



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 01:23 AM UTC

PDB ID : 6MSH / pdb_00006msh
EMDB ID : EMD-9220
Title : Cryo-EM structures and dynamics of substrate-engaged human 26S proteasome
Authors : Mao, Y.D.
Deposited on : 2018-10-16
Resolution : 3.60 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 ⓘ symbol.

The types of validation reports are described at

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

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

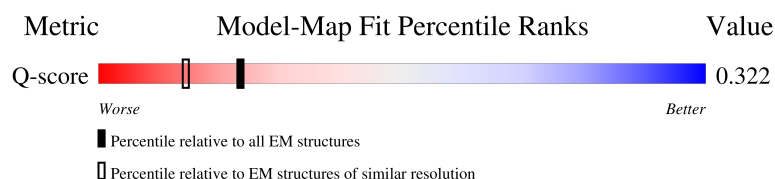
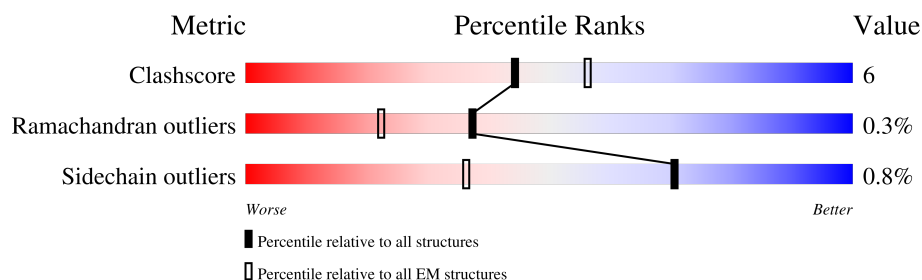
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.60 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12797 (3.10 - 4.10)

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

Mol	Chain	Length	Quality of chain
1	U	953	64% 72% 14% 14%
2	V	533	75% 76% 14% 10%
3	W	456	71% 76% 22% .
4	X	422	17% 81% 9% 10%

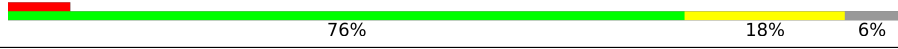
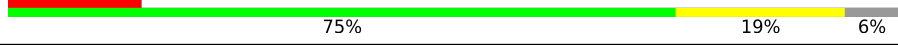
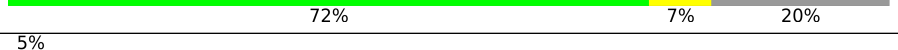
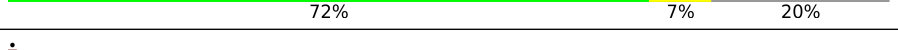
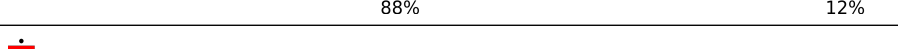
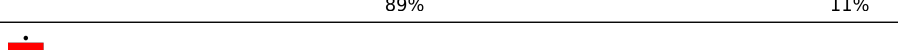
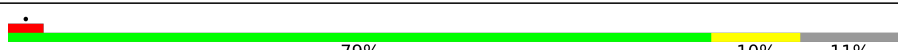
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Mol	Chain	Length	Quality of chain
5	Y	389	
6	Z	324	
7	a	376	
8	b	377	
9	c	309	
10	d	349	
11	e	70	
12	f	892	
13	A	433	
14	B	440	
15	C	398	
16	D	418	
17	E	403	
18	F	439	
19	v	22	
20	G	245	
20	g	245	
21	H	233	
21	h	233	
22	I	260	
22	i	260	
23	J	247	
23	j	247	
24	K	240	
24	k	240	

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Mol	Chain	Length	Quality of chain
25	L	268	
25	l	268	
26	M	254	
26	m	254	
27	N	238	
27	n	238	
28	O	276	
28	o	276	
29	P	204	
29	p	204	
30	Q	201	
30	q	201	
31	R	262	
31	r	262	
32	S	240	
32	s	240	
33	T	263	
33	t	263	

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 103729 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	U	820	Total	C	N	O	S	0	0
			6398	4062	1086	1206	44		

- Molecule 2 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	V	480	Total	C	N	O	S	0	0
			3852	2444	684	710	14		

- Molecule 3 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

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

- Molecule 4 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	X	380	Total	C	N	O	S	0	0
			3009	1918	509	570	12		

- Molecule 5 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

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

- Molecule 6 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

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

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

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

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

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

- Molecule 9 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

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

- Molecule 10 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

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

- Molecule 11 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	e	40	Total	C	N	O	S	0	0
			334	200	55	77	2		

- Molecule 12 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	f	886	Total	C	N	O	S	0	0
			6840	4300	1171	1324	45		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	A	356	Total	C	N	O	S	0	0
			2767	1741	488	521	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	B	350	Total	C	N	O	S	0	0
			2706	1703	458	533	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	C	396	Total	C	N	O	S	0	0
			3105	1954	558	576	17		

- 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 proteasome regulatory subunit 10B.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	E	389	Total	C	N	O	S	0	0
			3097	1947	552	581	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	F	395	Total	C	N	O	S	0	0
			3098	1951	533	596	18		

- Molecule 19 is a protein called substrate.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	v	22	Total	C	N	O	0	0
			110	66	22	22		

- Molecule 20 is a protein called Proteasome subunit alpha type-6.

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

- Molecule 21 is a protein called Proteasome subunit alpha type-2.

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

- Molecule 22 is a protein called Proteasome subunit alpha type-4.

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

- Molecule 23 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	J	239	Total	C	N	O	S	0	0
			1704	1056	308	335	5		
23	j	239	Total	C	N	O	S	0	0
			1704	1056	308	335	5		

- Molecule 24 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	K	228	Total	C	N	O	S	0	0
			1722	1080	284	348	10		
24	k	228	Total	C	N	O	S	0	0
			1722	1080	284	348	10		

- Molecule 25 is a protein called Proteasome subunit alpha type-1.

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

- Molecule 26 is a protein called Proteasome subunit alpha type-3.

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

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

- Molecule 27 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	N	191	Total	C	N	O	S	0	0
			1430	893	245	280	12		
27	n	191	Total	C	N	O	S	0	0
			1430	893	245	280	12		

- Molecule 28 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	O	220	Total	C	N	O	S	0	0
			1643	1033	280	318	12		
28	o	220	Total	C	N	O	S	0	0
			1643	1033	280	318	12		

- Molecule 29 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	P	204	Total	C	N	O	S	0	0
			1585	1010	262	294	19		
29	p	204	Total	C	N	O	S	0	0
			1585	1010	262	294	19		

- Molecule 30 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Q	199	Total	C	N	O	S	0	0
			1570	1006	265	290	9		
30	q	199	Total	C	N	O	S	0	0
			1570	1006	265	290	9		

- Molecule 31 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	R	201	Total	C	N	O	S	0	0
			1548	974	273	292	9		
31	r	201	Total	C	N	O	S	0	0
			1548	974	273	292	9		

- Molecule 32 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	S	213	Total	C	N	O	S	0	0
			1641	1036	282	313	10		
32	s	213	Total	C	N	O	S	0	0
			1641	1036	282	313	10		

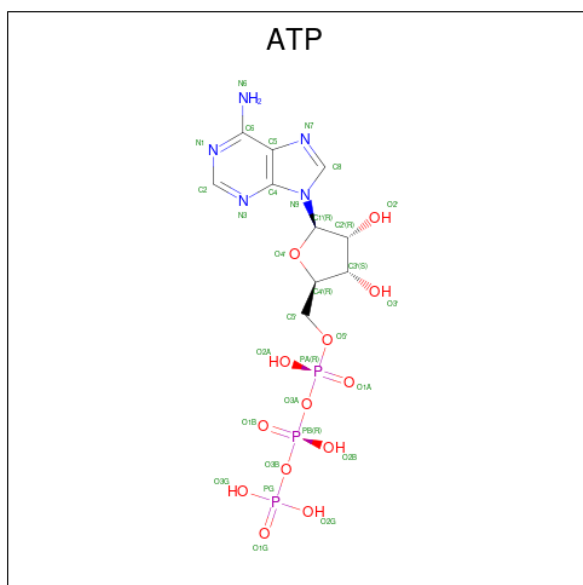
- Molecule 33 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	T	215	Total	C	N	O	S	0	0
			1667	1052	285	318	12		
33	t	215	Total	C	N	O	S	0	0
			1667	1052	285	318	12		

- Molecule 34 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

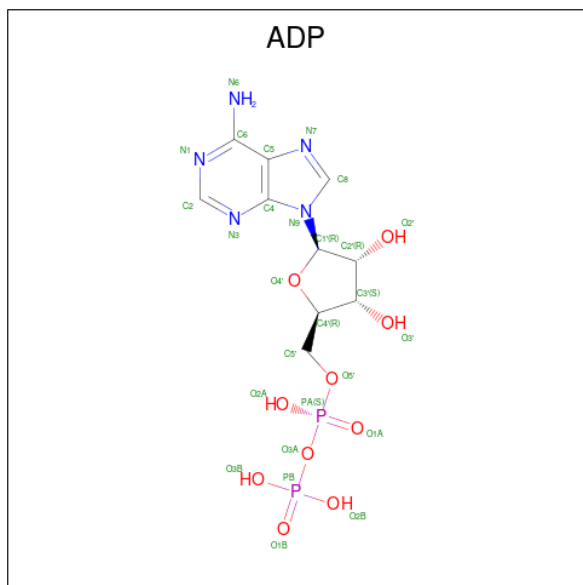
- Molecule 35 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

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

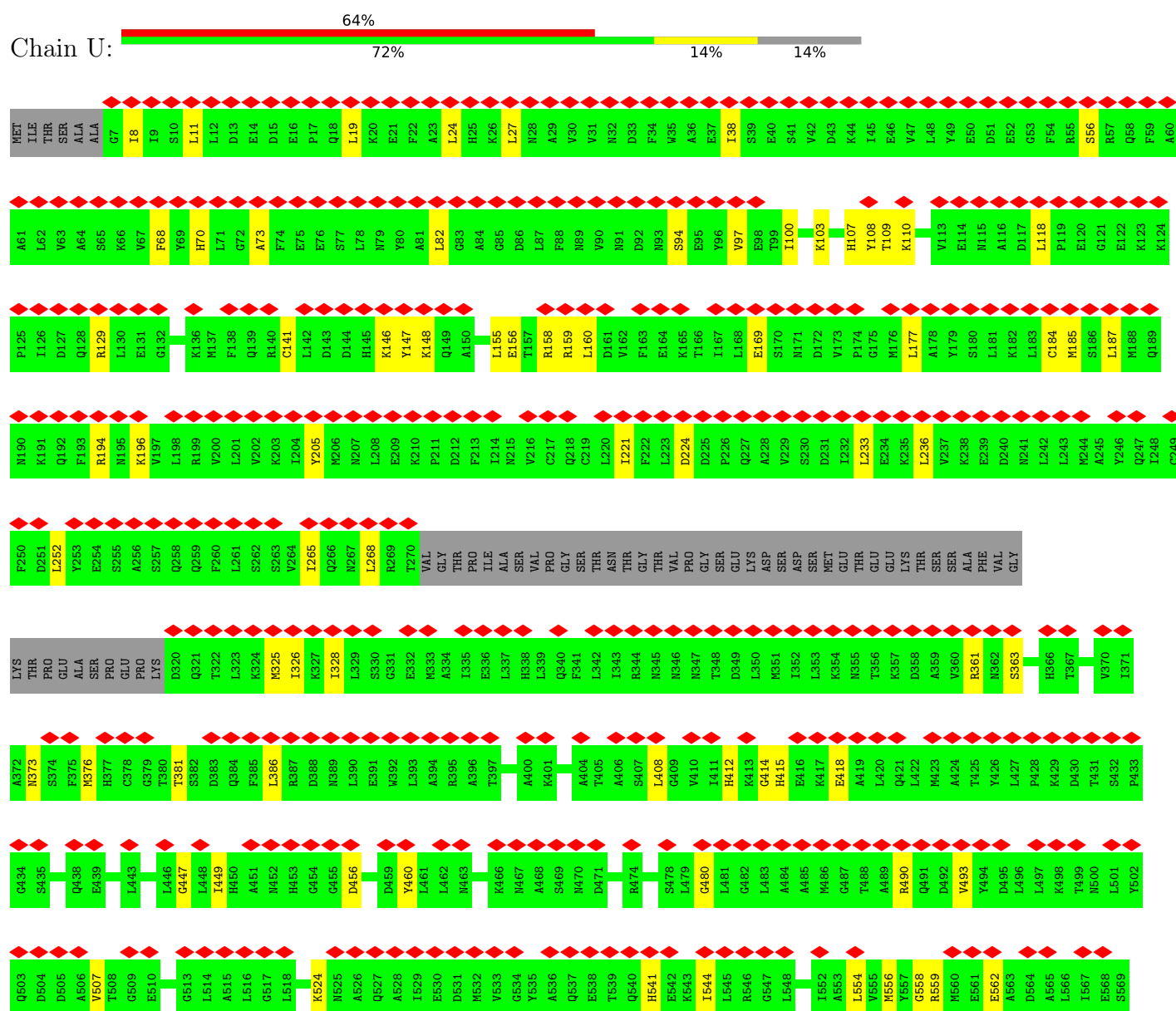


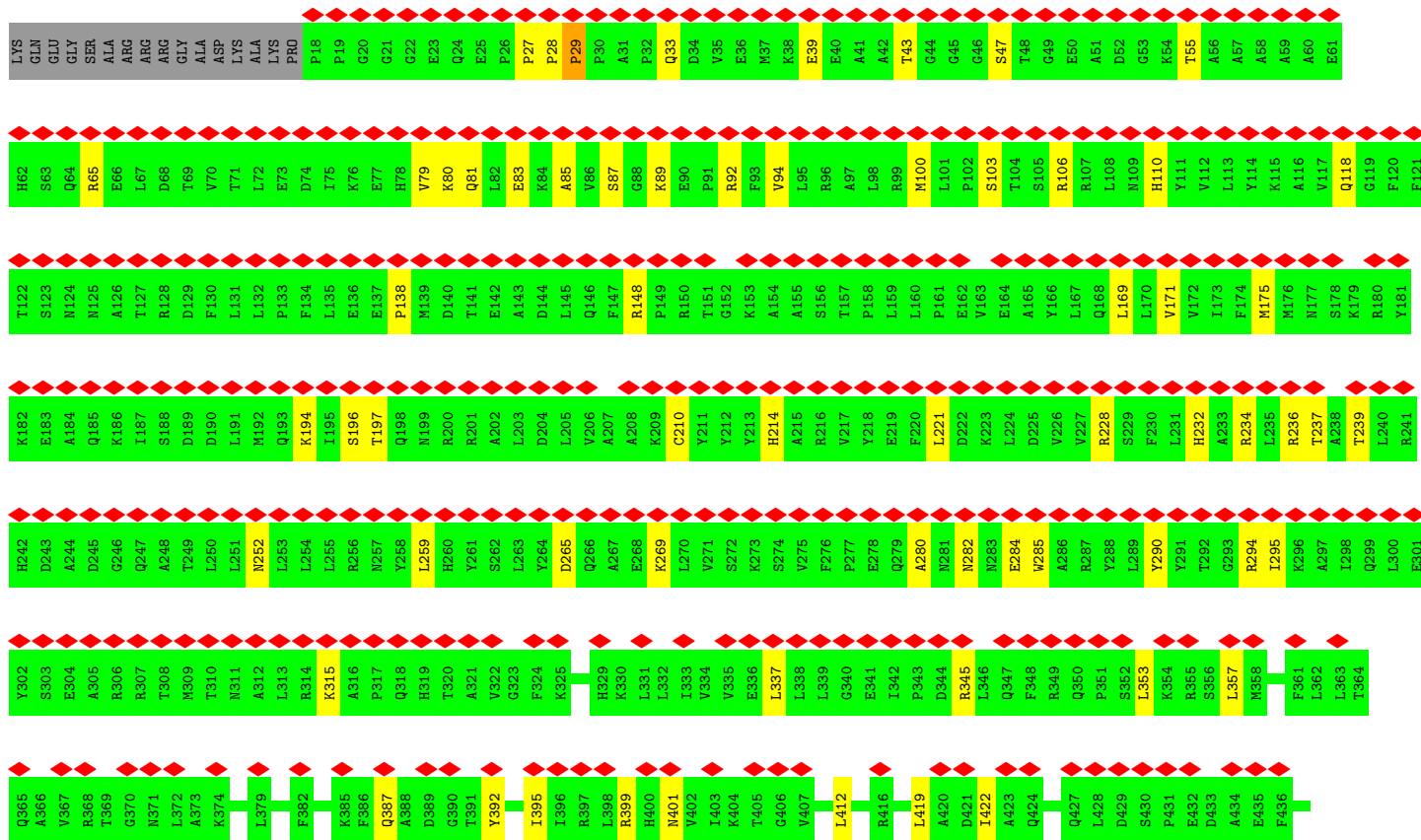
Mol	Chain	Residues	Atoms					AltConf
36	F	1	Total	C	N	O	P	0
			27	10	5	10	2	

