



## wwPDB EM Validation Summary Report ⓘ

Apr 6, 2026 – 12:15 AM UTC

PDB ID : 9W39 / pdb\_00009w39  
EMDB ID : EMD-65595  
Title : Structure of human 26S proteasome complexed with midnolin, 19S proteasome with Ubl bound  
Authors : Zhu, C.; Qin, L.; Liang, L.  
Deposited on : 2025-07-29  
Resolution : 3.65 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

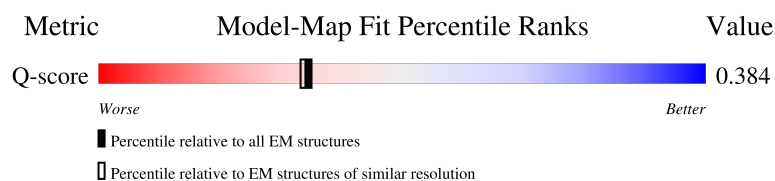
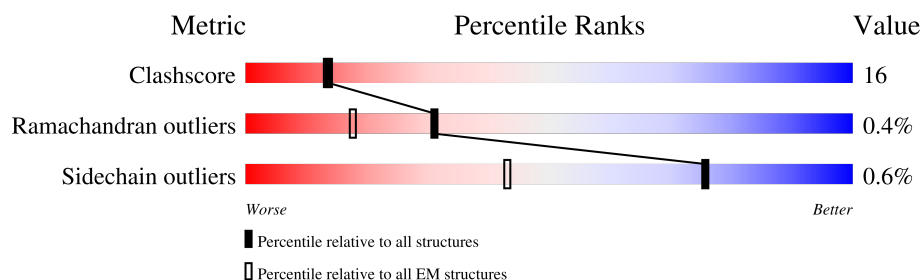
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (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) : 2.49

# 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 3.65 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	11564 ( 3.15 - 4.15 )

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  $\geq 3$ , 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	f	856	
2	C	406	
3	D	418	
4	V	534	

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Mol	Chain	Length	Quality of chain
5	W	456	
6	X	422	
7	Y	389	
8	Z	324	
9	a	376	
10	b	377	
11	d	350	
12	e	70	
13	v	7	
14	U	953	
15	c	590	
16	A	433	
17	B	440	
18	E	389	
19	F	439	

## 2 Entry composition

There are 23 unique types of molecules in this entry. The entry contains 49219 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 Maltose/maltodextrin-binding periplasmic protein, Midnolin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	f	84	Total	C	N	O	S	0	0
			632	394	115	121	2		

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
f	-387	MET	-	initiating methionine	UNP P0AEX9
f	-386	GLY	-	expression tag	UNP P0AEX9
f	-385	HIS	-	expression tag	UNP P0AEX9
f	-384	HIS	-	expression tag	UNP P0AEX9
f	-383	HIS	-	expression tag	UNP P0AEX9
f	-382	HIS	-	expression tag	UNP P0AEX9
f	-381	HIS	-	expression tag	UNP P0AEX9
f	-380	HIS	-	expression tag	UNP P0AEX9
f	-13	ASP	-	linker	UNP P0AEX9
f	-12	TYR	-	linker	UNP P0AEX9
f	-11	ASP	-	linker	UNP P0AEX9
f	-10	ILE	-	linker	UNP P0AEX9
f	-9	PRO	-	linker	UNP P0AEX9
f	-8	THR	-	linker	UNP P0AEX9
f	-7	THR	-	linker	UNP P0AEX9
f	-6	GLU	-	linker	UNP P0AEX9
f	-5	ASN	-	linker	UNP P0AEX9
f	-4	LEU	-	linker	UNP P0AEX9
f	-3	TYR	-	linker	UNP P0AEX9
f	-2	PHE	-	linker	UNP P0AEX9
f	-1	GLN	-	linker	UNP P0AEX9
f	0	GLY	-	linker	UNP P0AEX9

- Molecule 2 is a protein called 26S proteasome regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	364	Total	C	N	O	S	0	0
			2870	1811	516	527	16		

- Molecule 3 is a protein called 26S proteasome regulatory subunit 6B.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	380	Total	C	N	O	S	0	0
			3039	1923	524	579	13		

- Molecule 4 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	V	442	Total	C	N	O	S	0	0
			3592	2290	639	650	13		

- Molecule 5 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	W	440	Total	C	N	O	S	0	0
			3582	2269	609	681	23		

- Molecule 6 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	X	384	Total	C	N	O	S	0	0
			3040	1935	513	580	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Y	376	Total	C	N	O	S	0	0
			3103	1979	531	576	17		

- Molecule 8 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

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

- Molecule 9 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

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

- Molecule 10 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

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

- Molecule 11 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	d	270	Total	C	N	O	S	0	0
			2193	1417	360	407	9		

- Molecule 12 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	e	48	Total	C	N	O	0	0
			409	249	63	97		

- Molecule 13 is a protein called Substrate.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	v	7	Total	C	N	O	0	0
			35	21	7	7		

- Molecule 14 is a protein called 26S proteasome non-ATPase regulatory subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	U	818	Total	C	N	O	S	0	0
			6371	4046	1085	1196	44		

- Molecule 15 is a protein called Ubiquitin C-terminal hydrolase PSMD14, Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	c	293	Total	C	N	O	S	0	0
			2304	1457	396	432	19		

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
c	311	GLU	-	linker	UNP O00487
c	312	ASN	-	linker	UNP O00487
c	313	LEU	-	linker	UNP O00487
c	314	TYR	-	linker	UNP O00487
c	315	PHE	-	linker	UNP O00487
c	316	GLN	-	linker	UNP O00487
c	317	GLY	-	linker	UNP O00487
c	318	ALA	-	linker	UNP O00487
c	555	HIS	-	expression tag	UNP A0A2U3DNX3
c	556	HIS	-	expression tag	UNP A0A2U3DNX3
c	557	HIS	-	expression tag	UNP A0A2U3DNX3
c	558	HIS	-	expression tag	UNP A0A2U3DNX3
c	559	HIS	-	expression tag	UNP A0A2U3DNX3
c	560	HIS	-	expression tag	UNP A0A2U3DNX3
c	561	SER	-	expression tag	UNP A0A2U3DNX3
c	562	ALA	-	expression tag	UNP A0A2U3DNX3
c	563	TRP	-	expression tag	UNP A0A2U3DNX3
c	564	SER	-	expression tag	UNP A0A2U3DNX3
c	565	HIS	-	expression tag	UNP A0A2U3DNX3
c	566	PRO	-	expression tag	UNP A0A2U3DNX3
c	567	GLN	-	expression tag	UNP A0A2U3DNX3
c	568	PHE	-	expression tag	UNP A0A2U3DNX3
c	569	GLU	-	expression tag	UNP A0A2U3DNX3
c	570	LYS	-	expression tag	UNP A0A2U3DNX3
c	571	GLY	-	expression tag	UNP A0A2U3DNX3
c	572	GLY	-	expression tag	UNP A0A2U3DNX3
c	573	GLY	-	expression tag	UNP A0A2U3DNX3
c	574	SER	-	expression tag	UNP A0A2U3DNX3
c	575	GLY	-	expression tag	UNP A0A2U3DNX3
c	576	GLY	-	expression tag	UNP A0A2U3DNX3
c	577	GLY	-	expression tag	UNP A0A2U3DNX3
c	578	SER	-	expression tag	UNP A0A2U3DNX3
c	579	GLY	-	expression tag	UNP A0A2U3DNX3
c	580	GLY	-	expression tag	UNP A0A2U3DNX3
c	581	SER	-	expression tag	UNP A0A2U3DNX3
c	582	ALA	-	expression tag	UNP A0A2U3DNX3
c	583	TRP	-	expression tag	UNP A0A2U3DNX3
c	584	SER	-	expression tag	UNP A0A2U3DNX3
c	585	HIS	-	expression tag	UNP A0A2U3DNX3
c	586	PRO	-	expression tag	UNP A0A2U3DNX3
c	587	GLN	-	expression tag	UNP A0A2U3DNX3
c	588	PHE	-	expression tag	UNP A0A2U3DNX3
c	589	GLU	-	expression tag	UNP A0A2U3DNX3

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Chain	Residue	Modelled	Actual	Comment	Reference
c	590	LYS	-	expression tag	UNP A0A2U3DNX3

- Molecule 16 is a protein called 26S proteasome regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	A	366	Total	C	N	O	S	0	0
			2863	1805	503	537	18		

- Molecule 17 is a protein called 26S proteasome regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	B	340	Total	C	N	O	S	0	0
			2647	1663	451	521	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	E	347	Total	C	N	O	S	0	0
			2721	1713	484	508	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	F	372	Total	C	N	O	S	0	0
			2902	1823	501	562	16		

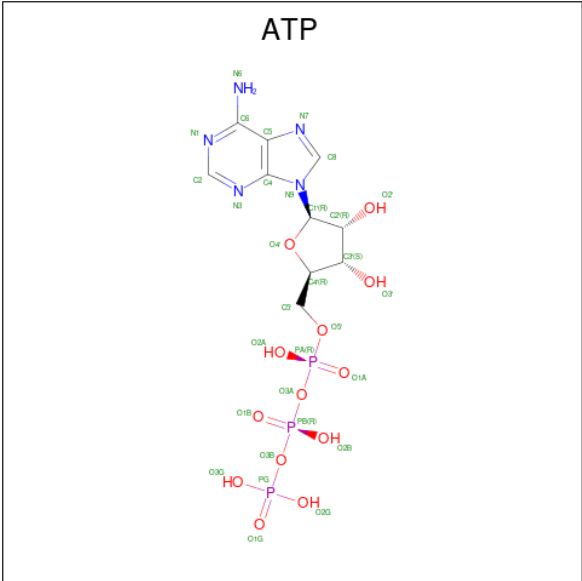
- Molecule 20 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).





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

- Molecule 21 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
21	D	1	Total	C	N	O	P	0
			31	10	5	13	3	

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

- Molecule 22 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 23 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

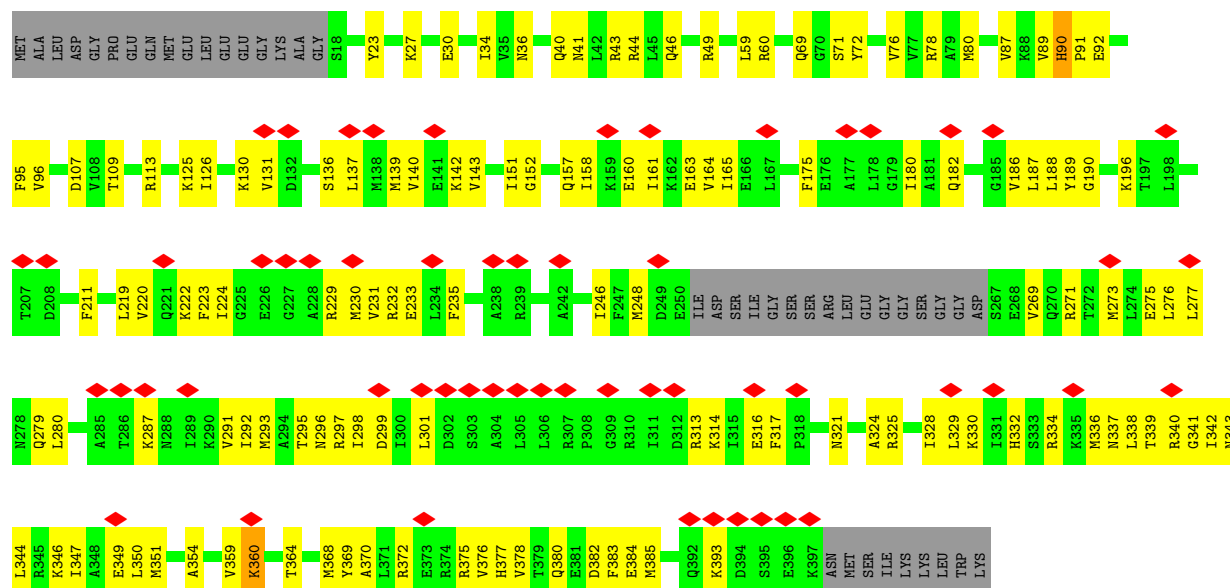
Mol	Chain	Residues	Atoms		AltConf
23	B	1	Total	Mg	0
			1	1	
23	E	1	Total	Mg	0
			1	1	
23	F	1	Total	Mg	0
			1	1	



GLY  
SER  
PRO  
SER  
GLY  
ALA  
SER  
GLY  
LEU  
GLY  
LEU  
ASP  
PHE  
GLU  
ASP  
SER  
VAL  
TRP  
LYS  
PRO  
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GLU  
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VAL  
VAL  
ALA

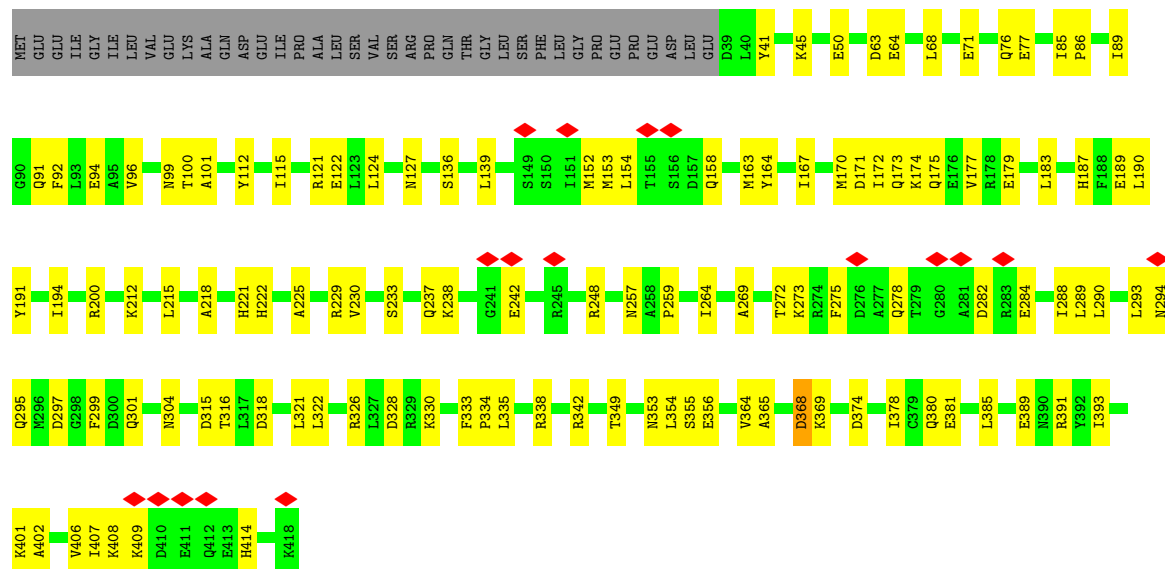
• Molecule 2: 26S proteasome regulatory subunit 8

