



wwPDB EM Validation Summary Report ⓘ

Apr 28, 2025 – 05:00 PM EDT

PDB ID : 9NKG / pdb_00009nkg
EMDB ID : EMD-49508
Title : Structure of substrate engaged MIDN-bound human 26S proteasome, EB-MIDN (Composite map)
Authors : Peddada, N.; Beutler, B.
Deposited on : 2025-02-28
Resolution : 2.80 Å(reported)
Based on initial model : 6mse

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.dev118
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

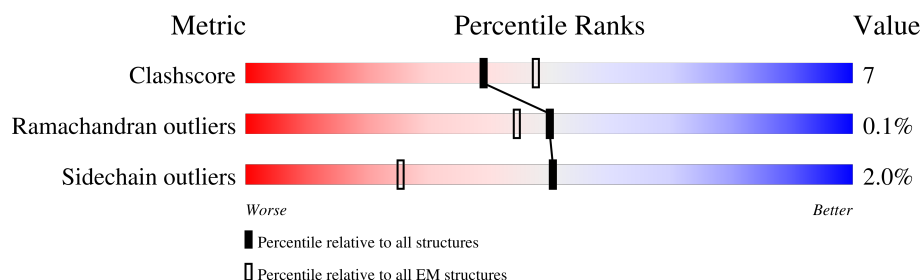
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 Å.

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




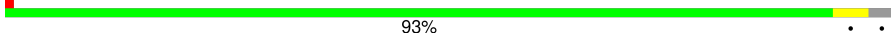




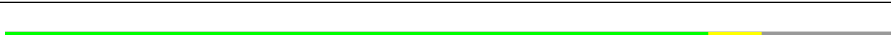
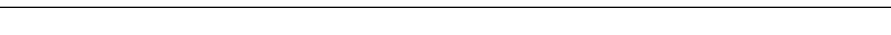
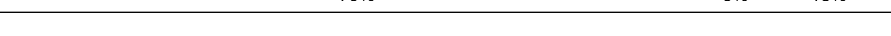
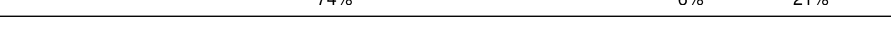
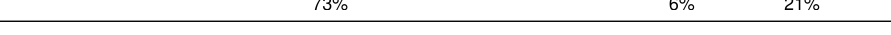
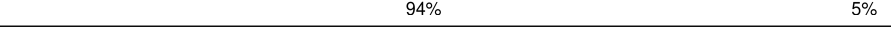
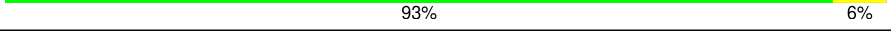

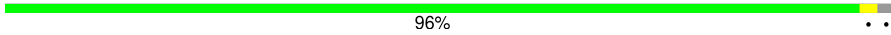










Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	G	246	
1	g	246	
2	H	234	
2	h	234	
3	I	261	
3	i	261	
4	J	248	
4	j	248	

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Mol	Chain	Length	Quality of chain
5	K	241	
5	k	241	
6	L	263	
6	l	263	
7	M	255	
7	m	255	
8	N	239	
8	n	239	
9	O	277	
9	o	277	
10	P	205	
10	p	205	
11	Q	201	
11	q	201	
12	R	263	
12	r	263	
13	S	241	
13	s	241	
14	T	264	
14	t	264	
15	A	433	
16	B	440	
17	C	406	
18	D	418	
19	E	403	

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Mol	Chain	Length	Quality of chain
20	F	439	
21	V	534	
22	W	456	
23	X	422	
24	Y	389	
25	Z	324	
26	a	376	
27	b	377	
28	d	350	
29	e	70	
30	v	12	
31	U	953	
32	c	310	
33	f	908	
34	z	468	

2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 201518 atoms, of which 98452 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 Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	G	240	Total	C	H	N	O	S	0	0
			3394	1106	1656	304	316	12		
1	g	240	Total	C	H	N	O	S	0	0
			3445	1124	1687	306	316	12		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
2	H	229	Total	C	H	N	O	S	0	0
			3252	1080	1590	288	288	6		
2	h	229	Total	C	H	N	O	S	0	0
			3252	1080	1590	288	288	6		

- Molecule 3 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	I	247	Total	C	H	N	O	S	0	0
			3543	1150	1741	322	320	10		
3	i	247	Total	C	H	N	O	S	0	0
			3503	1143	1717	320	313	10		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
4	J	232	Total	C	H	N	O	S	0	0
			3151	1038	1518	306	284	5		
4	j	232	Total	C	H	N	O	S	0	0
			3151	1038	1518	306	284	5		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
5	K	233	Total	C	H	N	O	S	0	0
			3264	1062	1597	287	307	11		
5	k	233	Total	C	H	N	O	S	0	0
			3249	1056	1589	287	306	11		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	9	TYR	ASP	conflict	UNP P28066
k	9	TYR	ASP	conflict	UNP P28066

- Molecule 6 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	L	233	Total	C	H	N	O	S	0	0
			3359	1090	1649	318	293	9		
6	l	233	Total	C	H	N	O	S	0	0
			3352	1089	1645	315	293	10		

- Molecule 7 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	M	239	Total	C	H	N	O	S	0	0
			3440	1131	1680	308	311	10		
7	m	239	Total	C	H	N	O	S	0	0
			3444	1131	1683	308	312	10		

- Molecule 8 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	N	202	Total	C	H	N	O	S	0	0
			2891	928	1422	257	272	12		
8	n	202	Total	C	H	N	O	S	0	0
			2881	926	1416	256	271	12		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
9	O	220	Total	C	H	N	O	S	0	0
			3139	1005	1559	272	294	9		
9	o	220	Total	C	H	N	O	S	0	0
			3131	1003	1555	272	292	9		

- Molecule 10 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	P	204	Total	C	H	N	O	S	0	0
			3096	992	1550	262	273	19		
10	p	204	Total	C	H	N	O	S	0	0
			3081	989	1543	263	268	18		

- Molecule 11 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	Q	196	Total	C	H	N	O	S	0	0
			2986	974	1477	259	268	8		
11	q	196	Total	C	H	N	O	S	0	0
			2981	973	1475	259	266	8		

- Molecule 12 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	R	200	Total	C	H	N	O	S	0	0
			2953	957	1449	271	267	9		
12	r	200	Total	C	H	N	O	S	0	0
			2938	954	1438	270	267	9		

- Molecule 13 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	S	212	Total	C	H	N	O	S	0	0
			3163	1016	1579	279	279	10		
13	s	212	Total	C	H	N	O	S	0	0
			3168	1017	1581	279	281	10		

- Molecule 14 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	T	212	Total	C	H	N	O	S	0	0
			3102	1003	1526	280	282	11		
14	t	212	Total	C	H	N	O	S	0	0
			3079	998	1511	279	280	11		

- Molecule 15 is a protein called 26S proteasome regulatory subunit 7.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	A	390	Total	C	H	N	O	S	0	0
			6166	1928	3106	537	578	17		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
16	B	393	Total	C	H	N	O	S	0	0
			6129	1936	3053	524	601	15		

- Molecule 17 is a protein called 26S protease regulatory subunit 8.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	C	389	Total	C	H	N	O	S	0	0
			6264	1932	3193	550	571	18		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
18	D	380	Total	C	H	N	O	S	0	0
			6114	1923	3075	524	579	13		

- Molecule 19 is a protein called 26S proteasome regulatory subunit 10B.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	E	389	Total	C	H	N	O	S	0	0
			6248	1947	3150	552	582	17		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
20	F	415	Total	C	H	N	O	S	0	0
			6569	2038	3318	561	634	18		

- Molecule 21 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	V	442	Total	C	H	N	O	S	0	0
			7239	2290	3647	639	650	13		

- Molecule 22 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	440	Total	C	N	O	S	0	0
			3588	2272	612	681	23		

- Molecule 23 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace	
23	X	384	Total	C	H	N	O	S	0	0
			6174	1935	3134	513	580	12		

- Molecule 24 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace	
24	Y	380	Total	C	H	N	O	S	0	0
			6260	1995	3133	535	580	17		

- Molecule 25 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	Z	286	Total	C	H	N	O	S	0	0
			4593	1457	2312	392	427	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
26	a	373	Total	C	H	N	O	S	0	0
			6007	1911	3012	510	559	15		

- Molecule 27 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	b	191	Total	C	H	N	O	S	0	0
			2963	910	1505	261	279	8		

- Molecule 28 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	d	270	Total	C	H	N	O	S	0	0
			4366	1407	2189	357	404	9		

- Molecule 29 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	e	48	Total	C	H	N	O	0	0
			687	236	298	62	91		

- Molecule 30 is a protein called unknown density (substrate density).

Mol	Chain	Residues	Atoms				AltConf	Trace
30	v	12	Total	C	N	O	0	0
			60	36	12	12		

- Molecule 31 is a protein called 26S proteasome non-ATPase regulatory subunit 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	U	814	Total	C	H	N	O	S	0	0
			12714	4028	6370	1080	1192	44		

- Molecule 32 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	c	283	Total	C	H	N	O	S	0	0
			4473	1412	2241	385	418	17		

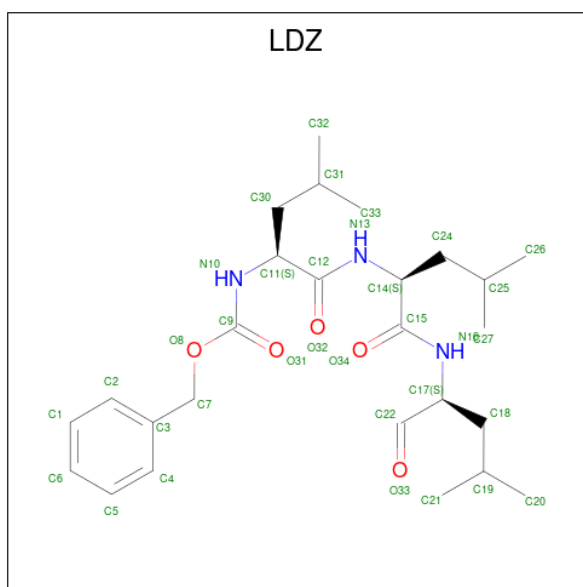
- Molecule 33 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	f	836	Total	C	H	N	O	S	0	0
			12946	4084	6486	1097	1234	45		

- Molecule 34 is a protein called Midnolin.

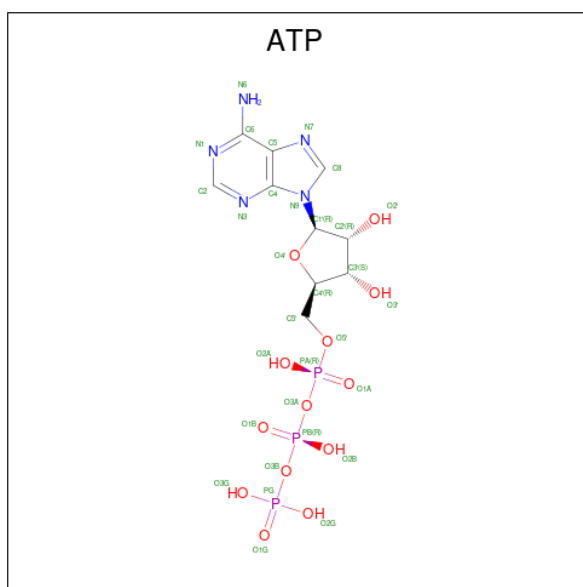
Mol	Chain	Residues	Atoms						AltConf	Trace
34	z	117	Total	C	H	N	O	S	0	0
			1904	566	983	185	167	3		

- Molecule 35 is N-[(benzyloxy)carbonyl]-L-leucyl-N-[(2S)-4-methyl-1-oxopentan-2-yl]-L-leucinamide (CCD ID: LDZ) (formula: C₂₆H₄₁N₃O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
35	N	1	Total	C	H	N	O	0
			75	26	41	3	5	
35	O	1	Total	C	H	N	O	0
			75	26	41	3	5	
35	R	1	Total	C	H	N	O	0
			75	26	41	3	5	
35	n	1	Total	C	H	N	O	0
			75	26	41	3	5	
35	o	1	Total	C	H	N	O	0
			75	26	41	3	5	
35	r	1	Total	C	H	N	O	0
			75	26	41	3	5	

- Molecule 36 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
36	A	1	Total	C	H	N	O	P
			43	10	12	5	13	3
36	B	1	Total	C	H	N	O	P
			43	10	12	5	13	3
36	D	1	Total	C	H	N	O	P
			43	10	12	5	13	3
36	F	1	Total	C	H	N	O	P
			43	10	12	5	13	3

- Molecule 37 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
37	A	1	Total	Mg	0
			1	1	
37	B	1	Total	Mg	0
			1	1	
37	D	1	Total	Mg	0
			1	1	
37	F	1	Total	Mg	0
			1	1	

- Molecule 38 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
38	E	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	


- Molecule 39 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

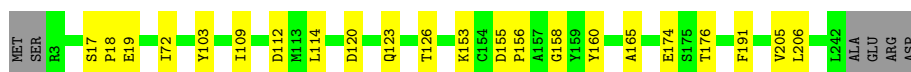
Mol	Chain	Residues	Atoms	AltConf
39	c	1	Total Zn 1 1	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Proteasome subunit alpha type-6

Chain G: 




- Molecule 1: Proteasome subunit alpha type-6

Chain g: 



- Molecule 2: Proteasome subunit alpha type-2

Chain H: 




- Molecule 2: Proteasome subunit alpha type-2

Chain h: 



- Molecule 3: Proteasome subunit alpha type-4

Chain I: 

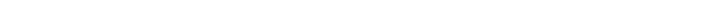


- Molecule 3: Proteasome subunit alpha type-4

[illegible]

- Chain J:  89% • 6%

[illegible]

- Chain j:  87% 6% 6%

MET
S2
S11
V42
V50
A51
V59
V69
D79
K115
T119
Q120
S121
R124
R125
P126
G140
L208
A209
R213
E233
LYU
LYS
LYS
GLU
GLU
GLU
ASN
GLU
LYS
LYS
LYS
GLN
LYS
LYS
ALA
ALA

- Chain K:  91% 5%

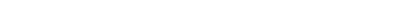
MET
PHE
LEU
THR
ARG
SER
GLU
TYR
Y9
E18
G19
E29
H99
N104
M107
I108
V109
E110
S111
M133
Q152
G171
S174
N225
E236
I241

- Chain k:  93%

Sequence logo for the 12th position. The y-axis represents information content in bits, ranging from 0 to 1. The x-axis shows amino acids: MET, PHE, LEU, THR, ARG, SER, GLU, TYR, Y9, E18, M73, I82, A85, S117, L121, D127, G131, V139, S180, I201, and I241. MET, PHE, LEU, THR, ARG, SER, GLU, and TYR are in a grey bar at the bottom. Y9, E18, M73, I82, A85, S117, L121, V139, S180, I201, and I241 are in yellow bars. D127 and G131 are in green bars and are the most frequent residues at this position, both reaching an information content of 1 bit. Red diamonds are placed above D127 and G131.


- Chain L: 83% 5% 11%

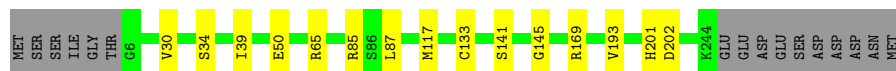
HIS
MET PHE ARG N4 Q16 H65 I72 S73 I74 A81 L84 K88 I112 L132 S150 A151 N152 Q166 T198 I223 L236 GLU GLU ARG PRO GLN GLN ARG LYS ALA GLN PRO PRO ALA ALA GLN PRO ASP GLY PRO ALA GLY LYS ALA ASP GLY PRO MET

- Chain 1:  83% 5% 11%


MET	PHE	ARG	N4	D9	T36	K62	I63	I74	A79	D80	A81	R82	L83	L84	M88	V130	G131	L132	M176	S211	L236	GLU	GLU	GLY	ARG	PRO	PRO	GLN	GLN	LYS	ALA	ALA	ALA	ALA	ALA	PRO	ALA	ASP	GLU	GLU	PRO	PRO	GLU	GLY	TRP
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- Molecule 7: Proteasome subunit alpha type-3

Chain M:  88% 6% 6%




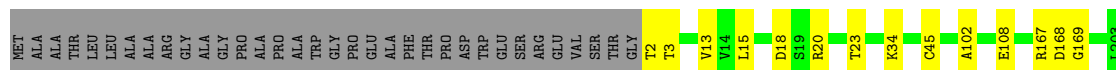
- Molecule 7: Proteasome subunit alpha type-3

Chain m:  89% 6% 5%




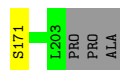
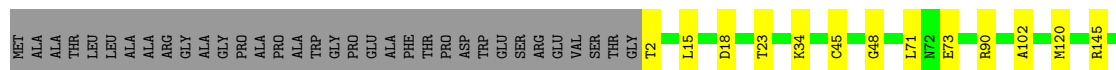
- Molecule 8: Proteasome subunit beta type-6

Chain N:  79% 6% 15%



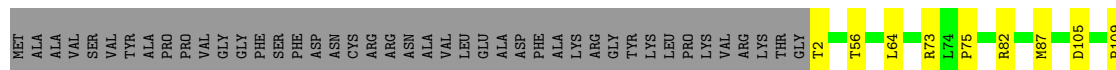
- Molecule 8: Proteasome subunit beta type-6

Chain n:  79% 6% 15%



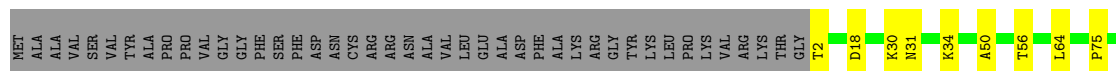
- Molecule 9: Proteasome subunit beta type-7

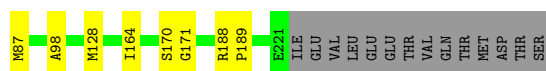
Chain O:  74% 6% 21%



- Molecule 9: Proteasome subunit beta type-7

Chain o:  73% 6% 21%





- Molecule 10: Proteasome subunit beta type-3

Chain P: 94% 5%



- Molecule 10: Proteasome subunit beta type-3

Chain p: 93% 6%



- Molecule 11: Proteasome subunit beta type-2

Chain Q: 90% 8% .



- Molecule 11: Proteasome subunit beta type-2

Chain q: 96% . .



