wwPDB EM Validation Summary Report (i)

Aug 7, 2023 – 03:24 PM EDT

PDB ID	:	5VHI
EMDB ID	:	EMD-8676
Title	:	Conformational Landscape of the p28-Bound Human Proteasome Regulatory Particle
Authors	:	Lu, Y.; Wu, J.; Dong, Y.; Chen, S.; Sun, S.; Ma, Y.B.; Ouyang, Q.; Finley, D.; Kirschner, M.W.; Mao, Y.
Deposited on	:	2017-04-13
Resolution	:	6.80 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

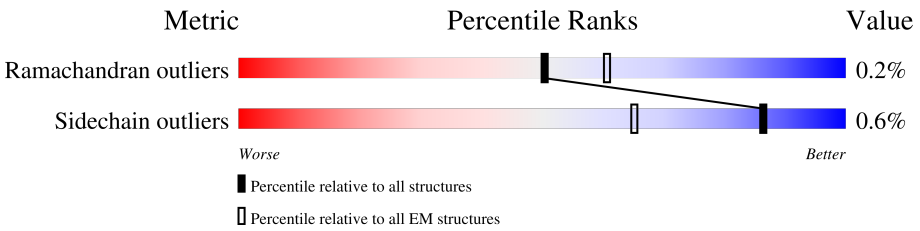
EMDB validation analysis	:	0.0.1.dev50
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 6.80 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	154571	4023
Sidechain outliers	154315	3826

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 <=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	352	22% 91% • 9%
2	B	341	30% 87% • 13%
3	C	385	38% 89% • 9%
4	D	368	46% 92% • 7%
5	E	379	24% 82% • 18%
6	F	380	20% 90% • 8%
7	U	935	8% 90% • 10%
8	V	488	29% 99% •
9	W	456	24% 100%

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Mol	Chain	Length	Quality of chain
10	X	385	44% / 100%
11	Y	378	7% / 99%
12	Z	286	10% / 100%
13	a	374	11% / 100%
14	b	191	11% / 100%
15	c	287	12% / 100%
16	d	257	20% / 100%
17	G	226	84% / 100%
18	e	70	41% / 100%
19	f	848	28% / 80% / 19%

2 Entry composition (i)

There are 20 unique types of molecules in this entry. The entry contains 54640 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 26S proteasome regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	321	2525	1596	451	463	15	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	298	2332	1464	400	457	11	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	350	2757	1728	501	514	14	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	343	2743	1739	479	516	9	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	311	2468	1548	445	460	15	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	351	2746	1733	476	520	17	0	0

- Molecule 7 is a protein called 26S proteasome non-ATPase regulatory subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	U	845	6568	4169	1118	1236	45	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	V	488	3919	2487	695	723	14	0	0

- Molecule 9 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	W	456	3703	2339	635	704	25	0	0

- Molecule 10 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	X	385	3048	1939	515	582	12	0	0

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

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

- Molecule 12 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	a	374	3003	1915	511	562	15	0	0

- Molecule 14 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

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

- Molecule 15 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

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

- Molecule 16 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	d	257	2116	1371	346	390	9	0	0

- Molecule 17 is a protein called 26S proteasome non-ATPase regulatory subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	G	226	1710	1063	302	334	11	0	0

- Molecule 18 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	e	70	583	357	89	135	2	0	0

- Molecule 19 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	f	686	5304	3335	901	1033	35	0	0

- Molecule 20 is ZINC ION (three-letter code: ZN) (formula: Zn).

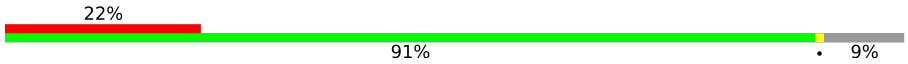
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
20	c	1	1	1	0

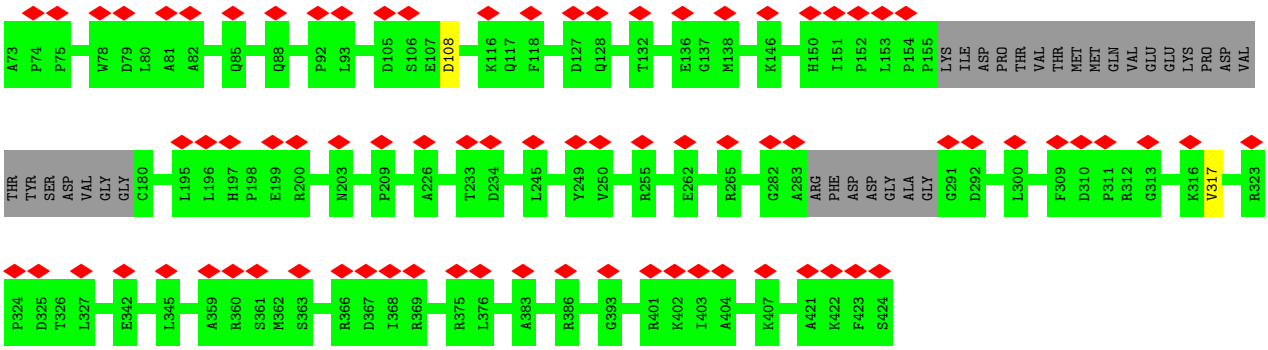
3 Residue-property plots (i)

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

- Molecule 1: 26S proteasome regulatory subunit 7

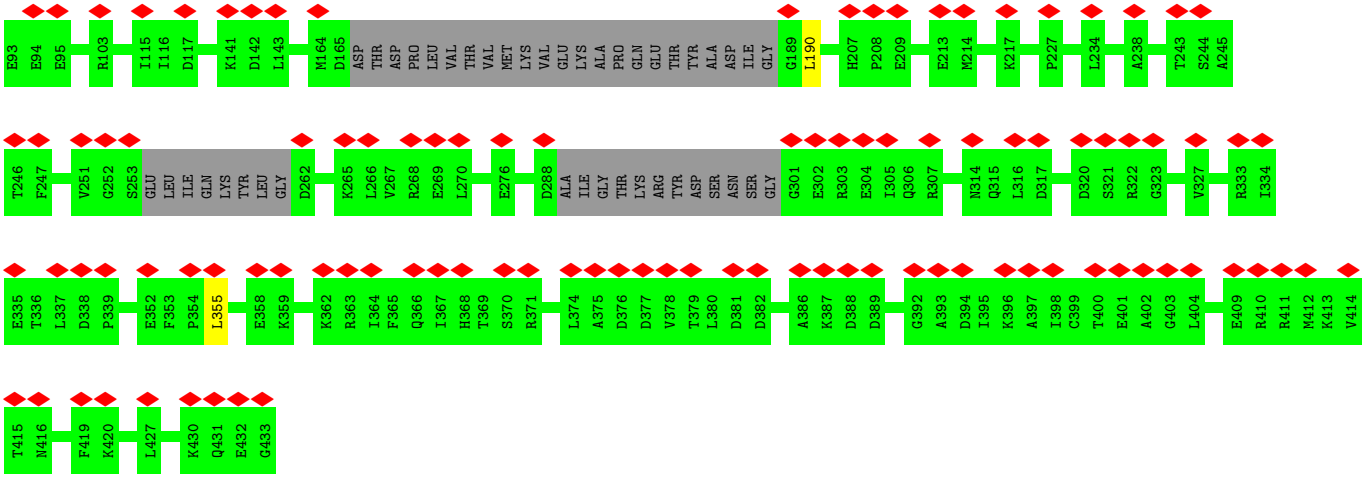
Chain A:





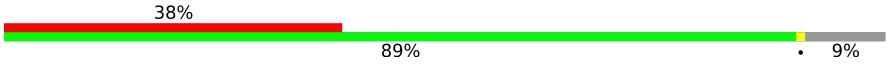
- Molecule 2: 26S proteasome regulatory subunit 4

