



wwPDB EM Validation Summary Report ⓘ

Apr 5, 2026 – 11:55 PM UTC

PDB ID : 9U3L / pdb_00009u3l
EMDB ID : EMD-63817
Title : Substrate-engaged human 26S proteasome bound to midnolin with RPT2 at top of spiral staircase
Authors : Zhu, C.; Qin, L.; Liang, L.
Deposited on : 2025-03-18
Resolution : 2.91 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

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

The types of validation reports are described at

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

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

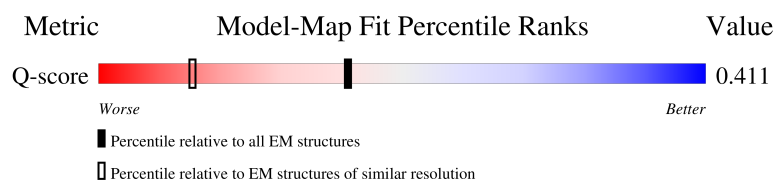
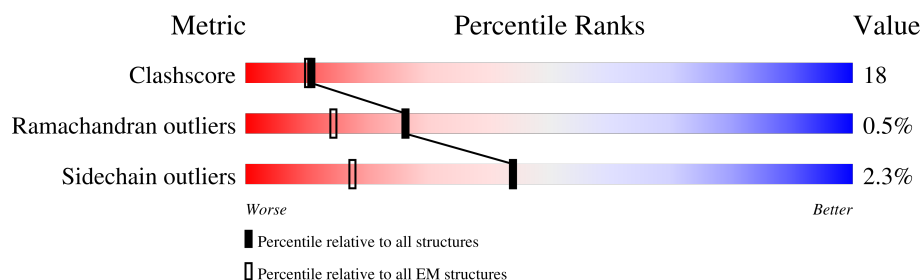
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.91 Å.

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



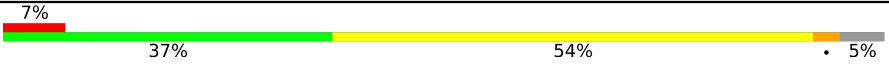







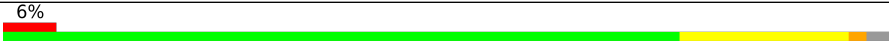

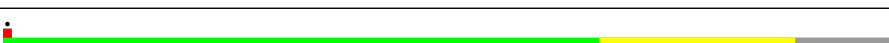


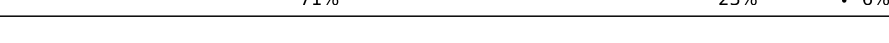
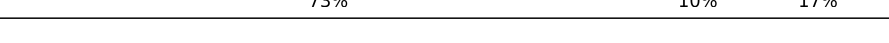
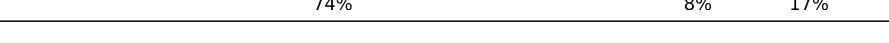
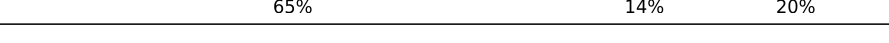
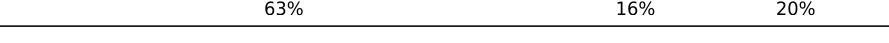
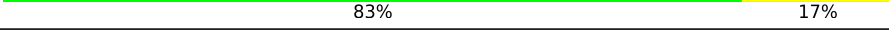






Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12972 (2.41 - 3.41)

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	A	433	
2	B	440	
3	C	398	
4	D	418	











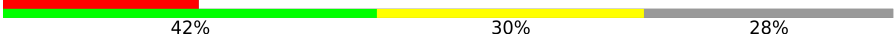


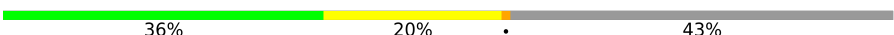




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Mol	Chain	Length	Quality of chain
5	E	403	
6	G	245	
6	g	245	
7	H	233	
7	h	233	
8	I	260	
8	i	260	
9	J	247	
9	j	247	
10	L	268	
10	l	268	
11	M	254	
11	m	254	
12	N	238	
12	n	238	
13	O	276	
13	o	276	
14	P	204	
14	p	204	
15	Q	201	
15	q	201	
16	R	262	
16	r	262	
17	S	240	
17	s	240	

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Mol	Chain	Length	Quality of chain
18	T	263	
18	t	263	
19	V	533	
20	W	456	
21	X	422	
22	Y	389	
23	Z	324	
24	a	376	
25	b	377	
26	c	309	
27	d	349	
28	u	908	
29	U	953	
30	e	70	
31	F	439	
32	K	240	
32	k	240	
33	v	15	

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 104750 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	413	Total	C	N	O	S	0	0
			3226	2033	565	610	18		

- Molecule 2 is a protein called 26S proteasome regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	411	Total	C	N	O	S	0	0
			3201	2019	545	622	15		

- Molecule 3 is a protein called 26S proteasome regulatory subunit 8.

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

- Molecule 4 is a protein called 26S proteasome regulatory subunit 6B.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	380	Total	C	N	O	S	0	0
			3034	1920	521	580	13		

- Molecule 5 is a protein called Proteasome 26S subunit, ATPase 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	381	Total	C	N	O	S	0	0
			3031	1903	542	569	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	237	Total	C	N	O	S	0	0
			1809	1151	302	343	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	g	240	Total	C	N	O	S	0	0
			1830	1163	306	348	13		

- Molecule 7 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	231	Total	C	N	O	S	0	0
			1703	1079	289	330	5		
7	h	232	Total	C	N	O	S	0	0
			1727	1096	292	334	5		

- Molecule 8 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	248	Total	C	N	O	S	0	0
			1895	1195	324	368	8		
8	i	250	Total	C	N	O	S	0	0
			1912	1204	329	371	8		

- Molecule 9 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	247	Total	C	N	O	S	0	0
			1844	1148	331	360	5		
9	j	239	Total	C	N	O	S	0	0
			1704	1056	308	335	5		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	240	Total	C	N	O	S	0	0
			1856	1178	314	353	11		
11	m	240	Total	C	N	O	S	0	0
			1862	1181	317	353	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	N	197	Total	C	N	O	S	0	0
			1482	928	253	289	12		
12	n	197	Total	C	N	O	S	0	0
			1482	928	253	289	12		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	P	204	Total	C	N	O	S	0	0
			1591	1013	265	294	19		
14	p	204	Total	C	N	O	S	0	0
			1591	1013	265	294	19		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Q	199	Total	C	N	O	S	0	0
			1570	1006	265	290	9		
15	q	199	Total	C	N	O	S	0	0
			1574	1009	266	290	9		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	215	Total	C	N	O	S	0	0
			1667	1052	285	318	12		
18	t	215	Total	C	N	O	S	0	0
			1673	1055	288	318	12		

- Molecule 19 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

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

- Molecule 20 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	W	455	Total	C	N	O	S	0	0
			3685	2329	632	699	25		

- Molecule 21 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	X	380	Total	C	N	O	S	0	0
			3003	1915	506	570	12		

- Molecule 22 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Y	377	Total	C	N	O	S	0	0
			3108	1982	532	577	17		

- Molecule 23 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Z	286	Total	C	N	O	S	0	0
			2277	1455	391	426	5		

- Molecule 24 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

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

- Molecule 25 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	c	287	Total	C	N	O	S	0	0
			2254	1427	386	422	19		

- Molecule 27 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	d	252	Total	C	N	O	S	0	0
			2074	1343	339	383	9		

- Molecule 28 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	u	842	Total	C	N	O	S	0	0
			6514	4118	1106	1246	44		

- Molecule 29 is a protein called 26S proteasome non-ATPase regulatory subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	U	837	Total	C	N	O	S	0	0
			6529	4143	1109	1233	44		

- Molecule 30 is a protein called 26S proteasome complex subunit SEM1.

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

- Molecule 31 is a protein called 26S proteasome regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	F	384	Total	C	N	O	S	0	0
			3005	1896	514	577	18		

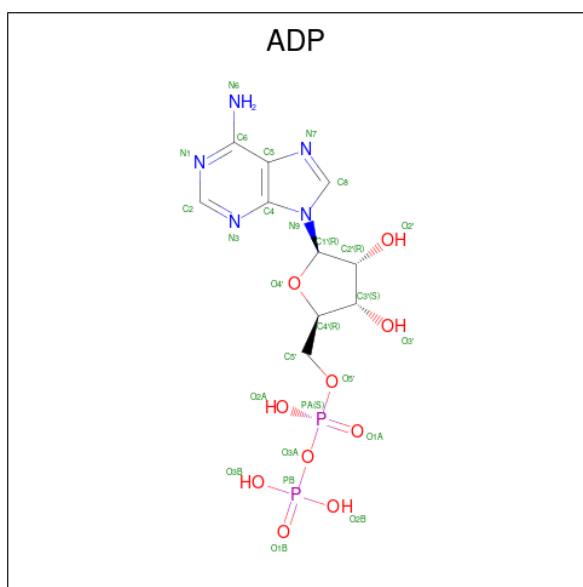
- Molecule 32 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	K	230	Total	C	N	O	S	0	0
			1750	1099	287	353	11		
32	k	228	Total	C	N	O	S	0	0
			1722	1080	284	348	10		

- Molecule 33 is a protein called substrate peptide.

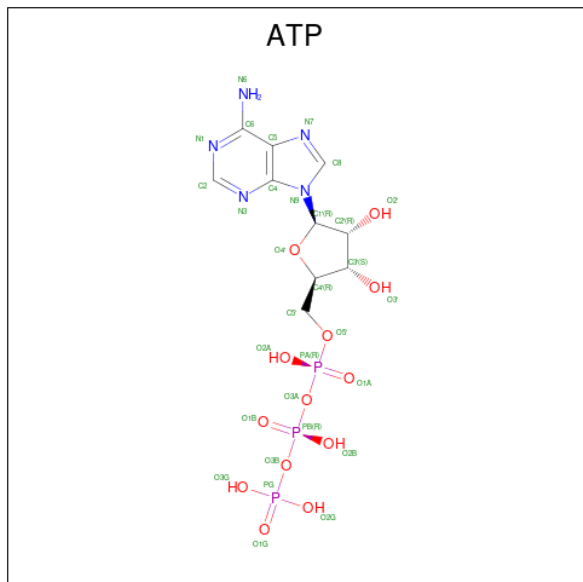
Mol	Chain	Residues	Atoms				AltConf	Trace
33	v	15	Total	C	N	O	0	0
			75	45	15	15		

- Molecule 34 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



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

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

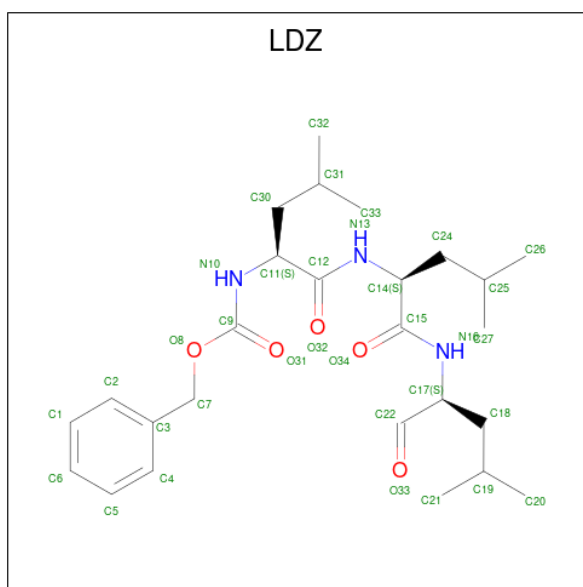


Mol	Chain	Residues	Atoms					AltConf
35	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
35	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
35	D	1	Total	C	N	O	P	0
			31	10	5	13	3	

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

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

- Molecule 37 is N-[(benzyloxy)carbonyl]-L-leucyl-N-[(2S)-4-methyl-1-oxopentan-2-yl]-L-leucinamide (CCD ID: LDZ) (formula: $C_{26}H_{41}N_3O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
37	N	1	Total	C	N	O	0
			34	26	3	5	
37	O	1	Total	C	N	O	0
			34	26	3	5	
37	R	1	Total	C	N	O	0
			34	26	3	5	
37	n	1	Total	C	N	O	0
			34	26	3	5	
37	o	1	Total	C	N	O	0
			34	26	3	5	
37	r	1	Total	C	N	O	0
			34	26	3	5	

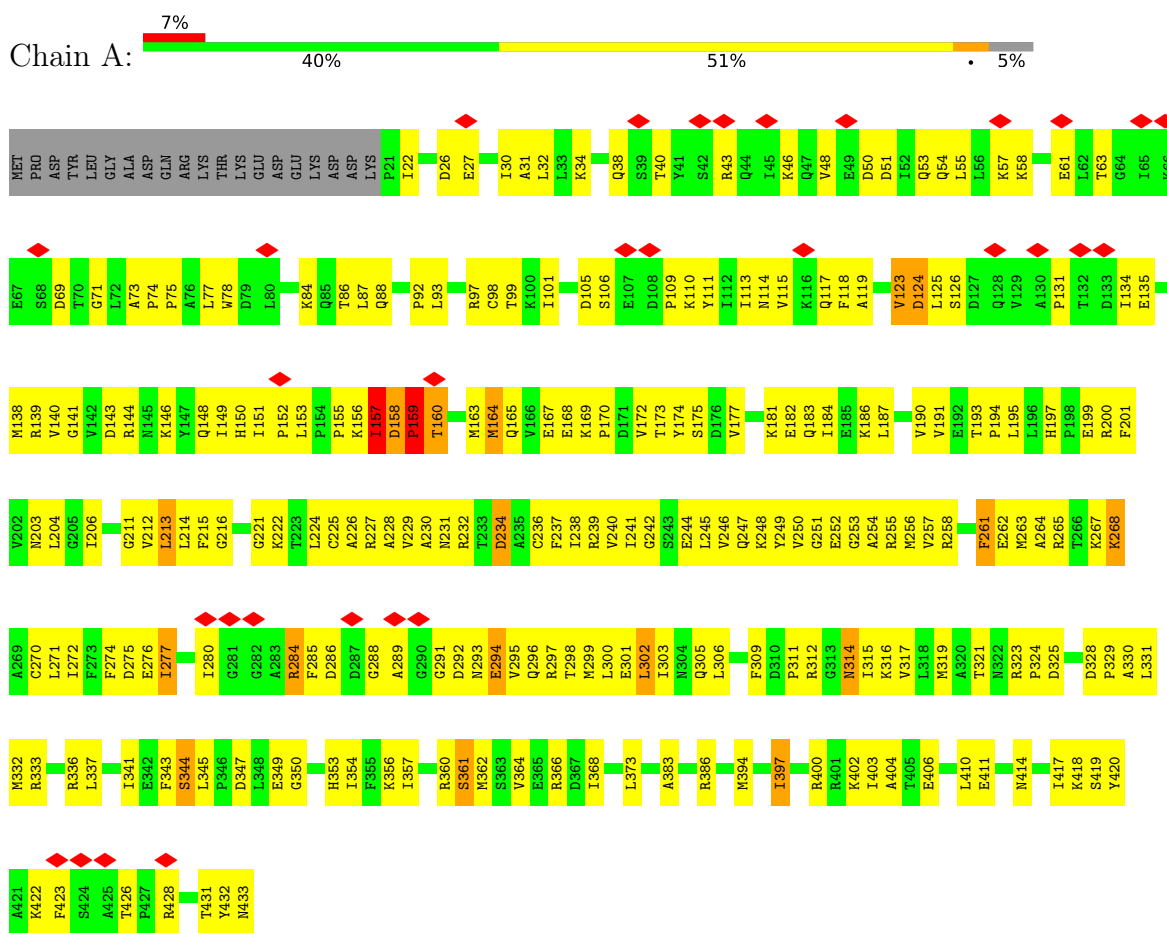
- Molecule 38 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

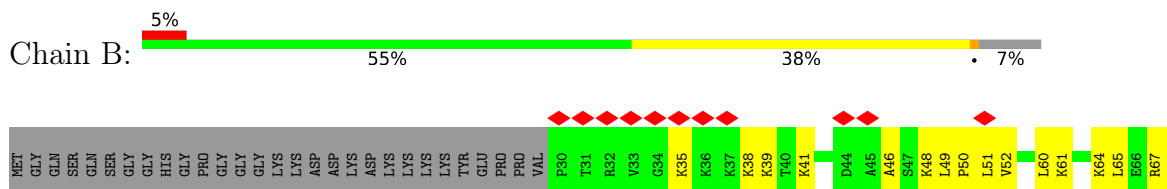
3 Residue-property plots

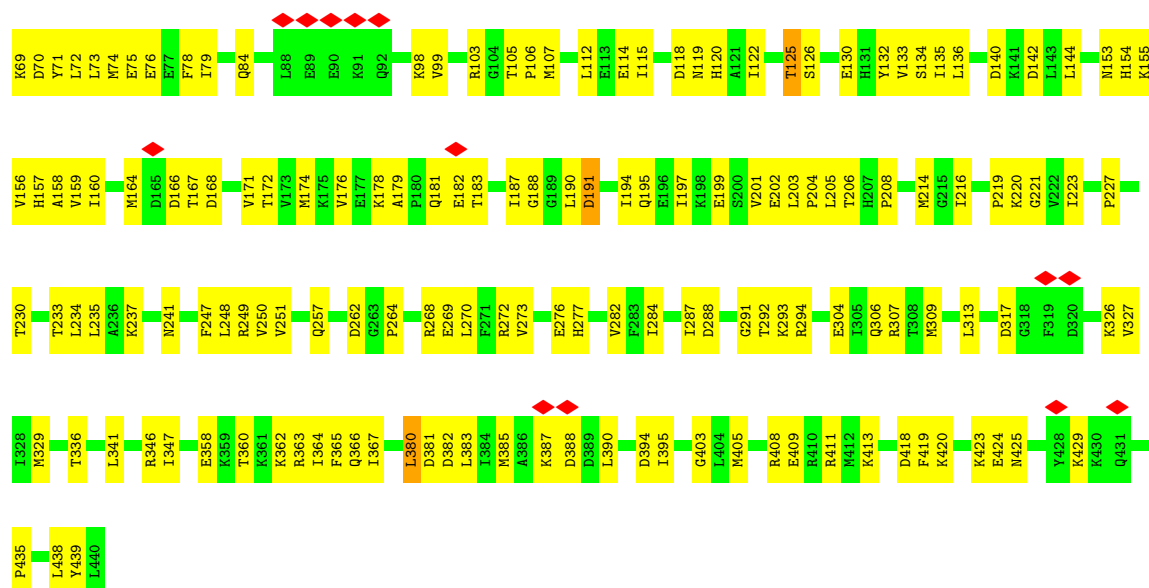
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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 regulatory subunit 7