3 Residue-property plots

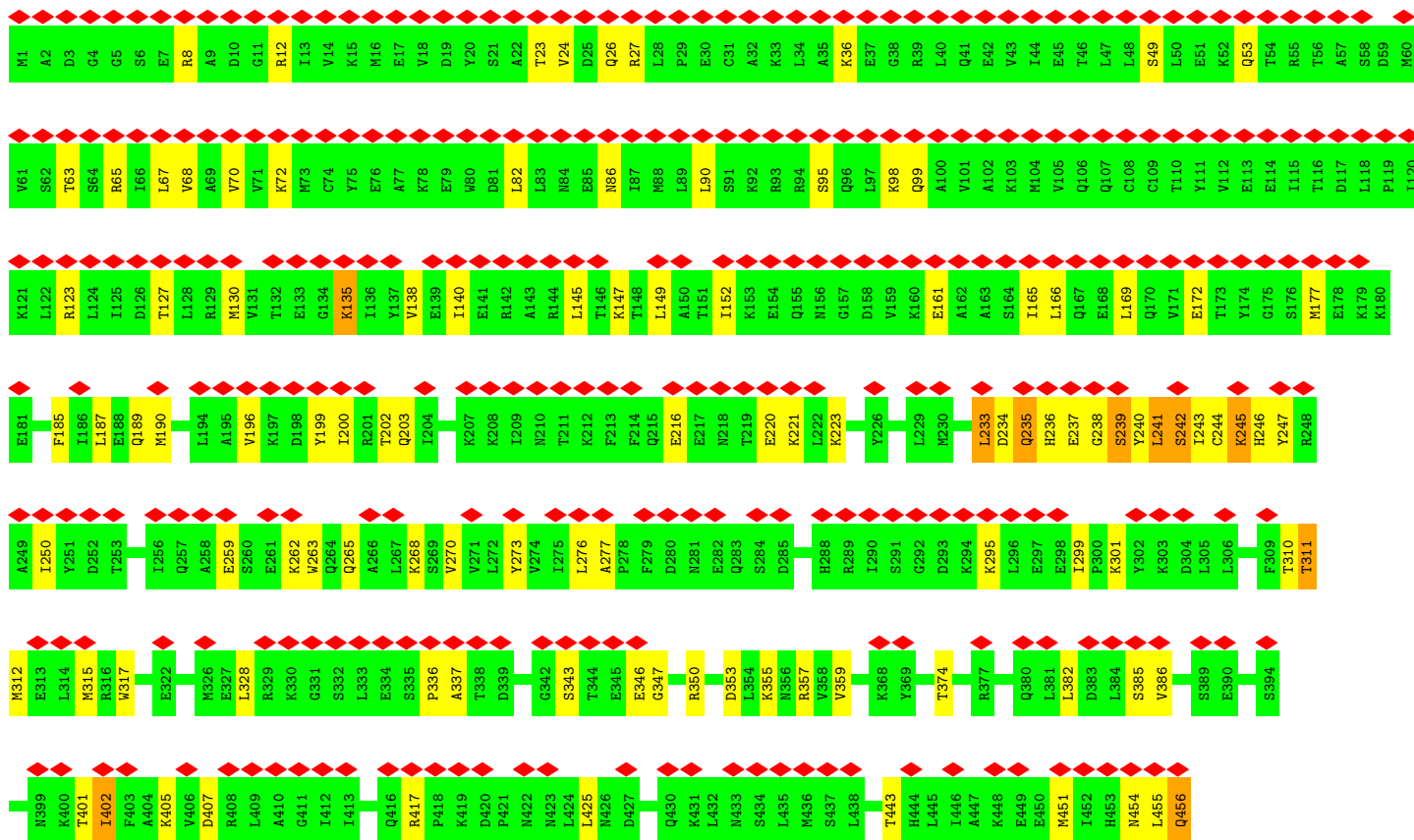
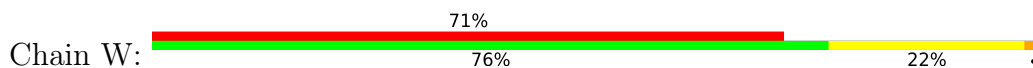
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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 non-ATPase regulatory subunit 1

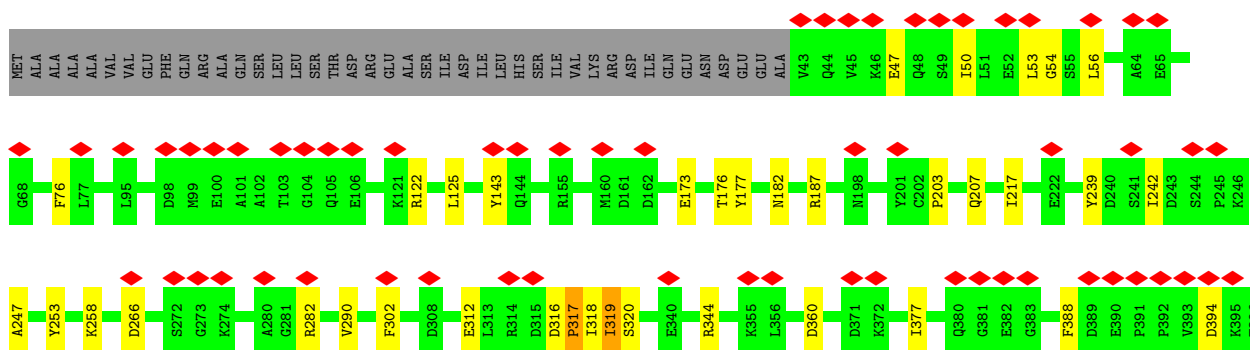
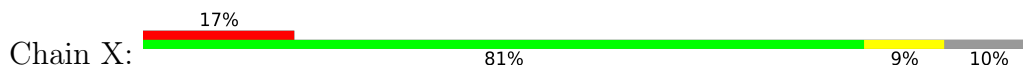


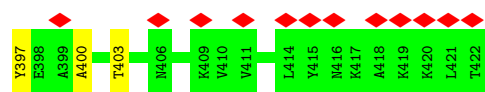


- Molecule 3: 26S proteasome non-ATPase regulatory subunit 12

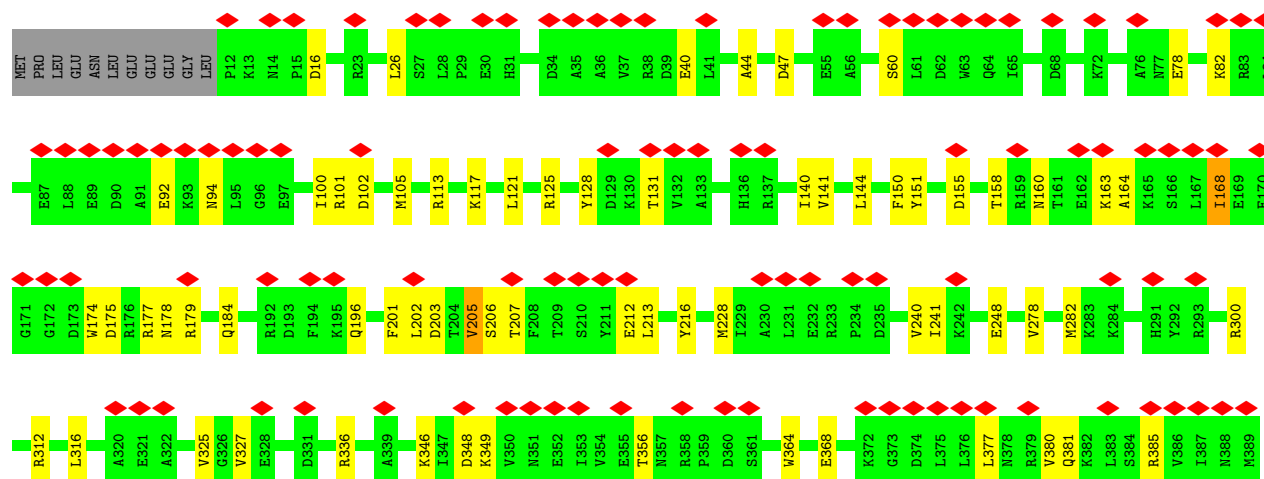
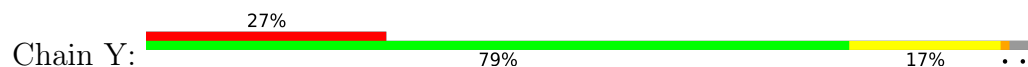


- Molecule 4: 26S proteasome non-ATPase regulatory subunit 11

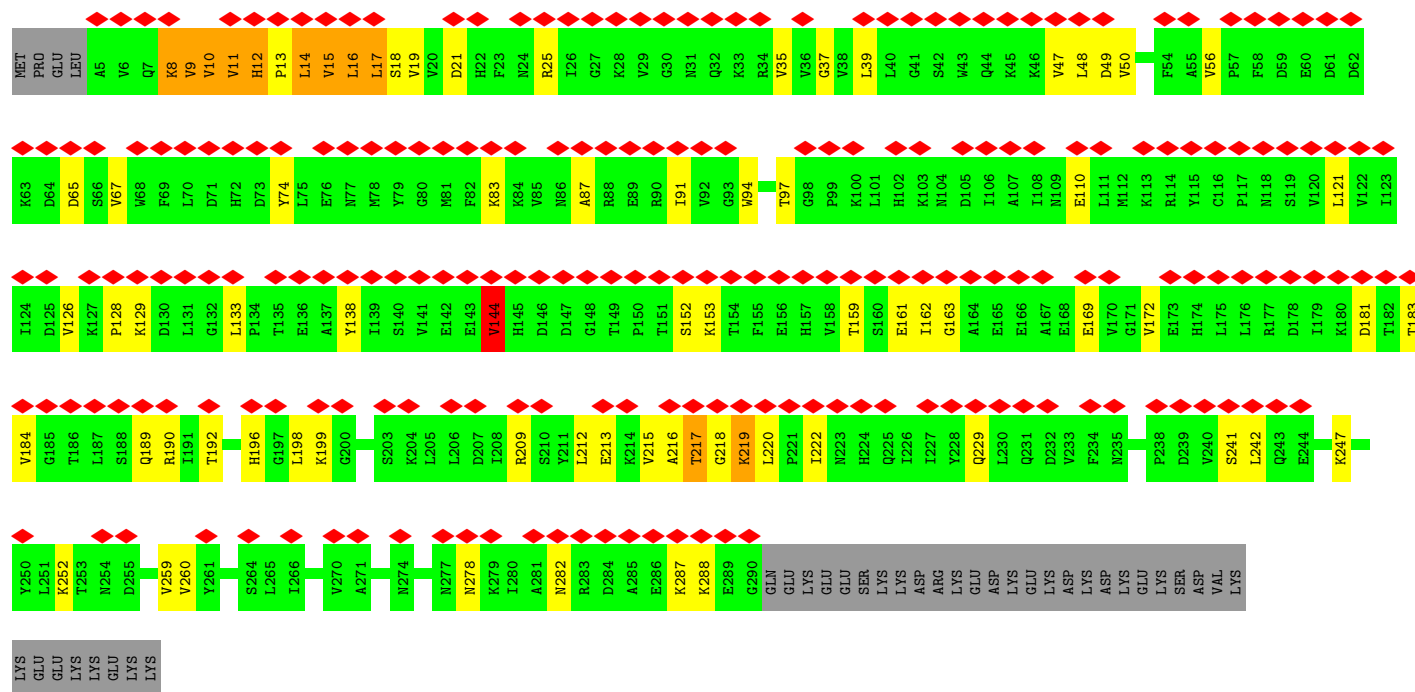




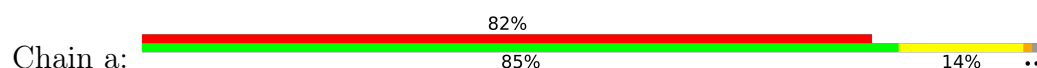
- Molecule 5: 26S proteasome non-ATPase regulatory subunit 6

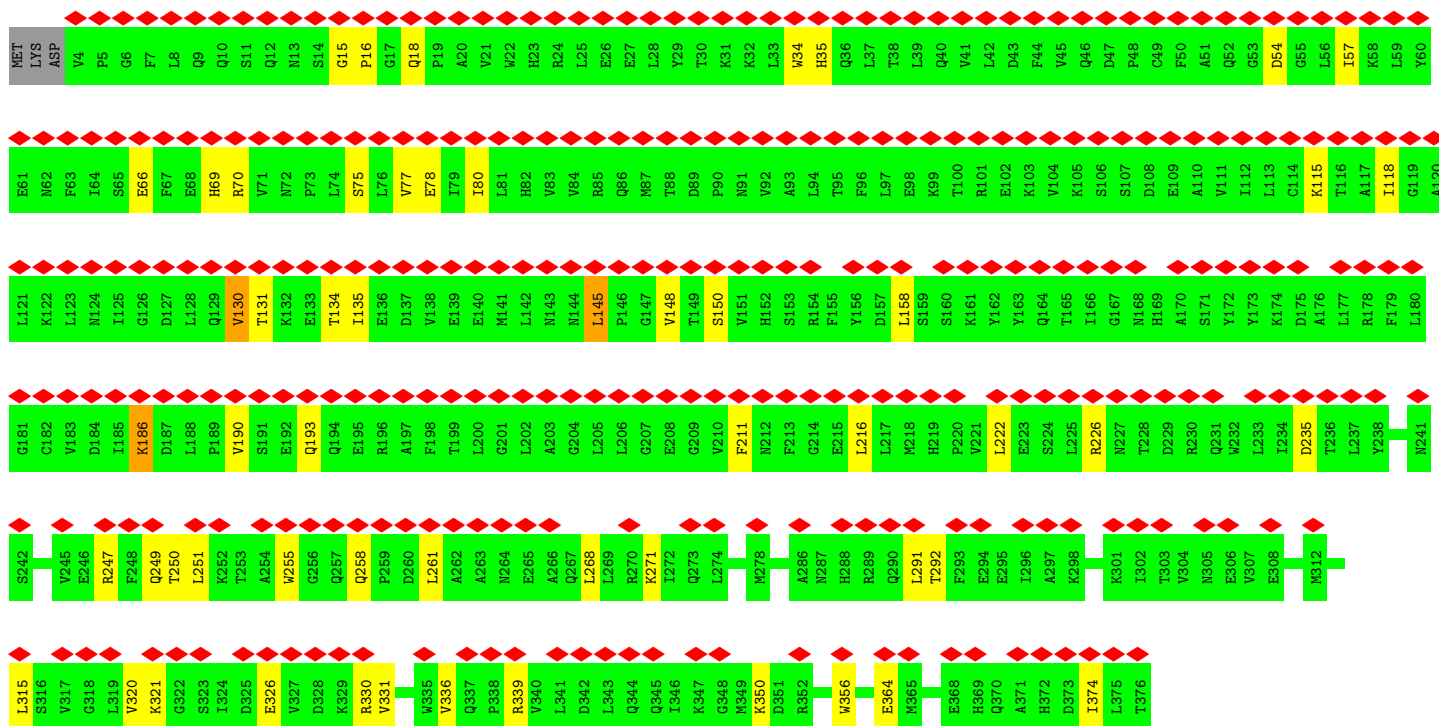


- Molecule 6: 26S proteasome non-ATPase regulatory subunit 7

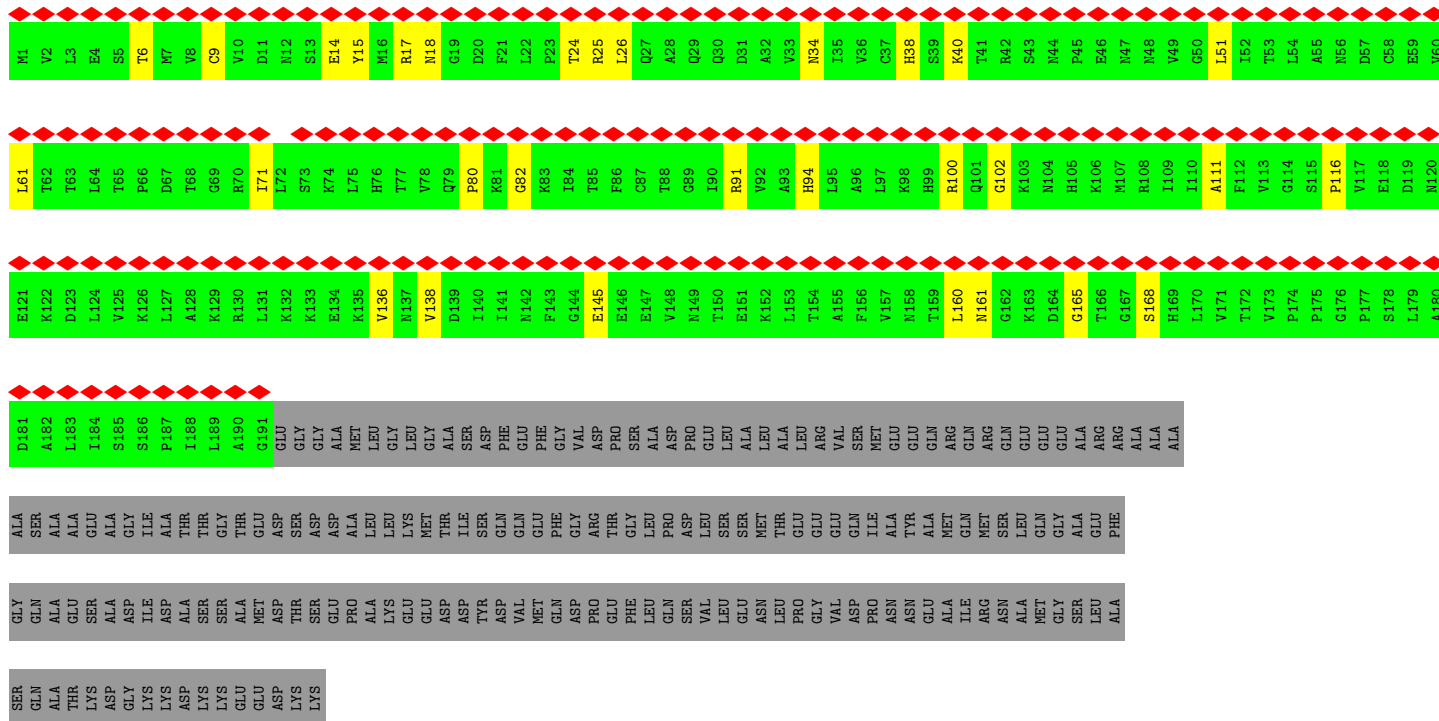
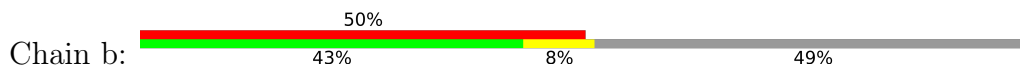


