



wwPDB EM Map/Model Validation Report ⓘ

Aug 30, 2016 – 11:18 AM EDT

PDB ID : 5GJR
EMDB ID: : EMD-9512
Title : An atomic structure of the human 26S proteasome
Authors : Huang, X.L.; Luan, B.; Wu, J.P.; Shi, Y.G.
Deposited on : 2016-07-01
Resolution : 3.50 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027939

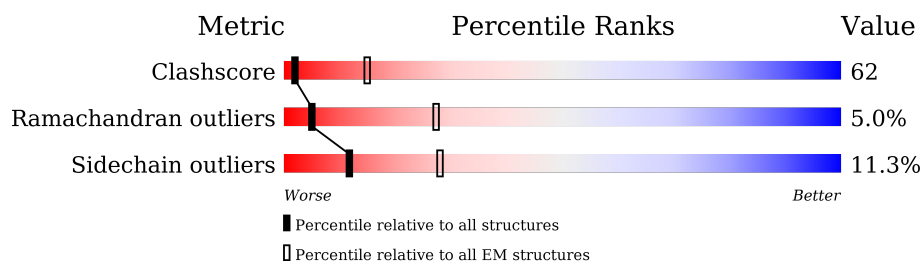
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





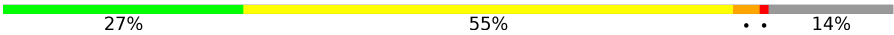
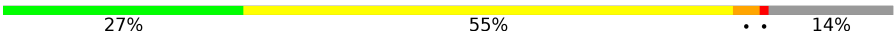


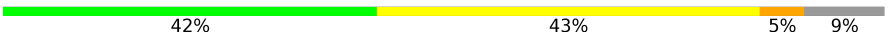
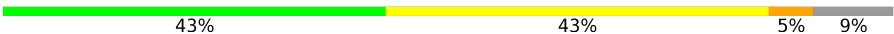
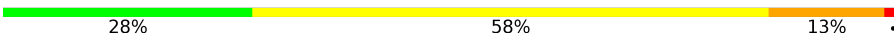
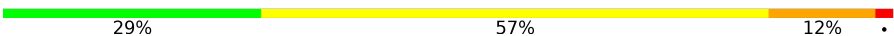
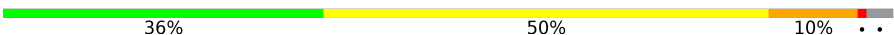
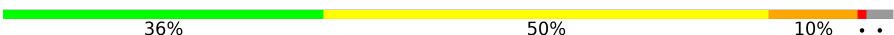


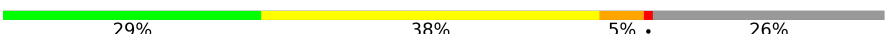
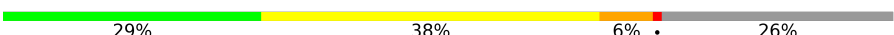


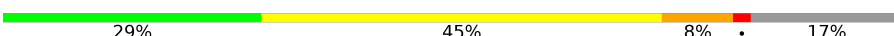




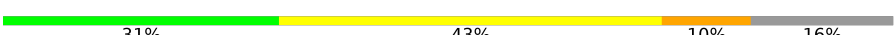
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	I	440	14% 52% 13% • 18%
1	w	440	61% 18% • 18%
2	H	433	18% 51% 16% • 12%
2	v	433	65% 20% • 12%
3	L	389	19% 58% 16% • •
3	z	389	73% 19% • •
4	0	439	20% 47% 17% • 14%
4	M	439	19% 48% 17% • 14%
5	J	406	17% 51% 17% • 12%




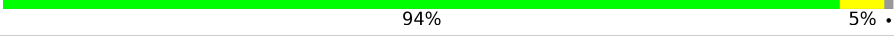




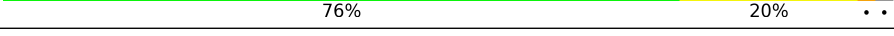
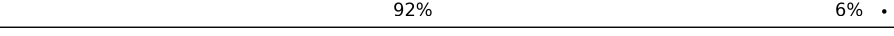
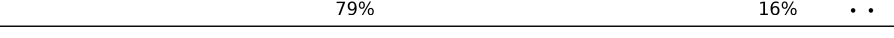
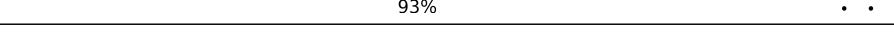

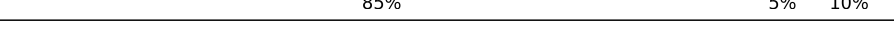


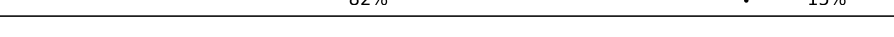

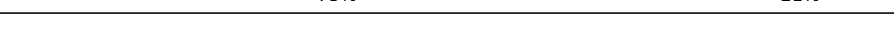






Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	x	406	
6	K	418	
6	y	418	
7	1	953	
7	N	953	
8	2	376	
8	O	376	
9	3	456	
9	P	456	
10	4	422	
10	Q	422	
11	5	389	
11	R	389	
12	6	525	
12	S	525	
13	7	350	
13	T	350	
14	8	324	
14	U	324	
15	9	310	
15	V	310	
16	AA	377	
16	W	377	
17	AB	70	
17	Y	70	




Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
18	AC	908	
18	Z	908	
19	B	246	
19	h	246	
20	C	234	
20	i	234	
21	D	261	
21	j	261	
22	E	248	
22	k	248	
23	F	241	
23	l	241	
24	G	263	
24	m	263	
25	X	255	
25	n	255	
26	a	239	
26	o	239	
27	b	277	
27	p	277	
28	c	205	
28	q	205	
29	d	201	
29	r	201	
30	e	263	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
30	s	263	 74% 24%
31	f	241	 85% 12%
31	t	241	 85% 12%
32	g	264	 77% 5% 18%
32	u	264	 77% 5% 18%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
33	ADP	0	501	-	-	X	-
33	ADP	I	501	-	-	X	-
33	ADP	J	501	-	-	X	-
33	ADP	K	501	-	-	X	-
33	ADP	L	401	-	-	X	-
33	ADP	M	501	-	-	X	-

2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 142753 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 protease regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	I	359	Total	C	N	O	S	0	0
			2720	1708	465	535	12		
1	w	359	Total	C	N	O	S	0	0
			2720	1708	465	535	12		

- Molecule 2 is a protein called 26S protease regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	380	Total	C	N	O	S	0	0
			2893	1817	515	543	18		
2	v	380	Total	C	N	O	S	0	0
			2893	1817	515	543	18		

- Molecule 3 is a protein called 26S protease regulatory subunit 10B.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	375	Total	C	N	O	S	0	0
			2860	1796	512	536	16		
3	z	375	Total	C	N	O	S	0	0
			2860	1796	512	536	16		

- Molecule 4 is a protein called 26S protease regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	M	376	Total	C	N	O	S	0	0
			2858	1802	496	545	15		
4	0	376	Total	C	N	O	S	0	0
			2858	1802	496	545	15		

- Molecule 5 is a protein called 26S protease regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	J	358	Total	C	N	O	S	0	0
			2820	1780	506	518	16		
5	x	358	Total	C	N	O	S	0	0
			2820	1780	506	518	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	K	380	Total	C	N	O	S	0	0
			3039	1923	524	579	13		
6	y	380	Total	C	N	O	S	0	0
			3039	1923	524	579	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	N	821	Total	C	N	O	S	0	0
			5449	3491	931	1009	18		
7	1	821	Total	C	N	O	S	0	0
			5449	3491	931	1009	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	O	372	Total	C	N	O	S	0	0
			2369	1515	405	438	11		
8	2	372	Total	C	N	O	S	0	0
			2375	1521	405	438	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	P	413	Total	C	N	O	S	0	0
			2832	1821	489	516	6		
9	3	413	Total	C	N	O	S	0	0
			2831	1820	489	516	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	Q	421	Total	C	N	O	S	0	0
			2956	1866	512	569	9		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
10	4	421	Total	C	N	O	S	0	0
			2956	1866	512	569	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	R	376	Total	C	N	O	S	0	0
			2767	1794	461	504	8		
11	5	376	Total	C	N	O	S	0	0
			2770	1796	461	504	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	S	421	Total	C	N	O	S	0	0
			2723	1737	484	499	3		
12	6	421	Total	C	N	O	S	0	0
			2732	1741	487	501	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	T	258	Total	C	N	O	S	0	0
			1699	1099	280	315	5		
13	7	258	Total	C	N	O	S	0	0
			1699	1099	280	315	5		

- Molecule 14 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	U	283	Total	C	N	O	S	0	0
			2131	1370	369	388	4		
14	8	283	Total	C	N	O	S	0	0
			2131	1370	369	388	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	V	257	Total	C	N	O	S	0	0
			2011	1276	341	377	17		
15	9	257	Total	C	N	O	S	0	0
			2009	1274	341	377	17		

- Molecule 16 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	W	193	Total	C	N	O	S	0	0
			1300	818	228	250	4		
16	AA	193	Total	C	N	O	S	0	0
			1300	818	228	250	4		

- Molecule 17 is a protein called 26S proteasome complex subunit DSS1.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	Y	59	Total	C	N	O	0	0
			316	191	60	65		
17	AB	59	Total	C	N	O	0	0
			316	191	60	65		

- Molecule 18 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	Z	732	Total	C	N	O	0	0
			3608	2144	732	732		
18	AC	732	Total	C	N	O	0	0
			3608	2144	732	732		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	B	244	Total	C	N	O	S	0	0
			1845	1171	309	352	13		
19	h	244	Total	C	N	O	S	0	0
			1853	1177	311	352	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	C	231	Total	C	N	O	S	0	0
			1737	1106	289	336	6		
20	i	231	Total	C	N	O	S	0	0
			1744	1112	290	336	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	D	250	Total	C	N	O	S	0	0
			1916	1206	330	372	8		
21	j	250	Total	C	N	O	S	0	0
			1913	1203	330	372	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	E	243	Total	C	N	O	S	0	0
			1724	1068	312	339	5		
22	k	243	Total	C	N	O	S	0	0
			1691	1051	309	327	4		

- Molecule 23 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	F	234	Total	C	N	O	S	0	0
			1766	1108	290	357	11		
23	l	234	Total	C	N	O	S	0	0
			1726	1107	291	317	11		

- Molecule 24 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	G	238	Total	C	N	O	S	0	0
			1850	1159	334	346	11		
24	m	238	Total	C	N	O	S	0	0
			1850	1159	334	346	11		

- Molecule 25 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	X	243	Total	C	N	O	S	0	0
			1873	1189	317	356	11		
25	n	243	Total	C	N	O	S	0	0
			1873	1189	317	356	11		

- Molecule 26 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	a	202	Total	C	N	O	S	0	0
			1509	945	258	294	12		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
26	o	202	Total	C	N	O	S	0	0
			1509	945	258	294	12		

- Molecule 27 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	220	Total	C	N	O	S	0	0
			1643	1033	280	318	12		
27	p	220	Total	C	N	O	S	0	0
			1643	1033	280	318	12		

- Molecule 28 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	c	204	Total	C	N	O	S	0	0
			1585	1010	262	294	19		
28	q	204	Total	C	N	O	S	0	0
			1585	1010	262	294	19		

- Molecule 29 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	d	199	Total	C	N	O	S	0	0
			1570	1006	265	290	9		
29	r	199	Total	C	N	O	S	0	0
			1570	1006	265	290	9		

- Molecule 30 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	e	201	Total	C	N	O	S	0	0
			1548	974	273	292	9		
30	s	201	Total	C	N	O	S	0	0
			1551	977	273	292	9		

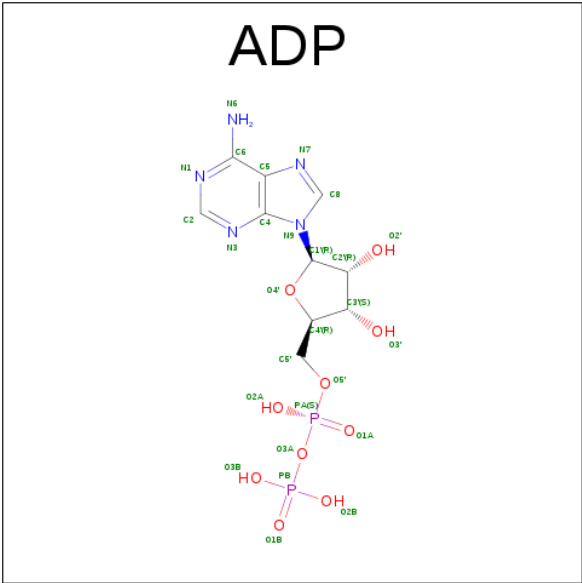
- Molecule 31 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	f	213	Total	C	N	O	S	0	0
			1644	1039	282	313	10		
31	t	213	Total	C	N	O	S	0	0
			1644	1039	282	313	10		

- Molecule 32 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	g	216	Total	C	N	O	S	0	0
			1672	1055	286	319	12		
32	u	217	Total	C	N	O	S	0	0
			1678	1058	290	318	12		

- Molecule 33 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
33	I	1	Total	C	N	O	P	0
			27	10	5	10	2	
33	H	1	Total	C	N	O	P	0
			27	10	5	10	2	
33	L	1	Total	C	N	O	P	0
			27	10	5	10	2	
33	M	1	Total	C	N	O	P	0
			27	10	5	10	2	
33	J	1	Total	C	N	O	P	0
			27	10	5	10	2	
33	K	1	Total	C	N	O	P	0
			27	10	5	10	2	
33	v	1	Total	C	N	O	P	0
			27	10	5	10	2	
33	w	1	Total	C	N	O	P	0
			27	10	5	10	2	

Continued on next page...

