



wwPDB EM Validation Summary Report ⓘ

Aug 27, 2026 – 12:18 am BST

PDB ID : 7ARD / pdb_00007ard
EMDB ID : EMD-11880
Title : Cryo-EM structure of Polytomella Complex-I (complete composition)
Authors : Klusch, N.; Kuehlbrandt, W.; Yildiz, O.
Deposited on : 2020-10-23
Resolution : 3.11 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:

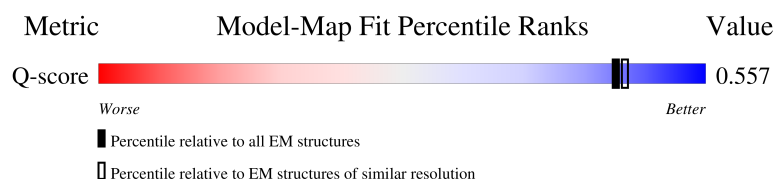
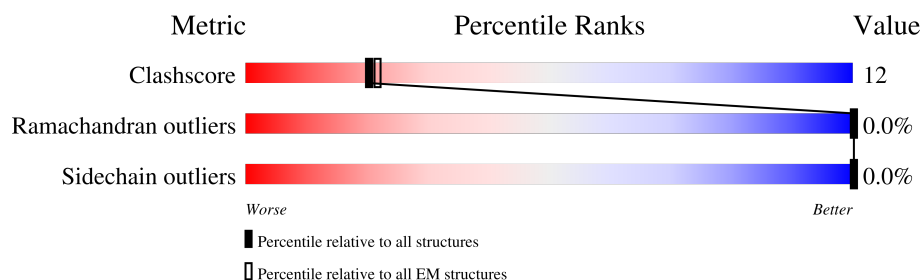
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.50

1 Overall quality at a glance

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

The reported resolution of this entry is 3.11 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	14465 (2.61 - 3.61)

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	154	12% 52% 27% 21%
2	B	164	18% 63% 31% 6%
3	C	217	6% 70% 30%
4	D	395	8% 65% 35%

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Mol	Chain	Length	Quality of chain
5	E	276	
6	F	469	
7	G	720	
8	H	293	
9	I	229	
10	J	145	
11	K	127	
12	L	536	
13	M	438	
14	N	375	
15	O	200	
16	P	370	
17	Q	185	
18	R	132	
19	S	98	
20	T	123	
21	U	122	
22	V	159	
23	W	137	
24	X	100	
25	Y	206	
26	Z	142	
27	a	71	
28	b	54	
29	c	110	

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Mol	Chain	Length	Quality of chain
30	d	83	
31	e	75	
32	f	121	
33	g	172	
34	h	81	
35	i	128	
36	j	87	
37	k	55	
38	l	151	
39	m	138	
40	n	121	
41	o	85	
42	p	156	
43	q	155	
44	r	121	
45	s	118	
46	t	134	
47	u	50	
48	w	41	
49	x	280	
50	y	310	
51	z	227	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
53	SF4	F	501	-	-	X	-

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 70559 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 ND3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	121	Total	C	N	O	S	0	0
			999	673	148	172	6		

- Molecule 2 is a protein called PSST.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	154	Total	C	N	O	S	0	0
			1206	774	208	211	13		

- Molecule 3 is a protein called ND9.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	216	Total	C	N	O	S	0	0
			1808	1169	302	332	5		

- Molecule 4 is a protein called ND7.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	395	Total	C	N	O	S	0	0
			3178	2029	557	569	23		

- Molecule 5 is a protein called 24 kDa.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	235	Total	C	N	O	S	0	0
			1806	1135	306	350	15		

- Molecule 6 is a protein called 51 kDa.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	430	Total	C	N	O	S	0	0
			3322	2088	594	617	23		

- Molecule 7 is a protein called 75 kDa.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	682	Total	C	N	O	S	0	0
			5166	3243	919	980	24		

- Molecule 8 is a protein called ND1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	293	Total	C	N	O	S	0	0
			2237	1487	346	387	17		

- Molecule 9 is a protein called TYKY.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	199	Total	C	N	O	S	0	0
			1602	1000	274	317	11		

- Molecule 10 is a protein called ND6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	145	Total	C	N	O	S	0	0
			1120	755	159	197	9		

- Molecule 11 is a protein called ND4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	104	Total	C	N	O	S	0	0
			798	518	128	145	7		

- Molecule 12 is a protein called ND5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	536	Total	C	N	O	S	0	0
			4111	2697	654	735	25		

- Molecule 13 is a protein called ND4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	438	Total	C	N	O	S	0	0
			3425	2314	520	572	19		

- Molecule 14 is a protein called ND2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	375	Total	C	N	O	S	0	0
			2967	1998	450	505	14		

- Molecule 15 is a protein called C1-FDX.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	161	Total	C	N	O	S	0	0
			1336	871	213	247	5		

- Molecule 16 is a protein called 39 kDa.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	347	Total	C	N	O	S	0	0
			2701	1713	464	514	10		

- Molecule 17 is a protein called 18 kDa.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	162	Total	C	N	O	S	0	0
			1276	812	227	233	4		

- Molecule 18 is a protein called 13 kDa.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	108	Total	C	N	O	S	0	0
			812	510	138	159	5		

- Molecule 19 is a protein called B8.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	S	95	Total	C	N	O	0	0
			716	450	124	142		

- Molecule 20 is a protein called SDAP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	83	Total	C	N	O	S	0	0
			645	406	103	134	2		

- Molecule 21 is a protein called SDAP2.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	U	84	Total	C	N	O		
			655	414	103	138	0	0

- Molecule 22 is a protein called B13.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	V	134	Total	C	N	O	S	
			1052	671	170	209	2	0

- Molecule 23 is a protein called B14.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	W	127	Total	C	N	O	S	
			1074	695	185	188	6	0

- Molecule 24 is a protein called PGIV.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	X	99	Total	C	N	O	S	
			816	522	139	149	6	0

- Molecule 25 is a protein called B14.7.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	Y	205	Total	C	N	O	S	
			1583	1027	259	293	4	0

- Molecule 26 is a protein called B16.6.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	Z	124	Total	C	N	O	S	
			1003	639	184	178	2	0

- Molecule 27 is a protein called MWFE.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	a	60	Total	C	N	O	S	
			515	335	89	90	1	0

- Molecule 28 is a protein called B9.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	b	54	Total	C	N	O	0	0
			270	162	54	54		

- Molecule 29 is a protein called KFYI.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	c	97	Total	C	N	O	S	0	0
			785	512	134	136	3		

- Molecule 30 is a protein called B14.5b.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	d	80	Total	C	N	O	S	0	0
			650	420	112	116	2		

- Molecule 31 is a protein called 15 kDa.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	e	71	Total	C	N	O	S	0	0
			592	370	103	112	7		

- Molecule 32 is a protein called MNLL.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	f	111	Total	C	N	O	S	0	0
			877	566	146	163	2		

- Molecule 33 is a protein called ESSS.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	g	147	Total	C	N	O	S	0	0
			1176	763	194	213	6		

- Molecule 34 is a protein called NUOP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	h	77	Total	C	N	O	S	0	0
			625	411	94	118	2		

- Molecule 35 is a protein called NUOP5.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	i	111	Total	C	N	O	0	0
			922	576	170	176		

- Molecule 36 is a protein called AGGG.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	j	87	Total	C	N	O	0	0
			435	261	87	87		

- Molecule 37 is a protein called B12.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	k	44	Total	C	N	O	S	0	0
			367	247	60	59	1		

- Molecule 38 is a protein called ASHL.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	l	127	Total	C	N	O	S	0	0
			1018	666	161	184	7		

- Molecule 39 is a protein called B15.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	m	111	Total	C	N	O	S	0	0
			934	601	158	172	3		

- Molecule 40 is a protein called Complex I-B22.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	n	120	Total	C	N	O	S	0	0
			1008	648	183	173	4		

- Molecule 41 is a protein called B18.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	o	83	Total	C	N	O	S	0	0
			704	448	129	120	7		

- Molecule 42 is a protein called PDSW.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	p	155	Total	C	N	O	S	0	0
			1287	803	242	238	4		

- Molecule 43 is a protein called B17.2.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	q	28	Total	C	N	O	S	0	0
			243	160	43	39	1		

- Molecule 44 is a protein called B14.5a.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	r	60	Total	C	N	O	S	0	0
			493	317	88	87	1		

- Molecule 45 is a protein called NUOP7.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	s	115	Total	C	N	O	S	0	0
			933	613	155	164	1		

- Molecule 46 is a protein called NUOP8.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	t	82	Total	C	N	O	S	0	0
			706	476	112	116	2		

- Molecule 47 is a protein called unknown.

Mol	Chain	Residues	Atoms				AltConf	Trace
47	u	50	Total	C	N	O	0	0
			250	150	50	50		

- Molecule 48 is a protein called unknown.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	w	41	Total	C	N	O	0	0
			204	122	41	41		

- Molecule 49 is a protein called CAL.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	x	250	Total	C	N	O	S	0	0
			1967	1240	346	375	6		

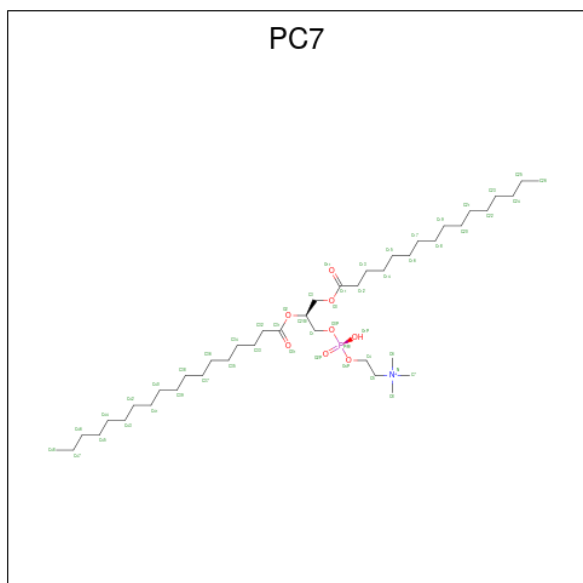
- Molecule 50 is a protein called CA2.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	y	308	Total	C	N	O	S	0	0
			2316	1470	401	438	7		

- Molecule 51 is a protein called CA3.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	z	226	Total	C	N	O	S	0	0
			1687	1069	279	334	5		

- Molecule 52 is (7S)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY) METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSAN-1-AMINIUM 4-OXIDE (CCD ID: PC7) (formula: $C_{42}H_{85}NO_8P$).



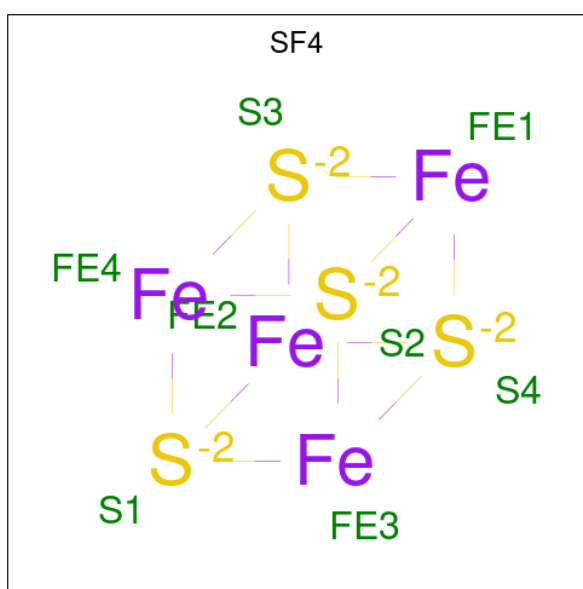
Mol	Chain	Residues	Atoms					AltConf
52	A	1	Total	C	N	O	P	0
			49	39	1	8	1	
52	L	1	Total	C	N	O	P	0
			48	38	1	8	1	
52	M	1	Total	C	N	O	P	0
			52	42	1	8	1	

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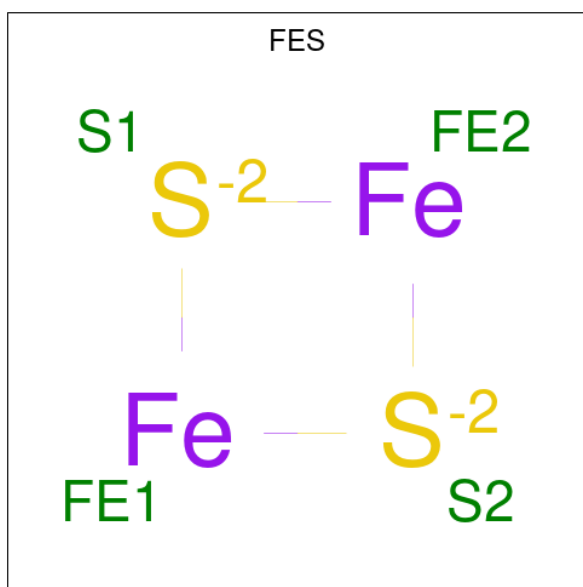
Mol	Chain	Residues	Atoms					AltConf
52	M	1	Total	C	N	O	P	0
			52	42	1	8	1	
52	N	1	Total	C	N	O	P	0
			52	42	1	8	1	
52	N	1	Total	C	N	O	P	0
			52	42	1	8	1	
52	z	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 53 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



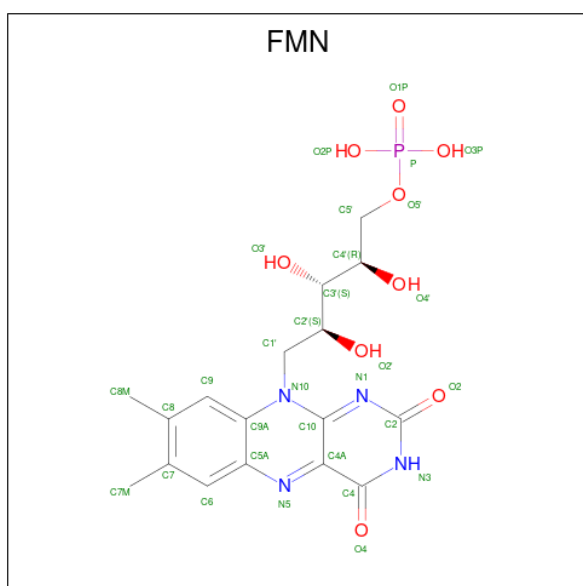
Mol	Chain	Residues	Atoms			AltConf
53	B	1	Total	Fe	S	0
			8	4	4	
53	F	1	Total	Fe	S	0
			8	4	4	
53	G	1	Total	Fe	S	0
			8	4	4	
53	G	1	Total	Fe	S	0
			8	4	4	
53	I	1	Total	Fe	S	0
			8	4	4	
53	I	1	Total	Fe	S	0
			8	4	4	

- Molecule 54 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



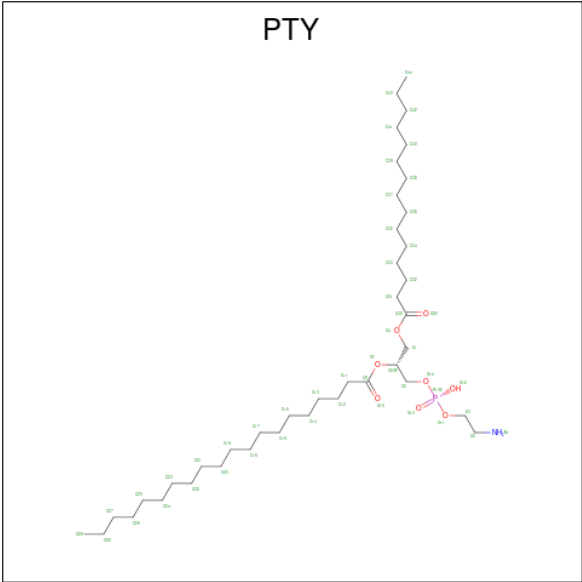
Mol	Chain	Residues	Atoms			AltConf
54	E	1	Total	Fe	S	0
			4	2	2	
54	G	1	Total	Fe	S	0
			4	2	2	

- Molecule 55 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



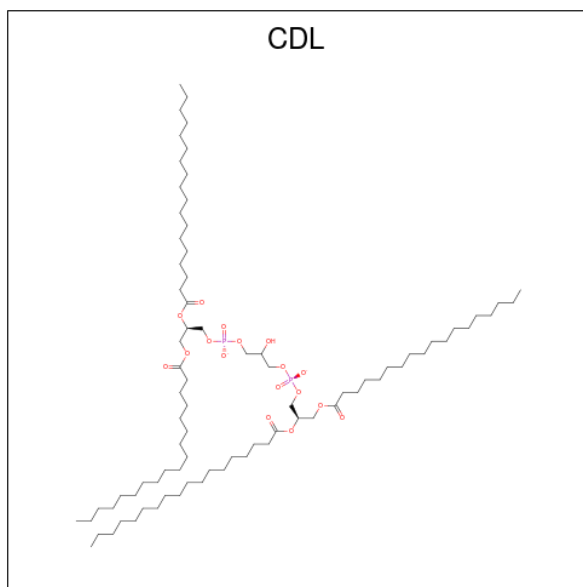
Mol	Chain	Residues	Atoms					AltConf
55	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 56 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: $C_{40}H_{80}NO_8P$).



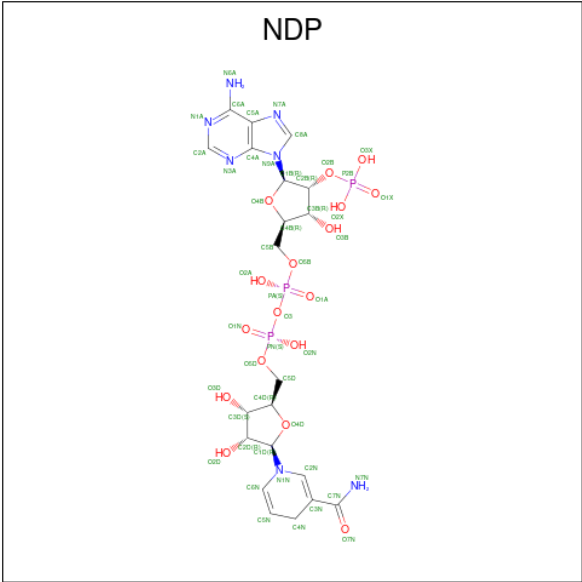
Mol	Chain	Residues	Atoms					AltConf
56	H	1	Total	C	N	O	P	0
			50	40	1	8	1	
56	L	1	Total	C	N	O	P	0
			50	40	1	8	1	
56	M	1	Total	C	N	O	P	0
			47	37	1	8	1	
56	N	1	Total	C	N	O	P	0
			50	40	1	8	1	
56	Y	1	Total	C	N	O	P	0
			50	40	1	8	1	
56	m	1	Total	C	N	O	P	0
			50	40	1	8	1	
56	m	1	Total	C	N	O	P	0
			50	40	1	8	1	

- Molecule 57 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



Mol	Chain	Residues	Atoms				AltConf
57	L	1	Total	C	O	P	0
			89	70	17	2	
57	M	1	Total	C	O	P	0
			100	81	17	2	
57	N	1	Total	C	O	P	0
			100	81	17	2	
57	d	1	Total	C	O	P	0
			100	81	17	2	
57	t	1	Total	C	O	P	0
			100	81	17	2	

- Molecule 58 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms						AltConf
60	W	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	
60	n	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	

- Molecule 61 is water.

Mol	Chain	Residues	Atoms		AltConf
61	A	6	Total	O	0
			6	6	
61	B	15	Total	O	0
			15	15	
61	C	37	Total	O	0
			37	37	
61	D	43	Total	O	0
			43	43	
61	E	15	Total	O	0
			15	15	
61	F	16	Total	O	0
			16	16	
61	G	114	Total	O	0
			114	114	
61	H	11	Total	O	0
			11	11	
61	I	33	Total	O	0
			33	33	
61	J	3	Total	O	0
			3	3	
61	K	5	Total	O	0
			5	5	
61	L	38	Total	O	0
			38	38	
61	M	39	Total	O	0
			39	39	
61	N	22	Total	O	0
			22	22	
61	O	15	Total	O	0
			15	15	
61	P	54	Total	O	0
			54	54	
61	Q	36	Total	O	0
			36	36	
61	R	9	Total	O	0
			9	9	

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Mol	Chain	Residues	Atoms		AltConf
61	S	7	Total 7	O 7	0
61	T	3	Total 3	O 3	0
61	V	8	Total 8	O 8	0
61	W	12	Total 12	O 12	0
61	X	2	Total 2	O 2	0
61	Y	13	Total 13	O 13	0
61	Z	10	Total 10	O 10	0
61	a	6	Total 6	O 6	0
61	c	7	Total 7	O 7	0
61	d	5	Total 5	O 5	0
61	e	6	Total 6	O 6	0
61	f	1	Total 1	O 1	0
61	g	9	Total 9	O 9	0
61	h	2	Total 2	O 2	0
61	i	9	Total 9	O 9	0
61	k	1	Total 1	O 1	0
61	l	21	Total 21	O 21	0
61	m	22	Total 22	O 22	0
61	n	5	Total 5	O 5	0
61	o	1	Total 1	O 1	0
61	p	14	Total 14	O 14	0

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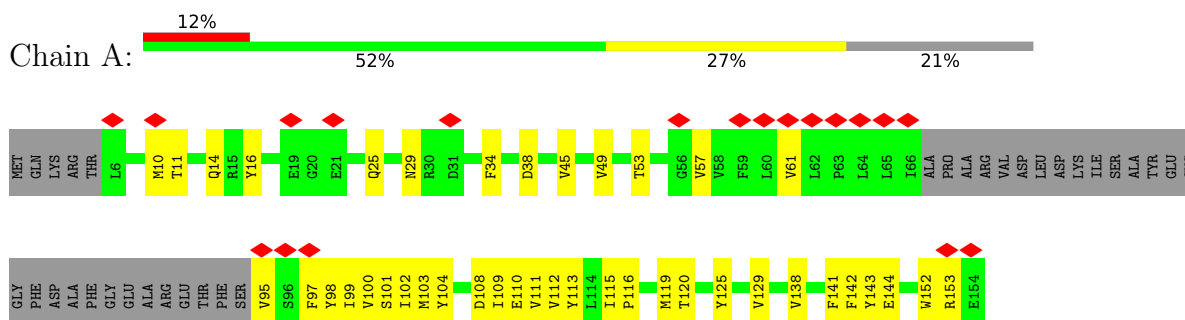
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Mol	Chain	Residues	Atoms		AltConf
61	q	8	Total 8	O 8	0
61	r	7	Total 7	O 7	0
61	s	8	Total 8	O 8	0
61	t	7	Total 7	O 7	0
61	x	25	Total 25	O 25	0
61	y	28	Total 28	O 28	0
61	z	24	Total 24	O 24	0

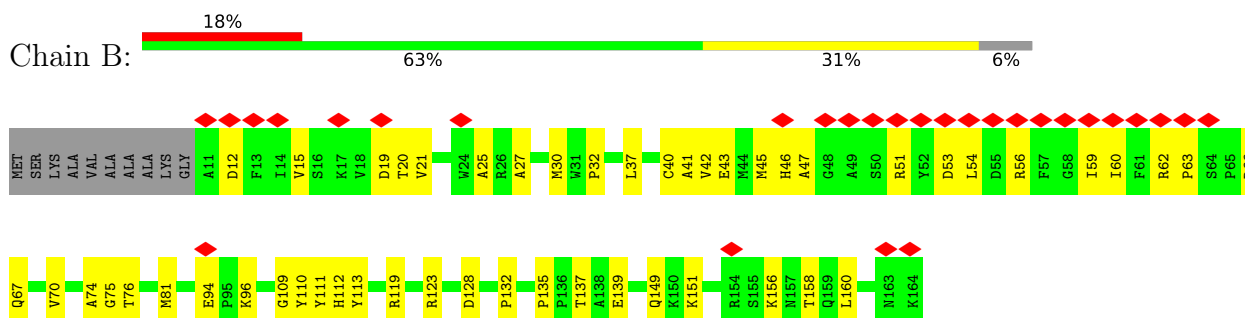
3 Residue-property plots [i](#)

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.

