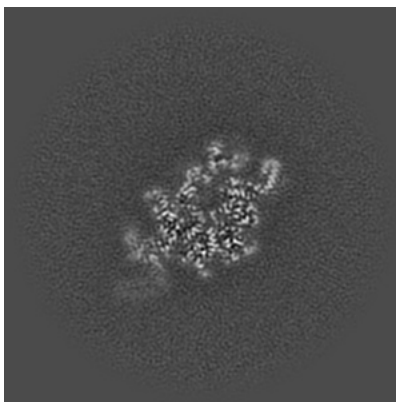
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

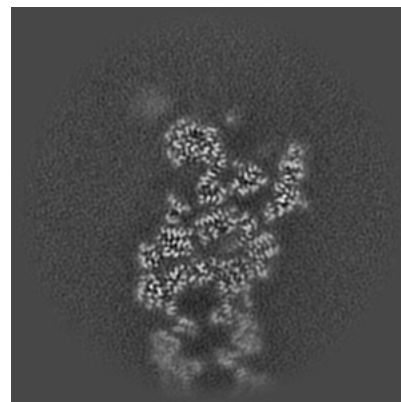
6.3.1 Primary map



X Index: 164

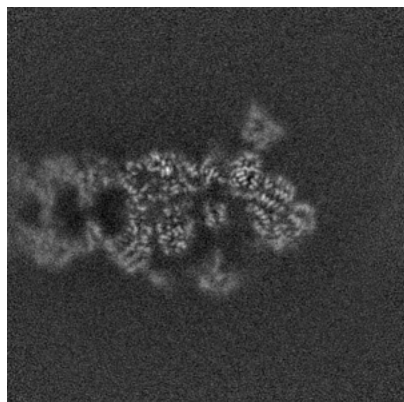


Y Index: 139

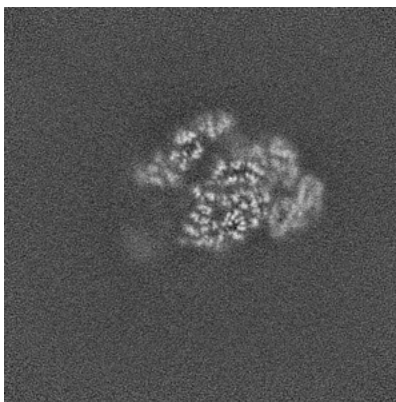


Z Index: 175

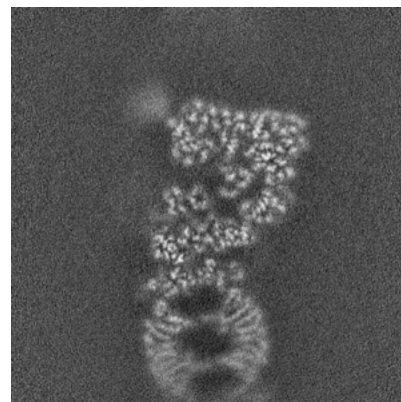
6.3.2 Raw map



X Index: 155



Y Index: 208

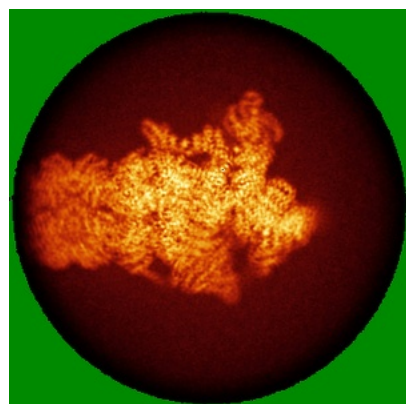


Z Index: 158

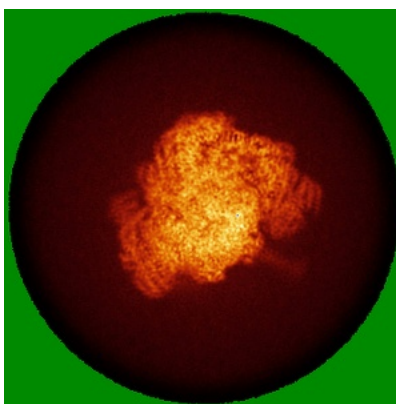
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

