



## wwPDB EM Validation Summary Report ⓘ

Apr 14, 2025 – 02:27 PM EDT

PDB ID : 8USB / pdb\_00008usb  
EMDB ID : EMD-42506  
Title : Non-substrate-engaged human 26S proteasome with Nub1/FAT10 bound to Rpn1  
Authors : Arkinson, C.; Gee, C.L.; Martin, A.  
Deposited on : 2023-10-27  
Resolution : 2.73 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>.

---

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

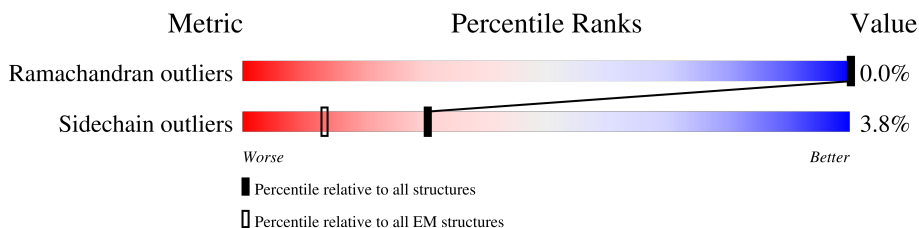
EMDB validation analysis : 0.0.1.dev117  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.42

# 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 2.73 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.





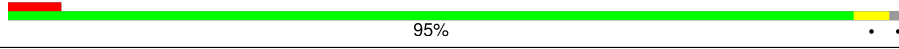
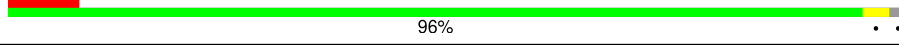

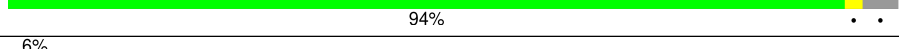
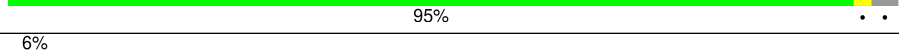
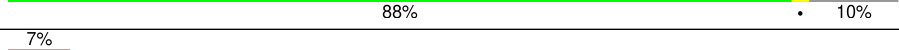
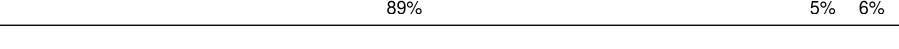
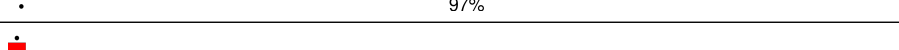



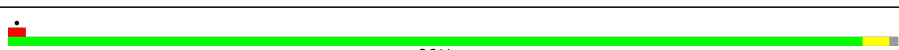
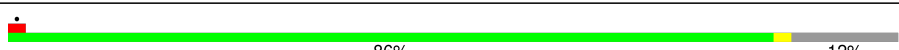
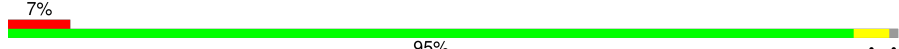


Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	W	456	94%
2	C	406	87%
3	b	377	47%
4	d	350	72%
5	f	908	88%
6	g	605	85%
7	B	440	89%
8	A	433	89%
9	D	418	89%

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
10	E	389	
11	F	439	
12	G	246	
13	H	234	
14	I	261	
15	J	248	
16	K	241	
17	L	263	
18	M	255	
19	O	277	
20	U	953	
21	V	534	
22	c	424	
23	e	70	
24	Y	389	
25	Z	324	
26	a	376	
27	X	422	

## 2 Entry composition

There are 31 unique types of molecules in this entry. The entry contains 70143 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	W	438	Total	C	N	O	S	0	0
			3570	2261	609	677	23		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	366	Total	C	N	O	S	0	0
			2895	1824	518	536	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	b	189	Total	C	N	O	S	0	0
			1446	903	259	277	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	265	Total	C	N	O	S	0	0
			2166	1402	355	400	9		

- Molecule 5 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	f	831	Total	C	N	O	S	0	0
			6433	4071	1089	1228	45		

- Molecule 6 is a protein called NEDD8 ultimate buster 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	g	91	Total	C	N	O	S	0	0
			736	466	134	135	1		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
g	-3	GLY	-	expression tag	UNP Q9Y5A7
g	-2	PRO	-	expression tag	UNP Q9Y5A7
g	-1	LEU	-	expression tag	UNP Q9Y5A7
g	0	GLY	-	expression tag	UNP Q9Y5A7

- Molecule 7 is a protein called 26S proteasome regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	B	405	Total	C	N	O	S	0	0
			3192	2012	546	619	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	A	395	Total	C	N	O	S	0	0
			3107	1956	547	586	18		

- Molecule 9 is a protein called 26S proteasome regulatory subunit 6B.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	E	354	Total	C	N	O	S	0	0
			2797	1761	495	525	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	F	351	Total	C	N	O	S	0	0
			2743	1733	472	522	16		

- Molecule 12 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	G	242	Total	C	N	O	S	0	0
			1886	1197	315	361	13		

- Molecule 13 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	H	230	Total	C	N	O	S	0	0
			1793	1147	302	338	6		

- Molecule 14 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	I	236	Total	C	N	O	S	1	0
			1841	1161	316	354	10		

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

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

- Molecule 16 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	K	234	Total	C	N	O	S	0	0
			1790	1125	295	359	11		

- Molecule 17 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	L	237	Total	C	N	O	S	0	0
			1864	1167	335	351	11		

- Molecule 18 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	M	240	Total	C	N	O	S	0	0
			1881	1193	321	356	11		

- Molecule 19 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	O	7	Total	C	N	O	0	0
			49	30	9	10		

- Molecule 20 is a protein called 26S proteasome non-ATPase regulatory subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	U	838	Total	C	N	O	S	0	0
			6515	4135	1106	1230	44		

- Molecule 21 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	470	Total	C	N	O	S	0	0
			3841	2438	685	704	14		

- Molecule 22 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	c	290	Total	C	N	O	S	0	0
			2282	1447	392	424	19		

There are 114 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
c	311	LEU	-	insertion	UNP O00487
c	312	ILE	-	expression tag	UNP O00487
c	313	ASN	-	expression tag	UNP O00487
c	314	HIS	-	expression tag	UNP O00487
c	315	HIS	-	expression tag	UNP O00487
c	316	HIS	-	expression tag	UNP O00487
c	317	HIS	-	expression tag	UNP O00487
c	318	HIS	-	expression tag	UNP O00487
c	319	HIS	-	expression tag	UNP O00487
c	320	ASP	-	expression tag	UNP O00487
c	321	TYR	-	expression tag	UNP O00487
c	322	ASP	-	expression tag	UNP O00487
c	323	ILE	-	expression tag	UNP O00487
c	324	PRO	-	expression tag	UNP O00487
c	325	THR	-	expression tag	UNP O00487
c	326	THR	-	expression tag	UNP O00487
c	327	ALA	-	expression tag	UNP O00487
c	328	SER	-	expression tag	UNP O00487
c	329	GLU	-	expression tag	UNP O00487
c	330	ASN	-	expression tag	UNP O00487
c	331	LEU	-	expression tag	UNP O00487
c	332	TYR	-	expression tag	UNP O00487
c	333	PHE	-	expression tag	UNP O00487
c	334	GLN	-	expression tag	UNP O00487
c	335	GLY	-	expression tag	UNP O00487

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
c	336	GLU	-	expression tag	UNP O00487
c	337	LEU	-	expression tag	UNP O00487
c	338	GLY	-	expression tag	UNP O00487
c	339	MET	-	expression tag	UNP O00487
c	340	ARG	-	expression tag	UNP O00487
c	341	GLY	-	expression tag	UNP O00487
c	342	SER	-	expression tag	UNP O00487
c	343	ALA	-	expression tag	UNP O00487
c	344	GLY	-	expression tag	UNP O00487
c	345	LYS	-	expression tag	UNP O00487
c	346	ALA	-	expression tag	UNP O00487
c	347	GLY	-	expression tag	UNP O00487
c	348	GLU	-	expression tag	UNP O00487
c	349	GLY	-	expression tag	UNP O00487
c	350	GLU	-	expression tag	UNP O00487
c	351	ILE	-	expression tag	UNP O00487
c	352	PRO	-	expression tag	UNP O00487
c	353	ALA	-	expression tag	UNP O00487
c	354	PRO	-	expression tag	UNP O00487
c	355	LEU	-	expression tag	UNP O00487
c	356	ALA	-	expression tag	UNP O00487
c	357	GLY	-	expression tag	UNP O00487
c	358	THR	-	expression tag	UNP O00487
c	359	VAL	-	expression tag	UNP O00487
c	360	SER	-	expression tag	UNP O00487
c	361	LYS	-	expression tag	UNP O00487
c	362	ILE	-	expression tag	UNP O00487
c	363	LEU	-	expression tag	UNP O00487
c	364	VAL	-	expression tag	UNP O00487
c	365	LYS	-	expression tag	UNP O00487
c	366	GLU	-	expression tag	UNP O00487
c	367	GLY	-	expression tag	UNP O00487
c	368	ASP	-	expression tag	UNP O00487
c	369	THR	-	expression tag	UNP O00487
c	370	VAL	-	expression tag	UNP O00487
c	371	LYS	-	expression tag	UNP O00487
c	372	ALA	-	expression tag	UNP O00487
c	373	GLY	-	expression tag	UNP O00487
c	374	GLN	-	expression tag	UNP O00487
c	375	THR	-	expression tag	UNP O00487
c	376	VAL	-	expression tag	UNP O00487
c	377	LEU	-	expression tag	UNP O00487

*Continued on next page...*



*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
c	378	VAL	-	expression tag	UNP O00487
c	379	LEU	-	expression tag	UNP O00487
c	380	GLU	-	expression tag	UNP O00487
c	381	ALA	-	expression tag	UNP O00487
c	382	MET	-	expression tag	UNP O00487
c	383	LYS	-	expression tag	UNP O00487
c	384	MET	-	expression tag	UNP O00487
c	385	GLU	-	expression tag	UNP O00487
c	386	THR	-	expression tag	UNP O00487
c	387	GLU	-	expression tag	UNP O00487
c	388	ILE	-	expression tag	UNP O00487
c	389	ASN	-	expression tag	UNP O00487
c	390	ALA	-	expression tag	UNP O00487
c	391	PRO	-	expression tag	UNP O00487
c	392	THR	-	expression tag	UNP O00487
c	393	ASP	-	expression tag	UNP O00487
c	394	GLY	-	expression tag	UNP O00487
c	395	LYS	-	expression tag	UNP O00487
c	396	VAL	-	expression tag	UNP O00487
c	397	GLU	-	expression tag	UNP O00487
c	398	LYS	-	expression tag	UNP O00487
c	399	VAL	-	expression tag	UNP O00487
c	400	LEU	-	expression tag	UNP O00487
c	401	VAL	-	expression tag	UNP O00487
c	402	LYS	-	expression tag	UNP O00487
c	403	GLU	-	expression tag	UNP O00487
c	404	ARG	-	expression tag	UNP O00487
c	405	ASP	-	expression tag	UNP O00487
c	406	ALA	-	expression tag	UNP O00487
c	407	VAL	-	expression tag	UNP O00487
c	408	GLN	-	expression tag	UNP O00487
c	409	GLY	-	expression tag	UNP O00487
c	410	GLY	-	expression tag	UNP O00487
c	411	GLN	-	expression tag	UNP O00487
c	412	GLY	-	expression tag	UNP O00487
c	413	LEU	-	expression tag	UNP O00487
c	414	ILE	-	expression tag	UNP O00487
c	415	LYS	-	expression tag	UNP O00487
c	416	ILE	-	expression tag	UNP O00487
c	417	GLY	-	expression tag	UNP O00487
c	418	VAL	-	expression tag	UNP O00487
c	419	HIS	-	expression tag	UNP O00487

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
c	420	HIS	-	expression tag	UNP O00487
c	421	HIS	-	expression tag	UNP O00487
c	422	HIS	-	expression tag	UNP O00487
c	423	HIS	-	expression tag	UNP O00487
c	424	HIS	-	expression tag	UNP O00487

- Molecule 23 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	e	50	Total	C	N	O	0	0
			425	260	65	100		

- Molecule 24 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	386	Total	C	N	O	S	0	0
			3179	2025	542	595	17		

- Molecule 25 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	286	Total	C	N	O	S	0	0
			2285	1461	392	427	5		