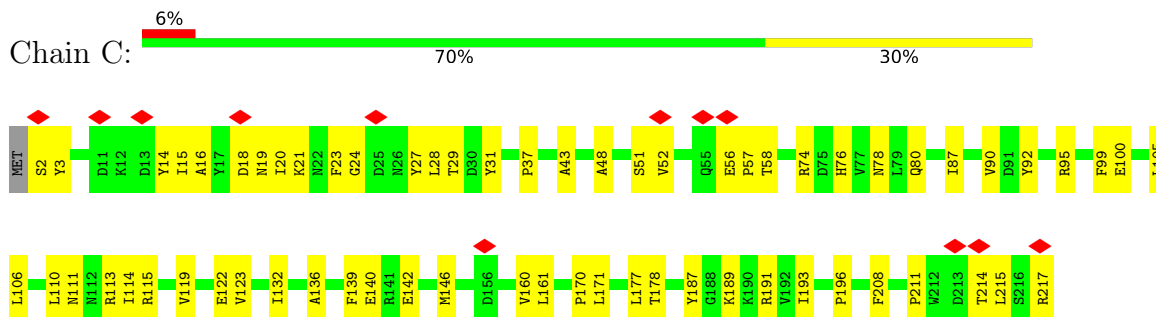
• Molecule 1: ND3



• Molecule 2: PSST

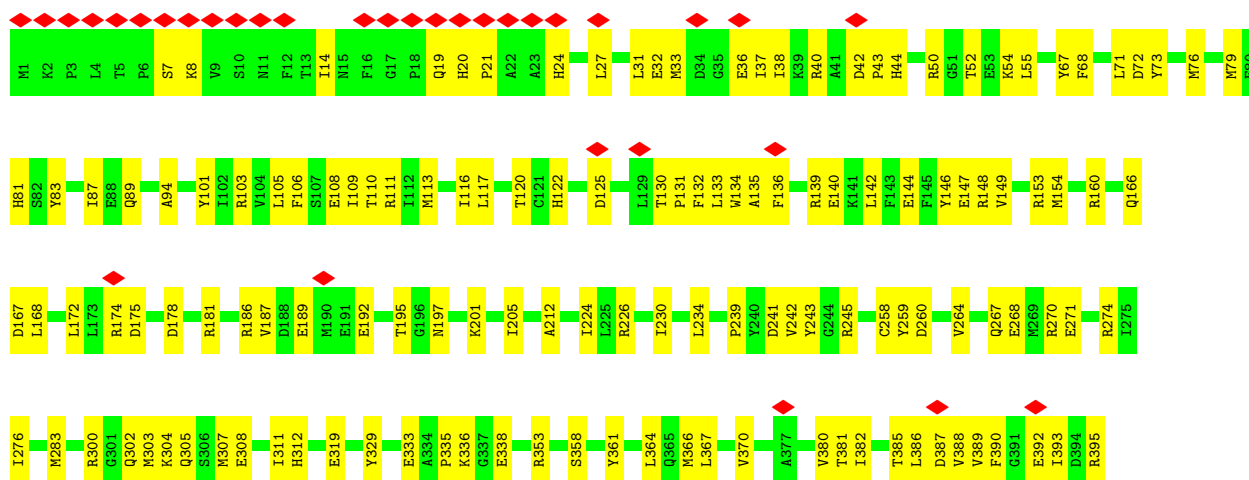


• Molecule 3: ND9

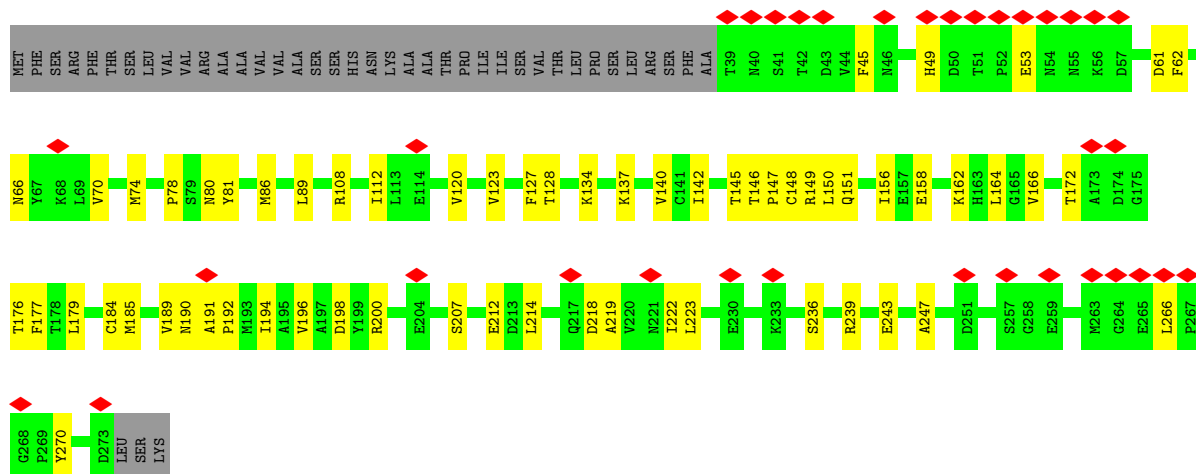


• Molecule 4: ND7

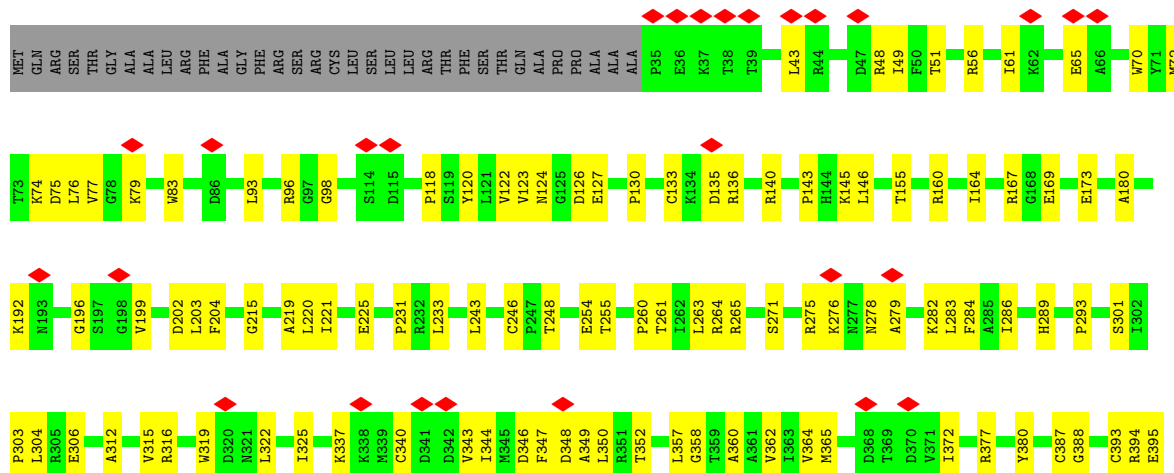


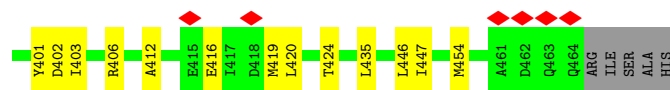


• Molecule 5: 24 kDa

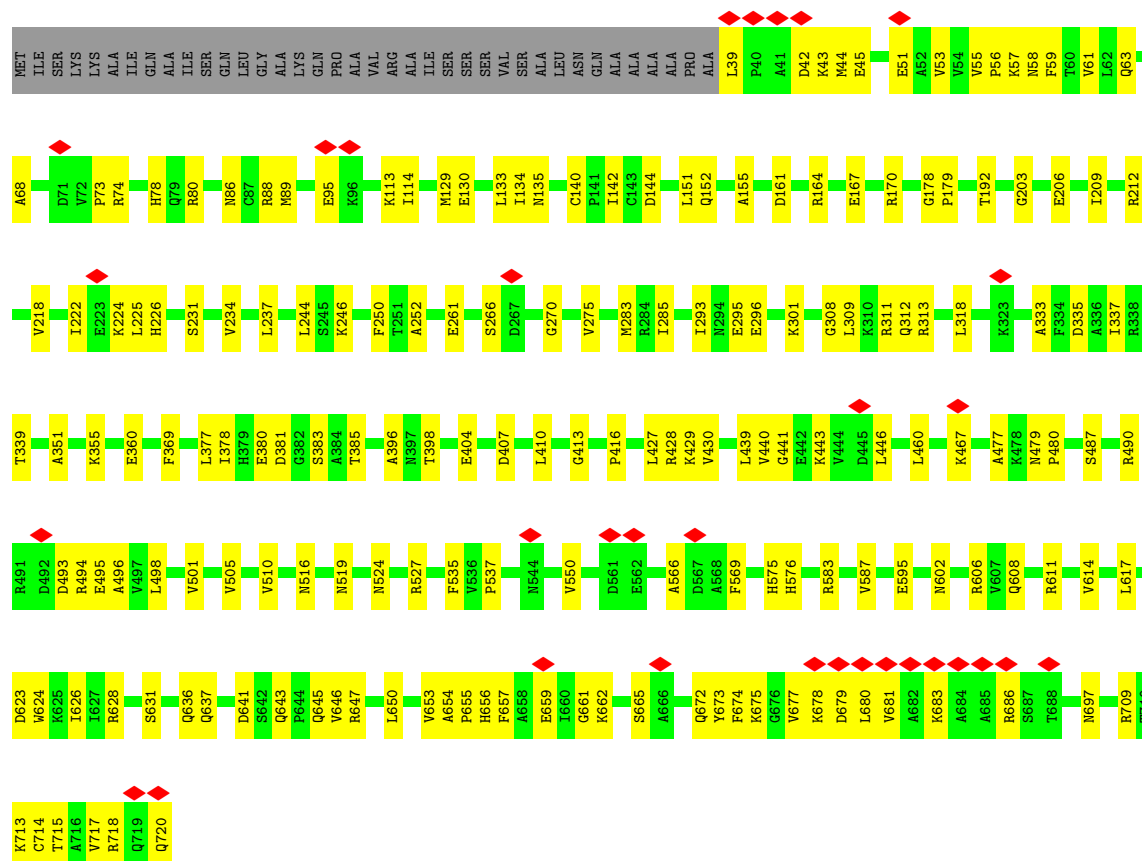


• Molecule 6: 51 kDa

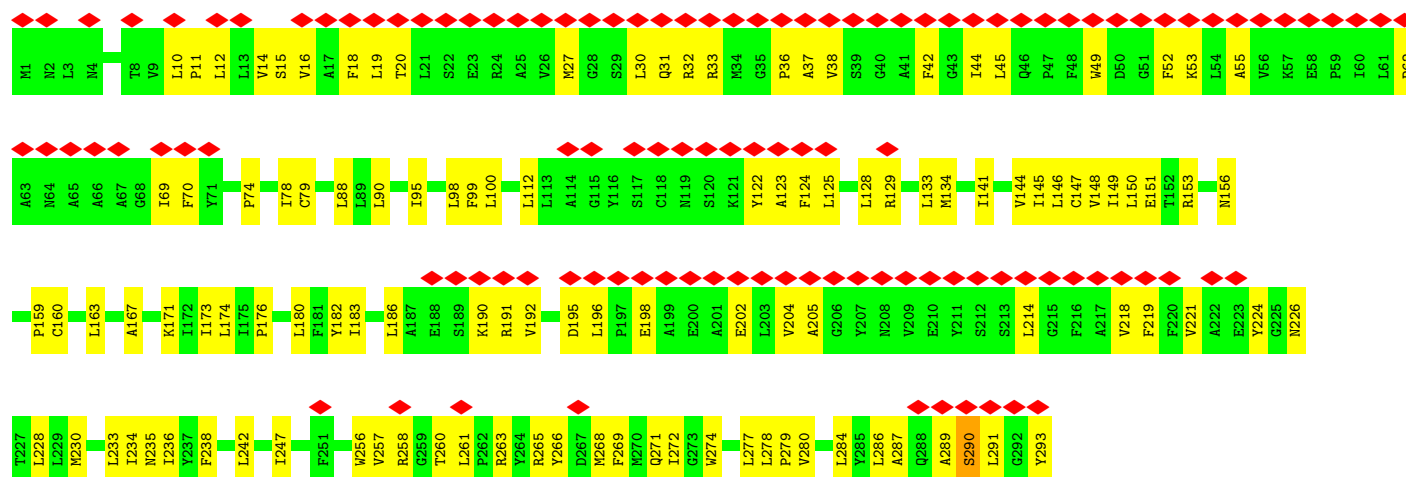
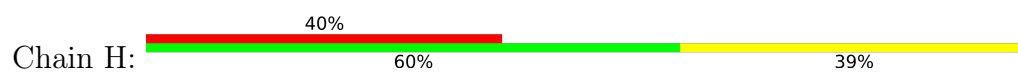




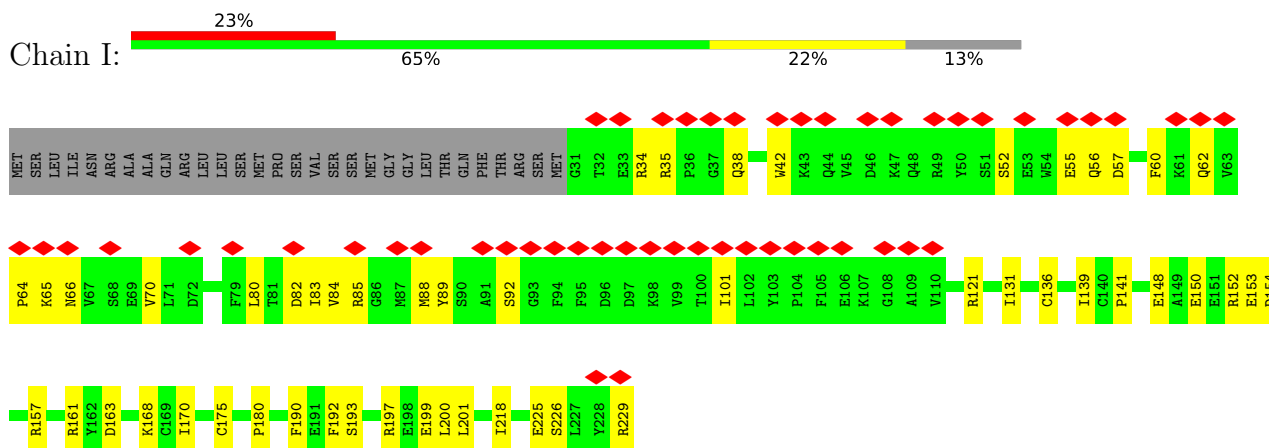
• Molecule 7: 75 kDa



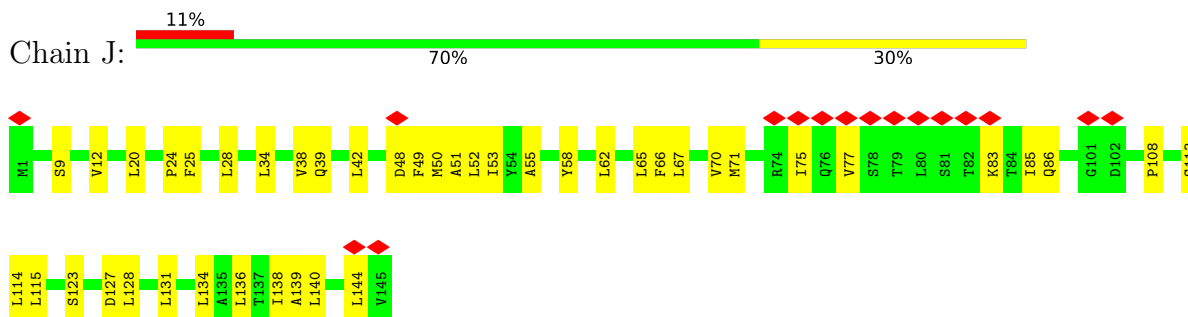
• Molecule 8: ND1



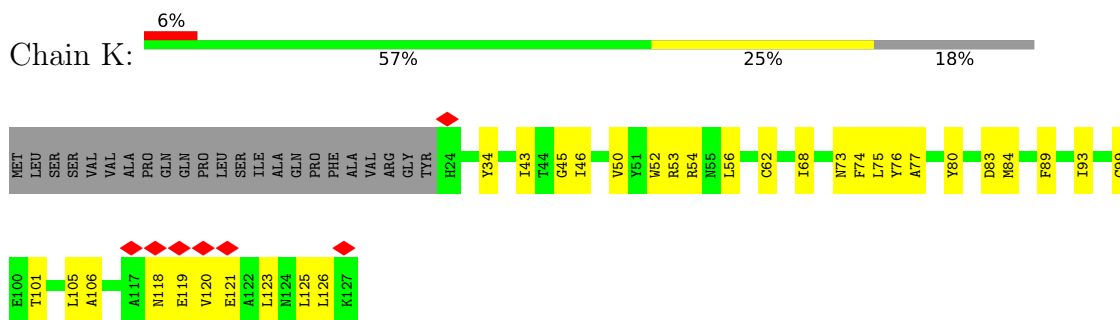
- Molecule 9: TYKY



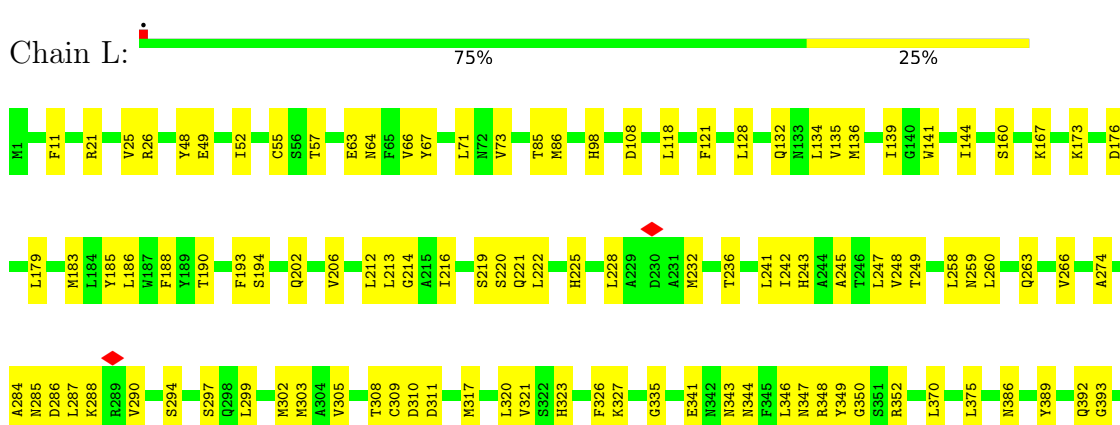
- Molecule 10: ND6



- Molecule 11: ND4L

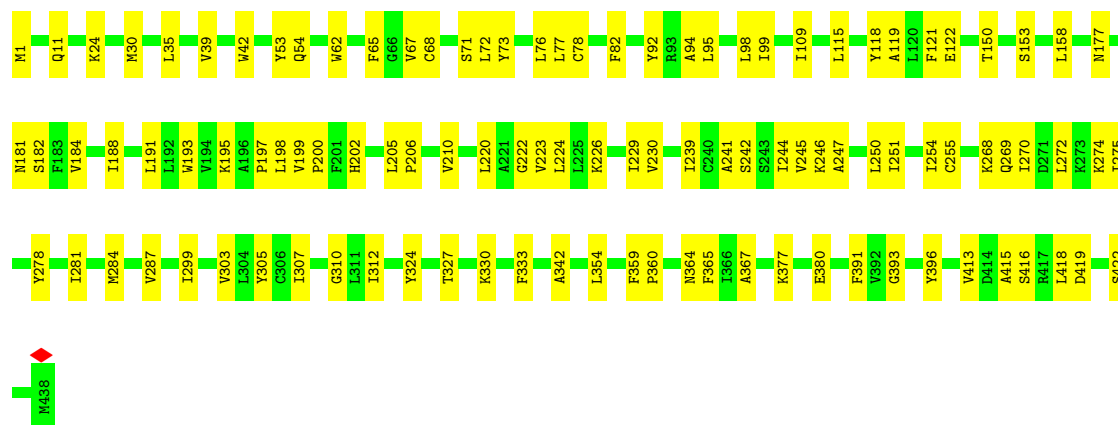
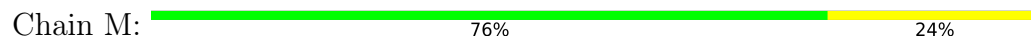


- Molecule 12: ND5

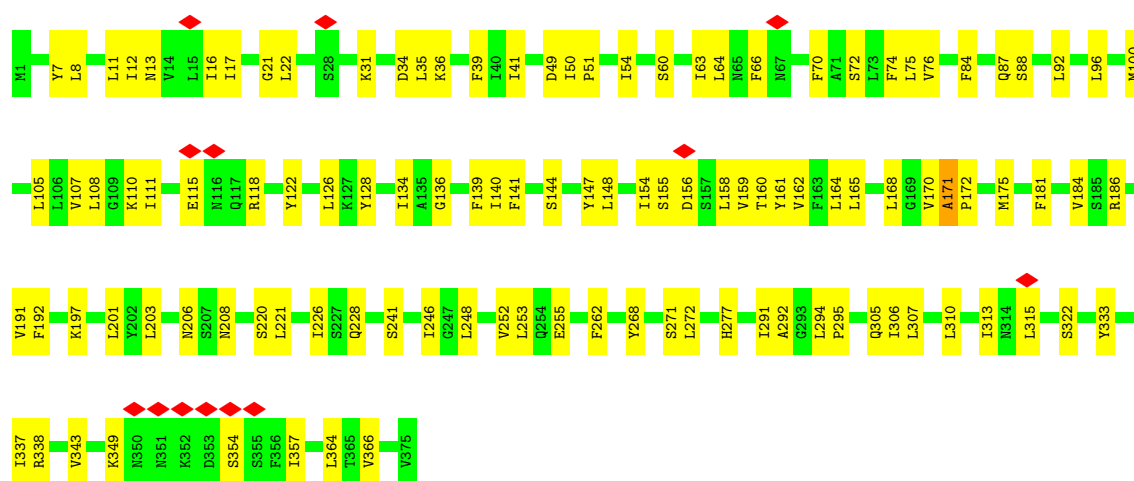




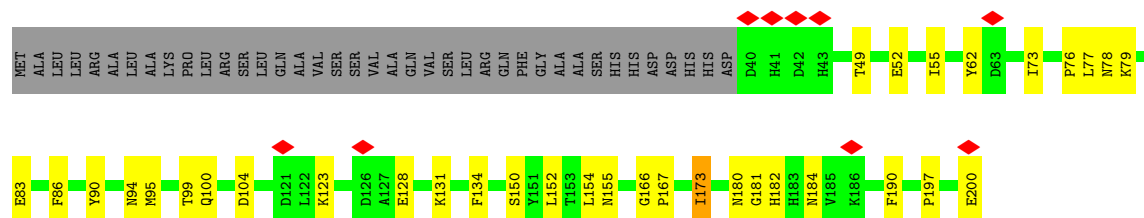
• Molecule 13: ND4



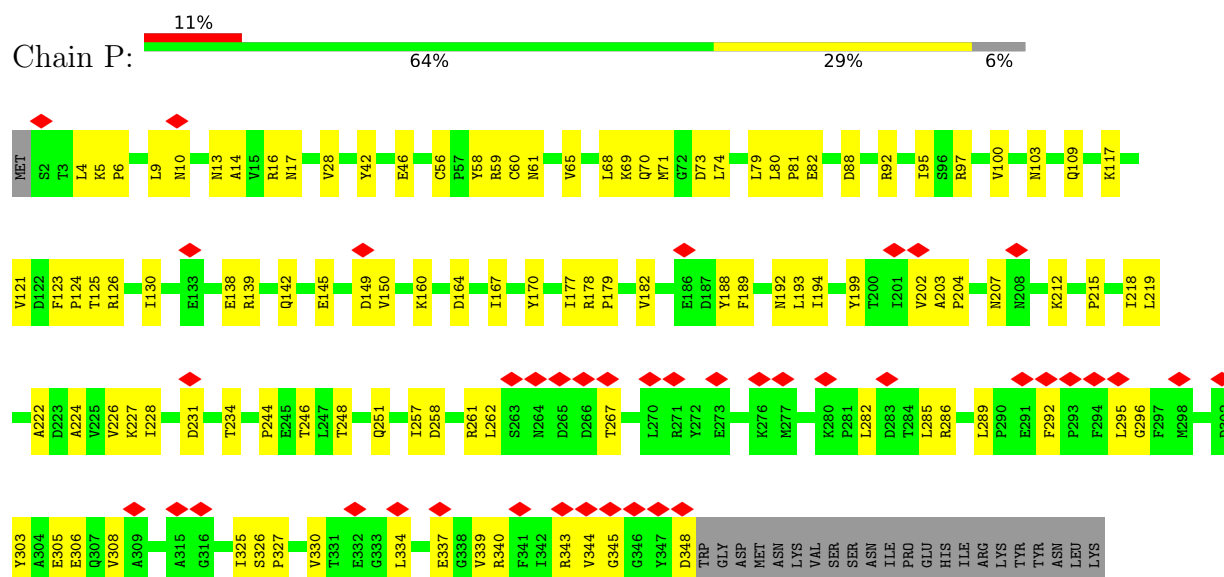
• Molecule 14: ND2



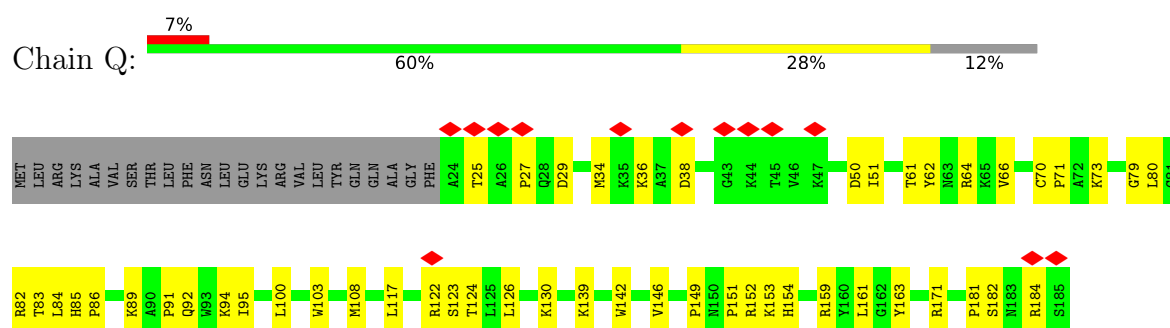
• Molecule 15: C1-FDX



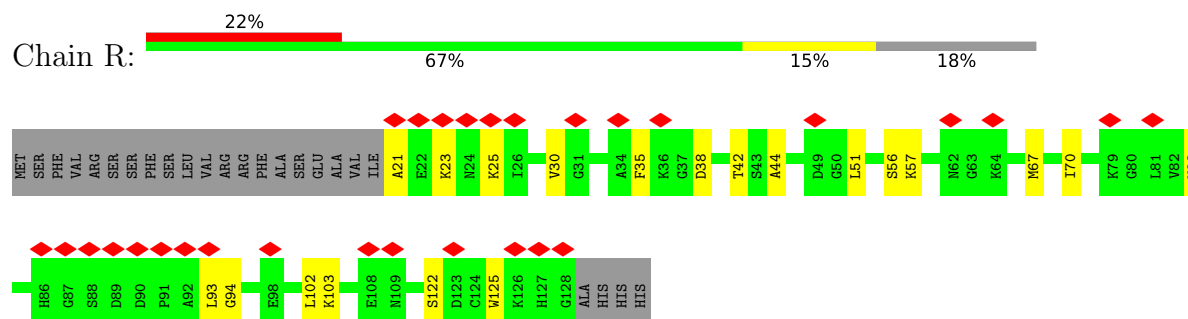
- Molecule 16: 39 kDa



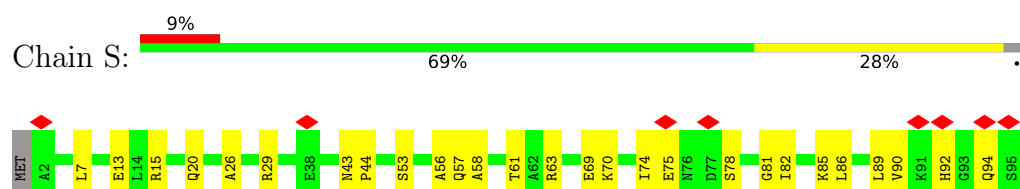
- Molecule 17: 18 kDa



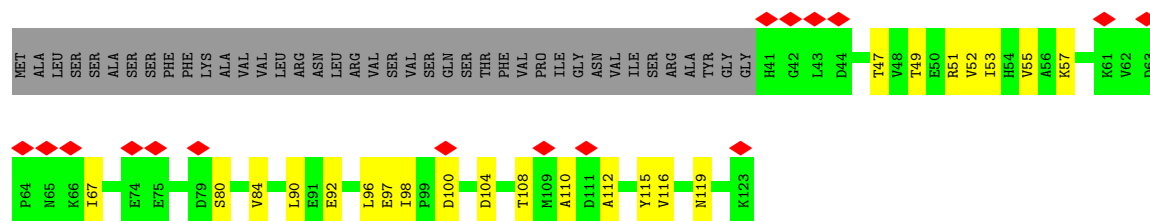
- Molecule 18: 13 kDa



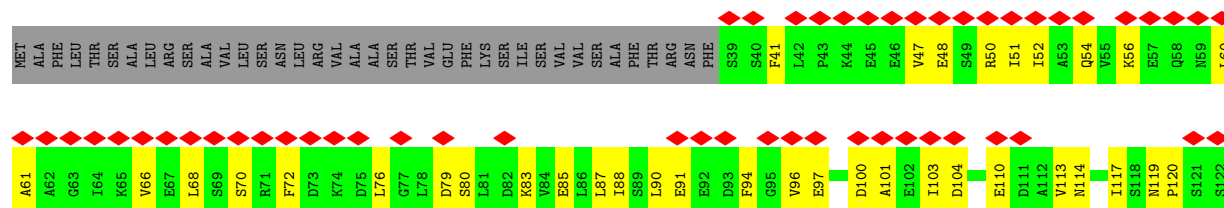
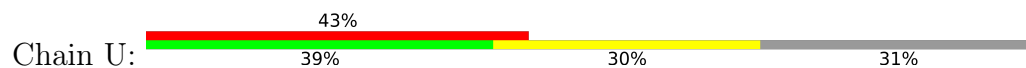
- Molecule 19: B8



