



## Full wwPDB EM Validation Report ⓘ

Dec 18, 2022 – 06:29 pm GMT

PDB ID : 7AR9  
EMDB ID : EMD-11877  
Title : Cryo-EM structure of Polytomella Complex-I (membrane arm)  
Authors : Klusch, N.; Kuehlbrandt, W.; Yildiz, O.  
Deposited on : 2020-10-23  
Resolution : 2.97 Å (reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

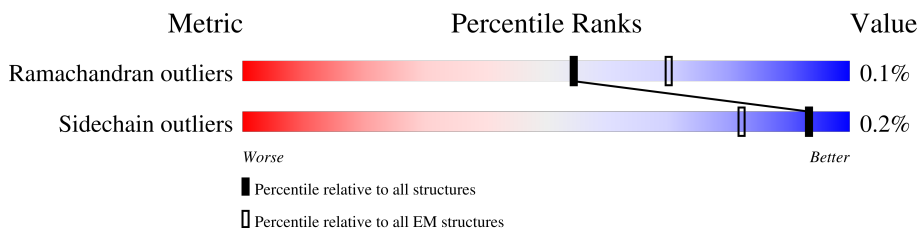
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 2.97 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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  $\geq 3$ , 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	11% (red), 79% (green), 21% (grey)
2	H	293	39% (red), 99% (green), . (yellow)
3	J	145	12% (red), 99% (green), . (yellow)
4	K	127	6% (red), 82% (green), 18% (grey)
5	L	536	. (red), 100% (green)
6	M	438	100% (green)
7	N	375	. (red), 99% (green), . (yellow)
8	O	200	6% (red), 80% (green), 20% (grey)
9	T	123	13% (red), 67% (green), 33% (grey)

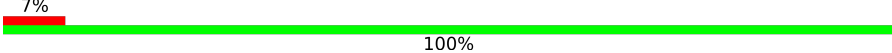
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Mol	Chain	Length	Quality of chain
10	X	100	8% 98% ..
11	Y	206	11% 100%
12	Z	142	35% 87% 13%
13	a	71	10% 83% 15%
14	b	54	35% 100%
15	c	110	5% 88% 12%
16	d	83	7% 96% .
17	e	75	9% 95% 5%
18	f	121	7% 91% 8%
19	g	172	8% 85% 15%
20	h	81	14% 95% 5%
21	i	128	12% 86% 13%
22	j	87	14% 100%
23	k	55	9% 80% 20%
24	l	151	6% 84% 16%
25	m	138	. 80% 20%
26	n	121	11% 99% .
27	o	85	6% 96% ..
28	p	156	5% 99% .
29	s	118	5% 97% .
30	t	134	5% 61% 39%
31	u	50	22% 100%
32	w	41	12% 100%
33	x	280	. 89% 11%
34	y	310	12% 99% ..

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Mol	Chain	Length	Quality of chain
35	z	227	 7% 100%

## 2 Entry composition [i](#)

There are 40 unique types of molecules in this entry. The entry contains 42861 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
			Total	C	N	O	S		
1	A	121	999	673	148	172	6	0	0

- Molecule 2 is a protein called ND1.

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

- Molecule 3 is a protein called ND6.

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

- Molecule 4 is a protein called ND4L.

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

- Molecule 5 is a protein called ND5.

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

- Molecule 6 is a protein called ND4.

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

- Molecule 7 is a protein called ND2.

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

- Molecule 8 is a protein called C1-FDX.

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

- Molecule 9 is a protein called SDAP1.

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

- Molecule 10 is a protein called PGIV.

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

- Molecule 11 is a protein called B14.7.

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

- Molecule 12 is a protein called B16.6.

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

- Molecule 13 is a protein called MWFE.

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

- Molecule 14 is a protein called B9.

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

- Molecule 15 is a protein called KFYI.

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

- Molecule 16 is a protein called B14.5b.

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

- Molecule 17 is a protein called 15 kDa.

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

- Molecule 18 is a protein called MNLL.

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

- Molecule 19 is a protein called ESSS.

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

- Molecule 20 is a protein called NUOP4.

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

- Molecule 21 is a protein called NUOP5.

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

- Molecule 22 is a protein called AGGG.

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

- Molecule 23 is a protein called B12.

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

- Molecule 24 is a protein called ASHI.

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

- Molecule 25 is a protein called B15.

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

- Molecule 26 is a protein called B22.

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

- Molecule 27 is a protein called B18.

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

- Molecule 28 is a protein called PDSW.



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

- Molecule 29 is a protein called NUOP7.

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

- Molecule 30 is a protein called NUOP8.

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

- Molecule 31 is a protein called unknown.

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

- Molecule 32 is a protein called unknown.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	w	41	Total	C	N	O	0	0
			205	123	41	41		

- Molecule 33 is a protein called CAL.

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

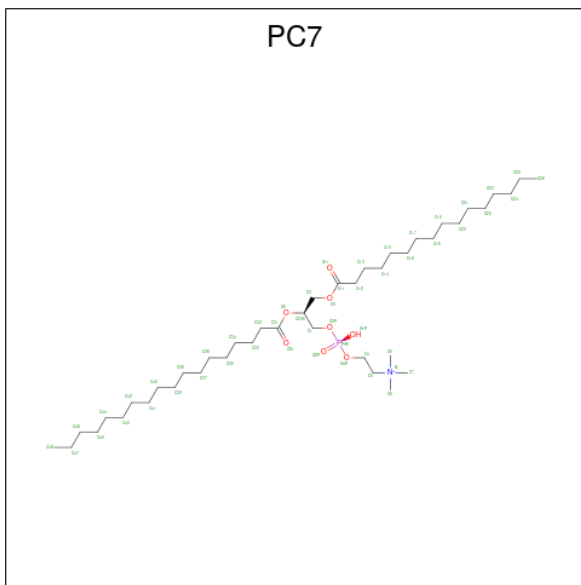
- Molecule 34 is a protein called CA2.

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

- Molecule 35 is a protein called CA3.

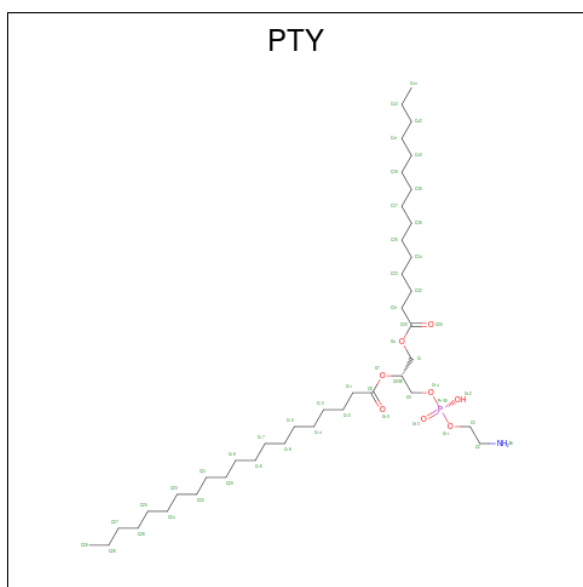
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	z	226	1687	1069	279	334	5	0	0

- Molecule 36 is (7S)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSAN-1-AMINIUM 4-OXIDE (three-letter code: PC7) (formula: C<sub>42</sub>H<sub>85</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
36	A	1	49	39	1	8	1	0
36	L	1	152	122	3	24	3	0
36	L	1	152	122	3	24	3	0
36	L	1	152	122	3	24	3	0
36	N	1	104	84	2	16	2	0
36	N	1	104	84	2	16	2	0
36	z	1	52	42	1	8	1	0

- Molecule 37 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula: C<sub>40</sub>H<sub>80</sub>NO<sub>8</sub>P).



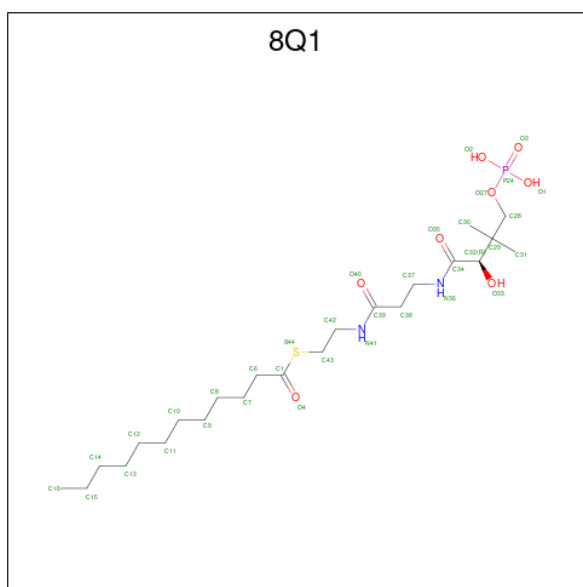
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
37	H	1	Total 50	C 40	N 1	O 8	P 1	0
37	L	1	Total 50	C 40	N 1	O 8	P 1	0
37	M	1	Total 47	C 37	N 1	O 8	P 1	0
37	N	1	Total 50	C 40	N 1	O 8	P 1	0
37	Y	1	Total 50	C 40	N 1	O 8	P 1	0
37	m	1	Total 100	C 80	N 2	O 16	P 2	0
37	m	1	Total 100	C 80	N 2	O 16	P 2	0

- Molecule 38 is CARDIOLIPIN (three-letter code: CDL) (formula: C<sub>81</sub>H<sub>156</sub>O<sub>17</sub>P<sub>2</sub>).



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

- Molecule 39 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonoxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (three-letter code: 8Q1) (formula: C<sub>23</sub>H<sub>45</sub>N<sub>2</sub>O<sub>8</sub>PS).



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

- Molecule 40 is water.

Mol	Chain	Residues	Atoms		AltConf
40	A	6	Total	O	0
			6	6	
40	H	10	Total	O	0
			10	10	
40	J	2	Total	O	0
			2	2	
40	K	5	Total	O	0
			5	5	
40	L	35	Total	O	0
			35	35	
40	M	41	Total	O	0
			41	41	
40	N	20	Total	O	0
			20	20	
40	O	16	Total	O	0
			16	16	
40	T	4	Total	O	0
			4	4	
40	X	2	Total	O	0
			2	2	
40	Y	13	Total	O	0
			13	13	

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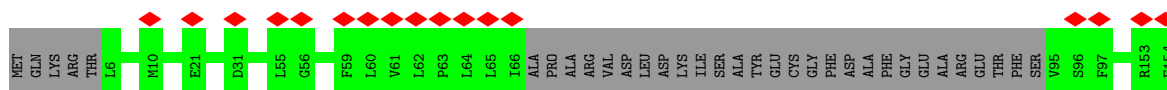
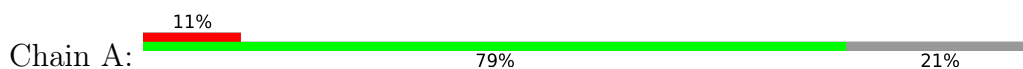
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Mol	Chain	Residues	Atoms		AltConf
40	Z	6	Total 6	O 6	0
40	a	6	Total 6	O 6	0
40	c	7	Total 7	O 7	0
40	d	5	Total 5	O 5	0
40	e	7	Total 7	O 7	0
40	f	4	Total 4	O 4	0
40	g	6	Total 6	O 6	0
40	h	3	Total 3	O 3	0
40	i	8	Total 8	O 8	0
40	k	1	Total 1	O 1	0
40	l	20	Total 20	O 20	0
40	m	22	Total 22	O 22	0
40	n	6	Total 6	O 6	0
40	o	2	Total 2	O 2	0
40	p	15	Total 15	O 15	0
40	s	9	Total 9	O 9	0
40	t	7	Total 7	O 7	0
40	x	26	Total 26	O 26	0
40	y	25	Total 25	O 25	0
40	z	25	Total 25	O 25	0

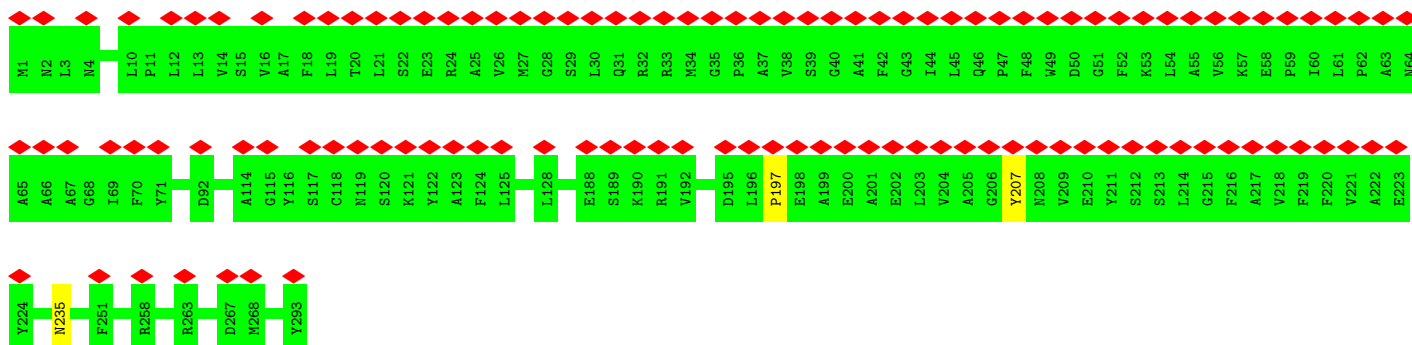
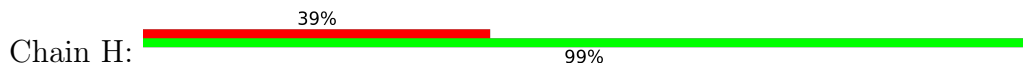
### 3 Residue-property plots [i](#)

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.

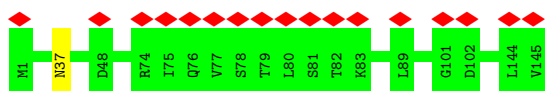
- Molecule 1: ND3



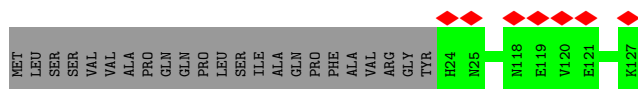
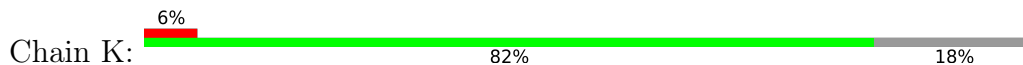
- Molecule 2: ND1



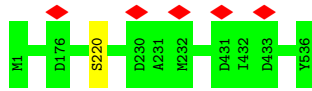
- Molecule 3: ND6



- Molecule 4: ND4L



- Molecule 5: ND5

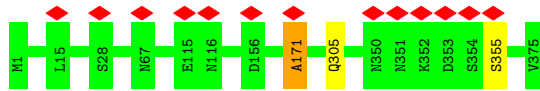


- Molecule 6: ND4

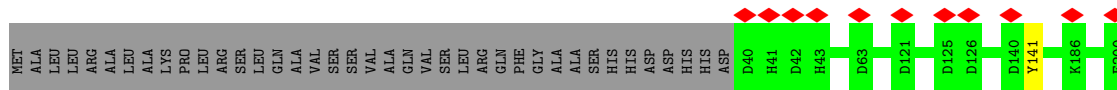
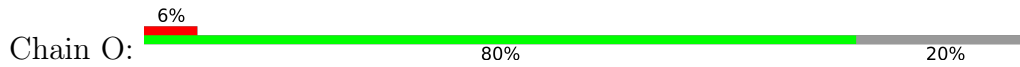


There are no outlier residues recorded for this chain.

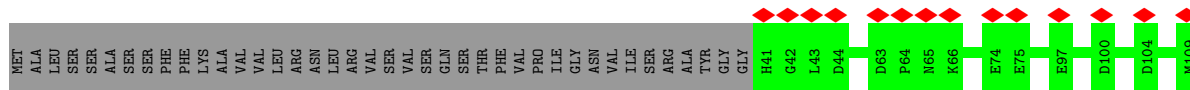
- Molecule 7: ND2



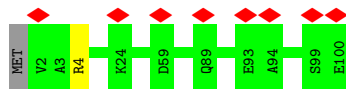
- Molecule 8: C1-FDX



- Molecule 9: SDAP1



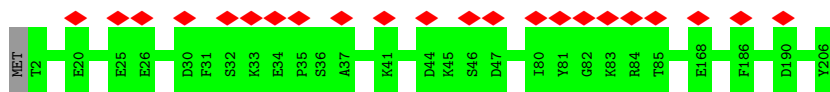
- Molecule 10: PGIV



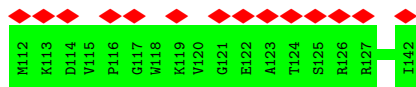
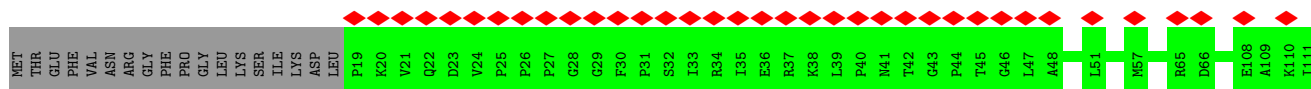
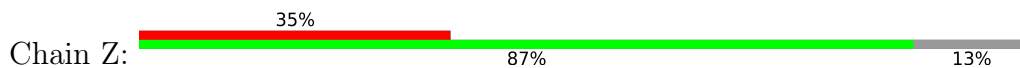
- Molecule 11: B14.7



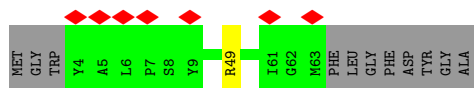
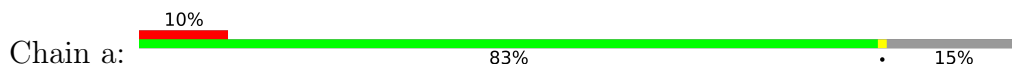




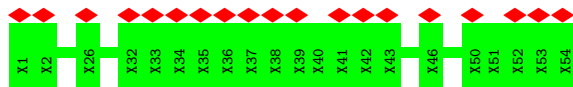
• Molecule 12: B16.6



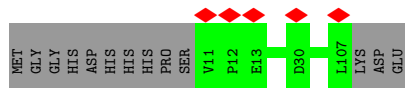
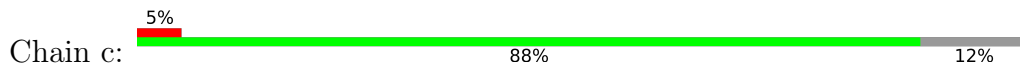
• Molecule 13: MWFE



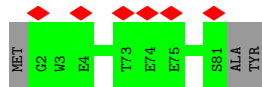
• Molecule 14: B9



• Molecule 15: KFYI

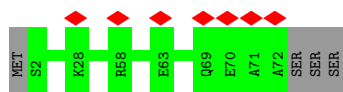


• Molecule 16: B14.5b

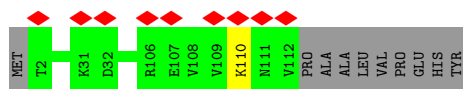
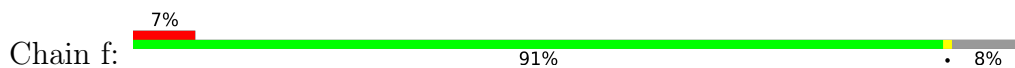


• Molecule 17: 15 kDa

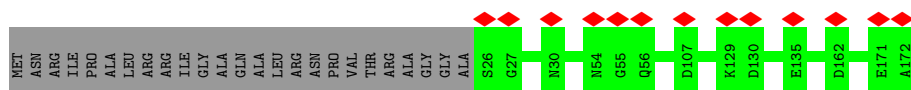
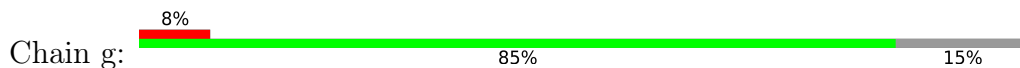