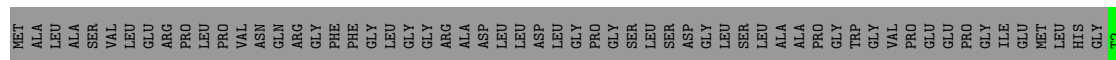
- Molecule 12: Proteasome subunit beta type-5

Chain R: 70% 6% 24%




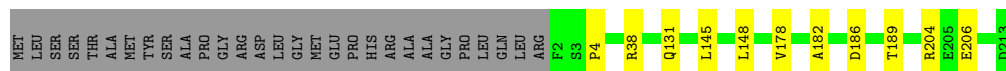
- Molecule 12: Proteasome subunit beta type-5

Chain r: 67% 9% 24%




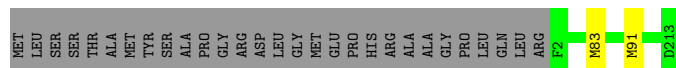
- Molecule 13: Proteasome subunit beta type-1

Chain S:  83% 5% 12%




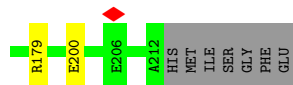
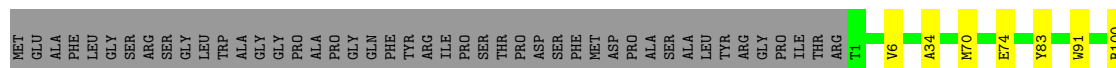
- Molecule 13: Proteasome subunit beta type-1

Chain s:  87% 12%



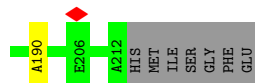
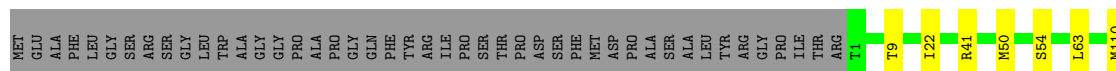
- Molecule 14: Proteasome subunit beta type-4

Chain T:  77% 20%




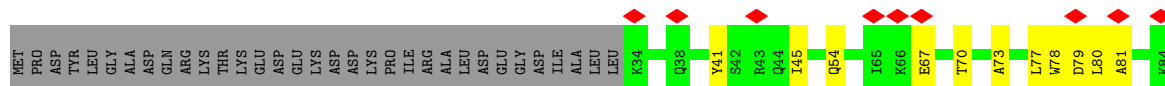
- Molecule 14: Proteasome subunit beta type-4

Chain t:  77% 20%



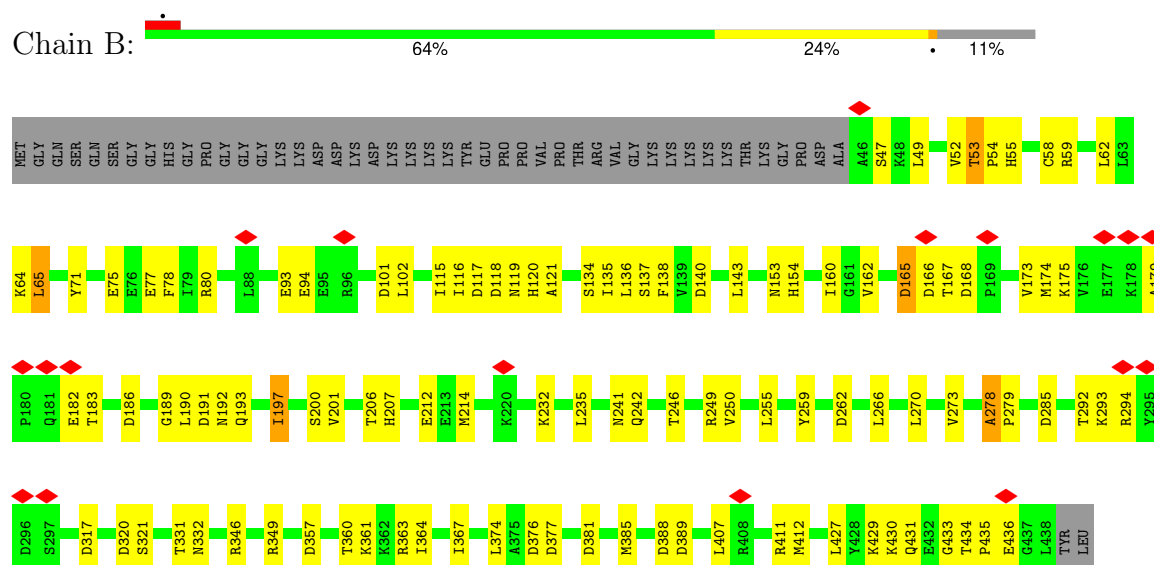
- Molecule 15: 26S proteasome regulatory subunit 7

Chain A:  76% 14% 10%



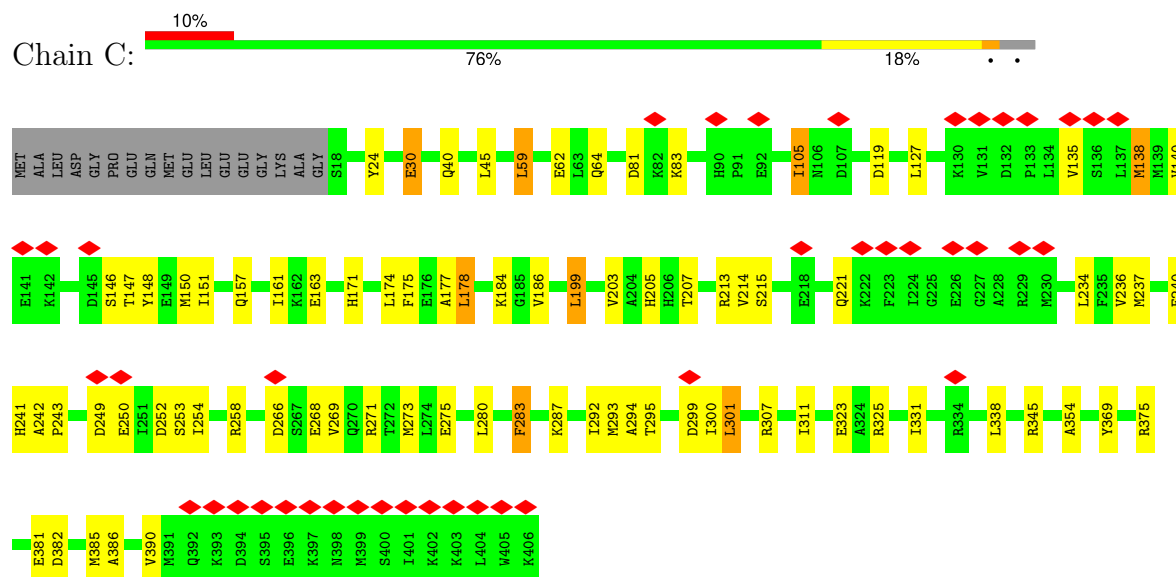
- Molecule 16: 26S proteasome regulatory subunit 4

Chain B:



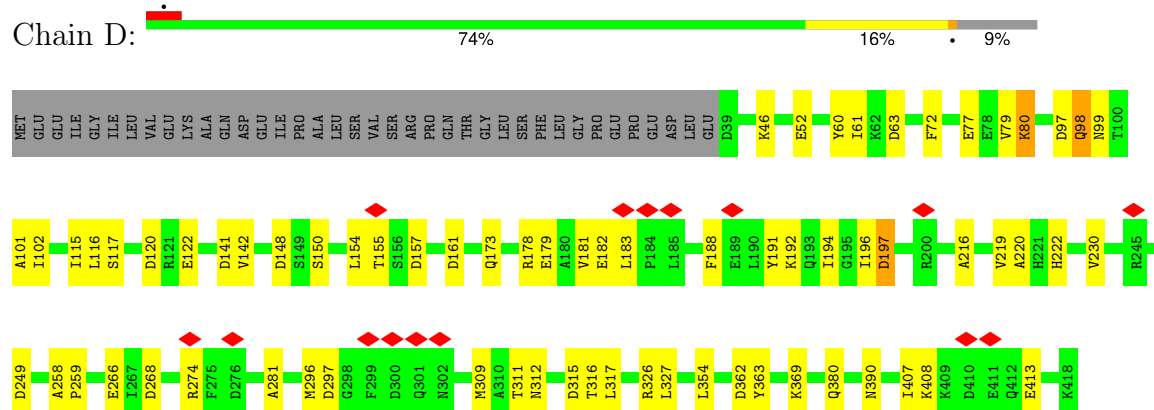
- Molecule 17: 26S protease regulatory subunit 8

Chain C:

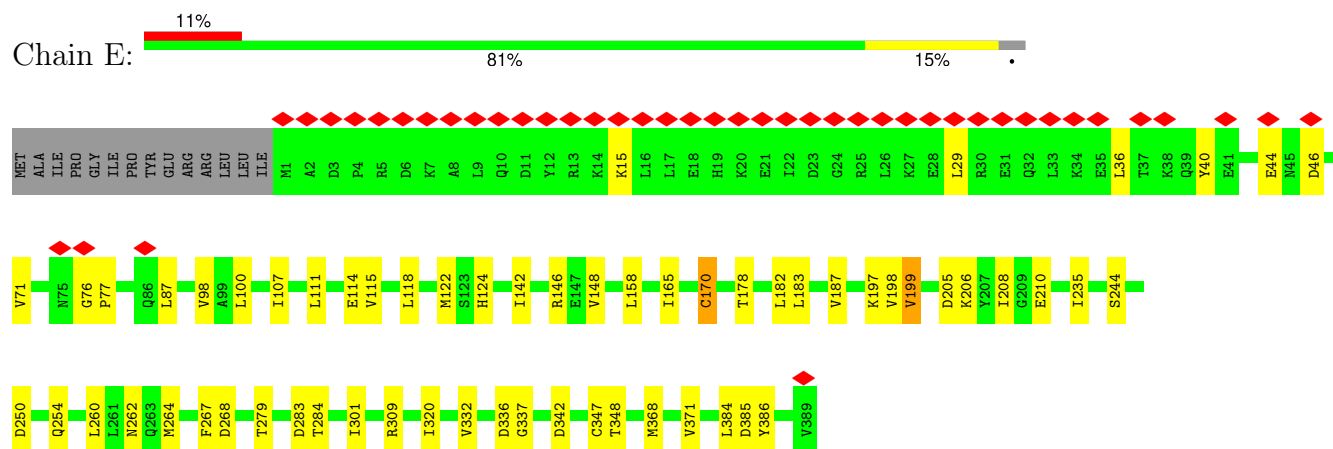


- Molecule 18: 26S proteasome regulatory subunit 6B

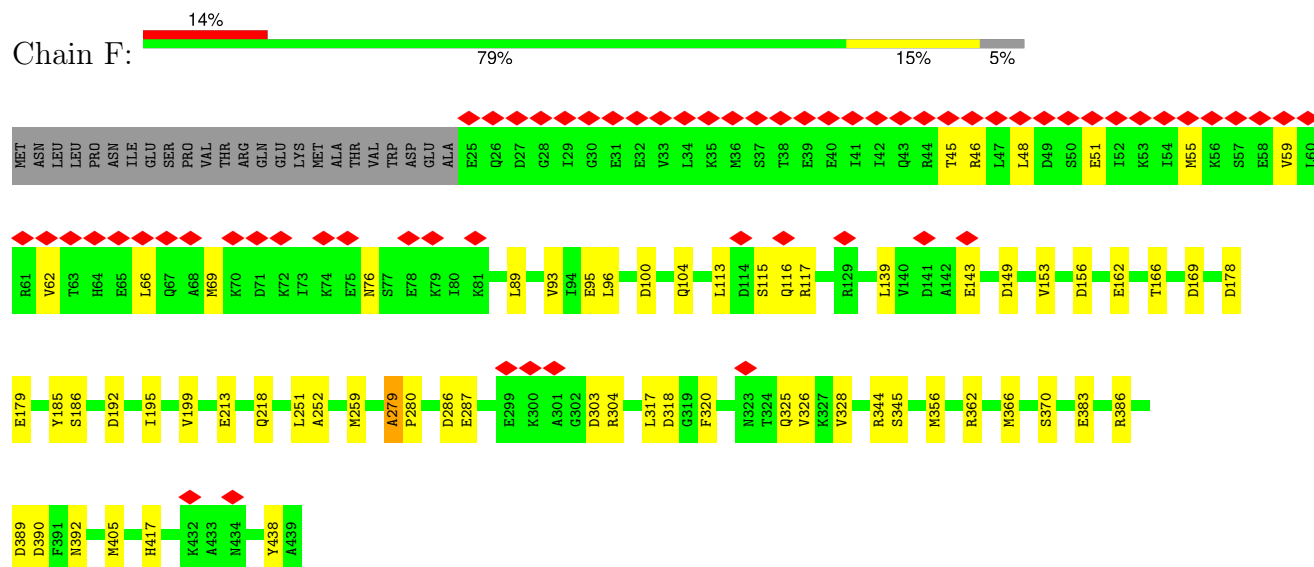
Chain D:



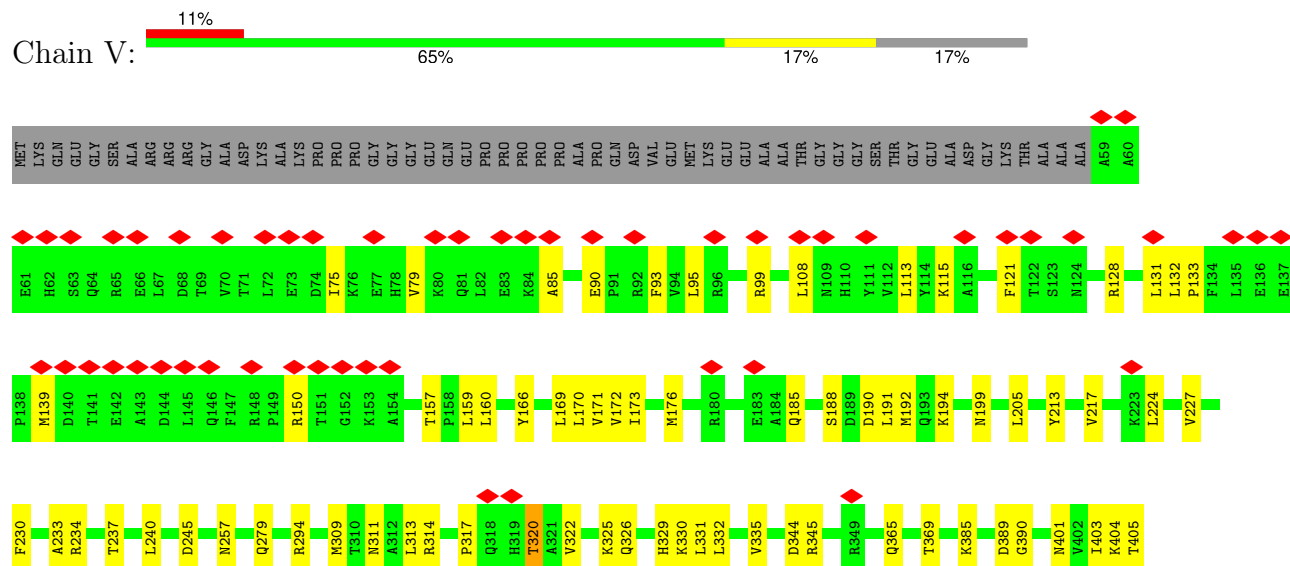
Chain E:

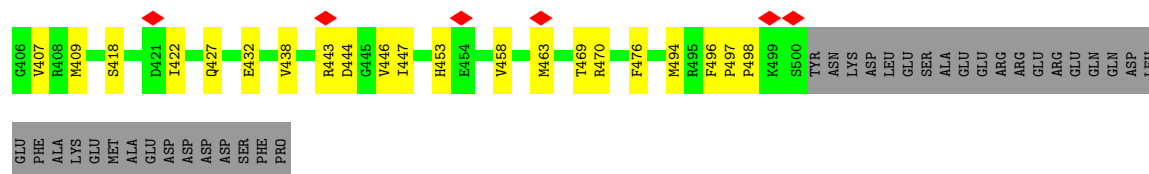


Chain F:

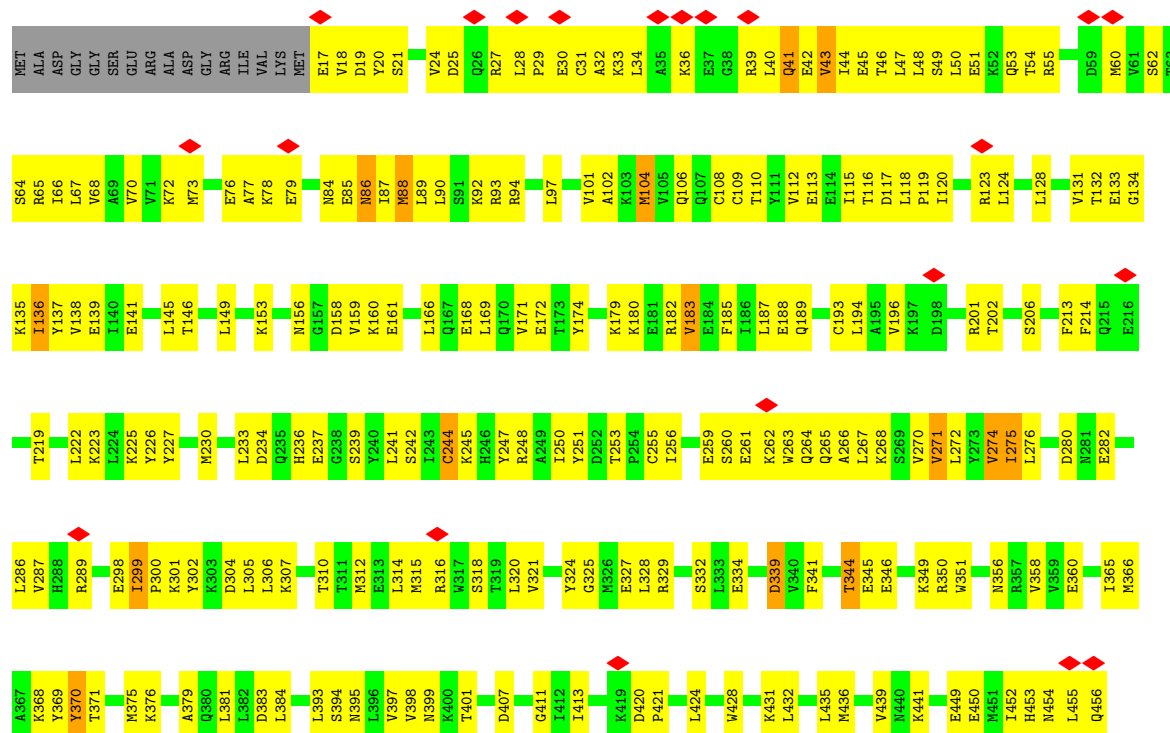


Chain V:

