wwPDB EM Validation Summary Report (i)

May 18, 2025 – 03:04 AM EDT

PDB ID	:	9E8O / pdb_00009e8o
EMDB ID	:	EMD-47726
Title	:	Nub1/Fat10-processing human 26S proteasome bound to Txnl1 with Rpt2 at top of spiral staircase and partially unfolded Eos
Authors	:	Arkinson, C.; Gee, C.L.; Martin, A.
Deposited on	:	2024-11-05
Resolution	:	3.10 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:

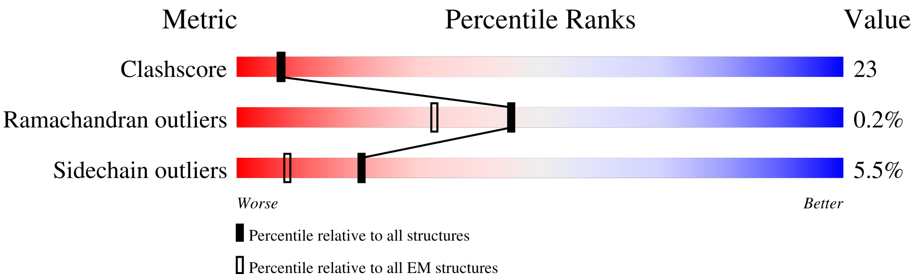
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal 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 3.10 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	B	440	6% / 52% 36% • 10%
2	C	406	55% 38% • 5%
3	D	418	• / 54% 35% • 9%
4	c	424	• / 35% 29% • 33%
5	G	246	15% / 58% 38% • •
6	H	234	• / 59% 38% • •
7	I	261	7% / 56% 39% • 5%
8	J	248	17% / 47% 47% • •

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Mol	Chain	Length	Quality of chain
9	K	241	20% / 49% 44% 6% •
10	L	263	27% / 48% 40% • 9%
11	M	255	30% / 47% 45% • 5%
12	N	239	28% / 44% 36% • 18%
13	O	277	29% / 47% 32% • 21%
14	P	205	36% / 44% 51% 5%
15	Q	201	40% / 47% 49% • •
16	R	263	34% / 41% 34% • 24%
17	S	241	42% / 46% 38% • 12%
18	T	264	34% / 42% 38% • 18%
19	X	422	13% / 55% 32% • 10%
20	Y	389	8% / 41% 50% 6% •
21	Z	324	• / 46% 38% 5% 12%
22	a	376	12% / 51% 45% • •
23	b	377	7% / 22% 26% • 49%
24	d	350	13% / 36% 35% • 29%
25	f	908	45% / 40% 54% • •
26	W	456	36% / 49% 45% • •
27	V	534	8% / 49% 31% • 19%
28	e	70	23% / 34% 30% 7% 29%
29	A	433	24% / 46% 40% • 10%
30	F	439	31% / 32% 46% • 18%
31	E	389	15% / 46% 46% • 6%
32	U	953	• / 58% 28% • 13%
33	g	390	34% / 27% 22% • 49%

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Mol	Chain	Length	Quality of chain
34	u	300	5% 31% 19% • 48%

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 83155 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 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B	397	3124	1968	530	611	15	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	386	3053	1921	547	567	18	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	c	282	2220	1407	380	414	19	0	0

There are 114 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
c	311	LEU	-	expression tag	UNP O00487
c	312	ILE	-	expression tag	UNP O00487
c	313	ASN	-	expression tag	UNP O00487
c	314	HIS	-	expression tag	UNP O00487
c	315	HIS	-	expression tag	UNP O00487
c	316	HIS	-	expression tag	UNP O00487
c	317	HIS	-	expression tag	UNP O00487
c	318	HIS	-	expression tag	UNP O00487
c	319	HIS	-	expression tag	UNP O00487

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Chain	Residue	Modelled	Actual	Comment	Reference
c	320	ASP	-	expression tag	UNP O00487
c	321	TYR	-	expression tag	UNP O00487
c	322	ASP	-	expression tag	UNP O00487
c	323	ILE	-	expression tag	UNP O00487
c	324	PRO	-	expression tag	UNP O00487
c	325	THR	-	expression tag	UNP O00487
c	326	THR	-	expression tag	UNP O00487
c	327	ALA	-	expression tag	UNP O00487
c	328	SER	-	expression tag	UNP O00487
c	329	GLU	-	expression tag	UNP O00487
c	330	ASN	-	expression tag	UNP O00487
c	331	LEU	-	expression tag	UNP O00487
c	332	TYR	-	expression tag	UNP O00487
c	333	PHE	-	expression tag	UNP O00487
c	334	GLN	-	expression tag	UNP O00487
c	335	GLY	-	expression tag	UNP O00487
c	336	GLU	-	expression tag	UNP O00487
c	337	LEU	-	expression tag	UNP O00487
c	338	GLY	-	expression tag	UNP O00487
c	339	MET	-	expression tag	UNP O00487
c	340	ARG	-	expression tag	UNP O00487
c	341	GLY	-	expression tag	UNP O00487
c	342	SER	-	expression tag	UNP O00487
c	343	ALA	-	expression tag	UNP O00487
c	344	GLY	-	expression tag	UNP O00487
c	345	LYS	-	expression tag	UNP O00487
c	346	ALA	-	expression tag	UNP O00487
c	347	GLY	-	expression tag	UNP O00487
c	348	GLU	-	expression tag	UNP O00487
c	349	GLY	-	expression tag	UNP O00487
c	350	GLU	-	expression tag	UNP O00487
c	351	ILE	-	expression tag	UNP O00487
c	352	PRO	-	expression tag	UNP O00487
c	353	ALA	-	expression tag	UNP O00487
c	354	PRO	-	expression tag	UNP O00487
c	355	LEU	-	expression tag	UNP O00487
c	356	ALA	-	expression tag	UNP O00487
c	357	GLY	-	expression tag	UNP O00487
c	358	THR	-	expression tag	UNP O00487
c	359	VAL	-	expression tag	UNP O00487
c	360	SER	-	expression tag	UNP O00487
c	361	LYS	-	expression tag	UNP O00487

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Chain	Residue	Modelled	Actual	Comment	Reference
c	362	ILE	-	expression tag	UNP O00487
c	363	LEU	-	expression tag	UNP O00487
c	364	VAL	-	expression tag	UNP O00487
c	365	LYS	-	expression tag	UNP O00487
c	366	GLU	-	expression tag	UNP O00487
c	367	GLY	-	expression tag	UNP O00487
c	368	ASP	-	expression tag	UNP O00487
c	369	THR	-	expression tag	UNP O00487
c	370	VAL	-	expression tag	UNP O00487
c	371	LYS	-	expression tag	UNP O00487
c	372	ALA	-	expression tag	UNP O00487
c	373	GLY	-	expression tag	UNP O00487
c	374	GLN	-	expression tag	UNP O00487
c	375	THR	-	expression tag	UNP O00487
c	376	VAL	-	expression tag	UNP O00487
c	377	LEU	-	expression tag	UNP O00487
c	378	VAL	-	expression tag	UNP O00487
c	379	LEU	-	expression tag	UNP O00487
c	380	GLU	-	expression tag	UNP O00487
c	381	ALA	-	expression tag	UNP O00487
c	382	MET	-	expression tag	UNP O00487
c	383	LYS	-	expression tag	UNP O00487
c	384	MET	-	expression tag	UNP O00487
c	385	GLU	-	expression tag	UNP O00487
c	386	THR	-	expression tag	UNP O00487
c	387	GLU	-	expression tag	UNP O00487
c	388	ILE	-	expression tag	UNP O00487
c	389	ASN	-	expression tag	UNP O00487
c	390	ALA	-	expression tag	UNP O00487
c	391	PRO	-	expression tag	UNP O00487
c	392	THR	-	expression tag	UNP O00487
c	393	ASP	-	expression tag	UNP O00487
c	394	GLY	-	expression tag	UNP O00487
c	395	LYS	-	expression tag	UNP O00487
c	396	VAL	-	expression tag	UNP O00487
c	397	GLU	-	expression tag	UNP O00487
c	398	LYS	-	expression tag	UNP O00487
c	399	VAL	-	expression tag	UNP O00487
c	400	LEU	-	expression tag	UNP O00487
c	401	VAL	-	expression tag	UNP O00487
c	402	LYS	-	expression tag	UNP O00487
c	403	GLU	-	expression tag	UNP O00487

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Chain	Residue	Modelled	Actual	Comment	Reference
c	404	ARG	-	expression tag	UNP O00487
c	405	ASP	-	expression tag	UNP O00487
c	406	ALA	-	expression tag	UNP O00487
c	407	VAL	-	expression tag	UNP O00487
c	408	GLN	-	expression tag	UNP O00487
c	409	GLY	-	expression tag	UNP O00487
c	410	GLY	-	expression tag	UNP O00487
c	411	GLN	-	expression tag	UNP O00487
c	412	GLY	-	expression tag	UNP O00487
c	413	LEU	-	expression tag	UNP O00487
c	414	ILE	-	expression tag	UNP O00487
c	415	LYS	-	expression tag	UNP O00487
c	416	ILE	-	expression tag	UNP O00487
c	417	GLY	-	expression tag	UNP O00487
c	418	VAL	-	expression tag	UNP O00487
c	419	HIS	-	expression tag	UNP O00487
c	420	HIS	-	expression tag	UNP O00487
c	421	HIS	-	expression tag	UNP O00487
c	422	HIS	-	expression tag	UNP O00487
c	423	HIS	-	expression tag	UNP O00487
c	424	HIS	-	expression tag	UNP O00487

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	240	Total 1867	C 1187	N 312	O 355	S 13	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	232	Total 1801	C 1149	N 304	O 342	S 6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	248	Total 1933	C 1222	N 330	O 371	S 10	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	J	239	1860	1166	327	362	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	K	238	1817	1142	303	361	11	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	83	LYS	ALA	conflict	UNP P28066

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	L	240	1876	1175	338	352	11	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	M	242	1890	1200	323	356	11	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	N	195	1462	913	250	287	12	0	0

- Molecule 13 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	O	220	1645	1035	278	320	12	0	0

- Molecule 14 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	P	204	Total 1587	C 1010	N 264	O 294	S 19	0	0

- Molecule 15 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Q	199	Total 1588	C 1017	N 270	O 292	S 9	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	R	201	Total 1559	C 982	N 274	O 294	S 9	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S	213	Total 1641	C 1041	N 281	O 309	S 10	0	0

- Molecule 18 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	216	Total 1683	C 1062	N 291	O 318	S 12	0	0

- Molecule 19 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	X	379	Total 3001	C 1914	N 508	O 567	S 12	0	0

- Molecule 20 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

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

- Molecule 21 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

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

- Molecule 22 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

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

- Molecule 23 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

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

- Molecule 24 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	d	250	Total 2048	C 1331	N 335	O 373	S 9	0	0

- Molecule 25 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	f	884	Total 6836	C 4298	N 1169	O 1323	S 46	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	W	437	Total 3564	C 2258	N 609	O 674	S 23	0	0

- Molecule 27 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	V	432	Total 3527	C 2252	N 628	O 634	S 13	0	0

- Molecule 28 is a protein called 26S proteasome complex subunit SEM1.

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

- Molecule 29 is a protein called 26S proteasome regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	A	391	Total 3074	C 1936	N 541	O 580	S 17	0	0

- Molecule 30 is a protein called 26S proteasome regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	F	359	Total 2803	C 1774	N 483	O 529	S 17	0	0

- Molecule 31 is a protein called 26S protease regulatory subunit 10B.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	E	364	Total 2887	C 1814	N 515	O 542	S 16	0	0

- Molecule 32 is a protein called 26S proteasome non-ATPase regulatory subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	U	829	Total 6459	C 4098	N 1098	O 1218	S 45	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	320	ASN	ASP	conflict	UNP Q99460

- Molecule 33 is a protein called Ubiquitin,Green to red photoconvertible GFP-like protein EosFP.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	g	200	Total 1622	C 1044	N 274	O 292	S 12	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
g	176	LYS	ASN	conflict	UNP Q5S6Z9
g	228	CR8	HIS	conflict	UNP Q5S6Z9
g	?	-	TYR	deletion	UNP Q5S6Z9
g	?	-	GLY	deletion	UNP Q5S6Z9
g	235	LYS	GLU	conflict	UNP Q5S6Z9
g	239	ASN	HIS	conflict	UNP Q5S6Z9
g	267	ASN	ILE	conflict	UNP Q5S6Z9
g	286	TYR	HIS	conflict	UNP Q5S6Z9
g	288	THR	VAL	conflict	UNP Q5S6Z9
g	323	GLU	THR	conflict	UNP Q5S6Z9
g	354	ALA	TYR	conflict	UNP Q5S6Z9
g	392	TYR	-	expression tag	UNP Q5S6Z9

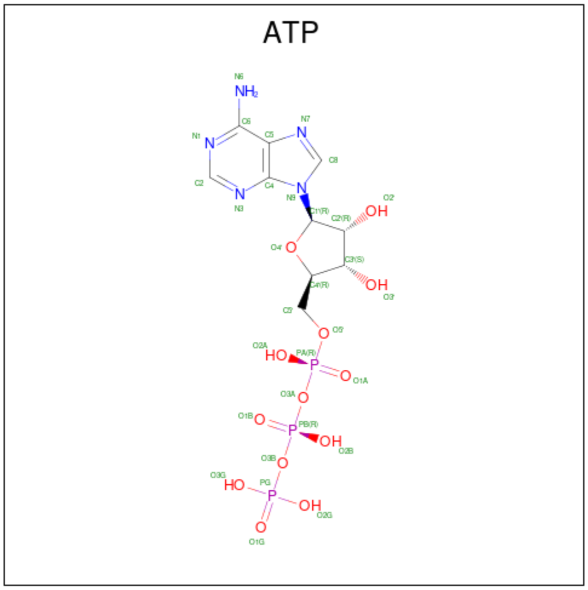
- Molecule 34 is a protein called Thioredoxin-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	u	155	Total 1240	C 783	N 199	O 250	S 8	0	0

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
u	-10	GLY	-	expression tag	UNP O43396
u	-9	HIS	-	expression tag	UNP O43396
u	-8	MET	-	expression tag	UNP O43396
u	-7	ASP	-	expression tag	UNP O43396
u	-6	TYR	-	expression tag	UNP O43396
u	-5	LYS	-	expression tag	UNP O43396
u	-4	ASP	-	expression tag	UNP O43396
u	-3	ASP	-	expression tag	UNP O43396
u	-2	ASP	-	expression tag	UNP O43396
u	-1	ASP	-	expression tag	UNP O43396
u	0	LYS	-	expression tag	UNP O43396

- Molecule 35 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).

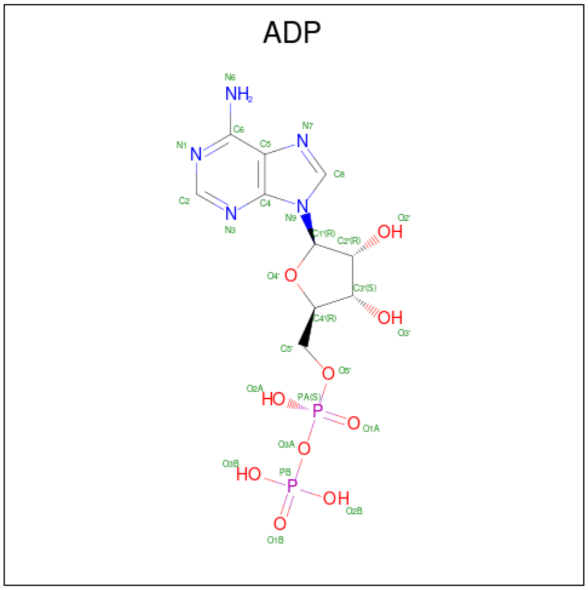


Mol	Chain	Residues	Atoms	AltConf
35	B	1	Total C N O P 31 10 5 13 3	0
35	C	1	Total C N O P 31 10 5 13 3	0

- Molecule 36 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
36	B	1	Total Mg 1 1	0
36	C	1	Total Mg 1 1	0
36	D	1	Total Mg 1 1	0

- Molecule 37 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
37	D	1	Total 27	C 10	N 5	O 10	P 2	0
37	A	1	Total 27	C 10	N 5	O 10	P 2	0
37	F	1	Total 27	C 10	N 5	O 10	P 2	0
37	E	1	Total 27	C 10	N 5	O 10	P 2	0

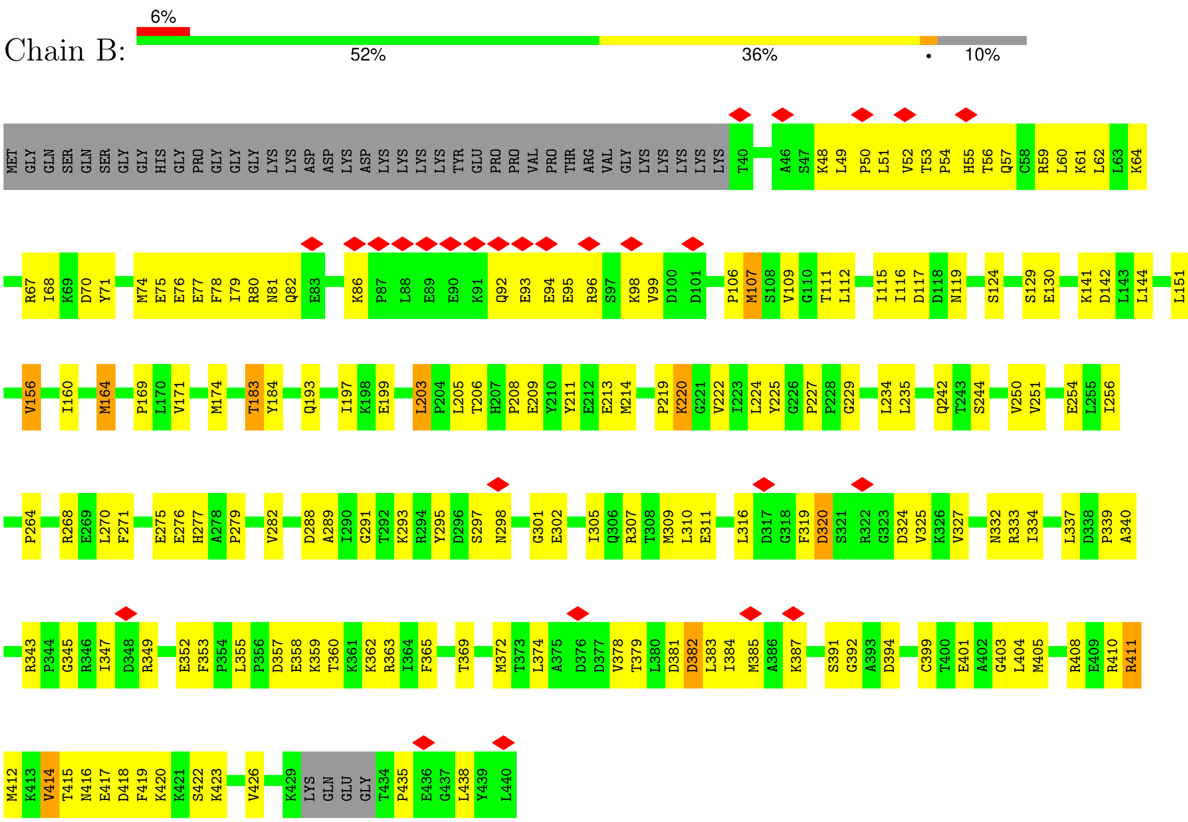
- Molecule 38 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

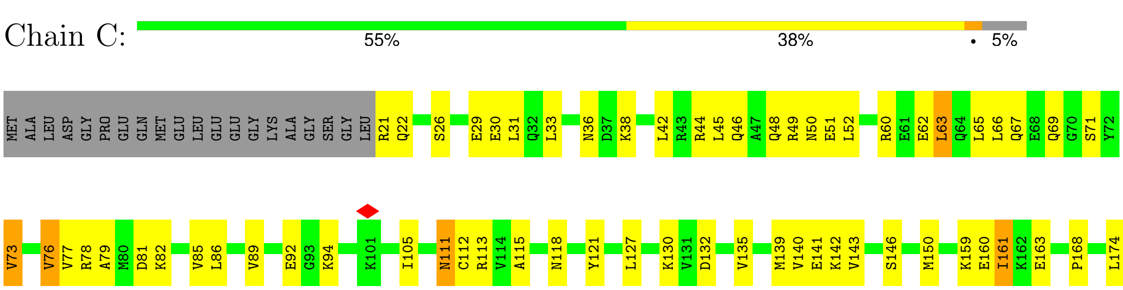
3 Residue-property plots (i)

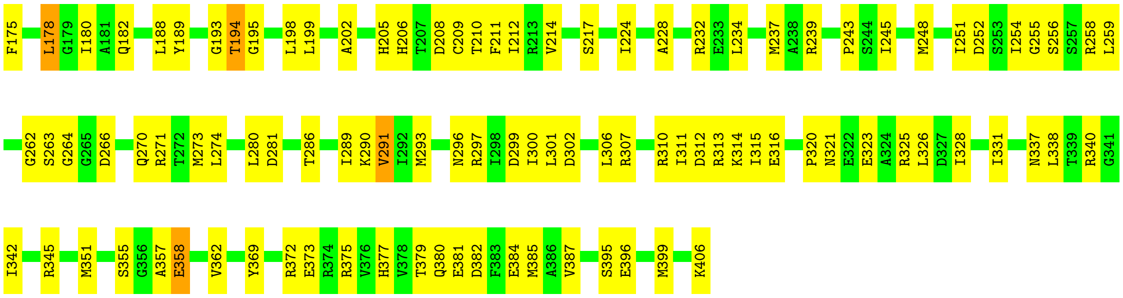
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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 4



