



wwPDB EM Validation Summary Report ⓘ

Jul 22, 2026 – 03:42 PM JST

PDB ID : 9M2W / pdb_00009m2w
EMDB ID : EMD-63592
Title : The cryo-EM structure of 26S proteasome-Midnolin complex in the MD state
Authors : Wang, H.Y.; Xu, W.Q.
Deposited on : 2025-02-28
Resolution : 3.31 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.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

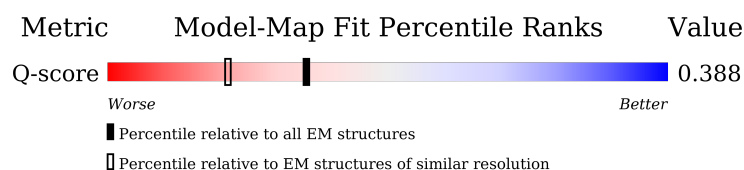
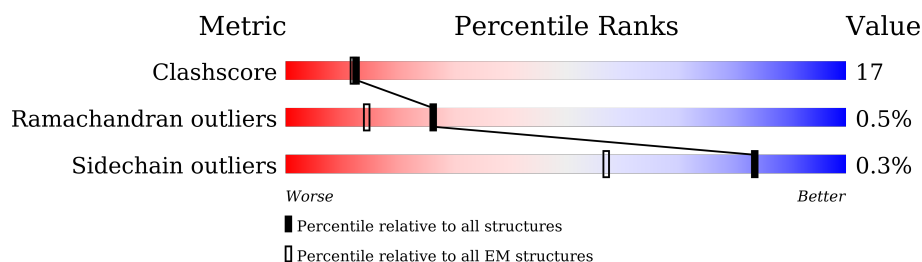
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.31 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14550 (2.81 - 3.81)

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

Mol	Chain	Length	Quality of chain
1	A	433	
2	B	440	
3	C	406	
4	D	418	

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Mol	Chain	Length	Quality of chain
5	E	389	
6	F	439	
7	G	246	
7	g	246	
8	H	234	
8	h	234	
9	I	261	
9	i	261	
10	J	248	
10	j	248	
11	K	241	
11	k	241	
12	L	263	
12	l	263	
13	M	255	
13	m	255	
14	N	239	
14	n	239	
15	O	277	
15	o	277	
16	P	205	
16	p	205	
17	Q	201	
17	q	201	
18	R	263	

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Mol	Chain	Length	Quality of chain
18	r	263	
19	S	241	
19	s	241	
20	T	264	
20	t	264	
21	U	953	
22	V	534	
23	W	456	
24	X	422	
25	Y	389	
26	Z	324	
27	a	376	
28	b	377	
29	c	310	
30	d	350	
31	e	70	
32	f	908	
33	v	15	
34	u	491	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
35	ATP	A	501	-	-	X	-
35	ATP	C	501	-	-	X	-
35	ATP	F	501	-	-	X	-
36	ADP	D	501	-	-	X	-

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 98427 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 regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	414	Total	C	N	O	S	0	0
			3062	1925	542	581	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	401	Total	C	N	O	S	0	0
			2901	1806	504	582	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	372	Total	C	N	O	S	0	0
			2723	1718	486	506	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	380	Total	C	N	O	S	0	0
			2777	1747	483	539	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	314	Total	C	N	O	S	0	0
			2324	1448	426	438	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	333	Total	C	N	O	S	0	0
			2421	1510	430	468	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	239	Total	C	N	O	S	0	0
			1798	1144	305	337	12		
7	g	235	Total	C	N	O	S	0	0
			1765	1124	297	332	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	230	Total	C	N	O	S	0	0
			1745	1117	294	329	5		
8	h	227	Total	C	N	O	S	0	0
			1679	1070	287	318	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	247	Total	C	N	O	S	0	0
			1900	1206	322	362	10		
9	i	246	Total	C	N	O	S	0	0
			1851	1165	319	359	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	239	Total	C	N	O	S	0	0
			1839	1152	327	355	5		
10	j	231	Total	C	N	O	S	0	0
			1622	1014	293	310	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	237	Total	C	N	O	S	0	0
			1773	1114	295	354	10		
11	k	227	Total	C	N	O	S	0	0
			1677	1059	275	335	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	238	Total	C	N	O	S	0	0
			1847	1157	332	347	11		
12	l	237	Total	C	N	O	S	0	0
			1831	1150	330	341	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	241	Total	C	N	O	S	0	0
			1843	1171	319	343	10		
13	m	240	Total	C	N	O	S	0	0
			1833	1164	311	348	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	200	Total	C	N	O	S	0	0
			1482	927	255	288	12		
14	n	201	Total	C	N	O	S	0	0
			1488	935	257	284	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	221	Total	C	N	O	S	0	0
			1637	1033	282	310	12		
15	o	220	Total	C	N	O	S	0	0
			1629	1027	278	312	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	204	Total	C	N	O	S	0	0
			1553	996	262	276	19		
16	p	204	Total	C	N	O	S	0	0
			1579	1006	264	290	19		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	197	Total	C	N	O	S	0	0
			1559	1002	267	281	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
17	q	197	Total	C	N	O	S	0	0
			1551	996	267	280	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	201	Total	C	N	O	S	0	0
			1536	970	271	286	9		
18	r	200	Total	C	N	O	S	0	0
			1540	973	273	285	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	213	Total	C	N	O	S	0	0
			1627	1032	284	301	10		
19	s	212	Total	C	N	O	S	0	0
			1620	1030	277	303	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	215	Total	C	N	O	S	0	0
			1674	1057	288	317	12		
20	t	215	Total	C	N	O	S	0	0
			1663	1052	289	310	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	803	Total	C	N	O	S	0	0
			5845	3671	1007	1130	37		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	420	Total	C	N	O	S	0	0
			3053	1923	532	593	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	456	Total	C	N	O	S	0	0
			3348	2085	584	663	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	381	Total	C	N	O	S	0	0
			2804	1765	480	550	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	379	Total	C	N	O	S	0	0
			2990	1901	512	564	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	287	Total	C	N	O	S	0	0
			2081	1318	361	399	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	a	373	Total	C	N	O	S	0	0
			2676	1691	456	518	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
28	b	189	Total	C	N	O	S	0	0
			1336	823	246	263	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
29	c	274	Total	C	N	O	S	0	0
			2008	1274	348	380	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	d	232	Total	C	N	O	S	0	0
			1772	1143	289	333	7		

- Molecule 31 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	e	38	Total	C	N	O	0	0
			280	165	49	66		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
32	f	879	Total	C	N	O	S	0	0
			6339	3965	1079	1264	31		

- Molecule 33 is a protein called Substrate.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	v	15	Total	C	N	O	0	0
			75	45	15	15		

- Molecule 34 is a protein called Midnolin.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	u	37	Total	C	N	O	S	0	0
			320	189	78	52	1		

There are 23 discrepancies between the modelled and reference sequences:

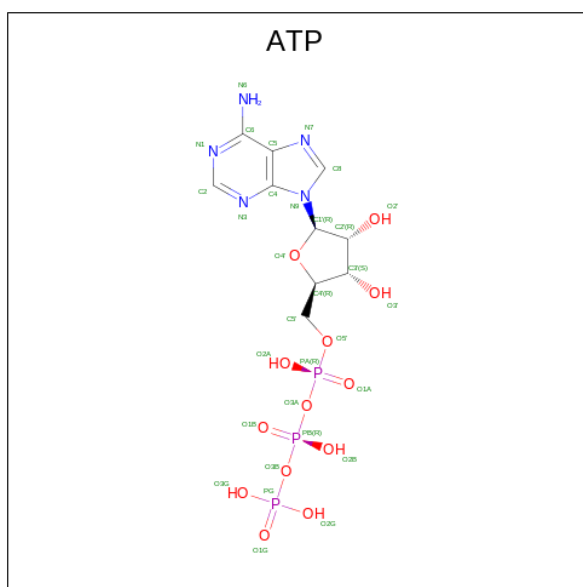
Chain	Residue	Modelled	Actual	Comment	Reference
u	0	MET	-	initiating methionine	UNP Q504T8
u	469	GLY	-	expression tag	UNP Q504T8
u	470	SER	-	expression tag	UNP Q504T8
u	471	ASP	-	expression tag	UNP Q504T8
u	472	TYR	-	expression tag	UNP Q504T8
u	473	LYS	-	expression tag	UNP Q504T8
u	474	ASP	-	expression tag	UNP Q504T8
u	475	ASP	-	expression tag	UNP Q504T8
u	476	ASP	-	expression tag	UNP Q504T8
u	477	ASP	-	expression tag	UNP Q504T8
u	478	LYS	-	expression tag	UNP Q504T8
u	479	GLY	-	expression tag	UNP Q504T8

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Chain	Residue	Modelled	Actual	Comment	Reference
u	480	SER	-	expression tag	UNP Q504T8
u	481	HIS	-	expression tag	UNP Q504T8
u	482	HIS	-	expression tag	UNP Q504T8
u	483	HIS	-	expression tag	UNP Q504T8
u	484	HIS	-	expression tag	UNP Q504T8
u	485	HIS	-	expression tag	UNP Q504T8
u	486	HIS	-	expression tag	UNP Q504T8
u	487	HIS	-	expression tag	UNP Q504T8
u	488	HIS	-	expression tag	UNP Q504T8
u	489	HIS	-	expression tag	UNP Q504T8
u	490	HIS	-	expression tag	UNP Q504T8

- Molecule 35 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).

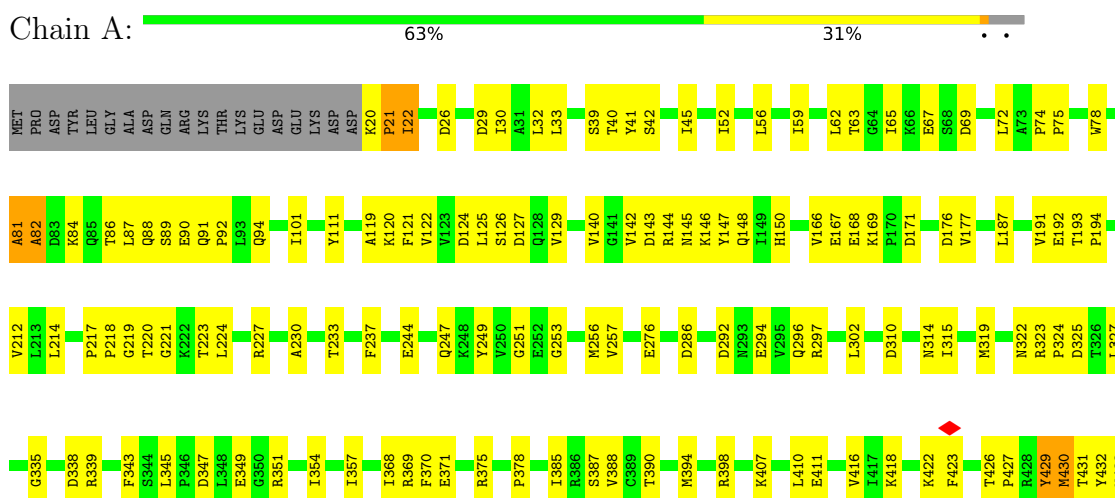




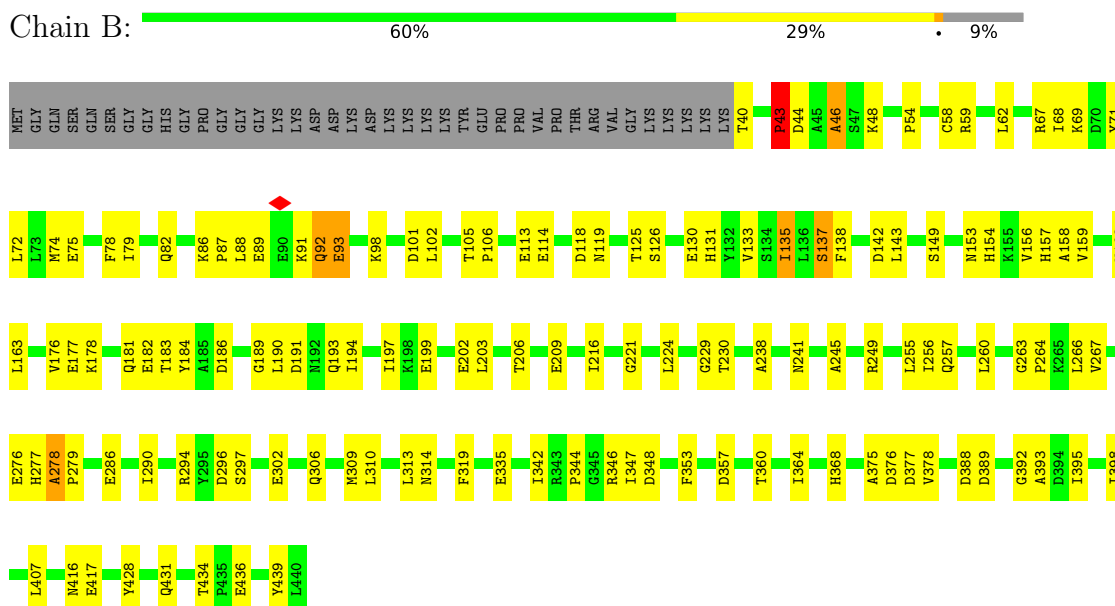
3 Residue-property plots [i](#)

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.

