



Full wwPDB EM Validation Report ⓘ

Oct 26, 2024 – 06:50 PM EDT

PDB ID : 6MSH
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 Full wwPDB EM Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

The types of validation reports are described at

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

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

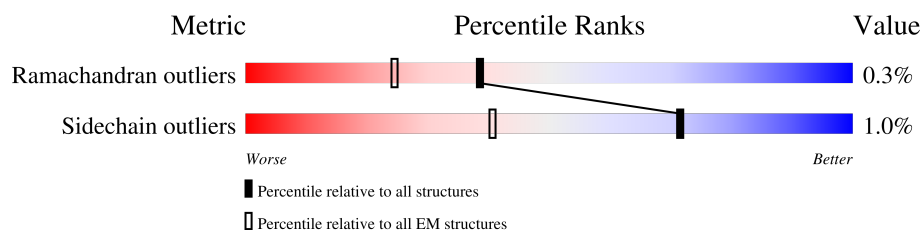
EMDB validation analysis : 0.0.1.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

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)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	U	953	<div> <div>64%</div> <div>85%</div> <div>14%</div> </div>
2	V	533	<div> <div>75%</div> <div>89%</div> <div>10%</div> </div>
3	W	456	<div> <div>71%</div> <div>97%</div> <div>.</div> </div>
4	X	422	<div> <div>17%</div> <div>90%</div> <div>10%</div> </div>
5	Y	389	<div> <div>27%</div> <div>96%</div> <div>..</div> </div>
6	Z	324	<div> <div>67%</div> <div>83%</div> <div>5%</div> <div>12%</div> </div>
7	a	376	<div> <div>82%</div> <div>98%</div> <div>..</div> </div>
8	b	377	<div> <div>50%</div> <div>51%</div> <div>49%</div> </div>
9	c	309	<div> <div>61%</div> <div>90%</div> <div>7%</div> </div>

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Mol	Chain	Length	Quality of chain
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	
25	L	268	
25	l	268	
26	M	254	
26	m	254	
27	N	238	

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Mol	Chain	Length	Quality of chain
27	n	238	 80%20%
28	O	276	 80%20%
28	o	276	 5%80%20%
29	P	204	 100%
29	p	204	 100%
30	Q	201	 98%..
30	q	201	 98%..
31	R	262	 76%23%
31	r	262	 76%23%
32	S	240	 5%89%11%
32	s	240	 89%11%
33	T	263	 82%18%
33	t	263	 82%18%

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		

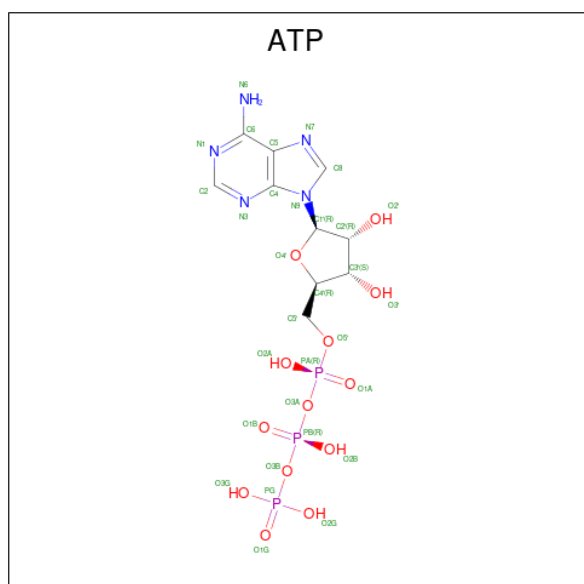
- Molecule 33 is a protein called Proteasome subunit beta type-4.

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 (three-letter code: ZN) (formula: Zn).

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

- Molecule 35 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



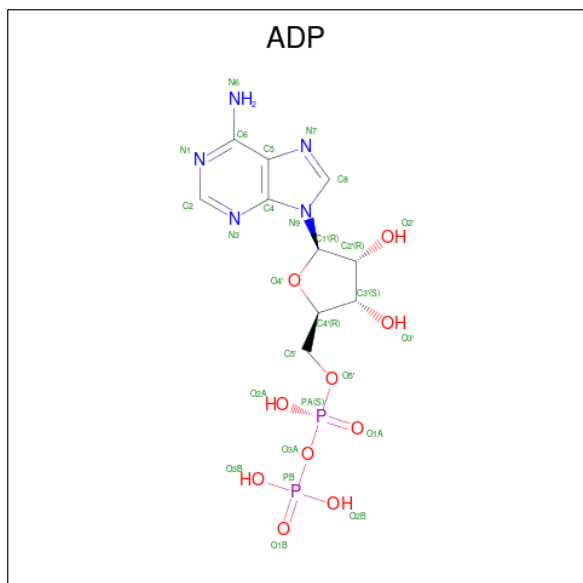
Mol	Chain	Residues	Atoms					AltConf
35	C	1	Total	C	N	O	P	0
			31	10	5	13	3	

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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	

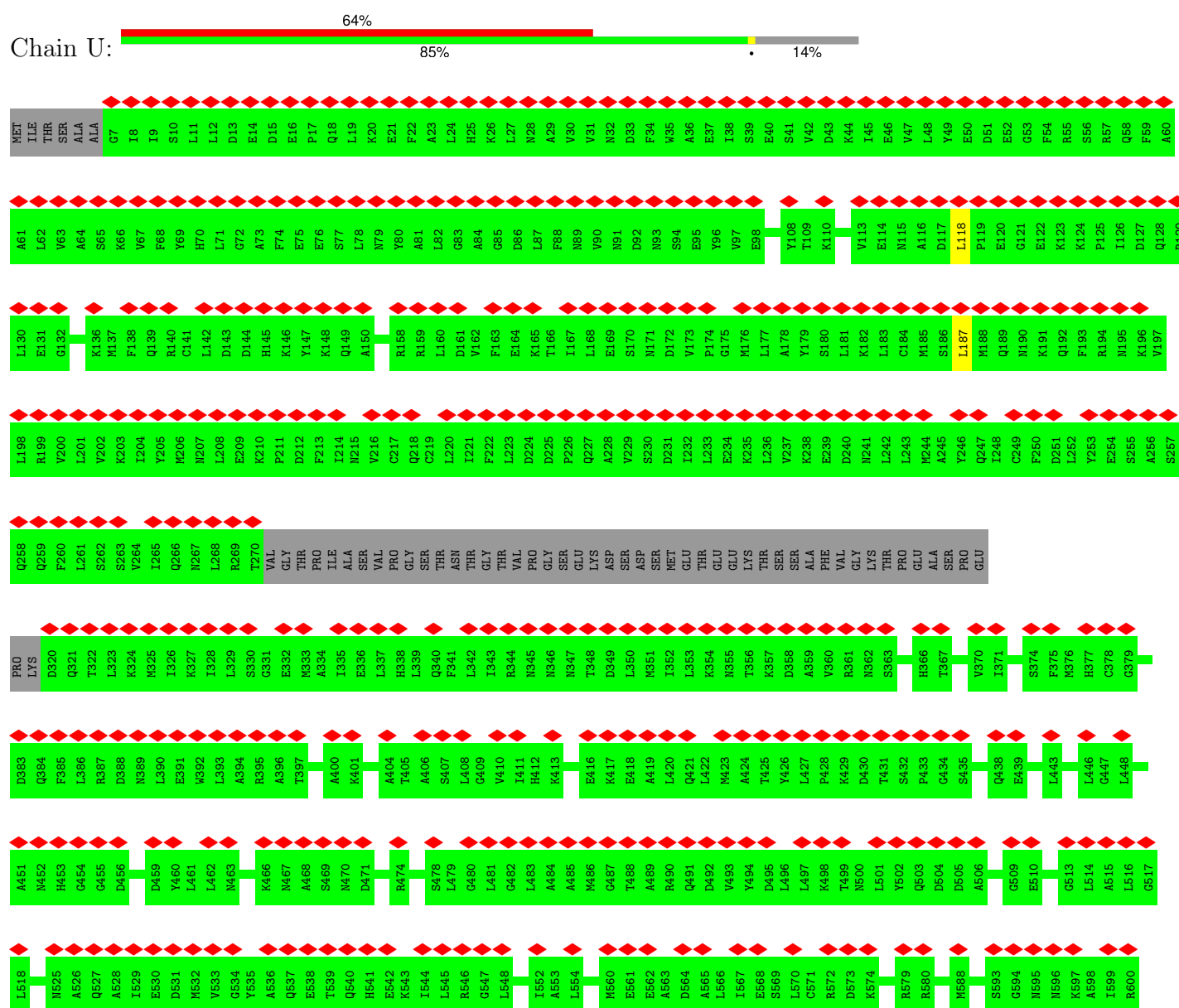
- Molecule 36 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

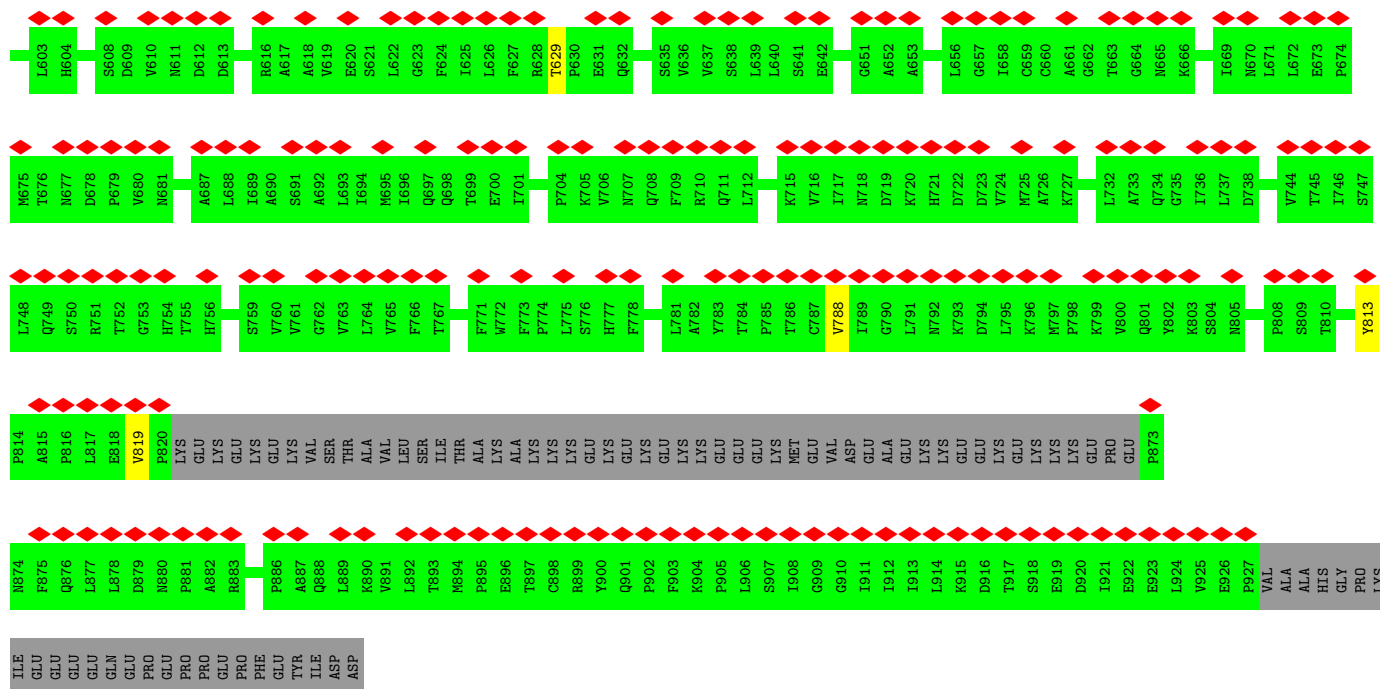


3 Residue-property plots

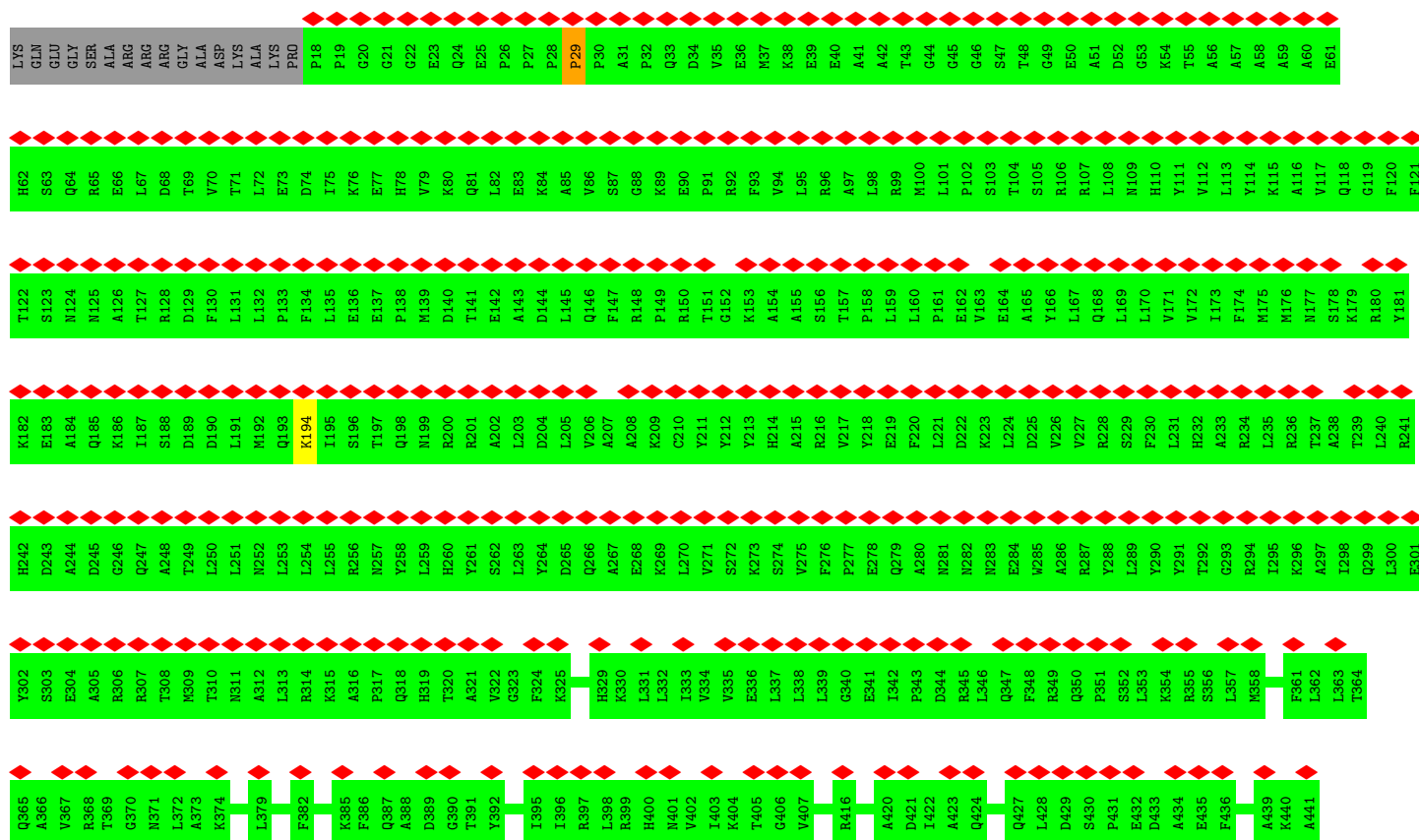
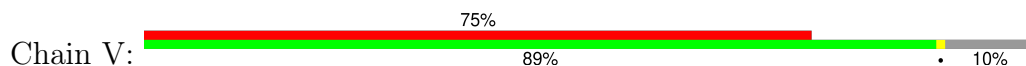
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

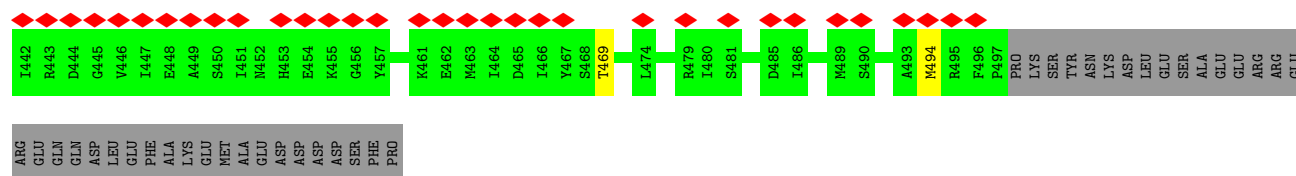
- Molecule 1: 26S proteasome non-ATPase regulatory subunit 1