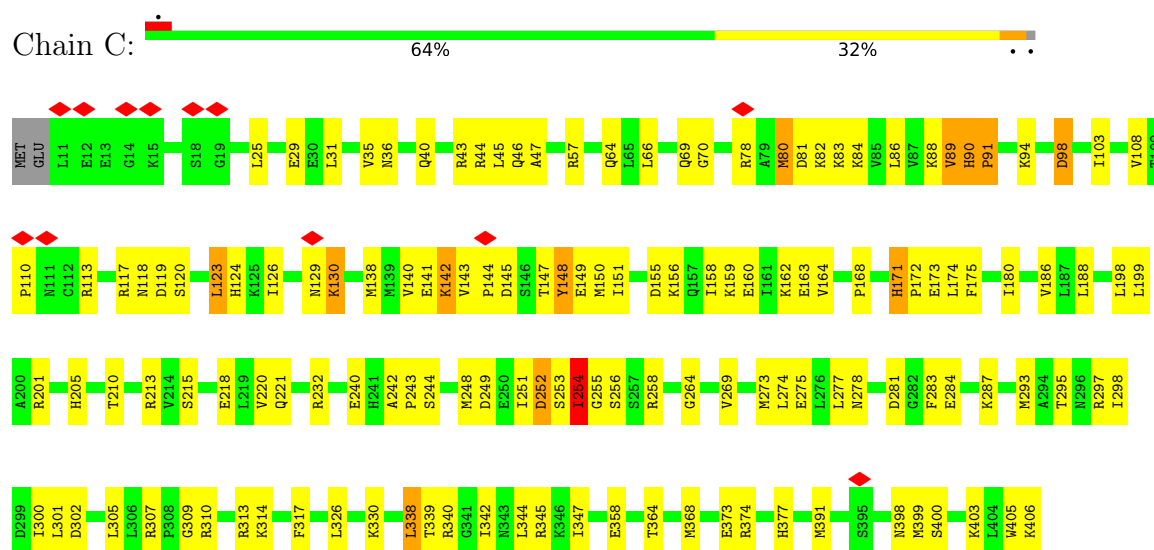


• Molecule 2: 26S proteasome regulatory subunit 4

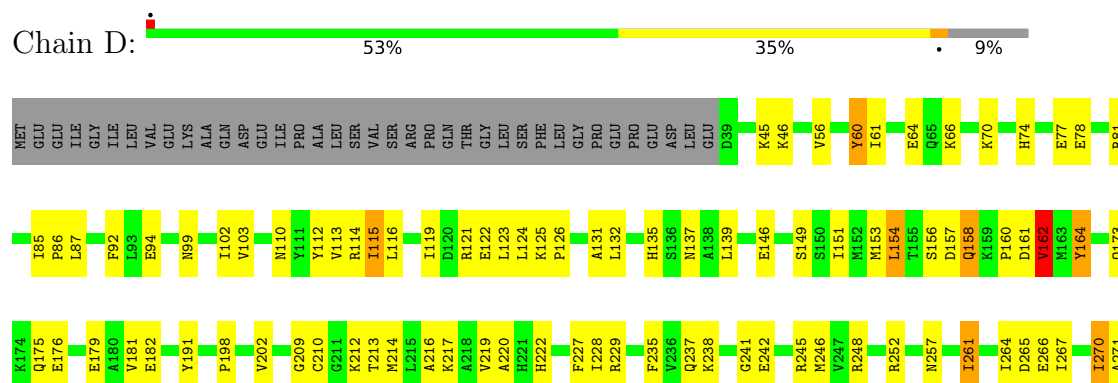


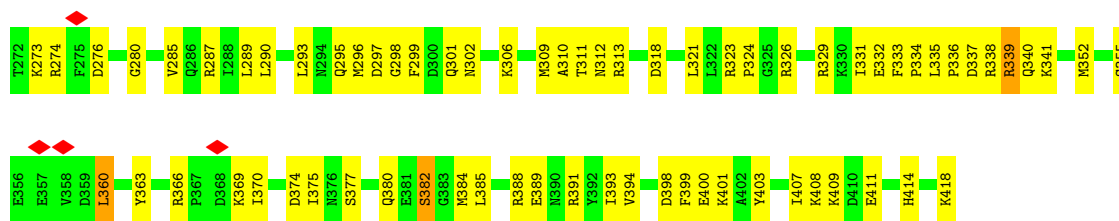


• Molecule 3: 26S proteasome regulatory subunit 8

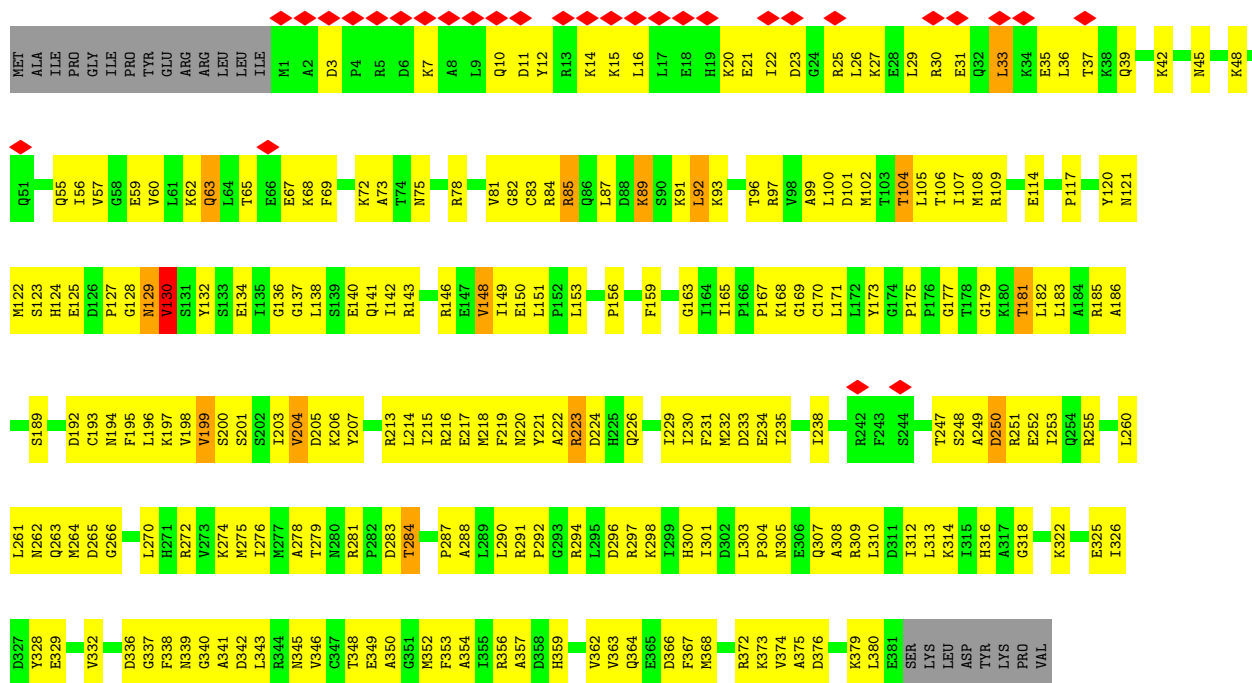


• Molecule 4: 26S proteasome regulatory subunit 6B

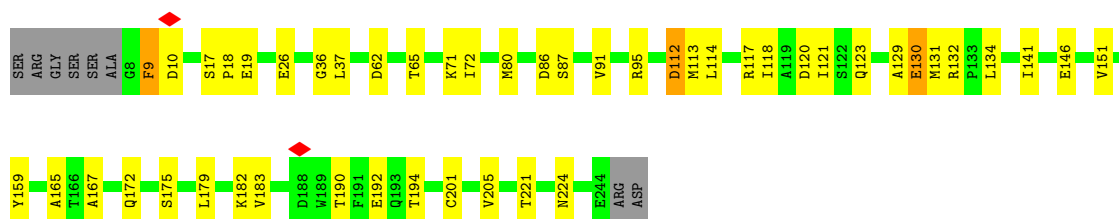
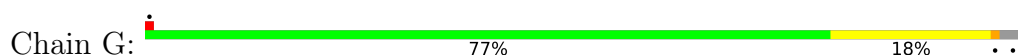




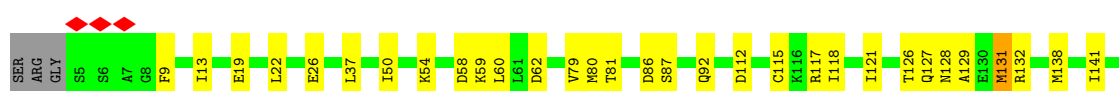
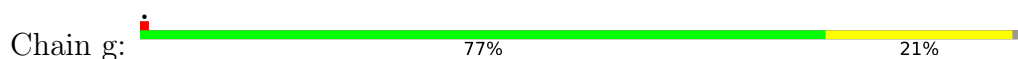
• Molecule 5: Proteasome 26S subunit, ATPase 6



• Molecule 6: Proteasome subunit alpha type-6



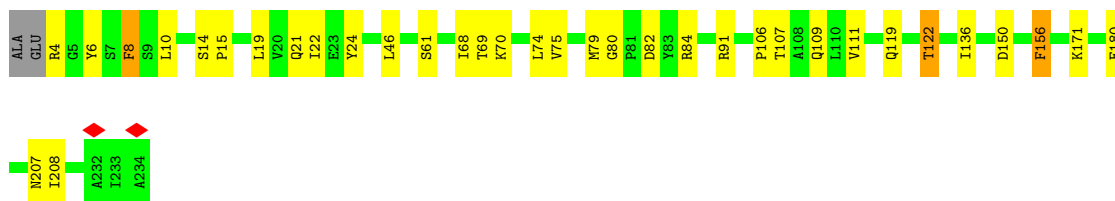
• Molecule 6: Proteasome subunit alpha type-6





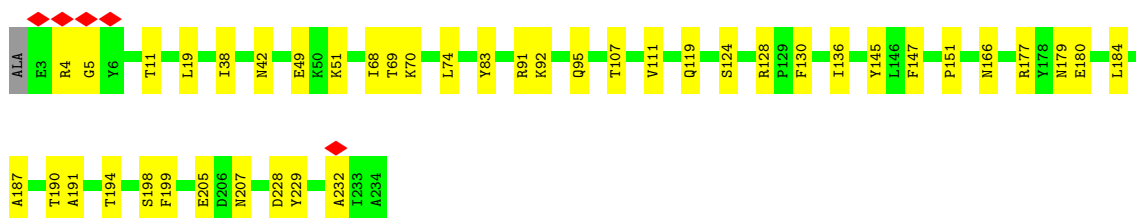
• Molecule 7: Proteasome subunit alpha type-2

Chain H: 84% 14% ..



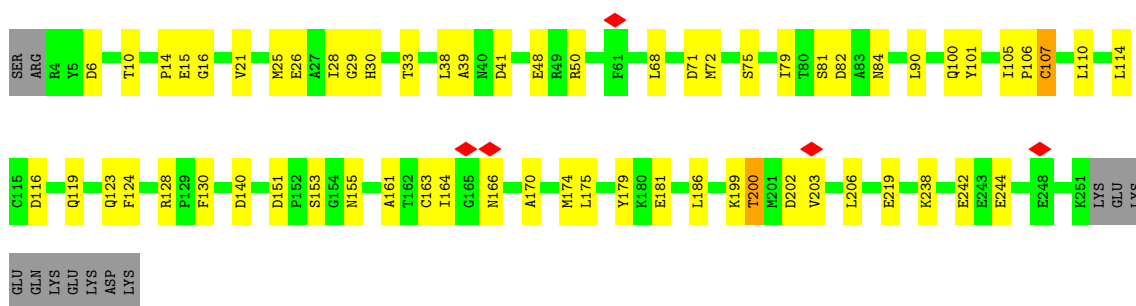
• Molecule 7: Proteasome subunit alpha type-2

Chain h: 82% 18%



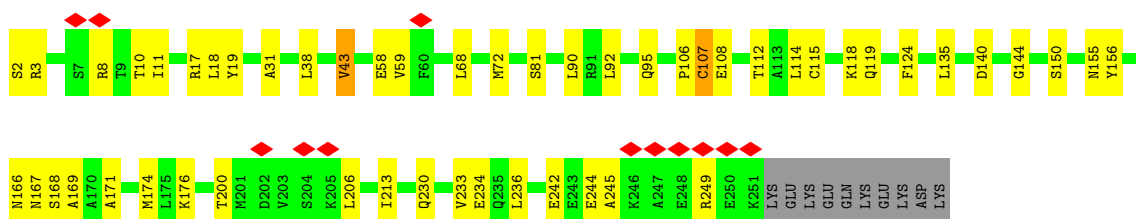
• Molecule 8: Proteasome subunit alpha type-4

Chain I: 72% 23% • 5%

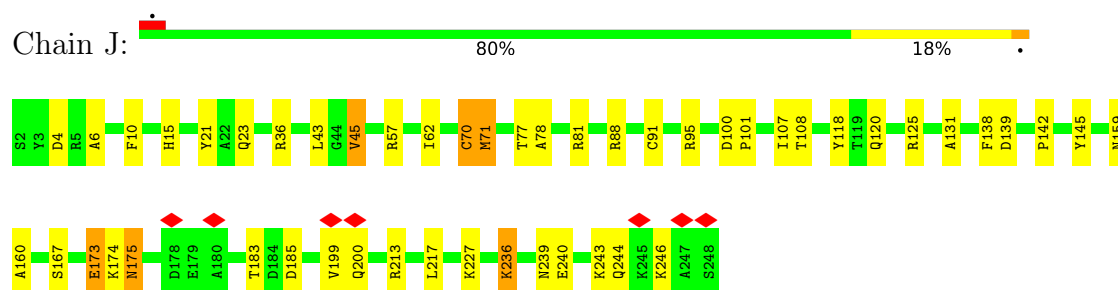


• Molecule 8: Proteasome subunit alpha type-4

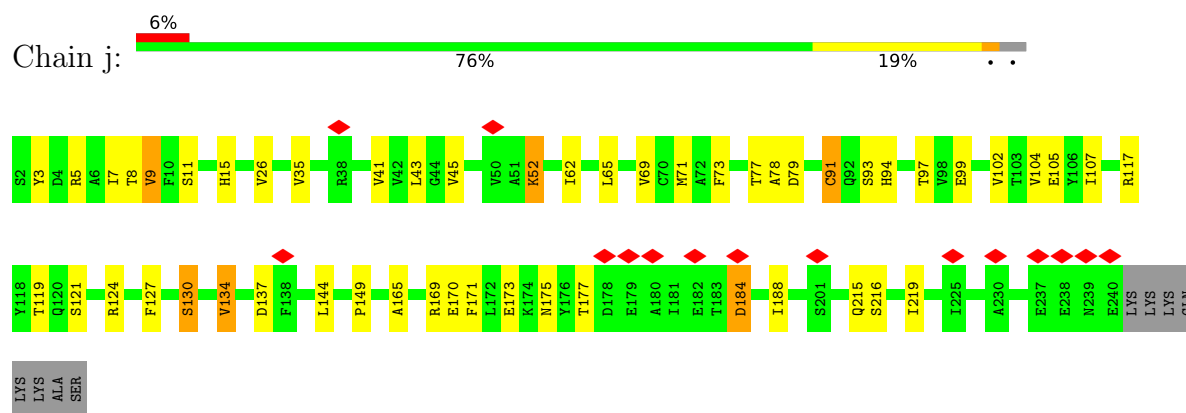
Chain i: 5% 76% 19% • •



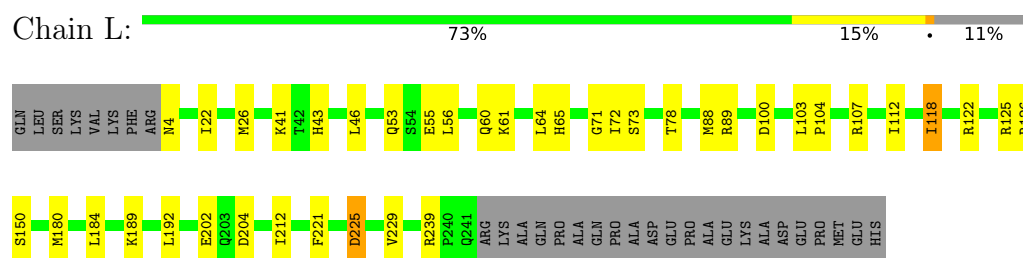
- Molecule 9: Proteasome subunit alpha type-7



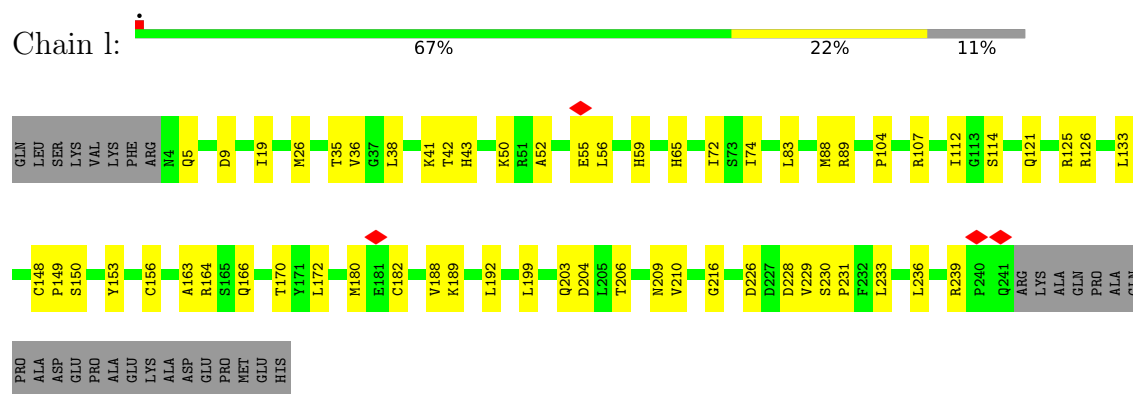
- Molecule 9: Proteasome subunit alpha type-7




- Molecule 10: Isoform Long of Proteasome subunit alpha type-1

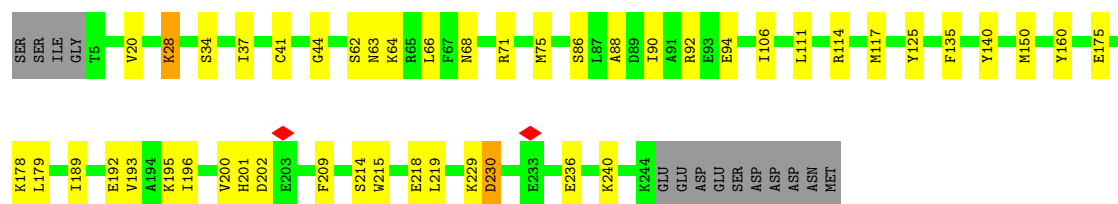


- Molecule 10: Isoform Long of Proteasome subunit alpha type-1



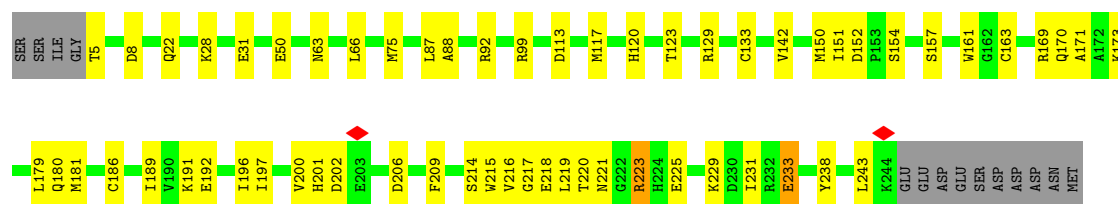
- Molecule 11: Proteasome subunit alpha type-3

Chain M:  76% 18% 6%



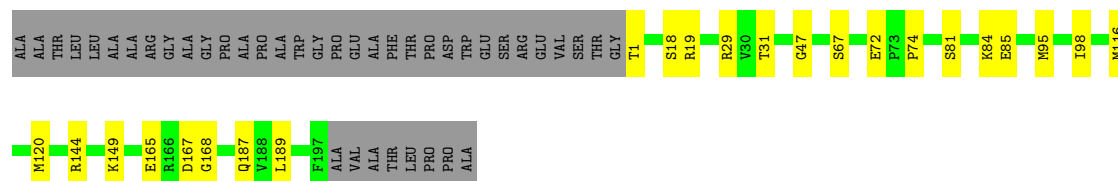
- Molecule 11: Proteasome subunit alpha type-3

Chain m:  71% 23% 6%




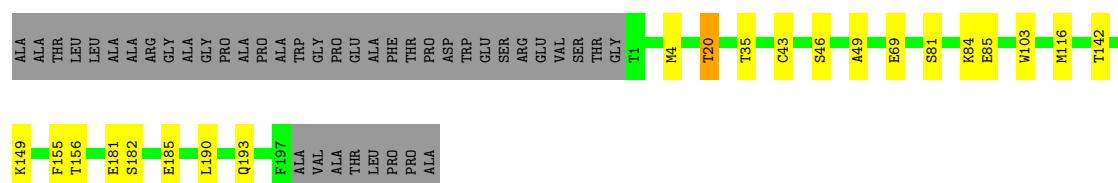
- Molecule 12: Proteasome subunit beta type-6

Chain N:  73% 10% 17%



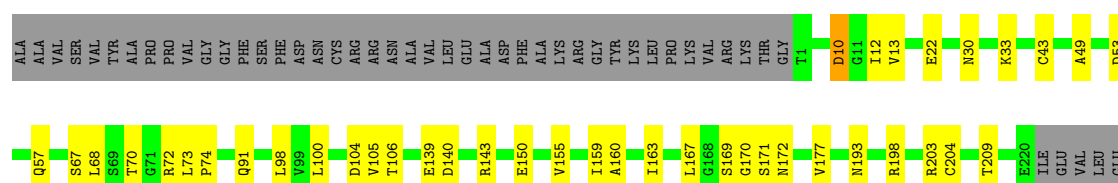
- Molecule 12: Proteasome subunit beta type-6

Chain n:  74% 8% 17%



- Molecule 13: Proteasome subunit beta type-7

Chain O:  65% 14% 20%



GLU
THR
VAL
GLN
THR
MET
ASP
THR
SER


• Molecule 13: Proteasome subunit beta type-7

Chain o:  63% 16% 20%

ALA
ALA
VAL
SER
VAL
TYR
ALA
PRO
VAL
GLY
PHE
SER
PHE
ASP
ASN
CYS
ARG
ASN
ALA
VAL
LEU
GLU
ALA
PHE
ASP
ALA
LYS
ARG
GLY
TYR
LYS
LEU
PRO
LYS
VAL
ARG
THR
GLY
T1
V7
G11
I12
T18
R19
A20
C43
A46
G47
T48
A49
A50


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

• Molecule 14: Proteasome subunit beta type-3

Chain P:  83% 17%


S2
M14
K15
Q31
A32
T58
Q61
T62
Q65
K77
R80
P107
D113
T116
F117
K118
P119
F120
I121
L124
D125
D126
D134
D135
C142
Q145
C150
E151
S152
H162
L163
F164
E165
N173
R177
I189
K201
D205

• Molecule 14: Proteasome subunit beta type-3

Chain p:  86% 13% .