- Molecule 7: 26S proteasome non-ATPase regulatory subunit 13

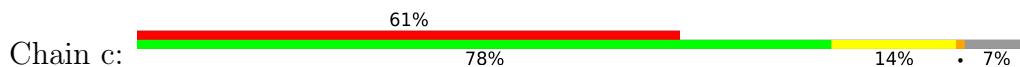


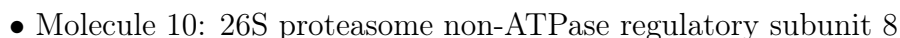


• Molecule 8: 26S proteasome non-ATPase regulatory subunit 4



• Molecule 9: 26S proteasome non-ATPase regulatory subunit 14





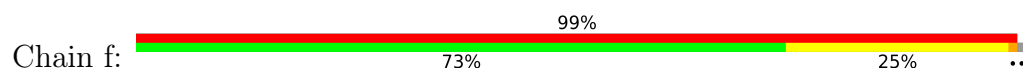
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M1	S2	E3	K4	K5	Q6	P7	V8	D9	LEU	GLY	LEU	LEU	LEU	GLU	GLU	GLU	ASP	ASP	PHE	GLU	GLU	PRO	ALA	ALA	GLU	ASP	TRP	GLY	LEU	ASP	ASP	GLU	ASP	ASP	HIS	VAL	TRP	E40	D41	N42	W43	D44	D45	D46	N47	V48	E49	D50	D61	F62	S63	N54	Q55	L56	R57	A58	E59
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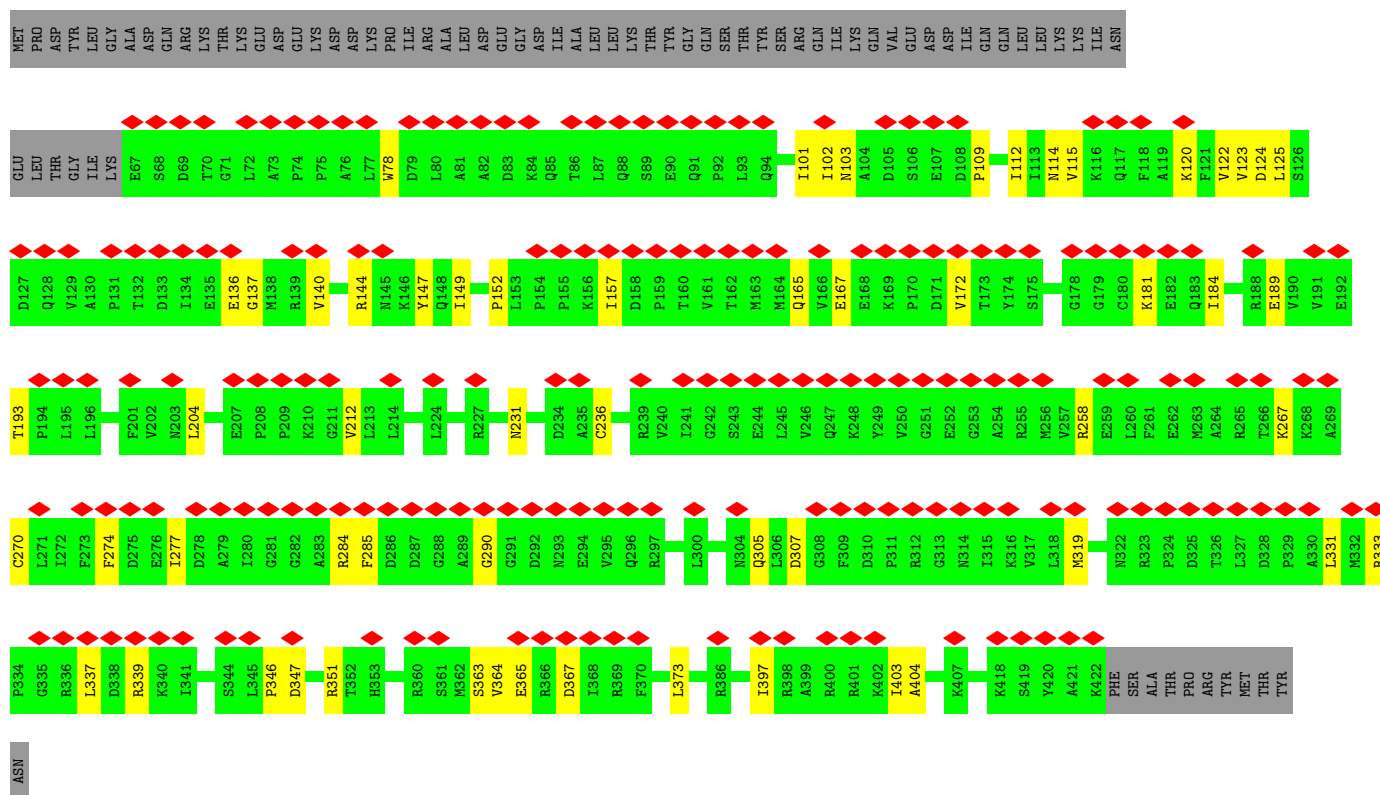
• Molecule 12: 26S proteasome non-ATPase regulatory subunit 2



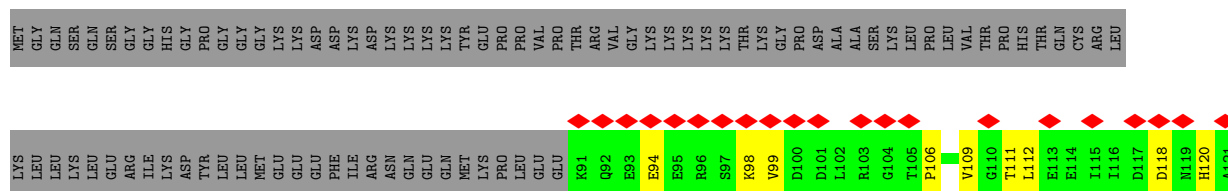
MET	GLU	GLU	K62	H63	K66	M67	E68	T69	S70
E61	R62	L63	G64	E65	R66	D67	T68	A69	P70
V71	Q72	P73	Q74	L75	E76	E77	L78	R79	R80
Q81	G82	G83	S84	S85	T86	T87	S88	M89	E90
E91	S92	R93	R94	P95	L96	K97	F98	L99	R100
K101	E102	Q103	G104	K105	L106	K107	E108	I109	P110
H111	N112	M113	D114	P115	G116	E117	N118	K119	R120
F121	A122	A123	D124	I125	S126	V127	V128	L129	A130
M131	T132	M133	A134	G135	E136	R137	E138	C139	L140
K141	Y142	R143	L144	V145	G146	S147	Q148	E149	E150
L151	V152	P153	V154	G155	H156	E157	Y158	V159	R160
H161	L162	A163	G164	E165	V166	A167	K168	E169	Y170
E171	N172	M173	D174	P175	G176	E177	N178	K179	R180
R181	E182	P183	L184	L185	T186	L187	V188	K189	E190
I191	V192	P193	Y194	N195	M196	A197	H198	N199	A200
S201	E202	E203	A204	C205	D206	L207	L208	M209	E210
I211	E212	Q213	V214	D215	M216	L217	E218	K219	D220
I221	D222	E223	N224	A225	V226	A227	K228	V229	C230
L231	V232	L233	T234	S235	C236	V237	L238	V239	V240
P241	E242	P243	E244	N245	S246	A247	L248	L249	R250
C251	A252	L253	G254	V255	P256	R257	K258	F259	S260
R261	P262	P263	E264	A265	L266	E267	L268	A269	L270
E271	L272	N273	D274	M275	E276	L277	V278	E279	D280
I281	P282	T283	S284	C285	K286	D287	V288	V289	V290
Q291	K292	Q293	M294	A295	P296	M297	L298	Q299	R300
H301	G302	V303	F304	L305	E306	L307	S308	E309	D310
V311	E312	E313	Y314	E315	D316	L317	T318	E319	I320
I321	S322	N323	V324	Q325	L326	N327	S328	N329	F330
L331	A332	L333	A334	R335	E336	L337	D338	L339	K340
E341	P342	K343	V344	P345	D346	D347	L348	S349	A350
A411	A412	S413	L414	G415	M416	L417	L418	L419	W420
D421	V422	D423	G424	G425	L426	T427	Q428	I429	D430
K431	Y432	L433	Y434	S435	S436	E437	D438	Y439	L440
K441	S442	G443	A444	L445	L446	A447	C448	G449	L450
L501	L502	P503	V504	M505	G506	D507	S508	K509	S510
S511	S512	M513	E514	A515	G516	V517	T518	A519	L520
A521	C522	G523	M524	I525	A526	V527	G528	S529	C530
N531	D532	D533	V534	T535	S536	T537	F538	A539	N540
H541	N542	T543	L544	N545	D546	F547	R548	S549	F550
A551	N552	T553	L554	V555	D556	V557	L558	P559	L560
G561	L562	G563	L564	N565	H566	L567	G568	K569	D570
K571	A572	I573	E574	A575	I576	L577	A578	A579	L580
L581	A582	V583	S584	E585	P586	F587	R588	S589	F590
A591	N592	T593	L594	V595	D596	V597	L598	A599	I600
A601	G602	S603	G604	K605	V606	L607	K608	V609	Q610
Q611	D612	L613	H614	L615	C616	S617	E618	H619	F620
D621	K623	E624	K625	E626	E627	D628	K629	D630	K631
K632	K633	K634	K635	D636	K637	D638	K639	K640	E641
A642	P643	A644	D645	M646	G647	D648	H649	Q650	G651
V652	A653	V654	L655	G656	I657	D658	L659	F660	E661
M662	G663	E664	E665	L666	G667	A668	E669	M670	Q671
A671	L672	R673	T674	F675	G676	H677	L678	L679	R680
Y681	G682	E683	P684	T685	L686	R687	R688	A689	V690
P691	L692	K693	L694	A695	L696	L697	S698	V699	S700
N701	P702	R703	L704	N705	L706	L707	D708	T709	L710
S711	K712	F713	S714	H715	D716	A717	D718	F719	E720

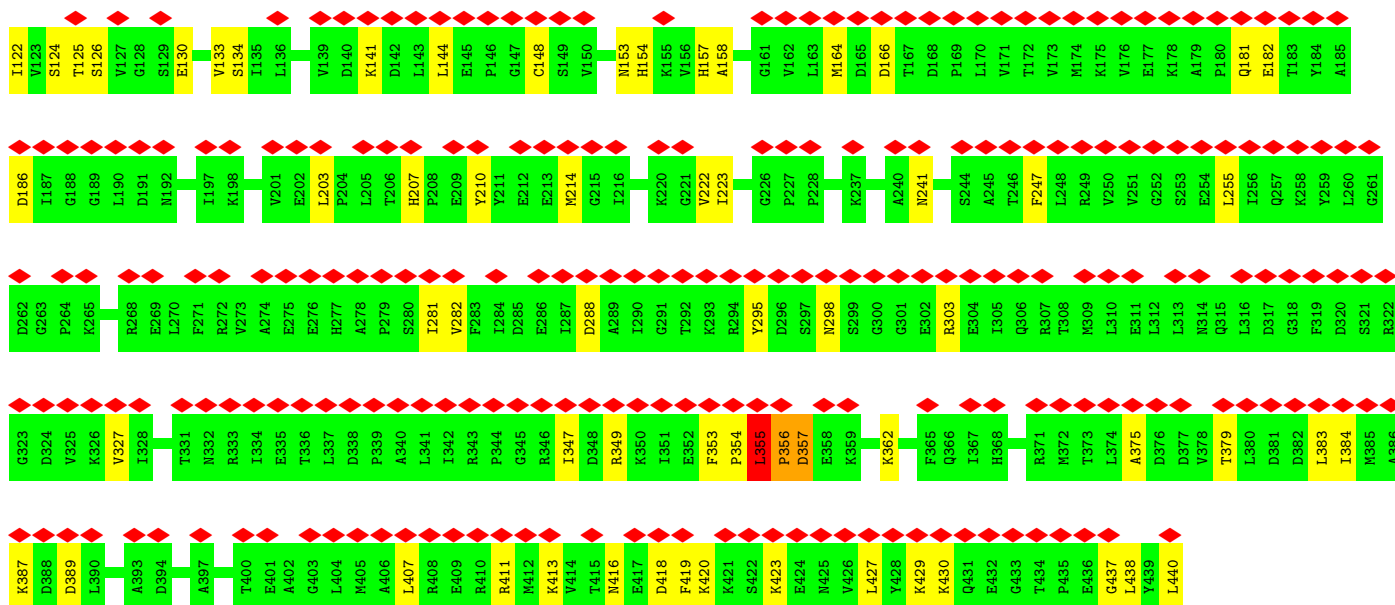


• Molecule 13: 26S proteasome regulatory subunit 7

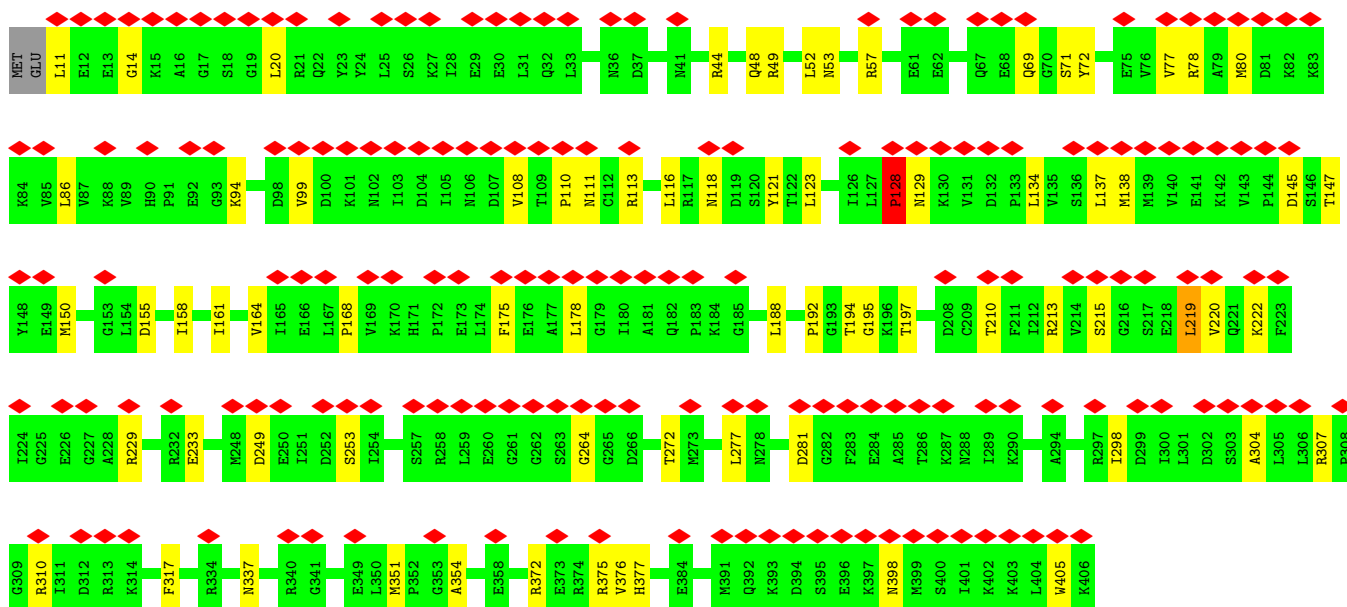
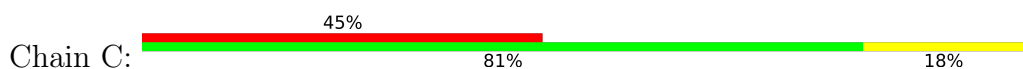


• Molecule 14: 26S proteasome regulatory subunit 4

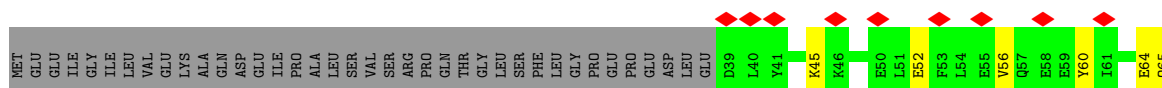


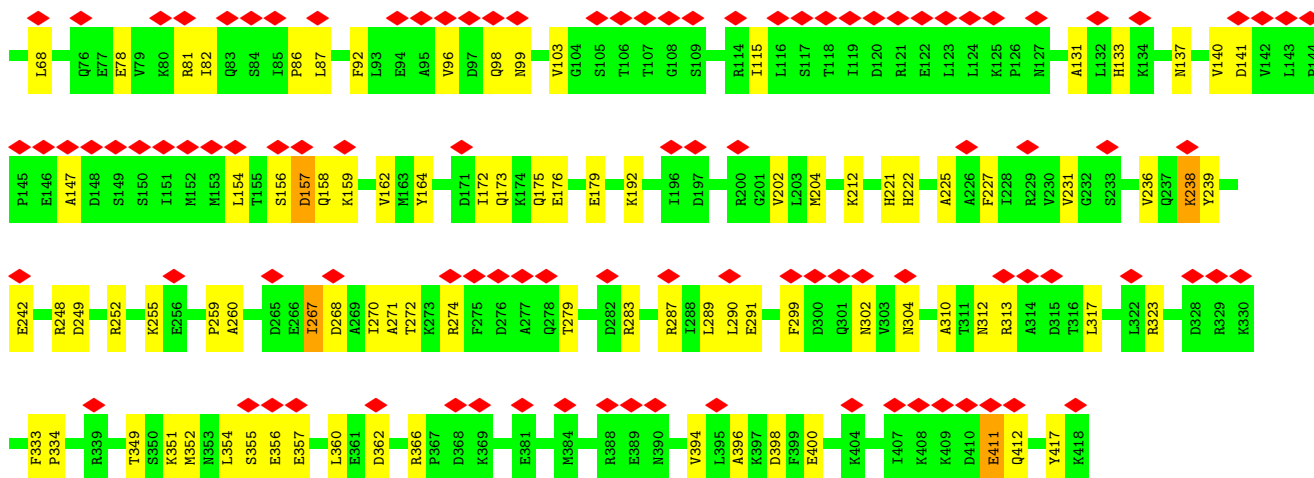


• Molecule 15: 26S proteasome regulatory subunit 8

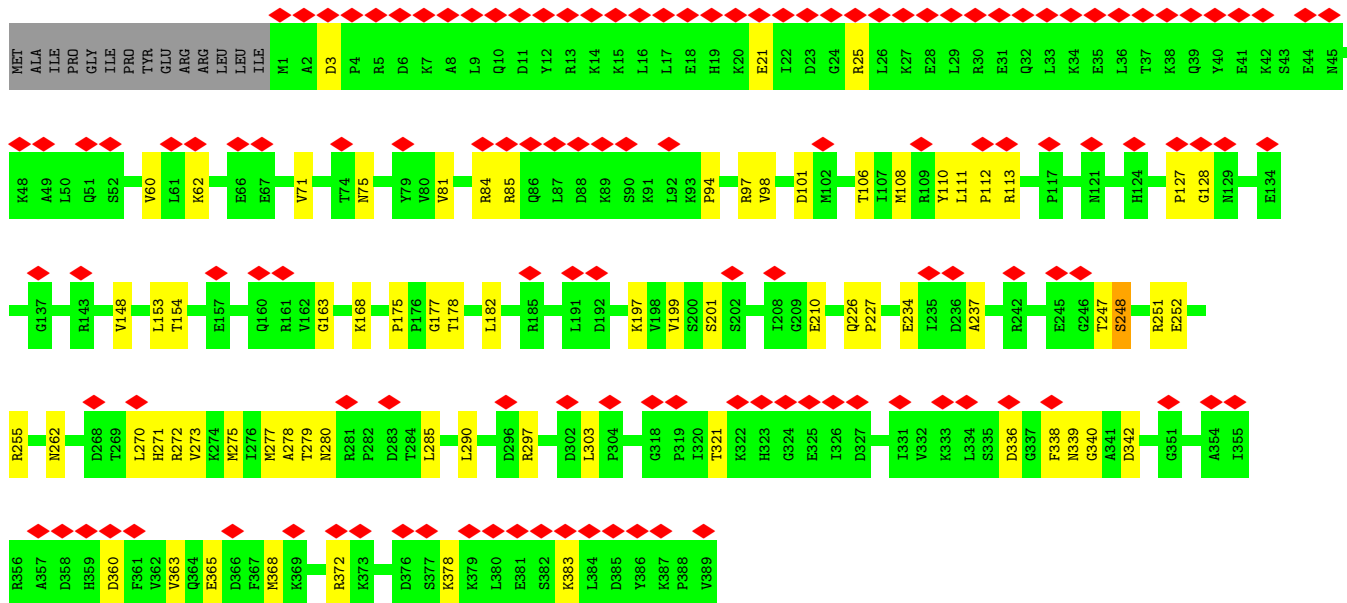
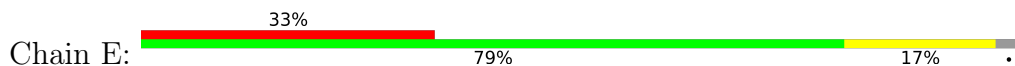