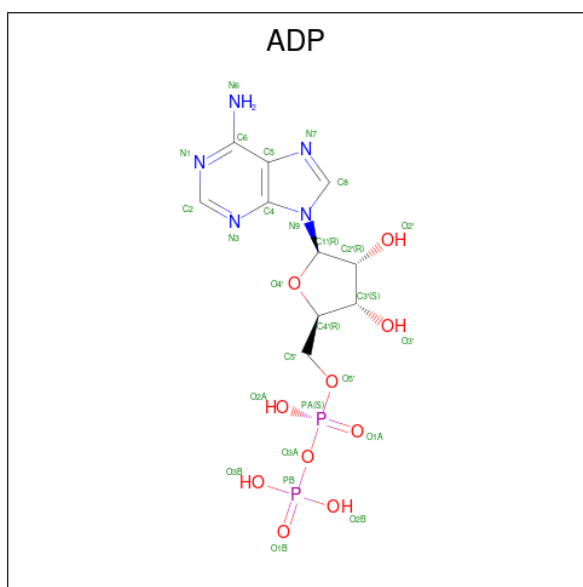
- Molecule 26 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

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

- Molecule 27 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	X	419	Total	C	N	O	S	0	0
			3317	2105	564	636	12		

- Molecule 28 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
28	C	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 29 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
29	C	1	Total	Mg	0
			1	1	
29	B	1	Total	Mg	0
			1	1	
29	A	1	Total	Mg	0
			1	1	
29	D	1	Total	Mg	0
			1	1	
29	E	1	Total	Mg	0
			1	1	
29	F	1	Total	Mg	0
			1	1	

- Molecule 30 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
30	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
30	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
30	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
30	E	1	Total	C	N	O	P	0
			31	10	5	13	3	
30	F	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 31 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

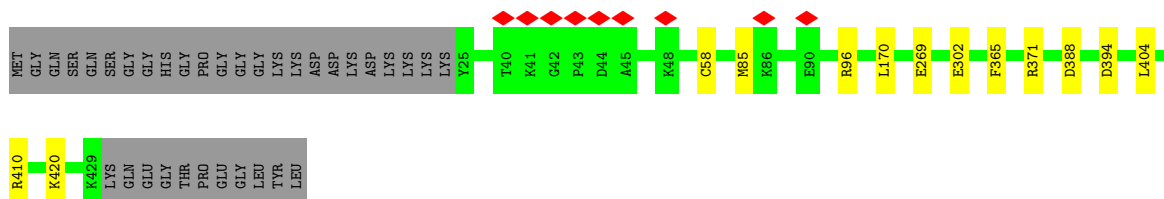
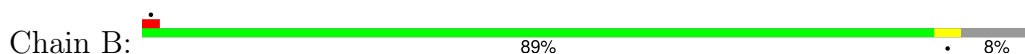
Mol	Chain	Residues	Atoms		AltConf
31	c	1	Total	Zn	0
			1	1	



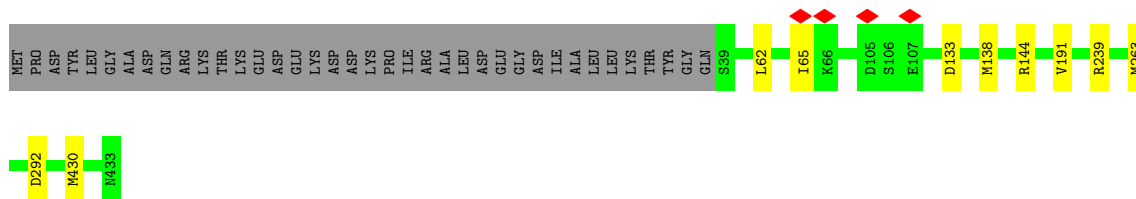
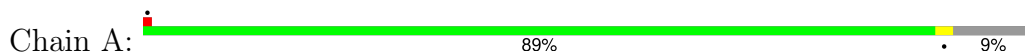


ASP	LEU	MET	ALA	PHE
GLU	PRO	TRP	CYS	LEU
GLU	PRO	TRP	ASP	ARG
ILE	LEU	LEU	GLY	LEU
ILE	PRO	ASN	ASN	TYR
ALA	LEU	ASP	VAL	LEU
GLU	SER	ASN	ASP	GLN
TYR	PRO	PRO	HIS	GLY
LEU	GLU	GLU	ALA	ILE
SER	ASP	THR	THR	ARG
TYR	SER	ASP	HIS	ASN
VAL	LEU	ASN	ILE	TYR
SER	SER	ARG	THR	HIS
ASN	PRO	GLN	ASN	SER
LYS	PRO	GLU	ARG	GLY
ARG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

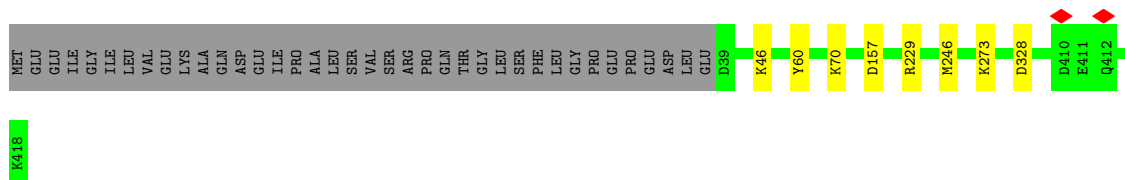
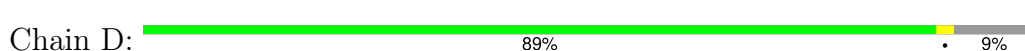
- Molecule 7: 26S proteasome regulatory subunit 4



- Molecule 8: 26S proteasome regulatory subunit 7



- Molecule 9: 26S proteasome regulatory subunit 6B

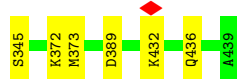


- Molecule 10: 26S protease regulatory subunit 10B





- Chain F:  75% 5% 20%




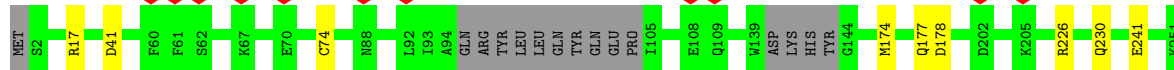
- Chain G:  6% 95%



- Chain H:  8% 96%



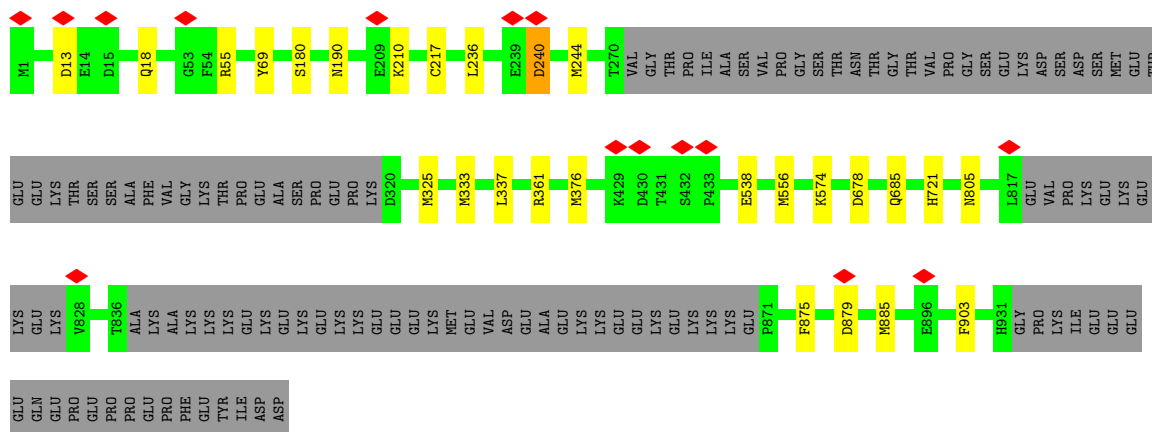
- Chain I:  87% 10%



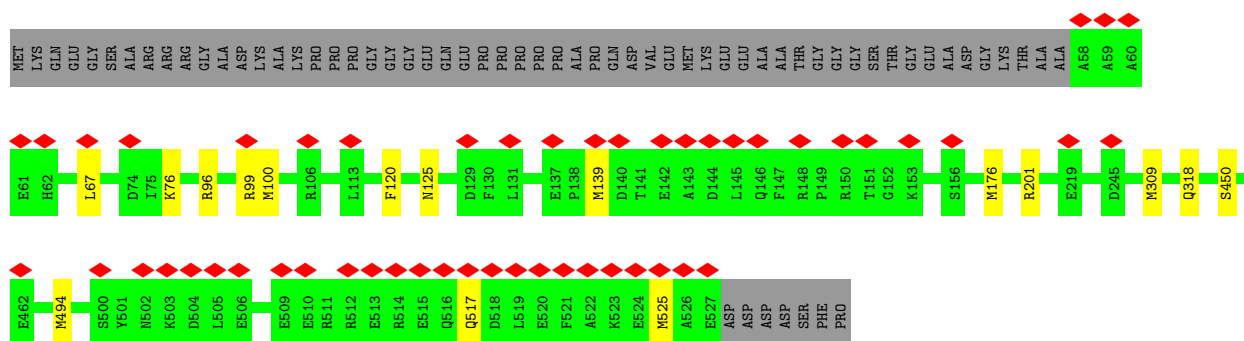
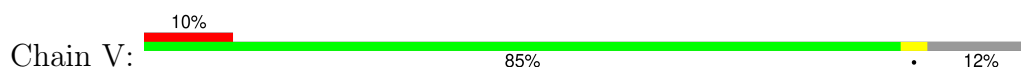
- Chain J:  8% 94% ...



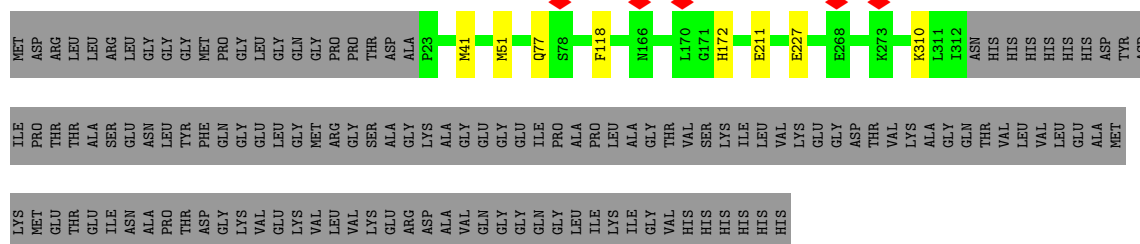




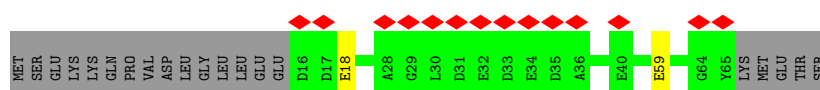
- Molecule 21: 26S proteasome non-ATPase regulatory subunit 3



- Molecule 22: 26S proteasome non-ATPase regulatory subunit 14

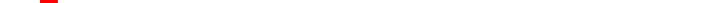


- Molecule 23: 26S proteasome complex subunit SEM1



- Molecule 24: 26S proteasome non-ATPase regulatory subunit 6

MET
PRO
LEU
E4
N5
L6
E7
E8
E9
E55
K59
N94
S98
Y143
W174
F272
M282
R385
M389

- Chain Z:  86% 12%

**Figure S6**

**A**

GLU  
LYS  
LYS

MET  
PRO  
GLU  
L4  
K28  
V29  
G30  
N31  
S42  
D62  
C116  
S119  
Q229  
E244  
R283  
D284  
K287  
K288  
E289  
GLY  
GLN  
GLU  
LYS  
GLU  
GLU  
SER  
LYS  
LYS  
ASP  
ARG  
LYS  
GLU  
ASP  
LYS  
GLU  
LYS  
ASP  
LYS  
ASP  
LYS  
GLU  
LYS  
SER  
ASP  
VAL  
LYS  
LYS  
GLU  
GLU  
LYS

- Chain a:  7% 95%

- Chain X:  8% 96%

The diagram illustrates the human genome with chromosomes 1 through 22, X, and Y. Each chromosome is represented by a colored bar with a diamond marker indicating a specific gene location. The markers are labeled with gene names: MET, ALA, ALA, A4, A5, V6, V7, E8, F9, Q10, R11, A12, Q13, S14, L15, L16, S17, T18, D19, R20, E21, A22, H28, R33, D34, I35, Q36, E37, N38, D39, E40, E41, S49, I50, L51, E52, L56, A64, E65, N78, L93, D98, H99, E100, E109, M112, H118, V122, K274, C289, L326, K395, Y415, K419, K420, L421, T422.