S2
V11
M12
A13
M14
A24
R27
Q31
L73
P107
D113
F114
K115
T116
F117
C122
S123
L124
I127
D135
F136
V137
V138
C142
M146
M171
V175
D176
R177
M183
I189
I190
I195
R203
M204
D205


• Molecule 15: Proteasome subunit beta type-2

Chain Q:  80% 19% .

H1
L4
Q8
L14
V20
A21
V26
Q27
M28
K29
M35
M38
V47
M69
A81
M82
F83
T84
R85
R86
N101
L102
L103
L104
D108
E111
G112
P113
M118
L124
H132
T150
I151
S152
R155
L160
R161
K162
C163
L164

L167
T177
R181
D184
K186
S195
F196
P197
K198
Q199
GLY
SER

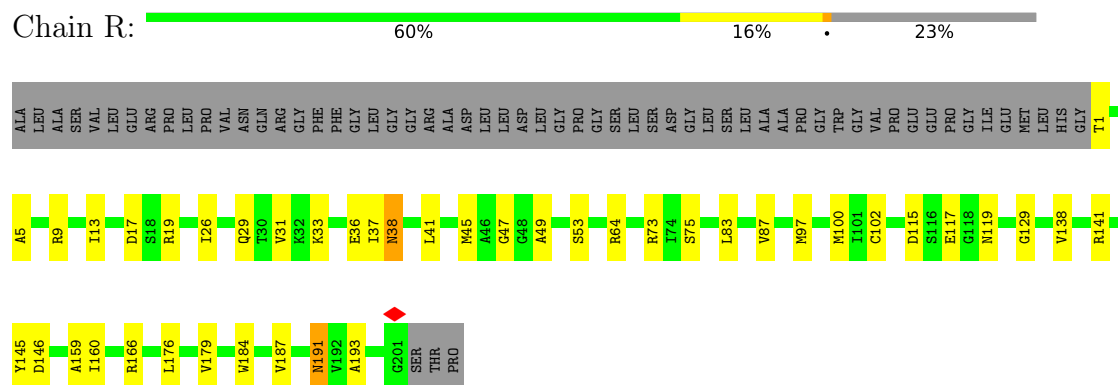
• Molecule 15: Proteasome subunit beta type-2

Chain q:  75% 24% .

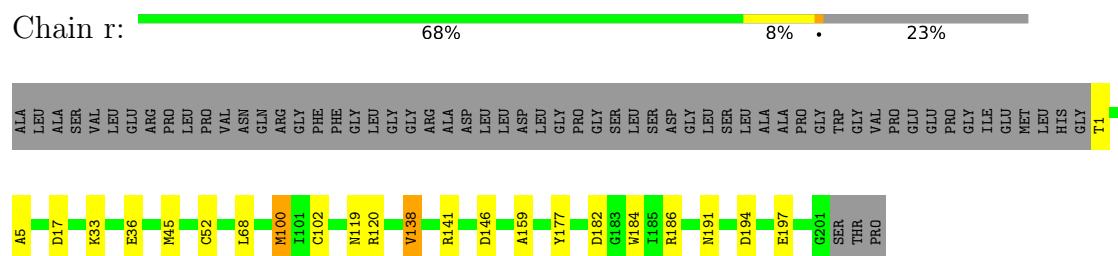
H1
L4
Q8
G9
V13
D18
N24
M38
L43
L44
L45
C46
V47
G48
E49
A50
G51
D52
T53
V54
E58
Y59
I60
V64
L88
S94
R95
Y98
N101
L102
L103
D108
E109
H110
E111
G112
P113
M118
D119
Y120
L121
A122
H132

L138
D144
T148
R156
L164
L167
P176
T177
I183
N186
H189
D190
L191
F196
P197
K198
Q199
GLY
SER

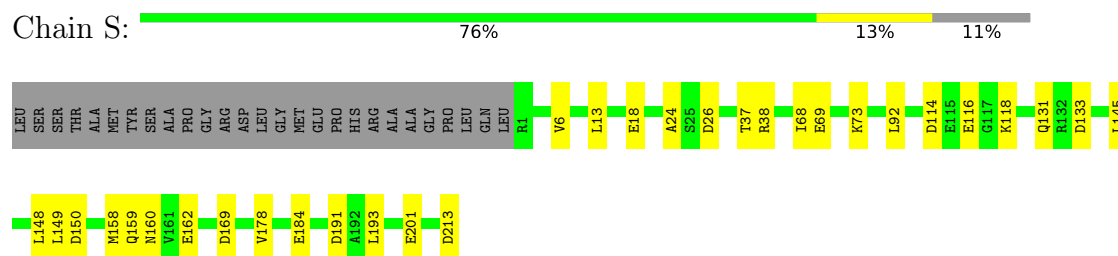
- Molecule 16: Proteasome subunit beta type-5



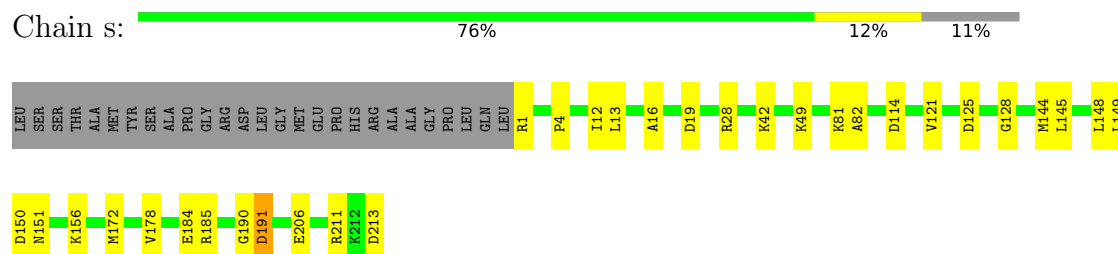
- Molecule 16: Proteasome subunit beta type-5



- Molecule 17: Proteasome subunit beta type-1

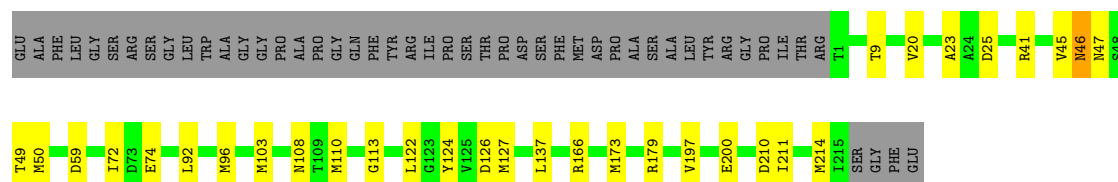


- Molecule 17: Proteasome subunit beta type-1

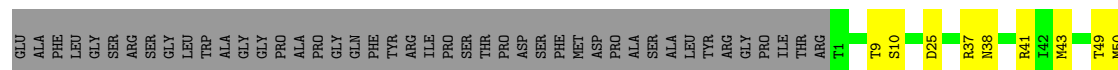


- Molecule 18: Proteasome subunit beta type-4

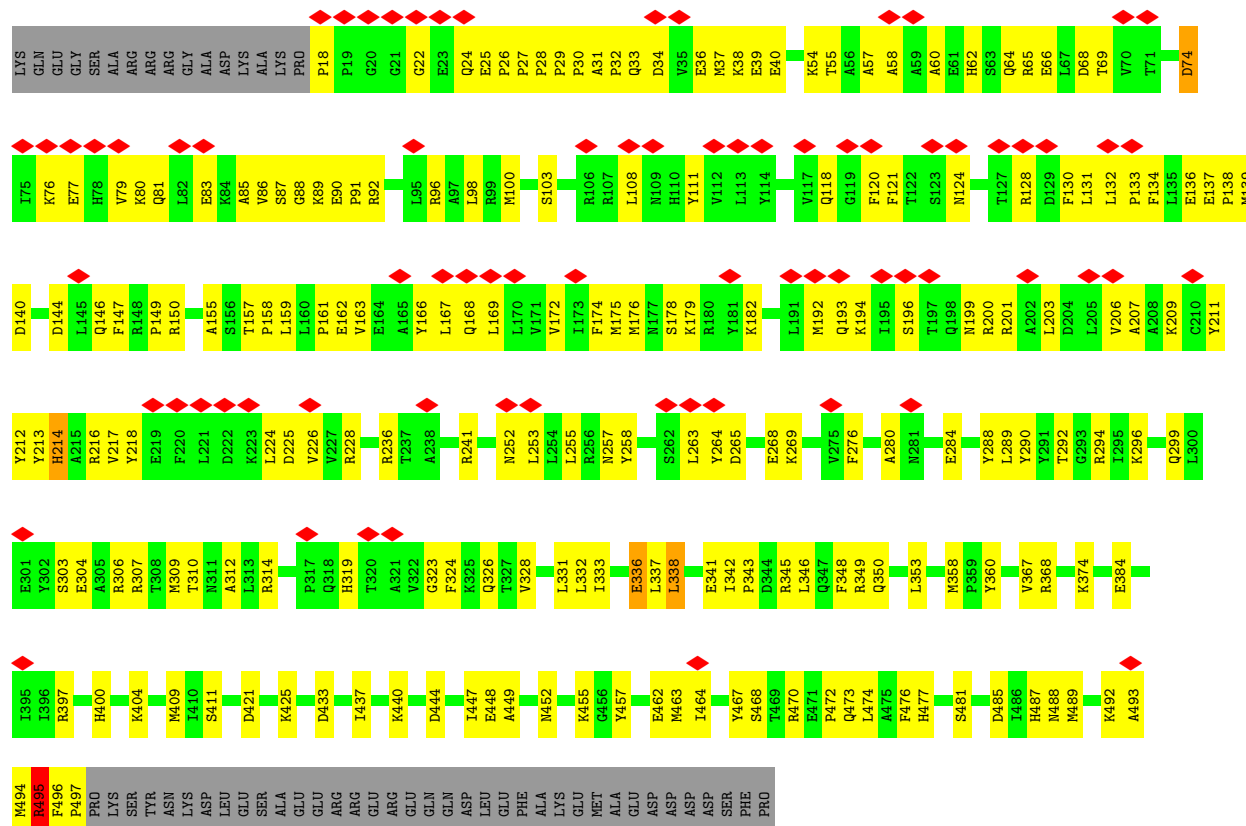




• Molecule 18: Proteasome subunit beta type-4

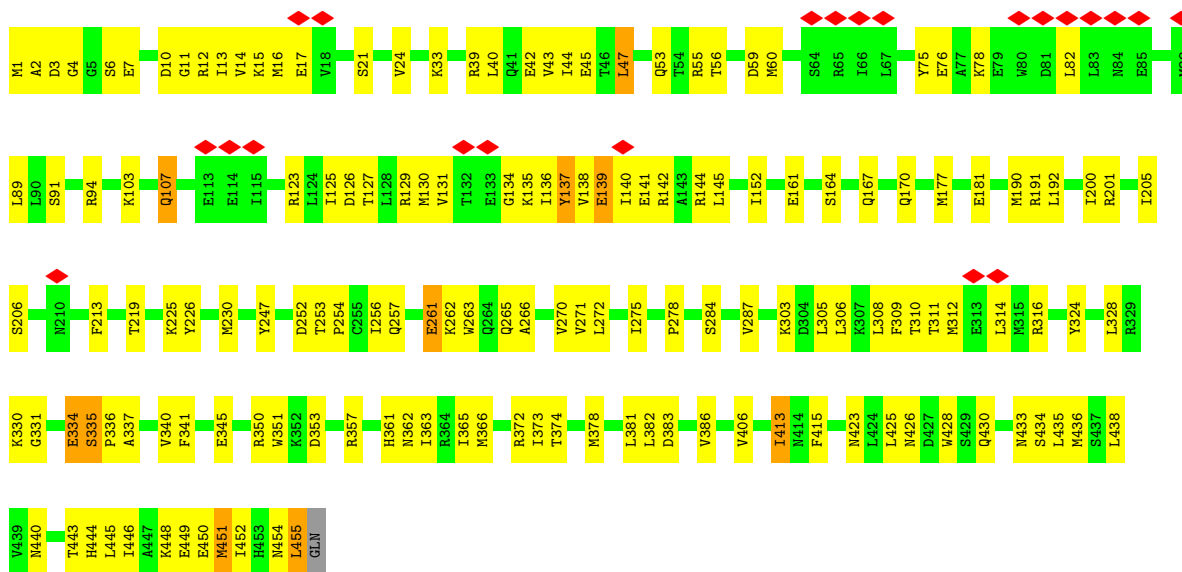


• Molecule 19: 26S proteasome non-ATPase regulatory subunit 3



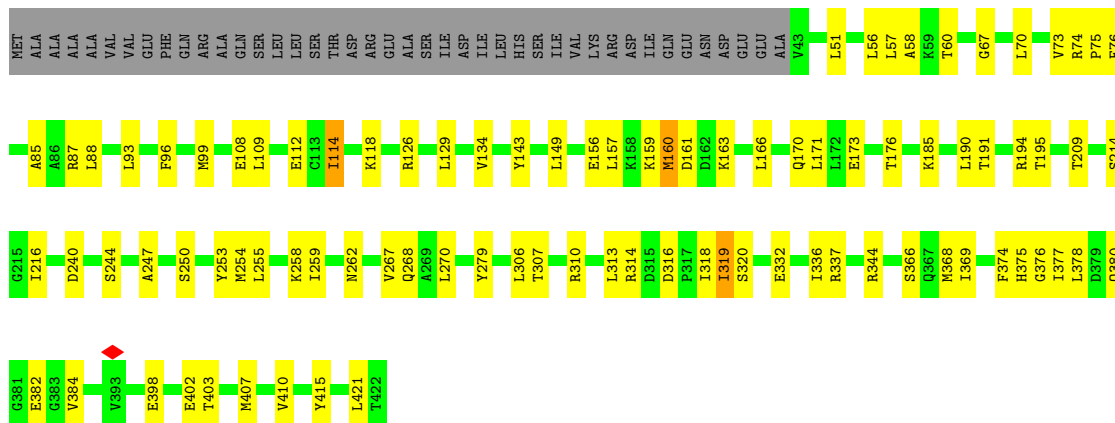
• Molecule 20: 26S proteasome non-ATPase regulatory subunit 12





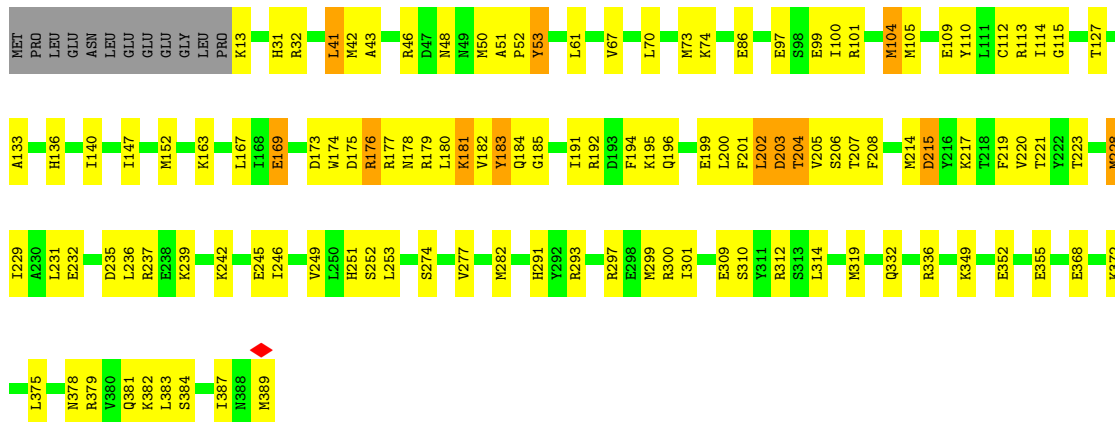
- Molecule 21: 26S proteasome non-ATPase regulatory subunit 11