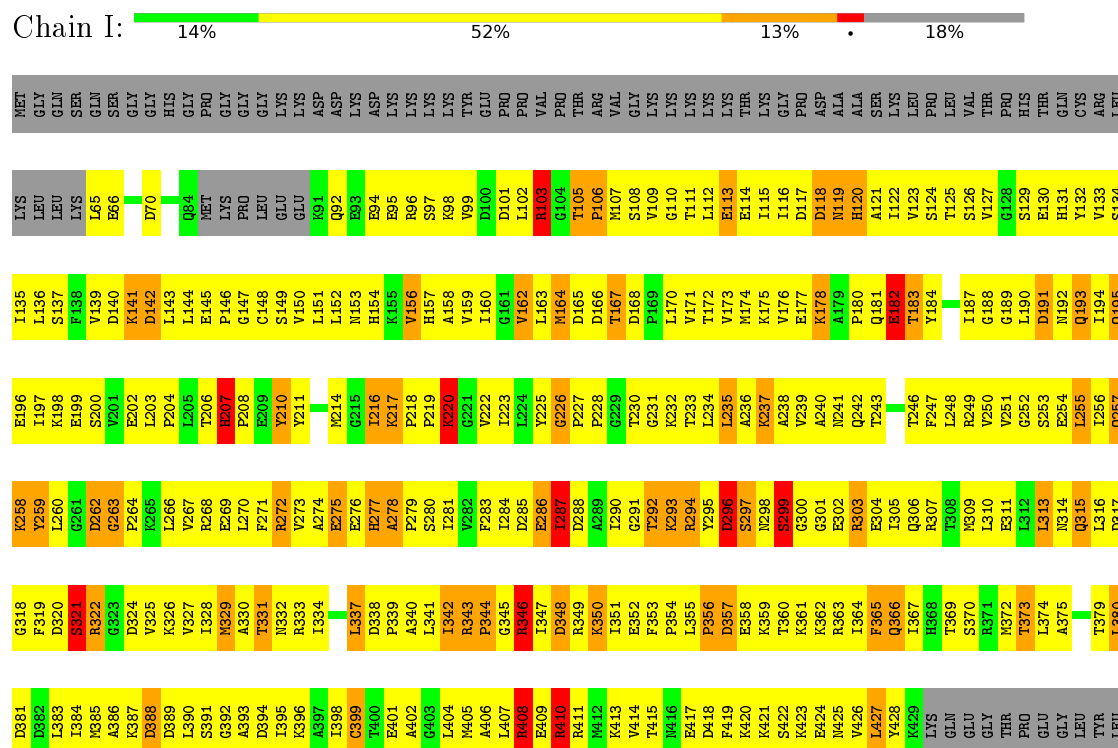
Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
33	x	1	Total	C	N	O	P	0
			27	10	5	10	2	
33	y	1	Total	C	N	O	P	0
			27	10	5	10	2	
33	z	1	Total	C	N	O	P	0
			27	10	5	10	2	
33	0	1	Total	C	N	O	P	0
			27	10	5	10	2	

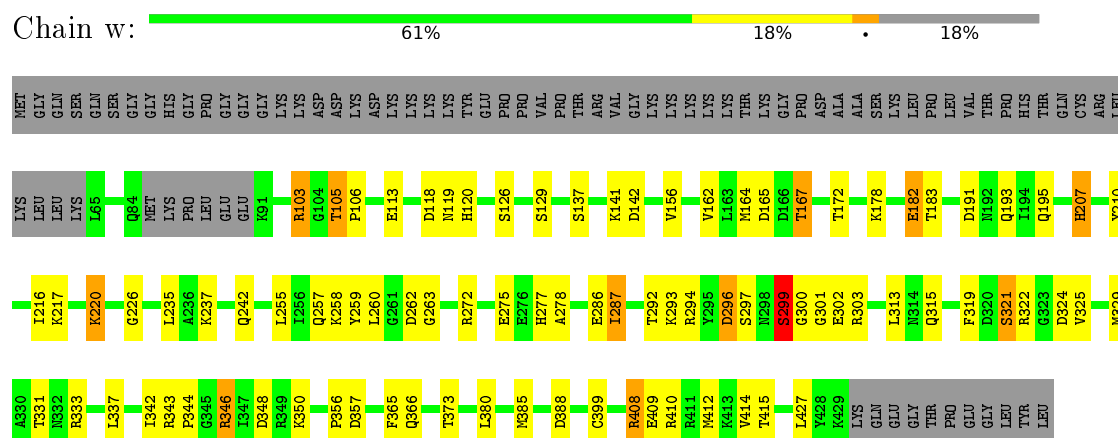
3 Residue-property plots

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

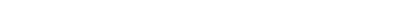
- Molecule 1: 26S protease regulatory subunit 4

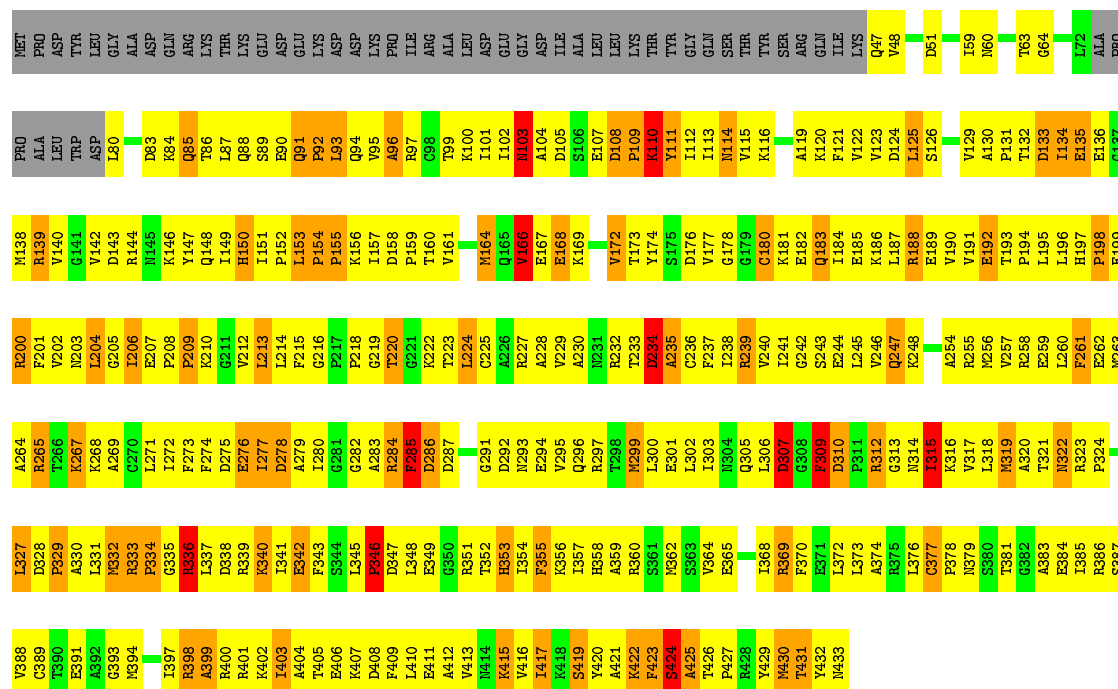


- Molecule 1: 26S protease regulatory subunit 4



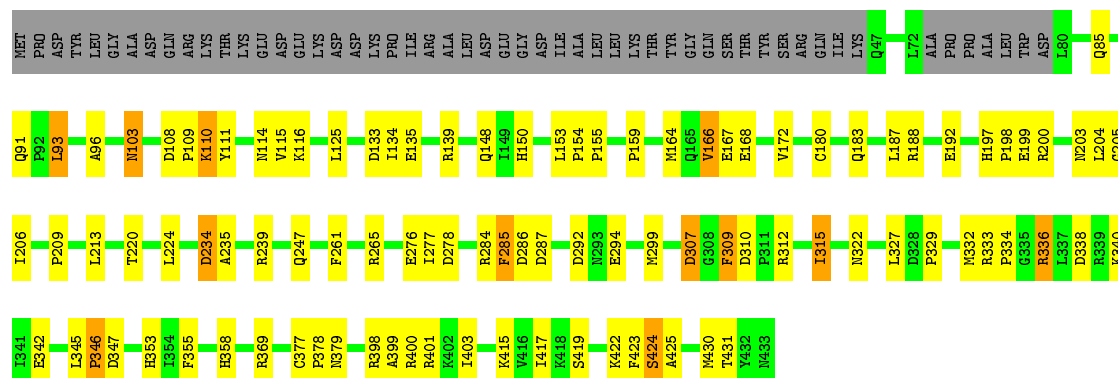
- Molecule 2: 26S protease regulatory subunit 7

Chain H:  18% 51% 16% • 12%



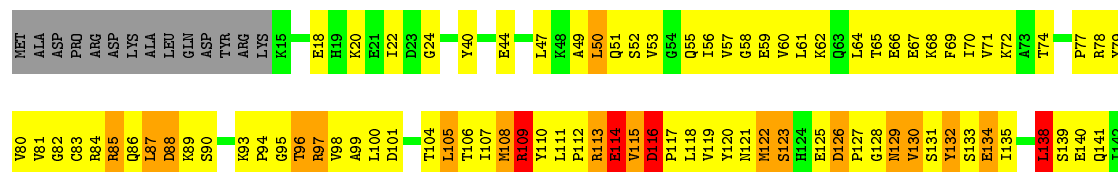
- Molecule 2: 26S protease regulatory subunit 7

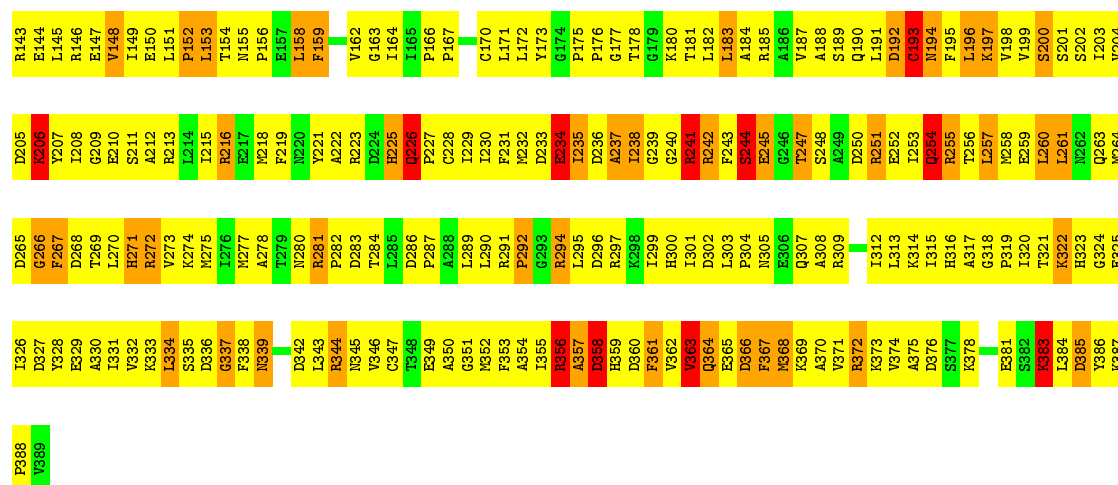
Chain v:  65% 20% • 12%



- Molecule 3: 26S protease regulatory subunit 10B

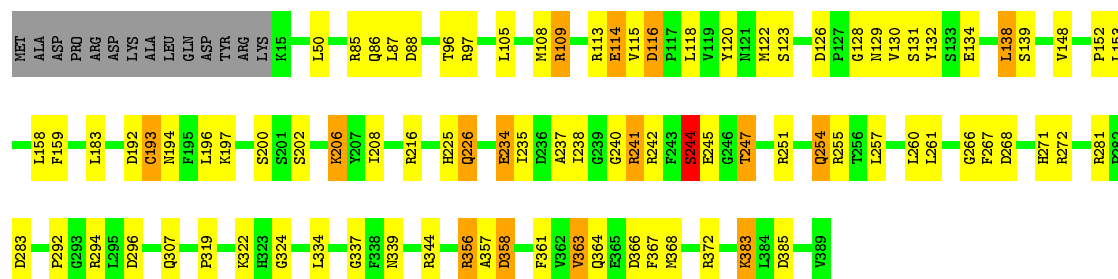
Chain L: 19% 58% 16% . .





