



Full wwPDB EM Validation Report ⓘ

Dec 31, 2024 – 06:00 PM EST

PDB ID : 8JRI
EMDB ID : EMD-36598
Title : Cryo-EM structure of human 26S proteasomal RP subcomplex (Ea state) without any bound substrate.
Authors : Hsu, S.T.D.; Draczkowski, P.; Wang, Y.S.
Deposited on : 2023-06-16
Resolution : 3.40 Å(reported)
Based on initial model : 6MSB

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

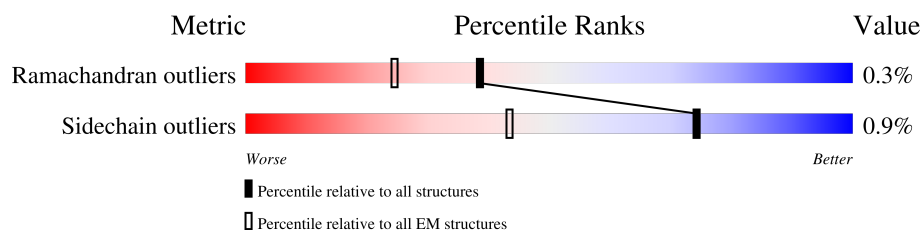
EMDB validation analysis : 0.0.1.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 Å.

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







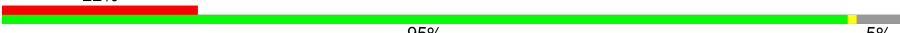









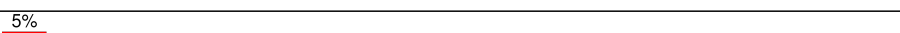
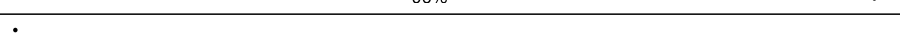
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	433	<div> <div>7%</div> <div>90%</div> <div>9%</div> </div>
2	B	440	<div> <div>7%</div> <div>87%</div> <div>13%</div> </div>
3	C	406	<div> <div>5%</div> <div>93%</div> <div>7%</div> </div>
4	D	418	<div> <div>90%</div> <div>9%</div> </div>
5	G	246	<div> <div>97%</div> </div>
6	H	234	<div> <div>99%</div> </div>
7	I	261	<div> <div>95%</div> </div>
8	J	248	<div> <div>96%</div> </div>
9	K	241	<div> <div>96%</div> </div>

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Mol	Chain	Length	Quality of chain
10	L	263	
11	M	255	
12	U	953	
13	c	310	
14	V	534	
15	W	456	
16	X	422	
17	Y	389	
18	Z	324	
19	a	376	
20	b	377	
21	d	350	
22	e	70	
23	f	908	
24	E	389	
25	F	439	

2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 62679 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 protease regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	394	Total	C	N	O	S	0	0
			2996	1886	531	561	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	384	Total	C	N	O	S	0	0
			2851	1786	493	560	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	379	Total	C	N	O	S	0	0
			2938	1850	531	541	16		

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

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

- Molecule 5 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	240	Total	C	N	O	S	0	0
			1826	1160	305	348	13		

- Molecule 6 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	232	Total	C	N	O	S	0	0
			1708	1081	289	333	5		

- Molecule 7 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	250	Total	C	N	O	S	0	0
			1912	1204	329	371	8		

- Molecule 8 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	239	Total	C	N	O	S	0	0
			1715	1064	311	335	5		

- Molecule 9 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	234	Total	C	N	O	S	0	0
			1759	1102	290	356	11		

- Molecule 10 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	238	Total	C	N	O	S	0	0
			1850	1159	334	346	11		

- Molecule 11 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	240	Total	C	N	O	S	0	0
			1856	1178	314	353	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	U	804	Total	C	N	O	S	0	0
			4492	2721	874	883	14		

- Molecule 13 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	c	287	Total	C	N	O	S	0	0
			2260	1430	389	422	19		

- Molecule 14 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	V	508	Total	C	N	O	S	0	0
			3121	1926	596	592	7		

- Molecule 15 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	W	456	Total	C	N	O	S	0	0
			3511	2216	609	665	21		

- Molecule 16 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	X	380	Total	C	N	O	S	0	0
			2932	1860	503	557	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Y	378	Total	C	N	O	S	0	0
			3115	1987	533	578	17		

- Molecule 18 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

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

- Molecule 19 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	a	373	Total	C	N	O	S	0	0
			2901	1843	497	546	15		

- Molecule 20 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

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

- Molecule 21 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	d	244	Total	C	N	O	S	0	0
			1692	1076	294	317	5		

- Molecule 22 is a protein called 26S proteasome complex subunit DSS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	e	40	Total	C	N	O	S	0	0
			248	148	47	52	1		

- Molecule 23 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	f	878	Total	C	N	O		0	0
			4328	2572	878	878			

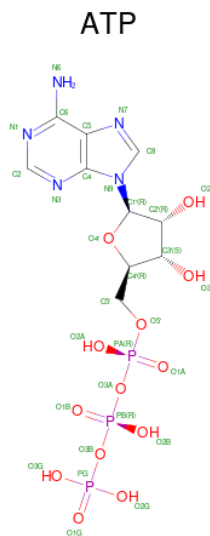
- Molecule 24 is a protein called 26S protease regulatory subunit 10B.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	E	375	Total	C	N	O	S	0	0
			2877	1806	514	541	16		

- Molecule 25 is a protein called 26S protease regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	F	377	Total	C	N	O	S	0	0
			2830	1783	491	541	15		

- Molecule 26 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 27 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 28 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$) (labeled as "Ligand of Interest" by depositor).

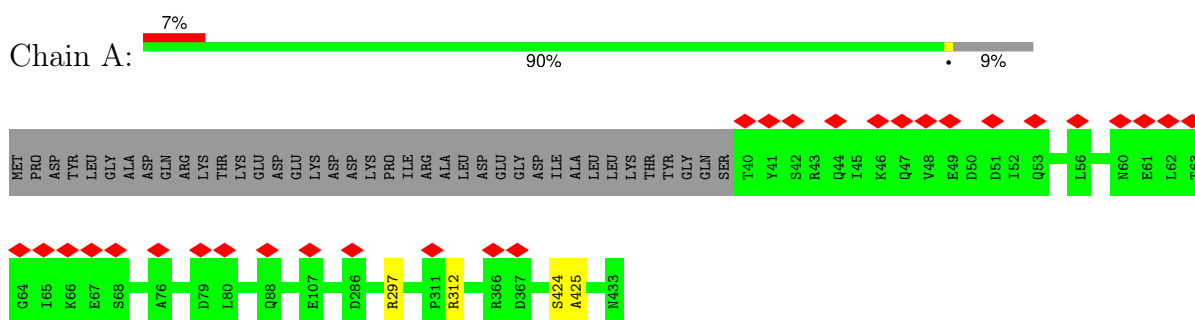


Mol	Chain	Residues	Atoms					AltConf
28	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
28	F	1	Total	C	N	O	P	0
			27	10	5	10	2	

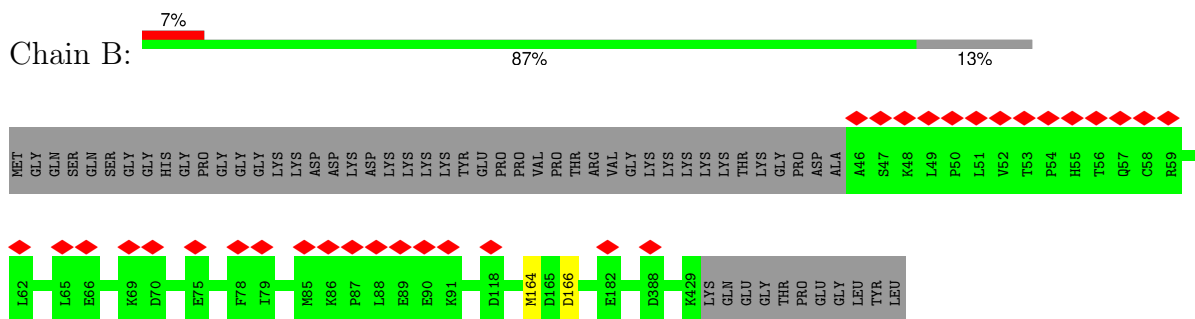
3 Residue-property plots [i](#)

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

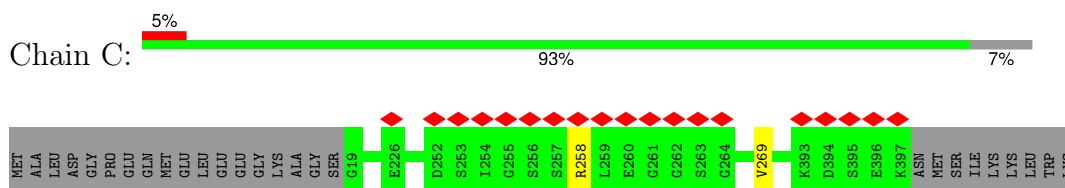
- Molecule 1: 26S protease regulatory subunit 7



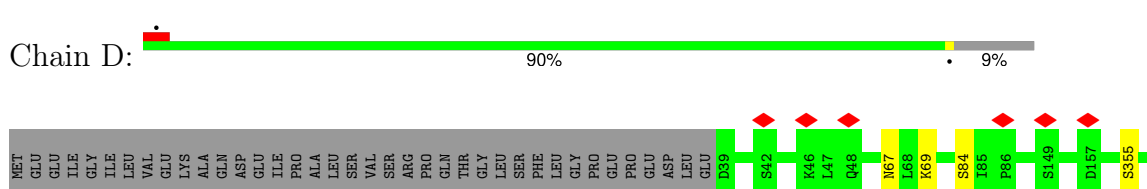
- Molecule 2: 26S protease regulatory subunit 4



- Molecule 3: 26S protease regulatory subunit 8



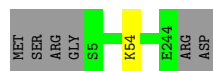
- Molecule 4: 26S protease regulatory subunit 6B





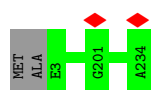
- Molecule 5: Proteasome subunit alpha type-6

Chain G: 97%



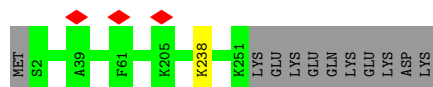
- Molecule 6: Proteasome subunit alpha type-2

Chain H: 99%



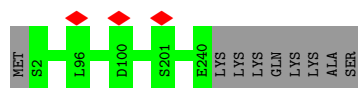
- Molecule 7: Proteasome subunit alpha type-4

Chain I: 95%



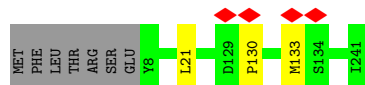
- Molecule 8: Proteasome subunit alpha type-7

Chain J: 96%



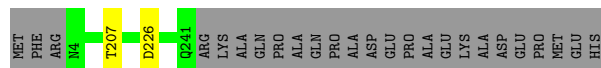
- Molecule 9: Proteasome subunit alpha type-5

Chain K: 96%



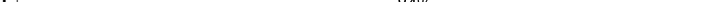
- Molecule 10: Proteasome subunit alpha type-1

Chain L: 90% 10%



- Molecule 11: Proteasome subunit alpha type-3

MET
SER
SER
ILE
GLY
T5
R40
K207
K244
GLU
GLU
ASP
GLU
SER
ASP
ASP
ASP
ASN
MET

- Chain U:  9% 84% 16%

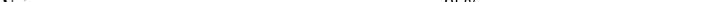
[illegible]