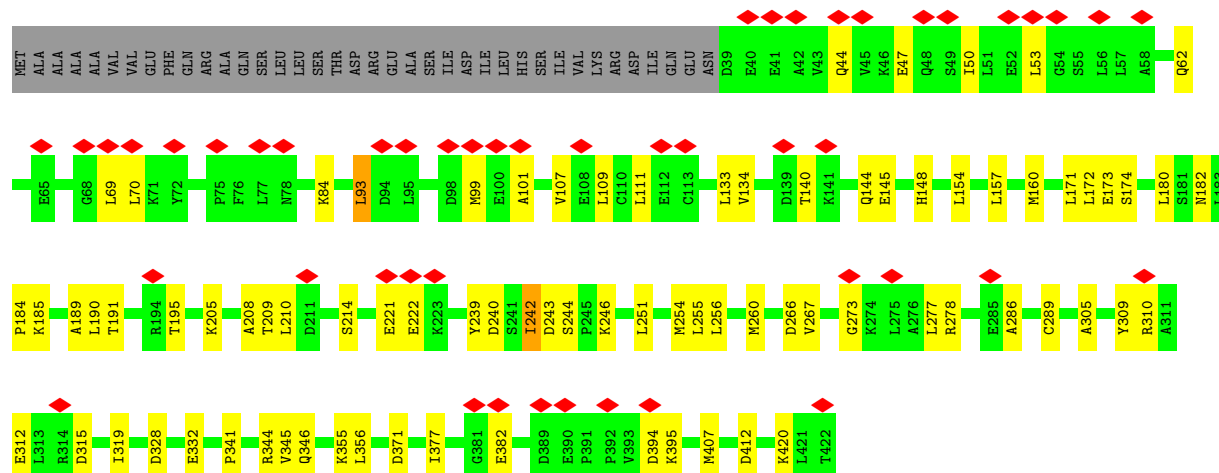




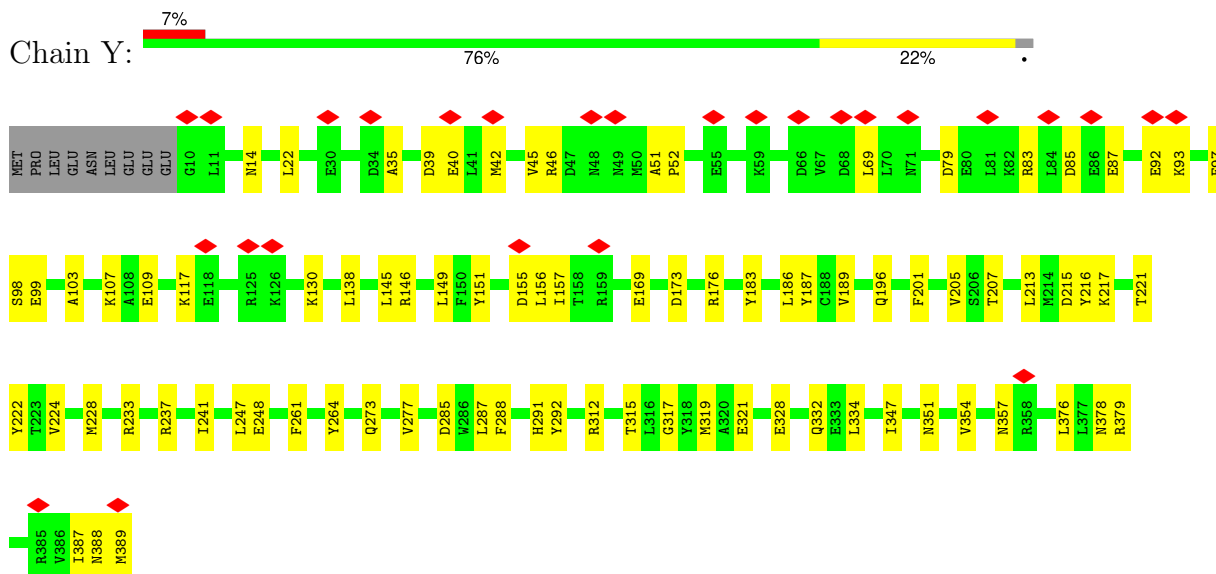
• Molecule 22: 26S proteasome non-ATPase regulatory subunit 12



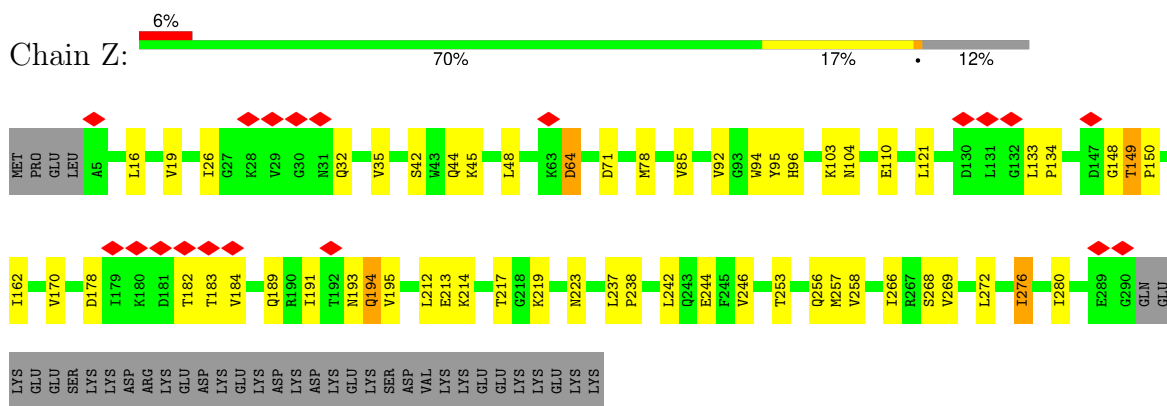
• Molecule 23: 26S proteasome non-ATPase regulatory subunit 11



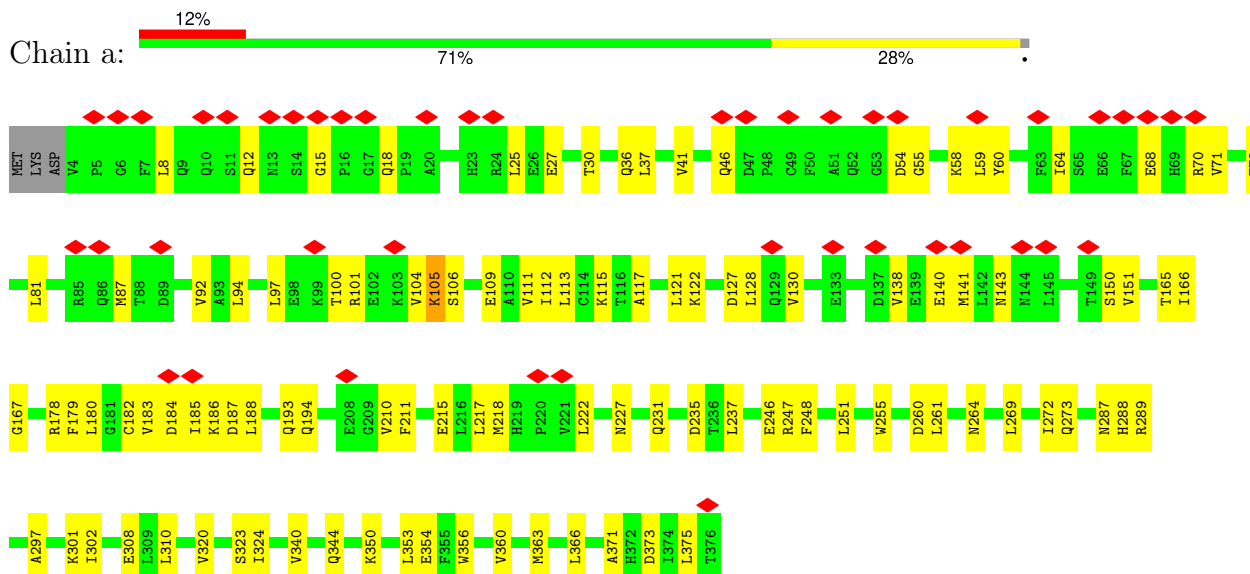
Chain Y:



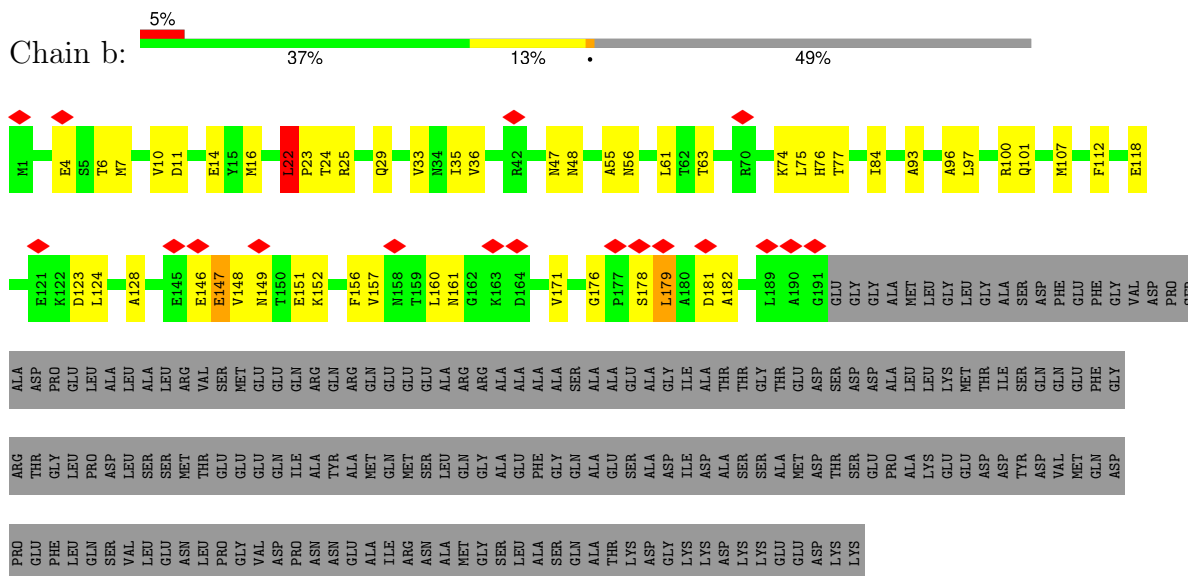
Chain Z:



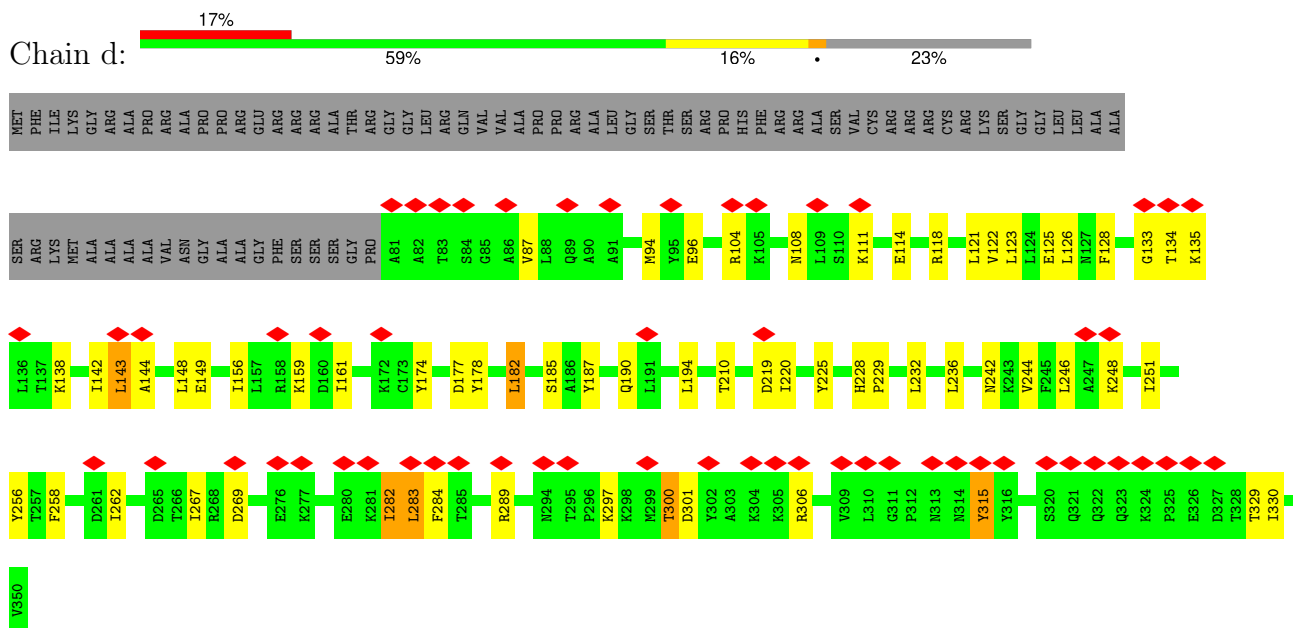
Chain a:



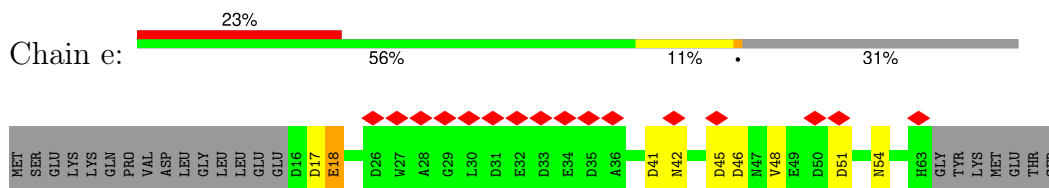
- Molecule 27: 26S proteasome non-ATPase regulatory subunit 4



- Molecule 28: 26S proteasome non-ATPase regulatory subunit 8



- Molecule 29: 26S proteasome complex subunit SEM1

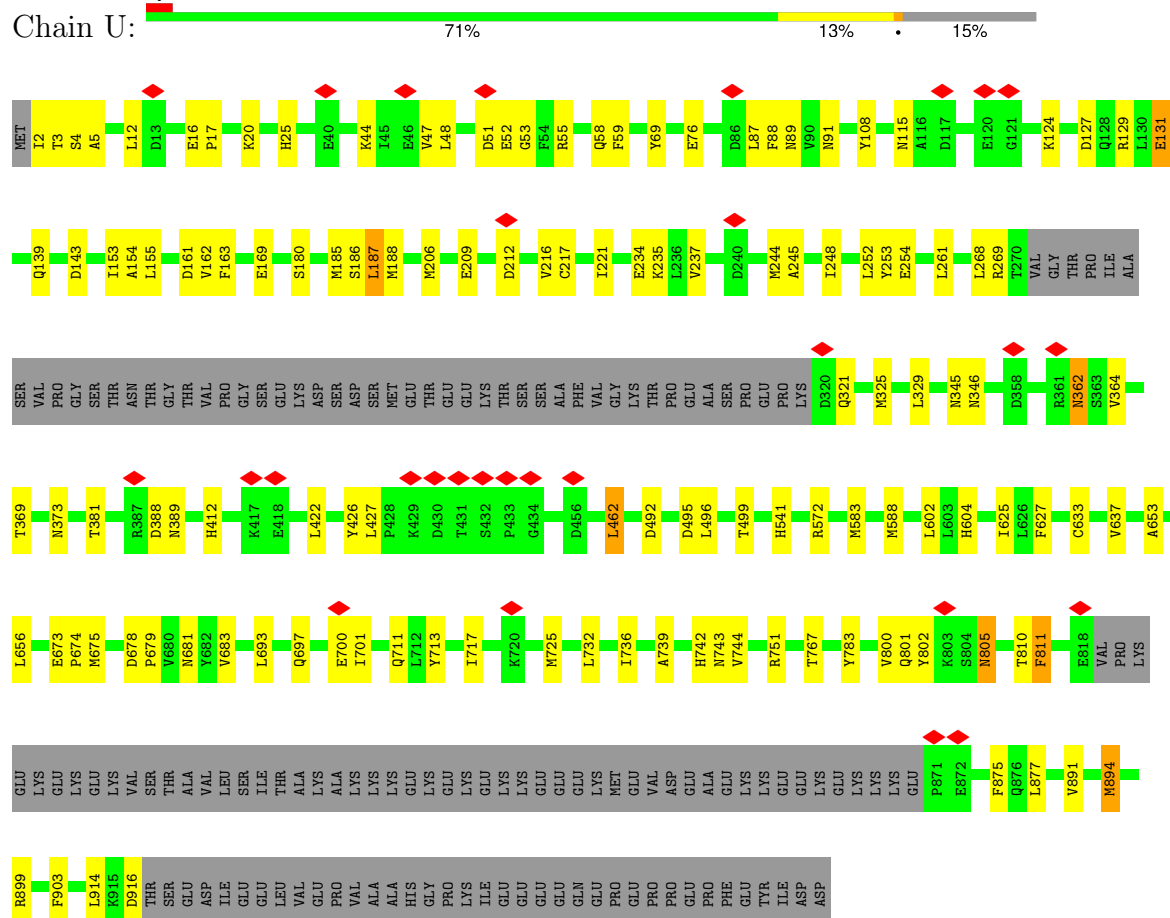


- Molecule 30: unknown density (substrate density)

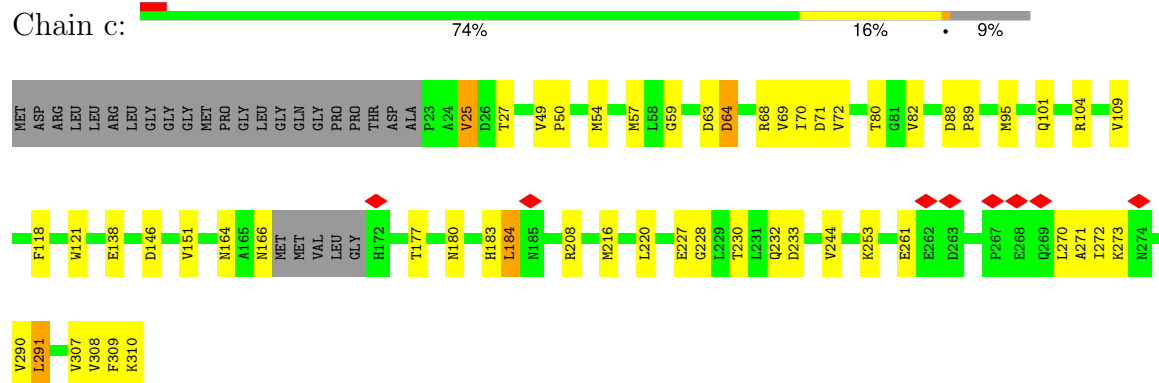


There are no outlier residues recorded for this chain.