• Molecule 16: 26S proteasome regulatory subunit 6B

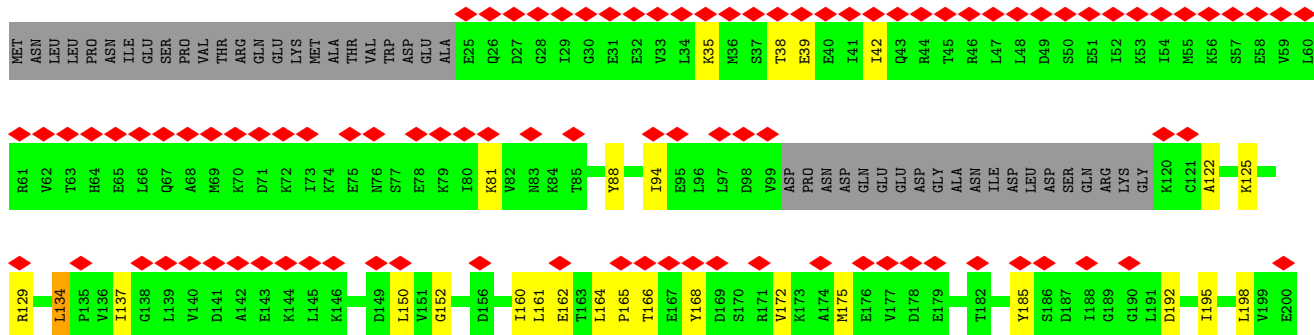
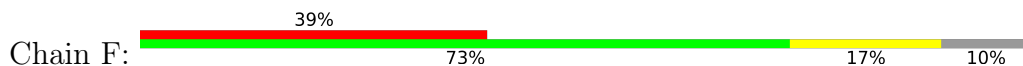


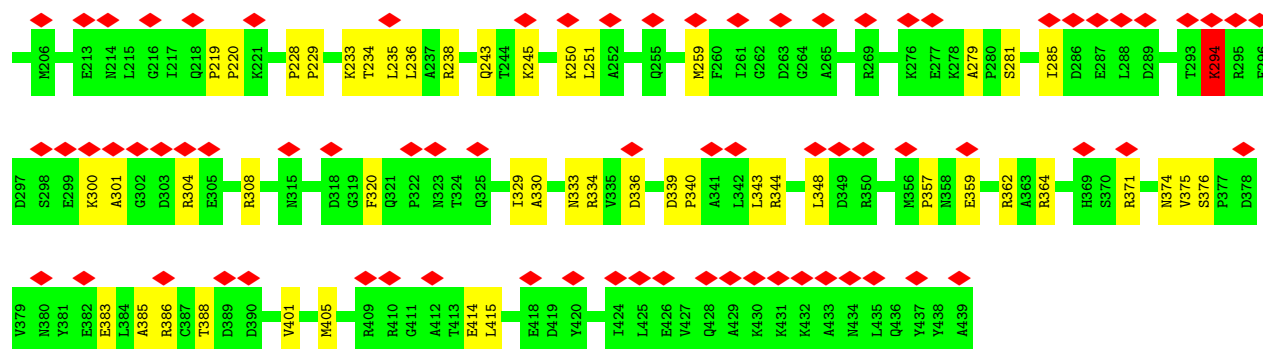


• Molecule 17: 26S proteasome regulatory subunit 10B

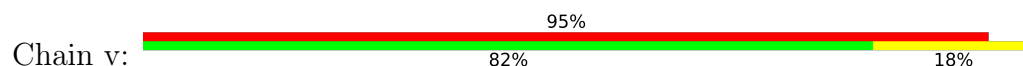


• Molecule 18: 26S proteasome regulatory subunit 6A

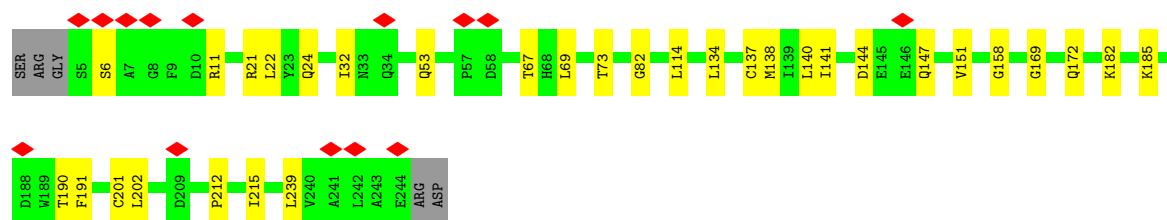
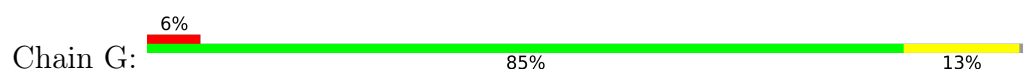




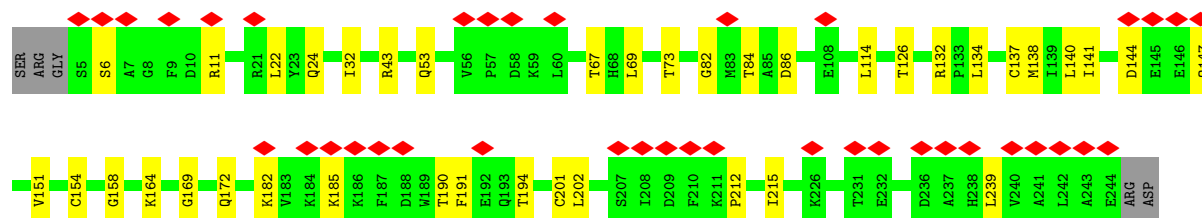
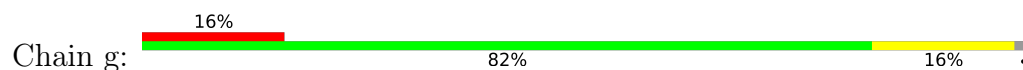
- Molecule 19: substrate



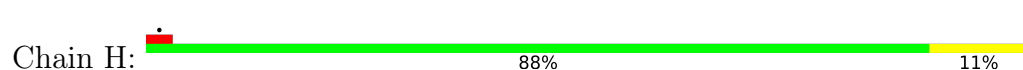
- Molecule 20: Proteasome subunit alpha type-6



- Molecule 20: Proteasome subunit alpha type-6

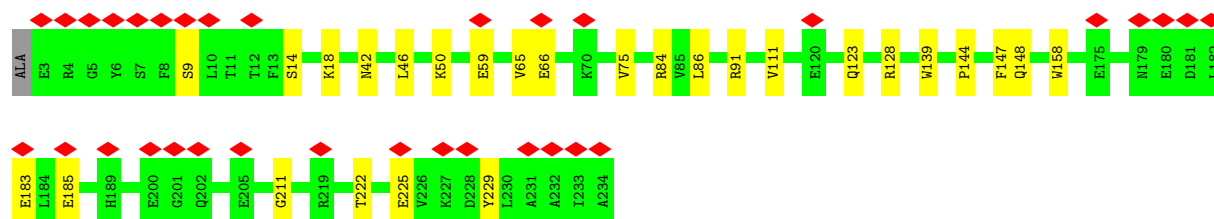
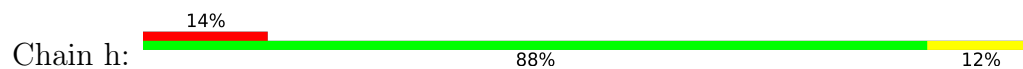


- Molecule 21: Proteasome subunit alpha type-2

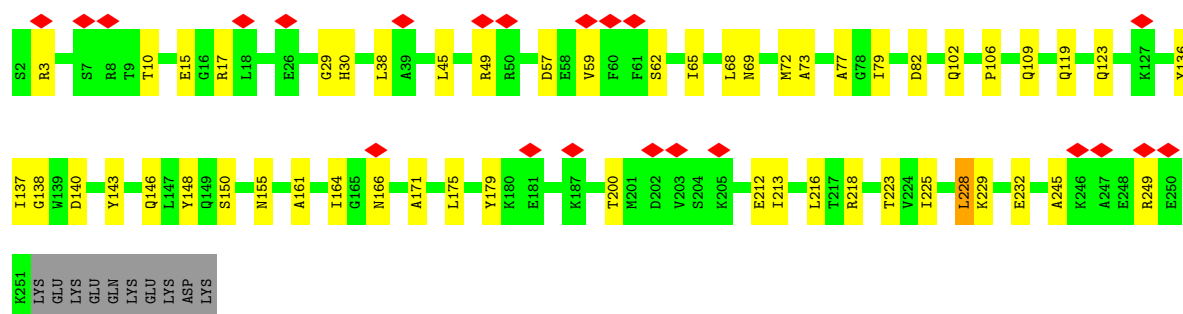
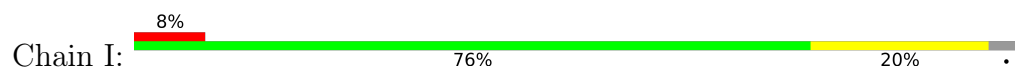




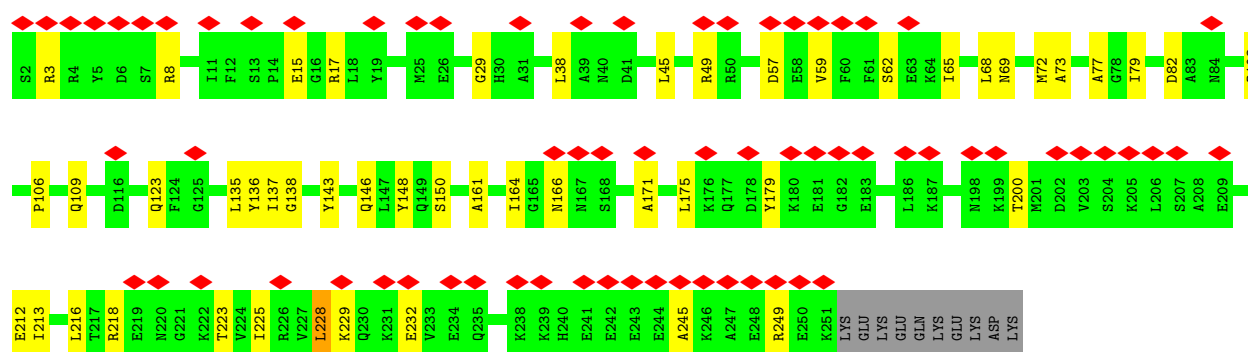
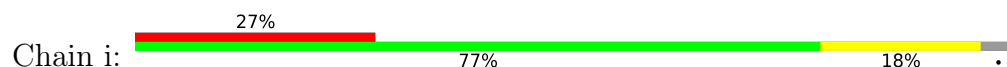
• Molecule 21: Proteasome subunit alpha type-2



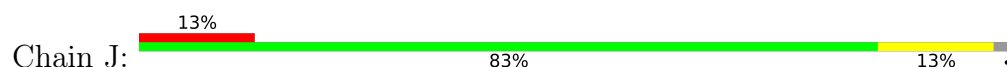
• Molecule 22: Proteasome subunit alpha type-4

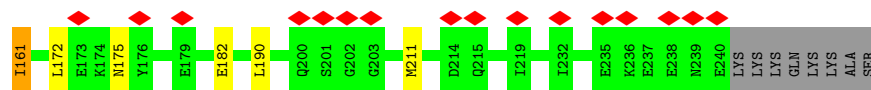


• Molecule 22: Proteasome subunit alpha type-4



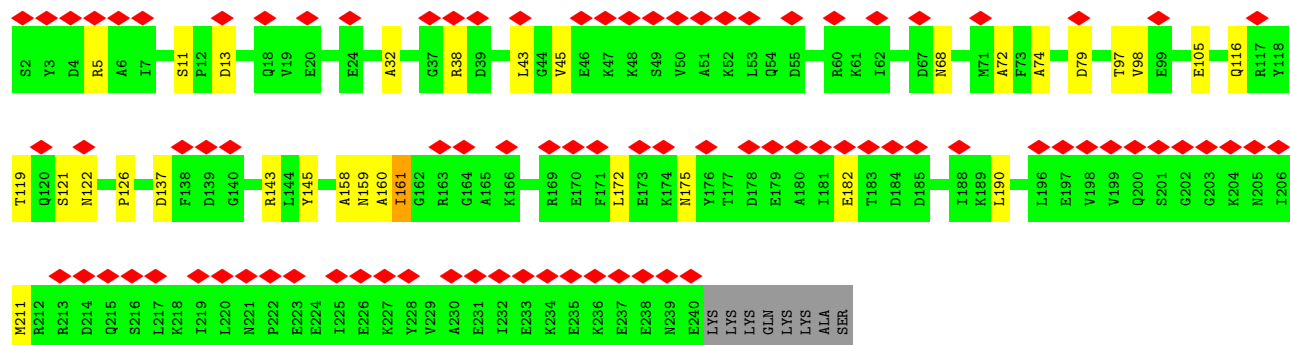
• Molecule 23: Proteasome subunit alpha type-7





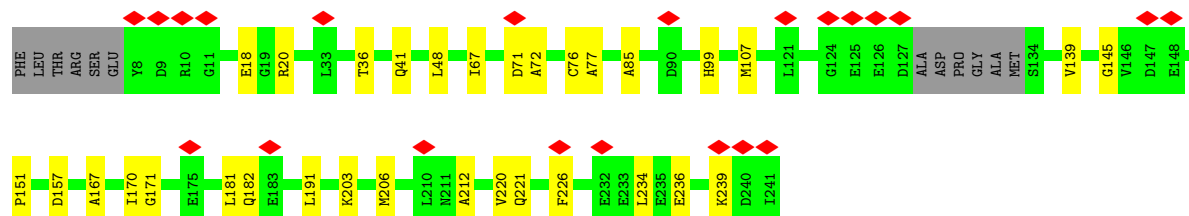
• Molecule 23: Proteasome subunit alpha type-7

Chain j: 36% 84% 12% .



