



## wwPDB EM Validation Summary Report ⓘ

Apr 18, 2024 – 06:51 pm BST

PDB ID : 8RGP  
EMDB ID : EMD-19145  
Title : Closed Complex I from murine brain  
Authors : Vercellino, I.; Sazanov, L.A.  
Deposited on : 2023-12-14  
Resolution : 3.00 Å(reported)  
Based on initial model : 6g2j

This is a wwPDB EM Validation Summary 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:

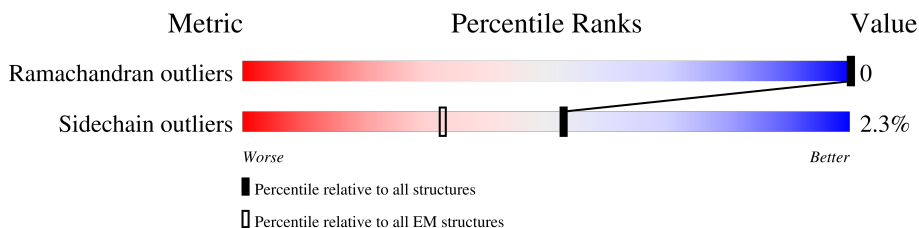
EMDB validation analysis : 0.0.1.dev92  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

# 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 3.00 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	6	224	67% (green), 31% (grey)
2	C	263	78% (green), 21% (grey), 5% (red)
3	D	463	92% (green), 7% (grey), 5% (red)
4	2	248	83% (green), 14% (grey)
5	1	464	91% (green), 7% (grey)
6	3	727	93% (green), 5% (grey)
7	9	212	83% (green), 16% (grey), 5% (red)
8	P	377	89% (green), 9% (grey), 5% (red)
9	Q	175	71% (green), 28% (grey)

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Mol	Chain	Length	Quality of chain
10	7	116	82% 17%
11	S	99	82% 15%
12	T	156	50% 49%
12	U	156	56% 44%
13	V	116	93%
14	W	131	85% 13%
15	q	145	98%
16	r	113	86% 12%
17	s	104	38% 61%
18	A	115	97%
19	H	318	97%
20	J	172	12% 97%
21	K	98	98%
22	L	607	97%
23	M	459	98%
24	N	345	97%
25	O	355	88% 10%
26	X	172	95% 5%
27	Y	141	95%
28	Z	144	97%
29	a	70	100%
30	b	84	5% 96%
31	c	76	62% 37%
32	d	120	98%
33	e	106	99%

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Mol	Chain	Length	Quality of chain
34	f	57	
35	g	151	
36	h	189	
37	i	128	
38	j	105	
39	k	104	
40	l	186	
41	m	129	
42	n	179	
43	o	137	
44	p	176	

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
37	SAC	i	1	-	X	-	-

## 2 Entry composition [i](#)

There are 57 unique types of molecules in this entry. The entry contains 67868 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 NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	6	155	1241	793	222	212	14	0	0

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	207	1721	1110	295	313	3	0	0

- Molecule 3 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	430	3464	2215	595	630	24	0	0

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	2	214	1660	1056	279	314	11	0	0

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	1	430	3321	2092	596	611	22	0	0

- Molecule 6 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	3	690	5305	3326	921	1017	41	0	0

- Molecule 7 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	9	178	1431	898	245	276	12	0	0

- Molecule 8 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	P	342	2748	1777	483	481	7	0	0

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	Q	126	1022	646	180	192	4	0	0

- Molecule 10 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	7	96	758	470	141	144	3	0	0

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	S	84	671	421	127	120	3	0	0

- Molecule 12 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	T	79	637	410	95	127	5	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	U	88	706	453	104	144	5	0	0

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	V	112	915	596	152	164	3	0	0

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	W	114	970	619	180	165	6	0	0

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	q	145	1209	777	215	212	5	0	0

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	r	99	796	504	148	141	3	0	0

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
17	s	41	344	215	61	68	0	0

- Molecule 18 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	A	115	Total	C	N	O	S	0	0
			932	633	132	160	7		