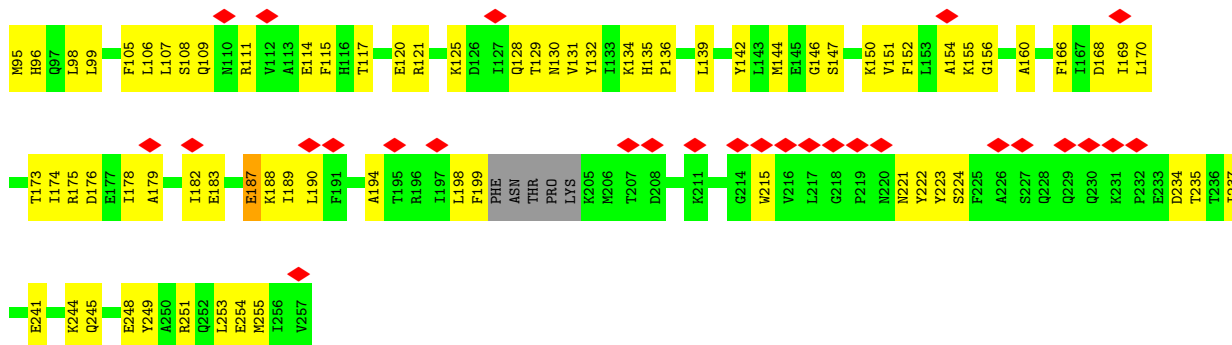
Chain X: 68% 21% 10%



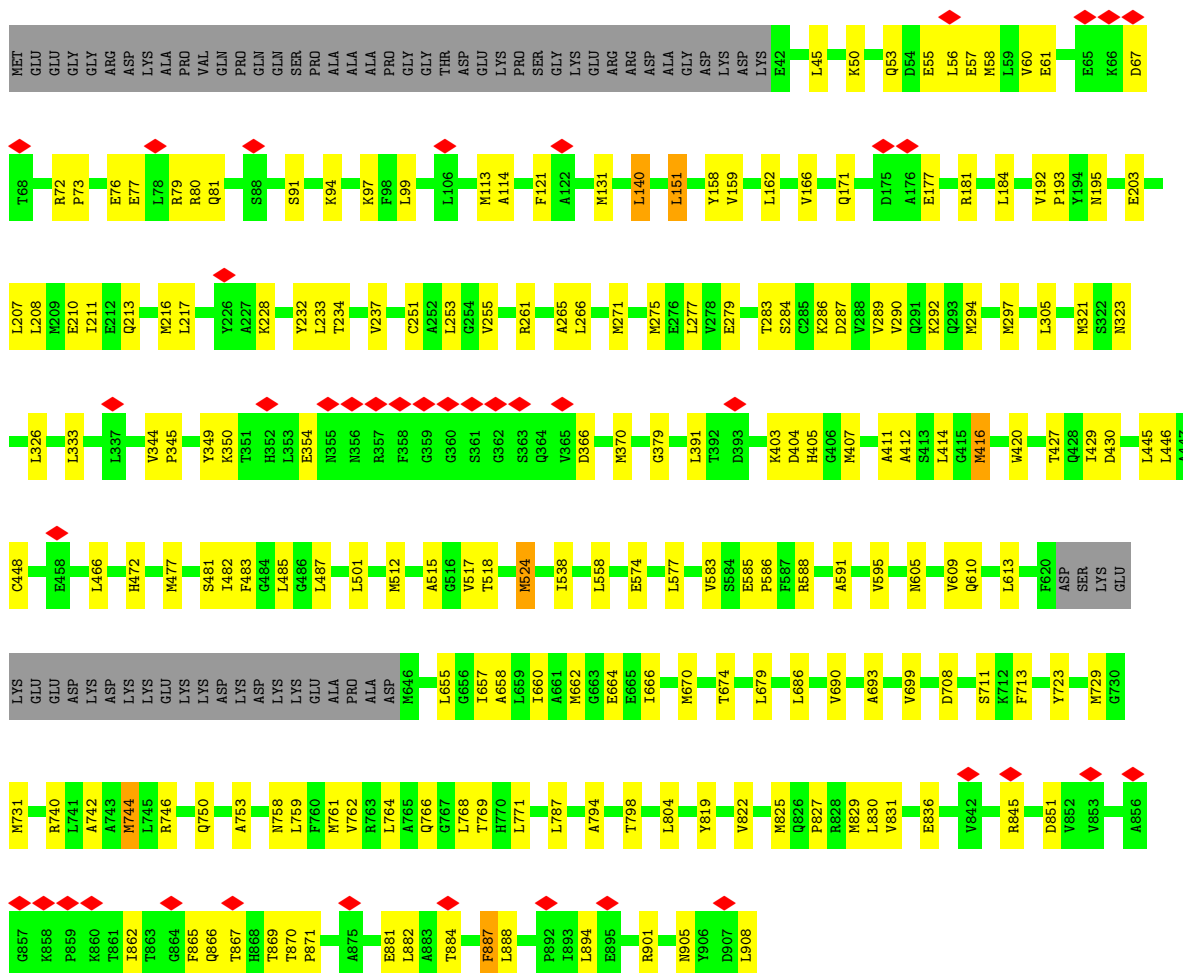
- Molecule 22: 26S proteasome non-ATPase regulatory subunit 6

Chain Y: 66% 28% 6%





• Molecule 28: 26S proteasome non-ATPase regulatory subunit 2

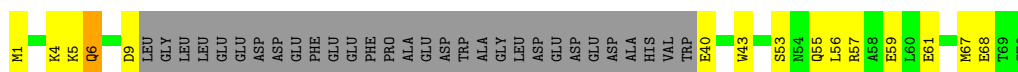


• Molecule 29: 26S proteasome non-ATPase regulatory subunit 1

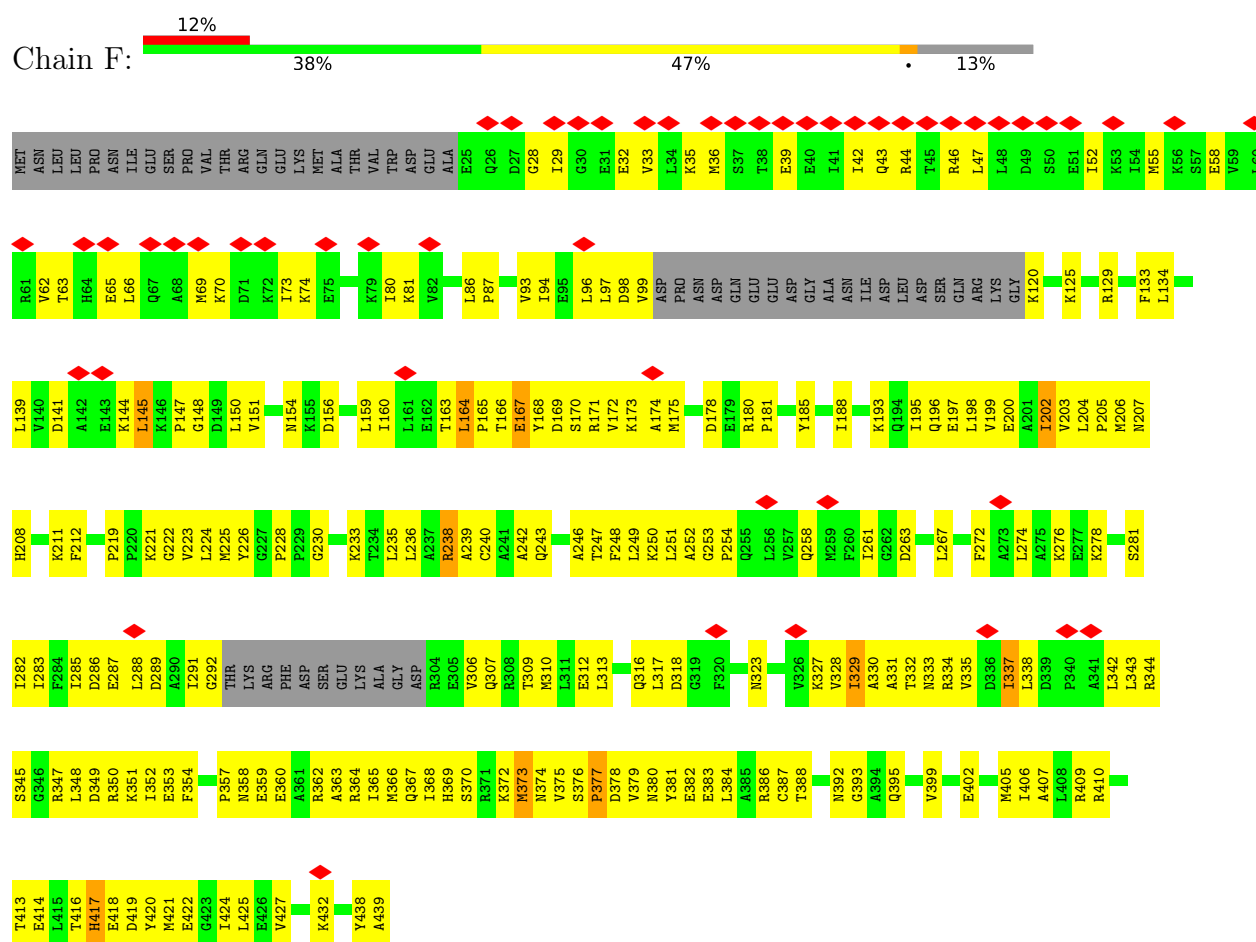


- Molecule 30: 26S proteasome complex subunit SEM1

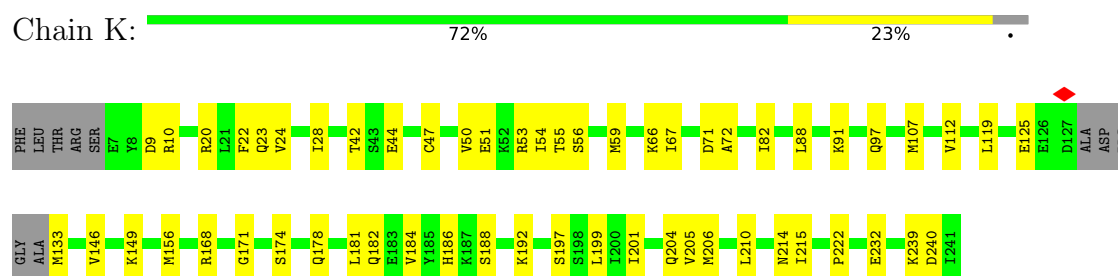
Chain e:



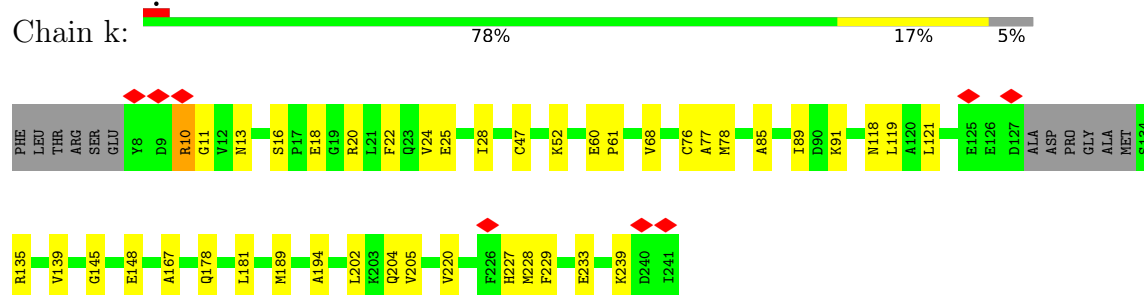
- Molecule 31: 26S proteasome regulatory subunit 6A



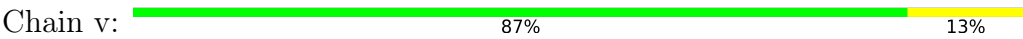
• Molecule 32: Proteasome subunit alpha type-5



• Molecule 32: Proteasome subunit alpha type-5



• Molecule 33: substrate peptide



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	25990	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.402	Depositor
Minimum map value	-1.074	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.083	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	510.0, 510.0, 510.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.85, 0.85, 0.85	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, LDZ, ZN, MG, 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	A	0.40	0/3280	0.66	2/4429 (0.0%)
2	B	0.27	0/3248	0.51	0/4381
3	C	0.27	0/3146	0.50	0/4226
4	D	0.39	0/3084	0.62	2/4161 (0.0%)
5	E	0.43	0/3077	0.61	0/4141
6	G	0.18	0/1842	0.46	0/2500
6	g	0.20	0/1863	0.41	0/2527
7	H	0.16	0/1738	0.39	0/2364
7	h	0.19	0/1764	0.41	0/2399
8	I	0.25	0/1925	0.52	0/2606
8	i	0.19	0/1942	0.49	0/2628
9	J	0.19	0/1869	0.50	0/2531
9	j	0.25	0/1728	0.54	0/2358
10	L	0.14	0/1885	0.36	0/2552
10	l	0.23	0/1885	0.42	0/2552
11	M	0.24	0/1891	0.47	1/2552 (0.0%)
11	m	0.24	0/1897	0.48	0/2559
12	N	0.16	0/1508	0.42	0/2040
12	n	0.15	0/1508	0.32	0/2040
13	O	0.35	0/1670	0.55	0/2265
13	o	0.17	0/1670	0.41	0/2265
14	P	0.18	0/1620	0.42	0/2184
14	p	0.19	0/1620	0.43	0/2184
15	Q	0.13	0/1603	0.37	0/2174
15	q	0.16	0/1607	0.39	0/2178
16	R	0.18	0/1579	0.36	0/2134
16	r	0.14	0/1579	0.35	0/2134
17	S	0.16	0/1671	0.39	0/2253
17	s	0.20	0/1671	0.40	0/2253
18	T	0.16	0/1700	0.39	0/2305
18	t	0.17	0/1706	0.39	0/2312
19	V	0.31	0/3929	0.58	1/5309 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
20	W	0.29	0/3733	0.52	0/5021
21	X	0.34	0/3047	0.51	0/4108
22	Y	0.39	0/3165	0.62	0/4262
23	Z	0.35	0/2320	0.62	0/3145
24	a	0.28	0/3053	0.52	0/4133
25	b	0.17	0/1478	0.41	0/2001
26	c	0.43	0/2296	0.68	0/3103
27	d	0.25	0/2117	0.49	0/2856
28	u	0.25	0/6625	0.43	0/8968
29	U	0.32	0/6642	0.54	0/8983
30	e	0.37	0/338	0.72	0/450
31	F	0.35	0/3042	0.61	0/4097
32	K	0.16	0/1776	0.39	0/2401
32	k	0.18	0/1747	0.45	0/2364
All	All	0.27	0/106084	0.50	6/143388 (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
8	I	0	1

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	123	LEU	N-CA-C	-6.93	105.38	114.31
1	A	159	PRO	N-CA-CB	-6.08	96.87	103.25
1	A	314	ASN	N-CA-C	-5.82	105.45	112.54
4	D	158	GLN	N-CA-C	-5.53	104.78	113.02
19	V	214	HIS	N-CA-C	-5.11	105.79	111.36

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	I	128	ARG	Sidechain

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	A	3226	0	3259	321	0
2	B	3201	0	3267	167	0
3	C	3105	0	3219	176	0
4	D	3034	0	3065	162	0
5	E	3031	0	3103	277	0
6	G	1809	0	1781	40	0
6	g	1830	0	1807	37	0
7	H	1703	0	1599	31	0
7	h	1727	0	1619	36	0
8	I	1895	0	1833	55	0
8	i	1912	0	1851	44	0
9	J	1844	0	1747	38	0
9	j	1704	0	1517	53	0
10	L	1850	0	1822	31	0
10	l	1850	0	1822	41	0
11	M	1856	0	1816	32	0
11	m	1862	0	1827	45	0
12	N	1482	0	1450	14	0
12	n	1482	0	1450	12	0
13	O	1643	0	1644	34	0
13	o	1643	0	1644	37	0
14	P	1591	0	1609	32	0
14	p	1591	0	1609	20	0
15	Q	1570	0	1547	26	0
15	q	1574	0	1558	31	0
16	R	1548	0	1499	30	0
16	r	1548	0	1499	15	0
17	S	1641	0	1618	21	0
17	s	1641	0	1618	25	0
18	T	1667	0	1628	25	0
18	t	1673	0	1639	23	0
19	V	3852	0	3893	227	0
20	W	3685	0	3799	192	0
21	X	3003	0	3102	88	0
22	Y	3108	0	3112	173	0
23	Z	2277	0	2306	169	0
24	a	2995	0	3012	176	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	b	1458	0	1505	74	0
26	c	2254	0	2265	160	0
27	d	2074	0	2103	125	0
28	u	6514	0	6527	178	0
29	U	6529	0	6572	362	0
30	e	334	0	294	24	0
31	F	3005	0	3093	246	0
32	K	1750	0	1706	50	0
32	k	1722	0	1673	39	0
33	v	75	0	20	1	0
34	A	27	0	12	2	0
34	E	27	0	12	3	0
34	F	27	0	12	2	0
35	B	31	0	12	1	0
35	C	31	0	12	0	0
35	D	31	0	12	3	0
36	B	1	0	0	0	0
36	C	1	0	0	0	0
36	D	1	0	0	0	0
37	N	34	0	41	2	0
37	O	34	0	41	5	0
37	R	34	0	41	4	0
37	n	34	0	41	2	0
37	o	34	0	41	4	0
37	r	34	0	41	1	0
38	c	1	0	0	0	0
All	All	104750	0	104266	3856	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 18.

The worst 5 of 3856 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)
29:U:623:GLY:HA2	29:U:659:CYS:SG	1.78	1.24
19:V:62:HIS:CE1	22:Y:389:MET:HE1	1.81	1.15
21:X:159:LYS:HA	21:X:159:LYS:HE3	1.19	1.15
22:Y:282:MET:HE3	22:Y:291:HIS:HB3	1.26	1.14
1:A:156:LYS:HE2	2:B:114:GLU:HB3	1.15	1.14

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	A	411/433 (95%)	346 (84%)	58 (14%)	7 (2%)	7	24
2	B	409/440 (93%)	359 (88%)	50 (12%)	0	100	100
3	C	394/398 (99%)	345 (88%)	42 (11%)	7 (2%)	6	23
4	D	378/418 (90%)	327 (86%)	47 (12%)	4 (1%)	11	35
5	E	379/403 (94%)	344 (91%)	32 (8%)	3 (1%)	16	43
6	G	235/245 (96%)	219 (93%)	13 (6%)	3 (1%)	9	30
6	g	238/245 (97%)	225 (94%)	12 (5%)	1 (0%)	30	58
7	H	229/233 (98%)	217 (95%)	10 (4%)	2 (1%)	14	40
7	h	230/233 (99%)	218 (95%)	11 (5%)	1 (0%)	30	58
8	I	246/260 (95%)	227 (92%)	18 (7%)	1 (0%)	30	58
8	i	248/260 (95%)	230 (93%)	17 (7%)	1 (0%)	30	58
9	J	245/247 (99%)	224 (91%)	17 (7%)	4 (2%)	7	25
9	j	237/247 (96%)	208 (88%)	27 (11%)	2 (1%)	16	43
10	L	236/268 (88%)	229 (97%)	7 (3%)	0	100	100
10	l	236/268 (88%)	225 (95%)	10 (4%)	1 (0%)	30	58
11	M	238/254 (94%)	227 (95%)	10 (4%)	1 (0%)	30	58
11	m	238/254 (94%)	221 (93%)	15 (6%)	2 (1%)	16	43
12	N	195/238 (82%)	188 (96%)	6 (3%)	1 (0%)	24	53
12	n	195/238 (82%)	189 (97%)	6 (3%)	0	100	100
13	O	218/276 (79%)	209 (96%)	8 (4%)	1 (0%)	24	53
13	o	218/276 (79%)	202 (93%)	16 (7%)	0	100	100
14	P	202/204 (99%)	192 (95%)	10 (5%)	0	100	100
14	p	202/204 (99%)	195 (96%)	6 (3%)	1 (0%)	24	53
15	Q	197/201 (98%)	186 (94%)	11 (6%)	0	100	100
15	q	197/201 (98%)	188 (95%)	8 (4%)	1 (0%)	24	53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	R	199/262 (76%)	190 (96%)	8 (4%)	1 (0%)	24	53
16	r	199/262 (76%)	189 (95%)	10 (5%)	0	100	100
17	S	211/240 (88%)	205 (97%)	5 (2%)	1 (0%)	24	53
17	s	211/240 (88%)	205 (97%)	5 (2%)	1 (0%)	24	53
18	T	213/263 (81%)	205 (96%)	7 (3%)	1 (0%)	24	53
18	t	213/263 (81%)	203 (95%)	10 (5%)	0	100	100
19	V	478/533 (90%)	425 (89%)	51 (11%)	2 (0%)	30	58
20	W	453/456 (99%)	415 (92%)	34 (8%)	4 (1%)	14	40
21	X	378/422 (90%)	360 (95%)	17 (4%)	1 (0%)	36	64
22	Y	375/389 (96%)	339 (90%)	35 (9%)	1 (0%)	36	64
23	Z	284/324 (88%)	245 (86%)	38 (13%)	1 (0%)	30	58
24	a	371/376 (99%)	343 (92%)	26 (7%)	2 (0%)	24	53
25	b	189/377 (50%)	166 (88%)	23 (12%)	0	100	100
26	c	285/309 (92%)	244 (86%)	37 (13%)	4 (1%)	9	29
27	d	248/349 (71%)	208 (84%)	40 (16%)	0	100	100
28	u	838/908 (92%)	799 (95%)	39 (5%)	0	100	100
29	U	829/953 (87%)	747 (90%)	77 (9%)	5 (1%)	21	50
30	e	36/70 (51%)	29 (81%)	7 (19%)	0	100	100
31	F	378/439 (86%)	328 (87%)	46 (12%)	4 (1%)	11	35
32	K	226/240 (94%)	219 (97%)	7 (3%)	0	100	100
32	k	224/240 (93%)	215 (96%)	9 (4%)	0	100	100
All	All	13289/14859 (89%)	12219 (92%)	998 (8%)	72 (0%)	26	53