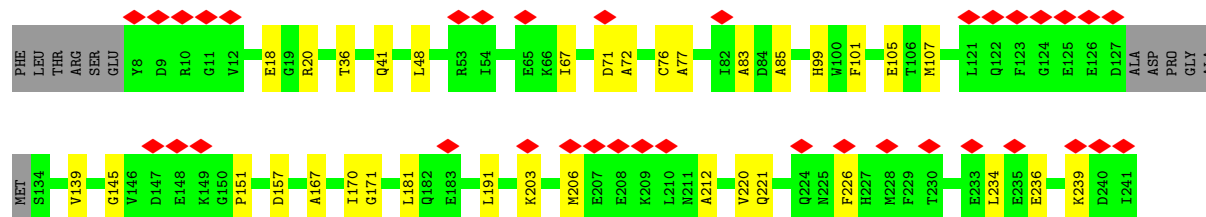
• Molecule 24: Proteasome subunit alpha type-5

Chain K: 9% 82% 13% 5%



• Molecule 24: Proteasome subunit alpha type-5

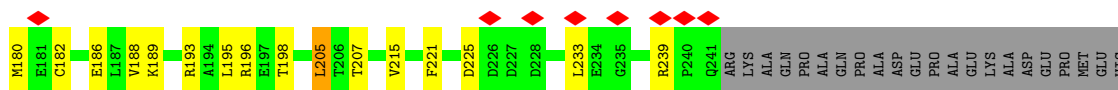
Chain k: 15% 81% 14% 5%



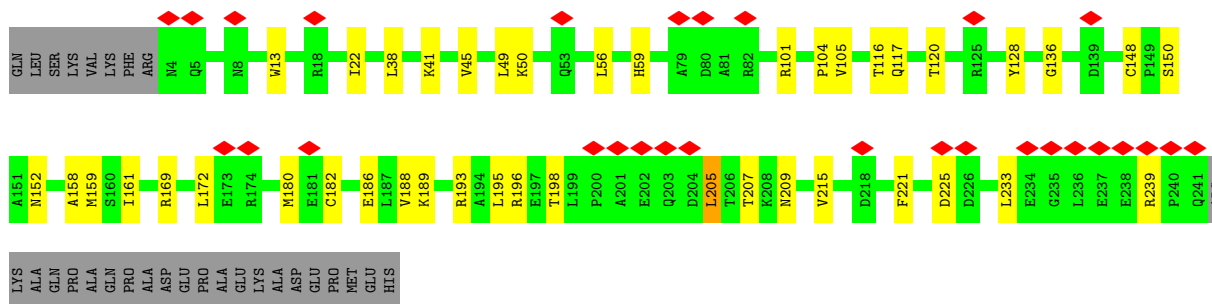
• Molecule 25: Proteasome subunit alpha type-1

Chain L: 74% 15% 11%

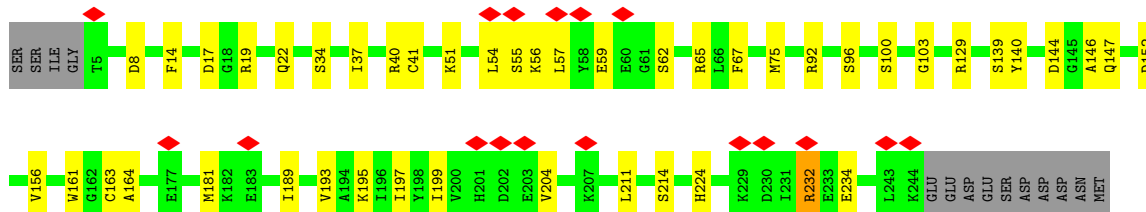
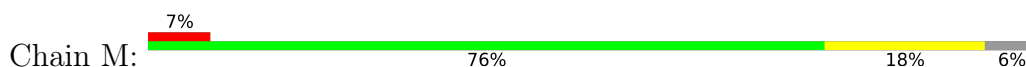




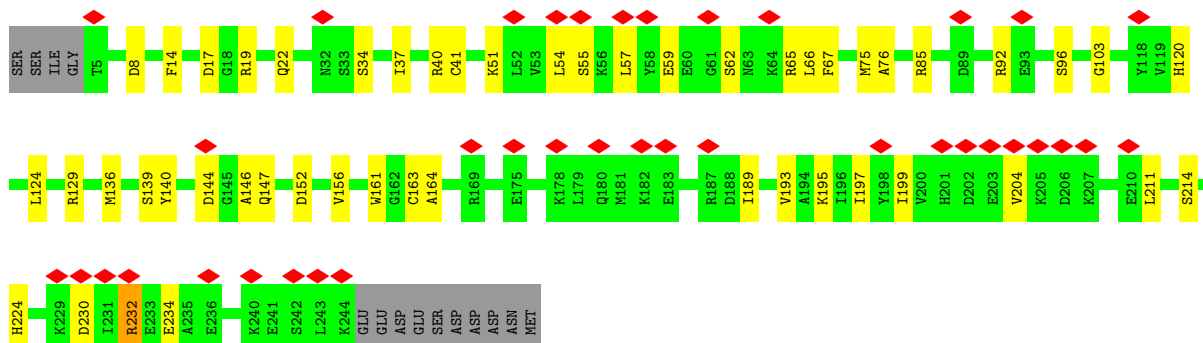
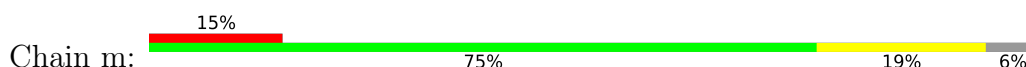
• Molecule 25: Proteasome subunit alpha type-1



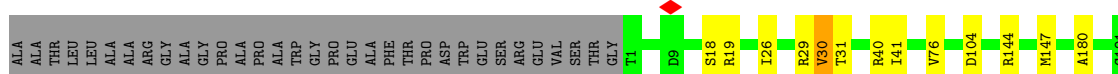
• Molecule 26: Proteasome subunit alpha type-3



• Molecule 26: Proteasome subunit alpha type-3



• Molecule 27: Proteasome subunit beta type-6



ASP
GLN
ILE
THR
PRO
PRO
LYS
PHE
PHE
ALA
VAL
ALA
THR
LEU
THR
PRO
PRO
PRO
ALA

• Molecule 27: Proteasome subunit beta type-6

Chain n:



ALA
ALA
THR
LEU
LEU
ALA
ALA
ARG
GLY
ALA
GLY
GLY
PRO
PRO
ALA
PRO
ALA
ALA
TRP
GLY
PRO
GLU
GLU
ALA
PHE
THR
THR
PRO
ASP
TSP
GLU
SER
ARG
GLU
VAL
SER
THR
GLY
T1
D9
S18
I26
V30
T31
D32
D39
R40
I41
E69
L70
N71
E72
V76
D104
R144

M147
A180
E185
G191
ASP
GLN
ILE
PRO
LYS
PHE
PHE
ALA
VAL
ALA
ASP
ASN
THR
LEU
PRO
PRO
ALA

• Molecule 28: Proteasome subunit beta type-7

Chain O:



ALA
ALA
VAL
SER
VAL
TYR
ALA
PRO
PRO
VAL
GLY
GLY
PHE
SER
PHE
ASP
ASN
CYS
ARG
ASN
ASN
ALA
VAL
LEU
GLU
ALA
ASP
PHE
ALA
LYS
ARG
GLY
TYR
LYS
LEU
PRO
LYS
VAL
ARG
LYS
THR
GLY
T1
V6
V13
R19
E22
G23
M24
C31
S32
Q57
A96

L100
Y111
P115
Y124
E139
P144
F164
G170
D174
V177
R187
L199
G200
R201
Y202
R203
C204
E205
K206
G207
I216
E220
ILE
GLU
VAL
VAL
LEU
GLU
THR
VAL
GLN
THR
MET
ASP
THR
SER

• Molecule 28: Proteasome subunit beta type-7

Chain o:



ALA
ALA
VAL
SER
VAL
TYR
ALA
PRO
PRO
VAL
GLY
GLY
PHE
SER
PHE
ASP
ASN
CYS
ARG
ARG
ASN
ASN
ALA
VAL
LEU
GLU
ALA
ASP
PHE
ALA
LYS
ARG
GLY
TYR
LYS
LEU
PRO
LYS
VAL
ARG
LYS
THR
GLY
T1
V6
V13
R19
G23
M24
C31
S32
A96
L100

Y111
P115
Y124
F138
E139
D140
R143
F164
G170
S171
N172
I173
D174
V177
N181
D184
R187
K194
K195
G196
T197
R198
L199
G200
R201
E205
K206
G207
E220
ILE
GLU
VAL
VAL
LEU
GLU
THR
VAL
GLN
THR
MET
ASP
THR
SER

• Molecule 29: Proteasome subunit beta type-3

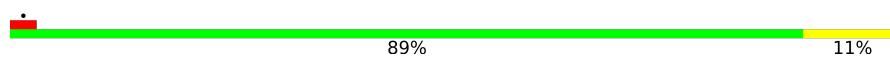
Chain P:

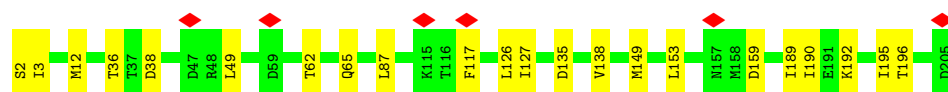


S2
I3
M12
T36
T37
D38
L49
L56
A57
T58
D59
T62
Q65
L87
F117
L126
I127
D135
V138
D159
I189
I190
E191
K192
K194
I195
T196
D205

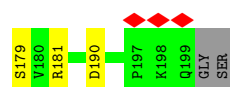
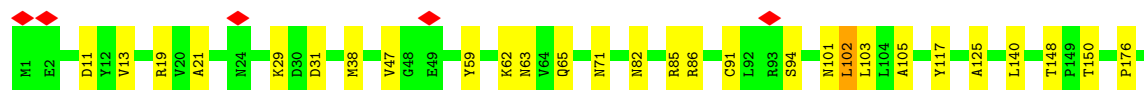
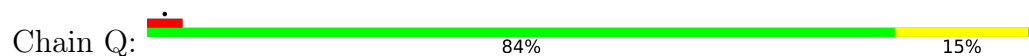
• Molecule 29: Proteasome subunit beta type-3

Chain p:

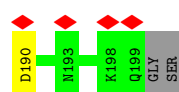
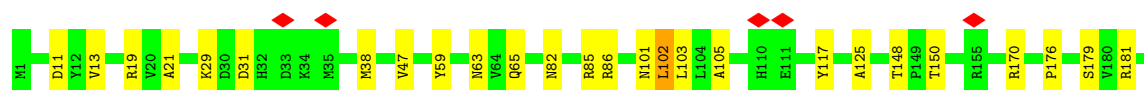
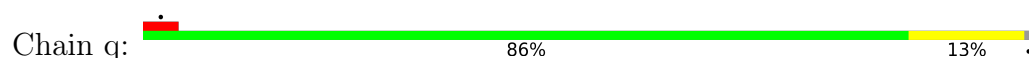




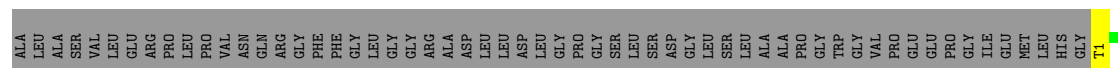
- Molecule 30: Proteasome subunit beta type-2



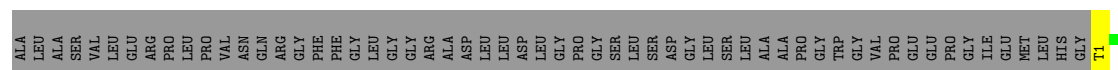
- Molecule 30: Proteasome subunit beta type-2



- Molecule 31: Proteasome subunit beta type-5

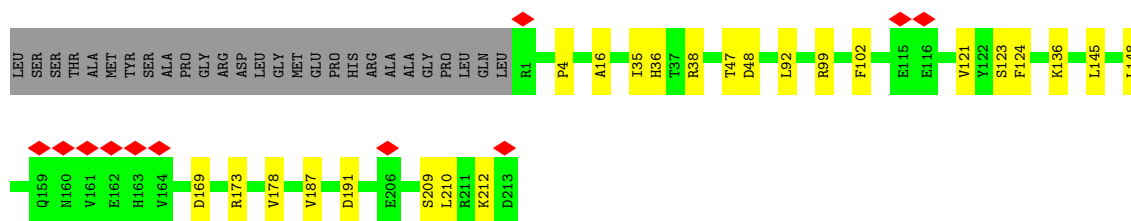


- Molecule 31: Proteasome subunit beta type-5



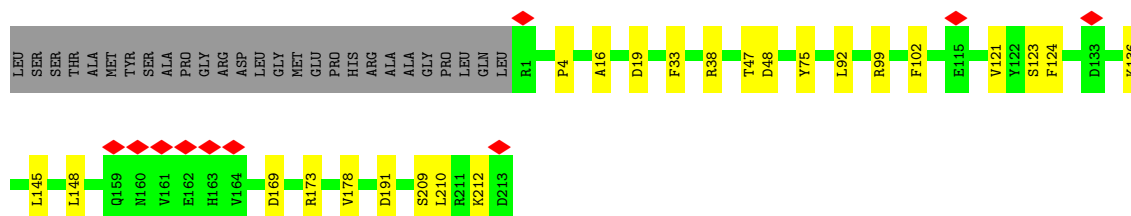
- Molecule 32: Proteasome subunit beta type-1

Chain S: 



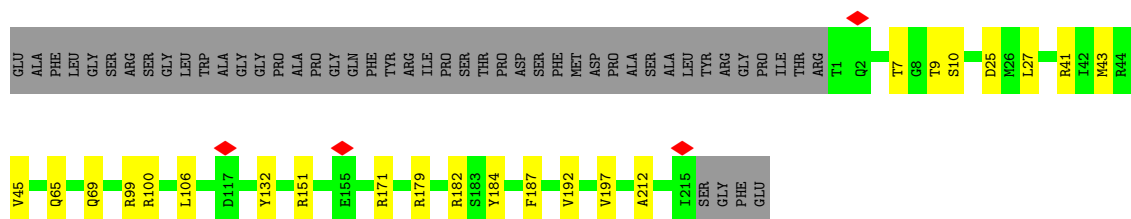
• Molecule 32: Proteasome subunit beta type-1

Chain s: 



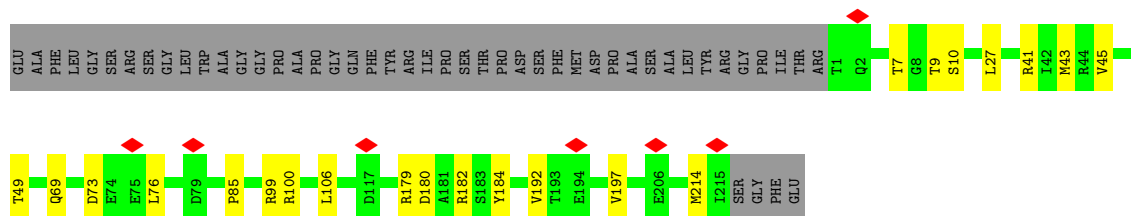
• Molecule 33: Proteasome subunit beta type-4

Chain T: 



• Molecule 33: Proteasome subunit beta type-4

Chain t: 



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	71651	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	44	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.016	Depositor
Minimum map value	-0.006	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.006	Depositor
Map size ($\text{\AA}$)	411.0, 411.0, 411.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.685, 0.685, 0.685	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	U	0.26	0/6513	0.62	2/8816 (0.0%)
2	V	0.31	0/3929	0.71	3/5309 (0.1%)
3	W	0.27	0/3751	0.66	3/5042 (0.1%)
4	X	0.35	0/3053	0.61	1/4115 (0.0%)
5	Y	0.34	0/3173	0.71	1/4273 (0.0%)
6	Z	0.27	0/2324	0.68	0/3150
7	a	0.26	0/3053	0.67	4/4133 (0.1%)
8	b	0.25	0/1478	0.62	0/2001
9	c	0.29	0/2302	0.67	0/3110
10	d	0.27	0/2162	0.70	6/2919 (0.2%)
11	e	0.30	0/338	0.76	1/450 (0.2%)
12	f	0.30	0/6954	0.80	11/9399 (0.1%)
13	A	0.30	0/2814	0.62	2/3801 (0.1%)
14	B	0.27	0/2745	0.66	4/3709 (0.1%)
15	C	0.33	0/3146	0.69	2/4226 (0.0%)
16	D	0.38	0/3090	0.73	4/4168 (0.1%)
17	E	0.35	0/3145	0.71	1/4233 (0.0%)
18	F	0.35	0/3137	0.69	2/4223 (0.0%)
20	G	0.40	0/1859	0.63	1/2523 (0.0%)
20	g	0.40	0/1859	0.63	1/2523 (0.0%)
21	H	0.43	0/1743	0.62	0/2372
21	h	0.43	0/1743	0.62	0/2372
22	I	0.39	0/1942	0.67	0/2628
22	i	0.39	0/1942	0.67	0/2628
23	J	0.36	0/1728	0.58	0/2358
23	j	0.36	0/1728	0.58	0/2358
24	K	0.35	0/1747	0.58	0/2364
24	k	0.35	0/1747	0.58	0/2364
25	L	0.42	0/1885	0.63	0/2552
25	l	0.42	0/1885	0.63	0/2552
26	M	0.41	1/1891 (0.1%)	0.70	3/2552 (0.1%)
26	m	0.41	1/1891 (0.1%)	0.70	3/2552 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
27	N	0.40	0/1454	0.52	0/1967
27	n	0.40	0/1454	0.52	0/1967
28	O	0.38	0/1670	0.59	0/2265
28	o	0.38	0/1670	0.59	0/2265
29	P	0.40	0/1614	0.56	0/2177
29	p	0.40	0/1614	0.56	0/2177
30	Q	0.45	0/1603	0.67	2/2174 (0.1%)
30	q	0.45	0/1603	0.67	2/2174 (0.1%)
31	R	0.39	0/1579	0.50	0/2134
31	r	0.39	0/1579	0.50	0/2134
32	S	0.39	0/1671	0.54	0/2253
32	s	0.39	0/1671	0.54	0/2253
33	T	0.39	0/1700	0.56	0/2305
33	t	0.39	0/1700	0.56	0/2305
All	All	0.35	2/105279 (0.0%)	0.65	59/142325 (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
2	V	0	1
6	Z	0	2
7	a	0	1
10	d	0	1
12	f	0	12
13	A	0	2
15	C	0	2
16	D	0	2
17	E	0	1
18	F	0	1
All	All	0	25

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	m	14	PHE	C-N	-5.18	1.23	1.33
26	M	14	PHE	C-N	-5.16	1.23	1.33

The worst 5 of 59 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	353	PHE	CA-C-N	8.03	129.87	119.84
14	B	353	PHE	C-N-CA	8.03	129.87	119.84
7	a	130	VAL	N-CA-C	-7.68	105.83	113.20
18	F	294	LYS	CA-C-N	7.21	135.30	121.54
18	F	294	LYS	C-N-CA	7.21	135.30	121.54

There are no chirality outliers.

5 of 25 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	V	29	PRO	Peptide
6	Z	144	VAL	Peptide
6	Z	183	THR	Peptide
7	a	18	GLN	Peptide
10	d	199	PHE	Peptide

5.2 Too-close contacts

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	U	6398	0	6422	82	0
2	V	3852	0	3893	44	0
3	W	3703	0	3822	103	0
4	X	3009	0	3113	24	0
5	Y	3115	0	3120	44	0
6	Z	2281	0	2312	105	0
7	a	2995	0	3012	35	0
8	b	1458	0	1505	21	0
9	c	2260	0	2276	41	0
10	d	2116	0	2146	21	0
11	e	334	0	294	6	0
12	f	6840	0	6842	142	0
13	A	2767	0	2787	41	0
14	B	2706	0	2731	61	0
15	C	3105	0	3219	53	0
16	D	3040	0	3076	63	0
17	E	3097	0	3174	42	0
18	F	3098	0	3187	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	v	110	0	32	7	0
20	G	1826	0	1796	16	0
20	g	1826	0	1796	22	0
21	H	1708	0	1594	16	0
21	h	1708	0	1594	14	0
22	I	1912	0	1851	34	0
22	i	1912	0	1851	29	0
23	J	1704	0	1517	22	0
23	j	1704	0	1517	19	0
24	K	1722	0	1673	18	0
24	k	1722	0	1673	21	0
25	L	1850	0	1822	23	0
25	l	1850	0	1822	24	0
26	M	1856	0	1814	29	0
26	m	1856	0	1814	32	0
27	N	1430	0	1398	10	0
27	n	1430	0	1398	8	0
28	O	1643	0	1644	15	0
28	o	1643	0	1644	13	0
29	P	1585	0	1598	17	0
29	p	1585	0	1598	13	0
30	Q	1570	0	1547	19	0
30	q	1570	0	1547	16	0
31	R	1548	0	1499	7	0
31	r	1548	0	1499	11	0
32	S	1641	0	1618	18	0
32	s	1641	0	1618	15	0
33	T	1667	0	1628	18	0
33	t	1667	0	1628	17	0
34	c	1	0	0	0	0
35	C	31	0	12	3	0
35	D	31	0	12	0	0
35	E	31	0	12	2	0
36	F	27	0	12	0	0
All	All	103729	0	103009	1327	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 6.