- Molecule 19 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	H	318	Total	C	N	O	S	0	0
			2540	1706	384	428	22		

- Molecule 20 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	J	172	Total	C	N	O	S	0	0
			1308	878	186	229	15		

- Molecule 21 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	K	98	Total	C	N	O	S	0	0
			737	477	112	137	11		

- Molecule 22 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	L	606	Total	C	N	O	S	0	0
			4800	3182	746	827	45		

- Molecule 23 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	M	459	Total	C	N	O	S	0	0
			3632	2408	567	617	40		

- Molecule 24 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	N	345	Total	C	N	O	S	0	0
			2703	1795	417	454	37		

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.



Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	O	320	2607	1674	431	492	10	0	0

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	X	171	1396	889	250	247	10	0	0

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	Y	140	1037	662	175	192	8	0	0

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	Z	141	1167	750	207	202	8	0	0

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	a	70	572	370	101	97	4	0	0

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	b	83	651	427	105	115	4	0	0

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	c	48	Total	C	N	O	S	0	0
			398	261	69	67	1		

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	d	120	Total	C	N	O	S	0	0
			996	651	171	165	9		

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	e	105	Total	C	N	O	S	0	0
			877	555	162	152	8		

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	f	53	Total	C	N	O	S	0	0
			456	295	82	77	2		

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	g	101	Total	C	N	O	S	0	0
			850	549	136	161	4		

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	h	139	Total	C	N	O	S	0	0
			1166	764	195	204	3		

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	i	98	Total	C	N	O	S	0	0
			828	537	146	142	3		

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	j	64	555	365	92	97	1	0	0

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	k	77	626	414	106	104	2	0	0

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	l	157	1323	855	220	237	11	0	0

- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
41	m	126	1050	676	189	185	0	0

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	n	178	1541	985	276	269	11	0	0

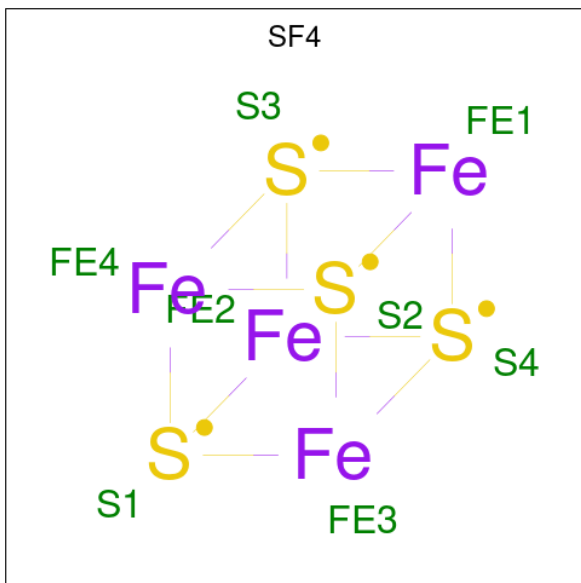
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	o	118	1014	639	190	177	8	0	0

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

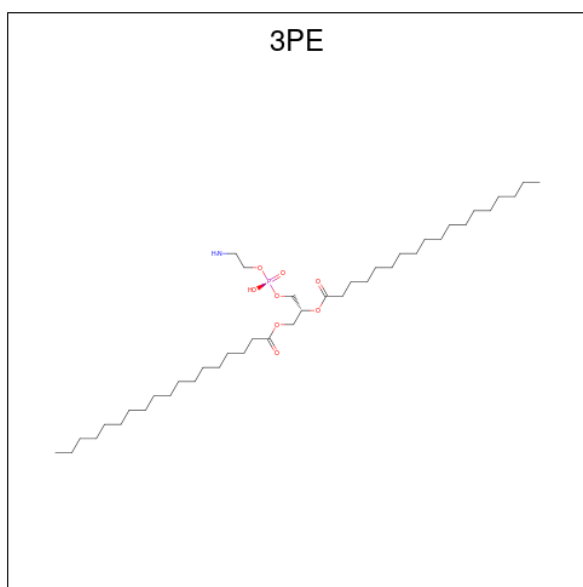
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	p	170	1438	903	258	269	8	0	0