Chain C: 



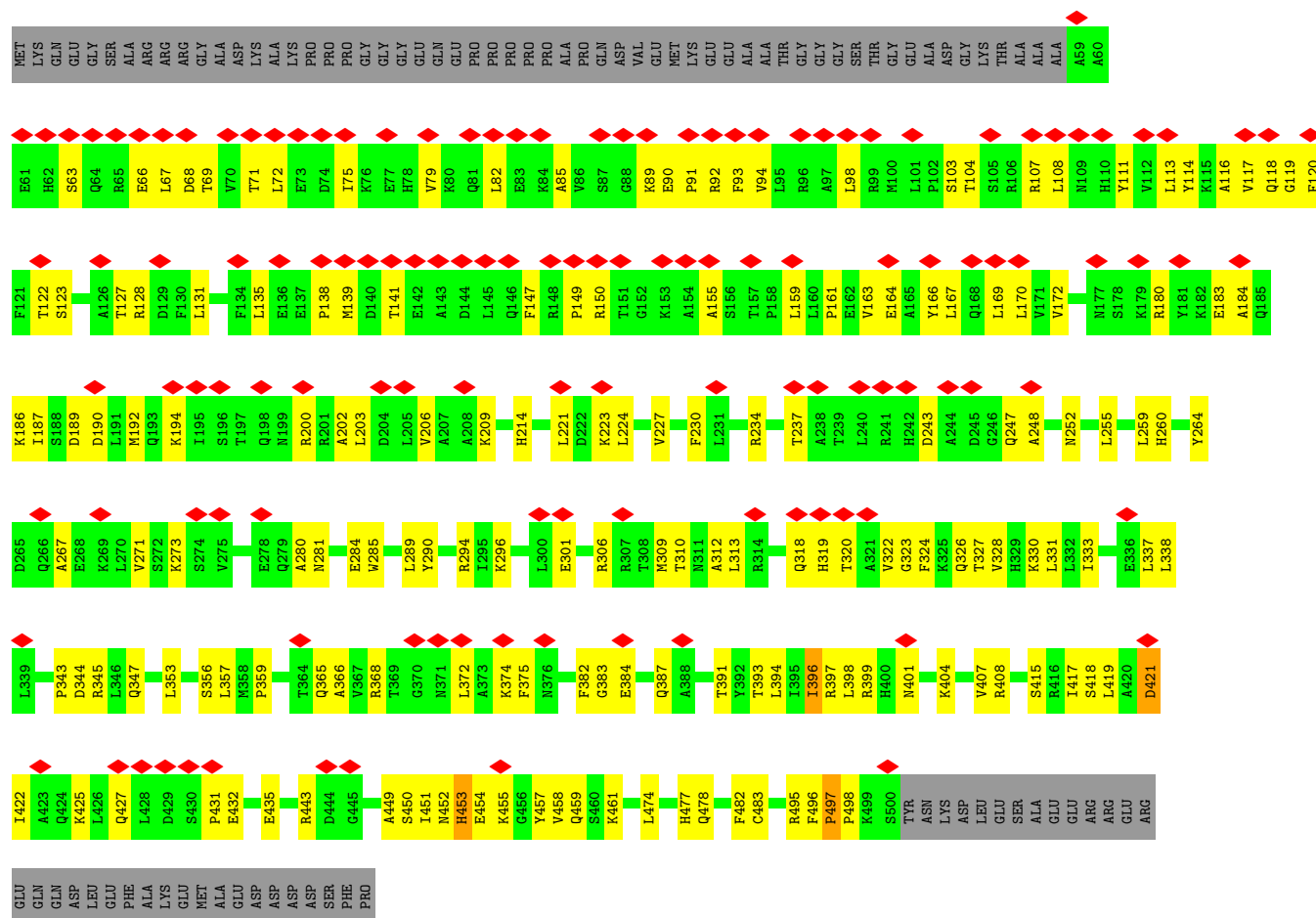
• Molecule 3: 26S proteasome regulatory subunit 6B

Chain D: 

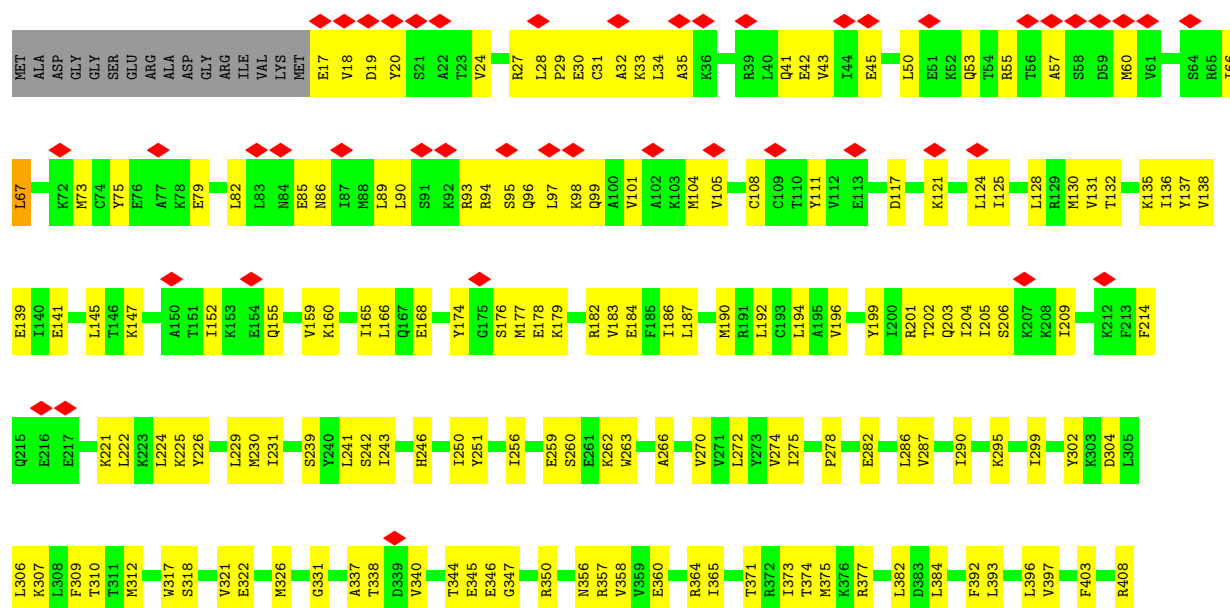


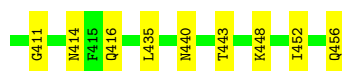
• Molecule 4: 26S proteasome non-ATPase regulatory subunit 3

Chain V: 

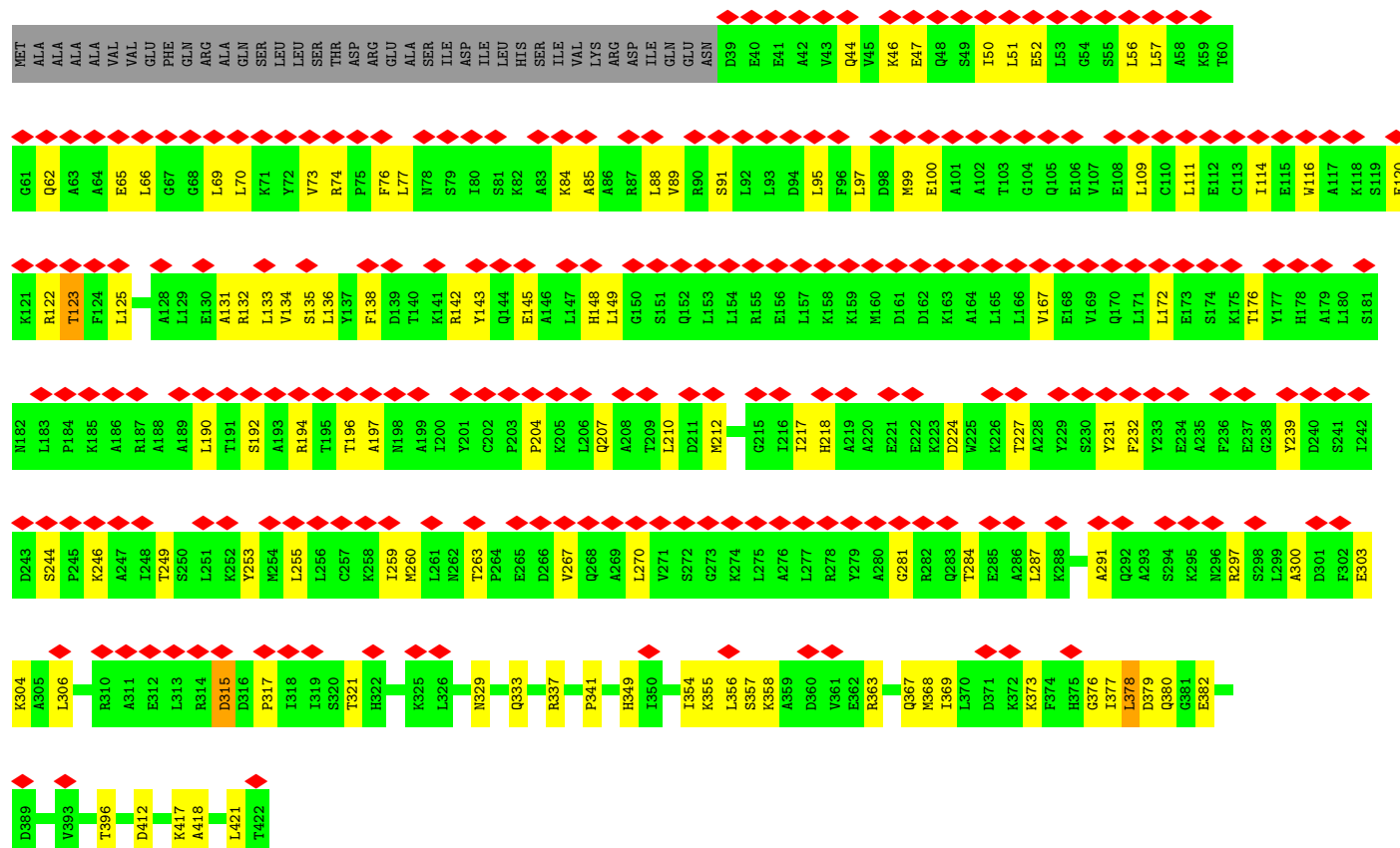


• Molecule 5: 26S proteasome non-ATPase regulatory subunit 12

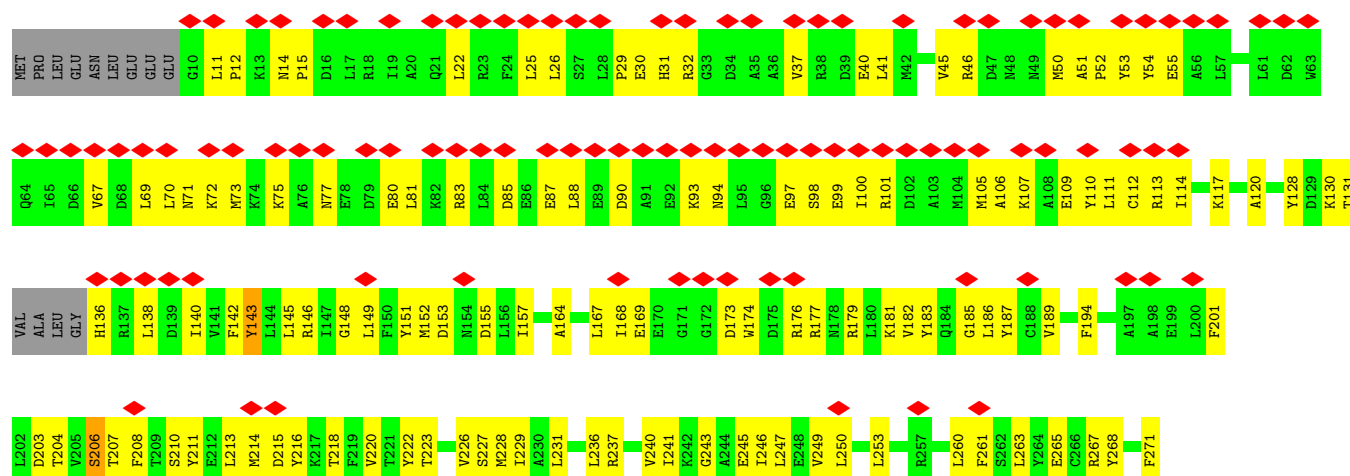


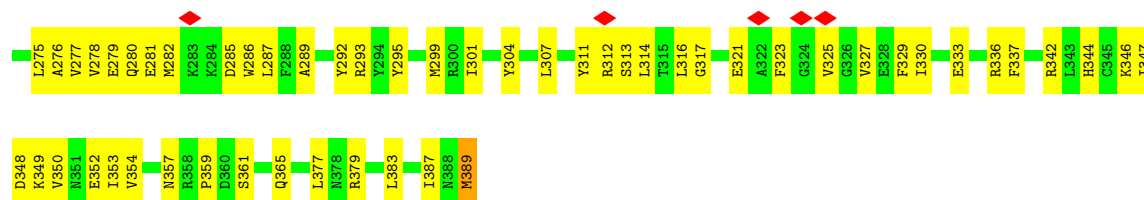


- Molecule 6: 26S proteasome non-ATPase regulatory subunit 11

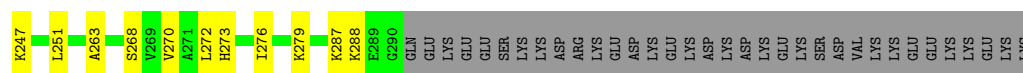
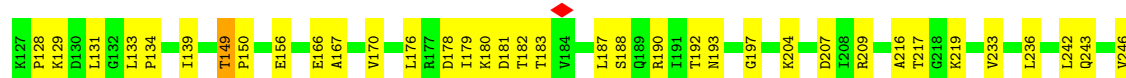


- Molecule 7: 26S proteasome non-ATPase regulatory subunit 6





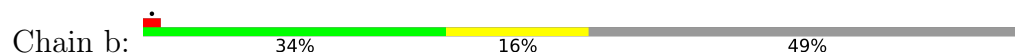
• Molecule 8: 26S proteasome non-ATPase regulatory subunit 7