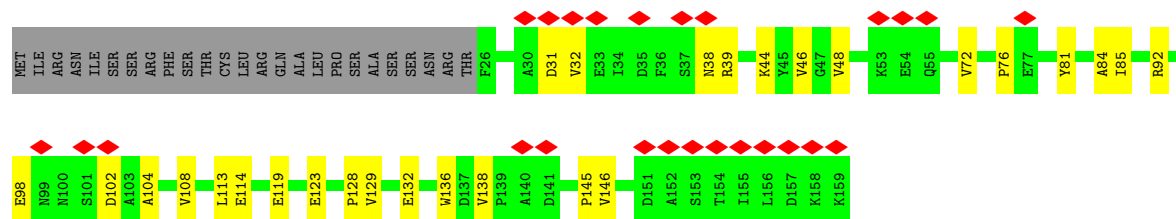
- Molecule 20: SDAP1



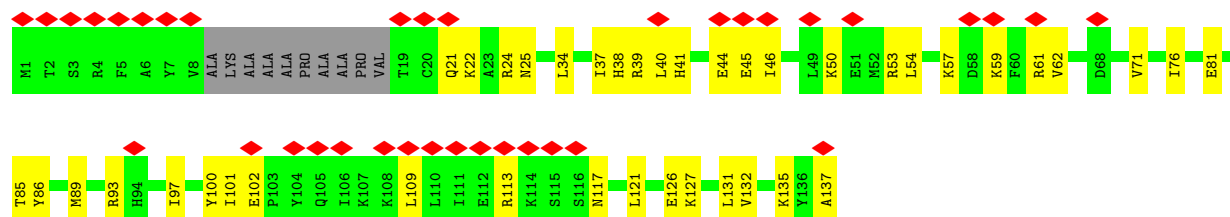
- Molecule 21: SDAP2



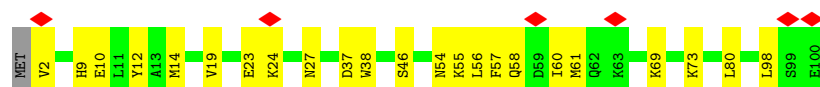
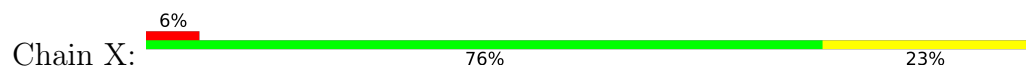
- Molecule 22: B13



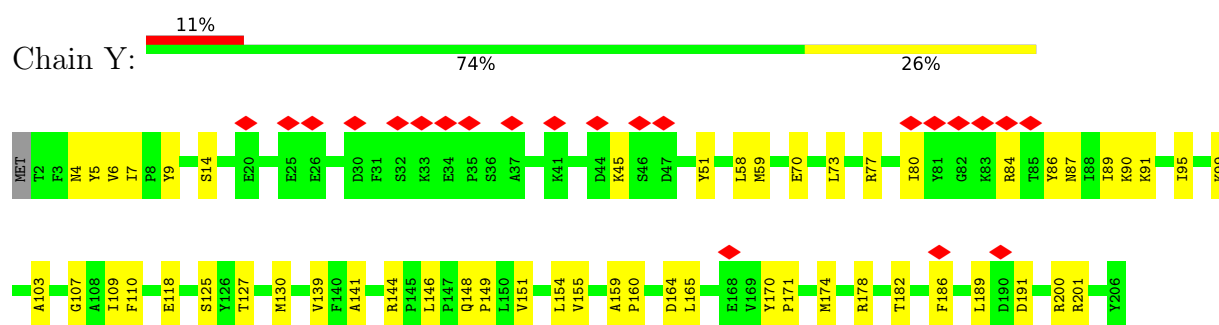
- Molecule 23: B14



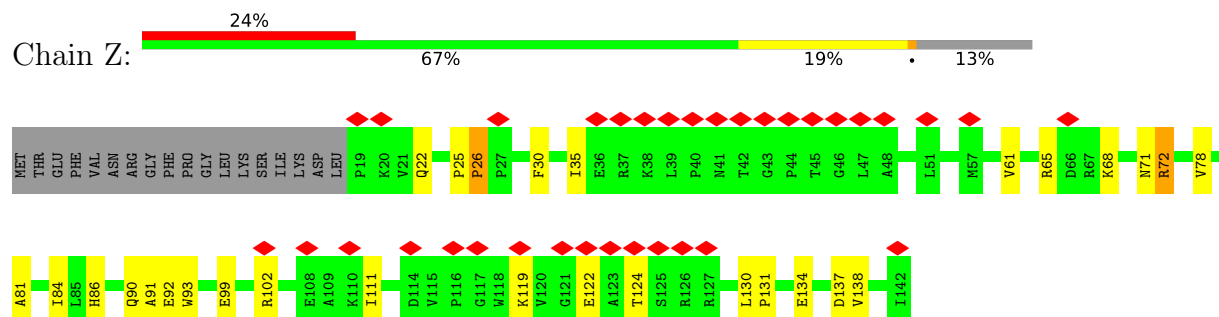
- Molecule 24: PGIV



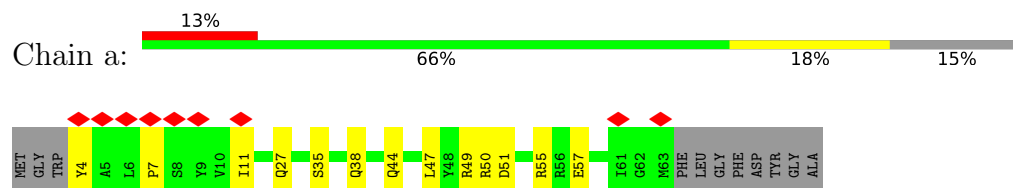
- Molecule 25: B14.7



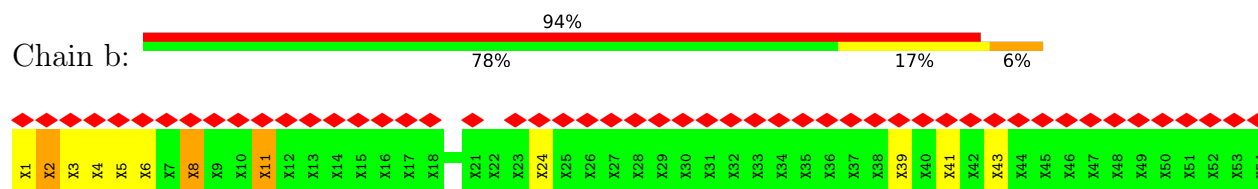
- Molecule 26: B16.6



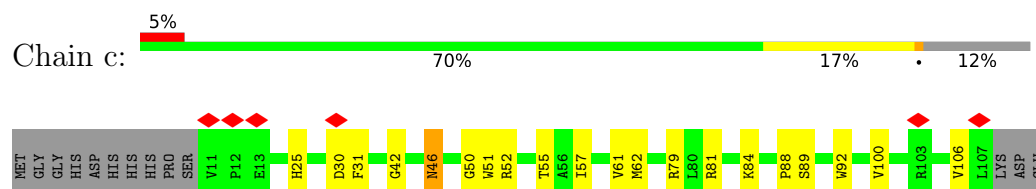
- Molecule 27: MWFE



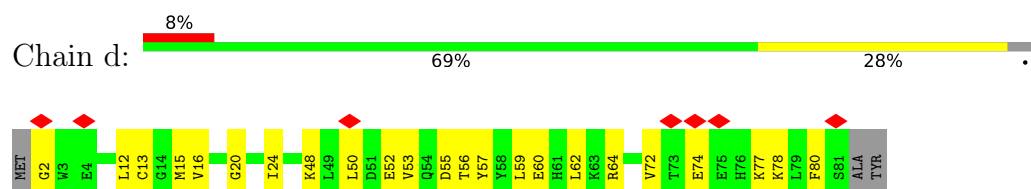
- Molecule 28: B9



- Molecule 29: KFYI



- Molecule 30: B14.5b



- Molecule 31: 15 kDa

Chain e: 



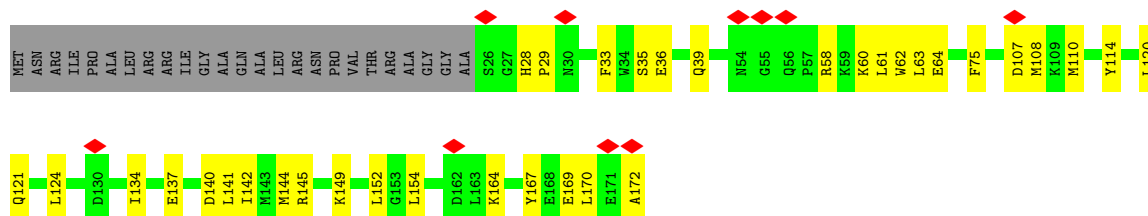
- Molecule 32: MNLL

Chain f: 



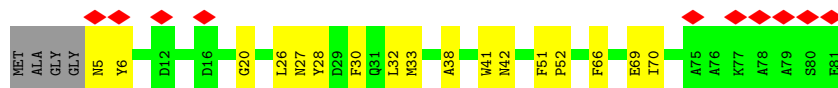
- Molecule 33: ESSS

Chain g: 



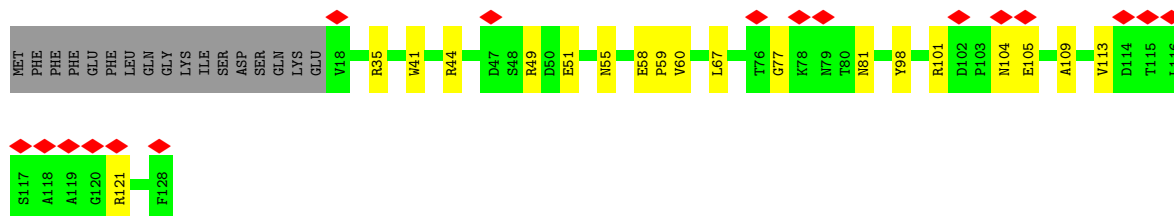
- Molecule 34: NUOP4

Chain h: 

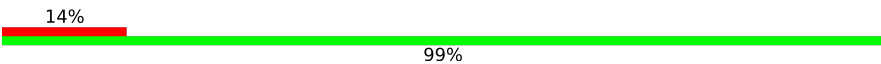


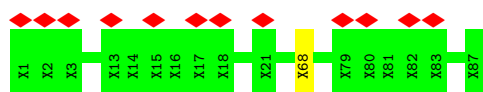
- Molecule 35: NUOP5

Chain i: 

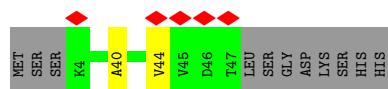
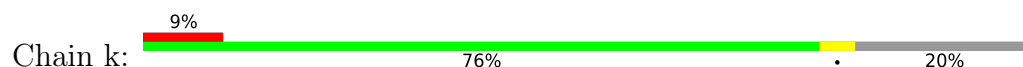


- Molecule 36: AGGG

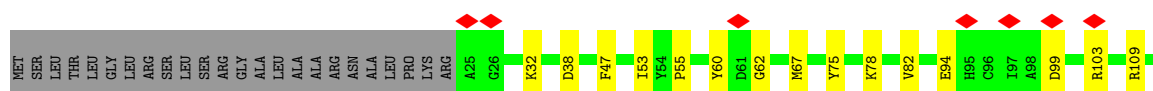
Chain j: 



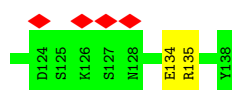
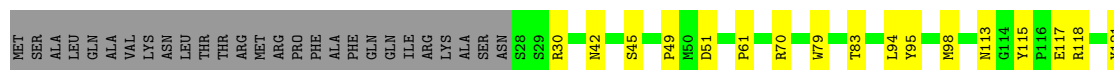
- Molecule 37: B12



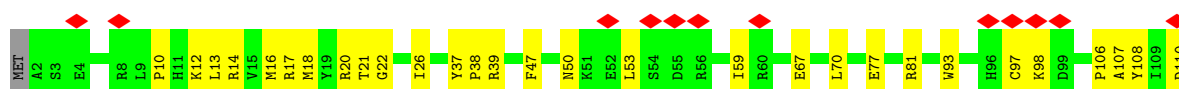
- Molecule 38: ASHI



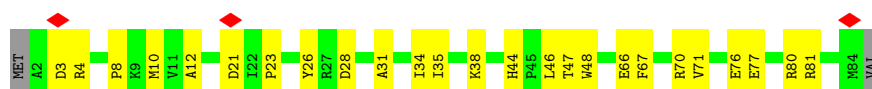
- Molecule 39: B15



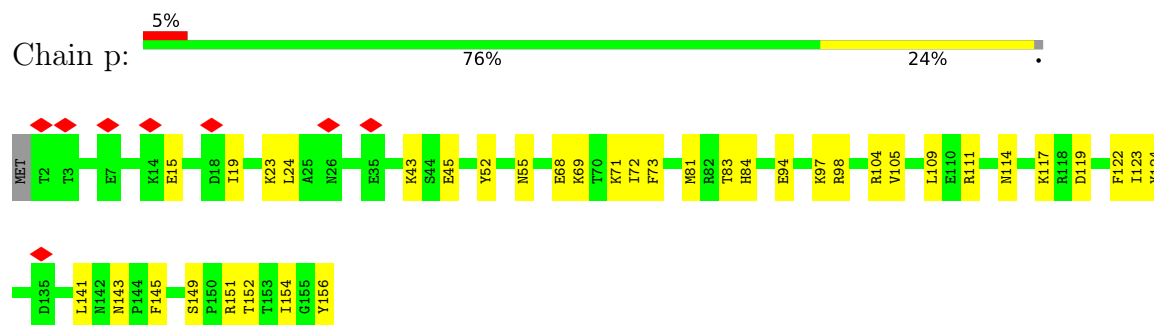
- Molecule 40: Complex I-B22



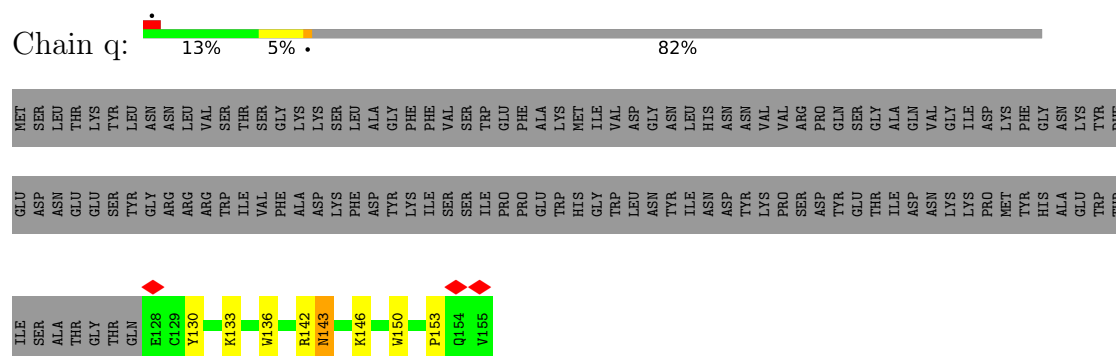
- Molecule 41: B18



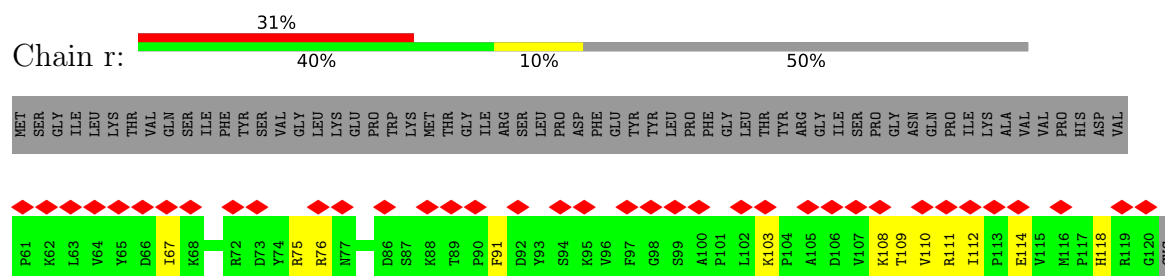
- Molecule 42: PDSW



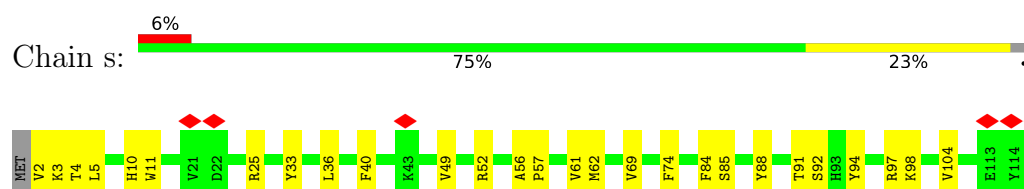
- Molecule 43: B17.2



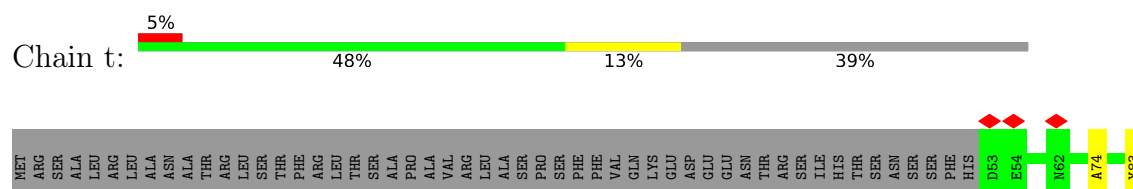
- Molecule 44: B14.5a

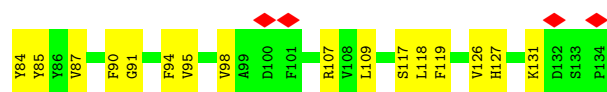


- Molecule 45: NUOP7

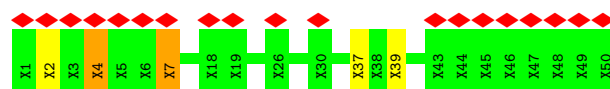
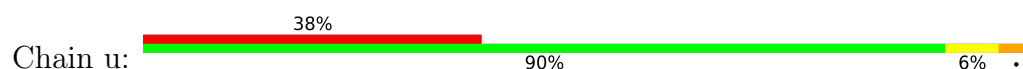


- Molecule 46: NUOP8

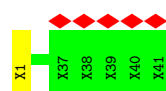




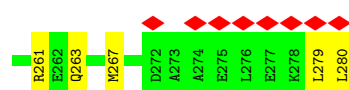
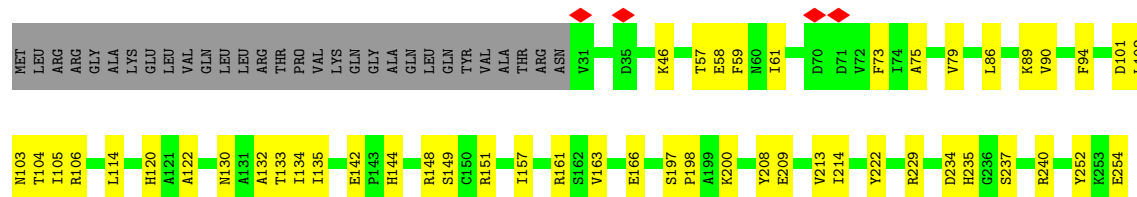
- Molecule 47: unknown



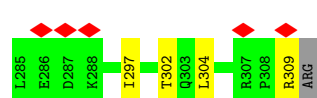
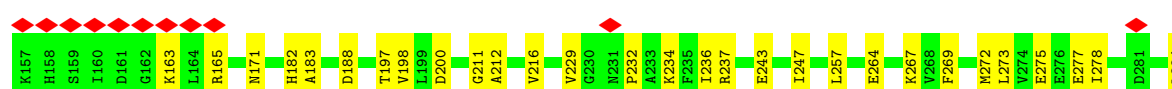
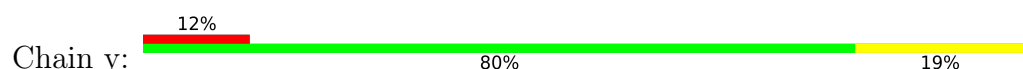
- Molecule 48: unknown



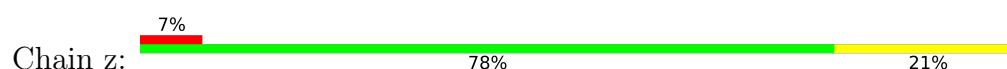
- Molecule 49: CAL

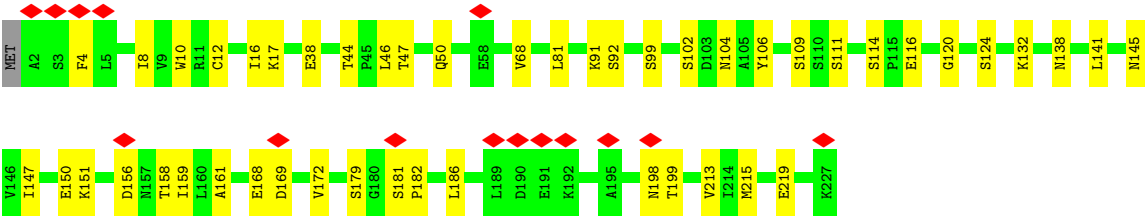


- Molecule 50: CA2



- Molecule 51: CA3





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	42350	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	64	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.119	Depositor
Minimum map value	-0.060	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.018	Depositor
Map size (Å)	502.2, 502.2, 502.2	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.837, 0.837, 0.837	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PC7, SF4, NDP, FMN, CDL, PTY, ZN, 8Q1, FES