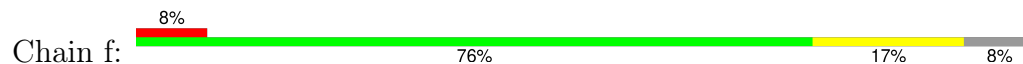
• Molecule 31: 26S proteasome non-ATPase regulatory subunit 1

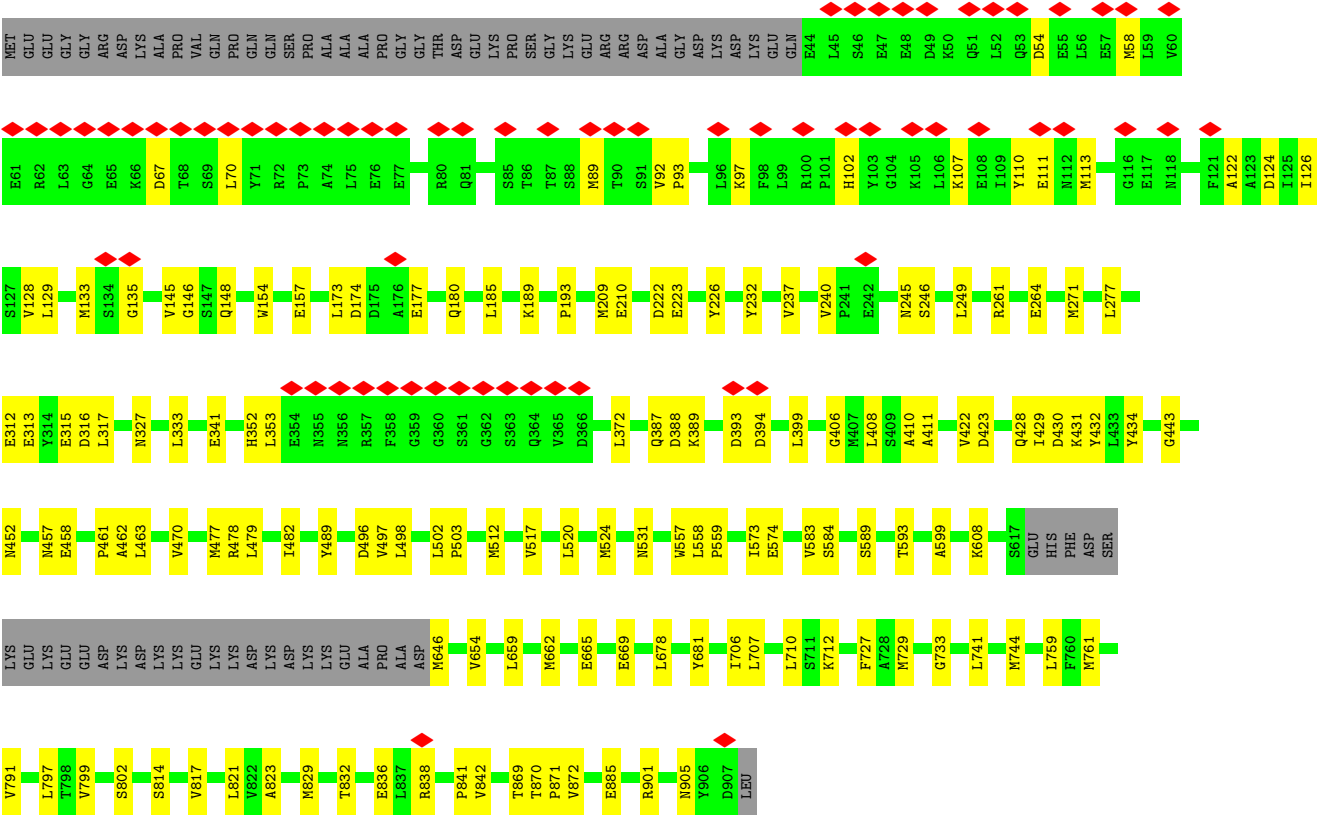


• Molecule 32: 26S proteasome non-ATPase regulatory subunit 14

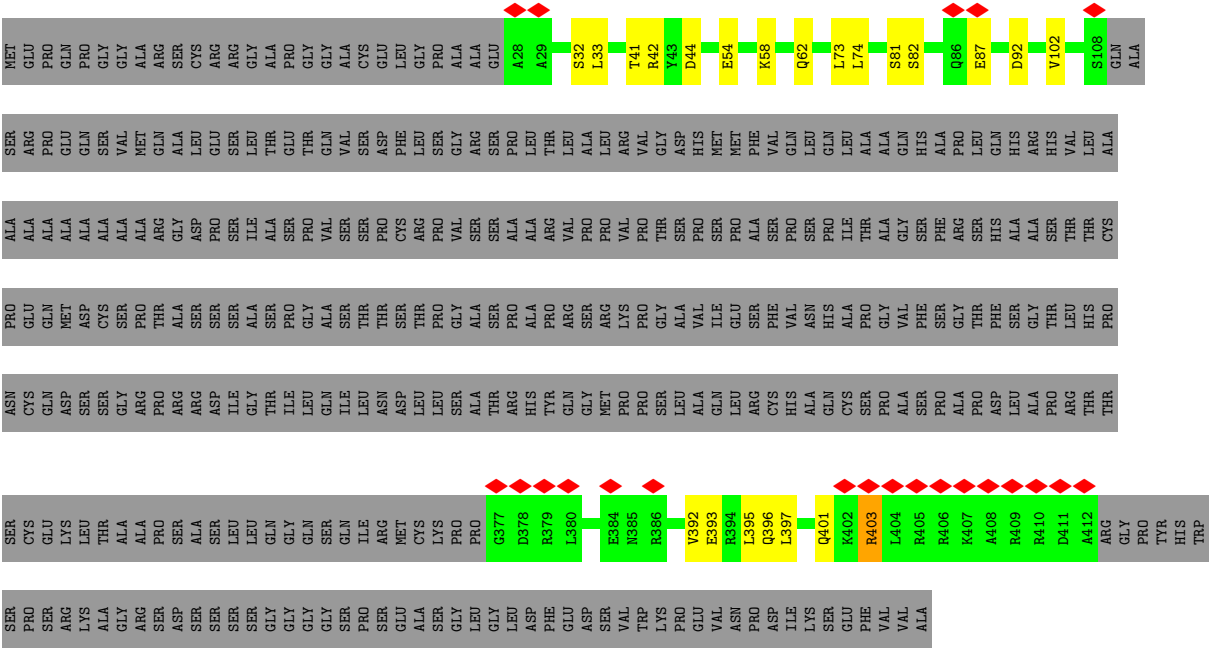


• Molecule 33: 26S proteasome non-ATPase regulatory subunit 2





● Molecule 34: Midnolin



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	232000	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.841	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.165	Depositor
Map size (Å)	687.36, 687.36, 687.36	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.074, 1.074, 1.074	Depositor

5 Model quality

5.1 Standard geometry

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

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	G	0.12	0/1767	0.27	0/2398
1	g	0.10	0/1790	0.22	0/2429
2	H	0.12	0/1701	0.29	0/2318
2	h	0.11	0/1701	0.25	0/2318
3	I	0.12	0/1831	0.29	0/2487
3	i	0.10	0/1815	0.23	0/2466
4	J	0.10	0/1657	0.25	0/2261
4	j	0.10	0/1657	0.25	0/2261
5	K	0.12	0/1694	0.28	0/2301
5	k	0.10	0/1686	0.22	0/2290
6	L	0.11	0/1744	0.26	0/2371
6	l	0.10	0/1741	0.27	0/2367
7	M	0.11	0/1795	0.26	0/2434
7	m	0.10	0/1796	0.22	0/2435
8	N	0.11	0/1495	0.23	0/2026
8	n	0.10	0/1491	0.21	0/2021
9	O	0.10	0/1607	0.24	0/2185
9	o	0.11	0/1603	0.23	0/2180
10	P	0.12	0/1575	0.26	0/2128
10	p	0.12	0/1567	0.25	0/2118
11	Q	0.10	0/1541	0.22	0/2092
11	q	0.11	0/1538	0.26	0/2088
12	R	0.10	0/1535	0.22	0/2080
12	r	0.11	0/1531	0.25	0/2076
13	S	0.10	0/1614	0.24	0/2178
13	s	0.10	0/1617	0.24	0/2182
14	T	0.12	0/1606	0.26	0/2179
14	t	0.11	0/1598	0.25	0/2170
15	A	0.15	0/3110	0.34	0/4196
16	B	0.15	0/3120	0.35	0/4210
17	C	0.15	0/3112	0.34	0/4182
18	D	0.15	0/3089	0.33	0/4168

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
19	E	0.14	0/3146	0.26	0/4233
20	F	0.13	0/3292	0.27	0/4435
21	V	0.14	0/3662	0.37	2/4946 (0.0%)
22	W	0.13	0/3636	0.25	0/4891
23	X	0.14	0/3084	0.34	0/4157
24	Y	0.14	0/3185	0.30	0/4290
25	Z	0.15	0/2324	0.31	0/3150
26	a	0.14	0/3053	0.33	0/4133
27	b	0.14	0/1478	0.33	0/2001
28	d	0.15	0/2223	0.34	0/3007
29	e	0.12	0/398	0.31	0/542
31	U	0.15	0/6458	0.30	0/8740
32	c	0.15	0/2274	0.31	0/3072
33	f	0.14	0/6569	0.32	0/8893
34	z	0.11	0/928	0.25	0/1241
All	All	0.13	0/104434	0.29	2/141326 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	V	494	MET	CA-C-N	10.40	137.66	122.99
21	V	494	MET	C-N-CA	10.40	137.66	122.99

There are no chirality outliers.

There are no planarity outliers.

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	G	1738	1656	1656	17	0
1	g	1758	1687	1687	4	0
2	H	1662	1590	1590	18	0
2	h	1662	1590	1590	12	0
3	I	1802	1741	1741	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	i	1786	1717	1717	5	0
4	J	1633	1518	1518	7	0
4	j	1633	1518	1518	10	0
5	K	1667	1597	1596	11	0
5	k	1660	1589	1589	6	0
6	L	1710	1649	1649	13	0
6	l	1707	1645	1645	9	0
7	M	1760	1680	1680	10	0
7	m	1761	1683	1683	7	0
8	N	1469	1422	1422	10	0
8	n	1465	1416	1416	10	0
9	O	1580	1559	1559	12	0
9	o	1576	1555	1555	12	0
10	P	1546	1550	1552	7	0
10	p	1538	1543	1545	9	0
11	Q	1509	1477	1477	9	0
11	q	1506	1475	1475	3	0
12	R	1504	1449	1449	12	0
12	r	1500	1438	1438	15	0
13	S	1584	1579	1579	7	0
13	s	1587	1581	1581	1	0
14	T	1576	1526	1528	6	0
14	t	1568	1511	1513	4	0
15	A	3060	3106	3106	61	0
16	B	3076	3053	3128	103	0
17	C	3071	3193	3193	69	0
18	D	3039	3075	3075	49	0
19	E	3098	3150	3174	45	0
20	F	3251	3318	3318	46	0
21	V	3592	3647	3647	66	0
22	W	3588	0	3704	254	0
23	X	3040	3134	3134	70	0
24	Y	3127	3133	3133	56	0
25	Z	2281	2312	2312	50	0
26	a	2995	3012	3012	84	0
27	b	1458	1505	1505	37	0
28	d	2177	2189	2189	55	0
29	e	389	298	298	10	0
30	v	60	0	15	0	0
31	U	6344	6370	6374	95	0
32	c	2232	2241	2242	42	0
33	f	6460	6486	6487	112	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	z	921	983	983	13	0
35	N	34	41	41	2	0
35	O	34	41	41	2	0
35	R	34	41	41	4	0
35	n	34	41	41	5	0
35	o	34	41	41	2	0
35	r	34	41	41	1	0
36	A	31	12	12	1	0
36	B	31	12	12	1	0
36	D	31	12	12	0	0
36	F	31	12	12	0	0
37	A	1	0	0	0	0
37	B	1	0	0	0	0
37	D	1	0	0	0	0
37	F	1	0	0	0	0
38	E	27	12	12	2	0
39	c	1	0	0	0	0
All	All	103066	98452	102283	1442	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 7.

The worst 5 of 1442 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)
22:W:47:LEU:HD22	22:W:70:VAL:HG22	1.41	0.98
22:W:67:LEU:HD12	22:W:104:MET:HE3	1.50	0.92
16:B:434:THR:HB	16:B:435:PRO:HD3	1.52	0.91
22:W:115:ILE:HD12	22:W:116:THR:H	1.35	0.91
22:W:264:GLN:HG2	22:W:299:ILE:HD11	1.53	0.90

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	238/246 (97%)	226 (95%)	12 (5%)	0	100	100
1	g	238/246 (97%)	232 (98%)	6 (2%)	0	100	100
2	H	227/234 (97%)	224 (99%)	3 (1%)	0	100	100
2	h	227/234 (97%)	223 (98%)	4 (2%)	0	100	100
3	I	245/261 (94%)	237 (97%)	8 (3%)	0	100	100
3	i	245/261 (94%)	240 (98%)	5 (2%)	0	100	100
4	J	230/248 (93%)	225 (98%)	5 (2%)	0	100	100
4	j	230/248 (93%)	222 (96%)	8 (4%)	0	100	100
5	K	231/241 (96%)	228 (99%)	3 (1%)	0	100	100
5	k	231/241 (96%)	228 (99%)	3 (1%)	0	100	100
6	L	231/263 (88%)	221 (96%)	10 (4%)	0	100	100
6	l	231/263 (88%)	229 (99%)	2 (1%)	0	100	100
7	M	237/255 (93%)	233 (98%)	4 (2%)	0	100	100
7	m	237/255 (93%)	234 (99%)	3 (1%)	0	100	100
8	N	200/239 (84%)	198 (99%)	2 (1%)	0	100	100
8	n	200/239 (84%)	195 (98%)	5 (2%)	0	100	100
9	O	218/277 (79%)	213 (98%)	5 (2%)	0	100	100
9	o	218/277 (79%)	213 (98%)	5 (2%)	0	100	100
10	P	202/205 (98%)	197 (98%)	5 (2%)	0	100	100
10	p	202/205 (98%)	197 (98%)	5 (2%)	0	100	100
11	Q	194/201 (96%)	187 (96%)	7 (4%)	0	100	100
11	q	194/201 (96%)	188 (97%)	6 (3%)	0	100	100
12	R	198/263 (75%)	198 (100%)	0	0	100	100
12	r	198/263 (75%)	196 (99%)	2 (1%)	0	100	100
13	S	210/241 (87%)	207 (99%)	3 (1%)	0	100	100
13	s	210/241 (87%)	209 (100%)	1 (0%)	0	100	100
14	T	210/264 (80%)	198 (94%)	12 (6%)	0	100	100
14	t	210/264 (80%)	201 (96%)	9 (4%)	0	100	100
15	A	388/433 (90%)	366 (94%)	22 (6%)	0	100	100
16	B	391/440 (89%)	361 (92%)	27 (7%)	3 (1%)	16	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	C	387/406 (95%)	357 (92%)	30 (8%)	0	100	100
18	D	378/418 (90%)	350 (93%)	27 (7%)	1 (0%)	37	67
19	E	387/403 (96%)	368 (95%)	19 (5%)	0	100	100
20	F	413/439 (94%)	398 (96%)	14 (3%)	1 (0%)	44	73
21	V	440/534 (82%)	420 (96%)	20 (4%)	0	100	100
22	W	438/456 (96%)	420 (96%)	17 (4%)	1 (0%)	44	73
23	X	382/422 (90%)	366 (96%)	16 (4%)	0	100	100
24	Y	378/389 (97%)	364 (96%)	13 (3%)	1 (0%)	37	67
25	Z	284/324 (88%)	268 (94%)	14 (5%)	2 (1%)	19	48
26	a	371/376 (99%)	330 (89%)	40 (11%)	1 (0%)	37	67
27	b	189/377 (50%)	160 (85%)	28 (15%)	1 (0%)	25	56
28	d	268/350 (77%)	238 (89%)	28 (10%)	2 (1%)	19	48
29	e	46/70 (66%)	36 (78%)	10 (22%)	0	100	100
31	U	808/953 (85%)	762 (94%)	44 (5%)	2 (0%)	44	73
32	c	279/310 (90%)	262 (94%)	16 (6%)	1 (0%)	30	61
33	f	832/908 (92%)	786 (94%)	46 (6%)	0	100	100
34	z	113/468 (24%)	111 (98%)	2 (2%)	0	100	100
All	All	13314/15352 (87%)	12722 (96%)	576 (4%)	16 (0%)	50	77

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
22	W	370	TYR
25	Z	149	THR
26	a	105	LYS
16	B	65	LEU
16	B	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	G	164/210 (78%)	163 (99%)	1 (1%)	84	95
1	g	168/210 (80%)	167 (99%)	1 (1%)	84	95
2	H	150/191 (78%)	148 (99%)	2 (1%)	65	88
2	h	150/191 (78%)	149 (99%)	1 (1%)	81	94
3	I	166/221 (75%)	165 (99%)	1 (1%)	84	95
3	i	160/221 (72%)	159 (99%)	1 (1%)	84	95
4	J	136/211 (64%)	136 (100%)	0	100	100
4	j	136/211 (64%)	134 (98%)	2 (2%)	60	86
5	K	159/203 (78%)	158 (99%)	1 (1%)	84	95
5	k	158/203 (78%)	158 (100%)	0	100	100
6	L	161/224 (72%)	160 (99%)	1 (1%)	84	95
6	l	161/224 (72%)	158 (98%)	3 (2%)	52	82
7	M	162/212 (76%)	162 (100%)	0	100	100
7	m	163/212 (77%)	162 (99%)	1 (1%)	84	95
8	N	141/181 (78%)	140 (99%)	1 (1%)	81	94
8	n	140/181 (77%)	139 (99%)	1 (1%)	81	94
9	O	158/228 (69%)	158 (100%)	0	100	100
9	o	157/228 (69%)	157 (100%)	0	100	100
10	P	159/174 (91%)	157 (99%)	2 (1%)	65	88
10	p	156/174 (90%)	156 (100%)	0	100	100
11	Q	149/171 (87%)	148 (99%)	1 (1%)	81	94
11	q	148/171 (86%)	148 (100%)	0	100	100
12	R	139/202 (69%)	139 (100%)	0	100	100
12	r	138/202 (68%)	138 (100%)	0	100	100
13	S	158/199 (79%)	158 (100%)	0	100	100
13	s	159/199 (80%)	159 (100%)	0	100	100
14	T	151/215 (70%)	150 (99%)	1 (1%)	81	94
14	t	149/215 (69%)	148 (99%)	1 (1%)	81	94
15	A	333/372 (90%)	329 (99%)	4 (1%)	67	89
16	B	344/385 (89%)	330 (96%)	14 (4%)	26	59
17	C	340/352 (97%)	330 (97%)	10 (3%)	37	71
18	D	333/366 (91%)	319 (96%)	14 (4%)	25	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	E	341/353 (97%)	331 (97%)	10 (3%)	37	71
20	F	357/379 (94%)	347 (97%)	10 (3%)	38	72
21	V	388/460 (84%)	380 (98%)	8 (2%)	48	80
22	W	405/416 (97%)	383 (95%)	22 (5%)	18	48
23	X	330/362 (91%)	323 (98%)	7 (2%)	48	80
24	Y	335/344 (97%)	326 (97%)	9 (3%)	40	74
25	Z	257/295 (87%)	247 (96%)	10 (4%)	27	61
26	a	333/336 (99%)	322 (97%)	11 (3%)	33	67
27	b	167/312 (54%)	159 (95%)	8 (5%)	21	53
28	d	233/294 (79%)	224 (96%)	9 (4%)	27	61
29	e	39/63 (62%)	38 (97%)	1 (3%)	41	75
31	U	692/816 (85%)	676 (98%)	16 (2%)	45	78
32	c	249/268 (93%)	241 (97%)	8 (3%)	34	68
33	f	704/763 (92%)	692 (98%)	12 (2%)	56	84
34	z	100/377 (26%)	96 (96%)	4 (4%)	27	60
All	All	10576/12997 (81%)	10367 (98%)	209 (2%)	50	81