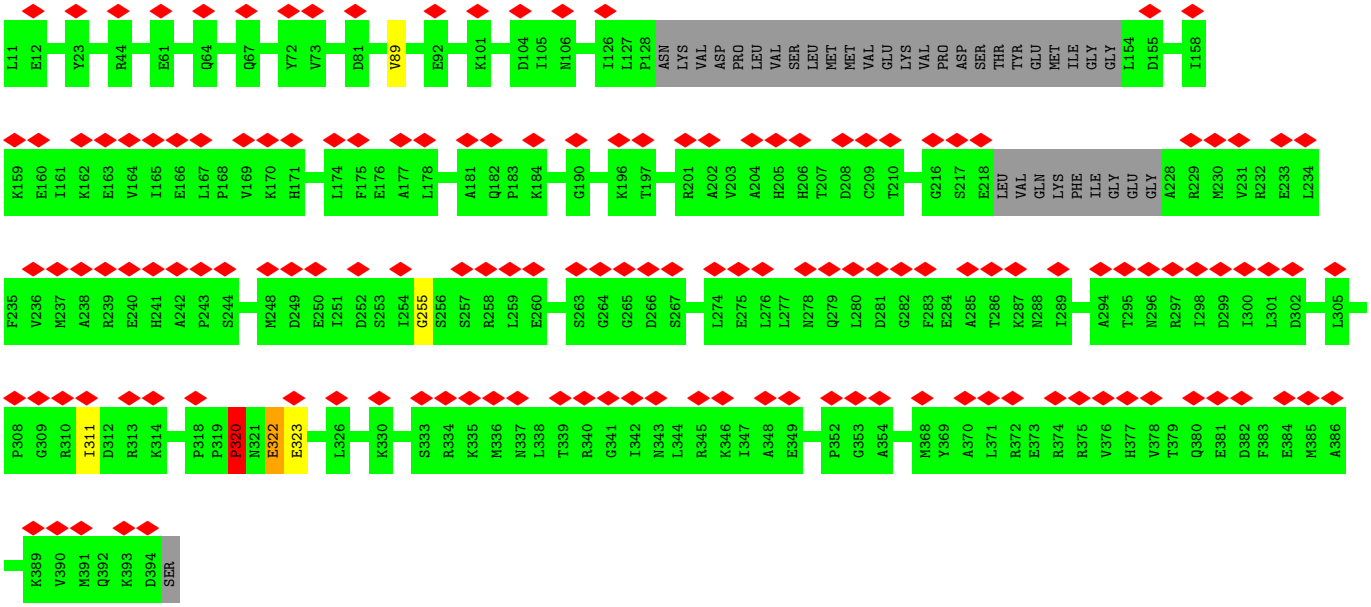
Chain B:



- Molecule 3: 26S proteasome regulatory subunit 8

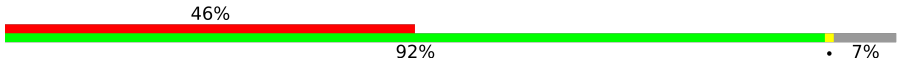
Chain C:

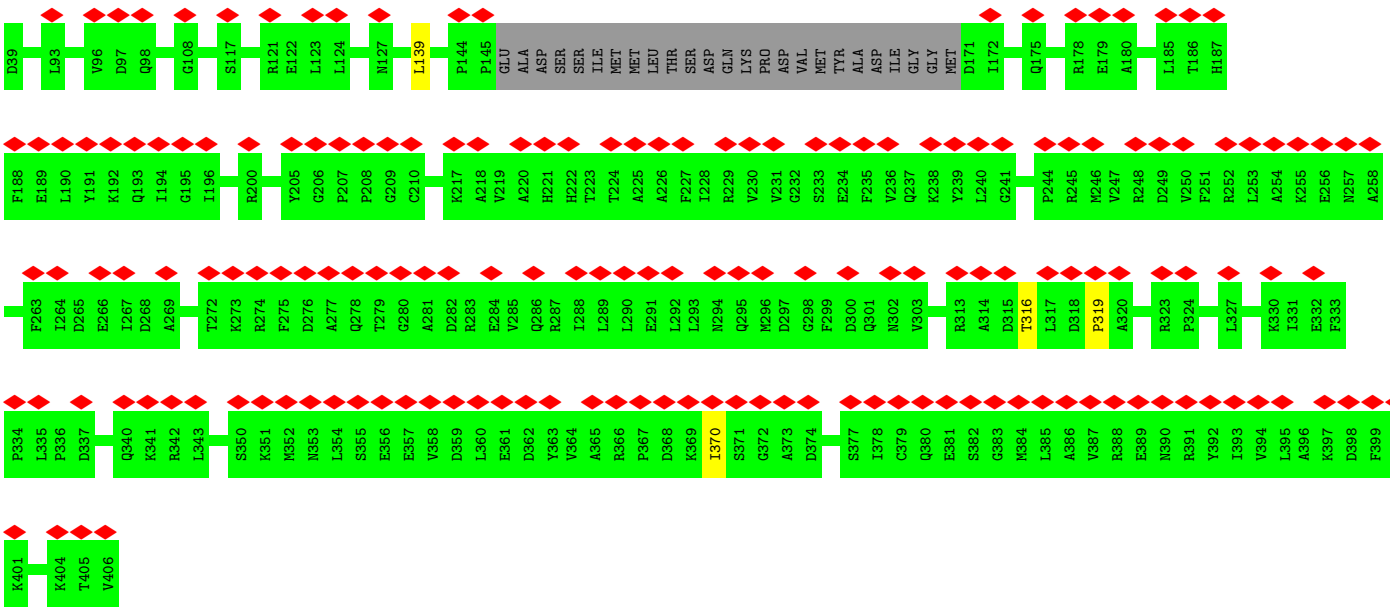




- Molecule 4: 26S proteasome regulatory subunit 6B

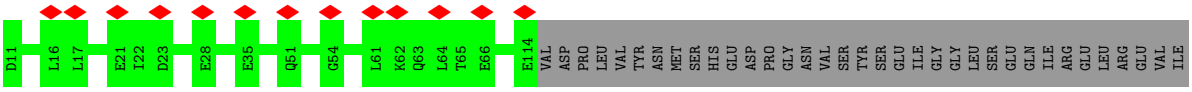
Chain D:

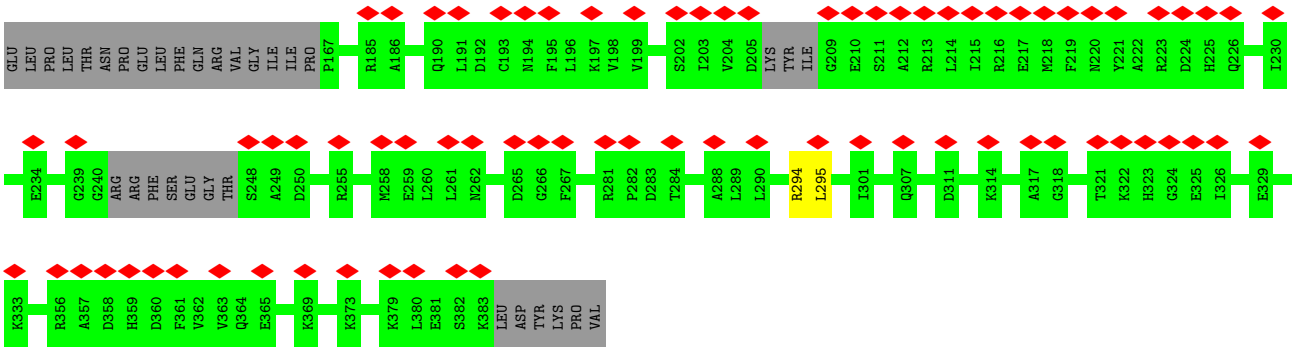




- Molecule 5: 26S proteasome regulatory subunit 10B

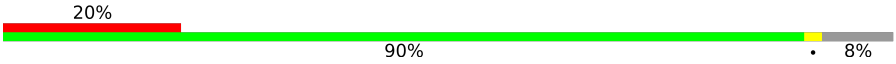
Chain E:

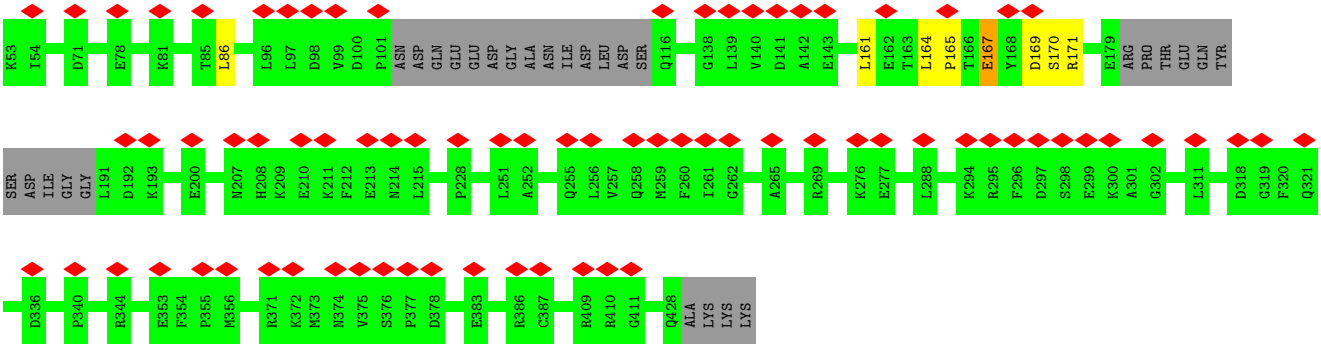




• Molecule 6: 26S proteasome regulatory subunit 6A

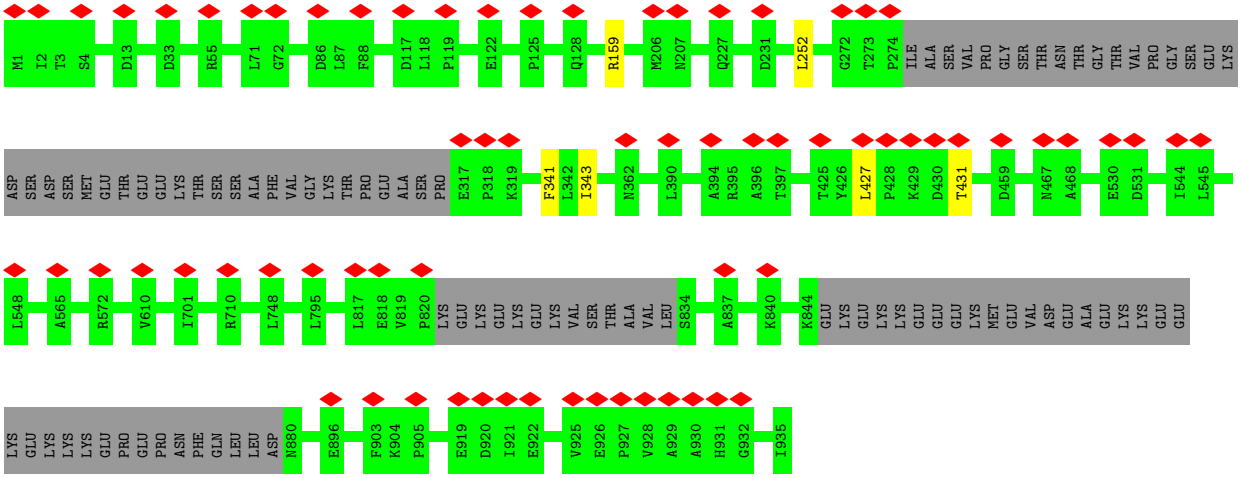
Chain F:





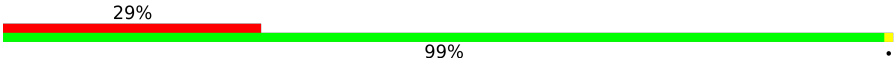
• Molecule 7: 26S proteasome non-ATPase regulatory subunit 1

Chain U:



• Molecule 8: 26S proteasome non-ATPase regulatory subunit 3

Chain V:



P18 P19 G20 G21 G22 E23 Q24 V35 E39 G49 E50 A51 D52 G53 K54 T55 A56 A57 I75 K76 E77 H78 V79 K80 Q81 L82 E83 K84 A85 V86 A97 L98 R99 M100 L101 P102 S103 T104 S105 R106 R107 L108 N109 H110 Y111 V112 L113 A116 V117 Q118 G119 F120 F121 T122

S123 N124 N125 A126 T127 R128 D129 F130 M139 D140 T141 E142 Q146 F147 R148 P149 A155 L159 Q168 L169 L170 I173 F174 R180 Y181 A184 Q185 K186 I187 S188 D189 D190 L191 M192 Q193 N199 E219 F220 L221 D222 D225 V226 F230 A233 T237

L240 Q266 A267 L270 V275 F276 P277 N282 A286 L289 A297 Y302 S303 R307 R314 A321 L346 Q347 F348 R349 M358 G370 N371 L372 A373 K374 Q377 Q381 F382 G390 T391 Y392 S411 S418 L419 A420 D421 I422 A423 Q424

L428 R443 E454 K455 G456 Y457 I464 D465 I466 Y467 R470 E471 L474 Q478 M494 P498 L505

- Molecule 9: 26S proteasome non-ATPase regulatory subunit 12

Chain W: 24% 100%

M1 A2 D3 G4 G5 S6 E7 R8 A9 D10 I13 V14 K15 M16 E17 V18 D19 A22 Q26 K33 G38 R39 L40 Q41 E42 V43 I44 E45 T46 S49 L50 Q53 A57 S58 V61 S64 R65 I66 L67 V68 D81 L82 L83 N84 E85 N86 I87 M88 L89

L90 S91 K92 R93 R94 S95 Q96 L97 K98 Q99 K103 Q106 E113 E114 I115 T116 D117 L118 T132 E133 G134 K135 T136 E154 G175 S176 M177 L194 Y199 N210 T211 K212 F213 F214 Q215 E216 E217 N218 T219 E220 K221 L224 D280 S284 D285 S291 G292

K303 F309 E313 L314 M315 R316 M326 R329 T338 D339 G342 Y370 I373 R377 Q380 L381 L382 D383 I402 L409 R417 P418 K419 L424 W428 L432 M436 Q456

- Molecule 10: 26S proteasome non-ATPase regulatory subunit 11

Chain X: 44% 100%

N38 D39 E40 E41 A42 V43 Q44 V45 K46 E47 Q48 S49 I50 L51 E52 L53 G54 S55 L56 L57 A58 K59 T60 G61 Q62 A63 A64 E65 L66 G67 G68 L69 L70 K71 Y72 V73 R74 P75 F76 L77 N78 S79 I80 S81 K82 A83 K84 A85 A86 R87 L88 V89 R90 S91 L92 L93 D94 L95 F96 L97

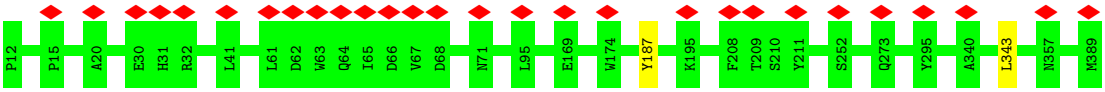
D98 M99 E100 A101 A102 T103 G104 Q105 E106 V107 E108 L109 C110 L111 E112 C113 I114 E115 W116 A117 K118 S119 E120 K121 R122 T123 R126 Q127 A128 L129 E130 A131 R132 L133 Y134 Y137 F138 D139 T140 K141 R142 Y143 Q144 E145 A146 L147 H148 L149 G150 S151 Q152 L153 L154 R155 E156 L157 K158 K159

M160 D161 D162 L165 L166 V167 E168 L171 A179 K185 A186 R187 S192 A193 R194 T195 T196 A197 P204 K205 L206 Q207 A220 E221 E222 T227 E237 D243 S244 P245 K246 A247 I248 L251 N262 E265 Q268 A269 S272 G273 K274 L275 A276 L277 R278

Y279 A280 G281 R282 Q292 N296 L306 T307 R310 L313 R314 D315 T321 K355 K372 F388 D394 Y397 E398 Y415 K419 T422

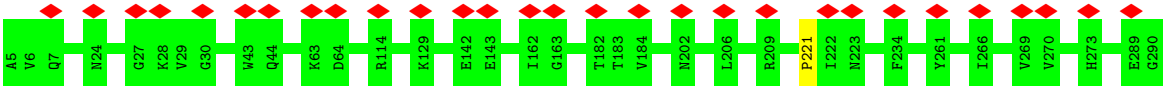
- Molecule 11: 26S proteasome non-ATPase regulatory subunit 6

Chain Y: 7% 99%



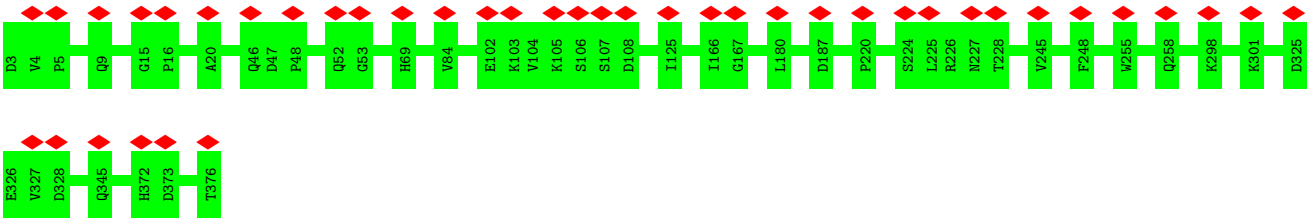
• Molecule 12: 26S proteasome non-ATPase regulatory subunit 7

Chain Z: 10% 100%



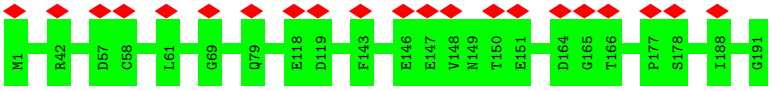
• Molecule 13: 26S proteasome non-ATPase regulatory subunit 13

Chain a: 11% 100%



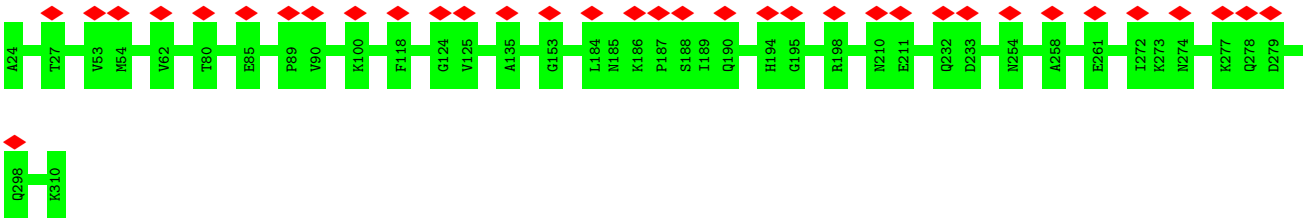
• Molecule 14: 26S proteasome non-ATPase regulatory subunit 4