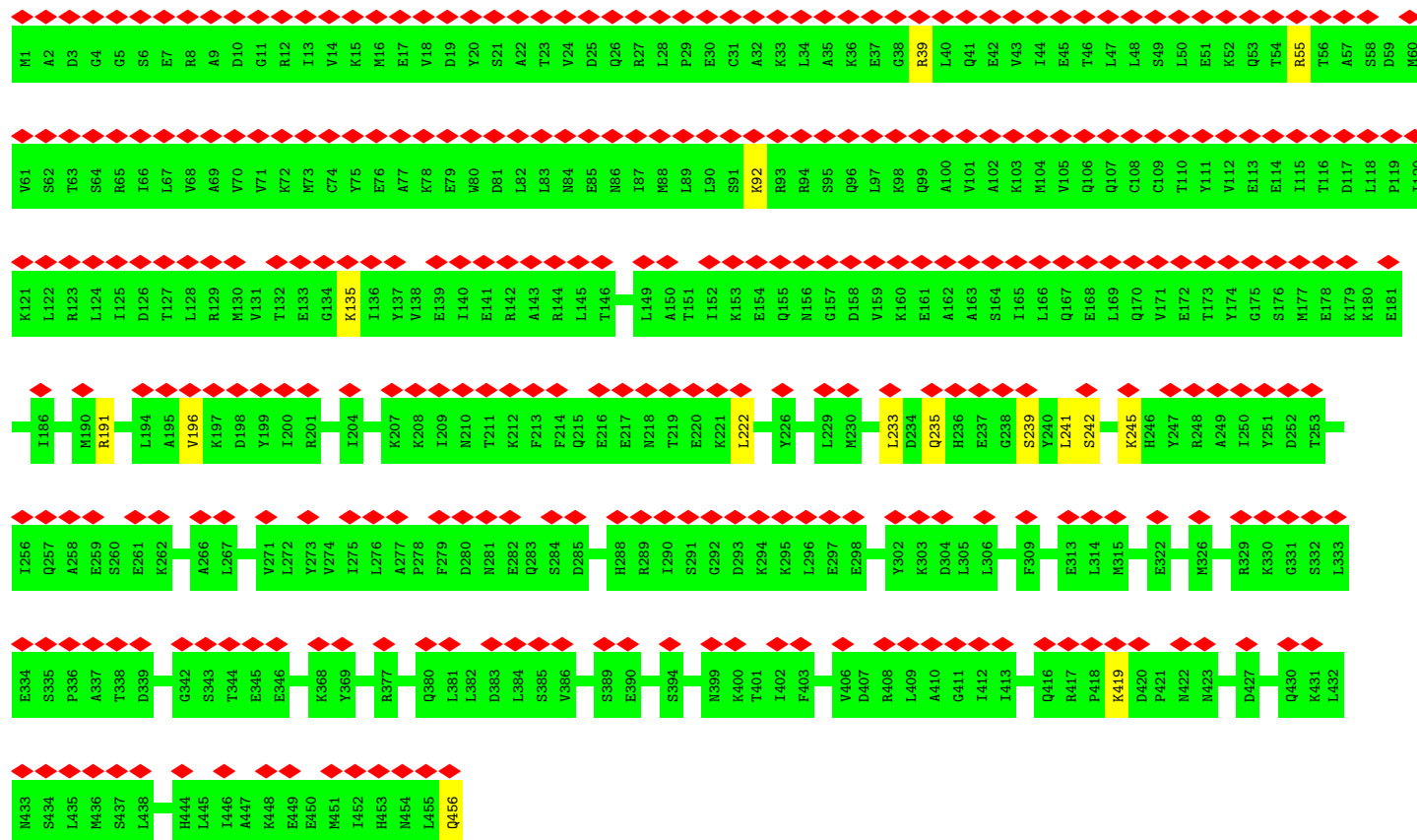
- Molecule 2: 26S proteasome non-ATPase regulatory subunit 3





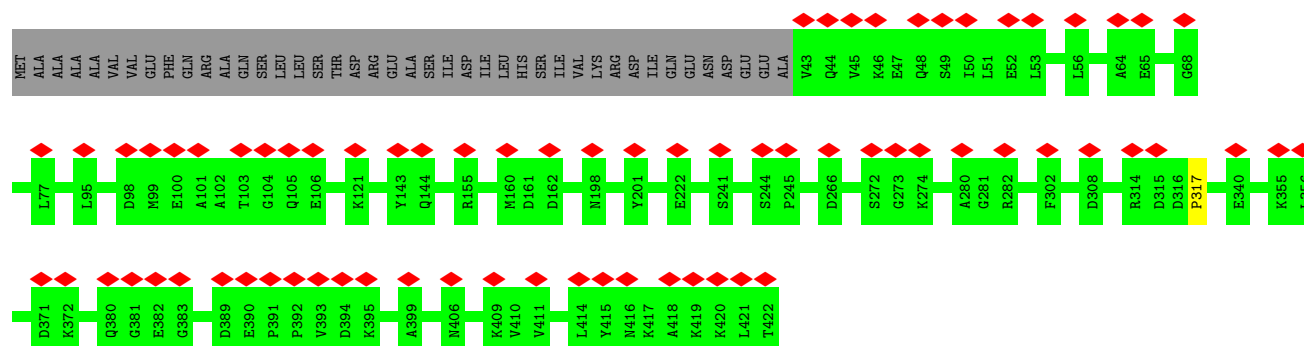
• Molecule 3: 26S proteasome non-ATPase regulatory subunit 12

Chain W:

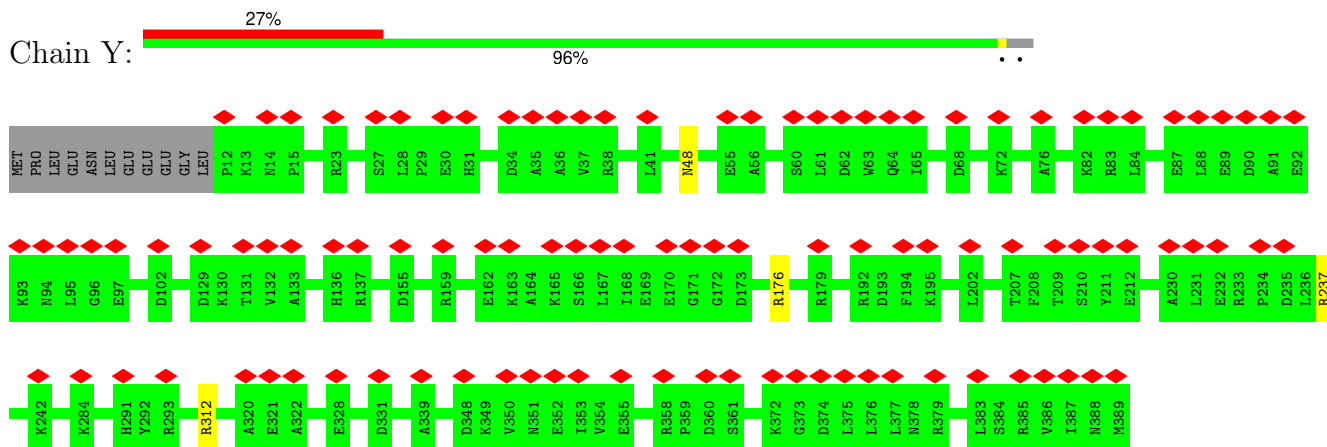


• Molecule 4: 26S proteasome non-ATPase regulatory subunit 11

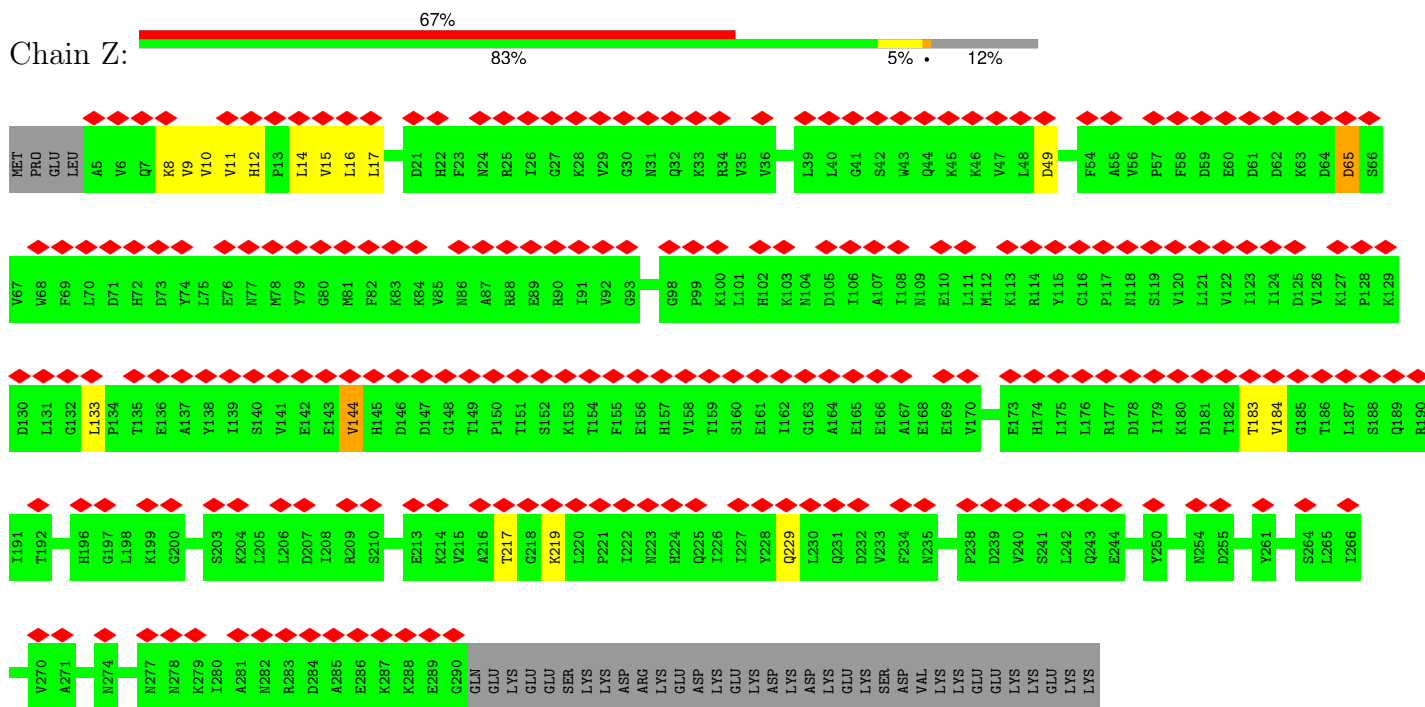
Chain X:

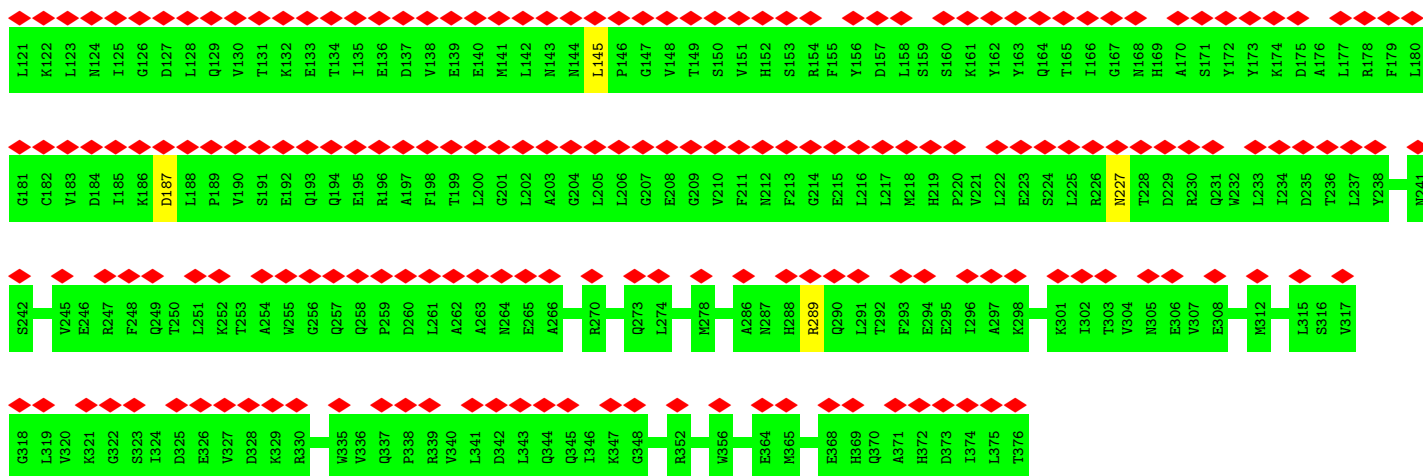


• Molecule 5: 26S proteasome non-ATPase regulatory subunit 6

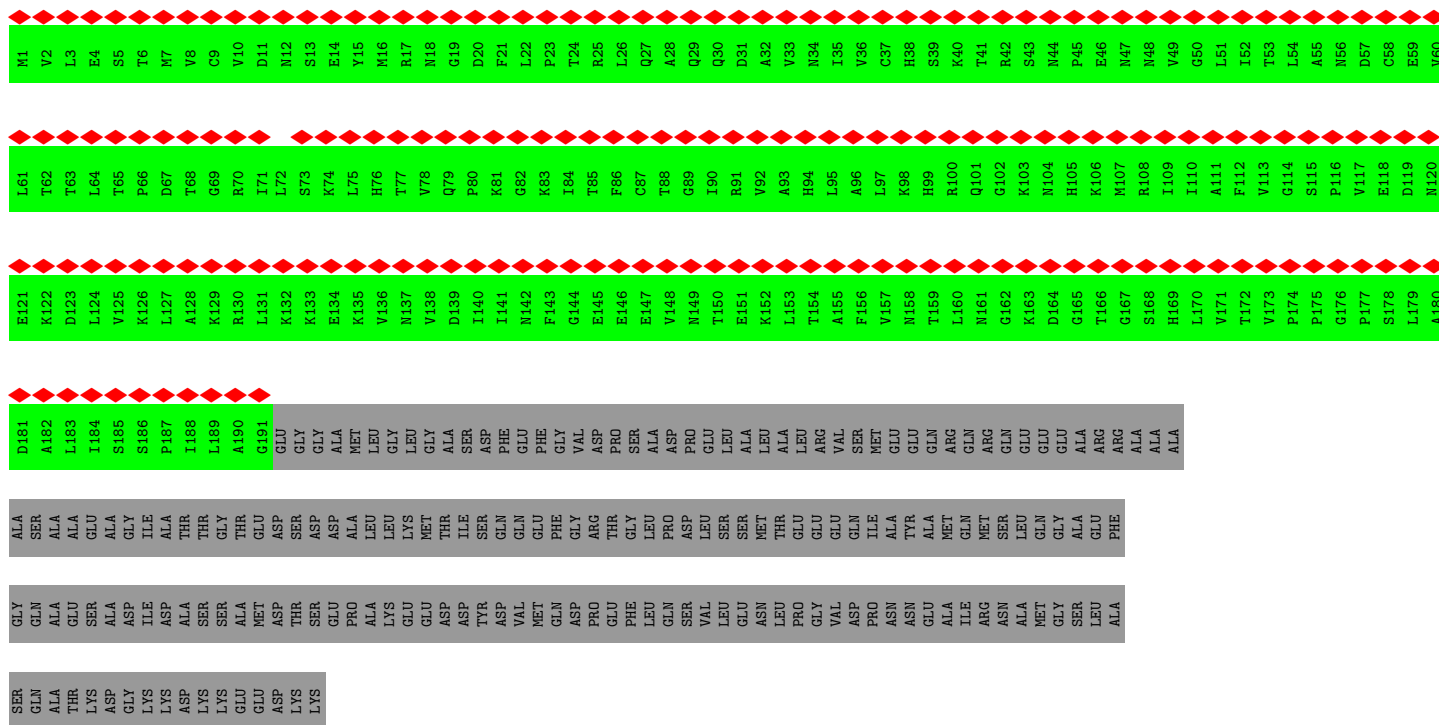


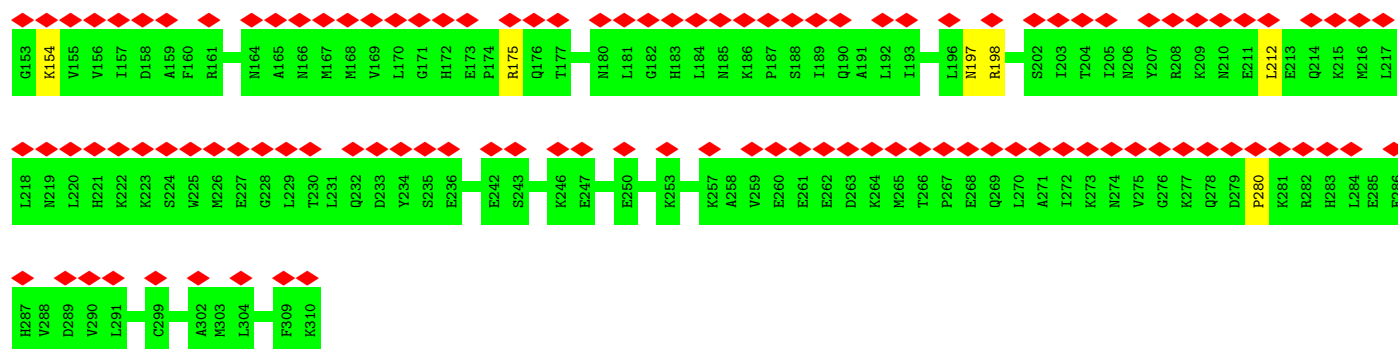
• Molecule 6: 26S proteasome non-ATPase regulatory subunit 7