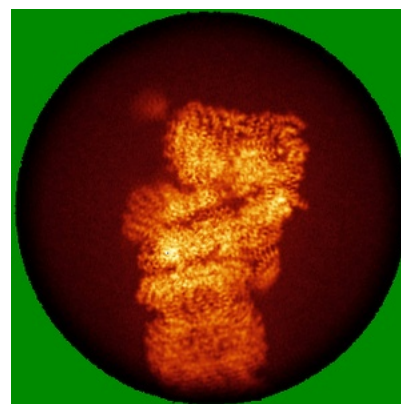
6.4.1 Primary map



X

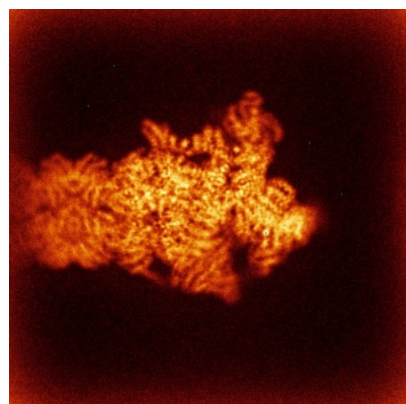


Y

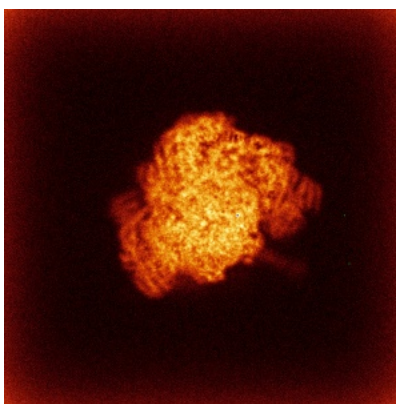


Z

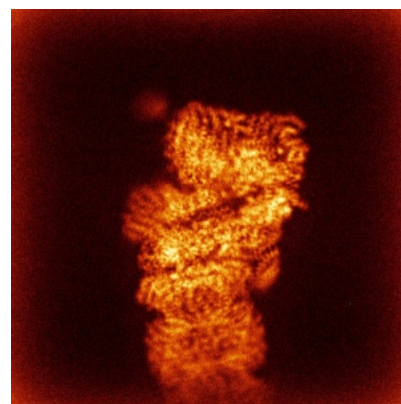
6.4.2 Raw map



X



Y

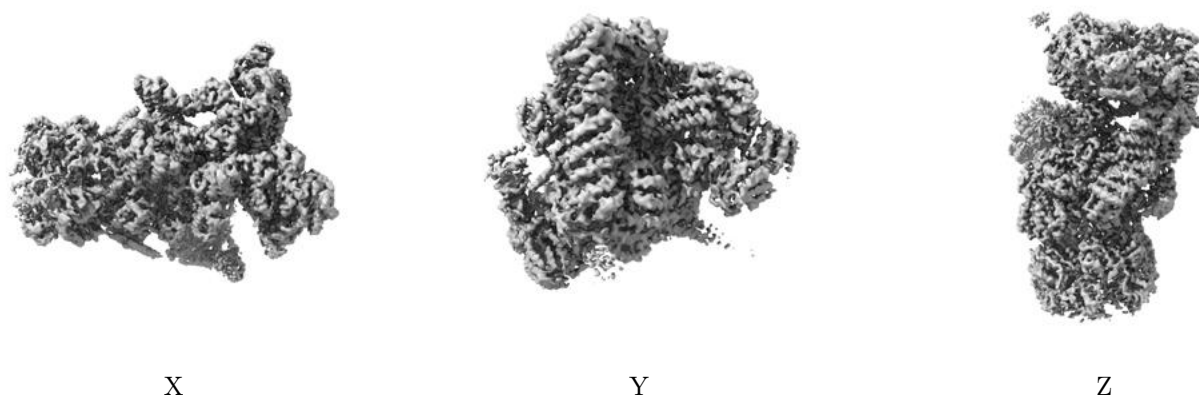


Z

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.

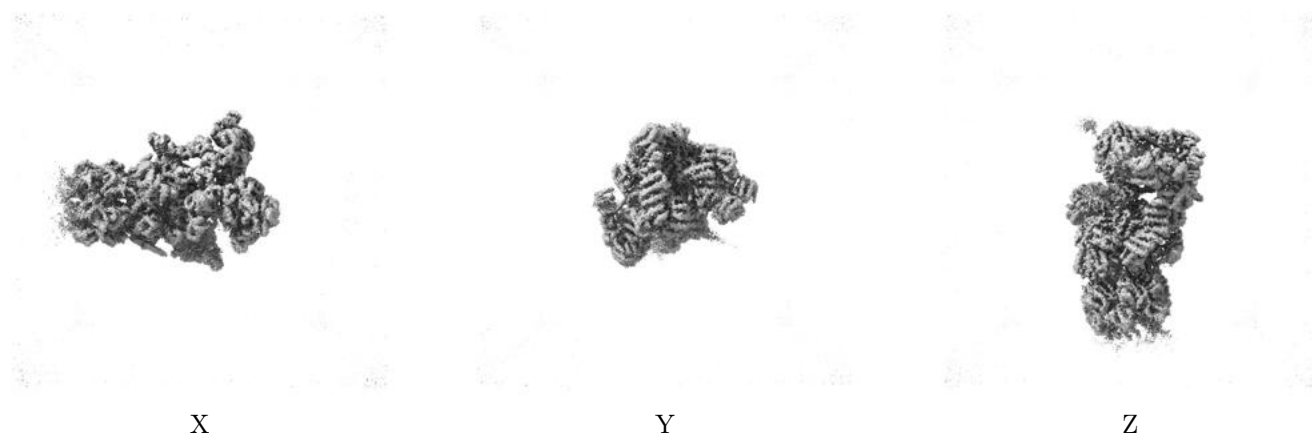
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.33. 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.