Chain b: 11% 100%



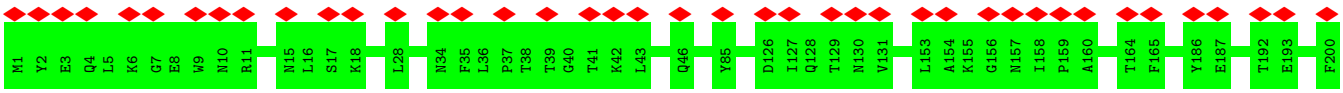
• Molecule 15: 26S proteasome non-ATPase regulatory subunit 14

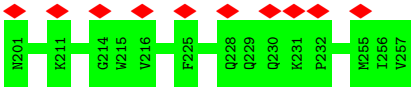
Chain c: 12% 100%



• Molecule 16: 26S proteasome non-ATPase regulatory subunit 8

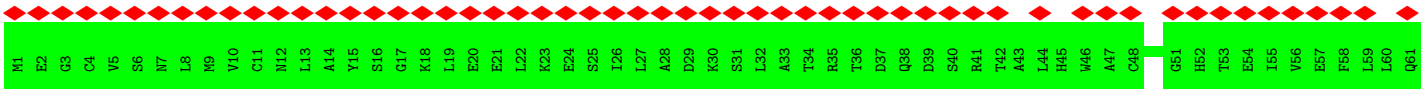
Chain d: 20% 100%

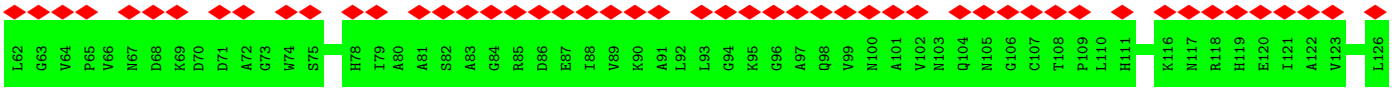


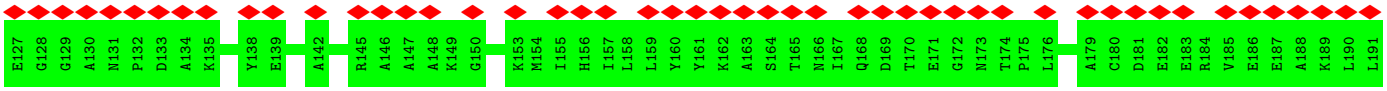


- Molecule 17: 26S proteasome non-ATPase regulatory subunit 10

Chain G:

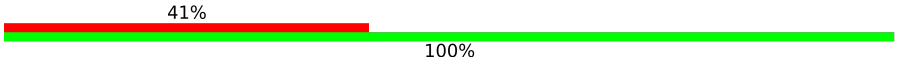


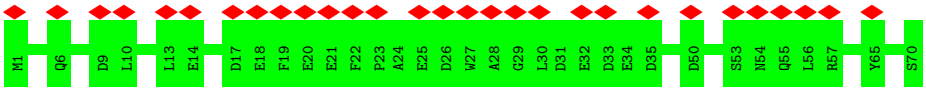




- Molecule 18: 26S proteasome complex subunit SEM1

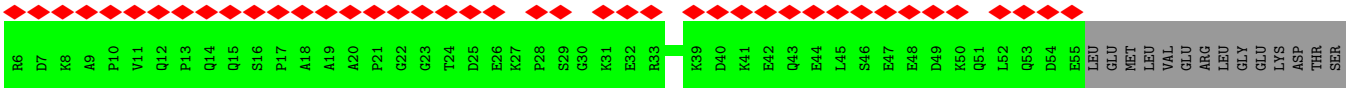
Chain e:

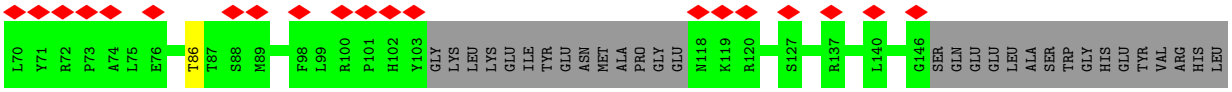


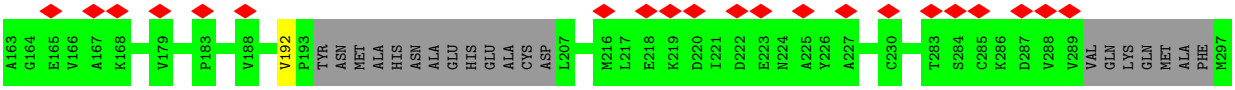


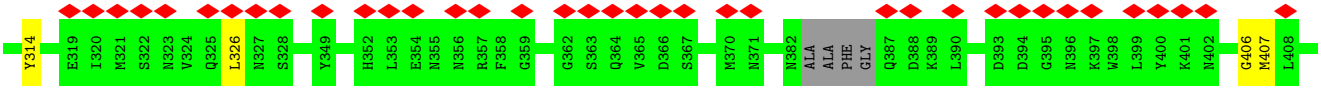
- Molecule 19: 26S proteasome non-ATPase regulatory subunit 2

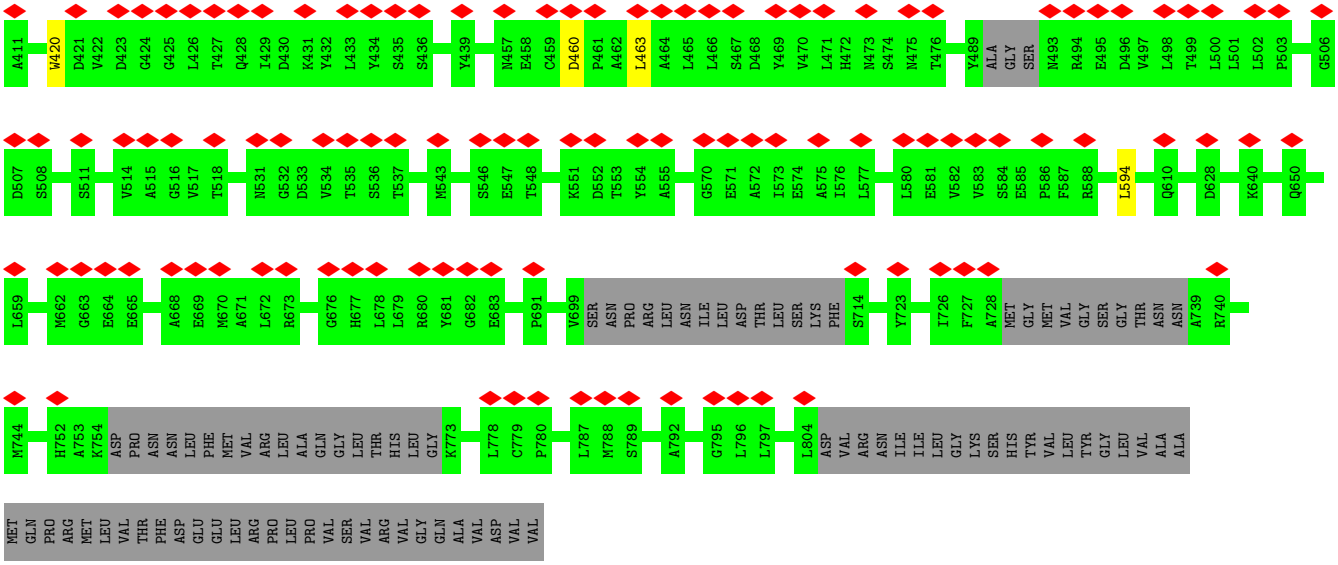
Chain f:










A411 W420 D421 V422 D423 G424 G425 L426 T427 Q428 I429 D430 K431 Y432 L433 Y434 S435 S436 Y439 N457 E458 C459 D460 P461 A462 L463 A464 L465 L466 S467 D468 Y469 V470 L471 H472 N473 S474 N475 T476 Y489 ALA GLY SER N493 R494 E495 D496 V497 L498 T499 L500 L501 L502 P503 G506
D507 S508 S511 V514 A515 G516 V517 T518 N531 G532 D533 V534 T535 S536 T537 M543 S546 E547 T548 K551 D552 T553 Y554 A555 G570 E571 A572 I573 E574 A575 I576 L577 L580 E581 V582 V583 S584 E585 P586 F587 R588 L594 Q610 D628 K640 Q650
L659 M662 G663 E664 E665 A668 E669 M670 A671 L672 R673 G676 H677 L678 L679 R680 Y681 G682 E683 P691 V699 SER ASN PRO ARG LEU ASN ILE LEU ASP THR LEU SER LYS PHE S714 Y723 I726 F727 A728 MET GLY MET VAL GLY SER GLY THR ASN ASN A739 R740
M744 H752 A753 K754 ASP PRO ASN ASN LEU PHE MET VAL ARG LEU ALA GLN GLY LEU THR HIS LEU GLY K773 L778 C779 P780 L787 M788 S789 A792 G795 L796 L797 L804 ASP VAL ARG ASN ILE ILE LEU GLY LYS SER HIS TYR VAL LEU TYR GLY LEU VAL ALA ALA
MET GLN PRO ARG MET LEU VAL THR PHE ASP GLU GLU LEU ARG PRO LEU PRO VAL SER VAL ARG VAL GLY GLN ALA VAL ASP VAL VAL