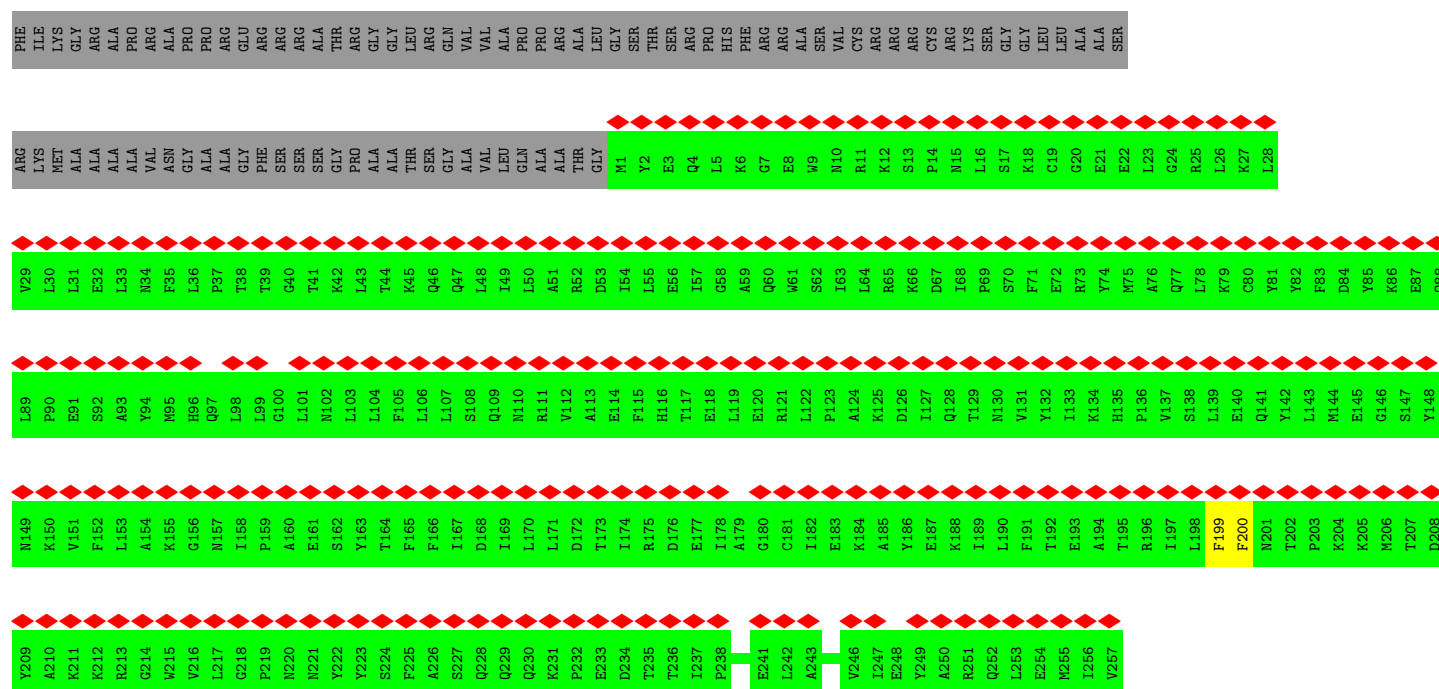
• Molecule 8: 26S proteasome non-ATPase regulatory subunit 4





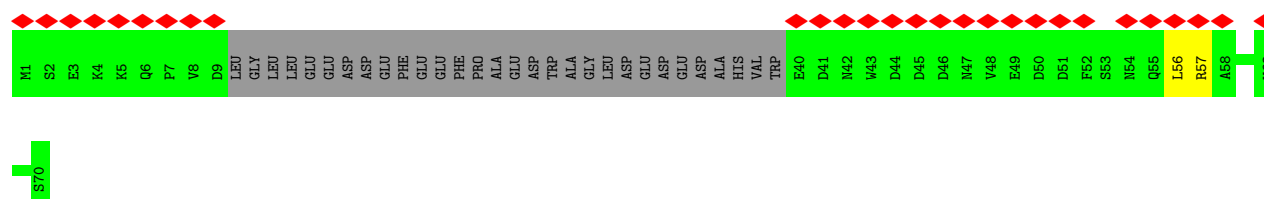
- Molecule 10: 26S proteasome non-ATPase regulatory subunit 8

Chain d: 71% 73% 26%



- Molecule 11: 26S proteasome complex subunit SEM1

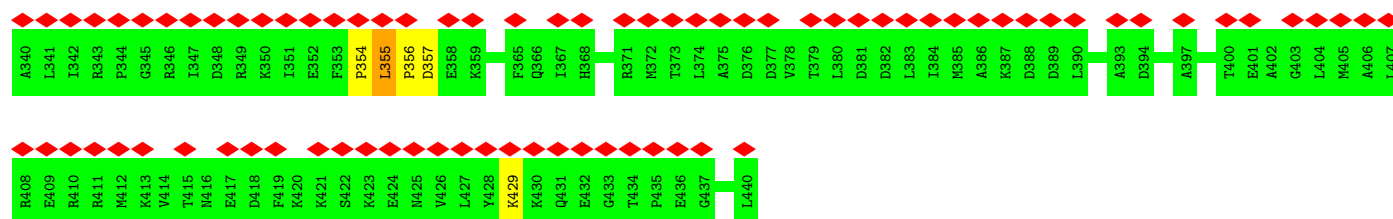
Chain e: 40% 54% 43%



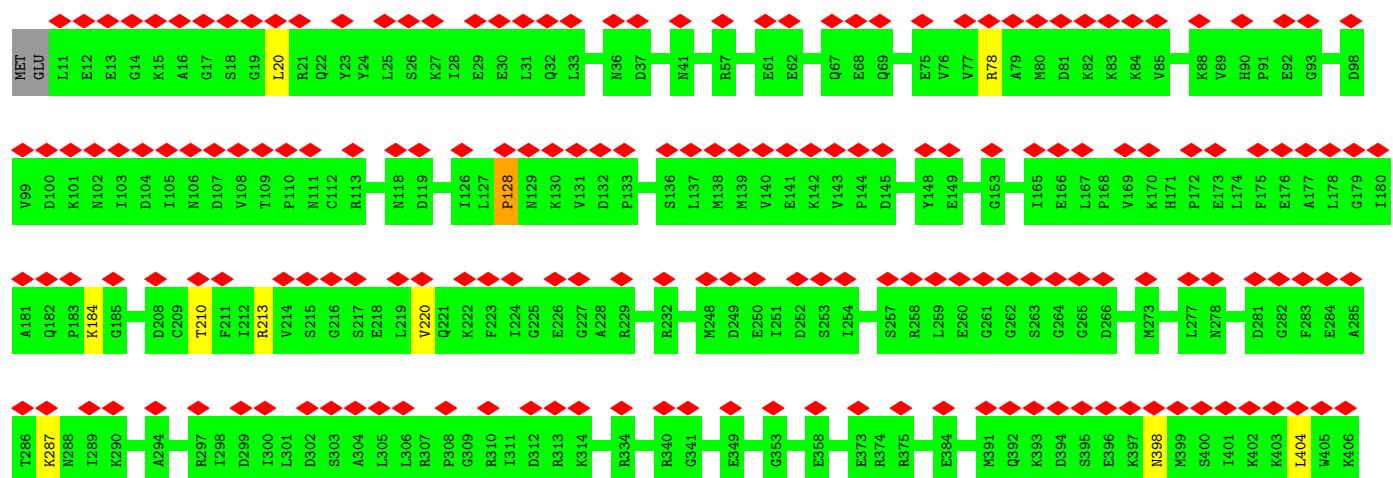
- Molecule 12: 26S proteasome non-ATPase regulatory subunit 2

Chain f: 99% 94%

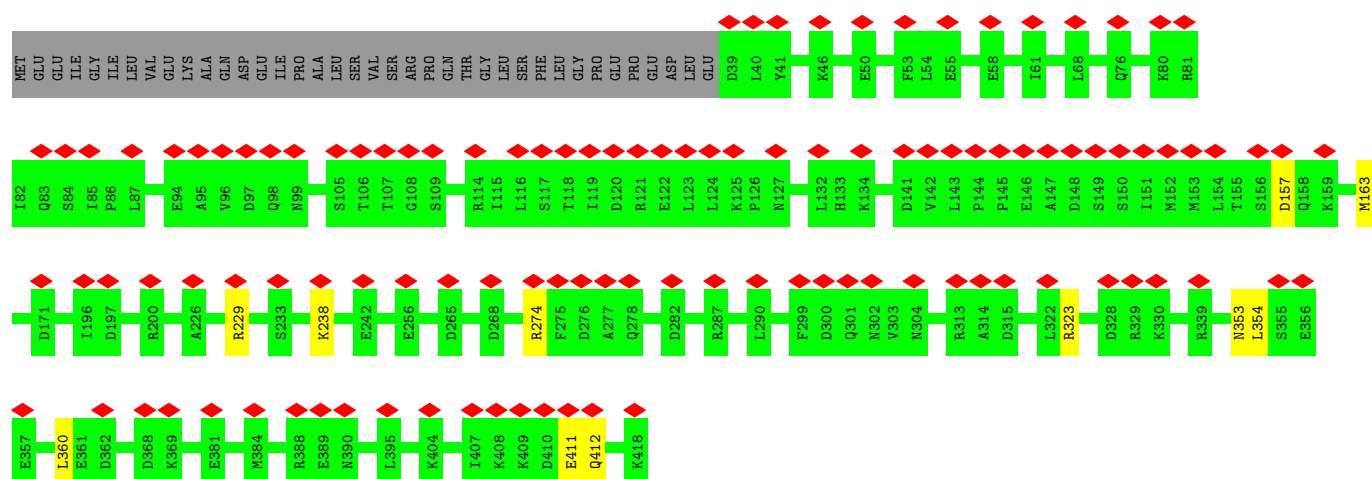
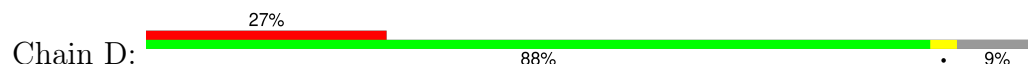
MET	GLU	GLU	G4	G5	R6	D7	K8	A9	P10	V11	Q12	P13	Q14	Q15	S16	P17	A18	A19	A20	P21	G22	G23	T24	D25	E26	K27	P28	S29	G30	K31	E32	R33	R34	D35	A36	G37	D38	K39	D40	K41	E42	Q43	E44	L45	S46	E47	E48	D49	K50	Q51	L52	Q53	D54	E55	L56	E57	M58	L59	V60	
E61	R62	L63	G64	E65	K66	D67	T68	S69	L70	V71	R72	P73	A74	L75	E76	L77	E78	L79	R80	Q81	I82	R83	S84	S85	T86	T87	S88	R89	T90	S91	V92	P93	K94	P95	L96	K97	P98	L99	R100	P101	H102	Y103	G104	L105	L106	K107	E108	I109	K110	Y110	E111	L112	M113	A114	P115	G116	E117	N118	K119	R120
F121	A122	A123	D124	L125	I126	S127	V128	L129	A130	M131	T132	M133	S134	G135	E136	L137	E138	C139	L140	K141	Y142	R143	L144	V145	G146	S147	Q148	E149	E150	L151	S152	S153	W154	G155	H156	E157	Y158	V159	R160	H161	L162	A163	G164	E165	L166	A167	K168	E169	I170	Q171	E172	L173	D174	D175	A176	E177	K178	V179	Q180	
R181	E182	P183	L184	L185	T186	L187	V188	K189	E190	I191	V192	P193	Y194	M195	M196	A197	H198	M199	A200	E201	H202	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	Y232	L233	T234	S235	C236	L237	N238	Y239	V240	
P241	E242	P243	E244	N245	S246	A247	L248	L249	R250	C251	A252	L253	G254	V255	P256	R257	K258	P259	S260	R261	F262	P263	E264	A265	L266	R267	L268	A269	L270	M271	L272	N273	D274	M275	E276	L277	V278	E279	D280	I281	F282	T283	S284	C285	K286	D287	L288	V289	V290	Q291	K292	Q293	M294	A295	F296	M297	L298	G299	R300	
H301	G302	V303	F304	L305	E306	L307	S308	E309	D310	V311	E312	E313	Y314	E315	D316	L317	T318	E319	I320	N321	S322	E323	V324	Q325	L326	N327	S328	N329	F330	L331	A332	L333	A334	R335	E336	L337	D338	I339	M340	E341	P342	K343	V344	P345	D346	D347	L348	Y349	K350	T351	H352	L353	E354	N355	N356	R357	G358	G359	G360	
S361	G362	S363	Q364	V365	D366	S367	A368	R369	M370	N371	L372	A373	Y374	S375	F376	V377	N378	G379	F380	V381	N382	A383	A384	F385	G386	Q387	D388	K389	L390	L391	T392	D393	D394	G395	N396	K397	W398	L399	Y400	K401	N402	K403	D404	H405	G406	M407	L408	S409	V410	A411	A412	S413	L414	G415	M416	I417	L418	L419	W420	
D421	V422	D423	Q424	G425	L426	T427	Q428	L429	D430	K431	Y432	A433	Y434	S435	S436	E437	L438	Y439	I440	K441	S442	G443	A444	L445	L446	A447	C448	G449	L450	V451	N452	S453	E454	V455	N456	M457	E458	C459	D460	P461	L462	L463	A464	L465	L466	S467	D468	Y469	V470	L471	H472	M473	S474	N475	T476	M477	L478	G480		
S481	I482	F483	Q484	L485	Q486	L487	A488	Y489	A490	G491	S492	M493	R494	E495	D496	V497	L498	T499	L500	L501	L502	P503	V504	M505	G506	D507	S508	K509	S510	S511	M512	E513	V514	A515	G516	V517	T518	A519	L520	A521	G522	G523	M524	I525	A526	V527	G528	S529	C530	N531	G532	D533	V534	T535	S536	T537	I538	L539	Q540	
T541	I542	M543	E544	K545	S546	E547	T548	E549	L550	K551	D552	T553	Y554	A555	R556	W557	L558	P559	L560	G561	L562	G563	E564	N565	H566	L567	G568	K569	G570	E571	A572	I573	E574	A575	I576	L577	A578	A579	L580	E581	V582	V583	S584	E585	P586	F587	S588	S589	F590	A591	N592	T593	L594	V595	D596	V597	C598	A599	Y600	
A601	G602	S603	G604	N605	V606	L607	K608	V609	Q610	Q611	L612	L613	H614	I615	C616	S617	E618	H619	F620	D621	S622	K623	E624	K625	E626	E627	D628	K629	D630	K631	K632	E633	K634	K635	D636	K637	D638	K639	K640	E641	A642	P643	A644	D645	M646	G647	A648	H649	Q650	G651	V652	A653	V654	L655	G656	I657	D658	L659	I660	
A661	M662	G663	E664	E665	I666	G667	A668	E669	M670	A671	L672	R673	T674	F675	G676	H677	L678	L679	B680	Y681	G682	E683	P684	T685	L686	R687	B688	A689	V690	P691	L692	A693	L694	A695	L696	I697	S698	V699	S700	N701	P702	R703	L704	A705	I706	L707	D708	T709	H710	S711	K712	F713	S714	H715	D716	A717	D718	F719	E720	
V721	S722	Y723	N724	S725	I726	F727	A728	M729	G730	M731	V732	G733	S734	G735	T736	N737	L738	A739	R740	L741	A742	A743	M744	L745	R746	Q747	L748	A749	Q750	Y751	H752	A753	K754	D755	P756	N757	L758	L759	F760	M761	V762	R763	L764	A765	Q766	G767	L768	T769	H770	L771	G772	K773	G774	T775	L776	T777	L778	C779	P780	
Y781	H782	S783	D784	R785	Q786	L787	M788	S789	Q790	V791	A792	V793	A794	G795	L796	L797	T798	V799	L800	N801	S802	F803	L804	D805	V806	R807	N808	I809	I810	L811	G812	R813	S814	K815	Y816	V817	L818	Y819	G820	L821	V822	A823	A824	M825	Q826	P827	R828	M829	V831	T832	F833	D834	E835	E836	L837	R838	P839	L840		