• Molecule 9: 26S proteasome non-ATPase regulatory subunit 13



• Molecule 10: 26S proteasome non-ATPase regulatory subunit 4

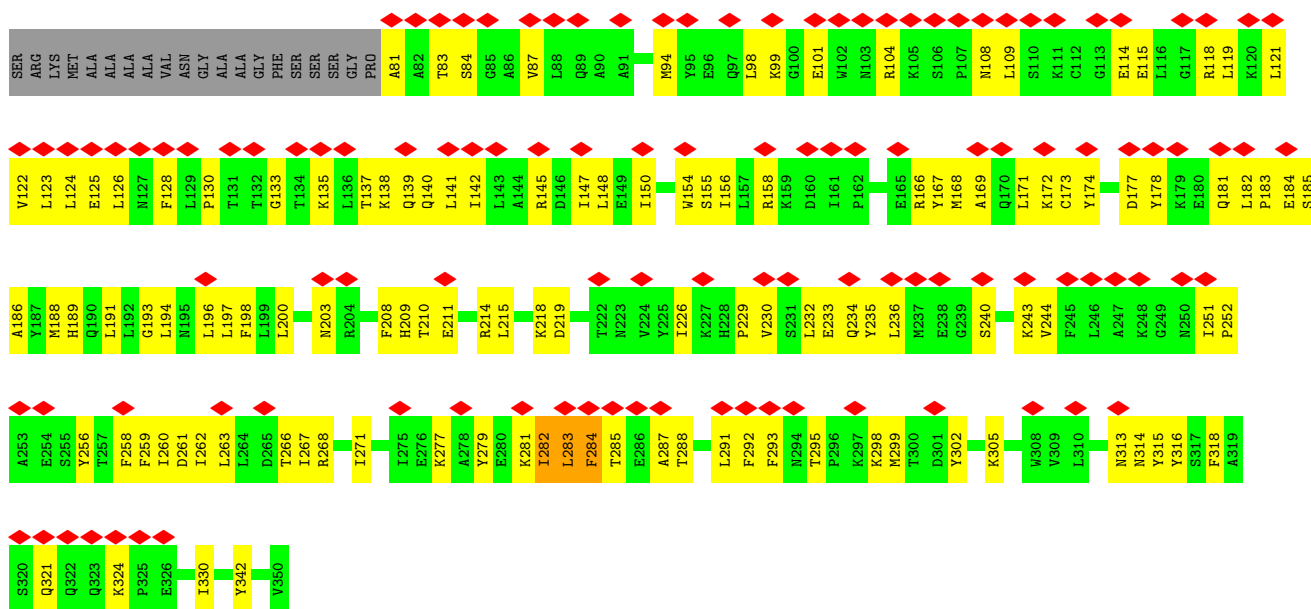


[illegible]

- Molecule 11: 26S proteasome non-ATPase regulatory subunit 8



MET	PHE	ILE	LYS	GLY	ARG	ALA	PRO	ARG	ALA	PRO	PRO	ARG	GLU	ARG	ARG	ARG	ALA	ALA	THR	ARG	GLY	GLY	LEU	ARG	GLN	VAL	VAL	ALA	PRO	PRO	PRO	ARG	ALA	ALA	LEU	GLY	SER	THR	SER	PRO	PRO	ARG	HIS	PHE	ARG	ARG	CYS	ARG	ARG	ARG	CYS	GLY	GLY	LEU	LEU	ALA	ALA
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- Molecule 12: 26S proteasome complex subunit SEM1



MET	SER	GLU	LYS	GLN	PRO	VAL	ASP	LEU	GLY	LEU	LEU	GLU	GLU	D16	E25	D26	W27	A28	G29	L30	D31	E32	D33	E34	D35	A36	H37	V38	V39	E40	D41	N42	W43	D44	D45	D46	D51	F52	S53	H63	GLY	TYR	LYS	MET	GLU	THR	SER
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- Molecule 13: Substrate

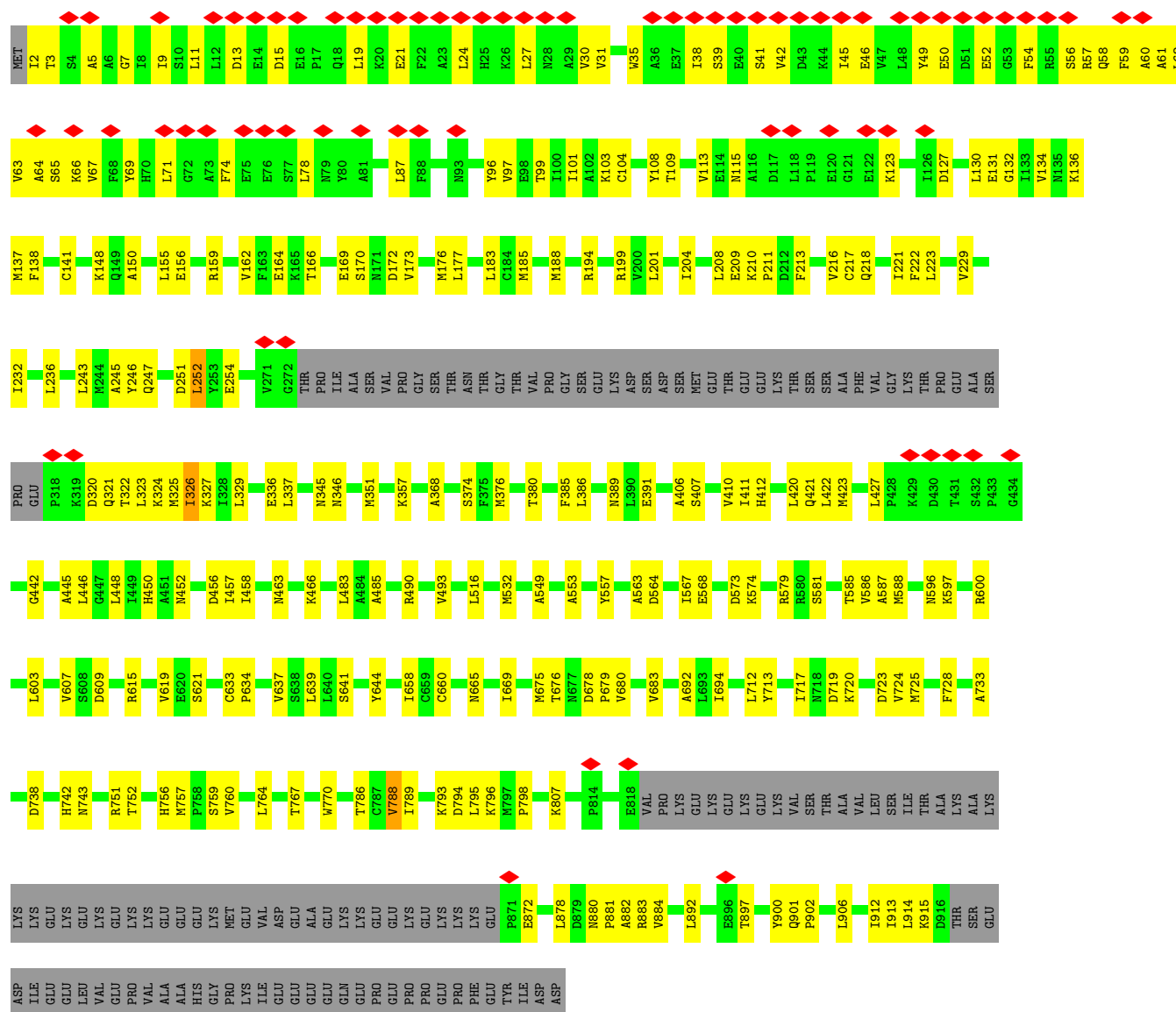


A diagram showing a 7x7 grid with columns labeled x1 through x7. Above column x3 is a red diamond, and above column x4 is another red diamond. The grid is currently empty.

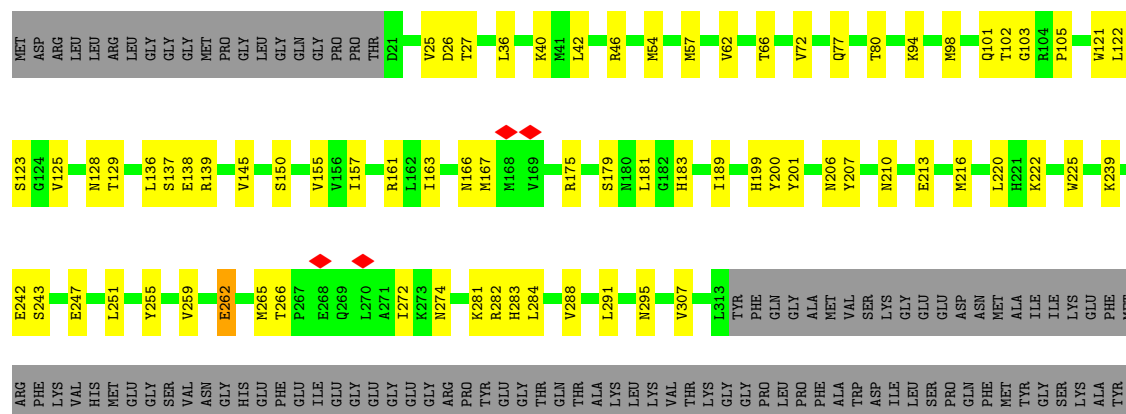
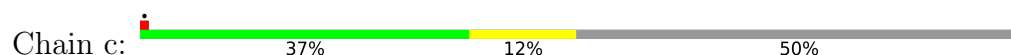
- Molecule 14: 26S proteasome non-ATPase regulatory subunit 1







● Molecule 15: Ubiquitin C-terminal hydrolase PSMD14, Uncharacterized protein



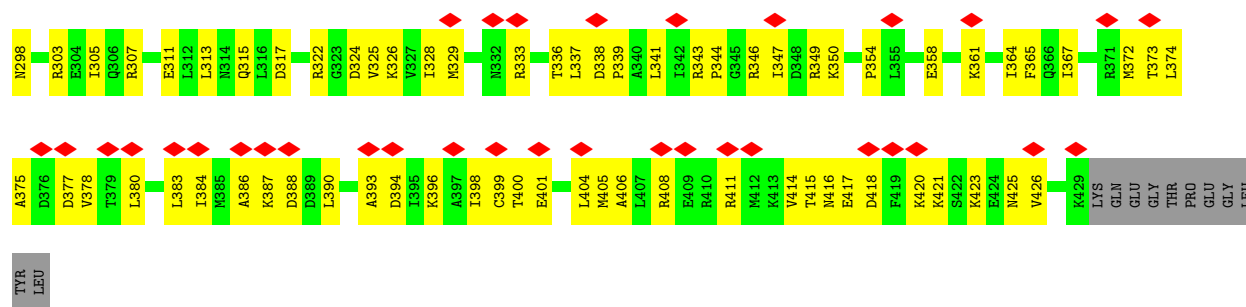
GLY	GLY	ASN	THR	GLY	VAL
GLY	SER	VAL	ASN	PRO	GLY
GLY	ASN	VAL	ASN	VAL	VAL
GLY	GLY	ASN	ILE	GLN	ASP
SER	SER	LYS	LYS	LYS	ILE
ALA	ALA	LEU	LEU	PRO	PRO
TRP	TRP	ASP	ASP	THR	THR
HIS	SER	ILE	THR	MET	ASP
PRO	PRO	THR	SER	TRP	LEU
GLN	GLN	HIS	HIS	GLU	LYS
PHE	PHE	ASN	ASN	ALA	LEU
GLU	GLU	GLU	GLU	SER	SER
LYS	LYS	ASP	ASP	ALA	PRO
		THR	THR	ARG	GLU
		ILE	ILE	MET	GLY
		VAL	VAL	THR	PHE
		GLU	GLU	PRO	LYS
		GLN	GLN	GLU	TRP
		TVR	TVR	ASP	GLU
		GLU	GLU	GLY	ARG
		ARG	ARG	ALA	VAL
		ALA	ALA	LEU	MET
		GLU	GLU	LYS	ASN
		GLY	GLY	GLY	PHE
		ARG	ARG	GLU	GLU
		HIS	HIS	ILE	ASP
		SER	SER	LYS	GLY
		THR	THR	GLN	GLY
		GLY	GLY	ARG	VAL
		GLY	GLY	LEU	VAL
		MET	MET	LYS	THR
		ASP	ASP	LEU	VAL
		GLU	GLU	LYS	THR
		LEU	LEU	ASP	GLN
		TVR	TVR	GLY	ASN
		LYS	LYS	GLY	ASP
		HIS	HIS	GLY	SER
		HIS	HIS	THR	LEU
		HIS	HIS	ASP	GLN
		HIS	HIS	ALA	ASP
		HIS	HIS	GLU	GLY
		HIS	HIS	VAL	GLY
		SER	SER	LYS	PHE
		ALA	ALA	THR	ILE
		TRP	TRP	THR	TYR
		SER	SER	THR	LYS
		HIS	HIS	LYS	VAL
		PRO	PRO	ALA	LYS
		GLN	GLN	LYS	LEU
		PHE	PHE	LYS	ARG
		GLU	GLU	PRO	GLY
		LYS	LYS	VAL	THR
		GLY	GLY	GLN	ASN
		GLY	GLY	LEU	PHE
		GLY	GLY	PRO	PRO
		SER	SER	GLY	ASP
		GLY	GLY	ALA	THR

- Molecule 16: 26S proteasome regulatory subunit 7

[illegible]

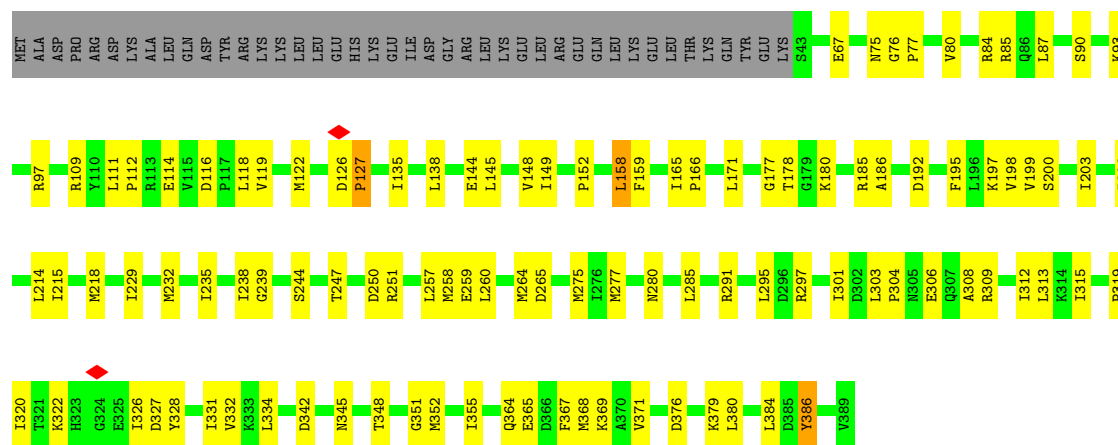
- Molecule 17: 26S proteasome regulatory subunit 4