- Chain c: 93% 7%

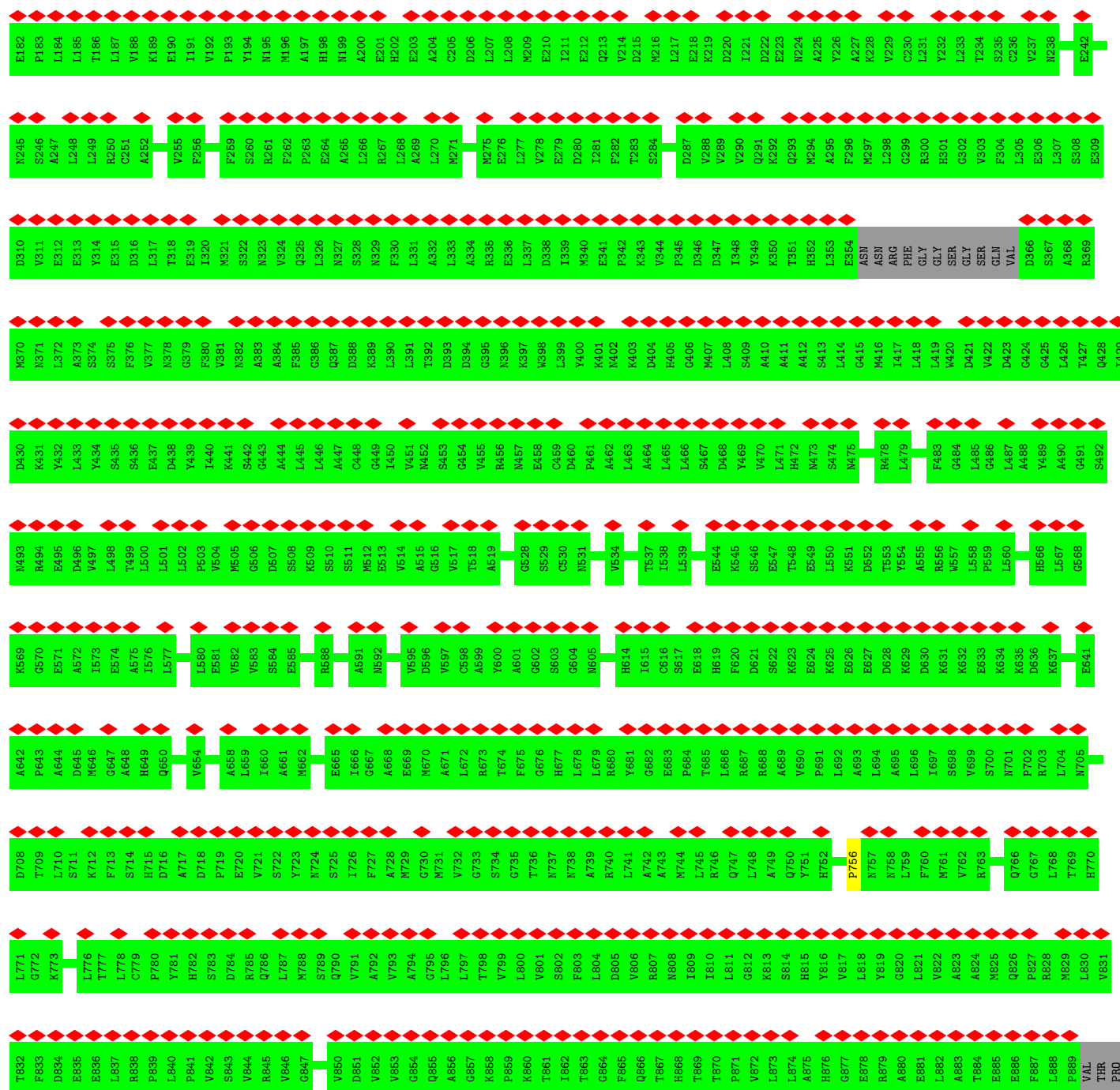
NET

ASP
ARG
LEU
LEU
ARG
LEU
GLY
GLY
GLY
MET
PRO
GLY
LEU
GLY
GLN
GLY
PRO
PRO
THR
ASP
ALA
PRD
A24

G81
V87
N166
V189
E288
K273
K310

- Chain V:  22% 95% 5%

N199	R200	R201	A202	L205	D243	A244	K273	S274	V275	F276	P277	N281	E304	V322	G323	F324	P343	D344	F348	P361	D429	I464	D465	P497	N502	K503	D504	L505	E506	S507	A508	E509	E510	R511	R512	K523	E524	M525	ALA	GLU	ASP	ASP	ASP	SER										
A97	L98	R99	M100	L101	P102	S103	T104	S105	R106	R107	L108	M109	H110	Y111	M112	L113	Y114	K115	A116	V117	Q118	G119	F120	F121	T122	S123	M124	M125	A126	T127	R128	D129	F130	P138	T141	E142	A143	D144	L145	Q146	Q168	L169	L170	V171	K186	I187	L191	M192	Q193	K194	I195	S196	T197	Q198
MET	LYS	GLN	GLY	SER	ALA	ARG	ARG	GLY	ALA	ASP	LYS	ALA	LYS	PRO	P18	P19	G20	G21	G22	Q23	Q24	E25	F32	E39	G49	E50	A51	D52	G53	K54	T55	A56	A57	A58	A59	H62	R65	D74	I76	K76	E77	H78	V79	K80	Q81	L82	E83	K84	A85	V86				



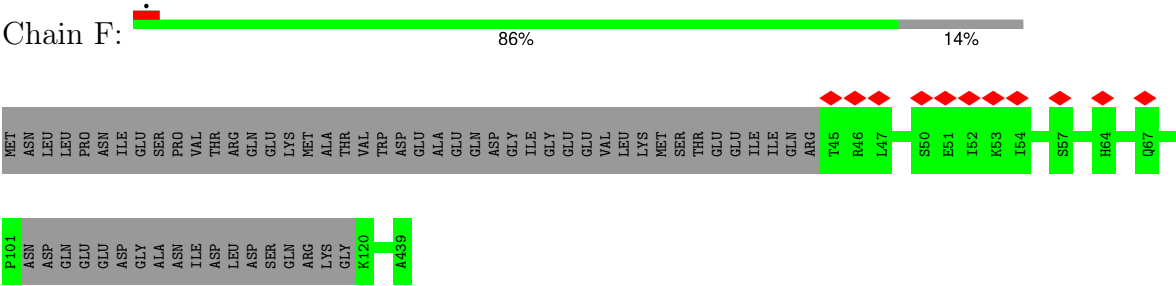
ILE
LEU
GLU
GLY
PRO
ARG
PHE
VAL
ILE
LEU
LEU
ARG
GLN
ASN
ASN
PRO
TYR
ASP
LEU

- Molecule 24: 26S protease regulatory subunit 10B

Chain E: 5% 96%

MET
ALA
ASP
PRO
ARG
ASP
LYS
ALA
LEU
LEU
GLN
ASP
TYR
PRO
ASP
LYS
K15
L16
L17
E18
H19
K20
E21
I22
D23
G24
R25
L26
K27
E28
L29
R30
E31
Q32
E35
K38
E41
P127
N262
V389

• Molecule 25: 26S protease regulatory subunit 6A



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	153646	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	49	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	70000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.931	Depositor
Minimum map value	-1.690	Depositor
Average map value	-0.003	Depositor
Map value standard deviation	0.087	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	560.0, 560.0, 560.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4, 1.4, 1.4	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, MG, 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	A	0.26	0/3047	0.54	0/4123
2	B	0.25	0/2888	0.50	0/3912
3	C	0.26	0/2977	0.51	0/4008
4	D	0.26	0/3089	0.53	0/4168
5	G	0.26	0/1859	0.49	0/2523
6	H	0.27	0/1743	0.48	0/2372
7	I	0.26	0/1942	0.52	0/2628
8	J	0.25	0/1739	0.52	0/2372
9	K	0.26	0/1786	0.52	0/2419
10	L	0.26	0/1885	0.55	0/2552
11	M	0.26	0/1891	0.49	0/2552
12	U	0.24	0/4510	0.44	0/6215
13	c	0.25	0/2302	0.49	0/3110
14	V	0.25	0/3149	0.49	0/4317
15	W	0.26	0/3557	0.56	0/4799
16	X	0.25	0/2975	0.48	0/4016
17	Y	0.26	0/3173	0.53	0/4273
18	Z	0.26	0/2324	0.47	0/3150
19	a	0.25	0/2951	0.50	0/3998
20	b	0.25	0/1478	0.53	0/2001
21	d	0.25	0/1717	0.47	0/2339
22	e	0.24	0/248	0.53	0/333
23	f	0.24	0/4326	0.42	0/6016
24	E	0.25	0/2921	0.51	0/3945
25	F	0.25	0/2869	0.48	0/3884
All	All	0.25	0/63346	0.50	0/86025

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](#)

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	A	392/433 (90%)	340 (87%)	50 (13%)	2 (0%)	25	54
2	B	382/440 (87%)	348 (91%)	34 (9%)	0	100	100
3	C	377/406 (93%)	344 (91%)	31 (8%)	2 (0%)	25	54
4	D	378/418 (90%)	334 (88%)	42 (11%)	2 (0%)	25	54
5	G	238/246 (97%)	223 (94%)	15 (6%)	0	100	100
6	H	230/234 (98%)	221 (96%)	9 (4%)	0	100	100
7	I	248/261 (95%)	233 (94%)	15 (6%)	0	100	100
8	J	237/248 (96%)	223 (94%)	14 (6%)	0	100	100
9	K	232/241 (96%)	216 (93%)	13 (6%)	3 (1%)	10	33
10	L	236/263 (90%)	221 (94%)	13 (6%)	2 (1%)	16	44
11	M	238/255 (93%)	224 (94%)	14 (6%)	0	100	100
12	U	798/953 (84%)	778 (98%)	20 (2%)	0	100	100
13	c	285/310 (92%)	274 (96%)	11 (4%)	0	100	100
14	V	506/534 (95%)	472 (93%)	31 (6%)	3 (1%)	22	50
15	W	454/456 (100%)	400 (88%)	47 (10%)	7 (2%)	8	30
16	X	378/422 (90%)	350 (93%)	28 (7%)	0	100	100
17	Y	376/389 (97%)	348 (93%)	27 (7%)	1 (0%)	37	66
18	Z	284/324 (88%)	269 (95%)	15 (5%)	0	100	100
19	a	371/376 (99%)	354 (95%)	17 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	b	189/377 (50%)	174 (92%)	15 (8%)	0	100	100
21	d	240/350 (69%)	217 (90%)	21 (9%)	2 (1%)	16	44
22	e	36/70 (51%)	25 (69%)	9 (25%)	2 (6%)	1	10
23	f	874/908 (96%)	766 (88%)	107 (12%)	1 (0%)	48	78
24	E	373/389 (96%)	359 (96%)	14 (4%)	0	100	100
25	F	373/439 (85%)	360 (96%)	13 (4%)	0	100	100
All	All	8725/9742 (90%)	8073 (92%)	625 (7%)	27 (0%)	38	66