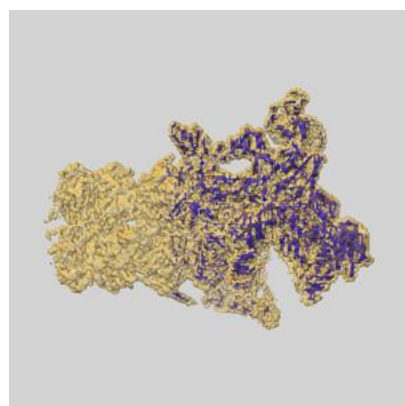
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

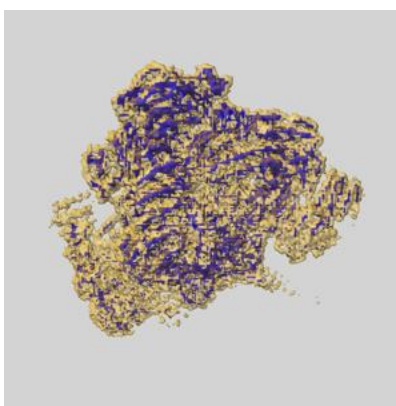
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

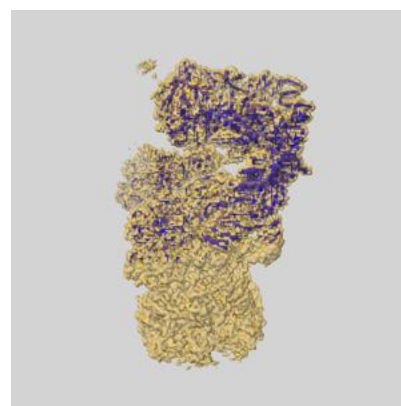
6.6.1 emd_45579_msk_1.map [i](#)