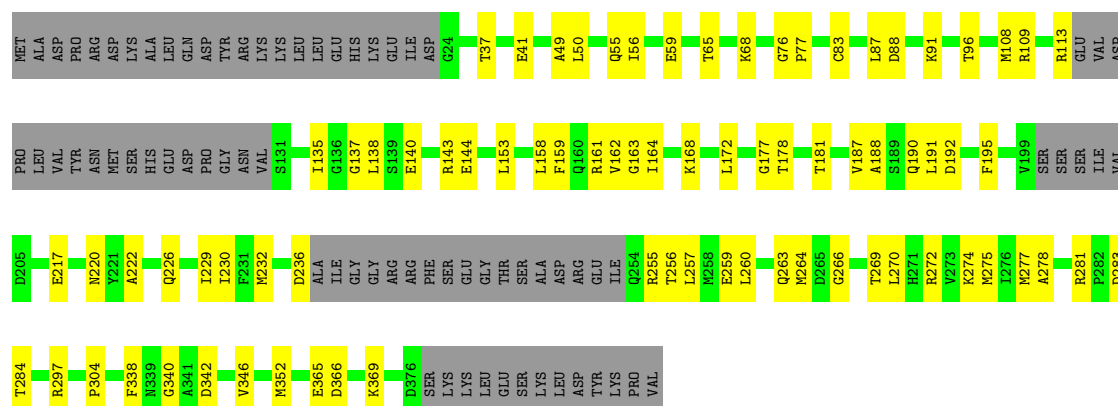
• Molecule 1: 26S proteasome regulatory subunit 7



• Molecule 2: 26S proteasome regulatory subunit 4



Chain C: 65% 27% 8%

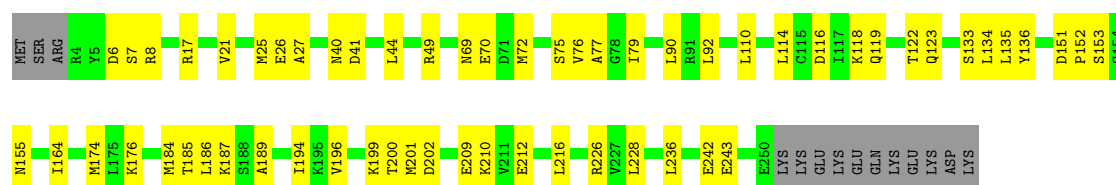


Chain h:  78% 19% .



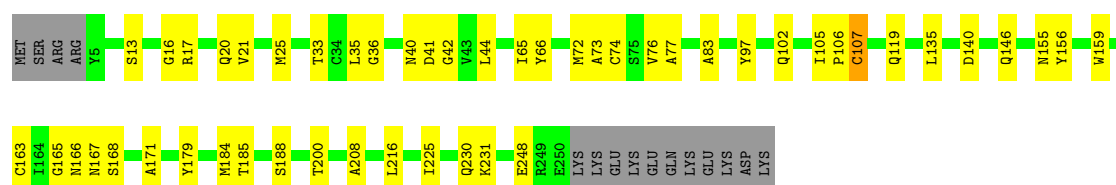
• Molecule 9: Proteasome subunit alpha type-4

Chain I:  72% 23% 5%



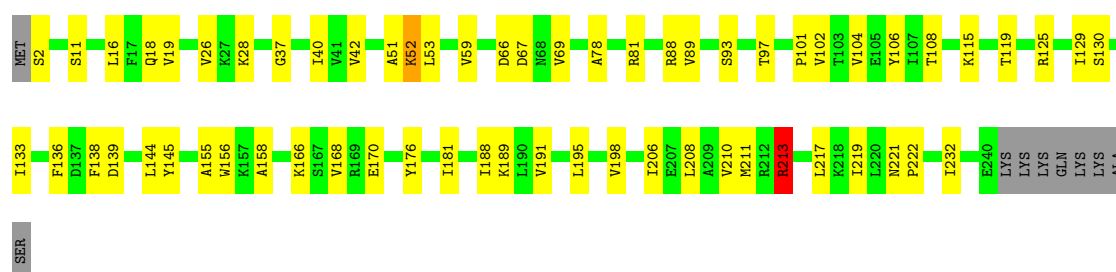
• Molecule 9: Proteasome subunit alpha type-4

Chain i:  75% 19% 6%



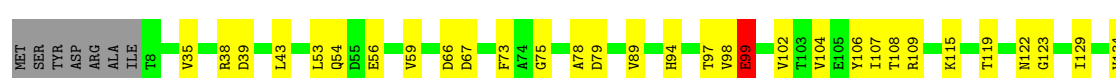
• Molecule 10: Proteasome subunit alpha type-7

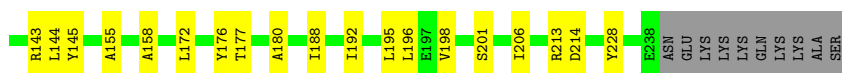
Chain J:  71% 24% .



• Molecule 10: Proteasome subunit alpha type-7

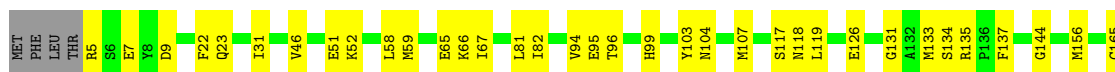
Chain j:  73% 20% 7%





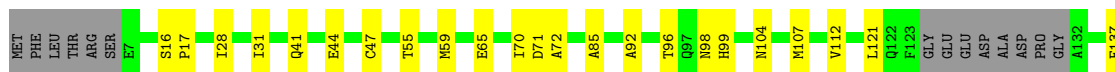
- Molecule 11: Proteasome subunit alpha type-5

Chain K: 74% 24%



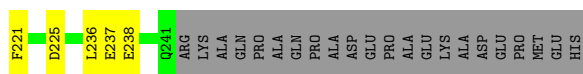
- Molecule 11: Proteasome subunit alpha type-5

Chain k: 75% 20% 6%



- Molecule 12: Proteasome subunit alpha type-1

Chain L: 62% 29% 10%



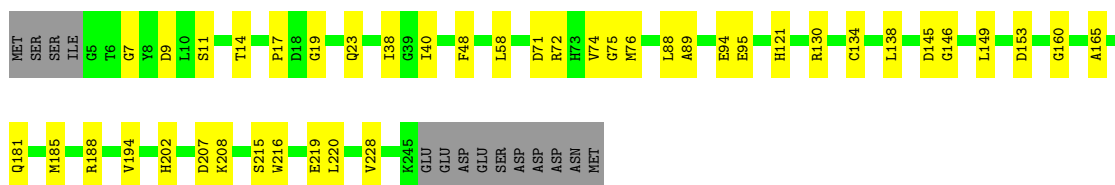
- Molecule 12: Proteasome subunit alpha type-1

Chain l: 70% 19% 10%



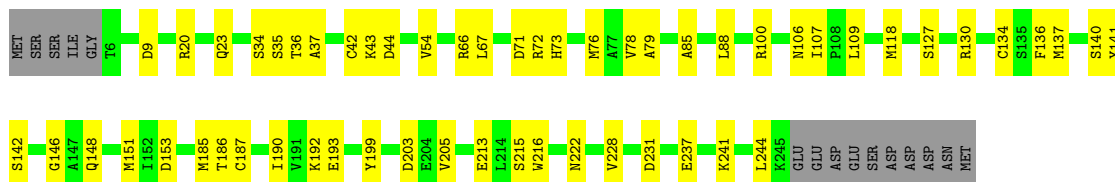
- Molecule 13: Proteasome subunit alpha type-3

Chain M: 78% 16% 5%



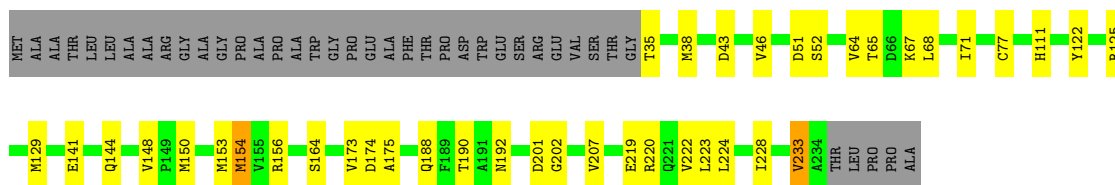
- Molecule 13: Proteasome subunit alpha type-3

Chain m: 72% 22% 6%



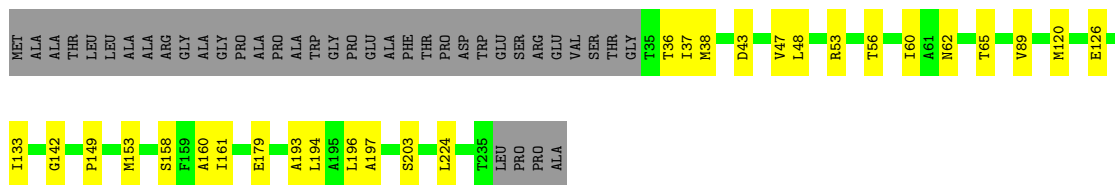
- Molecule 14: Proteasome subunit beta type-6

Chain N: 67% 16% 16%



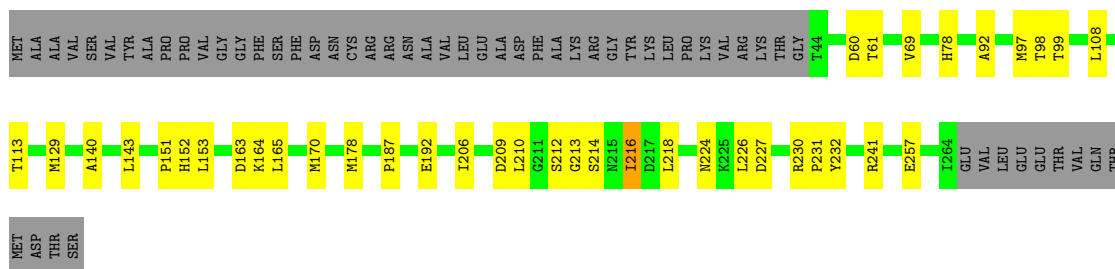
- Molecule 14: Proteasome subunit beta type-6

Chain n: 72% 12% 16%



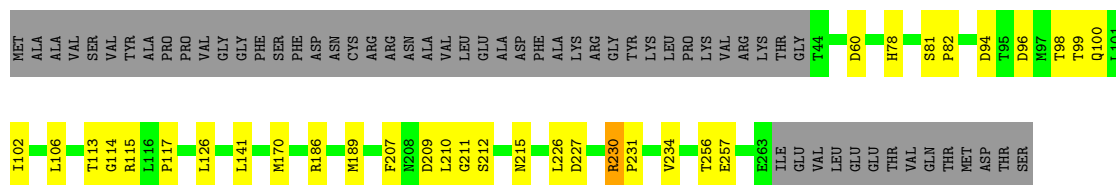
- Molecule 15: Proteasome subunit beta type-7

Chain O: 66% 14% 20%



- Molecule 15: Proteasome subunit beta type-7

Chain o:  68% 12% 21%



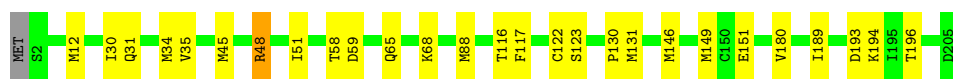
- Molecule 16: Proteasome subunit beta type-3

Chain P:  77% 23%



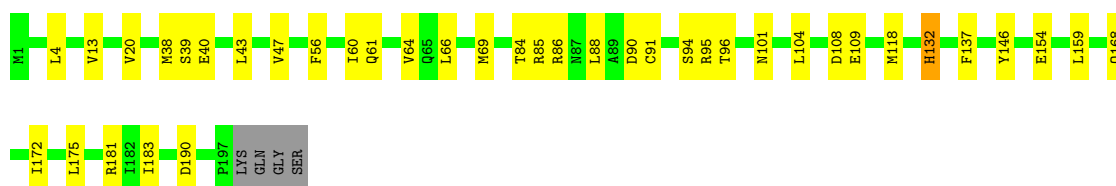
- Molecule 16: Proteasome subunit beta type-3

Chain p:  86% 13%



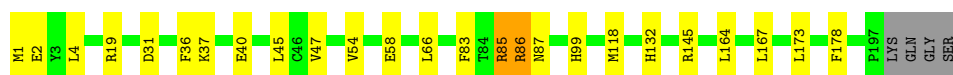
- Molecule 17: Proteasome subunit beta type-2

Chain Q:  79% 19%



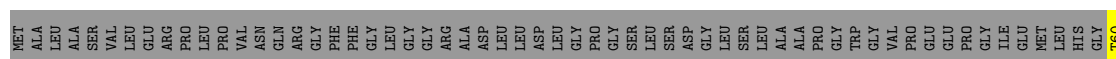
- Molecule 17: Proteasome subunit beta type-2

Chain q:  86% 11%



- Molecule 18: Proteasome subunit beta type-5

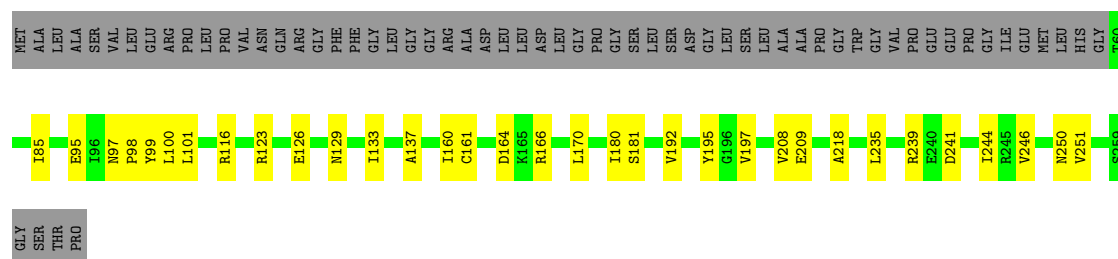
Chain R:  63% 14% 24%





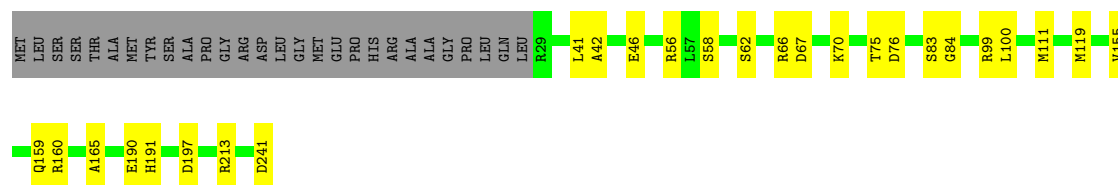
- Molecule 18: Proteasome subunit beta type-5