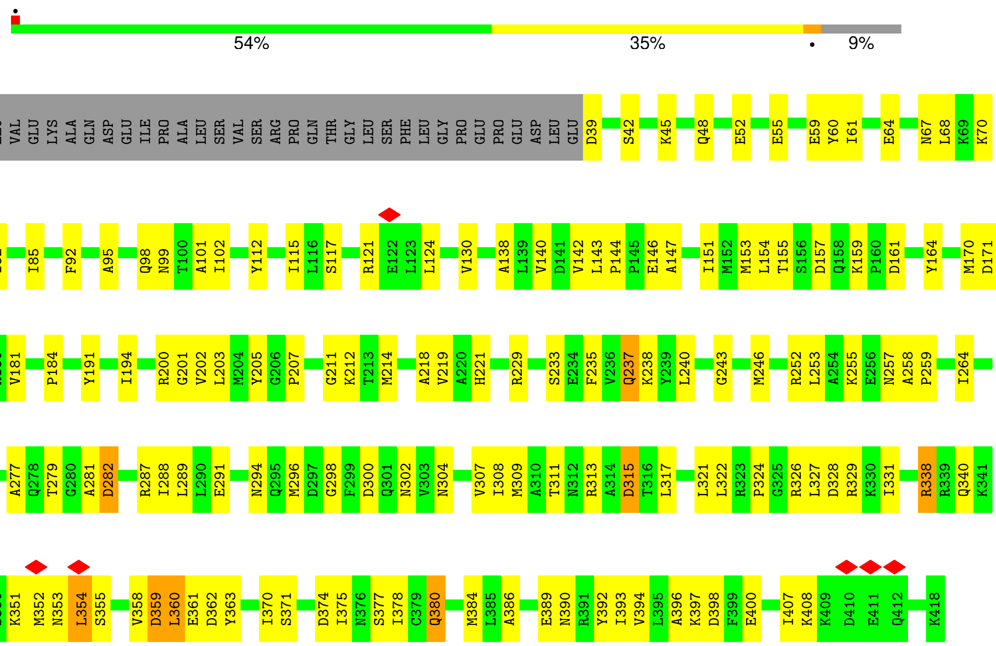
- Molecule 2: 26S protease regulatory subunit 8





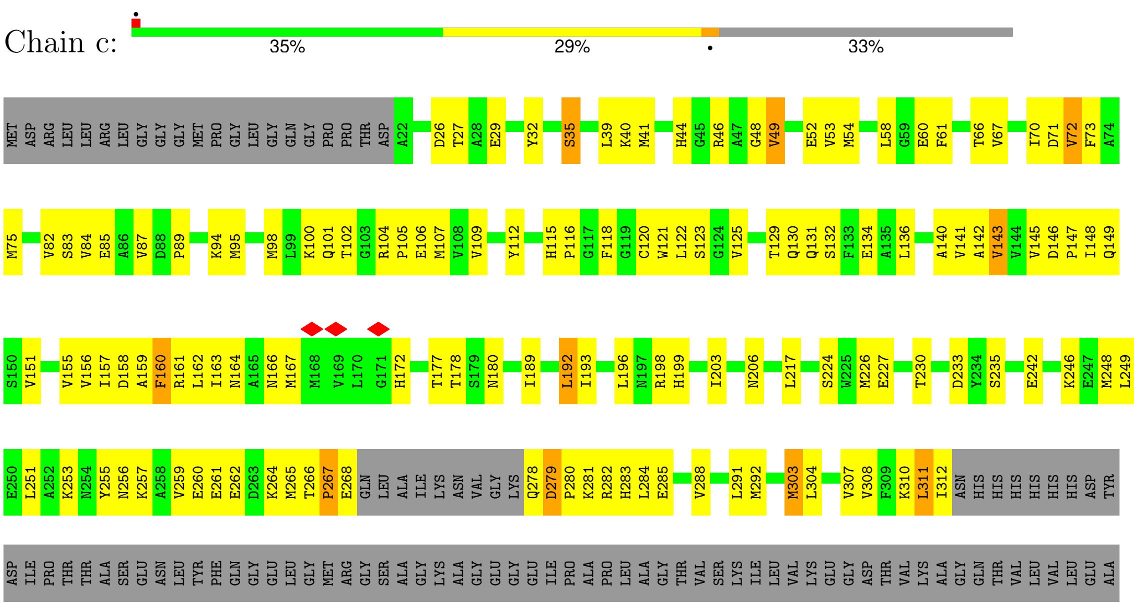
- Molecule 3: 26S proteasome regulatory subunit 6B

Chain D:

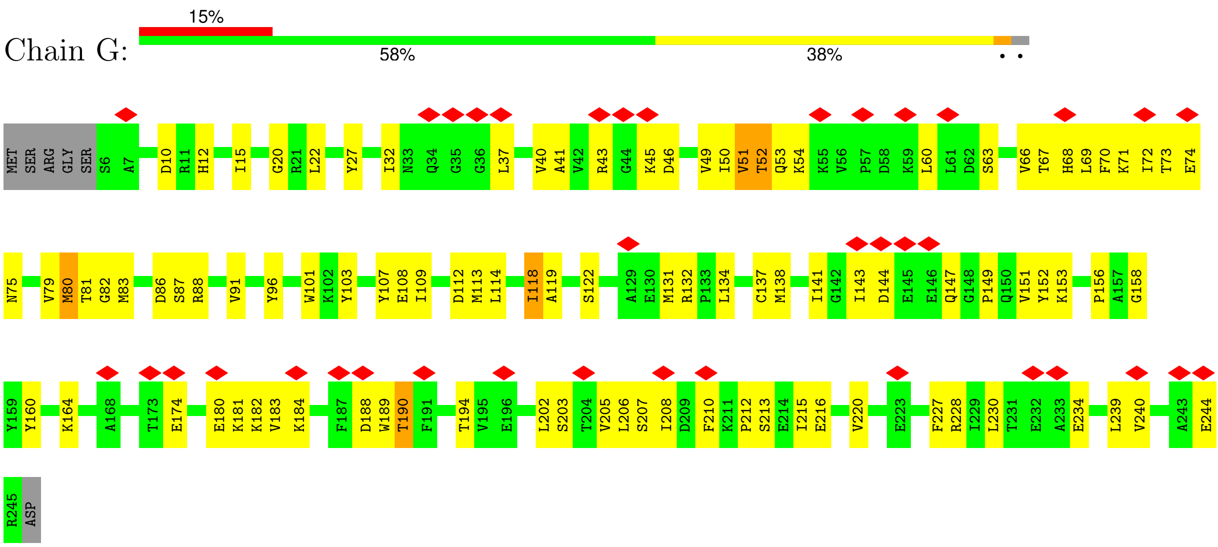


- Molecule 4: 26S proteasome non-ATPase regulatory subunit 14

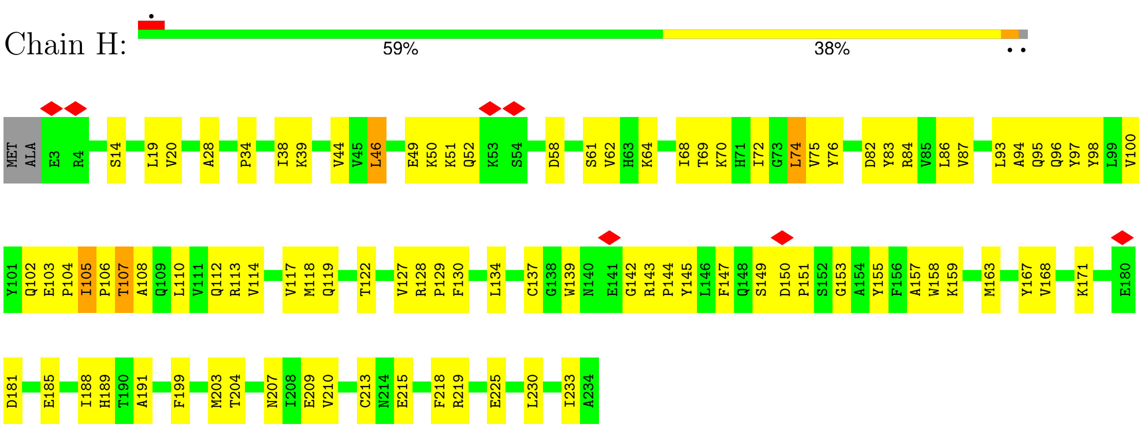
Chain c:



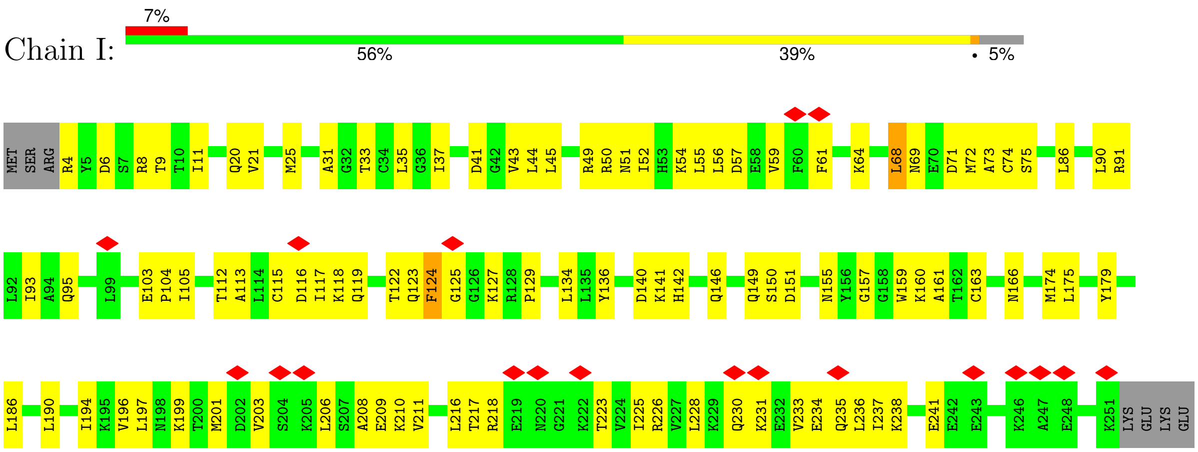
- Molecule 5: Proteasome subunit alpha type-6



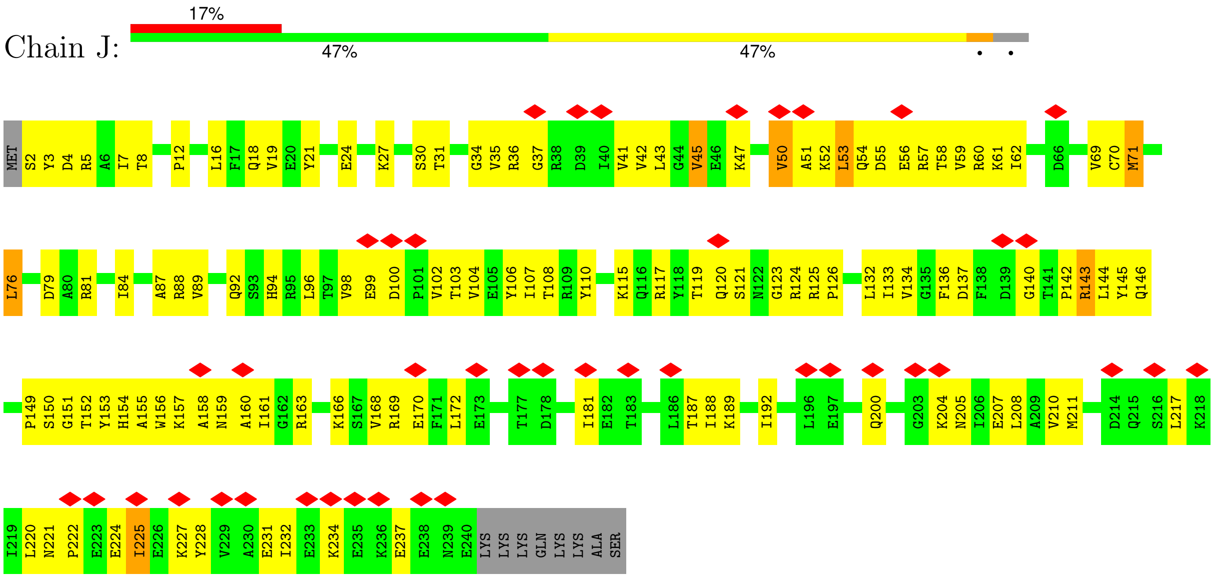
- Molecule 6: Proteasome subunit alpha type-2



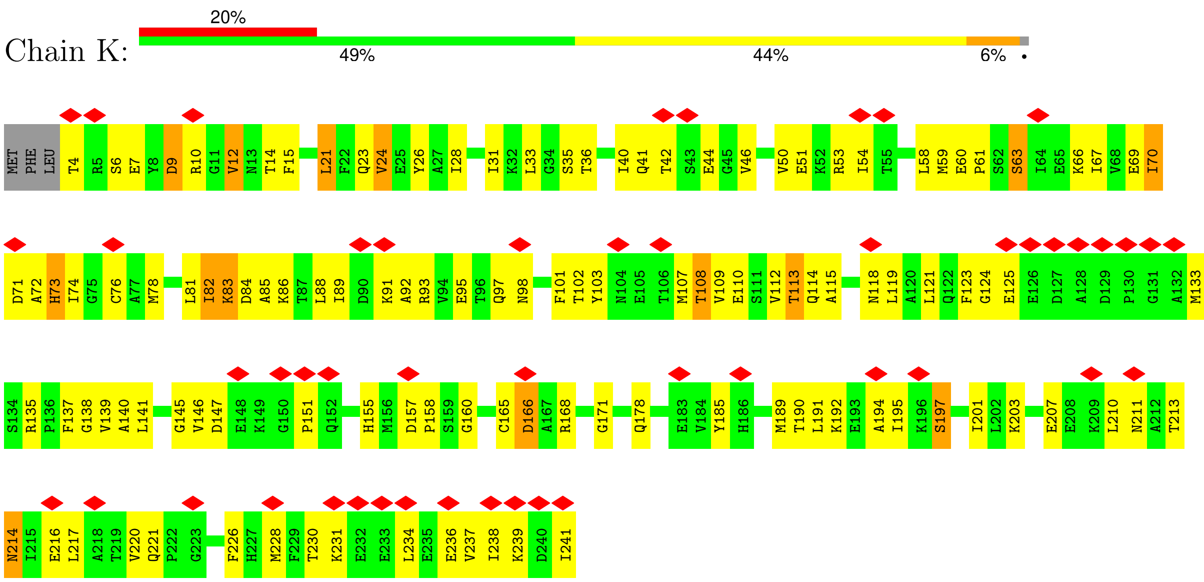
- Molecule 7: Proteasome subunit alpha type-4



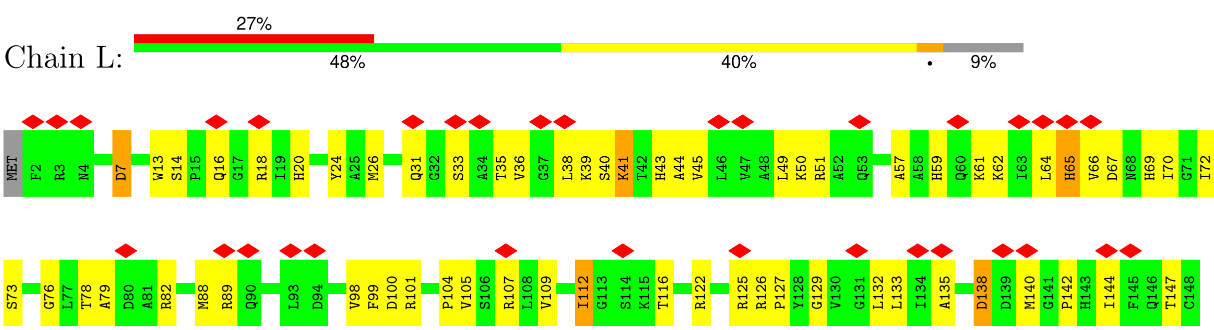
- Molecule 8: Proteasome subunit alpha type-7

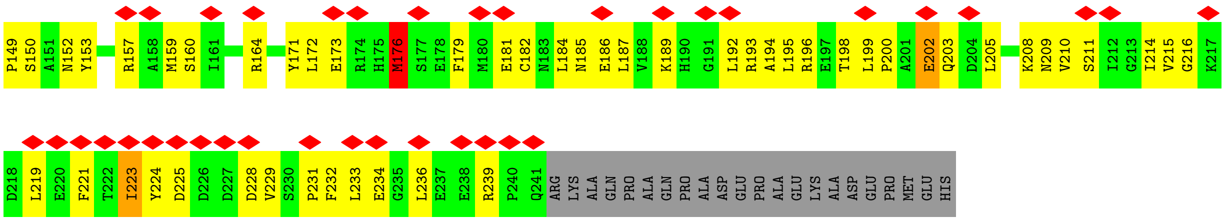


- Molecule 9: Proteasome subunit alpha type-5



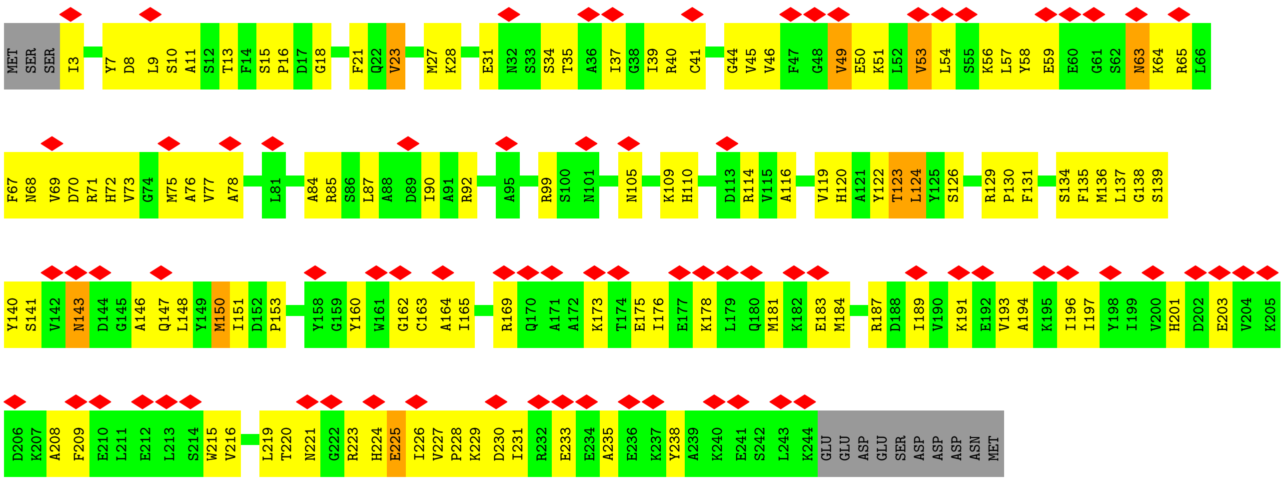
- Molecule 10: Proteasome subunit alpha type-1





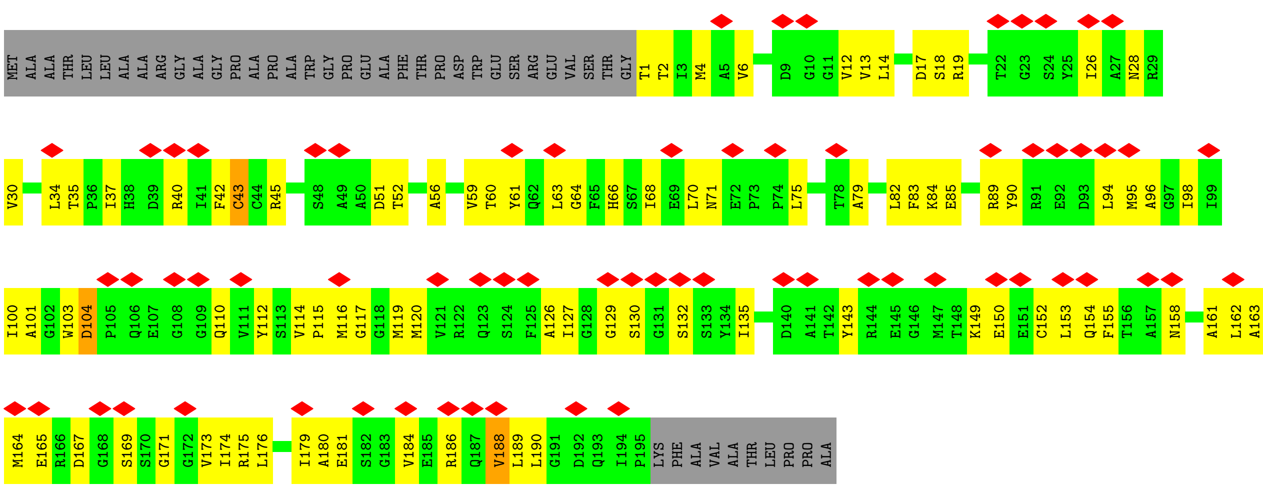
- Molecule 11: Proteasome subunit alpha type-3

Chain M:

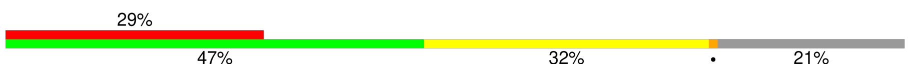



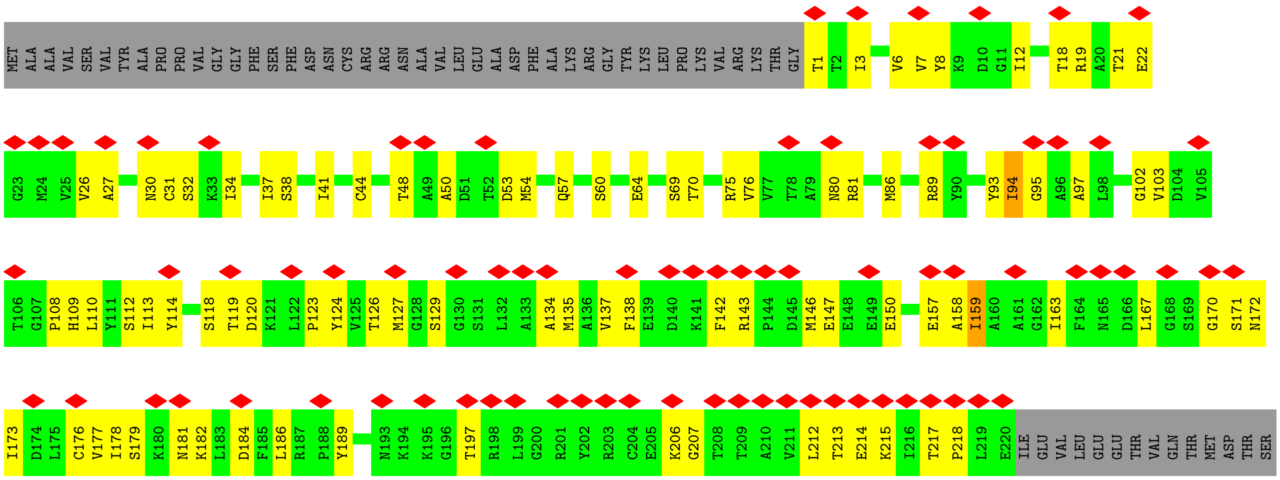
- Molecule 12: Proteasome subunit beta type-6