X



Y

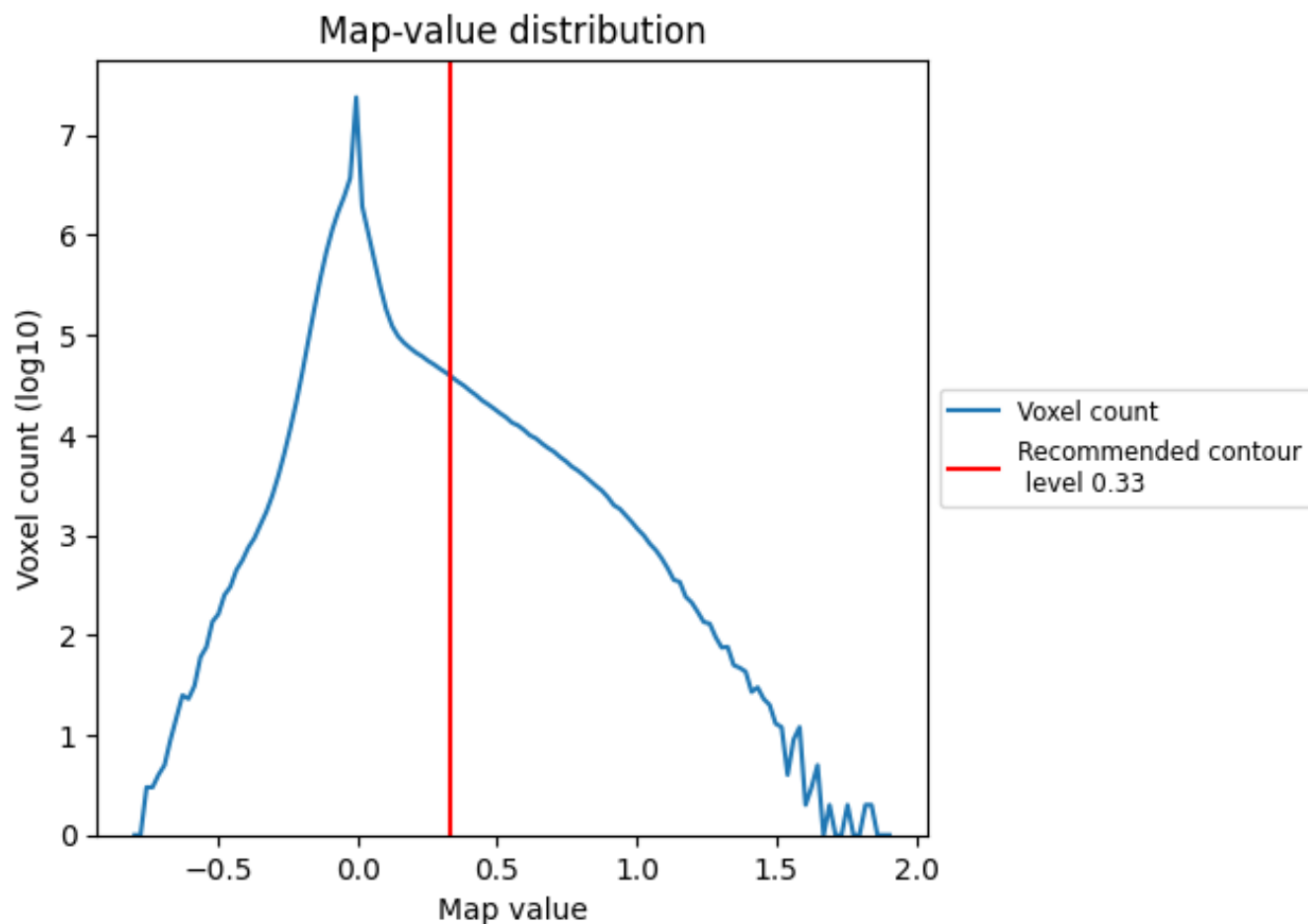


Z

7 Map analysis [i](#)

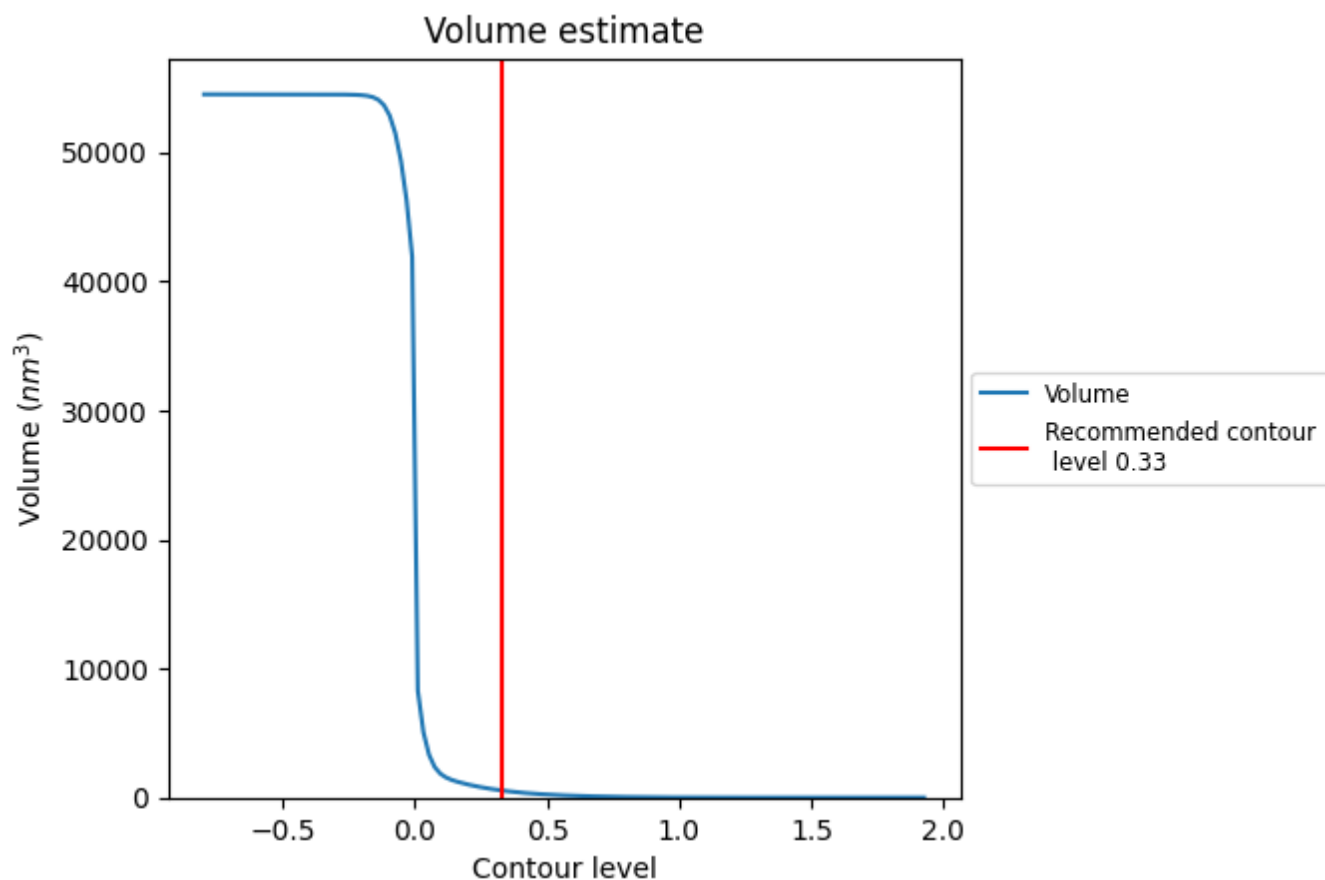
This section contains the results of statistical analysis of the map.