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	10891	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.015	Depositor
Minimum map value	-0.006	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.004	Depositor
Map size (Å)	250.88, 250.88, 250.88	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.98, 0.98, 0.98	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.21	0/2567	0.40	0/3462
2	B	0.20	0/2362	0.39	0/3182
3	C	0.26	0/2790	0.44	2/3748 (0.1%)
4	D	0.21	0/2787	0.39	0/3763
5	E	0.20	0/2499	0.37	0/3350
6	F	0.21	0/2781	0.42	1/3745 (0.0%)
7	U	0.20	0/6684	0.37	0/9043
8	V	0.22	0/3997	0.44	0/5399
9	W	0.21	0/3750	0.40	1/5039 (0.0%)
10	X	0.20	0/3092	0.35	0/4168
11	Y	0.20	0/3173	0.35	0/4273
12	Z	0.20	0/2324	0.37	0/3150
13	a	0.21	0/3061	0.37	0/4144
14	b	0.21	0/1478	0.37	0/2001
15	c	0.20	0/2302	0.35	0/3110
16	d	0.21	0/2162	0.38	0/2919
17	G	0.19	0/1735	0.33	0/2343
18	e	0.21	0/596	0.36	0/805
19	f	0.22	0/5377	0.43	1/7248 (0.0%)
All	All	0.21	0/55517	0.39	5/74892 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	320	PRO	CA-N-CD	-7.46	101.05	111.50
19	f	407	MET	N-CA-C	-6.27	94.06	111.00
6	F	164	LEU	C-N-CD	-5.61	108.25	120.60
3	C	255	GLY	N-CA-C	5.32	126.40	113.10
9	W	221	LYS	N-CA-C	-5.10	97.23	111.00

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	315/352 (90%)	285 (90%)	30 (10%)	0	100	100
2	B	290/341 (85%)	263 (91%)	27 (9%)	0	100	100
3	C	344/385 (89%)	324 (94%)	17 (5%)	3 (1%)	17	57
4	D	339/368 (92%)	321 (95%)	17 (5%)	1 (0%)	41	77
5	E	303/379 (80%)	283 (93%)	19 (6%)	1 (0%)	41	77
6	F	345/380 (91%)	316 (92%)	25 (7%)	4 (1%)	13	50
7	U	837/935 (90%)	791 (94%)	46 (6%)	0	100	100
8	V	484/488 (99%)	419 (87%)	65 (13%)	0	100	100
9	W	452/456 (99%)	411 (91%)	40 (9%)	1 (0%)	47	81
10	X	383/385 (100%)	364 (95%)	18 (5%)	1 (0%)	41	77
11	Y	376/378 (100%)	348 (93%)	28 (7%)	0	100	100
12	Z	284/286 (99%)	256 (90%)	27 (10%)	1 (0%)	34	72
13	a	372/374 (100%)	349 (94%)	23 (6%)	0	100	100
14	b	189/191 (99%)	171 (90%)	18 (10%)	0	100	100
15	c	285/287 (99%)	262 (92%)	23 (8%)	0	100	100
16	d	255/257 (99%)	236 (92%)	19 (8%)	0	100	100
17	G	224/226 (99%)	224 (100%)	0	0	100	100
18	e	68/70 (97%)	62 (91%)	6 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	f	664/848 (78%)	600 (90%)	62 (9%)	2 (0%)	41	77
All	All	6809/7386 (92%)	6285 (92%)	510 (8%)	14 (0%)	50	81

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	320	PRO
3	C	322	GLU
3	C	323	GLU
5	E	295	LEU
10	X	313	LEU

5.3.2 Protein sidechains (i)

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	274/300 (91%)	272 (99%)	2 (1%)	84	90
2	B	262/298 (88%)	260 (99%)	2 (1%)	81	89
3	C	302/333 (91%)	298 (99%)	4 (1%)	69	82
4	D	300/321 (94%)	297 (99%)	3 (1%)	76	86
5	E	270/333 (81%)	269 (100%)	1 (0%)	91	94
6	F	302/326 (93%)	298 (99%)	4 (1%)	69	82
7	U	717/798 (90%)	711 (99%)	6 (1%)	81	89
8	V	422/422 (100%)	419 (99%)	3 (1%)	84	90
9	W	416/416 (100%)	415 (100%)	1 (0%)	93	96
10	X	331/331 (100%)	331 (100%)	0	100	100
11	Y	334/334 (100%)	332 (99%)	2 (1%)	86	92
12	Z	257/257 (100%)	257 (100%)	0	100	100
13	a	334/334 (100%)	334 (100%)	0	100	100
14	b	167/167 (100%)	167 (100%)	0	100	100
15	c	252/252 (100%)	252 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	d	231/231 (100%)	231 (100%)	0	100	100
17	G	180/180 (100%)	180 (100%)	0	100	100
18	e	63/63 (100%)	63 (100%)	0	100	100
19	f	579/714 (81%)	572 (99%)	7 (1%)	71	83
All	All	5993/6410 (94%)	5958 (99%)	35 (1%)	86	92

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
19	f	86	THR
19	f	192	VAL
19	f	460	ASP
6	F	86	LEU
5	E	294	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 56 such sidechains are listed below:

Mol	Chain	Res	Type
9	W	257	GLN
19	f	750	GLN
12	Z	102	HIS
19	f	592	ASN
16	d	141	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
8	V	1
9	W	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	V	237:THR	C	238:ALA	N	3.31
1	W	205:ILE	C	206:SER	N	3.16

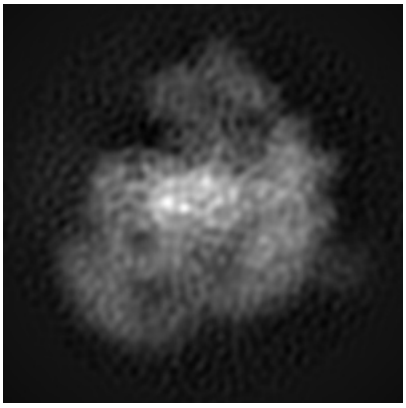
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-8676. These allow visual inspection of the internal detail of the map and identification of artifacts.

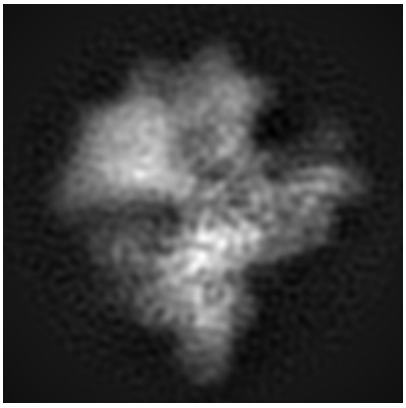
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

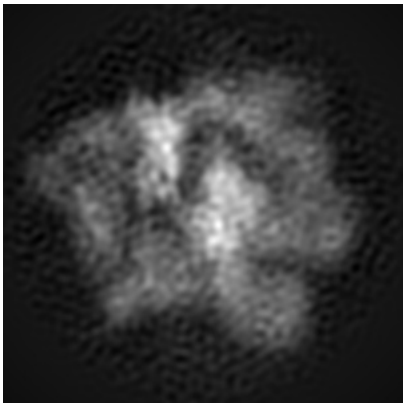
6.1.1 Primary map



X



Y

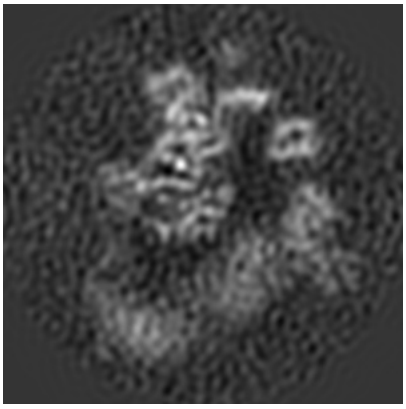


Z

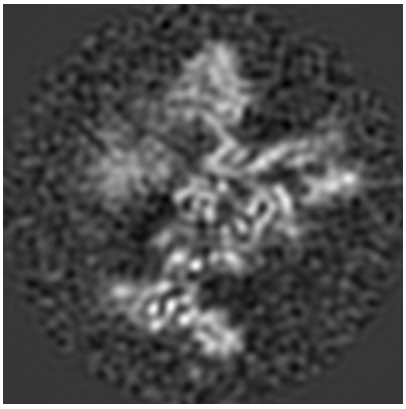
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