• Molecule 15: 26S proteasome regulatory subunit 8

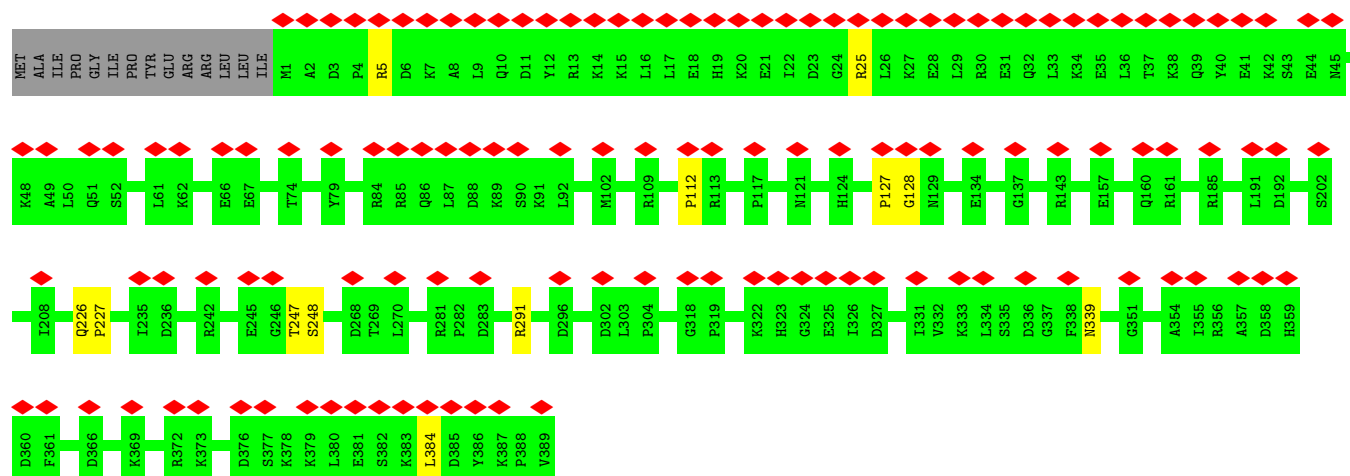


• Molecule 16: 26S proteasome regulatory subunit 6B

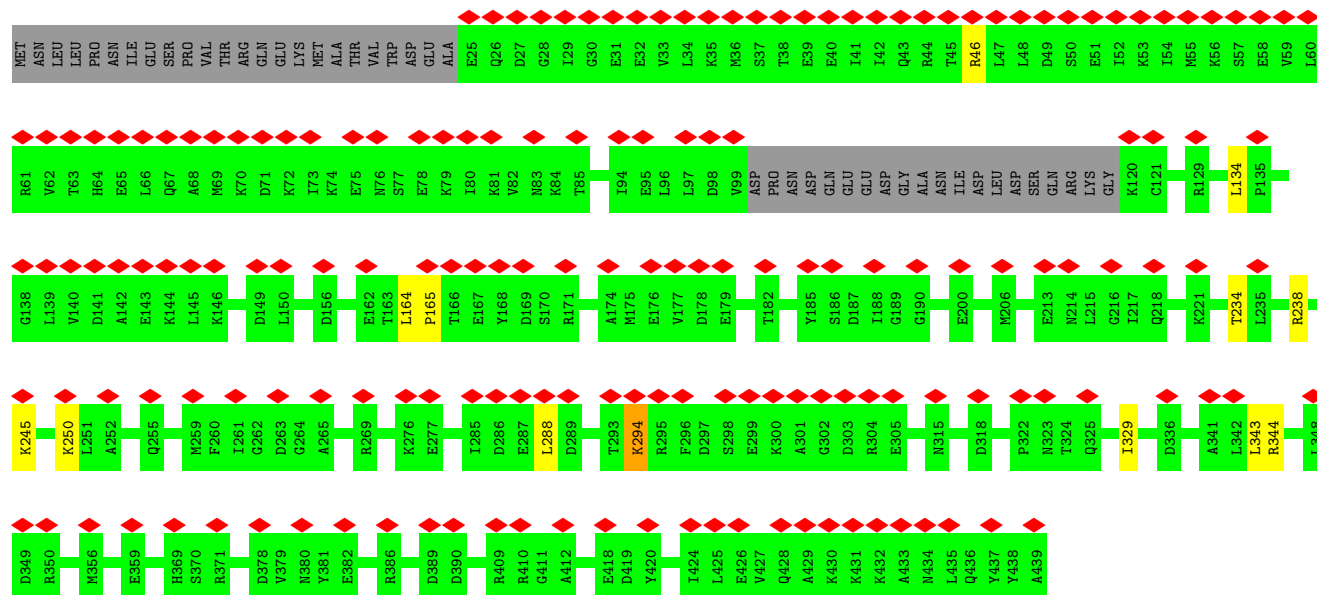
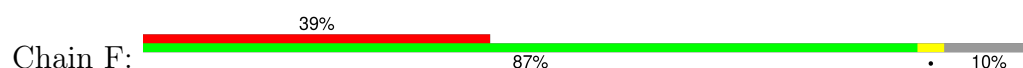


• Molecule 17: 26S proteasome regulatory subunit 10B

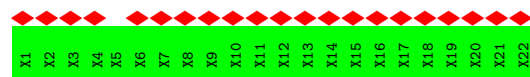




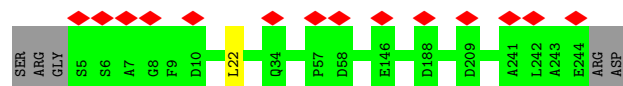
• Molecule 18: 26S proteasome regulatory subunit 6A



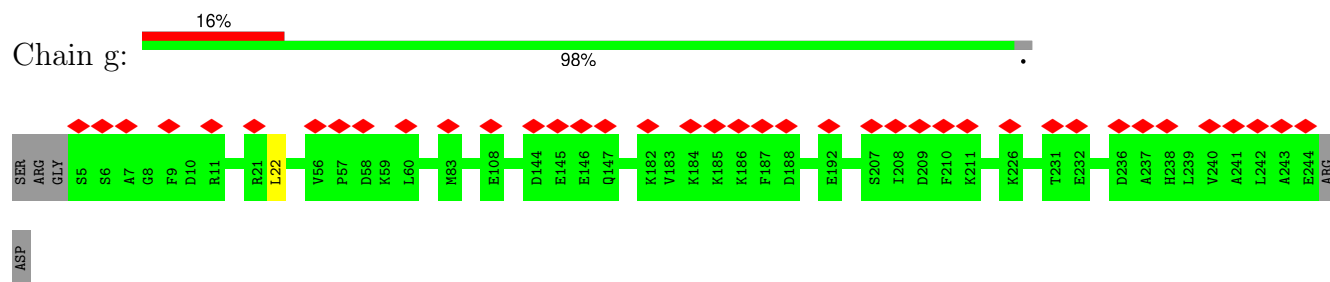
• Molecule 19: substrate



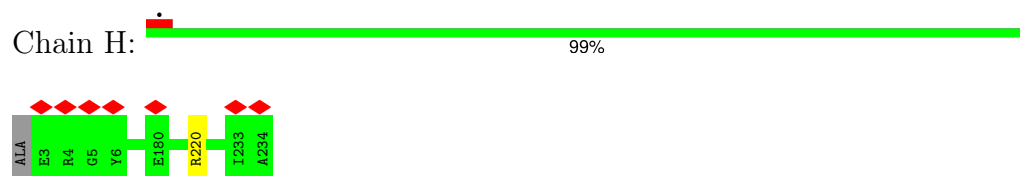
• Molecule 20: Proteasome subunit alpha type-6



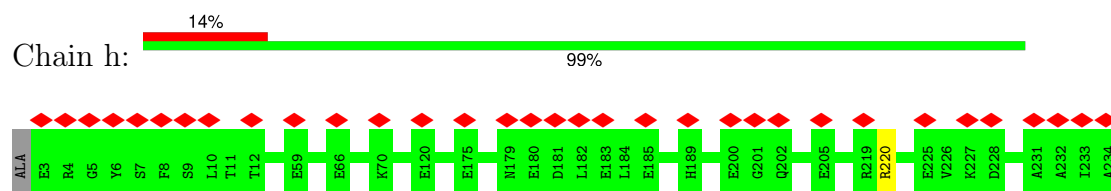
- Molecule 20: Proteasome subunit alpha type-6



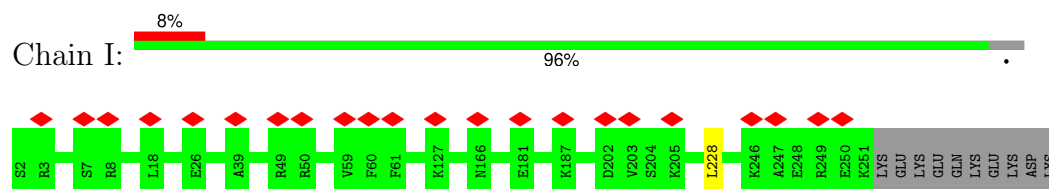
- Molecule 21: Proteasome subunit alpha type-2



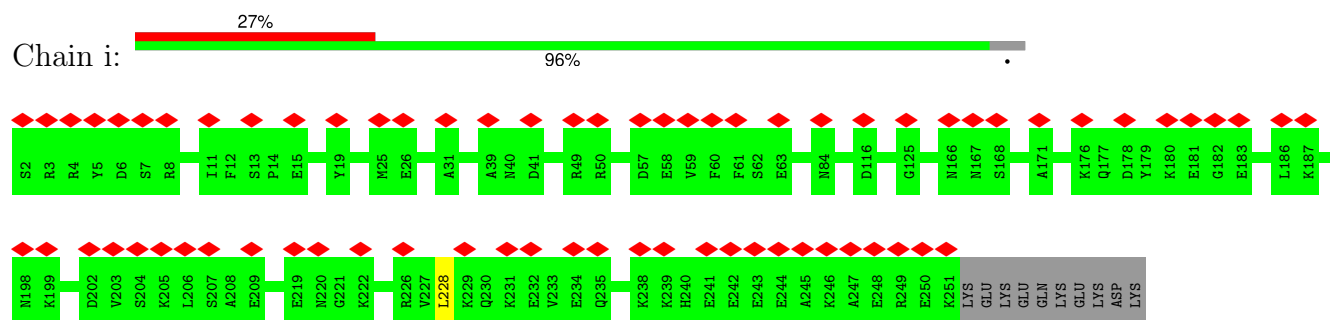
- Molecule 21: Proteasome subunit alpha type-2



- Molecule 22: Proteasome subunit alpha type-4

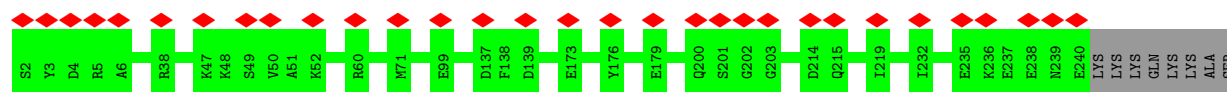


- Molecule 22: Proteasome subunit alpha type-4

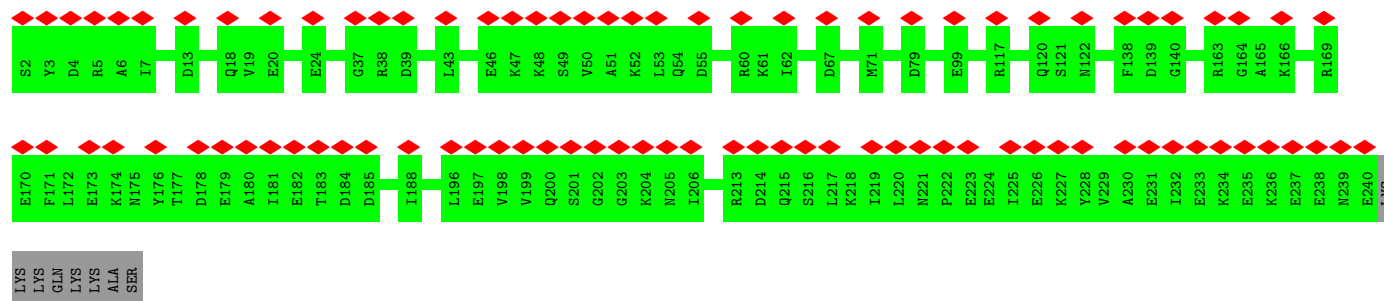


- Molecule 23: Proteasome subunit alpha type-7

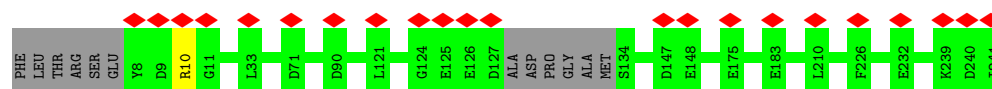




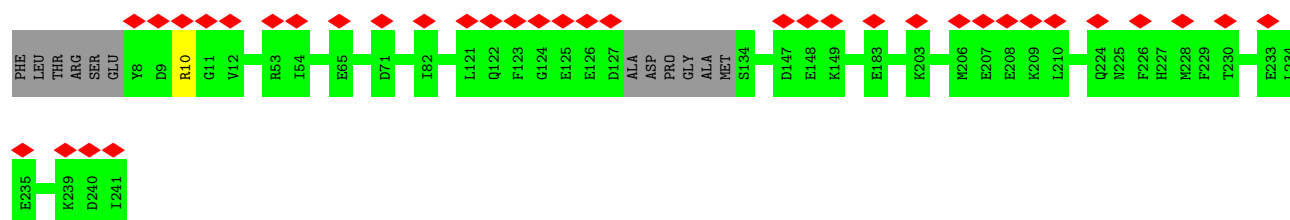
• Molecule 23: Proteasome subunit alpha type-7



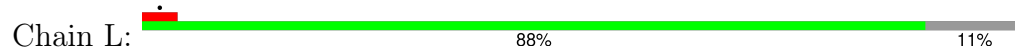
• Molecule 24: Proteasome subunit alpha type-5



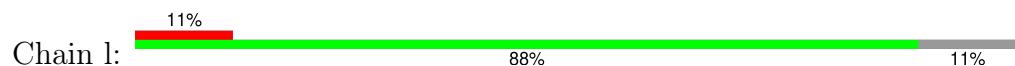
• Molecule 24: Proteasome subunit alpha type-5

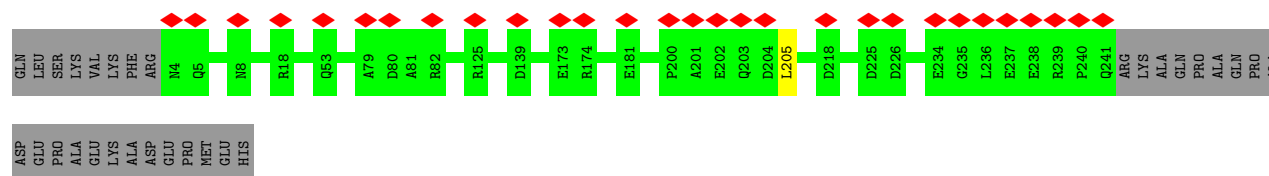


• Molecule 25: Proteasome subunit alpha type-1

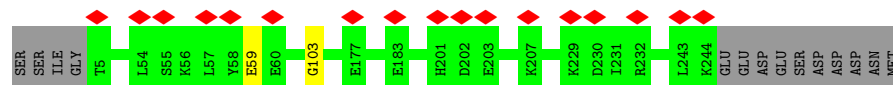


• Molecule 25: Proteasome subunit alpha type-1

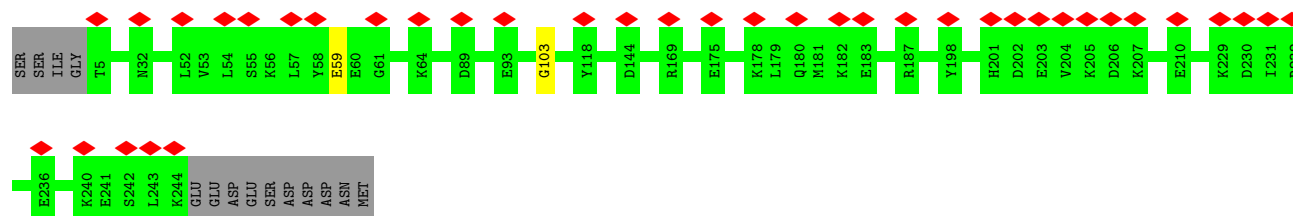




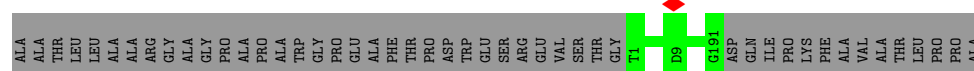
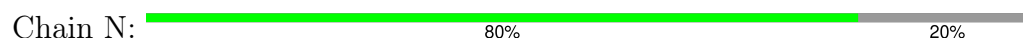
- Molecule 26: Proteasome subunit alpha type-3



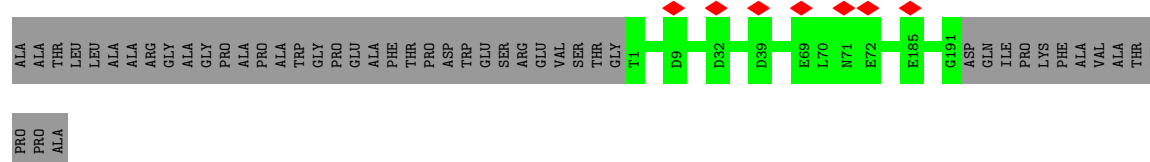
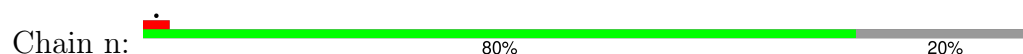
- Molecule 26: Proteasome subunit alpha type-3



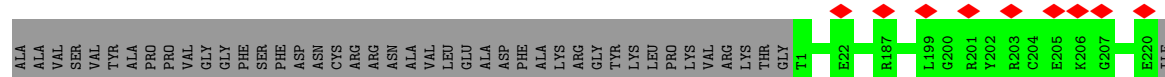
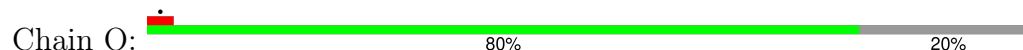
- Molecule 27: Proteasome subunit beta type-6



- Molecule 27: Proteasome subunit beta type-6




- Molecule 28: Proteasome subunit beta type-7



GLU
VAL
LEU
GLU
GLU
THR
VAL
GLN
THR
MET
ASP
THR
SER

- Molecule 28: Proteasome subunit beta type-7

Chain o:  5% 80% 20%

ALA
ALA
VAL
SER
VAL
TVR
ALA
PRO
PRO
VAL
VAL
GLY
GLY
PHE
SER
PHE
ASP
ASN
CYS
ARG
ARG
ASN
ALA
VAL
VAL
LEU
GLU
ALA
ASP
PHE
PHE
LYS
ARG
GLY
TYR
LYS
LYS
LEU
PRO
LYS
VAL
ARG
LYS
THR
GLY
T1
G23
R143
N181
D184
K194
K196
G196
T197
R198
L199
G200
R201

E205
K206
G207
E220
ILE
GLU
VAL
LEU
GLU
GLU
THR
VAL
GLN
THR
MET
ASP
THR
SER

- Molecule 29: Proteasome subunit beta type-3

Chain P:  100%

S2
F117
D205

- Molecule 29: Proteasome subunit beta type-3

Chain p:  100%

S2
D47
D59
K115
T116
F117
N157
D205

- Molecule 30: Proteasome subunit beta type-2

Chain Q:  98% ..