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	0.20	0/1028	0.42	0/1405
2	B	0.21	0/1240	0.46	0/1685
3	C	0.14	0/1862	0.36	0/2537
4	D	0.21	0/3257	0.47	0/4406
5	E	0.17	0/1843	0.42	0/2497
6	F	0.17	0/3394	0.42	0/4577
7	G	0.15	0/5254	0.36	0/7114
8	H	0.29	0/2287	0.59	1/3116 (0.0%)
9	I	0.17	0/1634	0.41	0/2204
10	J	0.17	0/1142	0.41	0/1558
11	K	0.17	0/812	0.38	0/1102
12	L	0.18	0/4210	0.41	0/5713
13	M	0.18	0/3529	0.41	0/4813
14	N	0.18	0/3050	0.43	0/4154
15	O	0.15	0/1380	0.41	1/1875 (0.1%)
16	P	0.17	0/2750	0.40	0/3726
17	Q	0.14	0/1311	0.35	0/1774
18	R	0.14	0/832	0.35	0/1125
19	S	0.15	0/725	0.36	0/979
20	T	0.17	0/655	0.42	0/891
21	U	0.22	0/663	0.51	0/895
22	V	0.15	0/1069	0.34	0/1448
23	W	0.19	0/1097	0.43	0/1472
24	X	0.18	0/838	0.42	0/1128
25	Y	0.19	0/1630	0.41	0/2227
26	Z	0.23	0/1029	0.50	1/1395 (0.1%)
27	a	0.19	0/532	0.42	0/722
29	c	0.13	0/816	0.39	1/1117 (0.1%)
30	d	0.17	0/667	0.38	0/902
31	e	0.14	0/602	0.41	0/803
32	f	0.17	0/906	0.32	0/1236
33	g	0.17	0/1210	0.38	0/1638

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
34	h	0.13	0/643	0.35	0/870
35	i	0.15	0/943	0.39	0/1275
37	k	0.14	0/381	0.31	0/517
38	l	0.15	0/1053	0.34	0/1435
39	m	0.15	0/967	0.36	0/1314
40	n	0.19	0/1036	0.39	0/1399
41	o	0.15	0/724	0.37	0/974
42	p	0.17	0/1314	0.38	0/1766
43	q	0.13	0/254	0.40	0/346
44	r	0.13	0/507	0.35	0/685
45	s	0.16	0/963	0.42	0/1317
46	t	0.17	0/736	0.36	0/1003
49	x	0.15	0/2010	0.37	0/2733
50	y	0.15	0/2363	0.37	0/3215
51	z	0.16	0/1713	0.34	0/2320
All	All	0.17	0/68861	0.41	4/93403 (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	H	0	1
26	Z	0	1
28	b	0	3
47	u	0	2
All	All	0	7

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	c	46	ASN	CB-CA-C	-6.17	109.45	116.54
15	O	173	ILE	N-CA-C	-5.99	106.89	111.62
26	Z	26	PRO	CA-N-CD	-5.35	104.51	112.00
8	H	30	LEU	CA-CB-CG	5.15	134.33	116.30

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	H	290	SER	Peptide
26	Z	72	ARG	Sidechain
28	b	11	UNK	Peptide
28	b	2	UNK	Peptide
28	b	8	UNK	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	999	0	989	40	0
2	B	1206	0	1193	59	0
3	C	1808	0	1750	61	0
4	D	3178	0	3148	118	0
5	E	1806	0	1769	52	0
6	F	3322	0	3278	87	0
7	G	5166	0	5193	141	0
8	H	2237	0	2336	113	0
9	I	1602	0	1534	49	0
10	J	1120	0	1189	42	0
11	K	798	0	801	31	0
12	L	4111	0	4124	120	0
13	M	3425	0	3509	86	0
14	N	2967	0	3053	99	0
15	O	1336	0	1273	25	0
16	P	2701	0	2719	84	0
17	Q	1276	0	1264	43	0
18	R	812	0	781	17	0
19	S	716	0	730	26	0
20	T	645	0	633	20	0
21	U	655	0	647	30	0
22	V	1052	0	1059	22	0
23	W	1074	0	1101	34	0
24	X	816	0	788	21	0
25	Y	1583	0	1559	50	0
26	Z	1003	0	1015	38	0
27	a	515	0	488	18	0
28	b	270	0	58	13	0
29	c	785	0	750	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	d	650	0	641	17	0
31	e	592	0	580	14	0
32	f	877	0	843	15	0
33	g	1176	0	1154	38	0
34	h	625	0	590	16	0
35	i	922	0	893	21	0
36	j	435	0	91	1	0
37	k	367	0	353	1	0
38	l	1018	0	982	31	0
39	m	934	0	861	20	0
40	n	1008	0	997	33	0
41	o	704	0	689	17	0
42	p	1287	0	1275	32	0
43	q	243	0	233	8	0
44	r	493	0	498	18	0
45	s	933	0	942	25	0
46	t	706	0	673	21	0
47	u	250	0	53	5	0
48	w	204	0	42	1	0
49	x	1967	0	1918	41	0
50	y	2316	0	2334	44	0
51	z	1687	0	1709	36	0
52	A	49	0	72	5	0
52	L	48	0	73	11	0
52	M	104	0	168	7	0
52	N	104	0	168	13	0
52	z	52	0	84	6	0
53	B	8	0	0	0	0
53	F	8	0	0	2	0
53	G	16	0	0	1	0
53	I	16	0	0	1	0
54	E	4	0	0	1	0
54	G	4	0	0	0	0
55	F	31	0	19	1	0
56	H	50	0	79	7	0
56	L	50	0	79	2	0
56	M	47	0	67	8	0
56	N	50	0	79	1	0
56	Y	50	0	79	4	0
56	m	100	0	158	8	0
57	L	89	0	128	9	0
57	M	100	0	156	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	N	100	0	156	10	0
57	d	100	0	156	3	0
57	t	100	0	156	9	0
58	P	48	0	26	1	0
59	R	1	0	0	0	0
60	W	35	0	0	1	0
60	n	35	0	0	0	0
61	A	6	0	0	0	0
61	B	15	0	0	2	0
61	C	37	0	0	0	0
61	D	43	0	0	3	0
61	E	15	0	0	0	0
61	F	16	0	0	0	0
61	G	114	0	0	3	0
61	H	11	0	0	0	0
61	I	33	0	0	1	0
61	J	3	0	0	0	0
61	K	5	0	0	0	0
61	L	38	0	0	1	0
61	M	39	0	0	0	0
61	N	22	0	0	0	0
61	O	15	0	0	1	0
61	P	54	0	0	2	0
61	Q	36	0	0	2	0
61	R	9	0	0	0	0
61	S	7	0	0	0	0
61	T	3	0	0	1	0
61	V	8	0	0	1	0
61	W	12	0	0	0	0
61	X	2	0	0	0	0
61	Y	13	0	0	0	0
61	Z	10	0	0	0	0
61	a	6	0	0	0	0
61	c	7	0	0	0	0
61	d	5	0	0	0	0
61	e	6	0	0	0	0
61	f	1	0	0	0	0
61	g	9	0	0	0	0
61	h	2	0	0	0	0
61	i	9	0	0	0	0
61	k	1	0	0	0	0
61	l	21	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	m	22	0	0	1	0
61	n	5	0	0	0	0
61	o	1	0	0	0	0
61	p	14	0	0	0	0
61	q	8	0	0	0	0
61	r	7	0	0	0	0
61	s	8	0	0	0	0
61	t	7	0	0	0	0
61	x	25	0	0	0	0
61	y	28	0	0	0	0
61	z	24	0	0	0	0
All	All	70559	0	68985	1689	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 12.

The worst 5 of 1689 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)
8:H:286:LEU:O	8:H:290:SER:OG	1.85	0.92
47:u:37:UNK:O	47:u:39:UNK:N	2.03	0.92
2:B:62:ARG:HE	2:B:63:PRO:HD2	1.32	0.91
28:b:41:UNK:O	28:b:43:UNK:N	2.03	0.91
12:L:26:ARG:HH21	33:g:29:PRO:HD2	1.37	0.89

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	A	117/154 (76%)	115 (98%)	2 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	152/164 (93%)	146 (96%)	6 (4%)	0	100	100
3	C	214/217 (99%)	211 (99%)	3 (1%)	0	100	100
4	D	393/395 (100%)	386 (98%)	6 (2%)	1 (0%)	36	65
5	E	233/276 (84%)	226 (97%)	7 (3%)	0	100	100
6	F	428/469 (91%)	415 (97%)	13 (3%)	0	100	100
7	G	680/720 (94%)	665 (98%)	15 (2%)	0	100	100
8	H	291/293 (99%)	283 (97%)	8 (3%)	0	100	100
9	I	197/229 (86%)	195 (99%)	2 (1%)	0	100	100
10	J	143/145 (99%)	138 (96%)	5 (4%)	0	100	100
11	K	102/127 (80%)	101 (99%)	1 (1%)	0	100	100
12	L	534/536 (100%)	525 (98%)	9 (2%)	0	100	100
13	M	436/438 (100%)	425 (98%)	11 (2%)	0	100	100
14	N	373/375 (100%)	369 (99%)	3 (1%)	1 (0%)	36	65
15	O	159/200 (80%)	154 (97%)	5 (3%)	0	100	100
16	P	345/370 (93%)	332 (96%)	13 (4%)	0	100	100
17	Q	160/185 (86%)	156 (98%)	4 (2%)	0	100	100
18	R	106/132 (80%)	103 (97%)	3 (3%)	0	100	100
19	S	93/98 (95%)	92 (99%)	1 (1%)	0	100	100
20	T	81/123 (66%)	81 (100%)	0	0	100	100
21	U	82/122 (67%)	72 (88%)	10 (12%)	0	100	100
22	V	132/159 (83%)	129 (98%)	3 (2%)	0	100	100
23	W	123/137 (90%)	121 (98%)	2 (2%)	0	100	100
24	X	97/100 (97%)	95 (98%)	2 (2%)	0	100	100
25	Y	203/206 (98%)	200 (98%)	3 (2%)	0	100	100
26	Z	122/142 (86%)	118 (97%)	4 (3%)	0	100	100
27	a	58/71 (82%)	57 (98%)	1 (2%)	0	100	100
29	c	95/110 (86%)	94 (99%)	1 (1%)	0	100	100
30	d	78/83 (94%)	77 (99%)	1 (1%)	0	100	100
31	e	69/75 (92%)	67 (97%)	2 (3%)	0	100	100
32	f	109/121 (90%)	109 (100%)	0	0	100	100
33	g	145/172 (84%)	143 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	h	75/81 (93%)	75 (100%)	0	0	100	100
35	i	109/128 (85%)	108 (99%)	1 (1%)	0	100	100
37	k	42/55 (76%)	41 (98%)	1 (2%)	0	100	100
38	l	125/151 (83%)	124 (99%)	1 (1%)	0	100	100
39	m	109/138 (79%)	107 (98%)	2 (2%)	0	100	100
40	n	118/121 (98%)	116 (98%)	2 (2%)	0	100	100
41	o	81/85 (95%)	81 (100%)	0	0	100	100
42	p	153/156 (98%)	152 (99%)	1 (1%)	0	100	100
43	q	26/155 (17%)	26 (100%)	0	0	100	100
44	r	58/121 (48%)	58 (100%)	0	0	100	100
45	s	113/118 (96%)	109 (96%)	4 (4%)	0	100	100
46	t	80/134 (60%)	80 (100%)	0	0	100	100
49	x	248/280 (89%)	245 (99%)	3 (1%)	0	100	100
50	y	306/310 (99%)	298 (97%)	8 (3%)	0	100	100
51	z	224/227 (99%)	219 (98%)	5 (2%)	0	100	100
All	All	8417/9404 (90%)	8239 (98%)	176 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
14	N	171	ALA
4	D	242	VAL

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	107/133 (80%)	107 (100%)	0	100	100
2	B	129/134 (96%)	129 (100%)	0	100	100
3	C	199/200 (100%)	199 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	339/339 (100%)	339 (100%)	0	100	100
5	E	197/232 (85%)	196 (100%)	1 (0%)	81	83
6	F	343/372 (92%)	343 (100%)	0	100	100
7	G	544/570 (95%)	544 (100%)	0	100	100
8	H	240/240 (100%)	240 (100%)	0	100	100
9	I	175/201 (87%)	175 (100%)	0	100	100
10	J	129/129 (100%)	129 (100%)	0	100	100
11	K	84/103 (82%)	84 (100%)	0	100	100
12	L	438/438 (100%)	438 (100%)	0	100	100
13	M	376/376 (100%)	376 (100%)	0	100	100
14	N	331/331 (100%)	330 (100%)	1 (0%)	86	86
15	O	146/177 (82%)	146 (100%)	0	100	100
16	P	296/318 (93%)	296 (100%)	0	100	100
17	Q	134/154 (87%)	134 (100%)	0	100	100
18	R	86/107 (80%)	86 (100%)	0	100	100
19	S	77/79 (98%)	77 (100%)	0	100	100
20	T	73/106 (69%)	73 (100%)	0	100	100
21	U	76/108 (70%)	76 (100%)	0	100	100
22	V	116/139 (84%)	116 (100%)	0	100	100
23	W	119/123 (97%)	119 (100%)	0	100	100
24	X	85/86 (99%)	85 (100%)	0	100	100
25	Y	165/166 (99%)	165 (100%)	0	100	100
26	Z	107/123 (87%)	107 (100%)	0	100	100
27	a	50/57 (88%)	50 (100%)	0	100	100
29	c	80/91 (88%)	80 (100%)	0	100	100
30	d	68/70 (97%)	68 (100%)	0	100	100
31	e	64/68 (94%)	64 (100%)	0	100	100
32	f	92/100 (92%)	92 (100%)	0	100	100
33	g	122/139 (88%)	122 (100%)	0	100	100
34	h	64/65 (98%)	64 (100%)	0	100	100
35	i	97/113 (86%)	97 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	k	35/45 (78%)	35 (100%)	0	100	100
38	l	110/128 (86%)	110 (100%)	0	100	100
39	m	100/123 (81%)	100 (100%)	0	100	100
40	n	106/107 (99%)	106 (100%)	0	100	100
41	o	74/76 (97%)	74 (100%)	0	100	100
42	p	140/141 (99%)	140 (100%)	0	100	100
43	q	26/138 (19%)	25 (96%)	1 (4%)	29	58
44	r	55/109 (50%)	55 (100%)	0	100	100
45	s	105/108 (97%)	105 (100%)	0	100	100
46	t	73/119 (61%)	73 (100%)	0	100	100
49	x	209/234 (89%)	209 (100%)	0	100	100
50	y	250/252 (99%)	250 (100%)	0	100	100
51	z	188/189 (100%)	188 (100%)	0	100	100
All	All	7219/7956 (91%)	7216 (100%)	3 (0%)	100	100

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	E	49	HIS
14	N	305	GLN
43	q	143	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 102 such sidechains are listed below:

Mol	Chain	Res	Type
17	Q	150	ASN
25	Y	205	HIS
50	y	244	ASN
18	R	86	HIS
23	W	21	GLN

5.3.3 RNA ⓘ

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 32 ligands modelled in this entry, 1 is monoatomic - leaving 31 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	$\# Z > 2$
52	PC7	z	301	-	51,51,51	0.95	4 (7%)	57,59,59	1.01	2 (3%)
57	CDL	M	502	-	99,99,99	0.87	6 (6%)	105,111,111	1.05	4 (3%)
56	PTY	Y	301	-	49,49,49	0.87	4 (8%)	52,54,54	1.11	2 (3%)
53	SF4	G	803	7	0,12,12	-	-	-		
52	PC7	M	503	-	51,51,51	0.98	4 (7%)	57,59,59	1.09	2 (3%)
60	8Q1	n	200	-	31,34,34	1.75	6 (19%)	40,43,43	1.74	6 (15%)
52	PC7	M	504	-	51,51,51	0.96	4 (7%)	57,59,59	1.08	2 (3%)
53	SF4	I	500	9	0,12,12	-	-	-		
57	CDL	d	101	-	99,99,99	0.88	8 (8%)	105,111,111	1.10	4 (3%)
52	PC7	L	602	-	47,47,51	1.02	3 (6%)	53,55,59	1.03	2 (3%)
57	CDL	L	601	-	88,88,99	0.93	7 (7%)	94,100,111	1.11	4 (4%)
54	FES	E	500	5	0,4,4	-	-	-		
57	CDL	N	401	-	99,99,99	0.89	6 (6%)	105,111,111	1.10	4 (3%)
53	SF4	G	802	7	0,12,12	-	-	-		
52	PC7	N	403	-	51,51,51	0.99	4 (7%)	57,59,59	1.06	2 (3%)
56	PTY	N	404	-	49,49,49	0.88	4 (8%)	52,54,54	1.10	2 (3%)
58	NDP	P	500	-	49,52,52	2.24	6 (12%)	66,80,80	1.64	13 (19%)
56	PTY	M	501	-	46,46,49	0.90	4 (8%)	49,51,54	1.14	2 (4%)
52	PC7	N	402	-	51,51,51	0.95	4 (7%)	57,59,59	1.04	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
55	FMN	F	500	-	33,33,33	1.05	2 (6%)	48,50,50	1.22	6 (12%)
56	PTY	L	603	-	49,49,49	0.87	4 (8%)	52,54,54	1.11	2 (3%)
52	PC7	A	201	-	48,48,51	0.97	4 (8%)	54,56,59	1.07	2 (3%)
56	PTY	m	201	-	49,49,49	0.87	4 (8%)	52,54,54	1.05	2 (3%)
53	SF4	I	501	9	0,12,12	-	-	-	-	-
57	CDL	t	201	-	99,99,99	0.88	7 (7%)	105,111,111	1.09	4 (3%)
60	8Q1	W	200	-	31,34,34	1.68	6 (19%)	40,43,43	1.56	5 (12%)
56	PTY	H	301	-	49,49,49	0.87	4 (8%)	52,54,54	1.05	2 (3%)
53	SF4	F	501	6	0,12,12	-	-	-	-	-
56	PTY	m	202	-	49,49,49	0.87	4 (8%)	52,54,54	1.06	2 (3%)
54	FES	G	801	7	0,4,4	-	-	-	-	-
53	SF4	B	500	2	0,12,12	-	-	-	-	-

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
52	PC7	z	301	-	-	30/55/55/55	-
57	CDL	M	502	-	-	66/110/110/110	-
56	PTY	Y	301	-	-	33/53/53/53	-
53	SF4	G	803	7	-	-	0/6/5/5
52	PC7	M	503	-	-	25/55/55/55	-
60	8Q1	n	200	-	-	17/41/41/41	-
52	PC7	M	504	-	-	32/55/55/55	-
53	SF4	I	500	9	-	-	0/6/5/5
57	CDL	d	101	-	-	59/110/110/110	-
52	PC7	L	602	-	-	34/51/51/55	-
57	CDL	L	601	-	-	53/99/99/110	-
54	FES	E	500	5	-	-	0/1/1/1
57	CDL	N	401	-	-	66/110/110/110	-
53	SF4	G	802	7	-	-	0/6/5/5
56	PTY	N	404	-	-	23/53/53/53	-
52	PC7	N	403	-	-	35/55/55/55	-
58	NDP	P	500	-	-	10/34/77/77	0/5/5/5
56	PTY	M	501	-	-	22/50/50/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
52	PC7	N	402	-	-	27/55/55/55	-
55	FMN	F	500	-	-	9/18/18/18	0/3/3/3
56	PTY	L	603	-	-	28/53/53/53	-
52	PC7	A	201	-	-	36/52/52/55	-
56	PTY	m	201	-	-	24/53/53/53	-
57	CDL	t	201	-	-	64/110/110/110	-
60	8Q1	W	200	-	-	11/41/41/41	-
53	SF4	I	501	9	-	-	0/6/5/5
56	PTY	H	301	-	-	32/53/53/53	-
53	SF4	F	501	6	-	-	0/6/5/5
56	PTY	m	202	-	-	25/53/53/53	-
54	FES	G	801	7	-	-	0/1/1/1
53	SF4	B	500	2	-	-	0/6/5/5

The worst 5 of 109 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	P	500	NDP	P2B-O2B	12.64	1.83	1.59
60	n	200	8Q1	C34-N36	5.72	1.46	1.33
60	n	200	8Q1	C39-N41	5.49	1.45	1.33
60	W	200	8Q1	C34-N36	5.43	1.45	1.33
60	W	200	8Q1	C39-N41	5.11	1.45	1.33

The worst 5 of 78 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	P	500	NDP	PN-O3-PA	-7.02	108.74	132.83
60	n	200	8Q1	C6-C1-S44	7.00	121.61	113.46
60	W	200	8Q1	C6-C1-S44	6.02	120.47	113.46
52	M	503	PC7	O2-C31-C32	4.76	121.76	111.50
57	N	401	CDL	OA6-CA5-C11	4.40	120.98	111.50

There are no chirality outliers.

5 of 761 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
52	A	201	PC7	O31-C31-O2-C2
52	A	201	PC7	C1-O3P-P-O1P
52	A	201	PC7	C1-O3P-P-O2P

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Mol	Chain	Res	Type	Atoms
52	A	201	PC7	C1-O3P-P-O4P
52	A	201	PC7	C4-O4P-P-O1P

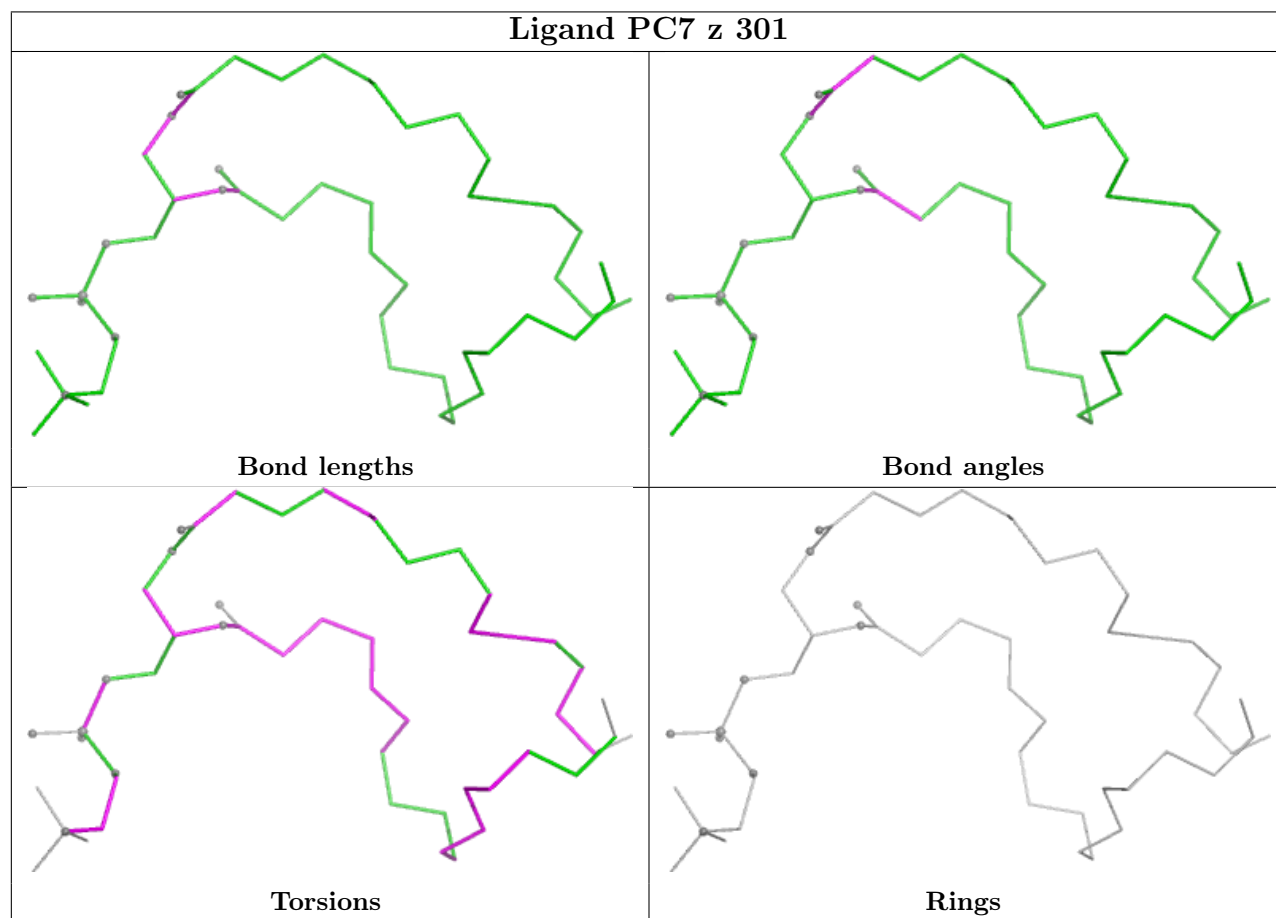
There are no ring outliers.