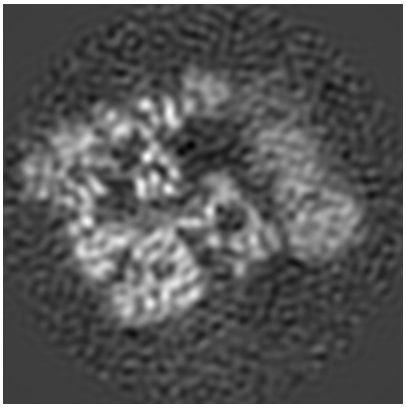
6.2.1 Primary map



X Index: 128



Y Index: 128

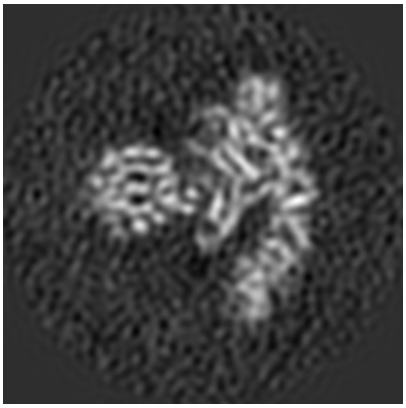


Z Index: 128

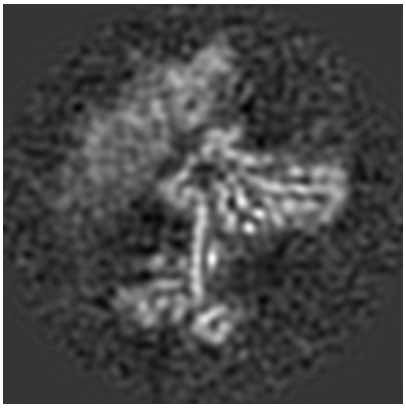
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

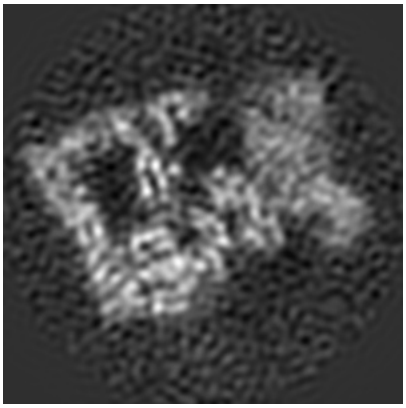
6.3.1 Primary map



X Index: 106



Y Index: 115

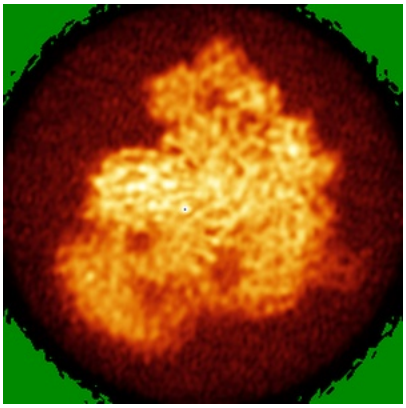


Z Index: 139

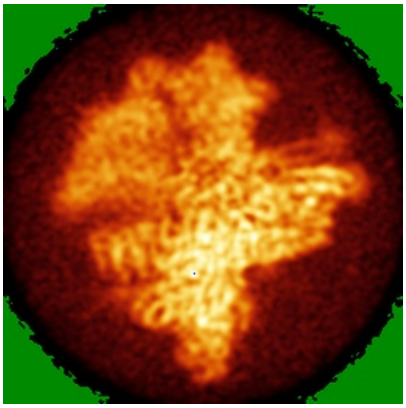
The images above show the largest variance slices of the map in three orthogonal directions.

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

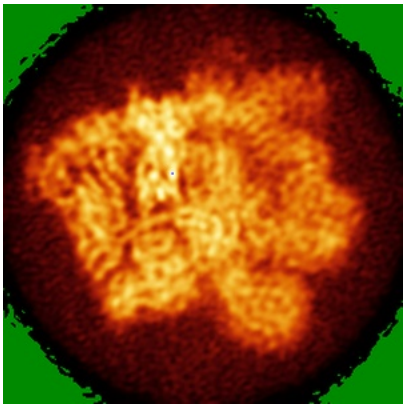
6.4.1 Primary map



X



Y

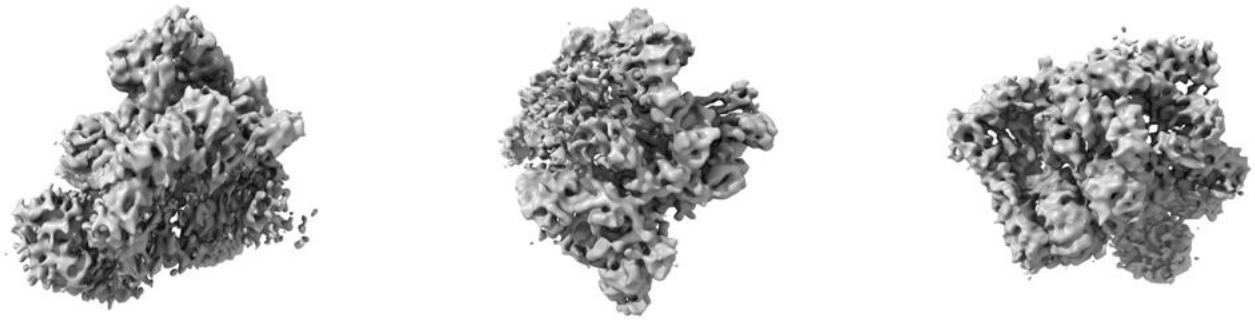


Z

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



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.004. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

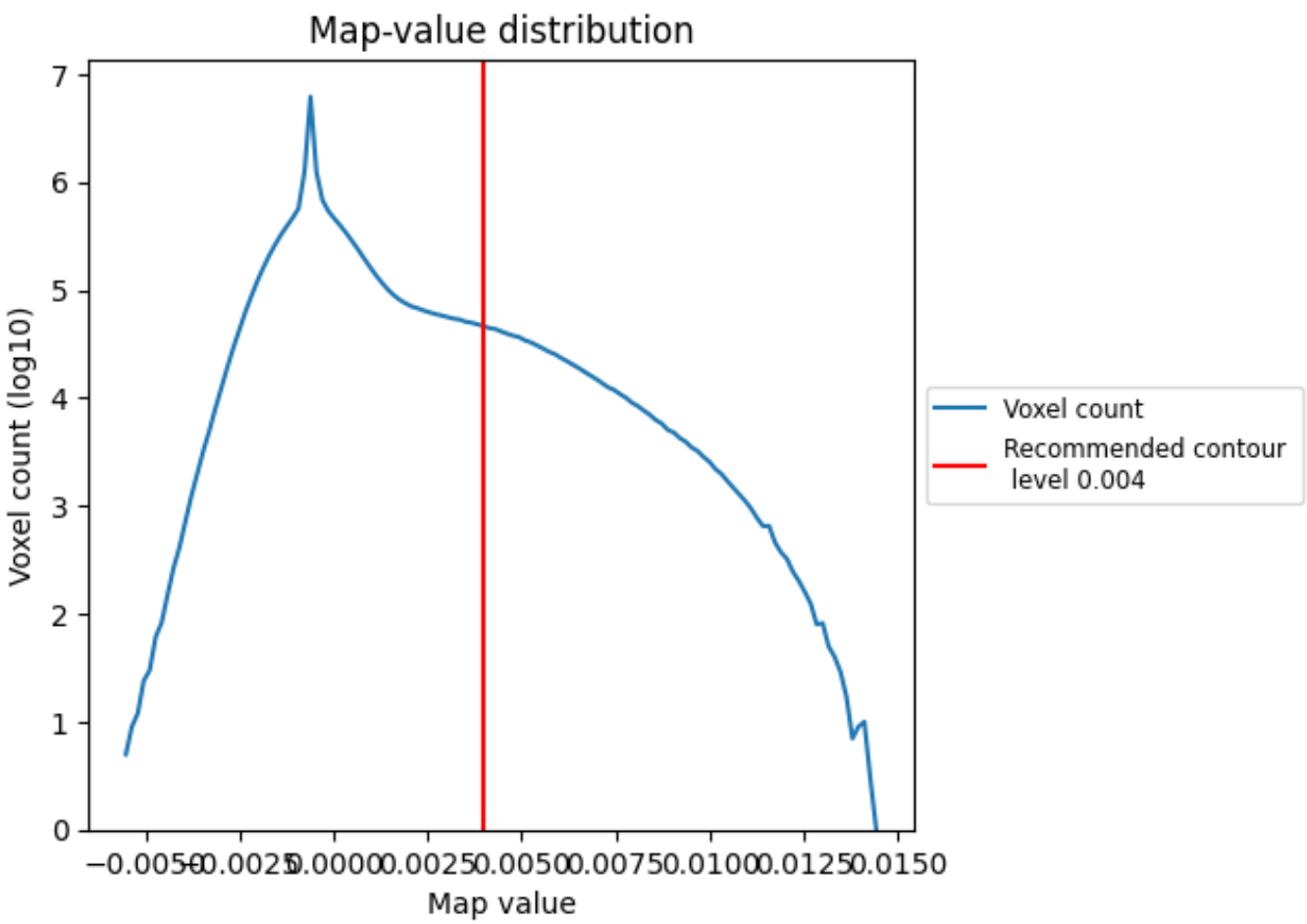
6.6 Mask visualisation (i)