M1
E2
N24
E49
R93
L102
P176
P197
K198
Q199
GLY
SER

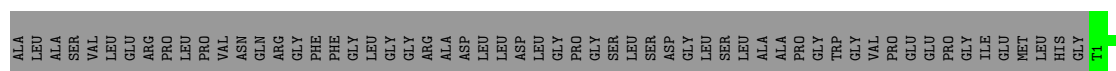
- Molecule 30: Proteasome subunit beta type-2

Chain q:  98% ..

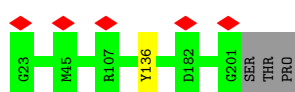
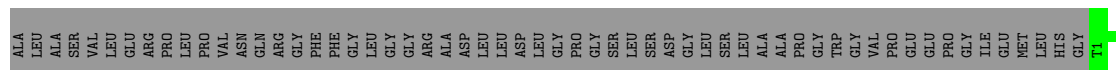
H1
D33
K34
K35
L102
H110
E111
R155
P176
D190
H193
K198
Q199
GLY
SER

- Molecule 31: Proteasome subunit beta type-5

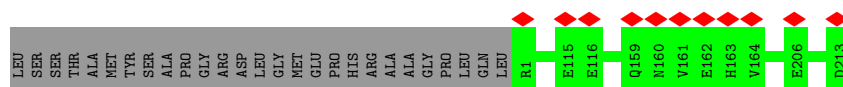
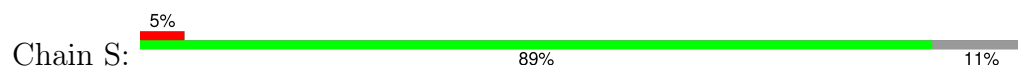
Chain R:  76% 23%



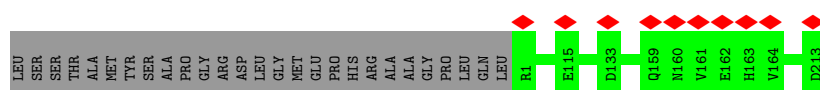
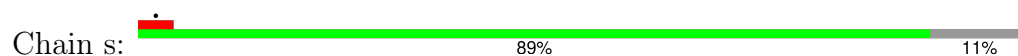
• Molecule 31: Proteasome subunit beta type-5



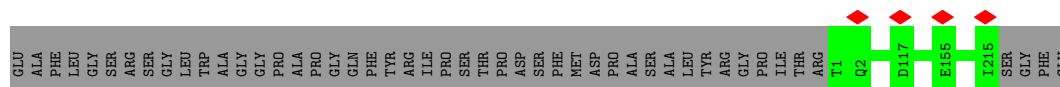
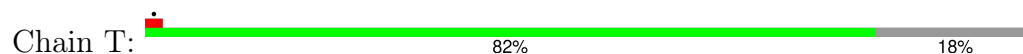
• Molecule 32: Proteasome subunit beta type-1



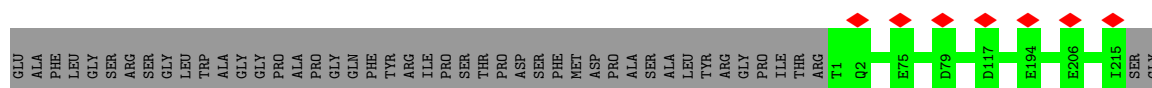
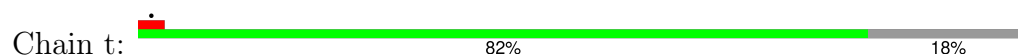
• Molecule 32: Proteasome subunit beta type-1



• Molecule 33: Proteasome subunit beta type-4



• Molecule 33: Proteasome subunit beta type-4



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 (Å)	411.0, 411.0, 411.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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: ZN, ATP, ADP

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	0.31	0/6513	0.56	1/8816 (0.0%)
2	V	0.34	0/3929	0.63	0/5309
3	W	0.31	0/3751	0.59	1/5042 (0.0%)
4	X	0.39	0/3053	0.57	0/4115
5	Y	0.38	0/3173	0.61	0/4273
6	Z	0.30	0/2324	0.61	2/3150 (0.1%)
7	a	0.31	0/3053	0.59	1/4133 (0.0%)
8	b	0.29	0/1478	0.58	0/2001
9	c	0.33	0/2302	0.63	1/3110 (0.0%)
10	d	0.32	0/2162	0.59	0/2919
11	e	0.32	0/338	0.65	1/450 (0.2%)
12	f	0.33	1/6954 (0.0%)	0.71	6/9399 (0.1%)
13	A	0.34	0/2814	0.55	0/3801
14	B	0.32	0/2745	0.57	0/3709
15	C	0.35	0/3146	0.60	1/4226 (0.0%)
16	D	0.41	0/3090	0.63	1/4168 (0.0%)
17	E	0.37	0/3145	0.62	1/4233 (0.0%)
18	F	0.37	0/3137	0.63	3/4223 (0.1%)
20	G	0.47	0/1859	0.57	0/2523
20	g	0.47	0/1859	0.57	0/2523
21	H	0.50	0/1743	0.59	1/2372 (0.0%)
21	h	0.50	0/1743	0.59	1/2372 (0.0%)
22	I	0.43	0/1942	0.59	0/2628
22	i	0.43	0/1942	0.59	0/2628
23	J	0.41	0/1728	0.54	0/2358
23	j	0.41	0/1728	0.54	0/2358
24	K	0.39	0/1747	0.56	0/2364
24	k	0.39	0/1747	0.56	0/2364
25	L	0.43	0/1885	0.59	0/2552
25	l	0.43	0/1885	0.59	0/2552
26	M	0.46	0/1891	0.59	0/2552
26	m	0.46	0/1891	0.59	0/2552

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
27	N	0.43	0/1454	0.53	0/1967
27	n	0.43	0/1454	0.53	0/1967
28	O	0.42	0/1670	0.55	0/2265
28	o	0.42	0/1670	0.55	0/2265
29	P	0.45	0/1614	0.54	0/2177
29	p	0.45	0/1614	0.54	0/2177
30	Q	0.47	0/1603	0.62	0/2174
30	q	0.47	0/1603	0.62	0/2174
31	R	0.46	0/1579	0.52	0/2134
31	r	0.46	0/1579	0.52	0/2134
32	S	0.42	0/1671	0.54	0/2253
32	s	0.42	0/1671	0.54	0/2253
33	T	0.44	0/1700	0.53	0/2305
33	t	0.44	0/1700	0.53	0/2305
All	All	0.39	1/105279 (0.0%)	0.59	21/142325 (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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	f	192	VAL	C-N	5.92	1.45	1.34

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	f	830	LEU	CA-CB-CG	7.96	133.61	115.30
18	F	343	LEU	CA-CB-CG	7.43	132.40	115.30
11	e	56	LEU	CA-CB-CG	7.33	132.15	115.30
12	f	759	LEU	CA-CB-CG	6.76	130.84	115.30
12	f	612	LEU	CA-CB-CG	6.74	130.79	115.30
6	Z	133	LEU	CA-CB-CG	6.52	130.30	115.30
7	a	187	ASP	CB-CG-OD1	6.16	123.85	118.30
12	f	811	LEU	CA-CB-CG	6.13	129.41	115.30
1	U	187	LEU	CA-CB-CG	6.11	129.34	115.30
9	c	212	LEU	CA-CB-CG	5.77	128.56	115.30
21	H	220	ARG	NE-CZ-NH2	-5.71	117.45	120.30
17	E	384	LEU	CA-CB-CG	5.61	128.19	115.30
21	h	220	ARG	NE-CZ-NH2	-5.57	117.51	120.30
15	C	404	LEU	CA-CB-CG	5.46	127.86	115.30
12	f	217	LEU	CA-CB-CG	5.45	127.84	115.30
18	F	294	LYS	C-N-CA	5.44	135.30	121.70
6	Z	65	ASP	CB-CG-OD1	5.37	123.14	118.30
16	D	354	LEU	CA-CB-CG	5.36	127.63	115.30
12	f	858	LYS	C-N-CD	5.15	139.21	128.40
3	W	222	LEU	CA-CB-CG	5.00	126.80	115.30
18	F	164	LEU	CA-CB-CG	5.00	126.80	115.30

There are no chirality outliers.

All (25) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	A	157	ILE	Peptide
13	A	284	ARG	Peptide
15	C	128	PRO	Peptide
15	C	220	VAL	Peptide
16	D	157	ASP	Peptide
16	D	411	GLU	Peptide
17	E	226	GLN	Peptide
18	F	294	LYS	Peptide
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
12	f	340	MET	Peptide
12	f	642	ALA	Peptide
12	f	737	ASN	Peptide
12	f	755	ASP	Peptide

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Mol	Chain	Res	Type	Group
12	f	807	ARG	Peptide
12	f	809	ILE	Peptide
12	f	816	TYR	Peptide
12	f	822	VAL	Peptide
12	f	823	ALA	Peptide
12	f	854	GLY	Peptide
12	f	870	THR	Peptide
12	f	875	ALA	Peptide

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	U	814/953 (85%)	760 (93%)	53 (6%)	1 (0%)	48	79
2	V	478/533 (90%)	436 (91%)	41 (9%)	1 (0%)	44	73
3	W	454/456 (100%)	420 (92%)	34 (8%)	0	100	100
4	X	378/422 (90%)	355 (94%)	22 (6%)	1 (0%)	37	67
5	Y	376/389 (97%)	340 (90%)	36 (10%)	0	100	100
6	Z	284/324 (88%)	240 (84%)	38 (13%)	6 (2%)	5	33
7	a	371/376 (99%)	338 (91%)	32 (9%)	1 (0%)	37	67
8	b	189/377 (50%)	171 (90%)	18 (10%)	0	100	100
9	c	285/309 (92%)	241 (85%)	43 (15%)	1 (0%)	30	63
10	d	255/349 (73%)	216 (85%)	38 (15%)	1 (0%)	30	63
11	e	36/70 (51%)	31 (86%)	5 (14%)	0	100	100
12	f	884/892 (99%)	709 (80%)	164 (19%)	11 (1%)	11	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	A	354/433 (82%)	310 (88%)	42 (12%)	2 (1%)	22	55
14	B	348/440 (79%)	300 (86%)	44 (13%)	4 (1%)	12	45
15	C	394/398 (99%)	342 (87%)	51 (13%)	1 (0%)	37	67
16	D	378/418 (90%)	335 (89%)	42 (11%)	1 (0%)	37	67
17	E	387/403 (96%)	338 (87%)	43 (11%)	6 (2%)	8	38
18	F	391/439 (89%)	350 (90%)	40 (10%)	1 (0%)	37	67
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	51
26	m	238/254 (94%)	216 (91%)	20 (8%)	2 (1%)	16	51
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%)	25	59
30	q	197/201 (98%)	181 (92%)	15 (8%)	1 (0%)	25	59
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	38	67

All (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
12	f	876	HIS
14	B	356	PRO
14	B	357	ASP
16	D	412	GLN
17	E	127	PRO
17	E	248	SER
7	a	69	HIS
12	f	118	ASN
12	f	476	THR
12	f	664	GLU
12	f	823	ALA
12	f	859	PRO
26	m	59	GLU
4	X	317	PRO
6	Z	10	VAL
12	f	809	ILE
13	A	109	PRO
17	E	247	THR
18	F	165	PRO
26	M	59	GLU
26	M	103	GLY
26	m	103	GLY
6	Z	65	ASP
9	c	280	PRO
12	f	475	ASN
15	C	128	PRO
30	Q	176	PRO
30	q	176	PRO

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Mol	Chain	Res	Type
6	Z	12	HIS
6	Z	184	VAL
12	f	755	ASP
13	A	285	PHE
17	E	112	PRO
6	Z	144	VAL
17	E	227	PRO
1	U	813	TYR
14	B	355	LEU
17	E	128	GLY
2	V	29	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%)	696 (99%)	4 (1%)	84	92
2	V	414/459 (90%)	411 (99%)	3 (1%)	81	90
3	W	416/416 (100%)	402 (97%)	14 (3%)	32	60
4	X	327/362 (90%)	327 (100%)	0	100	100
5	Y	334/344 (97%)	330 (99%)	4 (1%)	67	82
6	Z	257/295 (87%)	247 (96%)	10 (4%)	27	57
7	a	333/336 (99%)	330 (99%)	3 (1%)	75	87
8	b	167/312 (54%)	167 (100%)	0	100	100
9	c	252/267 (94%)	246 (98%)	6 (2%)	44	67
10	d	231/293 (79%)	231 (100%)	0	100	100
11	e	38/63 (60%)	37 (97%)	1 (3%)	41	65
12	f	742/748 (99%)	724 (98%)	18 (2%)	44	67
13	A	298/372 (80%)	293 (98%)	5 (2%)	56	75
14	B	300/385 (78%)	297 (99%)	3 (1%)	73	85
15	C	340/346 (98%)	333 (98%)	7 (2%)	48	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	D	333/366 (91%)	326 (98%)	7 (2%)	48	71
17	E	341/353 (97%)	337 (99%)	4 (1%)	67	82
18	F	340/379 (90%)	331 (97%)	9 (3%)	41	65
20	G	193/209 (92%)	192 (100%)	1 (0%)	86	93
20	g	193/209 (92%)	192 (100%)	1 (0%)	86	93
21	H	164/190 (86%)	164 (100%)	0	100	100
21	h	164/190 (86%)	164 (100%)	0	100	100
22	I	193/220 (88%)	192 (100%)	1 (0%)	86	93
22	i	193/220 (88%)	192 (100%)	1 (0%)	86	93
23	J	152/210 (72%)	152 (100%)	0	100	100
23	j	152/210 (72%)	152 (100%)	0	100	100
24	K	186/202 (92%)	185 (100%)	1 (0%)	86	93
24	k	186/202 (92%)	185 (100%)	1 (0%)	86	93
25	L	198/229 (86%)	197 (100%)	1 (0%)	86	93
25	l	198/229 (86%)	197 (100%)	1 (0%)	86	93
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%)	148 (100%)	0	100	100
27	n	148/180 (82%)	148 (100%)	0	100	100
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%)	84	92
30	q	164/171 (96%)	163 (99%)	1 (1%)	84	92
31	R	153/201 (76%)	152 (99%)	1 (1%)	81	90
31	r	153/201 (76%)	152 (99%)	1 (1%)	81	90
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	11045/12582 (88%)	10935 (99%)	110 (1%)	71	85

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	U	118	LEU
1	U	629	THR
1	U	788	VAL
1	U	819	VAL
2	V	194	LYS
2	V	469	THR
2	V	494	MET
3	W	39	ARG
3	W	55	ARG
3	W	92	LYS
3	W	135	LYS
3	W	191	ARG
3	W	196	VAL
3	W	233	LEU
3	W	235	GLN
3	W	239	SER
3	W	241	LEU
3	W	242	SER
3	W	245	LYS
3	W	419	LYS
3	W	456	GLN
5	Y	48	ASN
5	Y	176	ARG
5	Y	237	ARG
5	Y	312	ARG
6	Z	8	LYS
6	Z	9	VAL
6	Z	11	VAL
6	Z	14	LEU
6	Z	15	VAL
6	Z	16	LEU
6	Z	17	LEU
6	Z	49	ASP
6	Z	219	LYS
6	Z	229	GLN
7	a	145	LEU
7	a	227	ASN