Chain N:

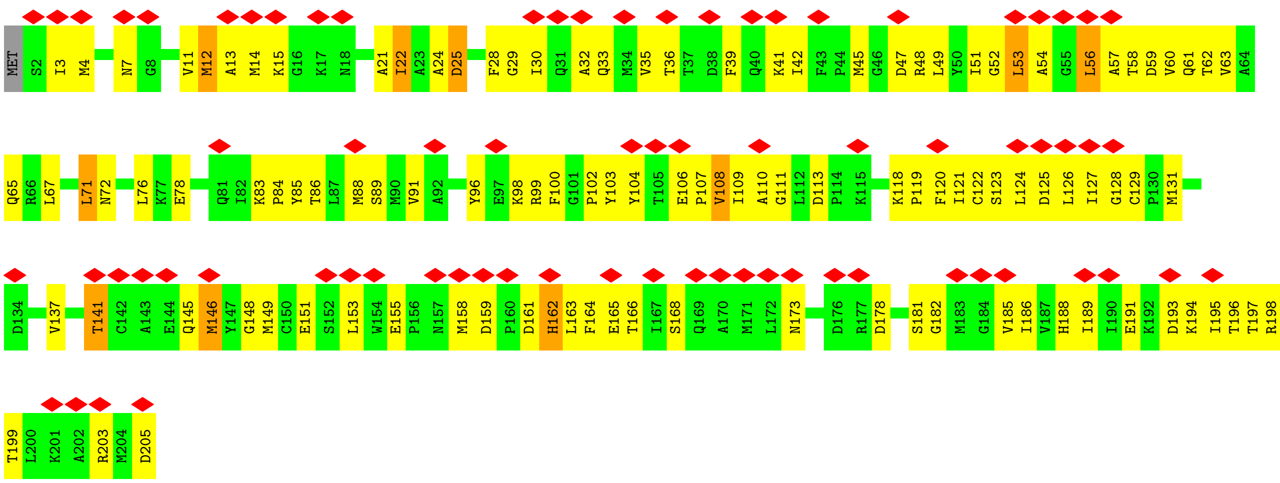
- Molecule 13: Proteasome subunit beta type-7

Chain O:




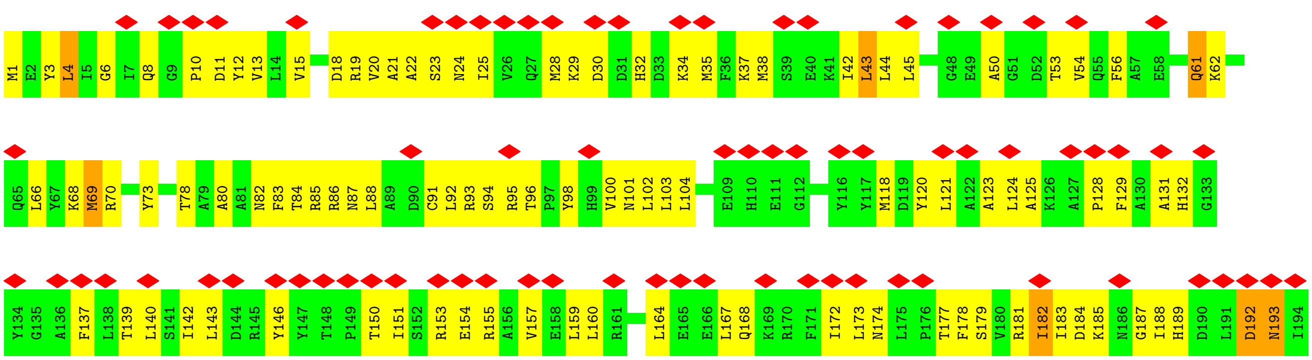
• Molecule 14: Proteasome subunit beta type-3

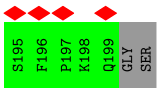
Chain P:



• Molecule 15: Proteasome subunit beta type-2

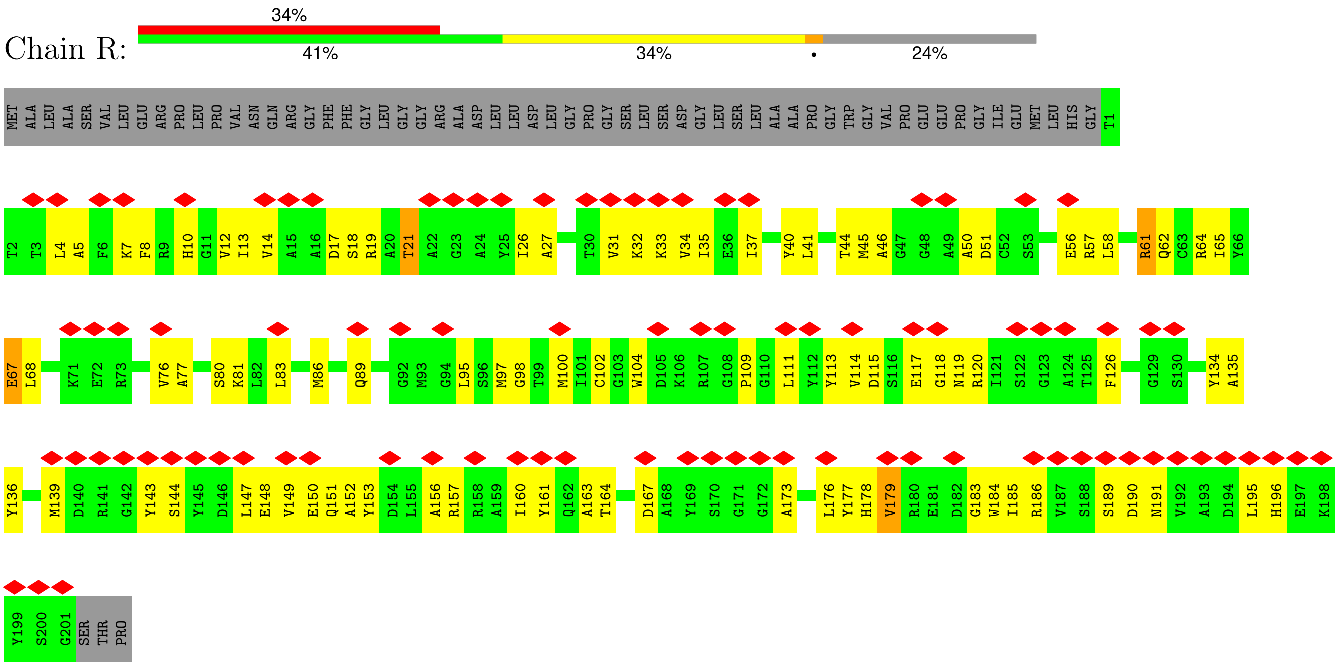
Chain Q:





• Molecule 16: Proteasome subunit beta type-5

Chain R:

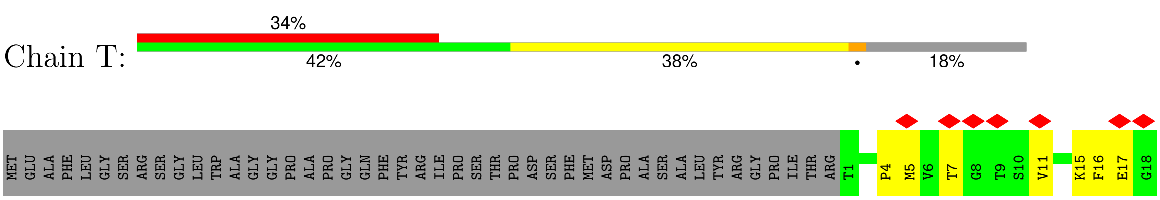


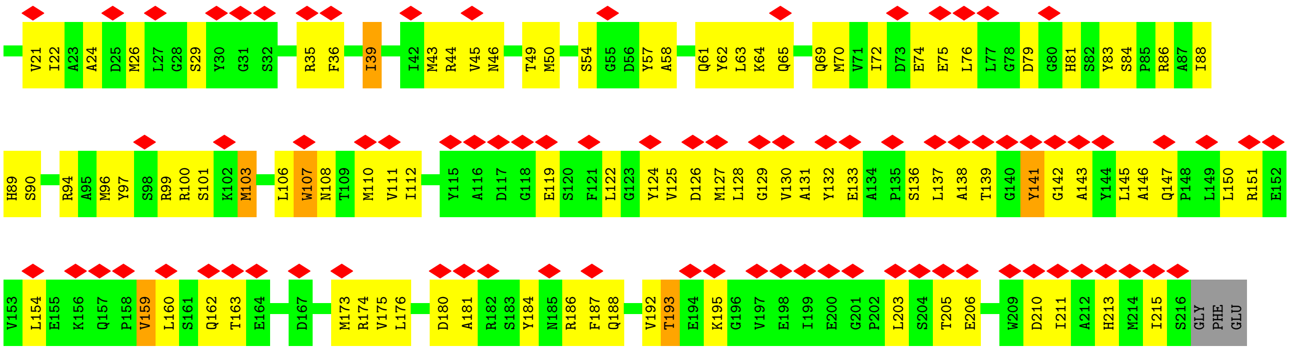
• Molecule 17: Proteasome subunit beta type-1

Chain S:

• Molecule 18: Proteasome subunit beta type-4

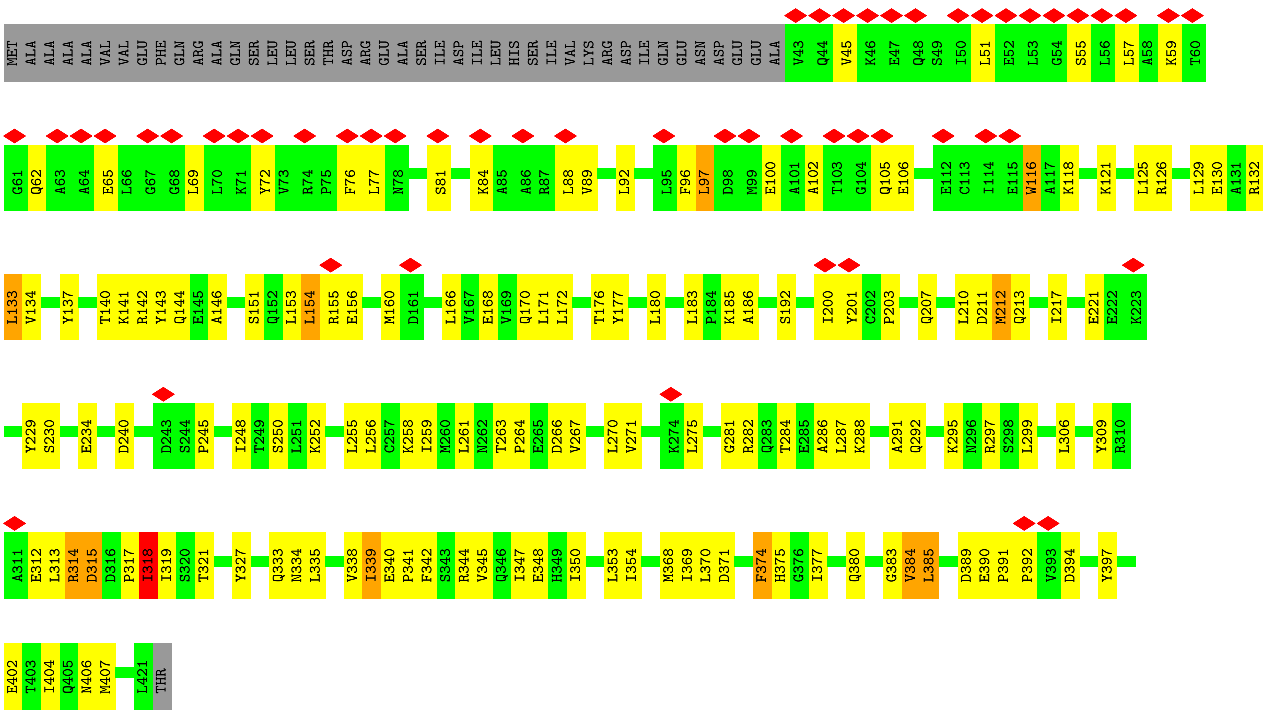
Chain T:





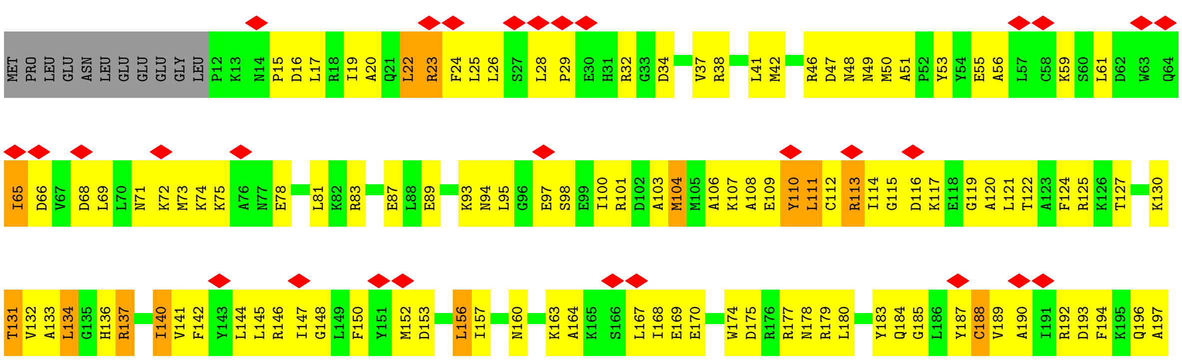
- Molecule 19: 26S proteasome non-ATPase regulatory subunit 11

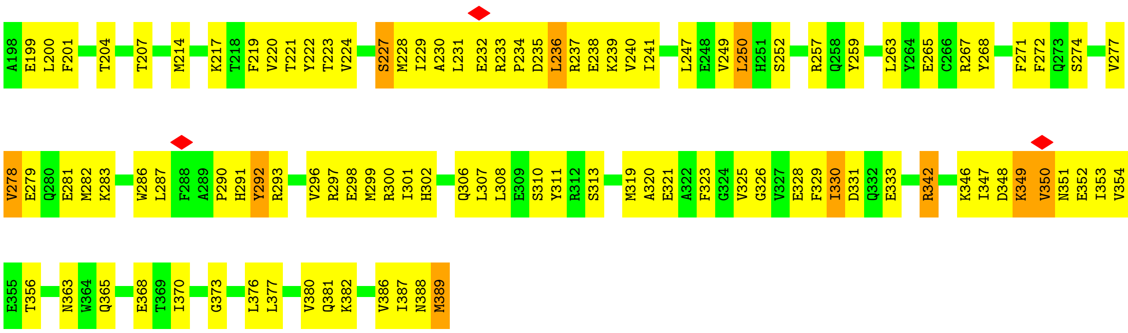
Chain X:



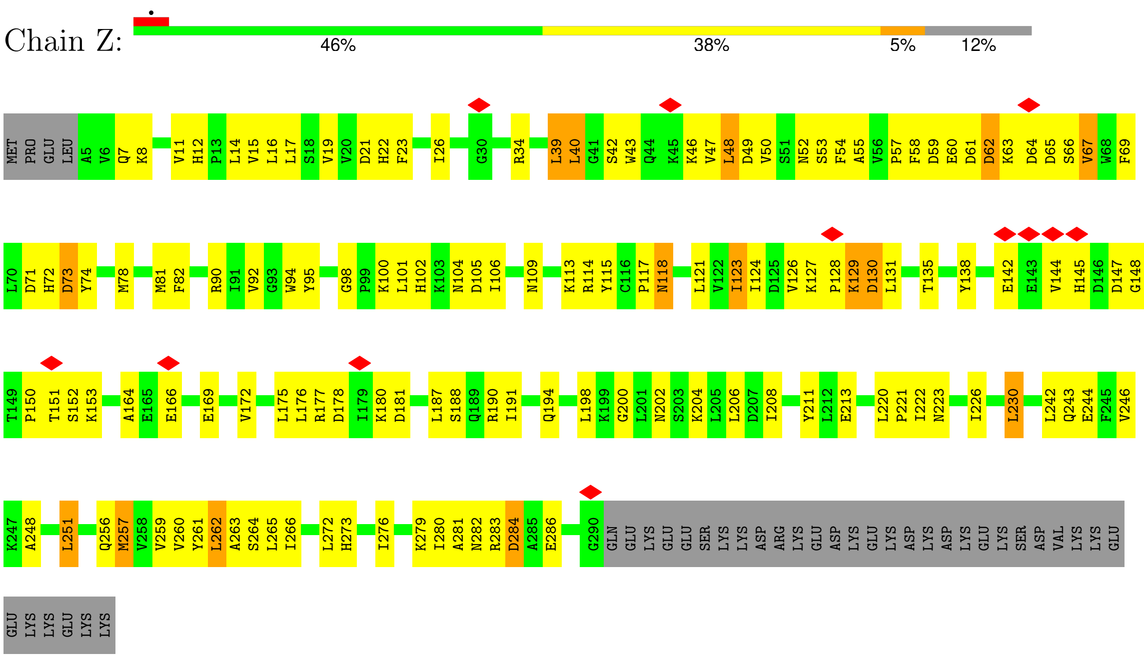
- Molecule 20: 26S proteasome non-ATPase regulatory subunit 6

Chain Y:

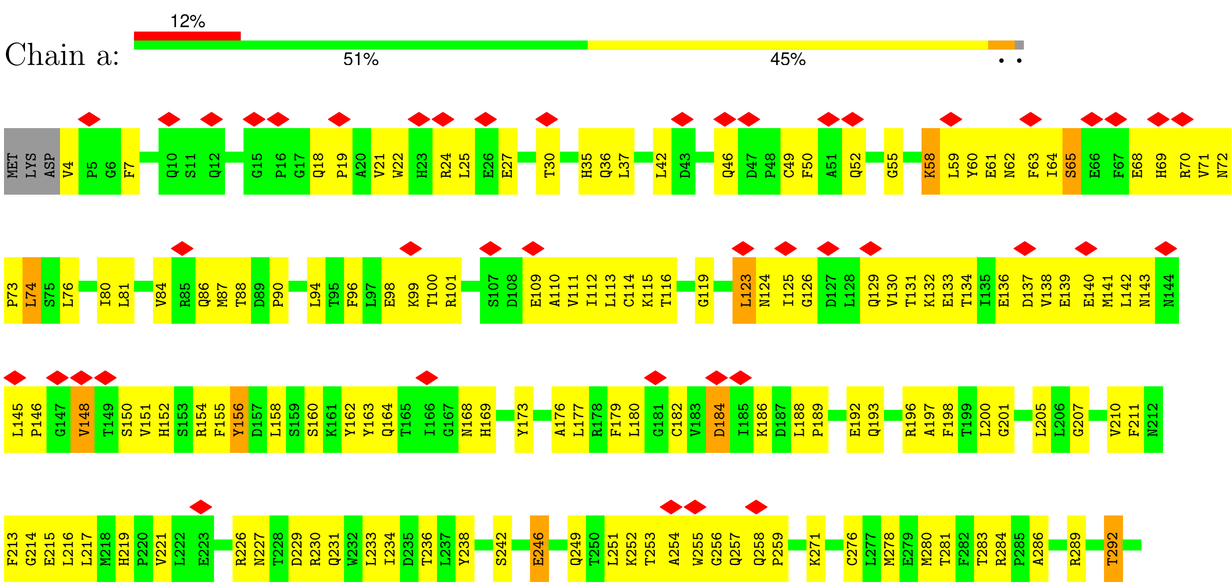


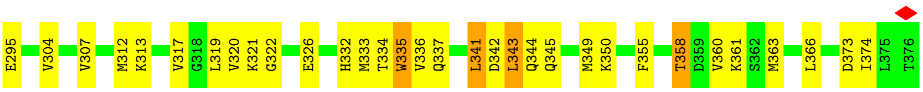


- Molecule 21: 26S proteasome non-ATPase regulatory subunit 7



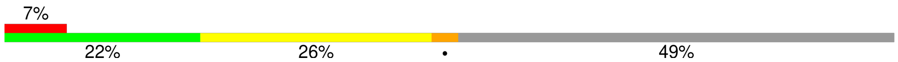
- Molecule 22: 26S proteasome non-ATPase regulatory subunit 13

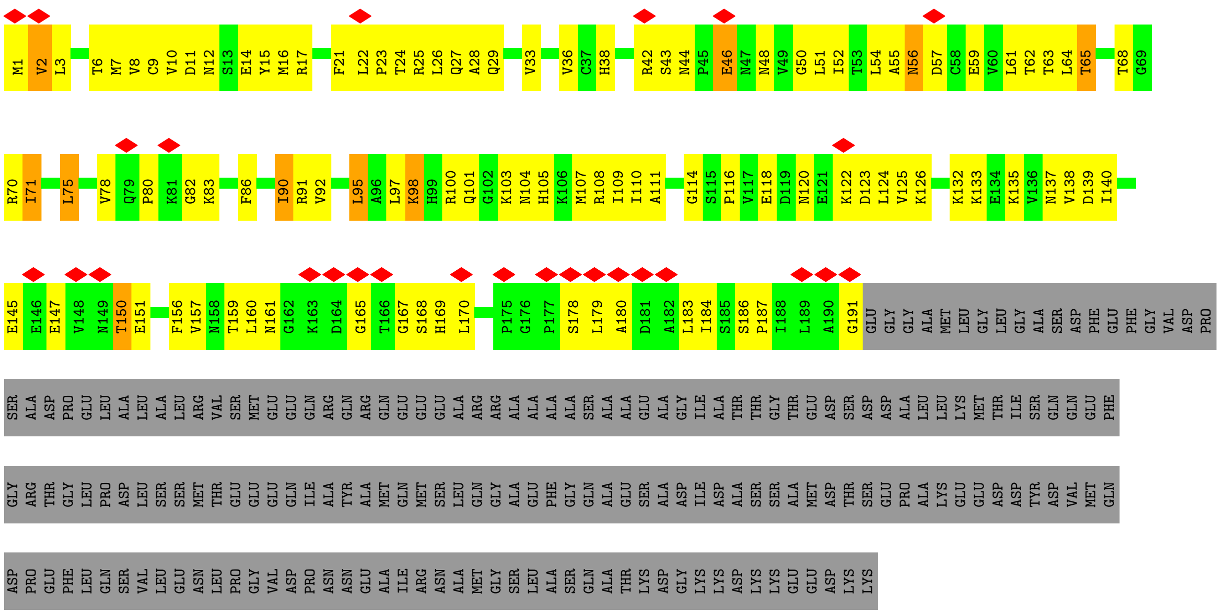




- Molecule 23: 26S proteasome non-ATPase regulatory subunit 4

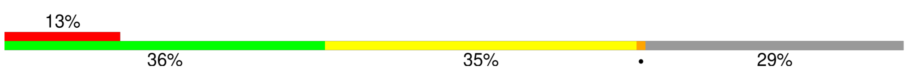
Chain b:

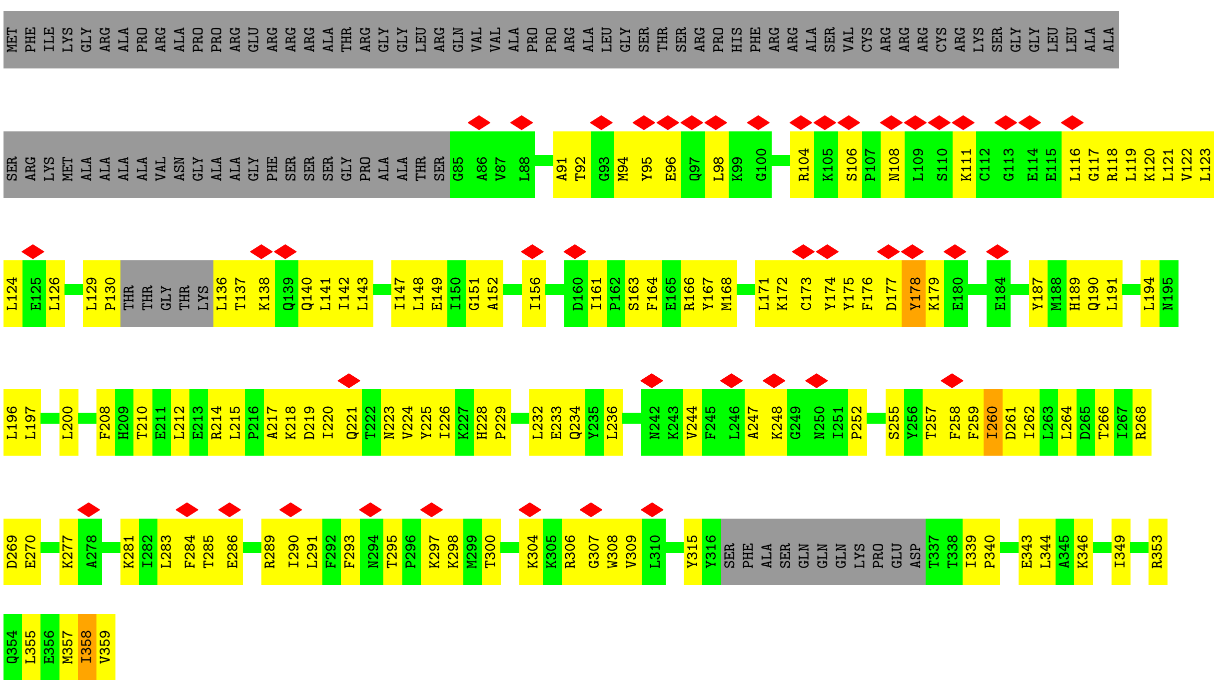




- Molecule 24: 26S proteasome non-ATPase regulatory subunit 8

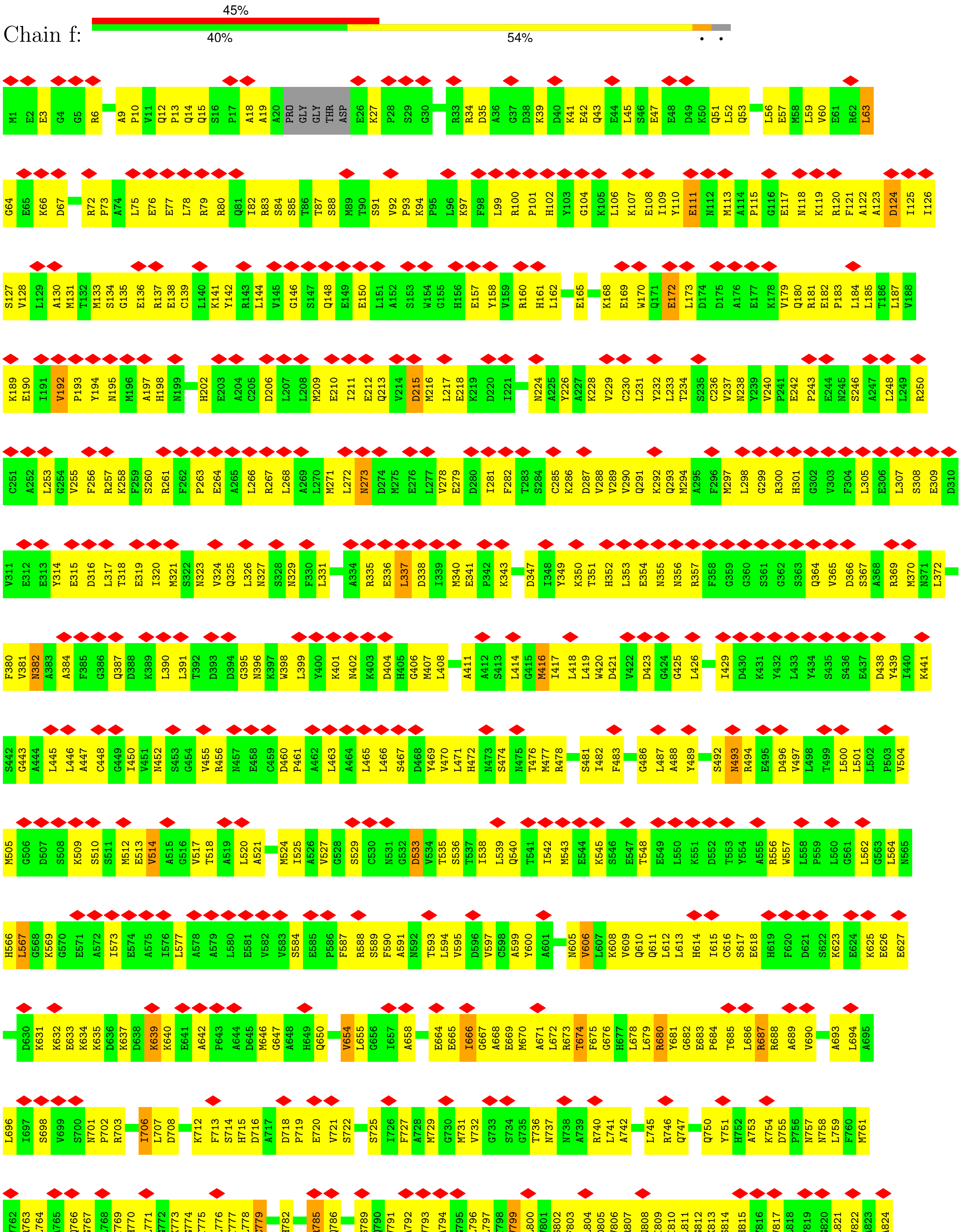
Chain d:

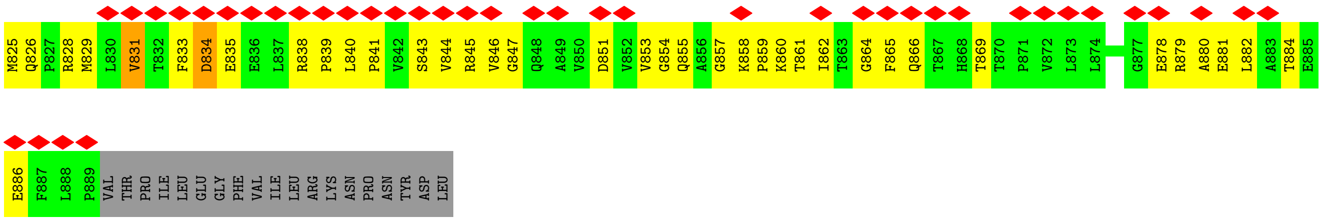




- Molecule 25: 26S proteasome non-ATPase regulatory subunit 2

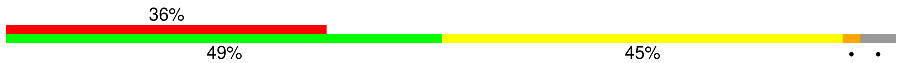
Chain f:

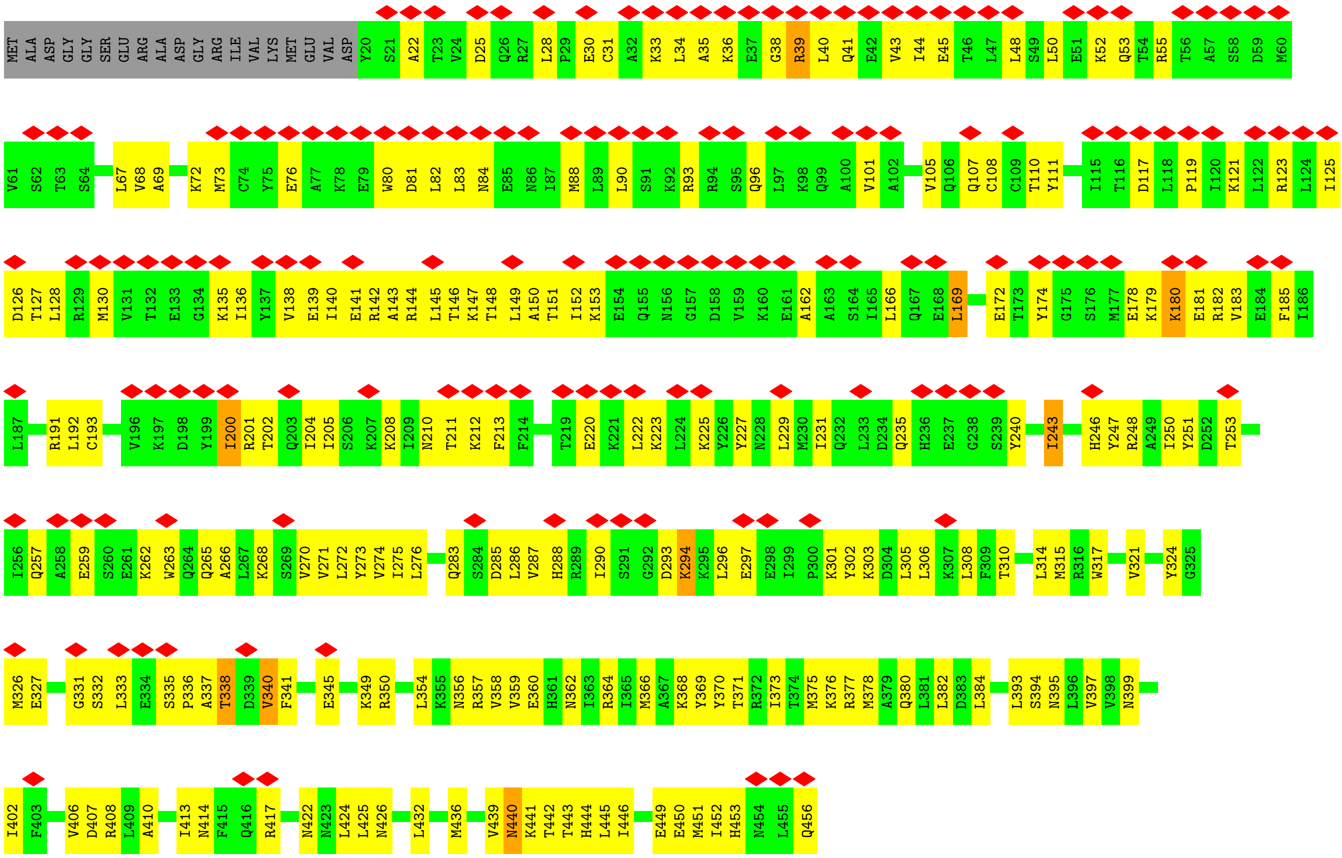




• Molecule 26: 26S proteasome non-ATPase regulatory subunit 12

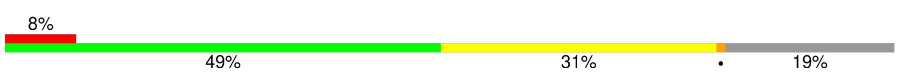
Chain W:

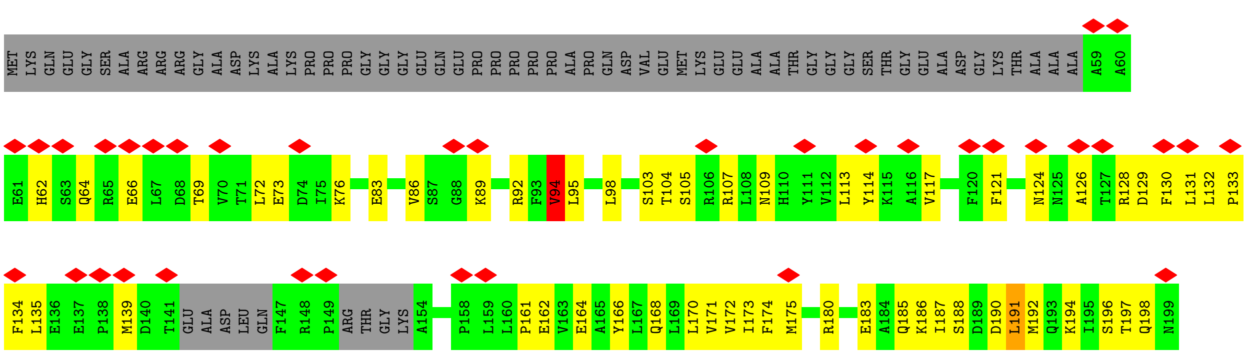


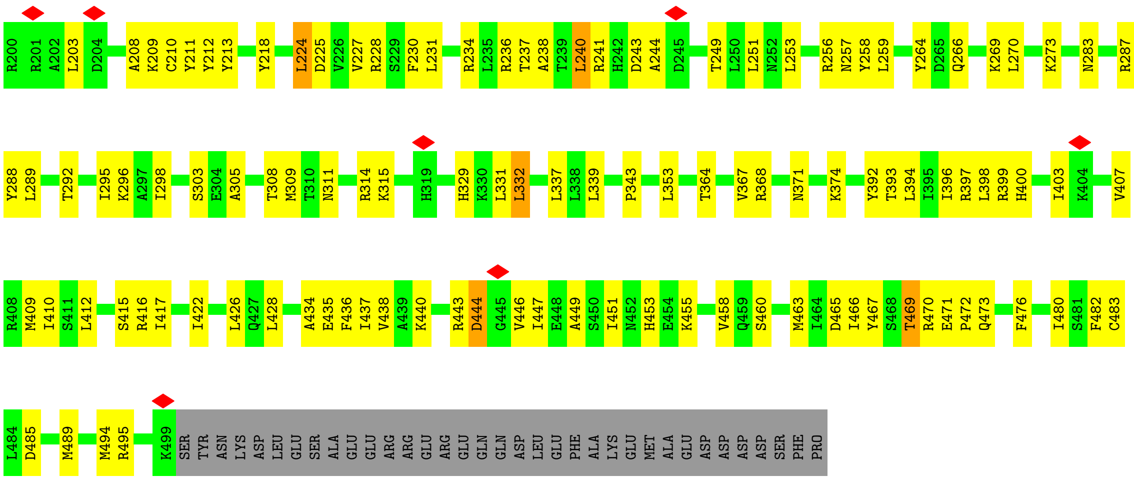


• Molecule 27: 26S proteasome non-ATPase regulatory subunit 3

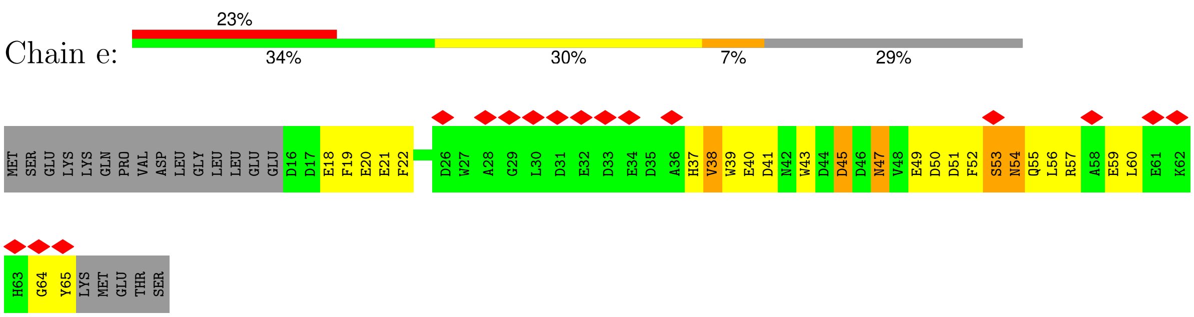
Chain V:



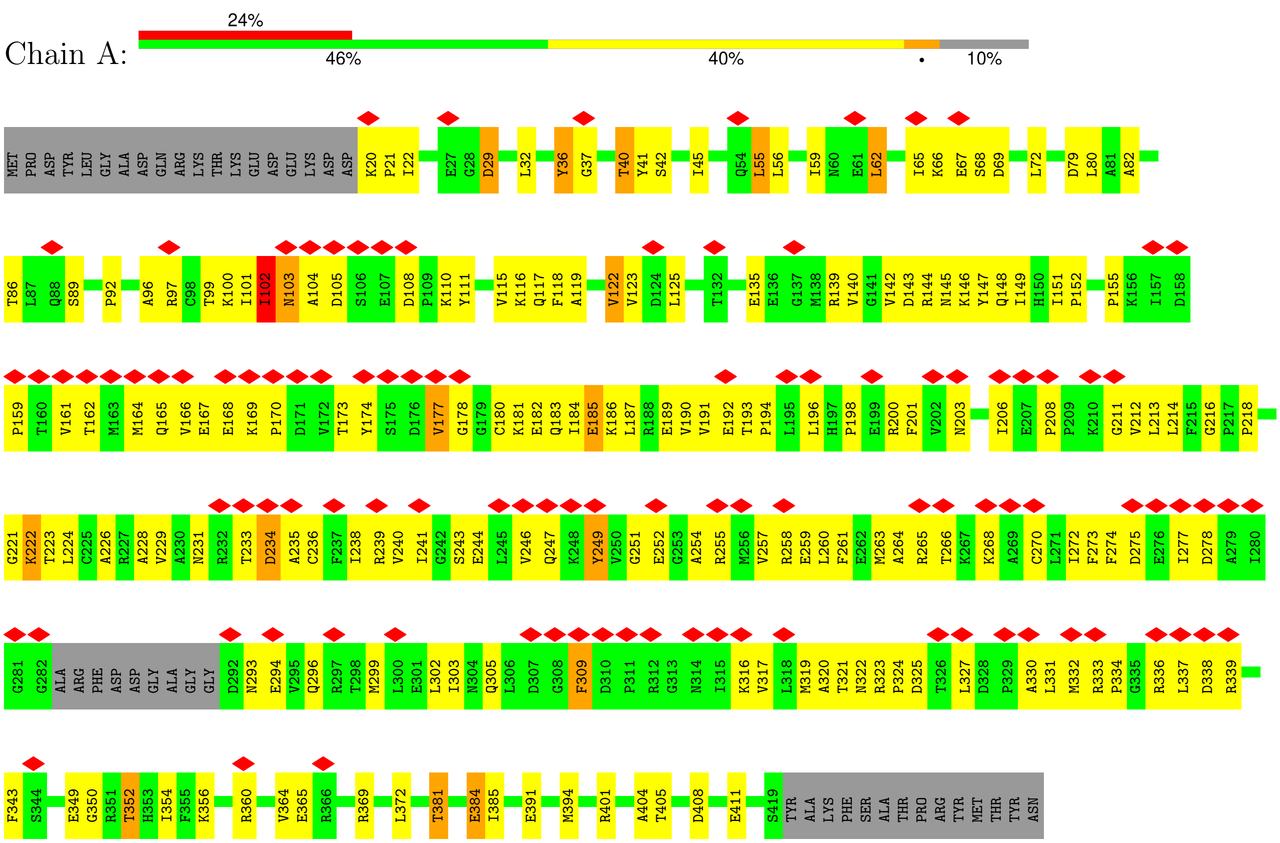




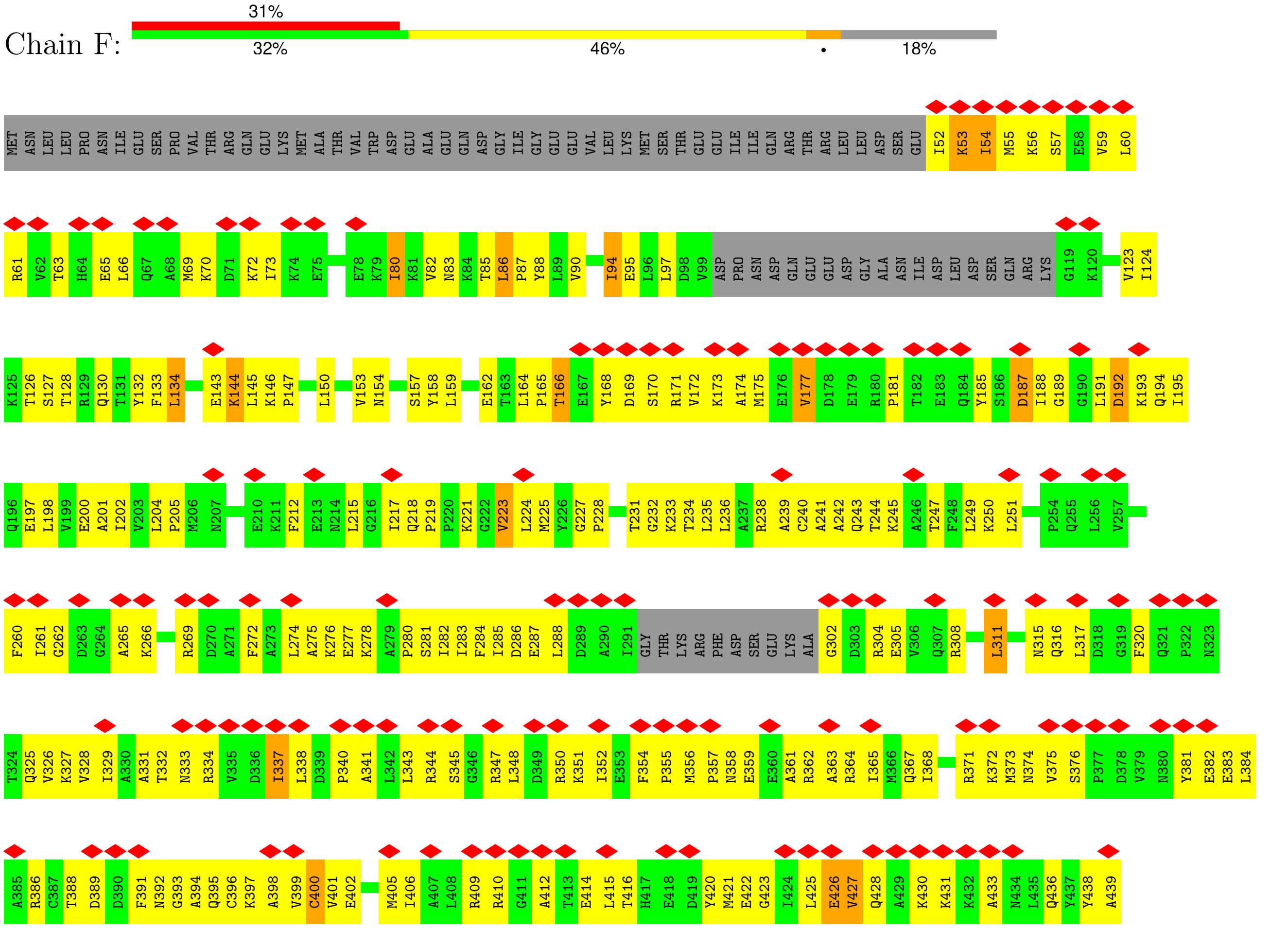
- Molecule 28: 26S proteasome complex subunit SEM1