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

7 Map analysis (i)

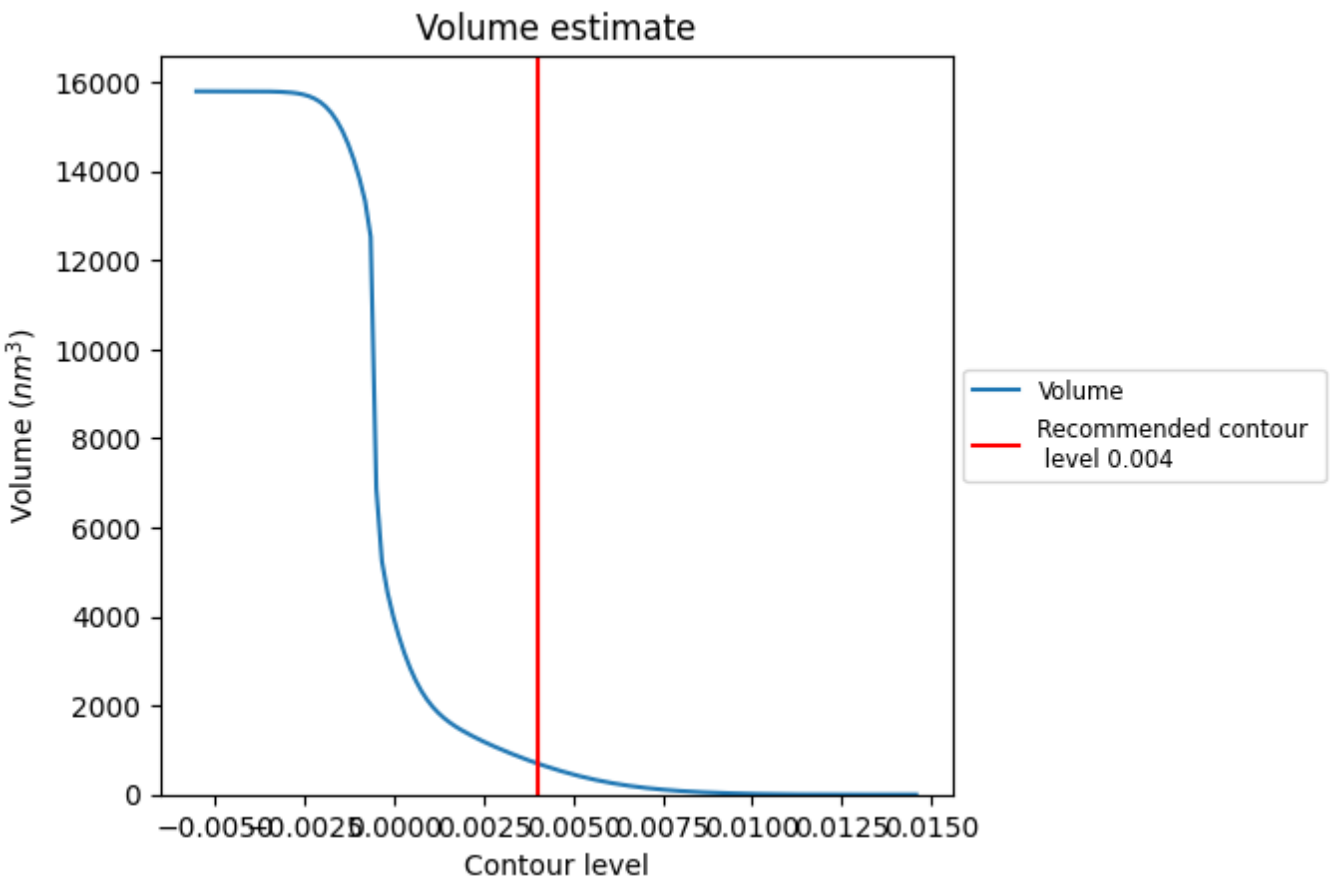
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

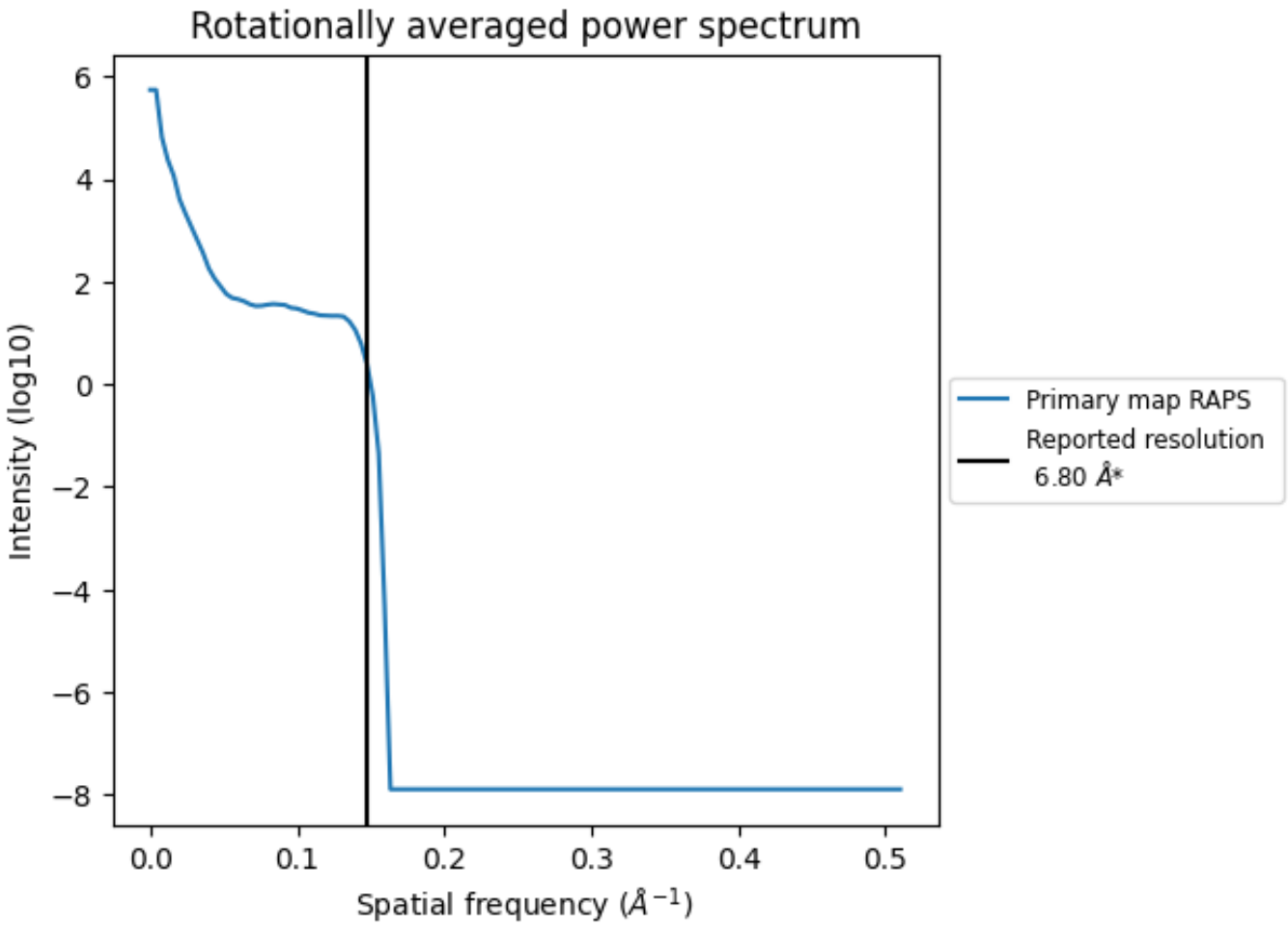
7.2 Volume estimate (i)



The volume at the recommended contour level is 699 nm^3; this corresponds to an approximate mass of 632 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 (i)



*Reported resolution corresponds to spatial frequency of 0.147 Å^{-1}

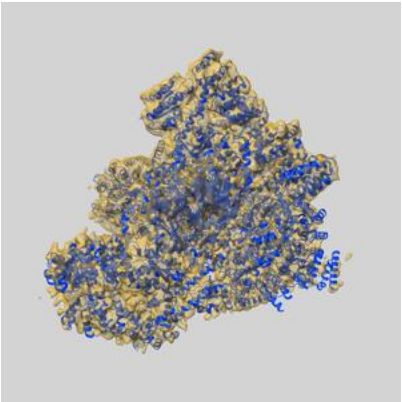
8 Fourier-Shell correlation (i)

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

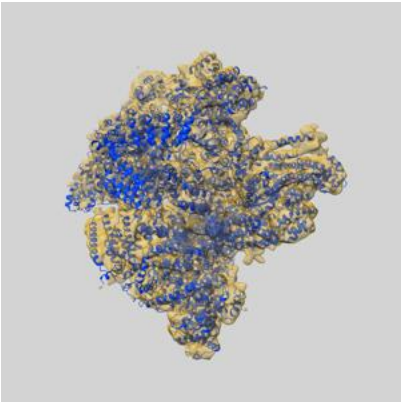
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-8676 and PDB model 5VHI. Per-residue inclusion information can be found in section 3 on page 7.