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	50918	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 ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1700	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.222	Depositor
Minimum map value	-0.487	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.051	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	293.44, 293.44, 293.44	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.048, 1.048, 1.048	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	W	0.24	0/3618	0.45	0/4868
2	C	0.25	0/2933	0.48	0/3946
3	b	0.25	0/1466	0.52	1/1986 (0.1%)
4	d	0.25	0/2212	0.45	1/2988 (0.0%)
5	f	0.26	0/6542	0.50	1/8856 (0.0%)
6	g	0.30	0/743	0.64	0/994
7	B	0.26	0/3241	0.50	0/4372
8	A	0.26	0/3159	0.51	0/4265
9	D	0.26	0/3089	0.48	0/4168
10	E	0.25	0/2842	0.50	0/3832
11	F	0.27	0/2781	0.48	0/3748
12	G	0.26	0/1920	0.47	0/2595
13	H	0.26	0/1832	0.47	0/2481
14	I	0.26	0/1867	0.51	1/2509 (0.0%)
15	J	0.26	0/1913	0.50	0/2581
16	K	0.25	0/1818	0.47	0/2455
17	L	0.25	0/1899	0.50	0/2567
18	M	0.26	0/1916	0.48	0/2580
19	O	0.18	0/49	0.33	0/65
20	U	0.25	0/6630	0.46	2/8977 (0.0%)
21	V	0.26	0/3913	0.52	1/5277 (0.0%)
22	c	0.25	0/2325	0.46	0/3143
23	e	0.26	0/437	0.51	0/595
24	Y	0.26	0/3237	0.48	0/4360
25	Z	0.25	0/2328	0.46	0/3156
26	a	0.24	0/3053	0.46	0/4133
27	X	0.24	0/3363	0.44	0/4534
All	All	0.25	0/71126	0.48	7/96031 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected

by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
10	E	0	1

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	U	337	LEU	CA-CB-CG	6.20	129.56	115.30
21	V	67	LEU	CA-CB-CG	5.58	128.13	115.30
3	b	119	ASP	CB-CG-OD2	5.36	123.13	118.30
5	f	390	LEU	CA-CB-CG	5.33	127.55	115.30
4	d	160	ASP	CB-CG-OD2	5.19	122.97	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	E	258	MET	Peptide

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

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 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	W	436/456 (96%)	427 (98%)	8 (2%)	1 (0%)	44	63
2	C	362/406 (89%)	353 (98%)	9 (2%)	0	100	100
3	b	187/377 (50%)	180 (96%)	7 (4%)	0	100	100

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	d	263/350 (75%)	250 (95%)	13 (5%)	0	100	100
5	f	825/908 (91%)	797 (97%)	28 (3%)	0	100	100
6	g	89/605 (15%)	85 (96%)	3 (3%)	1 (1%)	12	21
7	B	403/440 (92%)	392 (97%)	11 (3%)	0	100	100
8	A	393/433 (91%)	376 (96%)	16 (4%)	1 (0%)	37	55
9	D	378/418 (90%)	367 (97%)	11 (3%)	0	100	100
10	E	352/389 (90%)	344 (98%)	8 (2%)	0	100	100
11	F	347/439 (79%)	337 (97%)	10 (3%)	0	100	100
12	G	240/246 (98%)	233 (97%)	7 (3%)	0	100	100
13	H	228/234 (97%)	228 (100%)	0	0	100	100
14	I	231/261 (88%)	227 (98%)	4 (2%)	0	100	100
15	J	237/248 (96%)	236 (100%)	1 (0%)	0	100	100
16	K	232/241 (96%)	226 (97%)	6 (3%)	0	100	100
17	L	235/263 (89%)	231 (98%)	4 (2%)	0	100	100
18	M	238/255 (93%)	231 (97%)	7 (3%)	0	100	100
19	O	5/277 (2%)	5 (100%)	0	0	100	100
20	U	830/953 (87%)	814 (98%)	16 (2%)	0	100	100
21	V	468/534 (88%)	461 (98%)	7 (2%)	0	100	100
22	c	288/424 (68%)	285 (99%)	3 (1%)	0	100	100
23	e	48/70 (69%)	42 (88%)	6 (12%)	0	100	100
24	Y	384/389 (99%)	381 (99%)	3 (1%)	0	100	100
25	Z	284/324 (88%)	279 (98%)	5 (2%)	0	100	100
26	a	371/376 (99%)	368 (99%)	3 (1%)	0	100	100
27	X	417/422 (99%)	405 (97%)	12 (3%)	0	100	100
All	All	8771/10738 (82%)	8560 (98%)	208 (2%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	A	65	ILE
1	W	21	SER
6	g	160	GLN

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	W	403/416 (97%)	393 (98%)	10 (2%)	42	63
2	C	320/352 (91%)	307 (96%)	13 (4%)	26	45
3	b	166/312 (53%)	153 (92%)	13 (8%)	10	19
4	d	235/294 (80%)	223 (95%)	12 (5%)	20	36
5	f	701/763 (92%)	674 (96%)	27 (4%)	27	47
6	g	81/529 (15%)	70 (86%)	11 (14%)	3	4
7	B	359/385 (93%)	346 (96%)	13 (4%)	30	50
8	A	340/372 (91%)	331 (97%)	9 (3%)	41	62
9	D	333/366 (91%)	325 (98%)	8 (2%)	44	64
10	E	309/341 (91%)	301 (97%)	8 (3%)	41	62
11	F	299/379 (79%)	279 (93%)	20 (7%)	13	24
12	G	206/210 (98%)	197 (96%)	9 (4%)	24	42
13	H	188/191 (98%)	182 (97%)	6 (3%)	34	55
14	I	197/221 (89%)	189 (96%)	8 (4%)	26	45
15	J	203/211 (96%)	198 (98%)	5 (2%)	42	63
16	K	196/203 (97%)	190 (97%)	6 (3%)	35	56
17	L	203/224 (91%)	198 (98%)	5 (2%)	42	63
18	M	198/212 (93%)	184 (93%)	14 (7%)	12	22
19	O	6/228 (3%)	6 (100%)	0	100	100
20	U	712/816 (87%)	686 (96%)	26 (4%)	29	49
21	V	415/460 (90%)	400 (96%)	15 (4%)	30	50
22	c	255/359 (71%)	247 (97%)	8 (3%)	35	56
23	e	44/63 (70%)	42 (96%)	2 (4%)	23	41
24	Y	341/344 (99%)	330 (97%)	11 (3%)	34	55
25	Z	258/295 (88%)	251 (97%)	7 (3%)	40	60
26	a	333/336 (99%)	319 (96%)	14 (4%)	25	44

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
27	X	361/362 (100%)	349 (97%)	12 (3%)	33 54
All	All	7662/9244 (83%)	7370 (96%)	292 (4%)	30 48

5 of 292 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
21	V	201	ARG
27	X	223	LYS
22	c	41	MET
25	Z	116	CYS
7	B	410	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
25	Z	229	GLN
22	c	237	HIS
20	U	192	GLN
21	V	516	GLN
20	U	190	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 7 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
30	ATP	E	501	29	28,33,33	0.66	0	34,52,52	0.64	1 (2%)
28	ADP	C	501	29	24,29,29	0.87	0	29,45,45	1.19	2 (6%)
30	ATP	B	501	29	28,33,33	0.68	0	34,52,52	0.60	1 (2%)
30	ATP	F	501	29	28,33,33	0.65	0	34,52,52	0.64	1 (2%)
30	ATP	A	501	29	28,33,33	0.69	0	34,52,52	0.63	1 (2%)
30	ATP	D	501	29	28,33,33	0.67	0	34,52,52	0.76	2 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	ATP	E	501	29	-	3/18/38/38	0/3/3/3
28	ADP	C	501	29	-	4/12/32/32	0/3/3/3
30	ATP	B	501	29	-	3/18/38/38	0/3/3/3
30	ATP	F	501	29	-	7/18/38/38	0/3/3/3
30	ATP	A	501	29	-	1/18/38/38	0/3/3/3
30	ATP	D	501	29	-	5/18/38/38	0/3/3/3

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	C	501	ADP	N3-C2-N1	-3.60	123.78	128.67
28	C	501	ADP	C4-C5-N7	-2.54	106.65	109.34
30	A	501	ATP	C5-C6-N6	2.32	123.84	120.31
30	F	501	ATP	C5-C6-N6	2.32	123.84	120.31
30	E	501	ATP	C5-C6-N6	2.31	123.83	120.31

There are no chirality outliers.

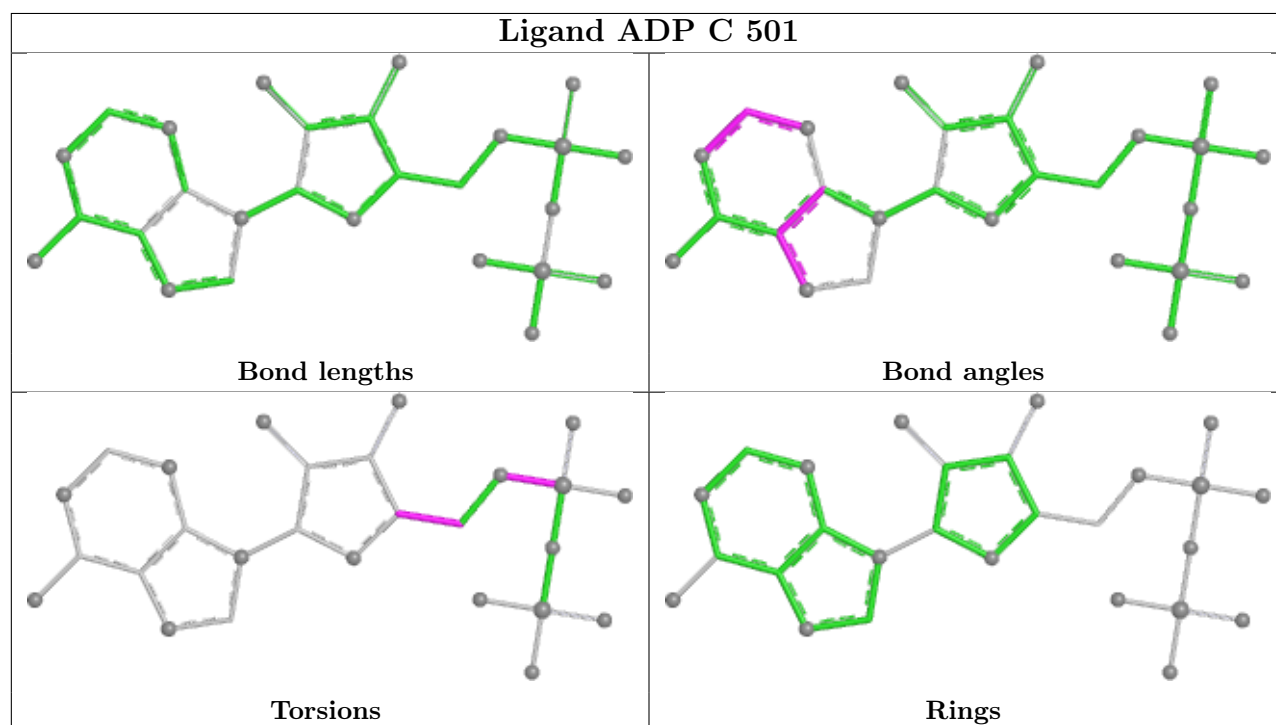
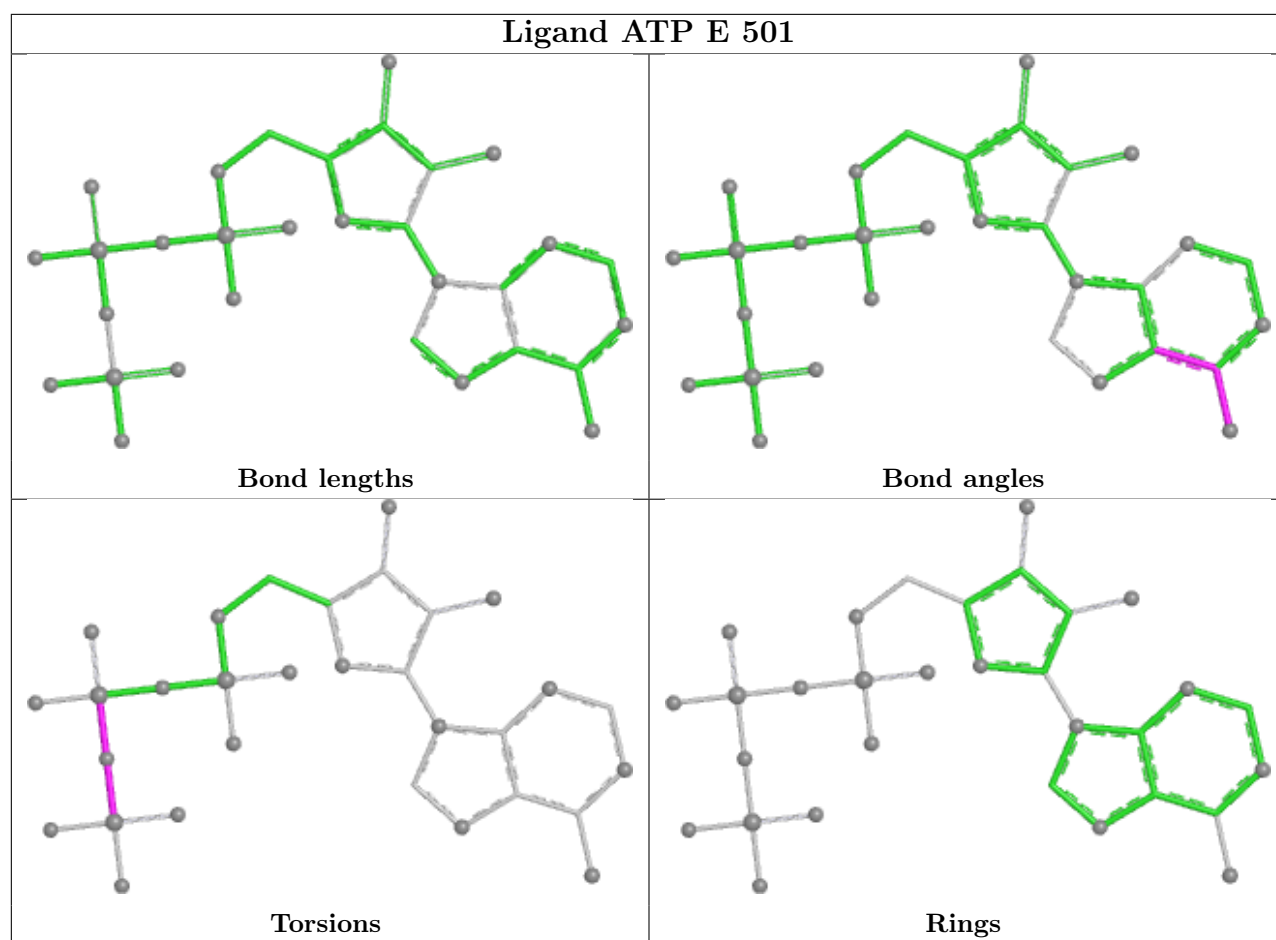
5 of 23 torsion outliers are listed below:

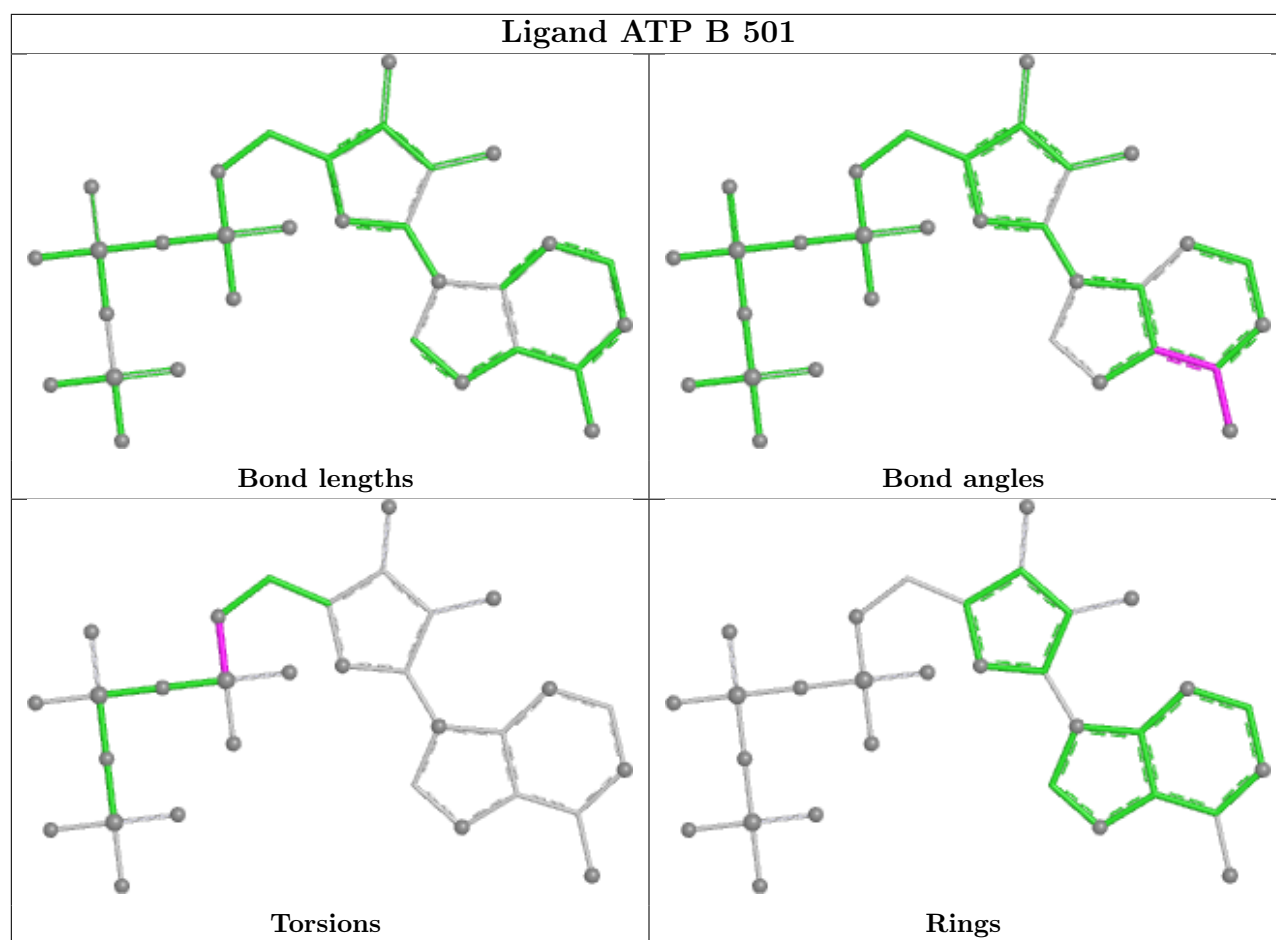
Mol	Chain	Res	Type	Atoms
28	C	501	ADP	C5'-O5'-PA-O1A
28	C	501	ADP	C5'-O5'-PA-O2A
28	C	501	ADP	C5'-O5'-PA-O3A
30	B	501	ATP	C5'-O5'-PA-O1A
30	B	501	ATP	C5'-O5'-PA-O2A

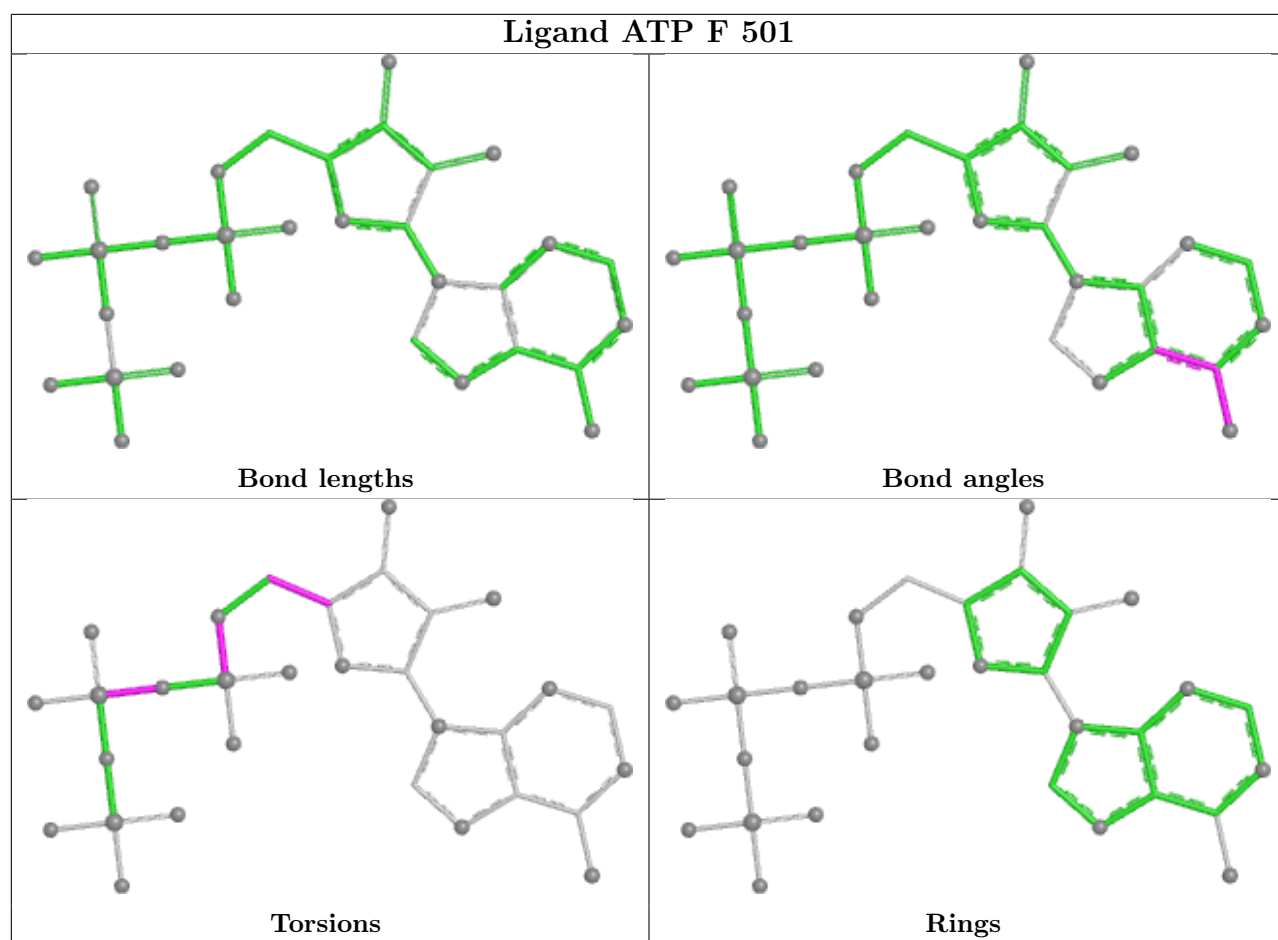
There are no ring outliers.