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
14	V	322	VAL
14	V	324	PHE
14	V	465	ASP
15	W	137	TYR
21	d	219	PRO
22	e	43	TRP
23	f	756	PRO
15	W	115	ILE
15	W	118	LEU
21	d	239	SER
1	A	425	ALA
15	W	84	ASN
22	e	56	LEU
4	D	84	SER
9	K	21	LEU
10	L	226	ASP
15	W	260	SER
15	W	316	ARG
17	Y	207	THR
1	A	424	SER
4	D	355	SER
10	L	207	THR
3	C	258	ARG
9	K	133	MET
9	K	130	PRO
3	C	269	VAL
15	W	138	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	307/372 (82%)	305 (99%)	2 (1%)	81	88
2	B	292/385 (76%)	290 (99%)	2 (1%)	81	88
3	C	314/352 (89%)	314 (100%)	0	100	100
4	D	333/366 (91%)	331 (99%)	2 (1%)	84	90
5	G	193/210 (92%)	192 (100%)	1 (0%)	86	91
6	H	164/191 (86%)	164 (100%)	0	100	100
7	I	193/221 (87%)	192 (100%)	1 (0%)	86	91
8	J	155/211 (74%)	155 (100%)	0	100	100
9	K	189/203 (93%)	189 (100%)	0	100	100
10	L	198/224 (88%)	198 (100%)	0	100	100
11	M	192/212 (91%)	191 (100%)	1 (0%)	86	91
12	U	159/816 (20%)	158 (99%)	1 (1%)	84	90
13	c	252/268 (94%)	252 (100%)	0	100	100
14	V	172/460 (37%)	172 (100%)	0	100	100
15	W	355/416 (85%)	328 (92%)	27 (8%)	11	34
16	X	303/362 (84%)	302 (100%)	1 (0%)	91	95
17	Y	334/344 (97%)	329 (98%)	5 (2%)	60	76
18	Z	257/295 (87%)	255 (99%)	2 (1%)	79	87
19	a	307/336 (91%)	305 (99%)	2 (1%)	81	88
20	b	167/312 (54%)	166 (99%)	1 (1%)	84	90
21	d	133/294 (45%)	132 (99%)	1 (1%)	79	87
22	e	12/63 (19%)	11 (92%)	1 (8%)	9	30
24	E	303/341 (89%)	302 (100%)	1 (0%)	91	95
25	F	286/379 (76%)	286 (100%)	0	100	100
All	All	5570/7633 (73%)	5519 (99%)	51 (1%)	74	86

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	297	ARG
1	A	312	ARG
2	B	164	MET
2	B	166	ASP
4	D	67	ASN
4	D	69	LYS
5	G	54	LYS
7	I	238	LYS
11	M	40	ARG
12	U	715	LYS
15	W	73	MET
15	W	75	TYR
15	W	79	GLU
15	W	80	TRP
15	W	83	LEU
15	W	85	GLU
15	W	89	LEU
15	W	93	ARG
15	W	96	GLN
15	W	99	GLN
15	W	101	VAL
15	W	104	MET
15	W	105	VAL
15	W	106	GLN
15	W	107	GLN
15	W	113	GLU
15	W	116	THR
15	W	124	LEU
15	W	135	LYS
15	W	137	TYR
15	W	140	ILE
15	W	141	GLU
15	W	154	GLU
15	W	159	VAL
15	W	169	LEU
15	W	173	THR
15	W	262	LYS
16	X	420	LYS
17	Y	202	LEU
17	Y	204	THR
17	Y	205	VAL
17	Y	207	THR
17	Y	213	LEU

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Mol	Chain	Res	Type
18	Z	109	ASN
18	Z	282	ASN
19	a	219	HIS
19	a	231	GLN
20	b	137	ASN
21	d	110	ASN
22	e	57	ARG
24	E	262	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
4	D	48	GLN
4	D	257	ASN
15	W	96	GLN
15	W	106	GLN
19	a	62	ASN
20	b	34	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 11 ligands modelled in this entry, 5 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
28	ADP	C	501	-	24,29,29	0.86	0	29,45,45	1.18	2 (6%)
26	ATP	E	401	27	28,33,33	0.66	0	34,52,52	0.72	2 (5%)
26	ATP	A	501	27	28,33,33	0.71	0	34,52,52	0.71	2 (5%)
26	ATP	D	501	27	28,33,33	0.68	0	34,52,52	0.61	1 (2%)
26	ATP	B	501	27	28,33,33	0.71	0	34,52,52	0.61	1 (2%)
28	ADP	F	501	27	24,29,29	0.88	1 (4%)	29,45,45	1.29	3 (10%)

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
28	ADP	C	501	-	-	4/12/32/32	0/3/3/3
26	ATP	E	401	27	-	12/18/38/38	0/3/3/3
26	ATP	A	501	27	-	5/18/38/38	0/3/3/3
26	ATP	D	501	27	-	9/18/38/38	0/3/3/3
26	ATP	B	501	27	-	6/18/38/38	0/3/3/3
28	ADP	F	501	27	-	5/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	F	501	ADP	O4'-C1'	2.06	1.43	1.40

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	C	501	ADP	N3-C2-N1	-3.52	123.90	128.67
28	F	501	ADP	O4'-C1'-N9	3.36	113.20	108.75
28	F	501	ADP	N3-C2-N1	-3.09	124.48	128.67
28	C	501	ADP	C4-C5-N7	-2.66	106.53	109.34
28	F	501	ADP	C4-C5-N7	-2.55	106.64	109.34
26	B	501	ATP	C5-C6-N6	2.34	123.88	120.31
26	A	501	ATP	C5-C6-N6	2.31	123.83	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	E	401	ATP	C5-C6-N6	2.29	123.80	120.31
26	D	501	ATP	C5-C6-N6	2.29	123.80	120.31
26	E	401	ATP	C4'-O4'-C1'	-2.27	107.84	109.92
26	A	501	ATP	C4'-O4'-C1'	-2.10	108.00	109.92

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	A	501	ATP	C5'-O5'-PA-O1A
26	A	501	ATP	C5'-O5'-PA-O2A
26	A	501	ATP	C5'-O5'-PA-O3A
26	B	501	ATP	C5'-O5'-PA-O1A
26	B	501	ATP	C5'-O5'-PA-O2A
26	B	501	ATP	C5'-O5'-PA-O3A
26	D	501	ATP	PB-O3B-PG-O2G
26	D	501	ATP	C5'-O5'-PA-O1A
26	E	401	ATP	PB-O3B-PG-O2G
26	E	401	ATP	C5'-O5'-PA-O1A
26	E	401	ATP	C5'-O5'-PA-O2A
26	E	401	ATP	C5'-O5'-PA-O3A
26	E	401	ATP	O4'-C4'-C5'-O5'
28	C	501	ADP	C5'-O5'-PA-O2A
28	C	501	ADP	C5'-O5'-PA-O3A
28	F	501	ADP	C5'-O5'-PA-O1A
28	F	501	ADP	C5'-O5'-PA-O3A
26	A	501	ATP	O4'-C4'-C5'-O5'
26	E	401	ATP	C3'-C4'-C5'-O5'
26	D	501	ATP	O4'-C4'-C5'-O5'
28	F	501	ADP	O4'-C4'-C5'-O5'
26	D	501	ATP	C3'-C4'-C5'-O5'
28	F	501	ADP	C3'-C4'-C5'-O5'
26	A	501	ATP	C3'-C4'-C5'-O5'
26	D	501	ATP	PB-O3A-PA-O1A
28	C	501	ADP	C3'-C4'-C5'-O5'
26	B	501	ATP	PA-O3A-PB-O2B
26	D	501	ATP	C5'-O5'-PA-O3A
26	B	501	ATP	PG-O3B-PB-O2B
28	F	501	ADP	C4'-C5'-O5'-PA
28	C	501	ADP	O4'-C4'-C5'-O5'
26	E	401	ATP	PG-O3B-PB-O1B
26	D	501	ATP	PB-O3B-PG-O3G

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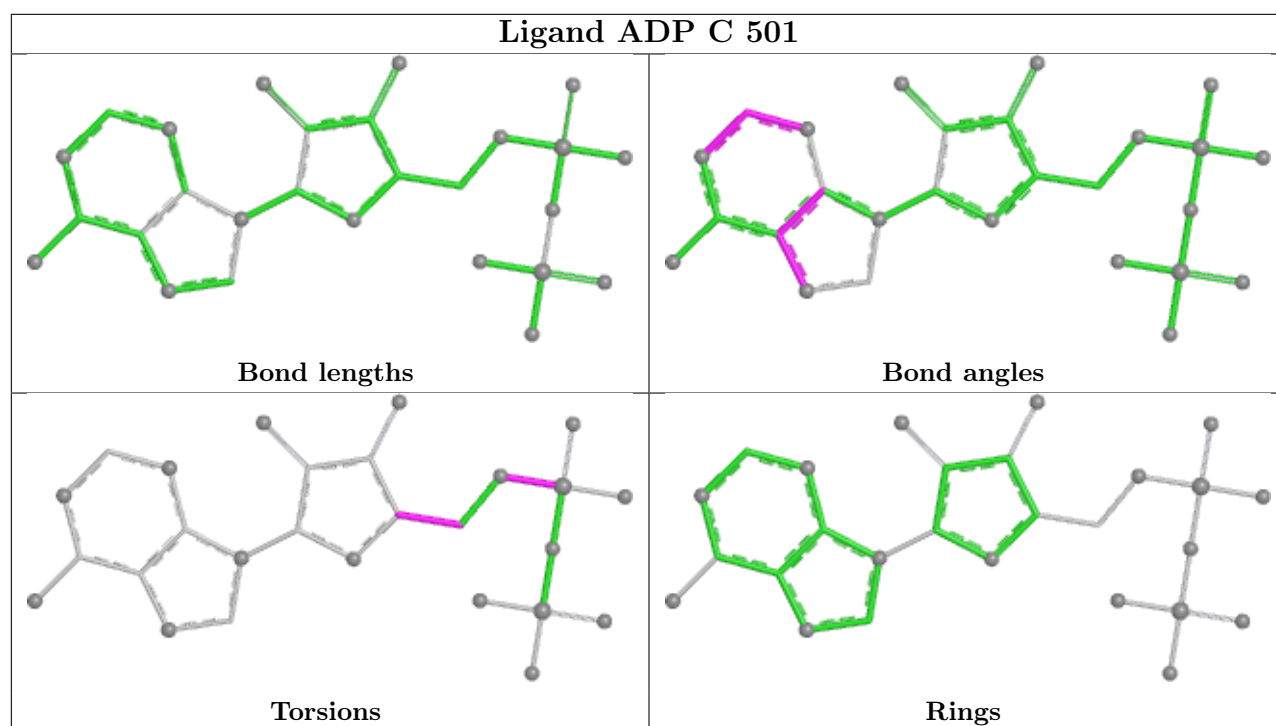
Continued from previous page...

