wwPDB EM Validation Summary Report (i)

Jun 3, 2025 – 04:20 PM EDT

PDB ID	:	9BV3 / pdb_00009bv3
EMDB ID	:	EMD-44930
Title	:	M1B Midnolin-Proteasome
Authors	:	Gao, J.; Yip, M.C.J.; Shao, S.
Deposited on	:	2024-05-19
Resolution	:	2.90 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:

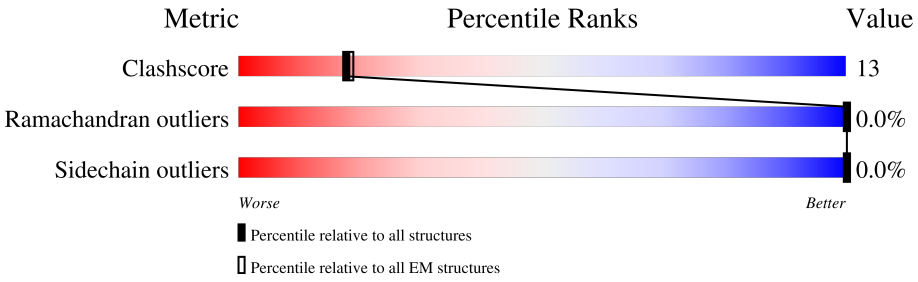
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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 2.90 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)
Clashscore	210492	15764
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 <=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	y	567	5% 95%
2	U	953	6% 61% 24% 15%
3	V	534	15% 57% 28% 14%
4	W	456	67% 29%
5	X	422	15% 70% 28%
6	Y	389	73% 25%
7	Z	324	6% 67% 22% 11%
8	a	376	20% 66% 33%

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Mol	Chain	Length	Quality of chain
9	b	377	19% 30% 20% 49%
10	c	310	6% 68% 25% 7%
11	d	350	12% 53% 22% 25%
12	e	70	7% 44% 11% 44%
13	A	433	67% 23% 10%
14	B	440	5% 58% 26% 16%
15	C	406	69% 19% 12%
16	D	418	68% 23% 9%
17	E	389	69% 24% 7%
18	F	439	54% 26% 21%
19	G	246	75% 22%
20	H	234	75% 23%
21	I	261	75% 23%
22	J	248	69% 28%
23	L	263	71% 19% 10%
24	M	255	71% 24% 5%
25	N	239	70% 13% 17%
25	n	239	59% 17% 23%
26	O	277	60% 20% 20%
26	o	277	8% 46% 18% 36%
27	P	205	70% 30%
27	p	205	20% 61% 19% 20%
28	Q	201	79% 19%
28	q	201	16% 62% 24% 14%
29	R	263	56% 20% 24%

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Mol	Chain	Length	Quality of chain
29	r	263	52% 19% 29%
30	S	241	70% 18% 12%
30	s	241	65% 21% 15%
31	T	264	58% 23% 19%
31	t	264	60% 18% 22%
32	K	241	74% 20% 6%
33	f	908	15% 47% 24% 29%

2 Entry composition (i)

There are 36 unique types of molecules in this entry. The entry contains 88575 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 Midnolin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	y	31	Total	C	N	O	S	0	0
			273	164	66	42	1		

There are 101 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
y	-98	MET	-	initiating methionine	UNP Q504T8
y	-97	ASP	-	expression tag	UNP Q504T8
y	-96	TYR	-	expression tag	UNP Q504T8
y	-95	LYS	-	expression tag	UNP Q504T8
y	-94	ASP	-	expression tag	UNP Q504T8
y	-93	ASP	-	expression tag	UNP Q504T8
y	-92	ASP	-	expression tag	UNP Q504T8
y	-91	ASP	-	expression tag	UNP Q504T8
y	-90	LYS	-	expression tag	UNP Q504T8
y	-89	ASP	-	expression tag	UNP Q504T8
y	-88	TYR	-	expression tag	UNP Q504T8
y	-87	LYS	-	expression tag	UNP Q504T8
y	-86	ASP	-	expression tag	UNP Q504T8
y	-85	ASP	-	expression tag	UNP Q504T8
y	-84	ASP	-	expression tag	UNP Q504T8
y	-83	ASP	-	expression tag	UNP Q504T8
y	-82	LYS	-	expression tag	UNP Q504T8
y	-81	GLY	-	expression tag	UNP Q504T8
y	-80	GLY	-	expression tag	UNP Q504T8
y	-79	GLY	-	expression tag	UNP Q504T8
y	-78	GLY	-	expression tag	UNP Q504T8
y	-77	SER	-	expression tag	UNP Q504T8
y	-76	GLY	-	expression tag	UNP Q504T8
y	-75	GLY	-	expression tag	UNP Q504T8
y	-74	GLY	-	expression tag	UNP Q504T8
y	-73	GLY	-	expression tag	UNP Q504T8
y	-72	PHE	-	expression tag	UNP Q504T8
y	-71	GLU	-	expression tag	UNP Q504T8

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Chain	Residue	Modelled	Actual	Comment	Reference
y	-70	THR	-	expression tag	UNP Q504T8
y	-69	SER	-	expression tag	UNP Q504T8
y	-68	LEU	-	expression tag	UNP Q504T8
y	-67	TYR	-	expression tag	UNP Q504T8
y	-66	LYS	-	expression tag	UNP Q504T8
y	-65	LYS	-	expression tag	UNP Q504T8
y	-64	ALA	-	expression tag	UNP Q504T8
y	-63	GLY	-	expression tag	UNP Q504T8
y	-62	LEU	-	expression tag	UNP Q504T8
y	-61	ALA	-	expression tag	UNP Q504T8
y	-60	THR	-	expression tag	UNP Q504T8
y	-59	MET	-	expression tag	UNP Q504T8
y	-58	GLU	-	expression tag	UNP Q504T8
y	-57	LYS	-	expression tag	UNP Q504T8
y	-56	VAL	-	expression tag	UNP Q504T8
y	-55	LEU	-	expression tag	UNP Q504T8
y	-54	VAL	-	expression tag	UNP Q504T8
y	-53	GLU	-	expression tag	UNP Q504T8
y	-52	THR	-	expression tag	UNP Q504T8
y	-51	SER	-	expression tag	UNP Q504T8
y	-50	TYR	-	expression tag	UNP Q504T8
y	-49	PRO	-	expression tag	UNP Q504T8
y	-48	SER	-	expression tag	UNP Q504T8
y	-47	GLN	-	expression tag	UNP Q504T8
y	-46	THR	-	expression tag	UNP Q504T8
y	-45	THR	-	expression tag	UNP Q504T8
y	-44	ARG	-	expression tag	UNP Q504T8
y	-43	LEU	-	expression tag	UNP Q504T8
y	-42	PRO	-	expression tag	UNP Q504T8
y	-41	PRO	-	expression tag	UNP Q504T8
y	-40	ILE	-	expression tag	UNP Q504T8
y	-39	THR	-	expression tag	UNP Q504T8
y	-38	TYR	-	expression tag	UNP Q504T8
y	-37	THR	-	expression tag	UNP Q504T8
y	-36	GLY	-	expression tag	UNP Q504T8
y	-35	ARG	-	expression tag	UNP Q504T8
y	-34	PHE	-	expression tag	UNP Q504T8
y	-33	SER	-	expression tag	UNP Q504T8
y	-32	LEU	-	expression tag	UNP Q504T8
y	-31	GLU	-	expression tag	UNP Q504T8
y	-30	PRO	-	expression tag	UNP Q504T8
y	-29	ALA	-	expression tag	UNP Q504T8

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Chain	Residue	Modelled	Actual	Comment	Reference
y	-28	PRO	-	expression tag	UNP Q504T8
y	-27	ASN	-	expression tag	UNP Q504T8
y	-26	SER	-	expression tag	UNP Q504T8
y	-25	GLY	-	expression tag	UNP Q504T8
y	-24	ASN	-	expression tag	UNP Q504T8
y	-23	THR	-	expression tag	UNP Q504T8
y	-22	LEU	-	expression tag	UNP Q504T8
y	-21	TRP	-	expression tag	UNP Q504T8
y	-20	PRO	-	expression tag	UNP Q504T8
y	-19	GLU	-	expression tag	UNP Q504T8
y	-18	PRO	-	expression tag	UNP Q504T8
y	-17	LEU	-	expression tag	UNP Q504T8
y	-16	PHE	-	expression tag	UNP Q504T8
y	-15	SER	-	expression tag	UNP Q504T8
y	-14	LEU	-	expression tag	UNP Q504T8
y	-13	VAL	-	expression tag	UNP Q504T8
y	-12	SER	-	expression tag	UNP Q504T8
y	-11	GLY	-	expression tag	UNP Q504T8
y	-10	LEU	-	expression tag	UNP Q504T8
y	-9	VAL	-	expression tag	UNP Q504T8
y	-8	SER	-	expression tag	UNP Q504T8
y	-7	MET	-	expression tag	UNP Q504T8
y	-6	THR	-	expression tag	UNP Q504T8
y	-5	ASN	-	expression tag	UNP Q504T8
y	-4	PRO	-	expression tag	UNP Q504T8
y	-3	PRO	-	expression tag	UNP Q504T8
y	-2	ALA	-	expression tag	UNP Q504T8
y	-1	SER	-	expression tag	UNP Q504T8
y	0	SER	-	expression tag	UNP Q504T8
y	1	SER	-	expression tag	UNP Q504T8
y	457	ALA	VAL	conflict	UNP Q504T8

- Molecule 2 is a protein called 26S proteasome non-ATPase regulatory subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	U	812	Total	C	N	O	S	0	0
			6334	4021	1078	1190	45		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	V	457	Total	C	N	O	S	0	0
			3725	2364	669	679	13		

- Molecule 4 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	W	438	Total	C	N	O	S	0	0
			3572	2262	610	677	23		

- Molecule 5 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	X	413	Total	C	N	O	S	0	0
			3259	2073	556	618	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Y	381	Total	C	N	O	S	0	0
			3135	2000	536	582	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Z	287	Total	C	N	O	S	0	0
			2290	1462	394	429	5		

- Molecule 8 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	a	375	Total	C	N	O	S	0	0
			3012	1921	513	563	15		

- Molecule 9 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	b	191	Total	C	N	O	S	0	0
			1459	910	261	281	7		

- Molecule 10 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	d	261	Total	C	N	O	S	0	0
			2124	1376	348	391	9		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
12	e	39	Total	C	N	O	0	0
			345	213	54	78		

- Molecule 13 is a protein called 26S proteasome regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	A	389	Total	C	N	O	S	0	0
			3057	1927	537	575	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	B	371	Total	C	N	O	S	0	0
			2933	1846	499	574	14		

- Molecule 15 is a protein called 26S protease regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	C	359	Total	C	N	O	S	0	0
			2834	1790	509	519	16		

- Molecule 16 is a protein called 26S proteasome regulatory subunit 6B.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	D	380	Total	C	N	O	S	0	0
			3040	1923	524	580	13		

- Molecule 17 is a protein called 26S protease regulatory subunit 10B.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	E	362	Total	C	N	O	S	0	0
			2869	1805	508	540	16		

- Molecule 18 is a protein called 26S proteasome regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	F	349	Total	C	N	O	S	0	0
			2724	1721	469	519	15		

- Molecule 19 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	G	238	Total	C	N	O	S	0	0
			1865	1186	311	355	13		

- Molecule 20 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	H	229	Total	C	N	O	S	0	0
			1789	1145	301	337	6		

- Molecule 21 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	I	254	Total	C	N	O	S	0	0
			2007	1267	345	385	10		

- Molecule 22 is a protein called Proteasome subunit alpha type-7.

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

- Molecule 23 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	L	237	Total	C	N	O	S	0	0
			1868	1168	338	351	11		

- Molecule 24 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	M	243	Total	C	N	O	S	0	0
			1909	1208	324	366	11		

- Molecule 25 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	N	198	Total	C	N	O	S	0	0
			1487	931	254	290	12		
25	n	183	Total	C	N	O	S	0	0
			1360	849	234	265	12		

- Molecule 26 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	O	221	Total	C	N	O	S	0	0
			1667	1050	284	321	12		
26	o	176	Total	C	N	O	S	0	0
			1315	823	228	253	11		

- Molecule 27 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	P	204	Total	C	N	O	S	0	0
			1591	1013	265	294	19		
27	p	165	Total	C	N	O	S	0	0
			1271	806	211	237	17		

- Molecule 28 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Q	197	Total	C	N	O	S	0	0
			1578	1011	268	290	9		
28	q	173	Total	C	N	O	S	0	0
			1380	890	234	248	8		

- Molecule 29 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	R	199	Total	C	N	O	S	0	0
			1549	977	272	291	9		
29	r	187	Total	C	N	O	S	0	0
			1432	904	248	271	9		

- Molecule 30 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	S	212	Total	C	N	O	S	0	0
			1643	1041	280	312	10		
30	s	206	Total	C	N	O	S	0	0
			1597	1015	269	303	10		

- Molecule 31 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	T	213	Total	C	N	O	S	0	0
			1665	1050	288	316	11		
31	t	206	Total	C	N	O	S	0	0
			1609	1016	279	302	12		

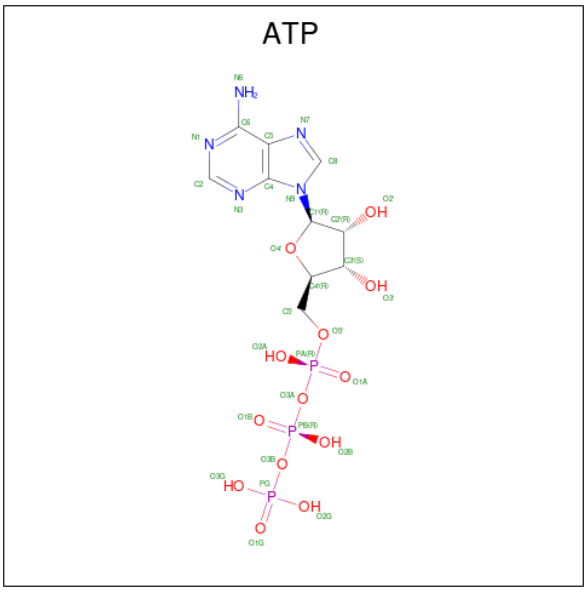
- Molecule 32 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	K	227	Total	C	N	O	S	0	0
			1736	1093	288	344	11		

- Molecule 33 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	f	647	Total	C	N	O	S	0	0
			4942	3141	835	932	34		

- Molecule 34 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

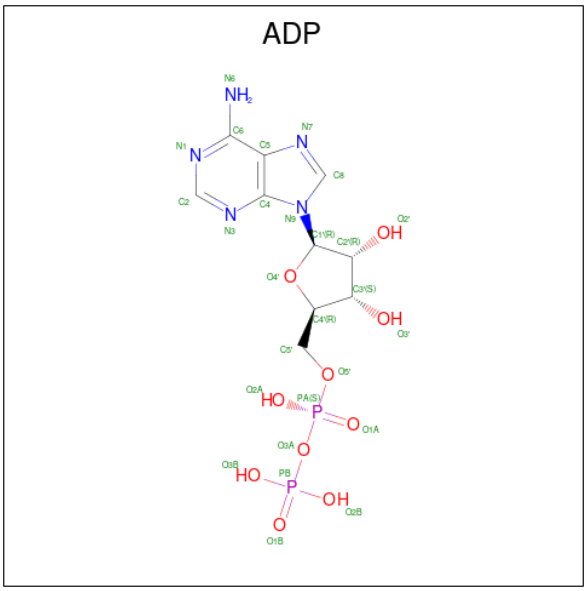


Mol	Chain	Residues	Atoms					AltConf
34	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
34	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
34	E	1	Total	C	N	O	P	0
			31	10	5	13	3	
34	F	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 35 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 36 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



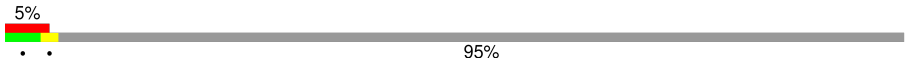
Mol	Chain	Residues	Atoms					AltConf
36	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
36	C	1	Total	C	N	O	P	0
			27	10	5	10	2	

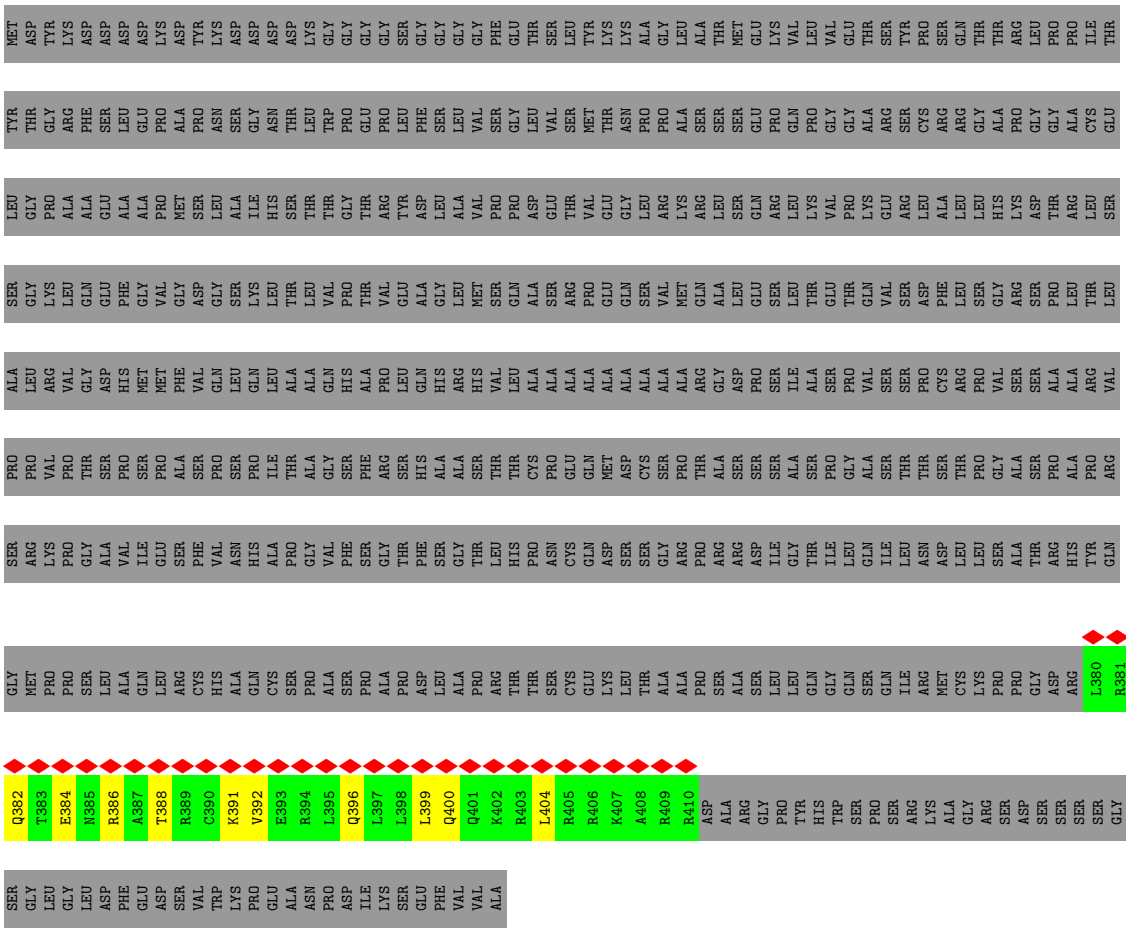
3 Residue-property plots (i)

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: Midnolin

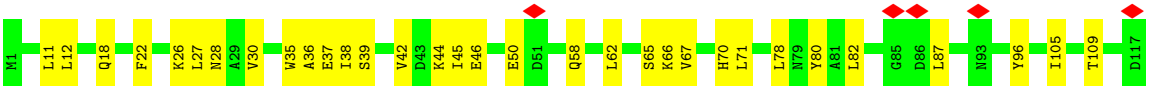
Chain y:

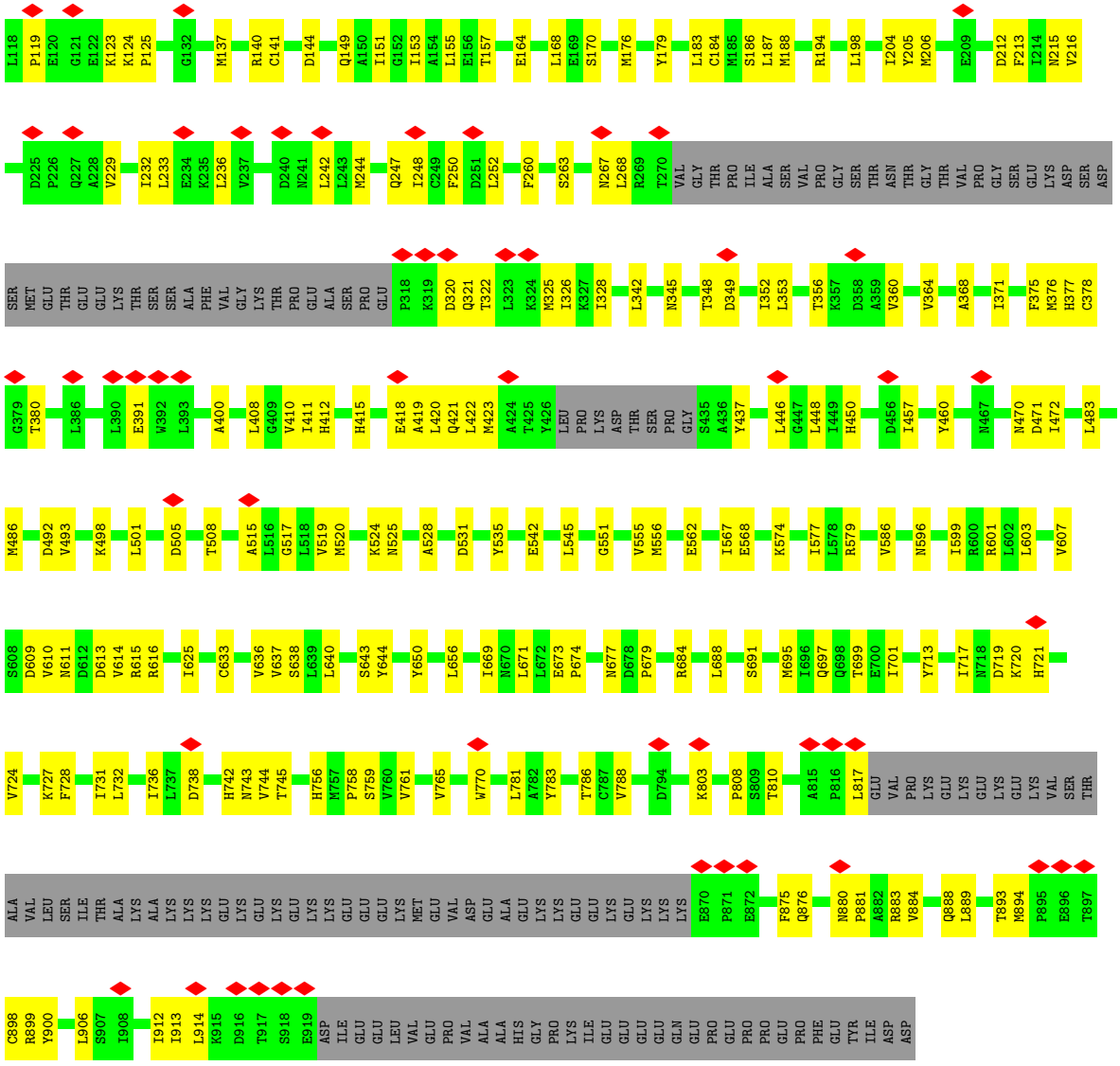




• Molecule 2: 26S proteasome non-ATPase regulatory subunit 1

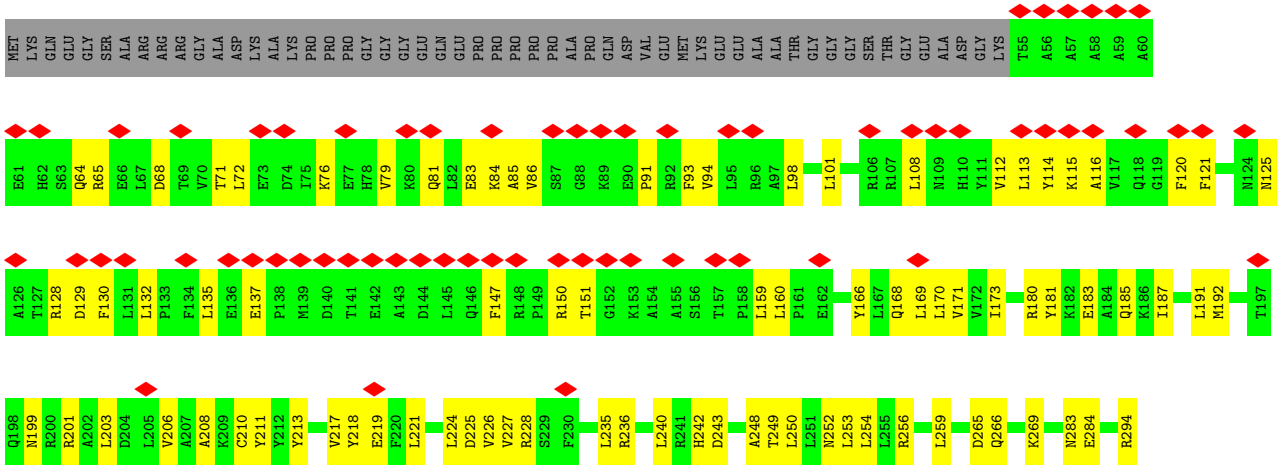
Chain U:

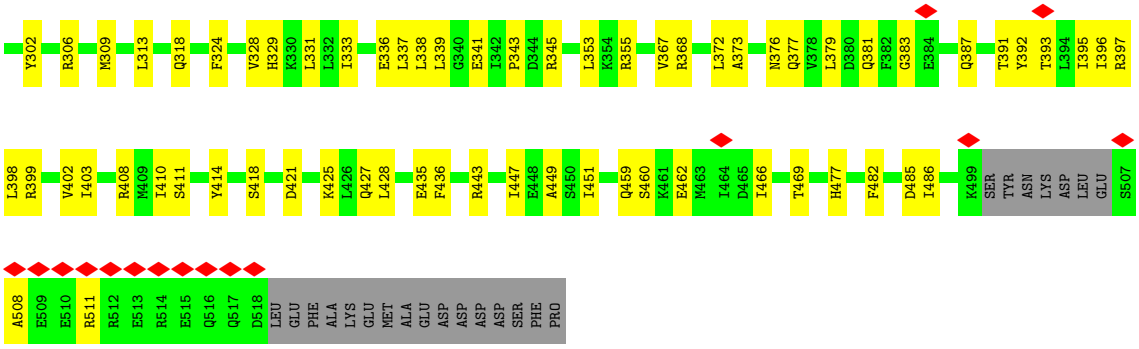




• Molecule 3: 26S proteasome non-ATPase regulatory subunit 3

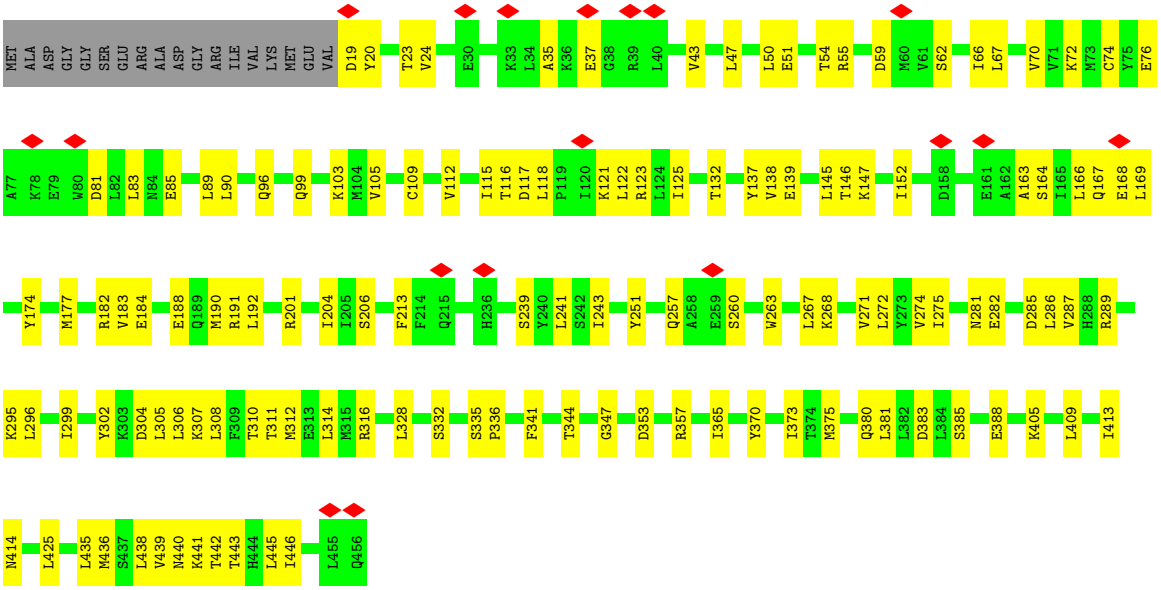
Chain V:





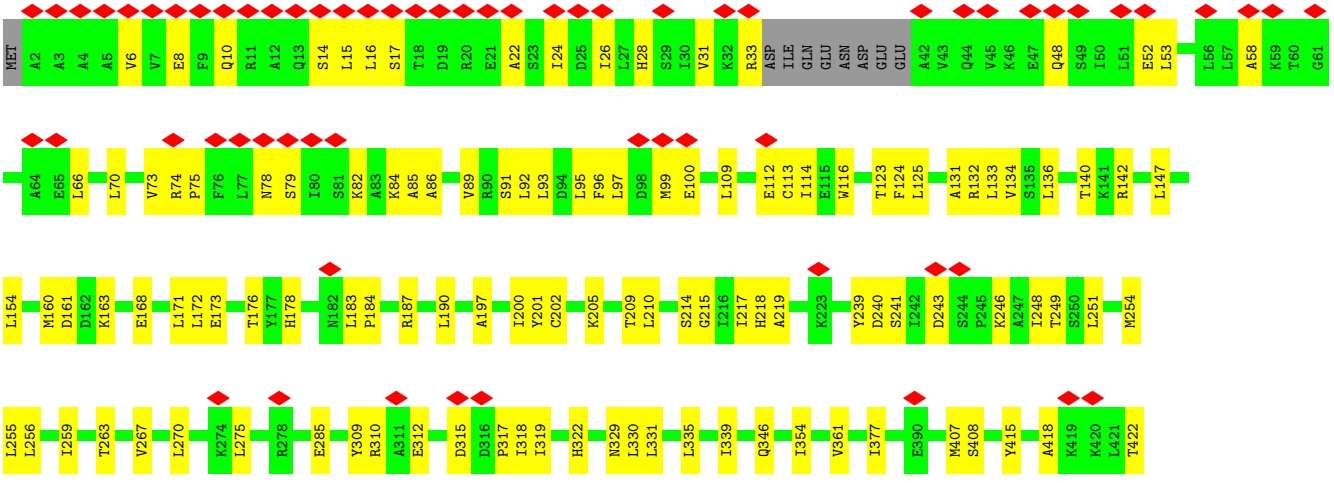
• Molecule 4: 26S proteasome non-ATPase regulatory subunit 12

Chain W:



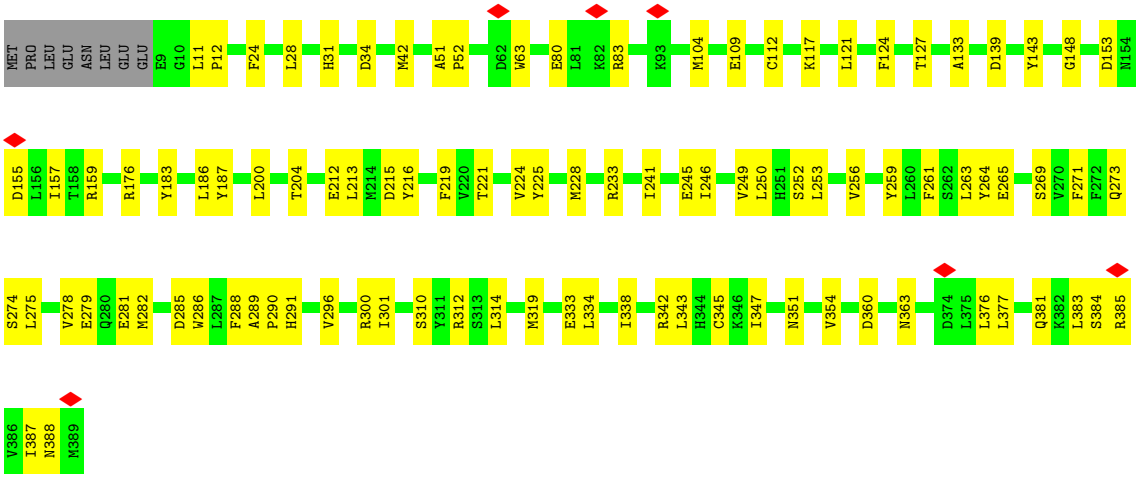
• Molecule 5: 26S proteasome non-ATPase regulatory subunit 11

Chain X:



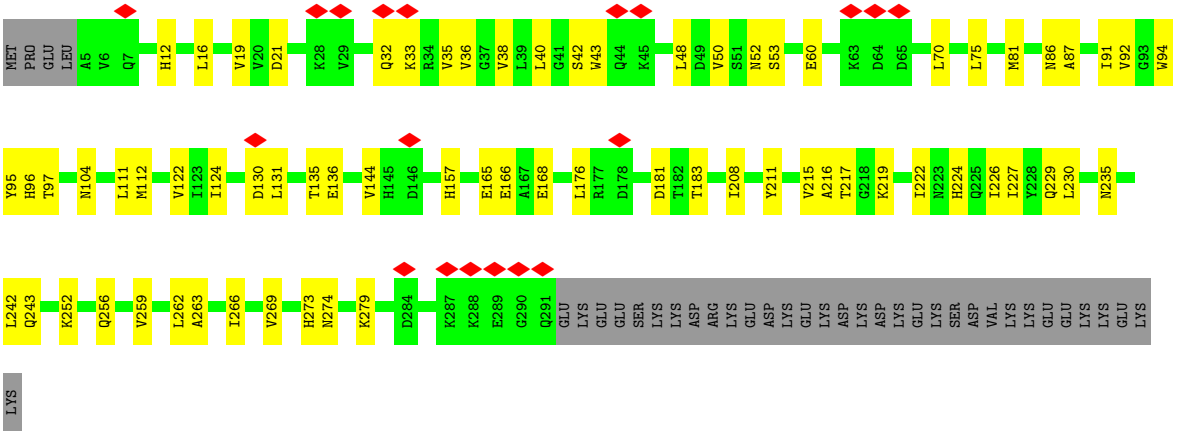
• Molecule 6: 26S proteasome non-ATPase regulatory subunit 6

Chain Y:



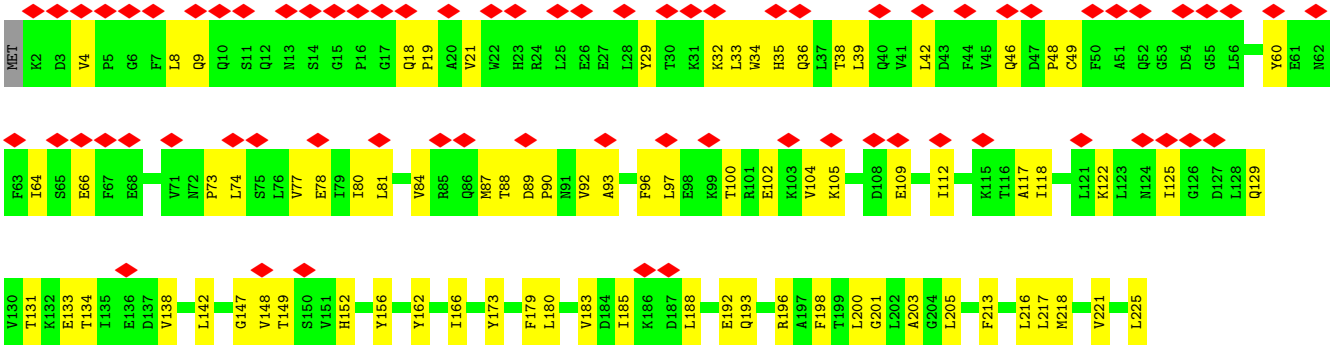
• Molecule 7: 26S proteasome non-ATPase regulatory subunit 7

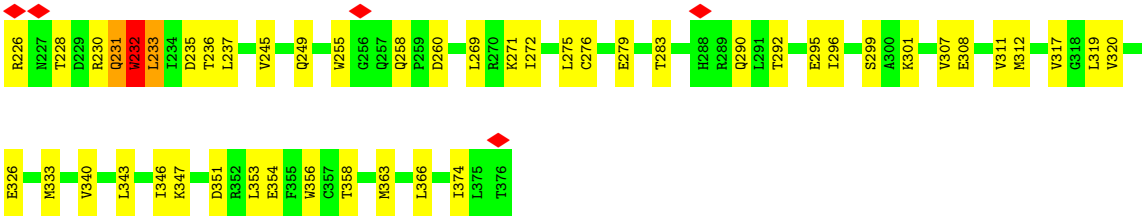
Chain Z:



• Molecule 8: 26S proteasome non-ATPase regulatory subunit 13

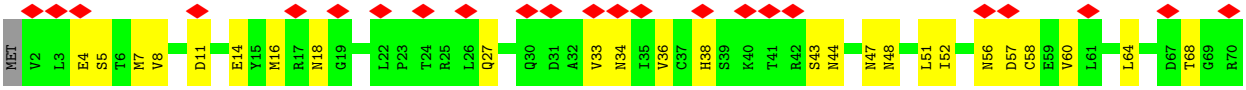
Chain a:

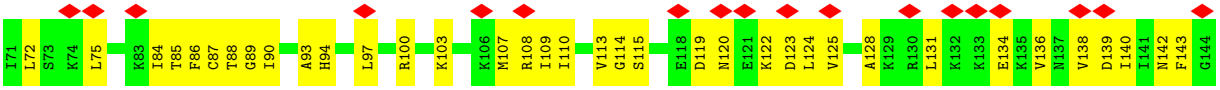


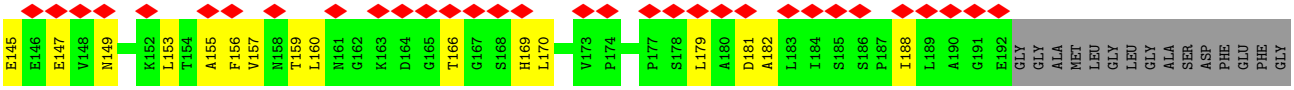


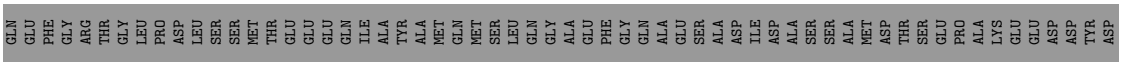
• Molecule 9: 26S proteasome non-ATPase regulatory subunit 4

Chain b:



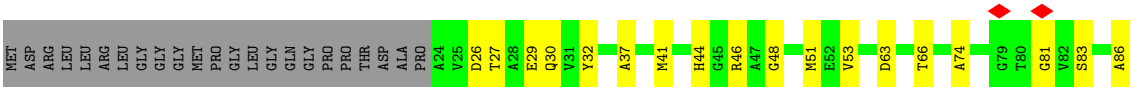


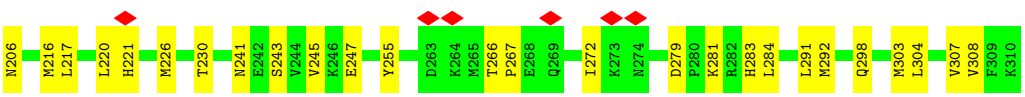




• Molecule 10: 26S proteasome non-ATPase regulatory subunit 14

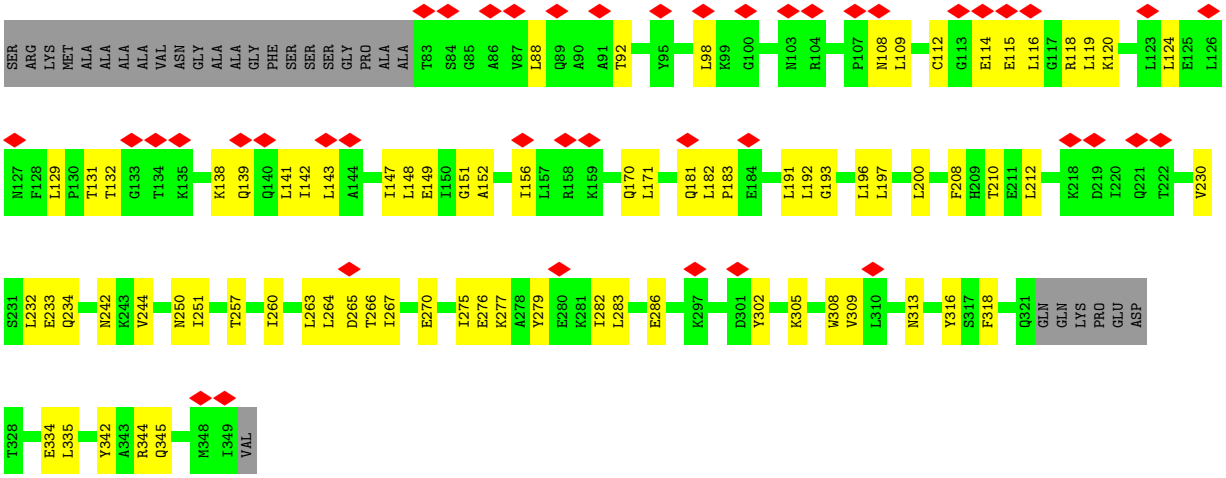
Chain c:





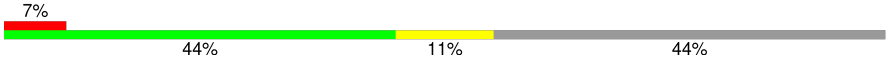
• Molecule 11: 26S proteasome non-ATPase regulatory subunit 8

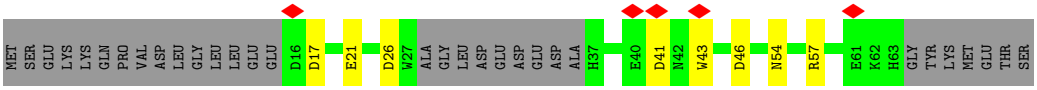
Chain d:



• Molecule 12: 26S proteasome complex subunit SEM1

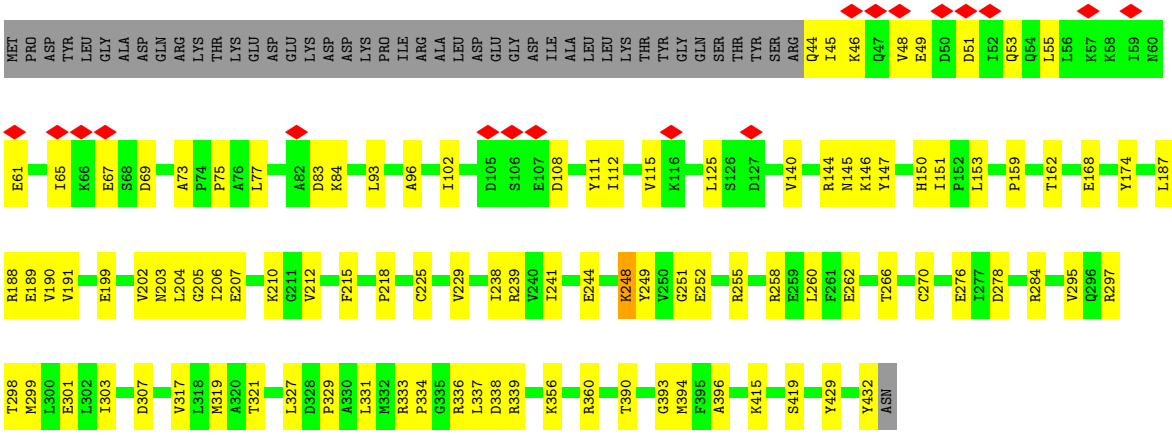
Chain e:





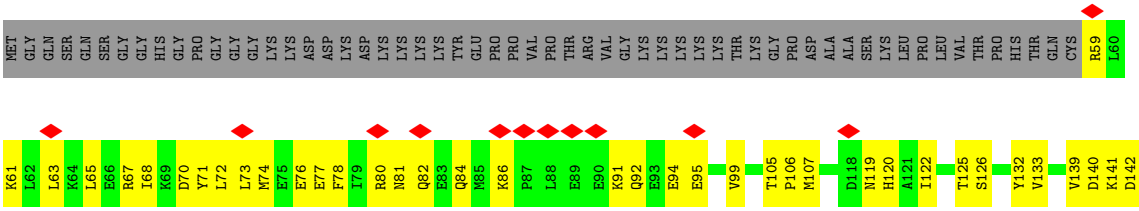
• Molecule 13: 26S proteasome regulatory subunit 7

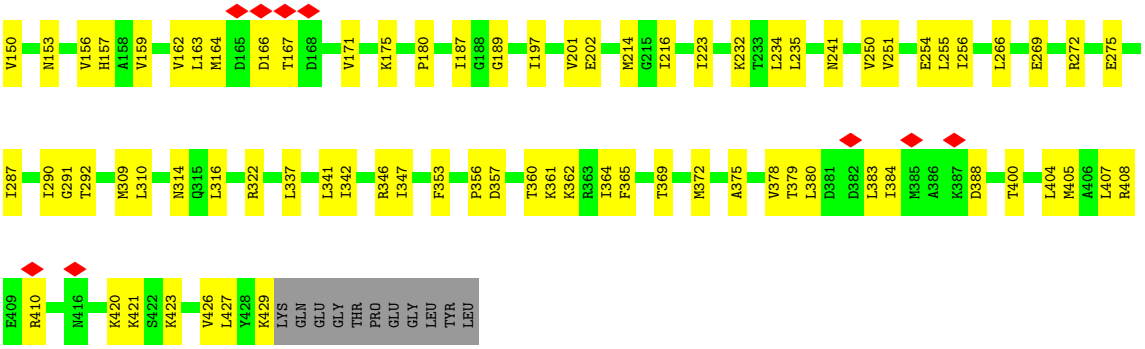
Chain A:



• Molecule 14: 26S proteasome regulatory subunit 4

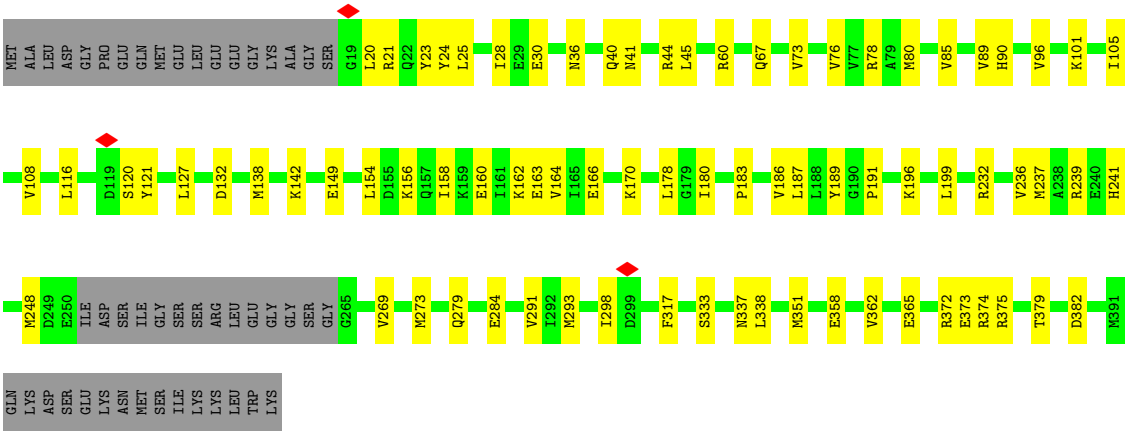
Chain B:





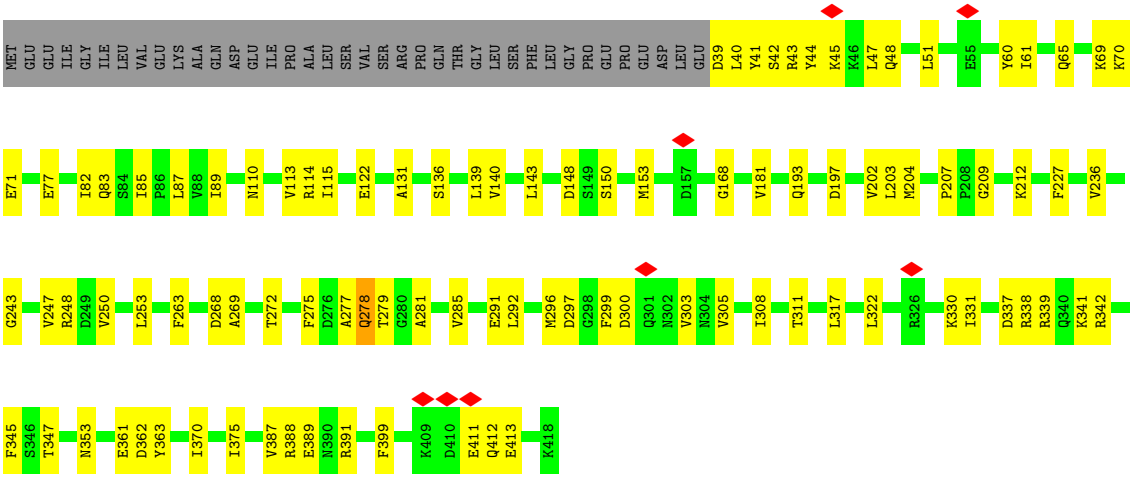
• Molecule 15: 26S protease regulatory subunit 8

Chain C:



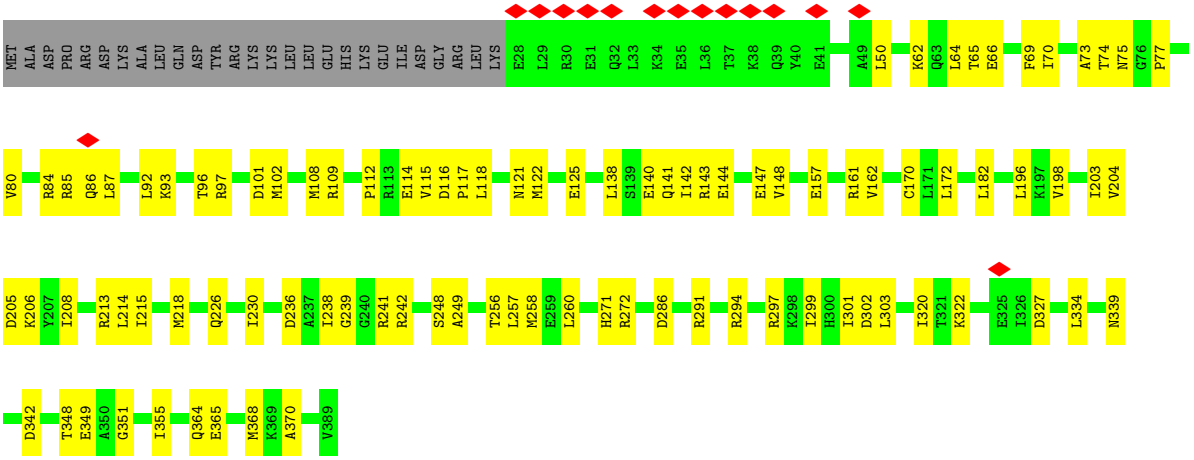
• Molecule 16: 26S proteasome regulatory subunit 6B

Chain D:



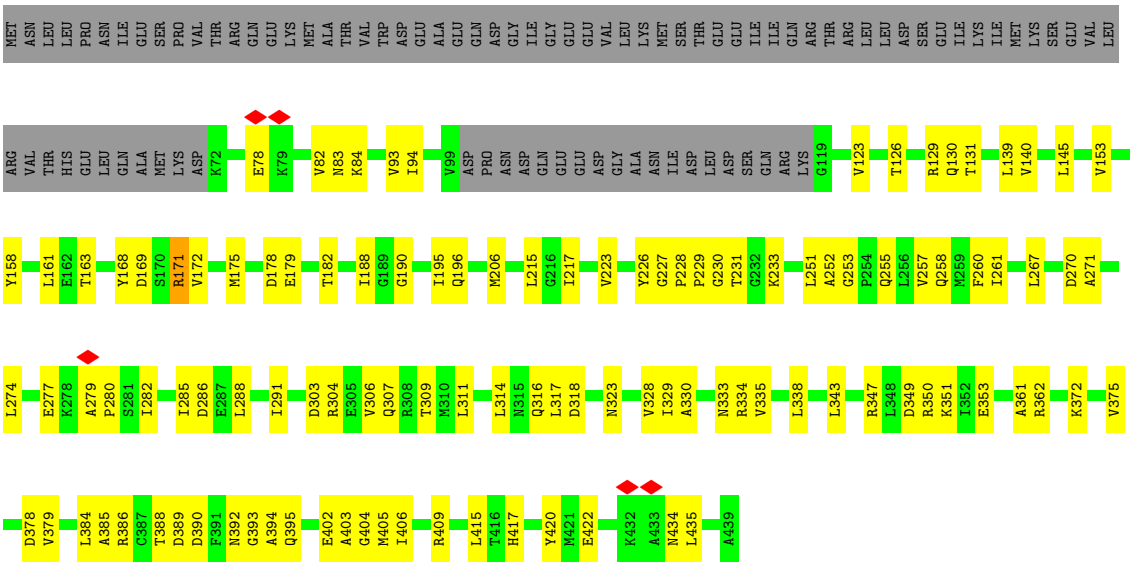
• Molecule 17: 26S protease regulatory subunit 10B

Chain E:



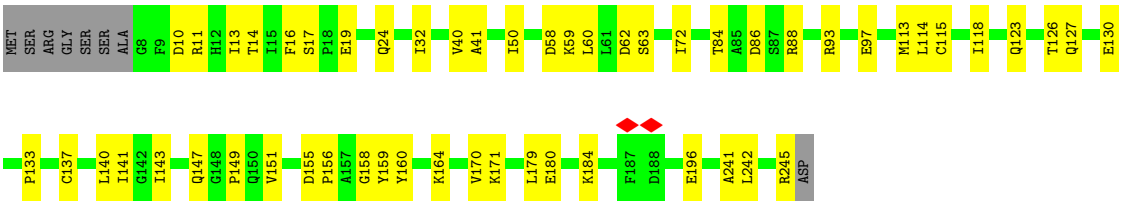
• Molecule 18: 26S proteasome regulatory subunit 6A

Chain F:



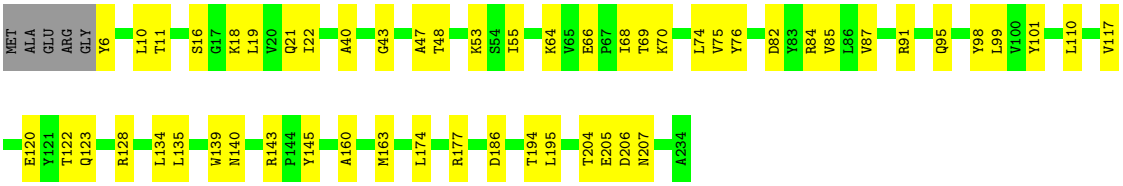
• Molecule 19: Proteasome subunit alpha type-6

Chain G:



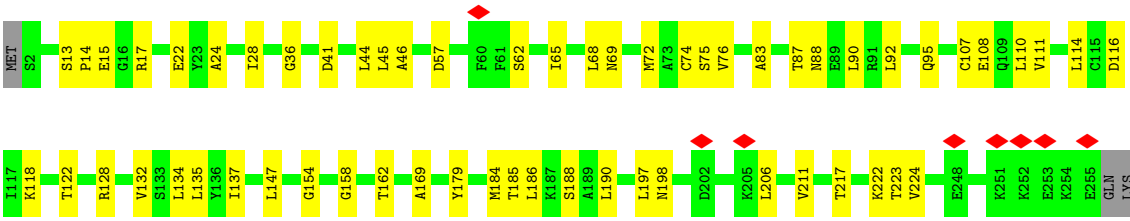
• Molecule 20: Proteasome subunit alpha type-2

Chain H:



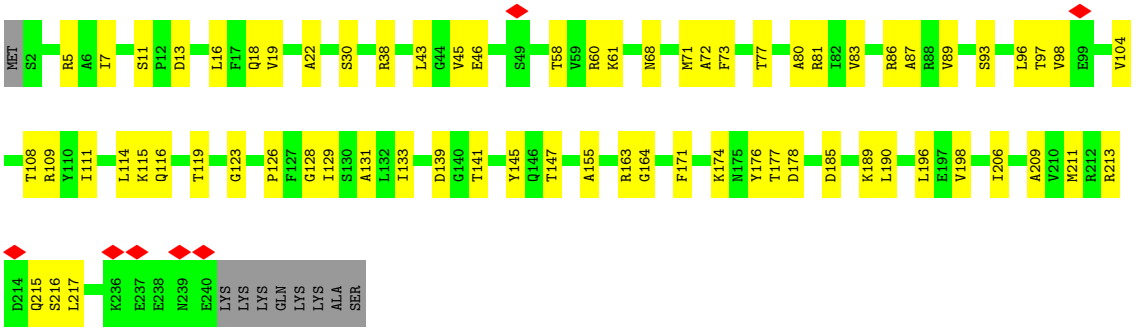
• Molecule 21: Proteasome subunit alpha type-4

Chain I:



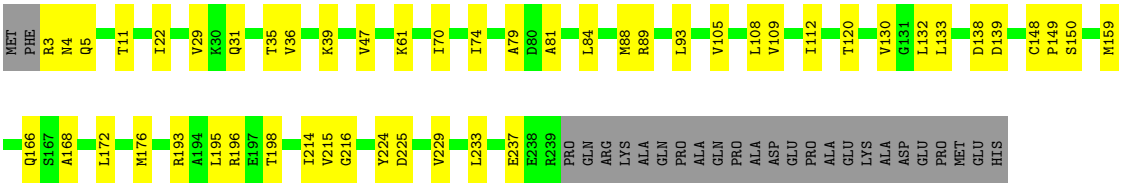
• Molecule 22: Proteasome subunit alpha type-7

Chain J:



• Molecule 23: Proteasome subunit alpha type-1

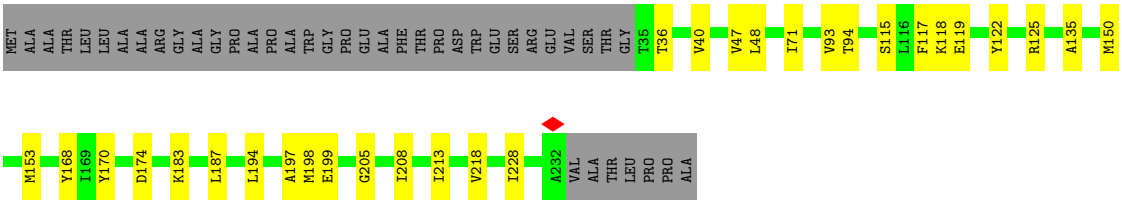
Chain L:



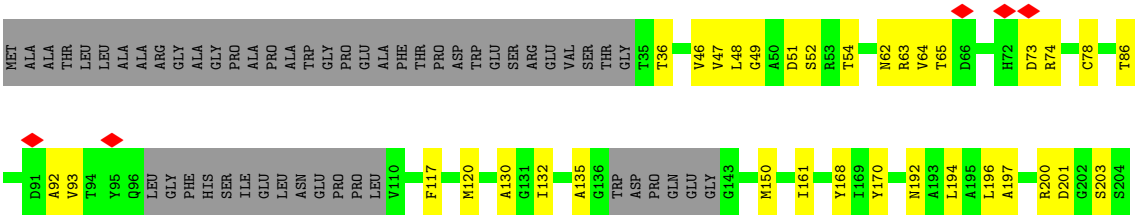
• Molecule 24: Proteasome subunit alpha type-3

Chain M:

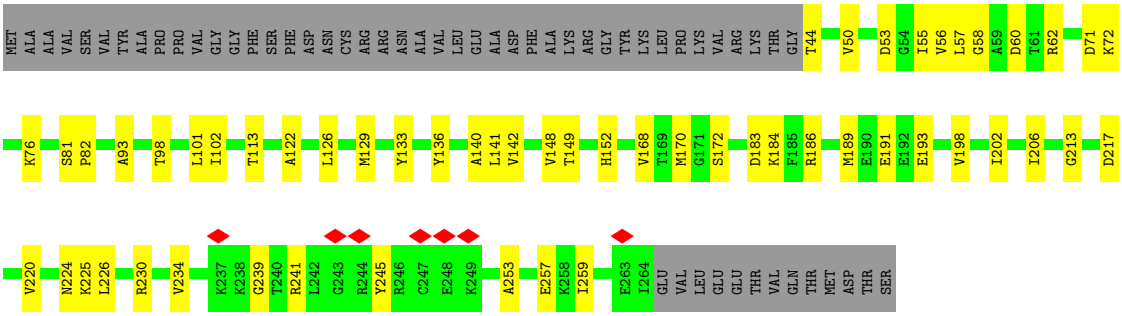
• Molecule 25: Proteasome subunit beta type-6



• Molecule 25: Proteasome subunit beta type-6

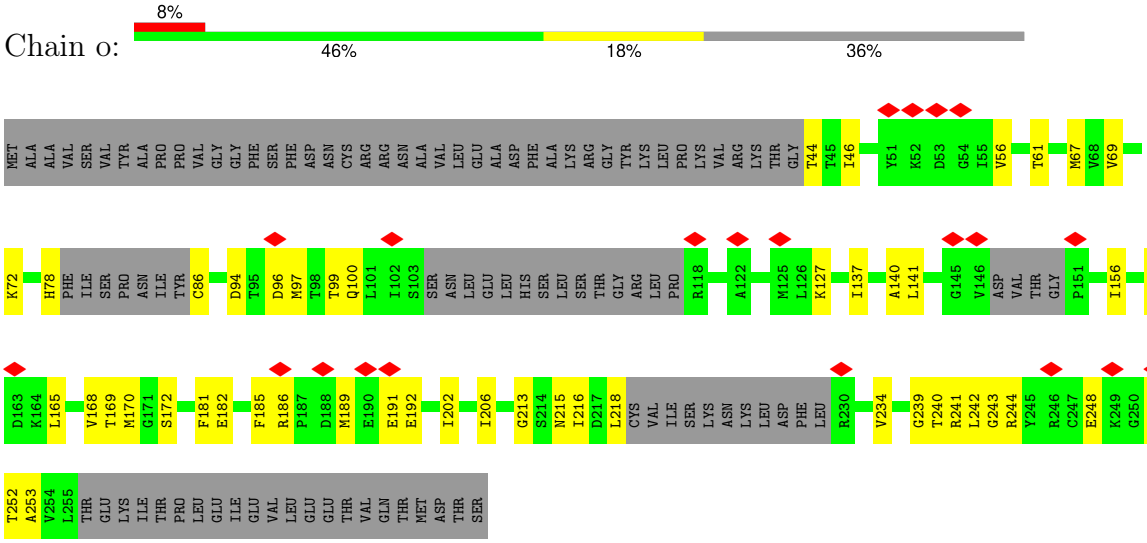


• Molecule 26: Proteasome subunit beta type-7



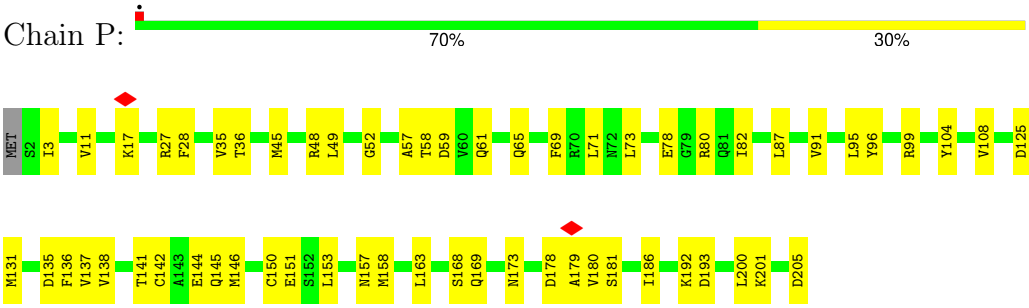
• Molecule 26: Proteasome subunit beta type-7

Chain o:



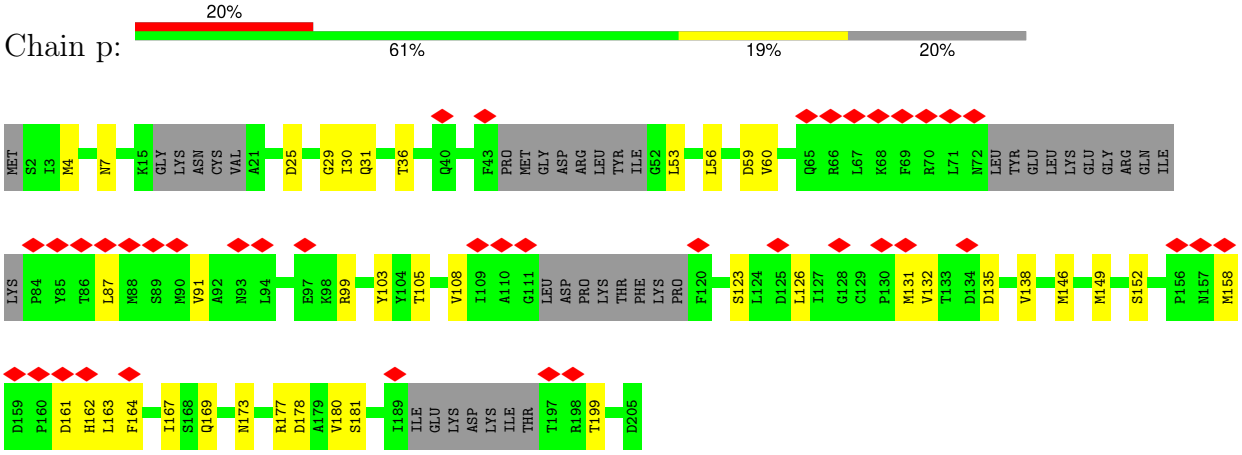
• Molecule 27: Proteasome subunit beta type-3

Chain P:



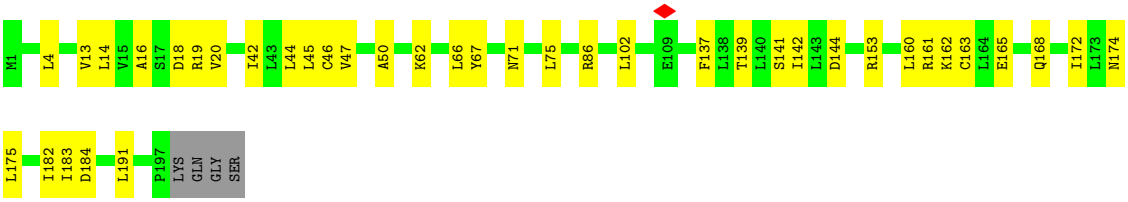
• Molecule 27: Proteasome subunit beta type-3

Chain p:



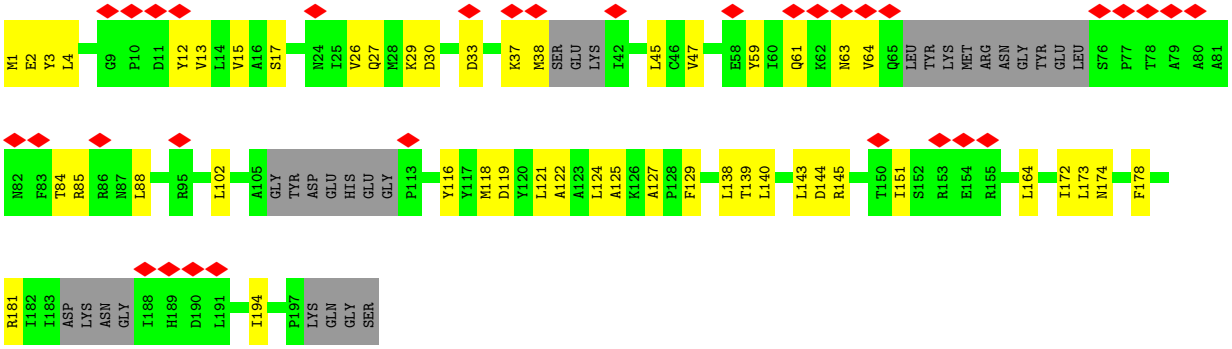
• Molecule 28: Proteasome subunit beta type-2

Chain Q:



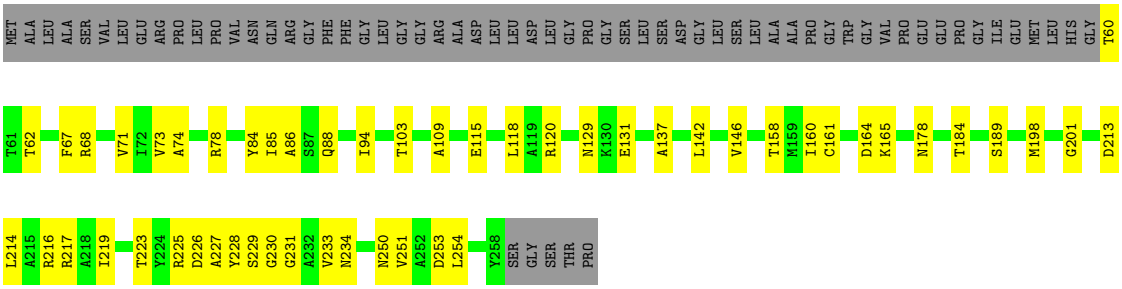
• Molecule 28: Proteasome subunit beta type-2

Chain q:



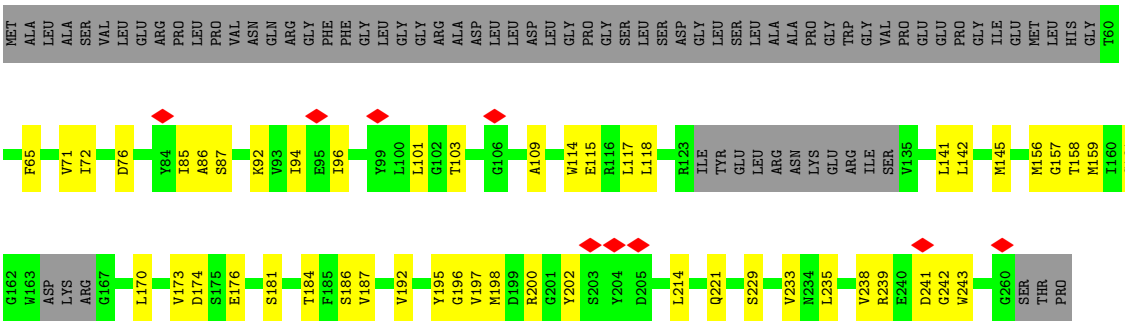
• Molecule 29: Proteasome subunit beta type-5

Chain R:



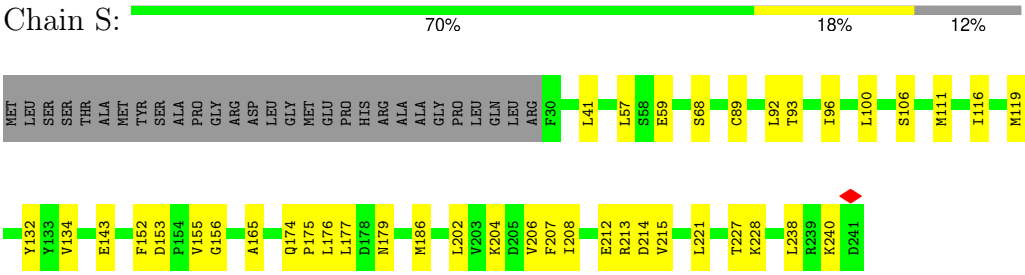
• Molecule 29: Proteasome subunit beta type-5

Chain r:



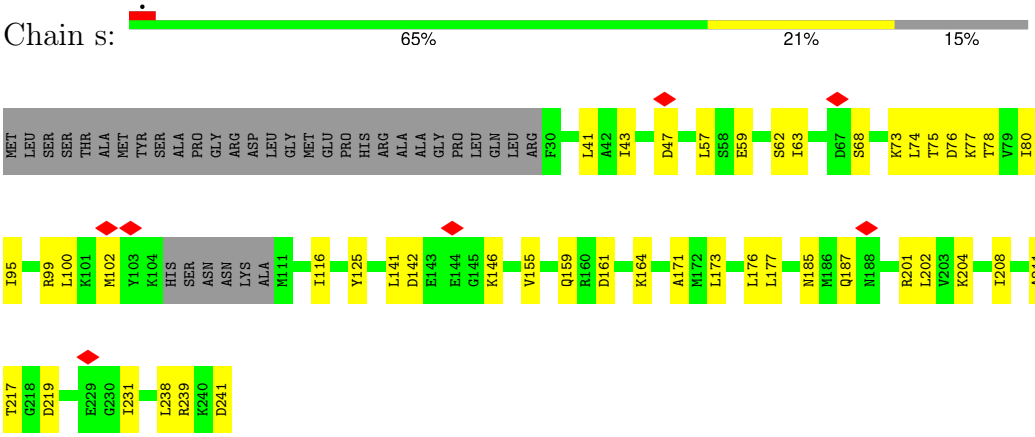
• Molecule 30: Proteasome subunit beta type-1

Chain S:



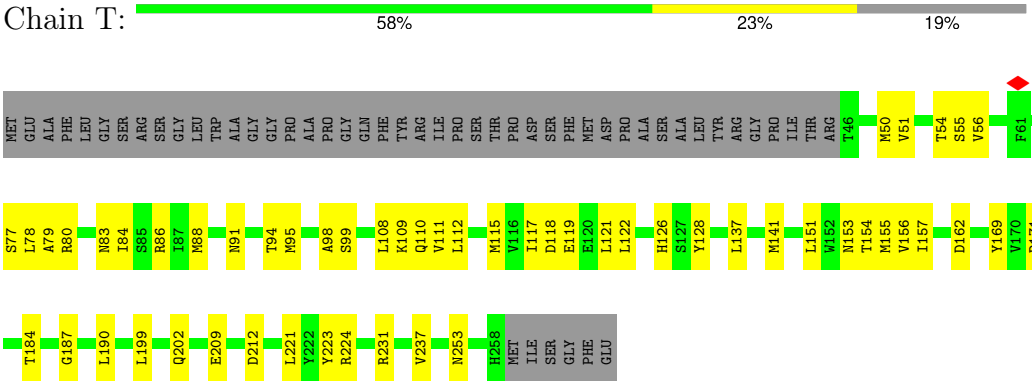
• Molecule 30: Proteasome subunit beta type-1

Chain s:



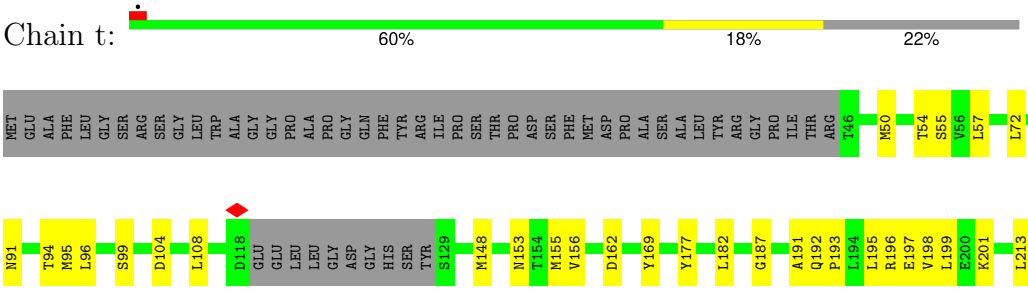
• Molecule 31: Proteasome subunit beta type-4

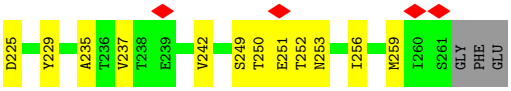
Chain T:



• Molecule 31: Proteasome subunit beta type-4

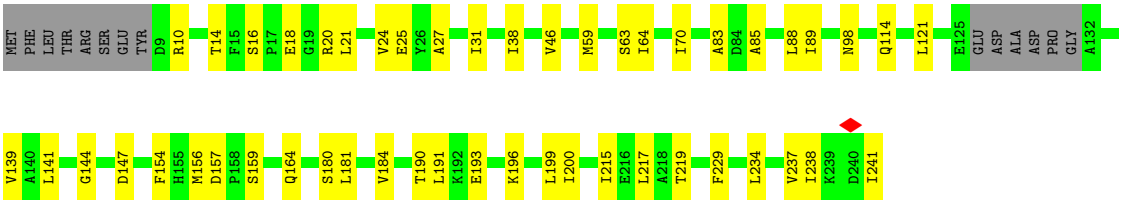
Chain t:





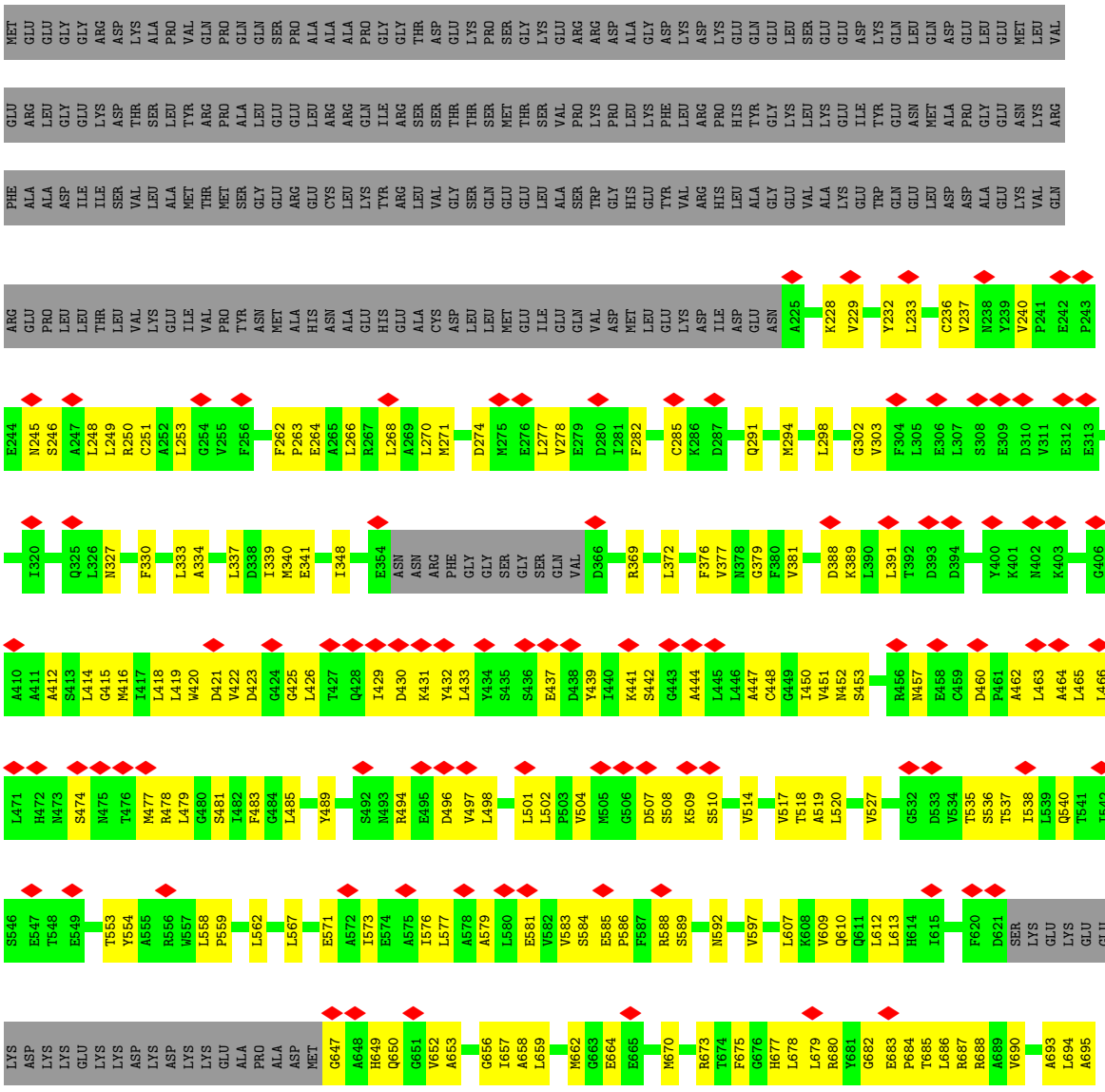
• Molecule 32: Proteasome subunit alpha type-5

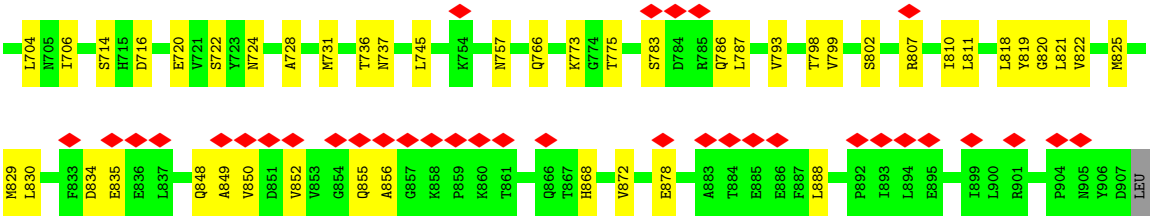
Chain K:



• Molecule 33: 26S proteasome non-ATPase regulatory subunit 2

Chain f:




L704
N705
I706
S714
H715
D716
E720
V721
S722
Y723
N724
A728
M731
T736
N737
L745
K754
N757
Q766
K773
G774
T775
S783
D784
R785
Q786
L787
V793
T798
V799
S802
R807
I810
L811
L818
Y819
G820
L821
V822
M825
M829
L830
F833
D834
E835
E836
L837
Q848
A849
V850
D851
V852
V853
G854
Q855
A856
G857
K858
P859
K860
T861
Q866
T867
H868
V872
E878
A883
T884
E885
E886
F887
L888
P892
I893
L894
E895
I899
L900
R901
P904
N905
Y906
D907
LEU

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	113946	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 ($e^-/Å^2$)	54	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	3.310	Depositor
Minimum map value	-1.762	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.113	Depositor
Recommended contour level	0.35	Depositor
Map size (Å)	363.0, 363.0, 363.0	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.825, 0.825, 0.825	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: ADP, ATP, MG

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	y	0.13	0/272	0.26	0/357
2	U	0.13	0/6446	0.32	1/8720 (0.0%)
3	V	0.14	0/3794	0.34	0/5118
4	W	0.12	0/3620	0.32	0/4869
5	X	0.13	0/3304	0.33	0/4453
6	Y	0.14	0/3193	0.31	0/4302
7	Z	0.13	0/2333	0.28	0/3162
8	a	0.17	0/3070	0.46	5/4155 (0.1%)
9	b	0.11	0/1479	0.32	0/2003
10	c	0.14	0/2302	0.36	0/3110
11	d	0.13	0/2168	0.32	0/2928
12	e	0.09	0/355	0.23	0/482
13	A	0.18	0/3108	0.38	1/4196 (0.0%)
14	B	0.17	0/2974	0.37	0/4009
15	C	0.14	0/2872	0.31	0/3866
16	D	0.17	0/3090	0.36	0/4168
17	E	0.20	0/2914	0.36	0/3927
18	F	0.19	0/2762	0.40	0/3723
19	G	0.14	0/1899	0.31	0/2567
20	H	0.13	0/1828	0.31	0/2476
21	I	0.14	0/2037	0.31	0/2740
22	J	0.14	0/1913	0.29	0/2581
23	L	0.14	0/1902	0.30	0/2569
24	M	0.13	0/1944	0.30	0/2617
25	N	0.13	0/1513	0.29	0/2047
25	n	0.11	0/1377	0.28	0/1857
26	O	0.14	0/1694	0.30	0/2293
26	o	0.11	0/1331	0.30	0/1791
27	P	0.15	0/1620	0.35	0/2184
27	p	0.13	0/1289	0.36	0/1732
28	Q	0.14	0/1611	0.30	0/2180
28	q	0.12	0/1405	0.28	0/1899

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
29	R	0.13	0/1580	0.30	0/2134
29	r	0.12	0/1460	0.32	0/1972
30	S	0.12	0/1673	0.28	0/2254
30	s	0.12	0/1625	0.32	0/2188
31	T	0.13	0/1698	0.33	0/2299
31	t	0.12	0/1639	0.29	0/2217
32	K	0.14	0/1761	0.32	0/2376
33	f	0.14	0/5027	0.36	0/6816
All	All	0.14	0/89882	0.33	7/121337 (0.0%)

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	a	233	LEU	N-CA-C	-6.58	105.39	113.41
8	a	232	TRP	N-CA-C	-6.38	97.20	110.80
8	a	231	GLN	N-CA-CB	5.67	118.71	109.69
8	a	231	GLN	N-CA-C	-5.62	102.32	110.24
13	A	252	GLU	N-CA-C	-5.33	106.91	113.41

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	y	273	0	309	10	0
2	U	6334	0	6368	193	0
3	V	3725	0	3781	130	0
4	W	3572	0	3689	102	0
5	X	3259	0	3371	97	0
6	Y	3135	0	3139	75	0
7	Z	2290	0	2320	65	0
8	a	3012	0	3029	110	0
9	b	1459	0	1499	68	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	c	2260	0	2276	69	0
11	d	2124	0	2155	69	0
12	e	345	0	267	7	0
13	A	3057	0	3114	76	0
14	B	2933	0	2994	107	0
15	C	2834	0	2948	63	0
16	D	3040	0	3075	97	0
17	E	2869	0	2930	88	0
18	F	2724	0	2800	114	0
19	G	1865	0	1875	46	0
20	H	1789	0	1784	47	0
21	I	2007	0	2030	48	0
22	J	1887	0	1905	46	0
23	L	1868	0	1858	42	0
24	M	1909	0	1883	57	0
25	N	1487	0	1452	21	0
25	n	1360	0	1344	35	0
26	O	1667	0	1689	43	0
26	o	1315	0	1321	38	0
27	P	1591	0	1609	56	0
27	p	1271	0	1262	36	0
28	Q	1578	0	1580	42	0
28	q	1380	0	1399	43	0
29	R	1549	0	1512	49	0
29	r	1432	0	1384	46	0
30	S	1643	0	1640	41	0
30	s	1597	0	1597	45	0
31	T	1665	0	1638	52	0
31	t	1609	0	1597	37	0
32	K	1736	0	1734	35	0
33	f	4942	0	4983	183	0
34	A	31	0	12	1	0
34	D	31	0	12	1	0
34	E	31	0	12	2	0
34	F	31	0	12	2	0
35	A	1	0	0	0	0
35	B	1	0	0	0	0
35	D	1	0	0	0	0
35	E	1	0	0	0	0
35	F	1	0	0	0	0
36	B	27	0	12	2	0
36	C	27	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	88575	0	89212	2340	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

The worst 5 of 2340 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:F:171:ARG:HH12	18:F:267:LEU:HD21	1.11	1.09
30:S:176:LEU:HD23	30:S:206:VAL:HG12	1.34	1.06
2:U:119:PRO:O	2:U:123:LYS:NZ	1.95	0.99
33:f:450:ILE:HD11	33:f:822:VAL:HG21	1.42	0.98
4:W:385:SER:OG	4:W:388:GLU:OE1	1.81	0.98

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	y	29/567 (5%)	29 (100%)	0	0	100	100
2	U	804/953 (84%)	745 (93%)	59 (7%)	0	100	100
3	V	453/534 (85%)	416 (92%)	37 (8%)	0	100	100
4	W	436/456 (96%)	406 (93%)	30 (7%)	0	100	100
5	X	409/422 (97%)	375 (92%)	34 (8%)	0	100	100
6	Y	379/389 (97%)	366 (97%)	13 (3%)	0	100	100
7	Z	285/324 (88%)	278 (98%)	7 (2%)	0	100	100
8	a	373/376 (99%)	347 (93%)	25 (7%)	1 (0%)	37	66
9	b	189/377 (50%)	172 (91%)	17 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	c	285/310 (92%)	258 (90%)	27 (10%)	0	100	100
11	d	257/350 (73%)	226 (88%)	31 (12%)	0	100	100
12	e	35/70 (50%)	34 (97%)	1 (3%)	0	100	100
13	A	387/433 (89%)	353 (91%)	34 (9%)	0	100	100
14	B	369/440 (84%)	348 (94%)	21 (6%)	0	100	100
15	C	355/406 (87%)	333 (94%)	22 (6%)	0	100	100
16	D	378/418 (90%)	353 (93%)	24 (6%)	1 (0%)	37	66
17	E	360/389 (92%)	337 (94%)	23 (6%)	0	100	100
18	F	345/439 (79%)	306 (89%)	39 (11%)	0	100	100
19	G	236/246 (96%)	218 (92%)	18 (8%)	0	100	100
20	H	227/234 (97%)	213 (94%)	14 (6%)	0	100	100
21	I	252/261 (97%)	237 (94%)	15 (6%)	0	100	100
22	J	237/248 (96%)	226 (95%)	11 (5%)	0	100	100
23	L	235/263 (89%)	223 (95%)	12 (5%)	0	100	100
24	M	241/255 (94%)	229 (95%)	11 (5%)	1 (0%)	30	60
25	N	196/239 (82%)	182 (93%)	14 (7%)	0	100	100
25	n	177/239 (74%)	166 (94%)	11 (6%)	0	100	100
26	O	219/277 (79%)	203 (93%)	16 (7%)	0	100	100
26	o	166/277 (60%)	157 (95%)	9 (5%)	0	100	100
27	P	202/205 (98%)	179 (89%)	23 (11%)	0	100	100
27	p	153/205 (75%)	137 (90%)	16 (10%)	0	100	100
28	Q	195/201 (97%)	186 (95%)	9 (5%)	0	100	100
28	q	163/201 (81%)	153 (94%)	10 (6%)	0	100	100
29	R	197/263 (75%)	186 (94%)	11 (6%)	0	100	100
29	r	181/263 (69%)	176 (97%)	5 (3%)	0	100	100
30	S	210/241 (87%)	199 (95%)	11 (5%)	0	100	100
30	s	202/241 (84%)	188 (93%)	14 (7%)	0	100	100
31	T	211/264 (80%)	195 (92%)	16 (8%)	0	100	100
31	t	202/264 (76%)	186 (92%)	16 (8%)	0	100	100
32	K	223/241 (92%)	213 (96%)	10 (4%)	0	100	100
33	f	641/908 (71%)	560 (87%)	80 (12%)	1 (0%)	44	73

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	11094/13689 (81%)	10294 (93%)	796 (7%)	4 (0%)	100 100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	a	232	TRP
16	D	278	GLN
24	M	208	LYS
33	f	855	GLN

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	y	29/459 (6%)	29 (100%)	0	100 100
2	U	691/816 (85%)	691 (100%)	0	100 100
3	V	402/460 (87%)	402 (100%)	0	100 100
4	W	403/416 (97%)	403 (100%)	0	100 100
5	X	353/362 (98%)	353 (100%)	0	100 100
6	Y	336/344 (98%)	336 (100%)	0	100 100
7	Z	258/295 (88%)	258 (100%)	0	100 100
8	a	335/336 (100%)	334 (100%)	1 (0%)	91 97
9	b	167/312 (54%)	167 (100%)	0	100 100
10	c	252/268 (94%)	252 (100%)	0	100 100
11	d	230/294 (78%)	230 (100%)	0	100 100
12	e	37/63 (59%)	37 (100%)	0	100 100
13	A	334/372 (90%)	333 (100%)	1 (0%)	91 97
14	B	329/385 (86%)	329 (100%)	0	100 100
15	C	311/352 (88%)	311 (100%)	0	100 100
16	D	333/366 (91%)	333 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	E	317/341 (93%)	317 (100%)	0	100	100
18	F	296/379 (78%)	295 (100%)	1 (0%)	91	97
19	G	204/210 (97%)	204 (100%)	0	100	100
20	H	188/191 (98%)	188 (100%)	0	100	100
21	I	214/221 (97%)	214 (100%)	0	100	100
22	J	203/211 (96%)	203 (100%)	0	100	100
23	L	203/224 (91%)	203 (100%)	0	100	100
24	M	201/212 (95%)	201 (100%)	0	100	100
25	N	154/181 (85%)	154 (100%)	0	100	100
25	n	140/181 (77%)	140 (100%)	0	100	100
26	O	182/228 (80%)	182 (100%)	0	100	100
26	o	139/228 (61%)	139 (100%)	0	100	100
27	P	173/174 (99%)	173 (100%)	0	100	100
27	p	137/174 (79%)	137 (100%)	0	100	100
28	Q	168/171 (98%)	168 (100%)	0	100	100
28	q	148/171 (86%)	148 (100%)	0	100	100
29	R	155/202 (77%)	155 (100%)	0	100	100
29	r	142/202 (70%)	142 (100%)	0	100	100
30	S	177/199 (89%)	177 (100%)	0	100	100
30	s	172/199 (86%)	172 (100%)	0	100	100
31	T	176/215 (82%)	176 (100%)	0	100	100
31	t	171/215 (80%)	171 (100%)	0	100	100
32	K	191/203 (94%)	191 (100%)	0	100	100
33	f	537/763 (70%)	537 (100%)	0	100	100
All	All	9588/11595 (83%)	9585 (100%)	3 (0%)	100	100

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	a	232	TRP
13	A	248	LYS
18	F	171	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 77

such sidechains are listed below:

Mol	Chain	Res	Type
27	P	33	GLN
33	f	396	ASN
28	Q	186	ASN
32	K	164	GLN
33	f	614	HIS

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	$\#\|Z\| > 2$
34	ATP	E	401	35	28,33,33	0.67	0	34,52,52	0.91	1 (2%)
34	ATP	A	501	35	28,33,33	0.69	0	34,52,52	0.93	2 (5%)
36	ADP	C	501	-	24,29,29	0.87	0	29,45,45	1.25	2 (6%)
34	ATP	D	501	35	28,33,33	0.74	0	34,52,52	0.95	1 (2%)
36	ADP	B	501	35	24,29,29	0.88	0	29,45,45	1.27	2 (6%)
34	ATP	F	501	35	28,33,33	0.71	0	34,52,52	0.89	1 (2%)

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
34	ATP	E	401	35	-	4/18/38/38	0/3/3/3
34	ATP	A	501	35	-	5/18/38/38	0/3/3/3
36	ADP	C	501	-	-	3/12/32/32	0/3/3/3
34	ATP	D	501	35	-	3/18/38/38	0/3/3/3
36	ADP	B	501	35	-	2/12/32/32	0/3/3/3
34	ATP	F	501	35	-	5/18/38/38	0/3/3/3

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	C	501	ADP	N3-C2-N1	-4.16	123.03	128.67
36	B	501	ADP	N3-C2-N1	-4.04	123.19	128.67
36	B	501	ADP	C4-C5-N7	-2.44	106.76	109.34
34	F	501	ATP	C5-C6-N6	2.42	123.99	120.31
36	C	501	ADP	C4-C5-N7	-2.36	106.84	109.34

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
34	A	501	ATP	PB-O3B-PG-O3G
34	A	501	ATP	C5'-O5'-PA-O1A
34	D	501	ATP	C5'-O5'-PA-O1A
34	D	501	ATP	C5'-O5'-PA-O3A
34	F	501	ATP	PB-O3B-PG-O2G

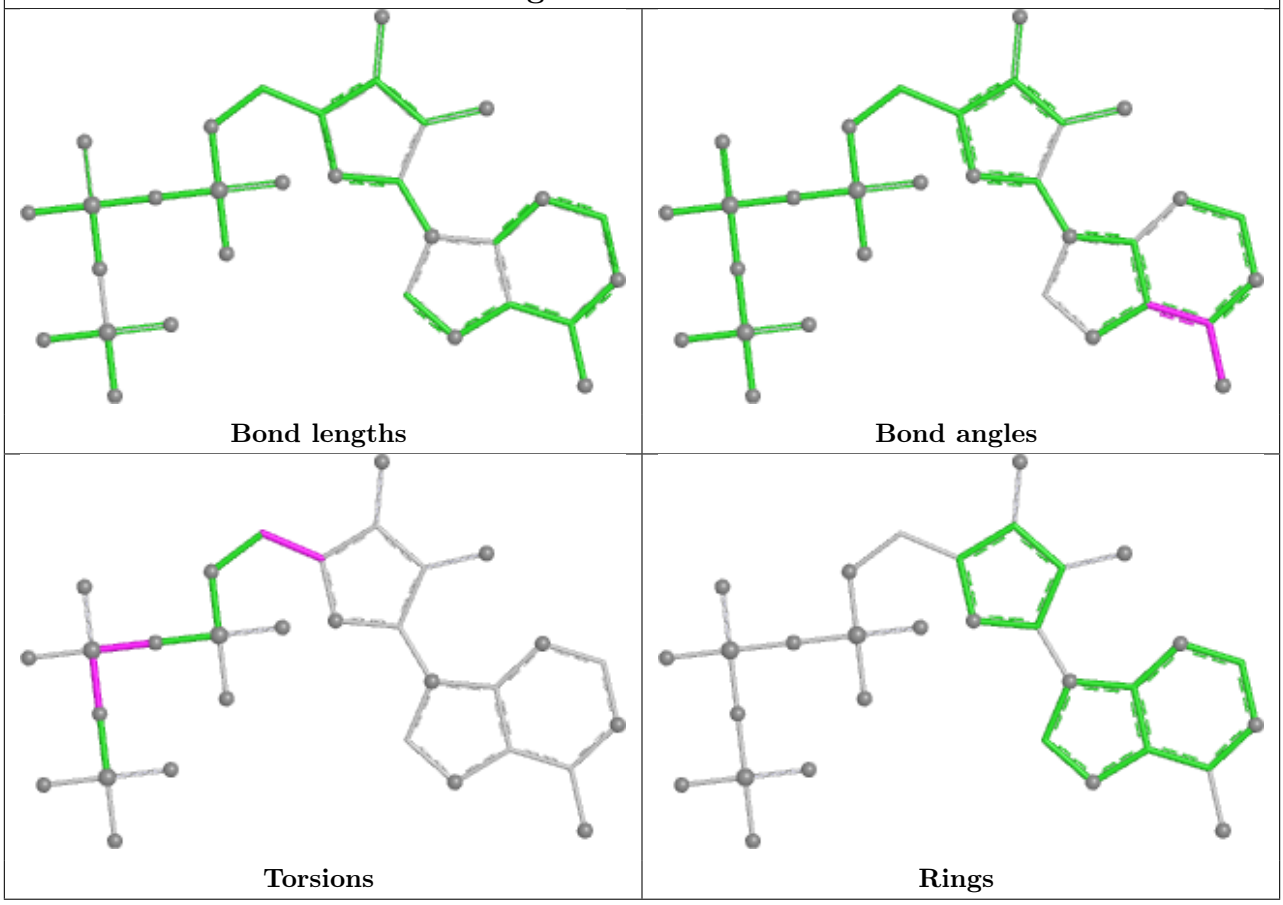
There are no ring outliers.