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.

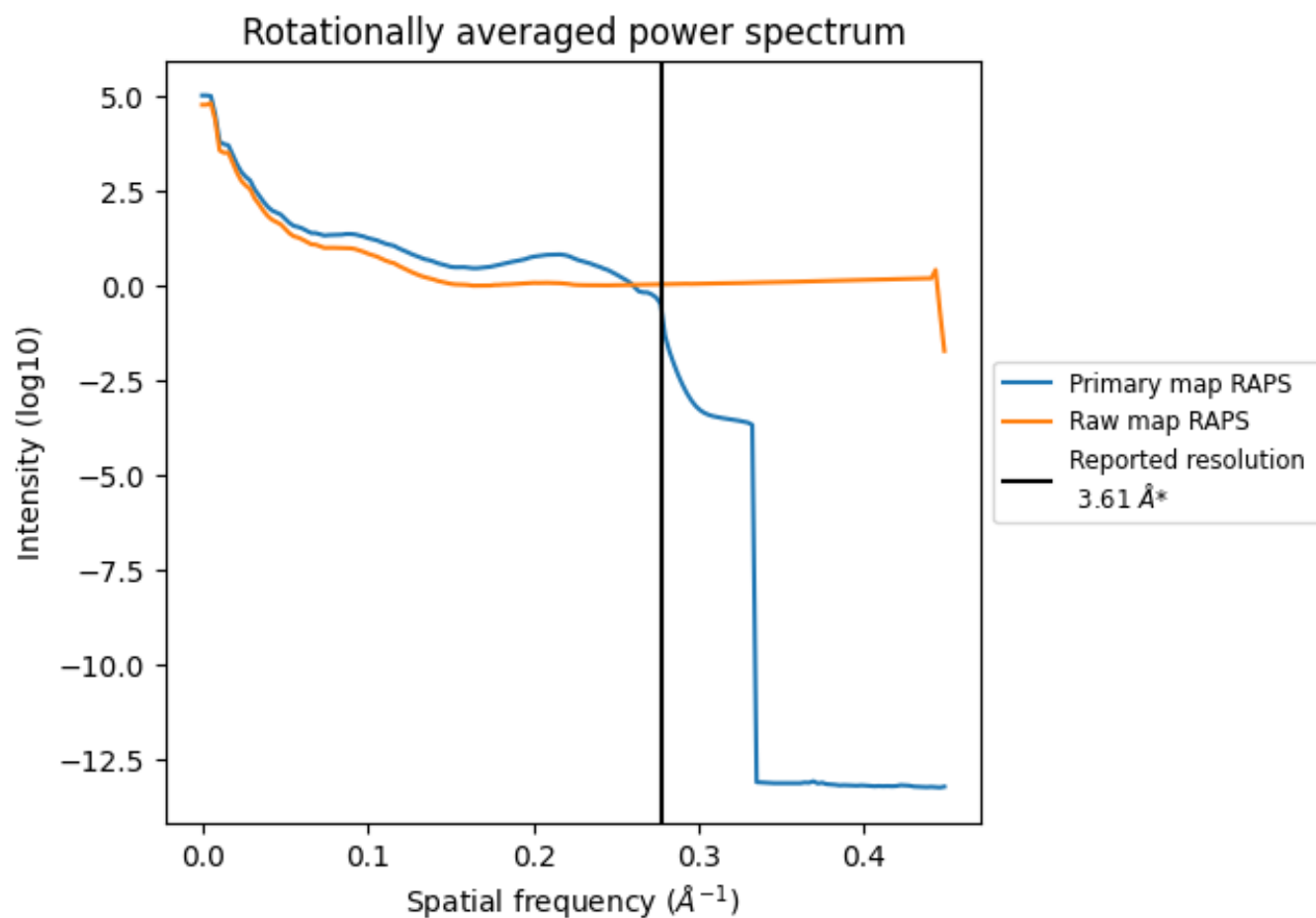
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 547 nm³; this corresponds to an approximate mass of 494 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 ⓘ