Chain r: 63% 13% 24%



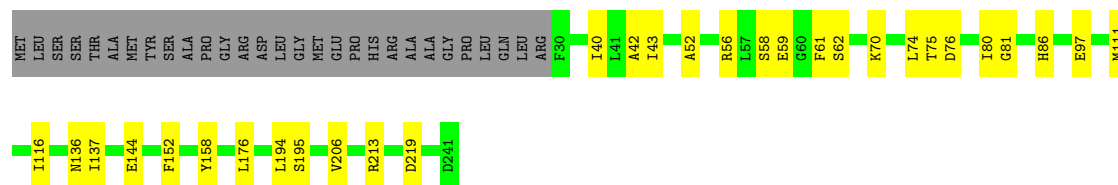
- Molecule 19: Proteasome subunit beta type-1

Chain S: 78% 11% 12%



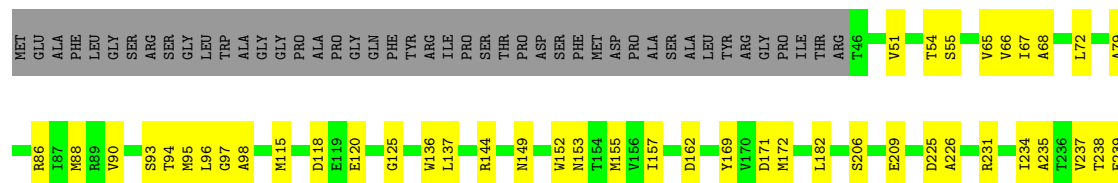
- Molecule 19: Proteasome subunit beta type-1

Chain s: 76% 12% 12%

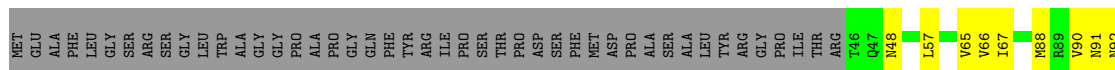


- Molecule 20: Proteasome subunit beta type-4

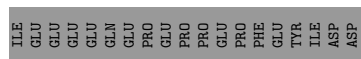
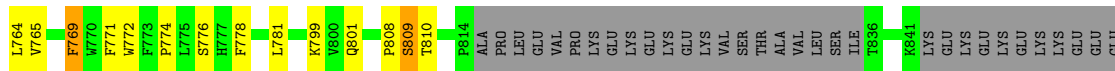
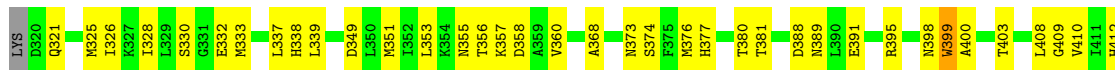
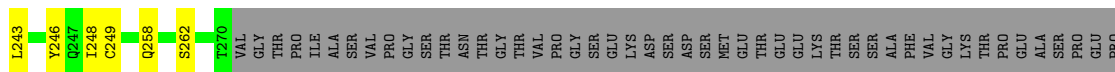
Chain T: 64% 17% 19%



- Molecule 20: Proteasome subunit beta type-4

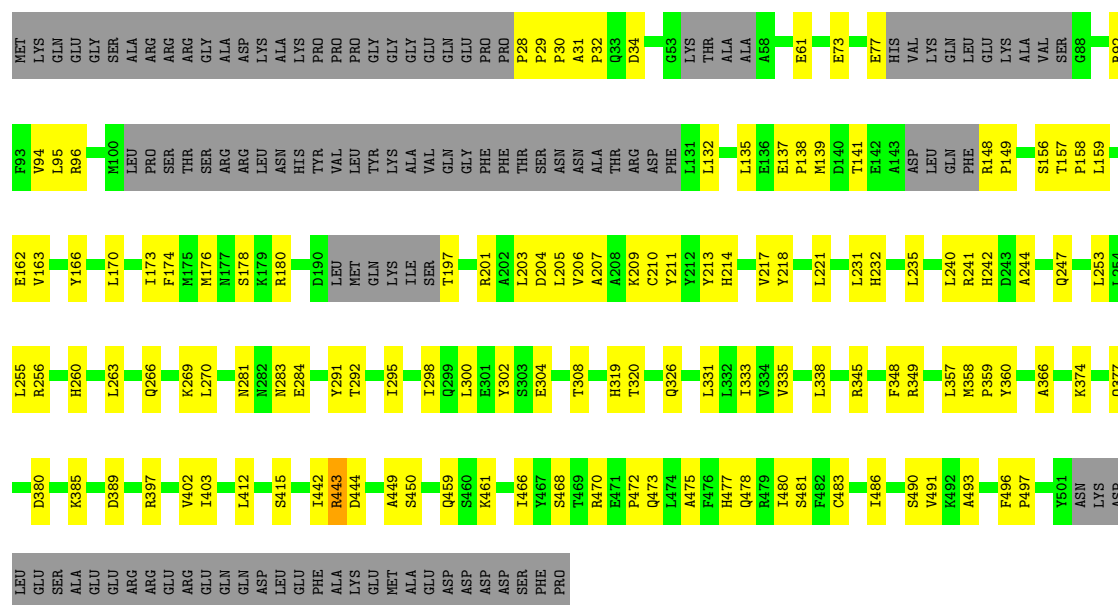


- Molecule 21: 26S proteasome non-ATPase regulatory subunit 1



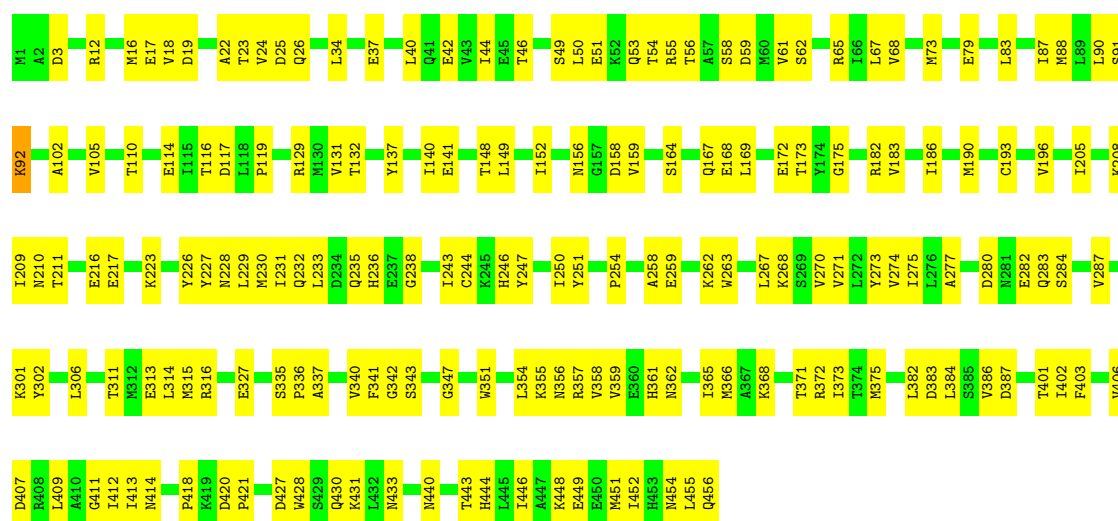
- Molecule 22: 26S proteasome non-ATPase regulatory subunit 3

Chain V:  55% 23% 21%



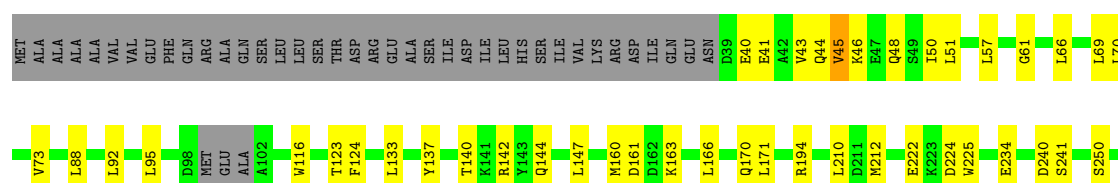
- Molecule 23: 26S proteasome non-ATPase regulatory subunit 12

Chain W:  60% 39%

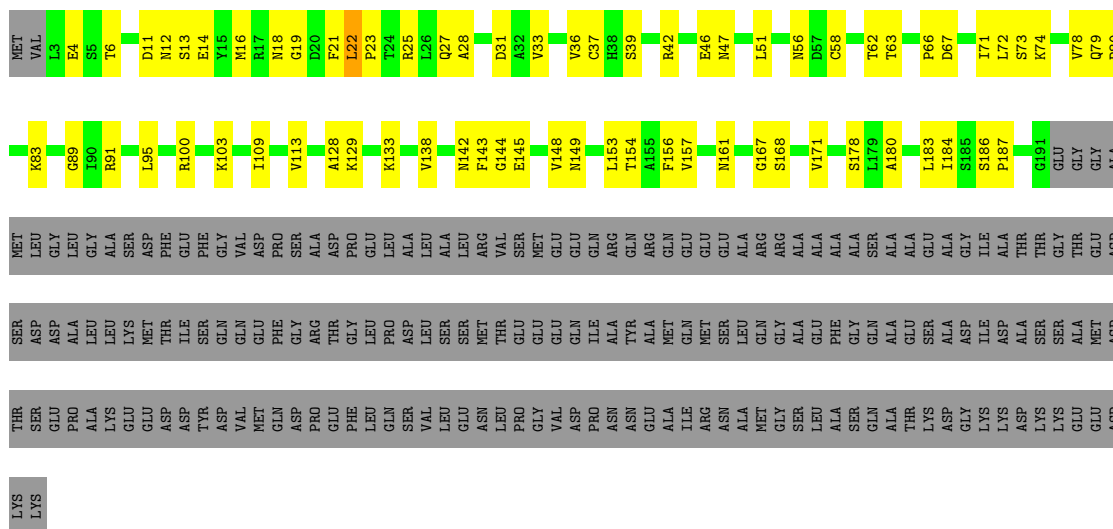
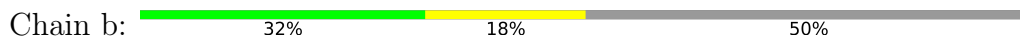


- Molecule 24: 26S proteasome non-ATPase regulatory subunit 11

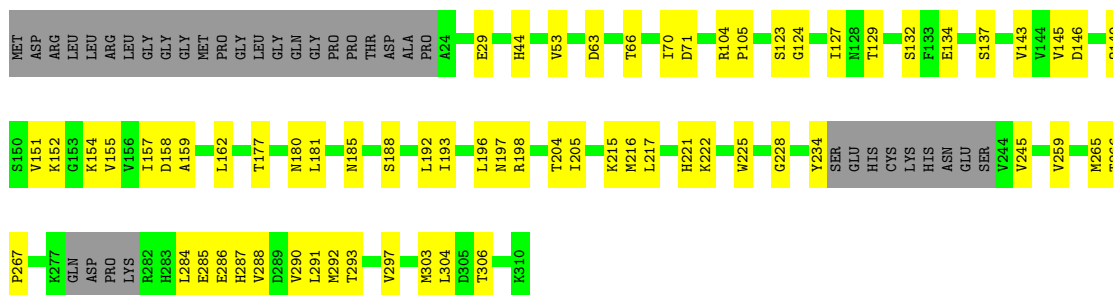
Chain X:  66% 23% 10%



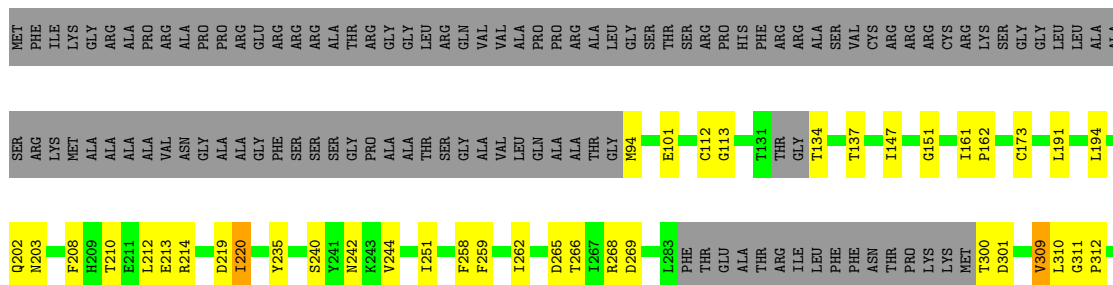
- Molecule 28: 26S proteasome non-ATPase regulatory subunit 4

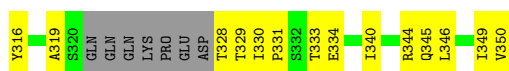


- Molecule 29: 26S proteasome non-ATPase regulatory subunit 14

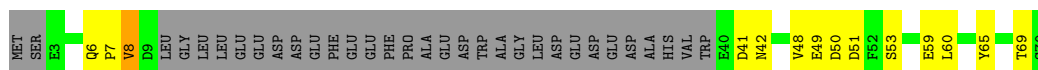
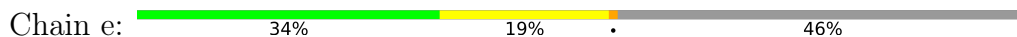