5 monomers are involved in 8 short contacts:

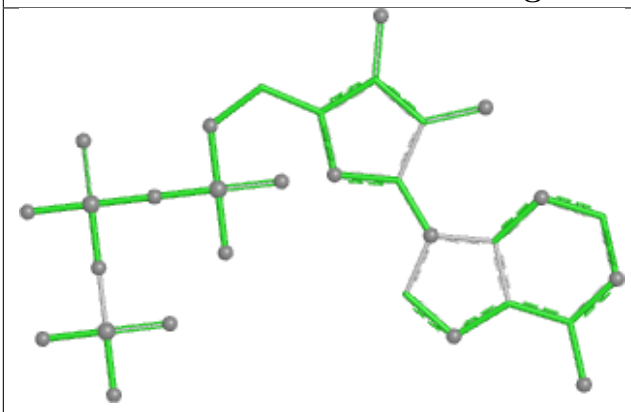
Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	E	401	ATP	2	0
34	A	501	ATP	1	0
34	D	501	ATP	1	0
36	B	501	ADP	2	0
34	F	501	ATP	2	0

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

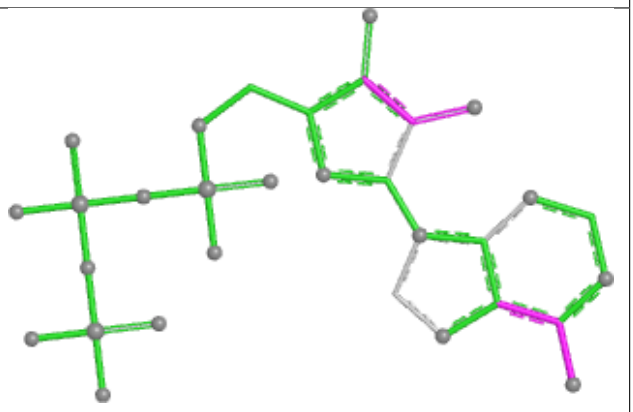
Ligand ATP E 401



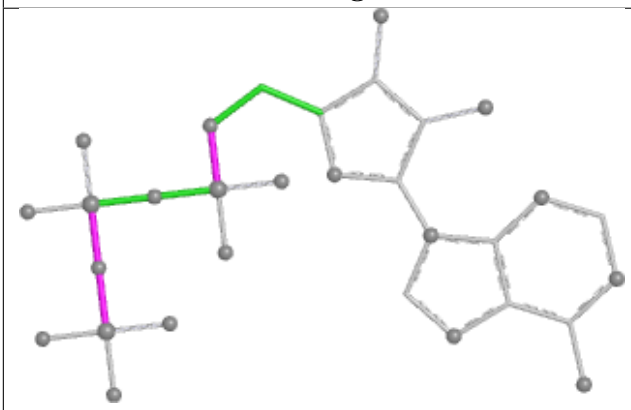
Ligand ATP A 501



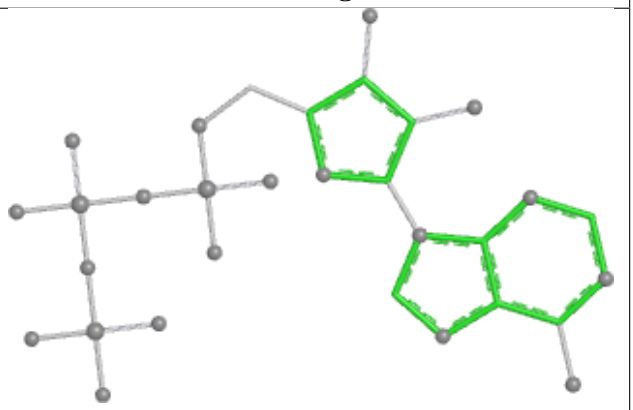
Bond lengths



Bond angles

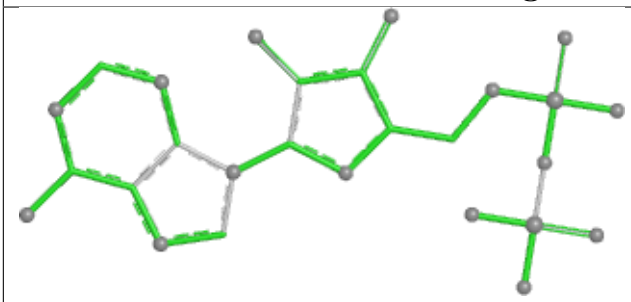


Torsions



Rings

Ligand ADP C 501



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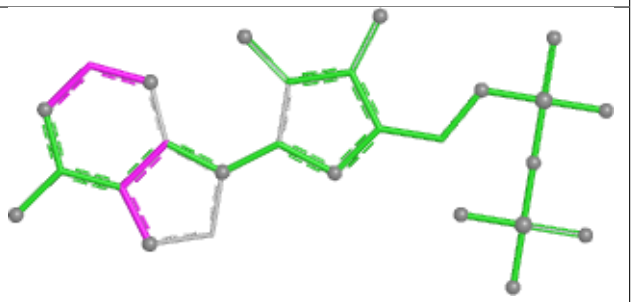

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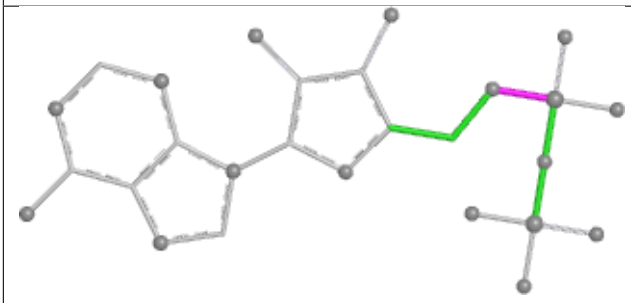

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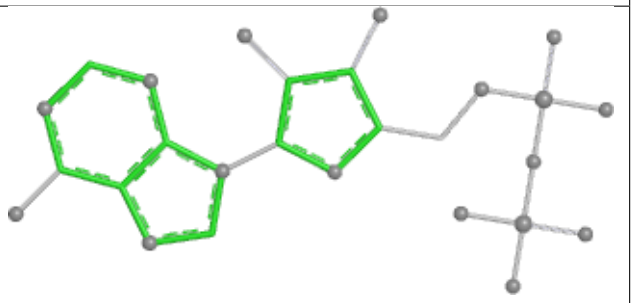
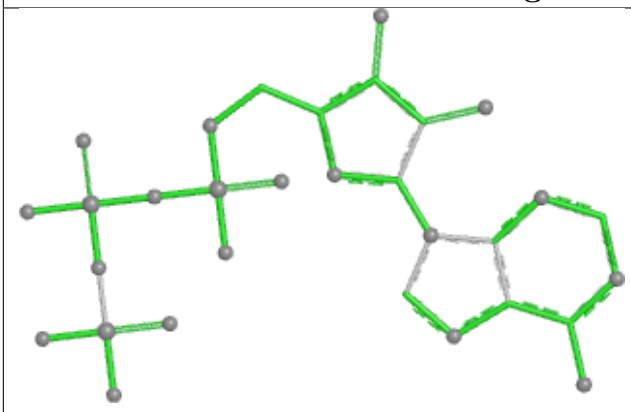
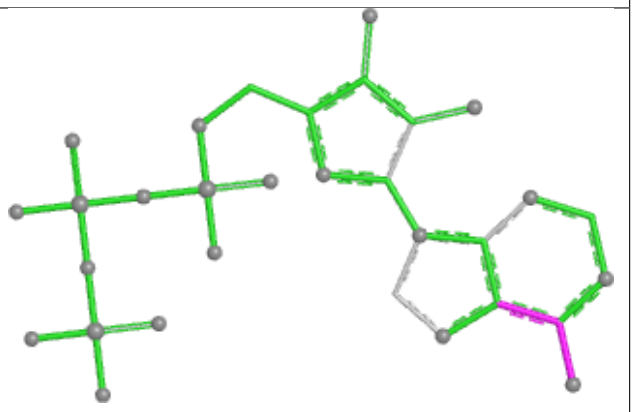


Rings

Ligand ATP D 501



Bond lengths



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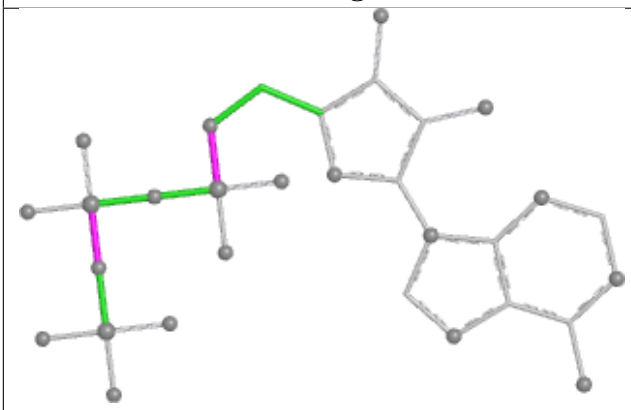
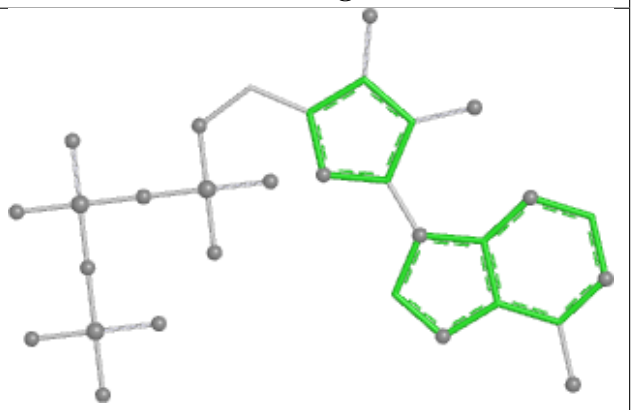
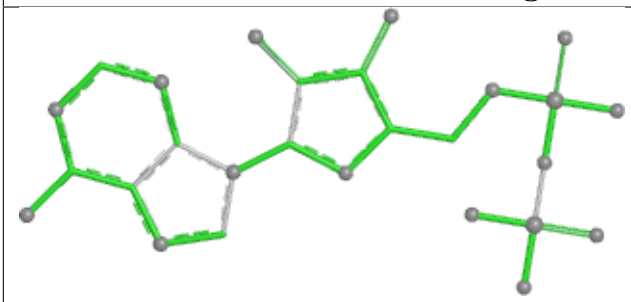


Torsions

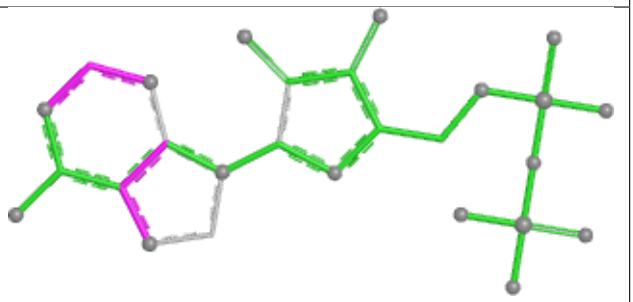


Rings

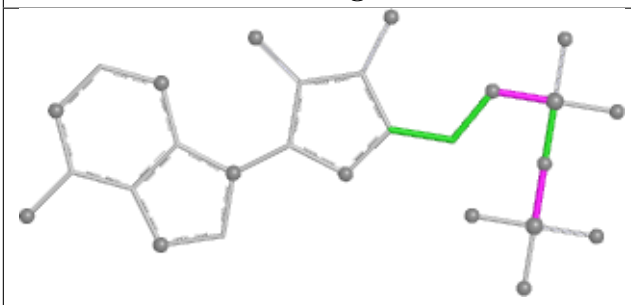
Ligand ADP B 501



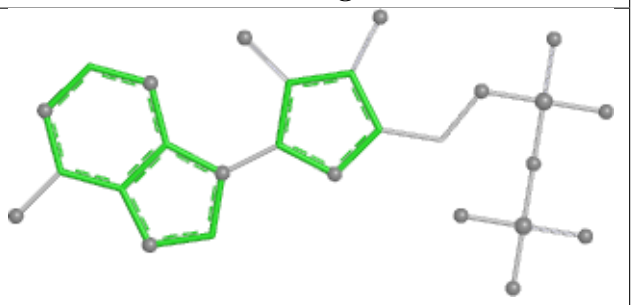
Bond lengths



Bond angles

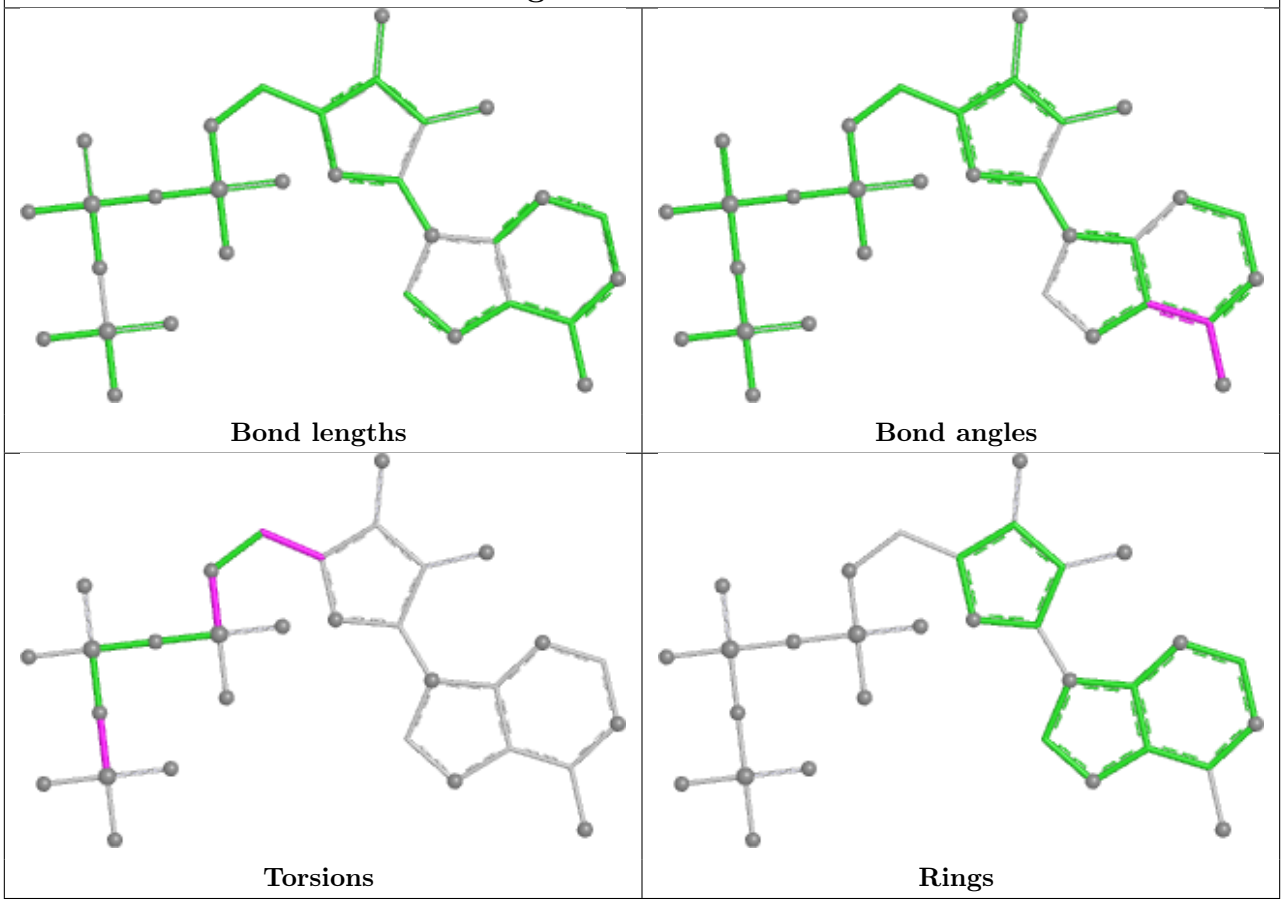


Torsions



Rings

Ligand ATP F 501



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

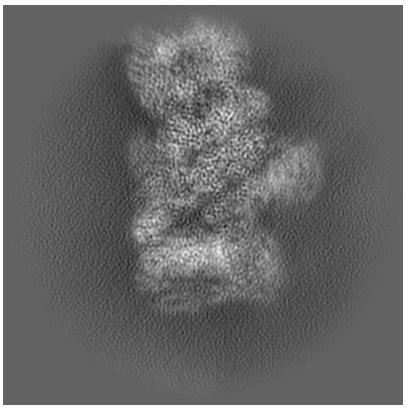
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-44930. These allow visual inspection of the internal detail of the map and identification of artifacts.