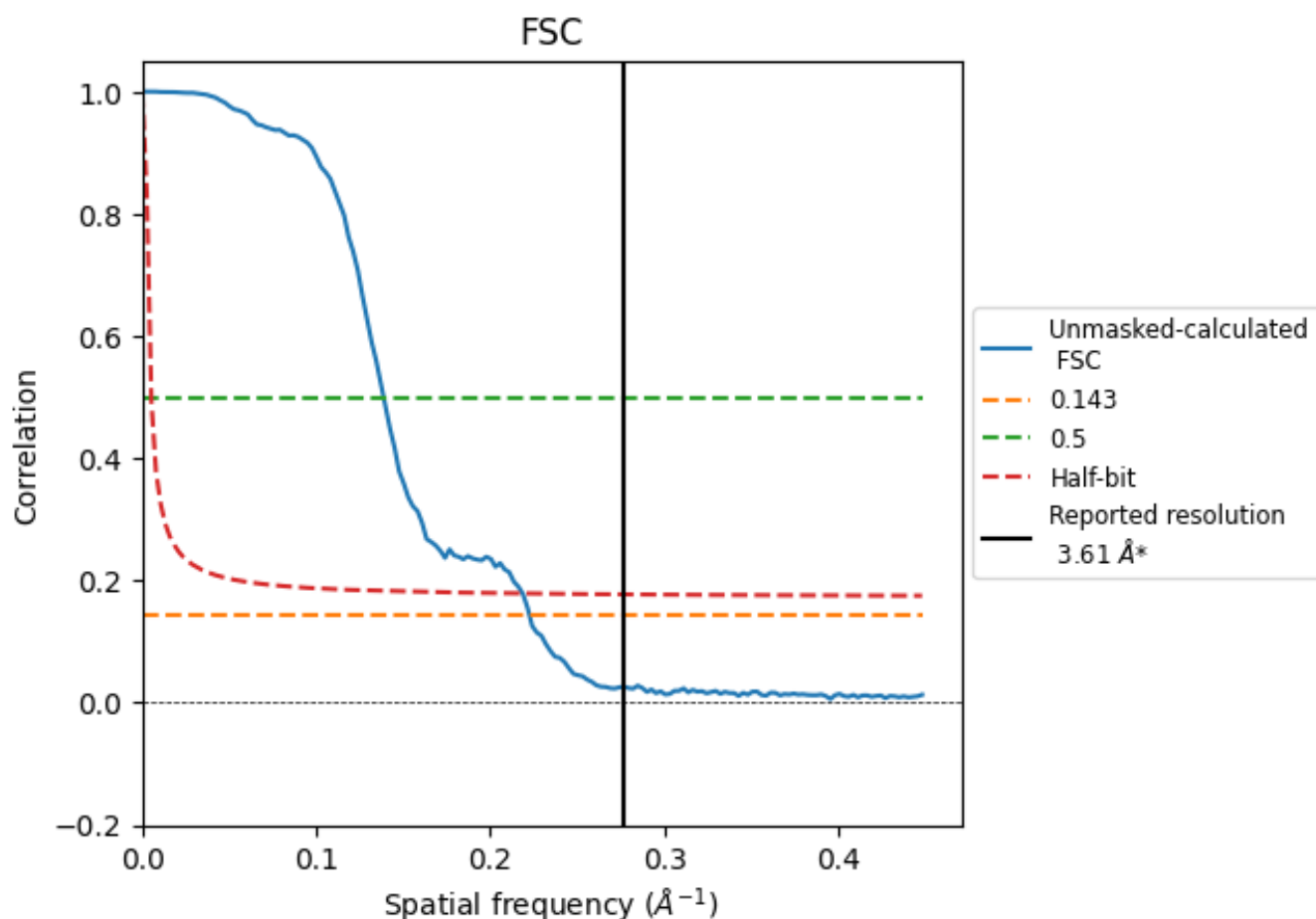


*Reported resolution corresponds to spatial frequency of 0.277 Å⁻¹

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 0.277 \AA^{-1}

8.2 Resolution estimates [i](#)

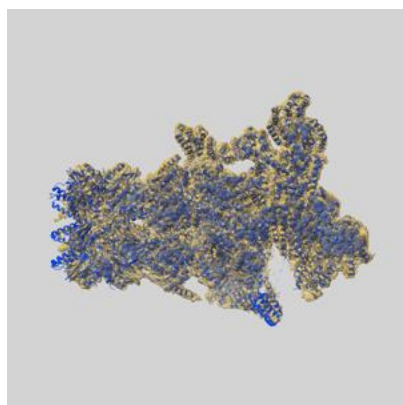
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.61	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.49	7.20	4.57

*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 4.49 differs from the reported value 3.61 by more than 10 %

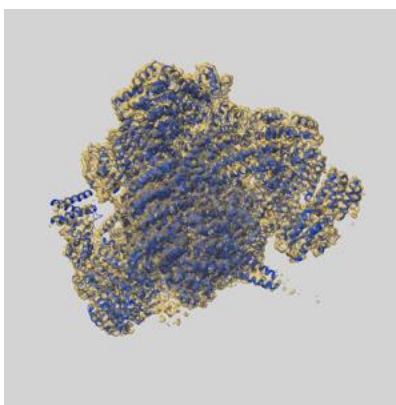
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-45579 and PDB model 9CGC. Per-residue inclusion information can be found in section [3](#) on page [12](#).