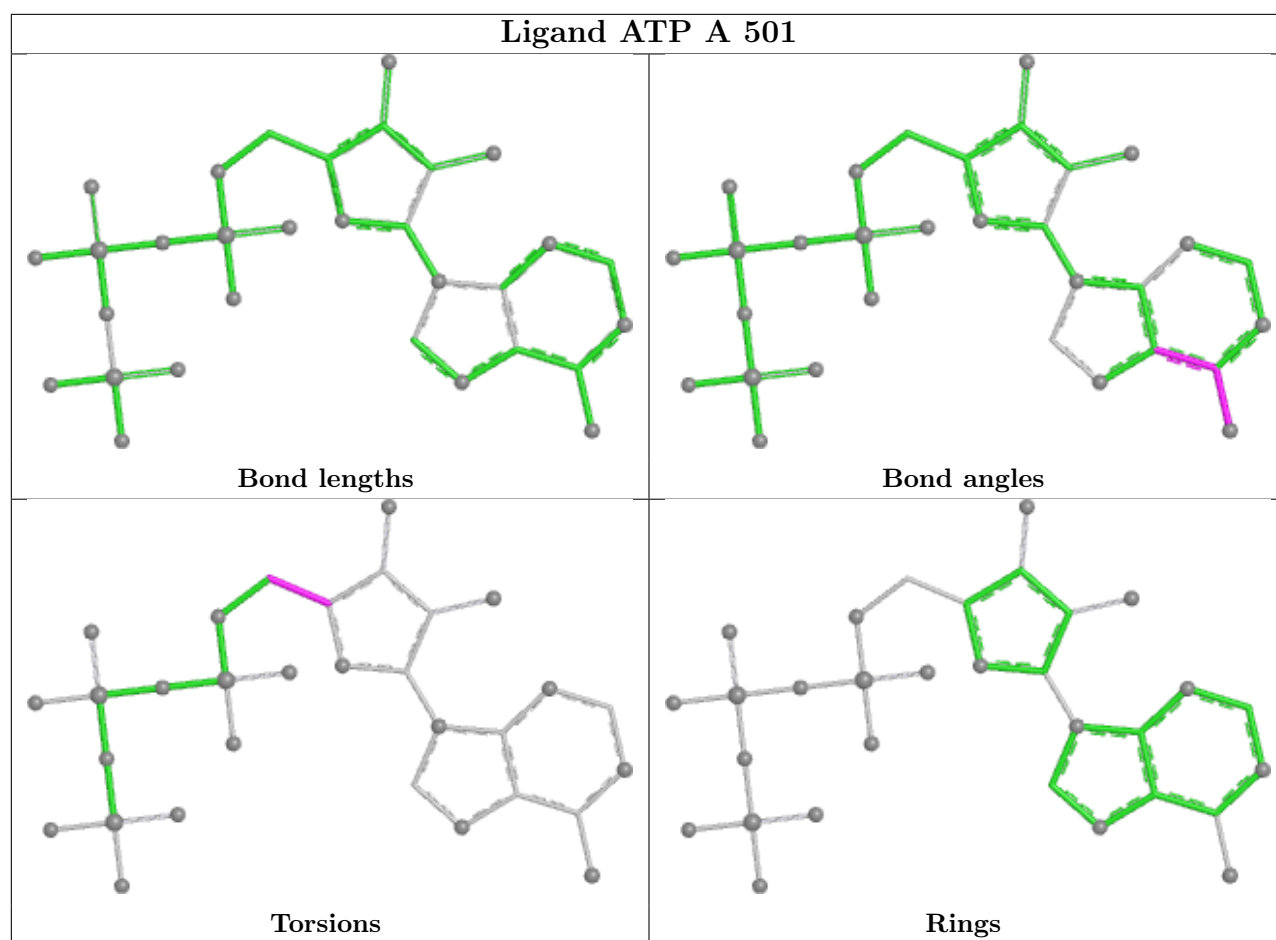
No monomer is involved in short contacts.

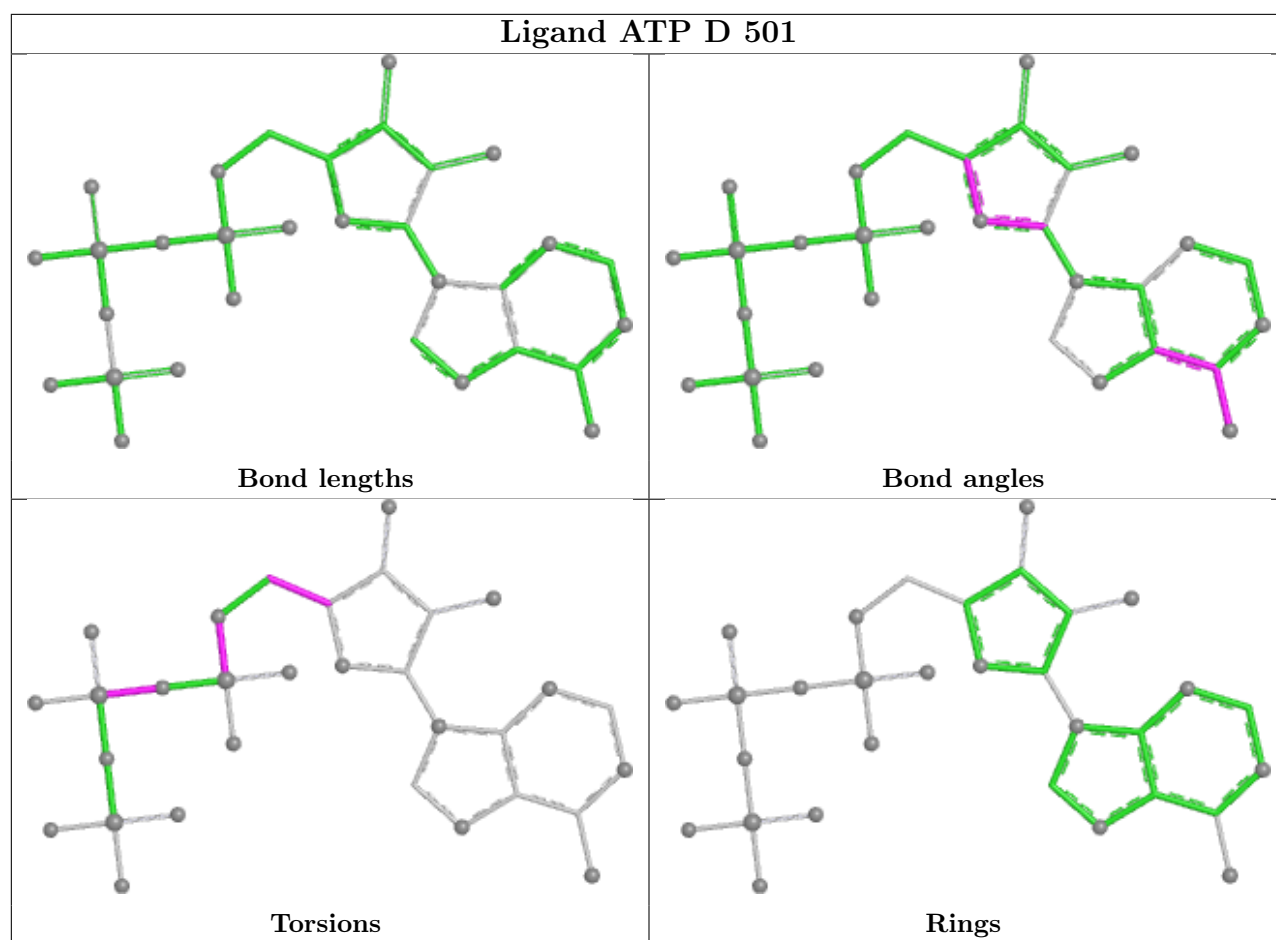
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



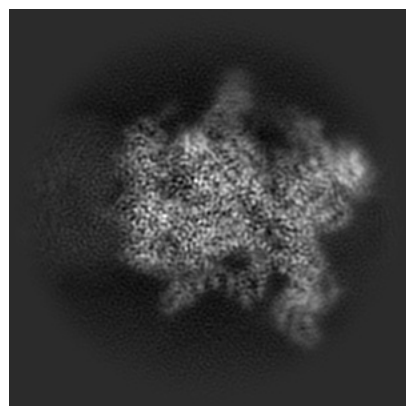
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42506. These allow visual inspection of the internal detail of the map and identification of artifacts.

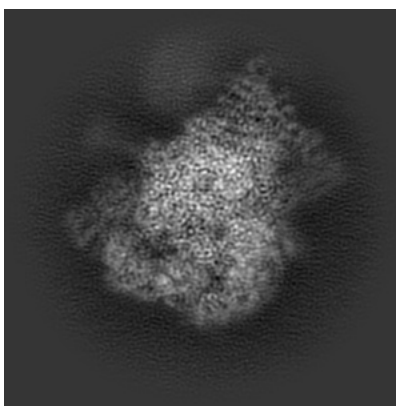
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

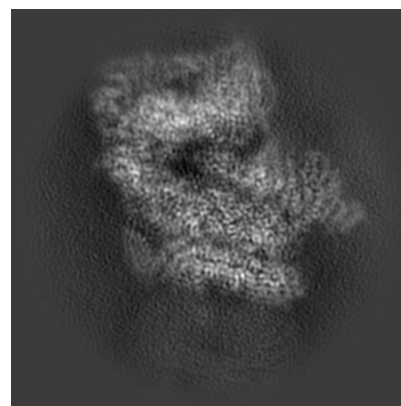
#### 6.1.1 Primary map



X

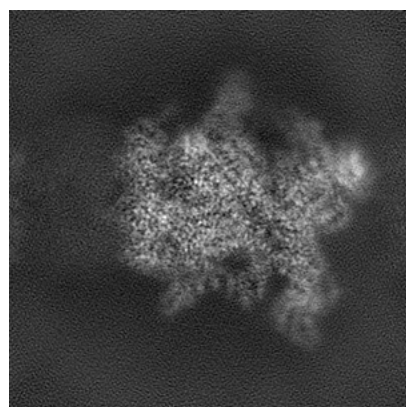


Y

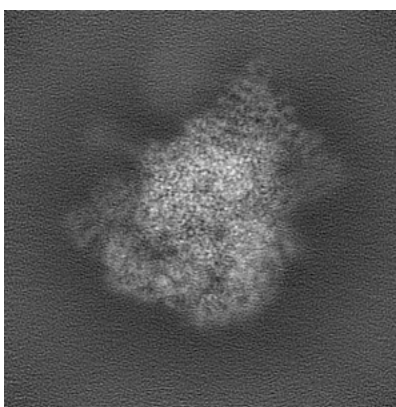


Z

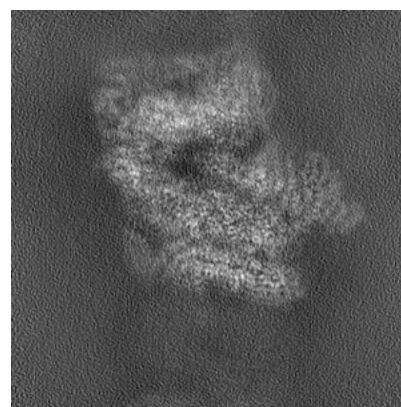
#### 6.1.2 Raw map



X



Y

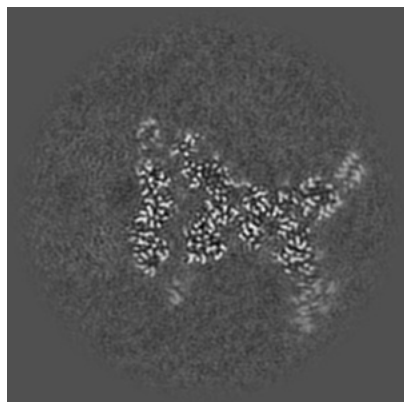


Z

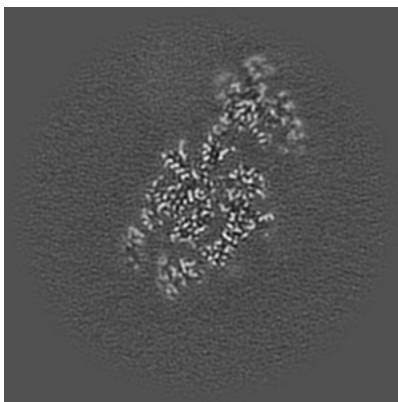
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