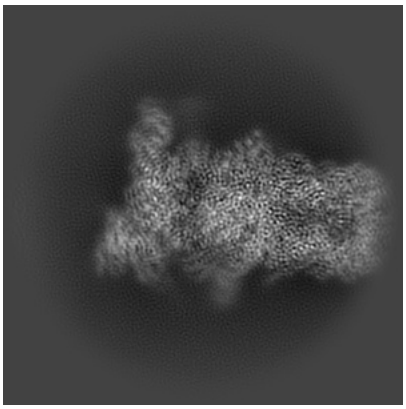
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

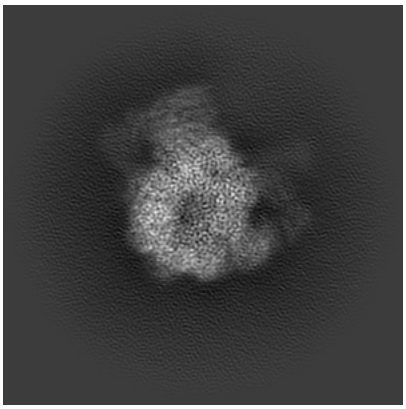
6.1.1 Primary map



X

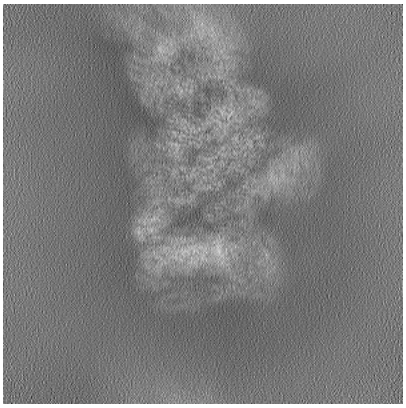


Y

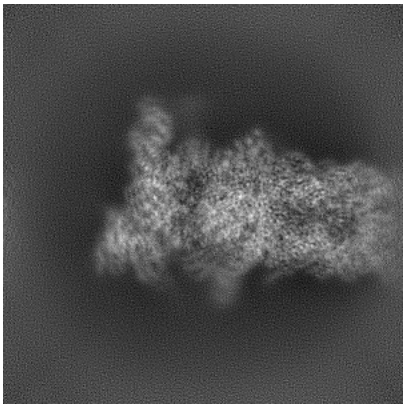


Z

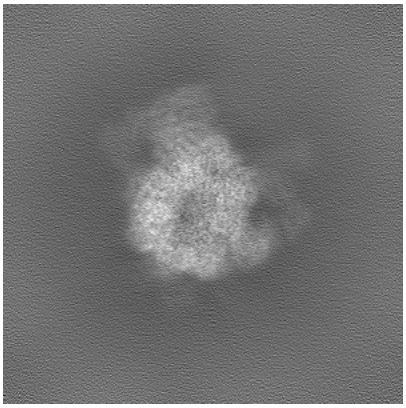
6.1.2 Raw map



X



Y

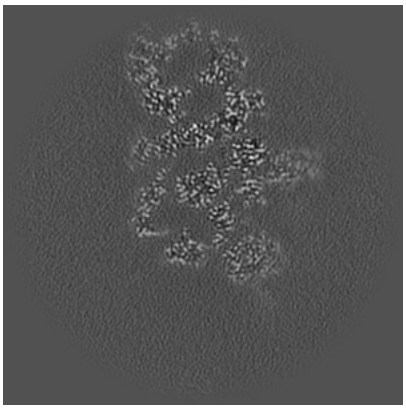


Z

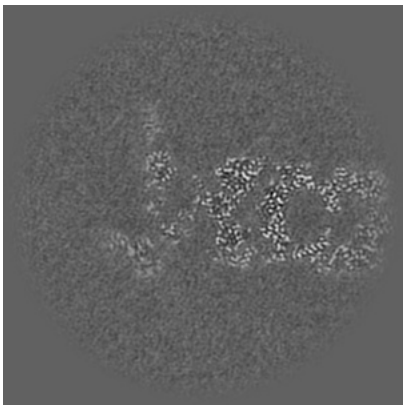
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map



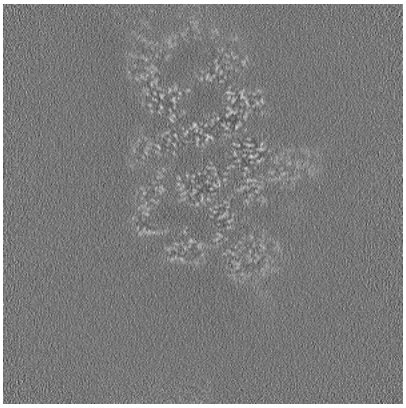
X Index: 220



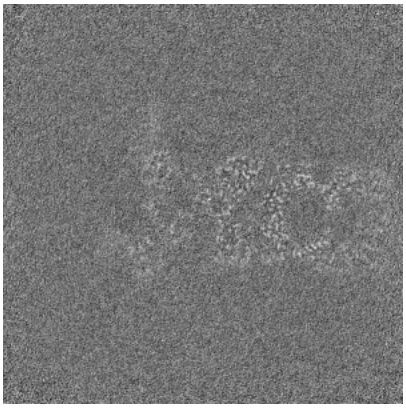
Y Index: 220

Z Index: 220

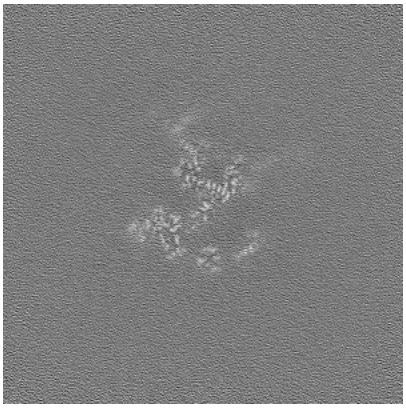
6.2.2 Raw map



X Index: 220



Y Index: 220

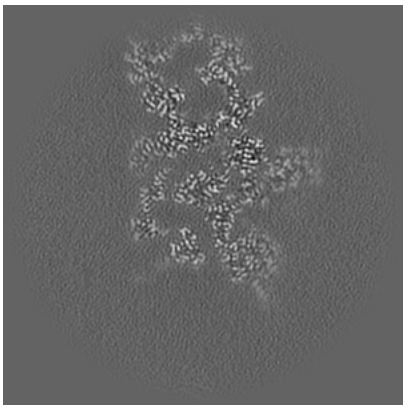


Z Index: 220

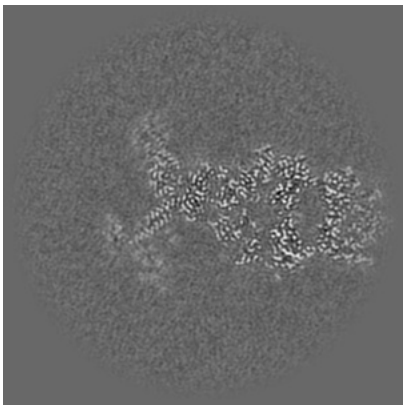
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

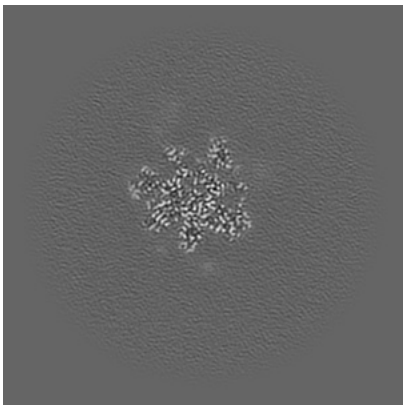
6.3.1 Primary map



X Index: 217

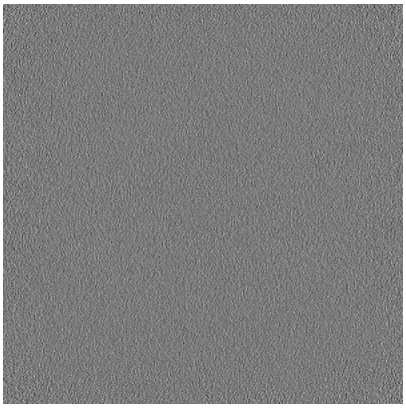


Y Index: 237

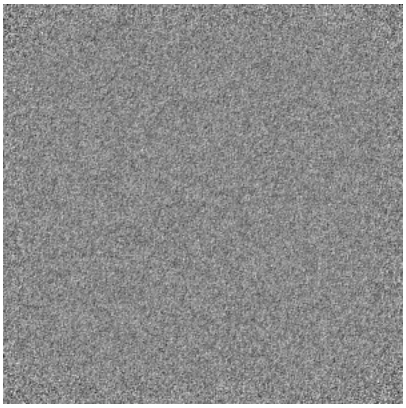


Z Index: 303

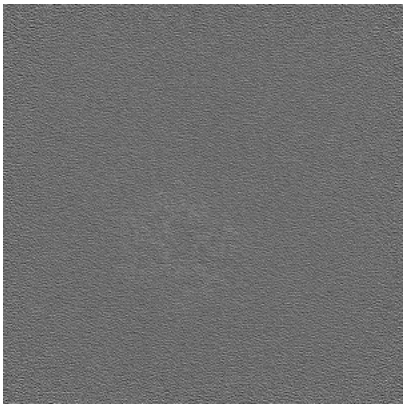
6.3.2 Raw map



X Index: 0



Y Index: 0

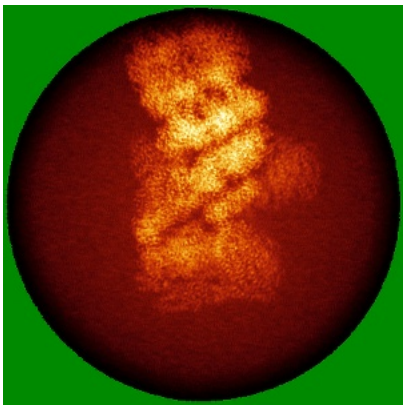


Z Index: 0

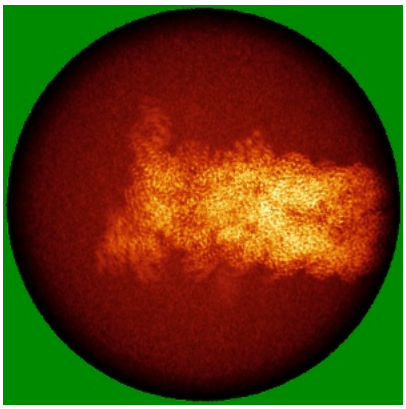
The images above show the largest variance slices of the map in three orthogonal directions.

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

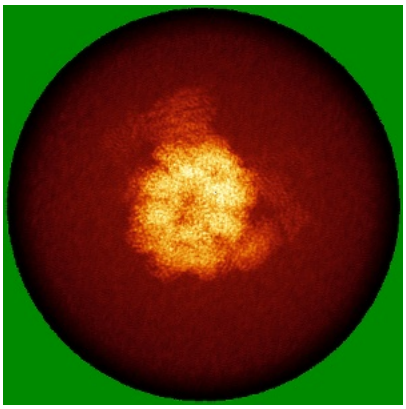
6.4.1 Primary map



X

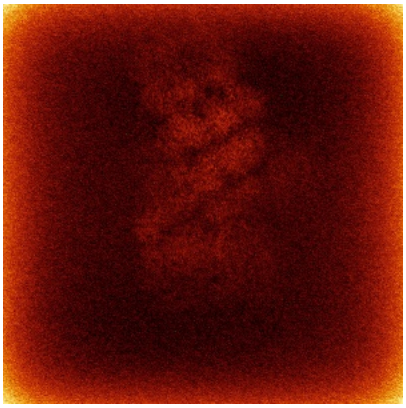


Y

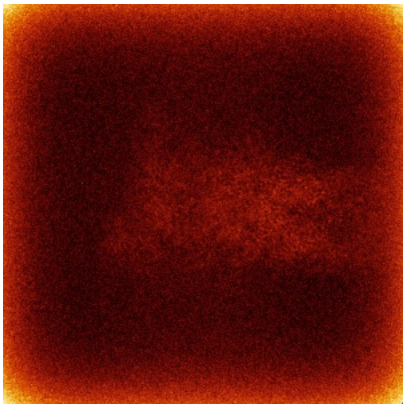


Z

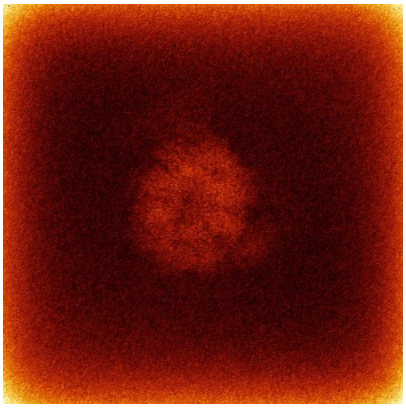
6.4.2 Raw map



X



Y

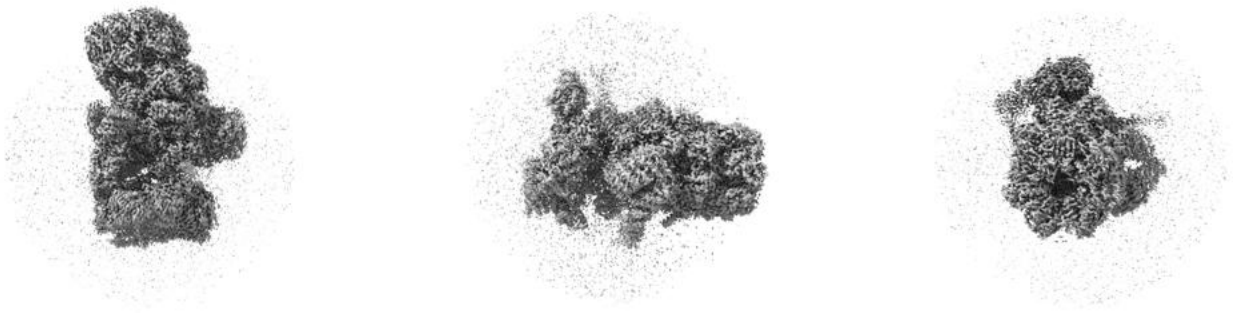


Z

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

6.5 Orthogonal surface views (i)

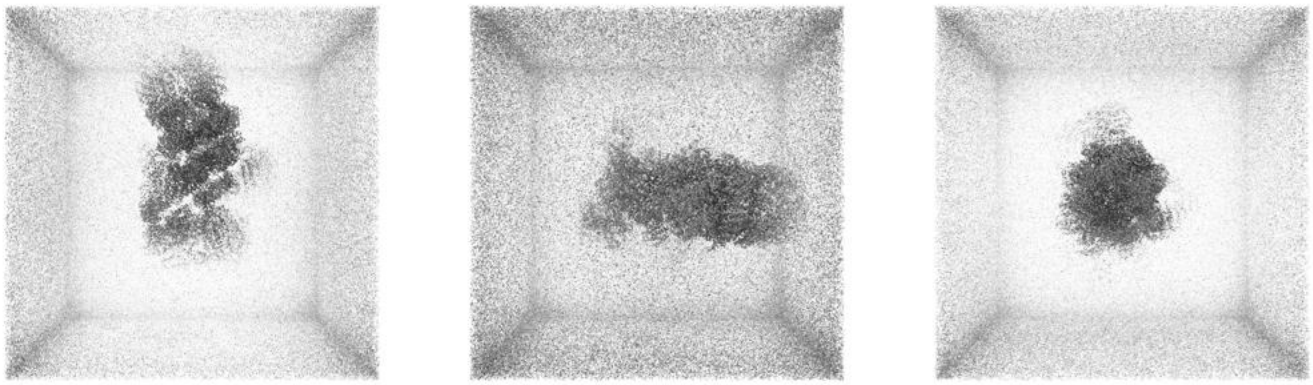
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.35. 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



X Y Z

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.

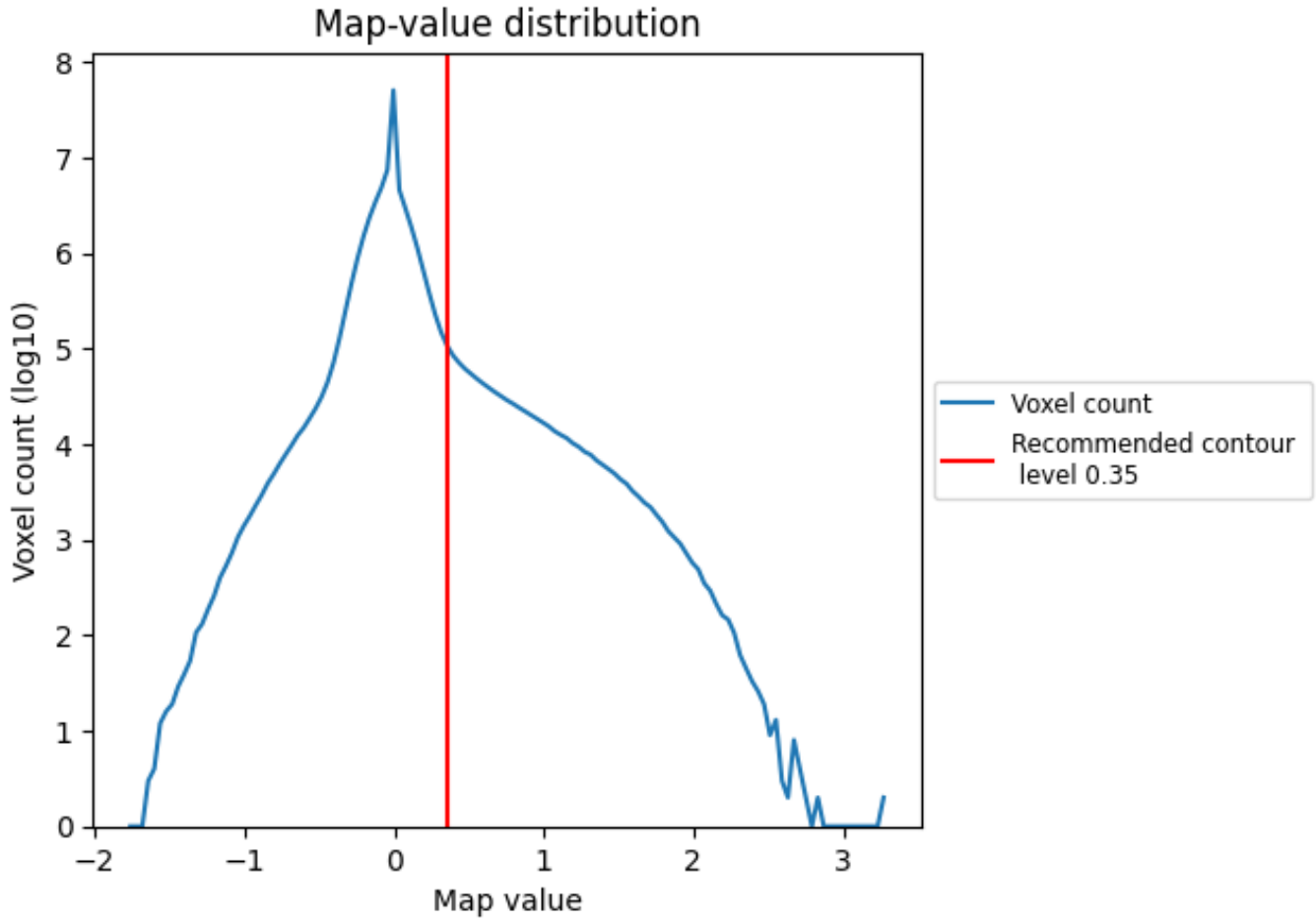
6.6 Mask visualisation (i)