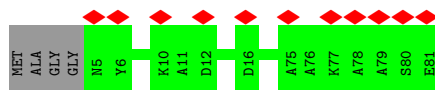
- Molecule 18: MNLL



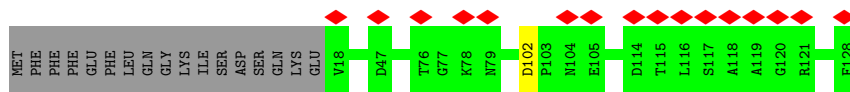
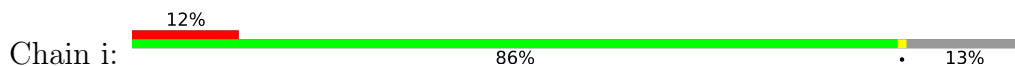
- Molecule 19: ESSS



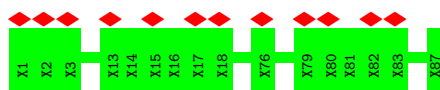
- Molecule 20: NUOP4



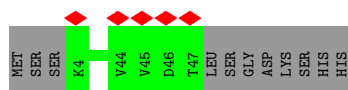
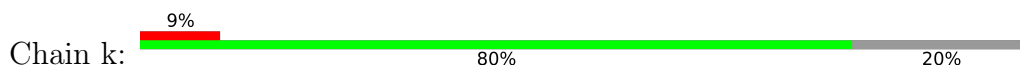
- Molecule 21: NUOP5



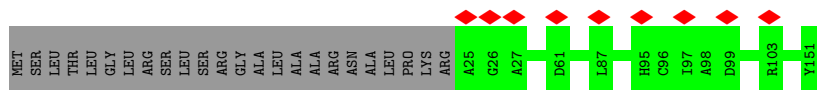
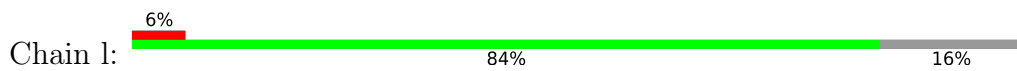
- Molecule 22: AGGG



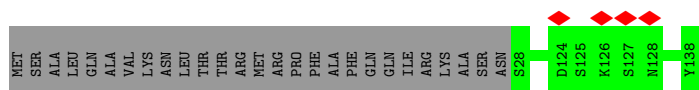
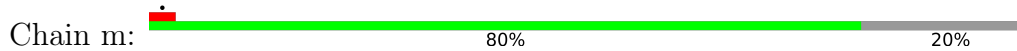
- Molecule 23: B12



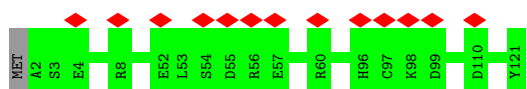
- Molecule 24: ASHI



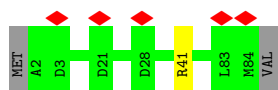
• Molecule 25: B15



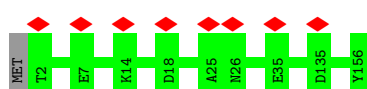
• Molecule 26: B22



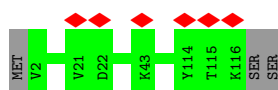
• Molecule 27: B18



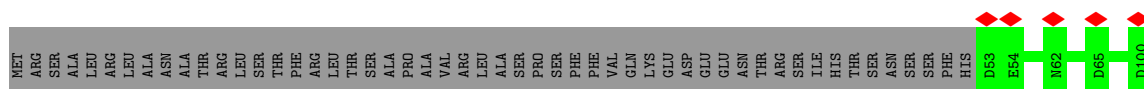
• Molecule 28: PDSW



• Molecule 29: NUOP7

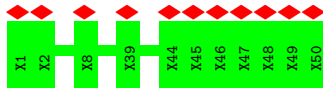


• Molecule 30: NUOP8

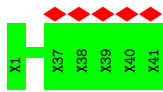




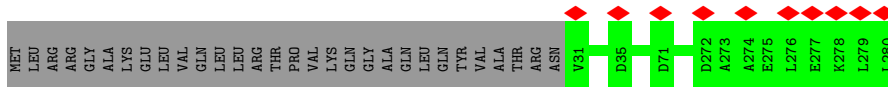
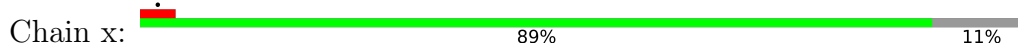
- Molecule 31: unknown



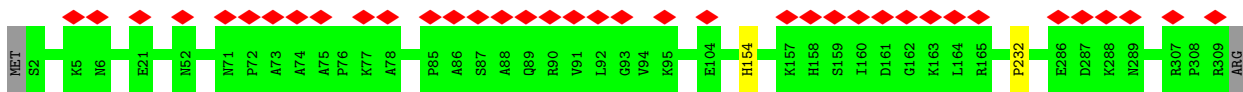
- Molecule 32: unknown



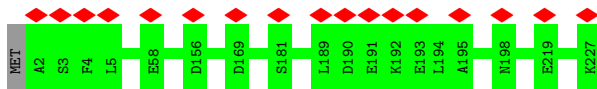
- Molecule 33: CAL



- Molecule 34: CA2



- Molecule 35: 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	0.083	Depositor
Minimum map value	-0.046	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	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: CDL, PTY, 8Q1, PC7

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	0.30	0/1028	0.51	0/1405
2	H	0.29	0/2287	0.55	0/3116
3	J	0.28	0/1142	0.51	0/1558
4	K	0.29	0/812	0.52	0/1102
5	L	0.29	0/4210	0.50	0/5713
6	M	0.31	0/3529	0.50	0/4813
7	N	0.29	0/3050	0.49	1/4154 (0.0%)
8	O	0.29	0/1380	0.48	0/1875
9	T	0.28	0/655	0.49	0/891
10	X	0.28	0/838	0.50	0/1128
11	Y	0.29	0/1630	0.51	0/2227
12	Z	0.30	0/1029	0.58	0/1395
13	a	0.27	0/532	0.50	0/722
15	c	0.26	0/816	0.48	0/1117
16	d	0.30	0/667	0.51	0/902
17	e	0.26	0/602	0.49	0/803
18	f	0.29	0/906	0.47	0/1236
19	g	0.28	0/1210	0.51	0/1638
20	h	0.27	0/643	0.44	0/870
21	i	0.30	0/943	0.60	1/1275 (0.1%)
23	k	0.26	0/381	0.44	0/517
24	l	0.28	0/1053	0.47	0/1435
25	m	0.27	0/967	0.48	0/1314
26	n	0.29	0/1036	0.54	0/1399
27	o	0.27	0/724	0.52	0/974
28	p	0.30	0/1314	0.52	0/1766
29	s	0.27	0/963	0.51	0/1317
30	t	0.28	0/736	0.46	0/1003
33	x	0.29	0/2010	0.54	0/2733
34	y	0.26	0/2363	0.50	0/3215
35	z	0.28	0/1713	0.49	0/2320
All	All	0.29	0/41169	0.51	2/55933 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	N	171	ALA	CB-CA-C	5.28	118.01	110.10
21	i	102	ASP	CB-CG-OD1	5.01	122.81	118.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	117/154 (76%)	114 (97%)	3 (3%)	0	100	100
2	H	291/293 (99%)	281 (97%)	8 (3%)	2 (1%)	22	58
3	J	143/145 (99%)	136 (95%)	7 (5%)	0	100	100
4	K	102/127 (80%)	101 (99%)	1 (1%)	0	100	100
5	L	534/536 (100%)	523 (98%)	10 (2%)	1 (0%)	47	80
6	M	436/438 (100%)	428 (98%)	8 (2%)	0	100	100
7	N	373/375 (100%)	363 (97%)	8 (2%)	2 (0%)	29	66
8	O	159/200 (80%)	153 (96%)	5 (3%)	1 (1%)	25	61
9	T	81/123 (66%)	78 (96%)	3 (4%)	0	100	100
10	X	97/100 (97%)	95 (98%)	2 (2%)	0	100	100
11	Y	203/206 (98%)	199 (98%)	4 (2%)	0	100	100
12	Z	122/142 (86%)	120 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	a	58/71 (82%)	58 (100%)	0	0	100	100
15	c	95/110 (86%)	94 (99%)	1 (1%)	0	100	100
16	d	78/83 (94%)	77 (99%)	1 (1%)	0	100	100
17	e	69/75 (92%)	68 (99%)	1 (1%)	0	100	100
18	f	109/121 (90%)	106 (97%)	3 (3%)	0	100	100
19	g	145/172 (84%)	142 (98%)	3 (2%)	0	100	100
20	h	75/81 (93%)	74 (99%)	1 (1%)	0	100	100
21	i	109/128 (85%)	107 (98%)	2 (2%)	0	100	100
23	k	42/55 (76%)	42 (100%)	0	0	100	100
24	l	125/151 (83%)	122 (98%)	3 (2%)	0	100	100
25	m	109/138 (79%)	105 (96%)	4 (4%)	0	100	100
26	n	118/121 (98%)	116 (98%)	2 (2%)	0	100	100
27	o	81/85 (95%)	79 (98%)	2 (2%)	0	100	100
28	p	153/156 (98%)	150 (98%)	3 (2%)	0	100	100
29	s	113/118 (96%)	111 (98%)	2 (2%)	0	100	100
30	t	80/134 (60%)	80 (100%)	0	0	100	100
33	x	248/280 (89%)	242 (98%)	6 (2%)	0	100	100
34	y	306/310 (99%)	301 (98%)	4 (1%)	1 (0%)	41	74
35	z	224/227 (99%)	219 (98%)	5 (2%)	0	100	100
All	All	4995/5455 (92%)	4884 (98%)	104 (2%)	7 (0%)	54	83

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	N	171	ALA
5	L	220	SER
2	H	207	TYR
8	O	141	TYR
7	N	355	SER
34	y	232	PRO
2	H	197	PRO



### 5.3.2 Protein sidechains [i](#)

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	H	240/240 (100%)	239 (100%)	1 (0%)	91	97
3	J	129/129 (100%)	128 (99%)	1 (1%)	81	92
4	K	84/103 (82%)	84 (100%)	0	100	100
5	L	438/438 (100%)	438 (100%)	0	100	100
6	M	376/376 (100%)	376 (100%)	0	100	100
7	N	331/331 (100%)	330 (100%)	1 (0%)	92	97
8	O	146/177 (82%)	146 (100%)	0	100	100
9	T	73/106 (69%)	73 (100%)	0	100	100
10	X	85/86 (99%)	84 (99%)	1 (1%)	71	89
11	Y	165/166 (99%)	165 (100%)	0	100	100
12	Z	107/123 (87%)	107 (100%)	0	100	100
13	a	50/57 (88%)	49 (98%)	1 (2%)	55	81
15	c	80/91 (88%)	80 (100%)	0	100	100
16	d	68/70 (97%)	68 (100%)	0	100	100
17	e	64/68 (94%)	64 (100%)	0	100	100
18	f	92/100 (92%)	91 (99%)	1 (1%)	73	90
19	g	122/139 (88%)	122 (100%)	0	100	100
20	h	64/65 (98%)	64 (100%)	0	100	100
21	i	97/113 (86%)	97 (100%)	0	100	100
23	k	35/45 (78%)	35 (100%)	0	100	100
24	l	110/128 (86%)	110 (100%)	0	100	100
25	m	100/123 (81%)	100 (100%)	0	100	100
26	n	106/107 (99%)	106 (100%)	0	100	100
27	o	74/76 (97%)	73 (99%)	1 (1%)	67	86
28	p	140/141 (99%)	140 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	s	105/108 (97%)	105 (100%)	0	100	100
30	t	73/119 (61%)	73 (100%)	0	100	100
33	x	209/234 (89%)	209 (100%)	0	100	100
34	y	250/252 (99%)	249 (100%)	1 (0%)	91	97
35	z	188/189 (100%)	188 (100%)	0	100	100
All	All	4308/4633 (93%)	4300 (100%)	8 (0%)	93	98

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	235	ASN
3	J	37	ASN
7	N	305	GLN
10	X	4	ARG
13	a	49	ARG
18	f	110	LYS
27	o	41	ARG
34	y	154	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
3	J	86	GLN
5	L	343	ASN
9	T	101	ASN
25	m	42	ASN
33	x	44	GLN
34	y	62	ASN
35	z	83	ASN
35	z	104	ASN
35	z	145	ASN

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

20 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
39	8Q1	n	200	-	31,34,34	1.73	6 (19%)	40,43,43	1.42	3 (7%)
38	CDL	d	101	-	99,99,99	0.88	8 (8%)	105,111,111	1.00	4 (3%)
38	CDL	L	601	-	88,88,99	0.93	8 (9%)	94,100,111	0.99	4 (4%)
36	PC7	L	603	-	47,47,51	1.02	4 (8%)	53,55,59	1.01	1 (1%)
38	CDL	t	201	-	99,99,99	0.88	8 (8%)	105,111,111	0.98	4 (3%)
36	PC7	z	301	-	51,51,51	0.96	4 (7%)	57,59,59	0.93	2 (3%)
36	PC7	L	604	-	51,51,51	0.96	4 (7%)	57,59,59	0.99	2 (3%)
37	PTY	m	201	-	49,49,49	0.88	4 (8%)	52,54,54	1.02	2 (3%)
37	PTY	H	301	-	49,49,49	0.86	4 (8%)	52,54,54	1.03	2 (3%)
37	PTY	Y	301	-	49,49,49	0.87	4 (8%)	52,54,54	1.11	2 (3%)
38	CDL	N	401	-	99,99,99	0.88	8 (8%)	105,111,111	1.00	4 (3%)
36	PC7	N	402	-	51,51,51	0.96	4 (7%)	57,59,59	0.97	2 (3%)
36	PC7	N	403	-	51,51,51	0.95	4 (7%)	57,59,59	1.20	3 (5%)
36	PC7	L	602	-	51,51,51	0.97	4 (7%)	57,59,59	0.97	2 (3%)
37	PTY	M	501	-	46,46,49	0.91	4 (8%)	49,51,54	1.04	2 (4%)
37	PTY	N	404	-	49,49,49	0.87	4 (8%)	52,54,54	0.97	2 (3%)
38	CDL	M	502	-	99,99,99	0.87	8 (8%)	105,111,111	1.13	6 (5%)
37	PTY	m	202	-	49,49,49	0.88	4 (8%)	52,54,54	1.06	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
37	PTY	L	605	-	49,49,49	0.88	4 (8%)	52,54,54	1.06	2 (3%)
36	PC7	A	201	-	48,48,51	0.98	4 (8%)	54,56,59	1.04	2 (3%)

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
39	8Q1	n	200	-	-	11/41/41/41	-
38	CDL	d	101	-	-	65/110/110/110	-
38	CDL	L	601	-	-	60/99/99/110	-
36	PC7	L	603	-	-	35/51/51/55	-
38	CDL	t	201	-	-	73/110/110/110	-
36	PC7	z	301	-	-	34/55/55/55	-
36	PC7	L	604	-	-	32/55/55/55	-
37	PTY	m	201	-	-	30/53/53/53	-
37	PTY	H	301	-	-	37/53/53/53	-
37	PTY	Y	301	-	-	33/53/53/53	-
38	CDL	N	401	-	-	67/110/110/110	-
36	PC7	N	402	-	-	29/55/55/55	-
36	PC7	N	403	-	-	32/55/55/55	-
36	PC7	L	602	-	-	30/55/55/55	-
37	PTY	M	501	-	-	26/50/50/53	-
37	PTY	N	404	-	-	28/53/53/53	-
38	CDL	M	502	-	-	73/110/110/110	-
37	PTY	m	202	-	-	33/53/53/53	-
37	PTY	L	605	-	-	30/53/53/53	-
36	PC7	A	201	-	-	32/52/52/55	-

All (102) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	n	200	8Q1	C34-N36	5.56	1.45	1.33
39	n	200	8Q1	C39-N41	5.45	1.45	1.33
38	t	201	CDL	OA6-CA4	-2.67	1.39	1.46
38	t	201	CDL	OB6-CB4	-2.64	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	d	101	CDL	OB6-CB4	-2.62	1.40	1.46
38	L	601	CDL	OA6-CA4	-2.60	1.40	1.46
38	d	101	CDL	OA6-CA4	-2.59	1.40	1.46
38	M	502	CDL	OB6-CB4	-2.59	1.40	1.46
38	L	601	CDL	OB6-CB4	-2.58	1.40	1.46
38	M	502	CDL	OA8-CA7	2.56	1.40	1.33
36	N	402	PC7	O2-C2	-2.54	1.40	1.46
37	M	501	PTY	O7-C6	-2.54	1.40	1.46
38	N	401	CDL	OB6-CB4	-2.54	1.40	1.46
37	N	404	PTY	O7-C6	-2.53	1.40	1.46
38	N	401	CDL	OA8-CA7	2.53	1.40	1.33
38	L	601	CDL	OB8-CB7	2.52	1.40	1.33
36	A	201	PC7	O2-C2	-2.52	1.40	1.46
37	m	202	PTY	O7-C6	-2.52	1.40	1.46
39	n	200	8Q1	C1-S44	2.51	1.82	1.76
36	L	603	PC7	O2-C2	-2.50	1.40	1.46
37	Y	301	PTY	O7-C6	-2.50	1.40	1.46
36	L	602	PC7	O2-C2	-2.49	1.40	1.46
38	t	201	CDL	OB8-CB7	2.49	1.40	1.33
36	L	604	PC7	O2-C2	-2.49	1.40	1.46
38	N	401	CDL	OA6-CA4	-2.48	1.40	1.46
38	d	101	CDL	OA8-CA7	2.47	1.40	1.33
37	m	201	PTY	O7-C6	-2.47	1.40	1.46
36	A	201	PC7	O3-C11	2.46	1.40	1.33
38	L	601	CDL	OA8-CA7	2.46	1.40	1.33
38	d	101	CDL	OB8-CB7	2.46	1.40	1.33
37	L	605	PTY	O7-C6	-2.44	1.40	1.46
38	t	201	CDL	OA8-CA7	2.44	1.40	1.33
36	z	301	PC7	O3-C11	2.43	1.40	1.33
37	M	501	PTY	O4-C30	2.42	1.40	1.33
37	L	605	PTY	O4-C30	2.41	1.40	1.33
38	M	502	CDL	OB8-CB7	2.41	1.40	1.33
38	N	401	CDL	OB8-CB7	2.41	1.40	1.33
36	L	604	PC7	O3-C11	2.40	1.40	1.33
36	L	602	PC7	O3-C11	2.40	1.40	1.33
37	H	301	PTY	O4-C30	2.40	1.40	1.33
36	N	402	PC7	O3-C11	2.39	1.40	1.33
37	m	202	PTY	O4-C30	2.39	1.40	1.33
37	Y	301	PTY	O4-C30	2.37	1.40	1.33
36	N	403	PC7	O3-C11	2.37	1.40	1.33
37	m	201	PTY	O4-C30	2.36	1.40	1.33
37	N	404	PTY	O4-C30	2.36	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	M	502	CDL	OA6-CA5	2.34	1.40	1.34
36	z	301	PC7	O2-C31	2.32	1.40	1.34
36	N	403	PC7	O2-C2	-2.32	1.40	1.46
36	L	603	PC7	O2-C31	2.32	1.40	1.34
36	L	603	PC7	O3-C11	2.32	1.40	1.33
37	H	301	PTY	O7-C8	2.27	1.40	1.34
36	L	603	PC7	O3-C3	-2.26	1.40	1.45
39	n	200	8Q1	O35-C34	-2.25	1.18	1.23
39	n	200	8Q1	C6-C1	2.23	1.53	1.50
37	m	201	PTY	O4-C1	-2.23	1.40	1.45
36	z	301	PC7	O2-C2	-2.23	1.41	1.46
37	M	501	PTY	O4-C1	-2.22	1.40	1.45
37	m	202	PTY	O4-C1	-2.22	1.40	1.45
36	L	602	PC7	O2-C31	2.22	1.40	1.34
36	L	602	PC7	O3-C3	-2.22	1.40	1.45
38	N	401	CDL	OA6-CA5	2.22	1.40	1.34
36	N	403	PC7	O3-C3	-2.21	1.40	1.45
36	L	604	PC7	O3-C3	-2.21	1.40	1.45
37	L	605	PTY	O7-C8	2.21	1.40	1.34
37	H	301	PTY	O7-C6	-2.20	1.41	1.46
37	N	404	PTY	O4-C1	-2.18	1.40	1.45
36	N	402	PC7	O2-C31	2.17	1.40	1.34
37	Y	301	PTY	O4-C1	-2.17	1.40	1.45
37	L	605	PTY	O4-C1	-2.17	1.40	1.45
39	n	200	8Q1	O40-C39	-2.17	1.18	1.23
38	N	401	CDL	OB6-CB5	2.16	1.40	1.34
36	A	201	PC7	O2-C31	2.15	1.40	1.34
37	m	201	PTY	O7-C8	2.15	1.40	1.34
36	L	604	PC7	O2-C31	2.15	1.40	1.34
37	H	301	PTY	O4-C1	-2.13	1.40	1.45
36	N	402	PC7	O3-C3	-2.13	1.40	1.45
38	L	601	CDL	OA6-CA5	2.13	1.40	1.34
38	L	601	CDL	OB6-CB5	2.13	1.40	1.34
37	M	501	PTY	O7-C8	2.12	1.40	1.34
36	N	403	PC7	O2-C31	2.12	1.40	1.34
38	d	101	CDL	OA6-CA5	2.11	1.40	1.34
38	t	201	CDL	OA8-CA6	-2.11	1.40	1.45
36	z	301	PC7	O3-C3	-2.11	1.40	1.45
37	Y	301	PTY	O7-C8	2.10	1.40	1.34
38	t	201	CDL	OB6-CB5	2.10	1.40	1.34
37	m	202	PTY	O7-C8	2.10	1.40	1.34
38	M	502	CDL	OB6-CB5	2.10	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	N	404	PTY	O7-C8	2.10	1.40	1.34
38	d	101	CDL	OA8-CA6	-2.10	1.40	1.45
38	d	101	CDL	OB6-CB5	2.10	1.40	1.34
36	A	201	PC7	O3-C3	-2.08	1.40	1.45
38	L	601	CDL	OA8-CA6	-2.08	1.40	1.45
38	M	502	CDL	OB8-CB6	-2.07	1.40	1.45
38	M	502	CDL	OA6-CA4	-2.07	1.41	1.46
38	N	401	CDL	OB8-CB6	-2.06	1.40	1.45
38	d	101	CDL	OB8-CB6	-2.06	1.40	1.45
38	t	201	CDL	OB8-CB6	-2.06	1.40	1.45
38	L	601	CDL	OB8-CB6	-2.05	1.40	1.45
38	t	201	CDL	OA6-CA5	2.05	1.40	1.34
38	N	401	CDL	OA8-CA6	-2.01	1.40	1.45
38	M	502	CDL	OA8-CA6	-2.01	1.40	1.45