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Mol	Chain	Res	Type
7	a	289	ARG
9	c	36	LEU
9	c	40	LYS
9	c	154	LYS
9	c	175	ARG
9	c	197	ASN
9	c	198	ARG
11	e	57	ARG
12	f	80	ARG
12	f	83	ARG
12	f	131	MET
12	f	267	ARG
12	f	297	MET
12	f	327	ASN
12	f	344	VAL
12	f	396	ASN
12	f	457	ASN
12	f	531	ASN
12	f	565	ASN
12	f	569	LYS
12	f	660	ILE
12	f	662	MET
12	f	703	ARG
12	f	746	ARG
12	f	822	VAL
12	f	826	GLN
13	A	284	ARG
13	A	360	ARG
13	A	369	ARG
13	A	373	LEU
13	A	403	ILE
14	B	164	MET
14	B	355	LEU
14	B	429	LYS
15	C	20	LEU
15	C	78	ARG
15	C	184	LYS
15	C	210	THR
15	C	213	ARG
15	C	287	LYS
15	C	398	ASN
16	D	163	MET

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Mol	Chain	Res	Type
16	D	229	ARG
16	D	238	LYS
16	D	274	ARG
16	D	323	ARG
16	D	353	ASN
16	D	360	LEU
17	E	5	ARG
17	E	25	ARG
17	E	291	ARG
17	E	339	ASN
18	F	46	ARG
18	F	134	LEU
18	F	234	THR
18	F	238	ARG
18	F	245	LYS
18	F	250	LYS
18	F	288	LEU
18	F	329	ILE
18	F	344	ARG
20	G	22	LEU
22	I	228	LEU
24	K	10	ARG
25	L	205	LEU
30	Q	102	LEU
31	R	136	TYR
20	g	22	LEU
22	i	228	LEU
24	k	10	ARG
25	l	205	LEU
30	q	102	LEU
31	r	136	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (102) such sidechains are listed below:

Mol	Chain	Res	Type
1	U	70	HIS
1	U	596	ASN
1	U	707	ASN
1	U	888	GLN
2	V	281	ASN
2	V	453	HIS
2	V	473	GLN

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Mol	Chain	Res	Type
3	W	86	ASN
3	W	107	GLN
3	W	203	GLN
3	W	257	GLN
3	W	362	ASN
3	W	456	GLN
4	X	148	HIS
4	X	178	HIS
4	X	292	GLN
4	X	296	ASN
5	Y	48	ASN
5	Y	71	ASN
5	Y	136	HIS
6	Z	72	HIS
6	Z	193	ASN
6	Z	229	GLN
6	Z	256	GLN
7	a	152	HIS
7	a	193	GLN
7	a	227	ASN
7	a	249	GLN
7	a	257	GLN
7	a	332	HIS
7	a	370	GLN
9	c	197	ASN
9	c	214	GLN
9	c	287	HIS
10	d	47	GLN
11	e	63	HIS
12	f	43	GLN
12	f	112	ASN
12	f	118	ASN
12	f	291	GLN
12	f	327	ASN
12	f	378	ASN
12	f	382	ASN
12	f	396	ASN
12	f	457	ASN
12	f	531	ASN
12	f	565	ASN
12	f	614	HIS
12	f	619	HIS

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Mol	Chain	Res	Type
12	f	737	ASN
12	f	815	HIS
13	A	85	GLN
13	A	117	GLN
13	A	165	GLN
13	A	358	HIS
14	B	207	HIS
14	B	241	ASN
14	B	277	HIS
14	B	332	ASN
14	B	416	ASN
15	C	53	ASN
15	C	279	GLN
15	C	337	ASN
15	C	398	ASN
16	D	65	GLN
16	D	187	HIS
16	D	222	HIS
16	D	302	ASN
16	D	353	ASN
17	E	194	ASN
17	E	262	ASN
17	E	271	HIS
17	E	300	HIS
17	E	339	ASN
17	E	364	GLN
18	F	243	GLN
18	F	315	ASN
18	F	333	ASN
21	H	102	GLN
21	H	112	GLN
22	I	109	GLN
23	J	116	GLN
23	J	175	ASN
24	K	99	HIS
24	K	214	ASN
27	N	154	GLN
30	Q	71	ASN
30	Q	82	ASN
30	Q	101	ASN
30	Q	132	HIS
31	R	38	ASN

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Mol	Chain	Res	Type
21	h	112	GLN
22	i	109	GLN
23	j	116	GLN
23	j	175	ASN
24	k	99	HIS
24	k	214	ASN
27	n	154	GLN
30	q	71	ASN
30	q	82	ASN
30	q	101	ASN
30	q	132	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	-	28,33,33	0.79	0	34,52,52	1.22	3 (8%)
35	ATP	D	501	-	28,33,33	0.78	0	34,52,52	1.37	4 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	ATP	E	401	-	28,33,33	0.82	0	34,52,52	1.42	6 (17%)
36	ADP	F	501	-	24,29,29	0.79	0	29,45,45	1.38	4 (13%)

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	-	-	2/18/38/38	0/3/3/3
35	ATP	D	501	-	-	6/18/38/38	0/3/3/3
35	ATP	E	401	-	-	1/18/38/38	0/3/3/3
36	ADP	F	501	-	-	7/12/32/32	0/3/3/3

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	C	501	ATP	N3-C2-N1	-4.16	123.03	128.67
36	F	501	ADP	N3-C2-N1	-3.87	123.41	128.67
35	E	401	ATP	N3-C2-N1	-3.42	124.03	128.67
35	D	501	ATP	N3-C2-N1	-3.40	124.06	128.67
35	D	501	ATP	O4'-C1'-N9	-2.77	105.07	108.75
36	F	501	ADP	C4-C5-N7	-2.38	106.82	109.34
35	E	401	ATP	O2A-PA-O1A	2.34	123.34	112.44
36	F	501	ADP	O2A-PA-O1A	2.27	122.99	112.44
35	C	501	ATP	C4-C5-N7	-2.26	106.95	109.34
35	C	501	ATP	O3G-PG-O2G	2.25	116.24	107.80
35	D	501	ATP	C4'-O4'-C1'	2.23	111.97	109.92
35	E	401	ATP	C1'-N9-C4	2.20	130.51	126.64
35	E	401	ATP	C4-C5-N7	-2.14	107.07	109.34
35	E	401	ATP	C5'-C4'-C3'	-2.13	107.56	115.21
35	E	401	ATP	O4'-C1'-N9	-2.09	105.97	108.75
35	D	501	ATP	C4-C5-N7	-2.06	107.16	109.34
36	F	501	ADP	C4'-O4'-C1'	-2.04	108.06	109.92

There are no chirality outliers.

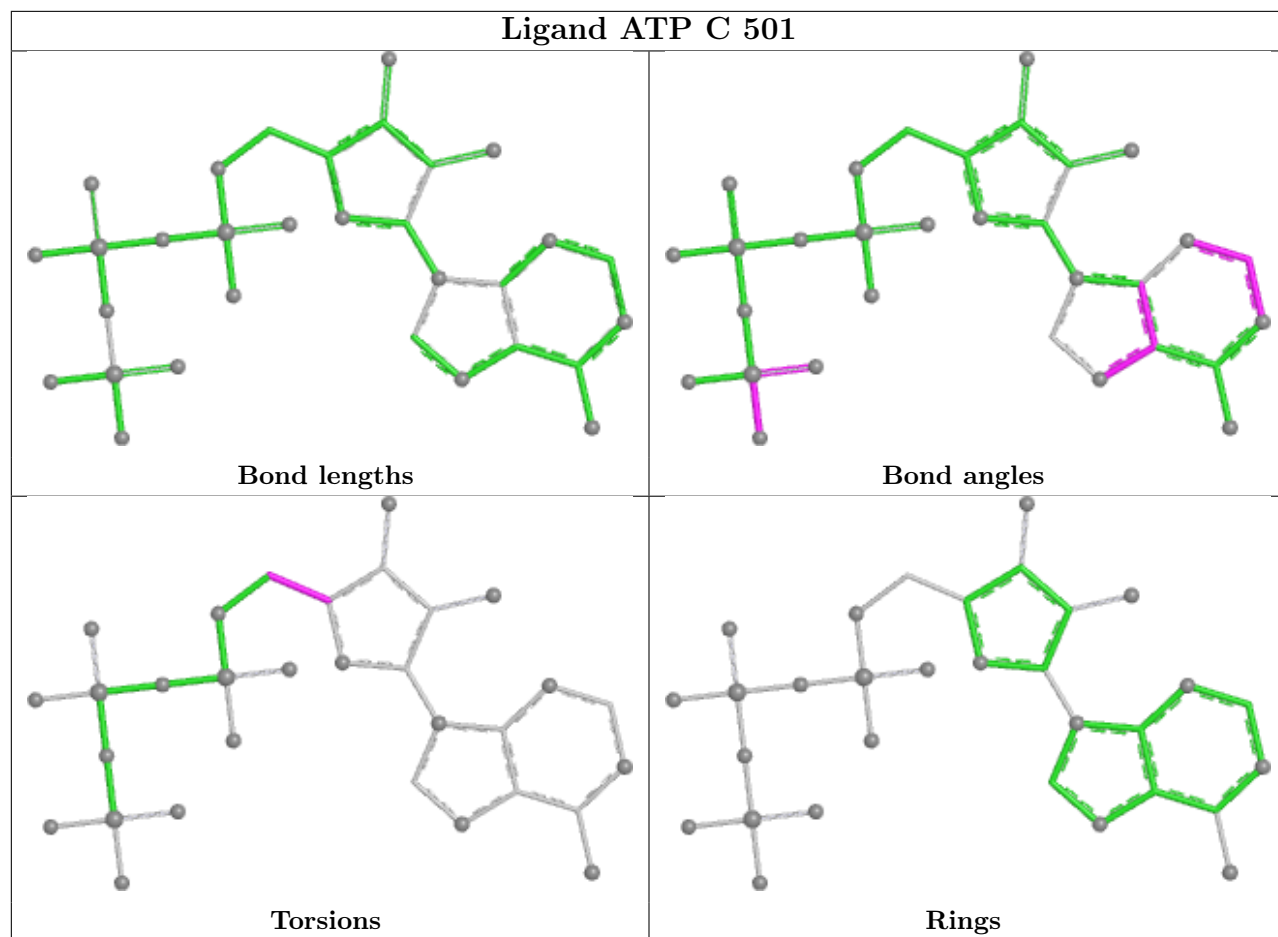
All (16) torsion outliers are listed below:

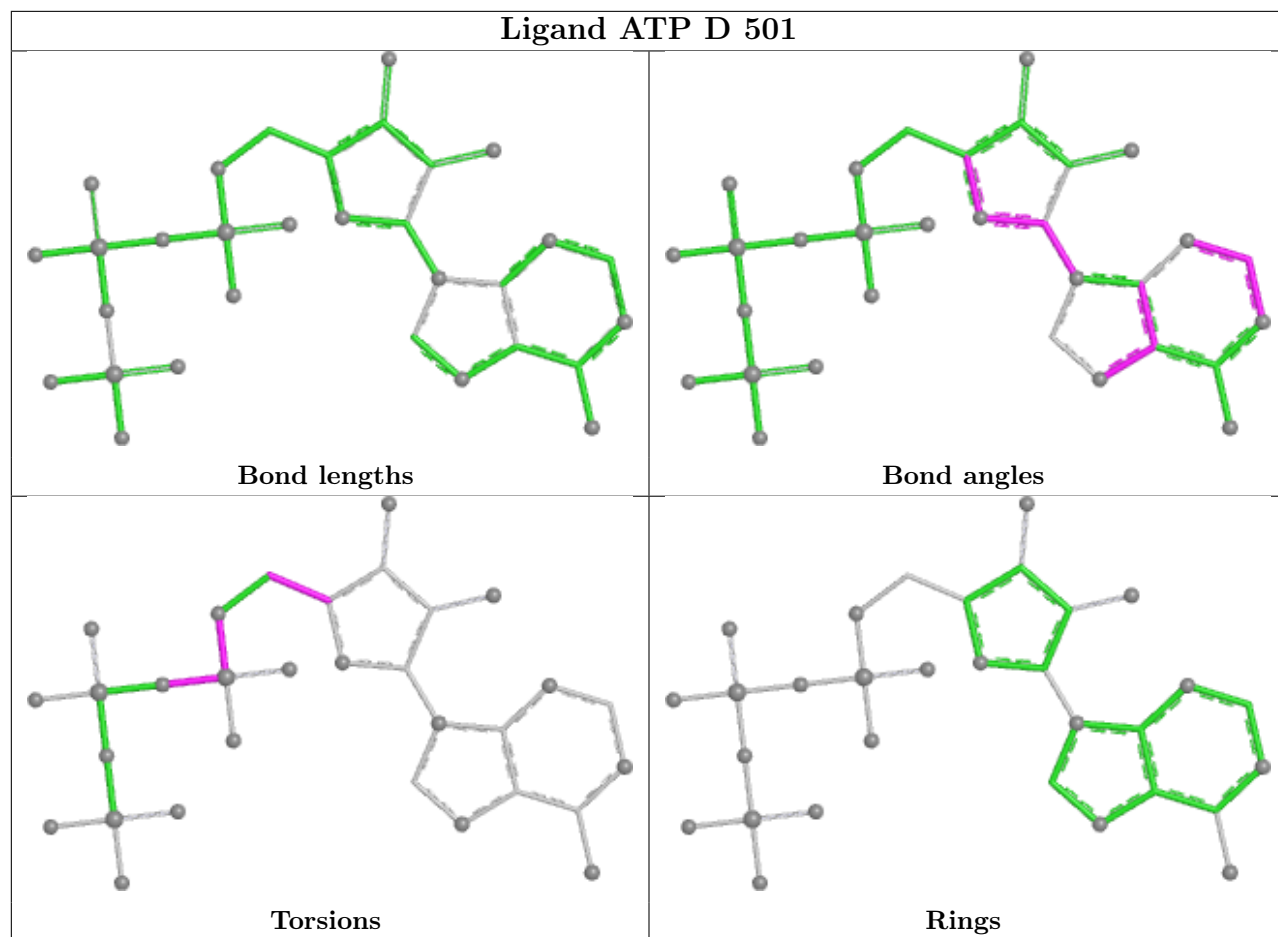
Mol	Chain	Res	Type	Atoms
35	D	501	ATP	C5'-O5'-PA-O1A
35	D	501	ATP	C5'-O5'-PA-O2A
35	D	501	ATP	C5'-O5'-PA-O3A
36	F	501	ADP	PA-O3A-PB-O2B
36	F	501	ADP	PA-O3A-PB-O3B
36	F	501	ADP	C5'-O5'-PA-O1A
36	F	501	ADP	C5'-O5'-PA-O2A
36	F	501	ADP	C5'-O5'-PA-O3A
36	F	501	ADP	O4'-C4'-C5'-O5'
36	F	501	ADP	C3'-C4'-C5'-O5'
35	C	501	ATP	O4'-C4'-C5'-O5'
35	C	501	ATP	C3'-C4'-C5'-O5'
35	E	401	ATP	C4'-C5'-O5'-PA
35	D	501	ATP	PB-O3A-PA-O5'
35	D	501	ATP	O4'-C4'-C5'-O5'
35	D	501	ATP	PB-O3A-PA-O2A

There are no ring outliers.