- Molecule 30: 26S proteasome non-ATPase regulatory subunit 8

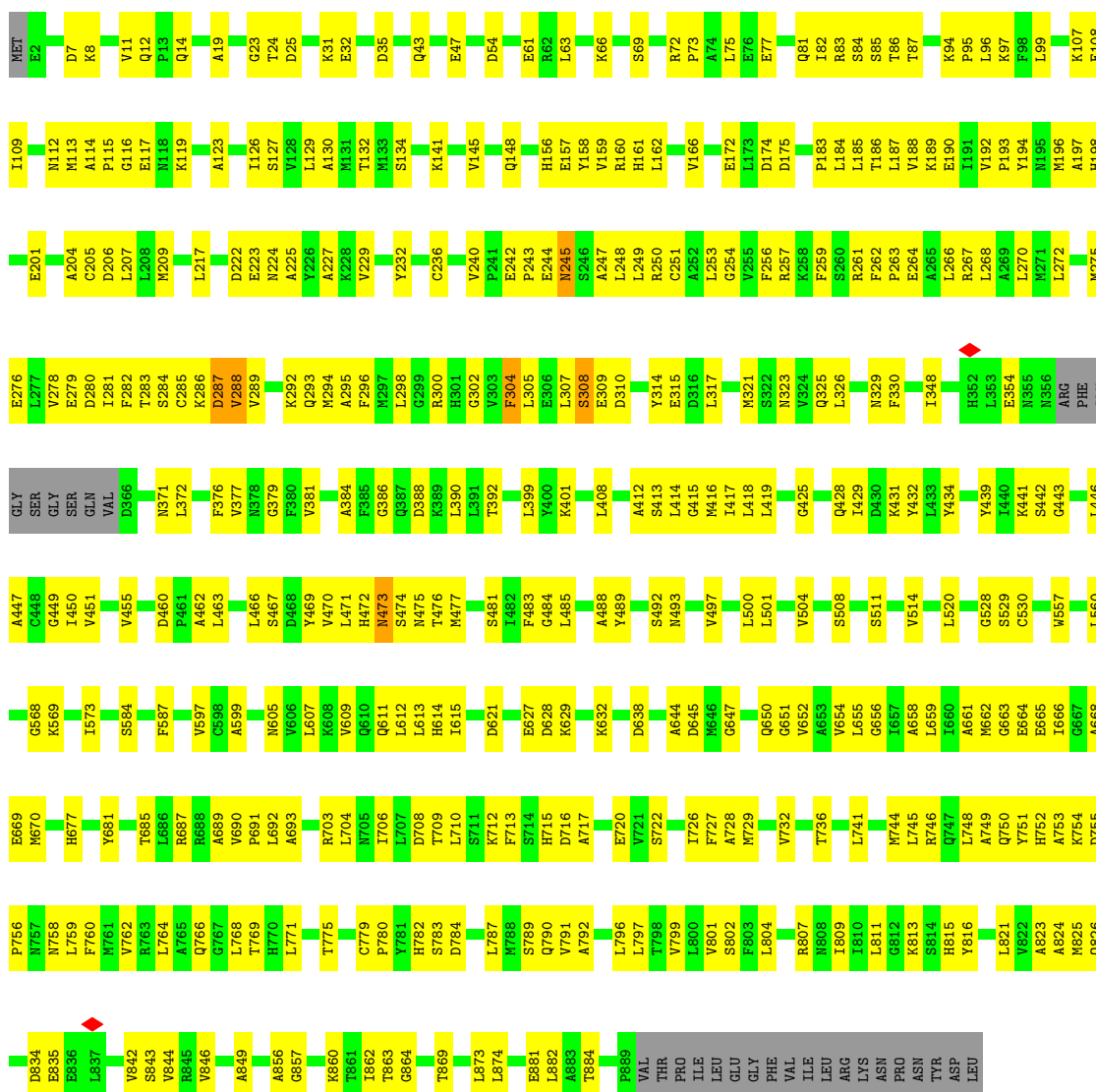




• Molecule 31: 26S proteasome complex subunit SEM1

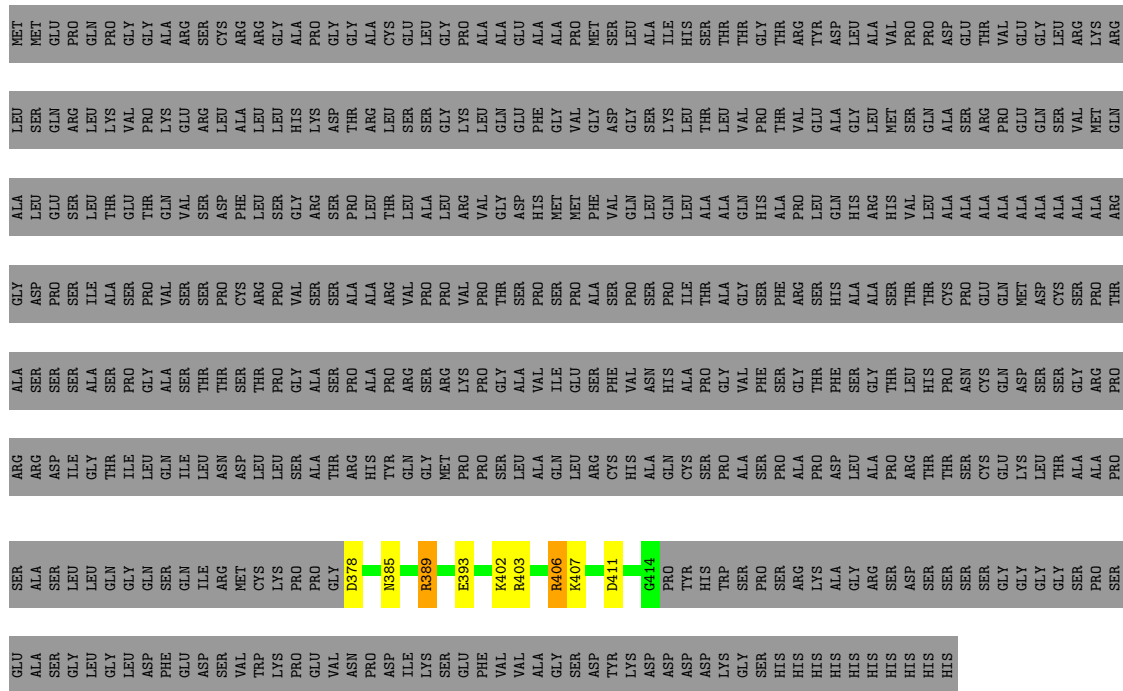


• Molecule 32: 26S proteasome non-ATPase regulatory subunit 2



• Molecule 33: Substrate





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	468422	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.551	Depositor
Minimum map value	-0.112	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.025	Depositor
Map size ($\text{\AA}$)	445.19998, 445.19998, 445.19998	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.06, 1.06, 1.06	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.39	0/3113	0.57	0/4227
2	B	0.38	0/2943	0.60	5/4005 (0.1%)
3	C	0.24	0/2759	0.45	1/3737 (0.0%)
4	D	0.19	0/2823	0.39	0/3838
5	E	0.13	0/2352	0.31	0/3179
6	F	0.23	0/2451	0.45	2/3322 (0.1%)
7	G	0.34	0/1830	0.42	0/2482
7	g	0.25	0/1797	0.33	0/2443
8	H	0.34	0/1784	0.41	0/2423
8	h	0.26	0/1715	0.36	0/2334
9	I	0.31	0/1930	0.39	0/2609
9	i	0.26	0/1879	0.39	0/2545
10	J	0.33	0/1865	0.43	0/2524
10	j	0.23	0/1645	0.32	0/2247
11	K	0.30	0/1800	0.37	0/2437
11	k	0.25	0/1702	0.34	0/2309
12	L	0.32	0/1882	0.43	0/2549
12	l	0.26	0/1866	0.35	0/2527
13	M	0.33	0/1878	0.43	0/2535
13	m	0.25	0/1868	0.30	0/2526
14	N	0.39	0/1507	0.44	0/2042
14	n	0.34	0/1514	0.42	2/2051 (0.1%)
15	O	0.31	0/1664	0.32	0/2257
15	o	0.31	0/1656	0.35	1/2246 (0.0%)
16	P	0.34	0/1581	0.37	0/2135
16	p	0.31	0/1608	0.38	0/2170
17	Q	0.34	0/1592	0.33	0/2156
17	q	0.32	0/1584	0.37	0/2148
18	R	0.32	0/1567	0.27	0/2118
18	r	0.32	0/1571	0.34	0/2123
19	S	0.33	0/1657	0.31	0/2233
19	s	0.36	0/1650	0.36	0/2227

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
20	T	0.34	0/1707	0.39	0/2312
20	t	0.34	0/1696	0.31	0/2297
21	U	0.16	0/5935	0.33	0/8069
22	V	0.18	0/3104	0.38	0/4225
23	W	0.17	0/3386	0.36	0/4596
24	X	0.25	0/2839	0.45	2/3851 (0.1%)
25	Y	0.20	0/3042	0.36	0/4110
26	Z	0.23	0/2118	0.42	1/2891 (0.0%)
27	a	0.20	0/2725	0.42	1/3722 (0.0%)
28	b	0.15	0/1353	0.36	0/1846
29	c	0.17	0/2043	0.36	0/2784
30	d	0.14	0/1803	0.33	0/2447
31	e	0.37	0/282	0.75	1/378 (0.3%)
32	f	0.51	1/6432 (0.0%)	0.89	8/8752 (0.1%)
34	u	0.84	0/319	1.44	0/419
All	All	0.30	1/99817 (0.0%)	0.45	24/135403 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	f	245	ASN	C-O	5.37	1.30	1.24

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	n	142	GLY	CA-C-N	7.91	127.52	119.92
14	n	142	GLY	C-N-CA	7.91	127.52	119.92
3	C	198	LEU	N-CA-C	-7.60	102.94	111.07
32	f	288	VAL	N-CA-C	6.83	116.96	110.74
32	f	287	ASP	N-CA-C	-6.58	104.11	111.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3062	0	2938	181	0
2	B	2901	0	2696	157	0
3	C	2723	0	2645	149	0
4	D	2777	0	2566	103	0
5	E	2324	0	2231	61	0
6	F	2421	0	2294	92	0
7	G	1798	0	1776	52	0
7	g	1765	0	1729	61	0
8	H	1745	0	1692	37	0
8	h	1679	0	1596	36	0
9	I	1900	0	1880	60	0
9	i	1851	0	1777	52	0
10	J	1839	0	1805	62	0
10	j	1622	0	1464	42	0
11	K	1773	0	1728	59	0
11	k	1677	0	1611	36	0
12	L	1847	0	1811	75	0
12	l	1831	0	1800	40	0
13	M	1843	0	1800	38	0
13	m	1833	0	1773	49	0
14	N	1482	0	1442	35	0
14	n	1488	0	1457	26	0
15	O	1637	0	1642	45	0
15	o	1629	0	1623	31	0
16	P	1553	0	1574	40	0
16	p	1579	0	1590	29	0
17	Q	1559	0	1560	32	0
17	q	1551	0	1542	24	0
18	R	1536	0	1488	38	0
18	r	1540	0	1503	22	0
19	S	1627	0	1617	20	0
19	s	1620	0	1609	34	0
20	T	1674	0	1643	47	0
20	t	1663	0	1629	32	0
21	U	5845	0	5485	210	0
22	V	3053	0	2786	109	0
23	W	3348	0	3119	151	0
24	X	2804	0	2685	79	0
25	Y	2990	0	2888	111	0
26	Z	2081	0	1915	99	0
27	a	2676	0	2390	126	0
28	b	1336	0	1269	61	0
29	c	2008	0	1887	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	d	1772	0	1701	63	0
31	e	280	0	213	17	0
32	f	6339	0	5975	508	0
33	v	75	0	17	6	0
34	u	320	0	351	24	0
35	A	31	0	12	15	0
35	B	31	0	12	6	0
35	C	31	0	12	19	0
35	F	31	0	12	11	0
36	D	27	0	12	13	0
All	All	98427	0	94272	3233	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 17.

The worst 5 of 3233 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)
32:f:282:PHE:CE1	32:f:317:LEU:HD21	1.34	1.59
9:I:134:LEU:HD11	9:I:136:TYR:CZ	1.46	1.47
32:f:282:PHE:CZ	32:f:317:LEU:HD21	1.58	1.36
21:U:772:TRP:CD1	21:U:774:PRO:HD2	1.61	1.35
7:g:210:PHE:CE1	7:g:215:ILE:HD13	1.69	1.27

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	412/433 (95%)	361 (88%)	45 (11%)	6 (2%)	8 33
2	B	399/440 (91%)	339 (85%)	50 (12%)	10 (2%)	4 24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	368/406 (91%)	311 (84%)	54 (15%)	3 (1%)	16	45
4	D	378/418 (90%)	313 (83%)	60 (16%)	5 (1%)	9	35
5	E	306/389 (79%)	274 (90%)	31 (10%)	1 (0%)	36	66
6	F	323/439 (74%)	296 (92%)	26 (8%)	1 (0%)	36	66
7	G	237/246 (96%)	219 (92%)	18 (8%)	0	100	100
7	g	233/246 (95%)	222 (95%)	10 (4%)	1 (0%)	30	60
8	H	228/234 (97%)	205 (90%)	21 (9%)	2 (1%)	14	43
8	h	225/234 (96%)	212 (94%)	13 (6%)	0	100	100
9	I	245/261 (94%)	227 (93%)	18 (7%)	0	100	100
9	i	244/261 (94%)	222 (91%)	21 (9%)	1 (0%)	30	60
10	J	237/248 (96%)	216 (91%)	19 (8%)	2 (1%)	16	45
10	j	229/248 (92%)	214 (93%)	14 (6%)	1 (0%)	30	60
11	K	235/241 (98%)	217 (92%)	18 (8%)	0	100	100
11	k	223/241 (92%)	212 (95%)	11 (5%)	0	100	100
12	L	236/263 (90%)	223 (94%)	13 (6%)	0	100	100
12	l	235/263 (89%)	226 (96%)	9 (4%)	0	100	100
13	M	239/255 (94%)	225 (94%)	14 (6%)	0	100	100
13	m	238/255 (93%)	219 (92%)	19 (8%)	0	100	100
14	N	198/239 (83%)	181 (91%)	16 (8%)	1 (0%)	24	56
14	n	199/239 (83%)	182 (92%)	17 (8%)	0	100	100
15	O	219/277 (79%)	201 (92%)	17 (8%)	1 (0%)	24	56
15	o	218/277 (79%)	207 (95%)	11 (5%)	0	100	100
16	P	202/205 (98%)	186 (92%)	16 (8%)	0	100	100
16	p	202/205 (98%)	188 (93%)	14 (7%)	0	100	100
17	Q	195/201 (97%)	182 (93%)	13 (7%)	0	100	100
17	q	195/201 (97%)	185 (95%)	10 (5%)	0	100	100
18	R	199/263 (76%)	190 (96%)	9 (4%)	0	100	100
18	r	198/263 (75%)	187 (94%)	11 (6%)	0	100	100
19	S	211/241 (88%)	202 (96%)	9 (4%)	0	100	100
19	s	210/241 (87%)	199 (95%)	11 (5%)	0	100	100
20	T	213/264 (81%)	200 (94%)	13 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	t	213/264 (81%)	199 (93%)	14 (7%)	0	100	100
21	U	795/953 (83%)	725 (91%)	68 (9%)	2 (0%)	36	66
22	V	408/534 (76%)	351 (86%)	56 (14%)	1 (0%)	43	72
23	W	454/456 (100%)	401 (88%)	51 (11%)	2 (0%)	30	60
24	X	377/422 (89%)	344 (91%)	29 (8%)	4 (1%)	11	40
25	Y	377/389 (97%)	329 (87%)	47 (12%)	1 (0%)	36	66
26	Z	285/324 (88%)	236 (83%)	49 (17%)	0	100	100
27	a	371/376 (99%)	308 (83%)	59 (16%)	4 (1%)	11	40
28	b	187/377 (50%)	163 (87%)	23 (12%)	1 (0%)	24	56
29	c	268/310 (86%)	238 (89%)	30 (11%)	0	100	100
30	d	224/350 (64%)	197 (88%)	25 (11%)	2 (1%)	14	43
31	e	34/70 (49%)	25 (74%)	7 (21%)	2 (6%)	1	9
32	f	875/908 (96%)	746 (85%)	122 (14%)	7 (1%)	16	45
34	u	35/491 (7%)	35 (100%)	0	0	100	100
All	All	13032/15361 (85%)	11740 (90%)	1231 (9%)	61 (0%)	26	56