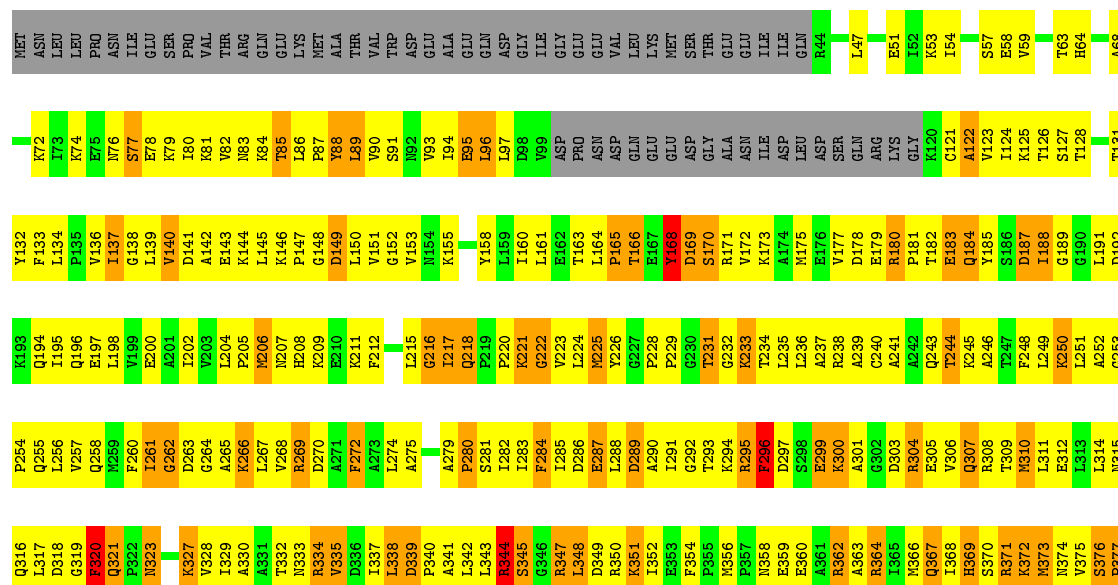
• Molecule 3: 26S protease regulatory subunit 10B

Chain z: 73% 19%



• Molecule 4: 26S protease regulatory subunit 6A

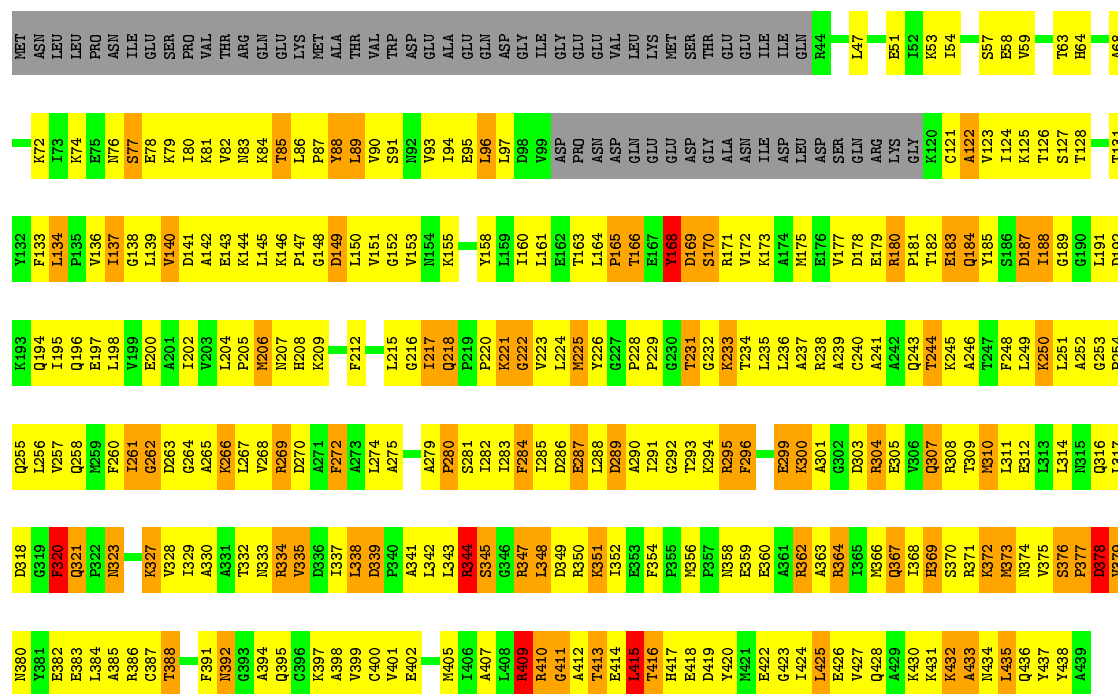
Chain M: 19% 48% 17% 14%





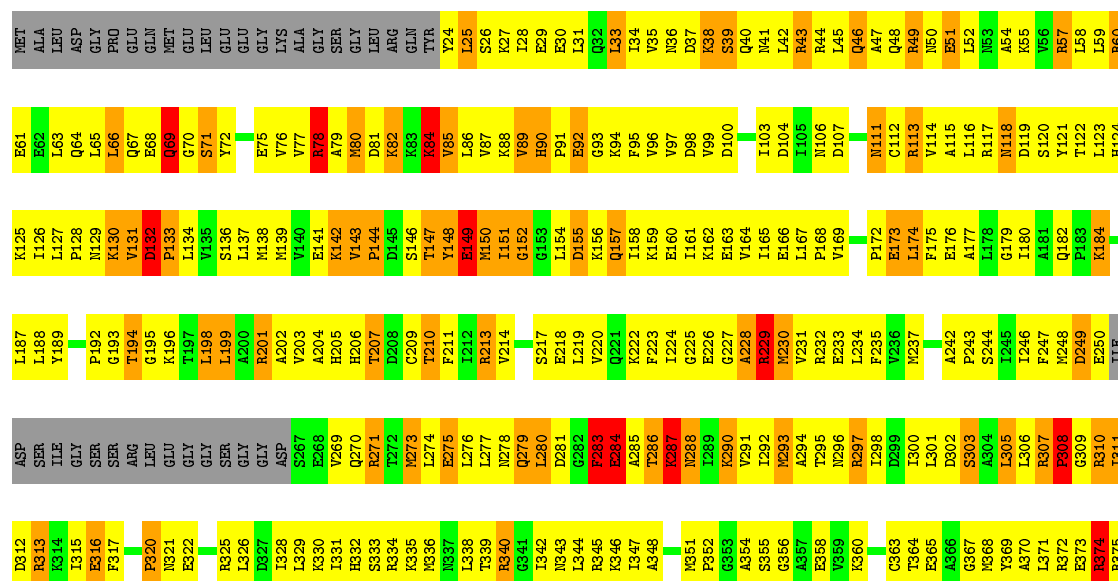
• Molecule 4: 26S protease regulatory subunit 6A

Chain 0: 20% 47% 17% 14%



• Molecule 5: 26S protease regulatory subunit 8

Chain J: 17% 51% 17% 12%



V376
H377
Q380
E381
D382
F383
V387
A388
K391
Q392
K393
S394
E396
K397
ASN
MET
SER
ILE
GLN
LYS
LEU
TRP
LYS

• Molecule 5: 26S protease regulatory subunit 8

Chain x: 66% 19% 12%

MET ALA ASP LEU GLY PRO GLU GLN MET MET LEU GLU GLU GLU GLY LYS LYS GLY SER GLY LEU ARG TTR Y24 L25 S26 R27 L33 D37 K38 S39 R43 Q46 R49 R50 E51 B57 R60 E61 L66 A69 Q69 G70 S71 R78 A79 R80 R81 R82 R83 R84
V85 V89 H90 P91 E92 M111 C112 R113 M118 K130 V131 D132 A133 P133 M139 K142 V143 P144 T147 Y148 E149 M150 I151 G152 D155 K156 Q157 E173 L174 Q182 P183 K184 P192 G193 T194 L198 L199 A200 R201 T207 T210 T213 S217 E226
R237 A238 R239 M230 A242 D249 E250 ILE ASP SER ILE GLY SER SER ARG LEU GLY GLY ASP S267 Q270 R271 T272 T273 L274 E275 Q279 L280 F283 E284 A285 T286 K287 N288 T289 K290 M293 R297 S303 A304 L305 L306 R307 P308 G309 R310 I311 D312
R313 E316 P320 R340 P352 R374 Q382 K397 ASN MET SER LEU ILE LYS LYS LEU TRP LYS