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	n	200	8Q1	C6-C1-S44	5.16	119.47	113.46
38	M	502	CDL	OA6-CA5-C11	5.13	122.56	111.50
36	L	602	PC7	O2-C31-C32	4.37	120.91	111.50
36	L	603	PC7	O2-C31-C32	4.33	120.83	111.50
36	N	403	PC7	O2-C31-C32	4.15	120.44	111.50
37	Y	301	PTY	O7-C8-C11	4.12	120.38	111.50
36	A	201	PC7	O2-C31-C32	4.12	120.37	111.50
38	L	601	CDL	OA6-CA5-C11	4.10	120.33	111.50
37	m	201	PTY	O7-C8-C11	4.03	120.19	111.50
37	L	605	PTY	O7-C8-C11	4.02	120.16	111.50
37	m	202	PTY	O7-C8-C11	3.98	120.07	111.50
37	H	301	PTY	O7-C8-C11	3.92	119.95	111.50
38	N	401	CDL	OA6-CA5-C11	3.92	119.95	111.50
36	L	604	PC7	O2-C31-C32	3.88	119.87	111.50
36	N	403	PC7	C2-O2-C31	-3.80	108.44	117.79
37	M	501	PTY	O7-C8-C11	3.80	119.69	111.50
38	d	101	CDL	OA6-CA5-C11	3.80	119.68	111.50
38	t	201	CDL	OB6-CB5-C51	3.77	119.62	111.50
38	M	502	CDL	OB6-CB5-C51	3.76	119.61	111.50
38	d	101	CDL	OB6-CB5-C51	3.74	119.57	111.50
36	N	402	PC7	O2-C31-C32	3.73	119.55	111.50
38	N	401	CDL	OB6-CB5-C51	3.62	119.31	111.50
37	N	404	PTY	O7-C8-C11	3.59	119.23	111.50
36	z	301	PC7	O2-C31-C32	3.52	119.08	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	t	201	CDL	OA6-CA5-C11	3.47	118.98	111.50
38	L	601	CDL	OB6-CB5-C51	3.43	118.89	111.50
39	n	200	8Q1	O4-C1-C6	-3.20	120.21	123.99
37	M	501	PTY	O4-C30-C31	2.92	121.08	111.91
36	N	403	PC7	O3-C11-C12	2.92	121.06	111.91
37	Y	301	PTY	O4-C30-C31	2.76	120.58	111.91
39	n	200	8Q1	C43-S44-C1	2.75	110.44	101.87
37	m	202	PTY	O4-C30-C31	2.72	120.44	111.91
36	A	201	PC7	O3-C11-C12	2.72	120.44	111.91
37	L	605	PTY	O4-C30-C31	2.64	120.20	111.91
38	M	502	CDL	OB8-CB7-C71	2.62	120.12	111.91
37	H	301	PTY	O4-C30-C31	2.61	120.10	111.91
38	t	201	CDL	OB8-CB7-C71	2.58	119.99	111.91
38	L	601	CDL	OA8-CA7-C31	2.51	119.78	111.91
36	L	604	PC7	O3-C11-C12	2.49	119.73	111.91
38	d	101	CDL	OB8-CB7-C71	2.49	119.71	111.91
36	z	301	PC7	O3-C11-C12	2.43	119.55	111.91
37	m	201	PTY	O4-C30-C31	2.42	119.51	111.91
36	N	402	PC7	O3-C11-C12	2.42	119.50	111.91
38	N	401	CDL	OB8-CB7-C71	2.36	119.31	111.91
38	N	401	CDL	OA8-CA7-C31	2.25	118.96	111.91
36	L	602	PC7	O3-C11-C12	2.24	118.95	111.91
38	M	502	CDL	OA8-CA7-C31	2.24	118.94	111.91
38	L	601	CDL	OB8-CB7-C71	2.23	118.90	111.91
38	d	101	CDL	OA8-CA7-C31	2.22	118.87	111.91
38	M	502	CDL	CA4-OA6-CA5	2.21	123.24	117.79
38	t	201	CDL	OA8-CA7-C31	2.12	118.57	111.91
37	N	404	PTY	O4-C30-C31	2.11	118.52	111.91
38	M	502	CDL	OA6-CA5-OA7	-2.00	118.86	123.70

There are no chirality outliers.

All (790) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
36	A	201	PC7	C32-C31-O2-C2
36	A	201	PC7	O31-C31-O2-C2
36	A	201	PC7	C1-O3P-P-O1P
36	A	201	PC7	C1-O3P-P-O2P
36	A	201	PC7	O4P-C4-C5-N
36	A	201	PC7	O11-C11-O3-C3
36	A	201	PC7	C12-C11-O3-C3
36	L	602	PC7	C32-C31-O2-C2

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Mol	Chain	Res	Type	Atoms
36	L	602	PC7	O31-C31-O2-C2
36	L	603	PC7	C32-C31-O2-C2
36	L	603	PC7	C1-O3P-P-O1P
36	L	603	PC7	C1-O3P-P-O2P
36	L	603	PC7	C1-O3P-P-O4P
36	L	603	PC7	C4-O4P-P-O2P
36	L	604	PC7	C1-O3P-P-O1P
36	L	604	PC7	C1-O3P-P-O2P
36	N	402	PC7	C4-O4P-P-O2P
36	N	403	PC7	C32-C31-O2-C2
36	N	403	PC7	C4-O4P-P-O1P
36	N	403	PC7	C4-O4P-P-O2P
36	N	403	PC7	O4P-C4-C5-N
36	z	301	PC7	O2-C2-C3-O3
36	z	301	PC7	O4P-C4-C5-N
37	H	301	PTY	C11-C8-O7-C6
37	H	301	PTY	C3-O11-P1-O12
37	H	301	PTY	C3-O11-P1-O14
37	H	301	PTY	C5-O14-P1-O11
37	H	301	PTY	C5-O14-P1-O12
37	H	301	PTY	C5-O14-P1-O13
37	L	605	PTY	N1-C2-C3-O11
37	L	605	PTY	O10-C8-O7-C6
37	L	605	PTY	C11-C8-O7-C6
37	M	501	PTY	C31-C30-O4-C1
37	M	501	PTY	O30-C30-O4-C1
37	M	501	PTY	C11-C8-O7-C6
37	M	501	PTY	C5-O14-P1-O11
37	M	501	PTY	C5-O14-P1-O12
37	N	404	PTY	O4-C1-C6-O7
37	N	404	PTY	N1-C2-C3-O11
37	N	404	PTY	C3-O11-P1-O12
37	N	404	PTY	C3-O11-P1-O13
37	N	404	PTY	C5-O14-P1-O12
37	Y	301	PTY	N1-C2-C3-O11
37	Y	301	PTY	C11-C8-O7-C6
37	Y	301	PTY	C3-O11-P1-O12
37	Y	301	PTY	C3-O11-P1-O13
37	m	201	PTY	N1-C2-C3-O11
37	m	201	PTY	C3-O11-P1-O12
37	m	201	PTY	C5-O14-P1-O11
37	m	201	PTY	C5-O14-P1-O12

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Mol	Chain	Res	Type	Atoms
37	m	201	PTY	C5-O14-P1-O13
37	m	202	PTY	C5-O14-P1-O11
37	m	202	PTY	C5-O14-P1-O13
38	L	601	CDL	CA2-OA2-PA1-OA3
38	L	601	CDL	CA3-OA5-PA1-OA3
38	L	601	CDL	CA3-OA5-PA1-OA4
38	L	601	CDL	C11-CA5-OA6-CA4
38	L	601	CDL	CB2-OB2-PB2-OB3
38	L	601	CDL	CB2-OB2-PB2-OB4
38	L	601	CDL	CB2-OB2-PB2-OB5
38	L	601	CDL	CB3-OB5-PB2-OB3
38	M	502	CDL	CA2-OA2-PA1-OA3
38	M	502	CDL	CA2-OA2-PA1-OA4
38	M	502	CDL	CA2-OA2-PA1-OA5
38	M	502	CDL	CA3-OA5-PA1-OA3
38	M	502	CDL	OA7-CA5-OA6-CA4
38	M	502	CDL	C11-CA5-OA6-CA4
38	M	502	CDL	CB3-OB5-PB2-OB3
38	N	401	CDL	CA2-OA2-PA1-OA3
38	N	401	CDL	CA2-OA2-PA1-OA4
38	N	401	CDL	CA3-OA5-PA1-OA4
38	N	401	CDL	OA7-CA5-OA6-CA4
38	N	401	CDL	C11-CA5-OA6-CA4
38	N	401	CDL	CB3-OB5-PB2-OB3
38	d	101	CDL	CA2-OA2-PA1-OA3
38	d	101	CDL	CA2-OA2-PA1-OA4
38	d	101	CDL	CA2-OA2-PA1-OA5
38	d	101	CDL	CA3-OA5-PA1-OA2
38	d	101	CDL	CA3-OA5-PA1-OA3
38	d	101	CDL	CA3-OA5-PA1-OA4
38	d	101	CDL	C11-CA5-OA6-CA4
38	d	101	CDL	OB6-CB4-CB6-OB8
38	t	201	CDL	O1-C1-CA2-OA2
38	t	201	CDL	CB2-C1-CA2-OA2
38	t	201	CDL	CA3-OA5-PA1-OA3
38	t	201	CDL	CB2-OB2-PB2-OB3
39	n	200	8Q1	C1-C6-C7-C8
39	n	200	8Q1	C42-C43-S44-C1
39	n	200	8Q1	C28-O27-P24-O2
39	n	200	8Q1	C28-O27-P24-O1
36	N	402	PC7	O11-C11-O3-C3
36	N	403	PC7	O11-C11-O3-C3

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Mol	Chain	Res	Type	Atoms
38	N	401	CDL	OB9-CB7-OB8-CB6
38	d	101	CDL	OB9-CB7-OB8-CB6
36	N	402	PC7	C12-C11-O3-C3
36	N	403	PC7	C12-C11-O3-C3
38	N	401	CDL	C71-CB7-OB8-CB6
38	d	101	CDL	C71-CB7-OB8-CB6
37	m	202	PTY	O30-C30-O4-C1
37	H	301	PTY	O10-C8-O7-C6
37	M	501	PTY	O10-C8-O7-C6
37	Y	301	PTY	O10-C8-O7-C6
38	L	601	CDL	OA7-CA5-OA6-CA4
38	d	101	CDL	OA7-CA5-OA6-CA4
38	d	101	CDL	C82-C83-C84-C85
37	H	301	PTY	C31-C30-O4-C1
37	m	202	PTY	C31-C30-O4-C1
36	L	602	PC7	C13-C14-C15-C16
38	t	201	CDL	C55-C56-C57-C58
36	L	603	PC7	O31-C31-O2-C2
37	H	301	PTY	O30-C30-O4-C1
36	L	602	PC7	C4-C5-N-C6
37	m	201	PTY	C22-C23-C24-C25
38	L	601	CDL	C17-C18-C19-C20
38	M	502	CDL	C38-C39-C40-C41
38	t	201	CDL	C77-C78-C79-C80
38	M	502	CDL	CA4-CA6-OA8-CA7
38	d	101	CDL	C19-C20-C21-C22
38	L	601	CDL	O1-C1-CB2-OB2
38	N	401	CDL	O1-C1-CB2-OB2
38	d	101	CDL	O1-C1-CA2-OA2
38	d	101	CDL	O1-C1-CB2-OB2
37	N	404	PTY	C38-C39-C40-C41
38	L	601	CDL	C75-C76-C77-C78
38	N	401	CDL	C82-C83-C84-C85
38	d	101	CDL	C22-C23-C24-C25
36	L	603	PC7	C40-C41-C42-C43
36	L	603	PC7	C35-C36-C37-C38
36	L	603	PC7	C19-C20-C21-C22
36	L	604	PC7	C15-C16-C17-C18
38	d	101	CDL	C51-C52-C53-C54
36	L	602	PC7	C35-C36-C37-C38
36	L	603	PC7	C37-C38-C39-C40
36	z	301	PC7	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
37	L	605	PTY	C11-C12-C13-C14
37	L	605	PTY	C24-C25-C26-C27
37	M	501	PTY	C22-C23-C24-C25
37	Y	301	PTY	C39-C40-C41-C42
37	m	201	PTY	C12-C13-C14-C15
37	m	201	PTY	C34-C35-C36-C37
38	L	601	CDL	C36-C37-C38-C39
38	L	601	CDL	C51-C52-C53-C54
38	N	401	CDL	C22-C23-C24-C25
38	d	101	CDL	C36-C37-C38-C39
36	A	201	PC7	C33-C34-C35-C36
36	L	603	PC7	C14-C15-C16-C17
36	N	402	PC7	C12-C13-C14-C15
37	M	501	PTY	C17-C18-C19-C20
37	N	404	PTY	C40-C41-C42-C43
37	m	201	PTY	C14-C15-C16-C17
37	m	201	PTY	C17-C18-C19-C20
37	m	202	PTY	C35-C36-C37-C38
38	L	601	CDL	C34-C35-C36-C37
38	L	601	CDL	C73-C74-C75-C76
38	M	502	CDL	C57-C58-C59-C60
38	t	201	CDL	C12-C13-C14-C15
38	t	201	CDL	C63-C64-C65-C66
38	t	201	CDL	C81-C82-C83-C84
36	L	603	PC7	C21-C22-C23-C24
36	N	403	PC7	C32-C33-C34-C35
37	L	605	PTY	C38-C39-C40-C41
38	N	401	CDL	C53-C54-C55-C56
38	t	201	CDL	C32-C33-C34-C35
36	N	403	PC7	O31-C31-O2-C2
37	N	404	PTY	C21-C22-C23-C24
38	N	401	CDL	C72-C73-C74-C75
36	N	402	PC7	C38-C39-C40-C41
38	L	601	CDL	C31-C32-C33-C34
38	t	201	CDL	C42-C43-C44-C45
36	z	301	PC7	C21-C22-C23-C24
37	m	202	PTY	C12-C13-C14-C15
38	L	601	CDL	C38-C39-C40-C41
38	d	101	CDL	C42-C43-C44-C45
38	L	601	CDL	CA2-C1-CB2-OB2
38	d	101	CDL	CA2-C1-CB2-OB2
38	t	201	CDL	CA2-C1-CB2-OB2

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Mol	Chain	Res	Type	Atoms
36	L	603	PC7	C4-C5-N-C7
37	Y	301	PTY	C31-C30-O4-C1
38	M	502	CDL	C31-CA7-OA8-CA6
36	z	301	PC7	C19-C20-C21-C22
37	M	501	PTY	C19-C20-C21-C22
38	M	502	CDL	C51-C52-C53-C54
36	L	602	PC7	C37-C38-C39-C40
36	N	403	PC7	C44-C45-C46-C47
38	L	601	CDL	O1-C1-CA2-OA2
38	t	201	CDL	O1-C1-CB2-OB2
36	L	604	PC7	C13-C14-C15-C16
37	m	201	PTY	C39-C40-C41-C42
37	Y	301	PTY	O30-C30-O4-C1
36	z	301	PC7	C17-C18-C19-C20
36	L	604	PC7	C32-C31-O2-C2
37	m	202	PTY	C19-C20-C21-C22
38	t	201	CDL	C74-C75-C76-C77
36	L	604	PC7	C31-C32-C33-C34
38	N	401	CDL	CB7-C71-C72-C73
38	t	201	CDL	CB5-C51-C52-C53
37	L	605	PTY	C31-C30-O4-C1
36	N	403	PC7	C14-C15-C16-C17
36	N	402	PC7	C11-C12-C13-C14
37	Y	301	PTY	C8-C11-C12-C13
37	Y	301	PTY	C30-C31-C32-C33
38	M	502	CDL	CB5-C51-C52-C53
38	M	502	CDL	C72-C73-C74-C75
38	N	401	CDL	C58-C59-C60-C61
36	L	602	PC7	C11-C12-C13-C14
36	L	603	PC7	C31-C32-C33-C34
37	L	605	PTY	C8-C11-C12-C13
37	L	605	PTY	C30-C31-C32-C33
36	N	402	PC7	C14-C15-C16-C17
38	N	401	CDL	CA4-CA3-OA5-PA1
37	N	404	PTY	C8-C11-C12-C13
38	N	401	CDL	CB5-C51-C52-C53
38	t	201	CDL	CA7-C31-C32-C33
37	M	501	PTY	C12-C13-C14-C15
38	t	201	CDL	C57-C58-C59-C60
36	L	602	PC7	C40-C41-C42-C43
37	H	301	PTY	C8-C11-C12-C13
38	L	601	CDL	CA5-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
38	M	502	CDL	O1-C1-CA2-OA2
36	A	201	PC7	C31-C32-C33-C34
38	d	101	CDL	C78-C79-C80-C81
36	A	201	PC7	C1-O3P-P-O4P
36	A	201	PC7	C4-O4P-P-O3P
36	L	603	PC7	C4-O4P-P-O3P
36	L	604	PC7	C1-O3P-P-O4P
36	L	604	PC7	C4-O4P-P-O3P
36	N	402	PC7	C1-O3P-P-O4P
36	N	403	PC7	C4-O4P-P-O3P
37	L	605	PTY	C5-O14-P1-O11
37	N	404	PTY	C3-O11-P1-O14
37	N	404	PTY	C5-O14-P1-O11
37	Y	301	PTY	C3-O11-P1-O14
38	L	601	CDL	CA3-OA5-PA1-OA2
38	L	601	CDL	CB3-OB5-PB2-OB2
38	M	502	CDL	CA3-OA5-PA1-OA2
38	M	502	CDL	CB3-OB5-PB2-OB2
38	N	401	CDL	CA2-OA2-PA1-OA5
38	N	401	CDL	CA3-OA5-PA1-OA2
38	t	201	CDL	CA3-OA5-PA1-OA2
38	t	201	CDL	CB2-OB2-PB2-OB5
38	t	201	CDL	CB7-C71-C72-C73
38	M	502	CDL	CB2-C1-CA2-OA2
38	N	401	CDL	CA2-C1-CB2-OB2
38	d	101	CDL	CB2-C1-CA2-OA2
36	L	604	PC7	O31-C31-O2-C2
36	z	301	PC7	O31-C31-O2-C2
37	m	202	PTY	C17-C18-C19-C20
36	A	201	PC7	C4-C5-N-C6
36	L	602	PC7	C4-C5-N-C8
36	N	402	PC7	C4-C5-N-C7
36	N	402	PC7	C4-C5-N-C6
36	N	403	PC7	C4-C5-N-C7
36	N	403	PC7	C4-C5-N-C8
36	z	301	PC7	C4-C5-N-C7
36	z	301	PC7	C4-C5-N-C6
36	L	602	PC7	C12-C11-O3-C3
36	N	403	PC7	C22-C23-C24-C25
36	L	604	PC7	C11-C12-C13-C14
36	L	604	PC7	C35-C36-C37-C38
38	t	201	CDL	C58-C59-C60-C61