5 of 61 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	43	PRO
2	B	88	LEU
2	B	92	GLN
2	B	162	VAL
3	C	219	LEU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	302/372 (81%)	301 (100%)	1 (0%)	86	85
2	B	284/385 (74%)	283 (100%)	1 (0%)	84	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	268/352 (76%)	267 (100%)	1 (0%)	84	83
4	D	263/366 (72%)	263 (100%)	0	100	100
5	E	228/341 (67%)	228 (100%)	0	100	100
6	F	233/379 (62%)	233 (100%)	0	100	100
7	G	187/210 (89%)	187 (100%)	0	100	100
7	g	183/210 (87%)	183 (100%)	0	100	100
8	H	175/191 (92%)	174 (99%)	1 (1%)	78	80
8	h	162/191 (85%)	161 (99%)	1 (1%)	78	80
9	I	195/221 (88%)	195 (100%)	0	100	100
9	i	183/221 (83%)	183 (100%)	0	100	100
10	J	189/211 (90%)	188 (100%)	1 (0%)	81	82
10	j	143/211 (68%)	142 (99%)	1 (1%)	76	79
11	K	188/203 (93%)	188 (100%)	0	100	100
11	k	174/203 (86%)	174 (100%)	0	100	100
12	L	197/224 (88%)	197 (100%)	0	100	100
12	l	194/224 (87%)	193 (100%)	1 (0%)	81	82
13	M	186/212 (88%)	186 (100%)	0	100	100
13	m	186/212 (88%)	186 (100%)	0	100	100
14	N	151/181 (83%)	150 (99%)	1 (1%)	76	79
14	n	151/181 (83%)	151 (100%)	0	100	100
15	O	174/228 (76%)	174 (100%)	0	100	100
15	o	173/228 (76%)	172 (99%)	1 (1%)	78	80
16	P	163/174 (94%)	163 (100%)	0	100	100
16	p	170/174 (98%)	169 (99%)	1 (1%)	78	80
17	Q	163/171 (95%)	162 (99%)	1 (1%)	78	80
17	q	161/171 (94%)	158 (98%)	3 (2%)	50	68
18	R	150/202 (74%)	150 (100%)	0	100	100
18	r	152/202 (75%)	151 (99%)	1 (1%)	76	79
19	S	170/199 (85%)	170 (100%)	0	100	100
19	s	171/199 (86%)	171 (100%)	0	100	100
20	T	176/215 (82%)	176 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	t	172/215 (80%)	172 (100%)	0	100	100
21	U	575/816 (70%)	573 (100%)	2 (0%)	86	85
22	V	283/460 (62%)	283 (100%)	0	100	100
23	W	326/416 (78%)	325 (100%)	1 (0%)	86	85
24	X	272/362 (75%)	271 (100%)	1 (0%)	84	83
25	Y	302/344 (88%)	300 (99%)	2 (1%)	76	79
26	Z	203/295 (69%)	203 (100%)	0	100	100
27	a	250/336 (74%)	250 (100%)	0	100	100
28	b	136/312 (44%)	136 (100%)	0	100	100
29	c	198/268 (74%)	197 (100%)	1 (0%)	81	82
30	d	177/294 (60%)	177 (100%)	0	100	100
31	e	26/63 (41%)	26 (100%)	0	100	100
32	f	629/763 (82%)	627 (100%)	2 (0%)	86	85
34	u	33/398 (8%)	30 (91%)	3 (9%)	9	32
All	All	9827/13006 (76%)	9799 (100%)	28 (0%)	84	85

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
32	f	390	LEU
34	u	406	ARG
10	j	99	GLU
18	r	195	TYR
8	h	156	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 54 such sidechains are listed below:

Mol	Chain	Res	Type
26	Z	243	GLN
32	f	475	ASN
16	p	65	GLN
27	a	169	HIS
32	f	53	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

5 ligands are modelled in this entry.

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	F	501	-	29,33,33	0.49	0	44,52,52	0.62	0
35	ATP	A	501	-	29,33,33	0.53	0	44,52,52	0.98	2 (4%)
35	ATP	B	501	-	29,33,33	0.53	0	44,52,52	0.68	1 (2%)
36	ADP	D	501	-	27,29,29	0.45	0	42,45,45	0.58	0
35	ATP	C	501	-	29,33,33	0.49	0	44,52,52	0.53	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	ATP	F	501	-	-	9/22/38/38	0/3/3/3
35	ATP	A	501	-	-	8/22/38/38	0/3/3/3
35	ATP	B	501	-	-	8/22/38/38	0/3/3/3
36	ADP	D	501	-	-	9/16/32/32	0/3/3/3

Continued on next page...

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	ATP	C	501	-	-	10/22/38/38	0/3/3/3

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	A	501	ATP	PA-O3A-PB	-3.63	120.38	132.83
35	A	501	ATP	PB-O3B-PG	-3.36	121.29	132.83
35	B	501	ATP	PB-O3B-PG	-2.20	125.27	132.83

There are no chirality outliers.

5 of 44 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
35	A	501	ATP	PB-O3A-PA-O5'
35	A	501	ATP	O4'-C1'-N9-C8
35	B	501	ATP	C5'-O5'-PA-O1A
35	B	501	ATP	C5'-O5'-PA-O2A
35	C	501	ATP	C5'-O5'-PA-O2A

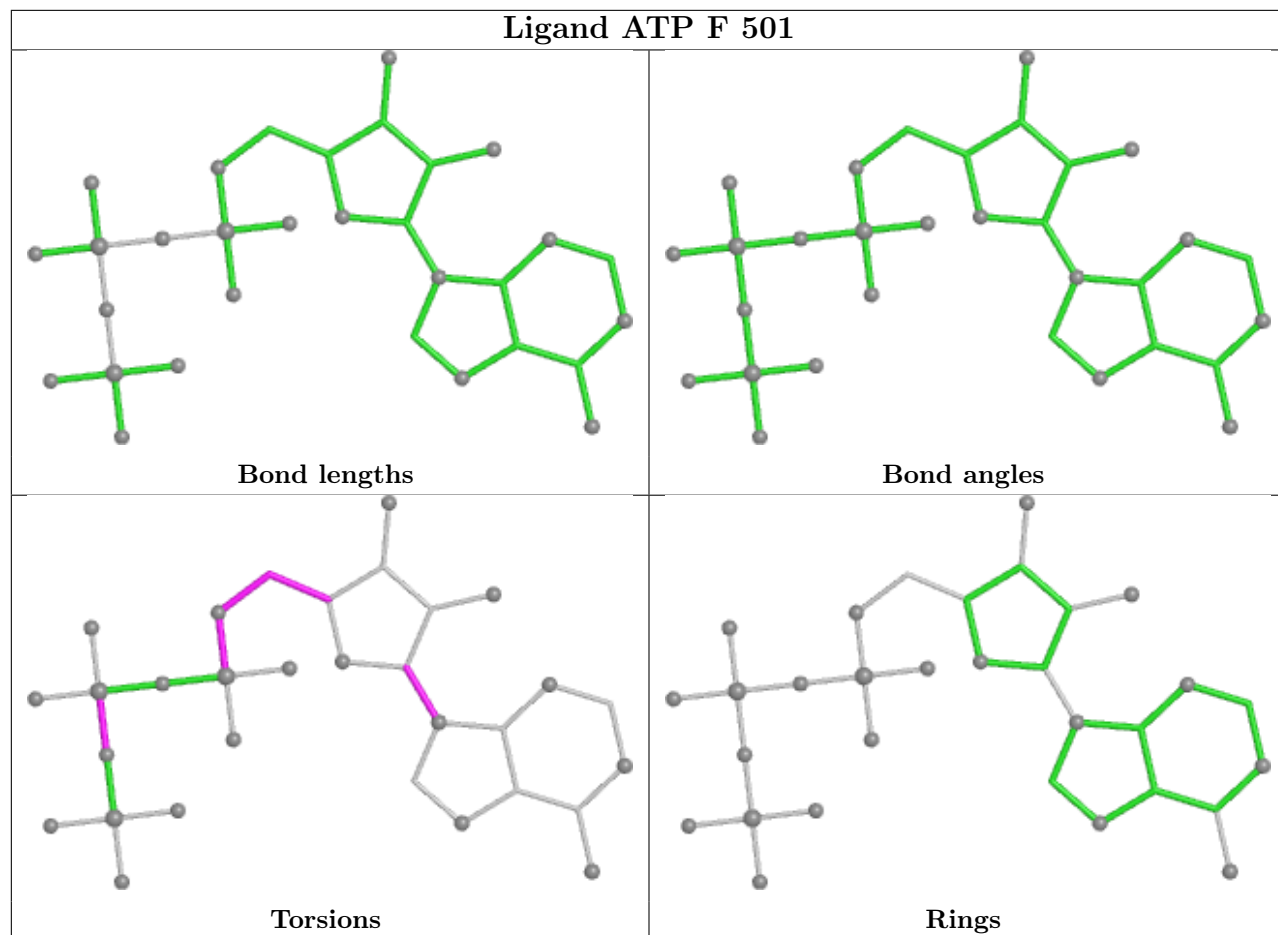
There are no ring outliers.

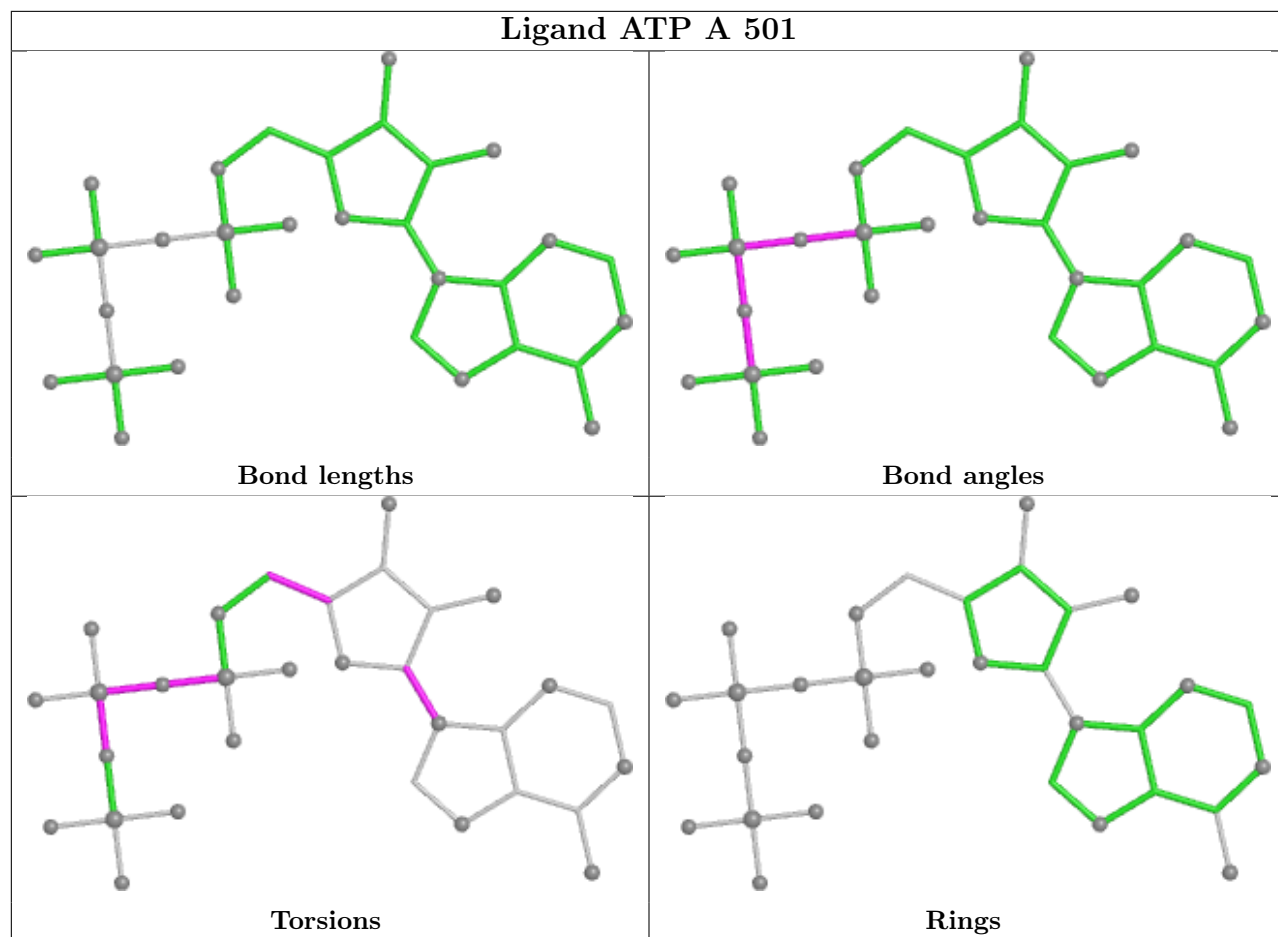
5 monomers are involved in 64 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	F	501	ATP	11	0
35	A	501	ATP	15	0
35	B	501	ATP	6	0
36	D	501	ADP	13	0
35	C	501	ATP	19	0