[illegible]



• Molecule 18: 26S proteasome regulatory subunit 10B

Chain E: 62% 26% 11%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	22385	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.571	Depositor
Minimum map value	-0.306	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.081	Depositor
Map size ( $\text{\AA}$ )	340.0, 340.0, 340.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.85, 0.85, 0.85	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	f	0.19	0/640	0.49	0/863
2	C	0.23	0/2908	0.51	0/3912
3	D	0.25	0/3089	0.50	0/4168
4	V	0.20	0/3662	0.46	0/4946
5	W	0.26	0/3630	0.55	0/4884
6	X	0.16	0/3084	0.41	0/4157
7	Y	0.24	0/3160	0.54	0/4254
8	Z	0.21	0/2324	0.44	0/3150
9	a	0.20	0/3053	0.50	0/4133
10	b	0.19	0/1478	0.47	0/2001
11	d	0.20	0/2239	0.51	0/3025
12	e	0.22	0/420	0.52	0/572
14	U	0.21	0/6486	0.43	0/8777
15	c	0.20	0/2347	0.39	0/3174
16	A	0.19	0/2914	0.48	0/3937
17	B	0.22	0/2684	0.53	0/3623
18	E	0.20	0/2765	0.46	0/3730
19	F	0.19	0/2942	0.43	0/3967
All	All	0.21	0/49825	0.48	0/67273

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	f	632	0	663	16	0
2	C	2870	0	2976	116	0
3	D	3039	0	3076	93	0
4	V	3592	0	3647	158	0
5	W	3582	0	3693	133	0
6	X	3040	0	3134	84	0
7	Y	3103	0	3104	163	0
8	Z	2281	0	2312	66	0
9	a	2995	0	3012	90	0
10	b	1458	0	1505	49	0
11	d	2193	0	2221	122	0
12	e	409	0	316	12	0
13	v	35	0	10	0	0
14	U	6371	0	6409	178	0
15	c	2304	0	2315	60	0
16	A	2863	0	2895	92	0
17	B	2647	0	2684	106	0
18	E	2721	0	2770	87	0
19	F	2902	0	2956	100	0
20	C	27	0	12	1	0
20	F	27	0	12	1	0
21	A	31	0	12	2	0
21	B	31	0	12	3	0
21	D	31	0	12	0	0
21	E	31	0	12	3	0
22	c	1	0	0	0	0
23	B	1	0	0	0	0
23	E	1	0	0	0	0
23	F	1	0	0	0	0
All	All	49219	0	49770	1574	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 16.

The worst 5 of 1574 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)
4:V:189:ASP:HA	4:V:192:MET:HE2	1.45	0.98
7:Y:14:ASN:HB2	7:Y:113:ARG:HH21	1.39	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:163:GLU:HB2	2:C:313:ARG:HH12	1.42	0.84
4:V:443:ARG:HA	11:d:277:LYS:HD2	1.58	0.84
18:E:322:LYS:HD2	18:E:326:ILE:HD11	1.60	0.83

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	f	82/856 (10%)	81 (99%)	1 (1%)	0	100	100
2	C	360/406 (89%)	325 (90%)	34 (9%)	1 (0%)	36	64
3	D	378/418 (90%)	351 (93%)	26 (7%)	1 (0%)	36	64
4	V	440/534 (82%)	418 (95%)	21 (5%)	1 (0%)	43	70
5	W	438/456 (96%)	411 (94%)	27 (6%)	0	100	100
6	X	382/422 (90%)	370 (97%)	11 (3%)	1 (0%)	36	64
7	Y	372/389 (96%)	349 (94%)	22 (6%)	1 (0%)	36	64
8	Z	284/324 (88%)	274 (96%)	9 (3%)	1 (0%)	30	58
9	a	371/376 (99%)	336 (91%)	31 (8%)	4 (1%)	11	39
10	b	189/377 (50%)	169 (89%)	18 (10%)	2 (1%)	11	39
11	d	268/350 (77%)	247 (92%)	18 (7%)	3 (1%)	11	39
12	e	46/70 (66%)	34 (74%)	10 (22%)	2 (4%)	2	16
14	U	812/953 (85%)	780 (96%)	32 (4%)	0	100	100
15	c	291/590 (49%)	278 (96%)	12 (4%)	1 (0%)	36	64
16	A	364/433 (84%)	324 (89%)	39 (11%)	1 (0%)	36	64
17	B	338/440 (77%)	303 (90%)	32 (10%)	3 (1%)	14	43
18	E	345/389 (89%)	326 (94%)	17 (5%)	2 (1%)	21	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	F	370/439 (84%)	337 (91%)	31 (8%)	2 (0%)	24	55
All	All	6130/8222 (75%)	5713 (93%)	391 (6%)	26 (0%)	31	58

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	Y	98	SER
8	Z	149	THR
11	d	283	LEU
15	c	262	GLU
16	A	82	ALA

### 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	f	70/690 (10%)	69 (99%)	1 (1%)	59	68
2	C	315/352 (90%)	313 (99%)	2 (1%)	78	78
3	D	333/366 (91%)	331 (99%)	2 (1%)	78	78
4	V	388/460 (84%)	385 (99%)	3 (1%)	73	74
5	W	404/416 (97%)	401 (99%)	3 (1%)	76	76
6	X	330/362 (91%)	328 (99%)	2 (1%)	78	78
7	Y	333/344 (97%)	330 (99%)	3 (1%)	70	73
8	Z	257/295 (87%)	257 (100%)	0	100	100
9	a	333/336 (99%)	332 (100%)	1 (0%)	86	81
10	b	167/312 (54%)	166 (99%)	1 (1%)	78	78
11	d	237/294 (81%)	236 (100%)	1 (0%)	84	79
12	e	43/63 (68%)	43 (100%)	0	100	100
14	U	695/816 (85%)	690 (99%)	5 (1%)	76	76
15	c	257/500 (51%)	257 (100%)	0	100	100
16	A	310/372 (83%)	307 (99%)	3 (1%)	68	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	B	296/385 (77%)	294 (99%)	2 (1%)	76	76
18	E	298/341 (87%)	296 (99%)	2 (1%)	76	76
19	F	316/379 (83%)	314 (99%)	2 (1%)	78	78
All	All	5382/7083 (76%)	5349 (99%)	33 (1%)	76	78

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	B	144	LEU
18	E	127	PRO
19	F	416	THR
6	X	378	LEU
6	X	315	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 100 such sidechains are listed below:

Mol	Chain	Res	Type
9	a	194	GLN
14	U	58	GLN
19	F	367	GLN
9	a	244	ASN
10	b	105	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 10 ligands modelled in this entry, 4 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
21	ATP	E	401	23	32,33,33	0.40	0	48,52,52	0.28	0
21	ATP	A	501	-	32,33,33	0.29	0	48,52,52	0.35	0
20	ADP	C	501	-	28,29,29	1.41	4 (14%)	43,45,45	1.82	7 (16%)
20	ADP	F	501	23	28,29,29	1.38	4 (14%)	43,45,45	1.87	9 (20%)
21	ATP	B	501	23	32,33,33	0.30	0	48,52,52	0.28	0
21	ATP	D	501	-	32,33,33	0.42	0	48,52,52	0.29	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
21	ATP	E	401	23	-	3/22/38/38	0/3/3/3
21	ATP	A	501	-	-	7/22/38/38	0/3/3/3
20	ADP	C	501	-	-	2/16/32/32	0/3/3/3
20	ADP	F	501	23	-	3/16/32/32	0/3/3/3
21	ATP	B	501	23	-	3/22/38/38	0/3/3/3
21	ATP	D	501	-	-	3/22/38/38	0/3/3/3

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	C	501	ADP	C5-C4	4.65	1.47	1.39
20	F	501	ADP	C5-C4	4.55	1.47	1.39
20	C	501	ADP	C5-C6	2.59	1.48	1.41
20	F	501	ADP	C5-C6	2.55	1.48	1.41
20	C	501	ADP	C5-N7	-2.42	1.34	1.39

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	C	501	ADP	C5-C4-N3	-6.13	118.28	126.72
20	F	501	ADP	C5-C4-N3	-5.94	118.54	126.72
20	C	501	ADP	N3-C4-N9	5.05	135.75	127.17
20	F	501	ADP	N3-C4-N9	4.86	135.44	127.17
20	F	501	ADP	C2-N3-C4	3.83	121.19	111.83

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

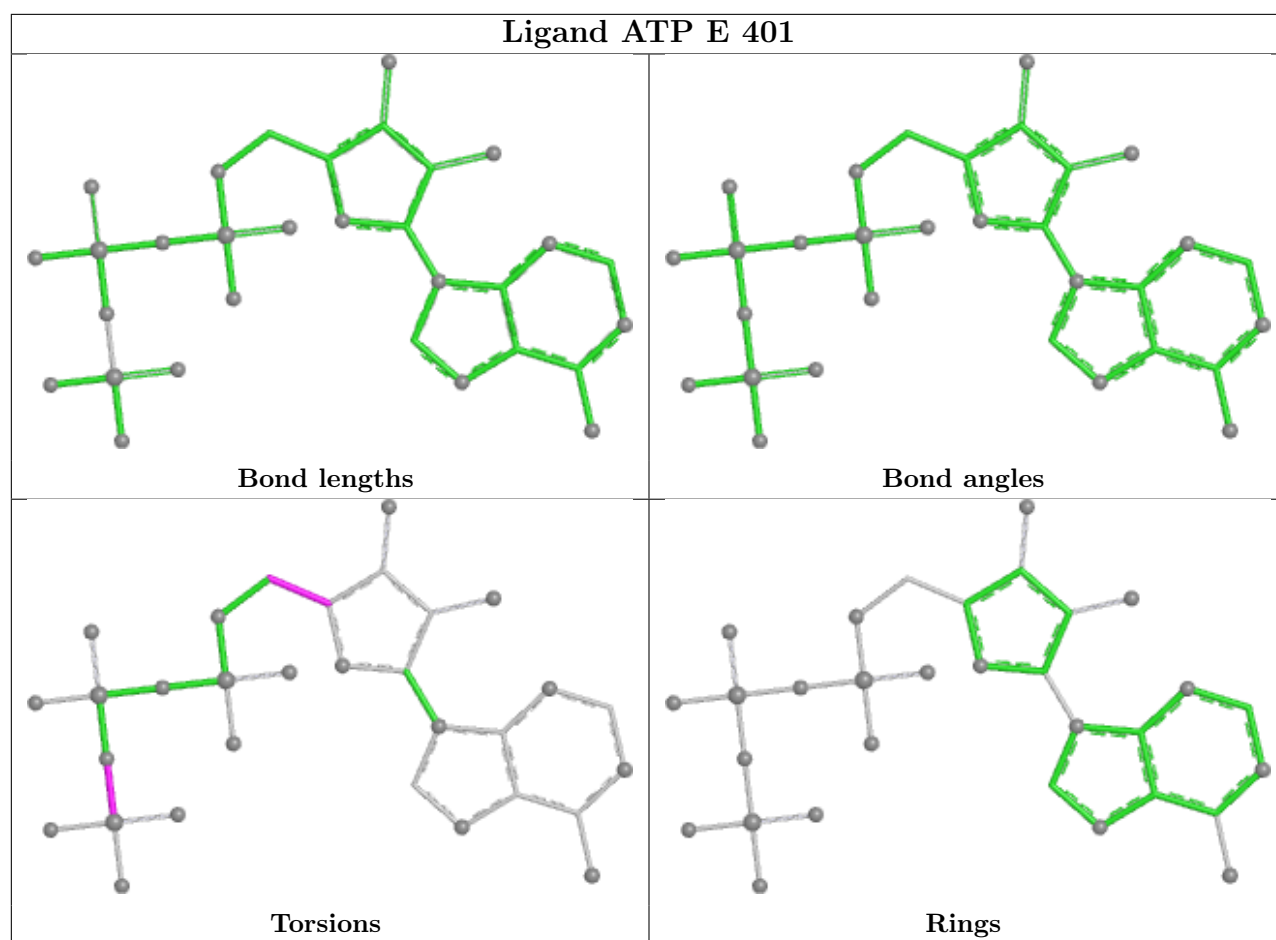
Mol	Chain	Res	Type	Atoms
20	F	501	ADP	C5'-O5'-PA-O1A
20	F	501	ADP	C5'-O5'-PA-O2A
20	F	501	ADP	C5'-O5'-PA-O3A
21	D	501	ATP	C5'-O5'-PA-O1A
21	A	501	ATP	C5'-O5'-PA-O2A