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Mol	Chain	Res	Type	Atoms
36	z	301	PC7	C32-C31-O2-C2
38	t	201	CDL	C11-CA5-OA6-CA4
36	L	604	PC7	C38-C39-C40-C41
36	N	403	PC7	C20-C21-C22-C23
37	H	301	PTY	C24-C25-C26-C27
37	M	501	PTY	C16-C17-C18-C19
37	M	501	PTY	C21-C22-C23-C24
37	Y	301	PTY	C12-C13-C14-C15
37	Y	301	PTY	C13-C14-C15-C16
38	L	601	CDL	C59-C60-C61-C62
38	M	502	CDL	C55-C56-C57-C58
38	N	401	CDL	C15-C16-C17-C18
38	t	201	CDL	C36-C37-C38-C39
38	t	201	CDL	C71-C72-C73-C74
36	L	602	PC7	C32-C33-C34-C35
36	L	604	PC7	C17-C18-C19-C20
36	N	403	PC7	C19-C20-C21-C22
36	z	301	PC7	C42-C43-C44-C45
37	L	605	PTY	C20-C21-C22-C23
37	N	404	PTY	C17-C18-C19-C20
37	N	404	PTY	C34-C35-C36-C37
38	M	502	CDL	C14-C15-C16-C17
38	N	401	CDL	C14-C15-C16-C17
38	N	401	CDL	C37-C38-C39-C40
38	N	401	CDL	C80-C81-C82-C83
38	t	201	CDL	OA7-CA5-OA6-CA4
36	L	603	PC7	C13-C14-C15-C16
36	L	604	PC7	C18-C19-C20-C21
37	Y	301	PTY	C21-C22-C23-C24
37	m	202	PTY	C21-C22-C23-C24
38	M	502	CDL	C13-C14-C15-C16
38	M	502	CDL	C52-C53-C54-C55
38	M	502	CDL	C83-C84-C85-C86
38	t	201	CDL	C19-C20-C21-C22
38	M	502	CDL	OA9-CA7-OA8-CA6
38	N	401	CDL	C54-C55-C56-C57
38	d	101	CDL	C41-C42-C43-C44
38	d	101	CDL	C80-C81-C82-C83
38	t	201	CDL	C20-C21-C22-C23
36	A	201	PC7	C40-C41-C42-C43
36	A	201	PC7	C13-C14-C15-C16
38	L	601	CDL	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
38	M	502	CDL	C82-C83-C84-C85
38	d	101	CDL	C71-C72-C73-C74
38	t	201	CDL	C17-C18-C19-C20
38	t	201	CDL	C52-C53-C54-C55
36	A	201	PC7	C41-C42-C43-C44
36	N	402	PC7	C21-C22-C23-C24
36	z	301	PC7	C43-C44-C45-C46
37	Y	301	PTY	C19-C20-C21-C22
38	M	502	CDL	C17-C18-C19-C20
38	M	502	CDL	C18-C19-C20-C21
38	M	502	CDL	C33-C34-C35-C36
38	N	401	CDL	C31-C32-C33-C34
38	N	401	CDL	C75-C76-C77-C78
38	N	401	CDL	C83-C84-C85-C86
36	L	602	PC7	C17-C18-C19-C20
36	L	602	PC7	C20-C21-C22-C23
36	L	603	PC7	C32-C33-C34-C35
37	Y	301	PTY	C35-C36-C37-C38
38	L	601	CDL	C21-C22-C23-C24
38	N	401	CDL	CA5-C11-C12-C13
36	A	201	PC7	C21-C22-C23-C24
36	L	602	PC7	C19-C20-C21-C22
36	L	604	PC7	C19-C20-C21-C22
36	N	402	PC7	C20-C21-C22-C23
36	z	301	PC7	C18-C19-C20-C21
37	L	605	PTY	C39-C40-C41-C42
37	N	404	PTY	C31-C32-C33-C34
37	m	201	PTY	C16-C17-C18-C19
37	m	202	PTY	C32-C33-C34-C35
38	M	502	CDL	C79-C80-C81-C82
38	N	401	CDL	C36-C37-C38-C39
38	d	101	CDL	C61-C62-C63-C64
38	d	101	CDL	C83-C84-C85-C86
37	L	605	PTY	O30-C30-O4-C1
37	H	301	PTY	C13-C14-C15-C16
37	M	501	PTY	C14-C15-C16-C17
38	N	401	CDL	C73-C74-C75-C76
38	d	101	CDL	C11-C12-C13-C14
38	M	502	CDL	C15-C16-C17-C18
38	M	502	CDL	C54-C55-C56-C57
38	t	201	CDL	C73-C74-C75-C76
37	m	202	PTY	C8-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
36	L	602	PC7	C36-C37-C38-C39
36	L	603	PC7	C38-C39-C40-C41
36	L	604	PC7	C32-C33-C34-C35
36	N	402	PC7	C32-C33-C34-C35
36	N	403	PC7	C21-C22-C23-C24
36	z	301	PC7	C35-C36-C37-C38
36	z	301	PC7	C34-C35-C36-C37
37	H	301	PTY	C18-C19-C20-C21
37	M	501	PTY	C39-C40-C41-C42
37	m	201	PTY	C18-C19-C20-C21
37	m	201	PTY	C32-C33-C34-C35
37	m	202	PTY	C34-C35-C36-C37
38	M	502	CDL	C71-C72-C73-C74
38	N	401	CDL	C74-C75-C76-C77
38	d	101	CDL	C56-C57-C58-C59
36	L	602	PC7	C4-C5-N-C7
36	L	603	PC7	C4-C5-N-C8
36	L	603	PC7	C4-C5-N-C6
36	N	402	PC7	C4-C5-N-C8
36	N	403	PC7	C4-C5-N-C6
36	z	301	PC7	C4-C5-N-C8
37	H	301	PTY	C19-C20-C21-C22
37	M	501	PTY	C13-C14-C15-C16
37	Y	301	PTY	C37-C38-C39-C40
39	n	200	8Q1	C12-C13-C14-C15
36	N	402	PC7	C22-C23-C24-C25
36	z	301	PC7	C40-C41-C42-C43
37	M	501	PTY	C37-C38-C39-C40
37	Y	301	PTY	C11-C12-C13-C14
38	L	601	CDL	C76-C77-C78-C79
38	M	502	CDL	C19-C20-C21-C22
38	N	401	CDL	C41-C42-C43-C44
38	d	101	CDL	C43-C44-C45-C46
38	t	201	CDL	C11-C12-C13-C14
38	t	201	CDL	C59-C60-C61-C62
36	N	403	PC7	C31-C32-C33-C34
36	L	603	PC7	C18-C19-C20-C21
36	z	301	PC7	C33-C34-C35-C36
38	N	401	CDL	C81-C82-C83-C84
37	H	301	PTY	C11-C12-C13-C14
37	M	501	PTY	C38-C39-C40-C41
38	d	101	CDL	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
36	A	201	PC7	C14-C15-C16-C17
38	N	401	CDL	C13-C14-C15-C16
38	N	401	CDL	C20-C21-C22-C23
38	d	101	CDL	C34-C35-C36-C37
36	L	602	PC7	C21-C22-C23-C24
36	N	402	PC7	C40-C41-C42-C43
38	M	502	CDL	C59-C60-C61-C62
38	d	101	CDL	C12-C13-C14-C15
38	t	201	CDL	C14-C15-C16-C17
39	n	200	8Q1	C9-C10-C11-C12
37	N	404	PTY	C30-C31-C32-C33
37	Y	301	PTY	C31-C32-C33-C34
38	t	201	CDL	C51-CB5-OB6-CB4
37	H	301	PTY	C33-C34-C35-C36
37	Y	301	PTY	C40-C41-C42-C43
38	M	502	CDL	C22-C23-C24-C25
36	N	402	PC7	C43-C44-C45-C46
37	Y	301	PTY	C25-C26-C27-C28
37	m	201	PTY	C33-C34-C35-C36
36	L	602	PC7	O11-C11-O3-C3
36	L	603	PC7	C23-C24-C25-C26
37	m	202	PTY	C15-C16-C17-C18
38	d	101	CDL	C31-C32-C33-C34
36	L	604	PC7	C37-C38-C39-C40
36	L	603	PC7	C20-C21-C22-C23
37	m	202	PTY	C39-C40-C41-C42
38	M	502	CDL	C64-C65-C66-C67
38	M	502	CDL	C78-C79-C80-C81
36	A	201	PC7	C4-C5-N-C7
36	A	201	PC7	C4-C5-N-C8
36	L	602	PC7	C31-C32-C33-C34
37	m	202	PTY	C16-C17-C18-C19
38	M	502	CDL	C36-C37-C38-C39
38	M	502	CDL	C42-C43-C44-C45
38	t	201	CDL	C75-C76-C77-C78
36	A	201	PC7	C37-C38-C39-C40
37	N	404	PTY	C11-C12-C13-C14
38	N	401	CDL	C34-C35-C36-C37
38	d	101	CDL	C24-C25-C26-C27
36	A	201	PC7	C43-C44-C45-C46
36	L	602	PC7	C45-C46-C47-C48
37	m	202	PTY	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
38	d	101	CDL	C77-C78-C79-C80
38	t	201	CDL	C61-C62-C63-C64
37	H	301	PTY	C41-C42-C43-C44
36	N	402	PC7	C31-C32-C33-C34
38	t	201	CDL	CA5-C11-C12-C13
38	t	201	CDL	C31-CA7-OA8-CA6
38	d	101	CDL	C52-C53-C54-C55
36	A	201	PC7	C32-C33-C34-C35
36	L	602	PC7	C18-C19-C20-C21
36	N	402	PC7	C23-C24-C25-C26
38	M	502	CDL	C53-C54-C55-C56
36	N	402	PC7	C44-C45-C46-C47
36	N	403	PC7	C15-C16-C17-C18
36	z	301	PC7	C45-C46-C47-C48
36	z	301	PC7	C39-C40-C41-C42
37	H	301	PTY	C23-C24-C25-C26
37	m	202	PTY	C11-C12-C13-C14
38	M	502	CDL	C73-C74-C75-C76
38	N	401	CDL	C78-C79-C80-C81
37	m	202	PTY	C37-C38-C39-C40
38	N	401	CDL	C39-C40-C41-C42
38	N	401	CDL	C55-C56-C57-C58
37	Y	301	PTY	C32-C33-C34-C35
37	L	605	PTY	C15-C16-C17-C18
37	Y	301	PTY	C14-C15-C16-C17
38	M	502	CDL	C37-C38-C39-C40
36	L	604	PC7	C14-C15-C16-C17
37	H	301	PTY	C32-C33-C34-C35
38	N	401	CDL	C71-C72-C73-C74
38	t	201	CDL	C13-C14-C15-C16
37	L	605	PTY	C35-C36-C37-C38
37	N	404	PTY	C33-C34-C35-C36
38	L	601	CDL	C33-C34-C35-C36
39	n	200	8Q1	C11-C10-C9-C8
38	t	201	CDL	OB7-CB5-OB6-CB4
37	M	501	PTY	C32-C33-C34-C35
36	L	602	PC7	O2-C2-C3-O3
38	N	401	CDL	OB6-CB4-CB6-OB8
36	L	603	PC7	C15-C16-C17-C18
37	L	605	PTY	C32-C33-C34-C35
38	M	502	CDL	C34-C35-C36-C37
37	Y	301	PTY	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
37	Y	301	PTY	C20-C21-C22-C23
38	M	502	CDL	C31-C32-C33-C34
38	M	502	CDL	C40-C41-C42-C43
38	t	201	CDL	C82-C83-C84-C85
37	m	201	PTY	C15-C16-C17-C18
38	M	502	CDL	C16-C17-C18-C19
38	N	401	CDL	C19-C20-C21-C22
38	N	401	CDL	C60-C61-C62-C63
39	n	200	8Q1	C10-C11-C12-C13
38	t	201	CDL	C71-CB7-OB8-CB6
37	N	404	PTY	C37-C38-C39-C40
38	t	201	CDL	C51-C52-C53-C54
37	L	605	PTY	C34-C35-C36-C37
37	m	201	PTY	C25-C26-C27-C28
38	M	502	CDL	C39-C40-C41-C42
37	M	501	PTY	C3-O11-P1-O14
37	m	201	PTY	C3-O11-P1-O14
38	N	401	CDL	CB2-OB2-PB2-OB5
38	N	401	CDL	CB3-OB5-PB2-OB2
37	L	605	PTY	C18-C19-C20-C21
37	N	404	PTY	C35-C36-C37-C38
37	H	301	PTY	O14-C5-C6-C1
37	Y	301	PTY	O14-C5-C6-C1
38	M	502	CDL	C43-C44-C45-C46
38	d	101	CDL	C18-C19-C20-C21
37	L	605	PTY	C41-C42-C43-C44
38	N	401	CDL	C62-C63-C64-C65
37	L	605	PTY	C31-C32-C33-C34
37	N	404	PTY	C19-C20-C21-C22
38	d	101	CDL	C59-C60-C61-C62
36	L	604	PC7	C39-C40-C41-C42
37	N	404	PTY	C32-C33-C34-C35
38	M	502	CDL	C41-C42-C43-C44
38	t	201	CDL	OA9-CA7-OA8-CA6
36	A	201	PC7	C15-C16-C17-C18
38	M	502	CDL	C35-C36-C37-C38
38	t	201	CDL	C54-C55-C56-C57
36	L	603	PC7	C1-C2-C3-O3
36	L	604	PC7	C1-C2-C3-O3
36	z	301	PC7	C1-C2-C3-O3
37	H	301	PTY	O4-C1-C6-C5
38	M	502	CDL	CB3-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
38	L	601	CDL	C56-C57-C58-C59
36	L	603	PC7	C22-C23-C24-C25
37	m	201	PTY	C21-C22-C23-C24
38	L	601	CDL	C20-C21-C22-C23
36	N	403	PC7	C23-C24-C25-C26
37	N	404	PTY	C15-C16-C17-C18
38	d	101	CDL	C84-C85-C86-C87
38	L	601	CDL	C19-C20-C21-C22
38	L	601	CDL	C23-C24-C25-C26
38	L	601	CDL	C61-C62-C63-C64
36	z	301	PC7	C41-C42-C43-C44
37	m	201	PTY	C24-C25-C26-C27
38	L	601	CDL	C55-C56-C57-C58
38	t	201	CDL	C84-C85-C86-C87
36	N	402	PC7	C15-C16-C17-C18
37	H	301	PTY	C15-C16-C17-C18
37	m	202	PTY	C11-C8-O7-C6
37	H	301	PTY	C26-C27-C28-C29
37	m	201	PTY	C26-C27-C28-C29
36	z	301	PC7	C31-C32-C33-C34
37	Y	301	PTY	C41-C42-C43-C44
36	z	301	PC7	C1-C2-O2-C31
38	M	502	CDL	CA3-CA4-OA6-CA5
38	t	201	CDL	C38-C39-C40-C41
39	n	200	8Q1	C28-O27-P24-O3
36	L	602	PC7	C23-C24-C25-C26
38	M	502	CDL	C71-CB7-OB8-CB6
38	t	201	CDL	C83-C84-C85-C86
37	Y	301	PTY	C36-C37-C38-C39
36	L	604	PC7	C41-C42-C43-C44
39	n	200	8Q1	C13-C14-C15-C16
37	m	201	PTY	C13-C14-C15-C16
38	L	601	CDL	C37-C38-C39-C40
36	N	403	PC7	C35-C36-C37-C38
37	N	404	PTY	C13-C14-C15-C16
38	M	502	CDL	OB9-CB7-OB8-CB6
36	L	603	PC7	C34-C35-C36-C37
38	L	601	CDL	C14-C15-C16-C17
37	H	301	PTY	C25-C26-C27-C28
38	L	601	CDL	C53-C54-C55-C56
38	M	502	CDL	C62-C63-C64-C65
36	L	603	PC7	O3P-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
38	M	502	CDL	OA5-CA3-CA4-CA6
38	t	201	CDL	OA5-CA3-CA4-CA6
36	z	301	PC7	C15-C16-C17-C18
37	H	301	PTY	C37-C38-C39-C40
38	d	101	CDL	CB7-C71-C72-C73
37	m	202	PTY	N1-C2-C3-O11
38	L	601	CDL	C64-C65-C66-C67
38	t	201	CDL	OB9-CB7-OB8-CB6
37	N	404	PTY	C36-C37-C38-C39
37	Y	301	PTY	C18-C19-C20-C21
38	t	201	CDL	C41-C42-C43-C44
38	t	201	CDL	C43-C44-C45-C46
36	L	604	PC7	C33-C34-C35-C36
37	Y	301	PTY	C26-C27-C28-C29
38	N	401	CDL	C35-C36-C37-C38
36	A	201	PC7	C11-C12-C13-C14
38	M	502	CDL	C44-C45-C46-C47
37	m	202	PTY	C25-C26-C27-C28
36	L	602	PC7	C1-C2-C3-O3
37	N	404	PTY	O4-C1-C6-C5
38	N	401	CDL	CA3-CA4-CA6-OA8
38	N	401	CDL	CB3-CB4-CB6-OB8
38	t	201	CDL	CA3-CA4-CA6-OA8
38	t	201	CDL	CB3-CB4-CB6-OB8
37	H	301	PTY	C40-C41-C42-C43
37	H	301	PTY	C12-C13-C14-C15
38	L	601	CDL	C77-C78-C79-C80
38	M	502	CDL	C21-C22-C23-C24
36	N	402	PC7	C45-C46-C47-C48
38	N	401	CDL	C76-C77-C78-C79
36	A	201	PC7	C12-C13-C14-C15
36	z	301	PC7	C23-C24-C25-C26
36	L	604	PC7	C22-C23-C24-C25
38	M	502	CDL	C24-C25-C26-C27
37	Y	301	PTY	O14-C5-C6-O7
37	m	201	PTY	O14-C5-C6-O7
38	M	502	CDL	OB5-CB3-CB4-OB6
38	t	201	CDL	OA5-CA3-CA4-OA6
38	d	101	CDL	C35-C36-C37-C38
36	L	603	PC7	O2-C2-C3-O3
38	L	601	CDL	OA6-CA4-CA6-OA8
38	M	502	CDL	OB6-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
38	N	401	CDL	OA6-CA4-CA6-OA8
38	d	101	CDL	OA6-CA4-CA6-OA8
38	t	201	CDL	OA6-CA4-CA6-OA8
38	t	201	CDL	C80-C81-C82-C83
36	A	201	PC7	C22-C23-C24-C25
36	N	403	PC7	C33-C34-C35-C36
38	t	201	CDL	C18-C19-C20-C21
37	m	202	PTY	O10-C8-O7-C6
38	M	502	CDL	C74-C75-C76-C77
37	m	202	PTY	C6-C5-O14-P1
36	L	602	PC7	C43-C44-C45-C46
36	N	402	PC7	C34-C35-C36-C37
37	N	404	PTY	C16-C17-C18-C19
38	M	502	CDL	C58-C59-C60-C61
37	L	605	PTY	C14-C15-C16-C17
38	d	101	CDL	C55-C56-C57-C58
36	A	201	PC7	O3P-C1-C2-C3
36	N	402	PC7	O3P-C1-C2-C3
38	M	502	CDL	OB5-CB3-CB4-CB6
38	N	401	CDL	OA5-CA3-CA4-CA6
37	Y	301	PTY	C23-C24-C25-C26
36	N	403	PC7	C40-C41-C42-C43
37	H	301	PTY	C1-C6-O7-C8
38	d	101	CDL	C62-C63-C64-C65
38	t	201	CDL	C24-C25-C26-C27
36	L	603	PC7	O3P-C1-C2-O2
36	N	402	PC7	O3P-C1-C2-O2
38	N	401	CDL	OA5-CA3-CA4-OA6
38	d	101	CDL	OA5-CA3-CA4-OA6
36	L	604	PC7	C16-C17-C18-C19
36	L	604	PC7	O2-C2-C3-O3
36	N	403	PC7	O2-C2-C3-O3
37	m	202	PTY	C20-C21-C22-C23
38	t	201	CDL	C60-C61-C62-C63
36	L	602	PC7	C41-C42-C43-C44
37	m	201	PTY	C20-C21-C22-C23
36	L	604	PC7	C42-C43-C44-C45
38	N	401	CDL	CB4-CB3-OB5-PB2
36	A	201	PC7	C4-O4P-P-O1P
36	L	602	PC7	C1-O3P-P-O1P
36	L	604	PC7	C4-O4P-P-O1P
36	N	402	PC7	C1-O3P-P-O1P