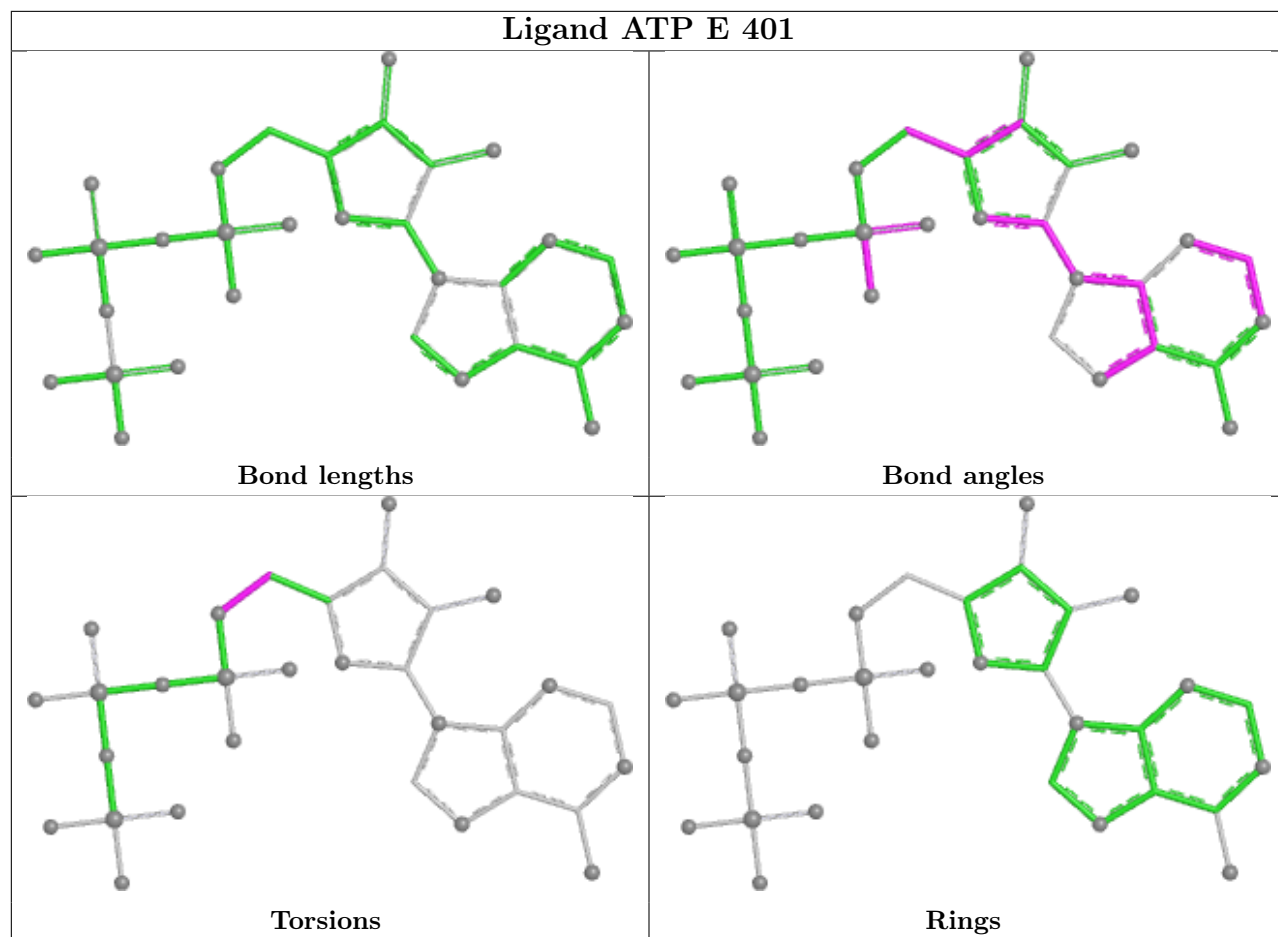
No monomer is involved in short contacts.

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

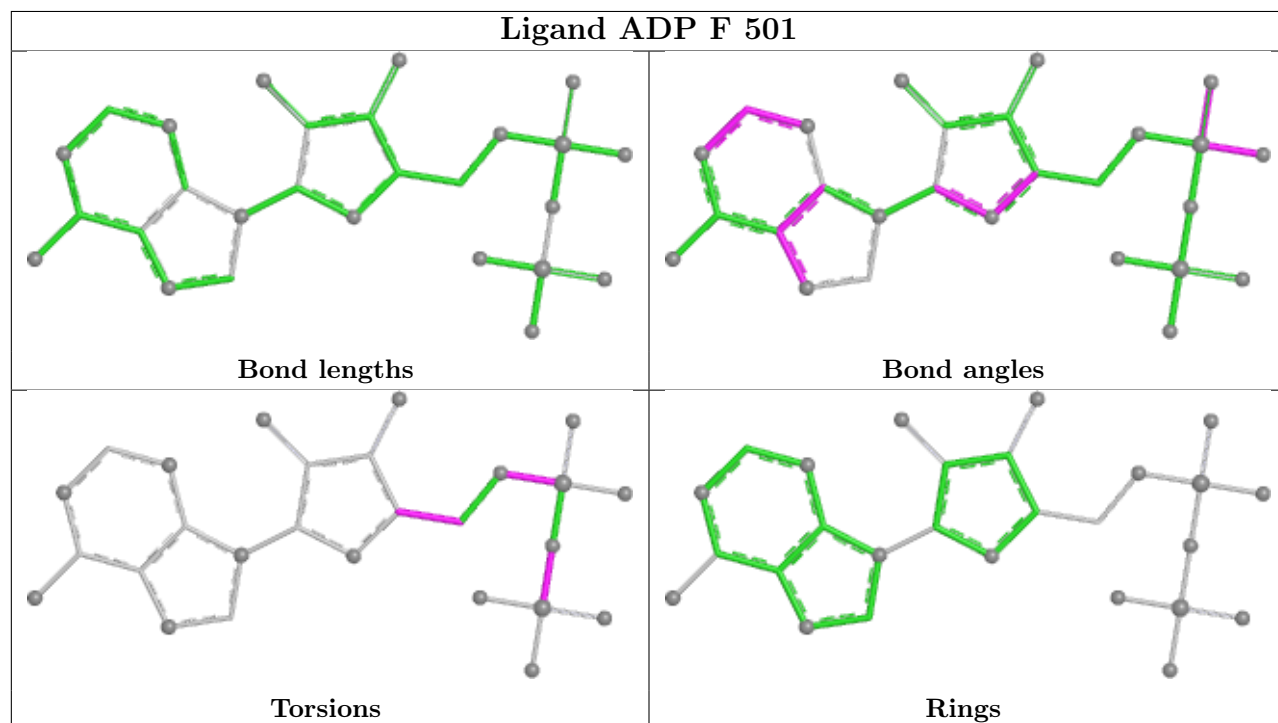




Ligand ATP E 401



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.

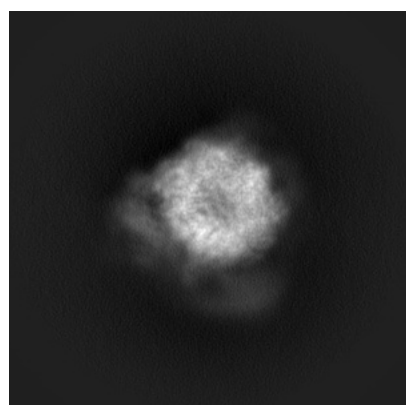
6 Map visualisation [i](#)

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.

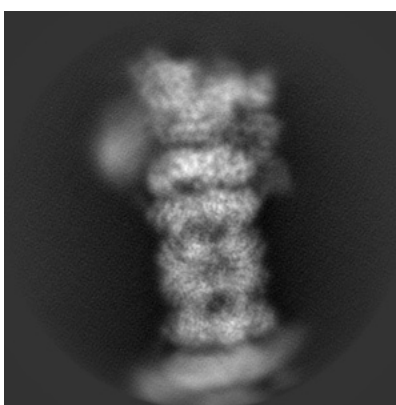
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

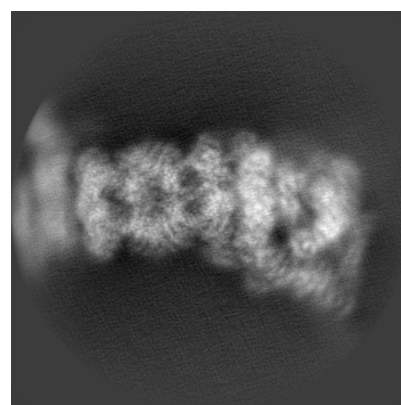
6.1.1 Primary map



X



Y

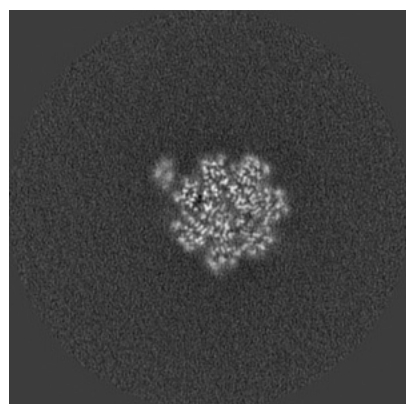


Z

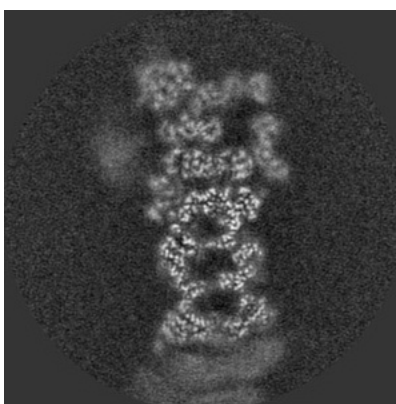
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

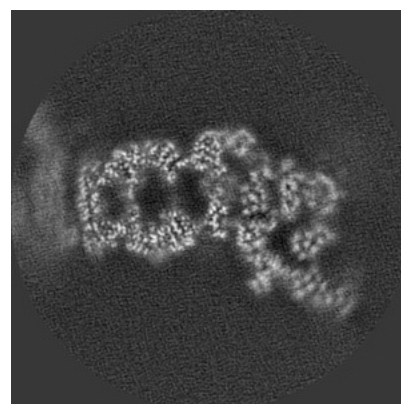
6.2.1 Primary map



X Index: 300



Y Index: 300

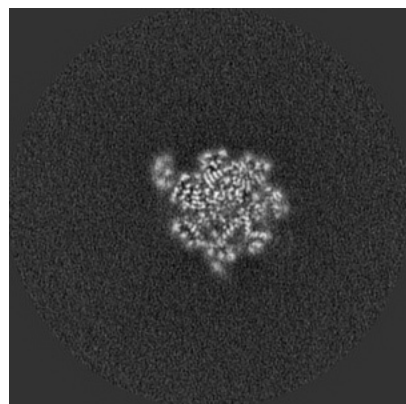


Z Index: 300

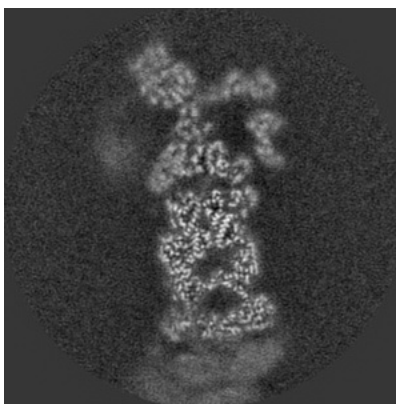
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

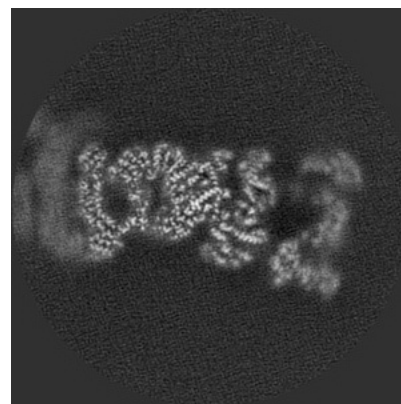
6.3.1 Primary map



X Index: 307



Y Index: 287

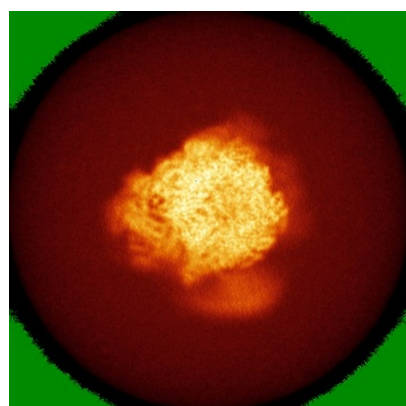


Z Index: 343

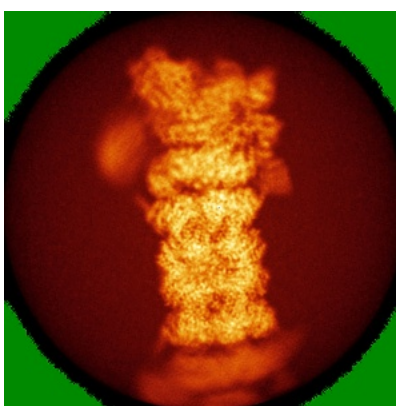
The images above show the largest variance slices of the map in three orthogonal directions.

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

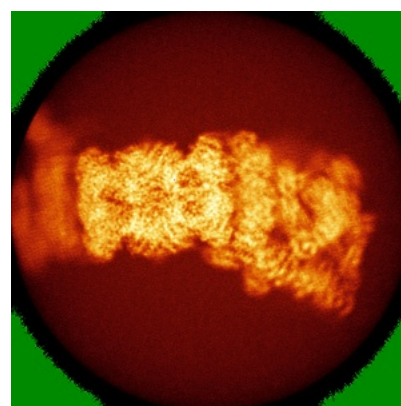
6.4.1 Primary map



X



Y

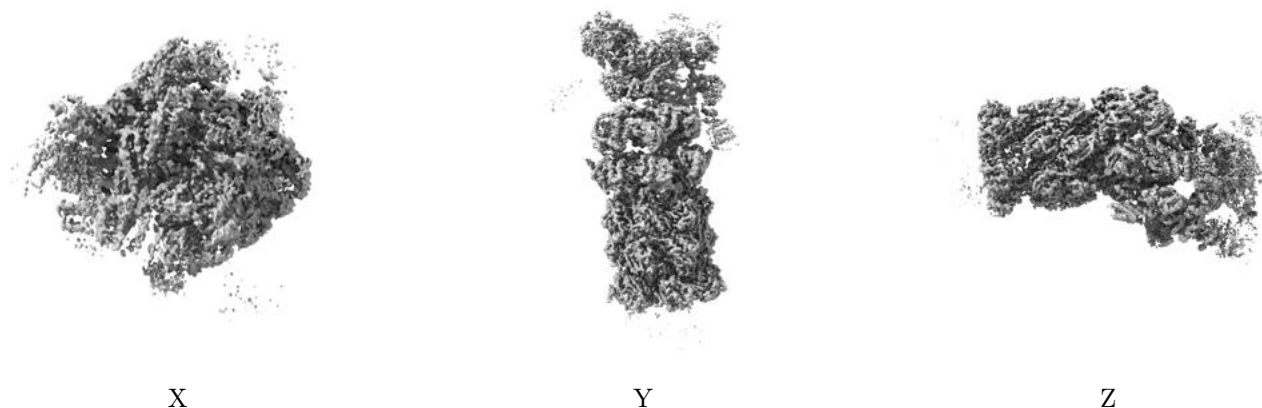


Z

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.

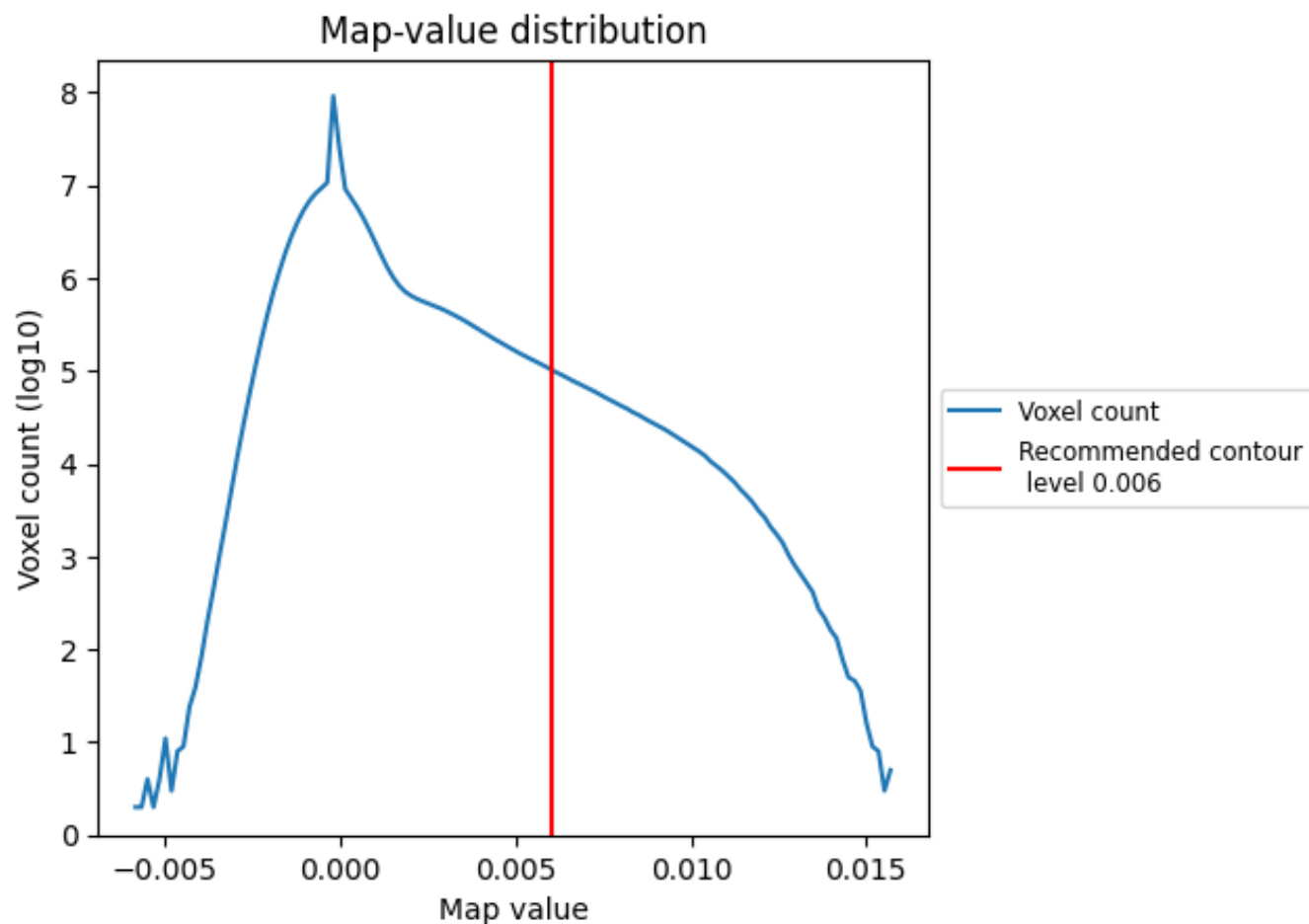
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