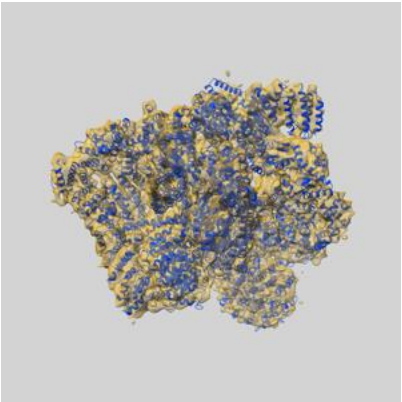
9.1 Map-model overlay (i)



X



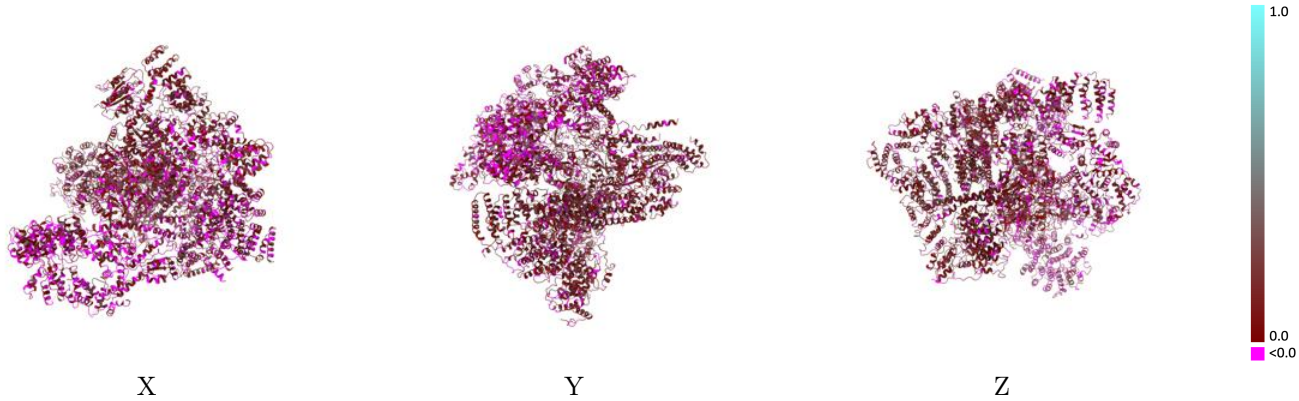
Y



Z

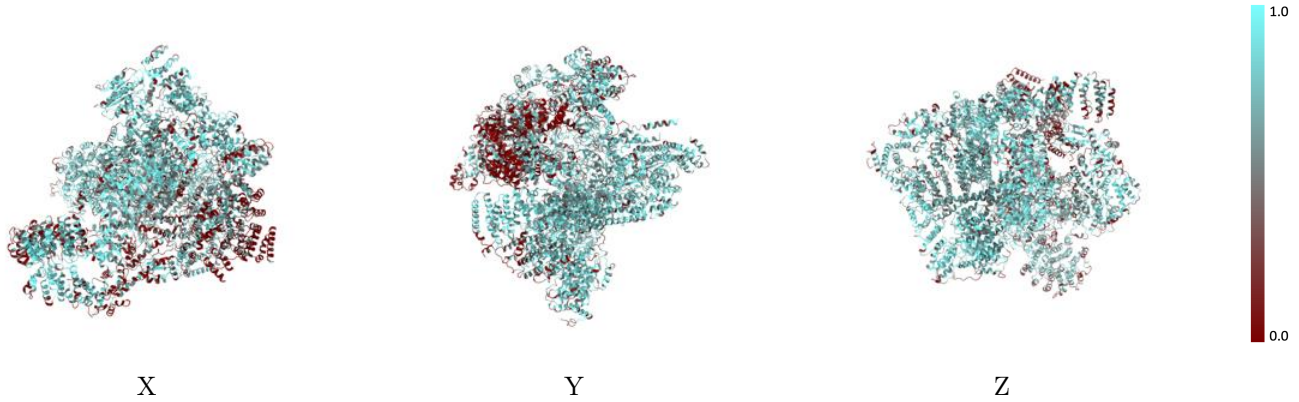
The images above show the 3D surface view of the map at the recommended contour level 0.004 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



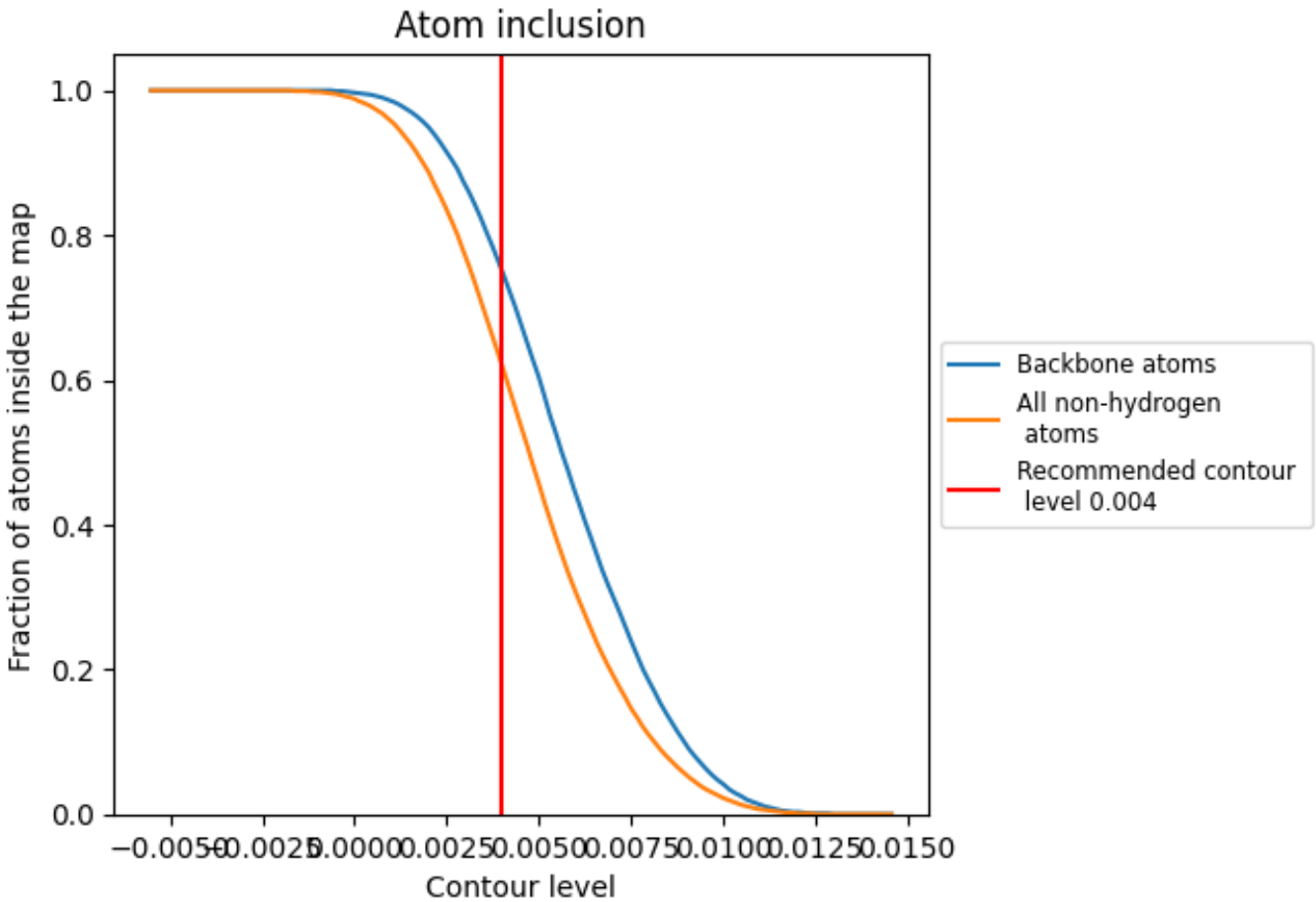
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.004).

9.4 Atom inclusion (i)



At the recommended contour level, 75% of all backbone atoms, 62% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.004) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6210	0.0990
A	0.6430	0.0840
B	0.5530	0.0660
C	0.4830	0.0670
D	0.4350	0.0610
E	0.6000	0.0810
F	0.6750	0.0940
G	0.1650	0.0280
U	0.7750	0.1400
V	0.6070	0.1070
W	0.6450	0.1100
X	0.4720	0.1030
Y	0.7680	0.1300
Z	0.7160	0.1330
a	0.7310	0.1330
b	0.7480	0.1270
c	0.6910	0.1340
d	0.6610	0.1290
e	0.4830	0.0680
f	0.5750	0.0410