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Mol	Chain	Res	Type	Atoms
36	N	403	PC7	C1-O3P-P-O1P
37	H	301	PTY	C3-O11-P1-O13
37	L	605	PTY	C5-O14-P1-O13
37	M	501	PTY	C3-O11-P1-O13
37	M	501	PTY	C5-O14-P1-O13
37	m	201	PTY	C3-O11-P1-O13
38	L	601	CDL	CB3-OB5-PB2-OB4
38	M	502	CDL	CA3-OA5-PA1-OA4
38	M	502	CDL	CB3-OB5-PB2-OB4
38	N	401	CDL	CA3-OA5-PA1-OA3
38	N	401	CDL	CB2-OB2-PB2-OB4
38	N	401	CDL	CB3-OB5-PB2-OB4
38	t	201	CDL	CA3-OA5-PA1-OA4
38	t	201	CDL	CB2-OB2-PB2-OB4
38	d	101	CDL	C21-C22-C23-C24
38	N	401	CDL	OB5-CB3-CB4-CB6
38	d	101	CDL	OA5-CA3-CA4-CA6
36	L	603	PC7	C12-C13-C14-C15
37	m	202	PTY	C14-C15-C16-C17
36	A	201	PC7	C5-C4-O4P-P
37	H	301	PTY	O14-C5-C6-O7
38	M	502	CDL	OA5-CA3-CA4-OA6
38	N	401	CDL	OB5-CB3-CB4-OB6
36	L	604	PC7	C4-C5-N-C6
38	t	201	CDL	C16-C17-C18-C19
36	N	402	PC7	O4P-C4-C5-N
37	M	501	PTY	C11-C12-C13-C14
38	L	601	CDL	C13-C14-C15-C16
38	d	101	CDL	CB3-CB4-CB6-OB8
38	t	201	CDL	OB6-CB4-CB6-OB8
37	H	301	PTY	C20-C21-C22-C23
37	L	605	PTY	C13-C14-C15-C16
37	m	202	PTY	C40-C41-C42-C43
38	L	601	CDL	C40-C41-C42-C43
38	L	601	CDL	C57-C58-C59-C60
37	M	501	PTY	C24-C25-C26-C27
37	m	202	PTY	C24-C25-C26-C27
37	m	201	PTY	C38-C39-C40-C41
38	d	101	CDL	C73-C74-C75-C76
38	L	601	CDL	C24-C25-C26-C27
38	L	601	CDL	C18-C19-C20-C21
36	A	201	PC7	O3P-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
36	L	604	PC7	C4-C5-N-C8
38	t	201	CDL	C33-C34-C35-C36
37	N	404	PTY	C11-C8-O7-C6
38	L	601	CDL	C74-C75-C76-C77
38	L	601	CDL	OB6-CB4-CB6-OB8
38	d	101	CDL	C64-C65-C66-C67
36	N	403	PC7	C1-O3P-P-O4P
37	L	605	PTY	C3-O11-P1-O14
38	d	101	CDL	CA5-C11-C12-C13
38	L	601	CDL	CB3-CB4-CB6-OB8
36	A	201	PC7	C35-C36-C37-C38
38	N	401	CDL	C1-CA2-OA2-PA1
38	t	201	CDL	C1-CA2-OA2-PA1
36	N	402	PC7	C41-C42-C43-C44
37	H	301	PTY	C17-C18-C19-C20
38	d	101	CDL	C75-C76-C77-C78
36	N	402	PC7	C13-C14-C15-C16
37	H	301	PTY	C22-C23-C24-C25
36	L	602	PC7	C12-C13-C14-C15
36	N	403	PC7	C36-C37-C38-C39
36	L	603	PC7	C39-C40-C41-C42
38	M	502	CDL	C76-C77-C78-C79
38	t	201	CDL	C53-C54-C55-C56
37	H	301	PTY	C39-C40-C41-C42
37	L	605	PTY	C17-C18-C19-C20
36	N	403	PC7	C1-C2-C3-O3
38	L	601	CDL	CA3-CA4-CA6-OA8
36	L	603	PC7	C11-C12-C13-C14
36	L	603	PC7	C3-C2-O2-C31
36	L	604	PC7	C4-C5-N-C7
36	L	602	PC7	C22-C23-C24-C25
38	t	201	CDL	C23-C24-C25-C26
37	H	301	PTY	C14-C15-C16-C17
38	L	601	CDL	OA5-CA3-CA4-OA6
36	A	201	PC7	C36-C37-C38-C39
38	L	601	CDL	C62-C63-C64-C65
38	d	101	CDL	C57-C58-C59-C60
38	t	201	CDL	C21-C22-C23-C24
38	d	101	CDL	C79-C80-C81-C82
36	L	602	PC7	C44-C45-C46-C47
36	N	403	PC7	C38-C39-C40-C41
37	L	605	PTY	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
37	M	501	PTY	C23-C24-C25-C26
38	L	601	CDL	CB2-C1-CA2-OA2
36	z	301	PC7	C37-C38-C39-C40
38	d	101	CDL	C20-C21-C22-C23
36	N	403	PC7	C16-C17-C18-C19
38	d	101	CDL	C76-C77-C78-C79
38	d	101	CDL	C37-C38-C39-C40
38	N	401	CDL	C18-C19-C20-C21
36	z	301	PC7	C22-C23-C24-C25
38	M	502	CDL	C75-C76-C77-C78
38	N	401	CDL	C56-C57-C58-C59
38	L	601	CDL	OA5-CA3-CA4-CA6
36	z	301	PC7	C20-C21-C22-C23
38	M	502	CDL	C81-C82-C83-C84
38	M	502	CDL	C20-C21-C22-C23
38	L	601	CDL	C12-C11-CA5-OA6
39	n	200	8Q1	O27-C28-C29-C31
38	d	101	CDL	C33-C34-C35-C36
38	d	101	CDL	C63-C64-C65-C66
38	N	401	CDL	CA7-C31-C32-C33
38	L	601	CDL	OB7-CB5-OB6-CB4
37	m	202	PTY	C12-C11-C8-O7
38	L	601	CDL	C32-C31-CA7-OA8
36	L	604	PC7	C43-C44-C45-C46
38	d	101	CDL	C53-C54-C55-C56
38	d	101	CDL	CA3-CA4-CA6-OA8
37	m	202	PTY	O14-C5-C6-O7
38	N	401	CDL	C52-C53-C54-C55
37	m	201	PTY	O14-C5-C6-C1
38	N	401	CDL	C77-C78-C79-C80
36	L	604	PC7	C45-C46-C47-C48
37	m	201	PTY	C12-C11-C8-O7
37	H	301	PTY	C31-C32-C33-C34
36	z	301	PC7	C13-C14-C15-C16
38	N	401	CDL	C33-C34-C35-C36
38	t	201	CDL	C35-C36-C37-C38
37	m	202	PTY	C12-C11-C8-O10
37	L	605	PTY	C37-C38-C39-C40
38	L	601	CDL	CA2-OA2-PA1-OA5
38	L	601	CDL	C12-C11-CA5-OA7
37	N	404	PTY	O10-C8-O7-C6
38	t	201	CDL	C31-C32-C33-C34

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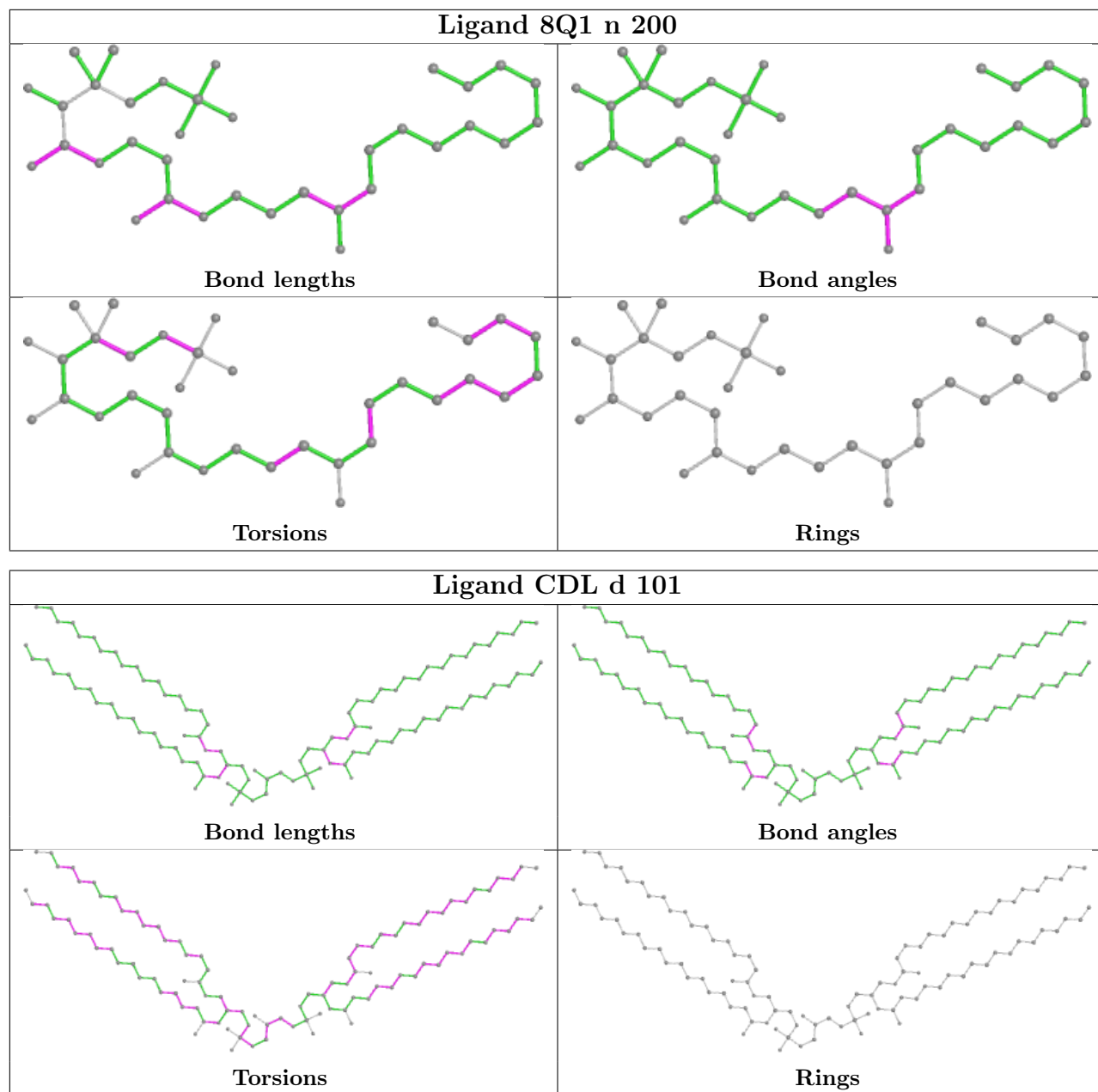
*Continued from previous page...*

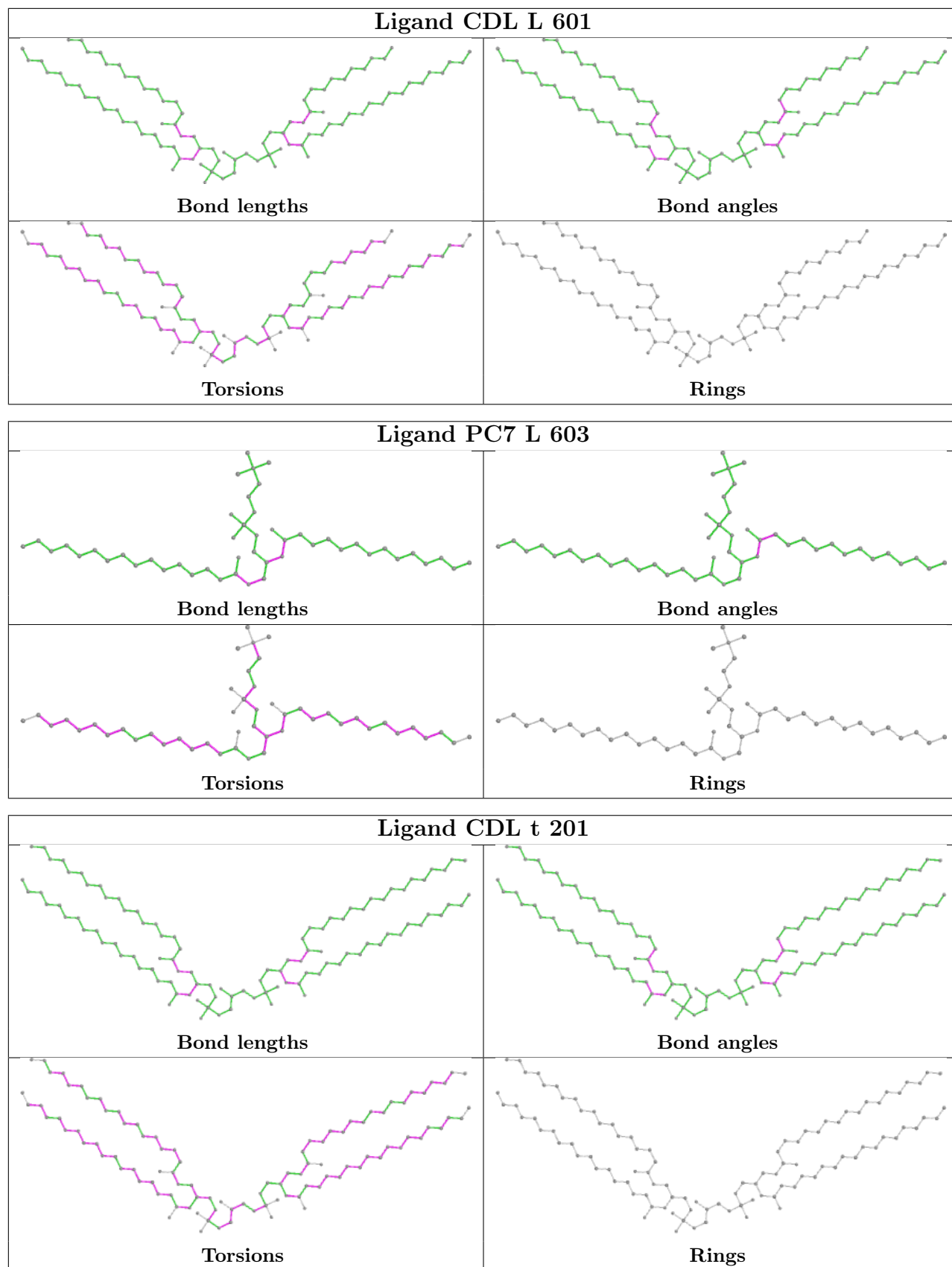
Mol	Chain	Res	Type	Atoms
36	z	301	PC7	C1-O3P-P-O2P
37	L	605	PTY	C3-O11-P1-O13
37	M	501	PTY	C3-O11-P1-O12
37	m	202	PTY	C3-O11-P1-O13
38	M	502	CDL	CB2-OB2-PB2-OB3
37	H	301	PTY	O4-C1-C6-O7
37	m	201	PTY	C12-C11-C8-O10
38	t	201	CDL	C56-C57-C58-C59
36	z	301	PC7	O2-C31-C32-C33
37	m	202	PTY	C36-C37-C38-C39
38	d	101	CDL	C58-C59-C60-C61
37	Y	301	PTY	C34-C35-C36-C37
36	L	603	PC7	C1-C2-O2-C31
36	N	403	PC7	C5-C4-O4P-P
37	M	501	PTY	C2-C3-O11-P1
38	L	601	CDL	C52-C51-CB5-OB6
37	m	201	PTY	C11-C12-C13-C14
37	L	605	PTY	C19-C20-C21-C22
38	d	101	CDL	C1-CB2-OB2-PB2
38	d	101	CDL	C72-C71-CB7-OB8
37	L	605	PTY	C26-C27-C28-C29
37	m	202	PTY	C33-C34-C35-C36
36	z	301	PC7	O3-C11-C12-C13
38	M	502	CDL	C12-C13-C14-C15
38	t	201	CDL	C72-C73-C74-C75
36	z	301	PC7	O31-C31-C32-C33

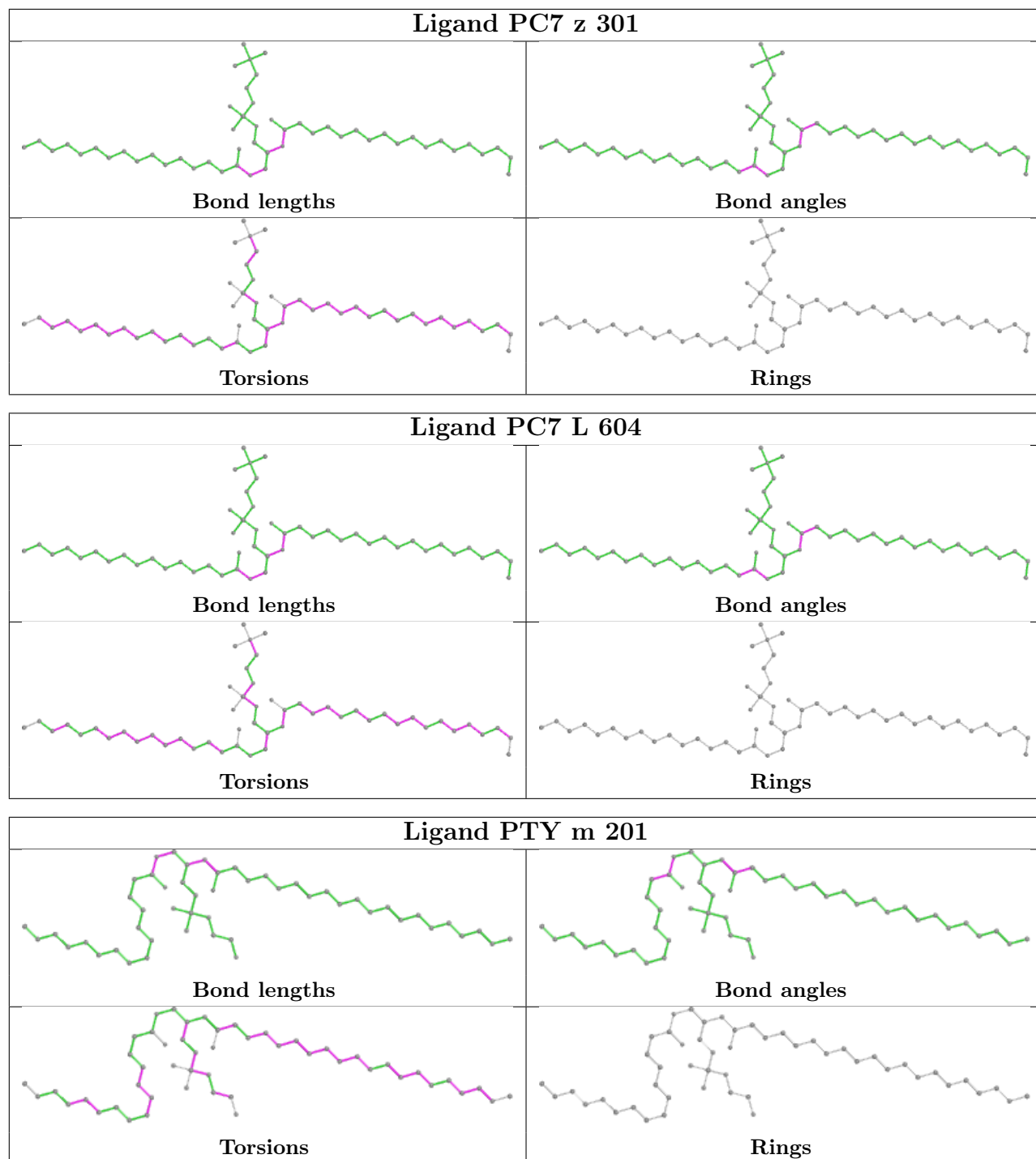
There are no ring outliers.