• Molecule 6: 26S protease regulatory subunit 6B

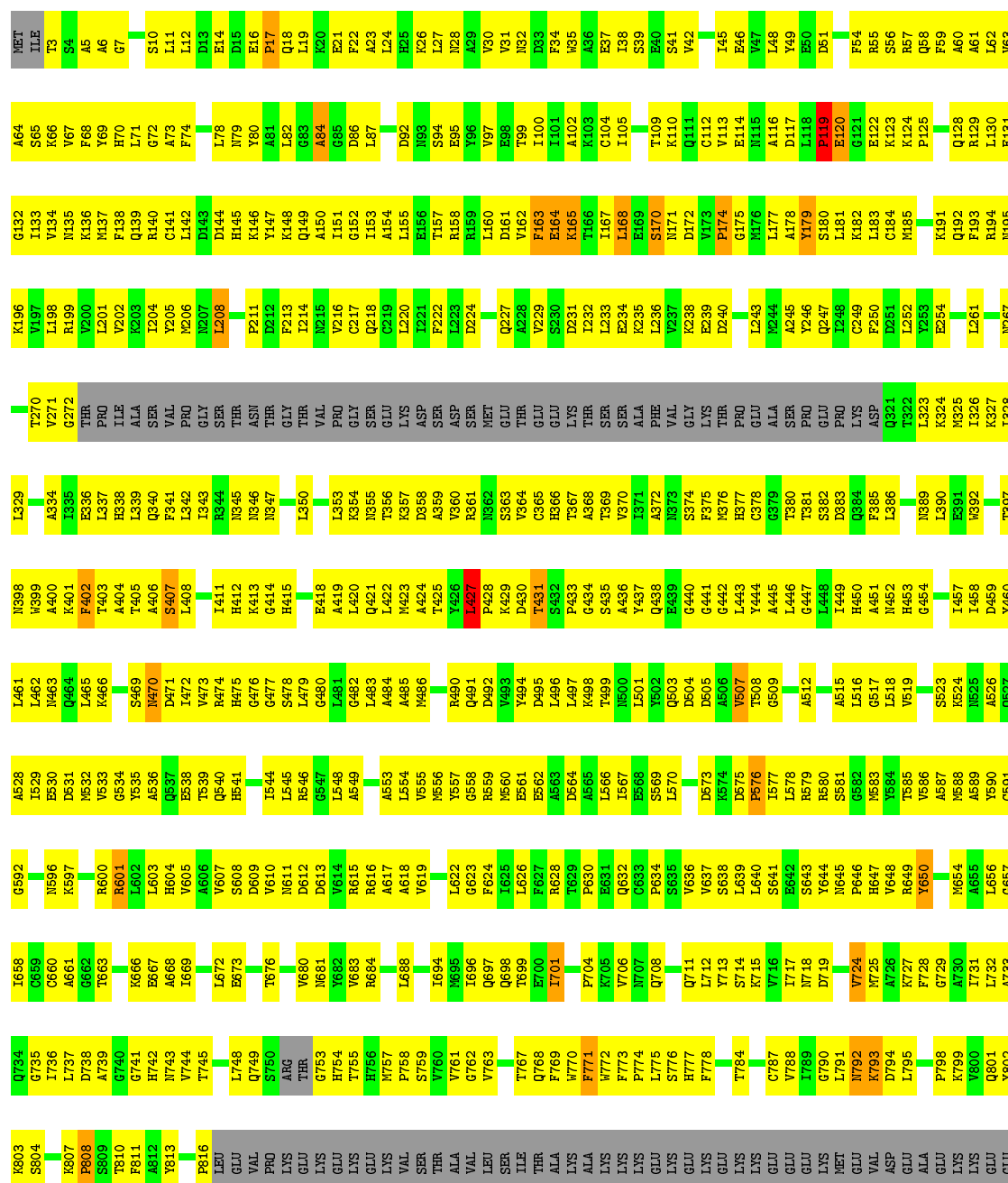
Chain K: 13% 56% 20% 9%

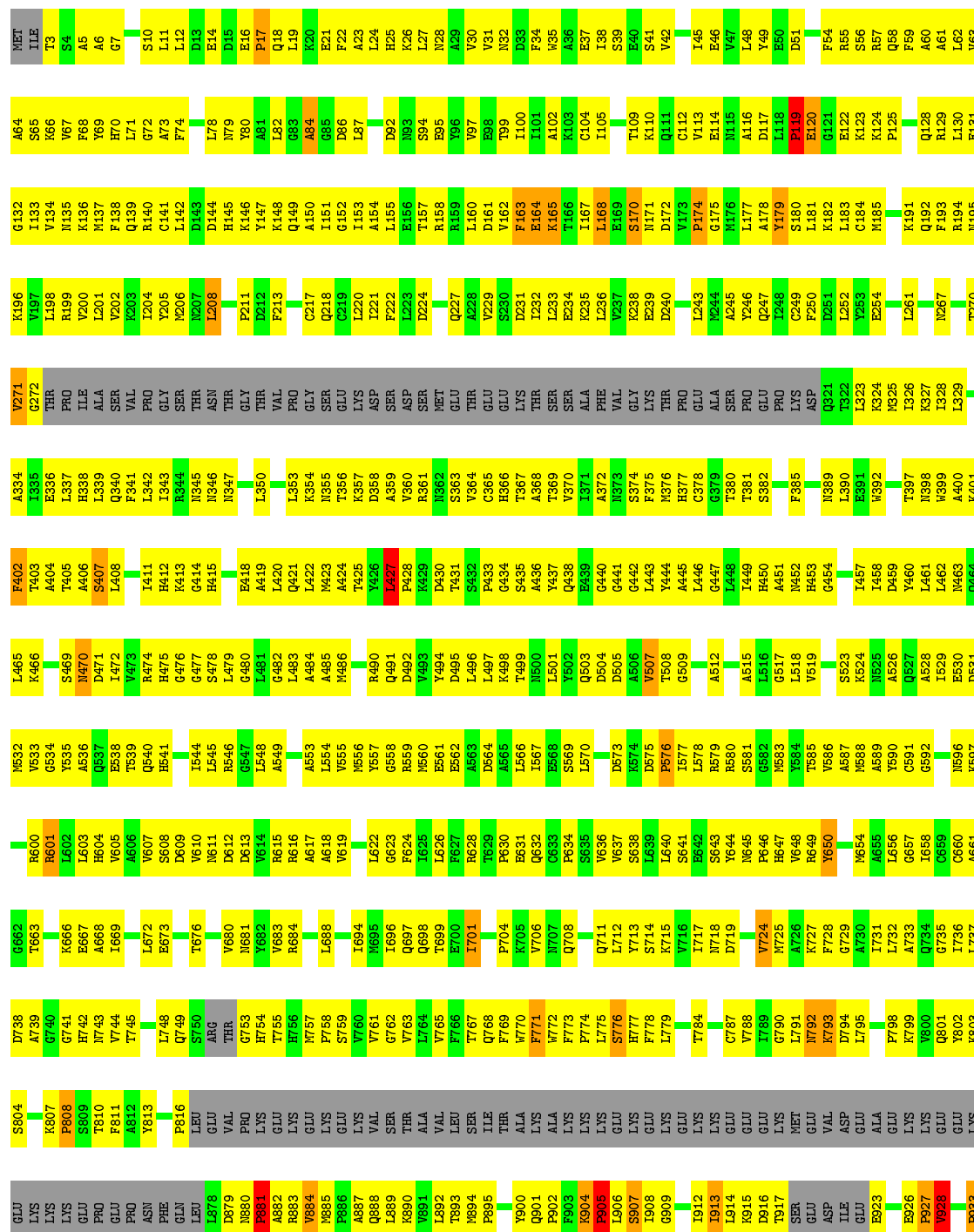
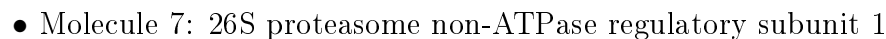
MET GLU GLU ILE GLY ILE VAL GLU LYS ALA ASP GLU ILE PRO ALA LEU SER VAL SER ARG PRO GLN THR GLY LEU SER LEU PHE LEU G90 G91 G92 L93 E94 A95 V96 D97 Q98 N99 T100 Y41 I102 S42 R43 Y44 K45 L46 T107 L47 G108 Q48 G109 M110 L51 L52 Y112 Y113 R114 L54 E55 V56 Q57 E58 T118 I119 D120
I61 K62 D63 E64 Q65 K66 M67 L68 K69 K70 E71 F72 L73 H74 Q76 E77 E78 V79 K80 R81 I82 Q83 S84 I85 P86 L87 V88 I89 G90 Q91 F92 L93 E94 A95 V96 D97 Q98 N99 T100 Y41 I102 S42 R43 Y44 K45 L46 T107 L47 G108 Q48 G109 M110 L51 L52 Y112 Y113 R114 L54 E55 V56 Q57 E58 T118 I119 D120
R121 E122 L123 L124 K125 P126 M127 A128 S129 V130 A131 L132 H133 K134 H135 H136 S136 M137 A138 L139 V140 D141 V142 L143 M144 P145 E146 A147 D148 S149 G150 T151 M152 M153 L154 T155 S156 K159 P160 D161 V162 M163 Y164 A165 D166 I167 G168 G169 M170 D171 I172 Q173 K174 Q175 Q176 V177 R178 E179 A180 V181
E182 L183 P184 L185 T186 H187 F188 E189 L190 K191 Q192 Q193 L194 G195 I196 D197 P198 P199 R200 G201 V202 L203 M204 Y205 G206 P207 P208 G209 C210 G211 T212 K213 M214 L215 A216 D217 A218 V219 A220 H221 R222 T223 T224 A225 A226 D227 T228 R229 G230 V231 G232 S233 E234 F235 V236 Q237 K238 Y239 L240 G241
E242 G243 P244 R245 V246 T247 M248 D249 A310 R311 R312 R313 A314 D315 T316 K255 E256 D257 A258 P259 A260 L261 L262 F263 G264 D265 D266 L267 D268 A269 L270 A271 T272 K273 L274 F275 D276 A277 Q278 T279 D282 R283 E284 V285 Q286 R287 T288 T289 L290 E291 L292 L293 T294 Q295 M296 D297 C298 F299 D300 Q301 N302
V303 N304 V305 K306 V307 I308 M309 A310 R311 R312 R313 A314 D315 T316 K255 E256 D257 A258 P259 A260 L261 L262 F263 G264 D265 D266 L267 D268 A269 L270 A271 T272 K273 L274 F275 D276 A277 Q278 T279 D282 R283 E284 V285 Q286 R287 T288 T289 L290 E291 L292 L293 T294 Q295 M296 D297 C298 F299 D300 Q301 N302
V364 A365 P366 R367 D368 K369 L370 S371 G372 A373 D374 L375 N376 S377 G383 G384 A385 A386 V387 R388 E389 R390 R391 Y392 K393 V394 L395 A396 K397 D398 F399 E400 K401 A402 Y403 T404 V405 L406 K407 K408 K409 D410 E411 Q412 K418

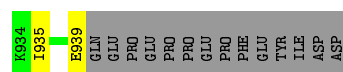
• Molecule 6: 26S protease regulatory subunit 6B

Chain y: 67% 22% 9%

MET GLU GLU ILE GLY ILE VAL GLU LYS ALA GLN ASP GLU ILE PRO ARG ARG GLN THR GLY LEU SER VAL SER ARG PRO LEU SER VAL PHE LEU GLY PRO L40 L51 E52 F53 L54 E58 Q65 F72 L73 I82 I85 P86 L87 L93

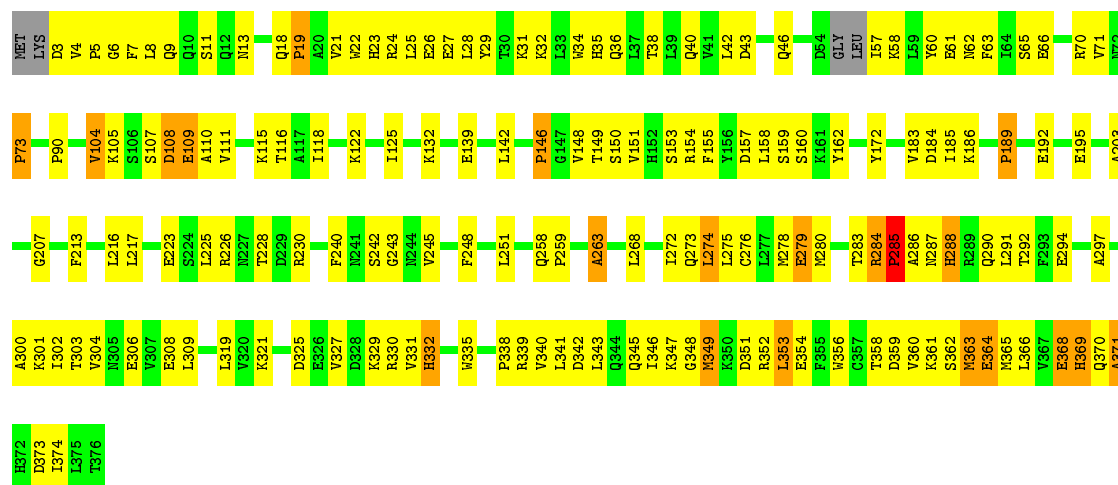






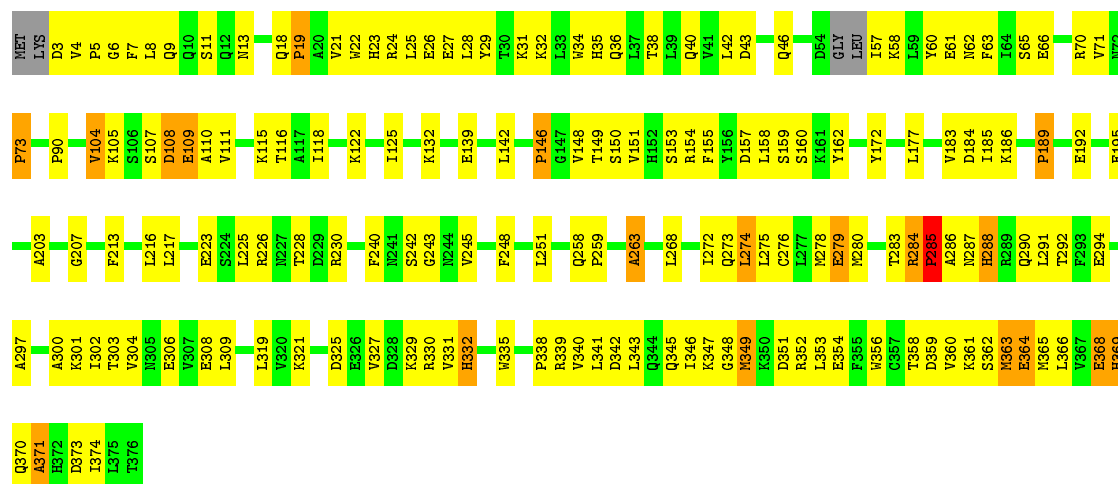
• Molecule 8: 26S proteasome non-ATPase regulatory subunit 13

Chain O: 55% 38% 5%



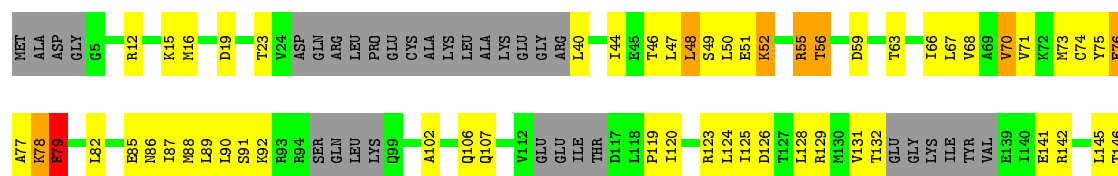
• Molecule 8: 26S proteasome non-ATPase regulatory subunit 13