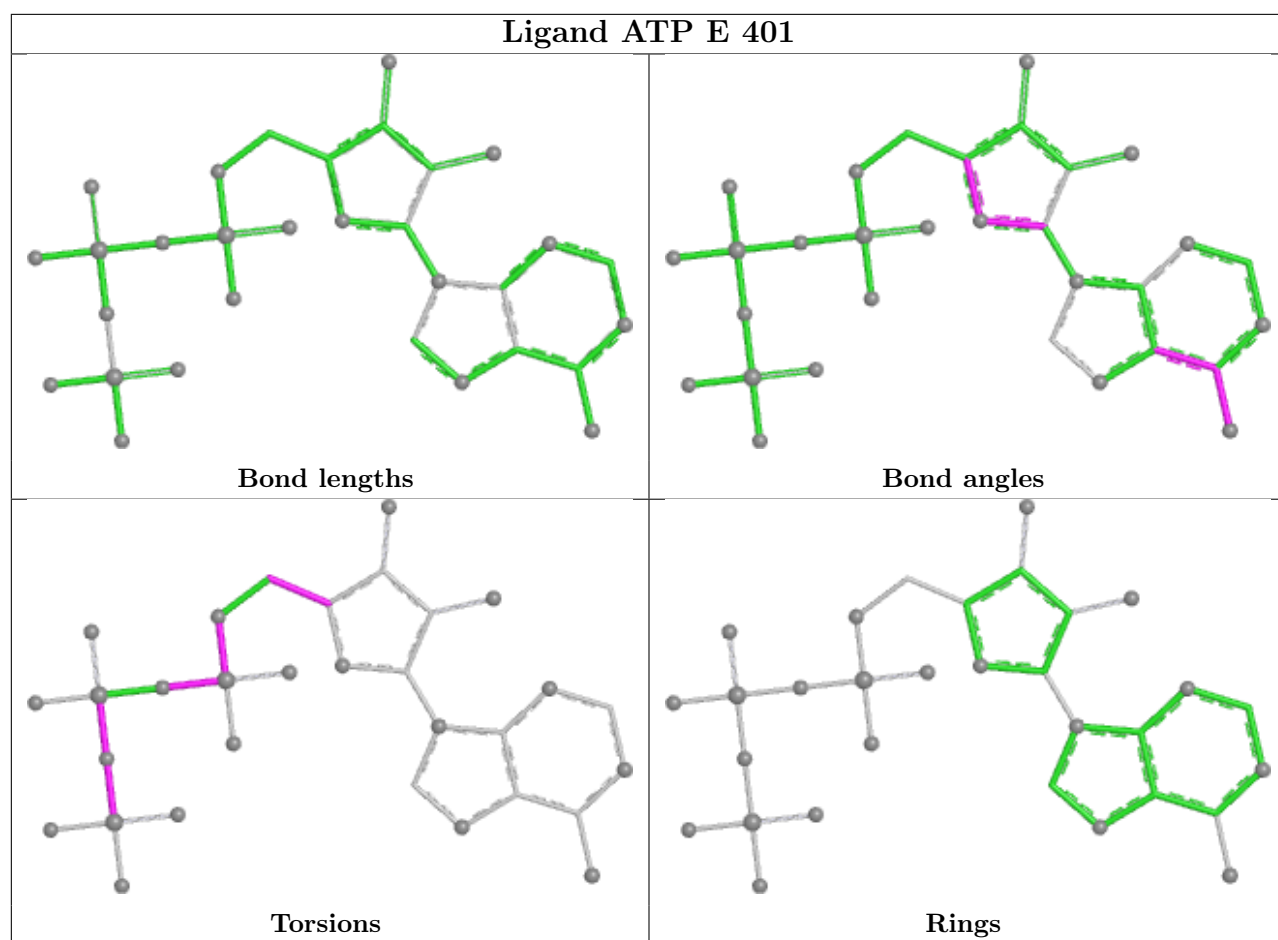
Mol	Chain	Res	Type	Atoms
26	E	401	ATP	PB-O3B-PG-O3G
26	B	501	ATP	PA-O3A-PB-O1B
26	D	501	ATP	PB-O3A-PA-O2A
26	E	401	ATP	PG-O3B-PB-O2B
26	D	501	ATP	PB-O3B-PG-O1G
26	E	401	ATP	PB-O3B-PG-O1G
26	E	401	ATP	PB-O3A-PA-O1A
26	E	401	ATP	PB-O3A-PA-O2A

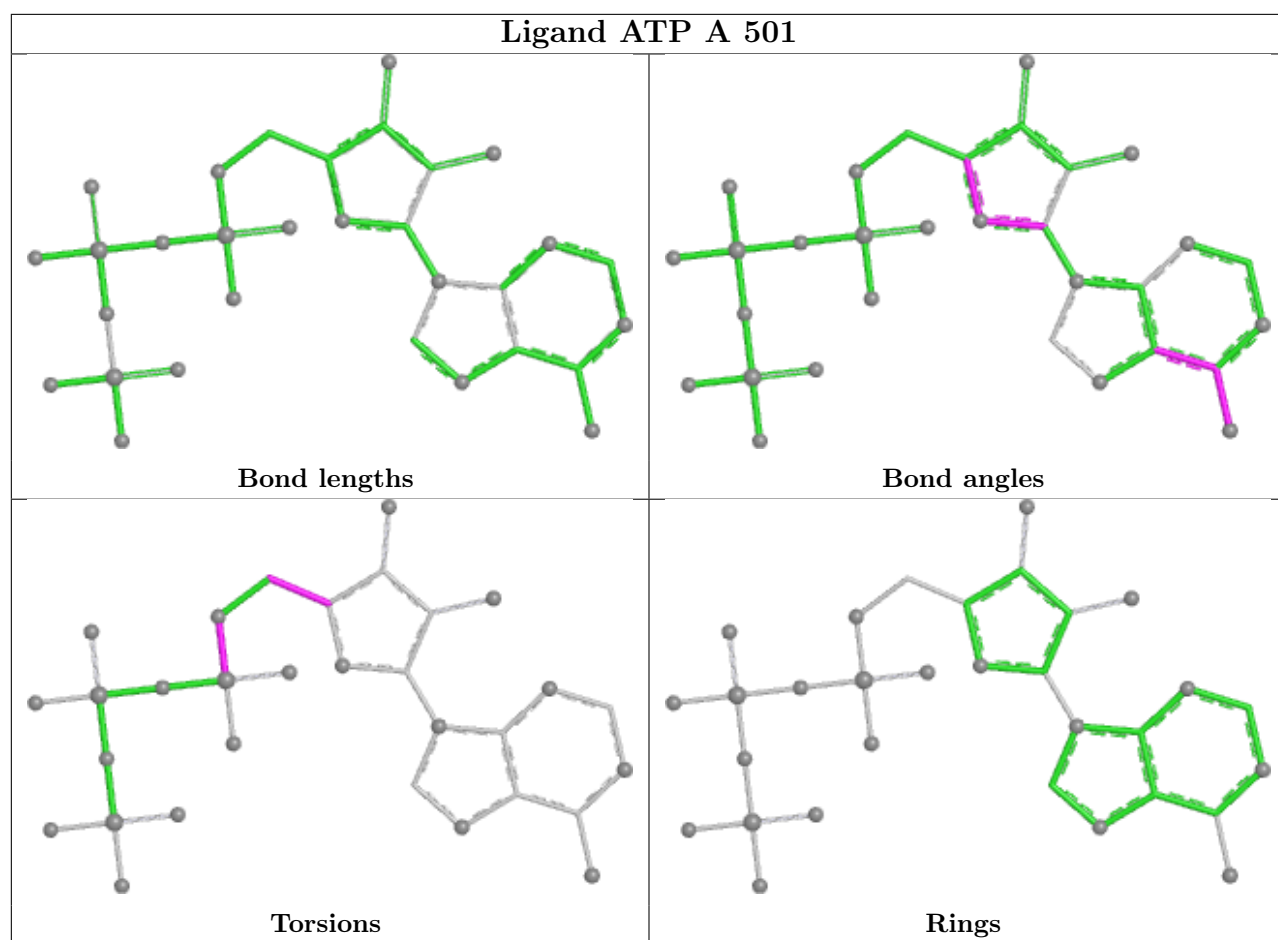
There are no ring outliers.

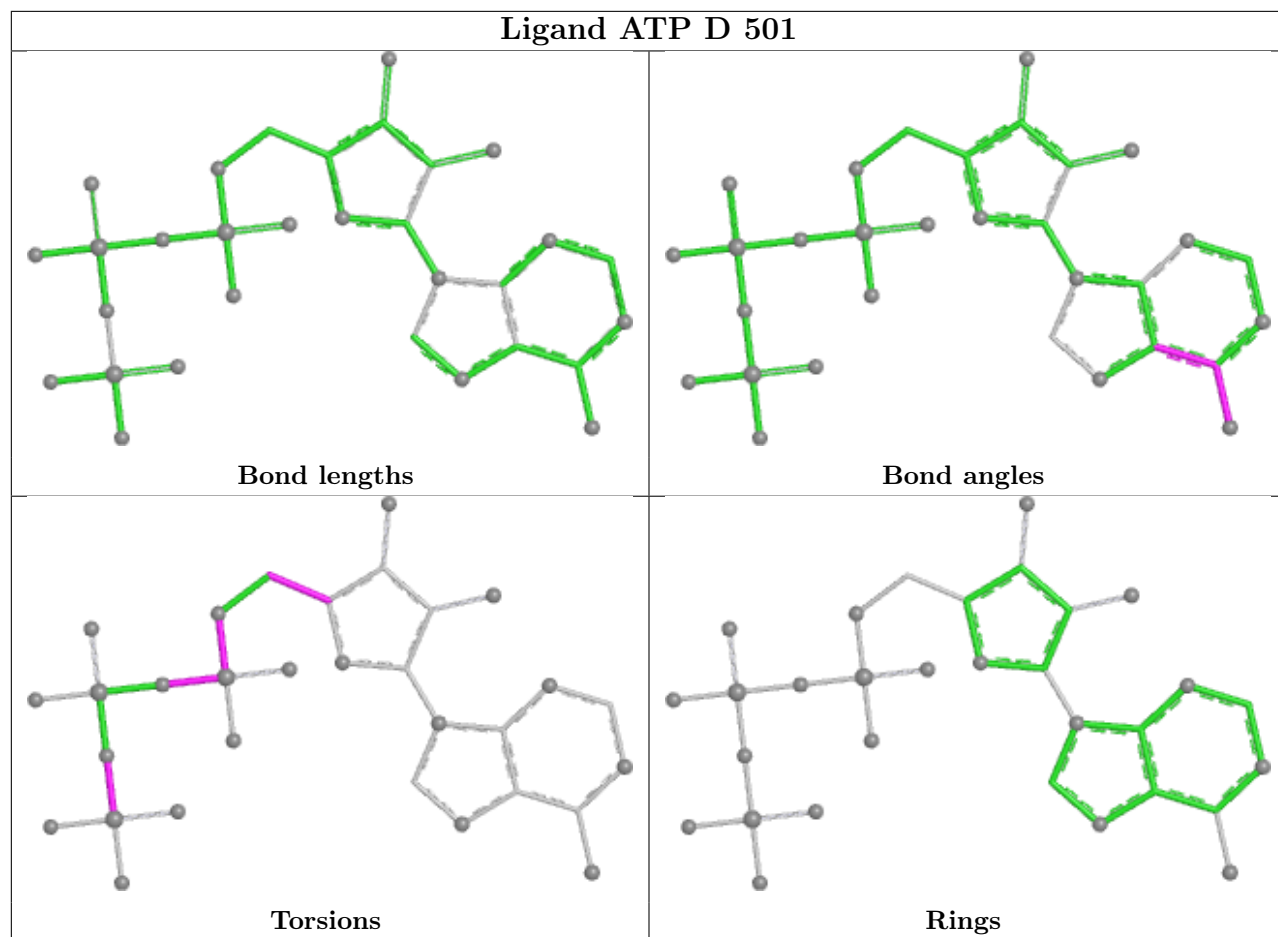
No monomer is involved in short contacts.

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.