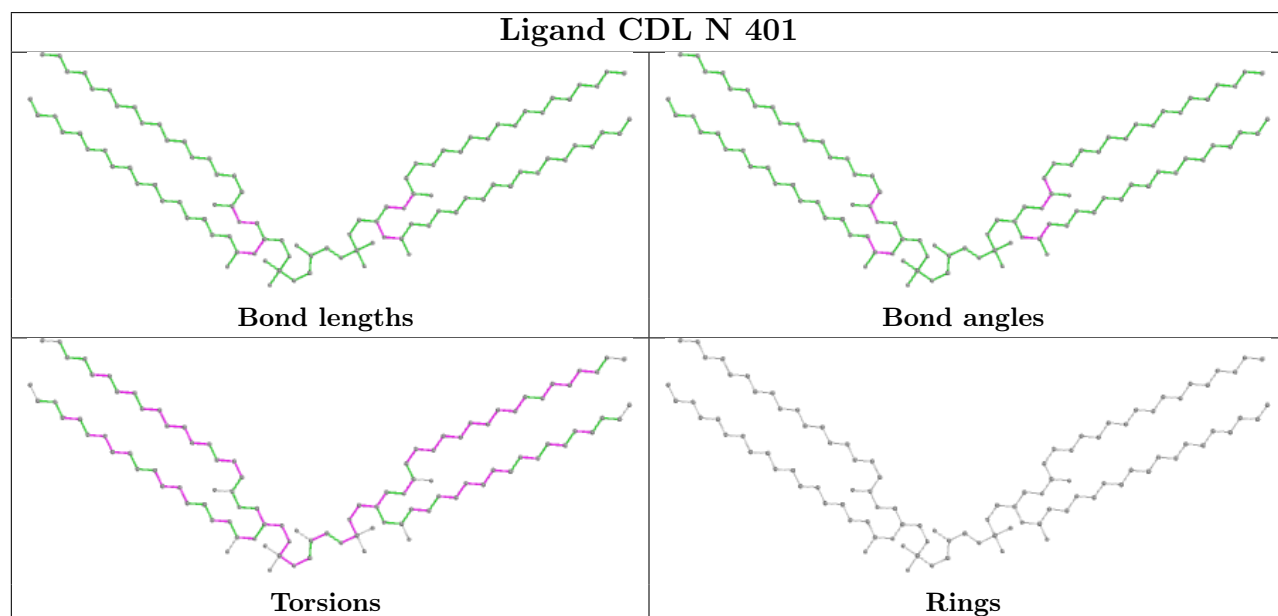
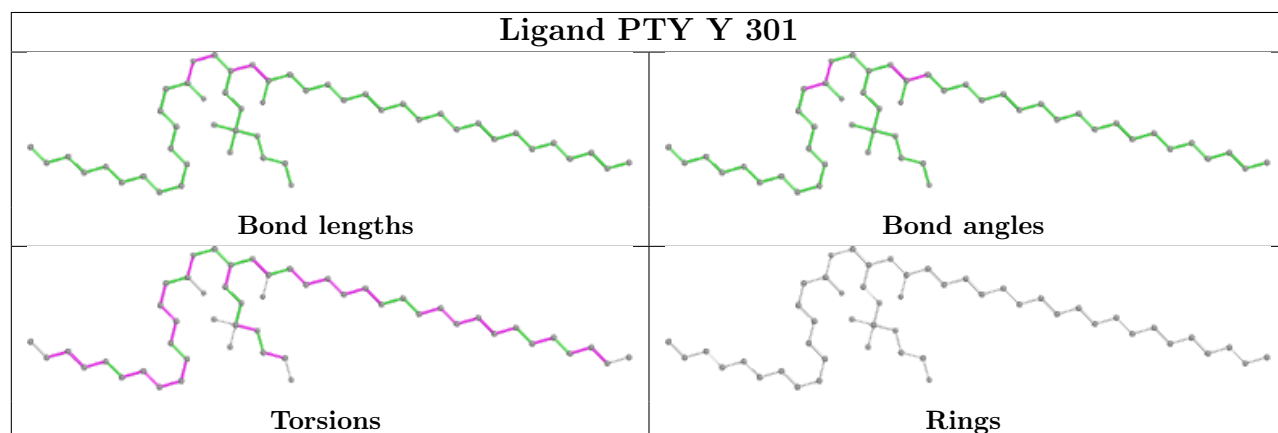
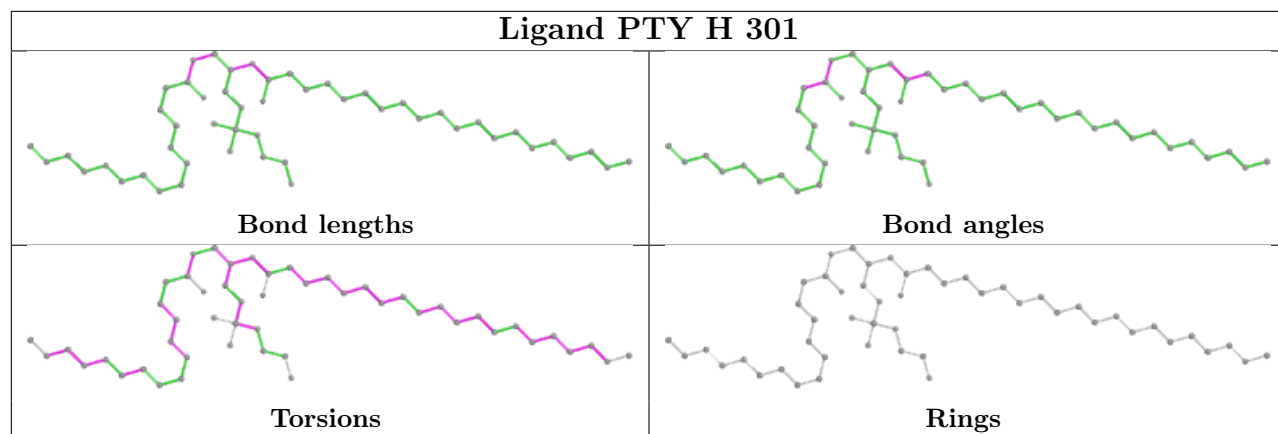
No monomer is involved in short contacts.

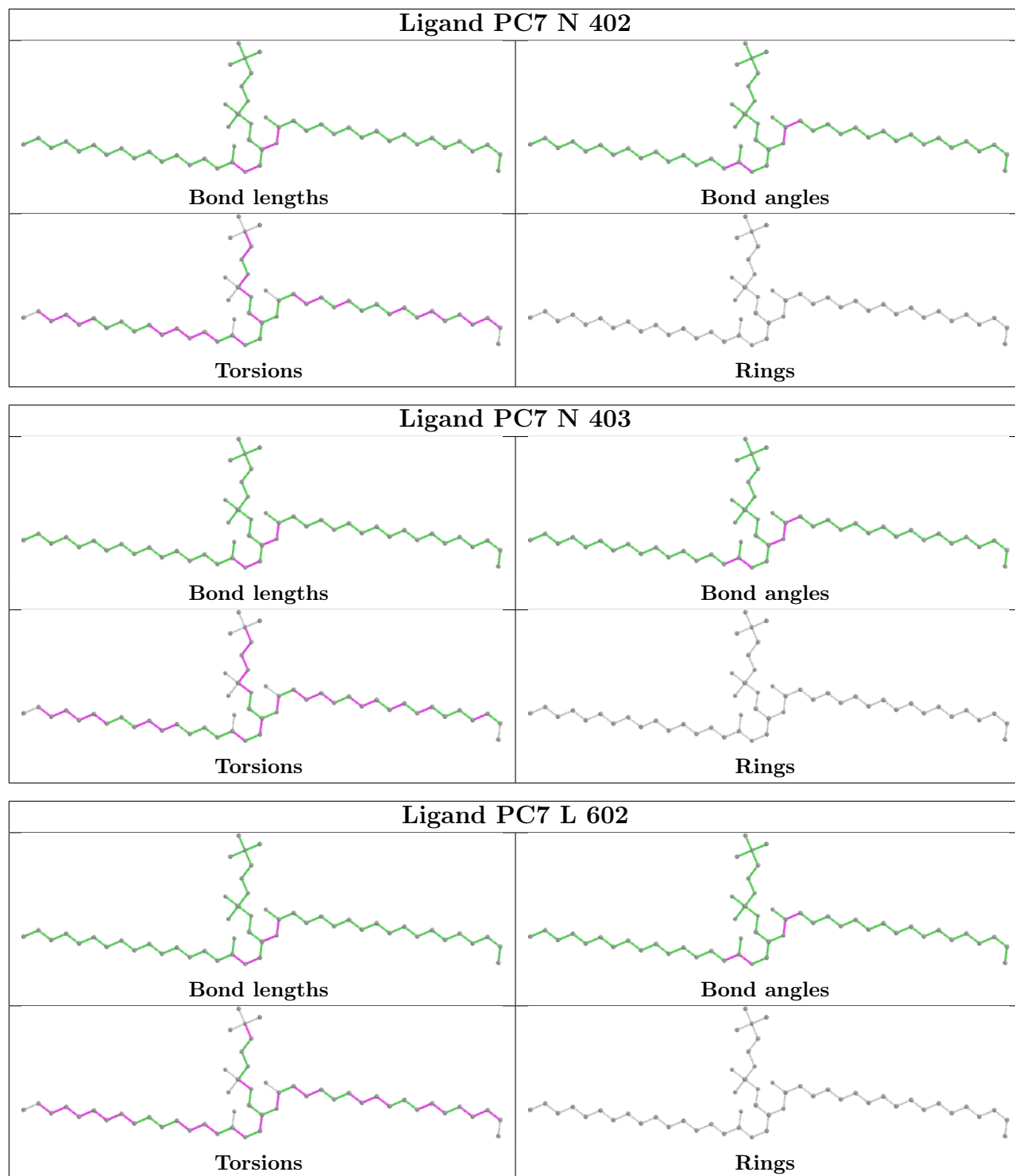
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



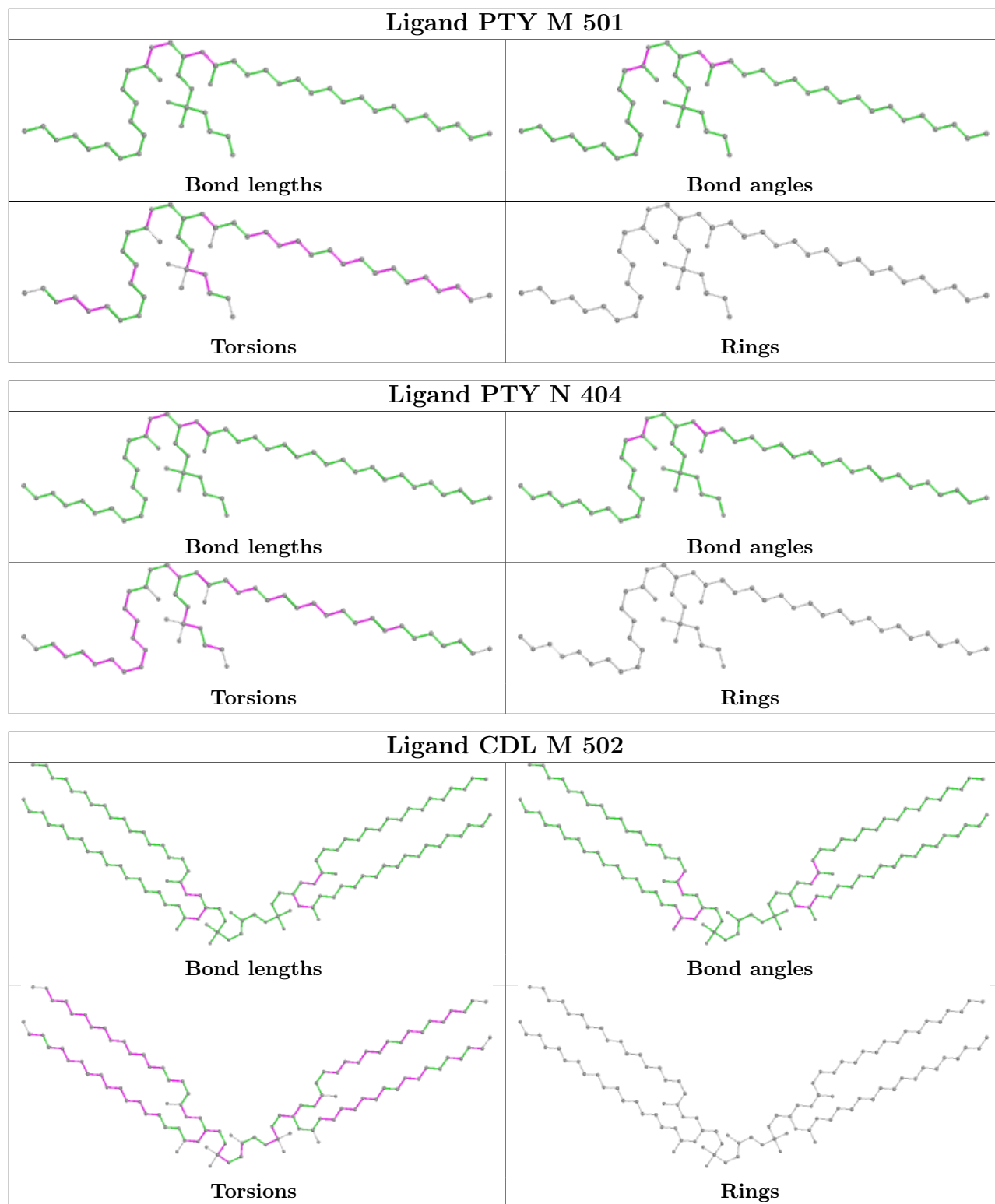


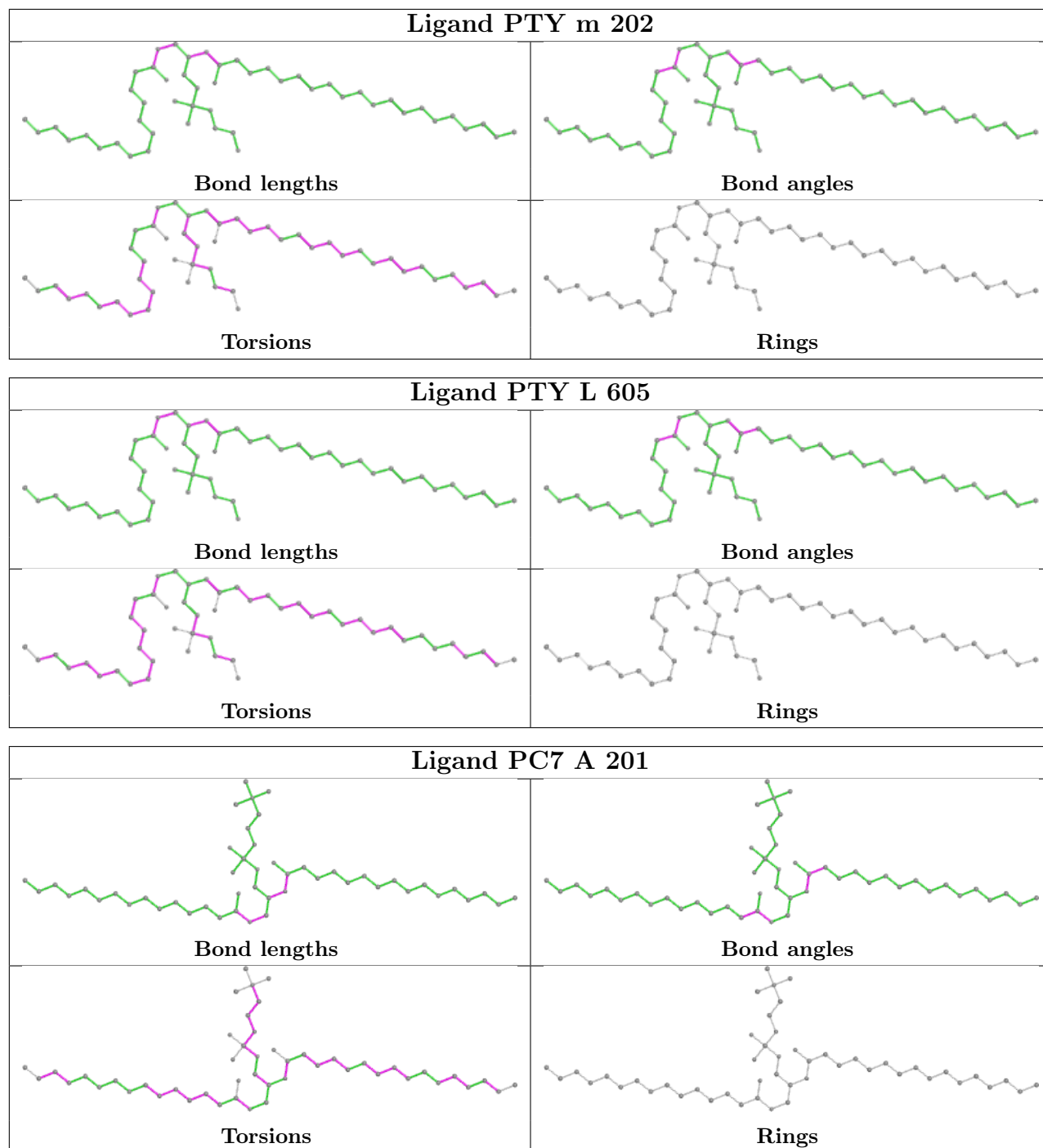












## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

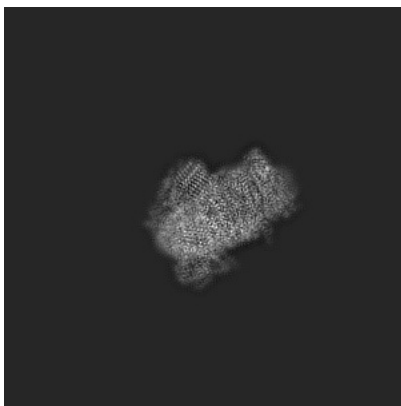
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11877. These allow visual inspection of the internal detail of the map and identification of artifacts.