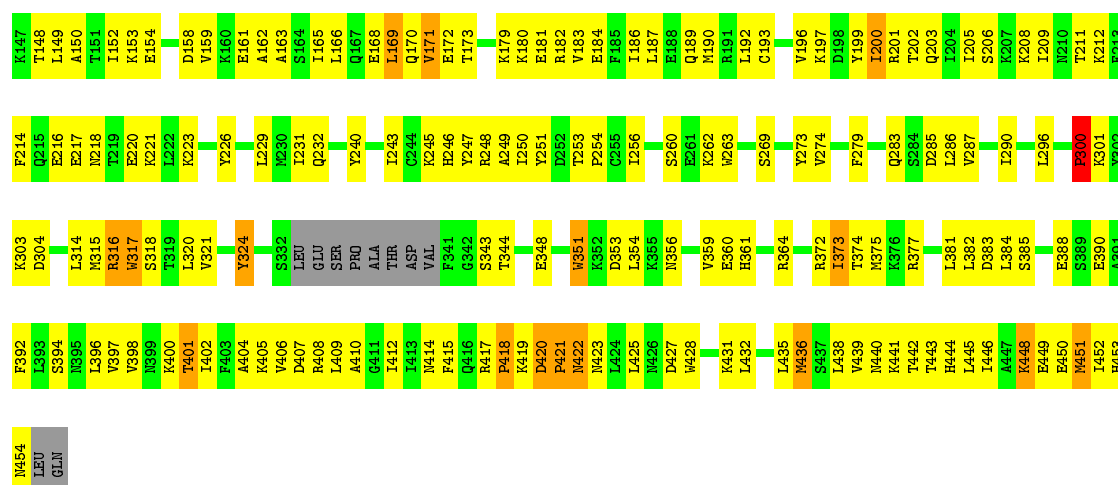
Chain 2: 55% 39% 5%



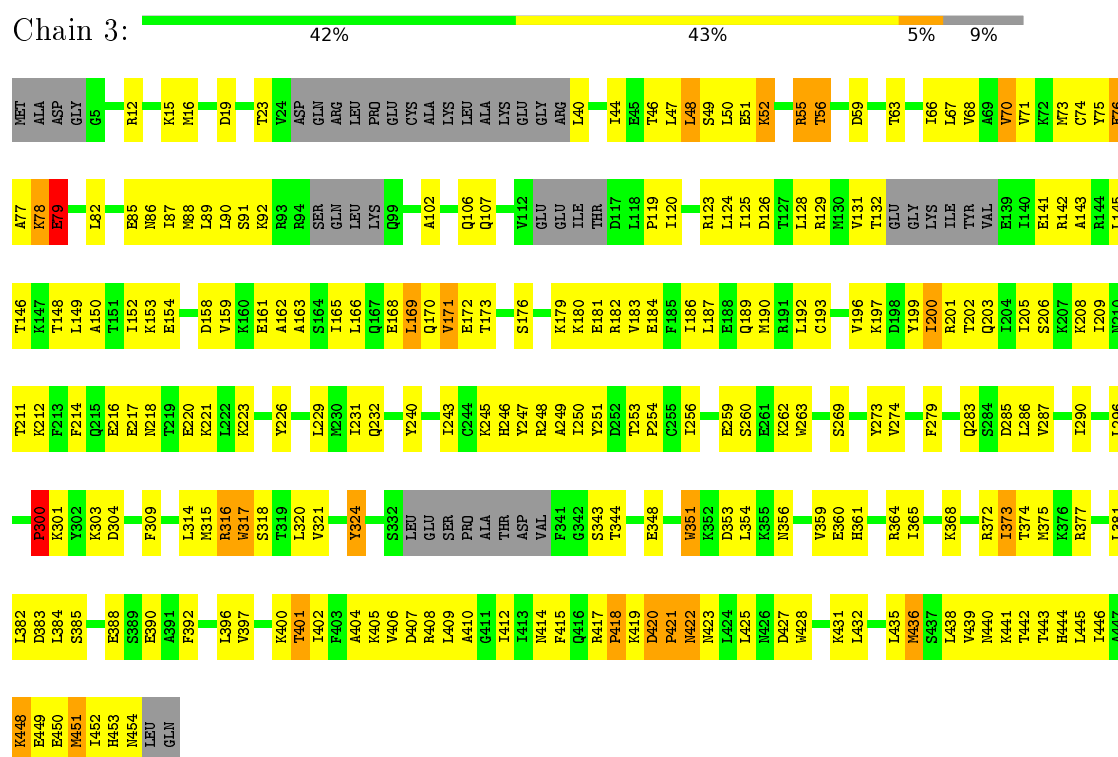
• Molecule 9: 26S proteasome non-ATPase regulatory subunit 12

Chain P: 43% 43% 5% 9%

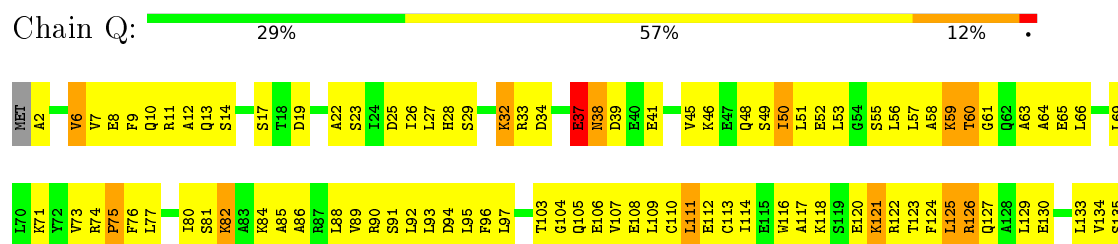


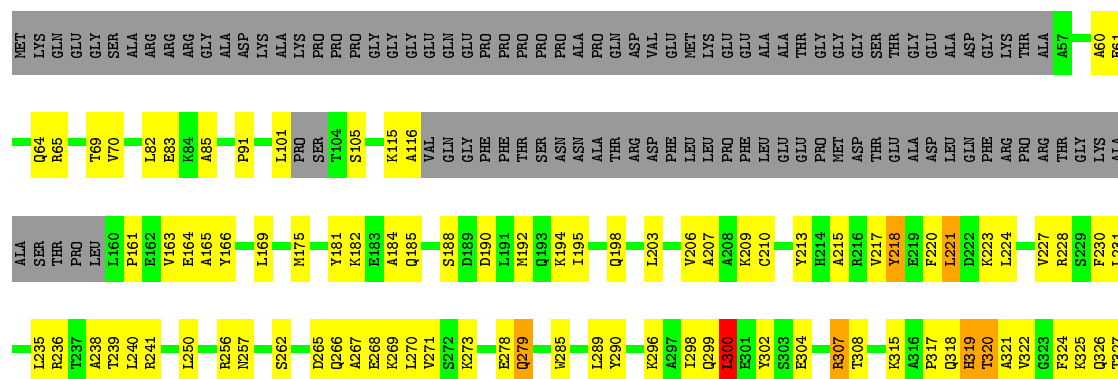


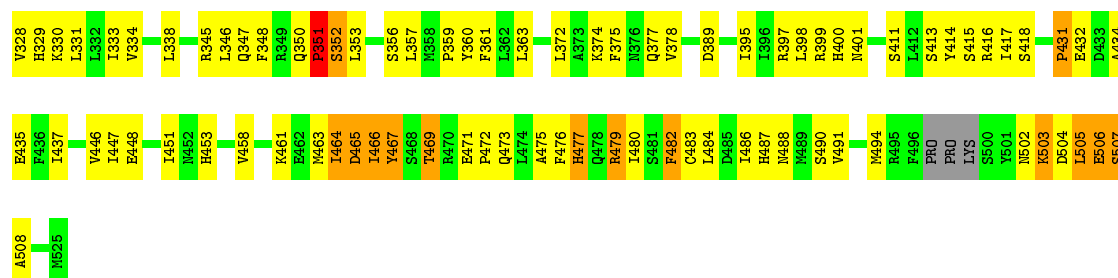
- Molecule 9: 26S proteasome non-ATPase regulatory subunit 12



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

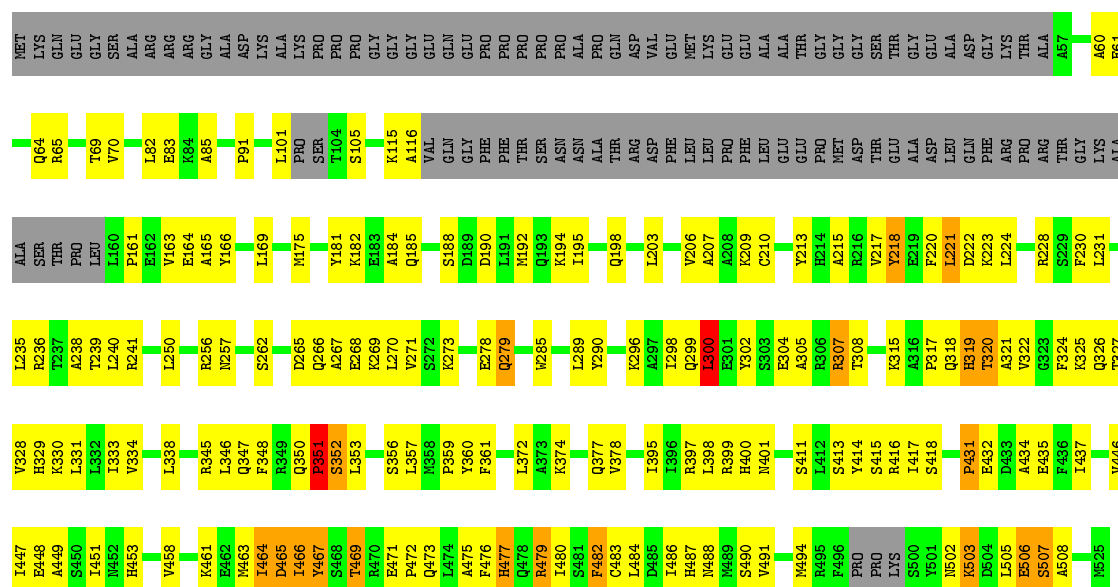






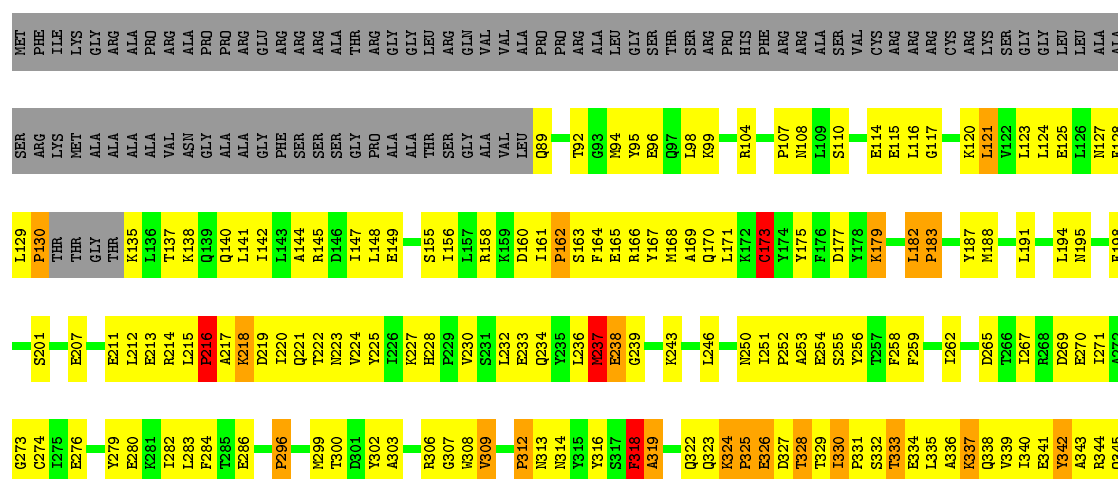
- Molecule 12: 26S proteasome non-ATPase regulatory subunit 3

Chain 6: 48% 28% 20%

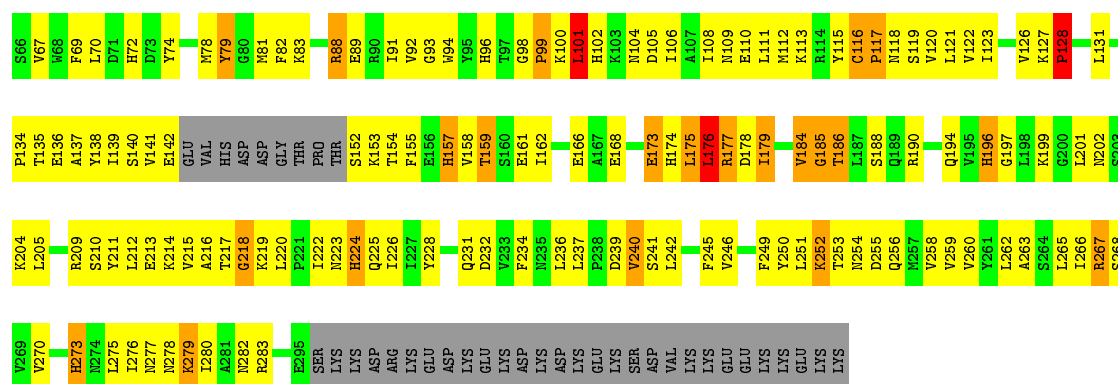


- Molecule 13: 26S proteasome non-ATPase regulatory subunit 8

Chain T: 29% 38% 6% 26%

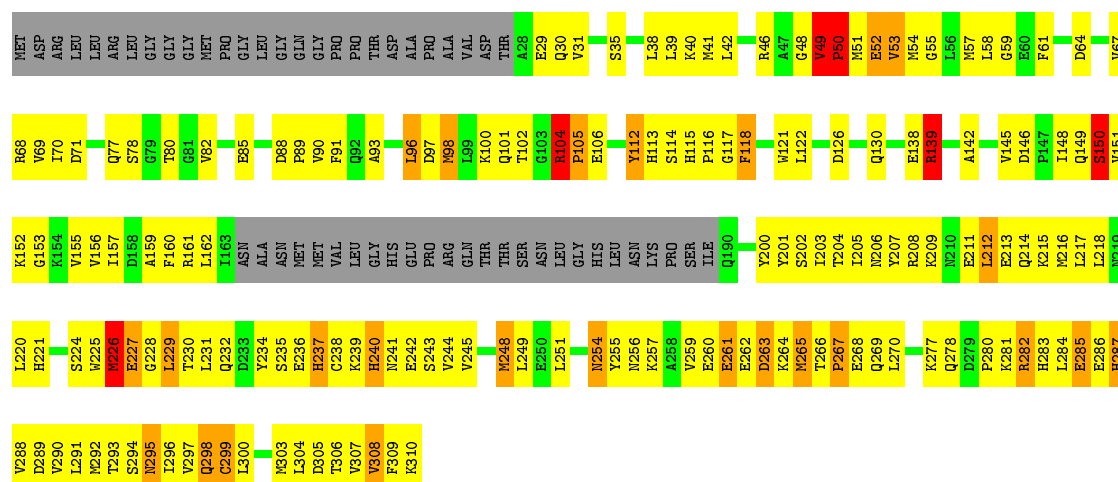






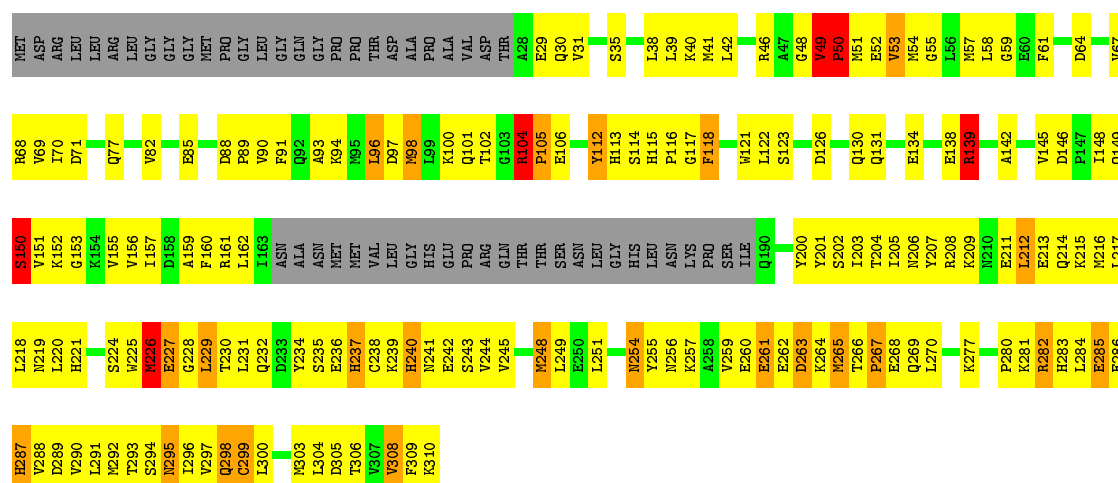
- Molecule 15: 26S proteasome non-ATPase regulatory subunit 14