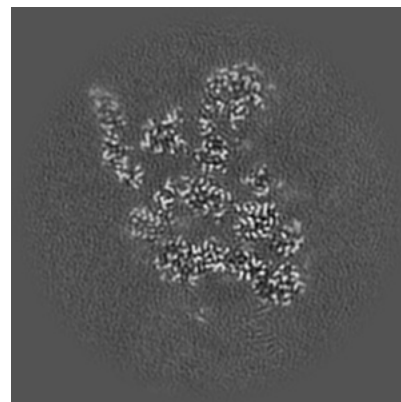
### 6.2.1 Primary map



X Index: 140

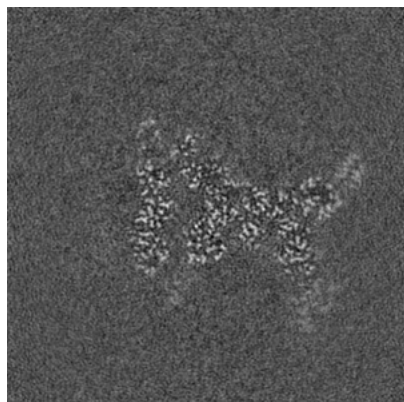


Y Index: 140

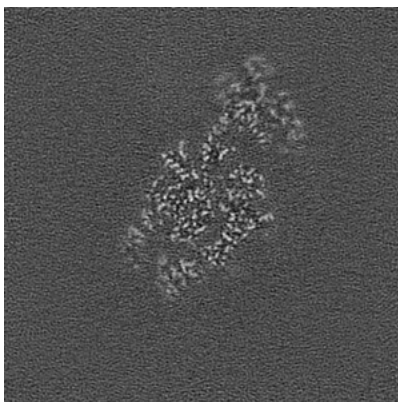


Z Index: 140

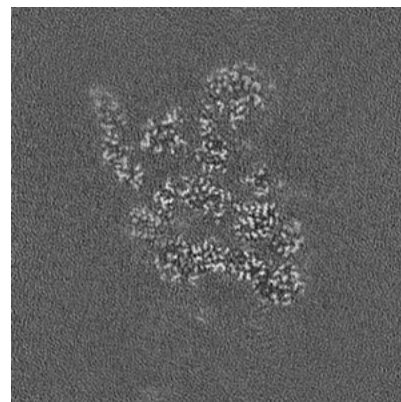
### 6.2.2 Raw map



X Index: 140



Y Index: 140

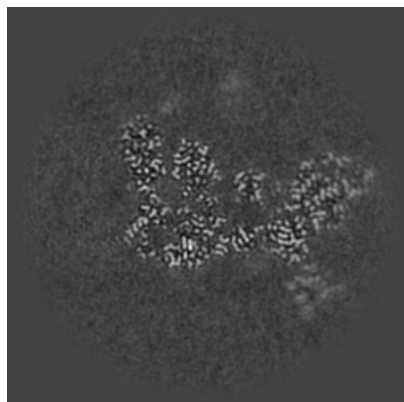


Z Index: 140

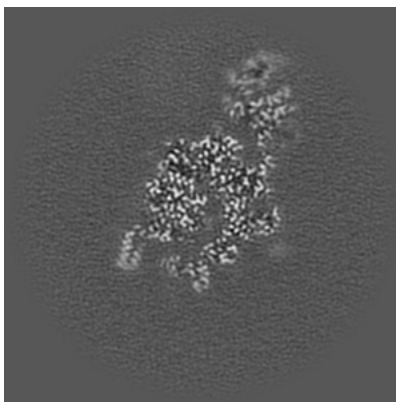
The images above show central slices of the map in three orthogonal directions.

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

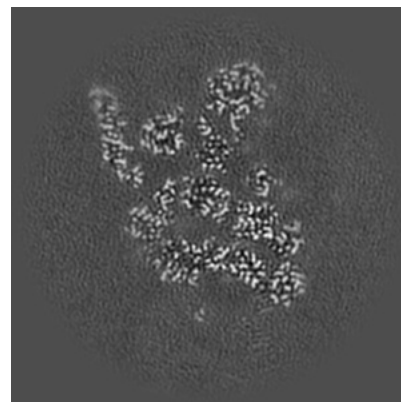
### 6.3.1 Primary map



X Index: 155

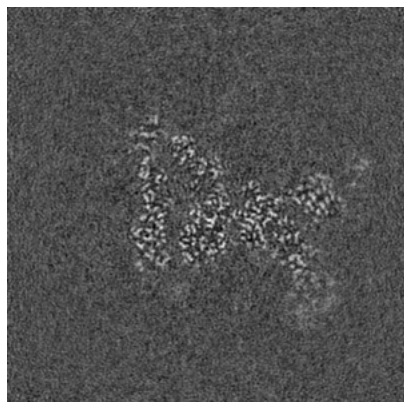


Y Index: 134

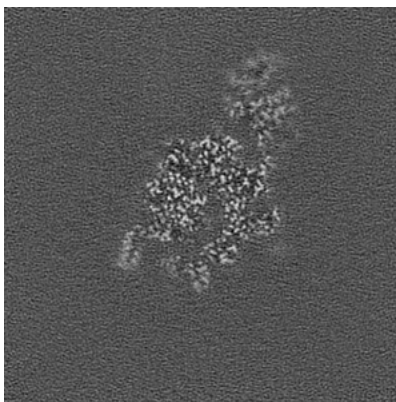


Z Index: 139

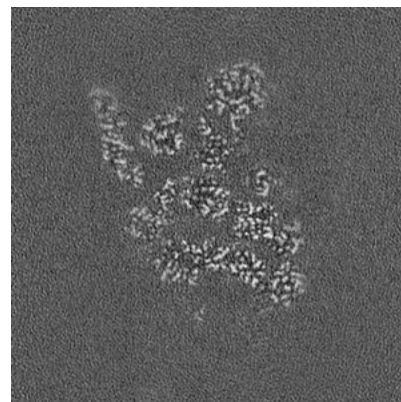
### 6.3.2 Raw map



X Index: 144



Y Index: 134



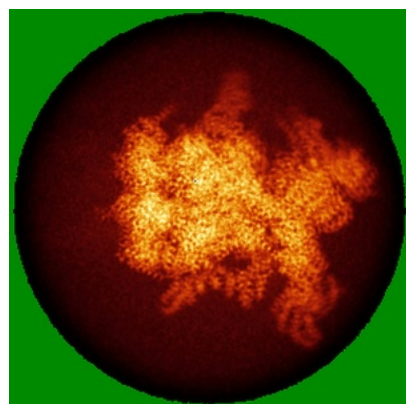
Z Index: 139

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

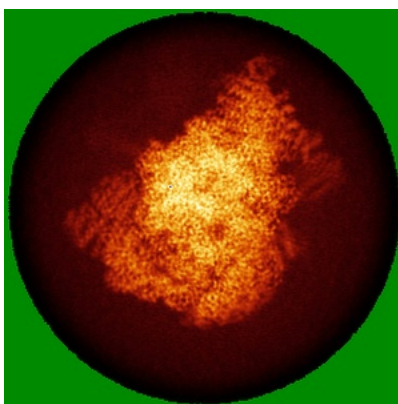


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

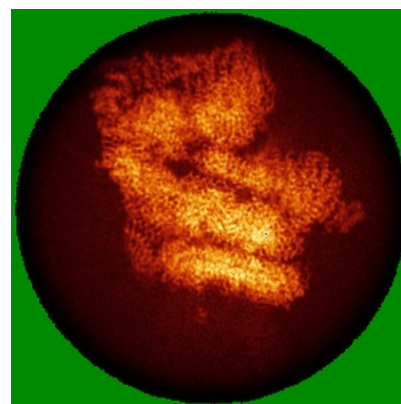
### 6.4.1 Primary map



X

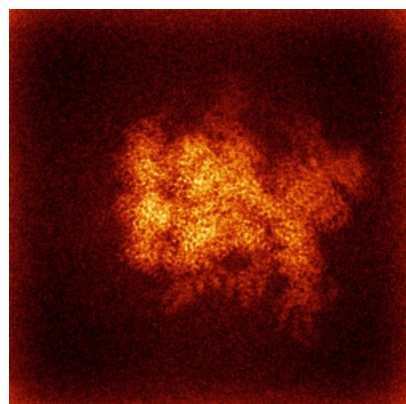


Y

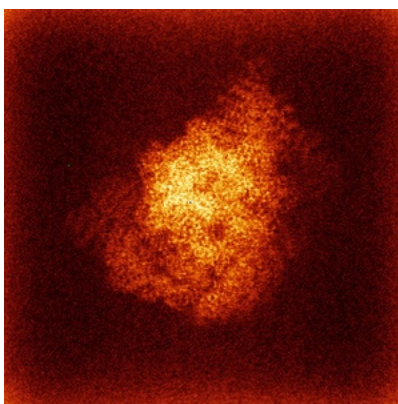


Z

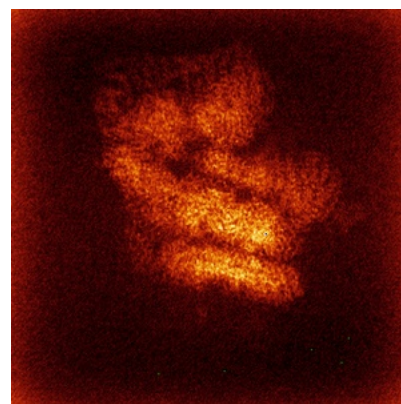
### 6.4.2 Raw map



X



Y

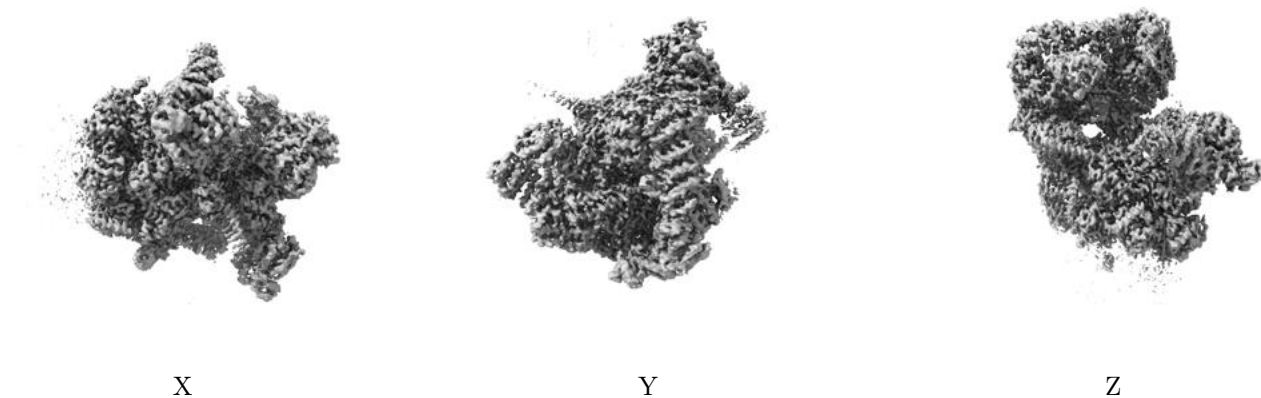


Z

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.

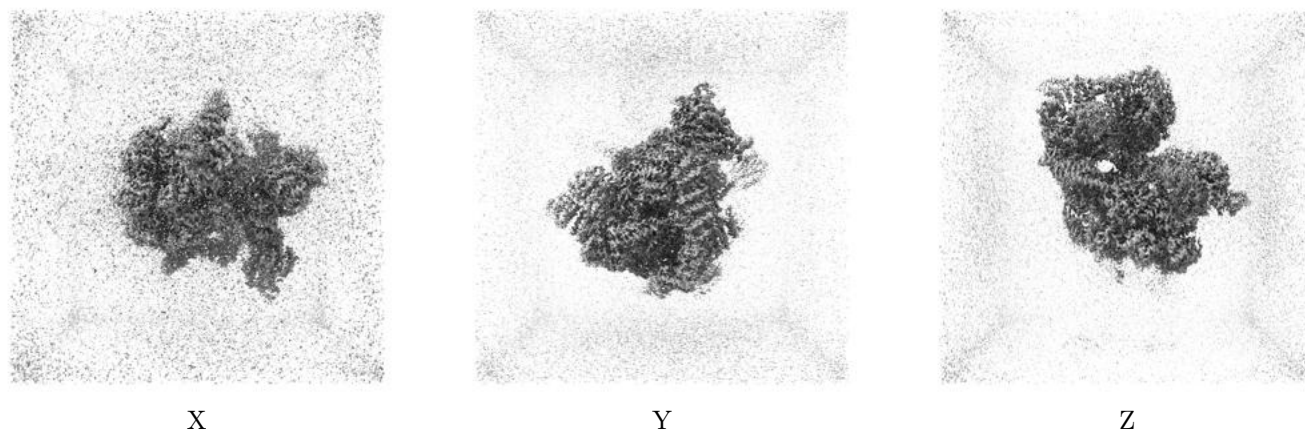
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