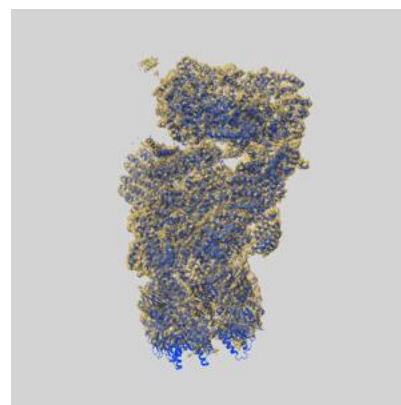
9.1 Map-model overlay [i](#)



X



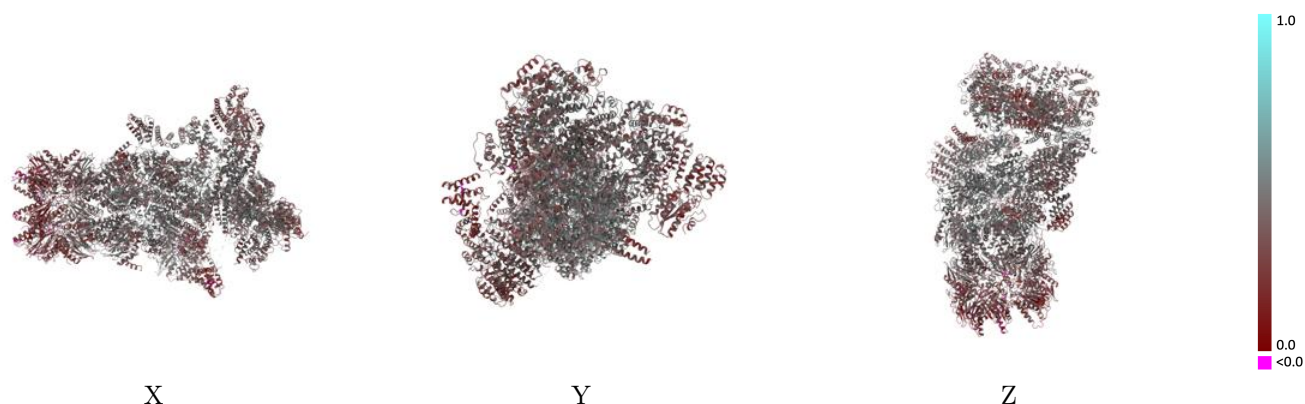
Y



Z

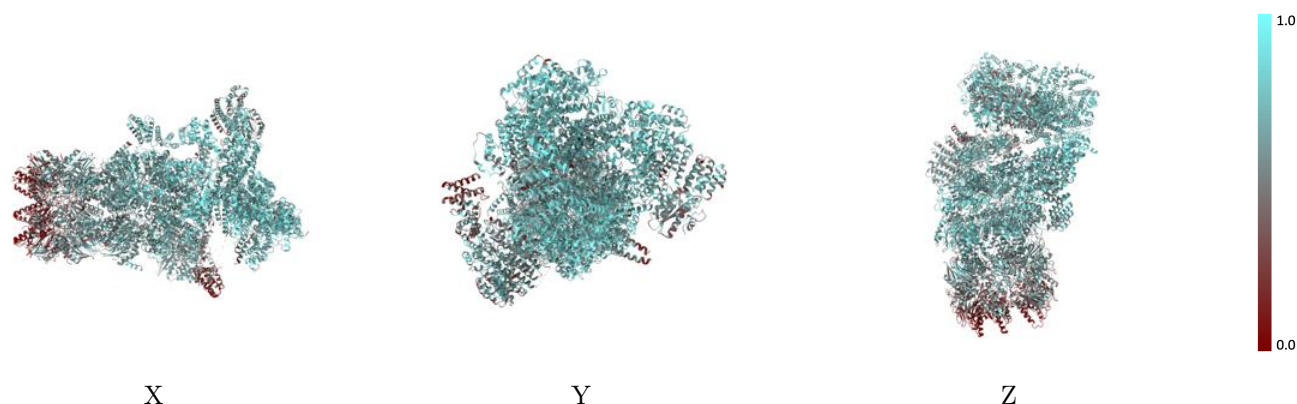
The images above show the 3D surface view of the map at the recommended contour level 0.33 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