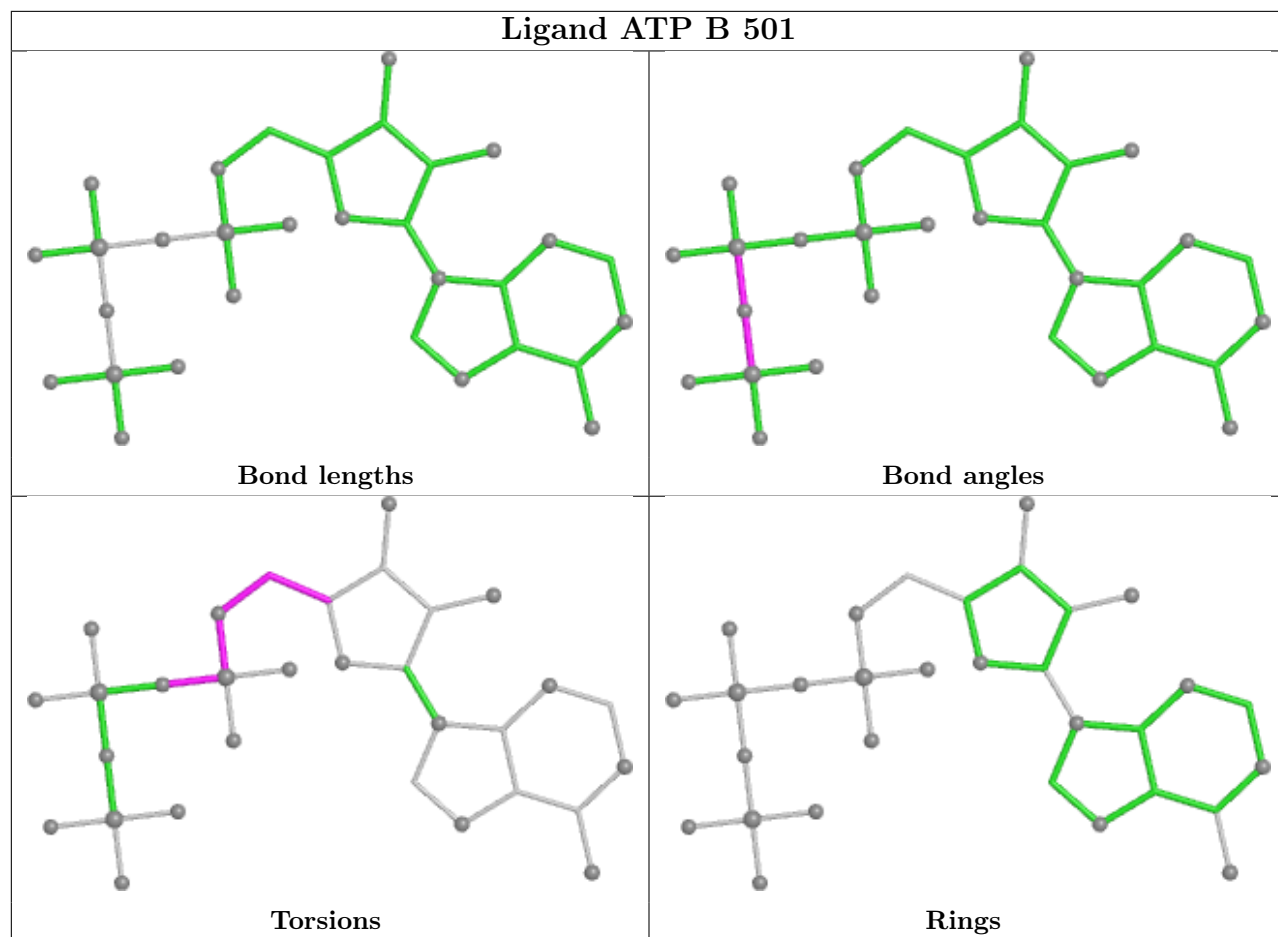
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

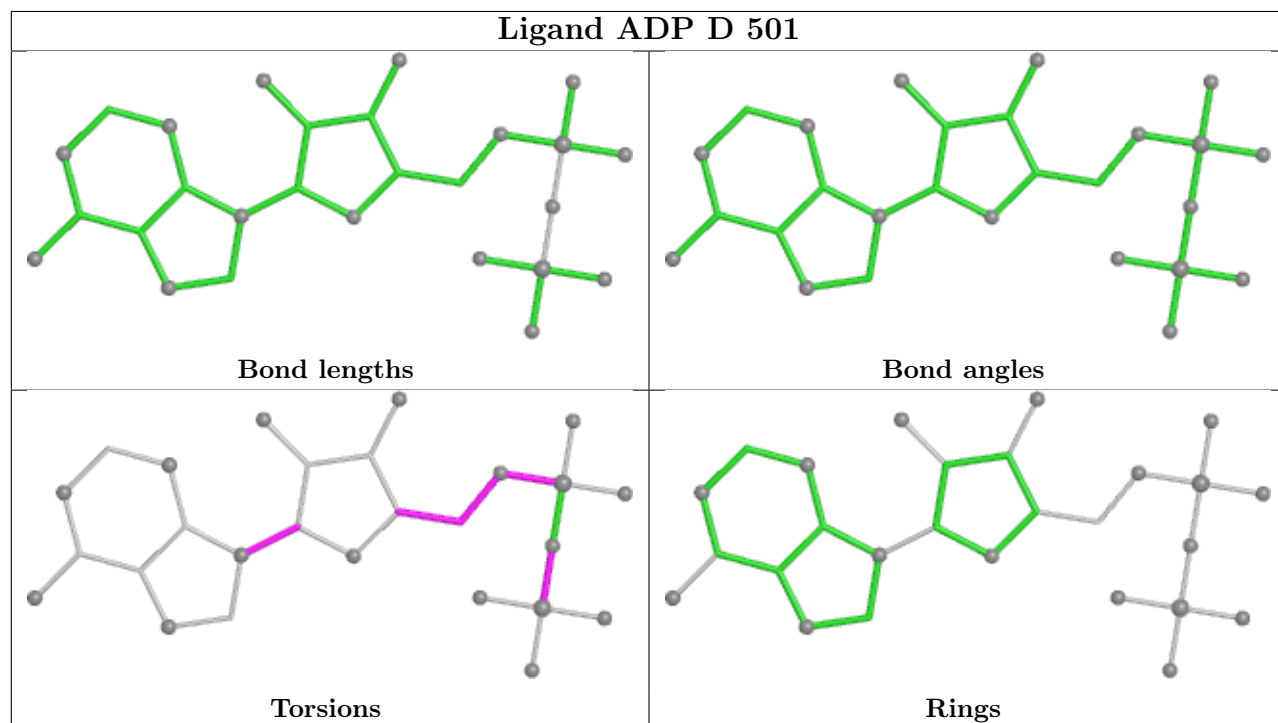


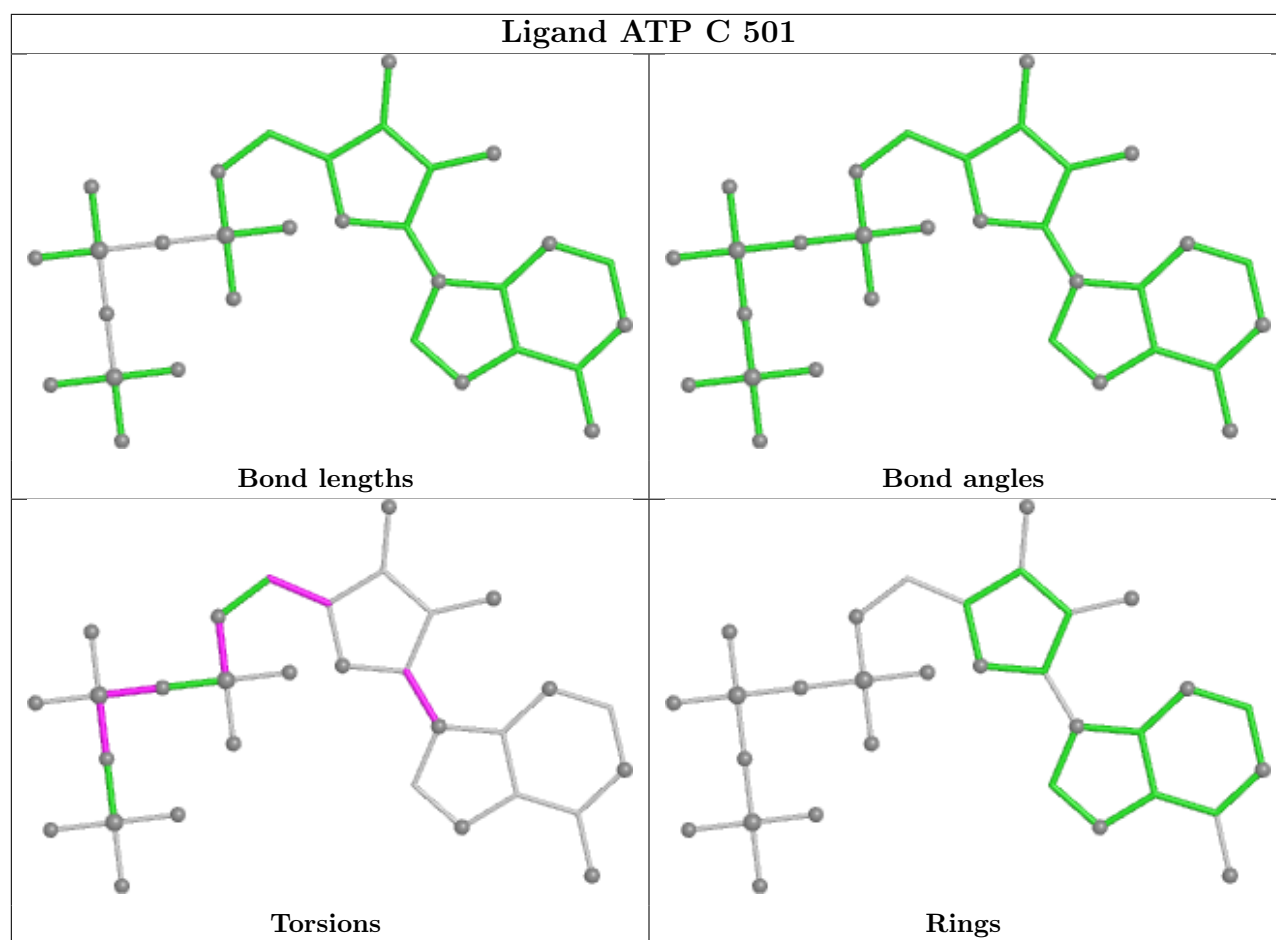


Ligand ATP B 501



Ligand ADP D 501





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

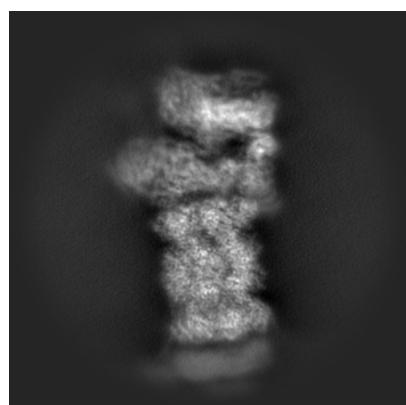
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-63592. These allow visual inspection of the internal detail of the map and identification of artifacts.

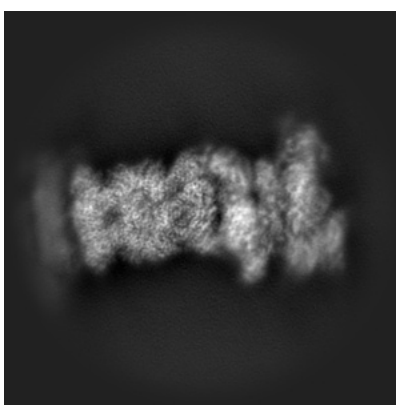
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

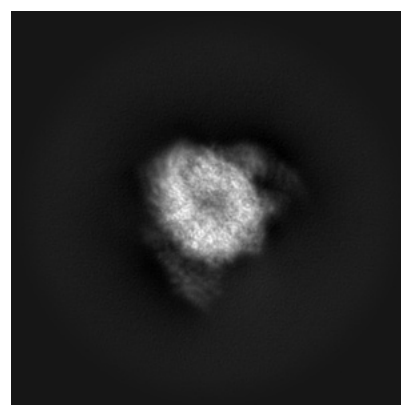
6.1.1 Primary map



X



Y

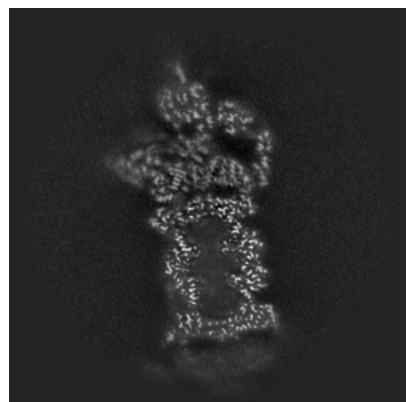


Z

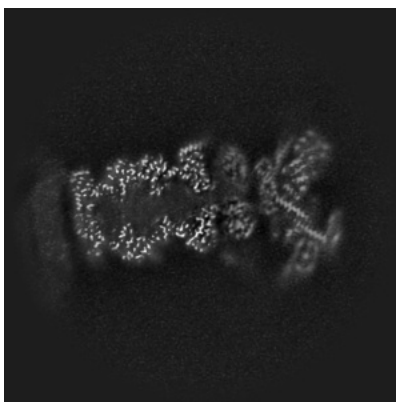
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