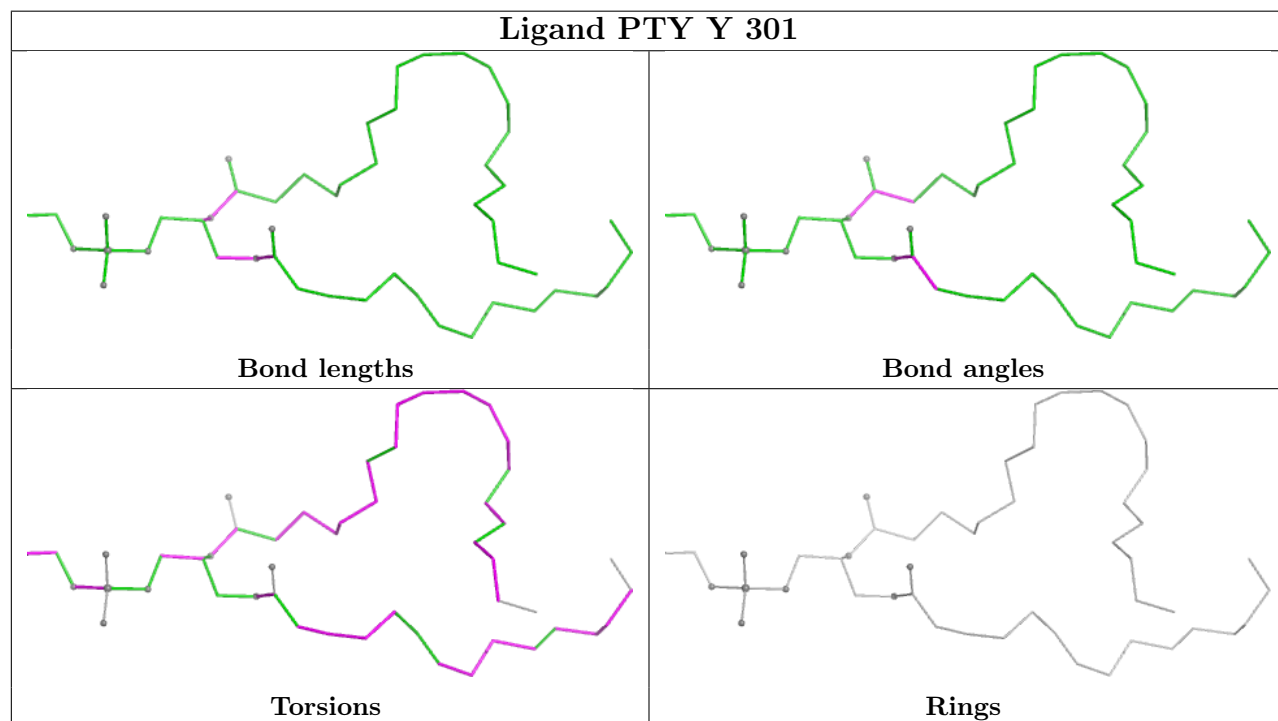
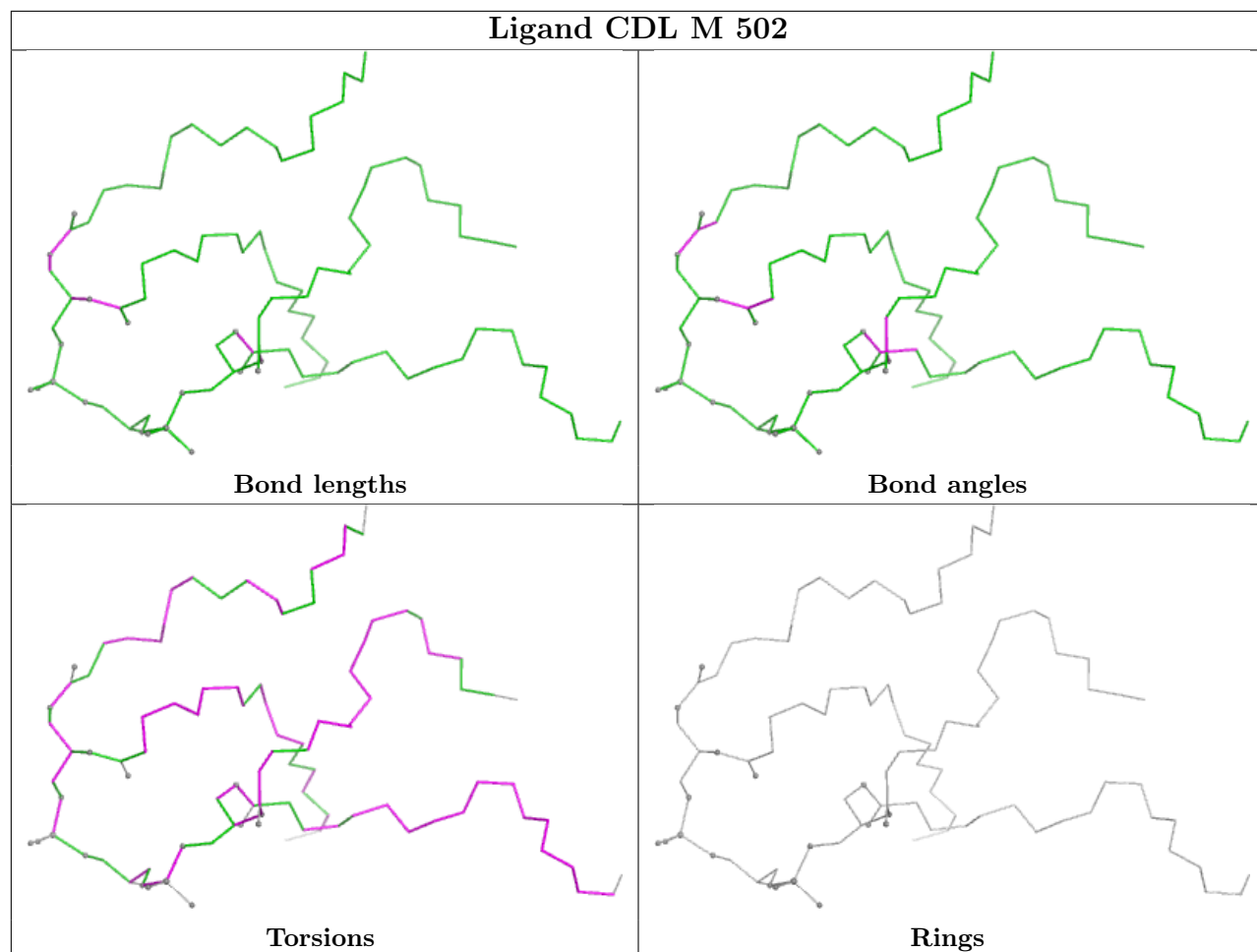
26 monomers are involved in 117 short contacts:

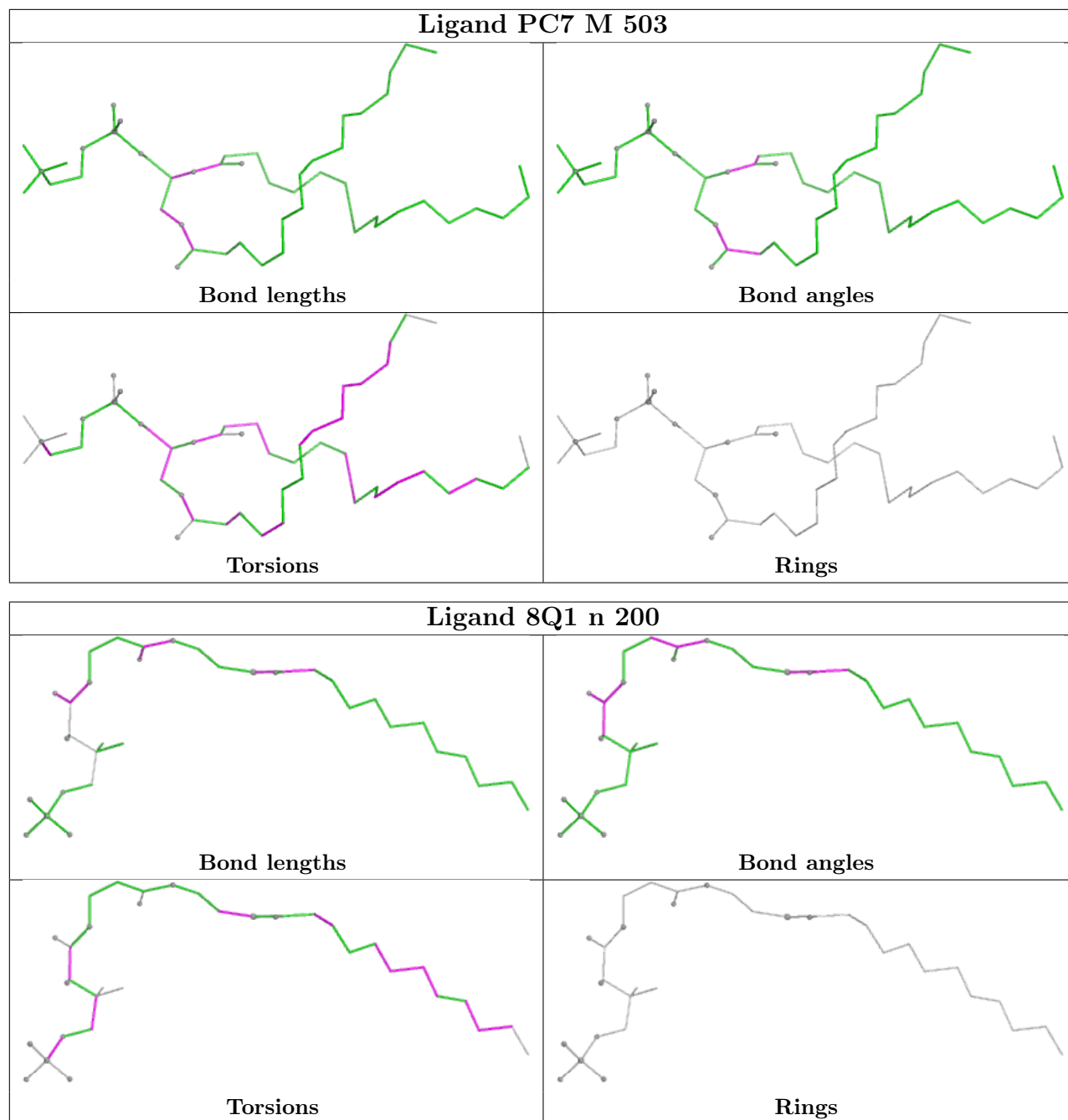
Mol	Chain	Res	Type	Clashes	Symm-Clashes
52	z	301	PC7	6	0
57	M	502	CDL	7	0
56	Y	301	PTY	4	0
52	M	503	PC7	5	0
52	M	504	PC7	2	0
53	I	500	SF4	1	0
57	d	101	CDL	3	0
52	L	602	PC7	11	0
57	L	601	CDL	9	0
54	E	500	FES	1	0
57	N	401	CDL	10	0
53	G	802	SF4	1	0
52	N	403	PC7	11	0
56	N	404	PTY	1	0
58	P	500	NDP	1	0
56	M	501	PTY	8	0
52	N	402	PC7	2	0
55	F	500	FMN	1	0
56	L	603	PTY	2	0
52	A	201	PC7	5	0
56	m	201	PTY	6	0
57	t	201	CDL	9	0
60	W	200	8Q1	1	0
56	H	301	PTY	7	0
53	F	501	SF4	2	0
56	m	202	PTY	2	0

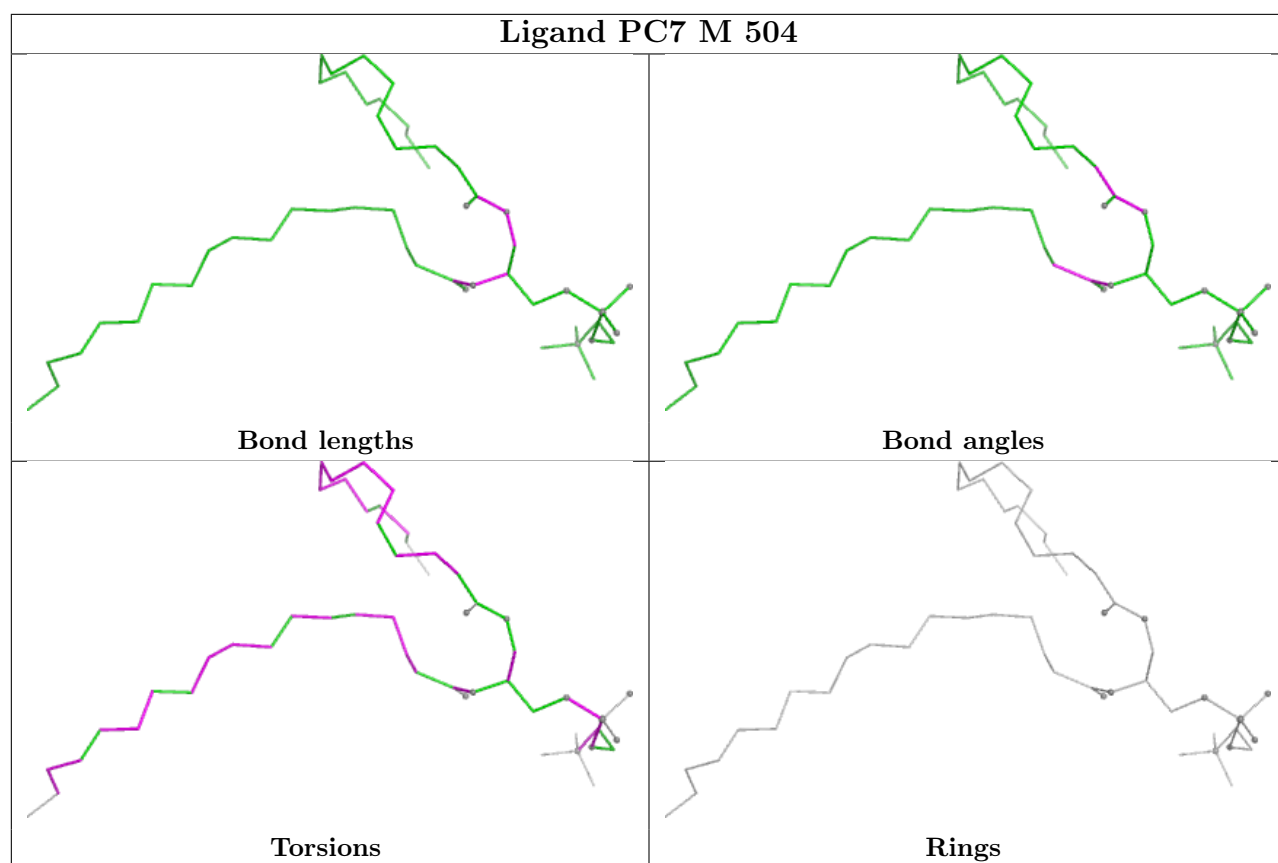
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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

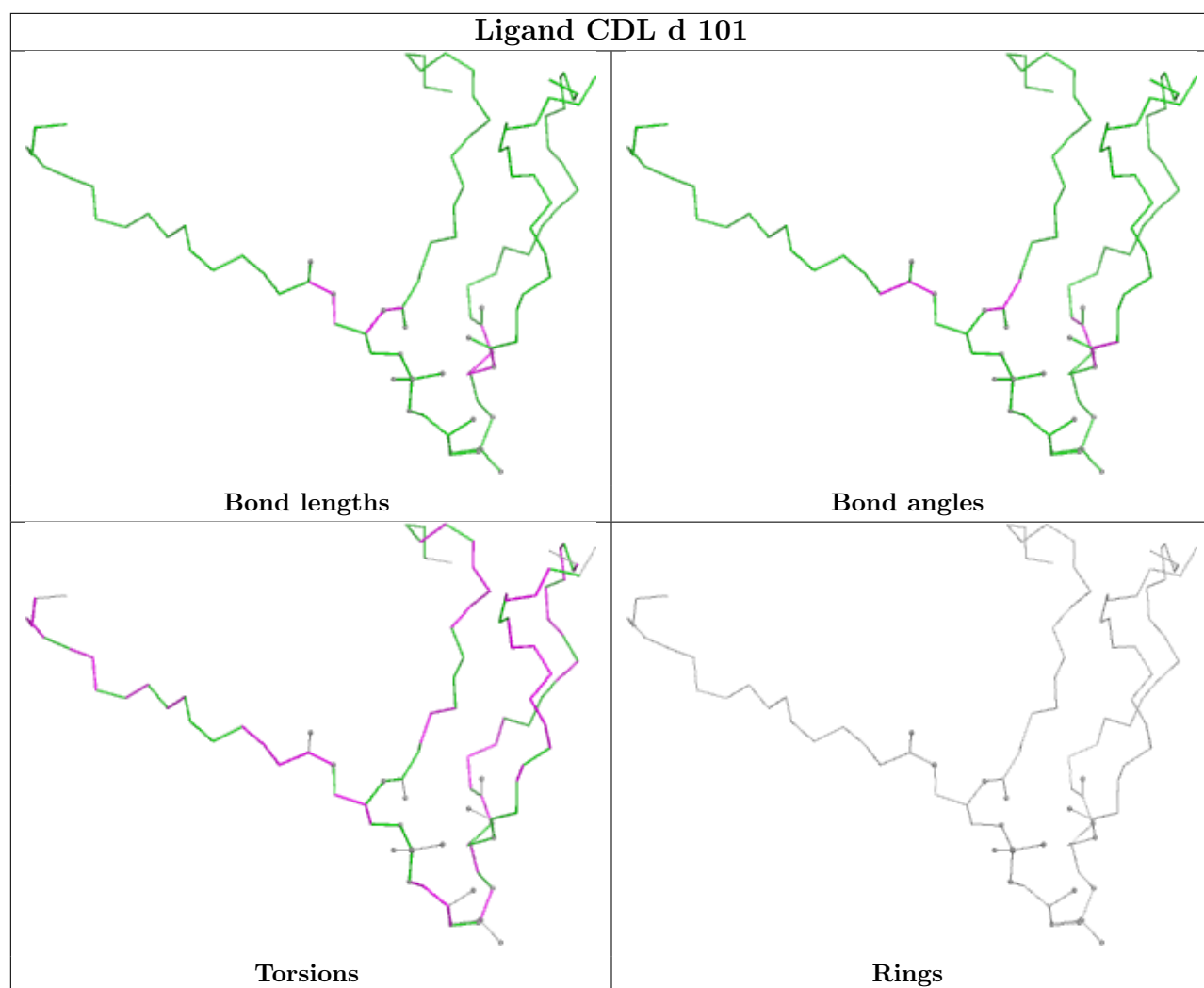
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