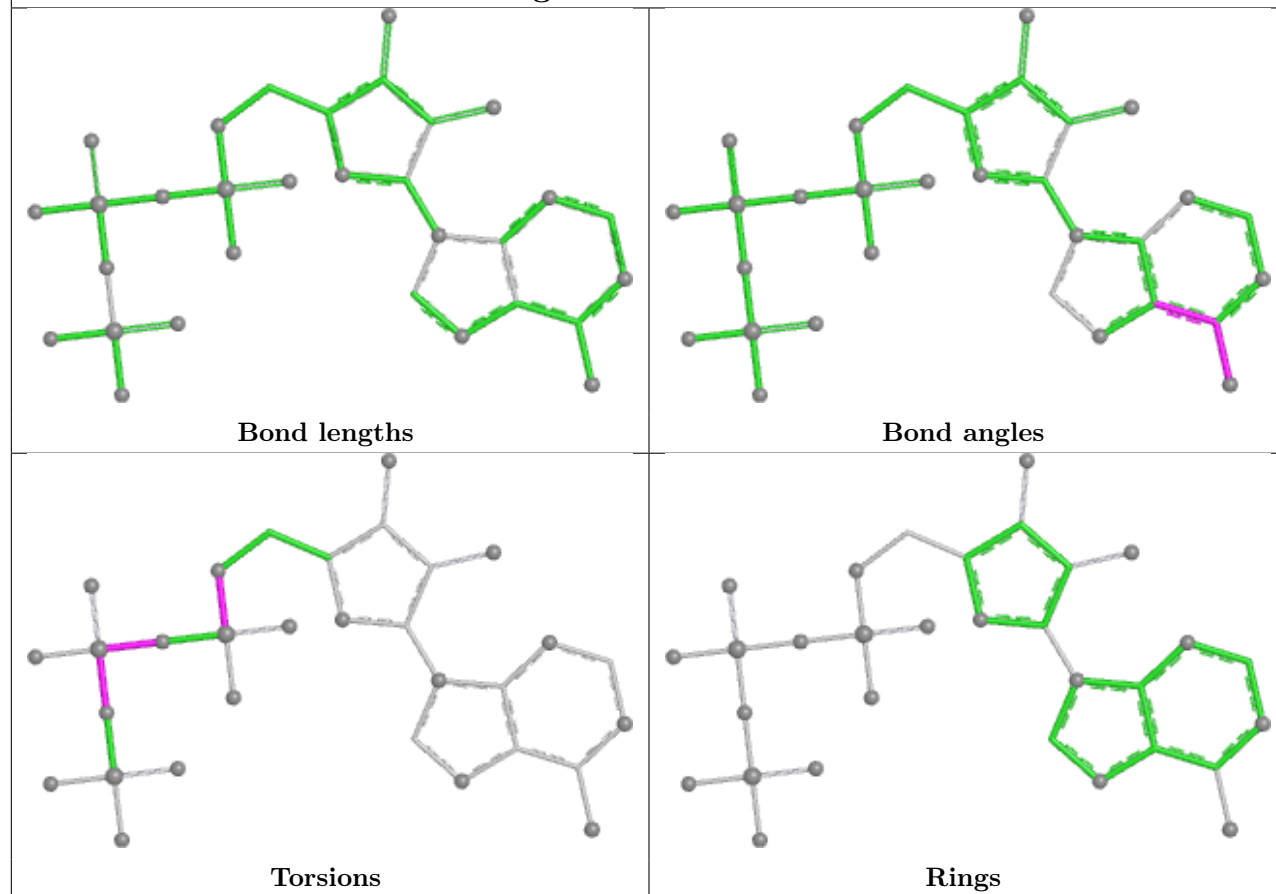




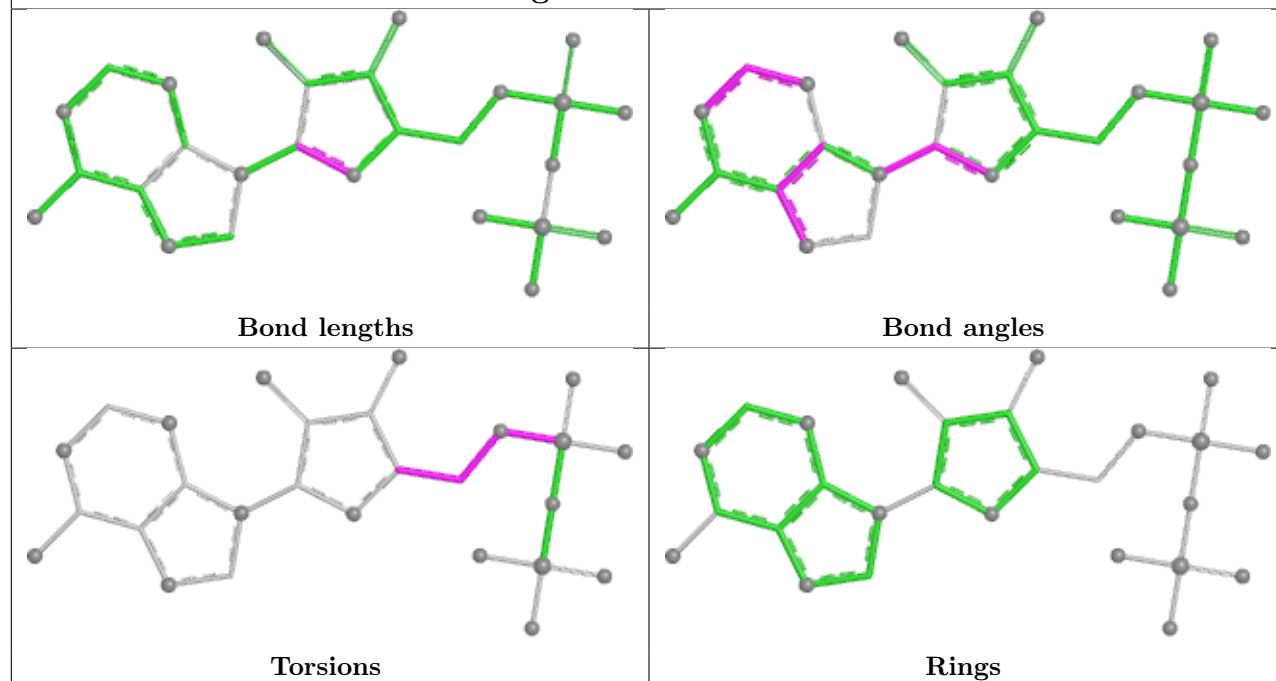




Ligand ATP B 501



Ligand ADP F 501



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

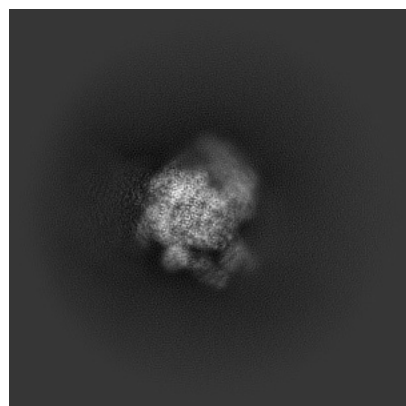
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36598. These allow visual inspection of the internal detail of the map and identification of artifacts.

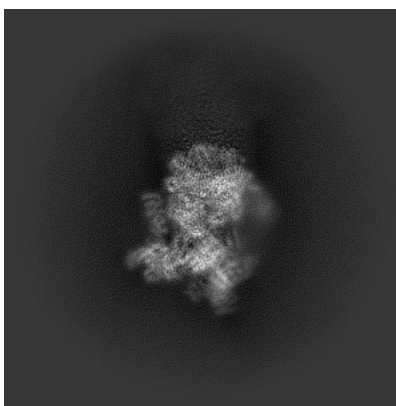
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

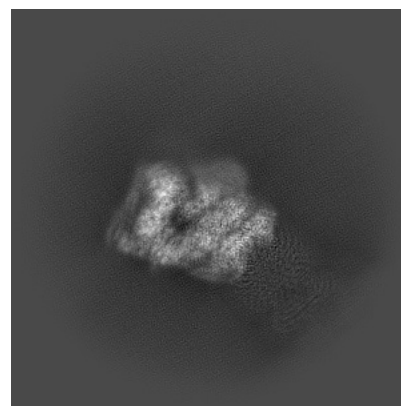
6.1.1 Primary map



X

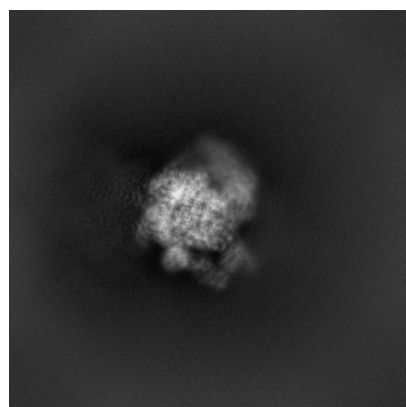


Y

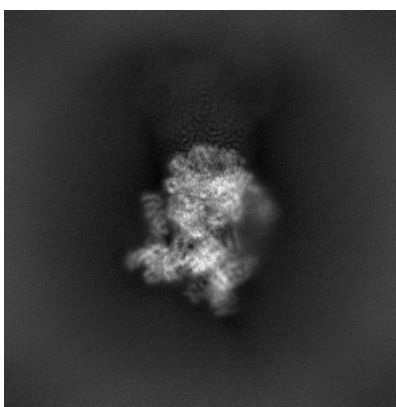


Z

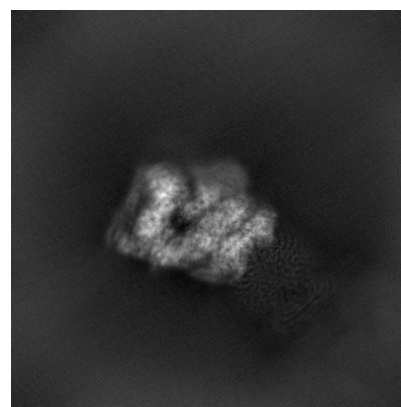
6.1.2 Raw map



X



Y

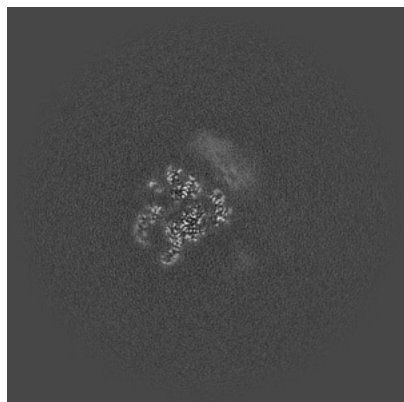


Z

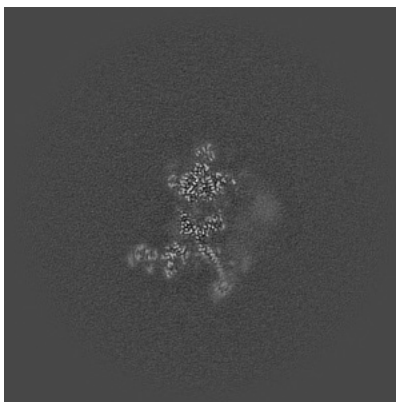
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