5 of 209 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
23	X	133	LEU
26	a	150	SER
33	f	434	TYR
23	X	242	ILE
25	Z	26	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 90 such sidechains are listed below:

Mol	Chain	Res	Type
23	X	322	HIS
26	a	332	HIS
23	X	406	ASN
25	Z	12	HIS
31	U	267	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 5 are monoatomic - leaving 11 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	$\# Z > 2$
36	ATP	F	501	37	28,33,33	0.70	0	34,52,52	1.06	3 (8%)
36	ATP	A	501	37	28,33,33	0.69	0	34,52,52	1.02	3 (8%)
36	ATP	D	502	37	28,33,33	0.72	0	34,52,52	1.14	3 (8%)
35	LDZ	r	301	-	33,34,34	0.51	0	42,44,44	0.88	1 (2%)
35	LDZ	R	301	-	33,34,34	0.46	0	42,44,44	0.71	1 (2%)
38	ADP	E	401	-	24,29,29	0.85	0	29,45,45	1.33	3 (10%)
36	ATP	B	501	37	28,33,33	0.76	0	34,52,52	1.12	3 (8%)
35	LDZ	O	301	-	33,34,34	0.49	1 (3%)	42,44,44	0.76	2 (4%)
35	LDZ	n	301	-	33,34,34	0.49	1 (3%)	42,44,44	0.67	0
35	LDZ	o	301	-	33,34,34	0.45	0	42,44,44	0.66	1 (2%)
35	LDZ	N	301	-	33,34,34	0.50	1 (3%)	42,44,44	0.65	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
36	ATP	F	501	37	-	4/18/38/38	0/3/3/3
36	ATP	A	501	37	-	3/18/38/38	0/3/3/3
36	ATP	D	502	37	-	4/18/38/38	0/3/3/3
35	LDZ	r	301	-	-	11/38/39/39	0/1/1/1
35	LDZ	R	301	-	-	7/38/39/39	0/1/1/1
38	ADP	E	401	-	-	4/12/32/32	0/3/3/3
36	ATP	B	501	37	-	5/18/38/38	0/3/3/3
35	LDZ	O	301	-	-	14/38/39/39	0/1/1/1
35	LDZ	n	301	-	-	4/38/39/39	0/1/1/1
35	LDZ	o	301	-	-	8/38/39/39	0/1/1/1
35	LDZ	N	301	-	-	8/38/39/39	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	O	301	LDZ	C17-N16	-2.07	1.43	1.46
35	N	301	LDZ	C17-N16	-2.06	1.43	1.46
35	n	301	LDZ	C17-N16	-2.00	1.43	1.46

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	E	401	ADP	N3-C2-N1	-4.14	123.06	128.67
35	r	301	LDZ	C14-N13-C12	3.73	129.67	121.65
36	D	502	ATP	C4'-O4'-C1'	-3.58	106.64	109.92
36	B	501	ATP	C4'-O4'-C1'	-3.40	106.81	109.92
35	O	301	LDZ	C14-N13-C12	2.83	127.73	121.65

There are no chirality outliers.

5 of 72 torsion outliers are listed below:

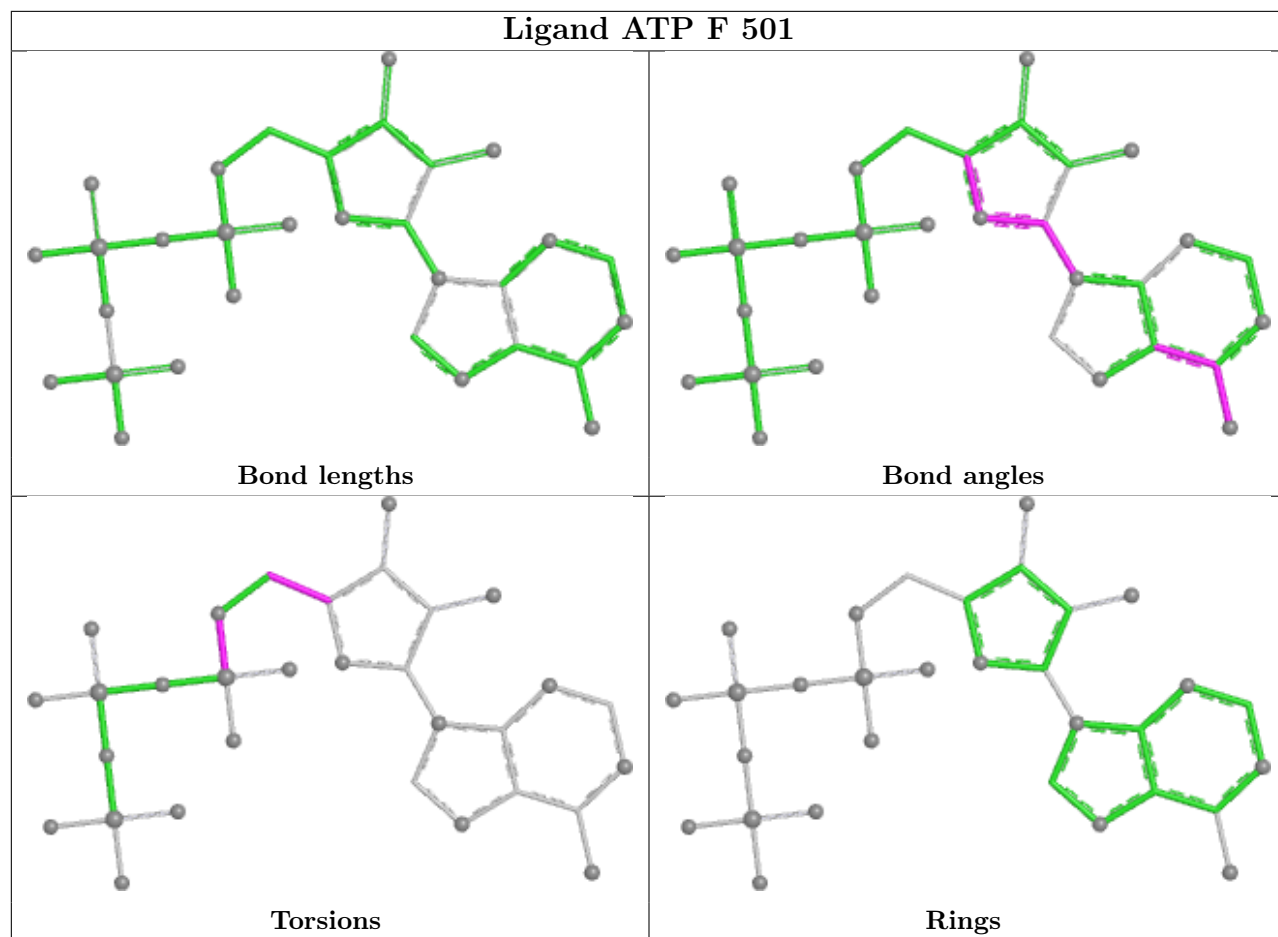
Mol	Chain	Res	Type	Atoms
35	N	301	LDZ	O8-C9-N10-C11
35	O	301	LDZ	C15-C14-N13-C12
35	R	301	LDZ	C22-C17-C18-C19
35	n	301	LDZ	O31-C9-O8-C7
35	n	301	LDZ	N10-C9-O8-C7

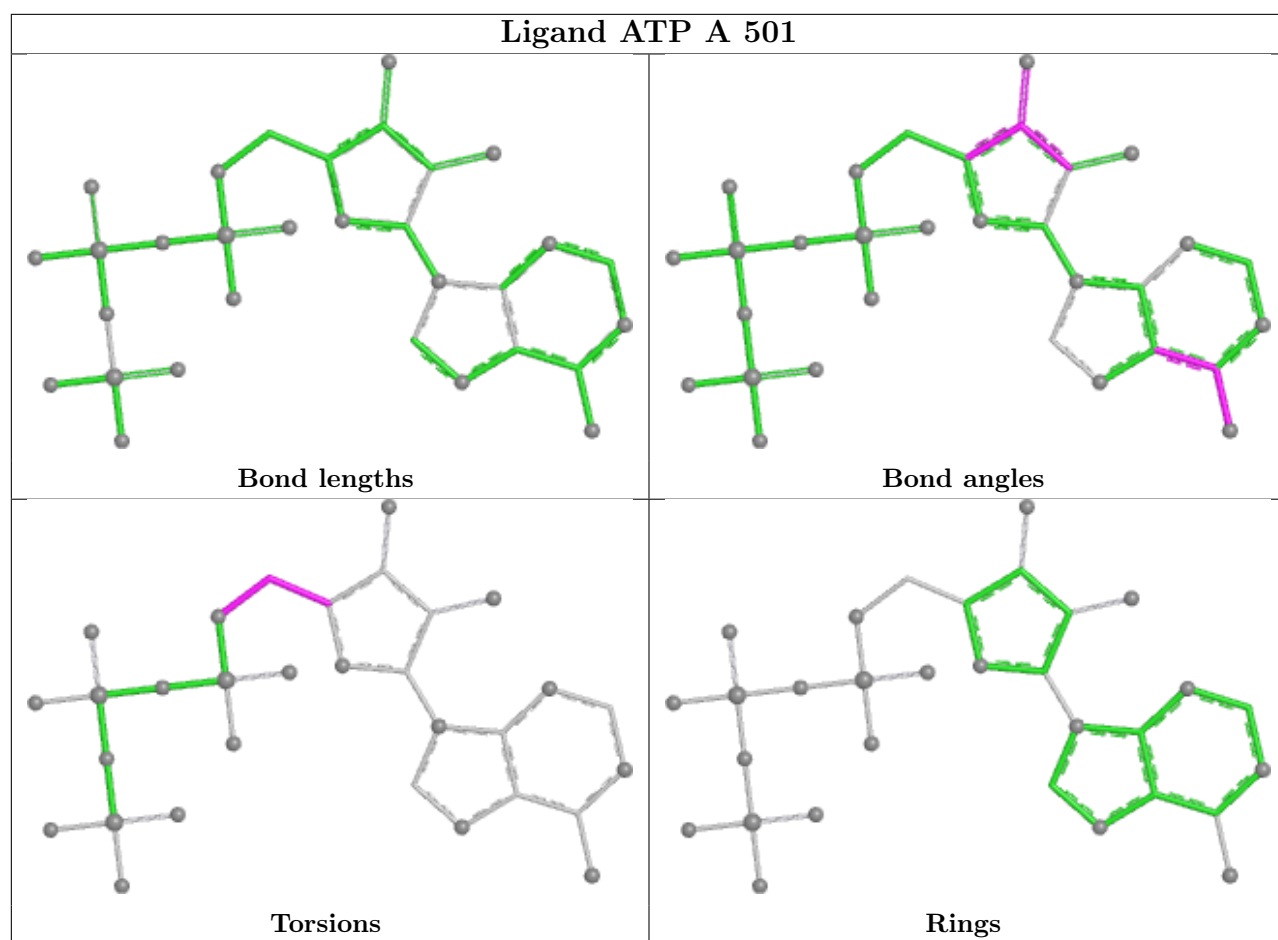
There are no ring outliers.

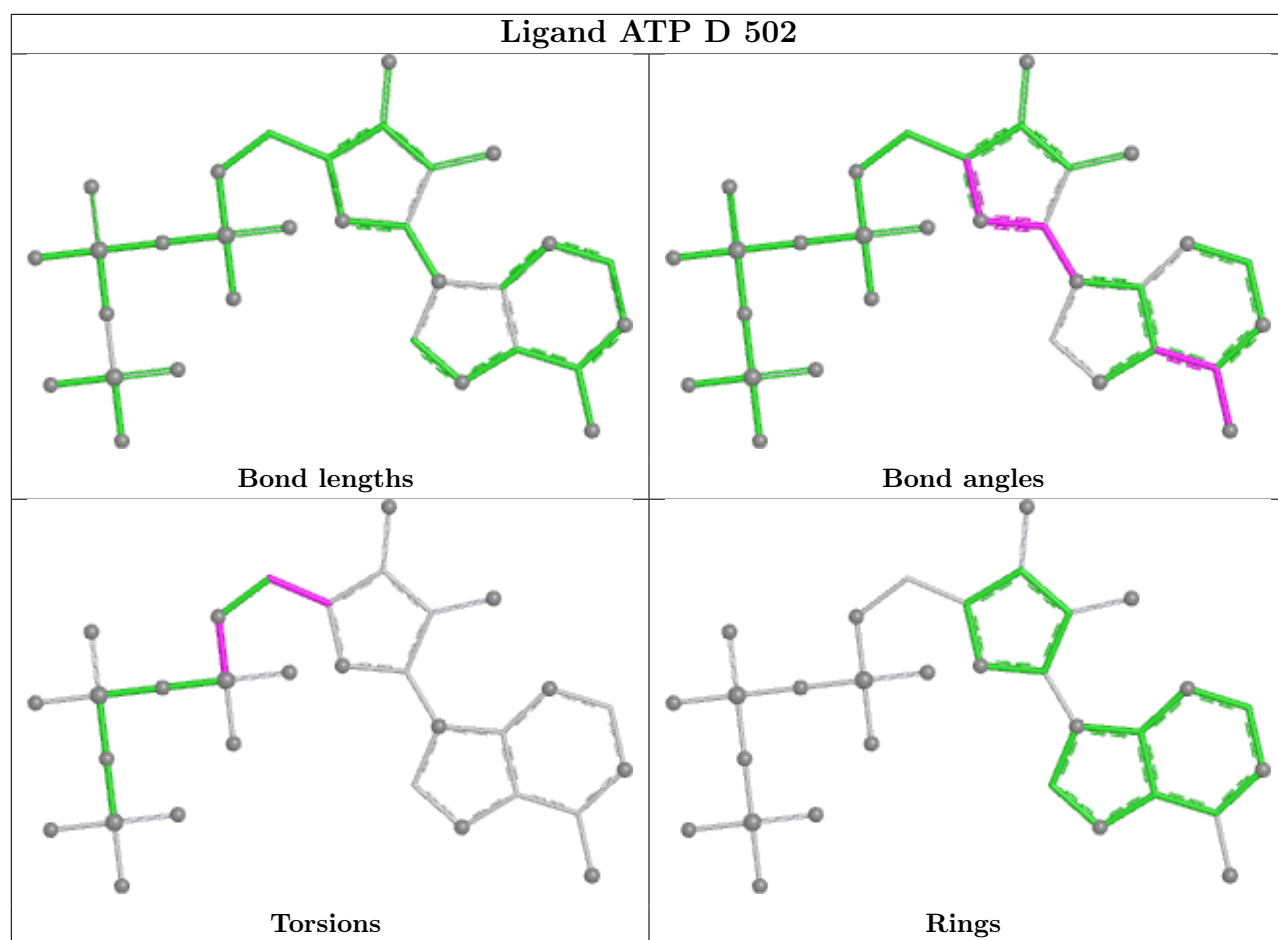
9 monomers are involved in 20 short contacts:

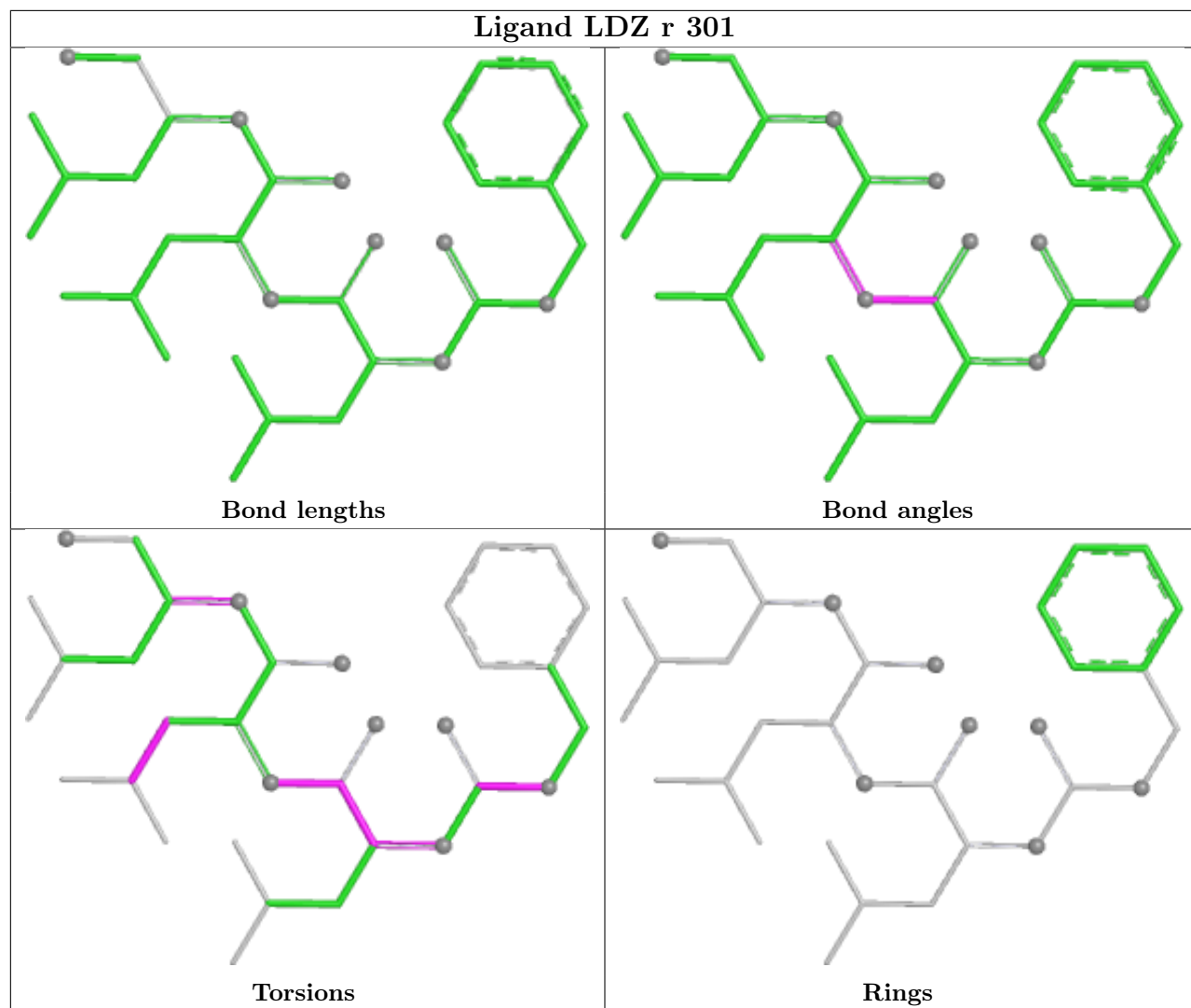
Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	A	501	ATP	1	0
35	r	301	LDZ	1	0
35	R	301	LDZ	4	0
38	E	401	ADP	2	0
36	B	501	ATP	1	0
35	O	301	LDZ	2	0
35	n	301	LDZ	5	0
35	o	301	LDZ	2	0
35	N	301	LDZ	2	0