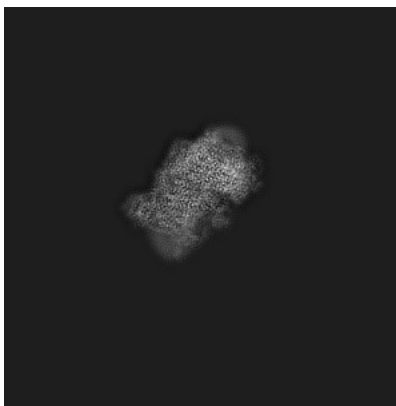
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

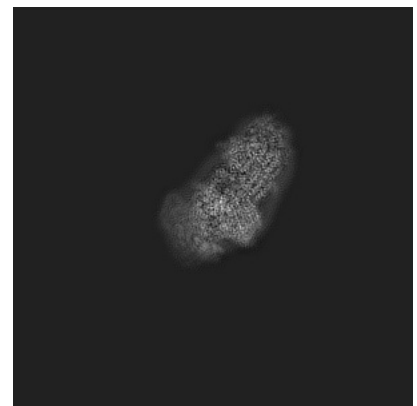
#### 6.1.1 Primary map



X

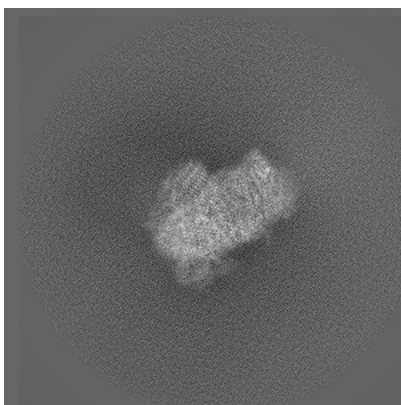


Y

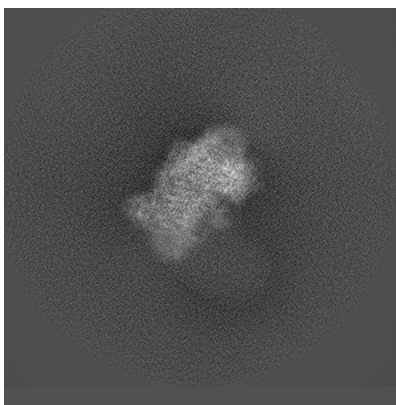


Z

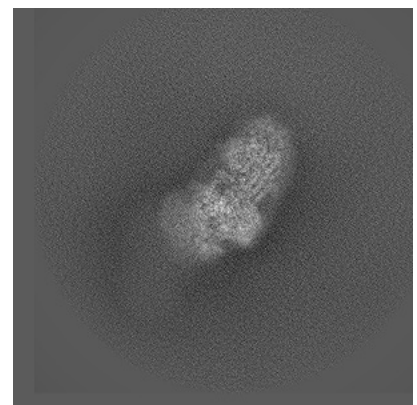
#### 6.1.2 Raw map



X



Y

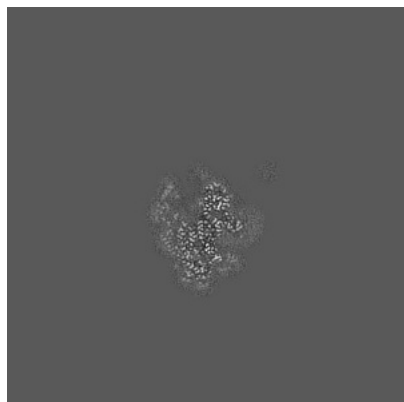


Z

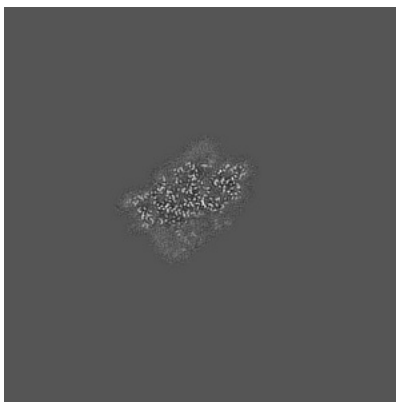
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

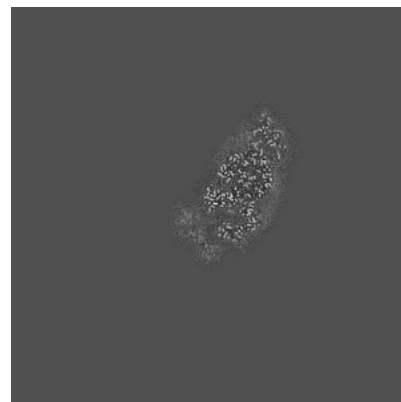
### 6.2.1 Primary map



X Index: 300

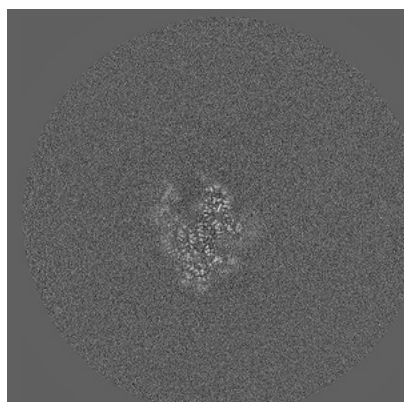


Y Index: 300

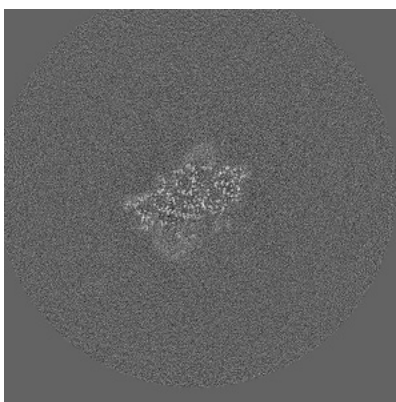


Z Index: 300

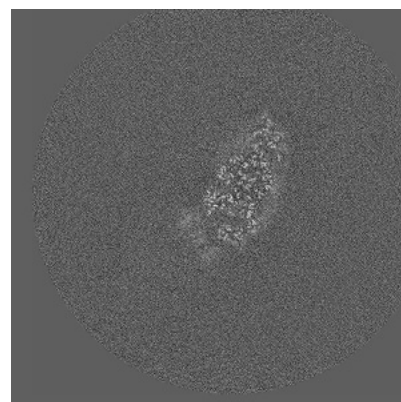
### 6.2.2 Raw map



X Index: 300



Y Index: 300

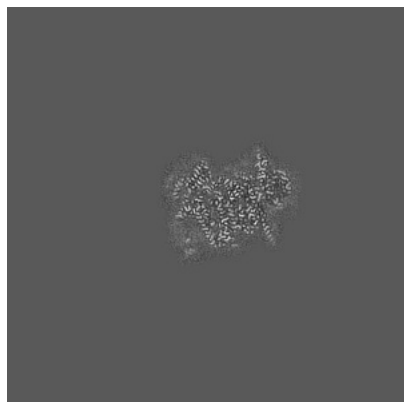


Z Index: 300

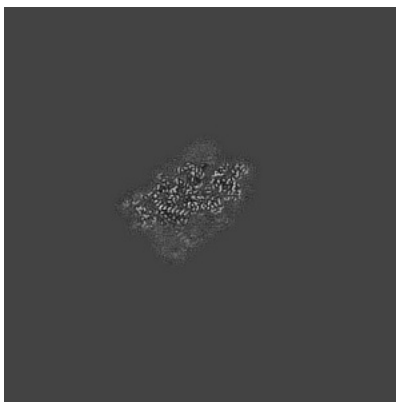
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

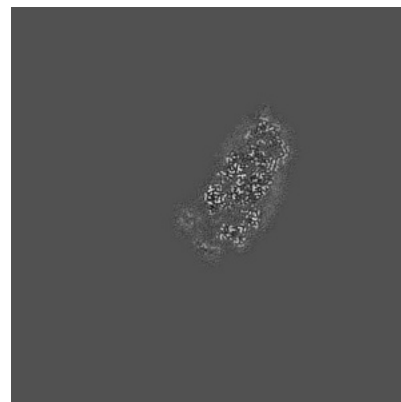
### 6.3.1 Primary map



X Index: 355

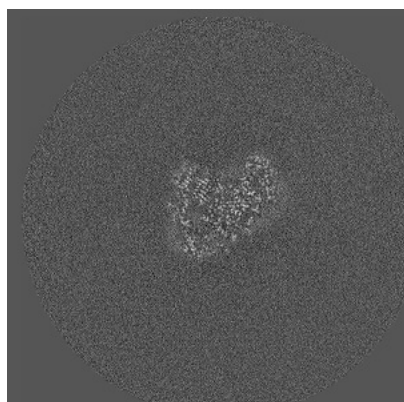


Y Index: 298

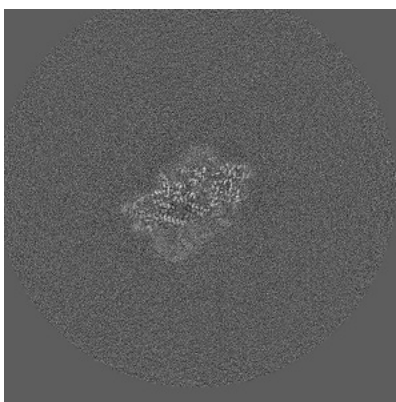


Z Index: 304

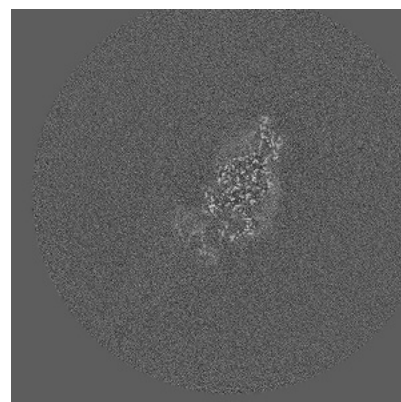
### 6.3.2 Raw map



X Index: 341



Y Index: 295

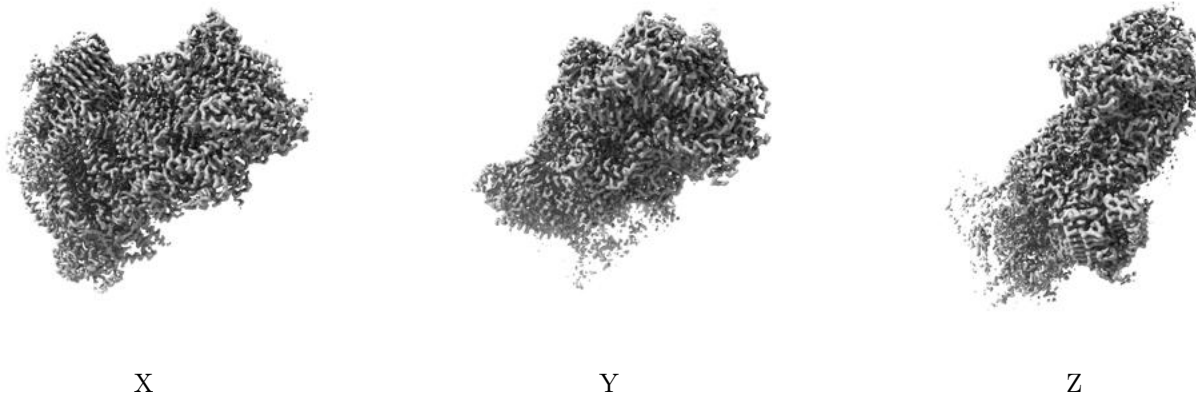


Z Index: 296

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

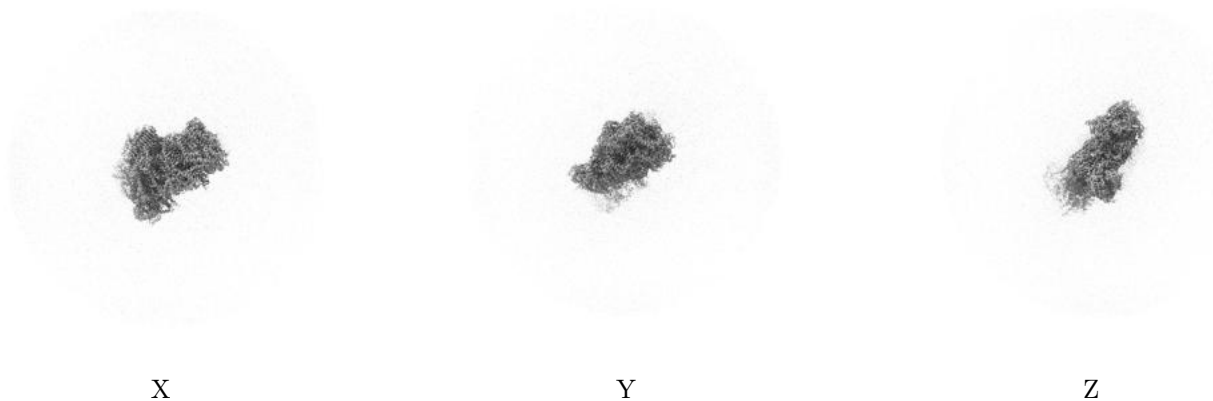
## 6.4 Orthogonal surface views [i](#)

### 6.4.1 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.

### 6.4.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

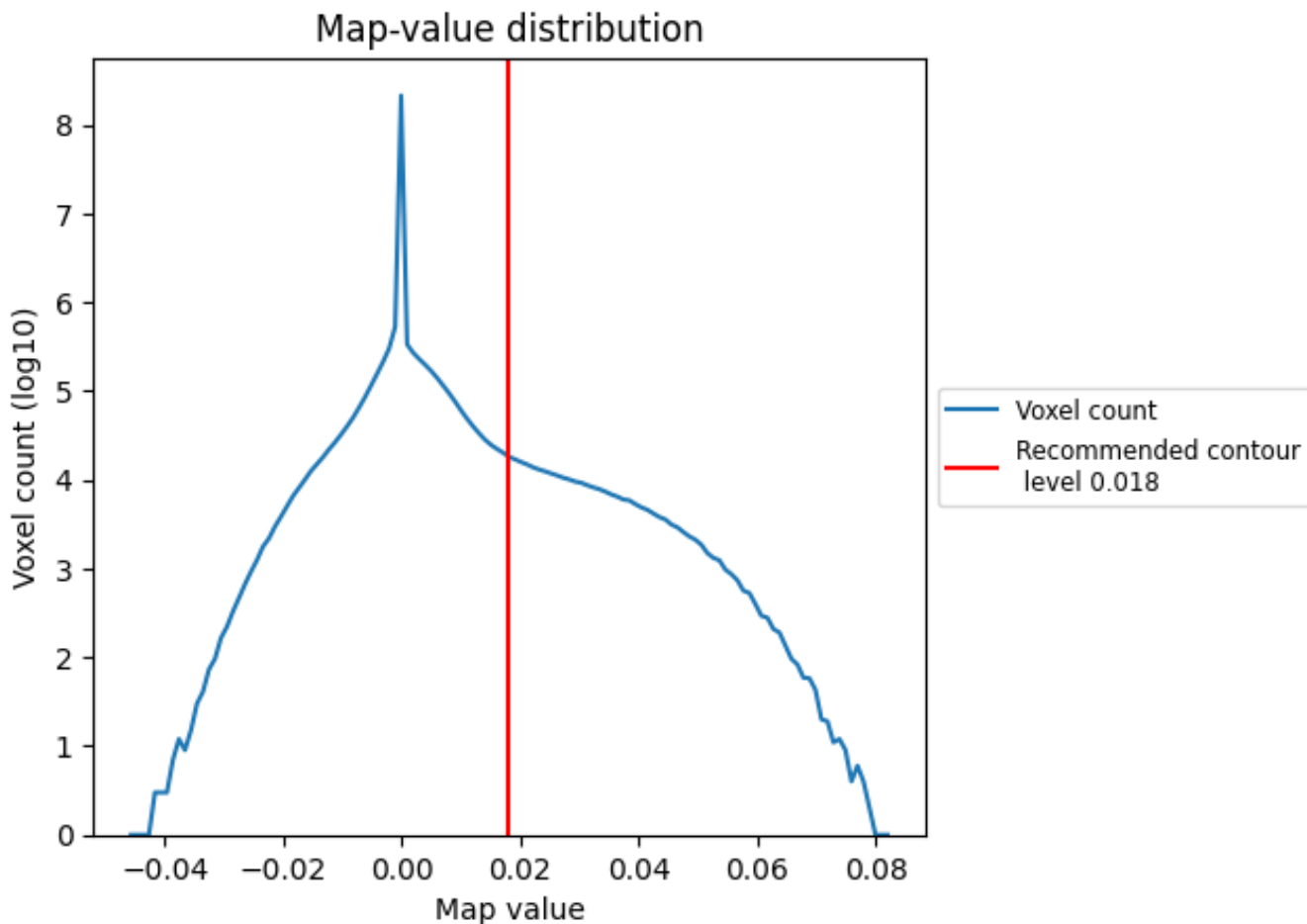
## 6.5 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

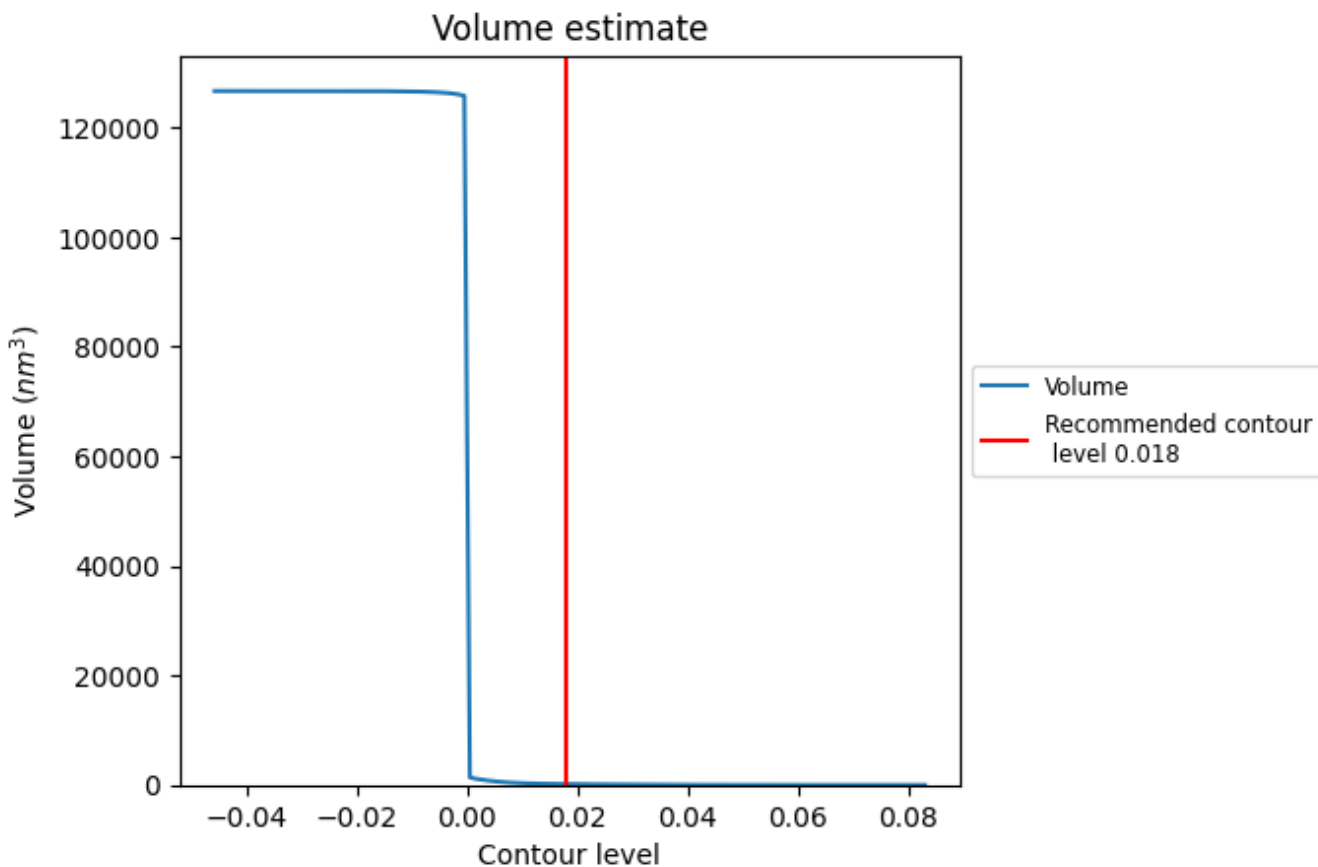
This section contains the results of statistical analysis of the map.