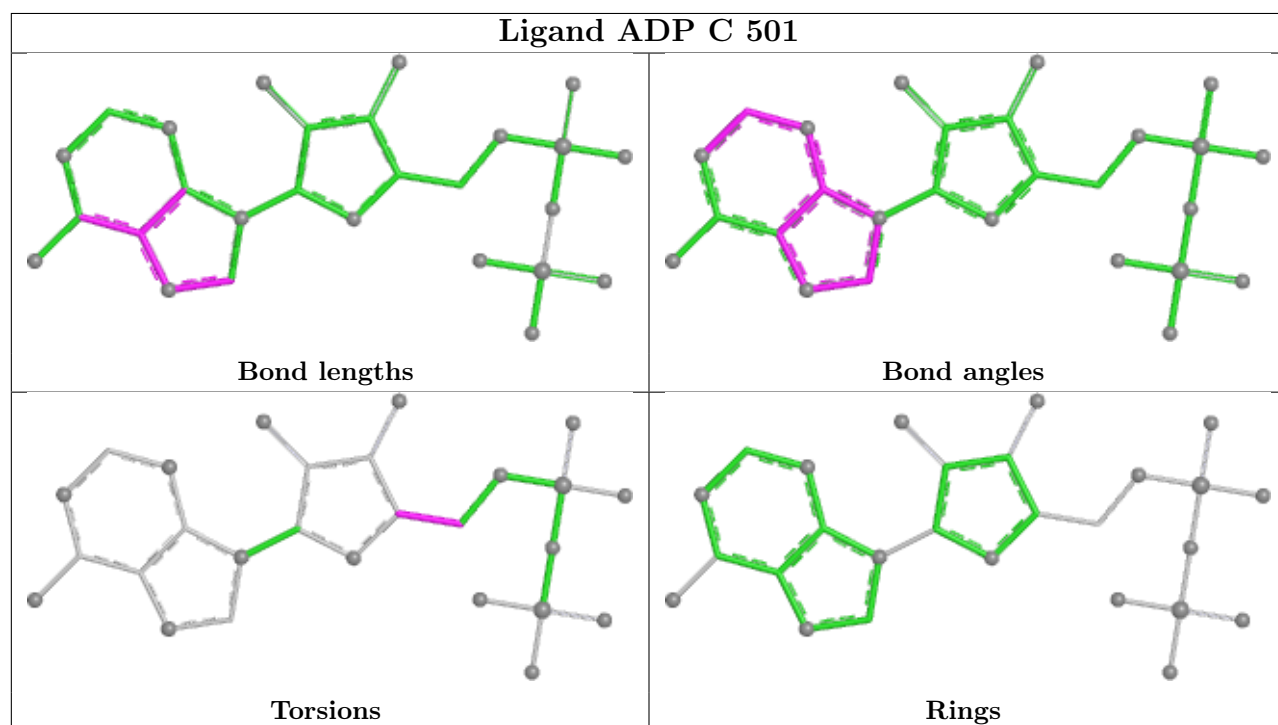
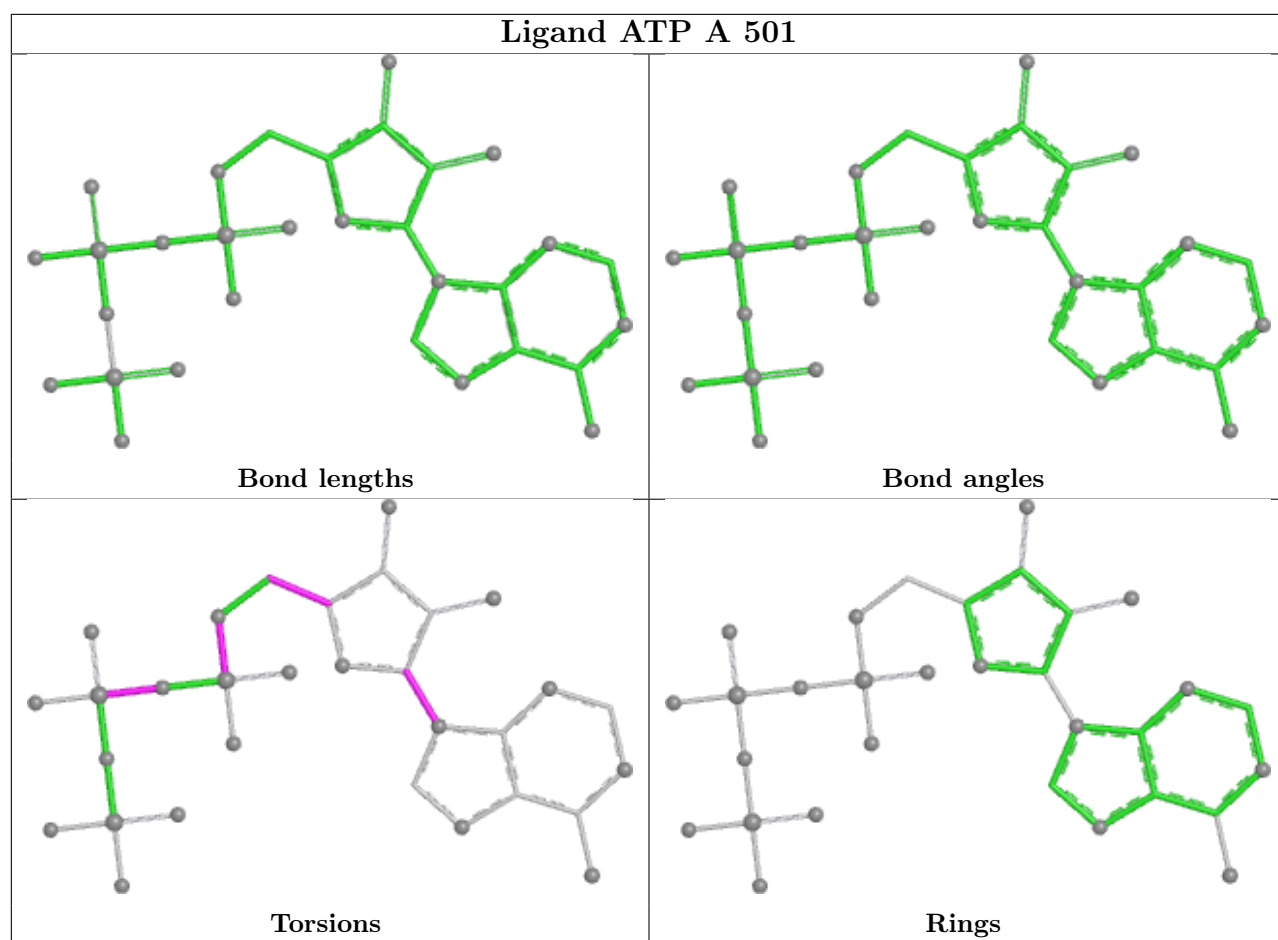
There are no ring outliers.

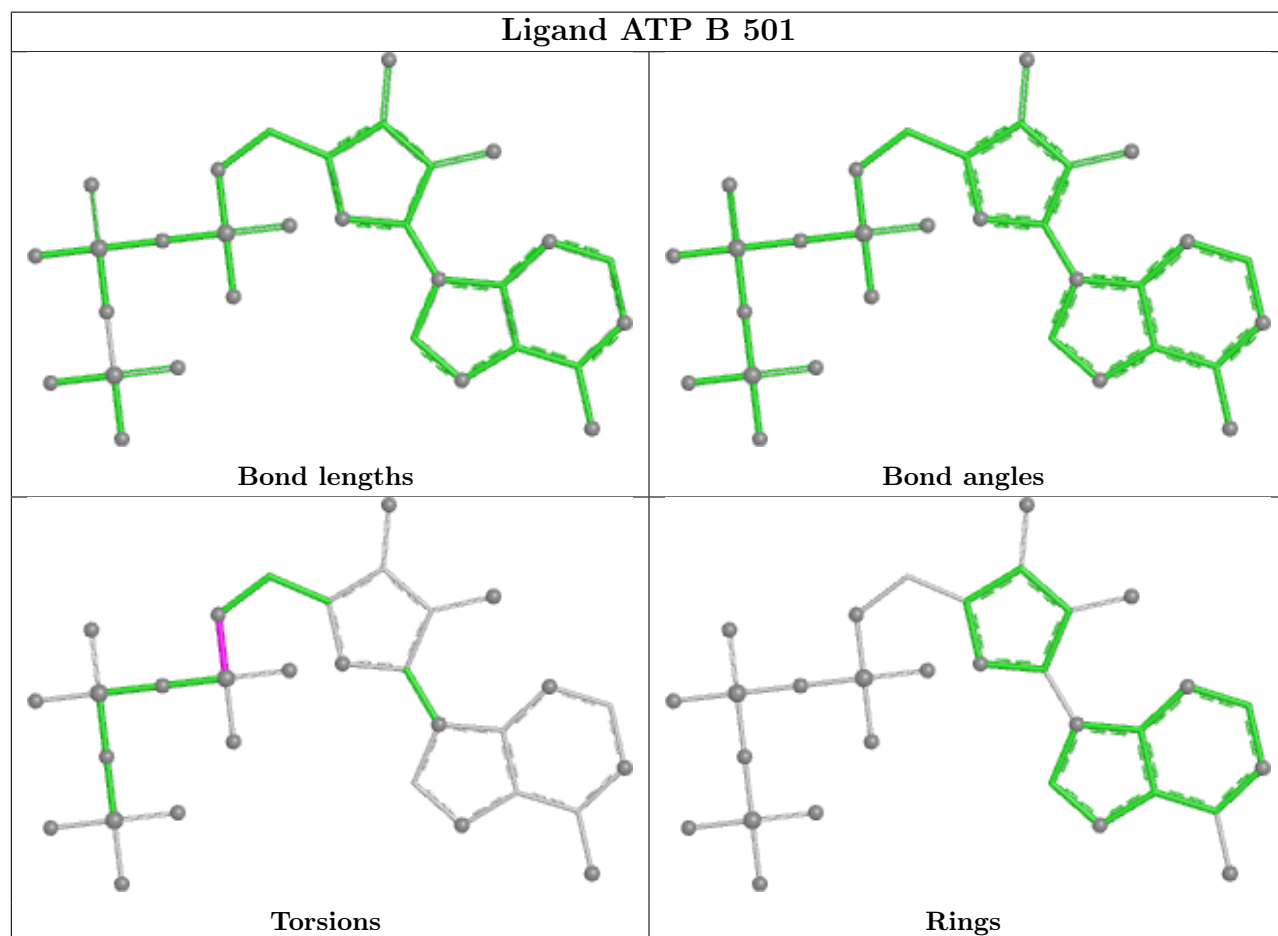
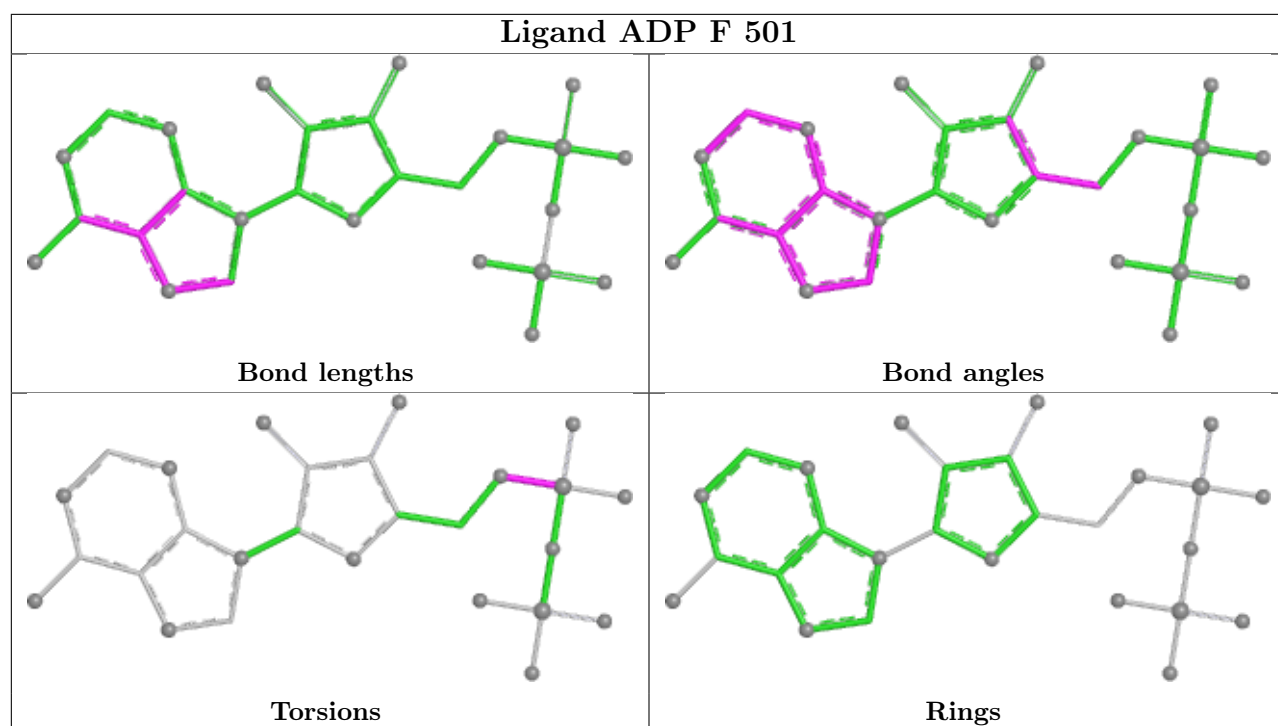
5 monomers are involved in 10 short contacts:

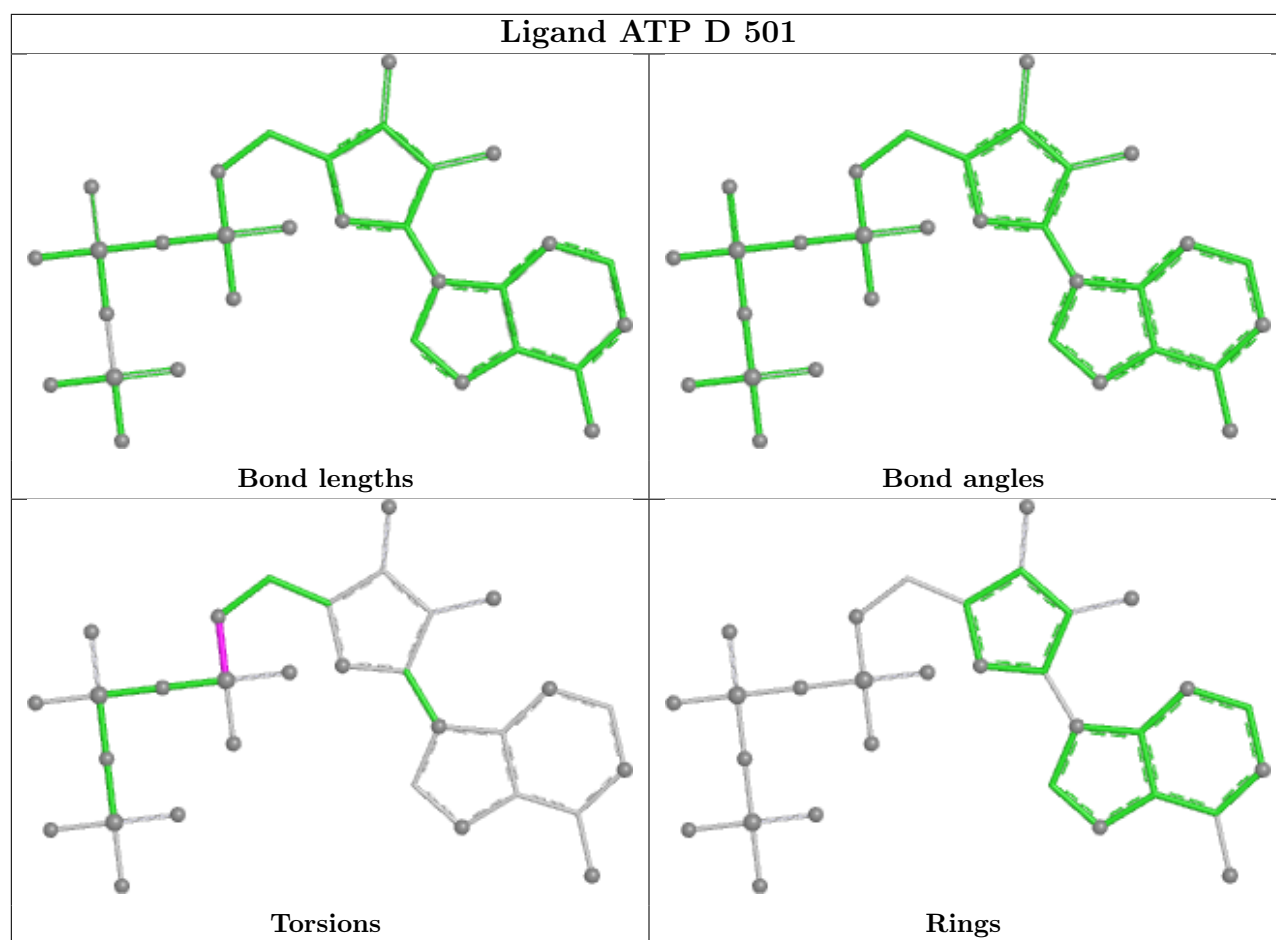
Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	E	401	ATP	3	0
21	A	501	ATP	2	0
20	C	501	ADP	1	0
20	F	501	ADP	1	0
21	B	501	ATP	3	0

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.