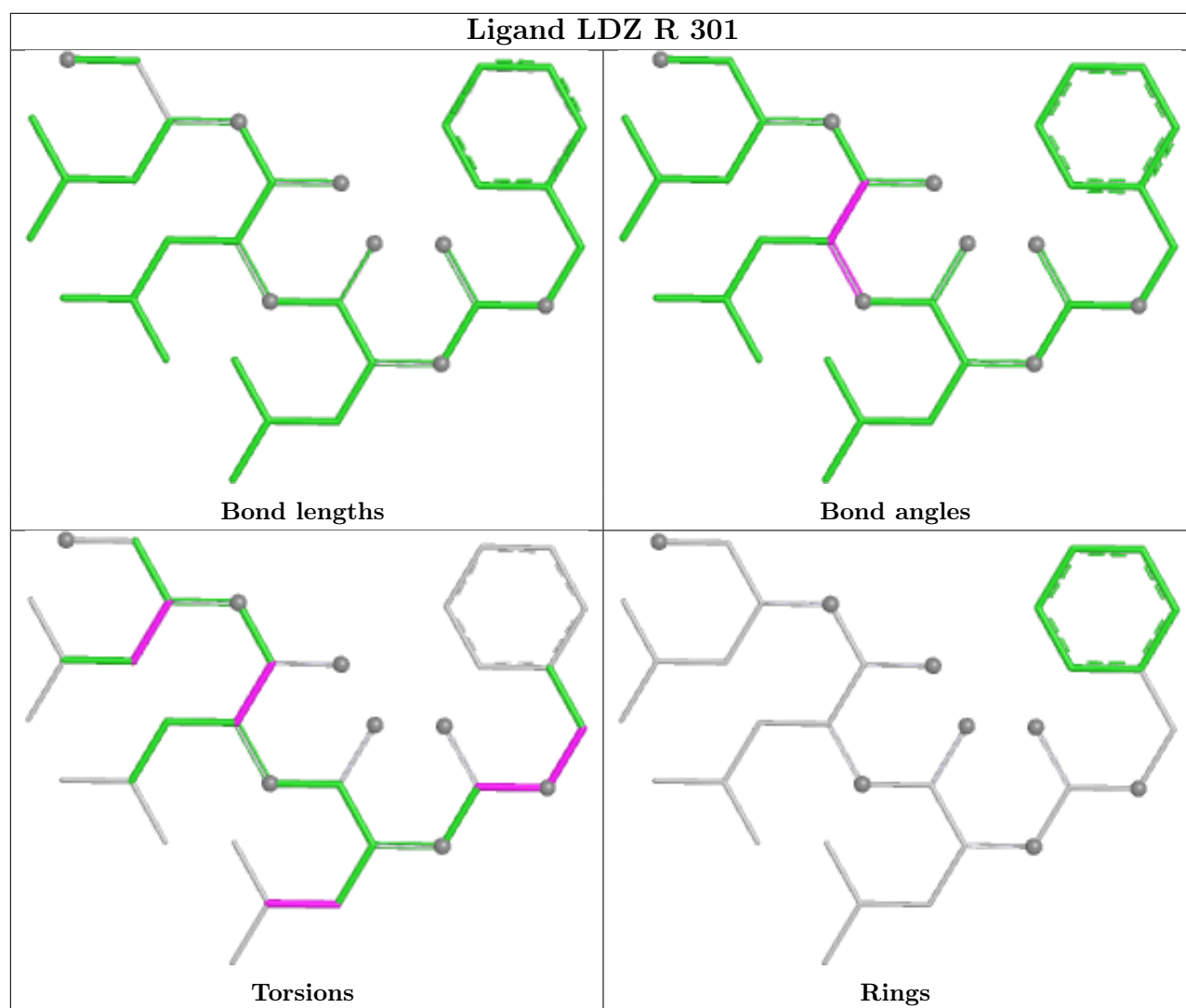
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

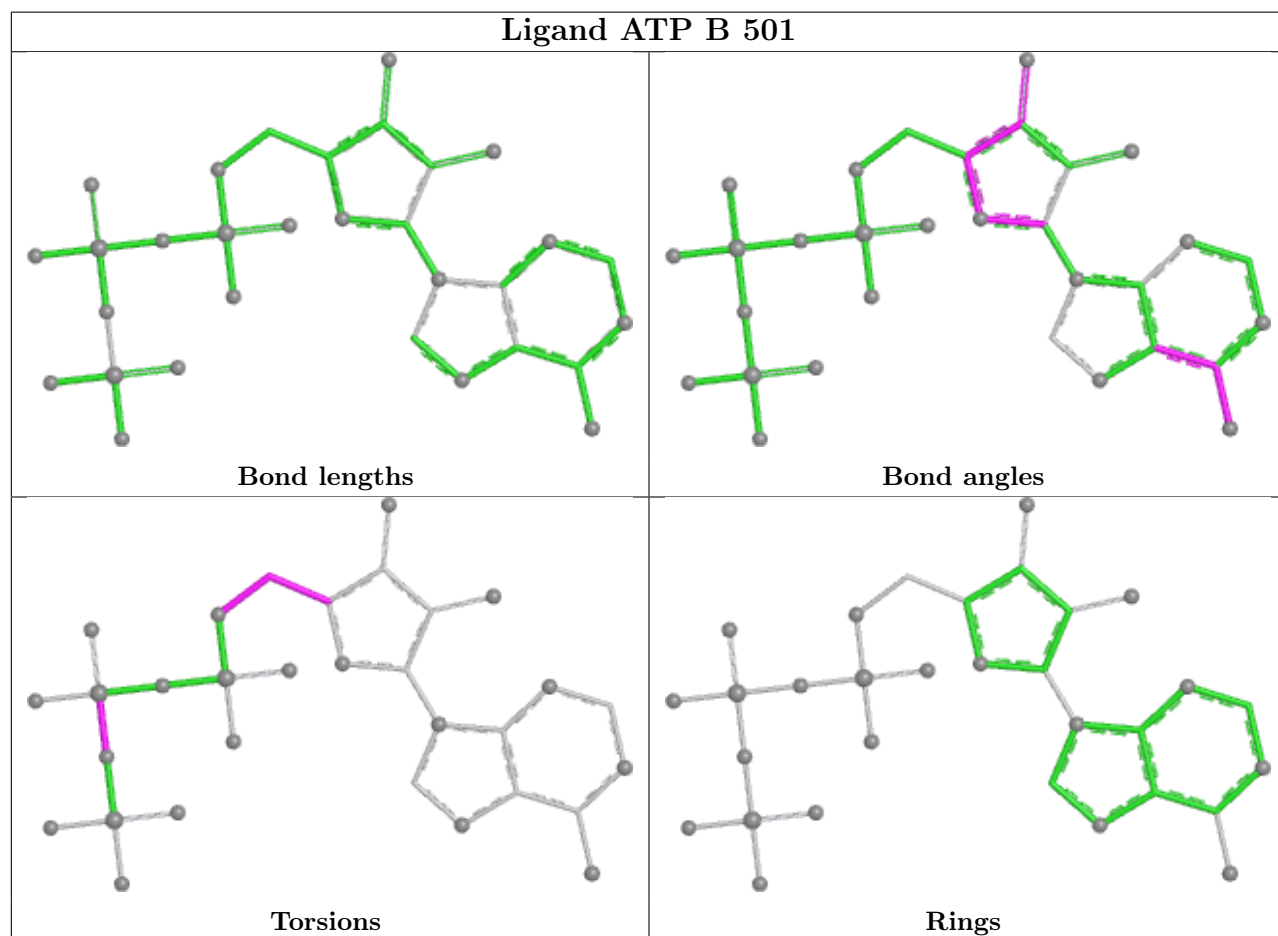
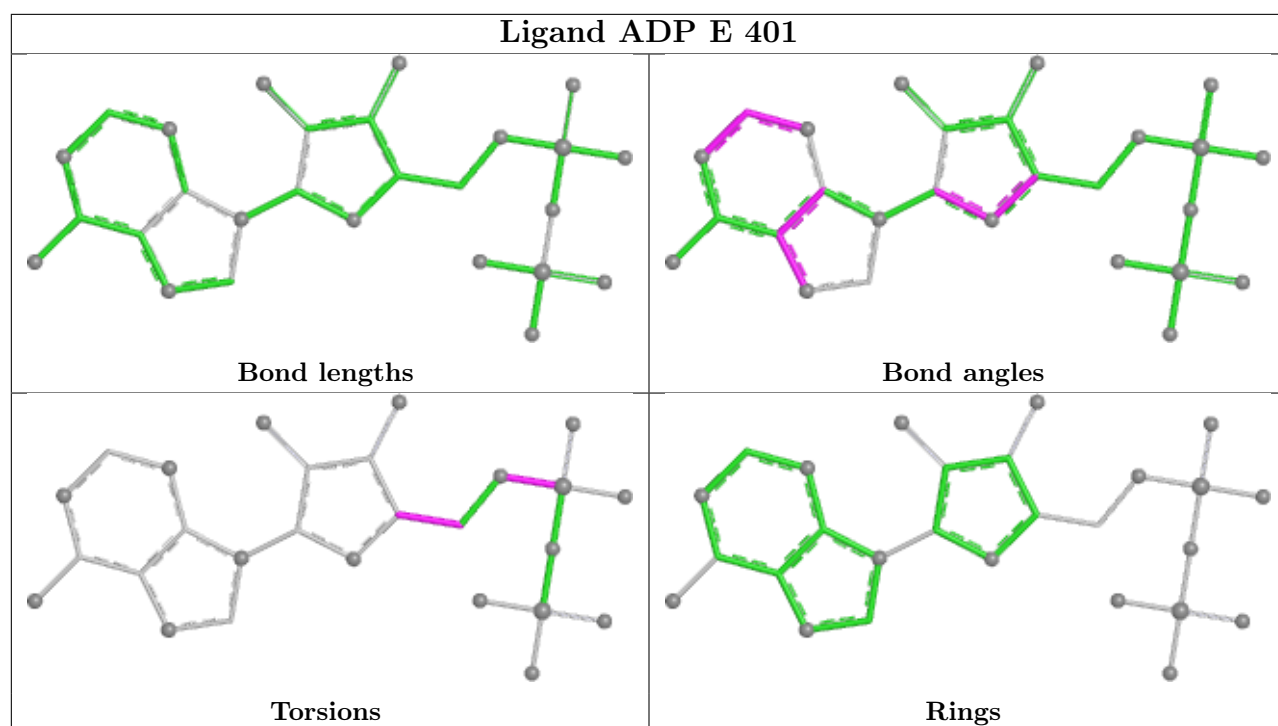