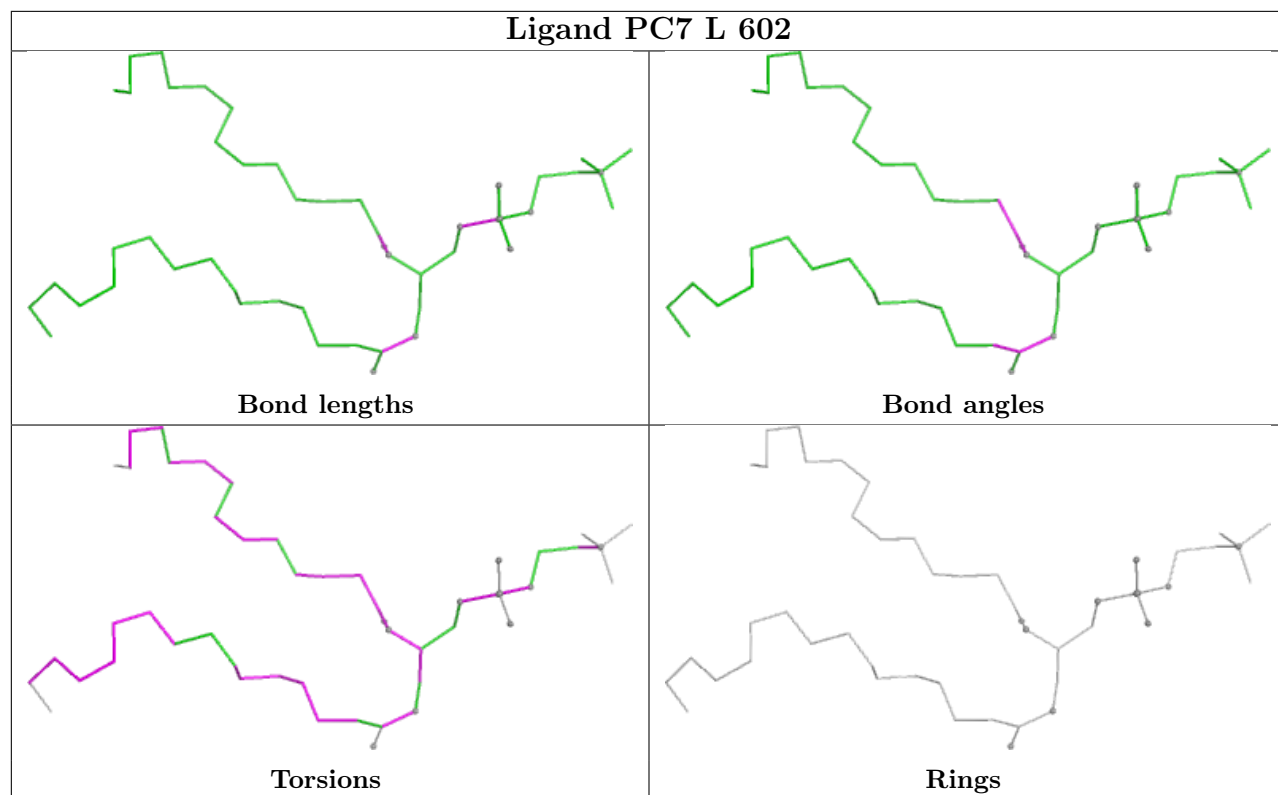


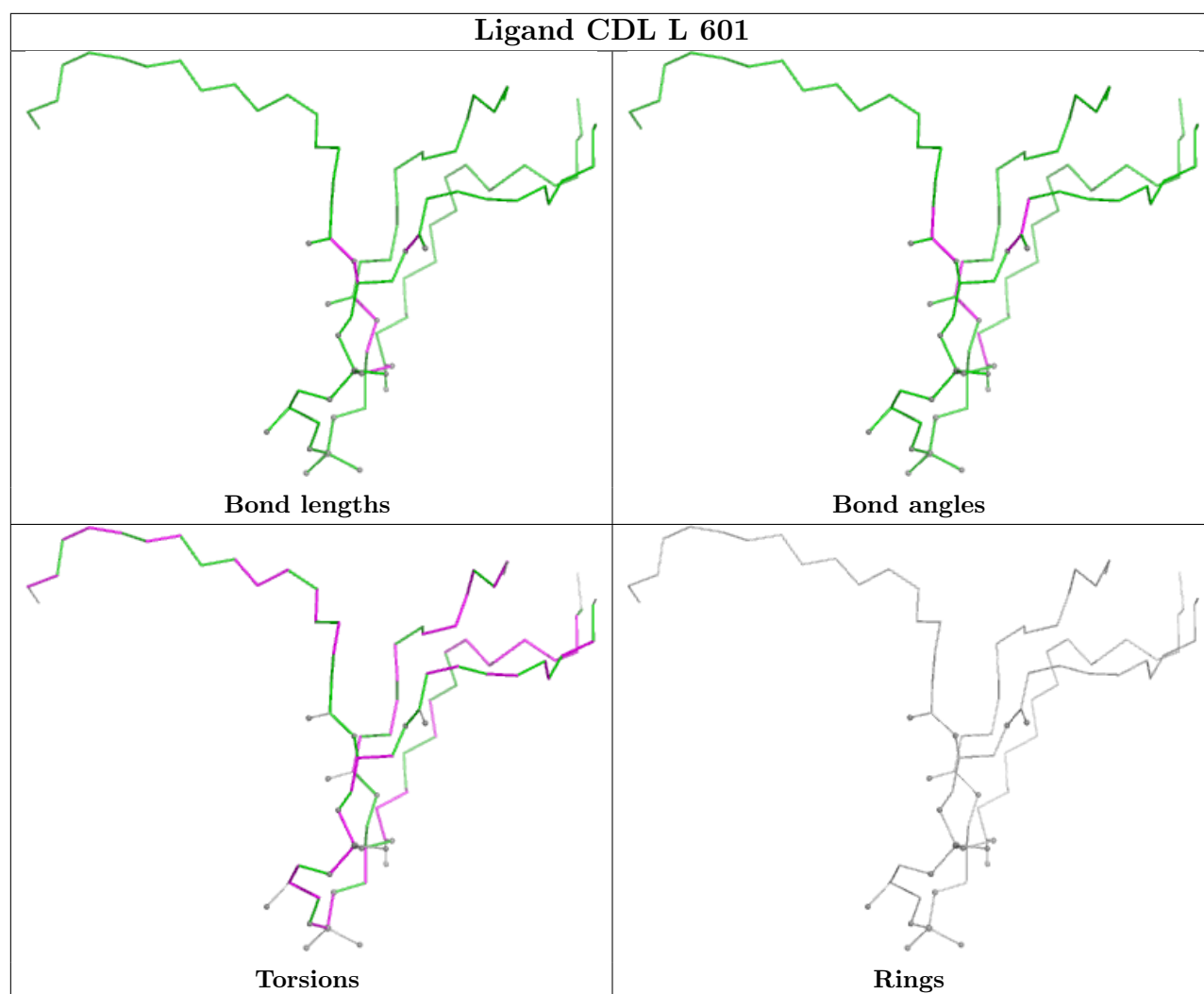


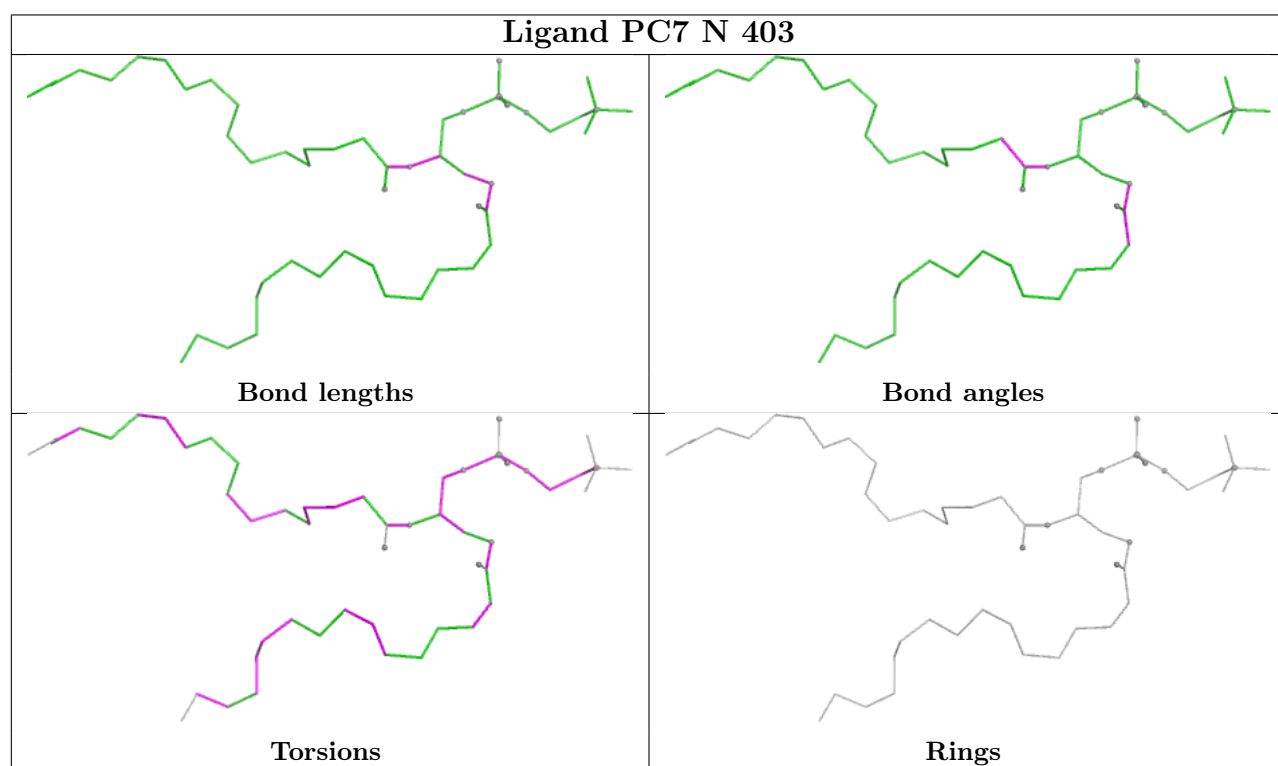
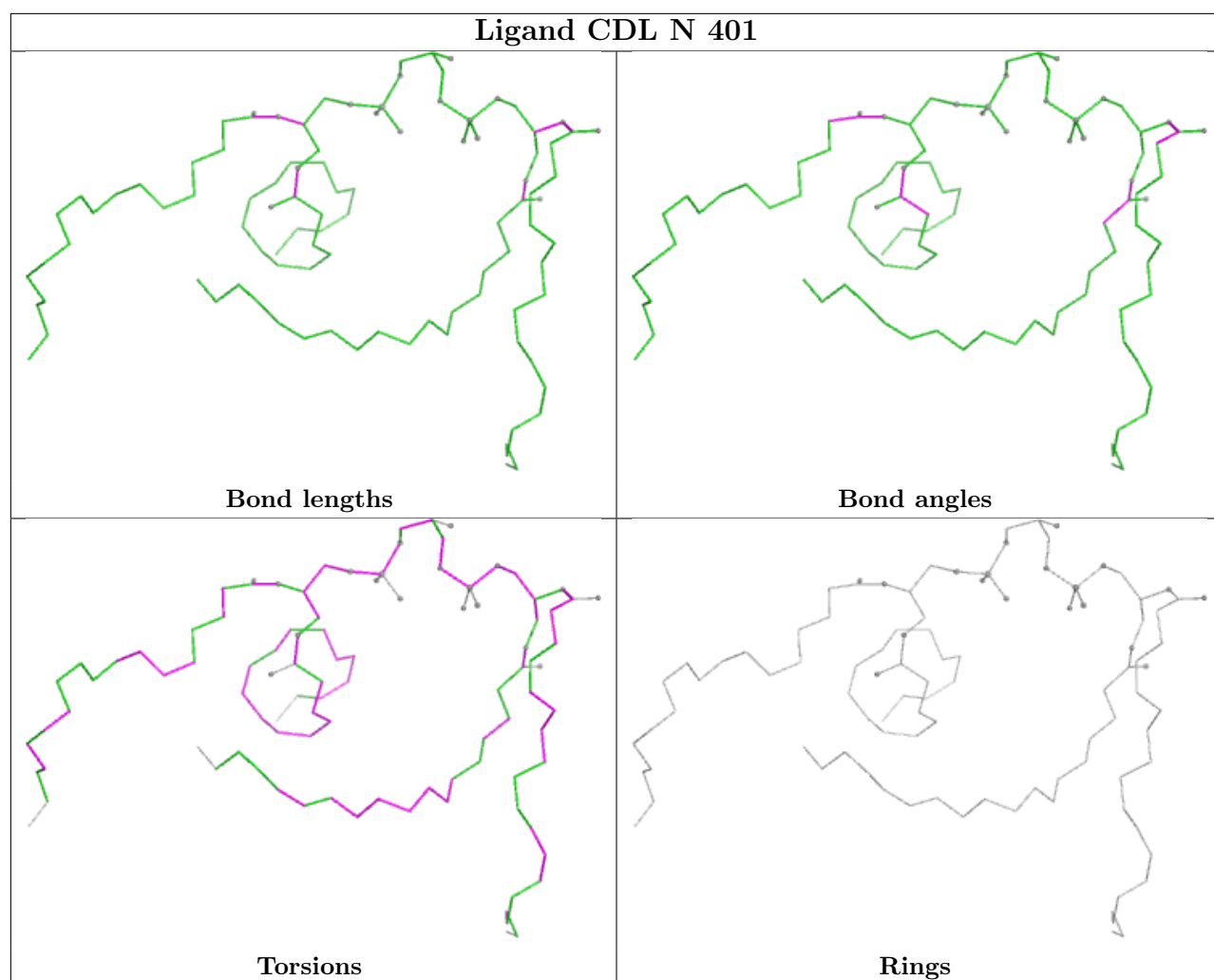


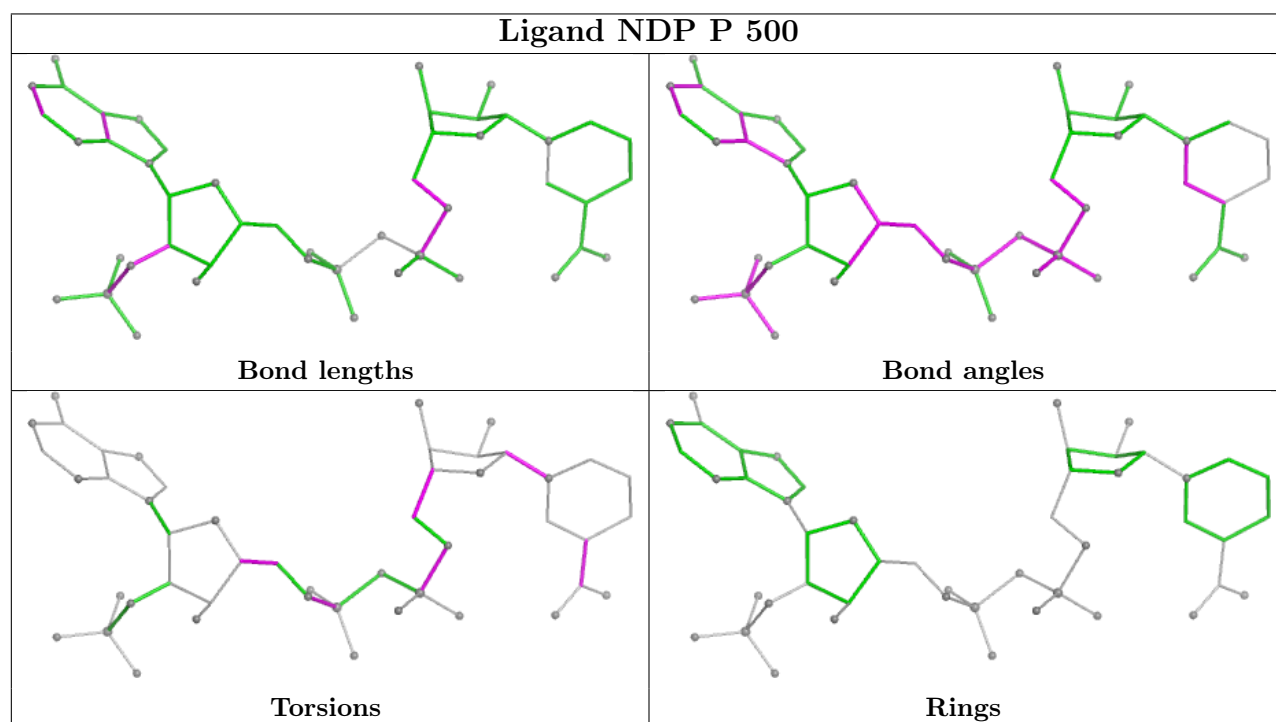
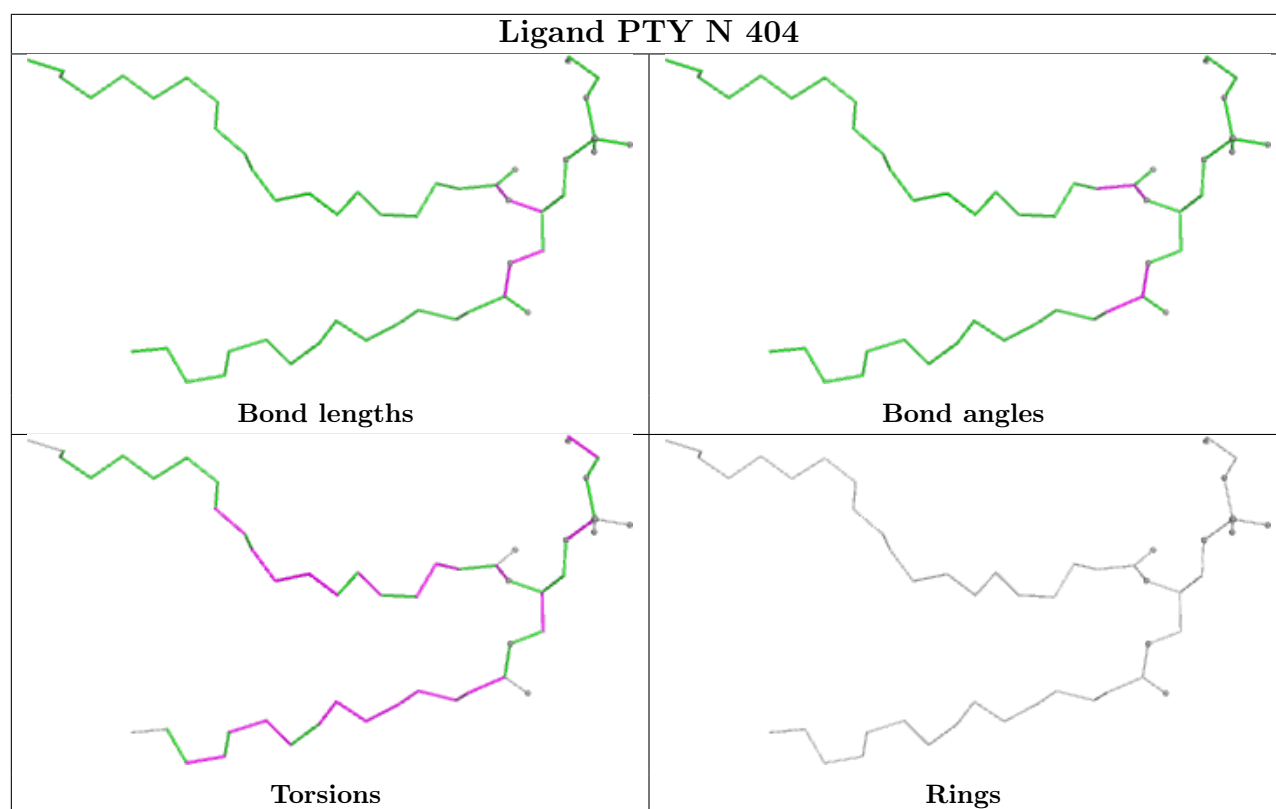


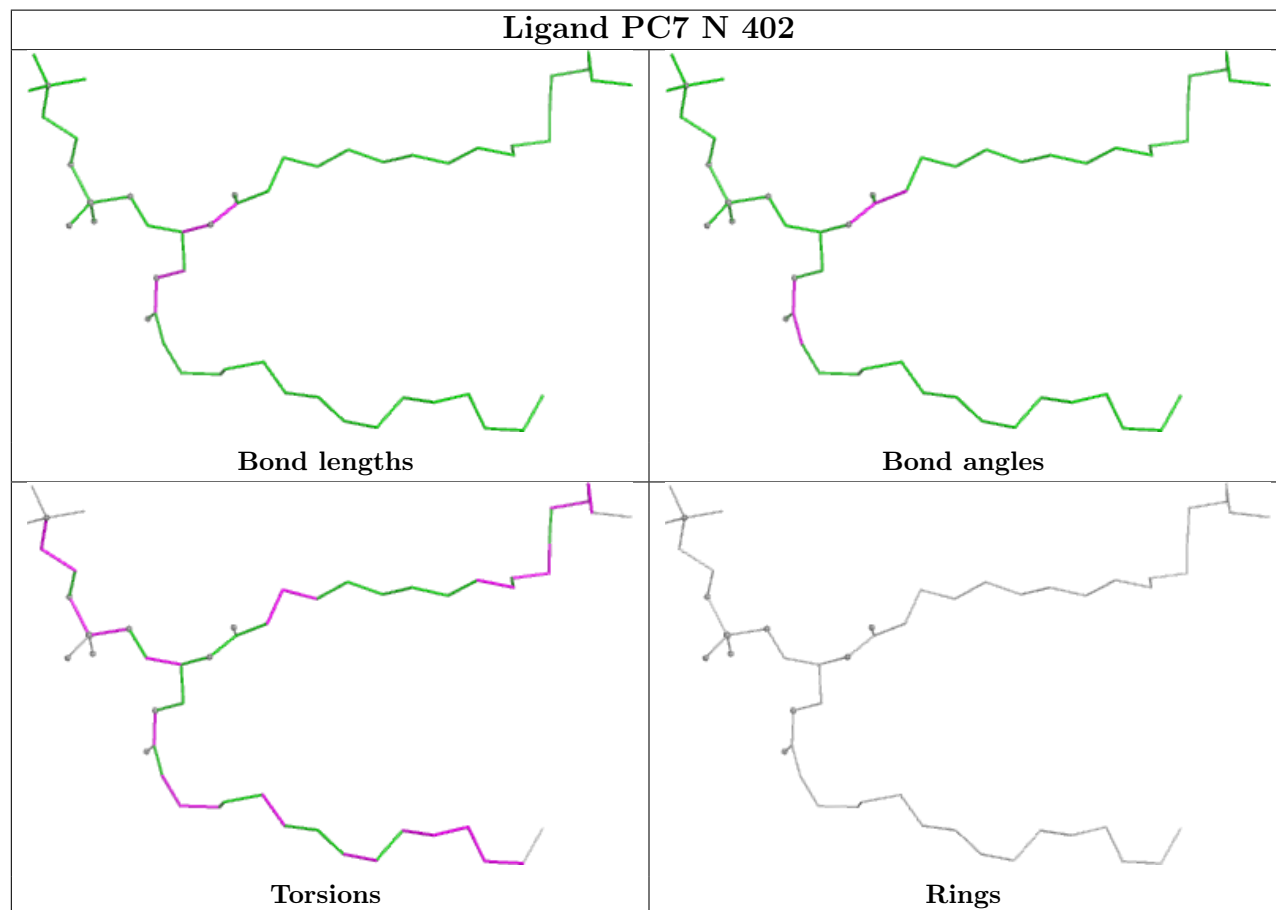
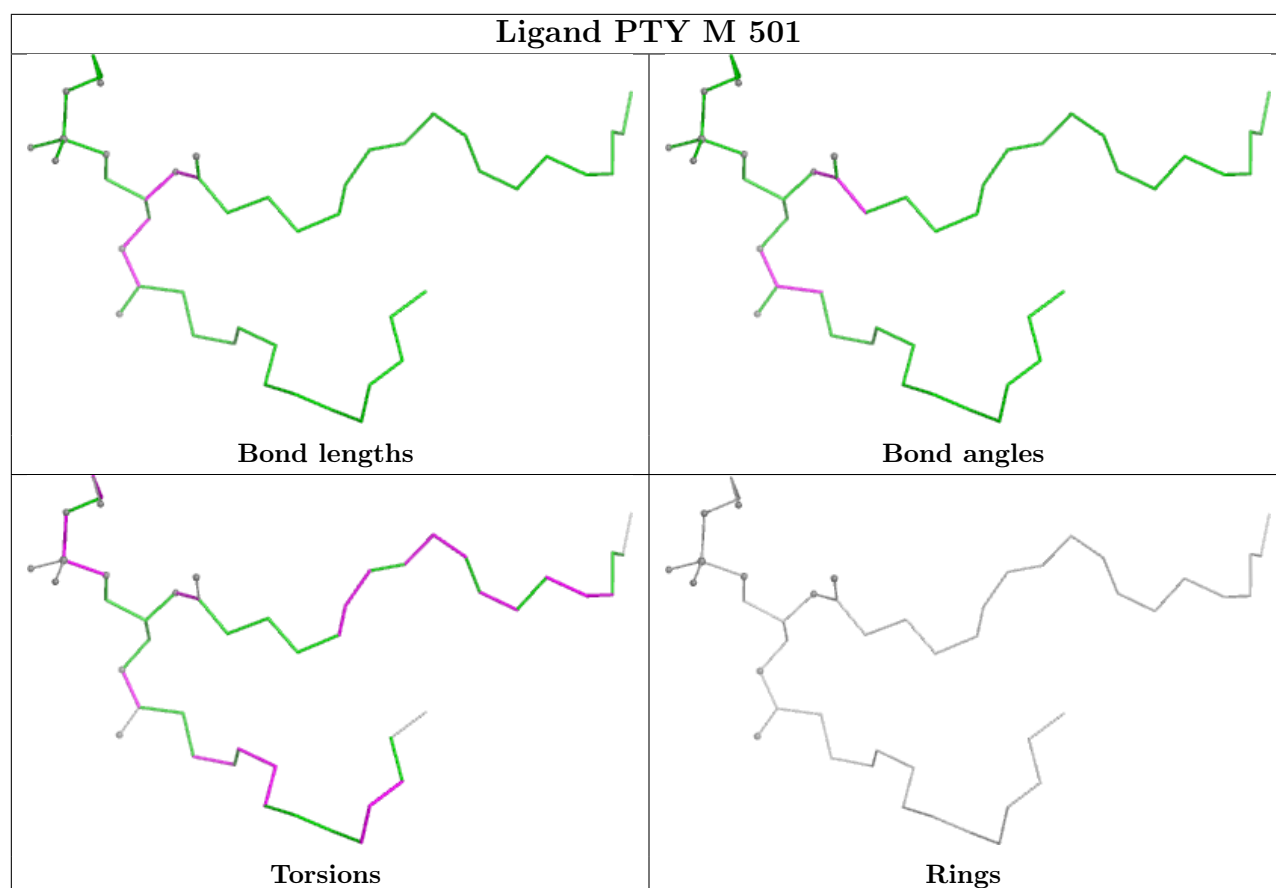


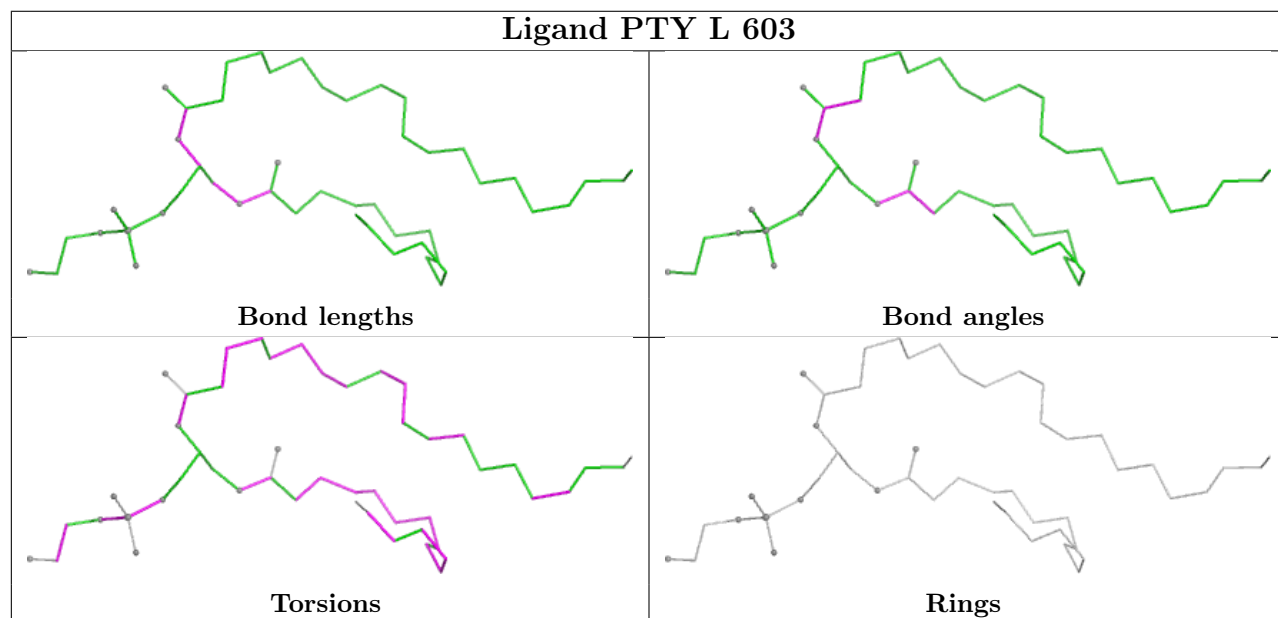
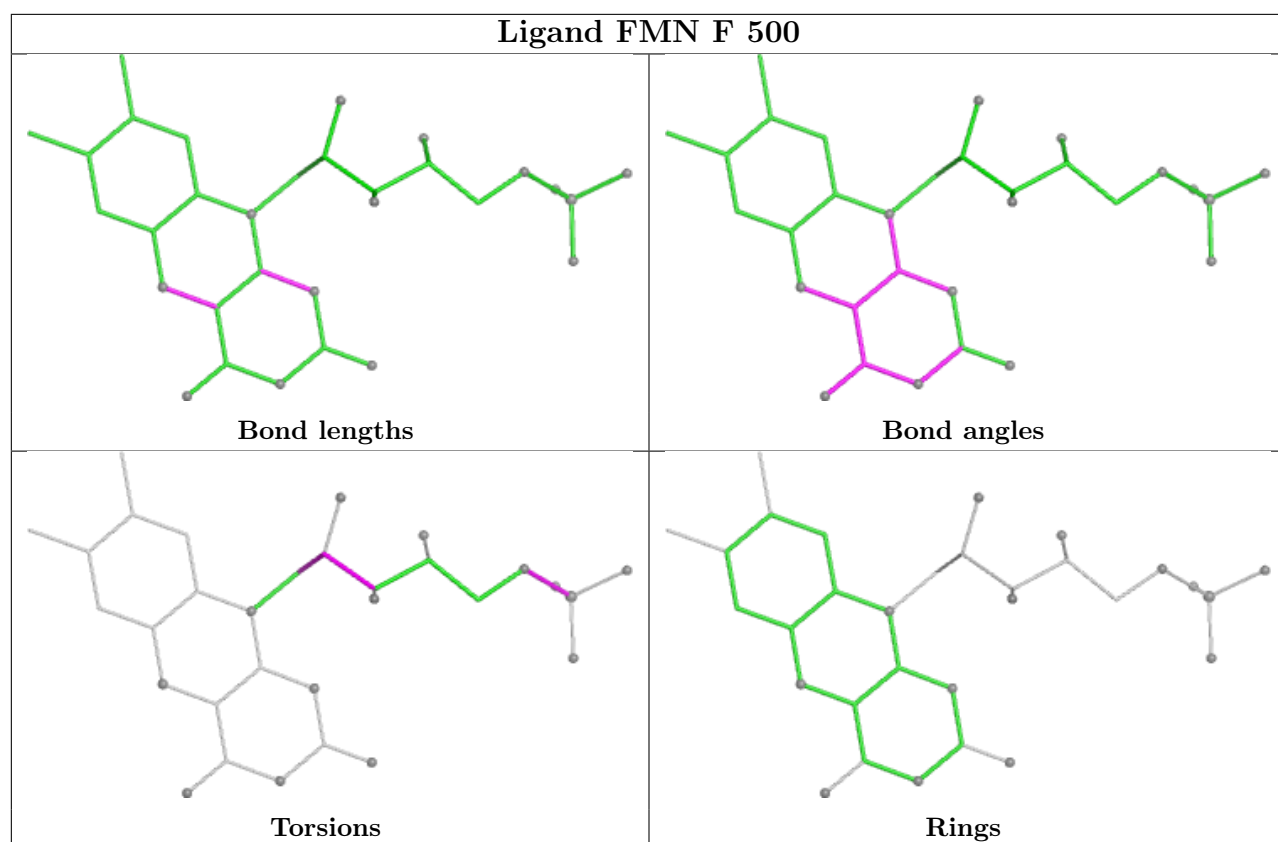