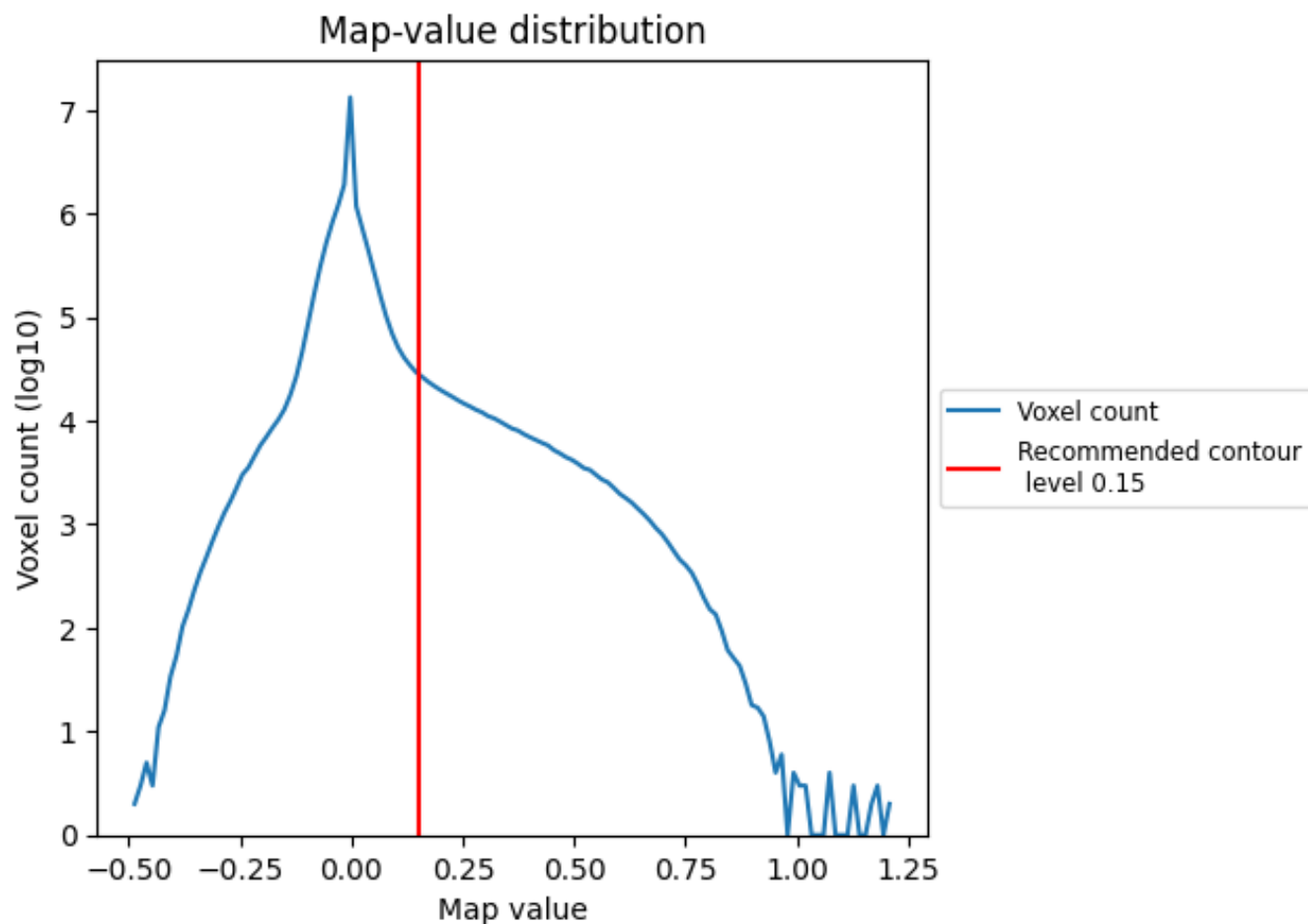
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

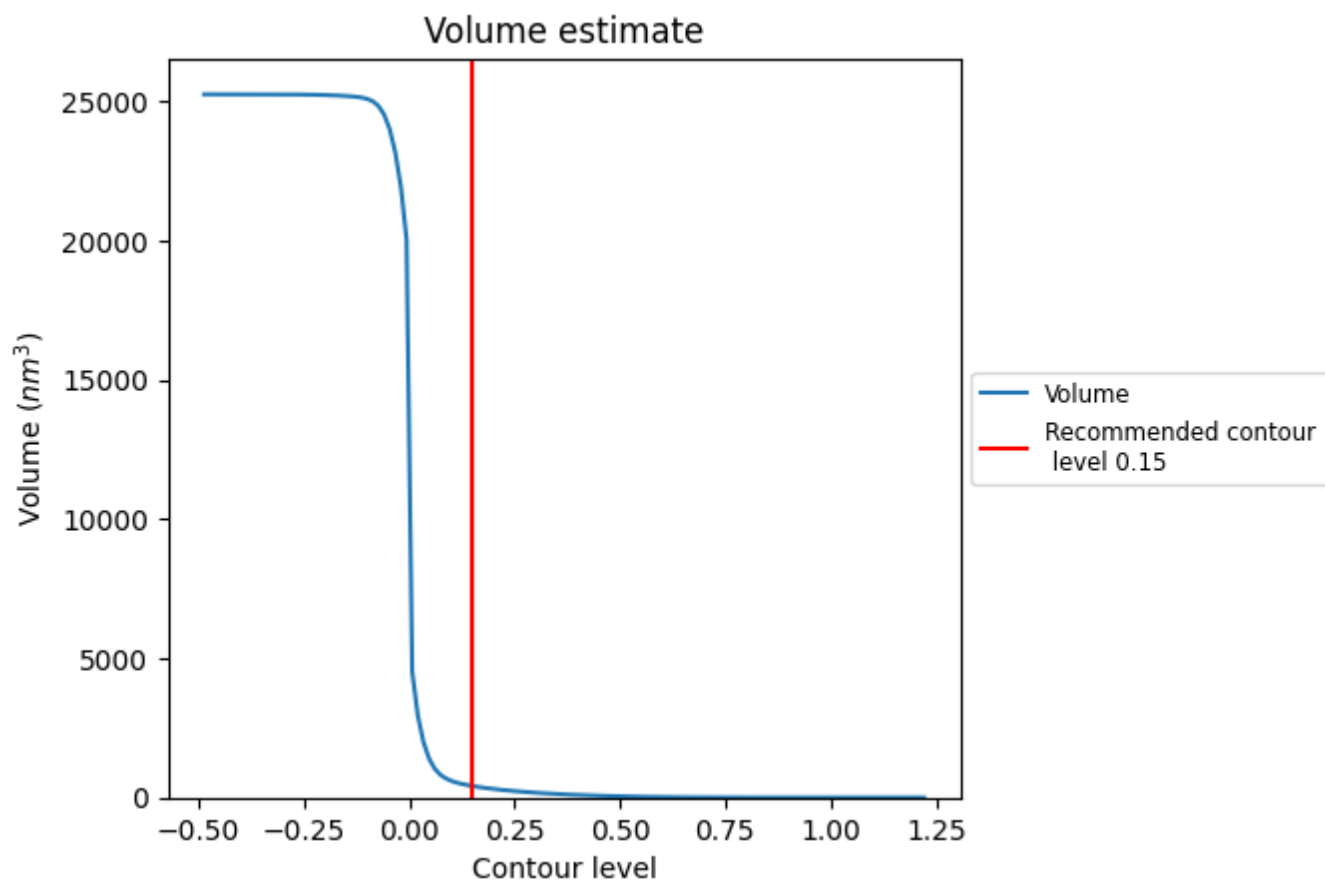
This section contains the results of statistical analysis of the map.

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



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

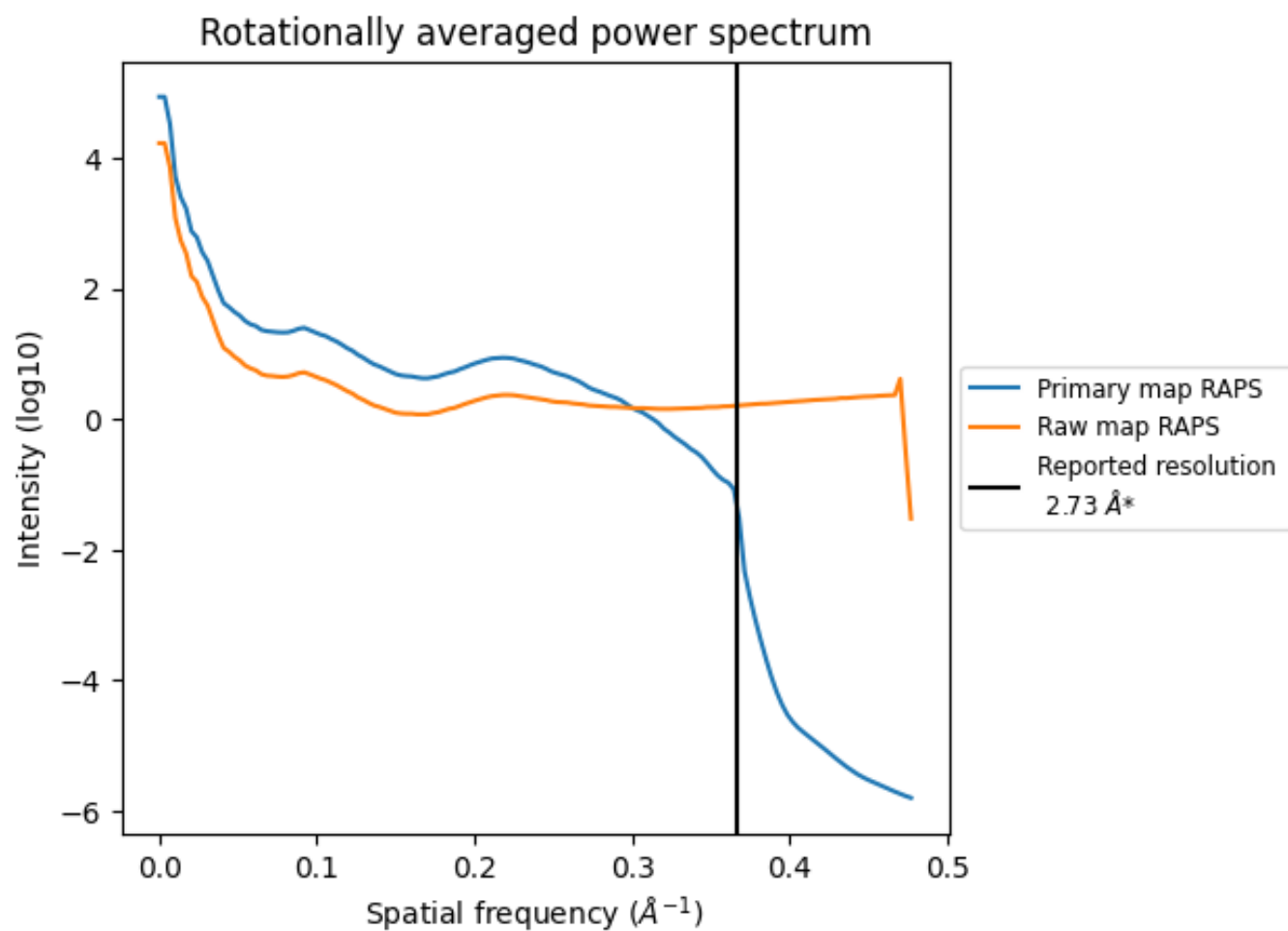
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 415 nm<sup>3</sup>; this corresponds to an approximate mass of 375 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ