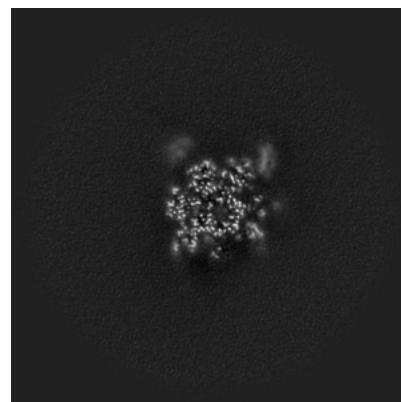
6.2.1 Primary map



X Index: 210



Y Index: 210

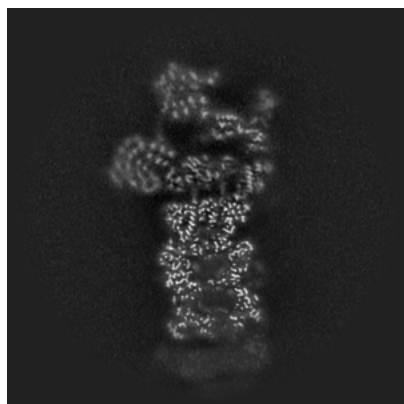


Z Index: 210

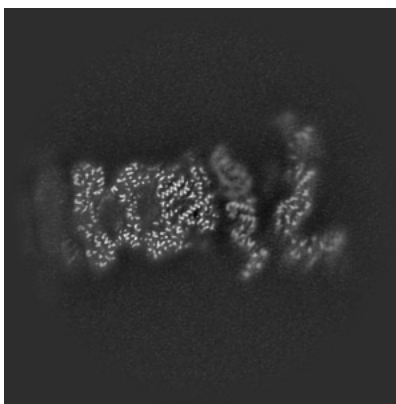
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

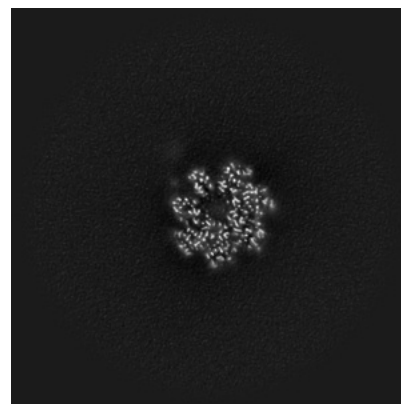
6.3.1 Primary map



X Index: 194



Y Index: 233

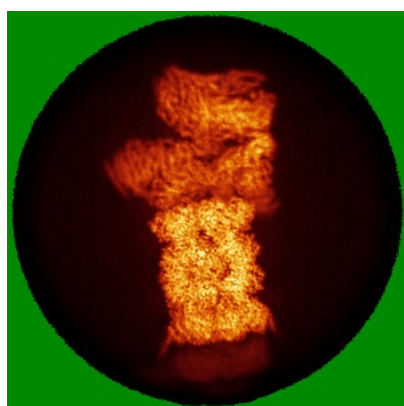


Z Index: 198

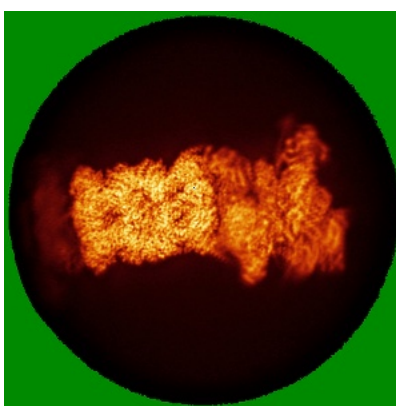
The images above show the largest variance slices of the map in three orthogonal directions.

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

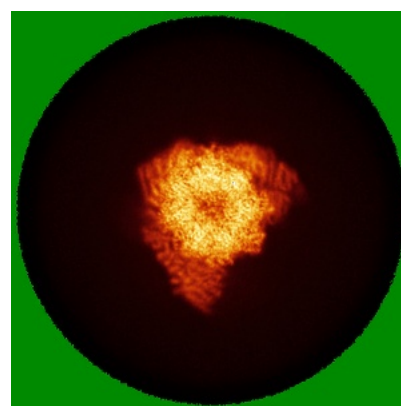
6.4.1 Primary map



X



Y

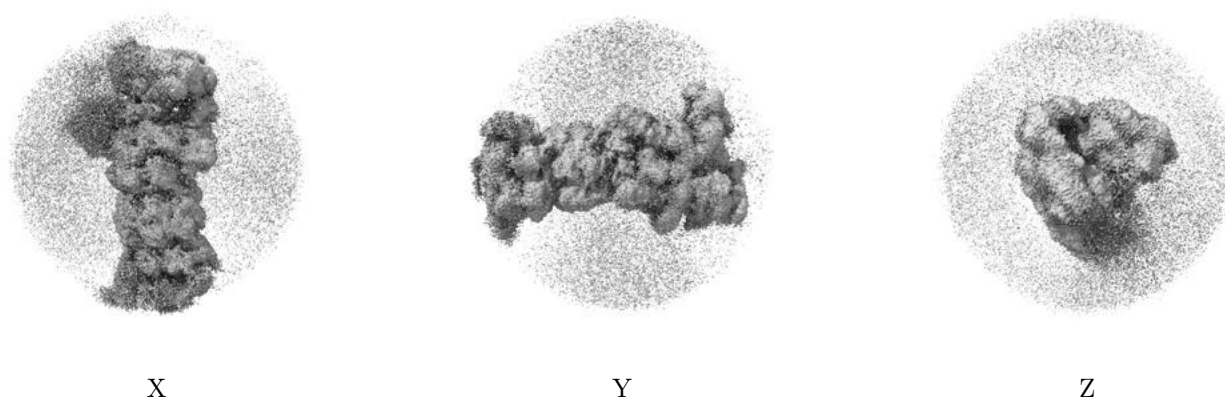


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

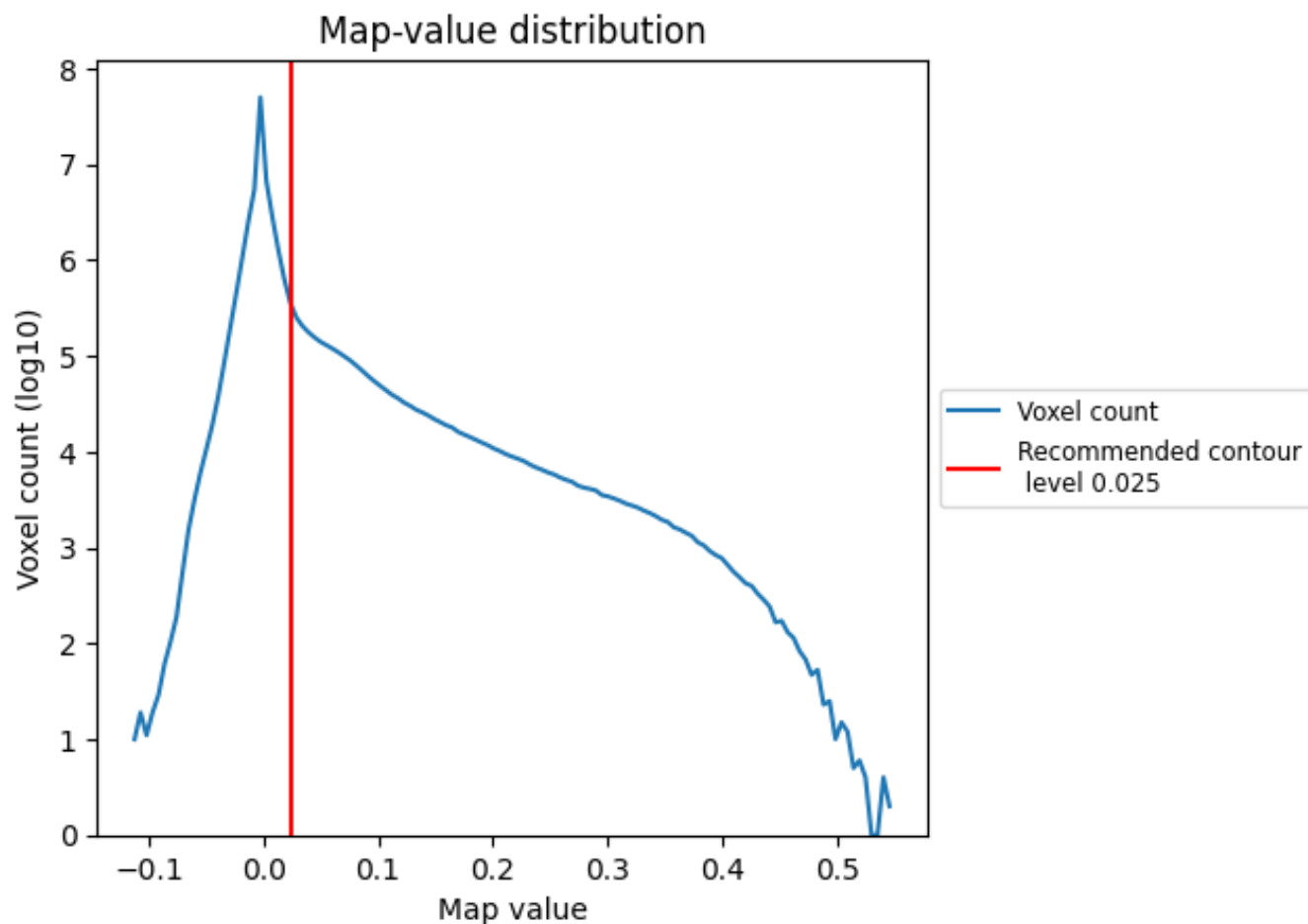
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

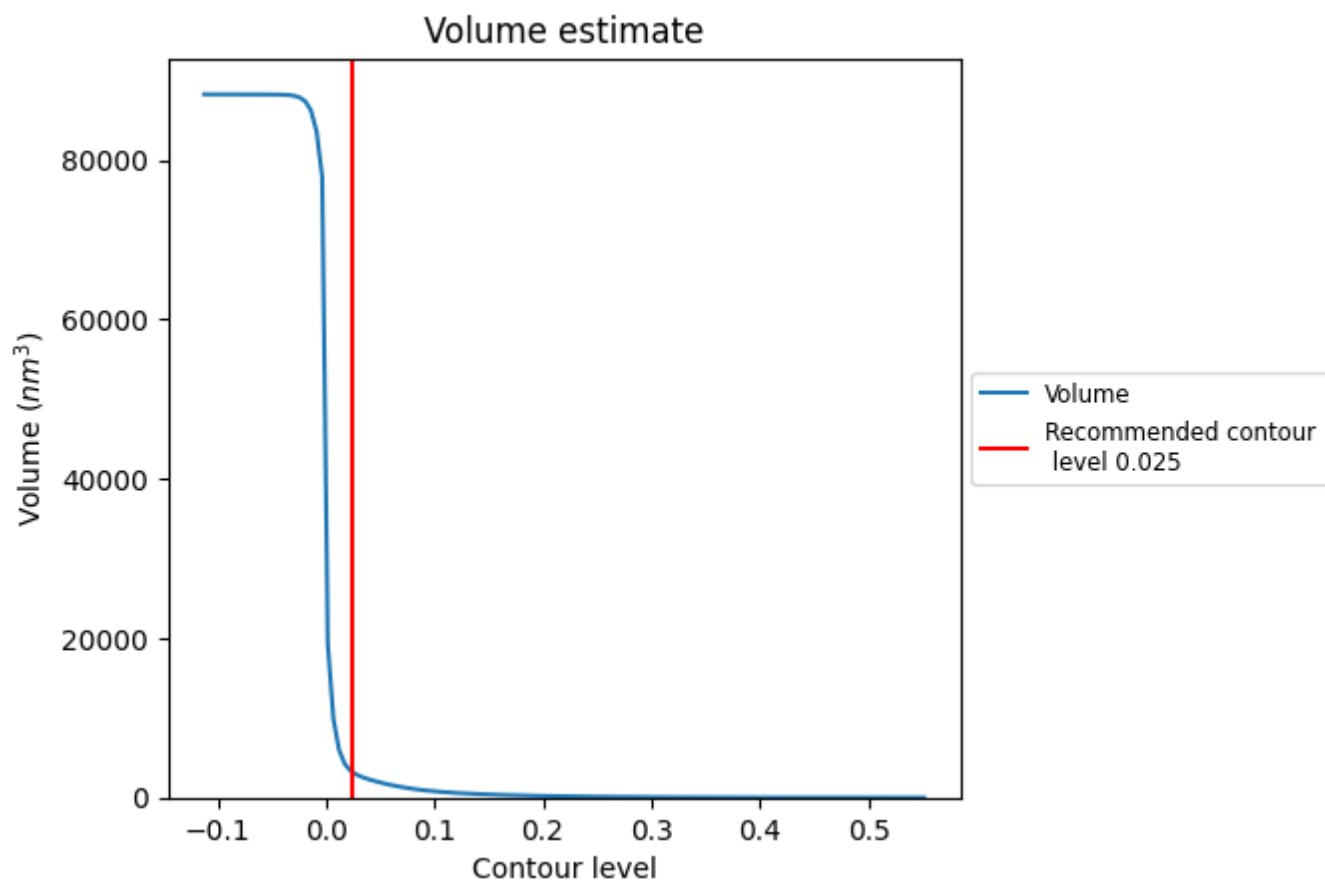
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