5 of 72 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	159	PRO
1	A	160	THR
1	A	164	MET
1	A	284	ARG
1	A	361	SER

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	A	348/372 (94%)	332 (95%)	16 (5%)	24	56
2	B	356/385 (92%)	353 (99%)	3 (1%)	73	89
3	C	340/346 (98%)	326 (96%)	14 (4%)	27	60
4	D	332/366 (91%)	318 (96%)	14 (4%)	26	59
5	E	333/353 (94%)	319 (96%)	14 (4%)	26	59
6	G	191/209 (91%)	190 (100%)	1 (0%)	81	93
6	g	194/209 (93%)	190 (98%)	4 (2%)	47	76
7	H	164/190 (86%)	161 (98%)	3 (2%)	51	79
7	h	167/190 (88%)	165 (99%)	2 (1%)	63	85
8	I	191/220 (87%)	186 (97%)	5 (3%)	40	72
8	i	193/220 (88%)	191 (99%)	2 (1%)	68	87
9	J	179/210 (85%)	172 (96%)	7 (4%)	28	61
9	j	152/210 (72%)	146 (96%)	6 (4%)	28	61
10	L	198/229 (86%)	193 (98%)	5 (2%)	42	73
10	l	198/229 (86%)	190 (96%)	8 (4%)	28	61
11	M	192/211 (91%)	188 (98%)	4 (2%)	47	76
11	m	193/211 (92%)	185 (96%)	8 (4%)	27	60
12	N	154/180 (86%)	150 (97%)	4 (3%)	40	72
12	n	154/180 (86%)	151 (98%)	3 (2%)	50	78
13	O	177/227 (78%)	173 (98%)	4 (2%)	44	74
13	o	177/227 (78%)	176 (99%)	1 (1%)	78	92
14	P	173/173 (100%)	172 (99%)	1 (1%)	78	92
14	p	173/173 (100%)	171 (99%)	2 (1%)	63	85
15	Q	164/171 (96%)	161 (98%)	3 (2%)	51	79
15	q	165/171 (96%)	162 (98%)	3 (2%)	51	79
16	R	153/201 (76%)	149 (97%)	4 (3%)	40	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	r	153/201 (76%)	149 (97%)	4 (3%)	40	72
17	S	174/198 (88%)	170 (98%)	4 (2%)	44	74
17	s	174/198 (88%)	173 (99%)	1 (1%)	78	92
18	T	175/214 (82%)	175 (100%)	0	100	100
18	t	176/214 (82%)	175 (99%)	1 (1%)	78	92
19	V	414/459 (90%)	407 (98%)	7 (2%)	53	80
20	W	413/416 (99%)	402 (97%)	11 (3%)	39	71
21	X	326/362 (90%)	320 (98%)	6 (2%)	51	79
22	Y	333/344 (97%)	321 (96%)	12 (4%)	31	63
23	Z	256/295 (87%)	248 (97%)	8 (3%)	35	67
24	a	333/336 (99%)	328 (98%)	5 (2%)	57	82
25	b	167/312 (54%)	165 (99%)	2 (1%)	63	85
26	c	251/267 (94%)	241 (96%)	10 (4%)	28	61
27	d	226/293 (77%)	220 (97%)	6 (3%)	39	71
28	u	709/763 (93%)	700 (99%)	9 (1%)	61	84
29	U	714/816 (88%)	697 (98%)	17 (2%)	43	73
30	e	38/63 (60%)	37 (97%)	1 (3%)	40	72
31	F	330/379 (87%)	322 (98%)	8 (2%)	43	73
32	K	190/202 (94%)	189 (100%)	1 (0%)	81	93
32	k	186/202 (92%)	181 (97%)	5 (3%)	39	71
All	All	11149/12597 (88%)	10890 (98%)	259 (2%)	44	74

5 of 259 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
29	U	459	ASP
29	U	788	VAL
15	Q	102	LEU
14	P	150	CYS
29	U	921	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 242 such sidechains are listed below:

Mol	Chain	Res	Type
22	Y	184	GLN
29	U	888	GLN
26	c	149	GLN
29	U	718	ASN
32	K	204	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
34	ADP	E	401	-	28,29,29	1.45	4 (14%)	43,45,45	1.80	9 (20%)
34	ADP	F	501	-	28,29,29	1.42	4 (14%)	43,45,45	1.84	9 (20%)
37	LDZ	N	301	-	33,34,34	0.40	0	42,44,44	0.78	2 (4%)
35	ATP	C	501	36	32,33,33	0.37	0	48,52,52	0.42	0
37	LDZ	n	301	-	33,34,34	0.51	1 (3%)	42,44,44	1.69	4 (9%)
35	ATP	B	501	36	32,33,33	1.88	1 (3%)	48,52,52	0.86	2 (4%)
37	LDZ	r	301	-	33,34,34	0.46	0	42,44,44	0.83	2 (4%)
37	LDZ	O	301	-	33,34,34	0.18	0	42,44,44	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	ADP	A	501	-	28,29,29	1.42	5 (17%)	43,45,45	1.83	8 (18%)
37	LDZ	o	301	-	33,34,34	0.45	0	42,44,44	1.22	4 (9%)
37	LDZ	R	301	-	33,34,34	0.55	1 (3%)	42,44,44	1.05	2 (4%)
35	ATP	D	501	36	32,33,33	0.32	0	48,52,52	0.30	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	ADP	E	401	-	-	5/16/32/32	0/3/3/3
34	ADP	F	501	-	-	5/16/32/32	0/3/3/3
37	LDZ	N	301	-	-	9/38/39/39	0/1/1/1
35	ATP	C	501	36	-	6/22/38/38	0/3/3/3
37	LDZ	n	301	-	-	24/38/39/39	0/1/1/1
35	ATP	B	501	36	-	3/22/38/38	0/3/3/3
37	LDZ	r	301	-	-	14/38/39/39	0/1/1/1
37	LDZ	O	301	-	-	15/38/39/39	0/1/1/1
34	ADP	A	501	-	-	4/16/32/32	0/3/3/3
37	LDZ	o	301	-	-	16/38/39/39	0/1/1/1
37	LDZ	R	301	-	-	10/38/39/39	0/1/1/1
35	ATP	D	501	36	-	2/22/38/38	0/3/3/3

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	B	501	ATP	PA-O3A	10.41	1.70	1.59
34	E	401	ADP	C5-C4	4.82	1.47	1.39
34	F	501	ADP	C5-C4	4.75	1.47	1.39
34	A	501	ADP	C5-C4	4.72	1.47	1.39
34	F	501	ADP	C5-C6	2.75	1.48	1.41

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	n	301	LDZ	C14-N13-C12	8.22	139.31	121.65
34	F	501	ADP	C5-C4-N3	-5.95	118.53	126.72
34	E	401	ADP	C5-C4-N3	-5.92	118.56	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	A	501	ADP	C5-C4-N3	-5.82	118.70	126.72
34	E	401	ADP	N3-C4-N9	4.77	135.28	127.17

There are no chirality outliers.

5 of 113 torsion outliers are listed below:

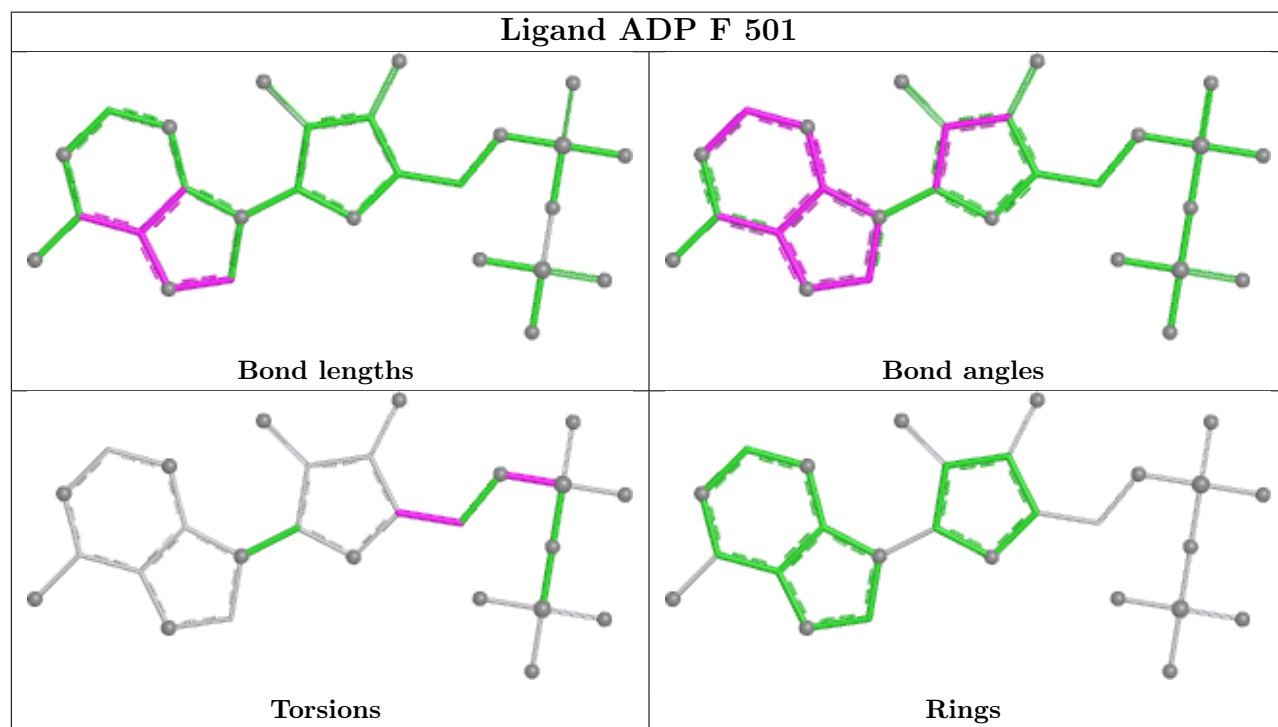
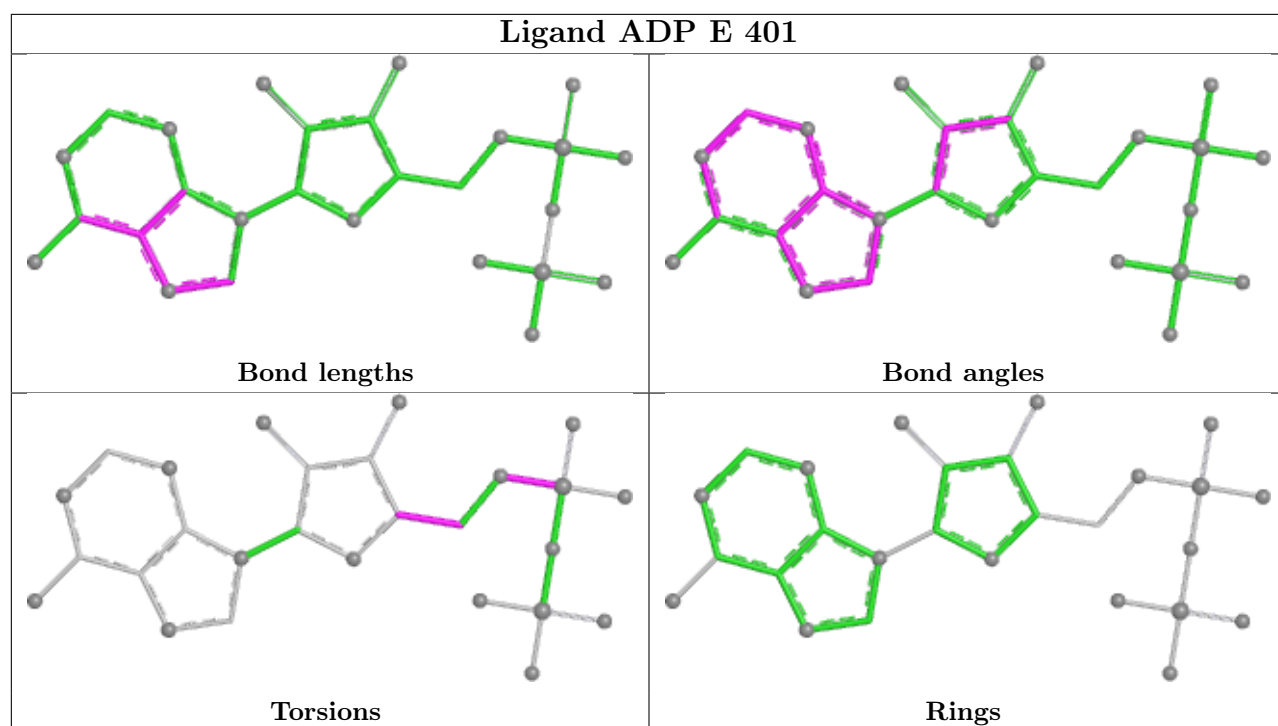
Mol	Chain	Res	Type	Atoms
34	A	501	ADP	C5'-O5'-PA-O3A
34	E	401	ADP	C5'-O5'-PA-O1A
34	E	401	ADP	C5'-O5'-PA-O3A
34	F	501	ADP	C5'-O5'-PA-O1A
34	F	501	ADP	C5'-O5'-PA-O2A

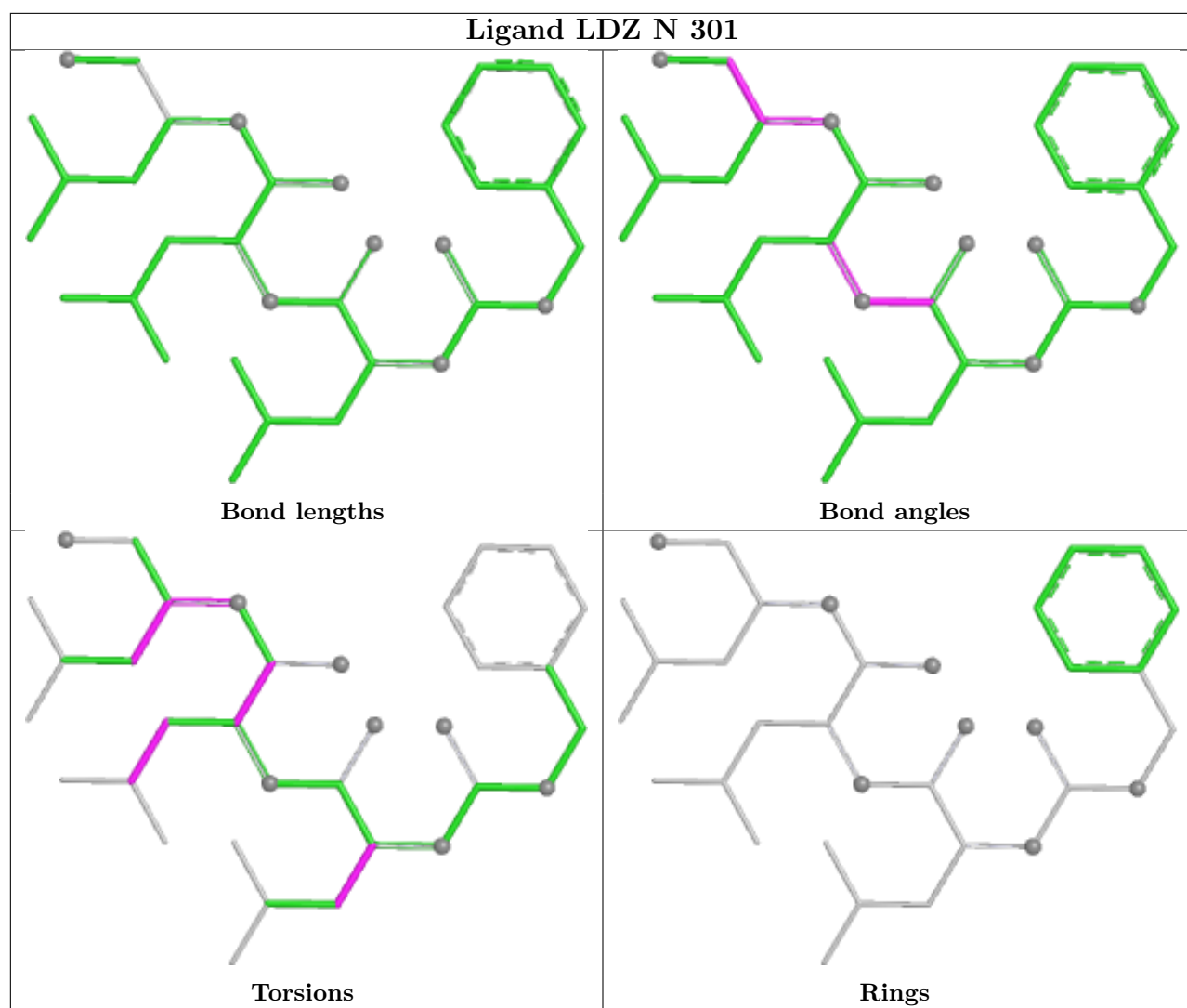
There are no ring outliers.