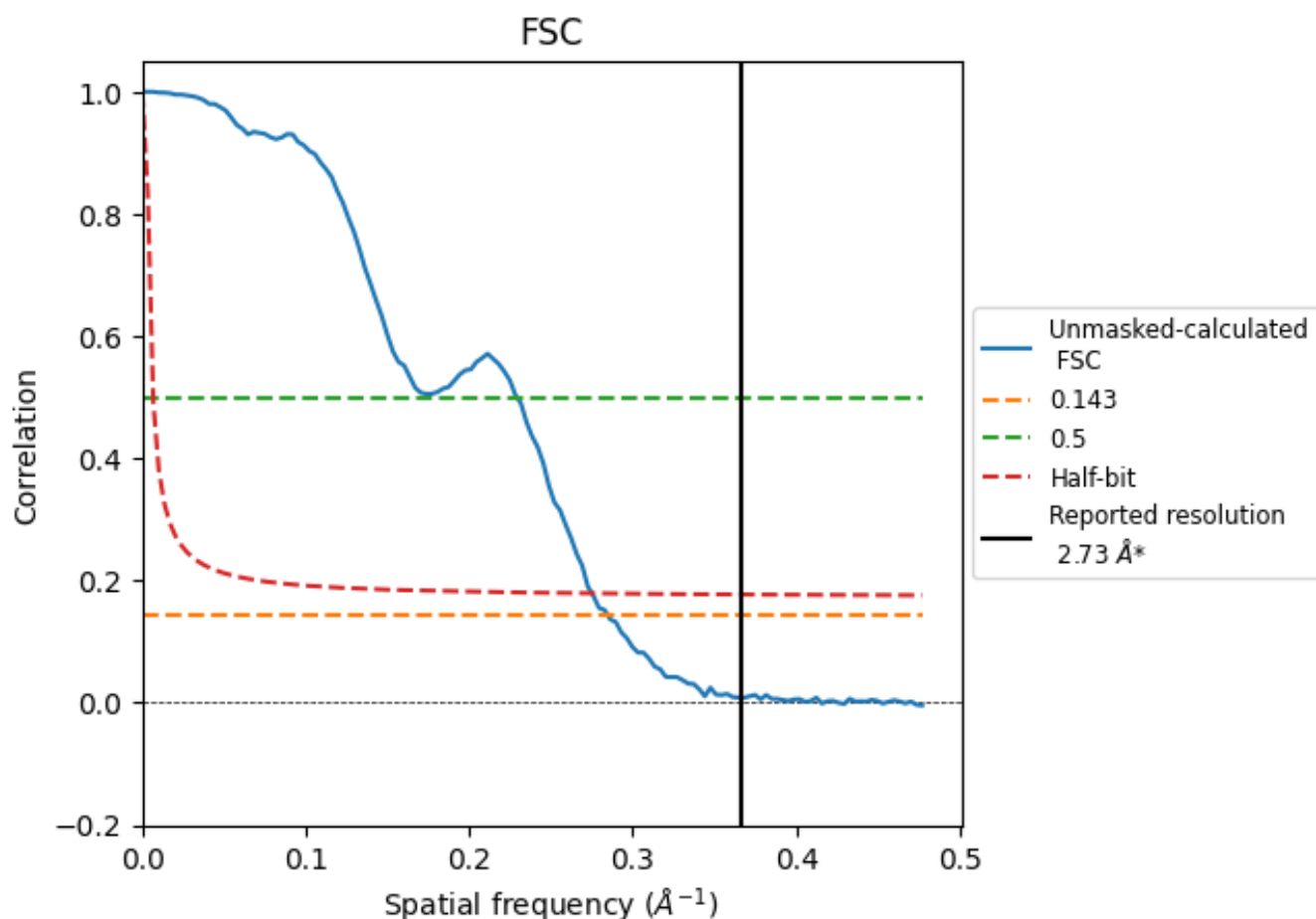
\*Reported resolution corresponds to spatial frequency of 0.366  $\text{\AA}^{-1}$



## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.366 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

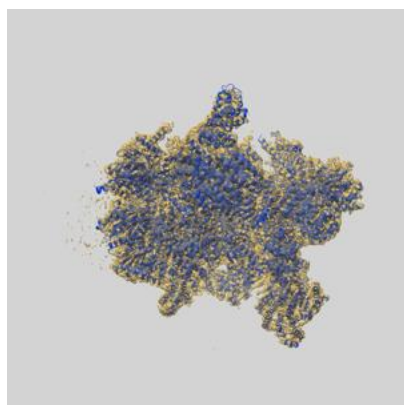
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.73	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.51	4.36	3.64

\*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 3.51 differs from the reported value 2.73 by more than 10 %

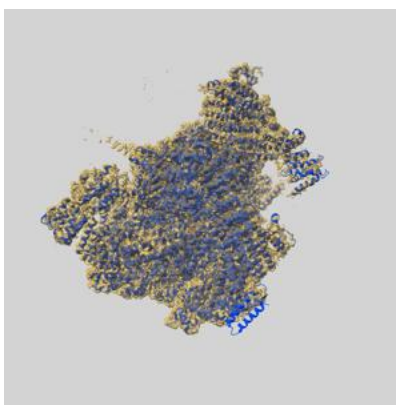
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-42506 and PDB model 8USB. Per-residue inclusion information can be found in [section 3](#) on [page 13](#).

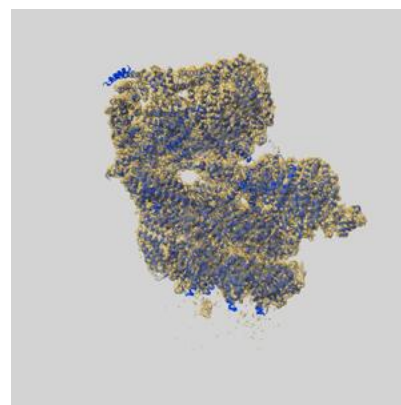
### 9.1 Map-model overlay [i](#)



X



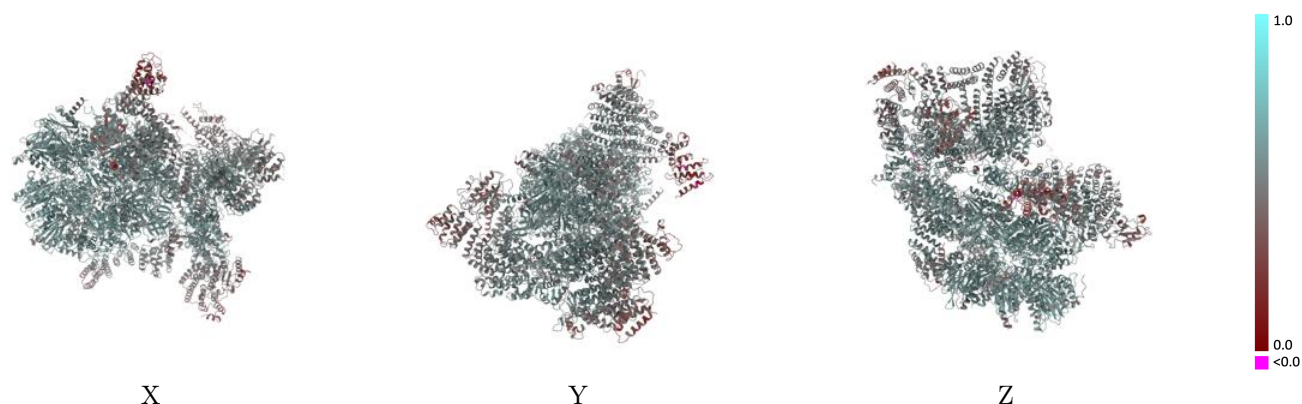
Y



Z

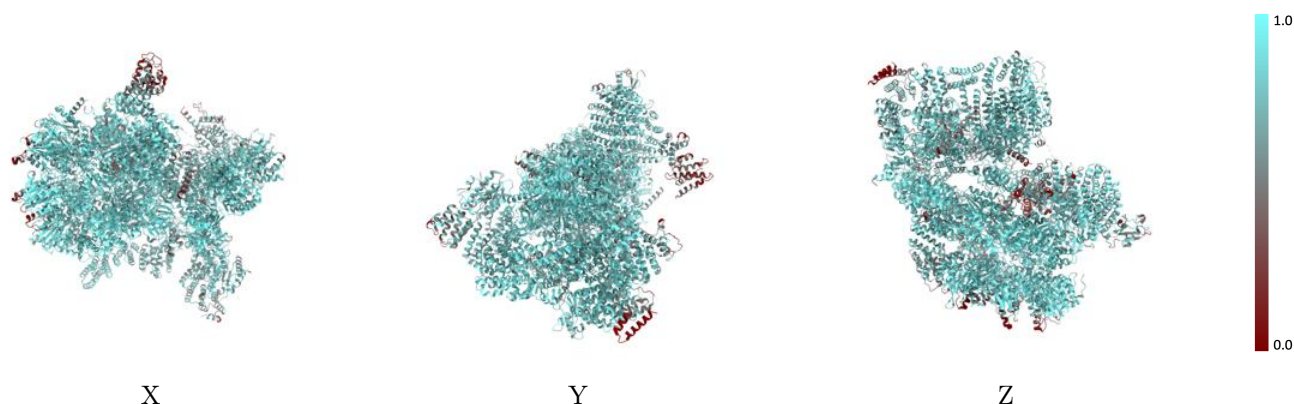
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



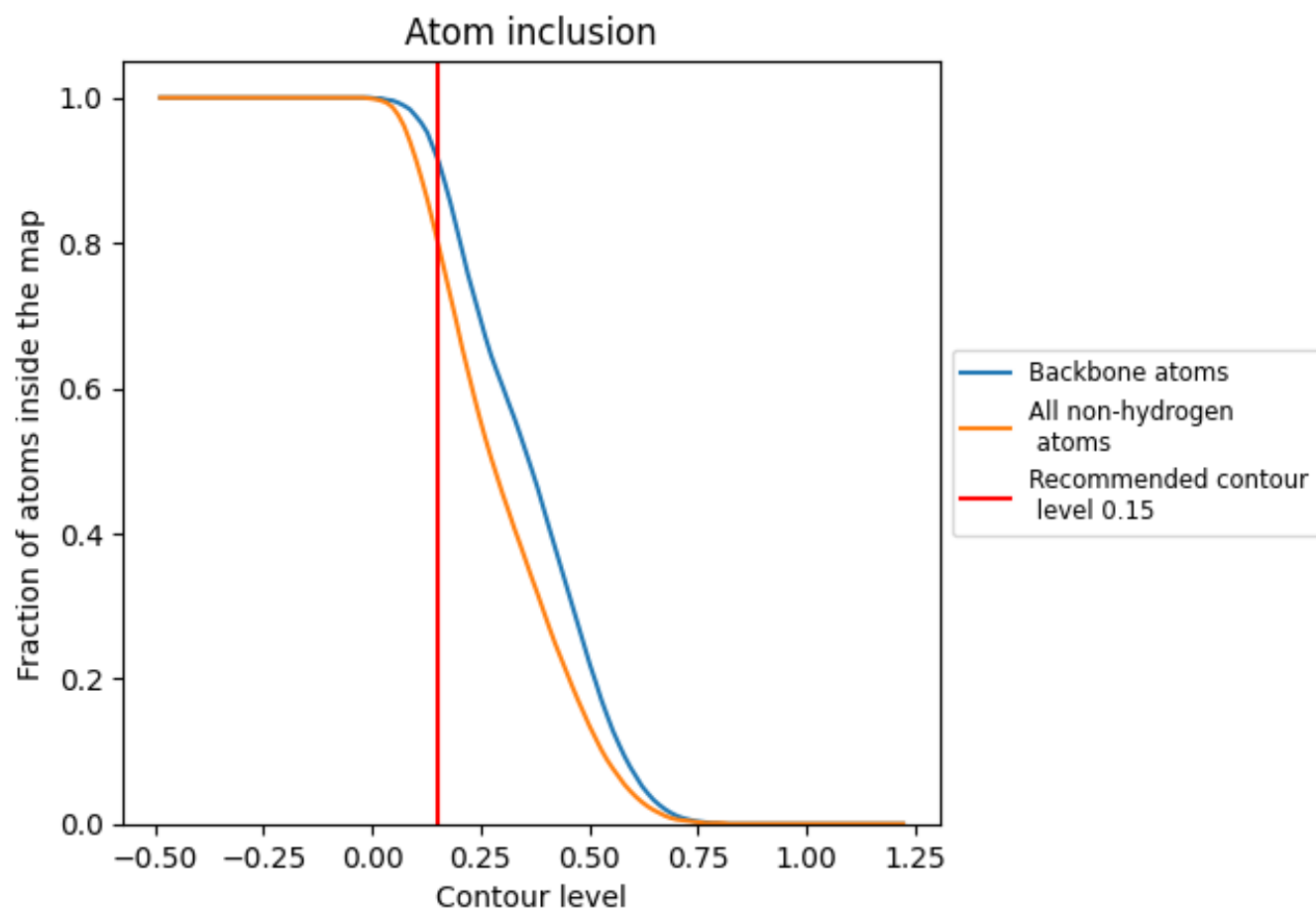
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.15).

























































## 9.4 Atom inclusion ⓘ



At the recommended contour level, 92% of all backbone atoms, 80% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8050	 0.5320
A	 0.8890	 0.5760
B	 0.8480	 0.5640
C	 0.8780	 0.5780
D	 0.8870	 0.5830
E	 0.9070	 0.5860
F	 0.8960	 0.5840
G	 0.8410	 0.5770
H	 0.8120	 0.5780
I	 0.8160	 0.5580
J	 0.7840	 0.5560
K	 0.8260	 0.5770
L	 0.8310	 0.5770
M	 0.8220	 0.5790
O	 0.7960	 0.5810
U	 0.8020	 0.5060
V	 0.7220	 0.4770
W	 0.8100	 0.5120
X	 0.7440	 0.5150
Y	 0.8670	 0.5540
Z	 0.8440	 0.5550
a	 0.7440	 0.4700
b	 0.6960	 0.4420
c	 0.8670	 0.5690
d	 0.6210	 0.4390
e	 0.6230	 0.4240
f	 0.7210	 0.4720
g	 0.5820	 0.4050