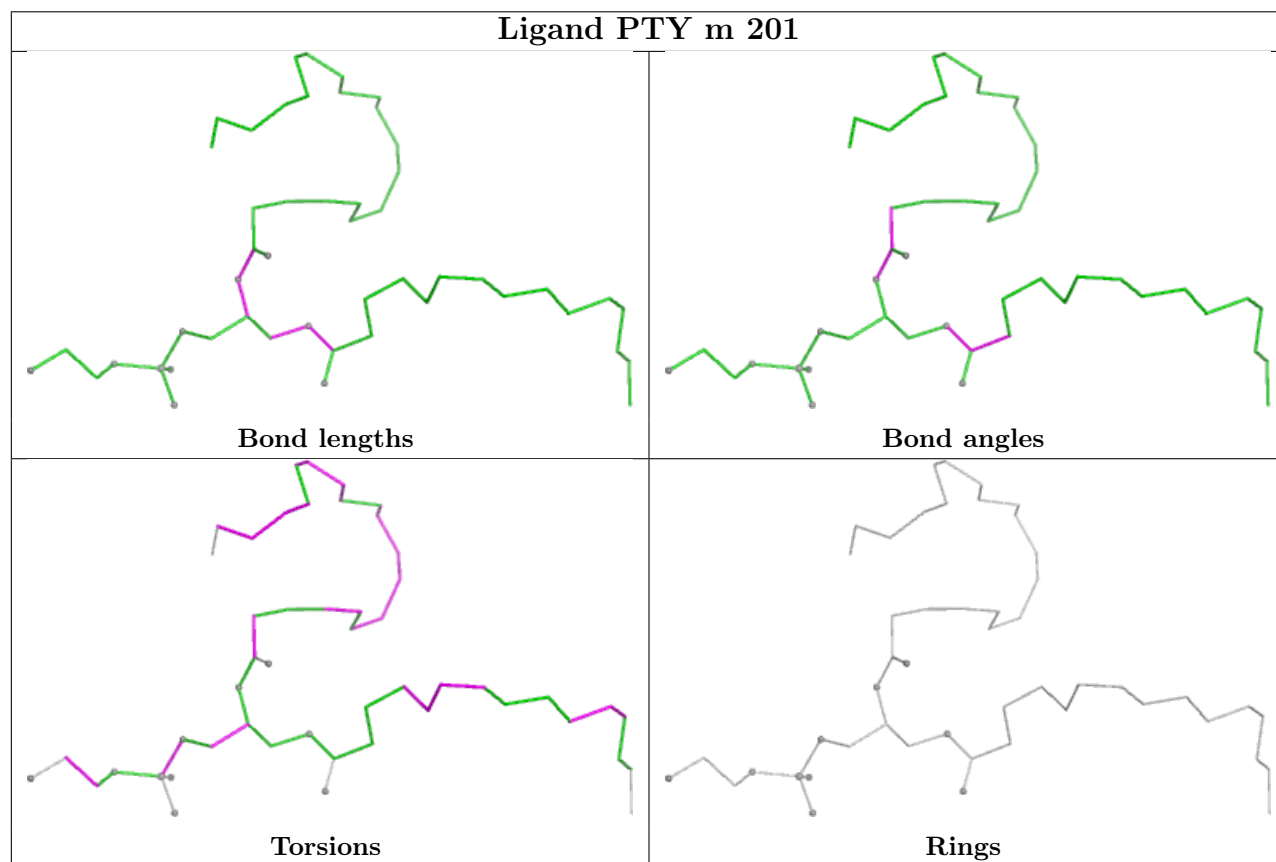
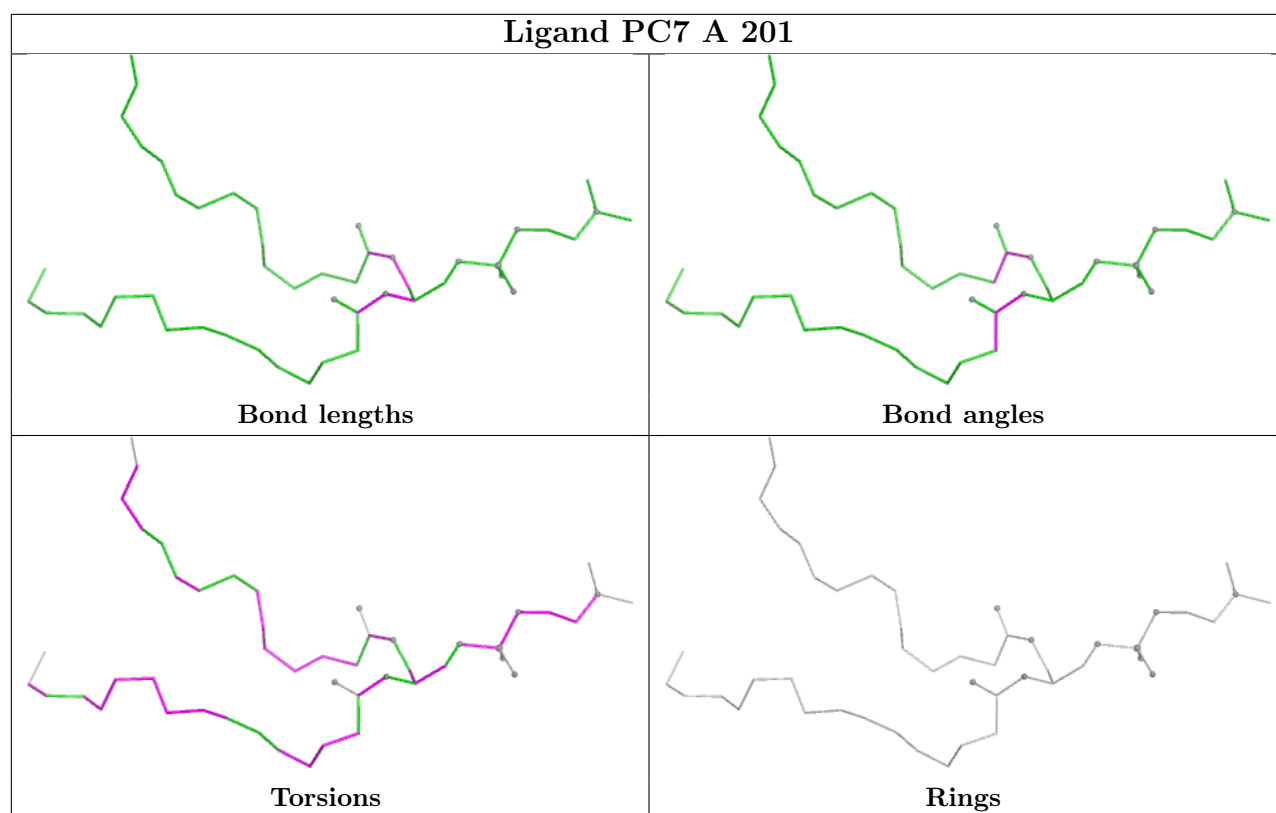


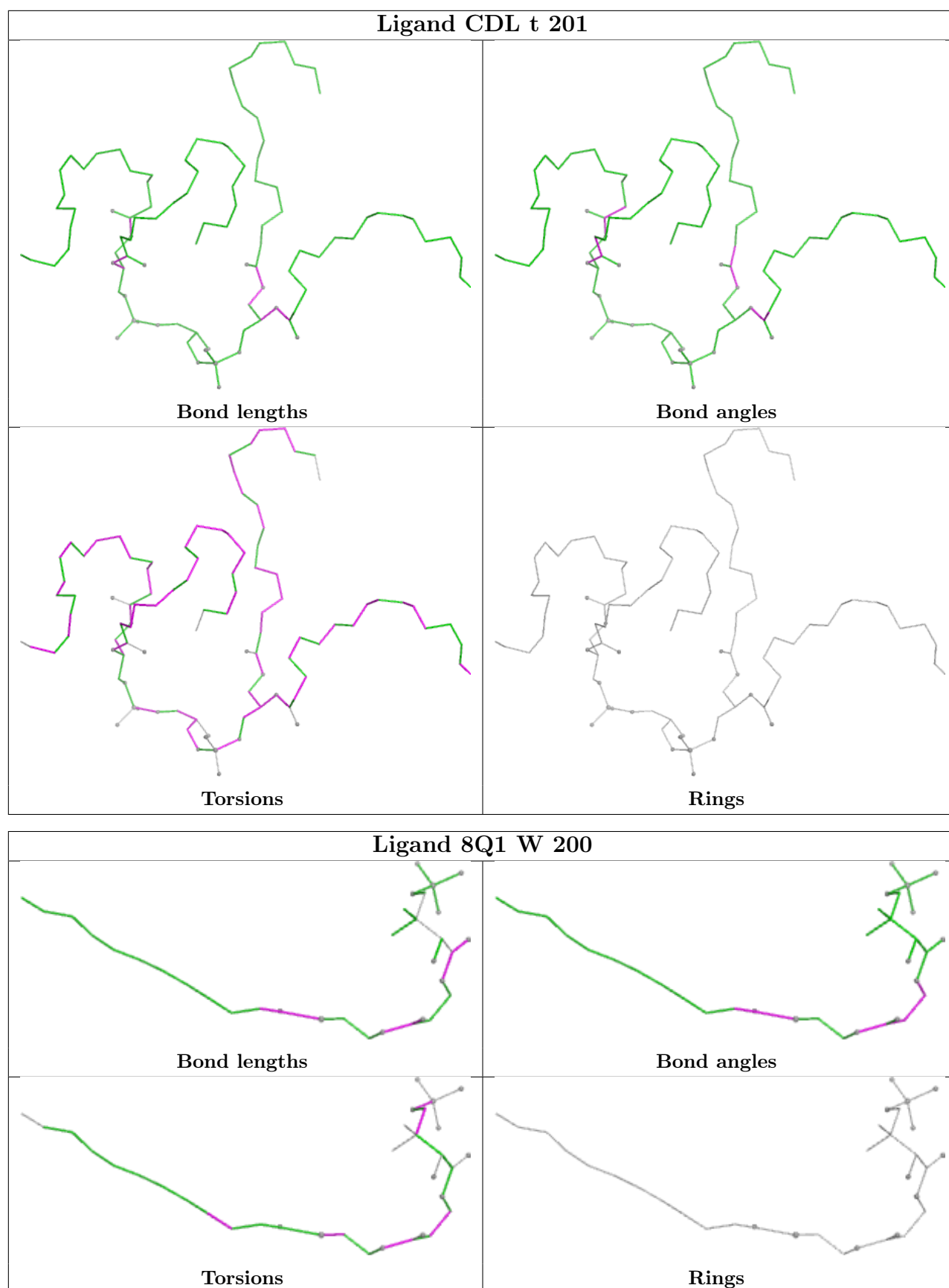


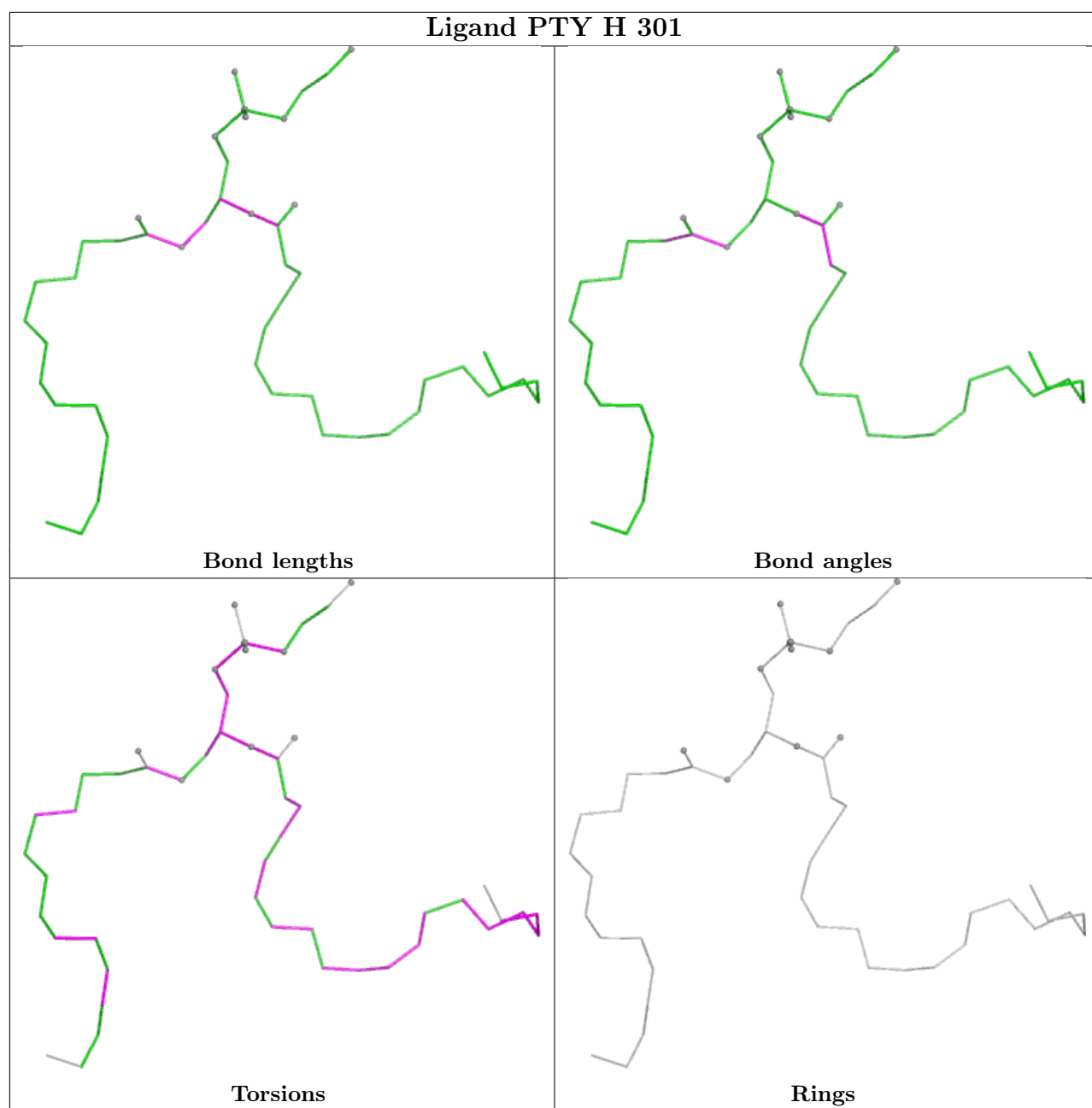


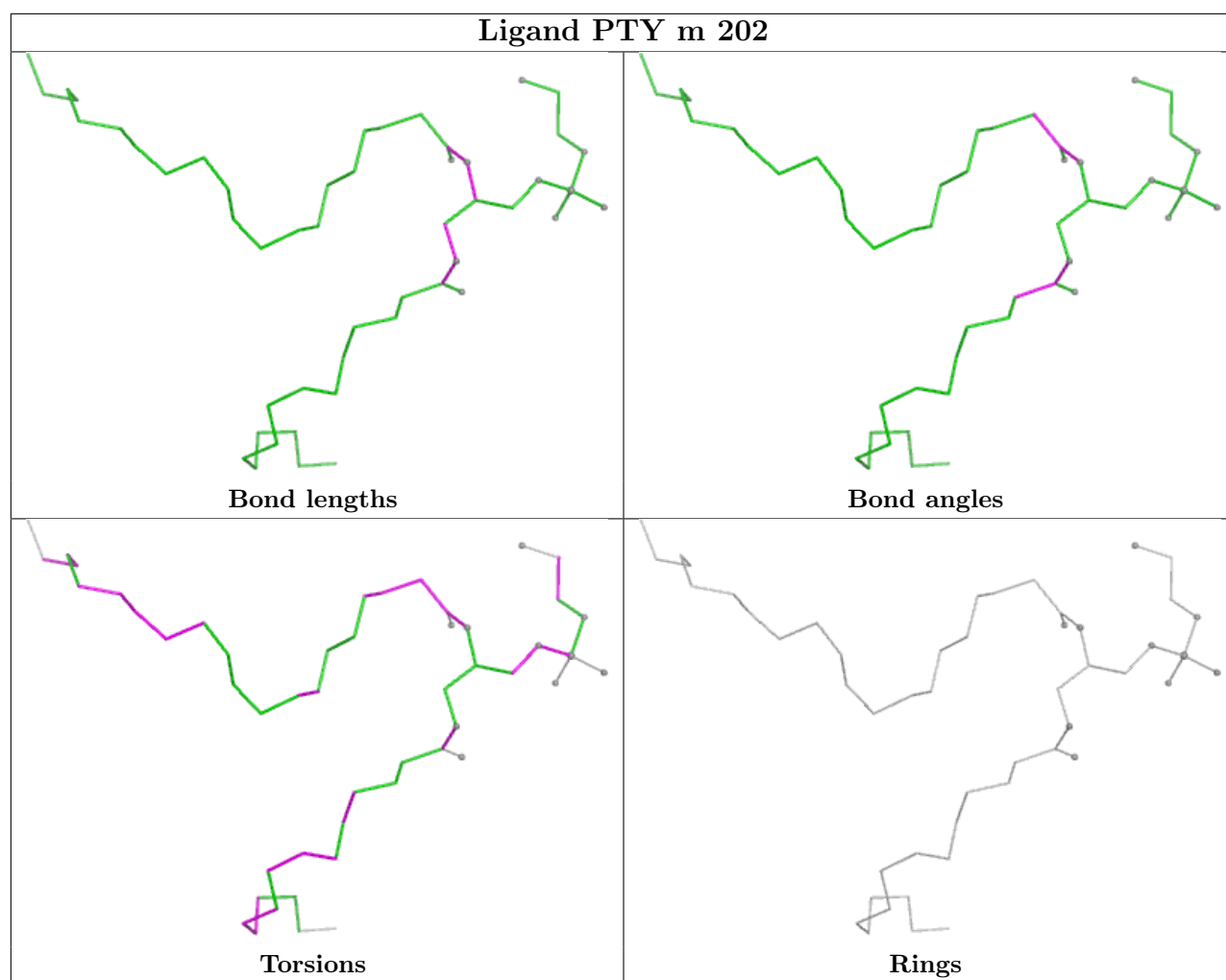












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

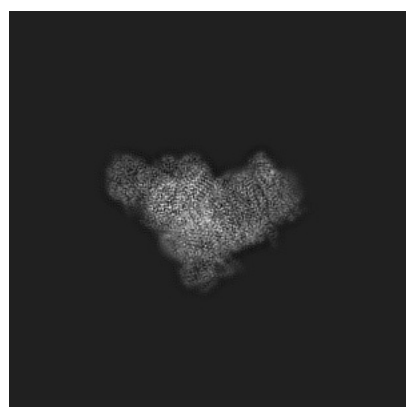
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11880. These allow visual inspection of the internal detail of the map and identification of artifacts.

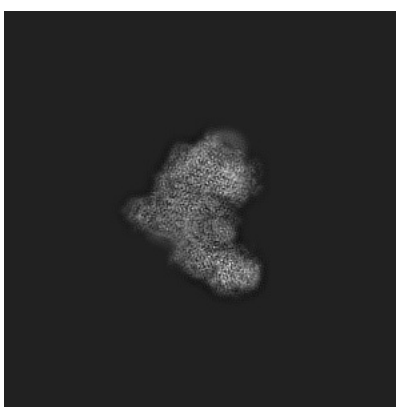
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X



Y

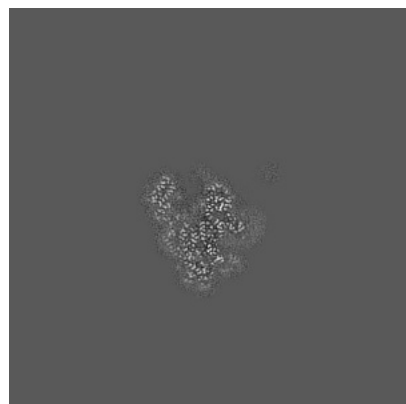


Z

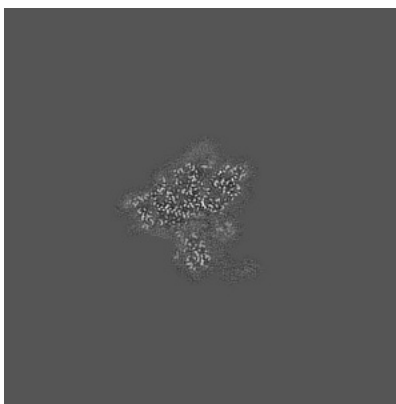
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

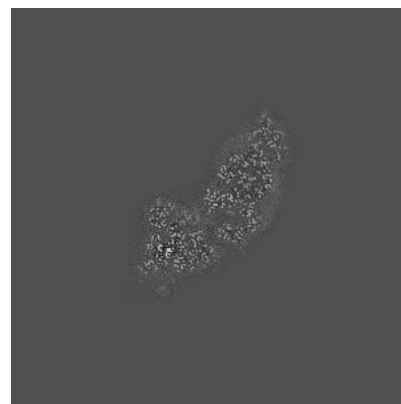
6.2.1 Primary map



X Index: 300



Y Index: 300

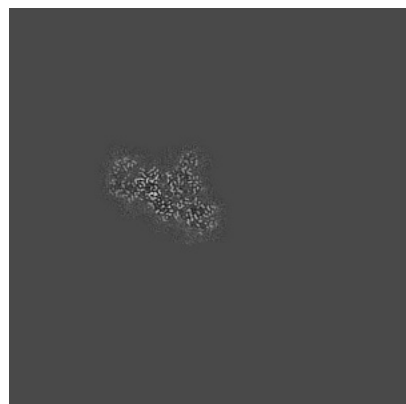


Z Index: 300

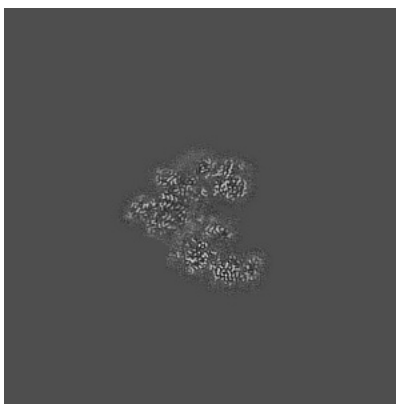
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

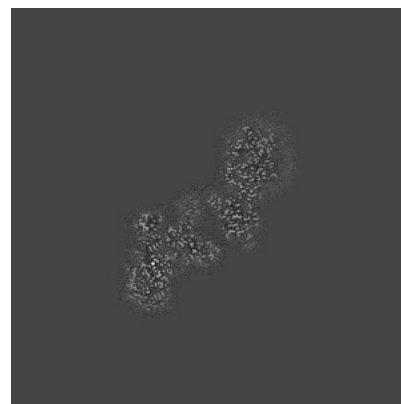
6.3.1 Primary map



X Index: 220



Y Index: 274

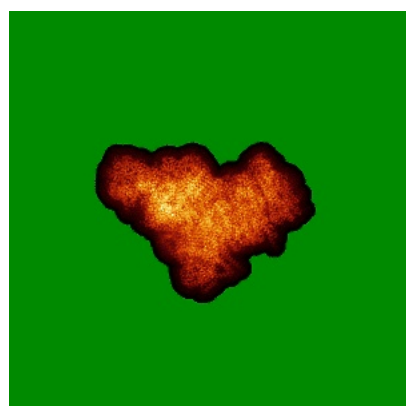


Z Index: 332

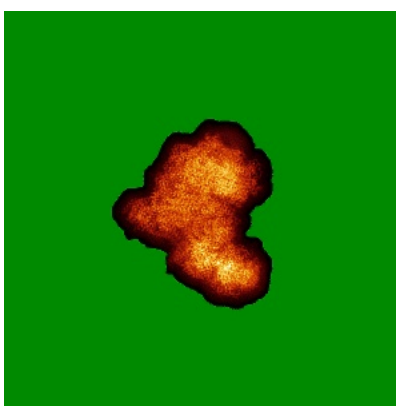
The images above show the largest variance slices of the map in three orthogonal directions.