Chain V: 29% 44% 8% 17%



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

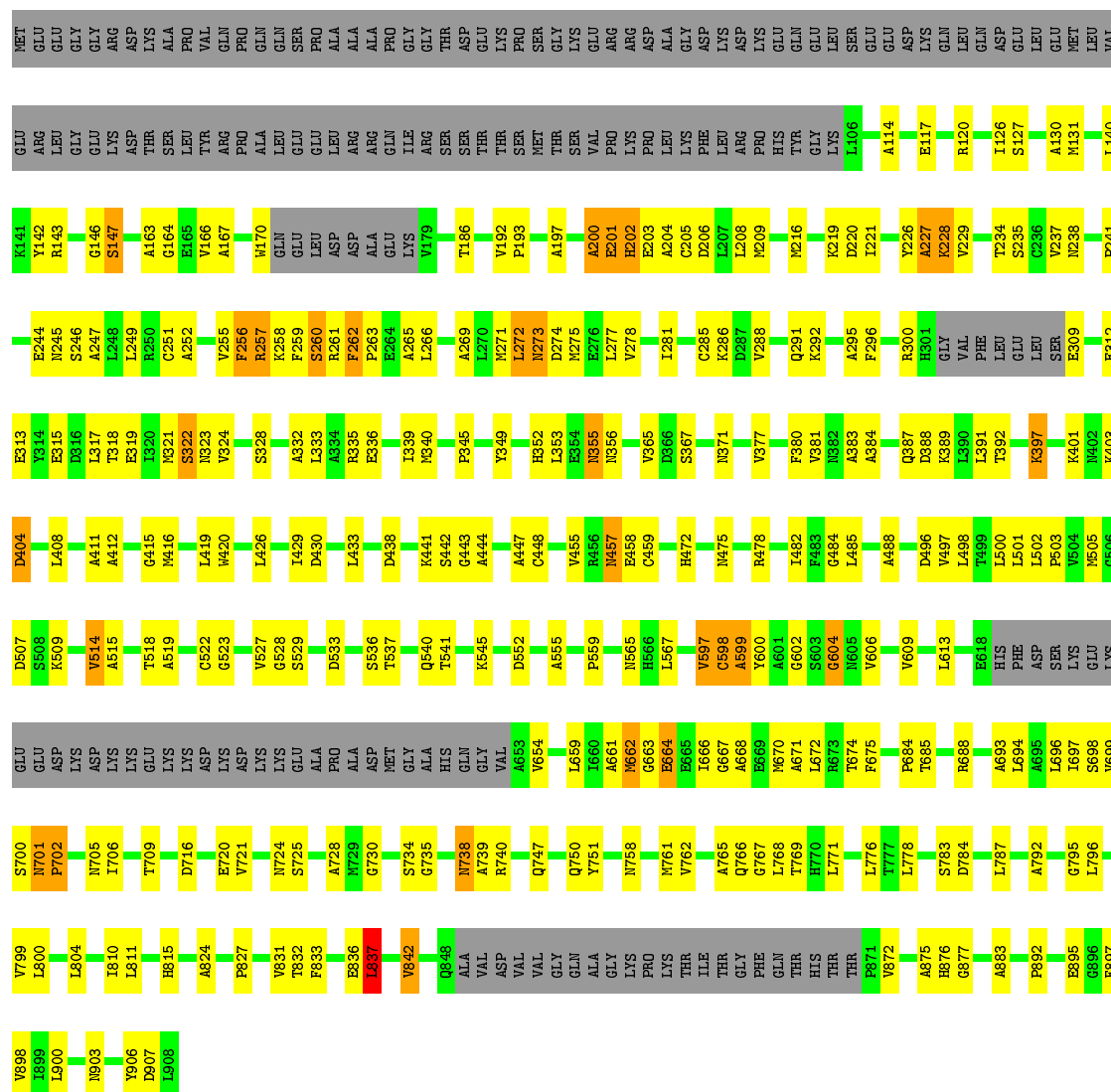
Chain 9: 29% 45% 8% 17%



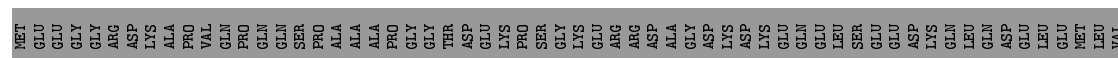
- Molecule 16: 26S proteasome non-ATPase regulatory subunit 4

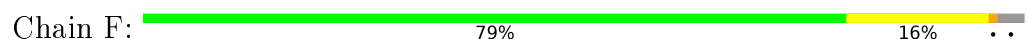


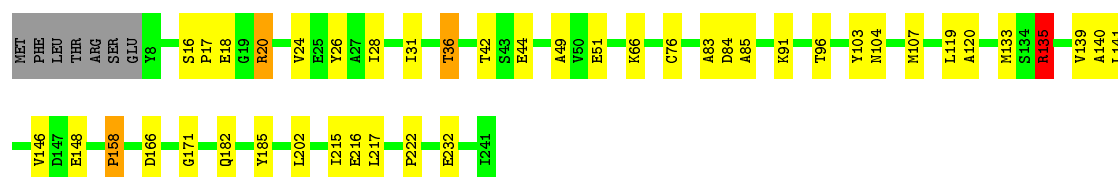
- Chain Z:  50% 27% . 19%



- Chain AC: 







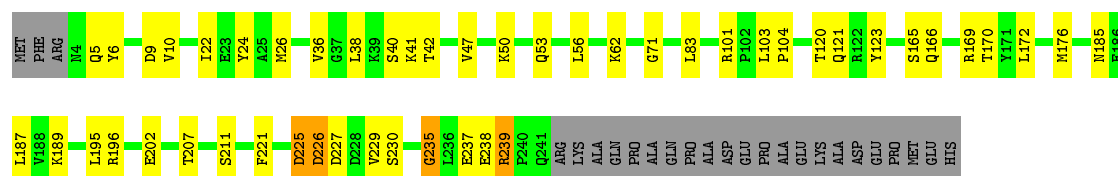
- Molecule 23: Proteasome subunit alpha type-5

Chain l:  93%




- Molecule 24: Proteasome subunit alpha type-1

Chain G:  72% 17% 10%



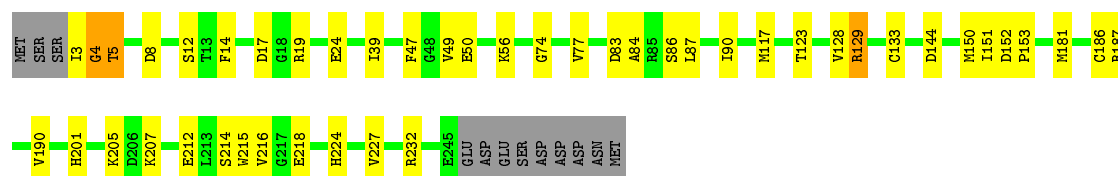
- Molecule 24: Proteasome subunit alpha type-1

Chain m:  85% 5% 10%




- Molecule 25: Proteasome subunit alpha type-3

Chain X:  77% 17% 5%




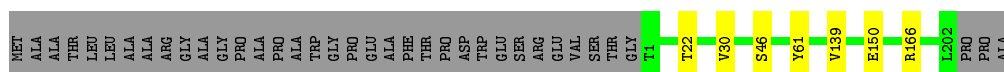
- Molecule 25: Proteasome subunit alpha type-3

Chain n:  91% 5% 5%



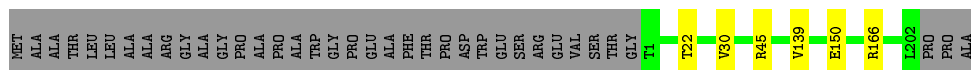
- Molecule 26: Proteasome subunit beta type-6

Chain a:  82% 15% 3%



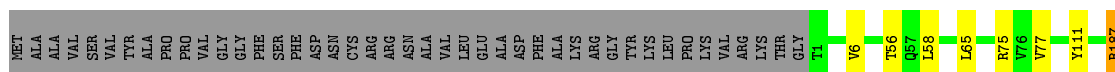
- Molecule 26: Proteasome subunit beta type-6

Chain o: 82% 15%



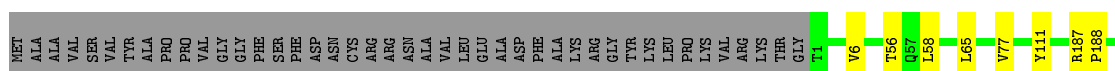
- Molecule 27: Proteasome subunit beta type-7

Chain b: 75% 21%



- Molecule 27: Proteasome subunit beta type-7

Chain p: 76% 21%



- Molecule 28: Proteasome subunit beta type-3

Chain c: 94% 5%



- Molecule 28: Proteasome subunit beta type-3

Chain q: 94% 5%

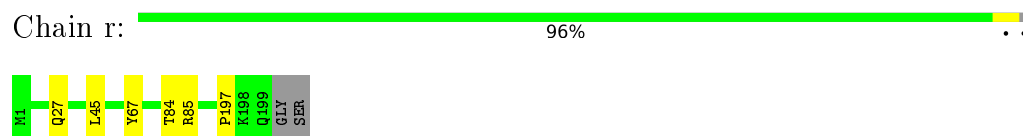


- Molecule 29: Proteasome subunit beta type-2

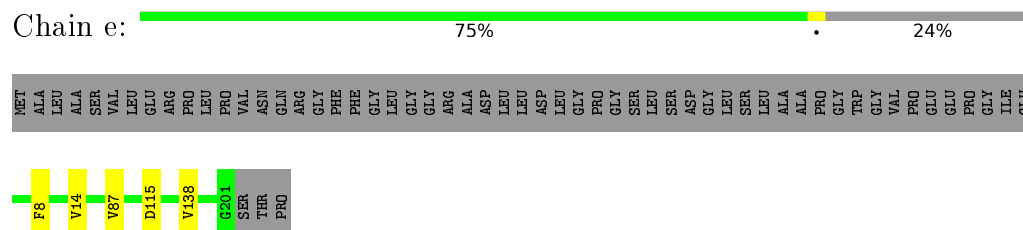
Chain d: 96% 2%



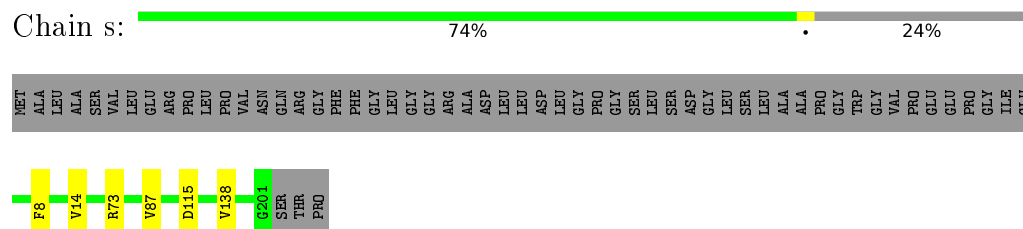
- Molecule 29: Proteasome subunit beta type-2



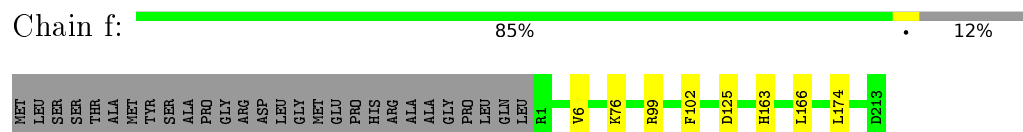
- Molecule 30: Proteasome subunit beta type-5