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

7 Map analysis

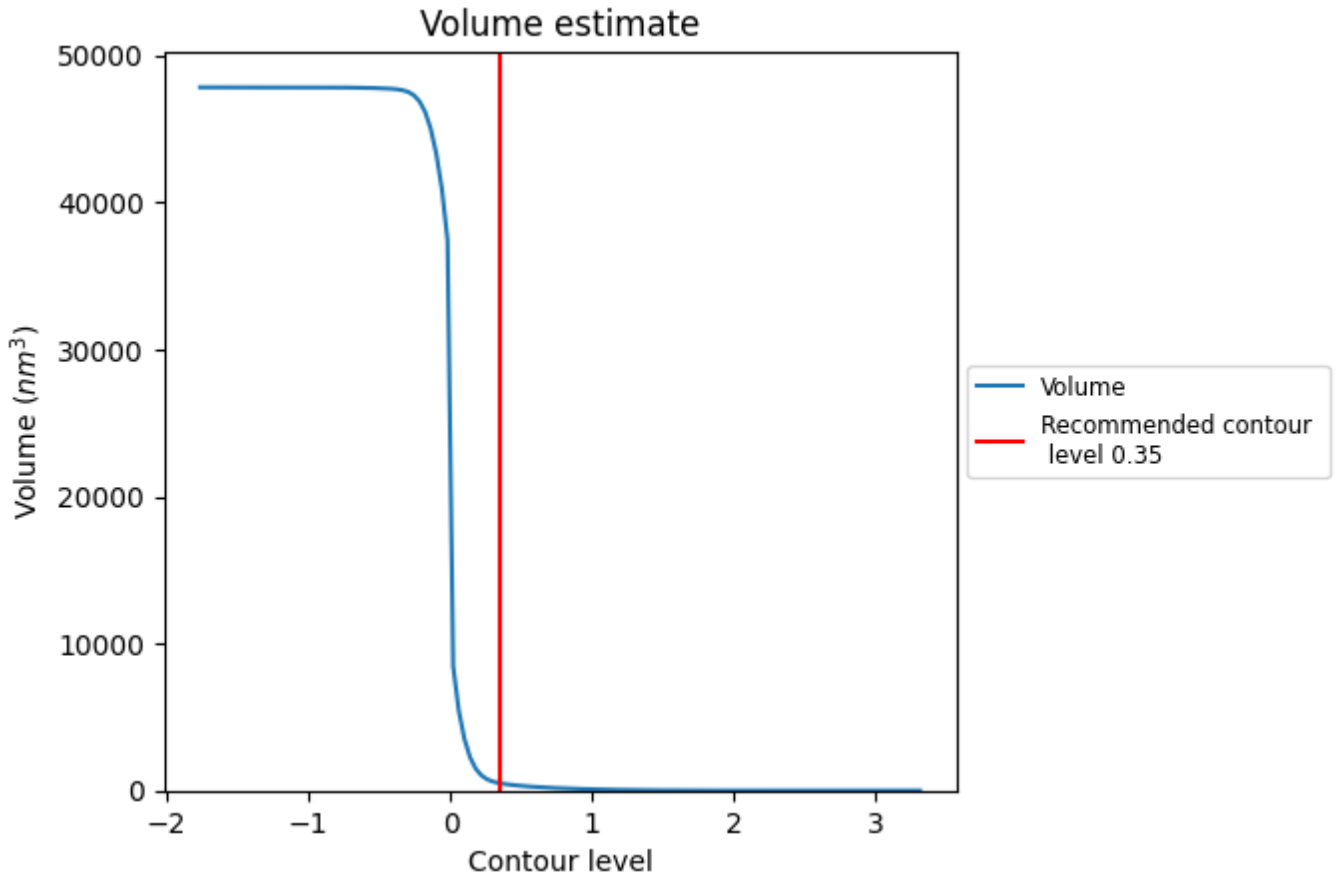
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

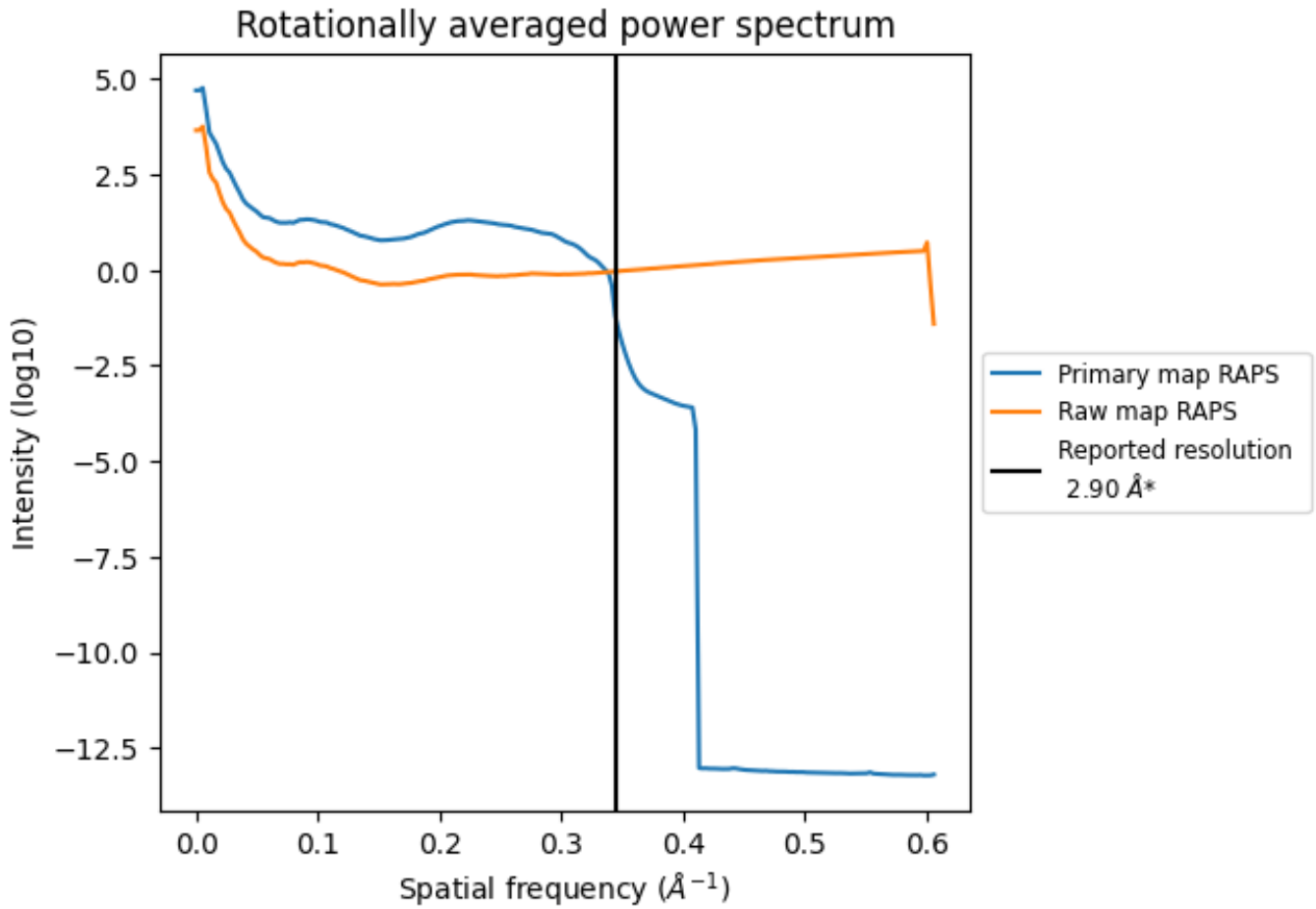
7.2 Volume estimate (i)



The volume at the recommended contour level is 501 nm^3; this corresponds to an approximate mass of 452 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)

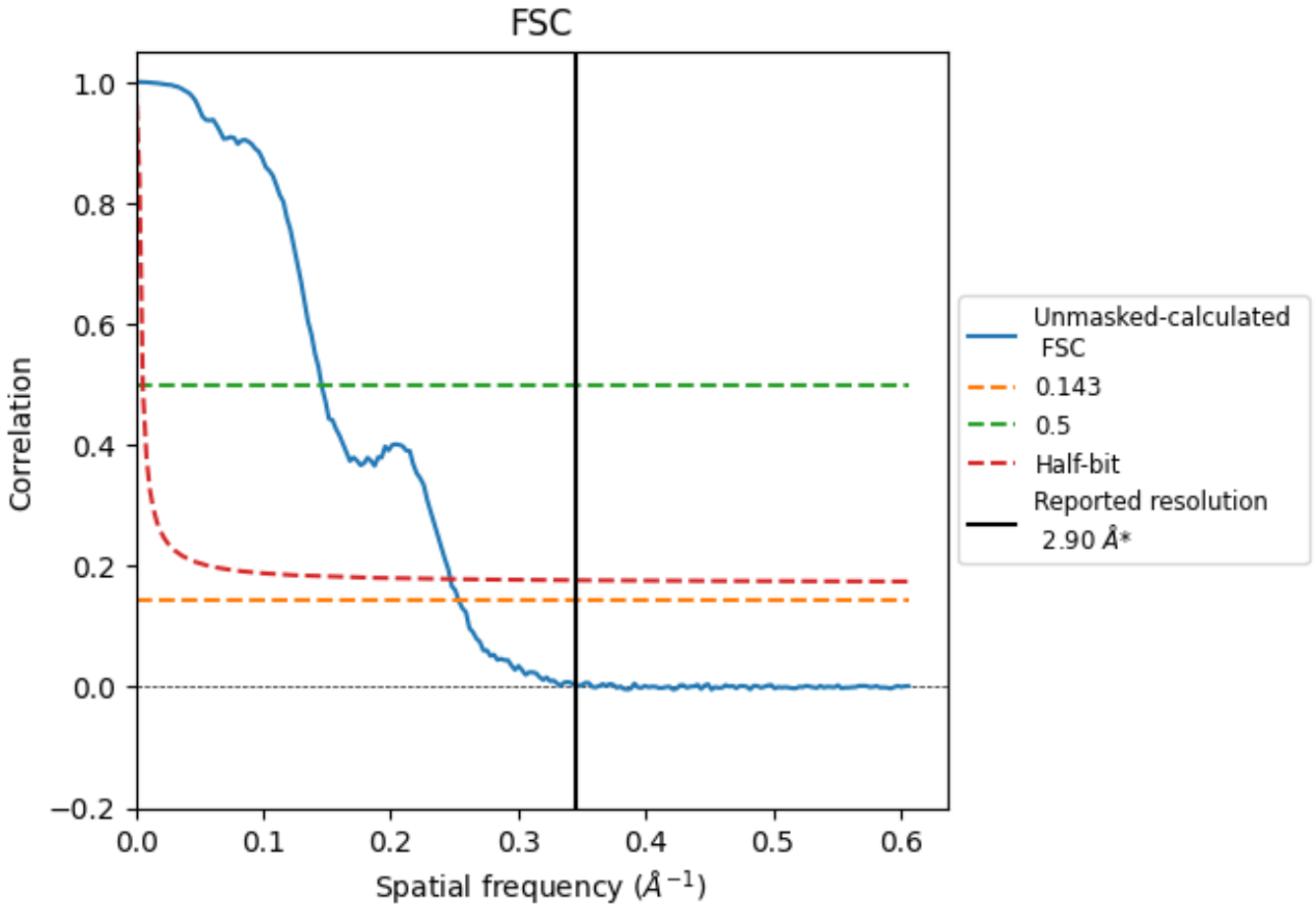


*Reported resolution corresponds to spatial frequency of 0.345 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.345 Å^{-1}

8.2 Resolution estimates (i)

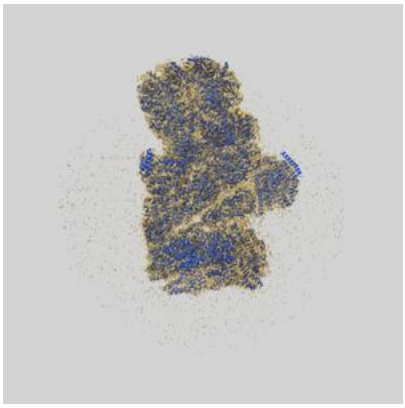
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.95	6.87	4.05

*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 3.95 differs from the reported value 2.9 by more than 10 %

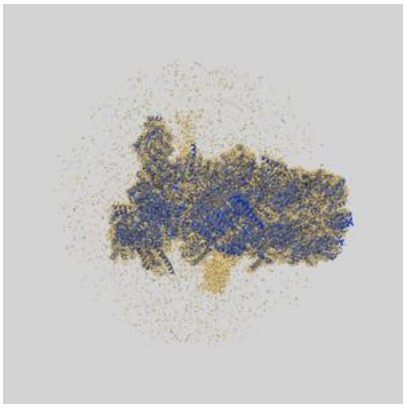
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-44930 and PDB model 9BV3. Per-residue inclusion information can be found in section 3 on page 15.

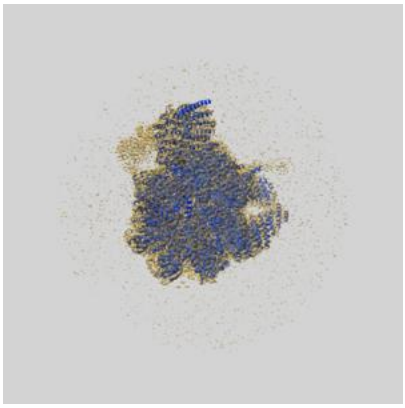
9.1 Map-model overlay



X



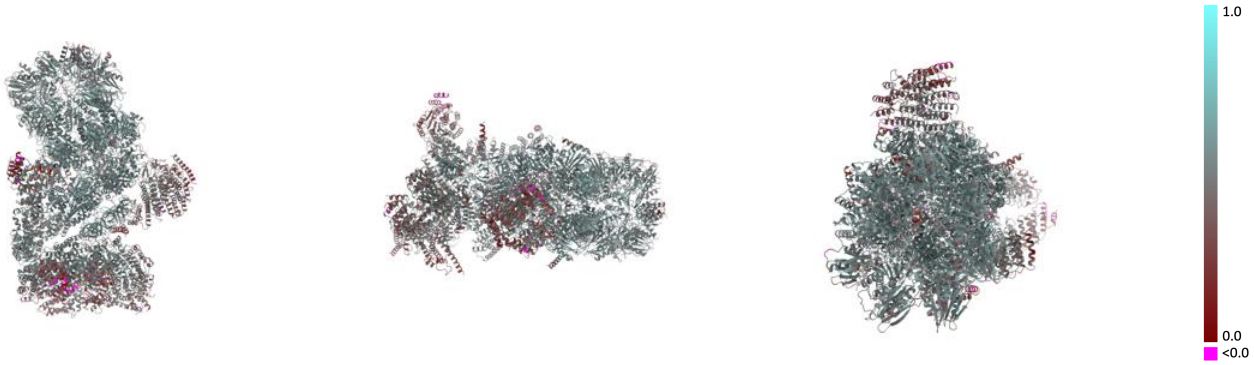
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.35 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.

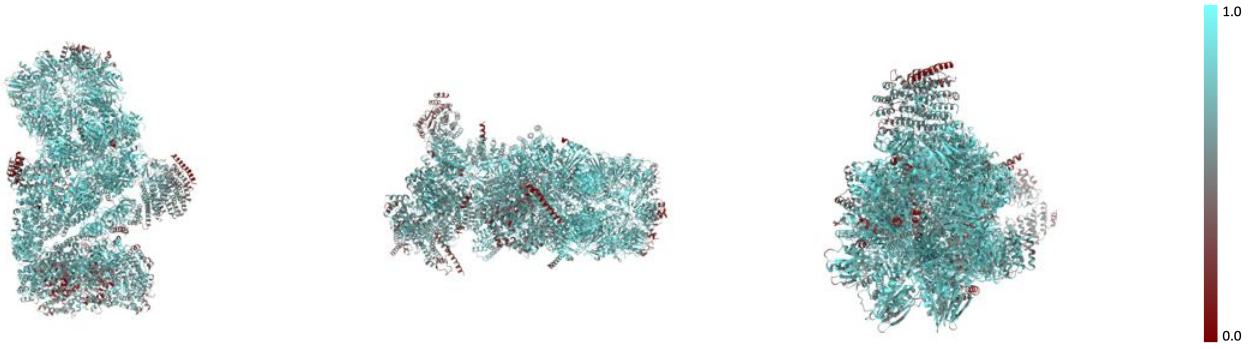
9.2 Q-score mapped to coordinate model



X Y Z

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.

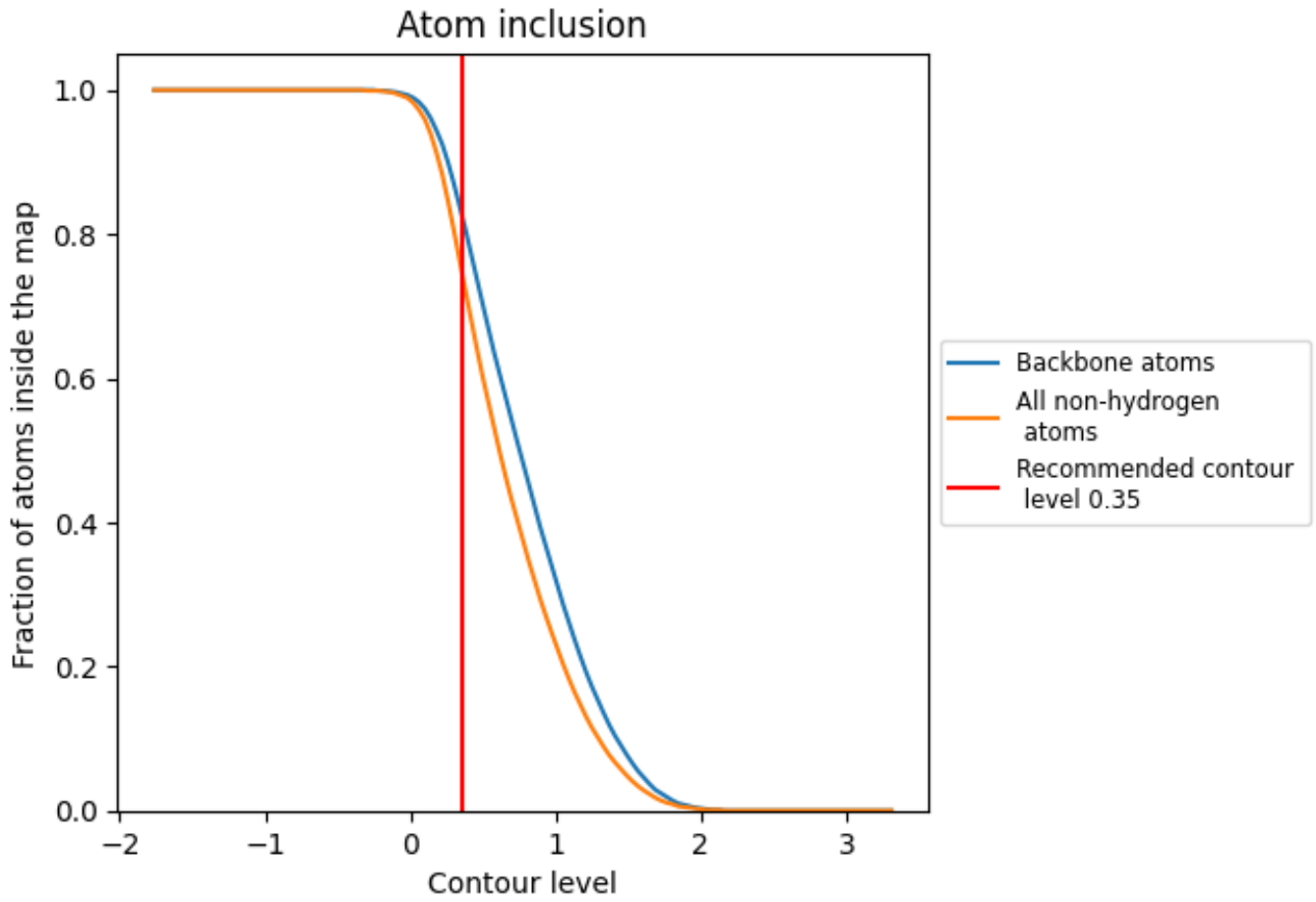
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.35).

9.4 Atom inclusion (i)



At the recommended contour level, 83% of all backbone atoms, 75% 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 (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7510	0.4970
A	0.8130	0.5260
B	0.7640	0.5050
C	0.8230	0.5450
D	0.8080	0.5330
E	0.8290	0.5460
F	0.8230	0.5360
G	0.8560	0.5510
H	0.8750	0.5660
I	0.8210	0.5410
J	0.8250	0.5360
K	0.8710	0.5590
L	0.8830	0.5660
M	0.8350	0.5480
N	0.8680	0.5580
O	0.8330	0.5390
P	0.8600	0.5490
Q	0.8640	0.5550
R	0.8530	0.5510
S	0.8380	0.5440
T	0.8440	0.5430
U	0.6860	0.4430
V	0.6420	0.4250
W	0.7400	0.4810
X	0.6610	0.4590
Y	0.8190	0.5260
Z	0.7480	0.5130
a	0.6290	0.4040
b	0.4580	0.3570
c	0.7720	0.5200
d	0.6150	0.4020
e	0.6710	0.4790
f	0.5930	0.3810
n	0.7530	0.5130
o	0.6710	0.4850

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
p	0.5890	0.4800
q	0.6330	0.5060
r	0.7390	0.4920
s	0.7580	0.5050
t	0.7650	0.5180
y	0.0470	0.2240