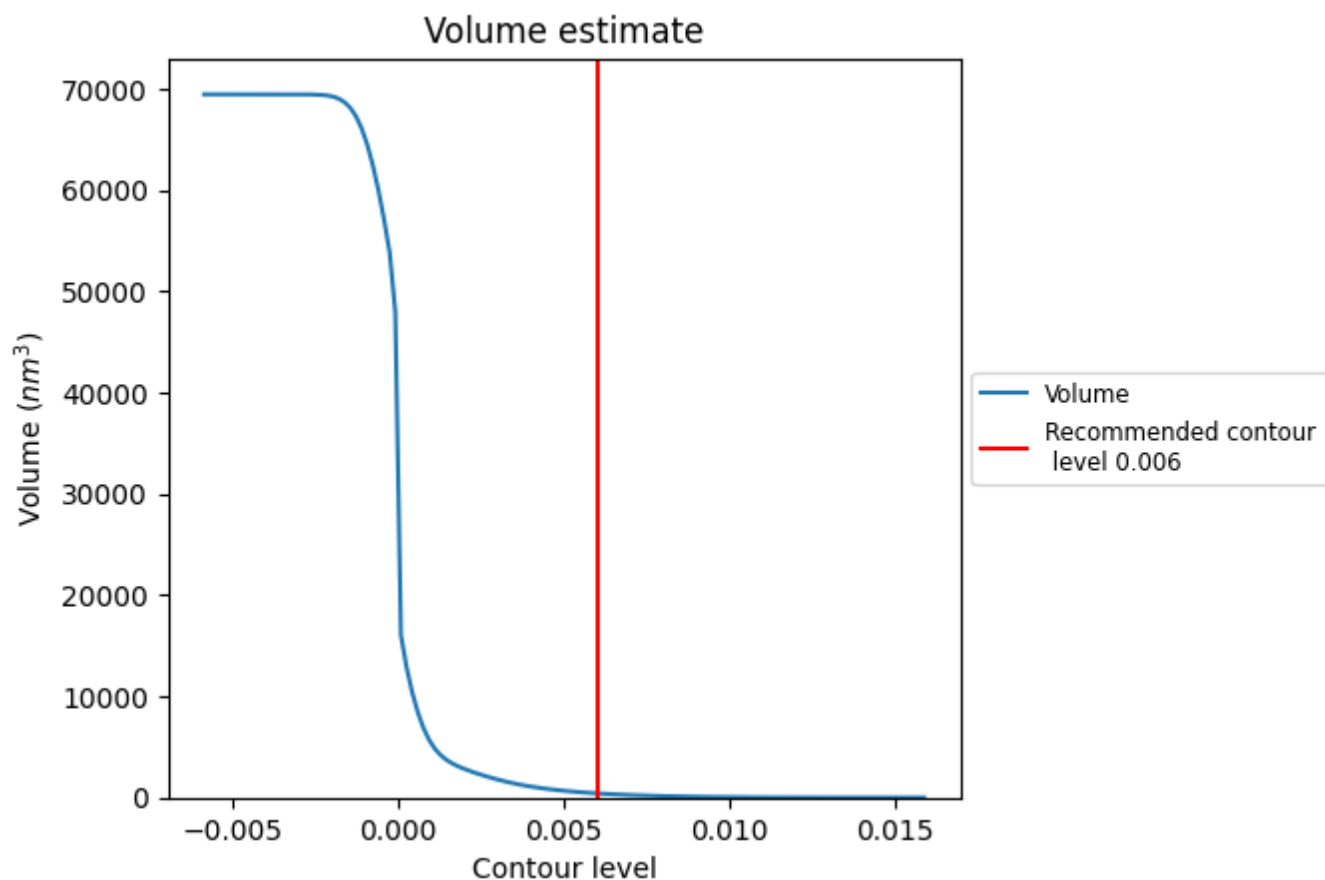
This section contains the results of statistical analysis of the map.

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.

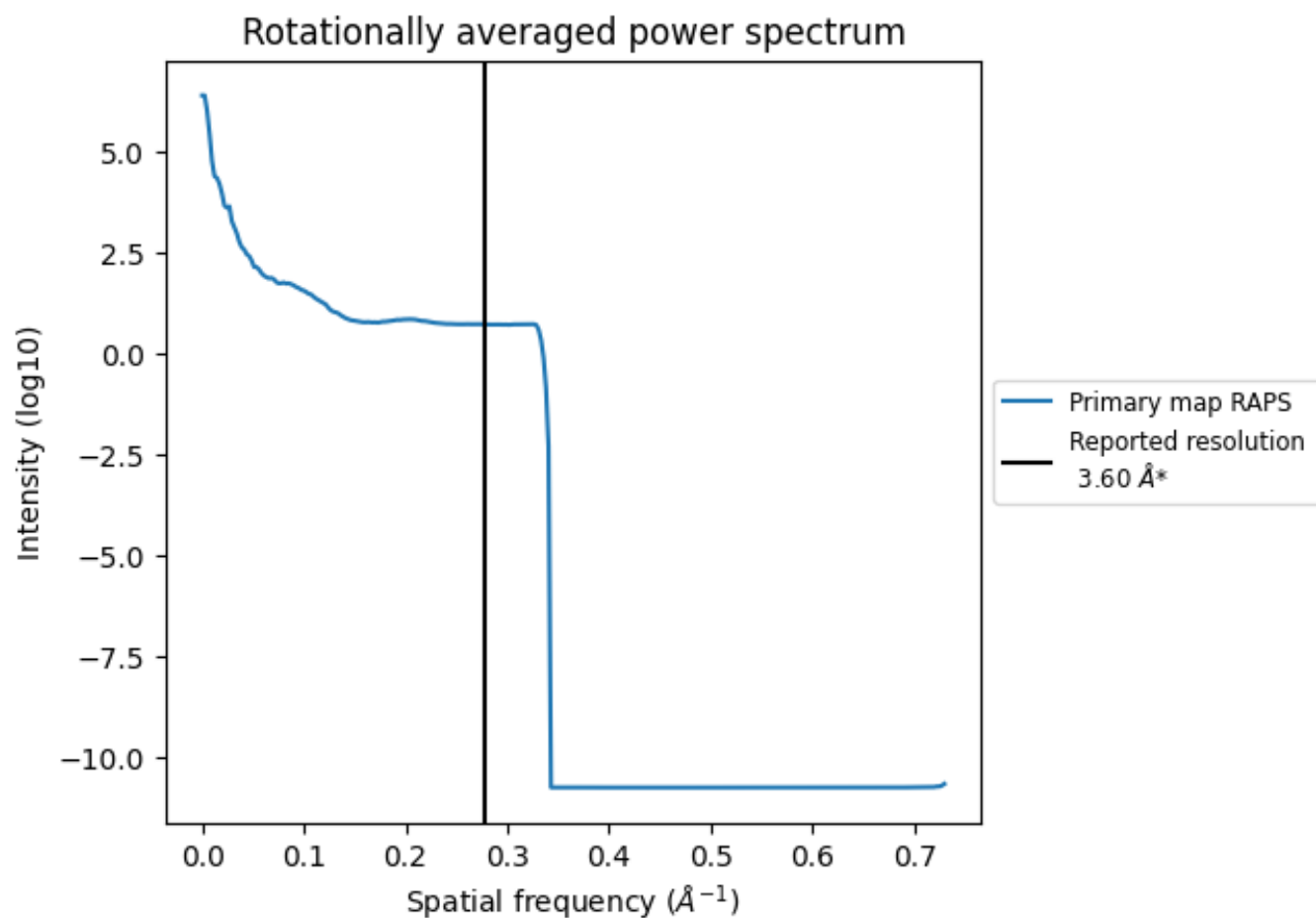
7.2 Volume estimate [i](#)



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

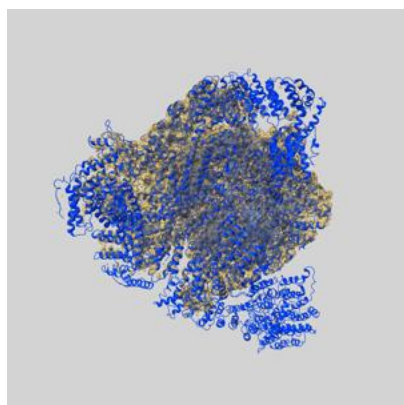
8 Fourier-Shell correlation

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

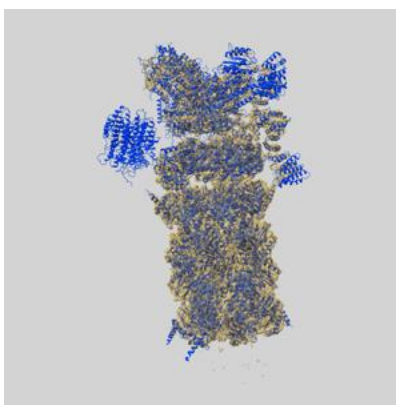
9 Map-model fit [i](#)

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](#).

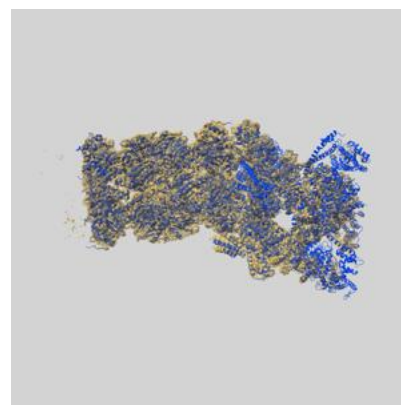
9.1 Map-model overlay [i](#)



X



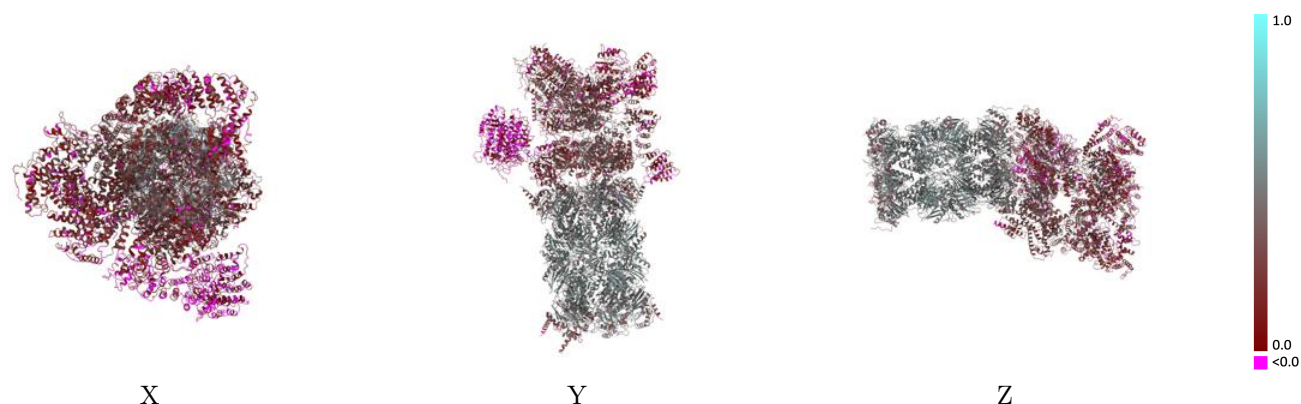
Y



Z

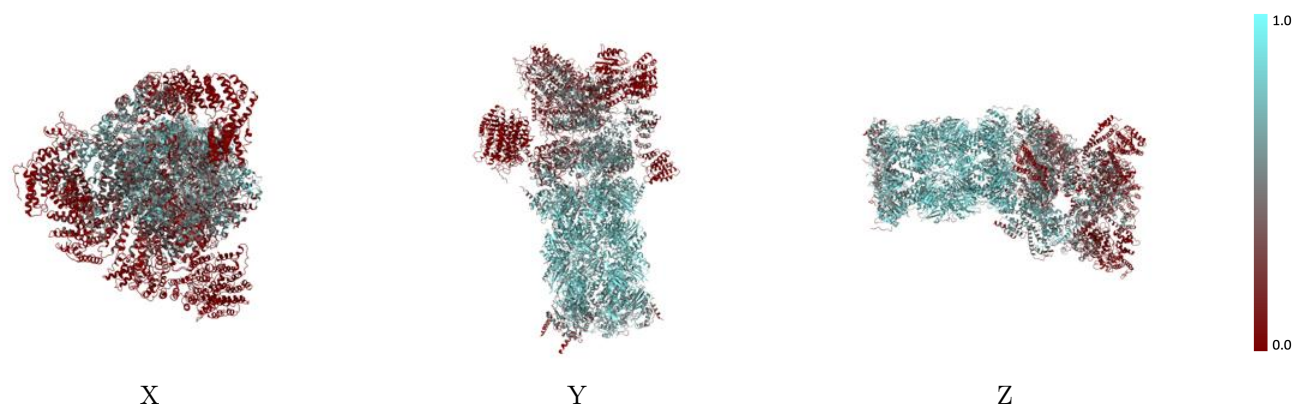
The images above show the 3D surface view of the map at the recommended contour level 0.006 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



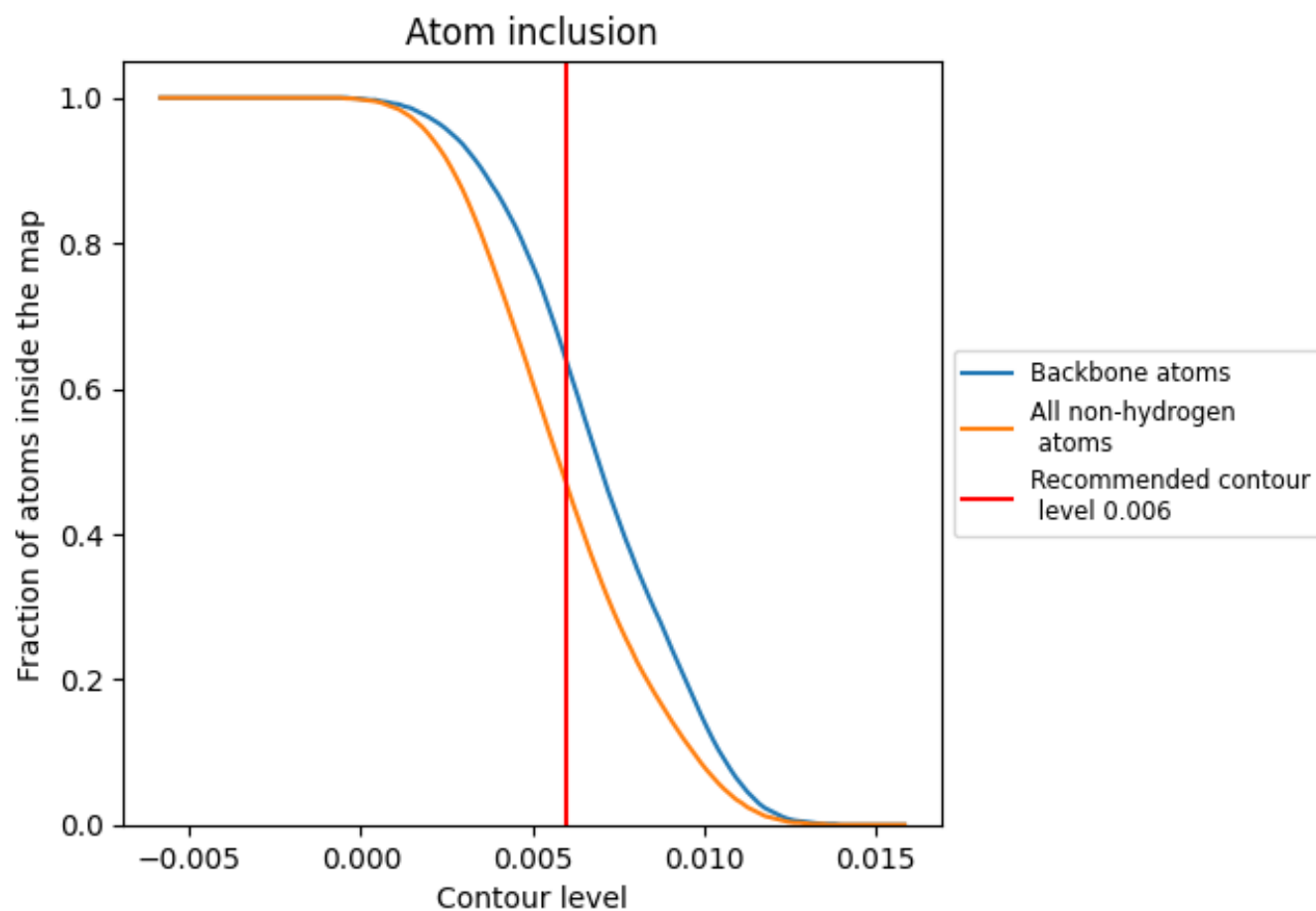
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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 (0.006).







































































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