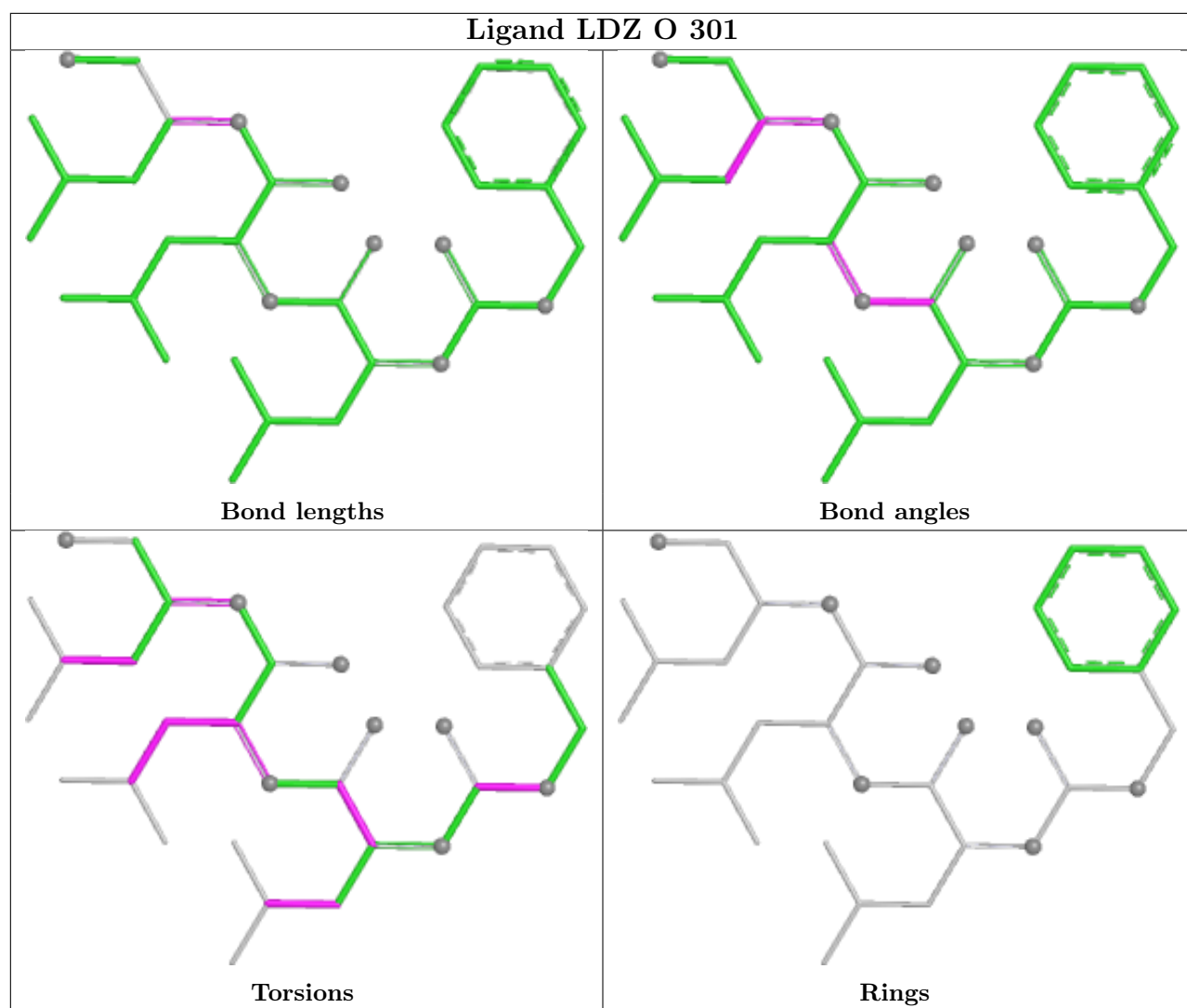


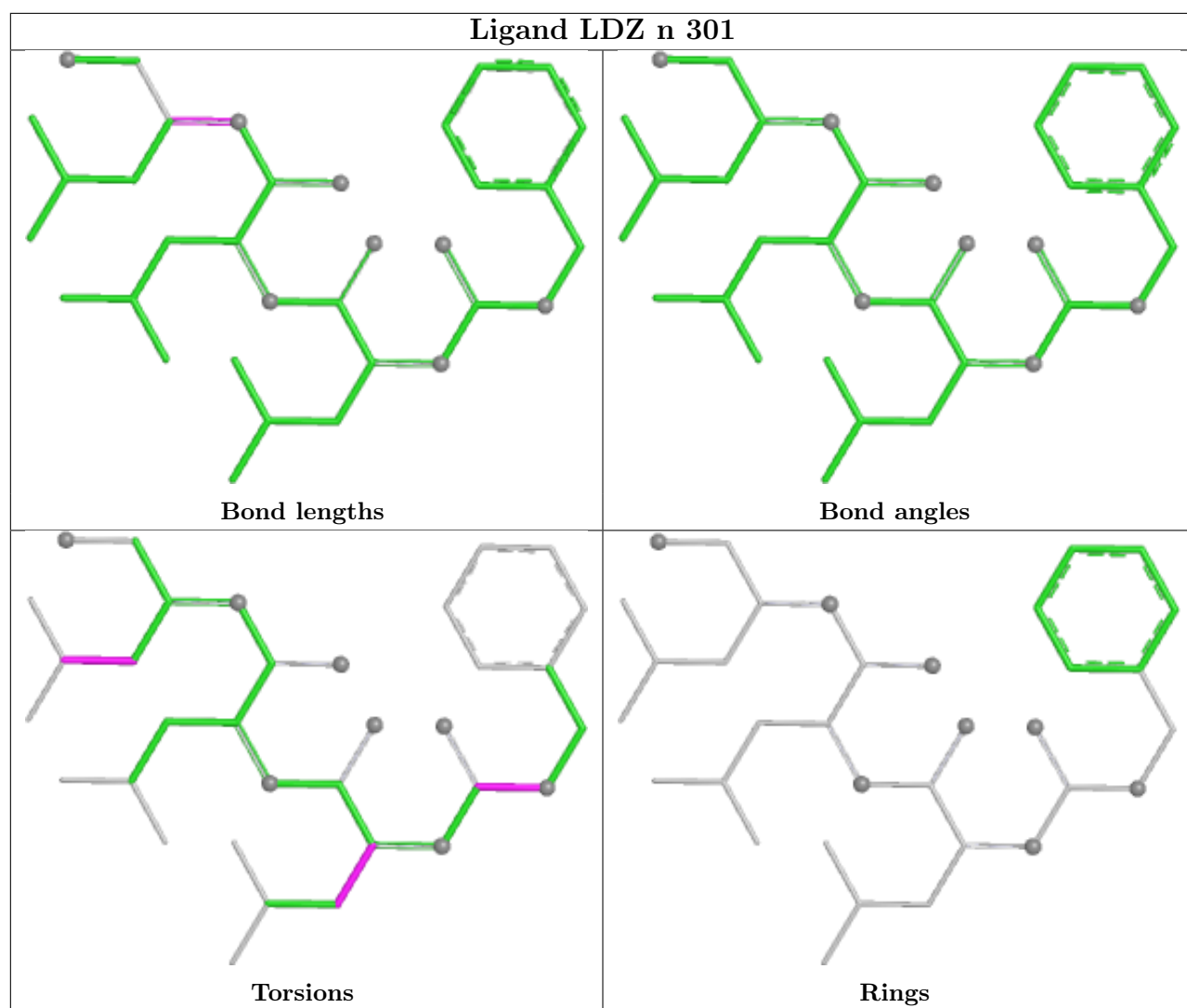


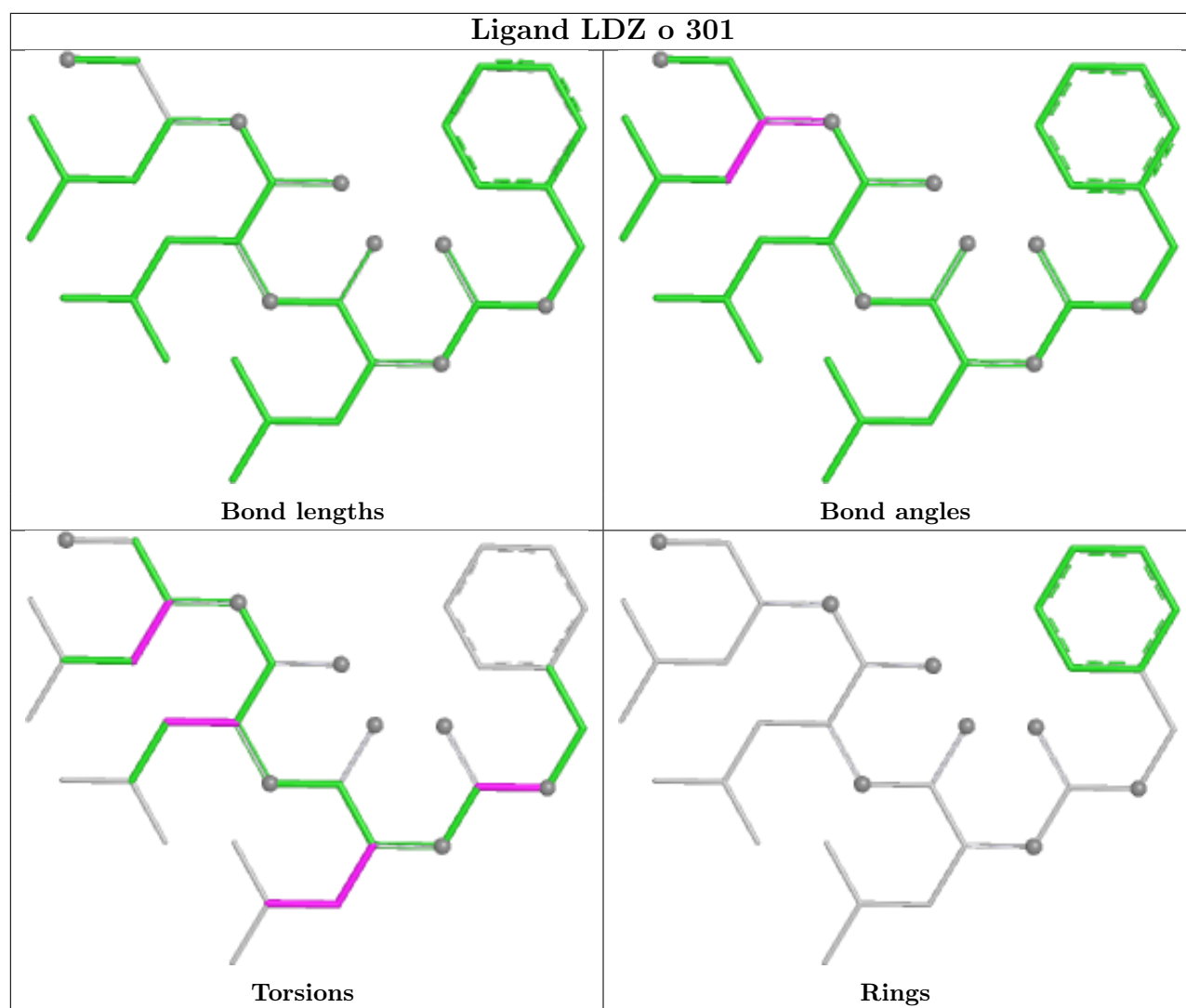


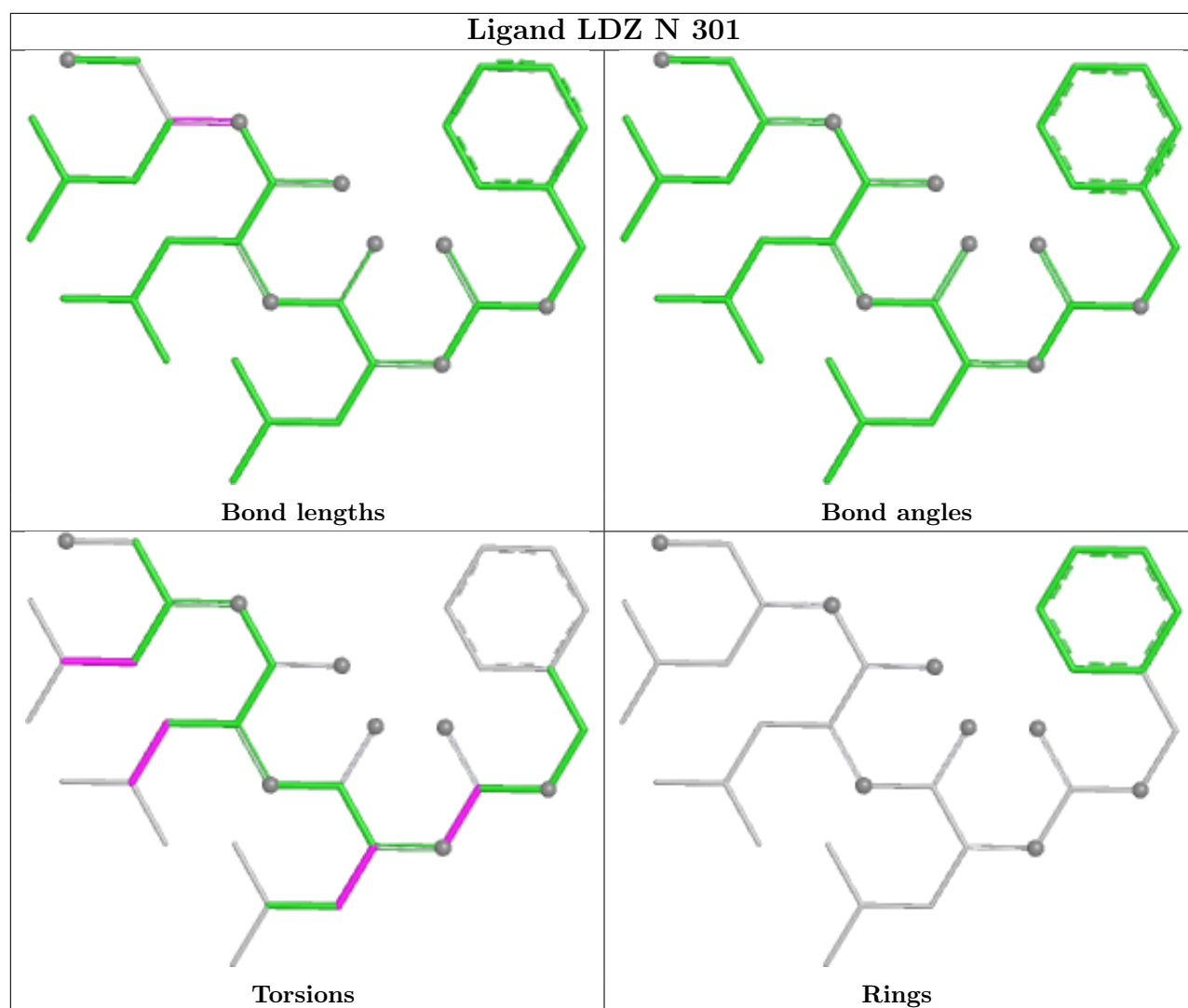












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

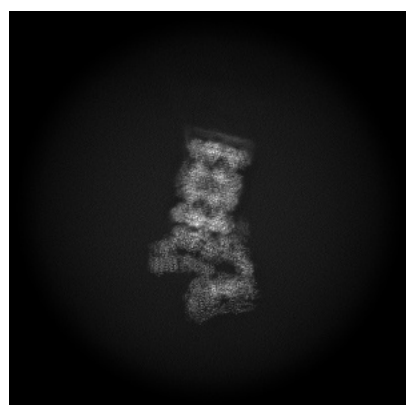
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49508. These allow visual inspection of the internal detail of the map and identification of artifacts.

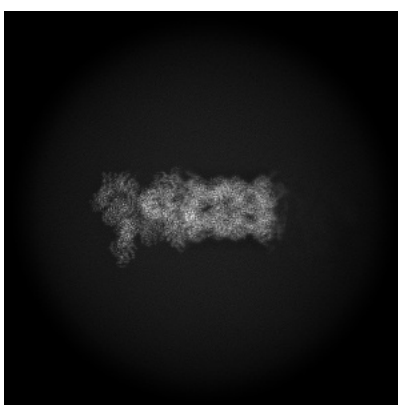
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

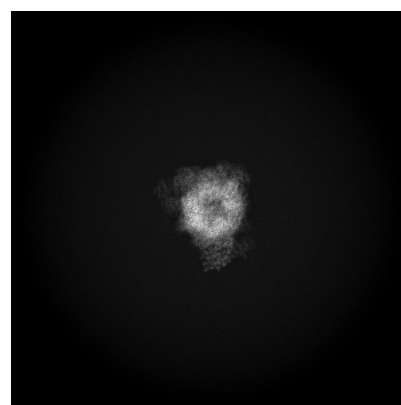
6.1.1 Primary map



X



Y

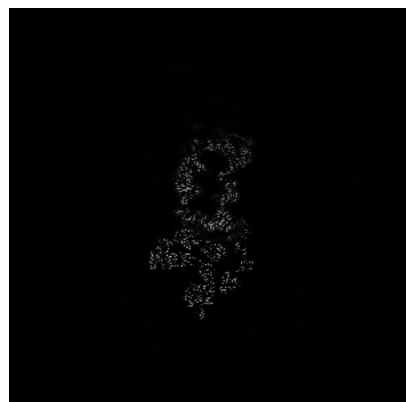


Z

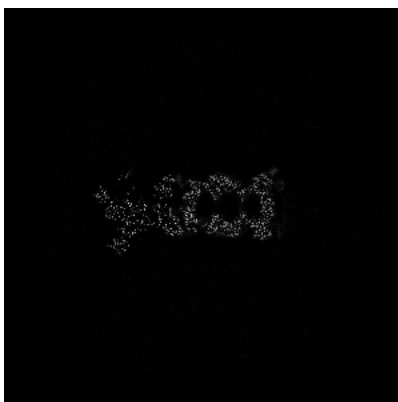
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

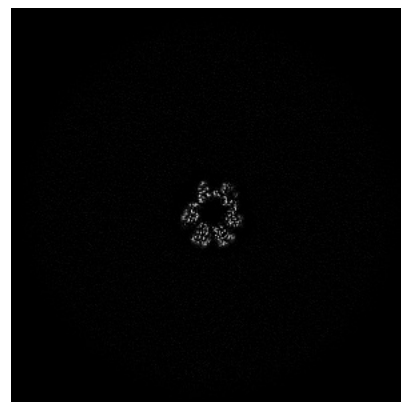
6.2.1 Primary map



X Index: 320



Y Index: 320

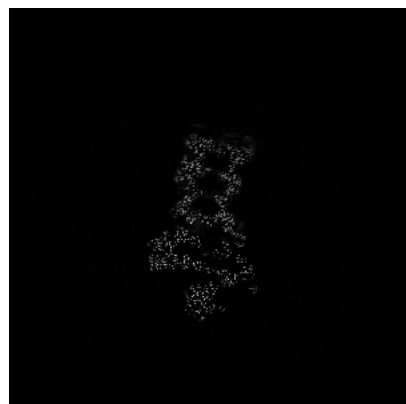


Z Index: 320

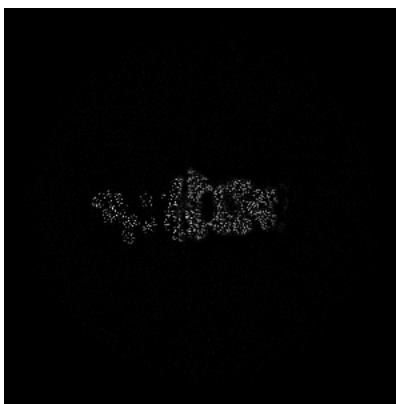
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

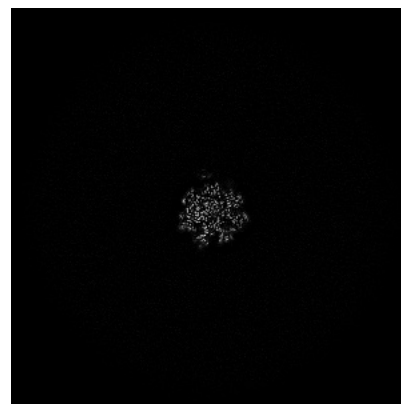
6.3.1 Primary map



X Index: 330



Y Index: 300



Z Index: 303

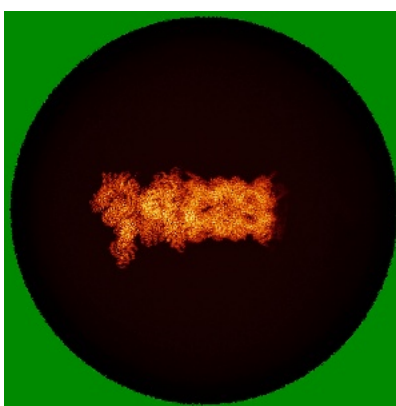
The images above show the largest variance slices of the map in three orthogonal directions.

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

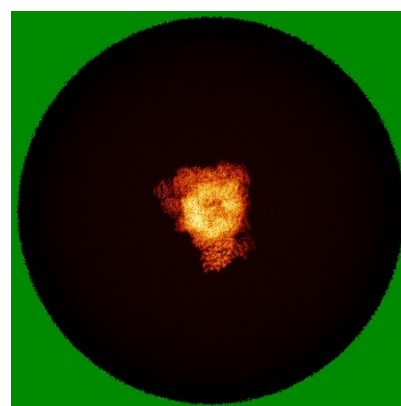
6.4.1 Primary map



X



Y

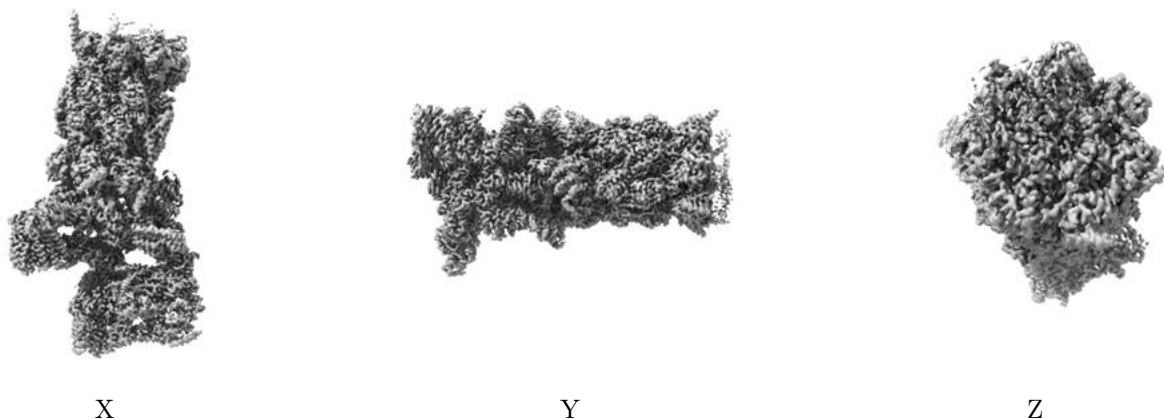


Z

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

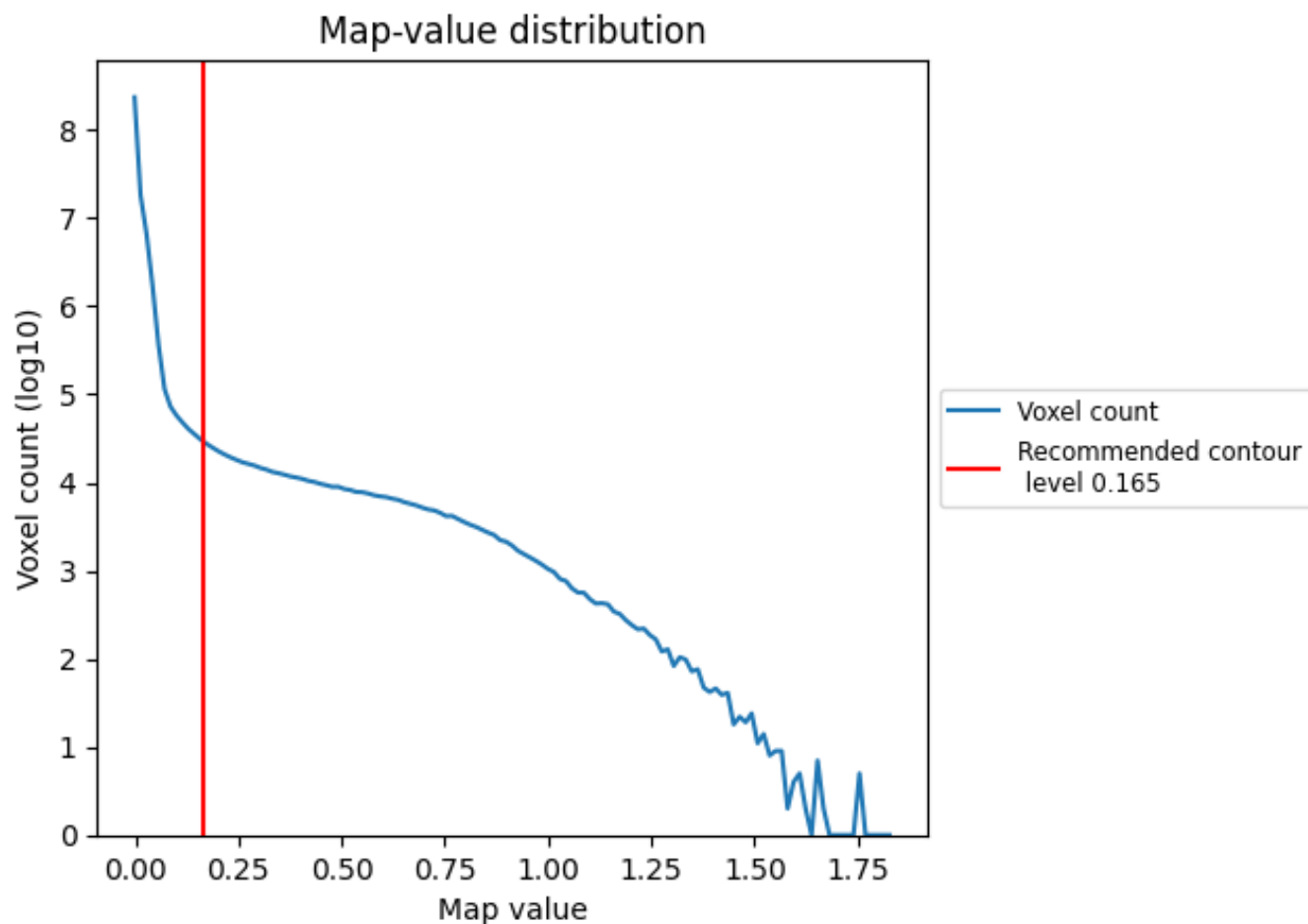
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