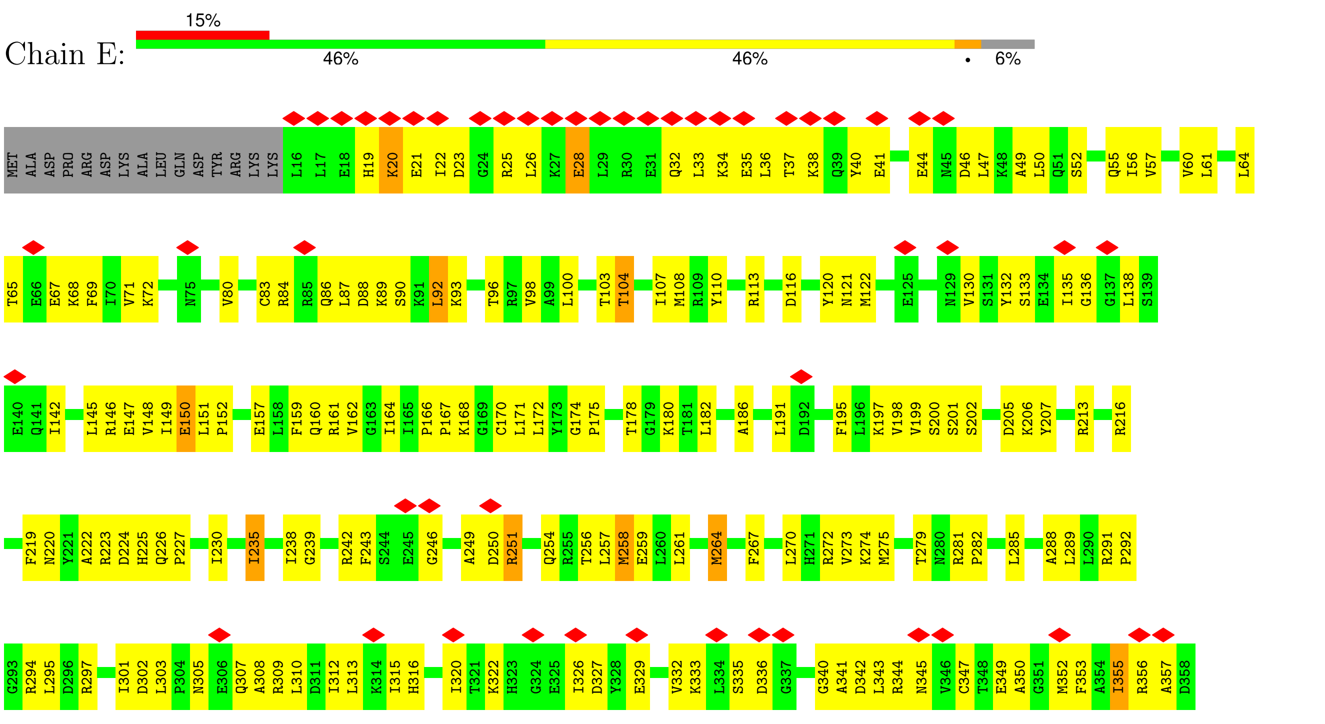
- Molecule 29: 26S proteasome regulatory subunit 7

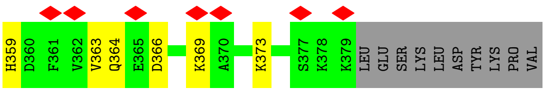


• Molecule 30: 26S proteasome regulatory subunit 6A



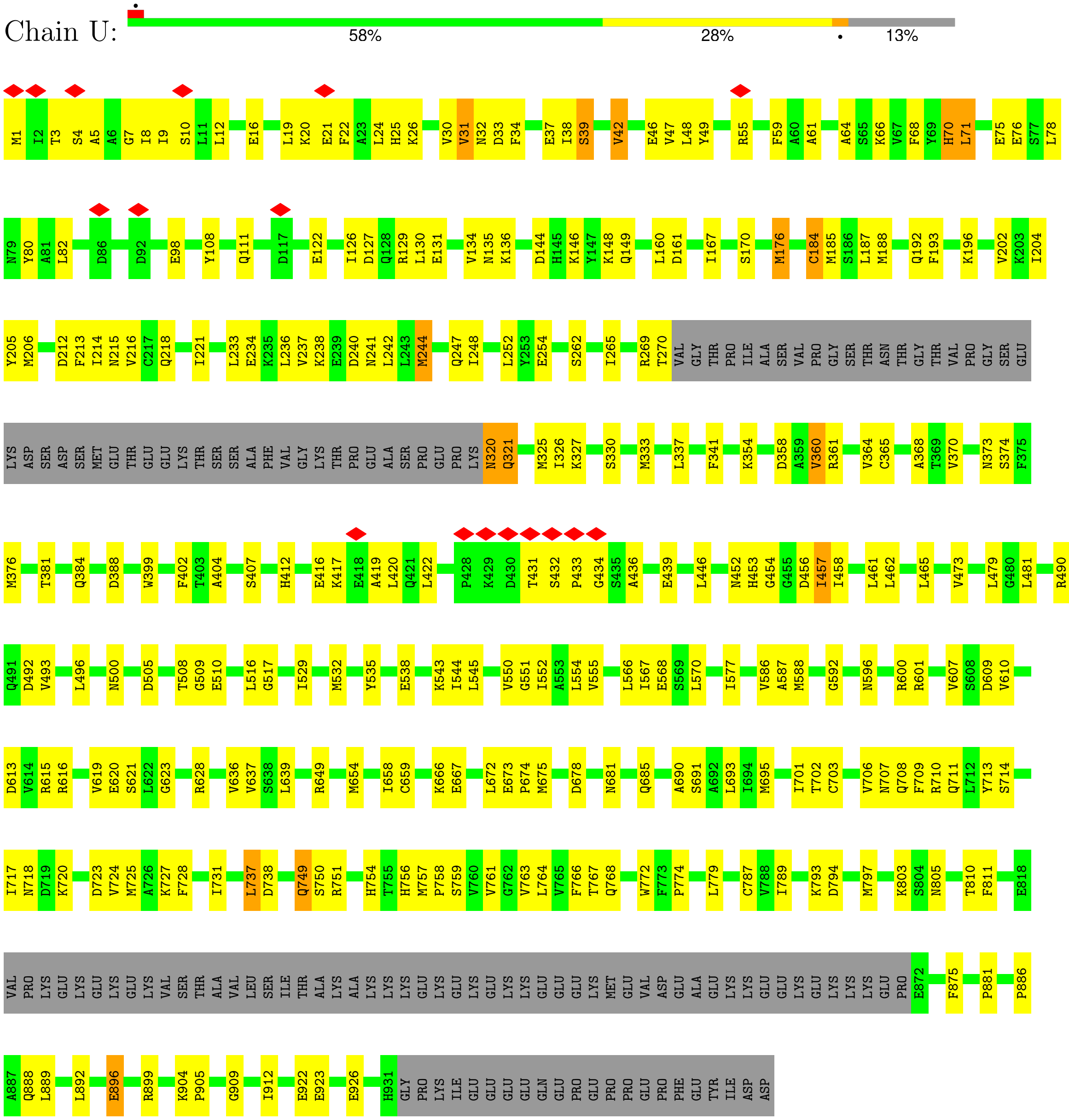
• Molecule 31: 26S protease regulatory subunit 10B





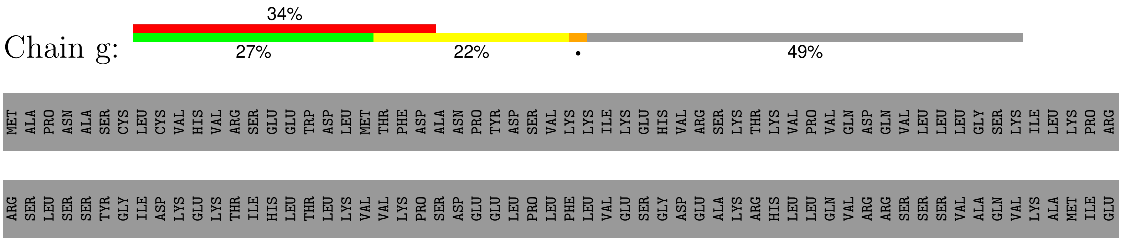
• Molecule 32: 26S proteasome non-ATPase regulatory subunit 1

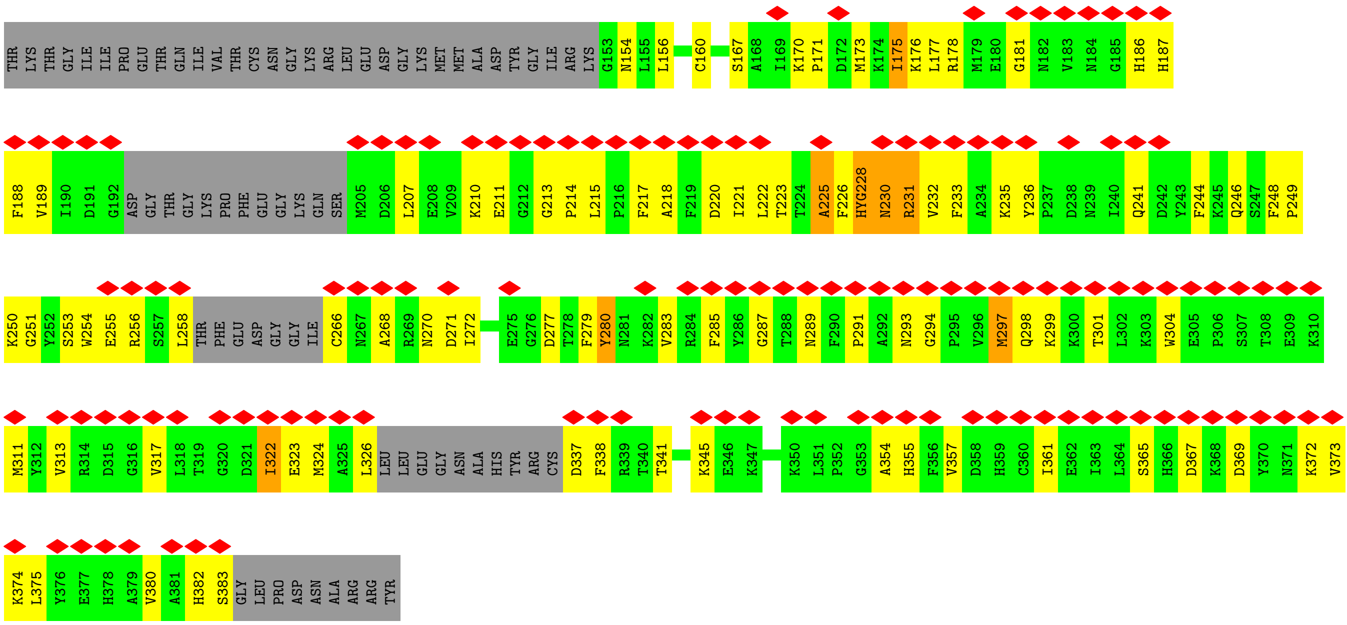
Chain U:



• Molecule 33: Ubiquitin,Green to red photoconvertible GFP-like protein EosFP

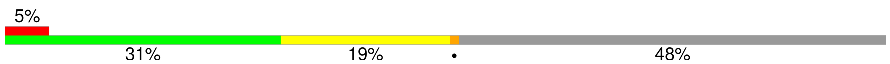
Chain g:

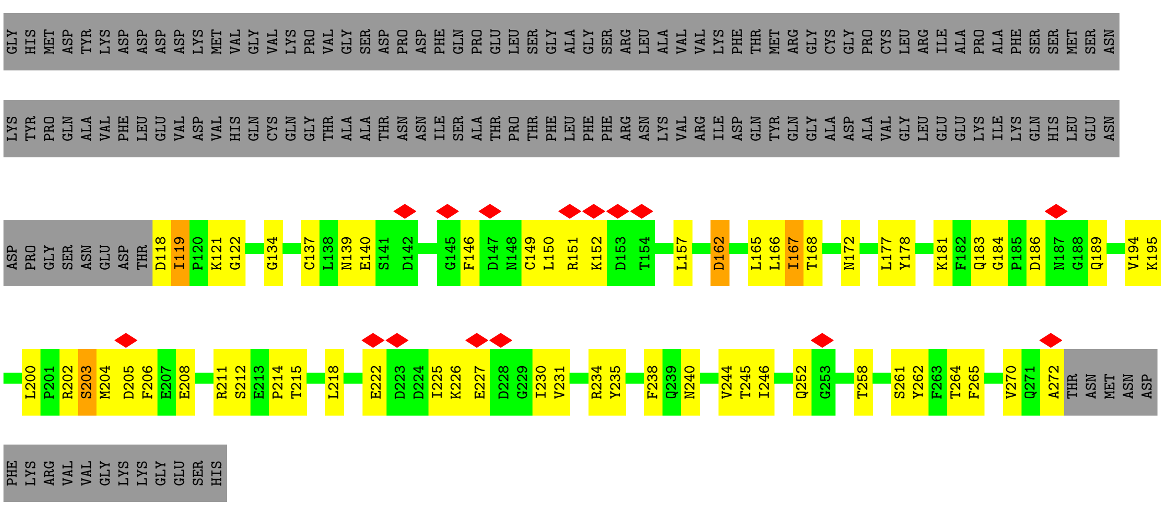




- Molecule 34: Thioredoxin-like protein 1

Chain u:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	73136	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1700	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.216	Depositor
Minimum map value	-0.584	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.044	Depositor
Recommended contour level	0.17	Depositor
Map size (Å)	356.32, 356.32, 356.32	wwPDB
Map dimensions	340, 340, 340	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.048, 1.048, 1.048	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: CR8, MG, ADP, ATP, 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	B	0.19	0/3170	0.37	0/4278
2	C	0.21	0/3094	0.34	0/4158
3	D	0.25	0/3090	0.42	1/4168 (0.0%)
4	c	0.35	0/2262	0.52	0/3059
5	G	0.16	0/1901	0.37	0/2572
6	H	0.15	0/1840	0.33	0/2495
7	I	0.16	0/1963	0.36	0/2650
8	J	0.14	0/1886	0.37	0/2551
9	K	0.20	0/1845	0.43	0/2490
10	L	0.14	0/1911	0.37	1/2584 (0.0%)
11	M	0.14	0/1925	0.38	0/2592
12	N	0.16	0/1487	0.40	0/2013
13	O	0.14	0/1672	0.37	0/2267
14	P	0.17	0/1616	0.44	0/2180
15	Q	0.13	0/1621	0.36	0/2194
16	R	0.13	0/1590	0.35	0/2147
17	S	0.12	0/1671	0.34	0/2252
18	T	0.16	0/1716	0.43	0/2323
19	X	0.17	0/3045	0.36	0/4105
20	Y	0.24	0/3173	0.52	0/4273
21	Z	0.28	0/2323	0.49	0/3147
22	a	0.17	0/3053	0.42	0/4133
23	b	0.18	0/1478	0.43	0/2001
24	d	0.17	0/2090	0.46	0/2820
25	f	0.18	0/6948	0.49	1/9387 (0.0%)
26	W	0.17	0/3611	0.45	1/4855 (0.0%)
27	V	0.17	0/3595	0.35	1/4851 (0.0%)
28	e	0.22	0/437	0.60	1/595 (0.2%)
29	A	0.21	0/3121	0.46	0/4212
30	F	0.19	0/2840	0.50	0/3828
31	E	0.17	0/2930	0.36	0/3944
32	U	0.24	0/6574	0.38	1/8899 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	g	0.60	3/1635 (0.2%)	0.57	6/2197 (0.3%)
34	u	0.15	0/1265	0.33	0/1711
All	All	0.21	3/84378 (0.0%)	0.42	13/113931 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
4	c	0	1
20	Y	0	3
22	a	0	1
All	All	0	5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	g	230	ASN	C-N	15.75	1.55	1.33
33	g	225	ALA	C-N	15.20	1.54	1.33
33	g	231	ARG	CA-C	8.85	1.64	1.52

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	g	225	ALA	O-C-N	10.99	136.04	122.63
33	g	232	VAL	N-CA-C	7.51	121.10	108.86
33	g	231	ARG	CA-C-O	6.72	130.12	120.51
33	g	232	VAL	N-CA-CB	-6.59	99.75	111.93
27	V	94	VAL	N-CA-C	-5.97	106.67	111.81

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
20	Y	110	TYR	Peptide
20	Y	113	ARG	Peptide
20	Y	349	LYS	Peptide
22	a	341	LEU	Peptide
4	c	49	VAL	Peptide

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	B	3124	0	3187	145	0
2	C	3053	0	3173	141	0
3	D	3040	0	3075	128	0
4	c	2220	0	2230	113	0
5	G	1867	0	1867	87	0
6	H	1801	0	1773	70	0
7	I	1933	0	1923	81	0
8	J	1860	0	1846	103	0
9	K	1817	0	1804	117	0
10	L	1876	0	1856	111	0
11	M	1890	0	1880	102	0
12	N	1462	0	1428	71	0
13	O	1645	0	1648	68	0
14	P	1587	0	1598	104	0
15	Q	1588	0	1584	90	0
16	R	1559	0	1523	84	0
17	S	1641	0	1639	83	0
18	T	1683	0	1662	94	0
19	X	3001	0	3106	115	0
20	Y	3115	0	3120	227	0
21	Z	2281	0	2311	129	0
22	a	2995	0	3012	158	0
23	b	1458	0	1505	93	0
24	d	2048	0	2082	113	0
25	f	6836	0	6841	476	0
26	W	3564	0	3684	180	0
27	V	3527	0	3595	127	0
28	e	425	0	328	34	0
29	A	3074	0	3152	169	0
30	F	2803	0	2896	201	0
31	E	2887	0	2951	169	0
32	U	6459	0	6484	200	0
33	g	1622	0	1565	71	0
34	u	1240	0	1189	41	0
35	B	31	0	12	3	0
35	C	31	0	12	4	0
36	B	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	C	1	0	0	0	0
36	D	1	0	0	0	0
37	A	27	0	12	3	0
37	D	27	0	12	4	0
37	E	27	0	12	4	0
37	F	27	0	12	7	0
38	c	1	0	0	0	0
All	All	83155	0	83589	3861	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 23.