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

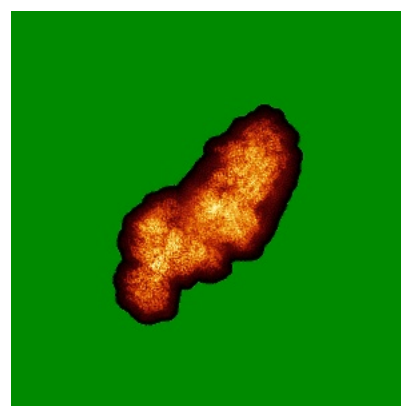
6.4.1 Primary map



X



Y

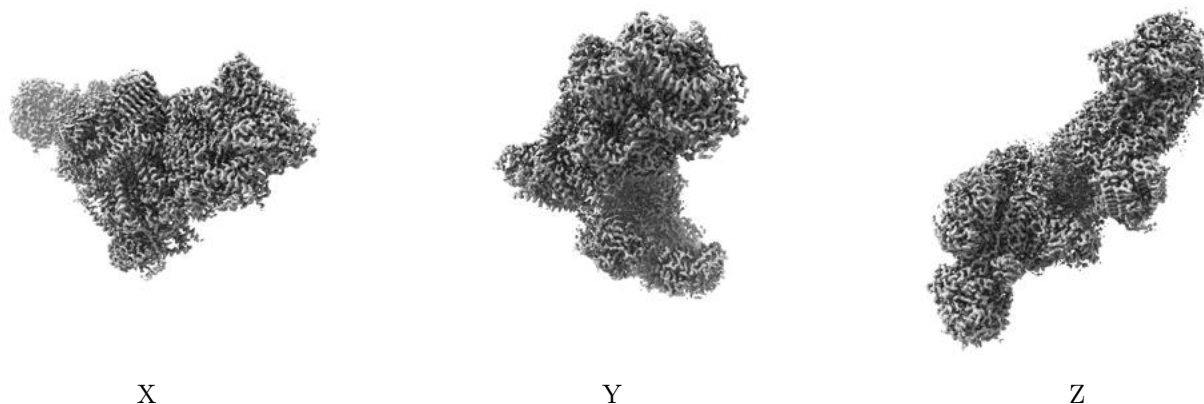


Z

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

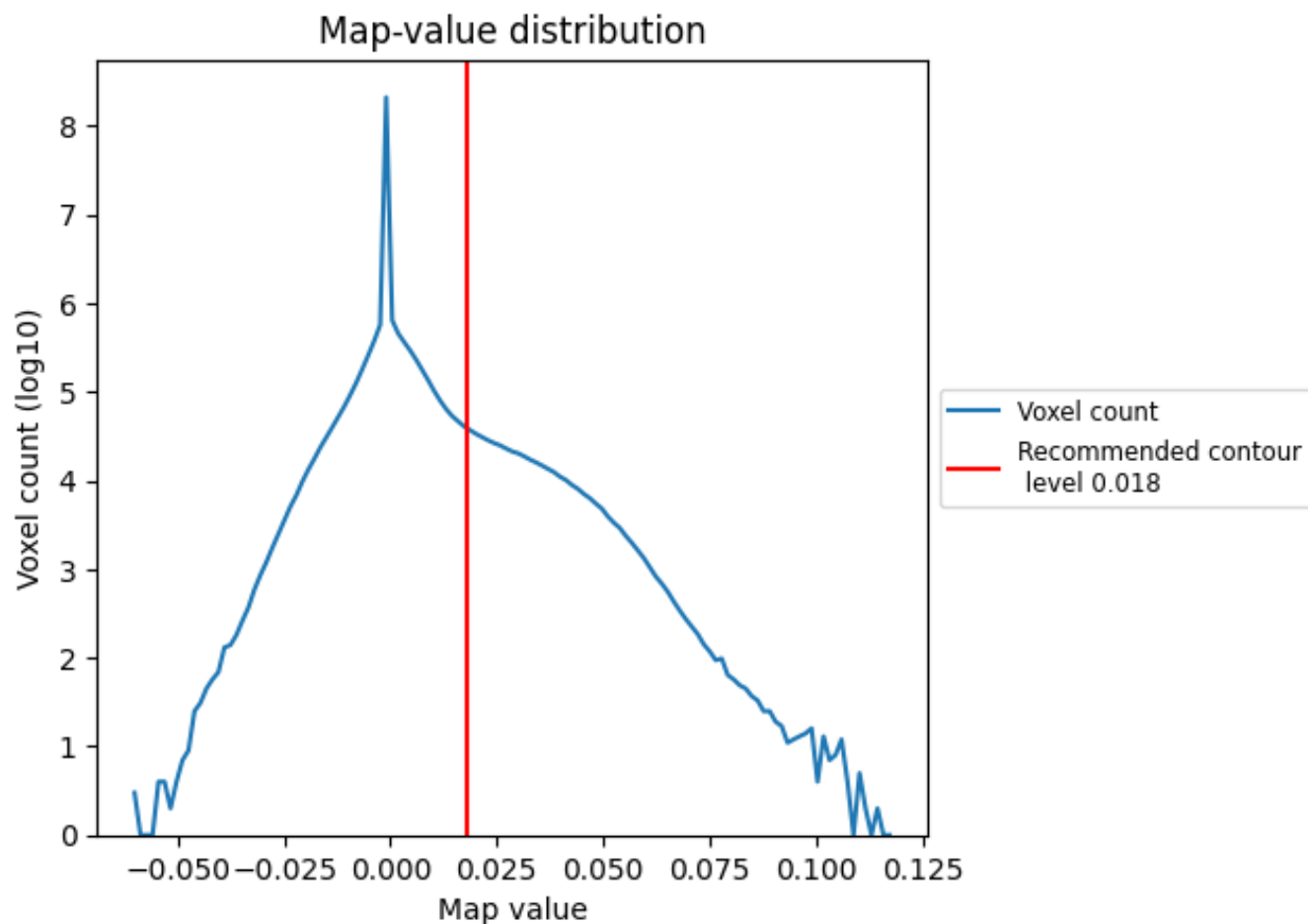
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

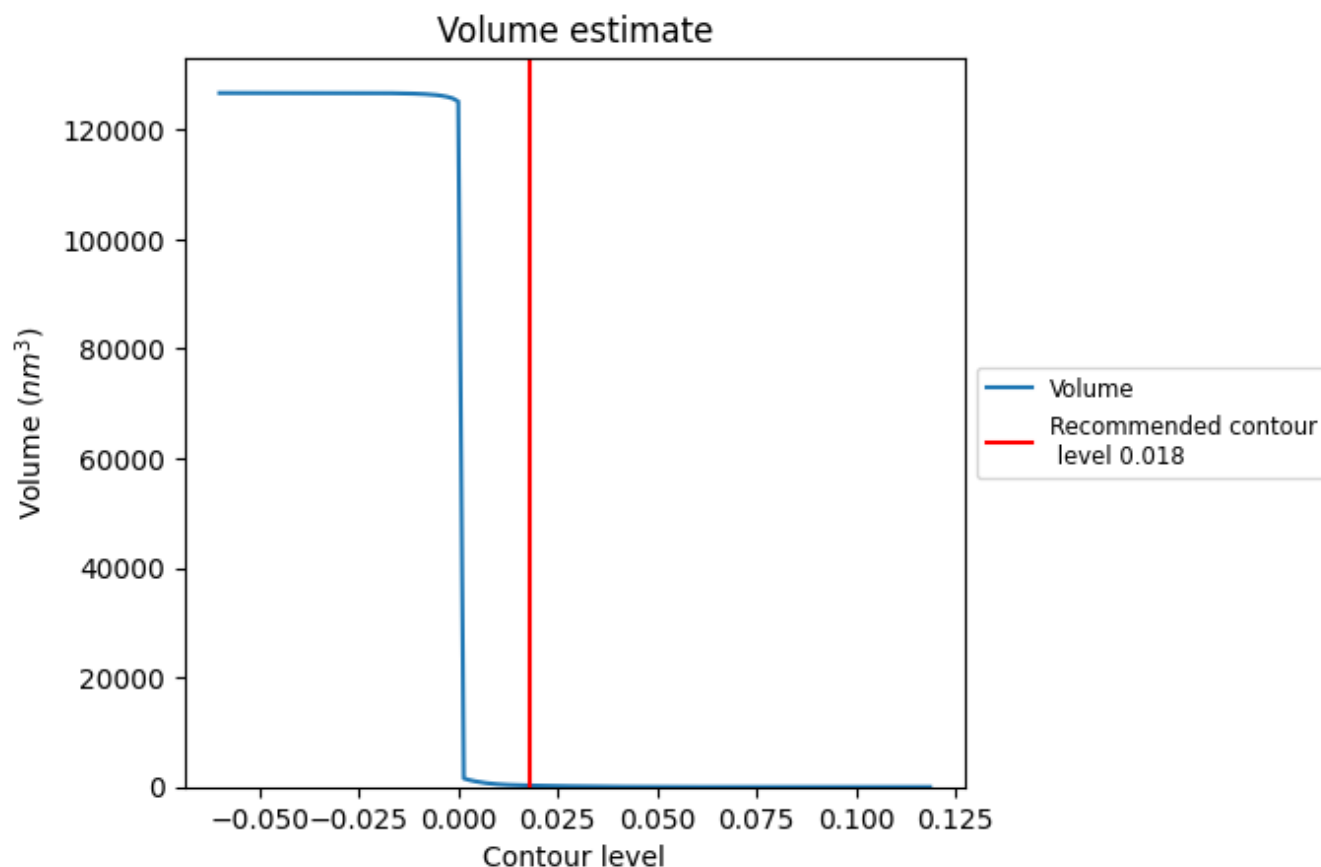
This section contains the results of statistical analysis of the map.

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.

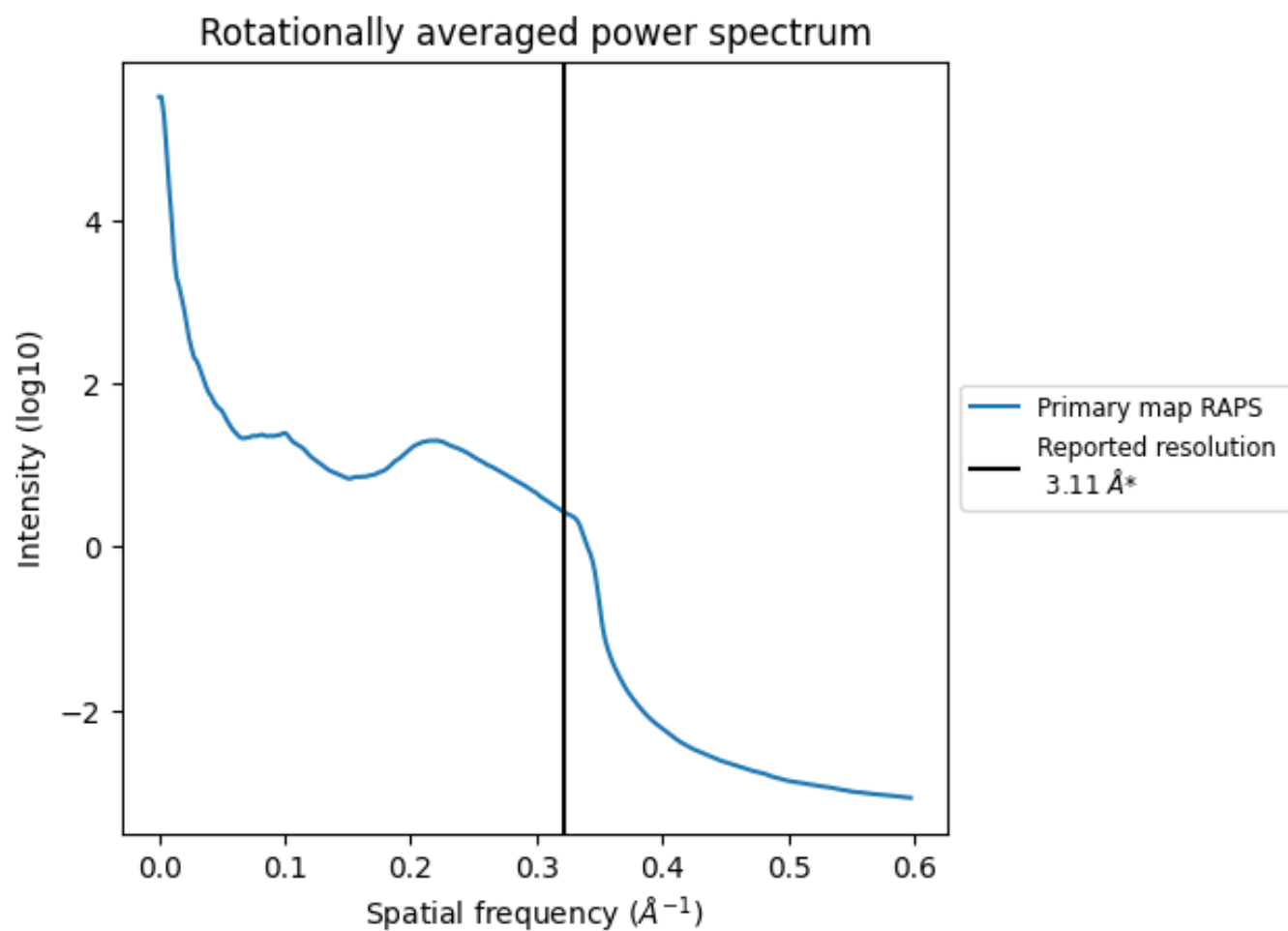
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 261 nm³; this corresponds to an approximate mass of 235 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 ⓘ

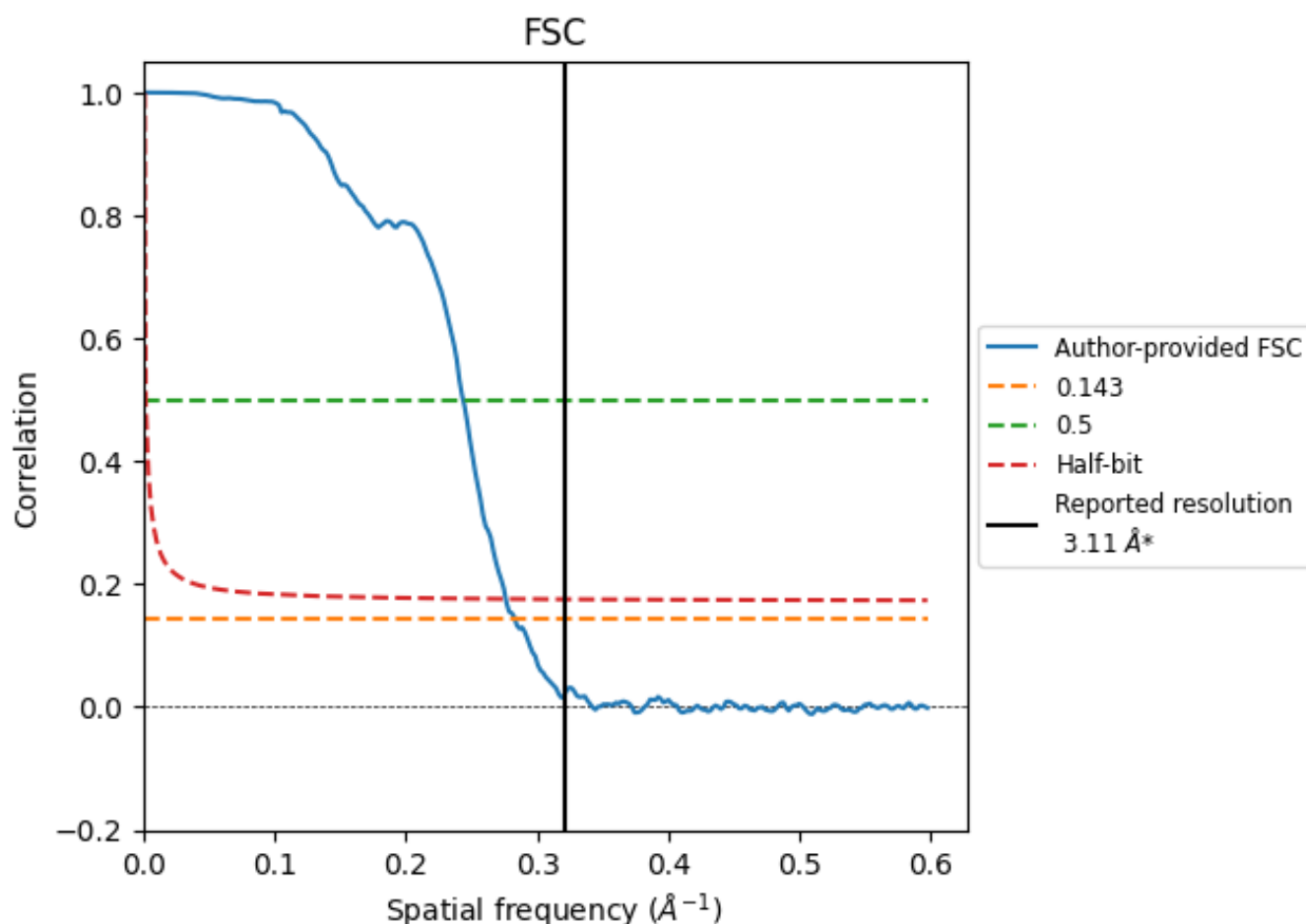


*Reported resolution corresponds to spatial frequency of 0.322 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.322 Å⁻¹

8.2 Resolution estimates [i](#)

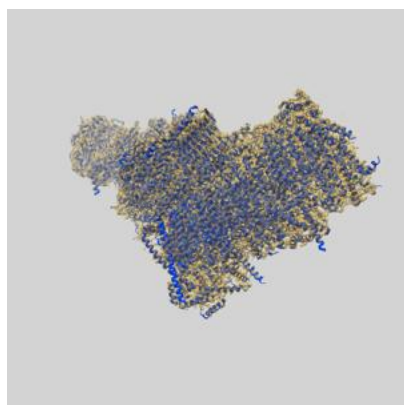
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.11	-	-
Author-provided FSC curve	3.53	4.10	3.62
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 3.53 differs from the reported value 3.11 by more than 10 %

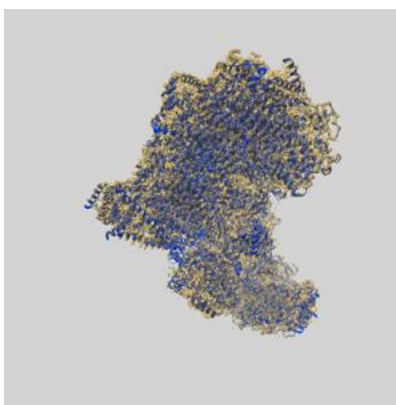
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-11880 and PDB model 7ARD. Per-residue inclusion information can be found in section [3](#) on page [22](#).

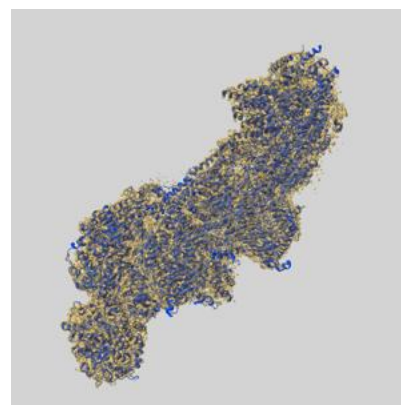
9.1 Map-model overlay [i](#)



X



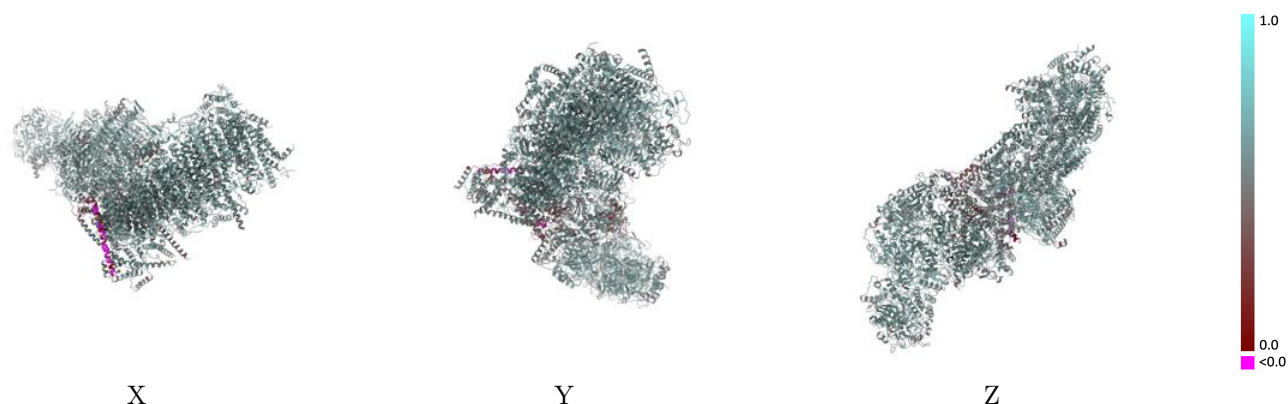
Y



Z

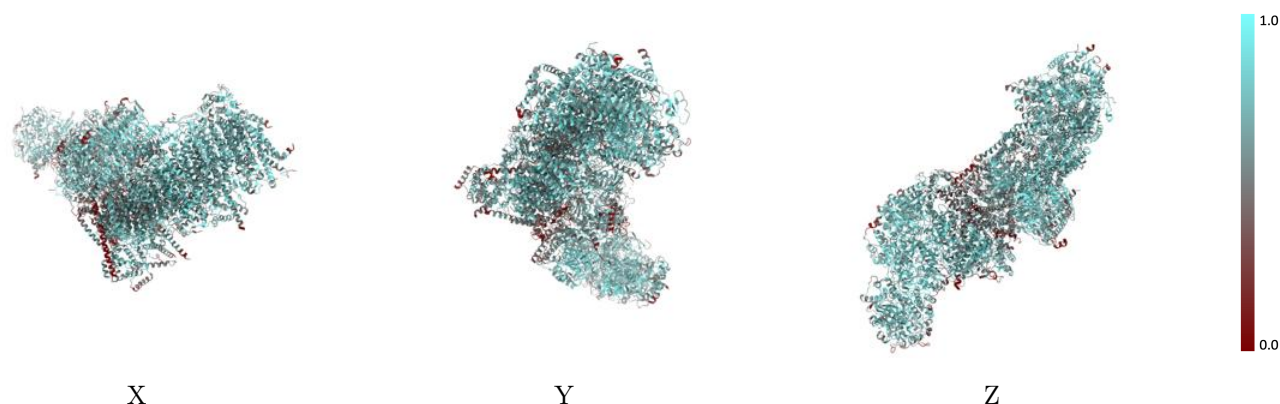
The images above show the 3D surface view of the map at the recommended contour level 0.018 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



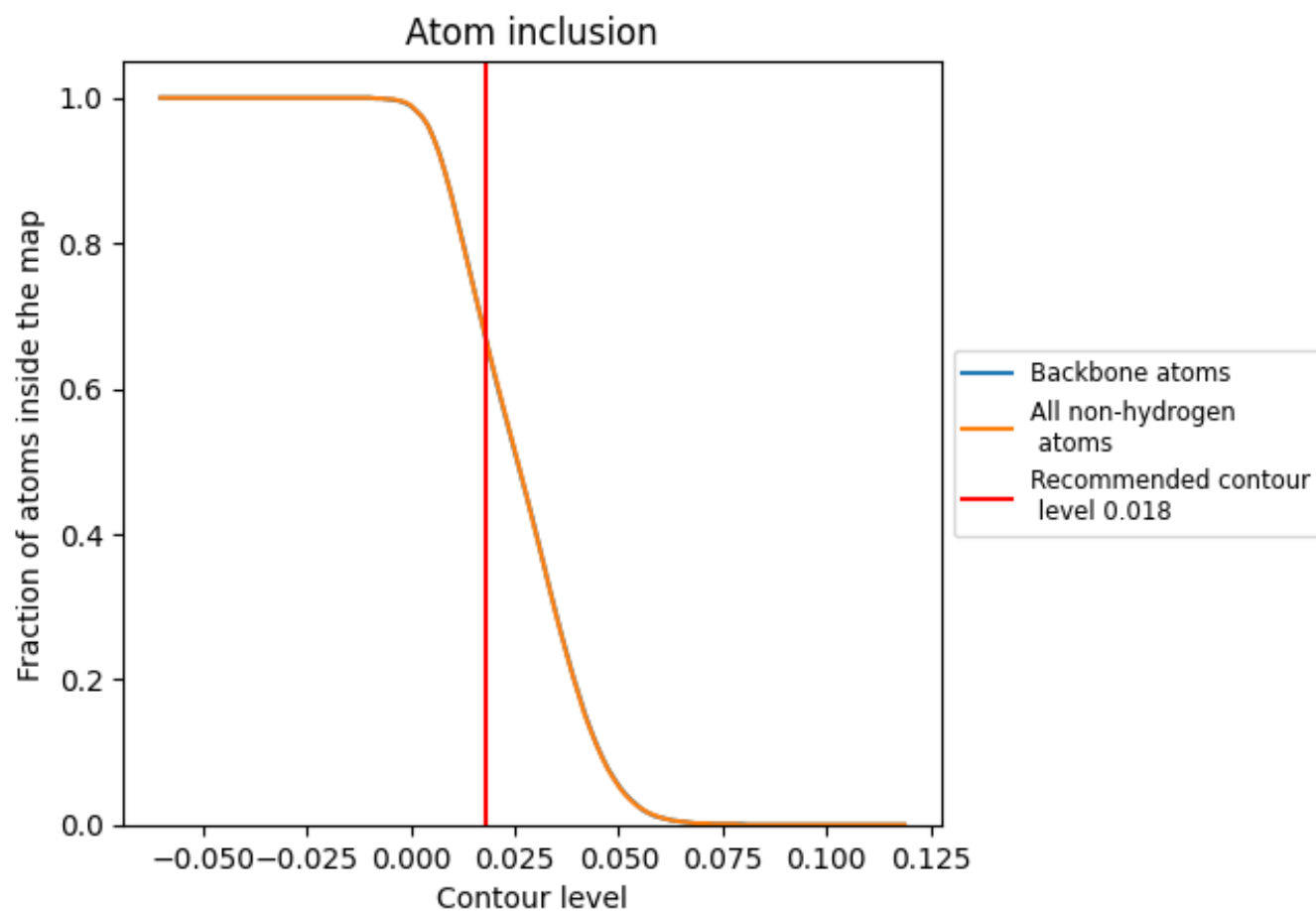
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.018).

9.4 Atom inclusion [i](#)



At the recommended contour level, 67% of all backbone atoms, 67% 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 (0.018) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6700	 0.5570
A	 0.6110	 0.5460
B	 0.6760	 0.5450
C	 0.7840	 0.5960
D	 0.7370	 0.5650
E	 0.6400	 0.5430
F	 0.6980	 0.5580
G	 0.7560	 0.5830
H	 0.4370	 0.4690
I	 0.6200	 0.5250
J	 0.6680	 0.5570
K	 0.7220	 0.5660
L	 0.7250	 0.5890
M	 0.7540	 0.5950
N	 0.7040	 0.5850
O	 0.7450	 0.5800
P	 0.6750	 0.5490
Q	 0.7110	 0.5810
R	 0.5850	 0.5360
S	 0.6580	 0.5420
T	 0.5840	 0.5220
U	 0.2990	 0.3850
V	 0.5760	 0.5250
W	 0.5510	 0.5010
X	 0.6420	 0.5480
Y	 0.6490	 0.5520
Z	 0.5640	 0.4950
a	 0.6240	 0.5280
b	 0.1000	 -0.0330
c	 0.7420	 0.5800
d	 0.6360	 0.5610
e	 0.6650	 0.5560
f	 0.6950	 0.5720
g	 0.7000	 0.5670
h	 0.6600	 0.5560



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
i	 0.6380	 0.5370
j	 0.6940	 0.5450
k	 0.6670	 0.5500
l	 0.7530	 0.5870
m	 0.7300	 0.5910
n	 0.6970	 0.5550
o	 0.7180	 0.5670
p	 0.7180	 0.5750
q	 0.7260	 0.5790
r	 0.3150	 0.5110
s	 0.6670	 0.5650
t	 0.6810	 0.5880
u	 0.5200	 0.3570
w	 0.6860	 0.5650
x	 0.7460	 0.5780
y	 0.6640	 0.5630
z	 0.6910	 0.5650