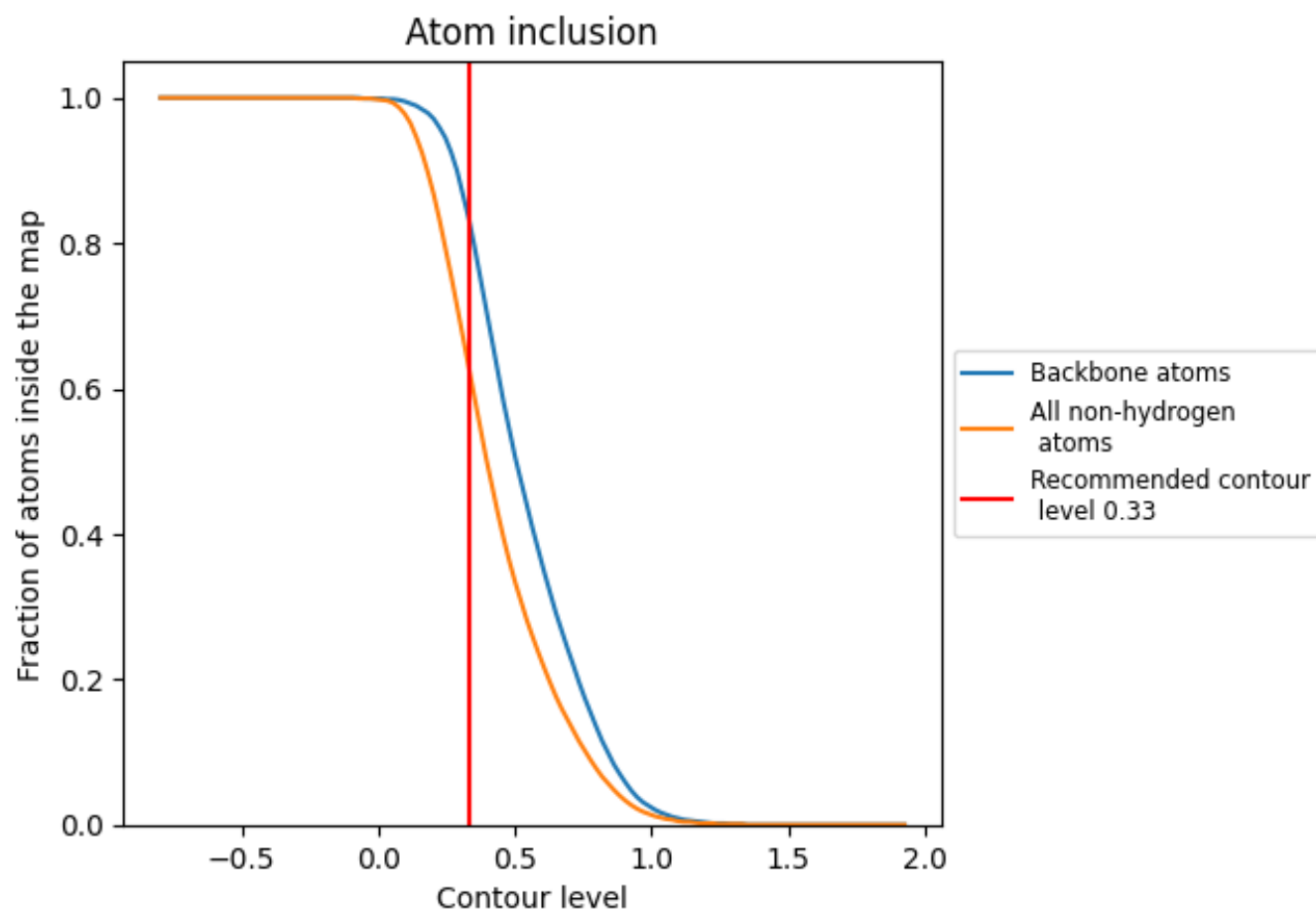
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.33).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 63% 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 (0.33) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6310	 0.3860
1	 0.5810	 0.3460
2	 0.5730	 0.3760
3	 0.5370	 0.3600
4	 0.5320	 0.3400
5	 0.5870	 0.3450
6	 0.5460	 0.3530
7	 0.5670	 0.3600
A	 0.7200	 0.4420
B	 0.6540	 0.4290
C	 0.6240	 0.4010
D	 0.6700	 0.4070
E	 0.6730	 0.4150
F	 0.7210	 0.4440
G	 0.7370	 0.4490
H	 0.7320	 0.4600
I	 0.6590	 0.4290
J	 0.6980	 0.4520
K	 0.7140	 0.4660
L	 0.7360	 0.4620
M	 0.7200	 0.4600
N	 0.7610	 0.4190
O	 0.6520	 0.3500
P	 0.7600	 0.4130
Q	 0.7200	 0.3870
R	 0.7190	 0.3880
S	 0.7450	 0.4140
T	 0.7320	 0.3810
U	 0.7020	 0.4300
V	 0.7380	 0.4550
W	 0.5530	 0.3320
Y	 0.7960	 0.4220
a	 0.3820	 0.2730
b	 0.3350	 0.2400
e	 0.3590	 0.2640



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Chain	Atom inclusion	Q-score
f	 0.3290	 0.2720
g	 0.2470	 0.2470
h	 0.2230	 0.2400
i	 0.2750	 0.2500
o	 0.5520	 0.3300