The worst 5 of 3861 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)
8:J:152:THR:HB	9:K:83:LYS:HE2	1.23	1.16
3:D:359:ASP:HB3	3:D:362:ASP:HB3	1.36	1.06
32:U:265:ILE:HD11	32:U:326:ILE:HG23	1.38	1.05
9:K:82:ILE:HB	9:K:83:LYS:HE3	1.30	1.05
3:D:201:GLY:HA2	3:D:307:VAL:O	1.62	0.96

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	B	393/440 (89%)	352 (90%)	38 (10%)	3 (1%)	16	48
2	C	384/406 (95%)	356 (93%)	28 (7%)	0	100	100
3	D	378/418 (90%)	354 (94%)	22 (6%)	2 (0%)	25	58
4	c	278/424 (66%)	252 (91%)	24 (9%)	2 (1%)	19	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	G	238/246 (97%)	227 (95%)	11 (5%)	0	100	100
6	H	230/234 (98%)	215 (94%)	15 (6%)	0	100	100
7	I	246/261 (94%)	237 (96%)	9 (4%)	0	100	100
8	J	237/248 (96%)	221 (93%)	16 (7%)	0	100	100
9	K	236/241 (98%)	227 (96%)	8 (3%)	1 (0%)	30	63
10	L	238/263 (90%)	227 (95%)	11 (5%)	0	100	100
11	M	240/255 (94%)	232 (97%)	8 (3%)	0	100	100
12	N	193/239 (81%)	186 (96%)	7 (4%)	0	100	100
13	O	218/277 (79%)	211 (97%)	7 (3%)	0	100	100
14	P	202/205 (98%)	192 (95%)	10 (5%)	0	100	100
15	Q	197/201 (98%)	190 (96%)	7 (4%)	0	100	100
16	R	199/263 (76%)	196 (98%)	3 (2%)	0	100	100
17	S	211/241 (88%)	205 (97%)	6 (3%)	0	100	100
18	T	214/264 (81%)	203 (95%)	11 (5%)	0	100	100
19	X	377/422 (89%)	362 (96%)	13 (3%)	2 (0%)	25	58
20	Y	376/389 (97%)	325 (86%)	49 (13%)	2 (0%)	25	58
21	Z	283/324 (87%)	240 (85%)	42 (15%)	1 (0%)	30	63
22	a	371/376 (99%)	339 (91%)	31 (8%)	1 (0%)	37	68
23	b	189/377 (50%)	168 (89%)	21 (11%)	0	100	100
24	d	244/350 (70%)	223 (91%)	20 (8%)	1 (0%)	30	63
25	f	880/908 (97%)	753 (86%)	126 (14%)	1 (0%)	48	79
26	W	433/456 (95%)	404 (93%)	29 (7%)	0	100	100
27	V	426/534 (80%)	404 (95%)	22 (5%)	0	100	100
28	e	48/70 (69%)	36 (75%)	12 (25%)	0	100	100
29	A	387/433 (89%)	346 (89%)	37 (10%)	4 (1%)	13	42
30	F	353/439 (80%)	310 (88%)	39 (11%)	4 (1%)	12	39
31	E	360/389 (92%)	336 (93%)	24 (7%)	0	100	100
32	U	823/953 (86%)	797 (97%)	26 (3%)	0	100	100
33	g	189/390 (48%)	167 (88%)	22 (12%)	0	100	100
34	u	153/300 (51%)	146 (95%)	7 (5%)	0	100	100
All	All	10424/12236 (85%)	9639 (92%)	761 (7%)	24 (0%)	45	74

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
19	X	318	ILE
19	X	339	ILE
24	d	358	ILE
29	A	222	LYS
30	F	86	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	B	351/385 (91%)	330 (94%)	21 (6%)	16	44
2	C	338/352 (96%)	320 (95%)	18 (5%)	19	48
3	D	333/366 (91%)	320 (96%)	13 (4%)	27	58
4	c	248/359 (69%)	235 (95%)	13 (5%)	19	48
5	G	202/210 (96%)	193 (96%)	9 (4%)	23	53
6	H	187/191 (98%)	178 (95%)	9 (5%)	21	51
7	I	202/221 (91%)	196 (97%)	6 (3%)	36	64
8	J	197/211 (93%)	188 (95%)	9 (5%)	23	52
9	K	198/204 (97%)	180 (91%)	18 (9%)	7	28
10	L	202/224 (90%)	191 (95%)	11 (5%)	18	47
11	M	198/212 (93%)	188 (95%)	10 (5%)	20	49
12	N	152/181 (84%)	145 (95%)	7 (5%)	23	52
13	O	178/228 (78%)	169 (95%)	9 (5%)	20	49
14	P	172/174 (99%)	160 (93%)	12 (7%)	12	39
15	Q	168/171 (98%)	156 (93%)	12 (7%)	12	39
16	R	156/202 (77%)	146 (94%)	10 (6%)	14	42
17	S	175/199 (88%)	164 (94%)	11 (6%)	15	42
18	T	178/215 (83%)	167 (94%)	11 (6%)	15	43
19	X	326/362 (90%)	308 (94%)	18 (6%)	18	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	Y	334/344 (97%)	303 (91%)	31 (9%)	7	27
21	Z	257/295 (87%)	235 (91%)	22 (9%)	8	31
22	a	333/336 (99%)	313 (94%)	20 (6%)	16	44
23	b	167/312 (54%)	153 (92%)	14 (8%)	9	32
24	d	221/294 (75%)	217 (98%)	4 (2%)	54	76
25	f	742/763 (97%)	701 (94%)	41 (6%)	18	47
26	W	402/416 (97%)	385 (96%)	17 (4%)	25	56
27	V	383/460 (83%)	371 (97%)	12 (3%)	35	63
28	e	44/63 (70%)	37 (84%)	7 (16%)	2	9
29	A	339/372 (91%)	319 (94%)	20 (6%)	16	44
30	F	306/379 (81%)	283 (92%)	23 (8%)	11	36
31	E	318/341 (93%)	304 (96%)	14 (4%)	24	54
32	U	705/816 (86%)	682 (97%)	23 (3%)	33	62
33	g	171/338 (51%)	157 (92%)	14 (8%)	9	33
34	u	141/263 (54%)	131 (93%)	10 (7%)	12	39
All	All	9024/10459 (86%)	8525 (94%)	499 (6%)	20	47

5 of 499 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
20	Y	81	LEU
31	E	104	THR
22	a	125	ILE
31	E	20	LYS
32	U	892	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 83 such sidechains are listed below:

Mol	Chain	Res	Type
26	W	156	ASN
31	E	225	HIS
26	W	235	GLN
29	A	247	GLN
32	U	347	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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	$\#\|Z\| > 2$
33	CR8	g	228	33	20,27,28	6.63	10 (50%)	15,37,39	4.18	7 (46%)

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
33	CR8	g	228	33	-	4/8/25/26	0/3/3/3

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	g	228	CR8	C4-C11	-17.95	1.01	1.46
33	g	228	CR8	C12-C11	-17.69	1.02	1.46
33	g	228	CR8	C5-C7	9.96	1.69	1.41
33	g	228	CR8	C6-C7	8.88	1.66	1.41
33	g	228	CR8	CA2-C2	-4.28	1.34	1.41

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	g	228	CR8	C6-C7-C5	-9.93	94.19	115.81
33	g	228	CR8	C4-C11-C12	7.44	130.50	116.67
33	g	228	CR8	C6-C12-C11	5.81	129.13	121.25
33	g	228	CR8	O13-C11-C12	-4.30	114.63	121.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	g	228	CR8	C5-C4-C11	4.25	127.02	121.25

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
33	g	228	CR8	C7-C8-CA2-C2
33	g	228	CR8	C7-C8-CA2-N2
33	g	228	CR8	CA1-C20-C21-N22
33	g	228	CR8	CA1-C20-C21-C23

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	g	228	CR8	5	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
37	ADP	F	501	-	24,29,29	0.87	1 (4%)	29,45,45	1.21	3 (10%)
35	ATP	C	501	36	28,33,33	0.82	0	34,52,52	0.62	1 (2%)
37	ADP	A	501	-	24,29,29	0.89	0	29,45,45	1.18	2 (6%)
35	ATP	B	501	36	28,33,33	0.90	2 (7%)	34,52,52	0.63	1 (2%)
37	ADP	E	501	-	24,29,29	0.87	0	29,45,45	1.23	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
37	ADP	D	501	36	24,29,29	0.84	0	29,45,45	1.32	3 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	ADP	F	501	-	-	3/12/32/32	0/3/3/3
35	ATP	C	501	36	-	5/18/38/38	0/3/3/3
37	ADP	A	501	-	-	0/12/32/32	0/3/3/3
35	ATP	B	501	36	-	4/18/38/38	0/3/3/3
37	ADP	E	501	-	-	4/12/32/32	0/3/3/3
37	ADP	D	501	36	-	3/12/32/32	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	B	501	ATP	PB-O3B	-2.43	1.56	1.59
35	B	501	ATP	PA-O3A	-2.00	1.57	1.59
37	F	501	ADP	O4'-C1'	2.00	1.43	1.40

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	A	501	ADP	N3-C2-N1	-3.64	123.73	128.67
37	D	501	ADP	N3-C2-N1	-3.59	123.79	128.67
37	F	501	ADP	N3-C2-N1	-3.58	123.81	128.67
37	E	501	ADP	N3-C2-N1	-3.37	124.10	128.67
37	E	501	ADP	C4-C5-N7	-2.90	106.27	109.34

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

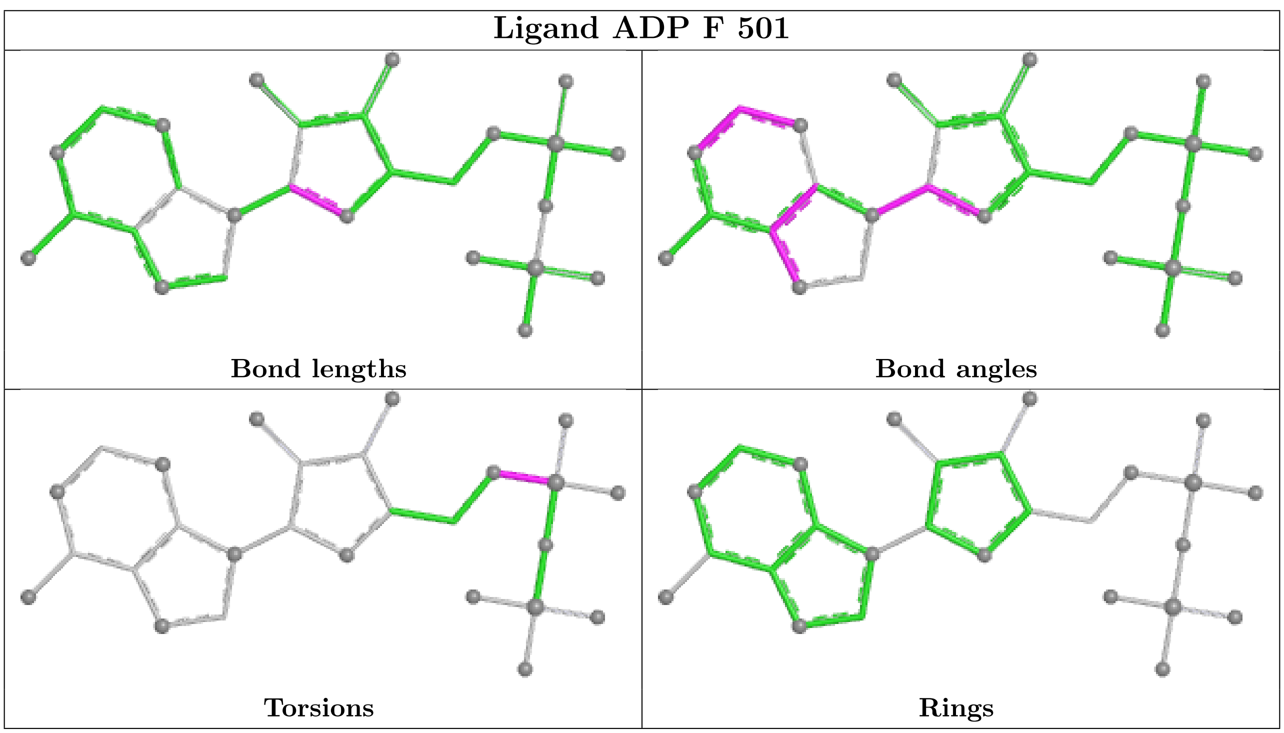
Mol	Chain	Res	Type	Atoms
35	B	501	ATP	C5'-O5'-PA-O1A
35	B	501	ATP	C5'-O5'-PA-O3A
35	C	501	ATP	PB-O3B-PG-O2G
37	D	501	ADP	C5'-O5'-PA-O1A
37	D	501	ADP	C5'-O5'-PA-O2A

There are no ring outliers.

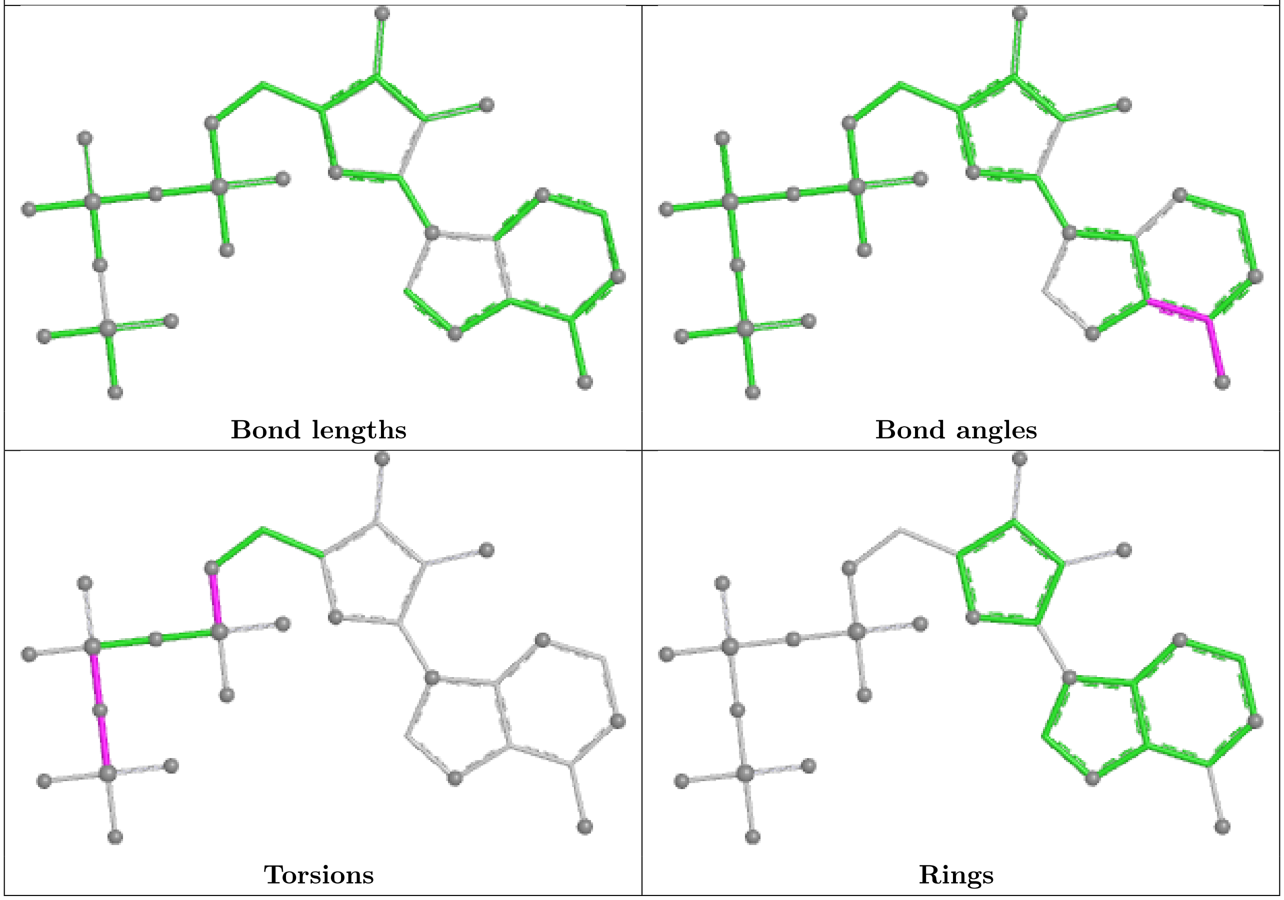
6 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	F	501	ADP	7	0
35	C	501	ATP	4	0
37	A	501	ADP	3	0
35	B	501	ATP	3	0
37	E	501	ADP	4	0
37	D	501	ADP	4	0

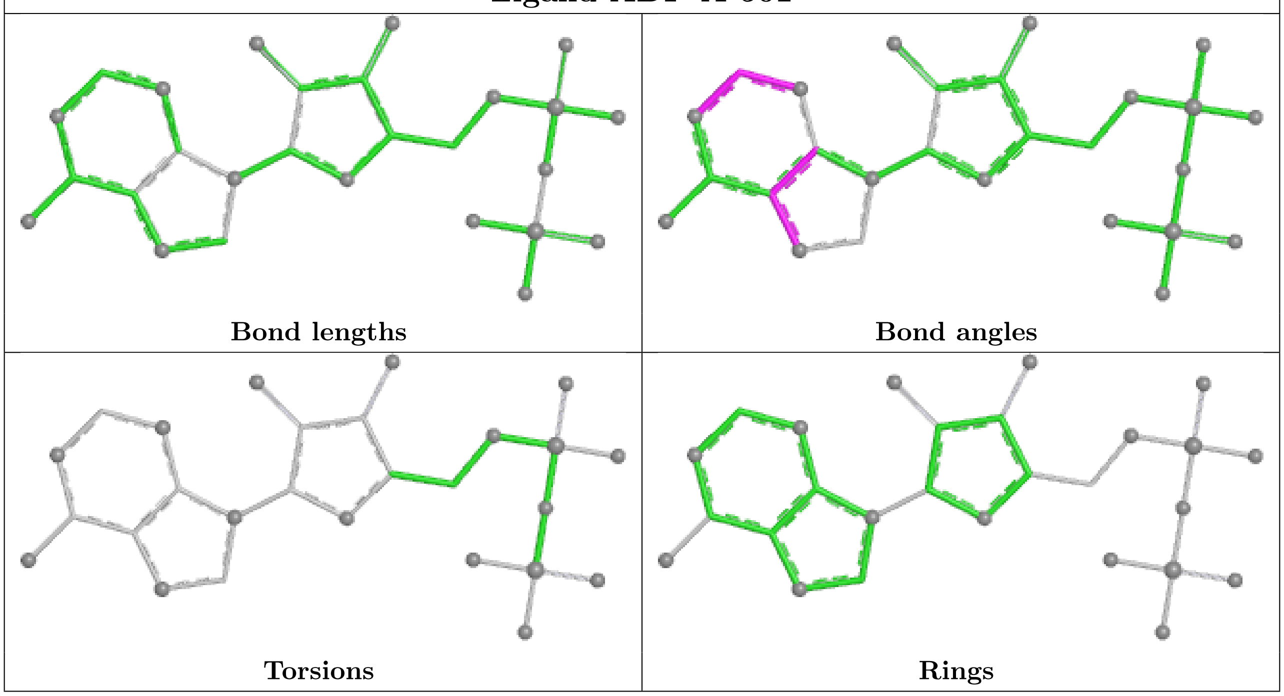
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