The worst 5 of 1327 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)
14:B:355:LEU:CD2	14:B:356:PRO:HD3	1.51	1.40
6:Z:10:VAL:HG22	6:Z:161:GLU:CG	1.73	1.17
12:f:657:ILE:O	12:f:661:ALA:HB3	1.44	1.16
14:B:355:LEU:HD22	14:B:356:PRO:CD	1.77	1.14
3:W:202:THR:CG2	3:W:233:LEU:HD21	1.77	1.13

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	U	814/953 (85%)	760 (93%)	53 (6%)	1 (0%)	48	79
2	V	478/533 (90%)	436 (91%)	41 (9%)	1 (0%)	43	72
3	W	454/456 (100%)	420 (92%)	34 (8%)	0	100	100
4	X	378/422 (90%)	355 (94%)	22 (6%)	1 (0%)	36	65
5	Y	376/389 (97%)	340 (90%)	36 (10%)	0	100	100
6	Z	284/324 (88%)	240 (84%)	38 (13%)	6 (2%)	5	31
7	a	371/376 (99%)	338 (91%)	32 (9%)	1 (0%)	36	65
8	b	189/377 (50%)	171 (90%)	18 (10%)	0	100	100
9	c	285/309 (92%)	241 (85%)	43 (15%)	1 (0%)	30	61
10	d	255/349 (73%)	216 (85%)	38 (15%)	1 (0%)	30	61
11	e	36/70 (51%)	31 (86%)	5 (14%)	0	100	100
12	f	884/892 (99%)	709 (80%)	164 (19%)	11 (1%)	10	41
13	A	354/433 (82%)	310 (88%)	42 (12%)	2 (1%)	21	54
14	B	348/440 (79%)	300 (86%)	44 (13%)	4 (1%)	11	43
15	C	394/398 (99%)	342 (87%)	51 (13%)	1 (0%)	36	65
16	D	378/418 (90%)	335 (89%)	42 (11%)	1 (0%)	36	65

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	E	387/403 (96%)	338 (87%)	43 (11%)	6 (2%)	7	36
18	F	391/439 (89%)	350 (90%)	40 (10%)	1 (0%)	36	65
20	G	238/245 (97%)	228 (96%)	10 (4%)	0	100	100
20	g	238/245 (97%)	228 (96%)	10 (4%)	0	100	100
21	H	230/233 (99%)	216 (94%)	14 (6%)	0	100	100
21	h	230/233 (99%)	216 (94%)	14 (6%)	0	100	100
22	I	248/260 (95%)	230 (93%)	18 (7%)	0	100	100
22	i	248/260 (95%)	230 (93%)	18 (7%)	0	100	100
23	J	237/247 (96%)	223 (94%)	14 (6%)	0	100	100
23	j	237/247 (96%)	223 (94%)	14 (6%)	0	100	100
24	K	224/240 (93%)	212 (95%)	12 (5%)	0	100	100
24	k	224/240 (93%)	212 (95%)	12 (5%)	0	100	100
25	L	236/268 (88%)	223 (94%)	13 (6%)	0	100	100
25	l	236/268 (88%)	223 (94%)	13 (6%)	0	100	100
26	M	238/254 (94%)	216 (91%)	20 (8%)	2 (1%)	16	49
26	m	238/254 (94%)	216 (91%)	20 (8%)	2 (1%)	16	49
27	N	189/238 (79%)	183 (97%)	6 (3%)	0	100	100
27	n	189/238 (79%)	183 (97%)	6 (3%)	0	100	100
28	O	218/276 (79%)	209 (96%)	9 (4%)	0	100	100
28	o	218/276 (79%)	209 (96%)	9 (4%)	0	100	100
29	P	202/204 (99%)	191 (95%)	11 (5%)	0	100	100
29	p	202/204 (99%)	191 (95%)	11 (5%)	0	100	100
30	Q	197/201 (98%)	181 (92%)	15 (8%)	1 (0%)	24	57
30	q	197/201 (98%)	181 (92%)	15 (8%)	1 (0%)	24	57
31	R	199/262 (76%)	190 (96%)	9 (4%)	0	100	100
31	r	199/262 (76%)	190 (96%)	9 (4%)	0	100	100
32	S	211/240 (88%)	202 (96%)	9 (4%)	0	100	100
32	s	211/240 (88%)	202 (96%)	9 (4%)	0	100	100
33	T	213/263 (81%)	198 (93%)	15 (7%)	0	100	100
33	t	213/263 (81%)	198 (93%)	15 (7%)	0	100	100
All	All	13216/14843 (89%)	12036 (91%)	1136 (9%)	44 (0%)	37	65

5 of 44 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	Z	217	THR
10	d	200	PHE
12	f	808	ASN
12	f	853	VAL
14	B	354	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	U	700/816 (86%)	695 (99%)	5 (1%)	76	78
2	V	414/459 (90%)	412 (100%)	2 (0%)	81	80
3	W	416/416 (100%)	405 (97%)	11 (3%)	40	62
4	X	327/362 (90%)	326 (100%)	1 (0%)	86	83
5	Y	334/344 (97%)	331 (99%)	3 (1%)	70	76
6	Z	257/295 (87%)	246 (96%)	11 (4%)	26	52
7	a	333/336 (99%)	332 (100%)	1 (0%)	86	83
8	b	167/312 (54%)	167 (100%)	0	100	100
9	c	252/267 (94%)	248 (98%)	4 (2%)	55	69
10	d	231/293 (79%)	230 (100%)	1 (0%)	84	81
11	e	38/63 (60%)	38 (100%)	0	100	100
12	f	742/748 (99%)	734 (99%)	8 (1%)	65	74
13	A	298/372 (80%)	296 (99%)	2 (1%)	76	78
14	B	300/385 (78%)	299 (100%)	1 (0%)	86	83
15	C	340/346 (98%)	337 (99%)	3 (1%)	70	76
16	D	333/366 (91%)	328 (98%)	5 (2%)	57	70
17	E	341/353 (97%)	341 (100%)	0	100	100
18	F	340/379 (90%)	333 (98%)	7 (2%)	47	65
20	G	193/209 (92%)	191 (99%)	2 (1%)	68	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	g	193/209 (92%)	191 (99%)	2 (1%)	68	75
21	H	164/190 (86%)	163 (99%)	1 (1%)	78	79
21	h	164/190 (86%)	163 (99%)	1 (1%)	78	79
22	I	193/220 (88%)	192 (100%)	1 (0%)	81	80
22	i	193/220 (88%)	192 (100%)	1 (0%)	81	80
23	J	152/210 (72%)	151 (99%)	1 (1%)	76	78
23	j	152/210 (72%)	151 (99%)	1 (1%)	76	78
24	K	186/202 (92%)	184 (99%)	2 (1%)	65	74
24	k	186/202 (92%)	184 (99%)	2 (1%)	65	74
25	L	198/229 (86%)	194 (98%)	4 (2%)	48	66
25	l	198/229 (86%)	194 (98%)	4 (2%)	48	66
26	M	192/211 (91%)	192 (100%)	0	100	100
26	m	192/211 (91%)	192 (100%)	0	100	100
27	N	148/180 (82%)	147 (99%)	1 (1%)	76	78
27	n	148/180 (82%)	147 (99%)	1 (1%)	76	78
28	O	177/227 (78%)	177 (100%)	0	100	100
28	o	177/227 (78%)	177 (100%)	0	100	100
29	P	172/173 (99%)	172 (100%)	0	100	100
29	p	172/173 (99%)	172 (100%)	0	100	100
30	Q	164/171 (96%)	163 (99%)	1 (1%)	78	79
30	q	164/171 (96%)	163 (99%)	1 (1%)	78	79
31	R	153/201 (76%)	153 (100%)	0	100	100
31	r	153/201 (76%)	153 (100%)	0	100	100
32	S	174/198 (88%)	174 (100%)	0	100	100
32	s	174/198 (88%)	174 (100%)	0	100	100
33	T	175/214 (82%)	175 (100%)	0	100	100
33	t	175/214 (82%)	175 (100%)	0	100	100
All	All	11045/12582 (88%)	10954 (99%)	91 (1%)	70	77

5 of 91 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
16	D	360	LEU

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Mol	Chain	Res	Type
24	K	170	ILE
18	F	198	LEU
20	G	22	LEU
25	L	205	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 177 such sidechains are listed below:

Mol	Chain	Res	Type
17	E	364	GLN
27	N	158	ASN
18	F	417	HIS
22	I	149	GLN
33	T	213	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 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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
35	ATP	C	501	-	32,33,33	1.30	5 (15%)	48,52,52	1.82	13 (27%)
36	ADP	F	501	-	28,29,29	1.35	5 (17%)	43,45,45	1.86	10 (23%)
35	ATP	E	401	-	32,33,33	1.32	3 (9%)	48,52,52	1.97	11 (22%)
35	ATP	D	501	-	32,33,33	1.31	4 (12%)	48,52,52	1.78	8 (16%)

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
35	ATP	C	501	-	-	2/22/38/38	0/3/3/3
36	ADP	F	501	-	-	7/16/32/32	0/3/3/3
35	ATP	E	401	-	-	1/22/38/38	0/3/3/3
35	ATP	D	501	-	-	6/22/38/38	0/3/3/3

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	E	401	ATP	C5-C4	4.63	1.47	1.39
35	D	501	ATP	C5-C4	4.48	1.47	1.39
35	C	501	ATP	C5-C4	4.25	1.46	1.39
36	F	501	ADP	C5-C4	4.18	1.46	1.39
35	D	501	ATP	C5-N7	-2.77	1.34	1.39

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	E	401	ATP	C5-C4-N3	-6.77	117.39	126.72
35	D	501	ATP	C5-C4-N3	-5.72	118.84	126.72
35	E	401	ATP	N3-C4-N9	5.63	136.74	127.17
35	C	501	ATP	C5-C4-N3	-5.53	119.11	126.72
36	F	501	ADP	C5-C4-N3	-5.16	119.61	126.72

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
35	D	501	ATP	C5'-O5'-PA-O1A
35	D	501	ATP	C5'-O5'-PA-O2A

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Mol	Chain	Res	Type	Atoms
35	D	501	ATP	C5'-O5'-PA-O3A
36	F	501	ADP	PA-O3A-PB-O2B
36	F	501	ADP	PA-O3A-PB-O3B

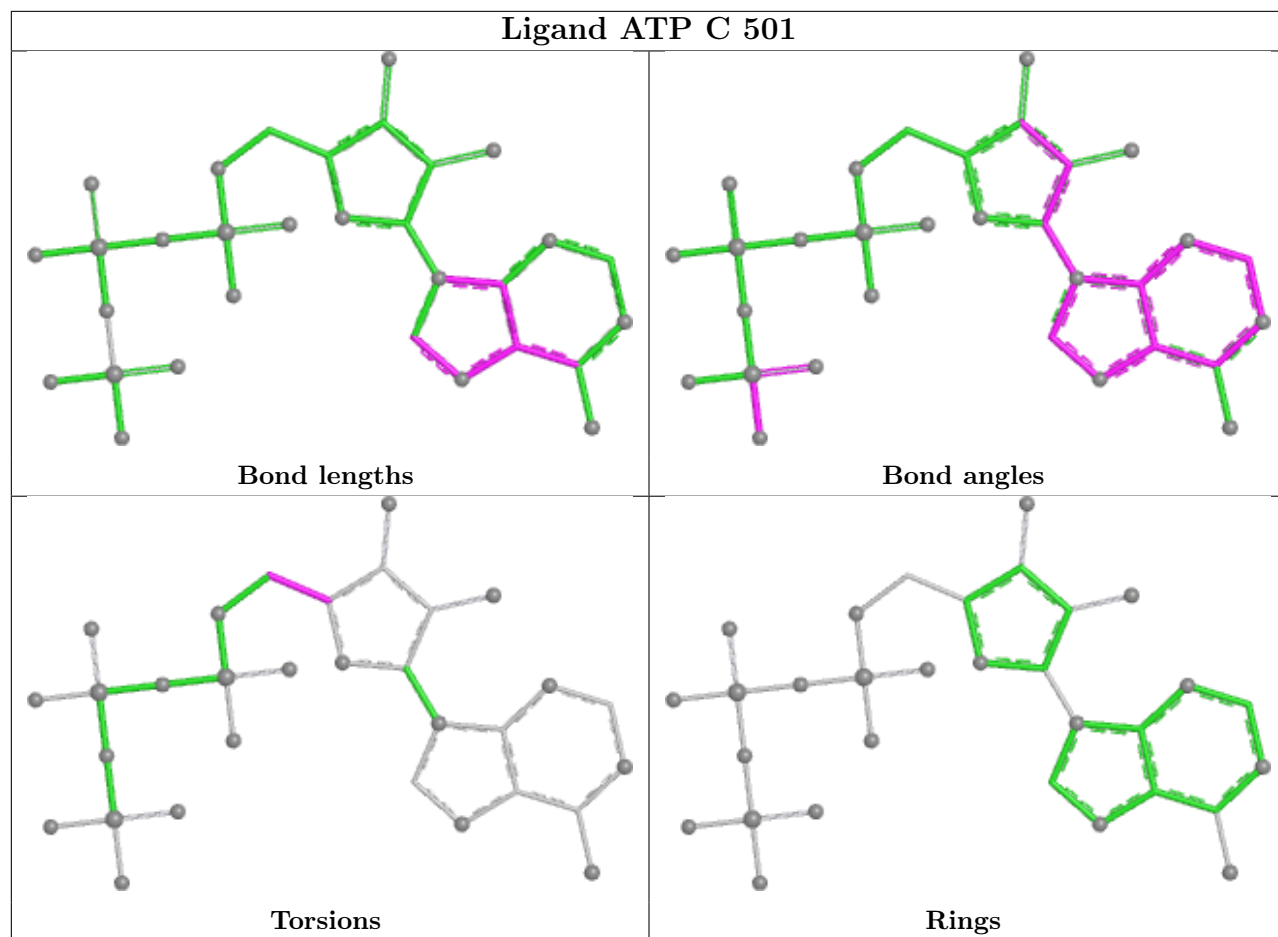
There are no ring outliers.

2 monomers are involved in 5 short contacts:

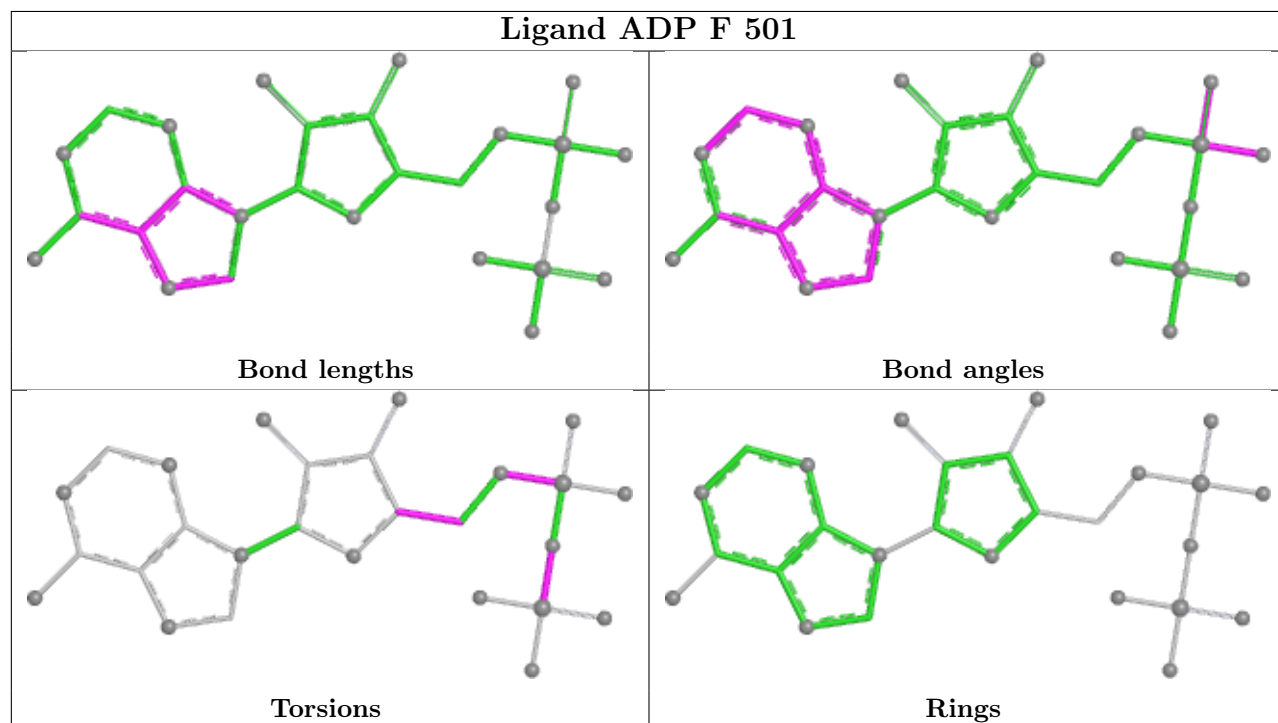
Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	C	501	ATP	3	0
35	E	401	ATP	2	0