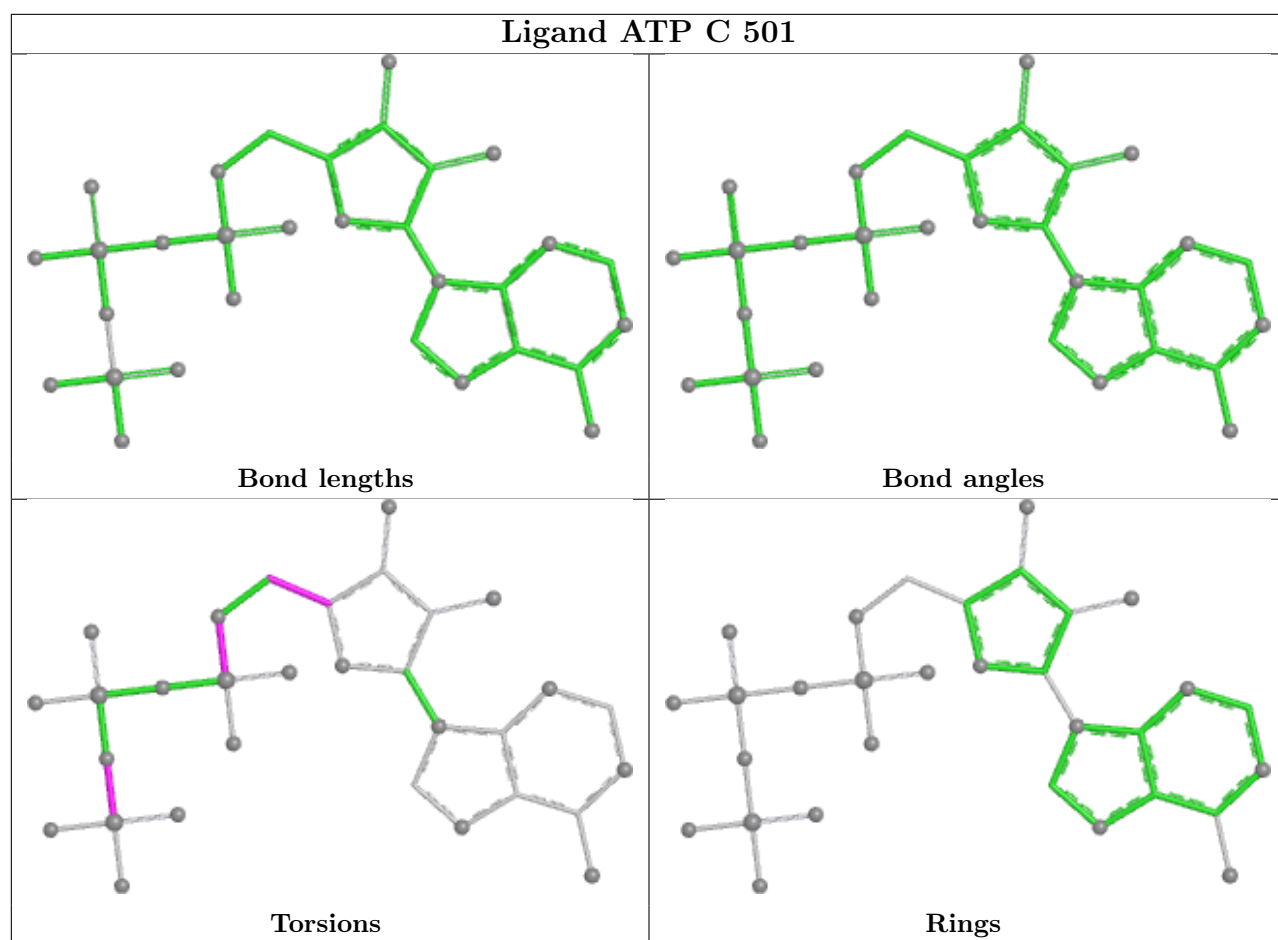
11 monomers are involved in 29 short contacts:

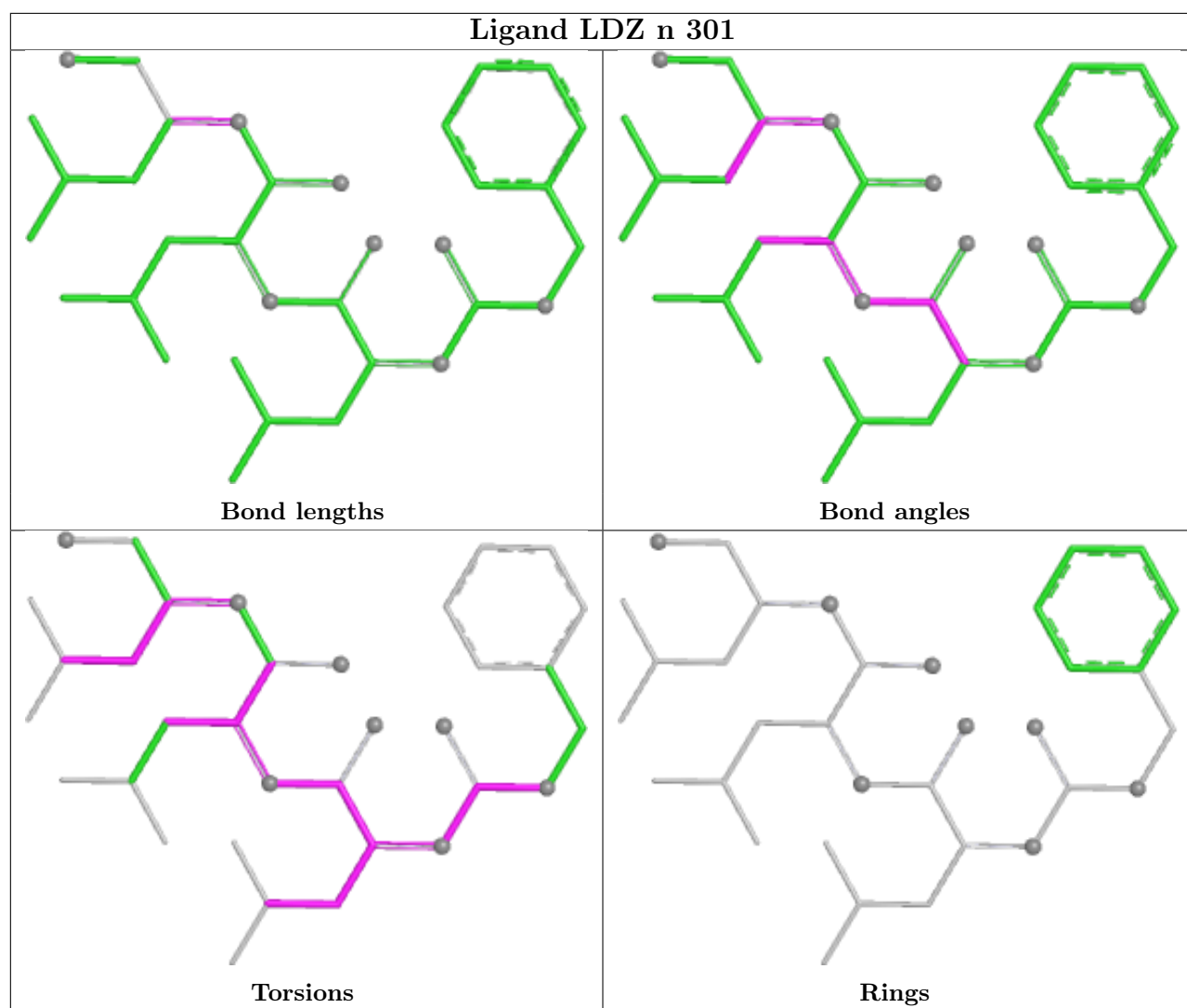
Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	E	401	ADP	3	0
34	F	501	ADP	2	0
37	N	301	LDZ	2	0
37	n	301	LDZ	2	0
35	B	501	ATP	1	0
37	r	301	LDZ	1	0
37	O	301	LDZ	5	0
34	A	501	ADP	2	0
37	o	301	LDZ	4	0
37	R	301	LDZ	4	0
35	D	501	ATP	3	0

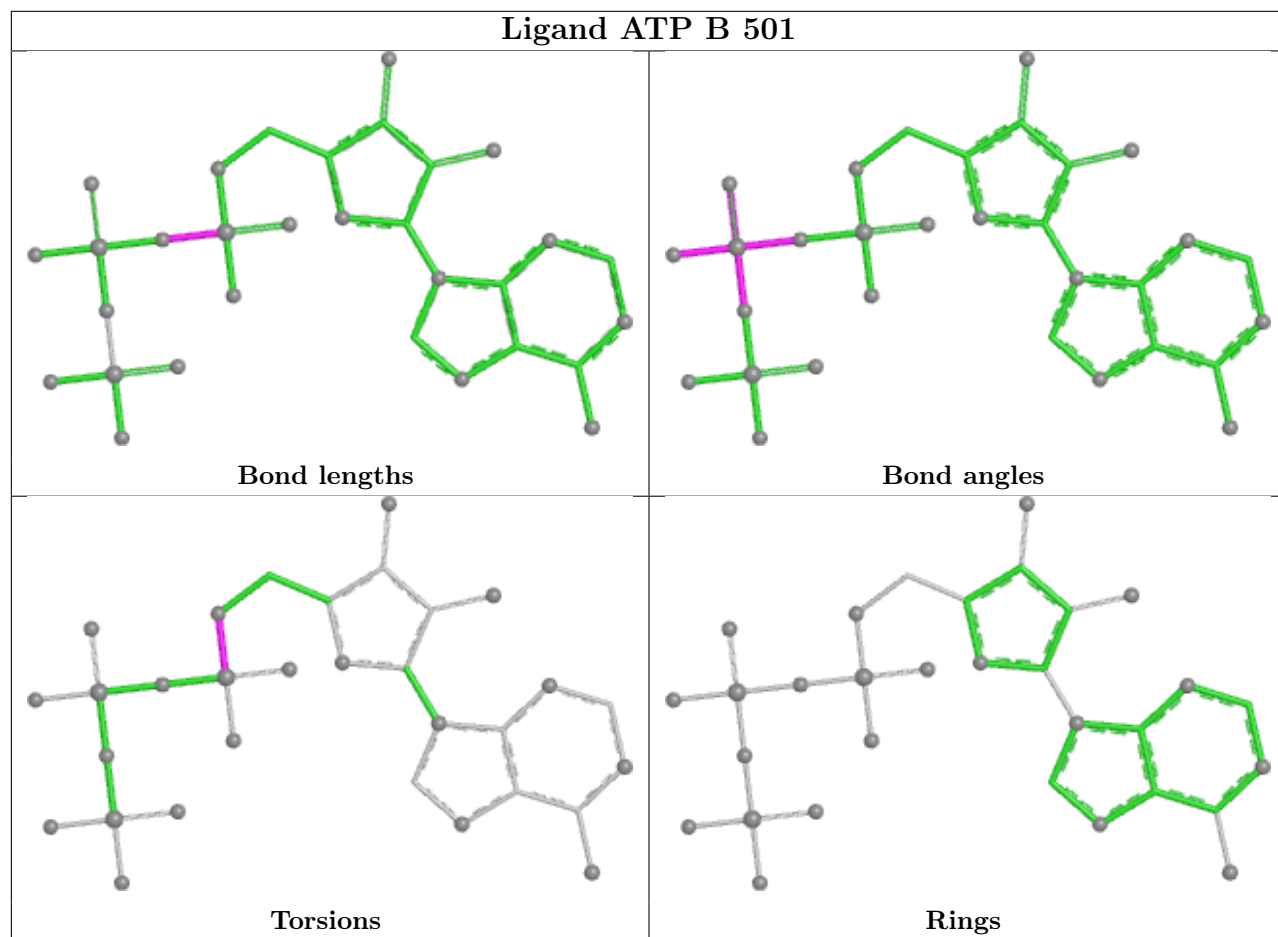
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