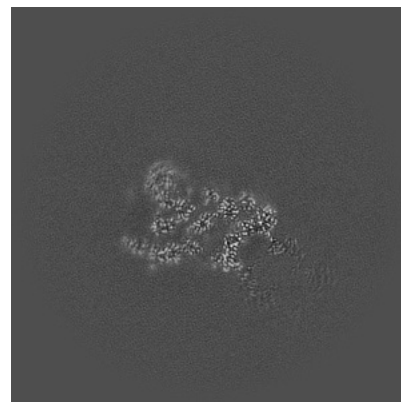
6.2.1 Primary map



X Index: 200

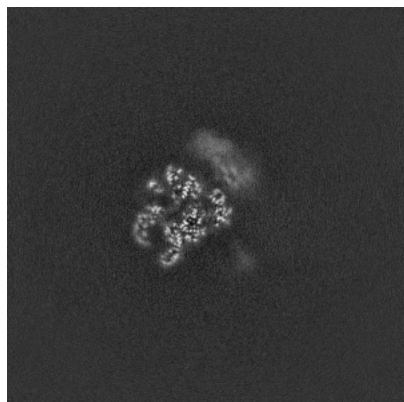


Y Index: 200

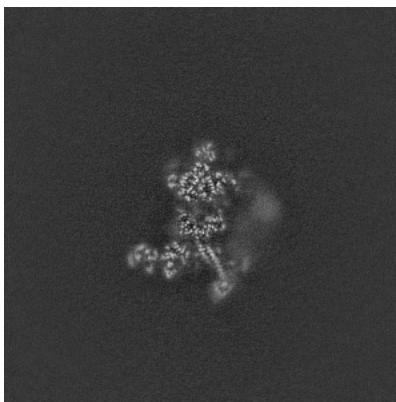


Z Index: 200

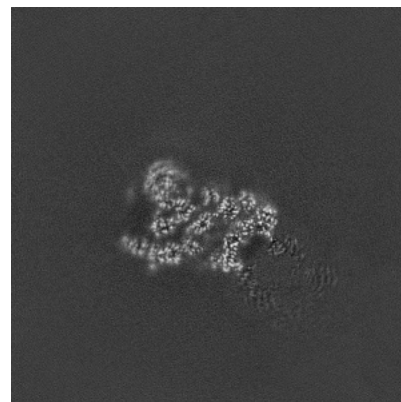
6.2.2 Raw map



X Index: 200



Y Index: 200

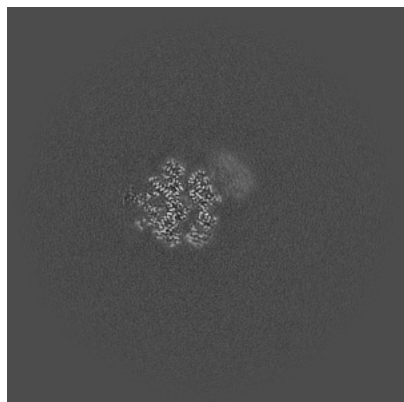


Z Index: 200

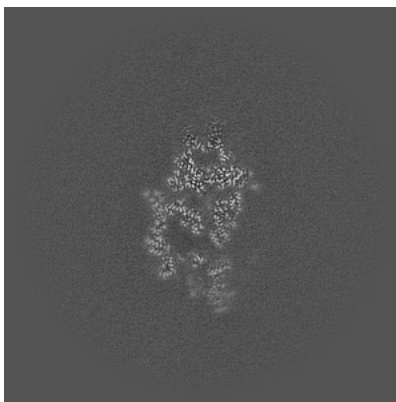
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

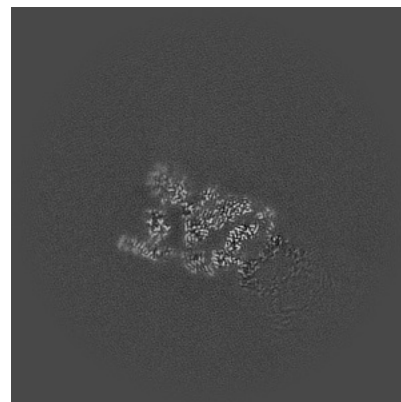
6.3.1 Primary map



X Index: 226

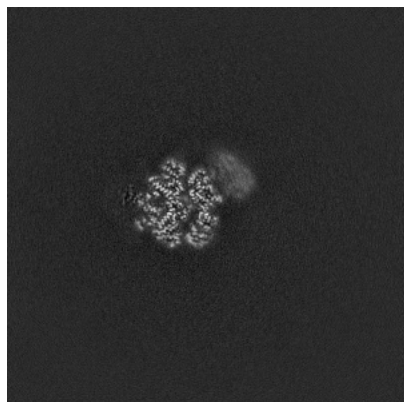


Y Index: 170

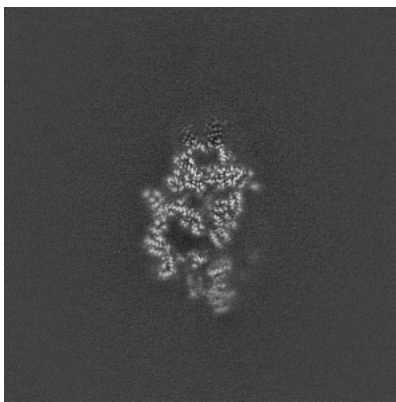


Z Index: 190

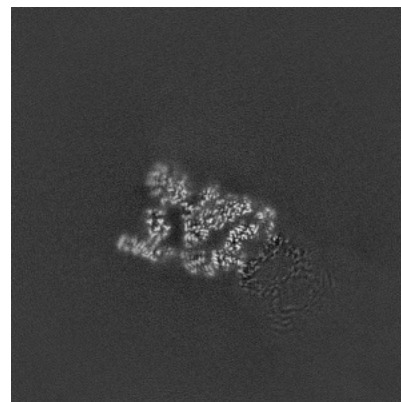
6.3.2 Raw map



X Index: 226



Y Index: 170

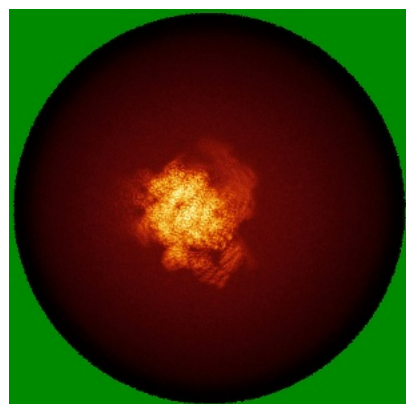


Z Index: 190

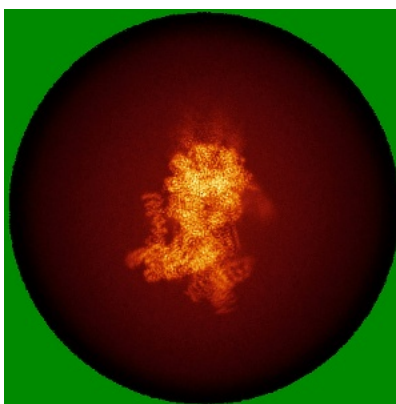
The images above show the largest variance slices of the map in three orthogonal directions.

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

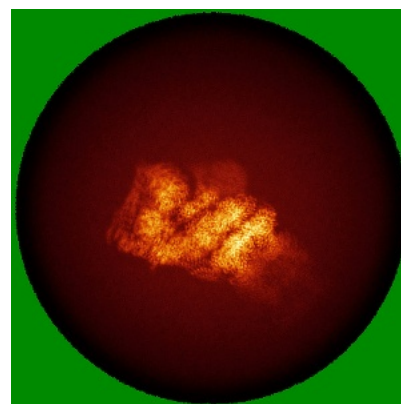
6.4.1 Primary map



X

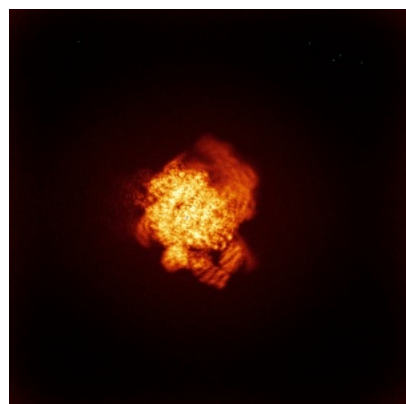


Y

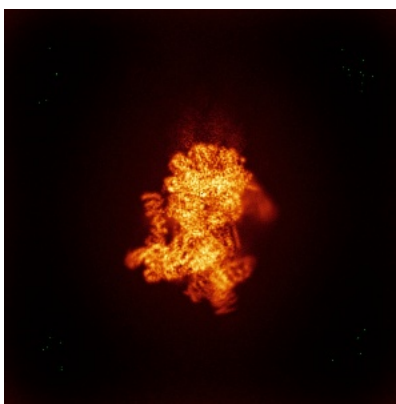


Z

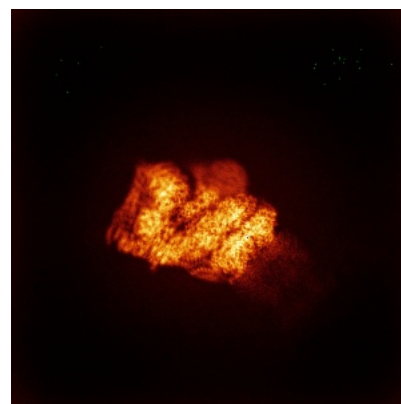
6.4.2 Raw map



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.

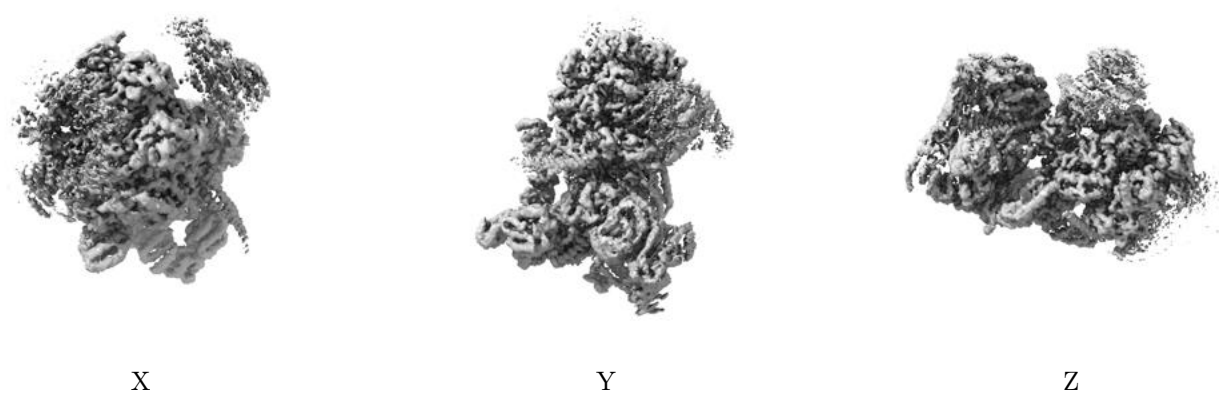
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.5. 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.

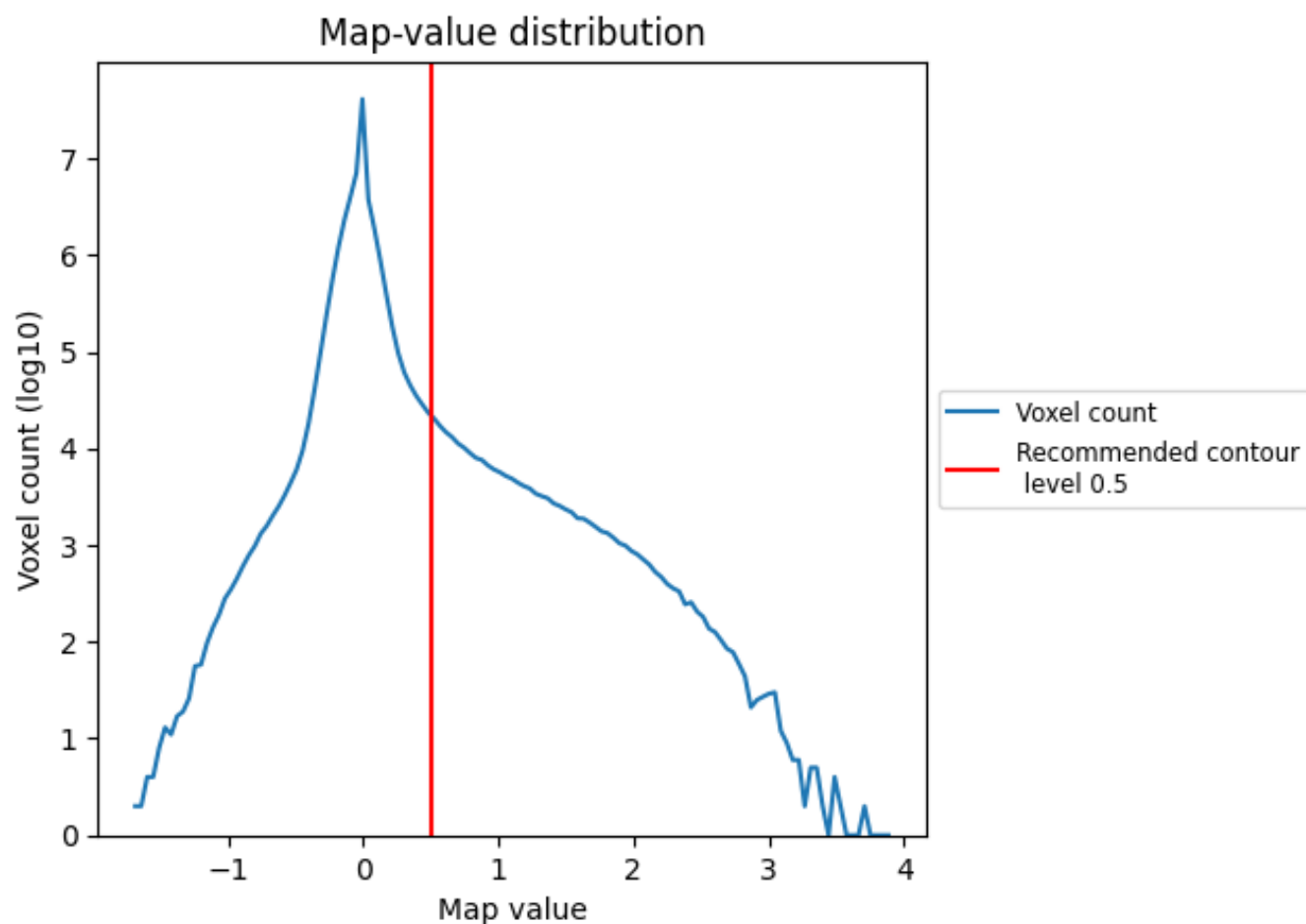
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