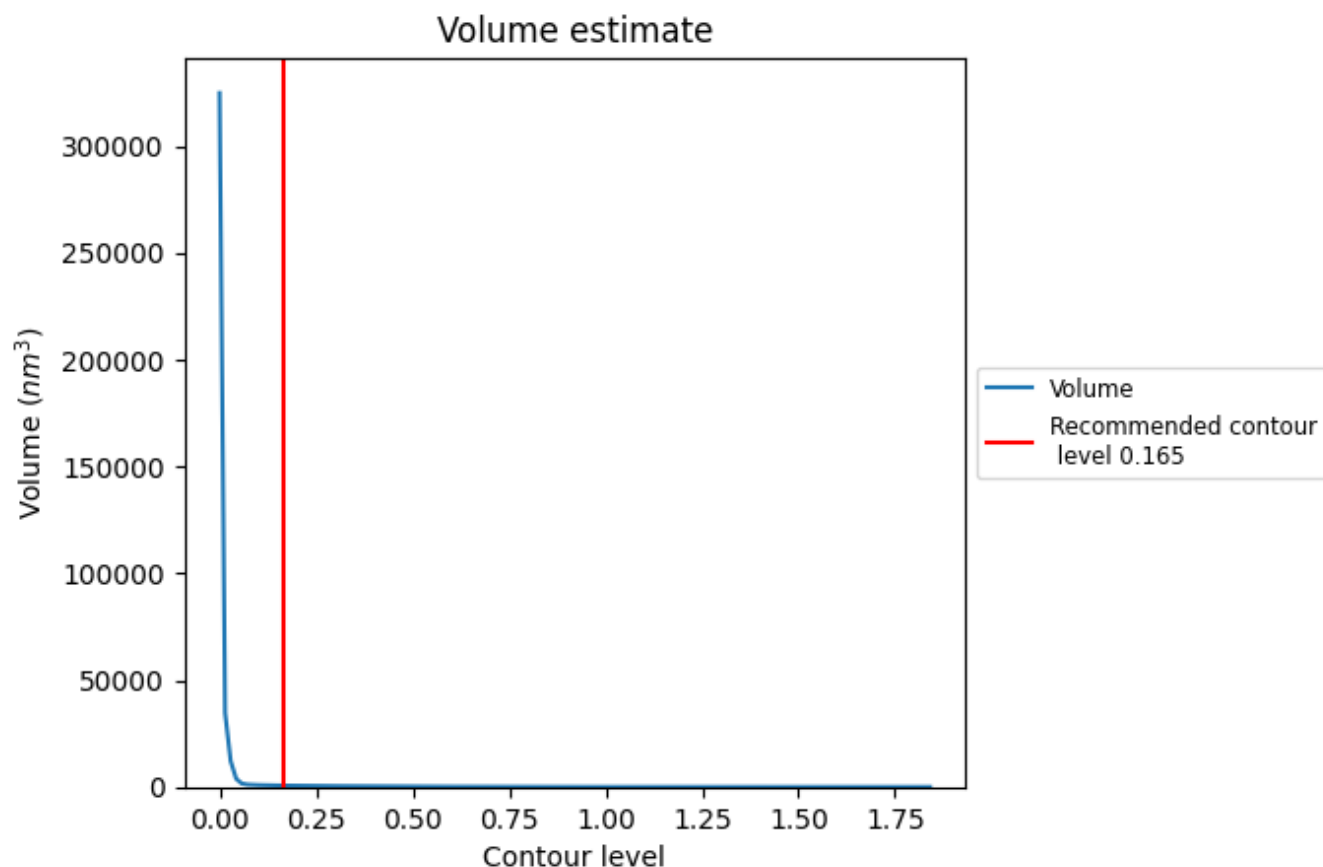
This section contains the results of statistical analysis of the map.

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.

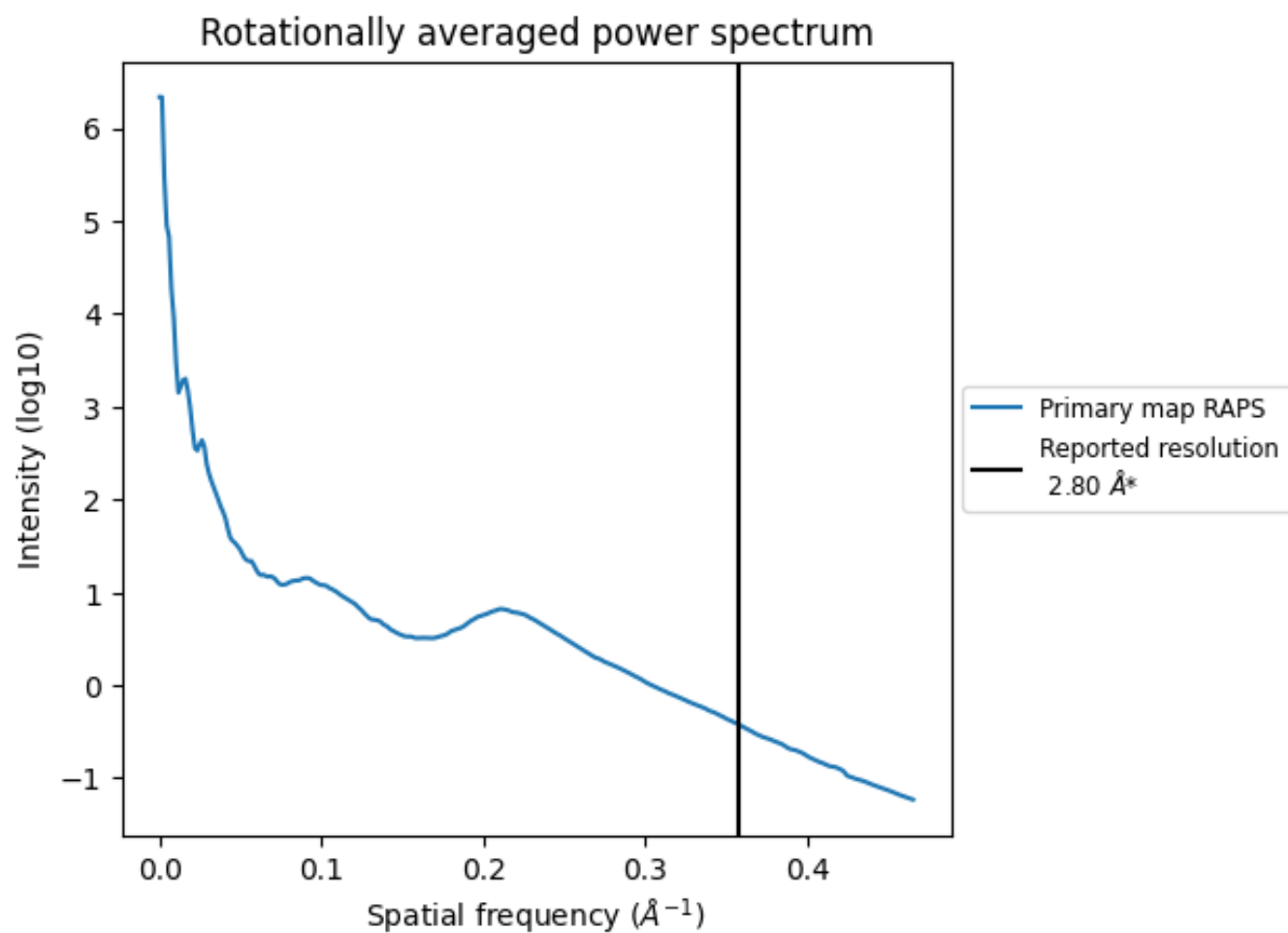
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 644 nm^3 ; this corresponds to an approximate mass of 582 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 0.357 Å⁻¹

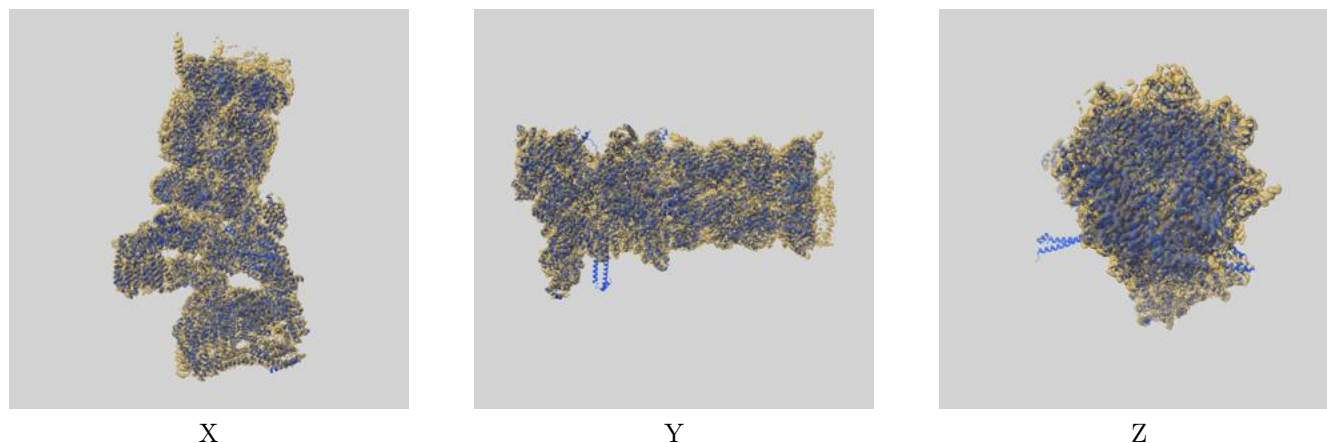
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

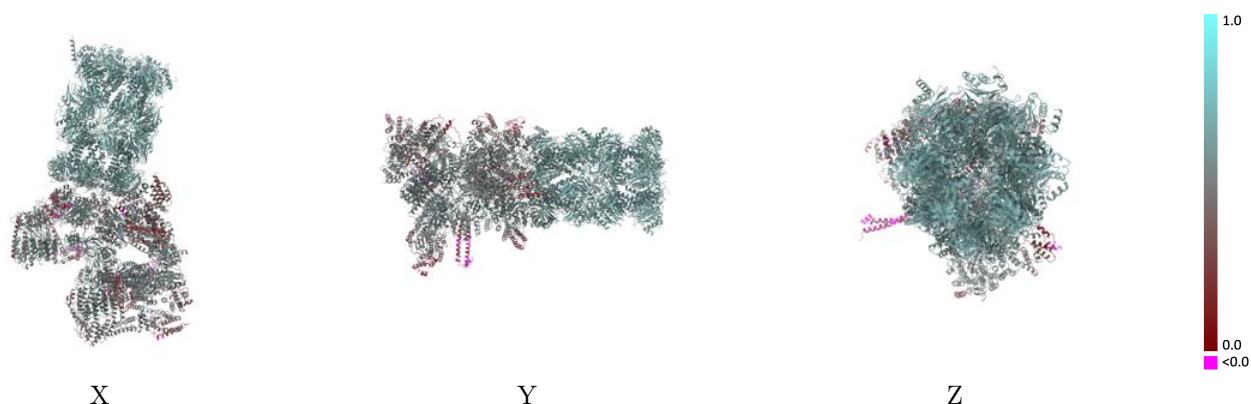
This section contains information regarding the fit between EMDB map EMD-49508 and PDB model 9NKG. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

9.1 Map-model overlay [i](#)



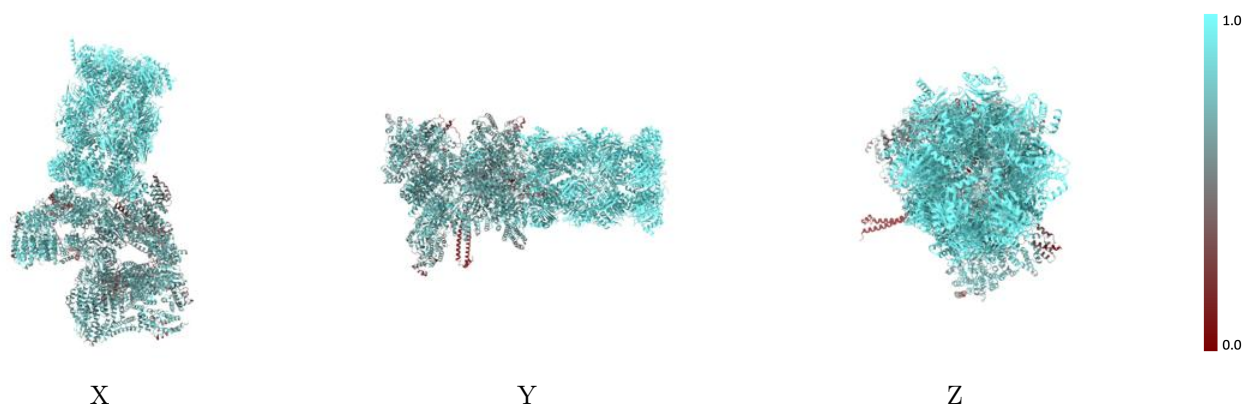
The images above show the 3D surface view of the map at the recommended contour level 0.165 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



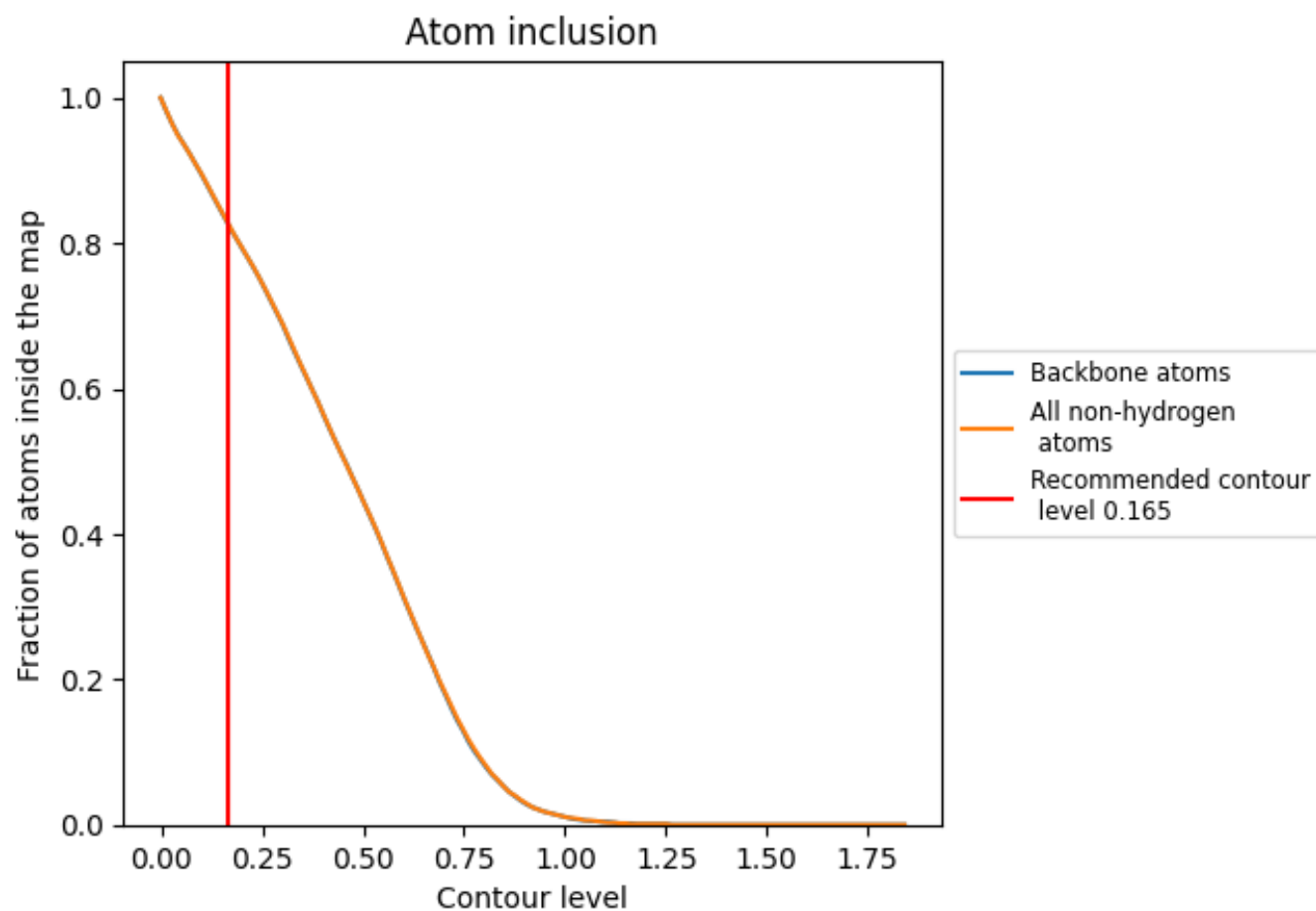
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.165).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 83% 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 (0.165) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8280	 0.5380
A	 0.7770	 0.5170
B	 0.7490	 0.4880
C	 0.6640	 0.4600
D	 0.7560	 0.5130
E	 0.7290	 0.4830
F	 0.6850	 0.4650
G	 0.9820	 0.5920
H	 0.9880	 0.6080
I	 0.9750	 0.5990
J	 0.9910	 0.6040
K	 0.9750	 0.5990
L	 0.9890	 0.6110
M	 0.9790	 0.5980
N	 0.9840	 0.6290
O	 0.9910	 0.6290
P	 0.9930	 0.6330
Q	 0.9900	 0.6440
R	 0.9900	 0.6410
S	 0.9900	 0.6380
T	 0.9880	 0.6360
U	 0.7370	 0.4920
V	 0.6700	 0.4490
W	 0.6890	 0.4730
X	 0.6390	 0.4240
Y	 0.7080	 0.4690
Z	 0.7310	 0.4960
a	 0.6640	 0.4240
b	 0.6630	 0.4240
c	 0.7740	 0.5340
d	 0.5960	 0.3690
e	 0.5250	 0.3600
f	 0.7610	 0.4760
g	 0.9780	 0.6250
h	 0.9880	 0.6330



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Chain	Atom inclusion	Q-score
i	 0.9770	 0.6200
j	 0.9880	 0.6120
k	 0.9660	 0.6140
l	 0.9890	 0.6230
m	 0.9740	 0.6220
n	 0.9850	 0.6360
o	 0.9940	 0.6360
p	 0.9890	 0.6390
q	 0.9880	 0.6410
r	 0.9850	 0.6410
s	 0.9880	 0.6340
t	 0.9900	 0.6280
v	 0.8000	 0.5970
z	 0.6120	 0.4320