## 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.

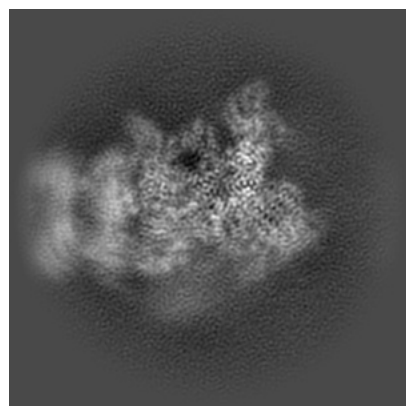
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-65595. These allow visual inspection of the internal detail of the map and identification of artifacts.

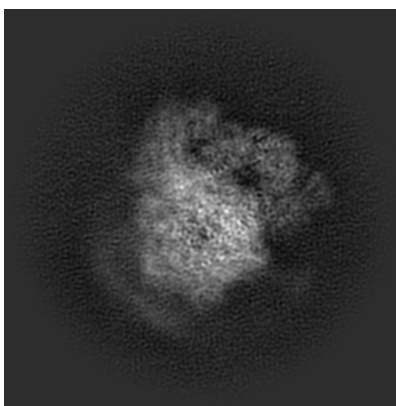
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

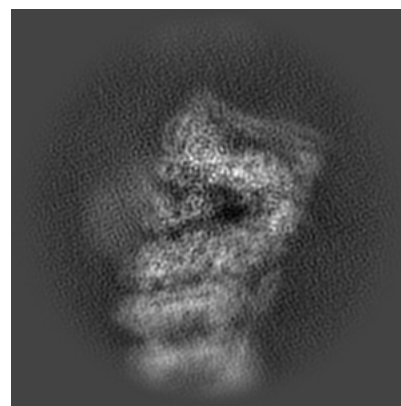
#### 6.1.1 Primary map



X

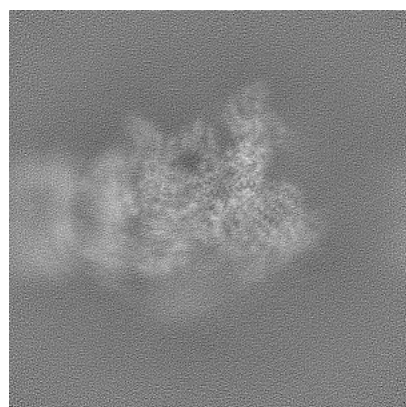


Y

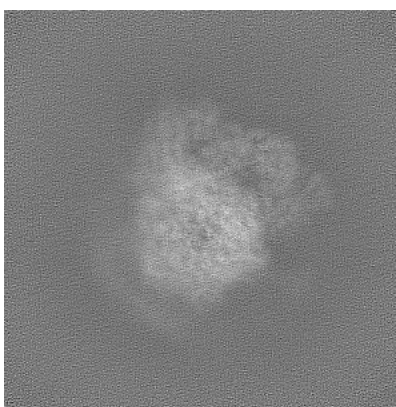


Z

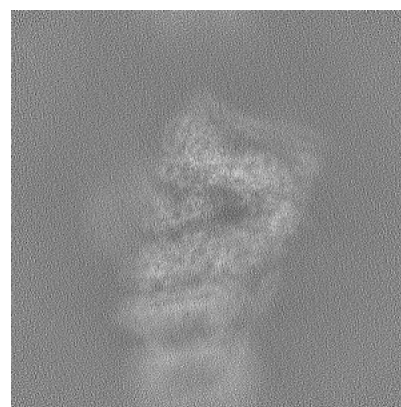
#### 6.1.2 Raw map



X



Y



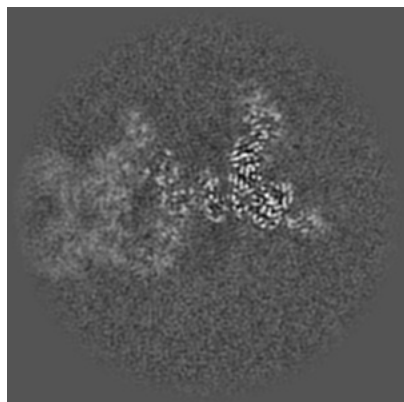
Z

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

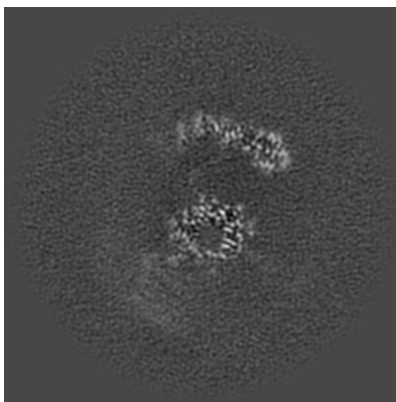


## 6.2 Central slices [i](#)

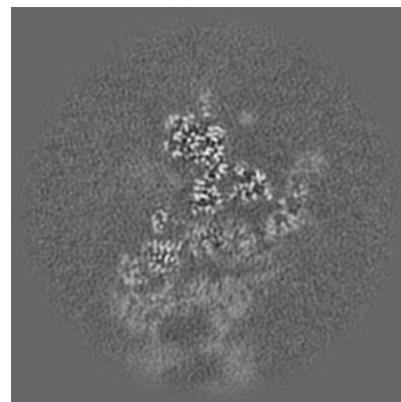
### 6.2.1 Primary map



X Index: 200

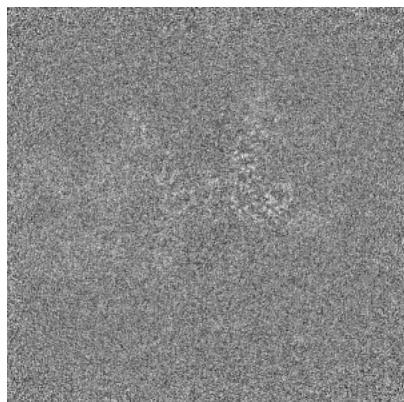


Y Index: 200

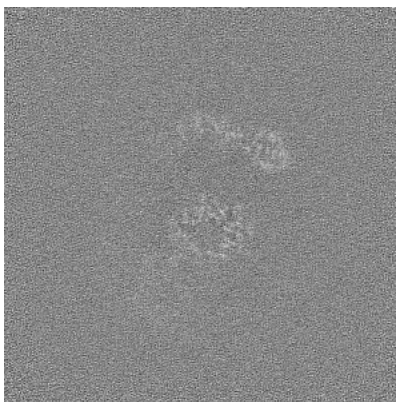


Z Index: 200

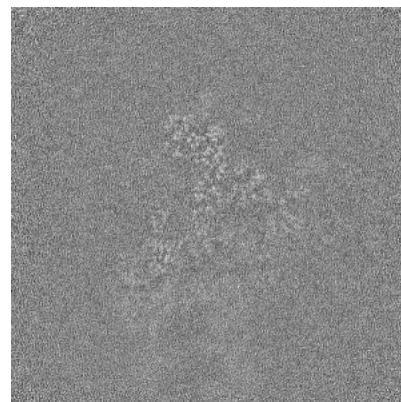
### 6.2.2 Raw map



X Index: 200



Y Index: 200

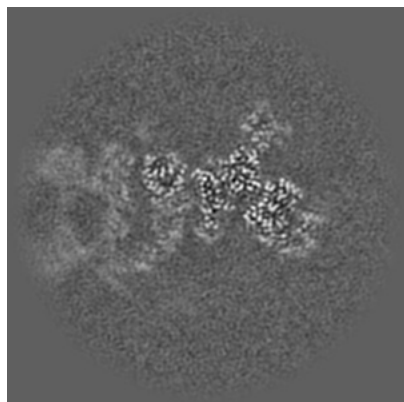


Z Index: 200

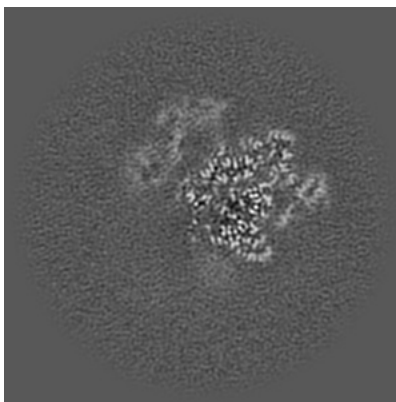
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

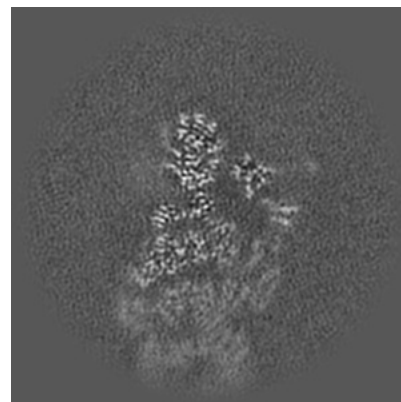
### 6.3.1 Primary map



X Index: 185

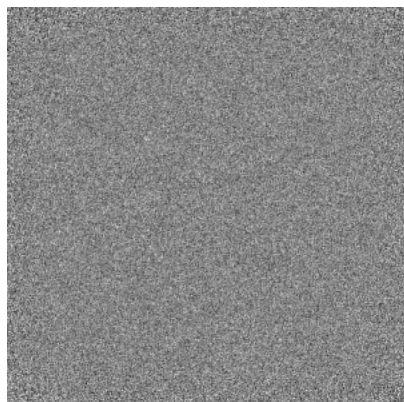


Y Index: 237

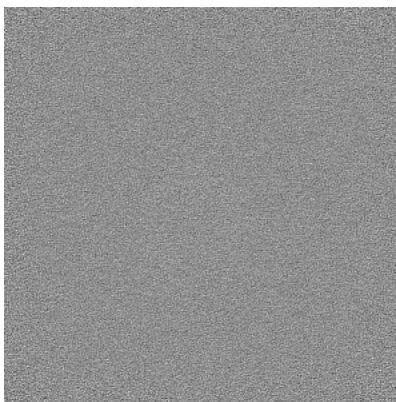


Z Index: 217

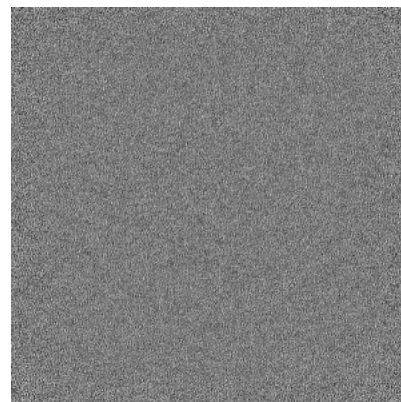
### 6.3.2 Raw map



X Index: 0



Y Index: 0

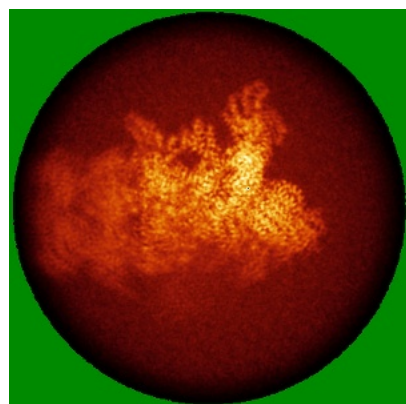


Z Index: 0

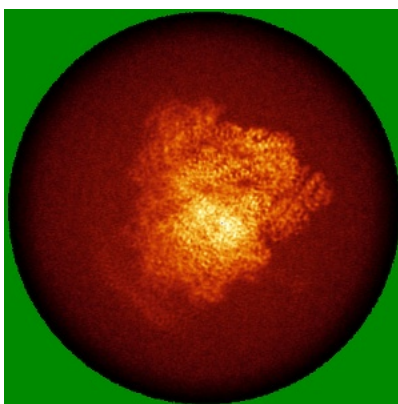
The images above show the largest variance slices of the map in three orthogonal directions.