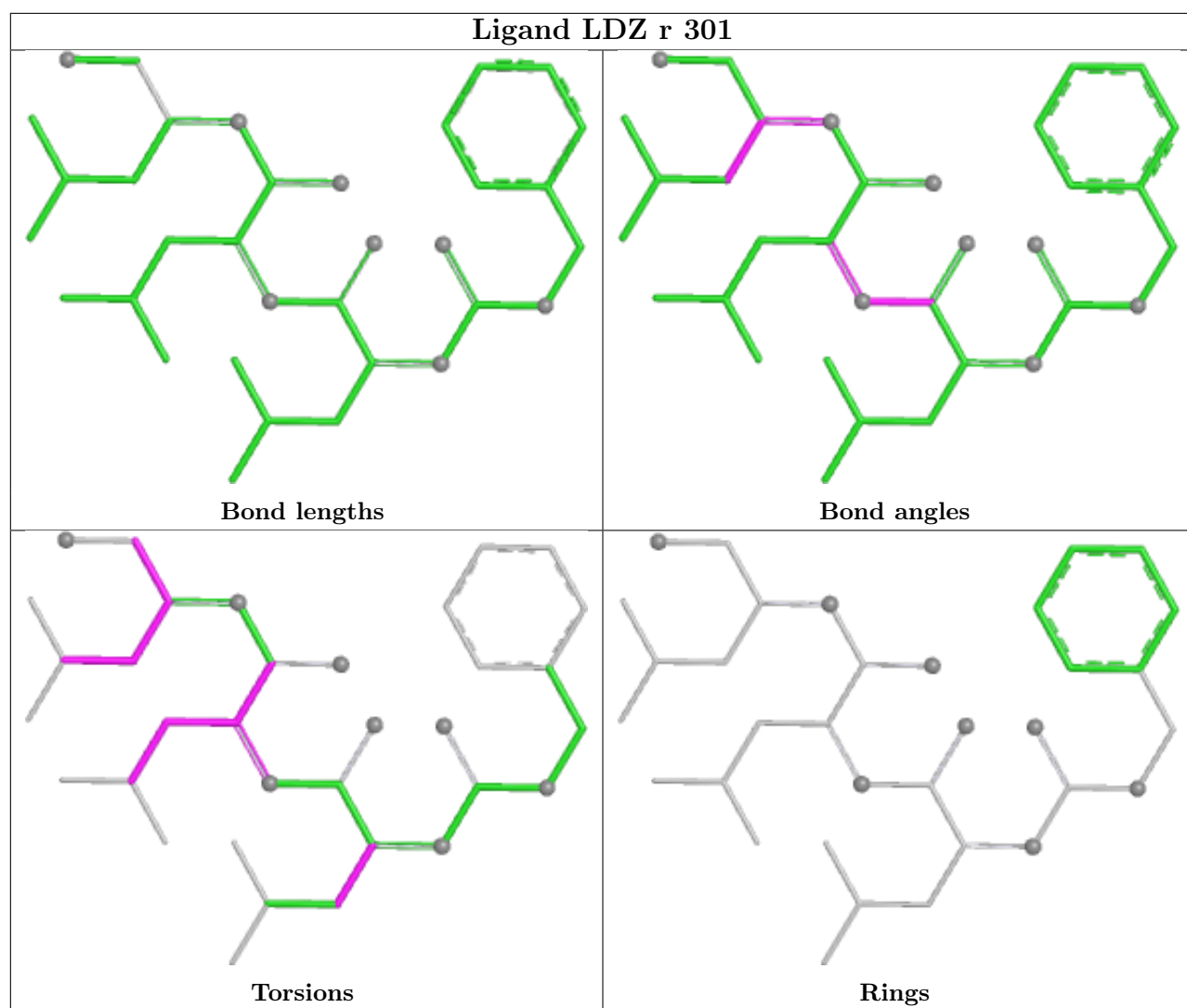


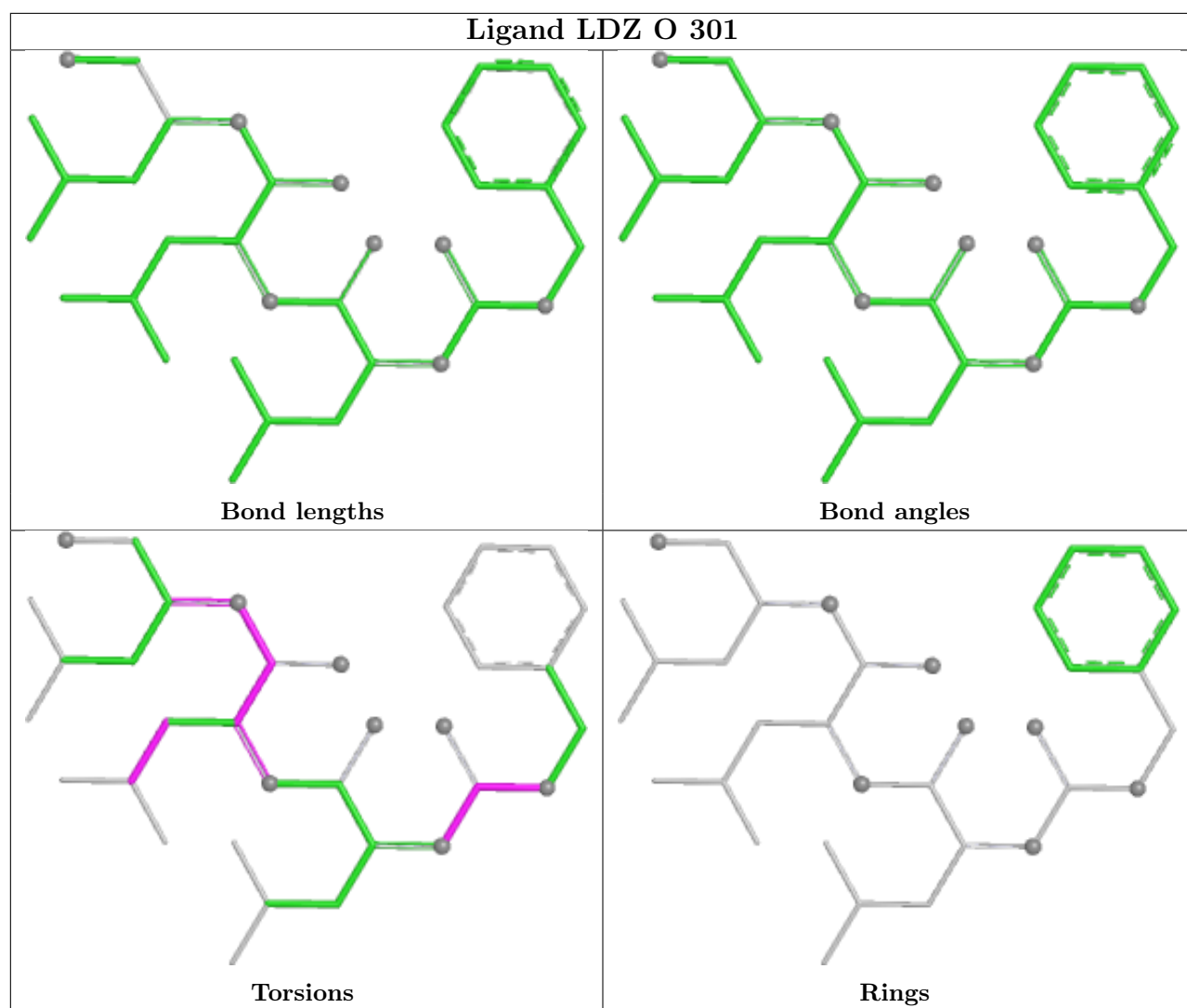


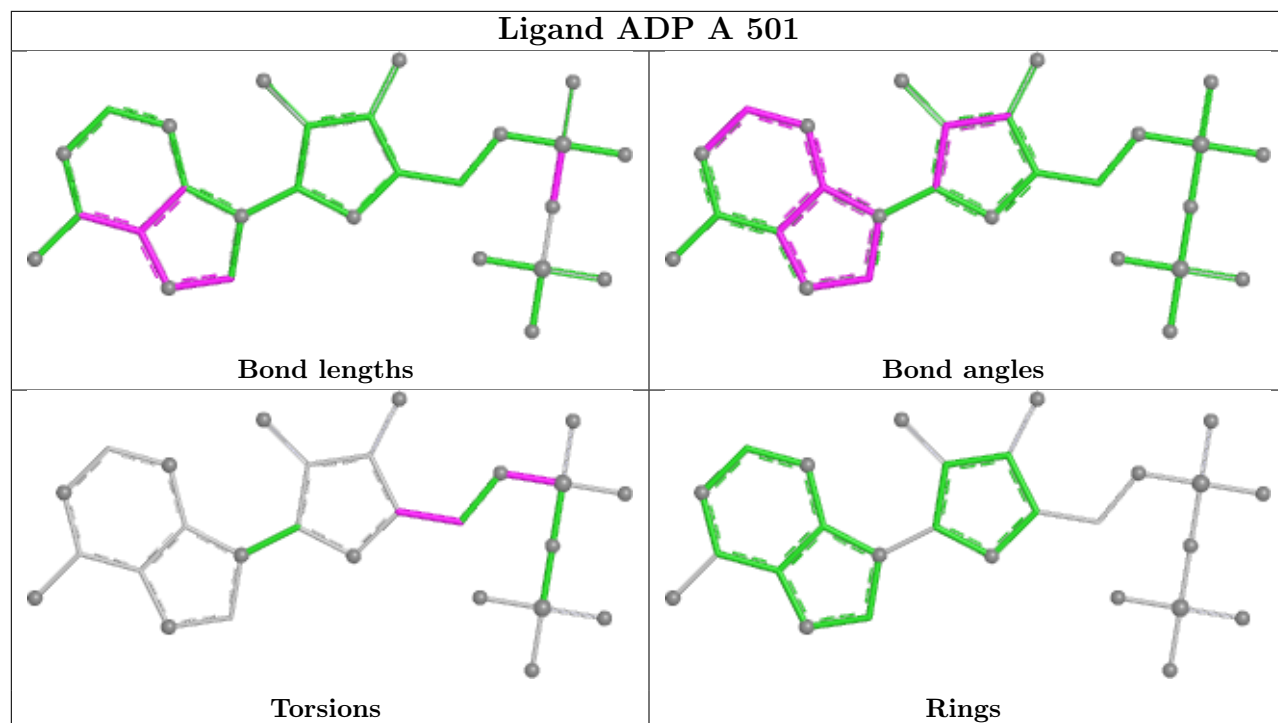


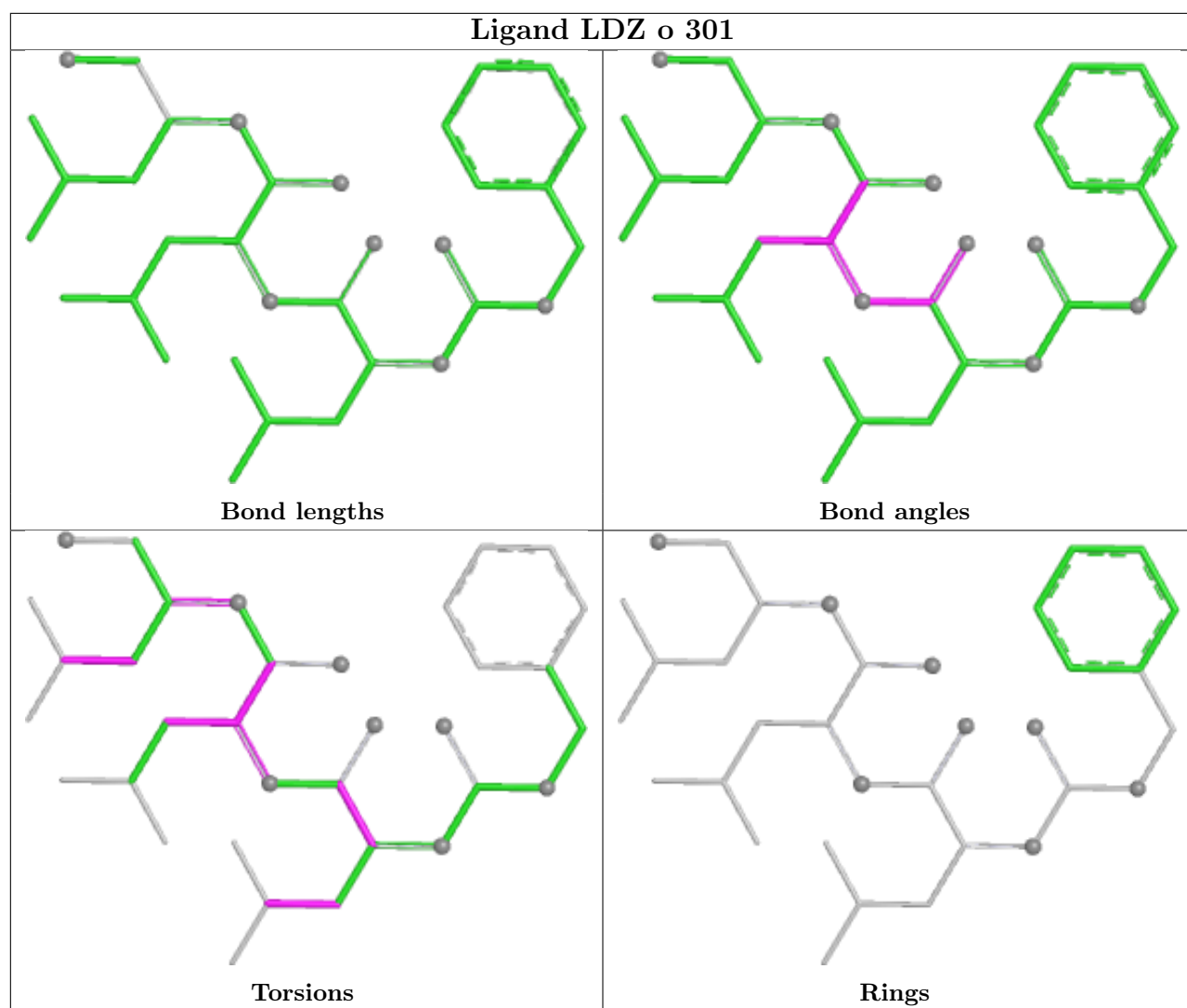


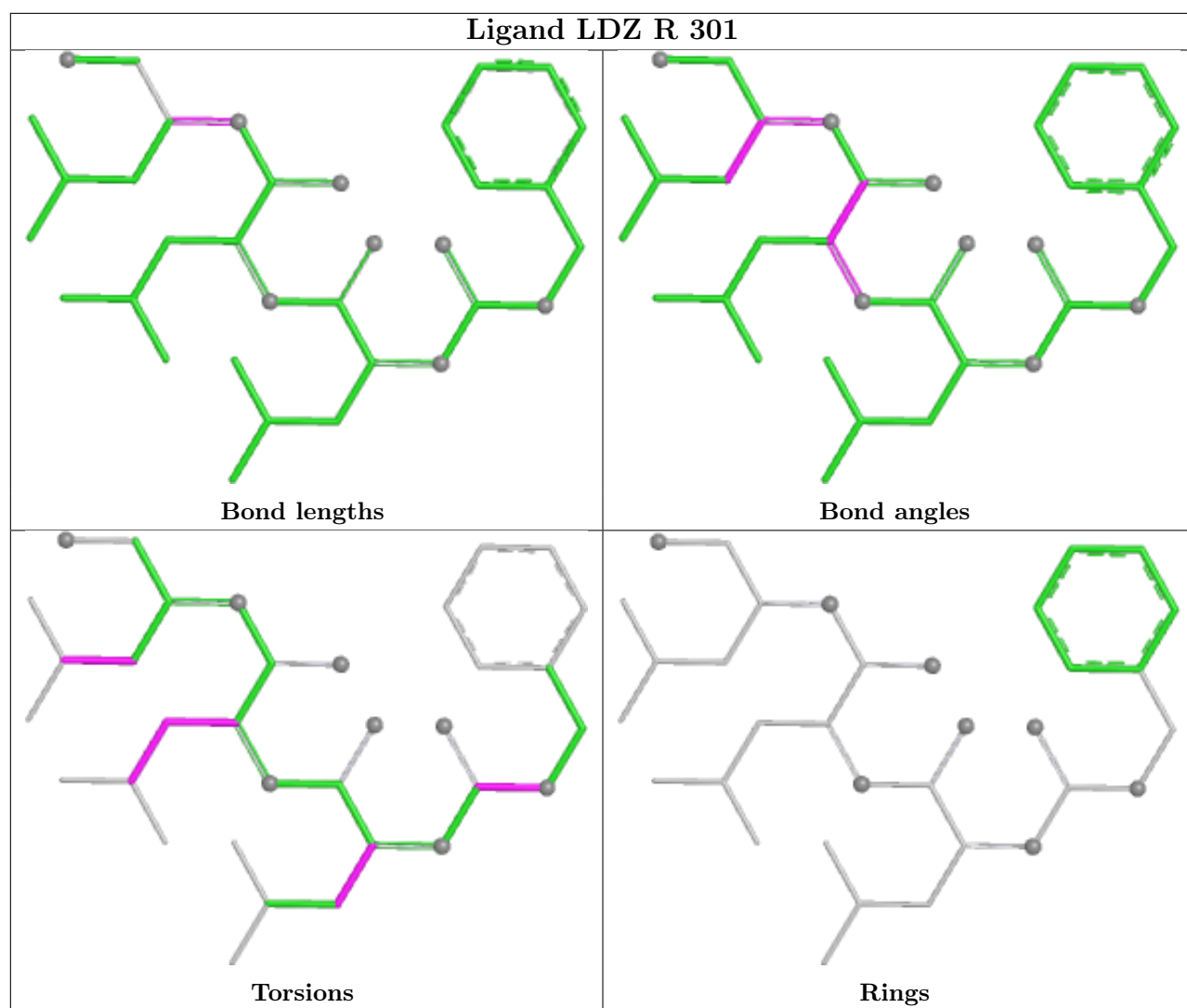


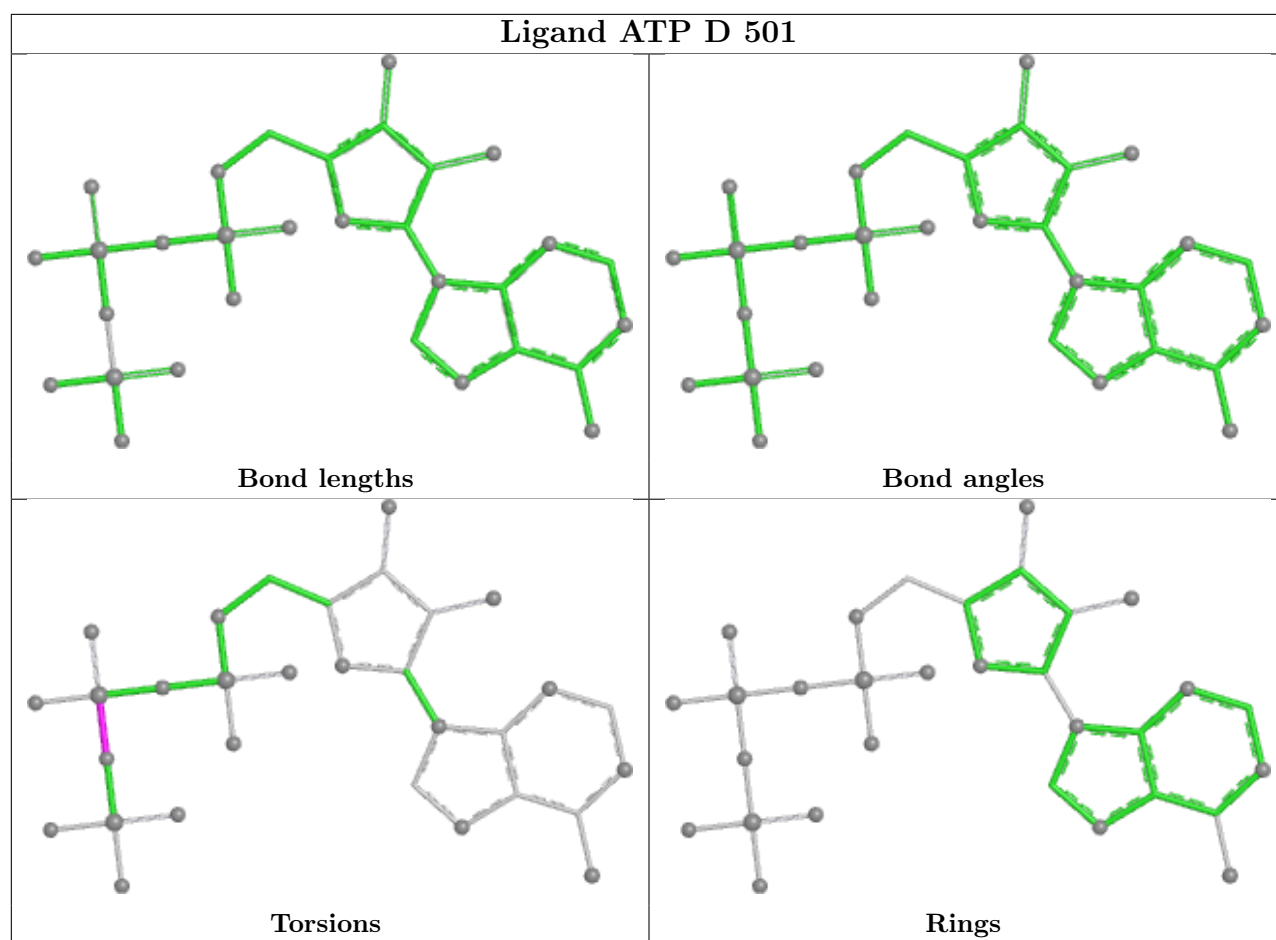












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

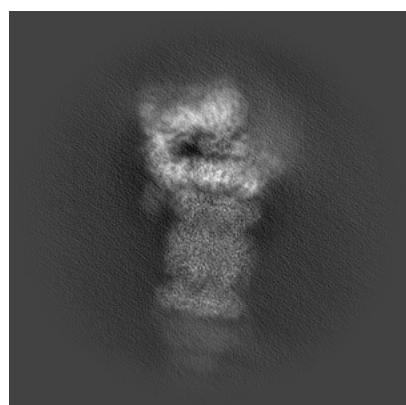
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-63817. These allow visual inspection of the internal detail of the map and identification of artifacts.

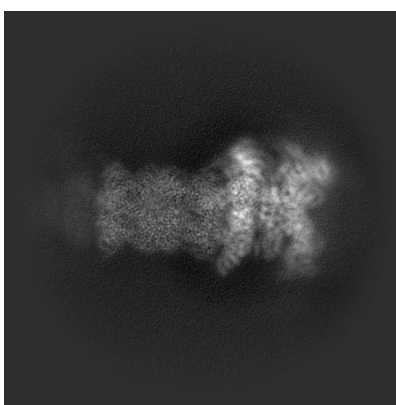
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

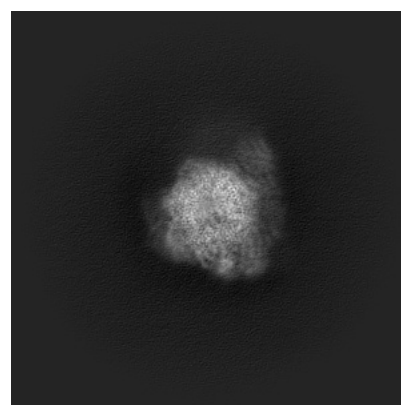
6.1.1 Primary map



X



Y



Z

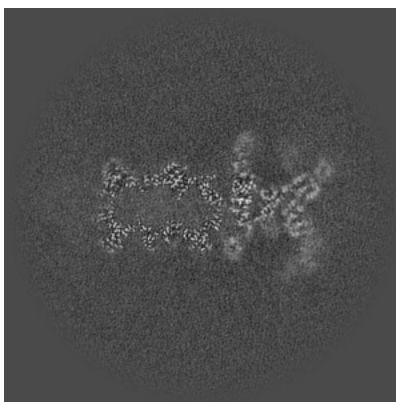
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

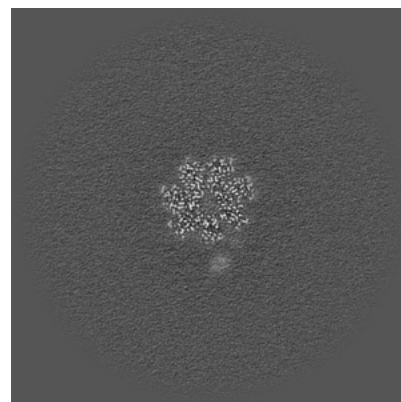
6.2.1 Primary map



X Index: 300



Y Index: 300

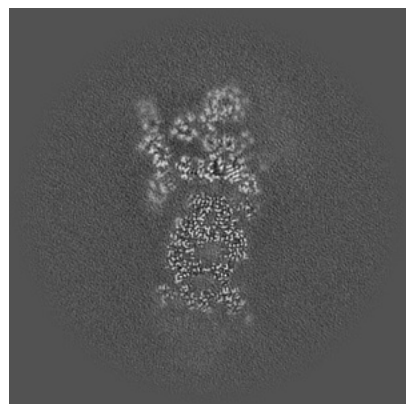


Z Index: 300

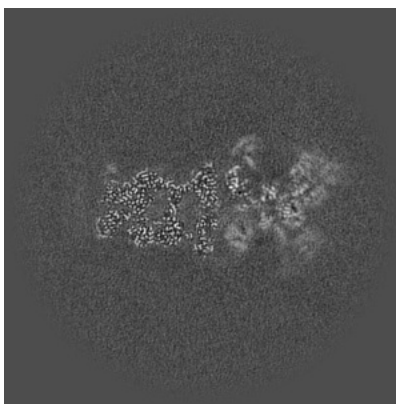
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

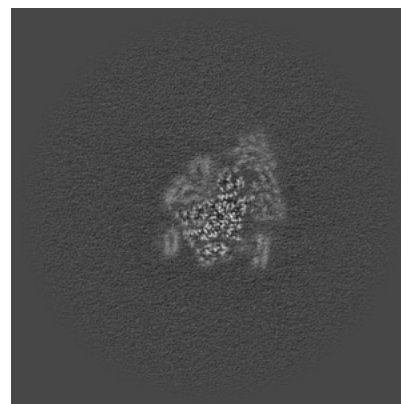
6.3.1 Primary map



X Index: 326



Y Index: 324

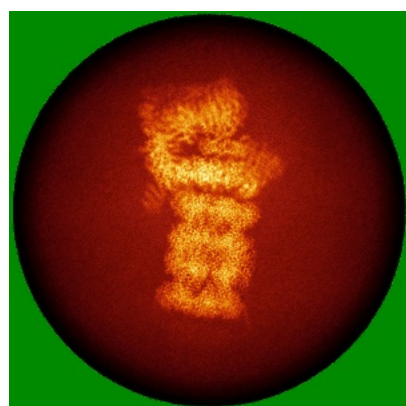


Z Index: 356

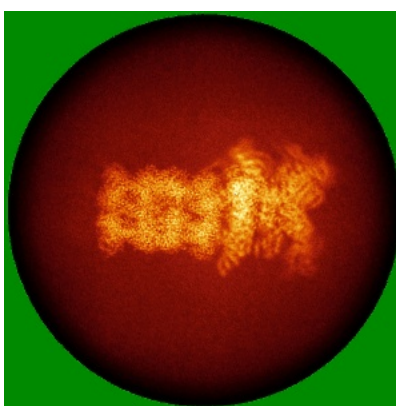
The images above show the largest variance slices of the map in three orthogonal directions.