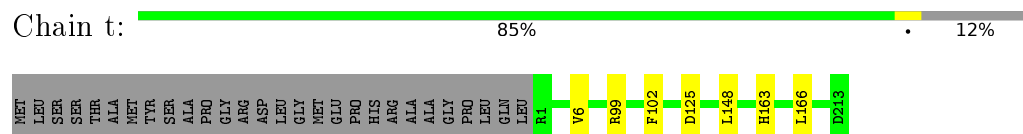
- Molecule 30: Proteasome subunit beta type-5



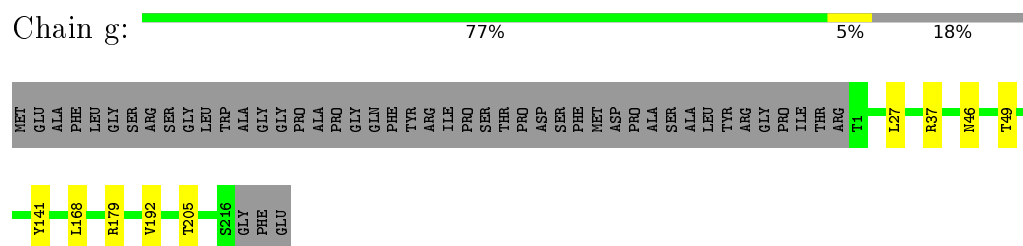
- Molecule 31: Proteasome subunit beta type-1



- Molecule 31: Proteasome subunit beta type-1



- Molecule 32: Proteasome subunit beta type-4



- Molecule 32: Proteasome subunit beta type-4

Chain u:



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	165699	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	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

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 >2	RMSZ	# Z >2
1	I	0.66	2/2756 (0.1%)	1.09	7/3727 (0.2%)
1	w	0.66	2/2756 (0.1%)	1.09	7/3727 (0.2%)
10	4	0.49	2/2989 (0.1%)	0.63	6/4054 (0.1%)
10	Q	0.48	1/2989 (0.0%)	0.63	6/4054 (0.1%)
11	5	0.48	0/2820	0.65	3/3815 (0.1%)
11	R	0.48	0/2817	0.65	3/3812 (0.1%)
12	6	0.41	0/2754	0.59	3/3728 (0.1%)
12	S	0.41	0/2745	0.58	2/3717 (0.1%)
13	7	0.41	0/1713	0.63	4/2306 (0.2%)
13	T	0.41	0/1713	0.63	4/2306 (0.2%)
14	8	0.46	0/2167	0.60	0/2936
14	U	0.46	0/2167	0.60	0/2936
15	9	0.47	0/2045	0.73	2/2760 (0.1%)
15	V	0.47	0/2047	0.72	2/2763 (0.1%)
16	AA	0.44	0/1312	0.76	4/1769 (0.2%)
16	W	0.44	0/1312	0.76	4/1769 (0.2%)
17	AB	0.43	0/315	0.74	1/433 (0.2%)
17	Y	0.43	0/315	0.74	1/433 (0.2%)
18	AC	0.32	0/3603	0.55	1/5005 (0.0%)
18	Z	0.32	0/3603	0.55	1/5005 (0.0%)
19	B	0.75	0/1878	0.74	0/2549
19	h	0.81	0/1886	0.77	0/2557
2	H	0.76	3/2939 (0.1%)	0.96	9/3970 (0.2%)
2	v	0.76	2/2939 (0.1%)	0.97	11/3970 (0.3%)
20	C	0.85	1/1773 (0.1%)	0.78	1/2409 (0.0%)
20	i	0.86	1/1780 (0.1%)	0.79	1/2417 (0.0%)
21	D	1.13	4/1946 (0.2%)	0.85	6/2633 (0.2%)
21	j	1.39	3/1943 (0.2%)	0.83	6/2629 (0.2%)
22	E	0.77	0/1748	0.77	0/2386
22	k	0.78	0/1716	0.80	1/2347 (0.0%)
23	F	0.78	1/1794 (0.1%)	0.79	1/2430 (0.0%)
23	l	0.80	1/1753 (0.1%)	0.83	2/2346 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
24	G	0.75	0/1885	0.77	0/2552
24	m	0.77	1/1885 (0.1%)	0.79	0/2552
25	X	0.83	2/1908 (0.1%)	0.76	0/2575
25	n	0.81	1/1908 (0.1%)	0.76	0/2575
26	a	0.88	5/1535 (0.3%)	0.86	4/2078 (0.2%)
26	o	0.86	3/1535 (0.2%)	0.87	4/2078 (0.2%)
27	b	0.79	1/1670 (0.1%)	0.84	3/2265 (0.1%)
27	p	0.80	1/1670 (0.1%)	0.82	2/2265 (0.1%)
28	c	0.87	0/1614	0.85	1/2177 (0.0%)
28	q	0.87	0/1614	0.85	1/2177 (0.0%)
29	d	0.87	1/1603 (0.1%)	0.83	0/2174
29	r	0.87	1/1603 (0.1%)	0.83	0/2174
3	L	0.66	0/2904	0.80	5/3924 (0.1%)
3	z	0.65	0/2904	0.79	4/3924 (0.1%)
30	e	0.92	0/1579	0.85	1/2134 (0.0%)
30	s	0.91	0/1582	0.84	1/2138 (0.0%)
31	f	0.85	0/1674	0.81	0/2257
31	t	0.85	0/1674	0.81	1/2257 (0.0%)
32	g	0.90	2/1705 (0.1%)	0.86	4/2312 (0.2%)
32	u	0.89	2/1711 (0.1%)	0.85	4/2319 (0.2%)
4	0	0.65	0/2896	0.81	6/3912 (0.2%)
4	M	0.65	0/2896	0.81	6/3912 (0.2%)
5	J	0.59	0/2857	0.75	3/3844 (0.1%)
5	x	0.59	0/2857	0.75	3/3844 (0.1%)
6	K	0.61	0/3089	0.80	3/4168 (0.1%)
6	y	0.61	0/3089	0.80	3/4168 (0.1%)
7	1	0.41	0/5506	0.60	1/7425 (0.0%)
7	N	0.41	0/5506	0.60	1/7425 (0.0%)
8	2	0.43	0/2390	0.65	2/3215 (0.1%)
8	O	0.43	0/2383	0.65	2/3206 (0.1%)
9	3	0.45	0/2860	0.67	3/3860 (0.1%)
9	P	0.45	0/2861	0.67	3/3861 (0.1%)
All	All	0.66	43/144386 (0.0%)	0.76	170/195445 (0.1%)

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
1	I	0	4
1	w	0	4

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
10	4	0	7
10	Q	0	7
11	5	0	9
11	R	0	9
13	7	0	2
13	T	0	2
14	8	0	1
14	U	0	1
15	9	0	3
15	V	0	3
16	AA	0	8
16	W	0	8
17	AB	0	2
17	Y	0	2
18	AC	0	7
18	Z	0	7
2	H	0	1
2	v	0	1
27	b	0	2
3	L	0	3
3	z	0	3
4	0	0	3
4	M	0	3
5	J	0	1
5	x	0	1
6	K	0	2
6	y	0	2
7	1	0	3
7	N	0	3
8	2	0	1
8	O	0	1
9	3	0	2
9	P	0	2
All	All	0	120

The worst 5 of 43 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	j	70	GLU	CD-OE1	44.40	1.74	1.25
21	D	70	GLU	CD-OE1	23.09	1.51	1.25
21	D	70	GLU	CD-OE2	22.37	1.50	1.25
21	j	70	GLU	CD-OE2	18.38	1.45	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	D	70	GLU	CG-CD	13.41	1.72	1.51

The worst 5 of 170 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	142	ASP	CB-CG-OD1	34.78	149.61	118.30
1	w	142	ASP	CB-CG-OD1	34.78	149.61	118.30
1	I	142	ASP	CB-CG-OD2	-25.59	95.27	118.30
1	w	142	ASP	CB-CG-OD2	-25.59	95.27	118.30
2	H	336	ARG	NE-CZ-NH1	-19.14	110.73	120.30

There are no chirality outliers.

5 of 120 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	336	ARG	Sidechain
1	I	105	THR	Peptide
1	I	137	SER	Peptide
1	I	299	SER	Mainchain,Peptide
3	L	226	GLN	Mainchain

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	I	2720	0	2686	879	0
1	w	2720	0	2686	0	0
2	H	2893	0	2843	712	0
2	v	2893	0	2843	0	0
3	L	2860	0	2826	796	0
3	z	2860	0	2826	0	0
4	0	2858	0	2853	623	0
4	M	2858	0	2853	691	0
5	J	2820	0	2927	756	0
5	x	2820	0	2927	0	0
6	K	3039	0	3076	951	0
6	y	3039	0	3076	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	1	5449	0	4576	626	0
7	N	5449	0	4576	642	0
8	2	2375	0	1869	215	0
8	O	2369	0	1862	201	0
9	3	2831	0	2386	358	0
9	P	2832	0	2388	347	0
10	4	2956	0	2669	567	0
10	Q	2956	0	2669	558	0
11	5	2770	0	2480	450	0
11	R	2767	0	2473	475	0
12	6	2732	0	2215	279	0
12	S	2723	0	2202	281	0
13	7	1699	0	1364	221	0
13	T	1699	0	1364	226	0
14	8	2131	0	2039	393	0
14	U	2131	0	2039	388	0
15	9	2009	0	1973	276	0
15	V	2011	0	1980	287	0
16	AA	1300	0	1134	200	0
16	W	1300	0	1134	215	0
17	AB	316	0	160	24	0
17	Y	316	0	160	25	0
18	AC	3608	0	1688	192	0
18	Z	3608	0	1688	203	0
19	B	1845	0	1805	62	0
19	h	1853	0	1827	0	0
20	C	1737	0	1673	67	0
20	i	1744	0	1693	0	0
21	D	1916	0	1857	37	0
21	j	1913	0	1848	0	0
22	E	1724	0	1525	43	0
22	k	1691	0	1468	0	0
23	F	1766	0	1714	40	0
23	l	1726	0	1722	0	0
24	G	1850	0	1822	48	0
24	m	1850	0	1822	0	0
25	X	1873	0	1832	43	0
25	n	1873	0	1832	0	0
26	a	1509	0	1473	0	0
26	o	1509	0	1473	0	0
27	b	1643	0	1644	0	0
27	p	1643	0	1644	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	c	1585	0	1598	0	0
28	q	1585	0	1598	0	0
29	d	1570	0	1547	0	0
29	r	1570	0	1547	0	0
30	e	1548	0	1499	0	0
30	s	1551	0	1508	0	0
31	f	1644	0	1627	0	0
31	t	1644	0	1627	0	0
32	g	1672	0	1630	0	0
32	u	1678	0	1640	0	0
33	0	27	0	12	9	0
33	H	27	0	12	6	0
33	I	27	0	12	23	0
33	J	27	0	12	21	0
33	K	27	0	12	23	0
33	L	27	0	12	16	0
33	M	27	0	12	11	0
33	v	27	0	12	0	0
33	w	27	0	12	0	0
33	x	27	0	12	0	0
33	y	27	0	12	0	0
33	z	27	0	12	0	0
All	All	142753	0	130149	12299	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 62.