### 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 [\(i\)](#)

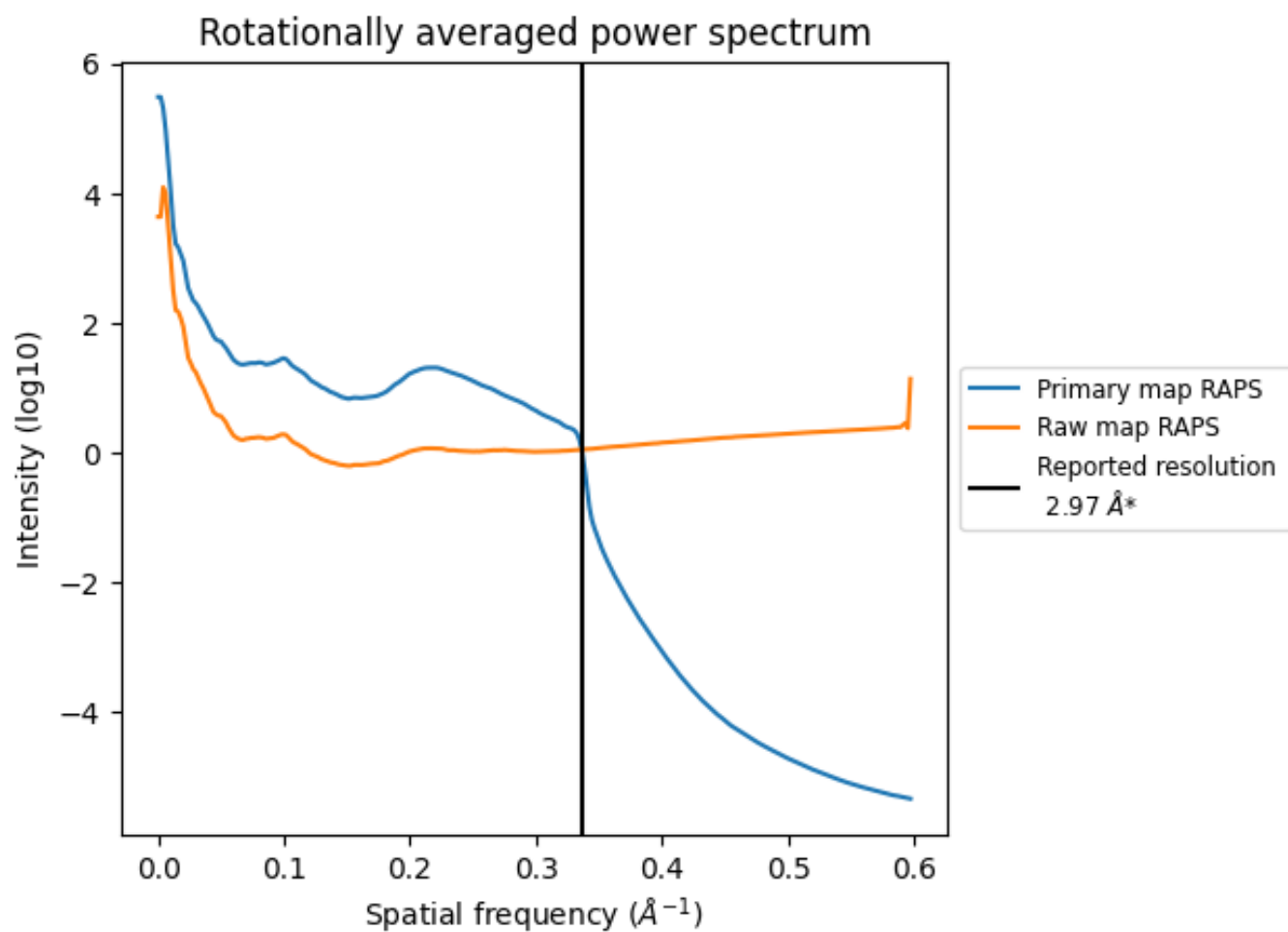


The volume at the recommended contour level is 162 nm<sup>3</sup>; this corresponds to an approximate mass of 147 kDa.

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 i

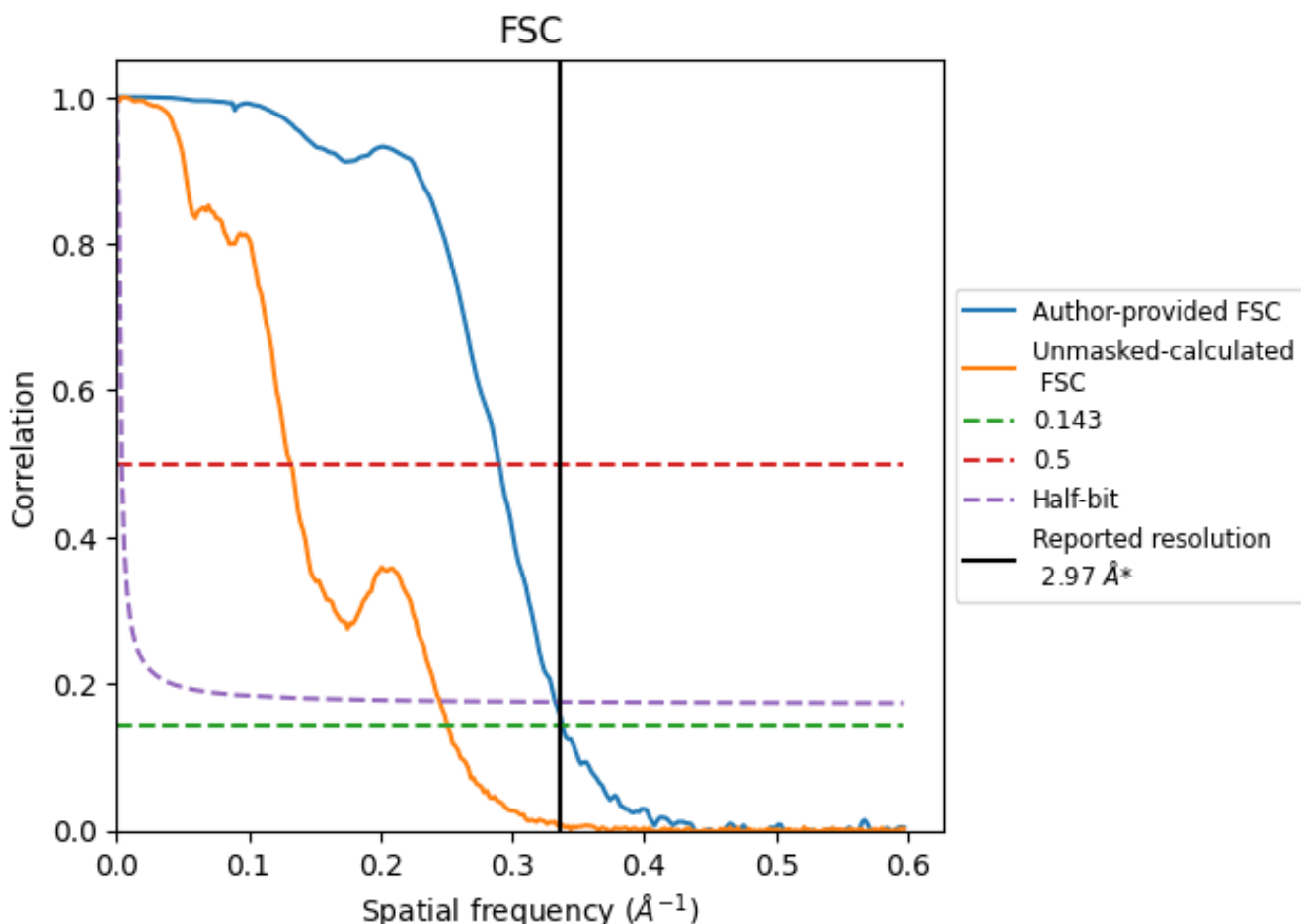


\*Reported resolution corresponds to spatial frequency of 0.337 Å<sup>-1</sup>

## 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 0.337 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

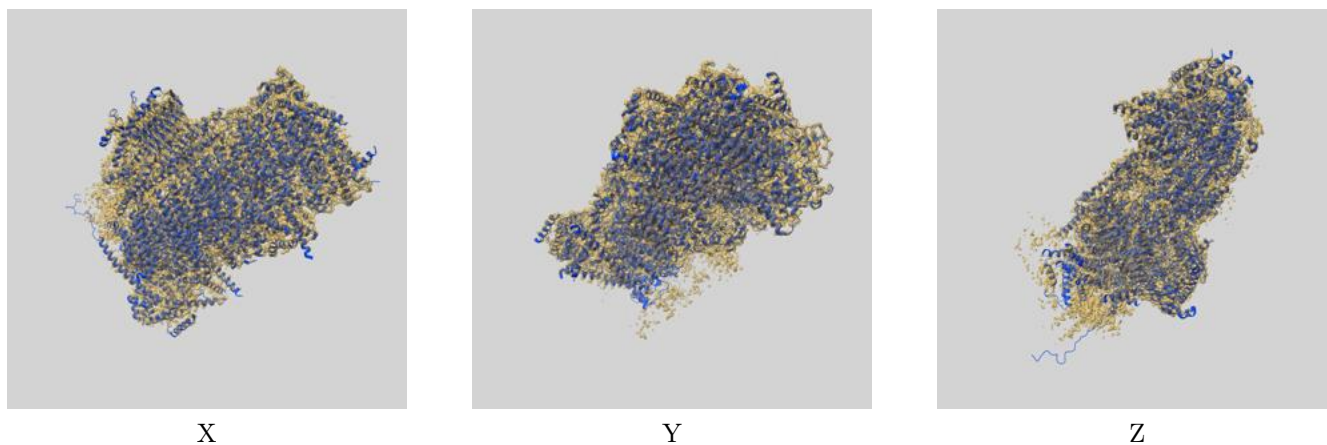
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.97	-	-
Author-provided FSC curve	2.96	3.44	3.00
Unmasked-calculated*	3.98	7.58	4.08

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.98 differs from the reported value 2.97 by more than 10 %

## 9 Map-model fit [i](#)

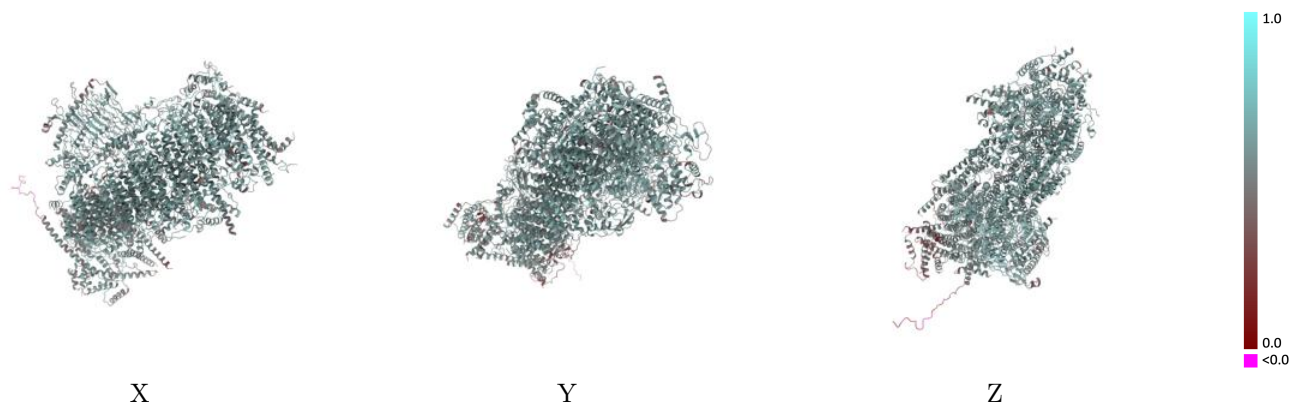
This section contains information regarding the fit between EMDB map EMD-11877 and PDB model 7AR9. Per-residue inclusion information can be found in section 3 on page 15.

### 9.1 Map-model overlay [i](#)



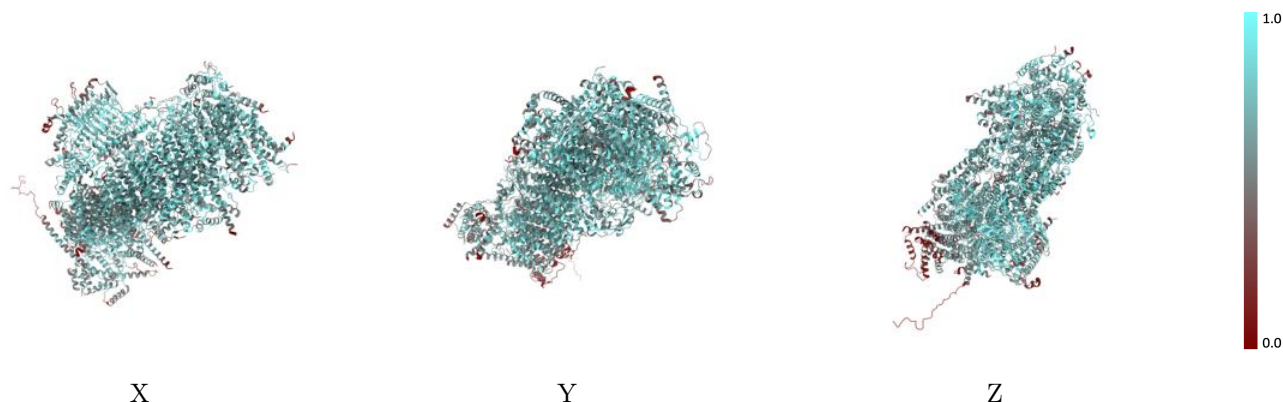
The images above show the 3D surface view of the map at the recommended contour level 0.018 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



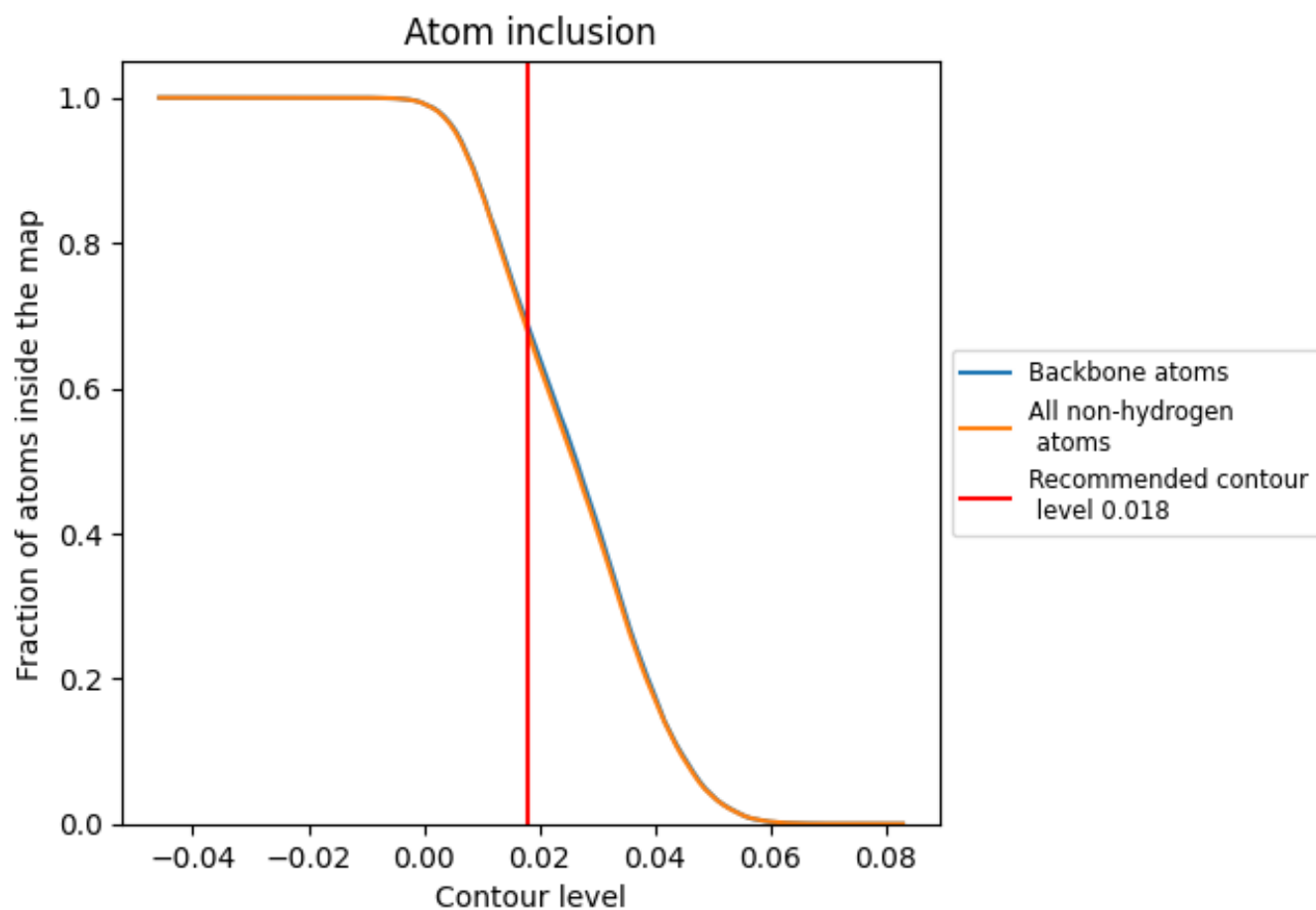
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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









































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 69% of all backbone atoms, 68% 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	 0.6779	 0.5650
A	 0.6267	 0.5490
H	 0.4411	 0.4750
J	 0.6670	 0.5590
K	 0.7283	 0.5720
L	 0.7304	 0.5920
M	 0.7686	 0.5980
N	 0.7106	 0.5850
O	 0.7532	 0.5830
T	 0.5813	 0.5230
X	 0.6334	 0.5450
Y	 0.6517	 0.5570
Z	 0.4650	 0.4250
a	 0.6303	 0.5410
b	 0.5407	 0.5320
c	 0.7569	 0.5870
d	 0.6580	 0.5610
e	 0.6632	 0.5600
f	 0.6923	 0.5700
g	 0.6990	 0.5720
h	 0.6618	 0.5520
i	 0.6528	 0.5470
j	 0.7149	 0.5460
k	 0.6611	 0.5510
l	 0.7520	 0.5870
m	 0.7453	 0.5940
n	 0.7099	 0.5680
o	 0.7166	 0.5730
p	 0.7231	 0.5780
s	 0.6835	 0.5660
t	 0.6879	 0.5870
u	 0.6440	 0.5170
w	 0.6780	 0.5650
x	 0.7556	 0.5840
y	 0.6753	 0.5630
z	 0.6911	 0.5680