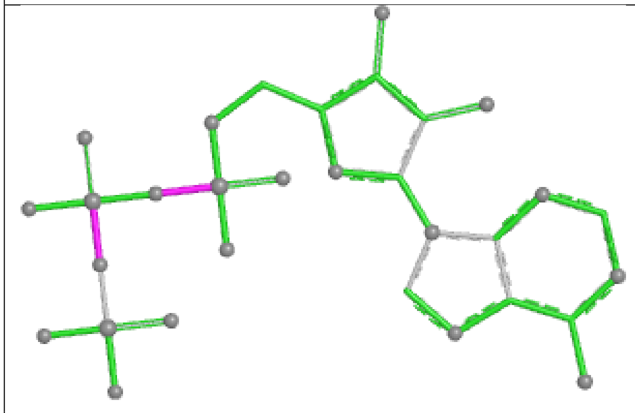
Ligand ATP C 501



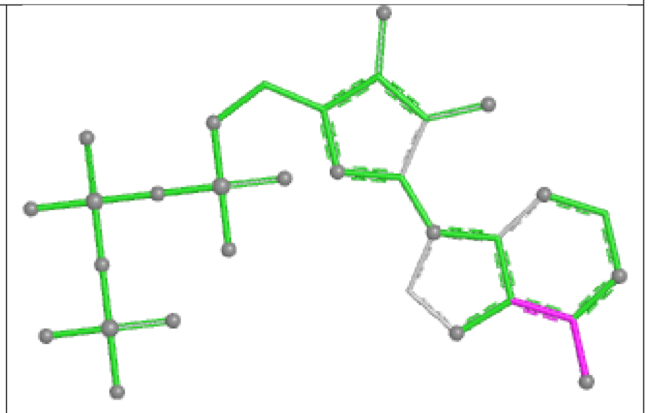
Ligand ADP A 501



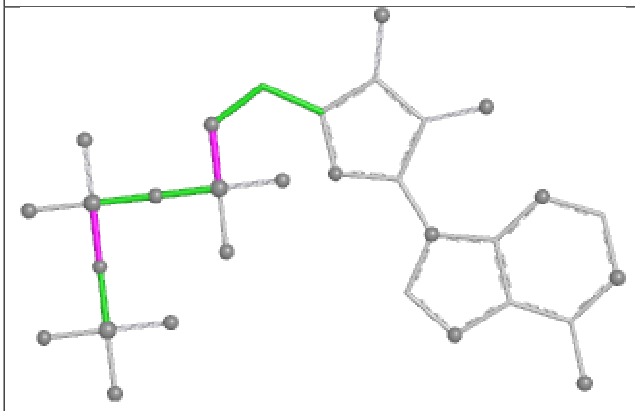
Ligand ATP B 501



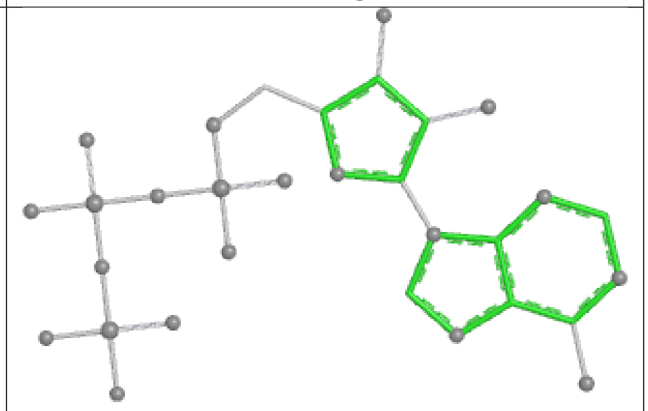
Bond lengths



Bond angles

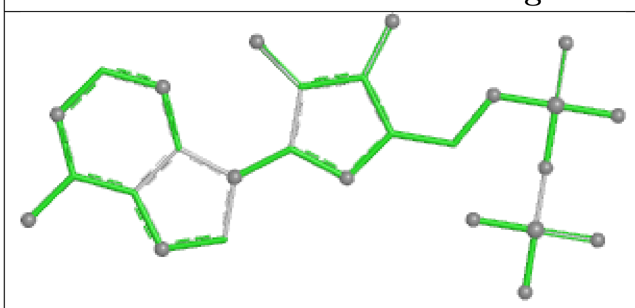


Torsions

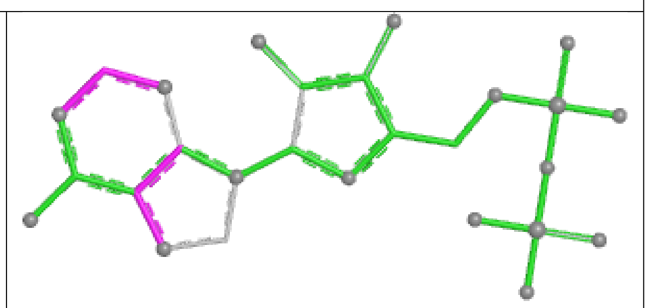


Rings

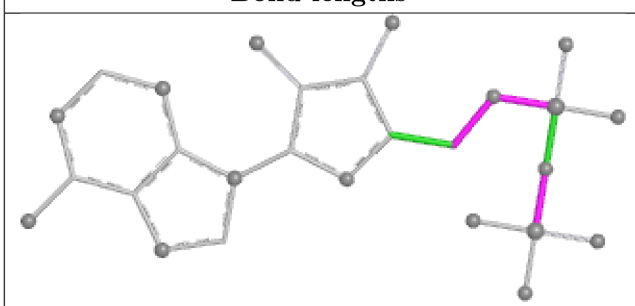
Ligand ADP E 501



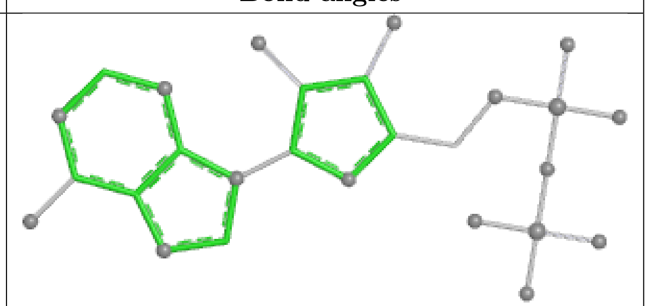
Bond lengths



Bond angles

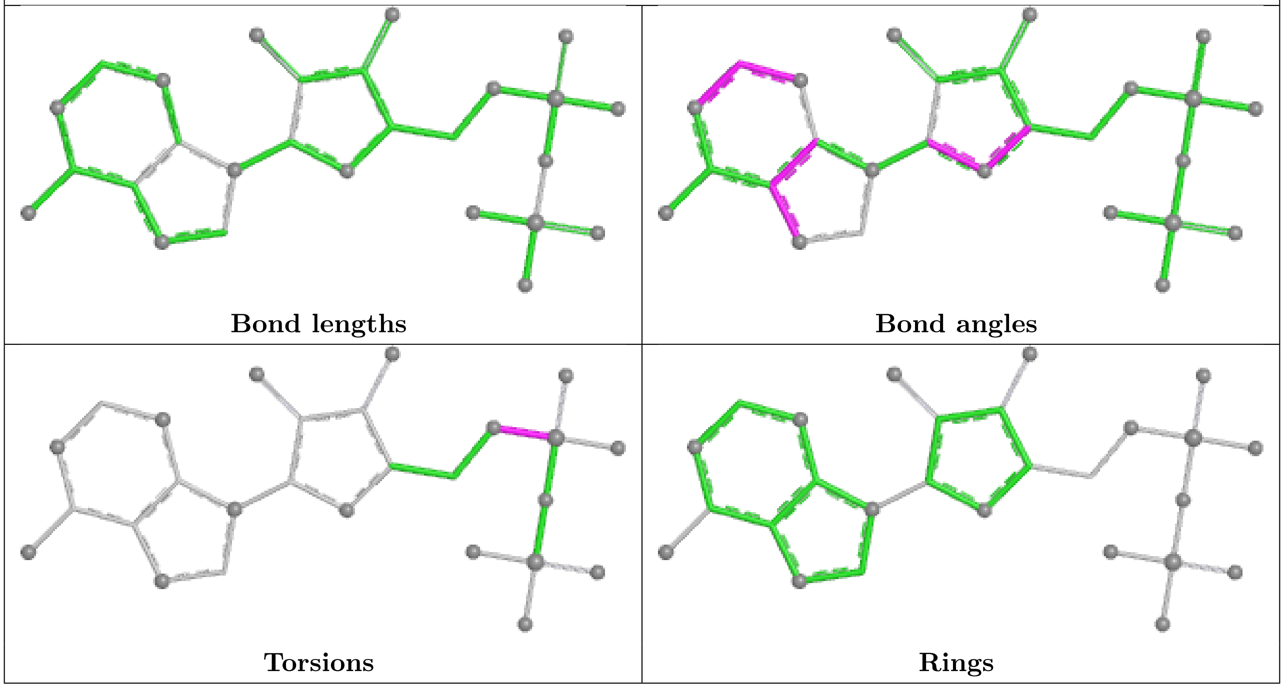


Torsions



Rings

Ligand ADP D 501



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
26	W	1
31	E	1
21	Z	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	W	416:GLN	C	417:ARG	N	6.76
1	E	273:VAL	C	274:LYS	N	5.62
1	Z	289:GLU	C	290:GLY	N	3.16

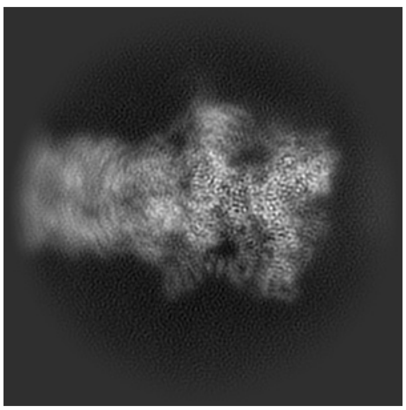
6 Map visualisation (i)

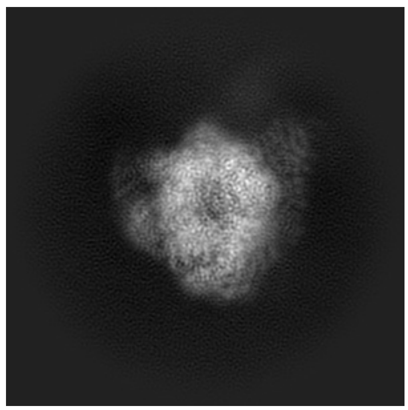
This section contains visualisations of the EMDB entry EMD-47726. These allow visual inspection of the internal detail of the map and identification of artifacts.

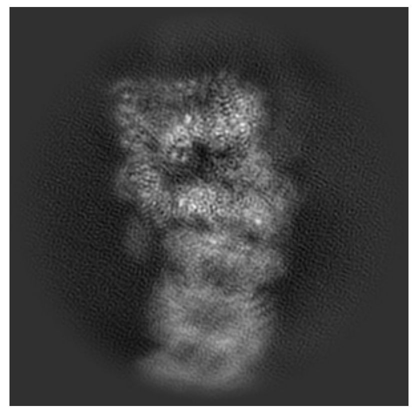
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

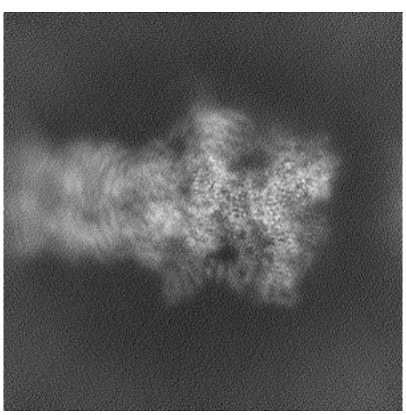
6.1.1 Primary map

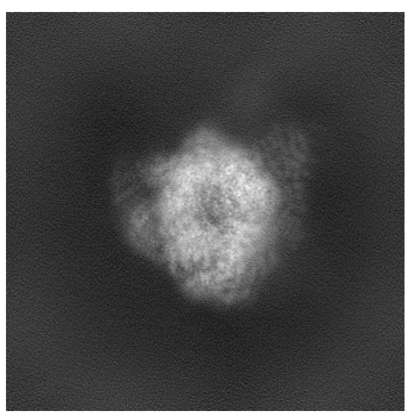

X

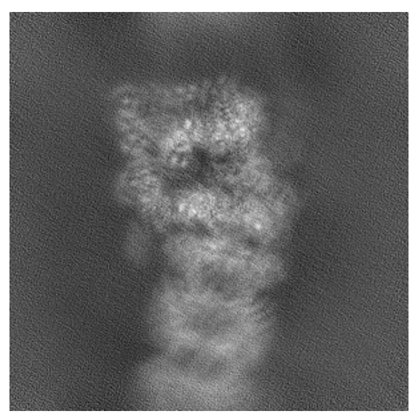

Y


Z

6.1.2 Raw map


X

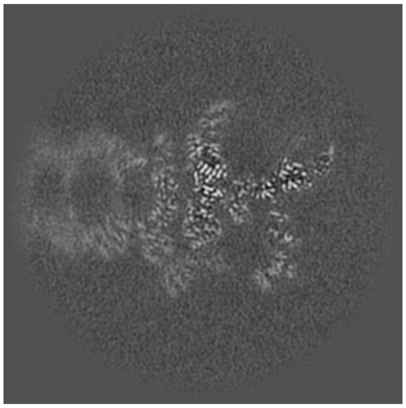

Y

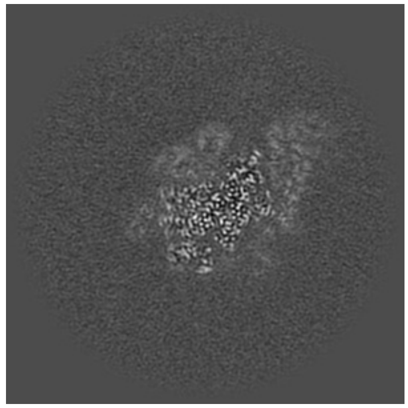

Z

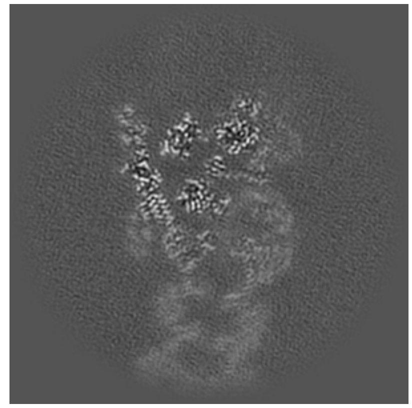
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

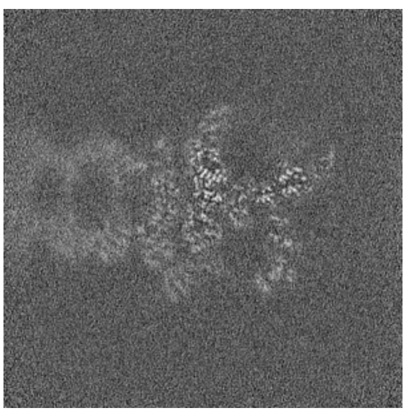
6.2.1 Primary map

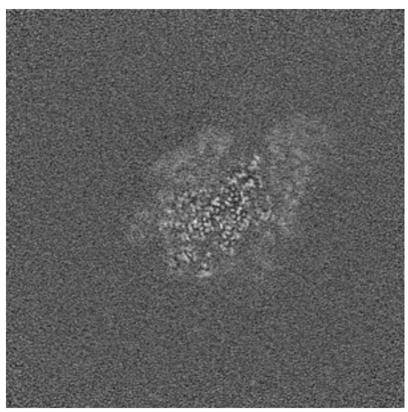

X Index: 170

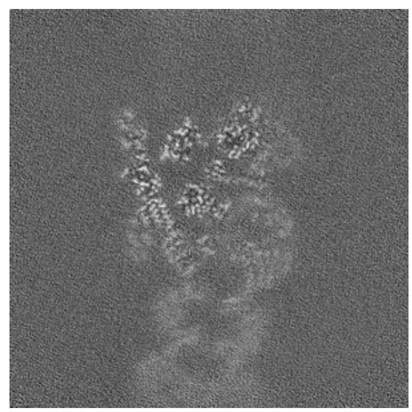

Y Index: 170


Z Index: 170

6.2.2 Raw map


X Index: 170

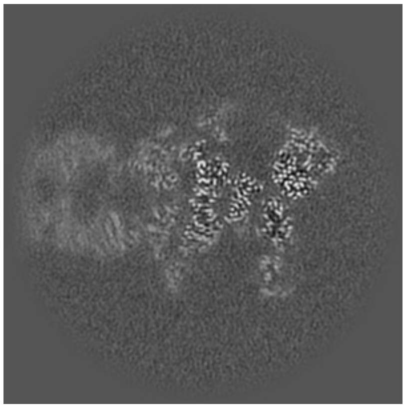

Y Index: 170

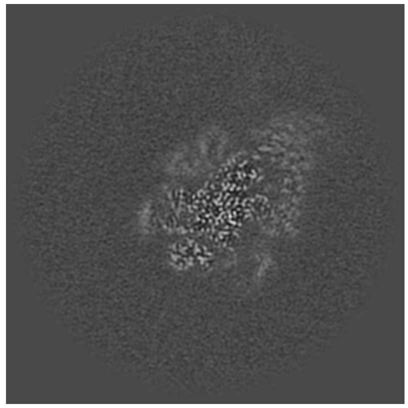

Z Index: 170

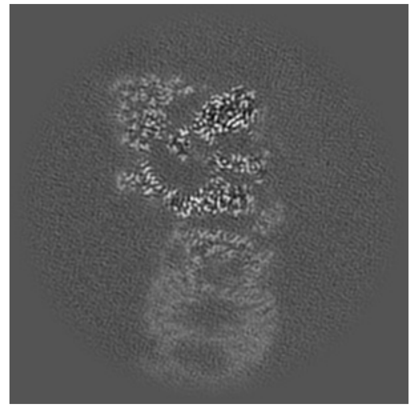
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

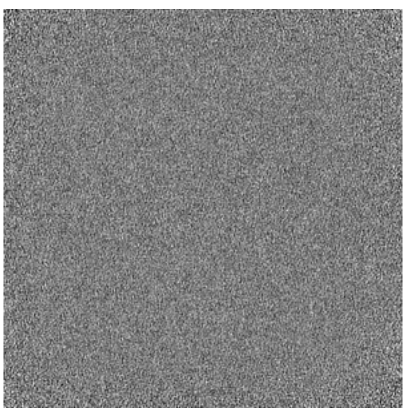
6.3.1 Primary map

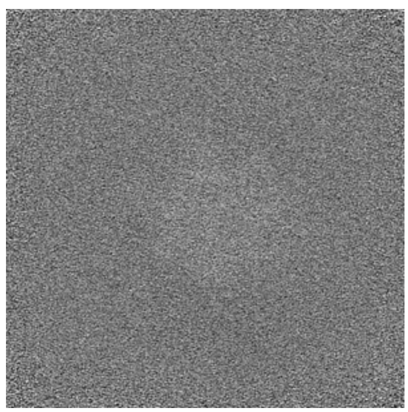

X Index: 178

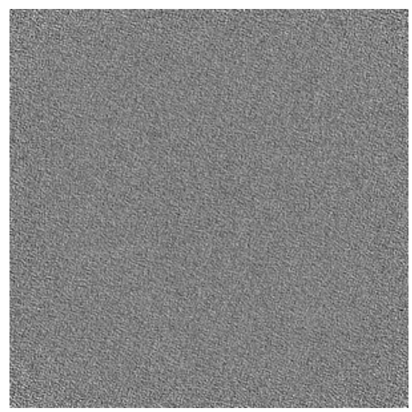

Y Index: 173


Z Index: 190

6.3.2 Raw map


X Index: 0

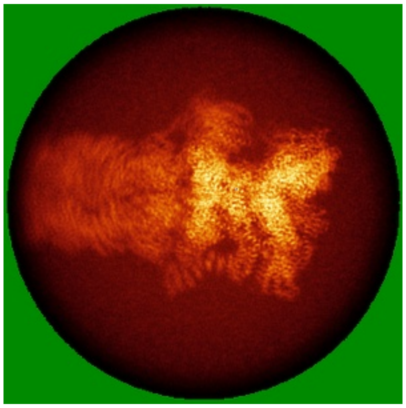

Y Index: 0

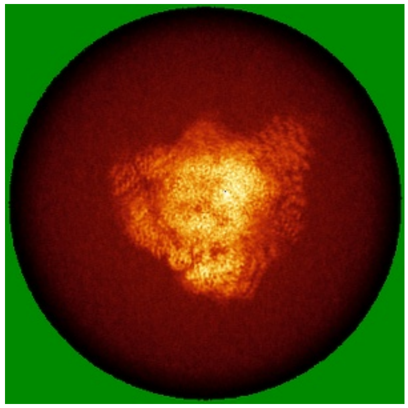

Z Index: 0

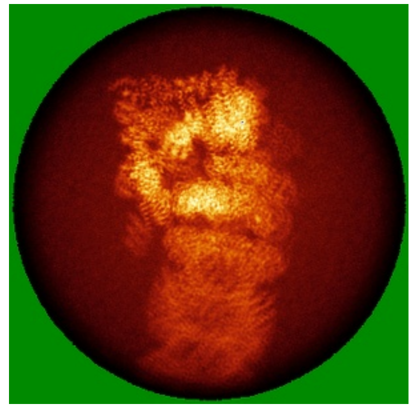
The images above show the largest variance slices of the map in three orthogonal directions.

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

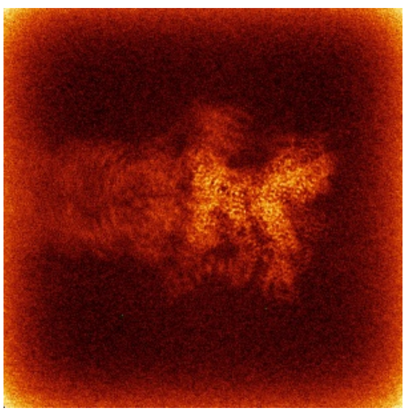
6.4.1 Primary map

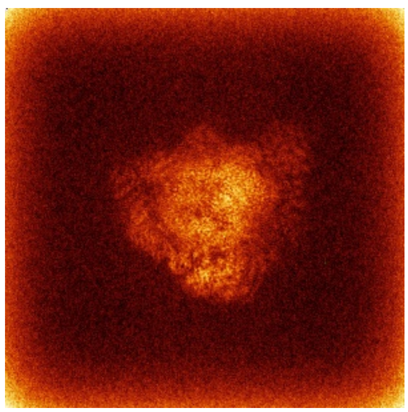

X

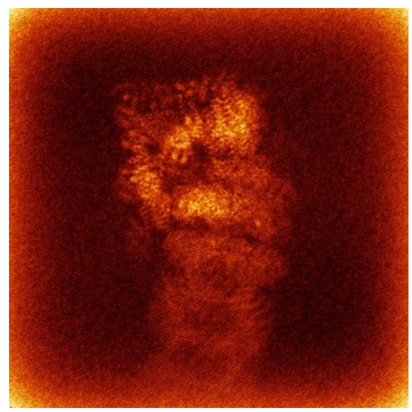

Y


Z

6.4.2 Raw map


X

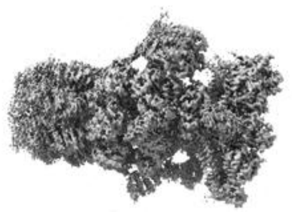

Y


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



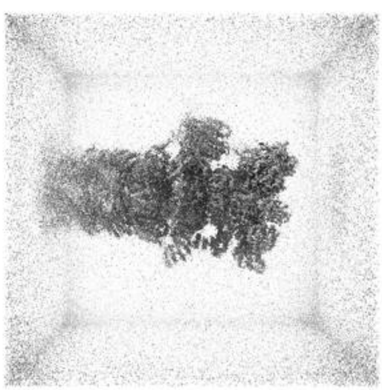
X

Y

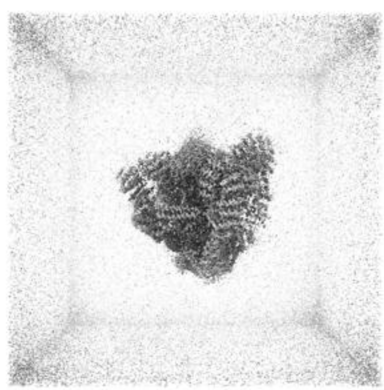
Z

The images above show the 3D surface view of the map at the recommended contour level 0.17. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

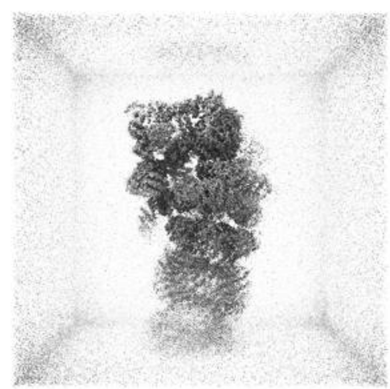
6.5.2 Raw map



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.