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

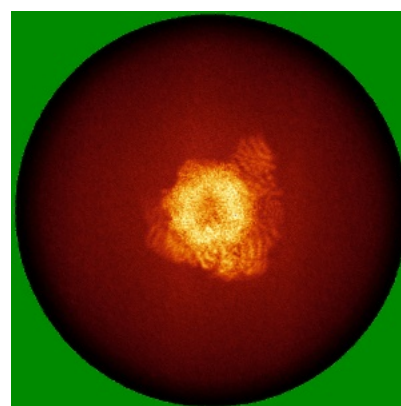
6.4.1 Primary map



X



Y

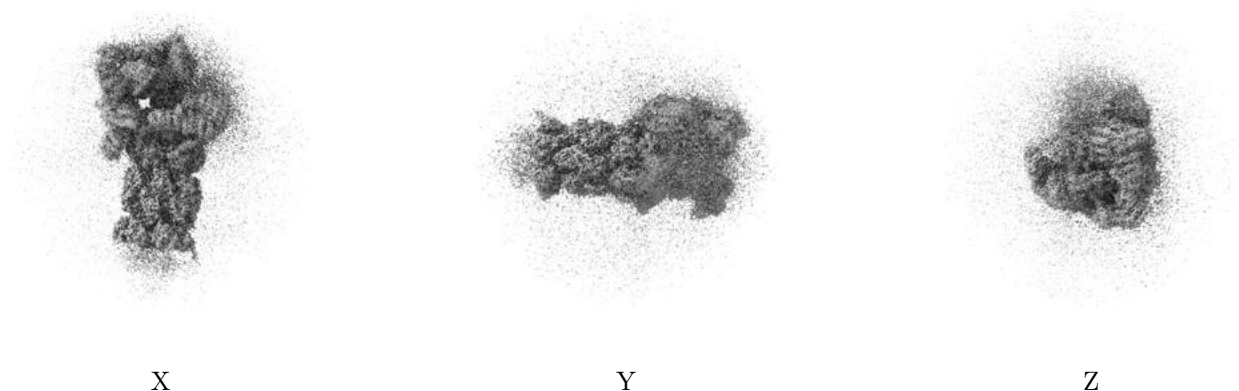


Z

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 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

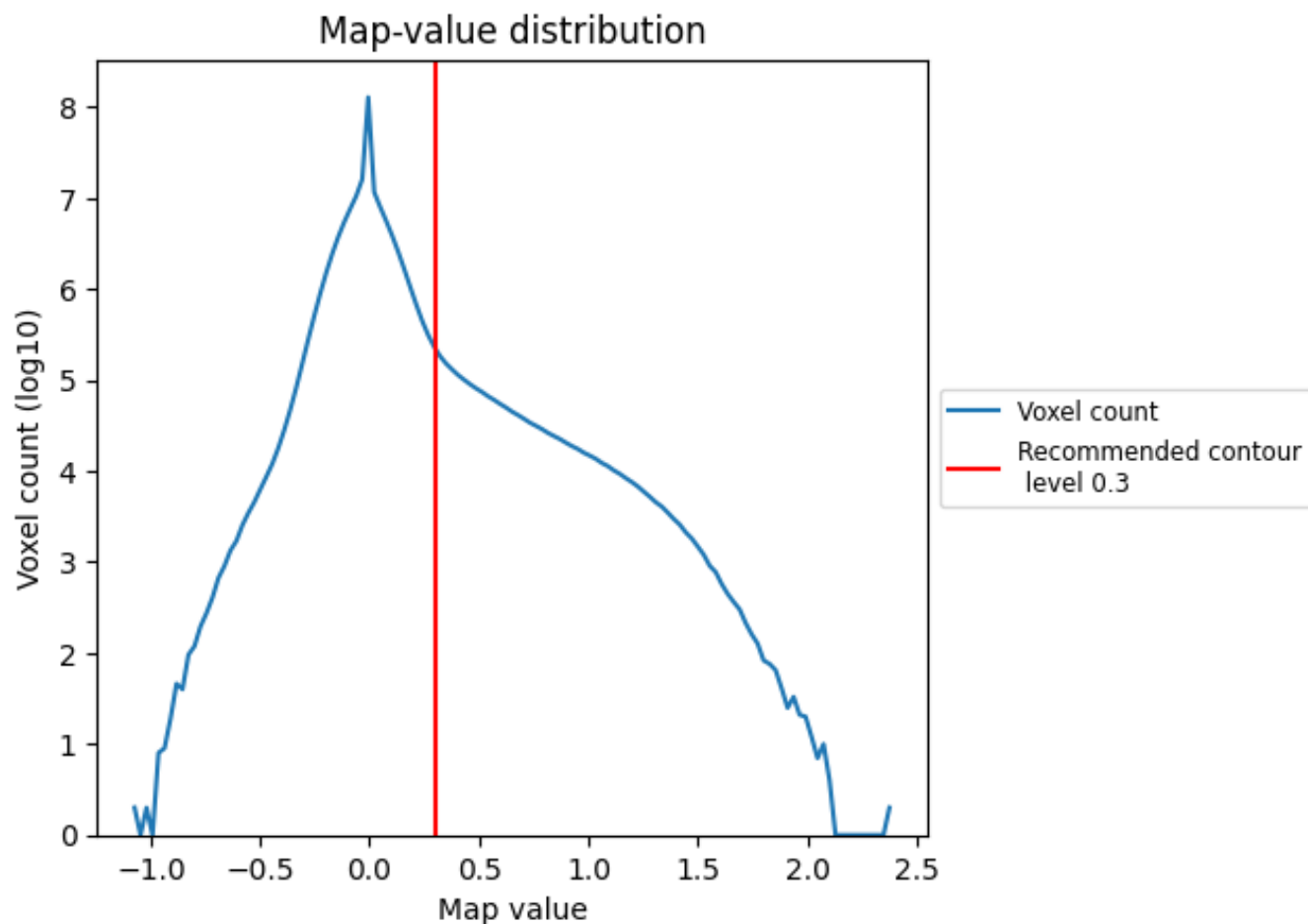
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

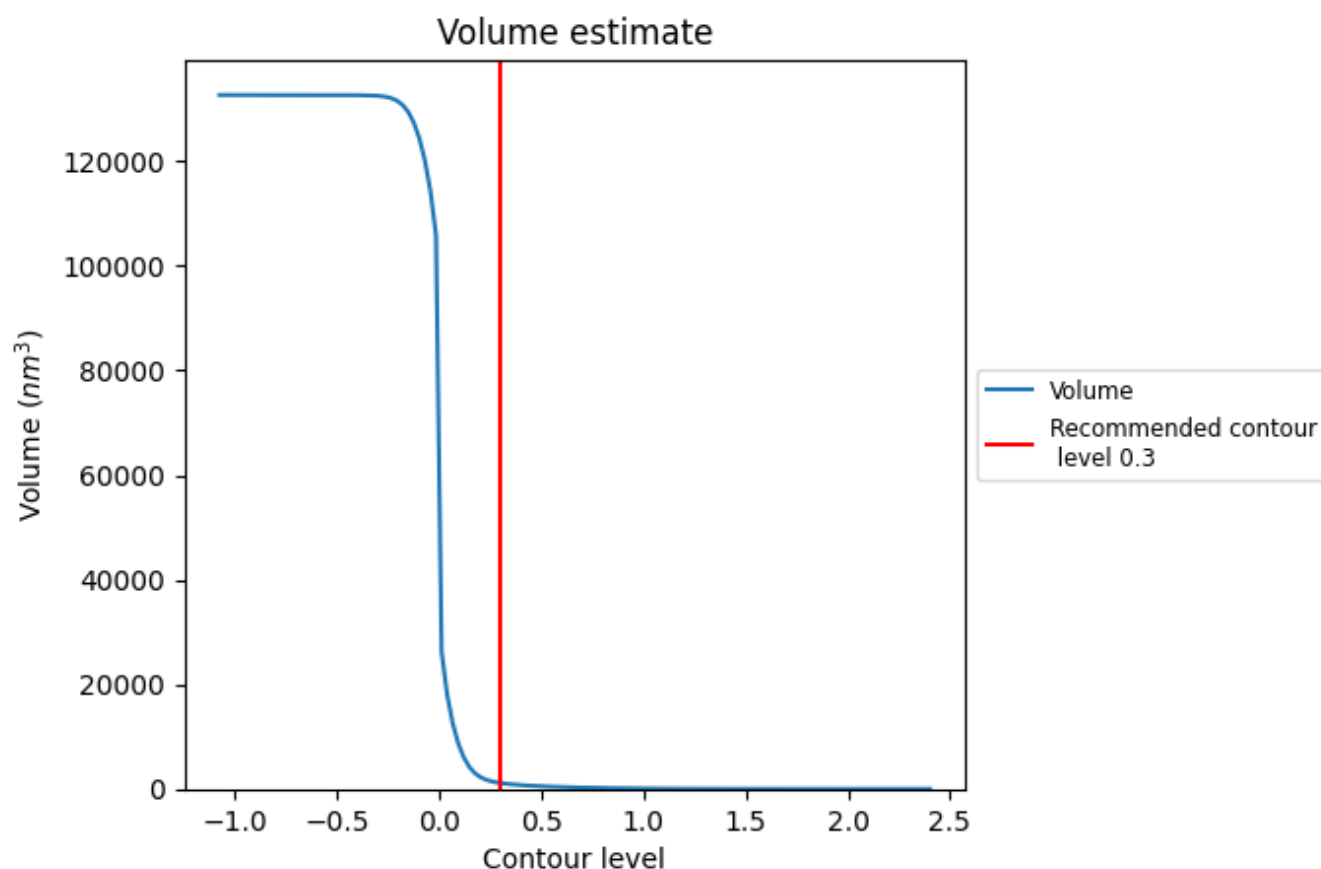
This section contains the results of statistical analysis of the map.

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.

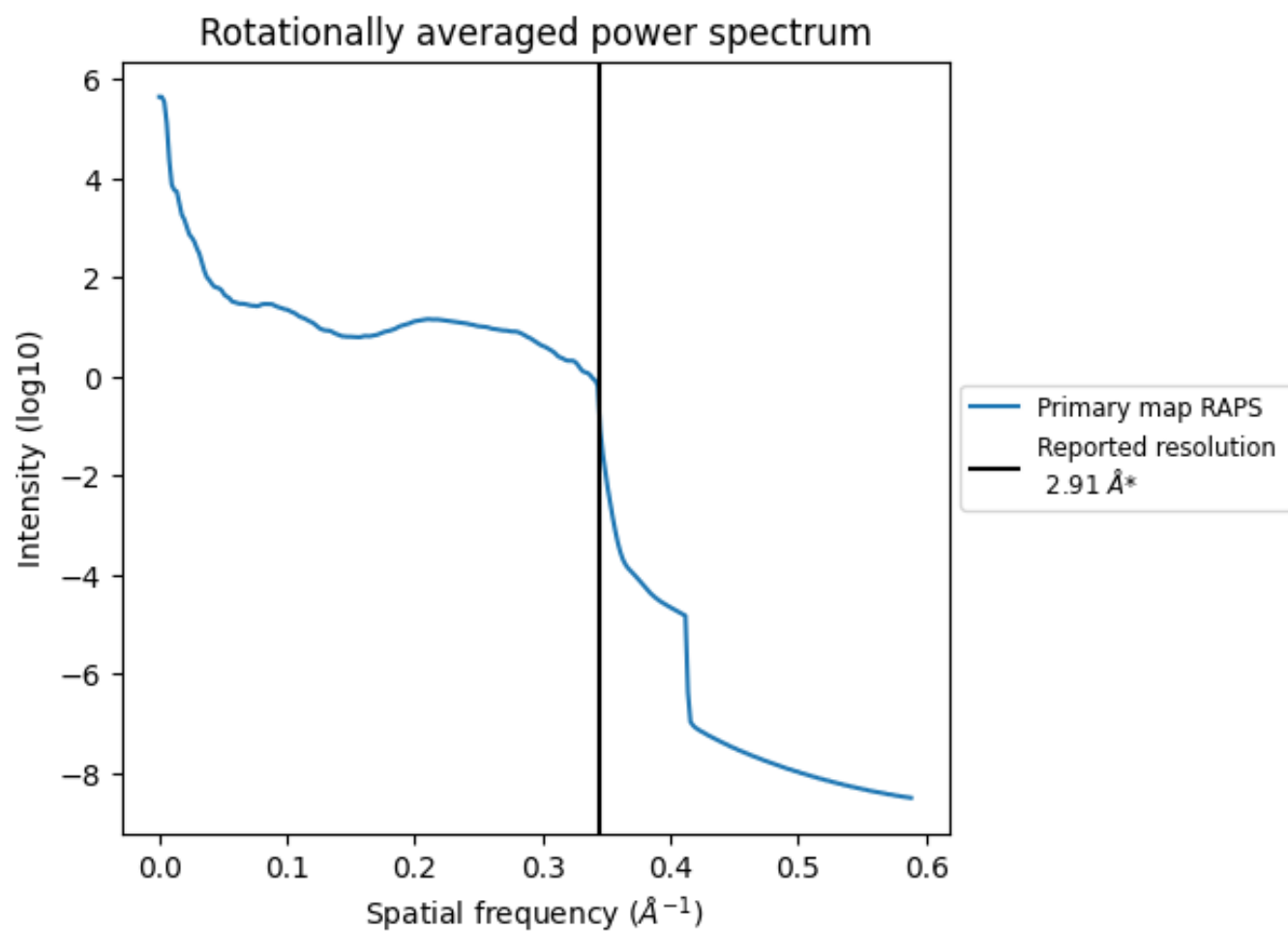
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1137 nm^3 ; this corresponds to an approximate mass of 1027 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 0.344 Å⁻¹

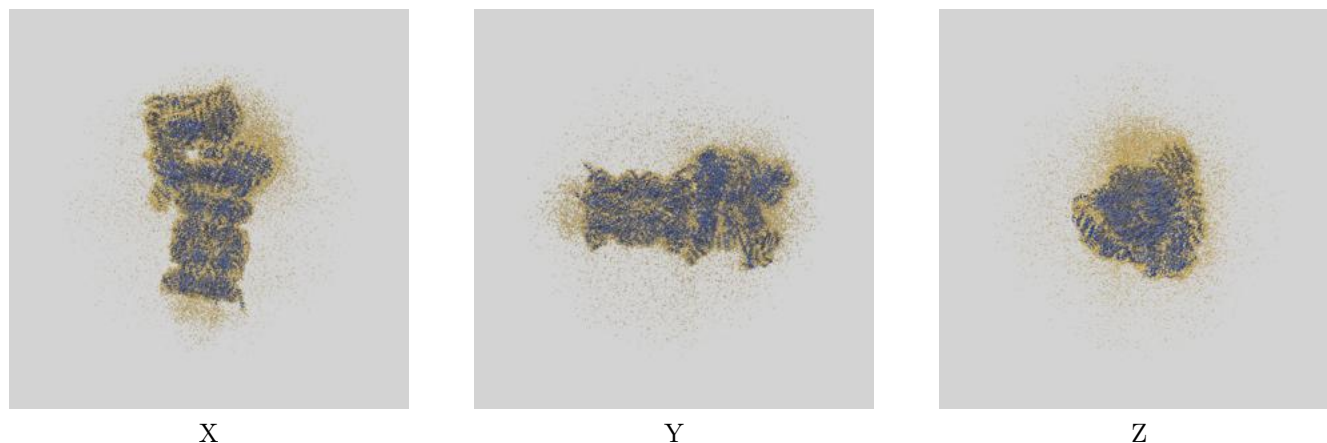
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

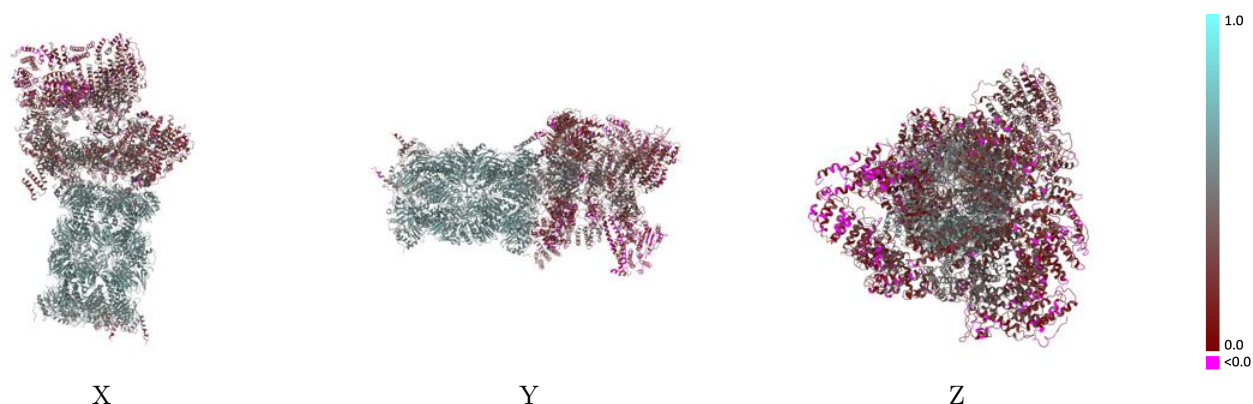
This section contains information regarding the fit between EMDB map EMD-63817 and PDB model 9U3L. Per-residue inclusion information can be found in section [3](#) on page [13](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

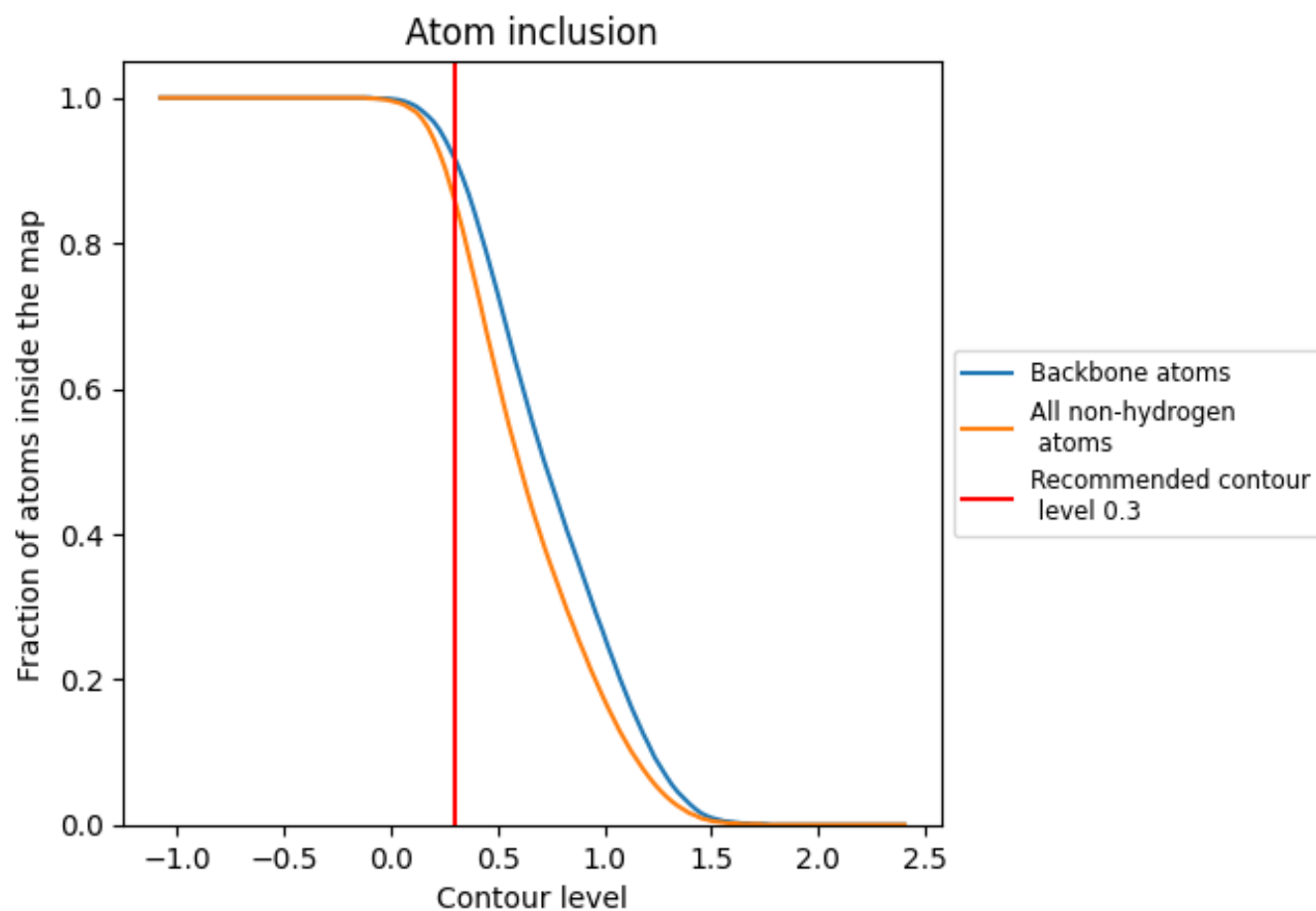


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 86% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8600	 0.4110
A	 0.8260	 0.2470
B	 0.8430	 0.3650
C	 0.9010	 0.4170
D	 0.9170	 0.4150
E	 0.8190	 0.2480
F	 0.7640	 0.1870
G	 0.9320	 0.5600
H	 0.9350	 0.5660
I	 0.9080	 0.5420
J	 0.8940	 0.5270
K	 0.9090	 0.5640
L	 0.9550	 0.5840
M	 0.9250	 0.5630
N	 0.9470	 0.5880
O	 0.9210	 0.5720
P	 0.9520	 0.5850
Q	 0.9480	 0.5810
R	 0.9470	 0.5850
S	 0.9410	 0.5870
T	 0.9560	 0.5900
U	 0.7880	 0.2500
V	 0.7140	 0.2030
W	 0.8640	 0.3020
X	 0.9180	 0.3930
Y	 0.9300	 0.3820
Z	 0.8560	 0.2600
a	 0.6650	 0.1430
b	 0.5800	 0.1500
c	 0.8900	 0.3620
d	 0.5940	 0.1730
e	 0.8730	 0.2710
g	 0.9020	 0.5460
h	 0.9050	 0.5540
i	 0.8220	 0.5090



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Chain	Atom inclusion	Q-score
j	 0.8150	 0.4720
k	 0.8350	 0.5150
l	 0.8740	 0.5450
m	 0.8910	 0.5490
n	 0.9540	 0.5890
o	 0.9390	 0.5750
p	 0.9460	 0.5870
q	 0.9340	 0.5850
r	 0.9410	 0.5800
s	 0.9330	 0.5860
t	 0.9470	 0.5860
u	 0.8040	 0.2810
v	 0.9870	 0.5280