The worst 5 of 12299 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)
14:8:70:LEU:HD21	14:8:111:LEU:CD2	1.28	1.64
3:L:238:ILE:HD11	3:L:257:LEU:CA	1.17	1.63
1:I:339:PRO:HB3	2:H:425:ALA:CB	1.28	1.61
18:Z:667:GLY:HA2	18:Z:671:ALA:CB	1.19	1.61
5:J:151:ILE:HD11	5:J:198:LEU:CD2	1.11	1.58

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	I	355/440 (81%)	255 (72%)	72 (20%)	28 (8%)	1	14
1	w	355/440 (81%)	255 (72%)	71 (20%)	29 (8%)	1	13
2	H	376/433 (87%)	248 (66%)	91 (24%)	37 (10%)	1	10
2	v	376/433 (87%)	249 (66%)	88 (23%)	39 (10%)	1	8
3	L	373/389 (96%)	264 (71%)	72 (19%)	37 (10%)	1	10
3	z	373/389 (96%)	263 (70%)	73 (20%)	37 (10%)	1	10
4	0	372/439 (85%)	255 (68%)	74 (20%)	43 (12%)	0	7
4	M	372/439 (85%)	255 (68%)	74 (20%)	43 (12%)	0	7
5	J	354/406 (87%)	255 (72%)	66 (19%)	33 (9%)	1	11
5	x	354/406 (87%)	255 (72%)	66 (19%)	33 (9%)	1	11
6	K	378/418 (90%)	266 (70%)	70 (18%)	42 (11%)	0	7
6	y	378/418 (90%)	266 (70%)	70 (18%)	42 (11%)	0	7
7	1	811/953 (85%)	607 (75%)	176 (22%)	28 (4%)	4	38
7	N	811/953 (85%)	607 (75%)	176 (22%)	28 (4%)	4	38
8	2	368/376 (98%)	287 (78%)	61 (17%)	20 (5%)	2	25
8	O	368/376 (98%)	287 (78%)	61 (17%)	20 (5%)	2	25
9	3	401/456 (88%)	338 (84%)	51 (13%)	12 (3%)	5	42
9	P	401/456 (88%)	338 (84%)	51 (13%)	12 (3%)	5	42
10	4	419/422 (99%)	331 (79%)	58 (14%)	30 (7%)	1	17
10	Q	419/422 (99%)	330 (79%)	58 (14%)	31 (7%)	1	16
11	5	374/389 (96%)	295 (79%)	54 (14%)	25 (7%)	1	19
11	R	374/389 (96%)	295 (79%)	54 (14%)	25 (7%)	1	19
12	6	413/525 (79%)	354 (86%)	42 (10%)	17 (4%)	3	33
12	S	413/525 (79%)	354 (86%)	42 (10%)	17 (4%)	3	33
13	7	254/350 (73%)	195 (77%)	43 (17%)	16 (6%)	2	21

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	T	254/350 (73%)	195 (77%)	43 (17%)	16 (6%)	2	21
14	8	279/324 (86%)	222 (80%)	42 (15%)	15 (5%)	2	25
14	U	279/324 (86%)	222 (80%)	42 (15%)	15 (5%)	2	25
15	9	253/310 (82%)	209 (83%)	32 (13%)	12 (5%)	3	29
15	V	253/310 (82%)	209 (83%)	32 (13%)	12 (5%)	3	29
16	AA	191/377 (51%)	145 (76%)	35 (18%)	11 (6%)	2	23
16	W	191/377 (51%)	145 (76%)	35 (18%)	11 (6%)	2	23
17	AB	55/70 (79%)	37 (67%)	10 (18%)	8 (14%)	0	4
17	Y	55/70 (79%)	37 (67%)	10 (18%)	8 (14%)	0	4
18	AC	722/908 (80%)	557 (77%)	116 (16%)	49 (7%)	1	19
18	Z	722/908 (80%)	558 (77%)	116 (16%)	48 (7%)	1	19
19	B	242/246 (98%)	230 (95%)	8 (3%)	4 (2%)	11	54
19	h	242/246 (98%)	229 (95%)	13 (5%)	0	100	100
20	C	229/234 (98%)	204 (89%)	23 (10%)	2 (1%)	21	68
20	i	229/234 (98%)	206 (90%)	21 (9%)	2 (1%)	21	68
21	D	248/261 (95%)	234 (94%)	13 (5%)	1 (0%)	39	81
21	j	248/261 (95%)	236 (95%)	11 (4%)	1 (0%)	39	81
22	E	241/248 (97%)	221 (92%)	15 (6%)	5 (2%)	9	50
22	k	241/248 (97%)	221 (92%)	15 (6%)	5 (2%)	9	50
23	F	232/241 (96%)	217 (94%)	13 (6%)	2 (1%)	21	68
23	l	232/241 (96%)	214 (92%)	17 (7%)	1 (0%)	39	81
24	G	236/263 (90%)	224 (95%)	9 (4%)	3 (1%)	15	60
24	m	236/263 (90%)	224 (95%)	9 (4%)	3 (1%)	15	60
25	X	241/255 (94%)	234 (97%)	4 (2%)	3 (1%)	16	61
25	n	241/255 (94%)	235 (98%)	4 (2%)	2 (1%)	24	70
26	a	200/239 (84%)	195 (98%)	4 (2%)	1 (0%)	34	78
26	o	200/239 (84%)	195 (98%)	4 (2%)	1 (0%)	34	78
27	b	218/277 (79%)	209 (96%)	8 (4%)	1 (0%)	34	78
27	p	218/277 (79%)	208 (95%)	8 (4%)	2 (1%)	21	68
28	c	202/205 (98%)	191 (95%)	9 (4%)	2 (1%)	19	66
28	q	202/205 (98%)	191 (95%)	9 (4%)	2 (1%)	19	66

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	d	197/201 (98%)	187 (95%)	9 (5%)	1 (0%)	34	78
29	r	197/201 (98%)	187 (95%)	9 (5%)	1 (0%)	34	78
30	e	199/263 (76%)	195 (98%)	4 (2%)	0	100	100
30	s	199/263 (76%)	195 (98%)	4 (2%)	0	100	100
31	f	211/241 (88%)	203 (96%)	8 (4%)	0	100	100
31	t	211/241 (88%)	203 (96%)	8 (4%)	0	100	100
32	g	214/264 (81%)	203 (95%)	10 (5%)	1 (0%)	34	78
32	u	215/264 (81%)	206 (96%)	8 (4%)	1 (0%)	34	78
All	All	19717/22846 (86%)	16137 (82%)	2604 (13%)	976 (5%)	5	27

5 of 976 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	165	ASP
1	I	207	HIS
1	I	220	LYS
1	I	277	HIS
1	I	278	ALA

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	I	291/385 (76%)	229 (79%)	62 (21%)	1	7
1	w	291/385 (76%)	227 (78%)	64 (22%)	1	7
2	H	298/372 (80%)	232 (78%)	66 (22%)	1	6
2	v	297/372 (80%)	232 (78%)	65 (22%)	1	7
3	L	298/341 (87%)	233 (78%)	65 (22%)	1	7
3	z	298/341 (87%)	233 (78%)	65 (22%)	1	7
4	0	296/379 (78%)	240 (81%)	56 (19%)	2	10
4	M	296/379 (78%)	240 (81%)	56 (19%)	2	10

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	J	310/352 (88%)	244 (79%)	66 (21%)	1	7
5	x	310/352 (88%)	244 (79%)	66 (21%)	1	7
6	K	333/366 (91%)	272 (82%)	61 (18%)	2	12
6	y	333/366 (91%)	270 (81%)	63 (19%)	2	10
7	1	376/816 (46%)	344 (92%)	32 (8%)	13	49
7	N	376/816 (46%)	344 (92%)	32 (8%)	13	49
8	2	142/336 (42%)	124 (87%)	18 (13%)	5	28
8	O	141/336 (42%)	123 (87%)	18 (13%)	5	28
9	3	201/416 (48%)	181 (90%)	20 (10%)	9	41
9	P	202/416 (49%)	181 (90%)	21 (10%)	9	39
10	4	250/362 (69%)	210 (84%)	40 (16%)	3	18
10	Q	249/362 (69%)	209 (84%)	40 (16%)	3	18
11	5	229/344 (67%)	202 (88%)	27 (12%)	6	31
11	R	228/344 (66%)	202 (89%)	26 (11%)	7	33
12	6	164/452 (36%)	153 (93%)	11 (7%)	20	61
12	S	163/452 (36%)	152 (93%)	11 (7%)	20	61
13	7	108/294 (37%)	91 (84%)	17 (16%)	3	19
13	T	109/294 (37%)	92 (84%)	17 (16%)	3	20
14	8	211/295 (72%)	186 (88%)	25 (12%)	6	31
14	U	212/295 (72%)	186 (88%)	26 (12%)	6	29
15	9	218/268 (81%)	187 (86%)	31 (14%)	4	24
15	V	219/268 (82%)	188 (86%)	31 (14%)	4	24
16	AA	111/312 (36%)	104 (94%)	7 (6%)	22	63
16	W	111/312 (36%)	103 (93%)	8 (7%)	18	57
17	AB	6/63 (10%)	6 (100%)	0	100	100
17	Y	6/63 (10%)	6 (100%)	0	100	100
19	B	193/210 (92%)	180 (93%)	13 (7%)	20	61
19	h	195/210 (93%)	182 (93%)	13 (7%)	20	61
20	C	175/191 (92%)	170 (97%)	5 (3%)	50	81
20	i	177/191 (93%)	164 (93%)	13 (7%)	17	57
21	D	194/221 (88%)	186 (96%)	8 (4%)	37	74

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	j	193/221 (87%)	186 (96%)	7 (4%)	42	77
22	E	152/211 (72%)	140 (92%)	12 (8%)	15	53
22	k	142/211 (67%)	132 (93%)	10 (7%)	19	59
23	F	190/203 (94%)	186 (98%)	4 (2%)	61	86
23	l	191/203 (94%)	184 (96%)	7 (4%)	41	76
24	G	198/224 (88%)	192 (97%)	6 (3%)	48	81
24	m	198/224 (88%)	188 (95%)	10 (5%)	29	69
25	X	193/212 (91%)	187 (97%)	6 (3%)	47	81
25	n	193/212 (91%)	184 (95%)	9 (5%)	32	72
26	a	155/181 (86%)	151 (97%)	4 (3%)	54	83
26	o	155/181 (86%)	152 (98%)	3 (2%)	65	87
27	b	177/228 (78%)	171 (97%)	6 (3%)	44	79
27	p	177/228 (78%)	172 (97%)	5 (3%)	51	82
28	c	172/174 (99%)	164 (95%)	8 (5%)	32	72
28	q	172/174 (99%)	164 (95%)	8 (5%)	32	72
29	d	164/171 (96%)	159 (97%)	5 (3%)	48	81
29	r	164/171 (96%)	160 (98%)	4 (2%)	57	85
30	e	153/202 (76%)	149 (97%)	4 (3%)	54	83
30	s	154/202 (76%)	149 (97%)	5 (3%)	46	80
31	f	175/199 (88%)	167 (95%)	8 (5%)	33	72
31	t	175/199 (88%)	169 (97%)	6 (3%)	44	79
32	g	175/215 (81%)	167 (95%)	8 (5%)	33	72
32	u	175/215 (81%)	165 (94%)	10 (6%)	25	66
All	All	12610/17990 (70%)	11190 (89%)	1420 (11%)	12	34

5 of 1420 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
22	E	146	GLN
30	s	87	VAL
11	5	212	GLU
26	a	46	SER
20	i	178	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 221 such sidechains are listed below:

Mol	Chain	Res	Type
16	W	101	GLN
32	u	81	HIS
14	8	102	HIS
19	B	75	ASN
29	d	71	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
33	ADP	0	501	-	24,29,29	0.95	1 (4%)	23,45,45	1.85	2 (8%)
33	ADP	H	501	-	24,29,29	1.00	1 (4%)	23,45,45	1.78	2 (8%)
33	ADP	I	501	-	24,29,29	1.00	1 (4%)	23,45,45	1.76	2 (8%)
33	ADP	J	501	-	24,29,29	0.92	1 (4%)	23,45,45	1.79	2 (8%)
33	ADP	K	501	-	24,29,29	0.98	1 (4%)	23,45,45	1.82	2 (8%)
33	ADP	L	401	-	24,29,29	0.98	1 (4%)	23,45,45	1.73	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	ADP	M	501	-	24,29,29	0.95	1 (4%)	23,45,45	1.85	2 (8%)
33	ADP	v	501	-	24,29,29	1.00	1 (4%)	23,45,45	1.78	2 (8%)
33	ADP	w	501	-	24,29,29	1.00	1 (4%)	23,45,45	1.76	2 (8%)
33	ADP	x	501	-	24,29,29	0.92	1 (4%)	23,45,45	1.79	2 (8%)
33	ADP	y	501	-	24,29,29	0.98	1 (4%)	23,45,45	1.82	2 (8%)
33	ADP	z	401	-	24,29,29	0.98	1 (4%)	23,45,45	1.73	1 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	ADP	0	501	-	-	0/12/32/32	0/3/3/3
33	ADP	H	501	-	-	0/12/32/32	0/3/3/3
33	ADP	I	501	-	-	0/12/32/32	0/3/3/3
33	ADP	J	501	-	-	0/12/32/32	0/3/3/3
33	ADP	K	501	-	-	0/12/32/32	0/3/3/3
33	ADP	L	401	-	-	0/12/32/32	0/3/3/3
33	ADP	M	501	-	-	0/12/32/32	0/3/3/3
33	ADP	v	501	-	-	0/12/32/32	0/3/3/3
33	ADP	w	501	-	-	0/12/32/32	0/3/3/3
33	ADP	x	501	-	-	0/12/32/32	0/3/3/3
33	ADP	y	501	-	-	0/12/32/32	0/3/3/3
33	ADP	z	401	-	-	0/12/32/32	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	x	501	ADP	C5-C4	2.77	1.46	1.40
33	J	501	ADP	C5-C4	2.77	1.46	1.40
33	0	501	ADP	C5-C4	2.84	1.46	1.40
33	M	501	ADP	C5-C4	2.84	1.46	1.40
33	K	501	ADP	C5-C4	2.96	1.47	1.40

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	0	501	ADP	N3-C2-N1	-6.78	123.54	128.87
33	M	501	ADP	N3-C2-N1	-6.78	123.54	128.87
33	v	501	ADP	N3-C2-N1	-6.68	123.62	128.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	H	501	ADP	N3-C2-N1	-6.68	123.62	128.87
33	x	501	ADP	N3-C2-N1	-6.68	123.63	128.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 109 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	0	501	ADP	9	0
33	H	501	ADP	6	0
33	I	501	ADP	23	0
33	J	501	ADP	21	0
33	K	501	ADP	23	0
33	L	401	ADP	16	0
33	M	501	ADP	11	0

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.