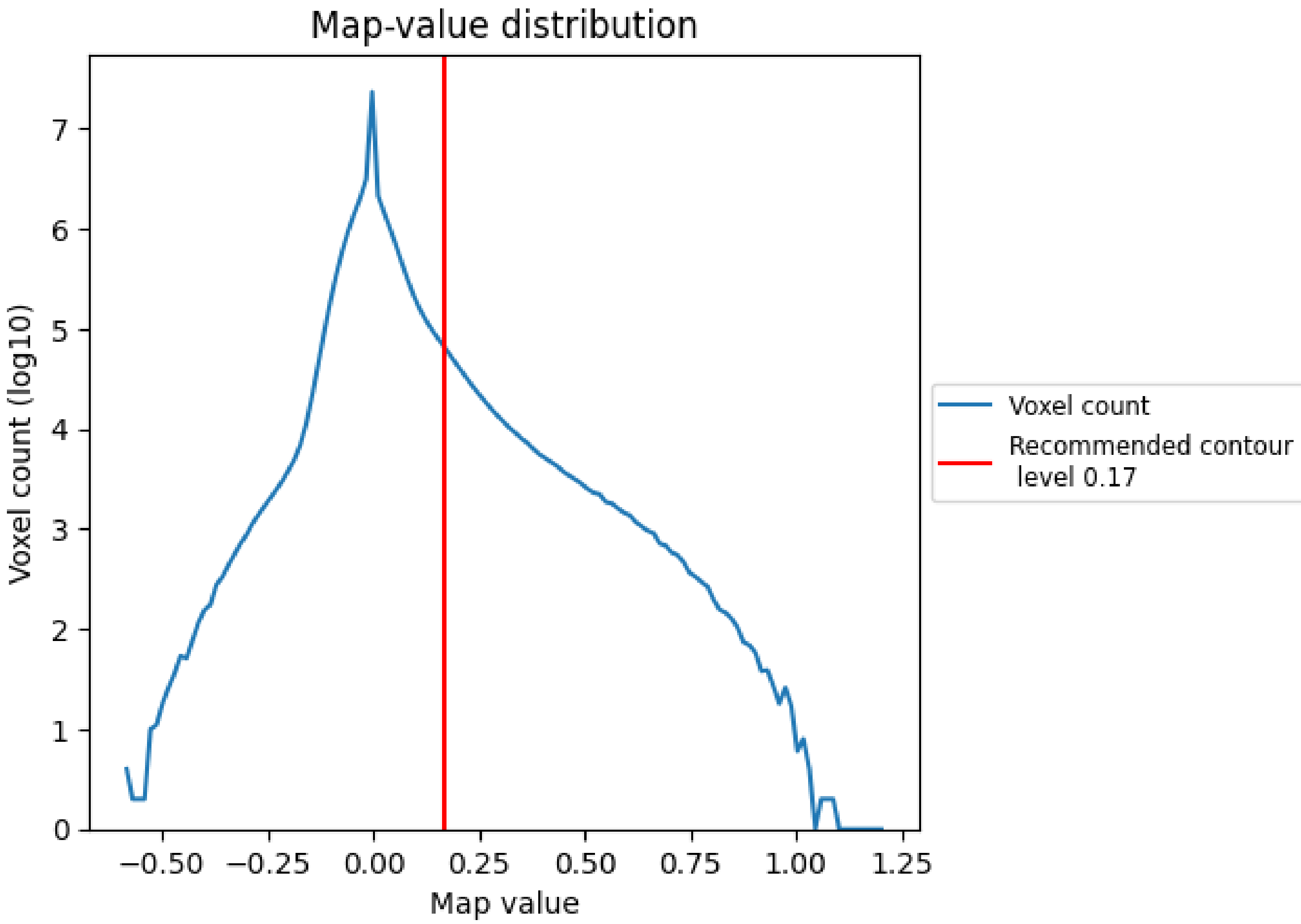
6.6 Mask visualisation (i)

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

7 Map analysis (i)

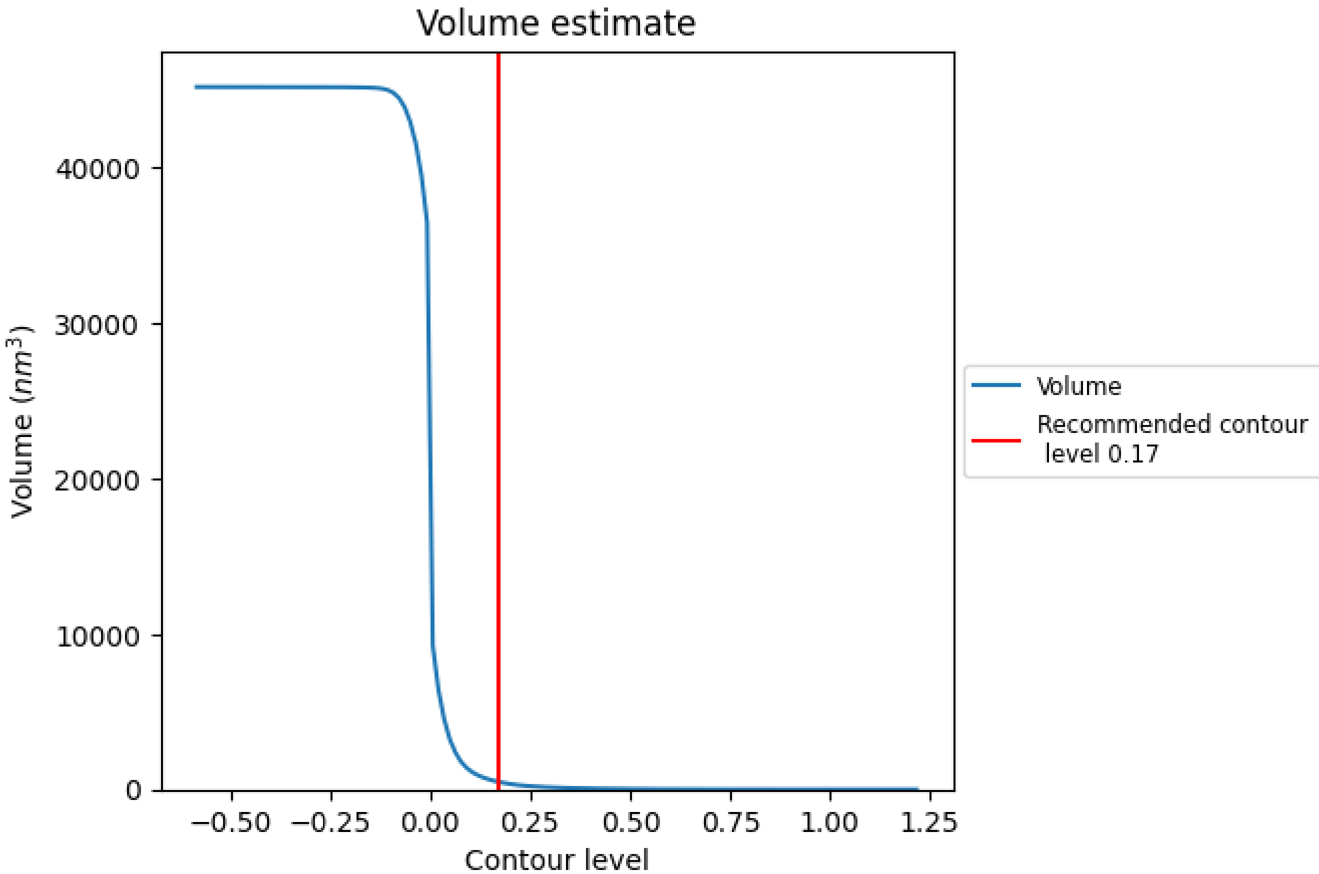
This section contains the results of statistical analysis of the map.

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.

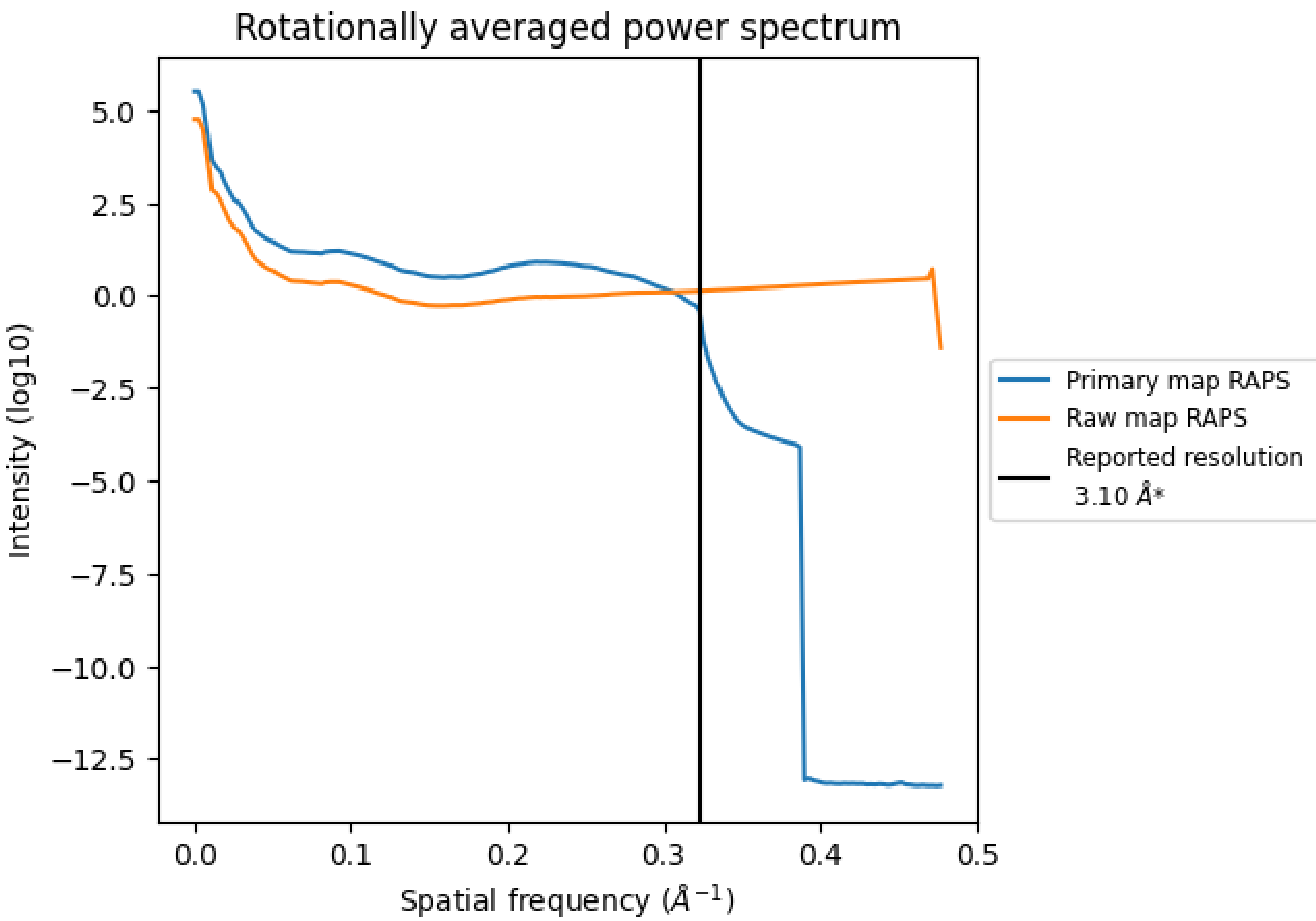
7.2 Volume estimate (i)



The volume at the recommended contour level is 493 nm^3; this corresponds to an approximate mass of 445 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)

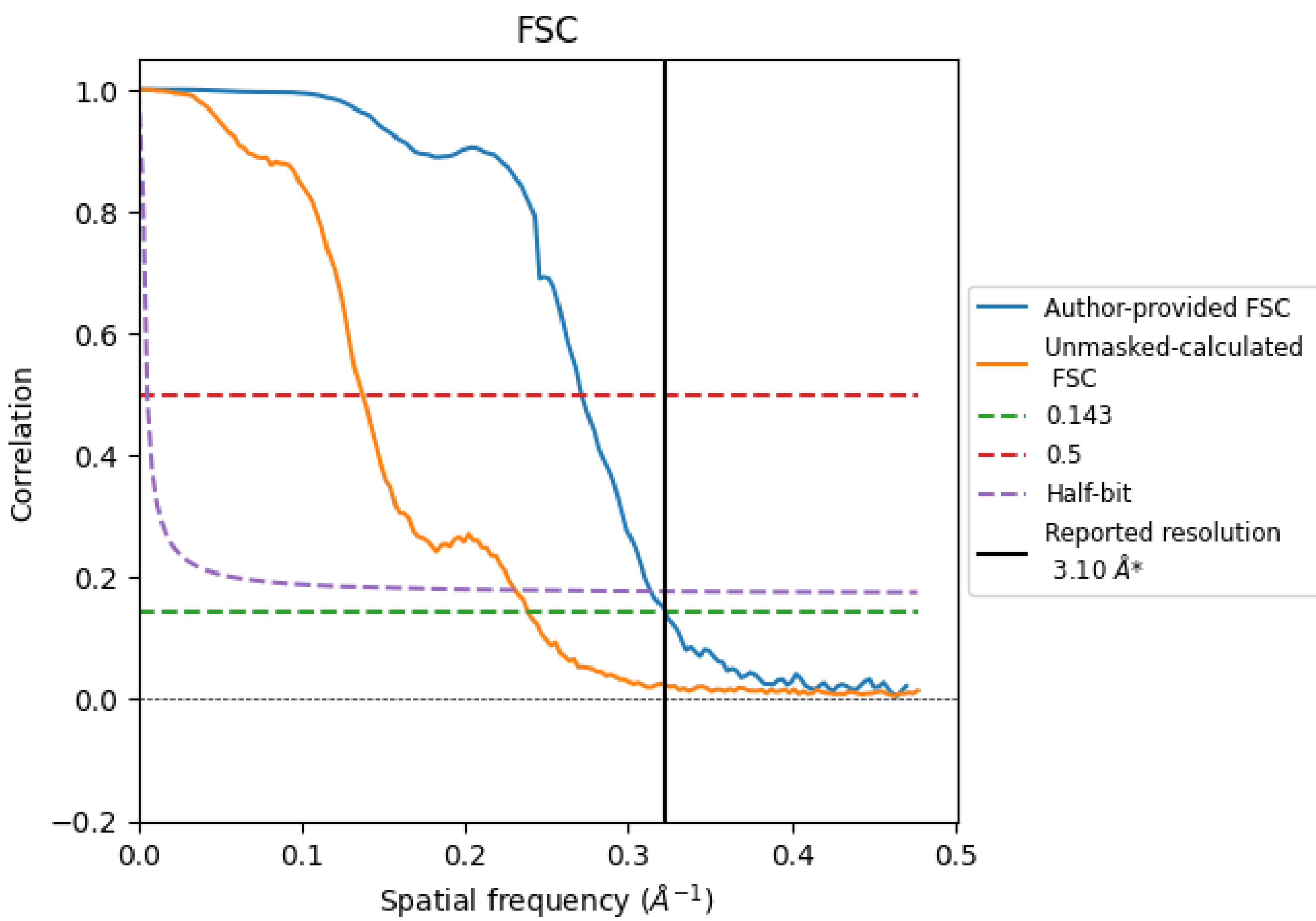


*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

8.2 Resolution estimates (i)

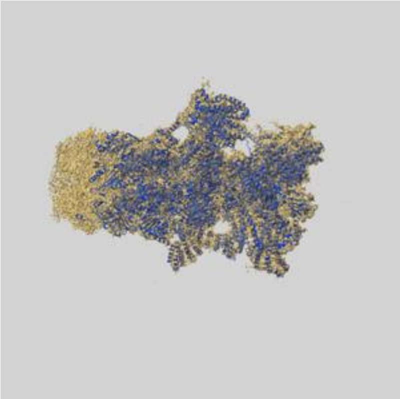
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.10	3.68	3.19
Unmasked-calculated*	4.19	7.28	4.33

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.19 differs from the reported value 3.1 by more than 10 %

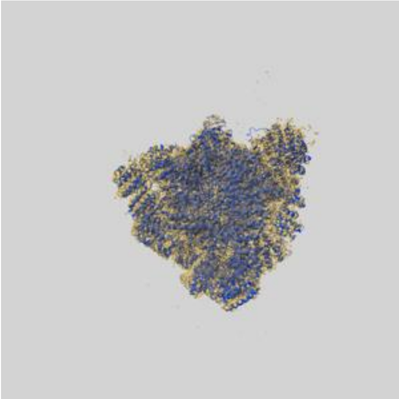
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-47726 and PDB model 9E8O. Per-residue inclusion information can be found in section 3 on page 16.

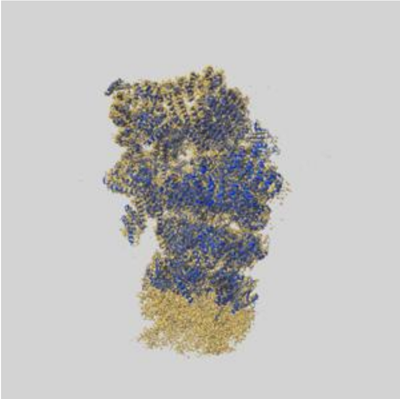
9.1 Map-model overlay (i)



X



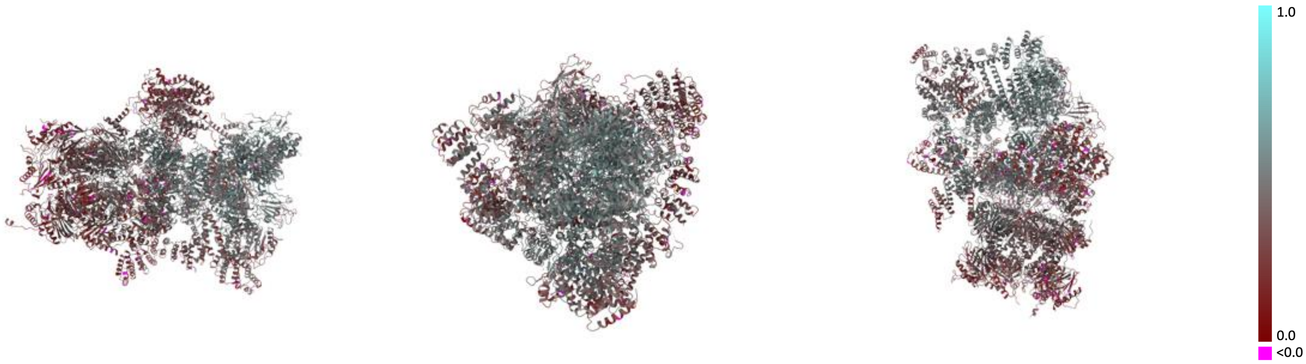
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.17 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.

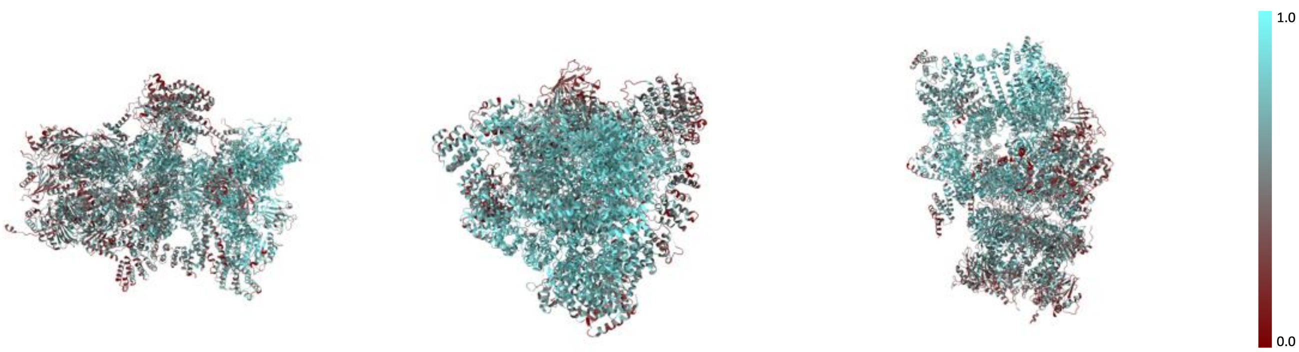
9.2 Q-score mapped to coordinate model (i)



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.

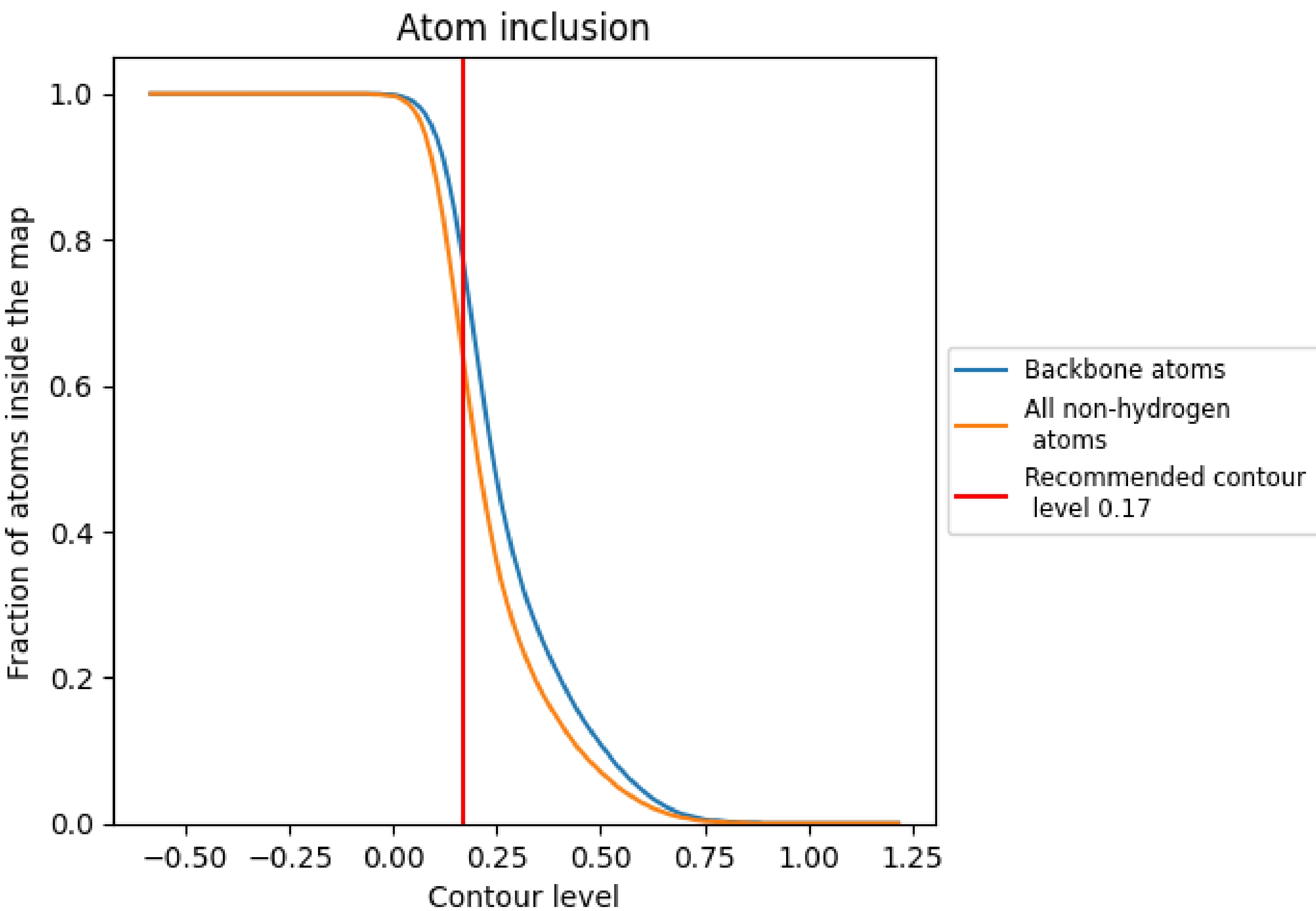
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.17).

9.4 Atom inclusion (i)



At the recommended contour level, 77% of all backbone atoms, 63% 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 (0.17) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6320	0.4010
A	0.5720	0.3890
B	0.7330	0.4860
C	0.8390	0.5360
D	0.8330	0.5250
E	0.6740	0.4320
F	0.4790	0.3320
G	0.6080	0.3840
H	0.7390	0.4610
I	0.6790	0.4310
J	0.6060	0.3930
K	0.5900	0.3820
L	0.5240	0.3390
M	0.5230	0.3310
N	0.5230	0.3090
O	0.5080	0.3290
P	0.4940	0.3140
Q	0.4660	0.2950
R	0.4560	0.2810
S	0.4210	0.2660
T	0.4690	0.2570
U	0.8200	0.5120
V	0.7070	0.4460
W	0.5220	0.3200
X	0.7150	0.4190
Y	0.7570	0.4110
Z	0.7930	0.4840
a	0.6840	0.3990
b	0.6800	0.4160
c	0.8400	0.5390
d	0.6170	0.3790
e	0.5800	0.3160
f	0.4330	0.2940
g	0.3200	0.4020
u	0.6860	0.4820