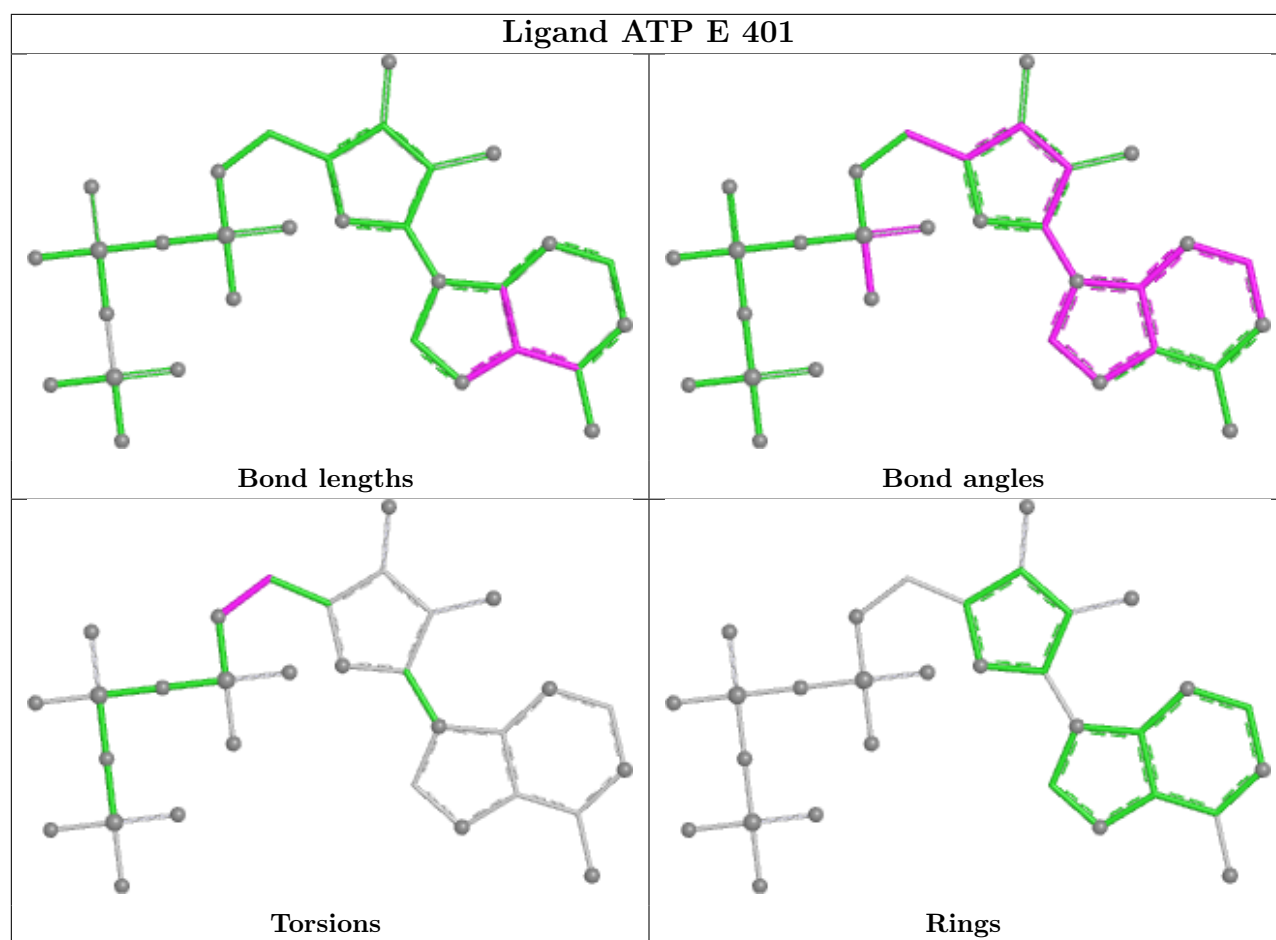
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

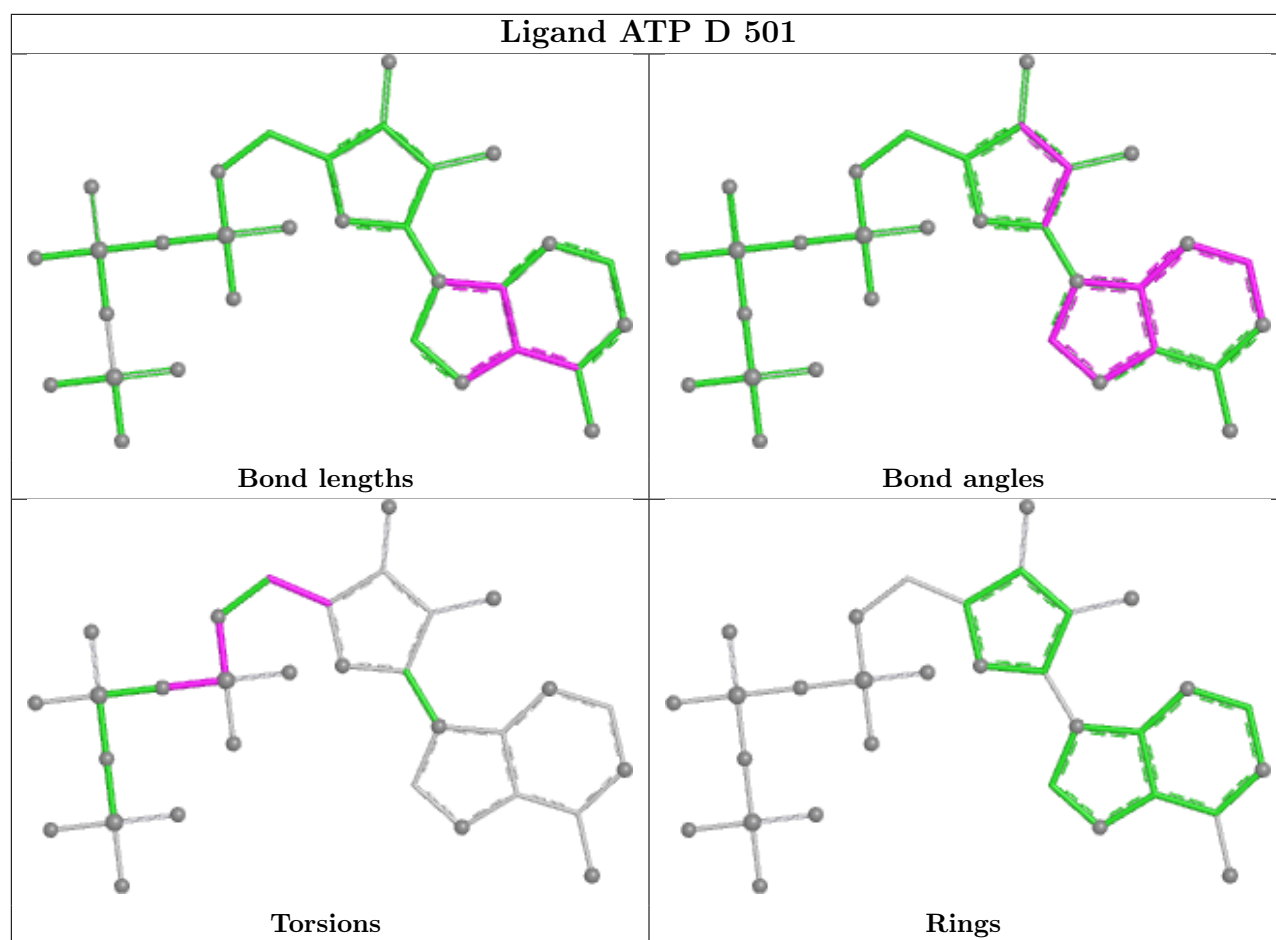
Ligand ATP C 501



Ligand ADP 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.

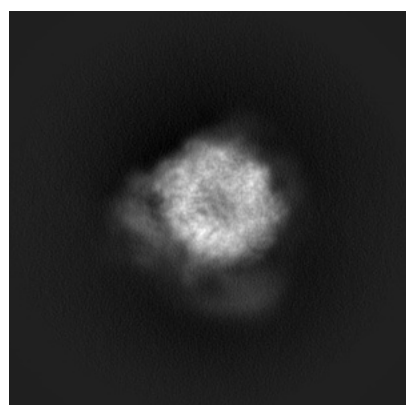
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9220. These allow visual inspection of the internal detail of the map and identification of artifacts.

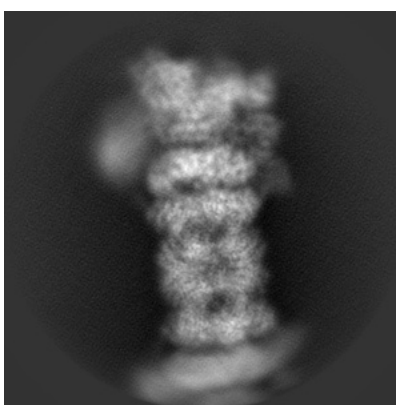
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

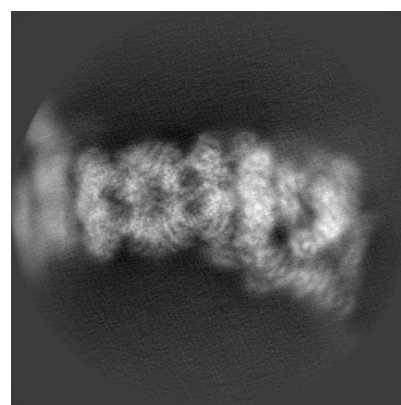
6.1.1 Primary map



X



Y

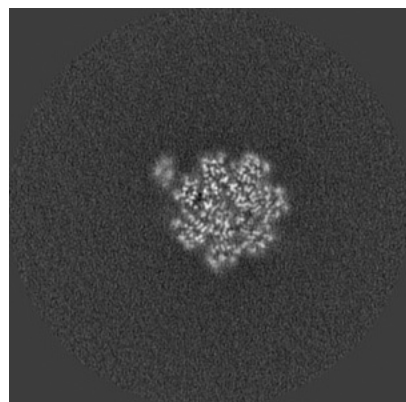


Z

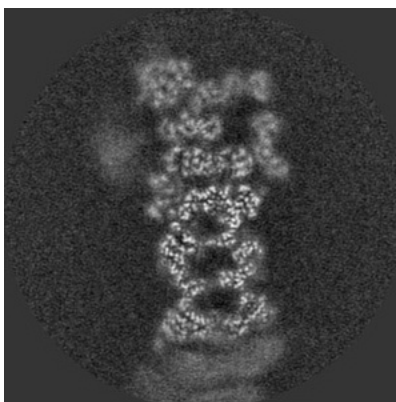
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

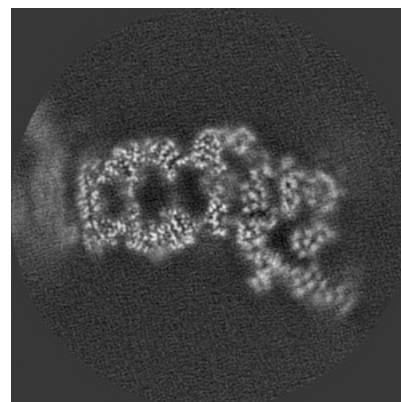
6.2.1 Primary map



X Index: 300



Y Index: 300

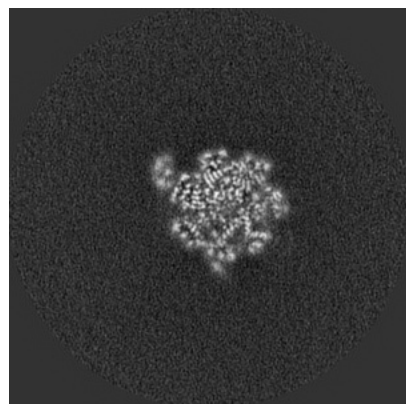


Z Index: 300

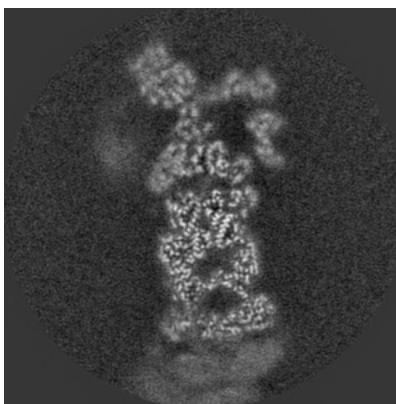
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

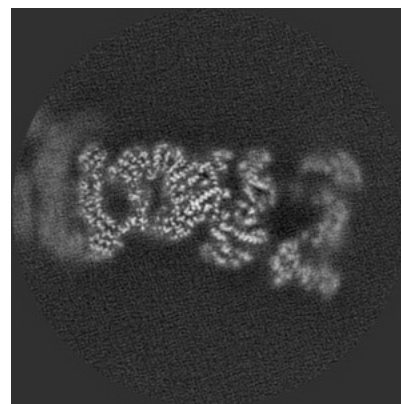
6.3.1 Primary map



X Index: 307



Y Index: 287

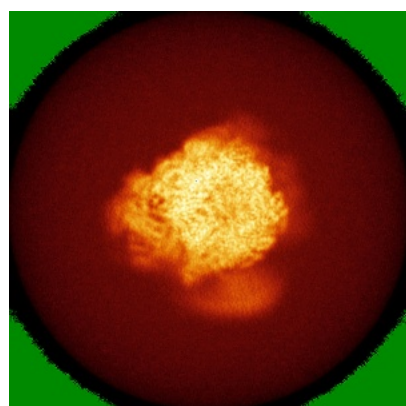


Z Index: 343

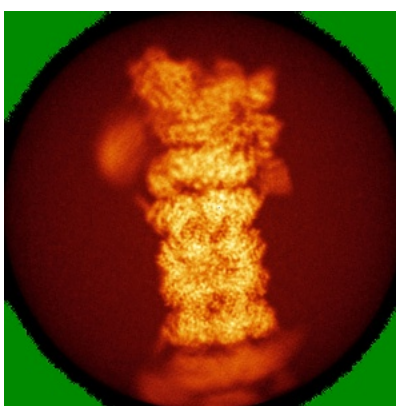
The images above show the largest variance slices of the map in three orthogonal directions.

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

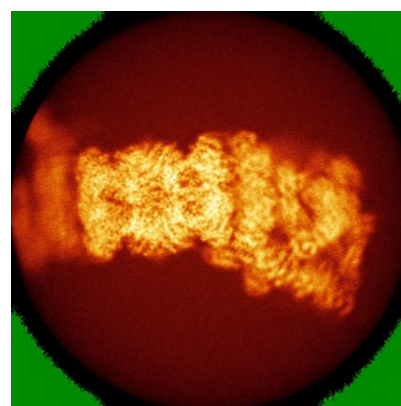
6.4.1 Primary map



X



Y

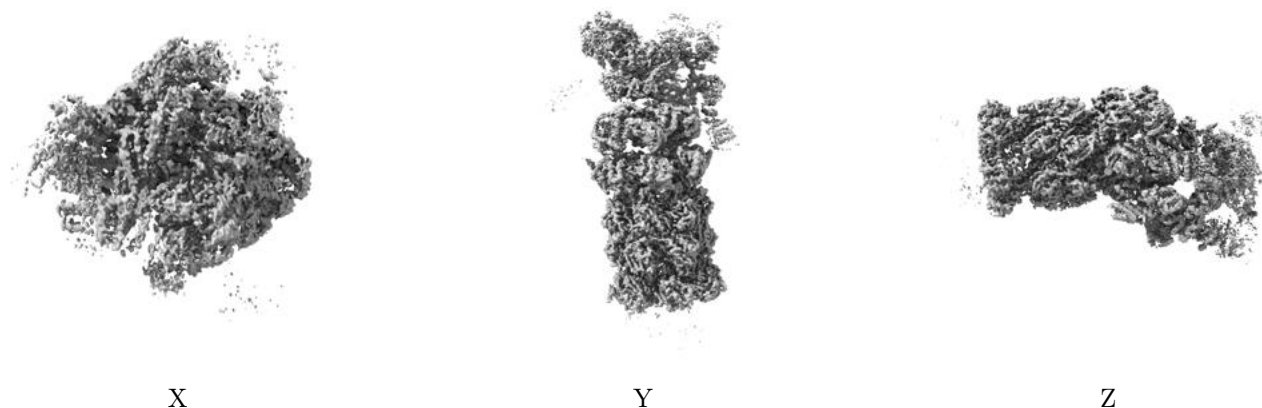


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.006. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

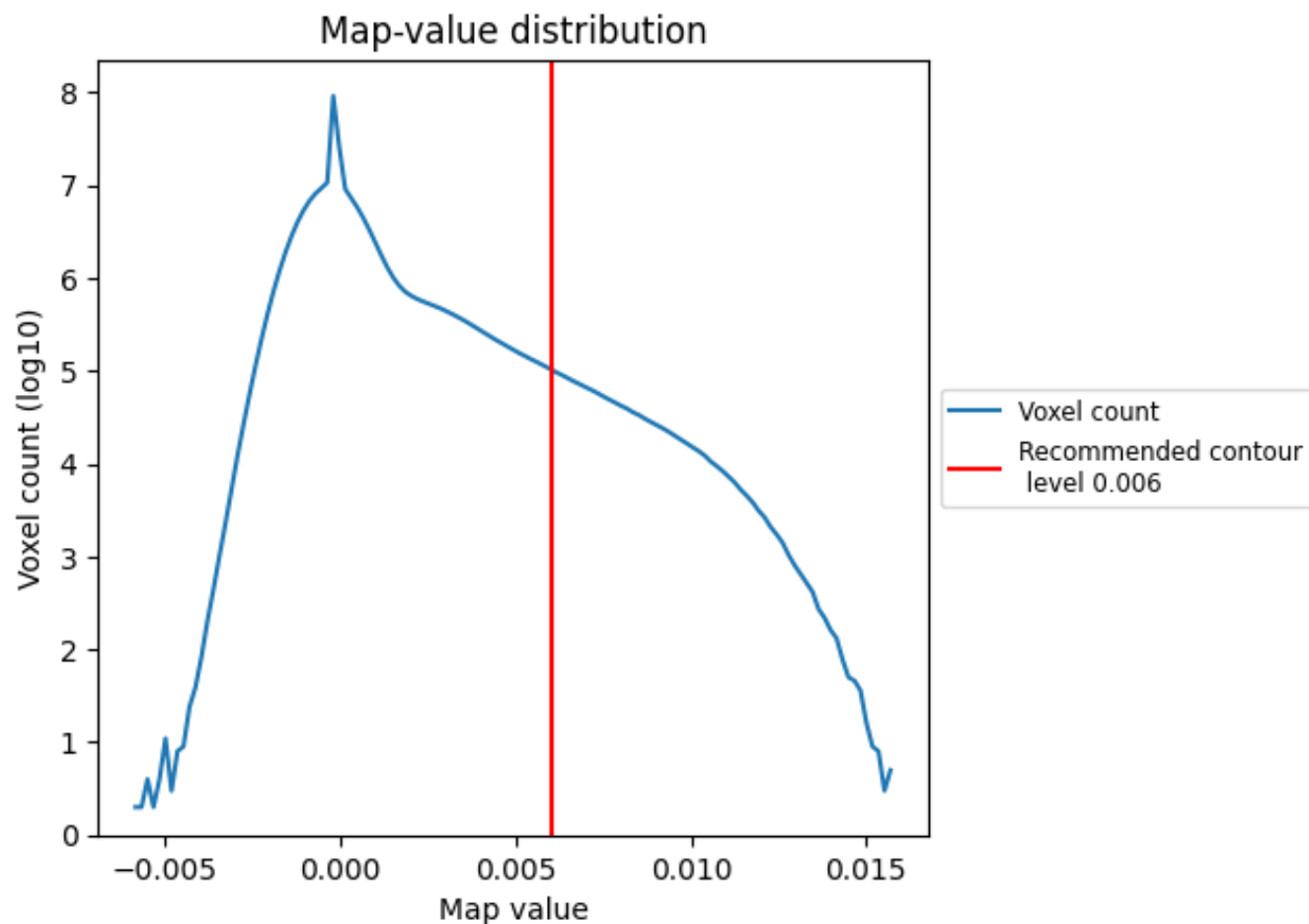
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