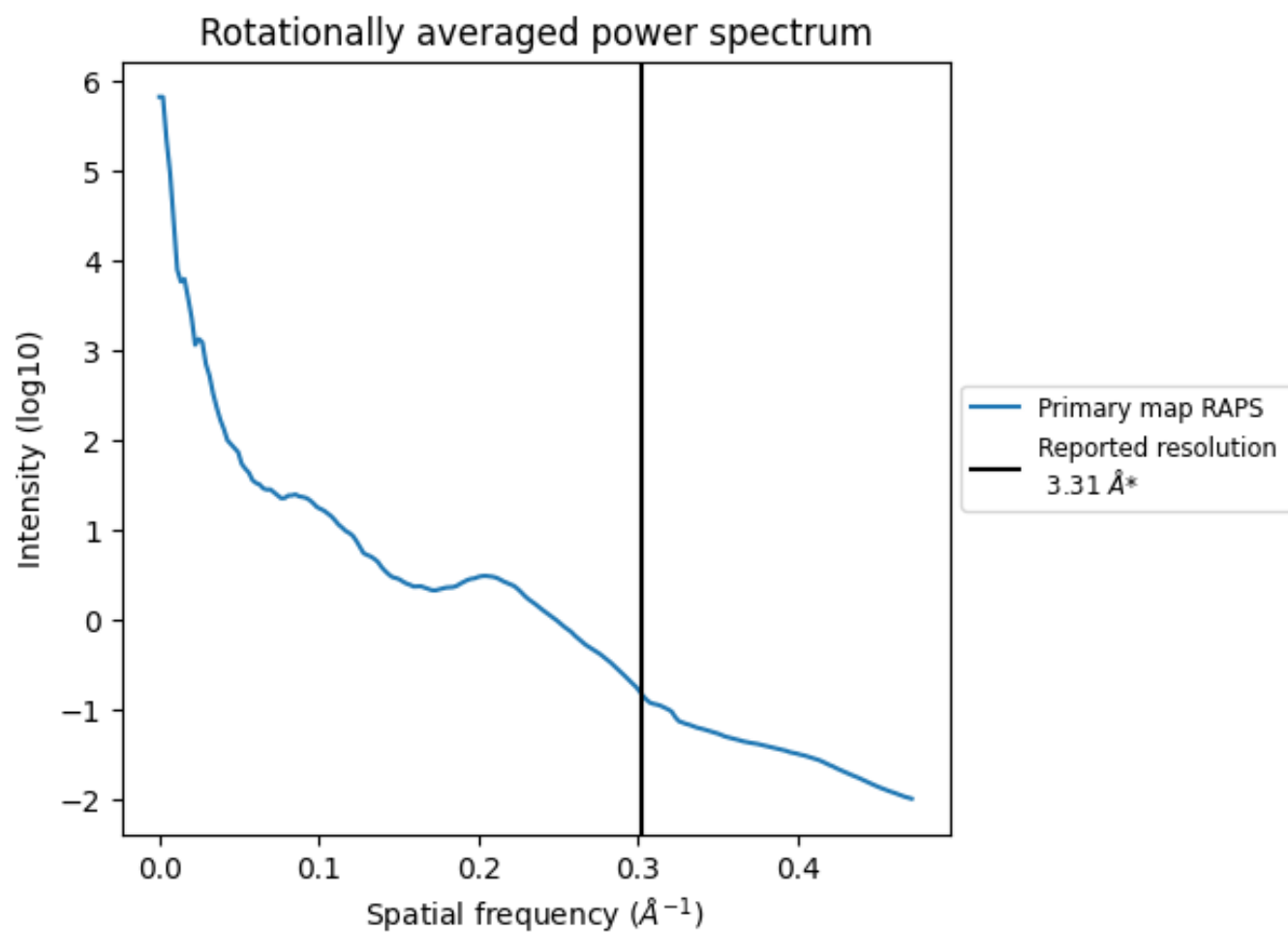
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3154 nm³; this corresponds to an approximate mass of 2849 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 0.302 Å⁻¹

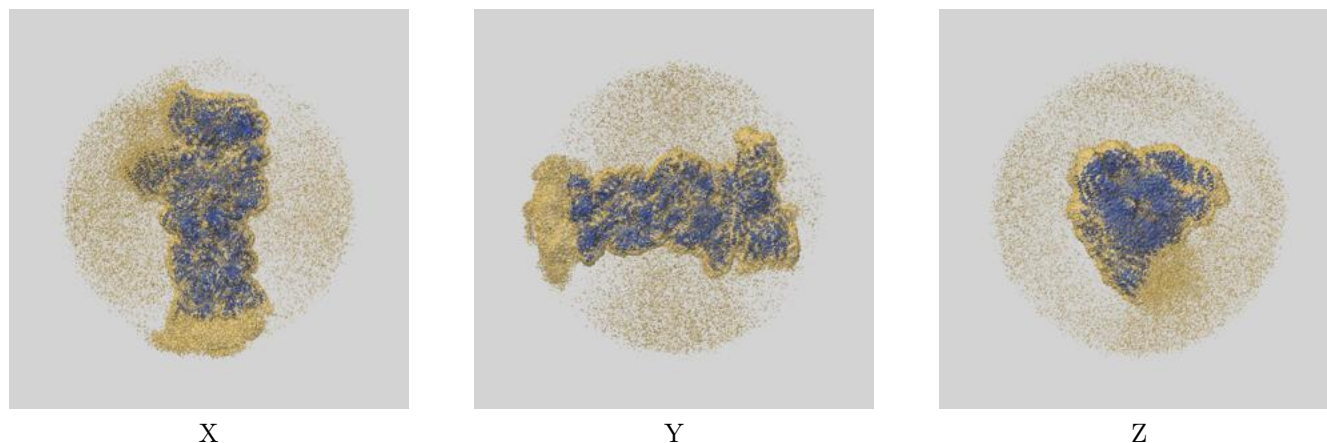
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

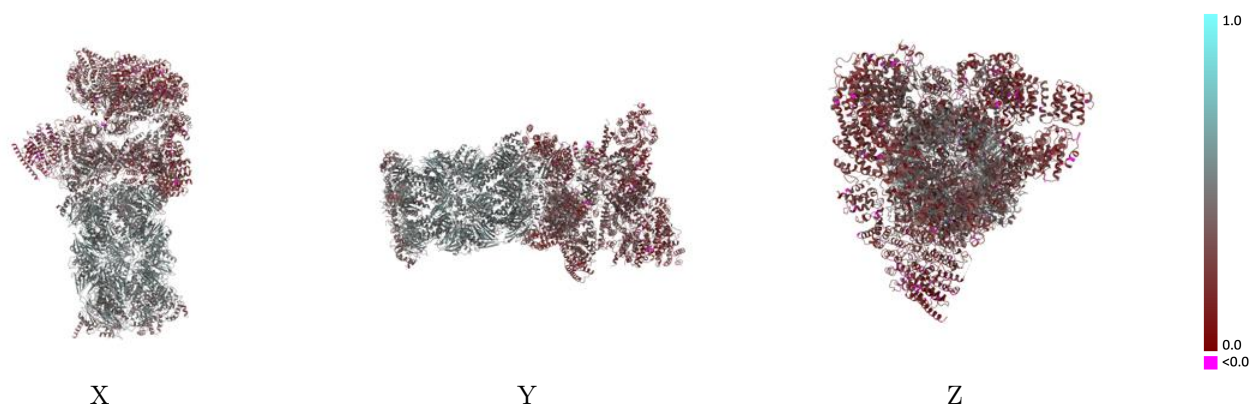
This section contains information regarding the fit between EMDB map EMD-63592 and PDB model 9M2W. Per-residue inclusion information can be found in section [3](#) on page [13](#).

9.1 Map-model overlay [i](#)



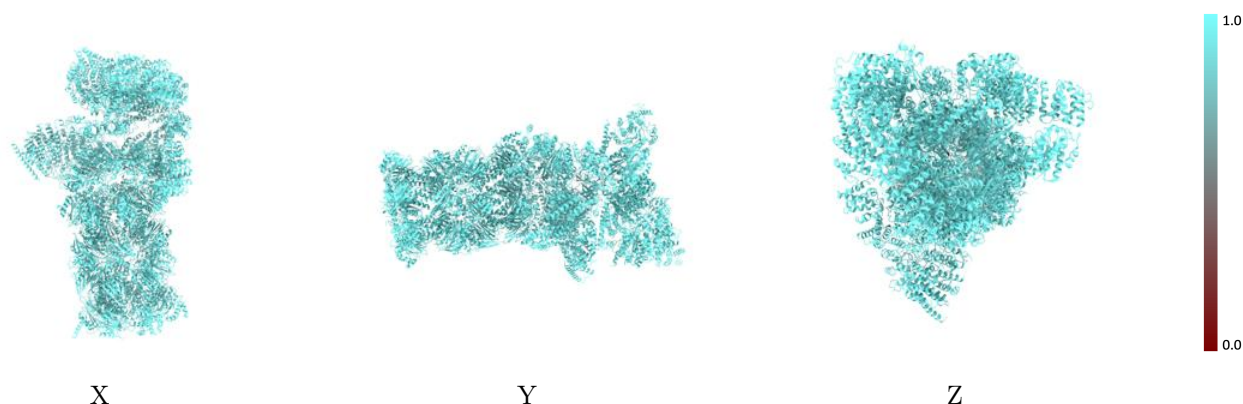
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



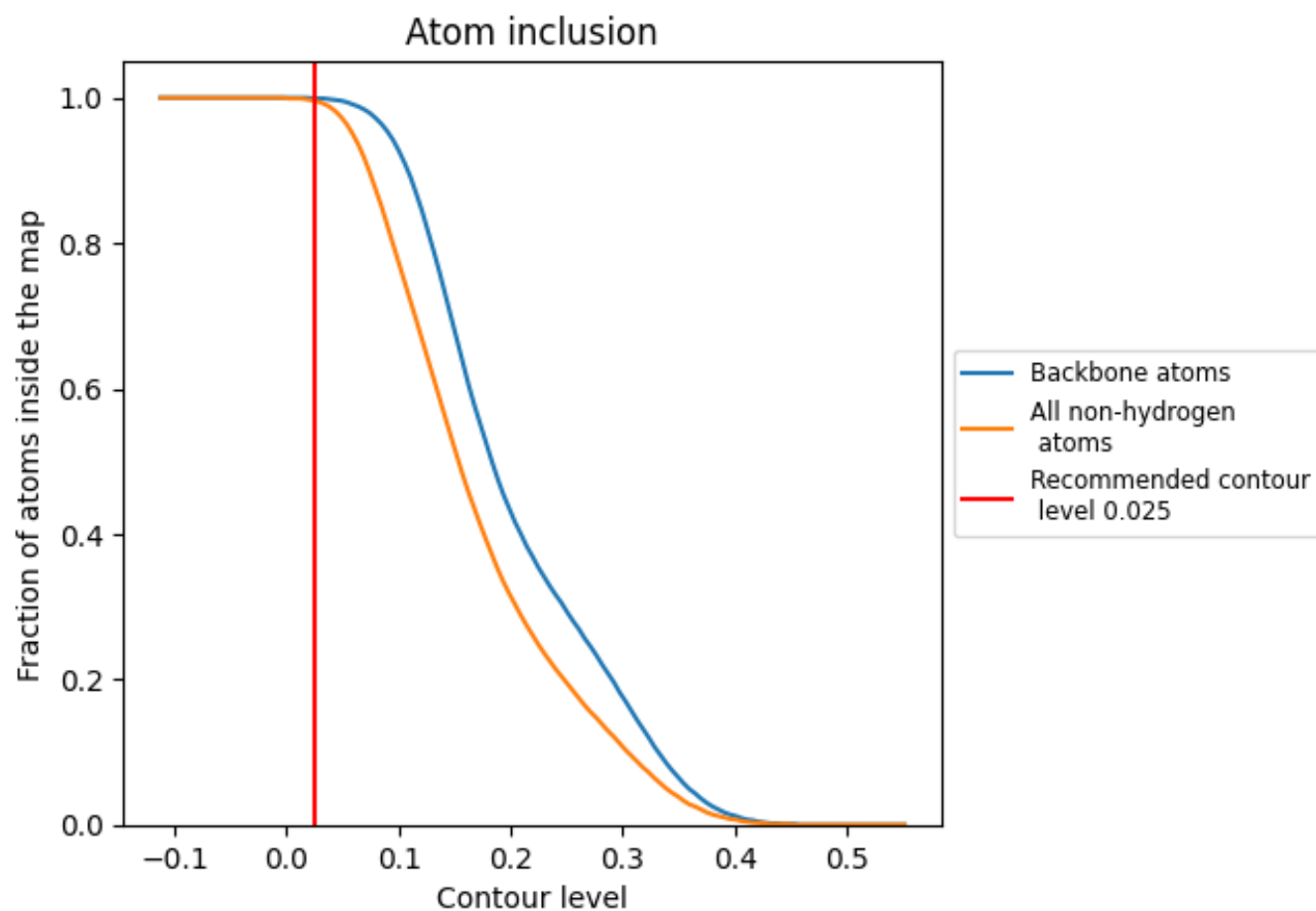
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.025).

9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 100% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9960	 0.3880
A	 0.9830	 0.3620
B	 0.9790	 0.3610
C	 0.9910	 0.3760
D	 0.9850	 0.3590
E	 0.9980	 0.2600
F	 0.9950	 0.3460
G	 0.9980	 0.4860
H	 0.9900	 0.4930
I	 0.9950	 0.4860
J	 0.9970	 0.4790
K	 0.9960	 0.4870
L	 0.9980	 0.4970
M	 0.9950	 0.4880
N	 0.9990	 0.5110
O	 0.9990	 0.5160
P	 1.0000	 0.5190
Q	 0.9990	 0.5210
R	 0.9990	 0.5230
S	 0.9980	 0.5170
T	 0.9990	 0.5130
U	 0.9990	 0.2940
V	 0.9970	 0.2690
W	 0.9950	 0.2530
X	 0.9980	 0.3150
Y	 0.9970	 0.3250
Z	 0.9970	 0.3030
a	 0.9990	 0.2410
b	 0.9990	 0.2280
c	 0.9890	 0.3120
d	 0.9960	 0.2420
e	 0.9960	 0.2740
f	 0.9920	 0.1960
g	 0.9990	 0.4570
h	 0.9960	 0.4660



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Chain	Atom inclusion	Q-score
i	 1.0000	 0.4440
j	 0.9990	 0.4450
k	 1.0000	 0.4600
l	 0.9990	 0.4730
m	 0.9980	 0.4680
n	 0.9990	 0.5090
o	 1.0000	 0.5140
p	 1.0000	 0.5050
q	 1.0000	 0.5120
r	 1.0000	 0.5180
s	 0.9990	 0.5200
t	 0.9990	 0.5150
u	 0.9870	 0.1290
v	 1.0000	 0.4210