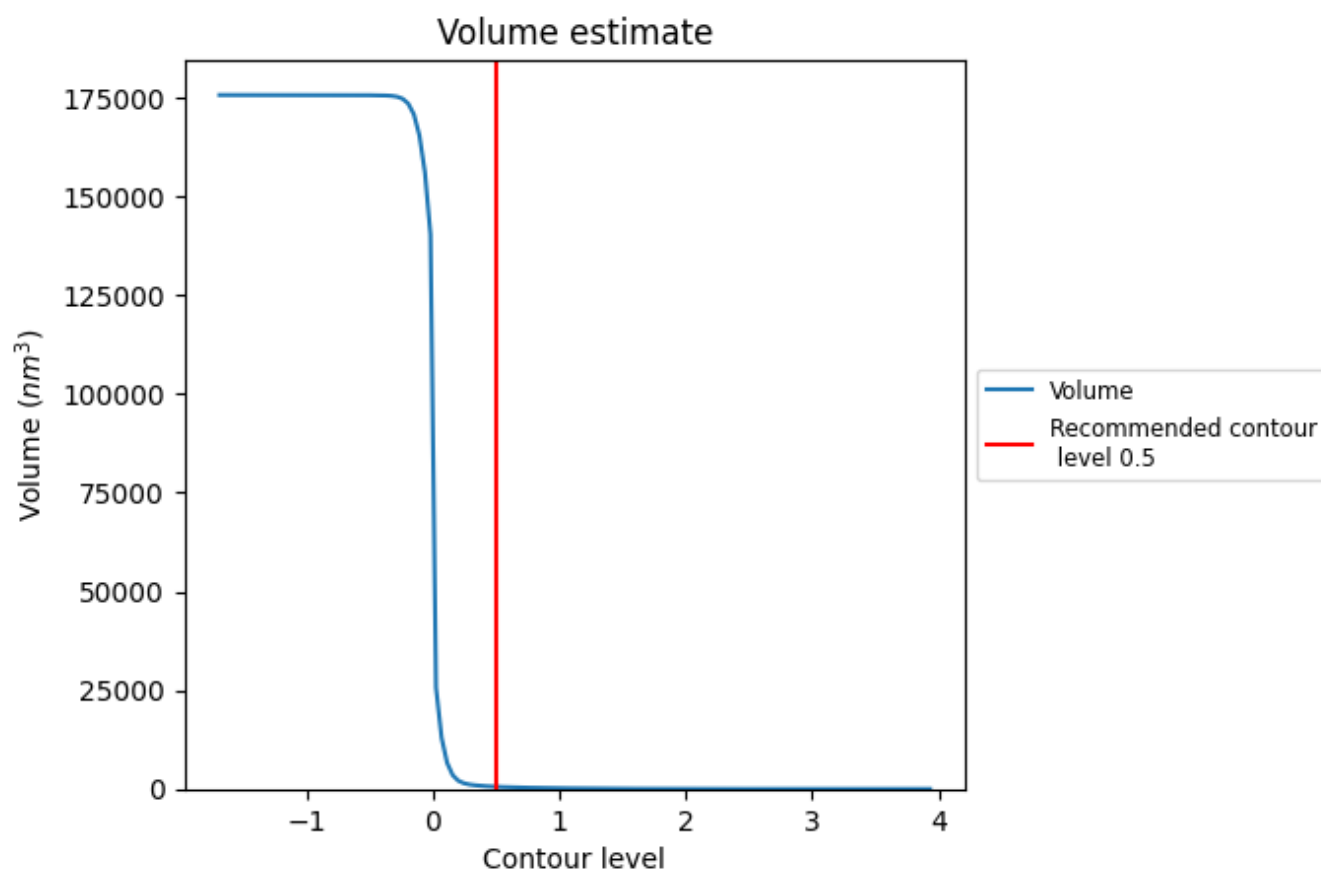
This section contains the results of statistical analysis of the map.

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.

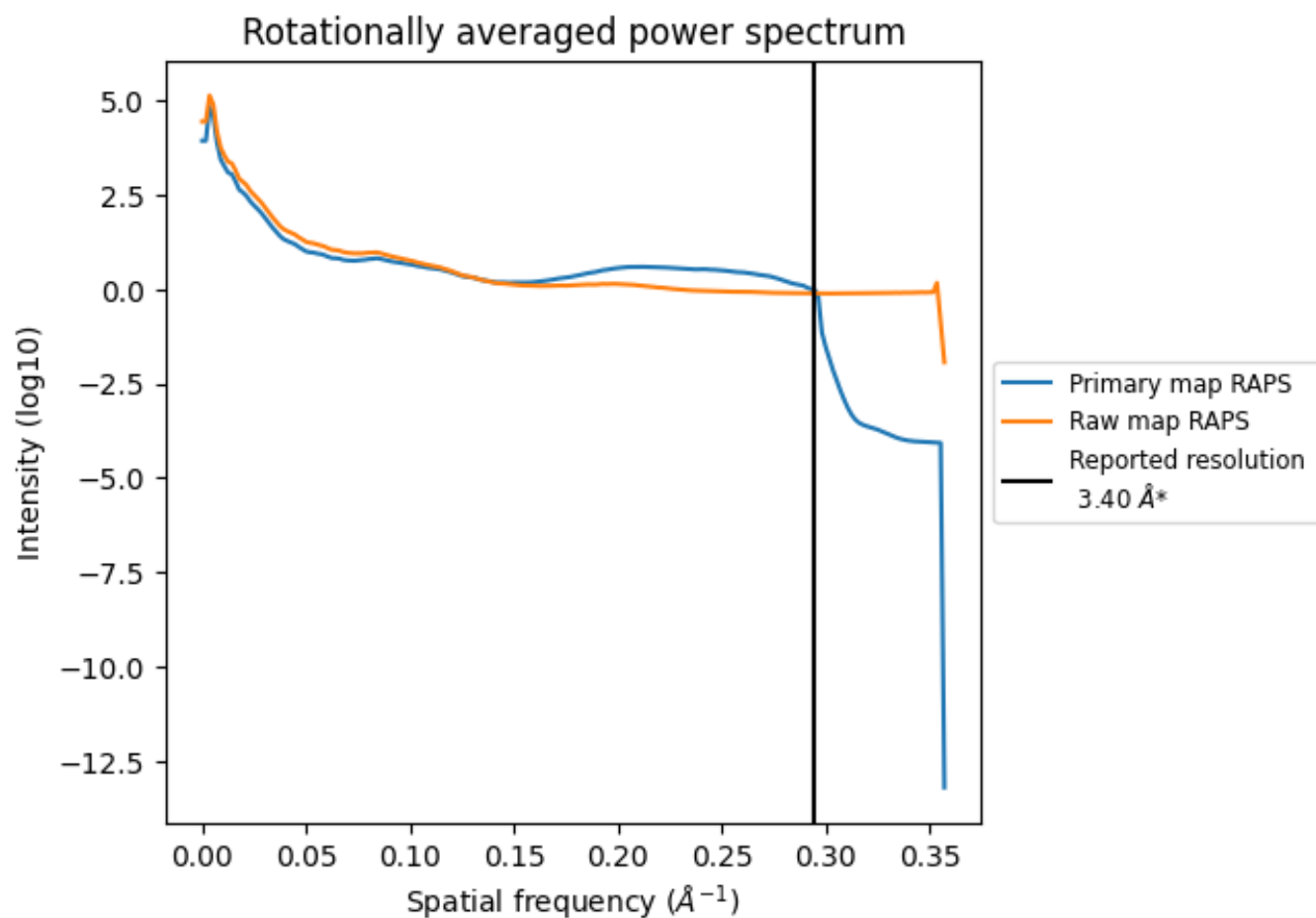
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 557 nm^3 ; this corresponds to an approximate mass of 504 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