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

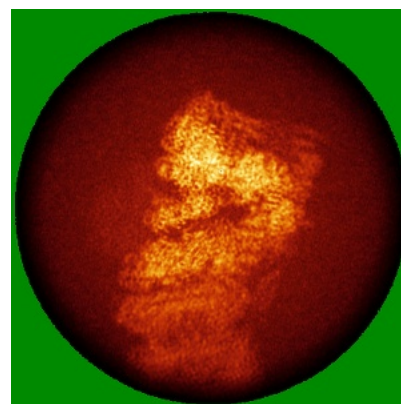
### 6.4.1 Primary map



X

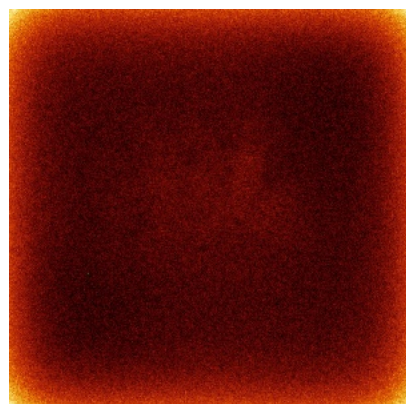


Y

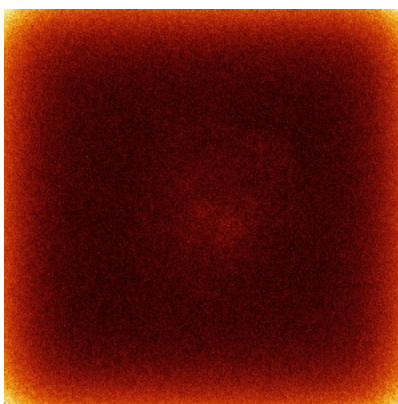


Z

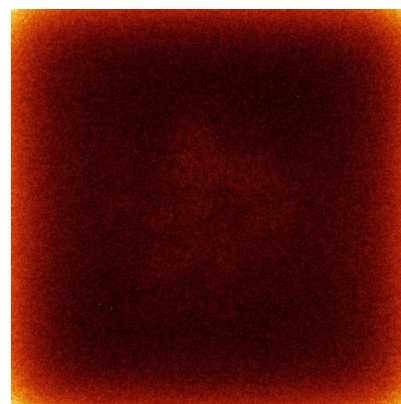
### 6.4.2 Raw map



X



Y



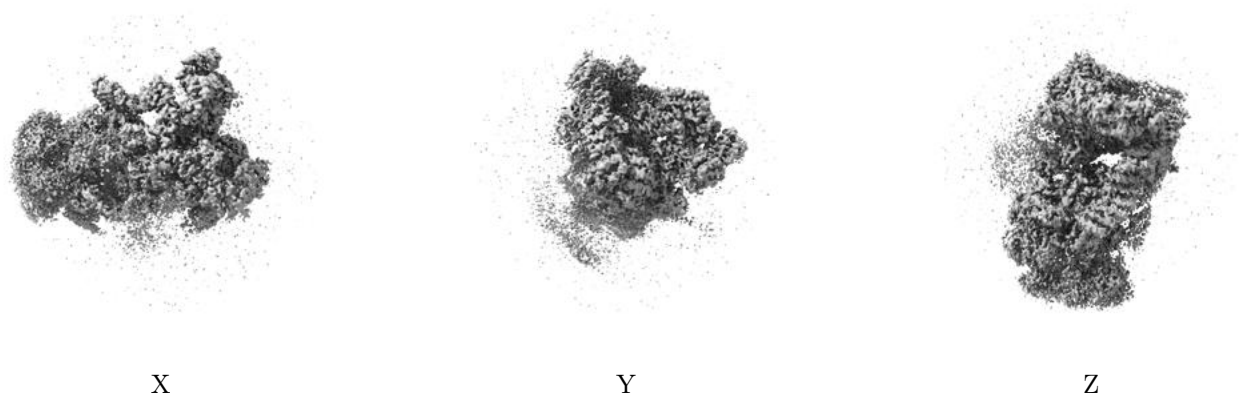
Z

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



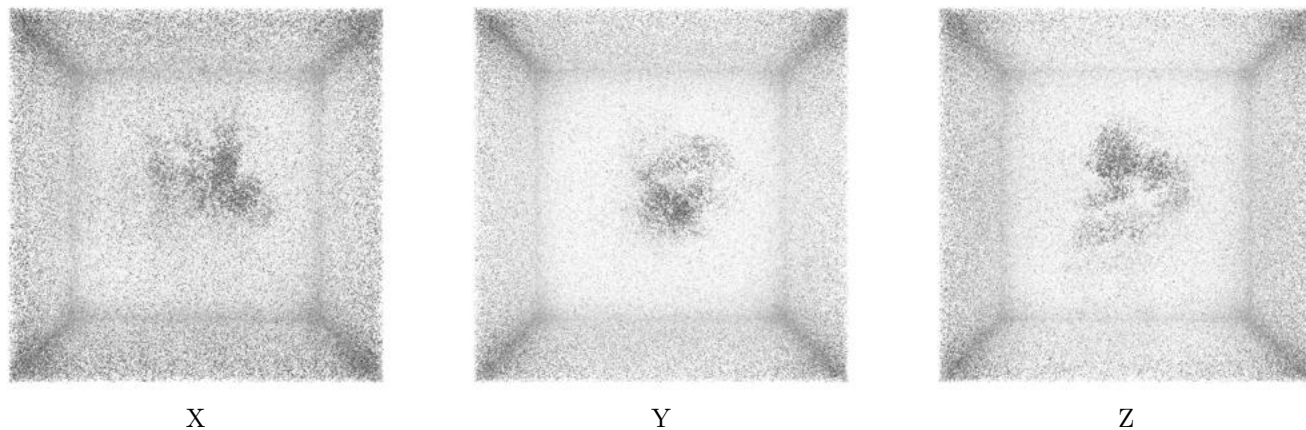
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.081. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

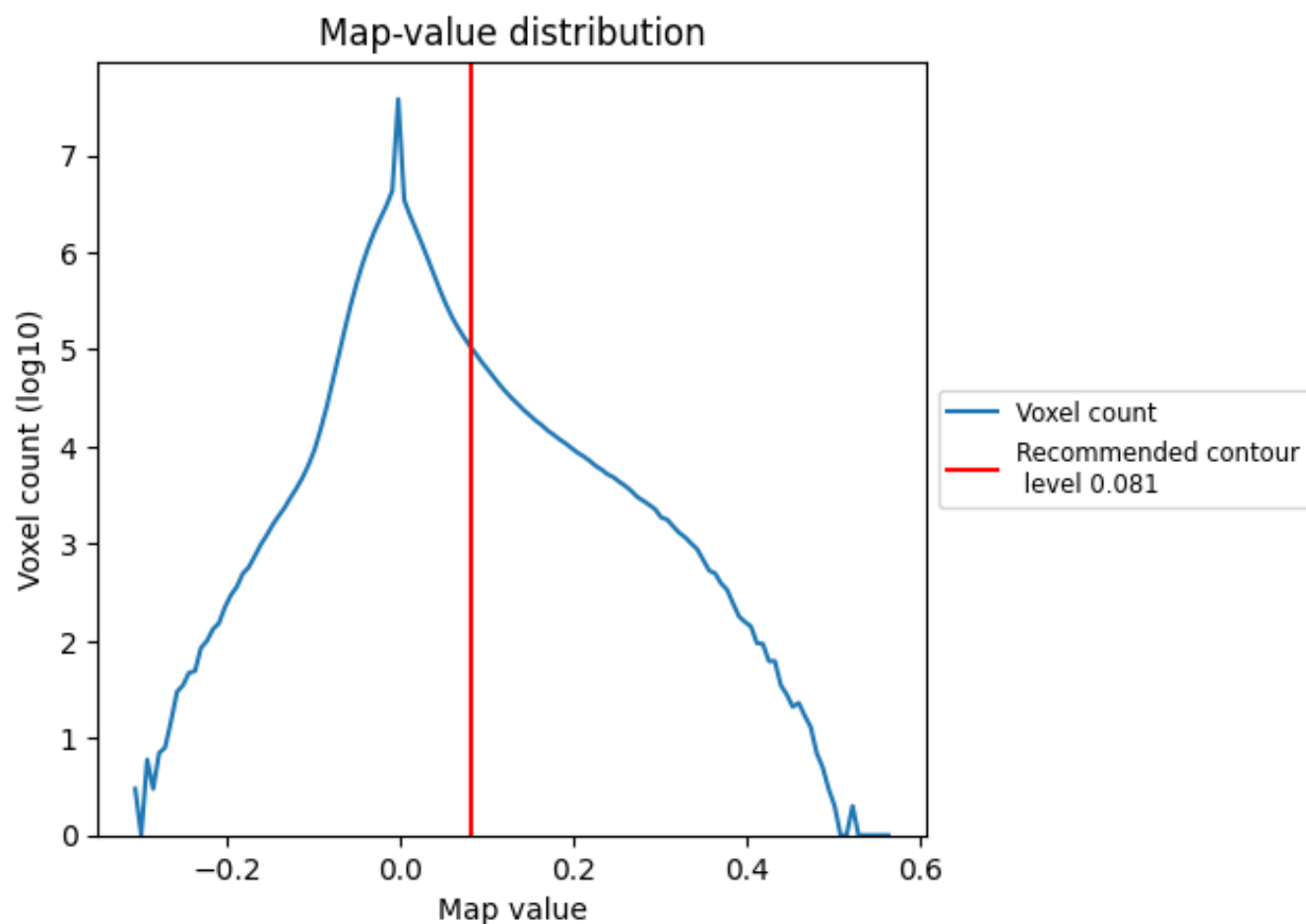
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

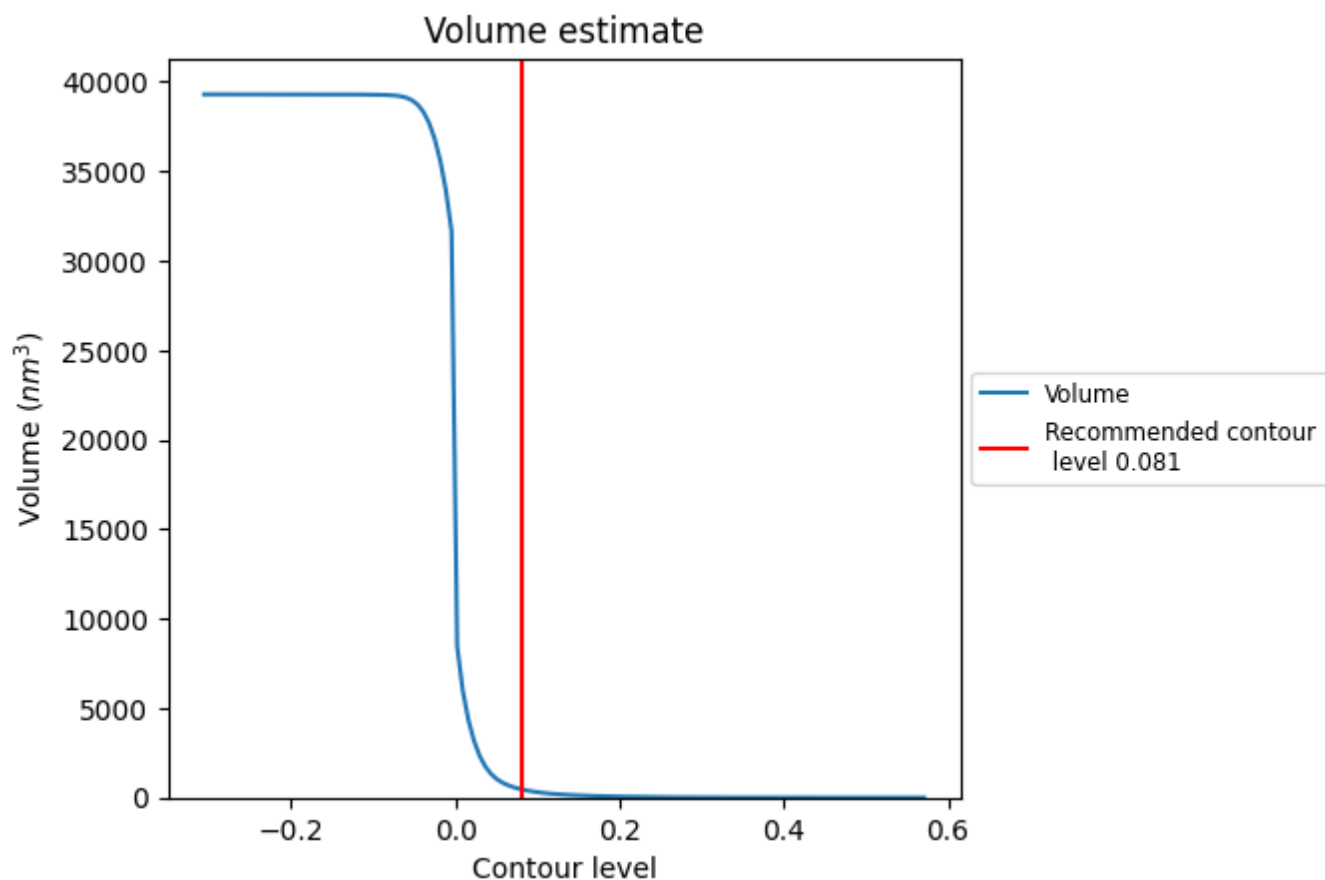
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

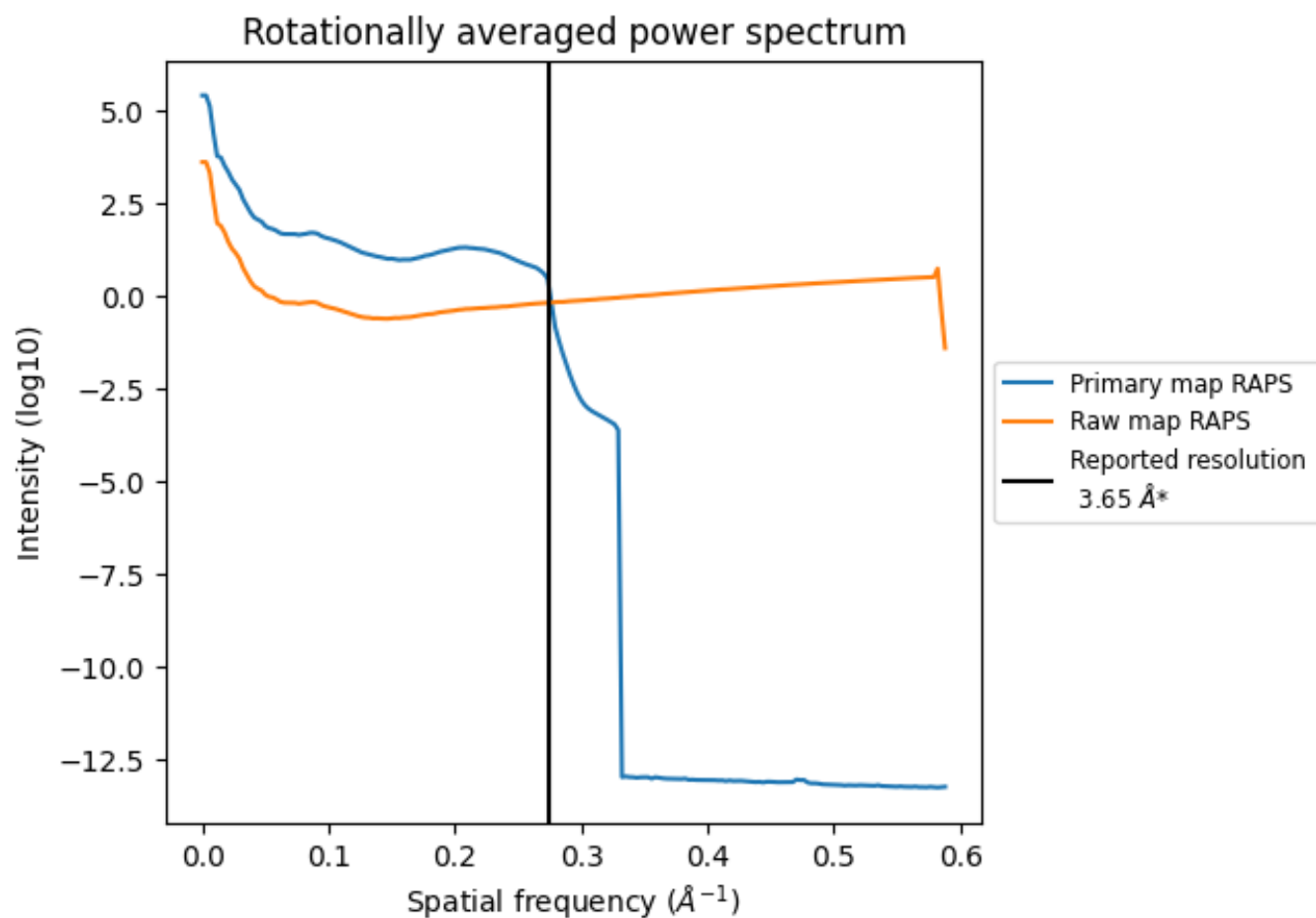
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 455 nm<sup>3</sup>; this corresponds to an approximate mass of 411 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 ⓘ