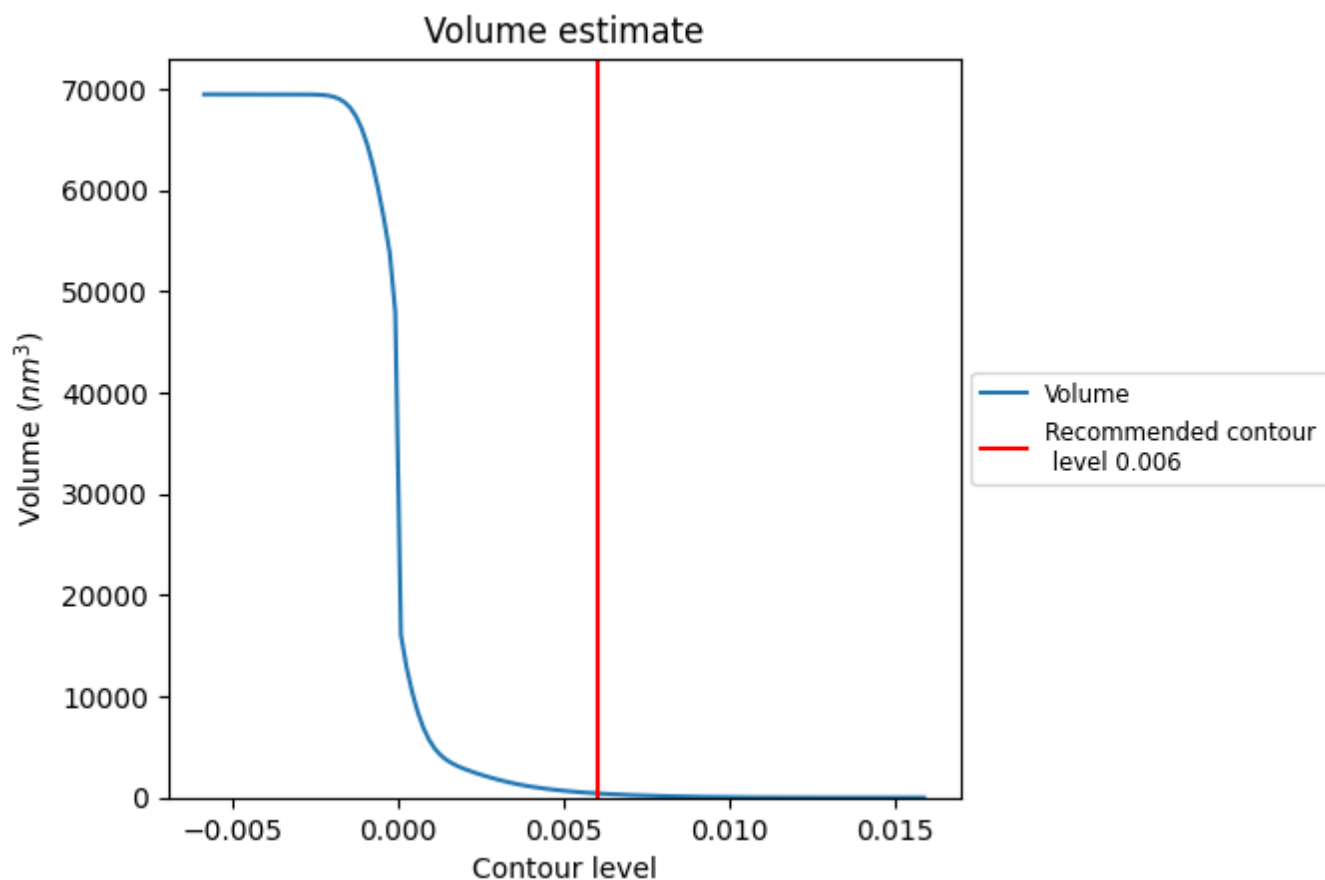
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

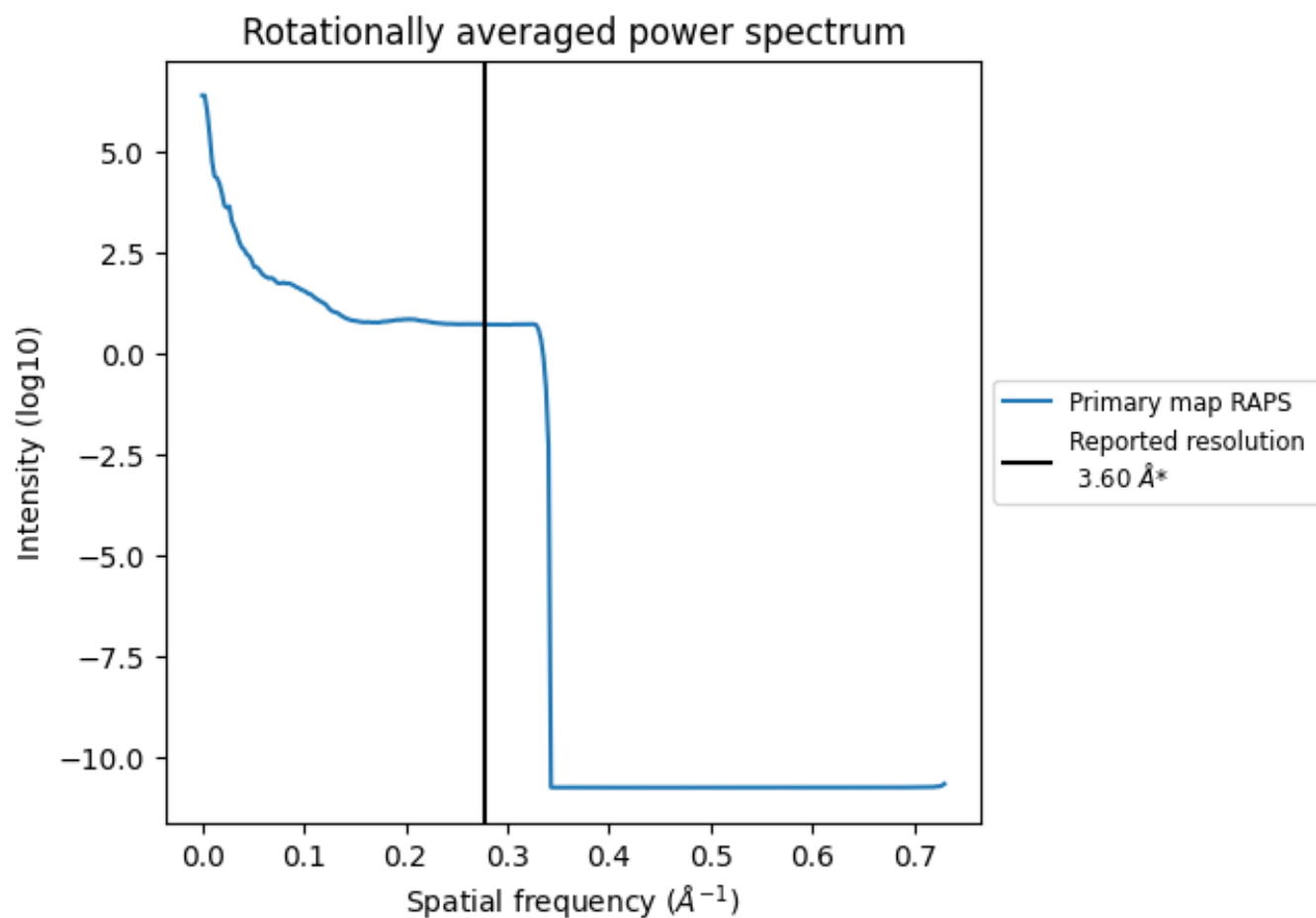
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 414 nm³; this corresponds to an approximate mass of 374 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

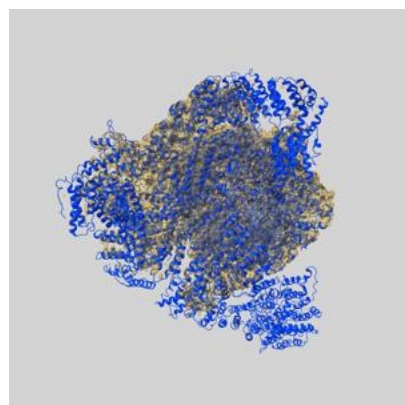
8 Fourier-Shell correlation

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

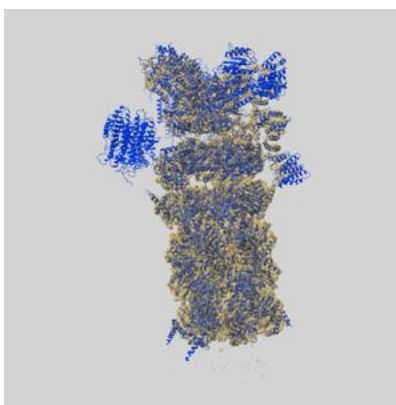
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-9220 and PDB model 6MSH. Per-residue inclusion information can be found in section [3](#) on page [12](#).

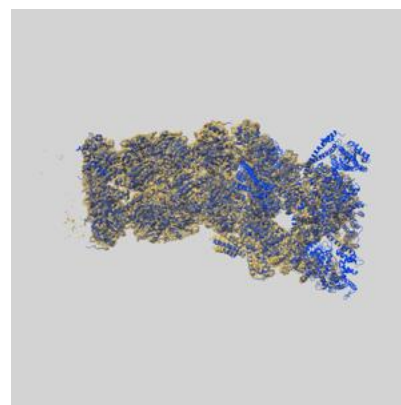
9.1 Map-model overlay [i](#)



X



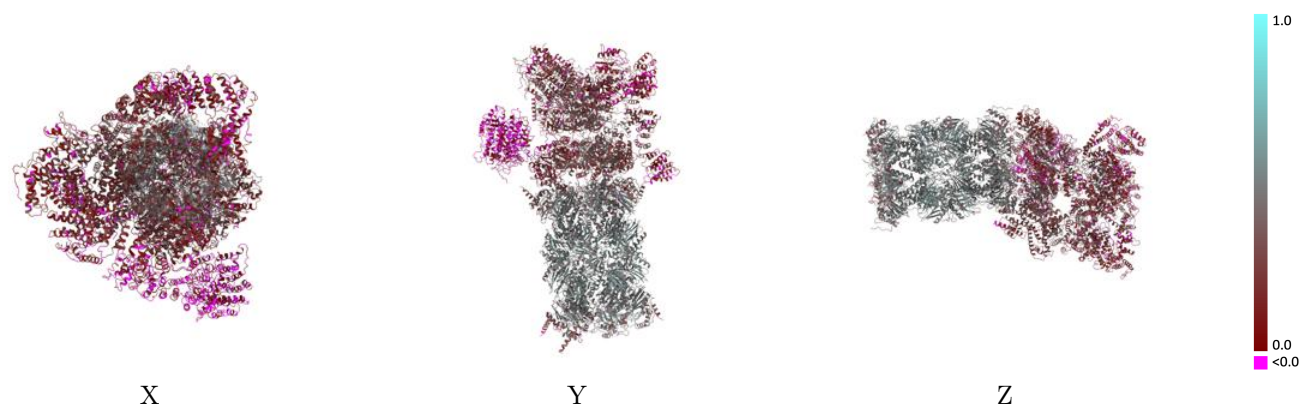
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.006 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

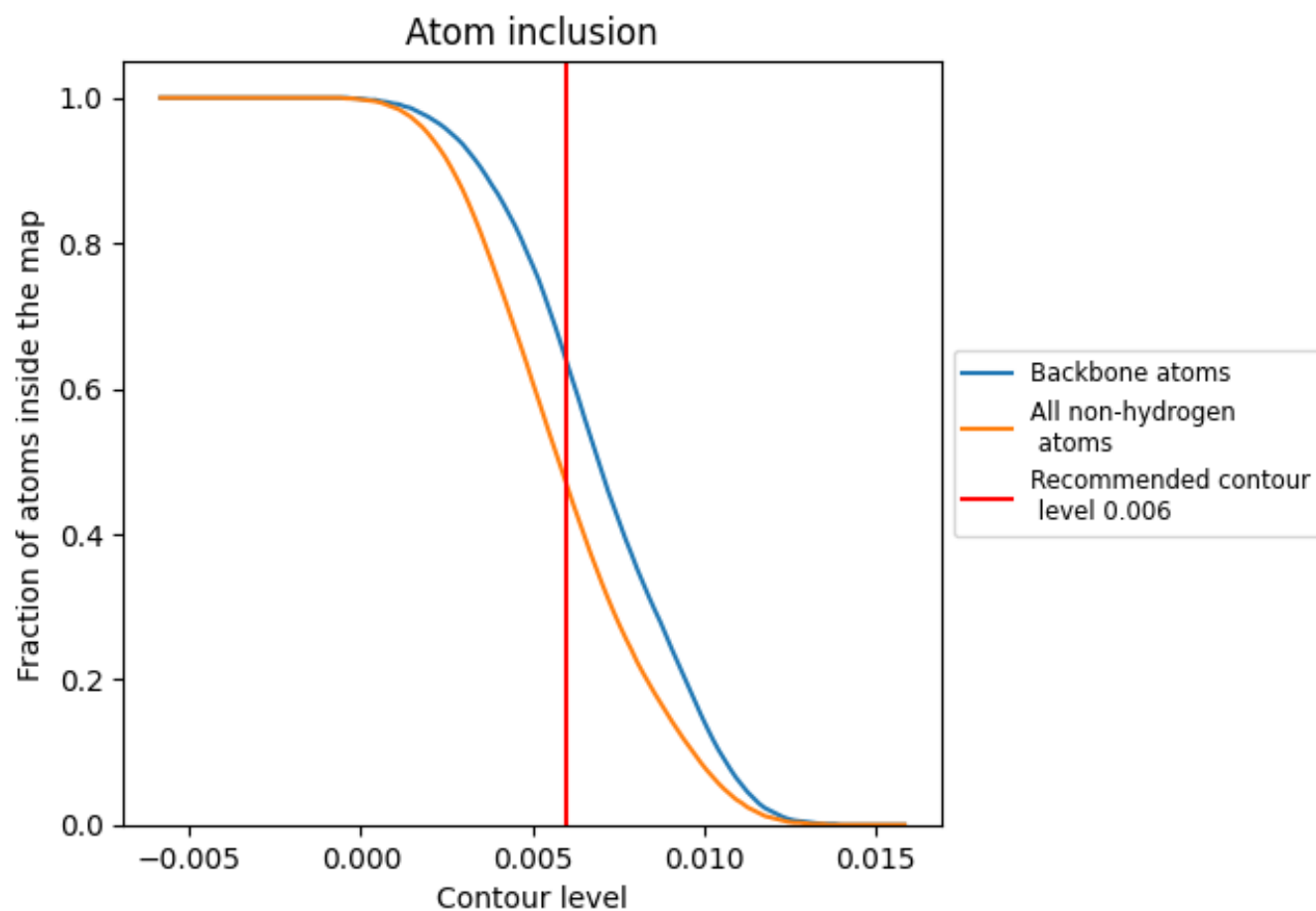


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 64% of all backbone atoms, 47% 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 (0.006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4680	 0.3220
A	 0.3550	 0.2230
B	 0.2200	 0.1930
C	 0.4110	 0.2770
D	 0.5110	 0.3430
E	 0.4630	 0.3010
F	 0.4250	 0.2540
G	 0.7230	 0.4480
H	 0.7700	 0.4580
I	 0.6950	 0.4170
J	 0.6640	 0.4090
K	 0.6590	 0.4270
L	 0.7160	 0.4530
M	 0.6960	 0.4230
N	 0.7810	 0.4940
O	 0.7640	 0.4890
P	 0.7680	 0.4970
Q	 0.7500	 0.4730
R	 0.7840	 0.5020
S	 0.7250	 0.4900
T	 0.7680	 0.4990
U	 0.2320	 0.2070
V	 0.1610	 0.1790
W	 0.2420	 0.1690
X	 0.5600	 0.2920
Y	 0.5320	 0.2640
Z	 0.2610	 0.2130
a	 0.1620	 0.1660
b	 0.0210	 0.1490
c	 0.3060	 0.2540
d	 0.0730	 0.1700
e	 0.2580	 0.1920
f	 0.0000	 0.0170
g	 0.6010	 0.4430
h	 0.6160	 0.4520



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Chain	Atom inclusion	Q-score
i	 0.5360	 0.4160
j	 0.4980	 0.3920
k	 0.5690	 0.4300
l	 0.6780	 0.4630
m	 0.6230	 0.4350
n	 0.7570	 0.5040
o	 0.7220	 0.4950
p	 0.7370	 0.5030
q	 0.7320	 0.4850
r	 0.7780	 0.5130
s	 0.7450	 0.4980
t	 0.7790	 0.5080
v	 0.0730	 0.2000