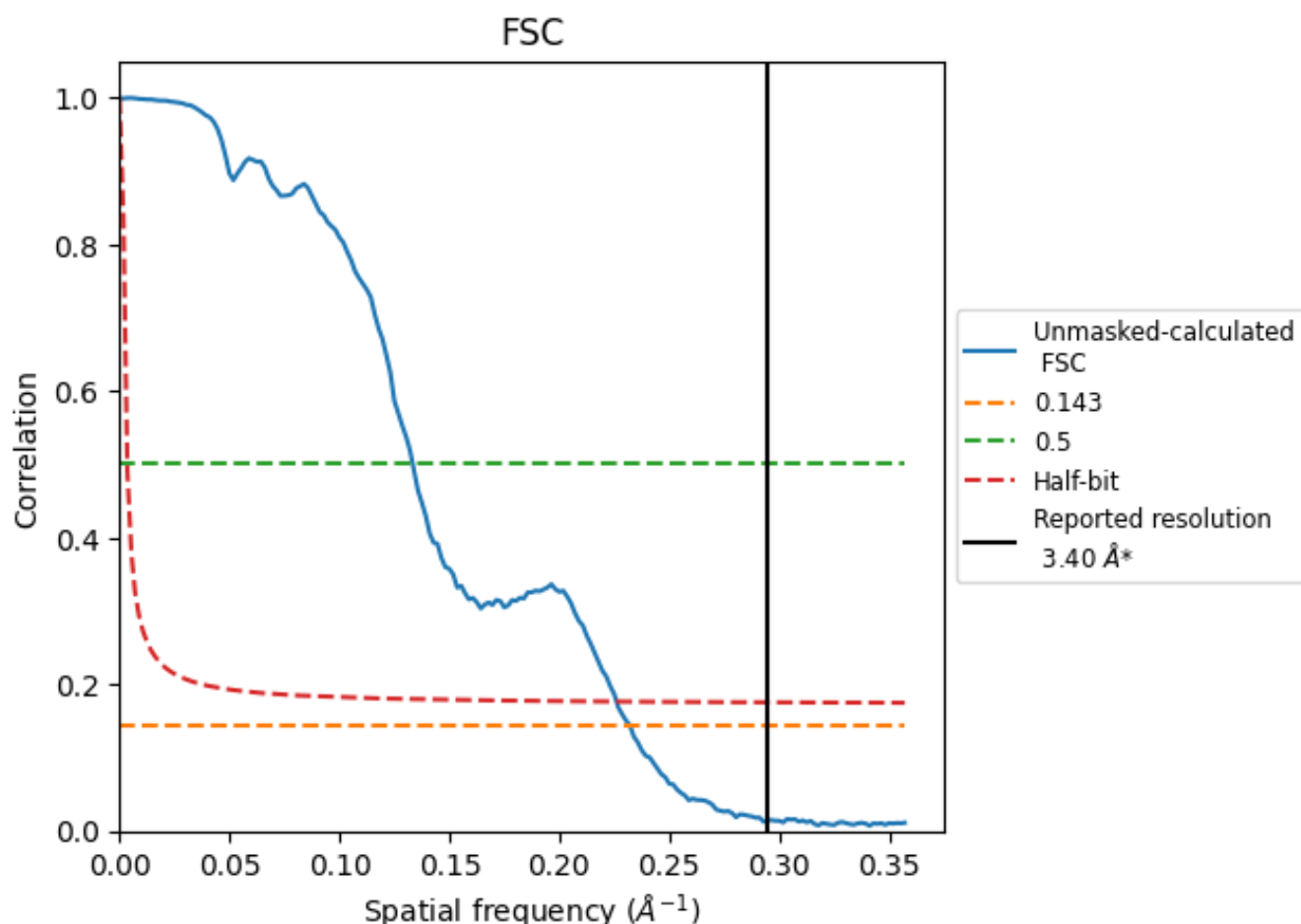


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.294 \AA^{-1}

8.2 Resolution estimates [i](#)

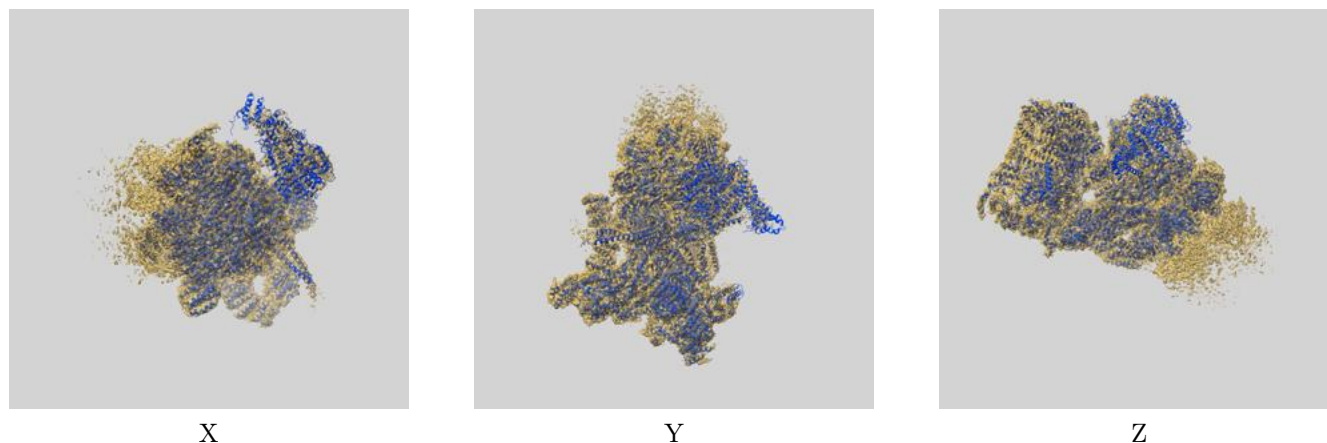
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.30	7.50	4.42

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.30 differs from the reported value 3.4 by more than 10 %

9 Map-model fit [i](#)

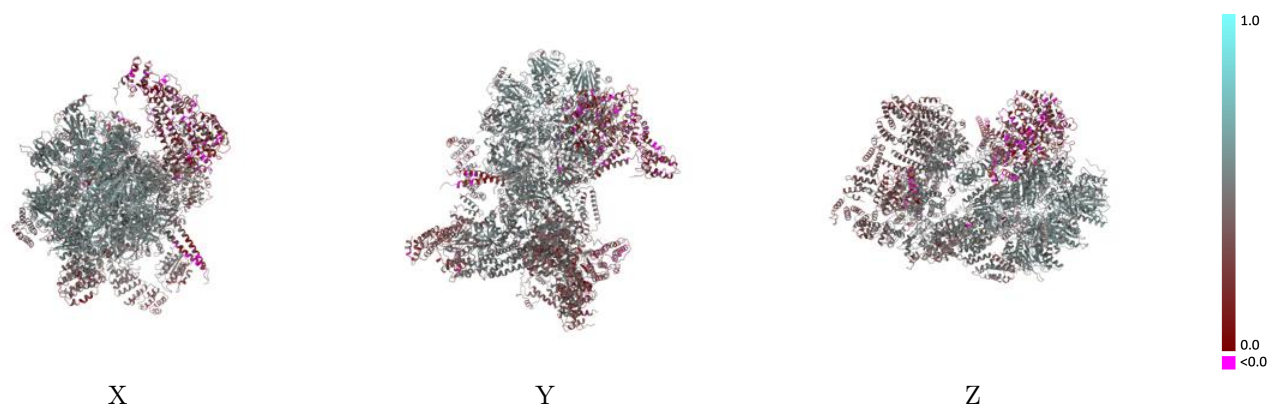
This section contains information regarding the fit between EMDB map EMD-36598 and PDB model 8JRI. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlay [i](#)



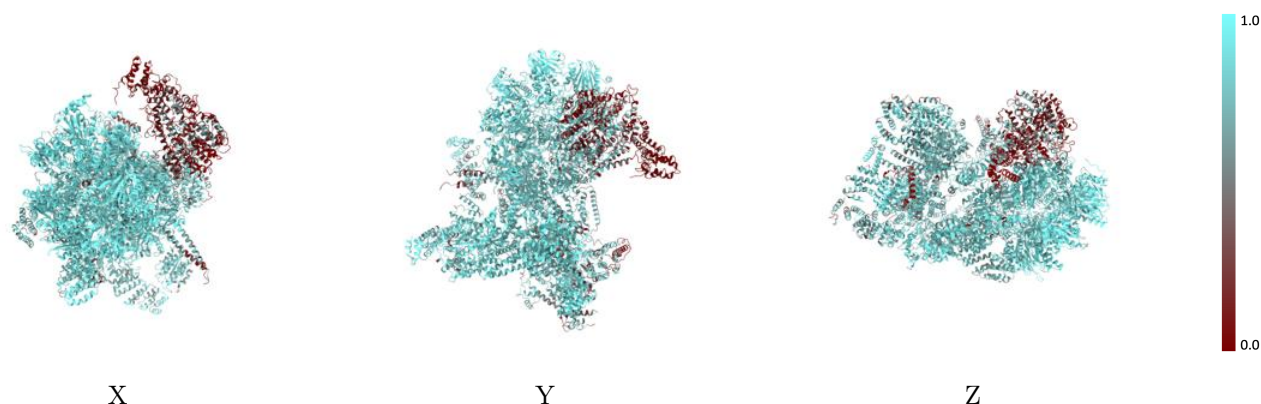
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



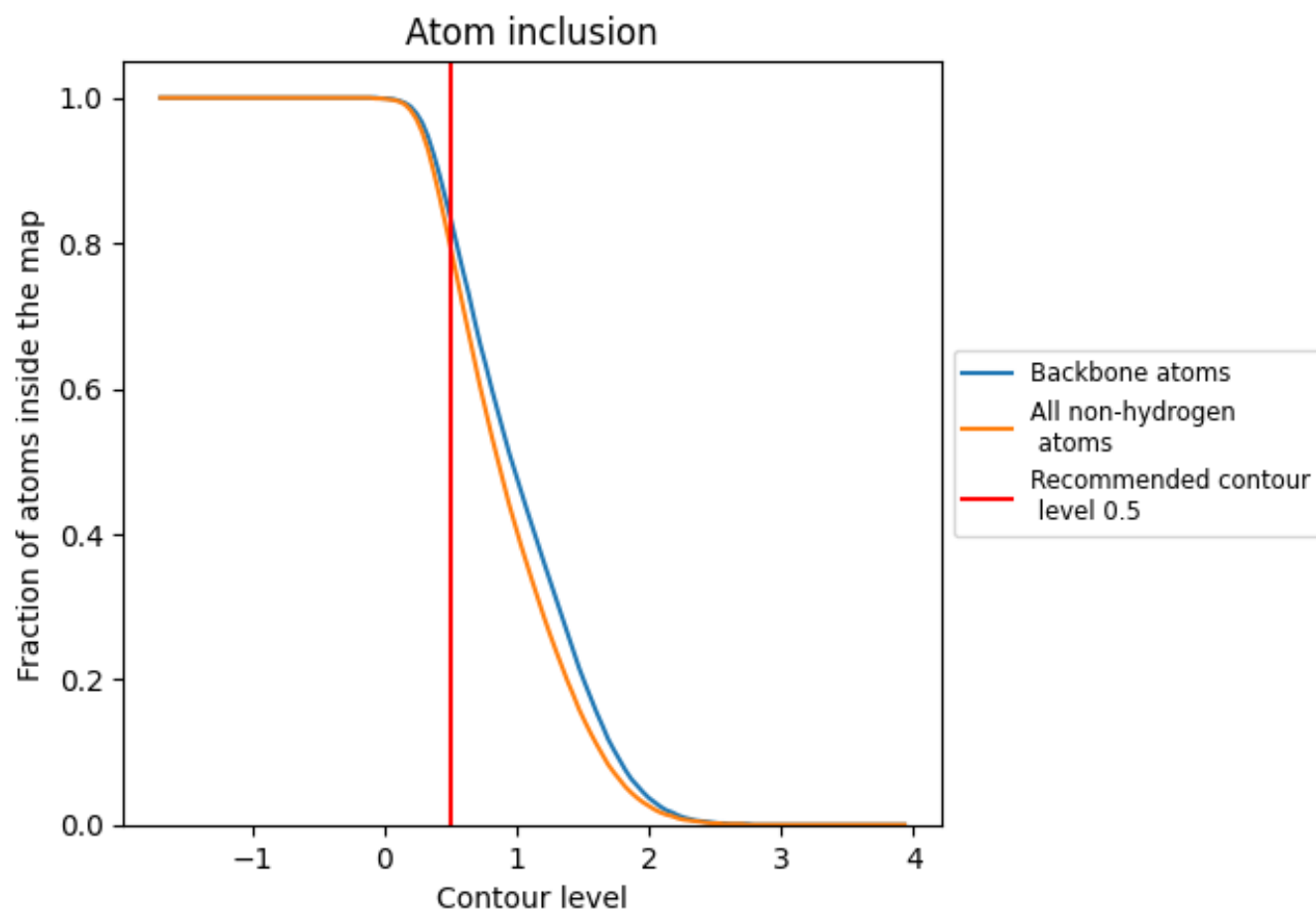
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.5).





















































9.4 Atom inclusion [i](#)



At the recommended contour level, 84% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7960	 0.4430
A	 0.8480	 0.4840
B	 0.8140	 0.4760
C	 0.8470	 0.4900
D	 0.8520	 0.4940
E	 0.8740	 0.4970
F	 0.8820	 0.5050
G	 0.9310	 0.5310
H	 0.9290	 0.5310
I	 0.8970	 0.5020
J	 0.9220	 0.5170
K	 0.9220	 0.5300
L	 0.9310	 0.5350
M	 0.9140	 0.5180
U	 0.7800	 0.3730
V	 0.7040	 0.3580
W	 0.8150	 0.4050
X	 0.7650	 0.4450
Y	 0.8510	 0.4470
Z	 0.8570	 0.4750
a	 0.8430	 0.4010
b	 0.7950	 0.3580
c	 0.8540	 0.4770
d	 0.6880	 0.3610
e	 0.7800	 0.3820
f	 0.2090	 0.2270