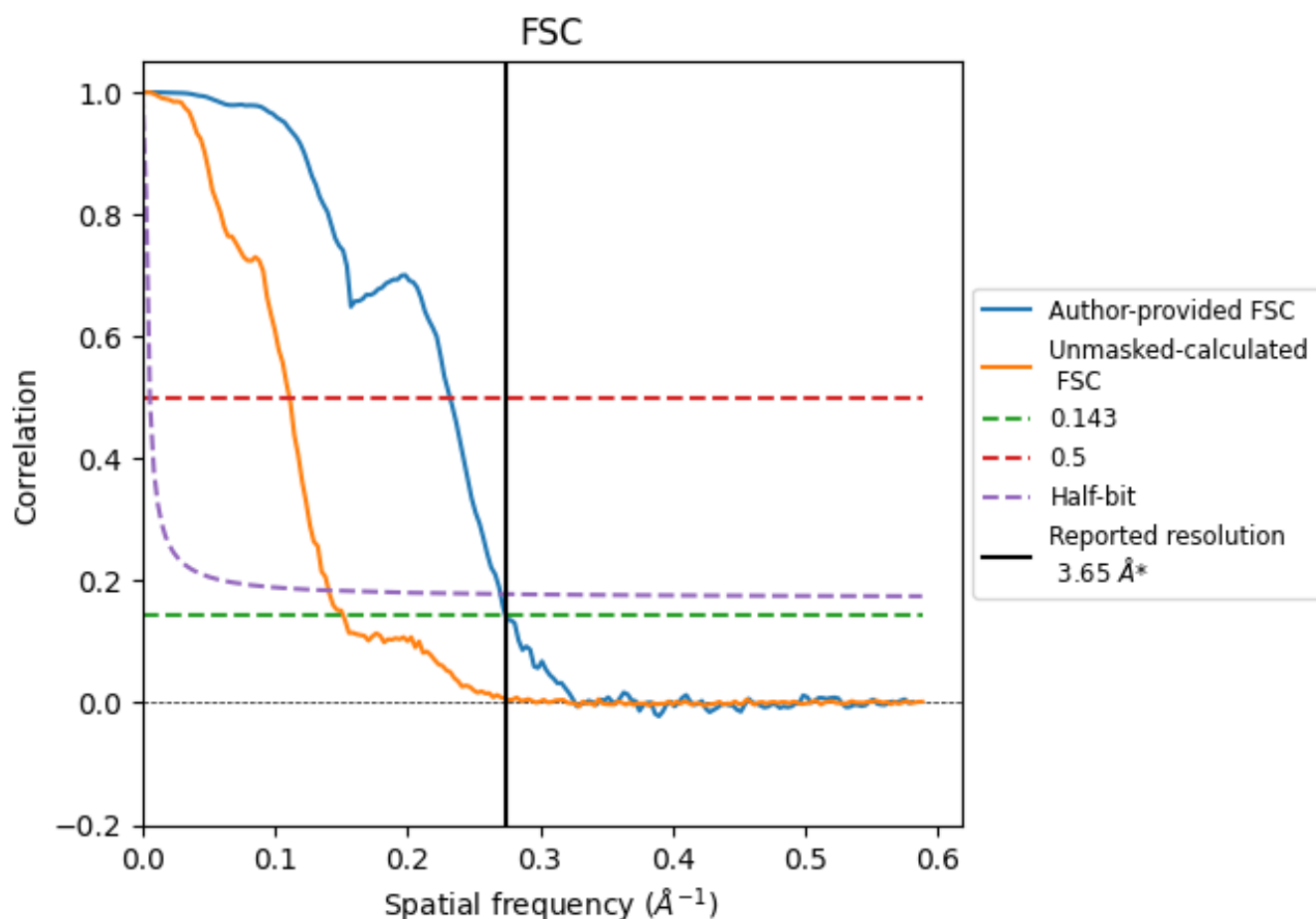


\*Reported resolution corresponds to spatial frequency of 0.274 Å<sup>-1</sup>

## 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  $0.274 \text{ \AA}^{-1}$



## 8.2 Resolution estimates [i](#)

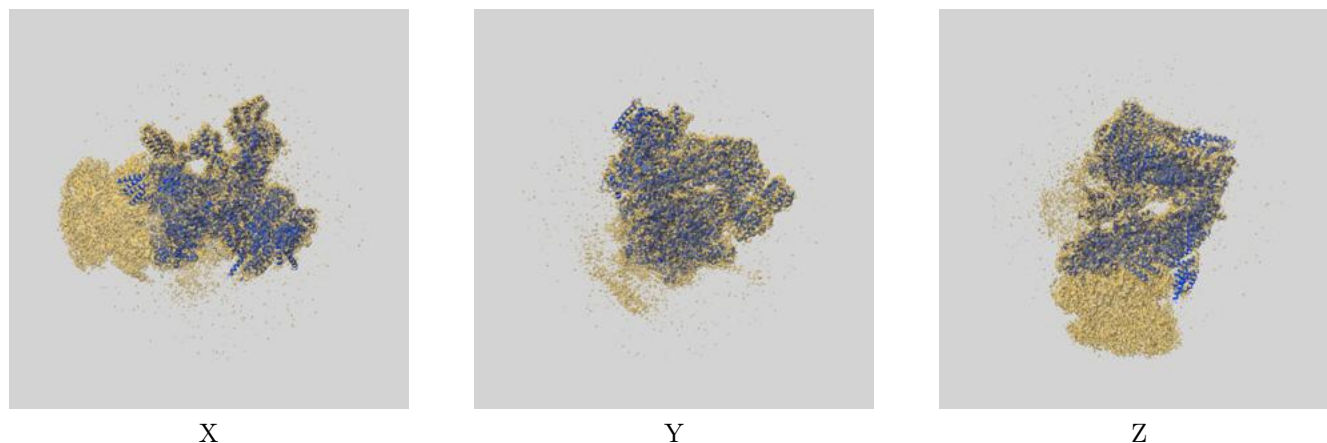
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.65	-	-
Author-provided FSC curve	3.65	4.31	3.70
Unmasked-calculated*	6.60	9.01	7.11

\*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 6.60 differs from the reported value 3.65 by more than 10 %

## 9 Map-model fit [i](#)

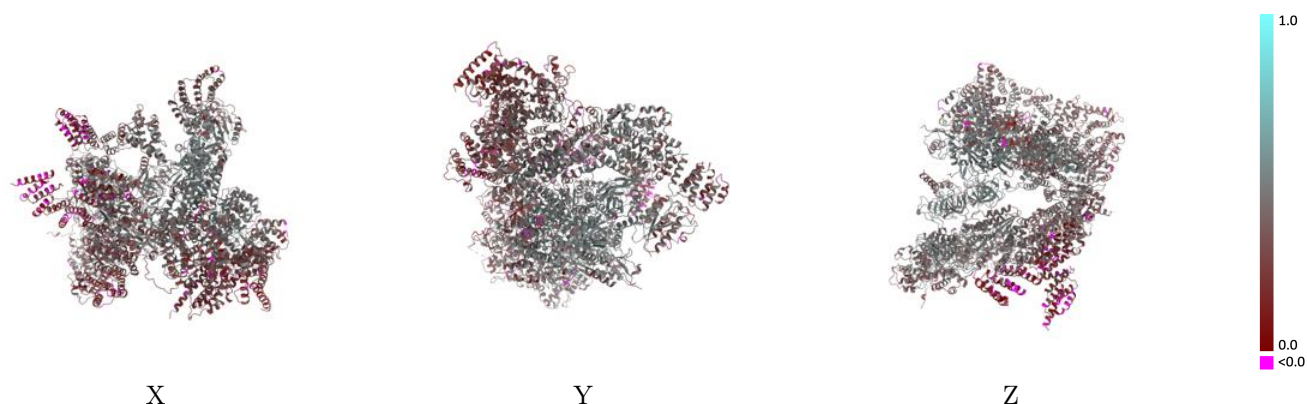
This section contains information regarding the fit between EMDB map EMD-65595 and PDB model 9W39. Per-residue inclusion information can be found in [section 3](#) on [page 11](#).

### 9.1 Map-model overlay [i](#)



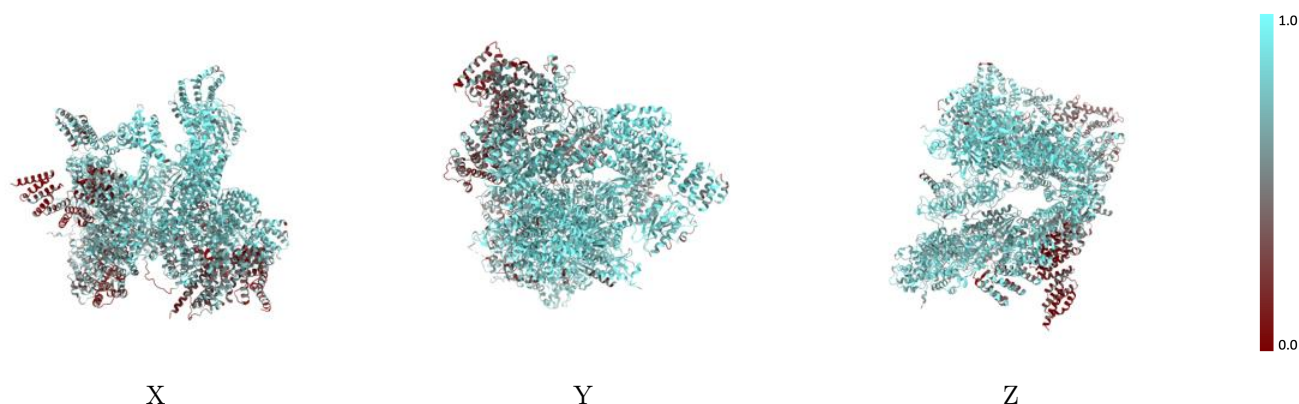
The images above show the 3D surface view of the map at the recommended contour level 0.081 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



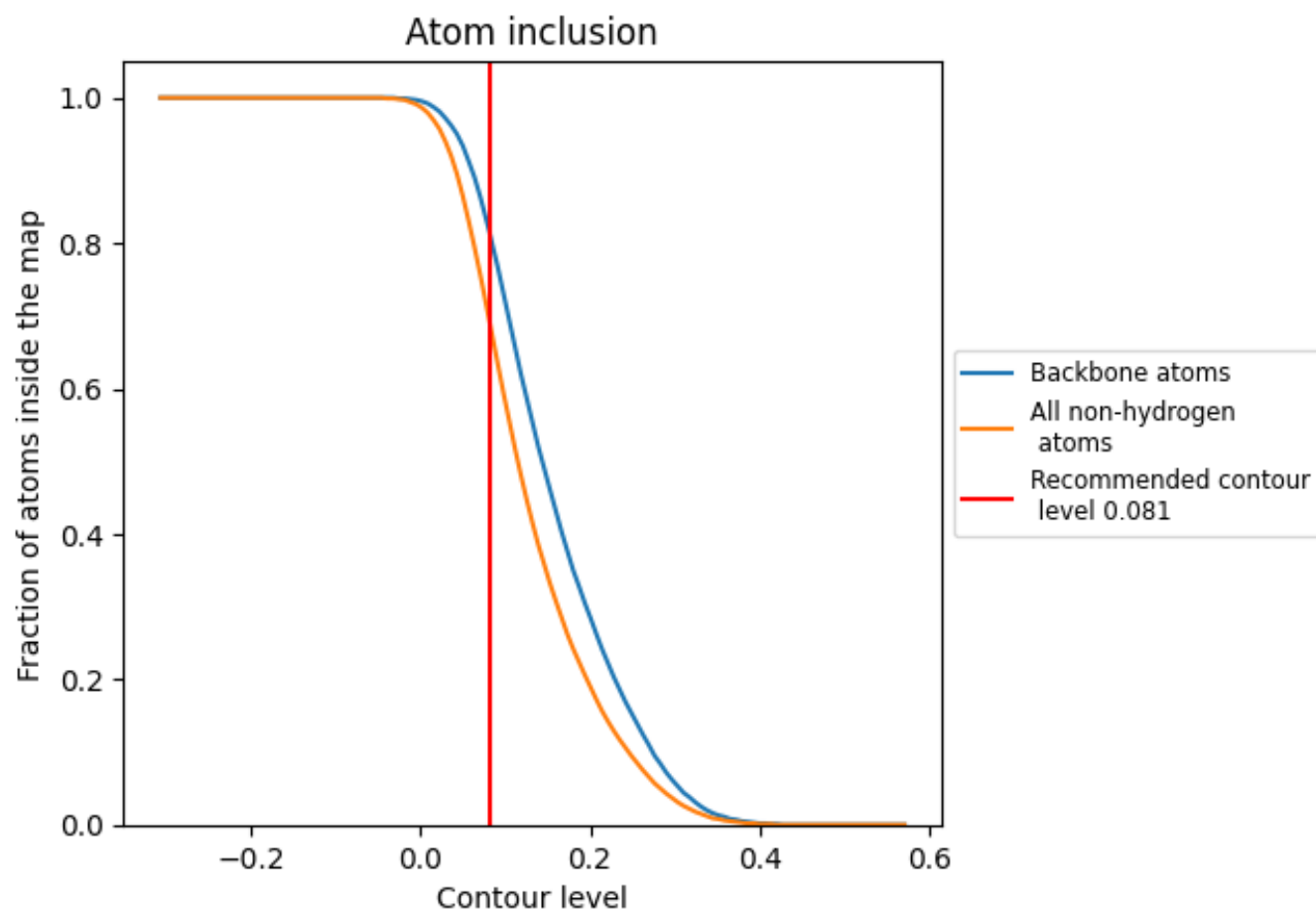
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.081).









































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 70% 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 (0.081) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6970	 0.3840
A	 0.7230	 0.4080
B	 0.5980	 0.3530
C	 0.6540	 0.3800
D	 0.7710	 0.4400
E	 0.8330	 0.4630
F	 0.7810	 0.4430
U	 0.7740	 0.4140
V	 0.5700	 0.3260
W	 0.7430	 0.3300
X	 0.3470	 0.2140
Y	 0.5700	 0.3180
Z	 0.8500	 0.4820
a	 0.8210	 0.4100
b	 0.7720	 0.4050
c	 0.8620	 0.5010
d	 0.4580	 0.2700
e	 0.5740	 0.3340
f	 0.8530	 0.4610
v	 0.5430	 0.3770