- Molecule 45 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



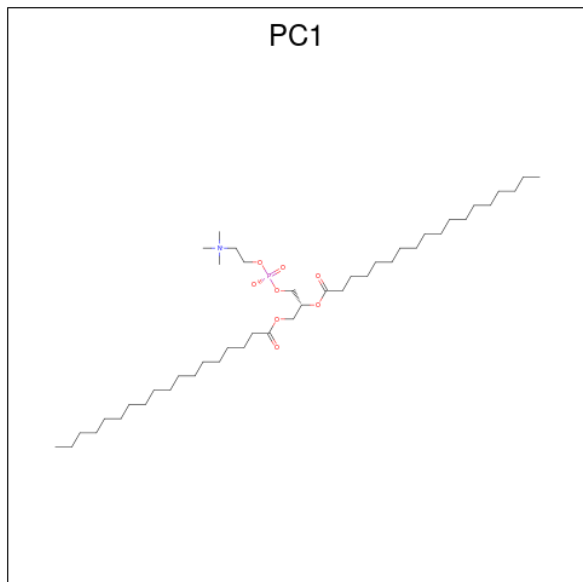
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
45	6	1	8	4	4	0
45	1	1	8	4	4	0
45	3	1	8	4	4	0
45	3	1	8	4	4	0
45	9	1	8	4	4	0
45	9	1	8	4	4	0

- Molecule 46 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: C<sub>41</sub>H<sub>82</sub>NO<sub>8</sub>P).



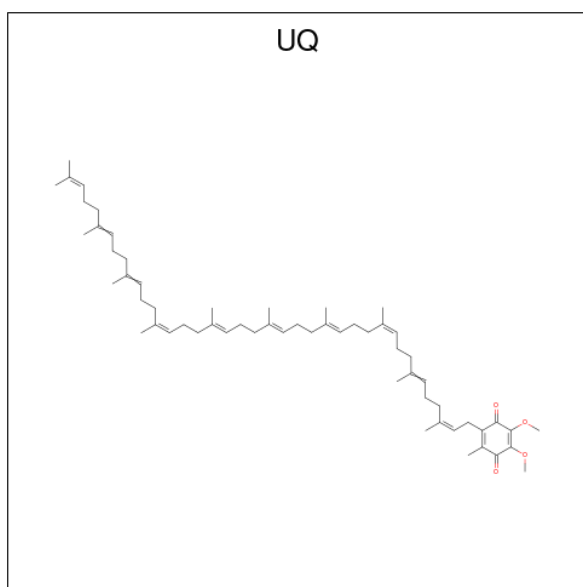
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
46	6	1	Total 32	22	1	8	1	0
46	D	1	Total 51	41	1	8	1	0
46	A	1	Total 43	33	1	8	1	0
46	K	1	Total 41	31	1	8	1	0
46	L	1	Total 51	41	1	8	1	0
46	L	1	Total 42	32	1	8	1	0
46	M	1	Total 51	41	1	8	1	0
46	M	1	Total 36	26	1	8	1	0
46	Y	1	Total 28	18	1	8	1	0
46	Z	1	Total 51	41	1	8	1	0
46	d	1	Total 31	21	1	8	1	0
46	h	1	Total 51	41	1	8	1	0
46	i	1	Total 42	32	1	8	1	0
46	m	1	Total 30	20	1	8	1	0

- Molecule 47 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula:  $C_{44}H_{88}NO_8P$ ).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
47	6	1	Total 43	33	1	8	1	0
47	9	1	Total 54	44	1	8	1	0
47	H	1	Total 42	32	1	8	1	0
47	M	1	Total 54	44	1	8	1	0
47	Z	1	Total 47	37	1	8	1	0

- Molecule 48 is Coenzyme Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-isomer (three-letter code: UQ) (formula:  $C_{59}H_{90}O_4$ ).



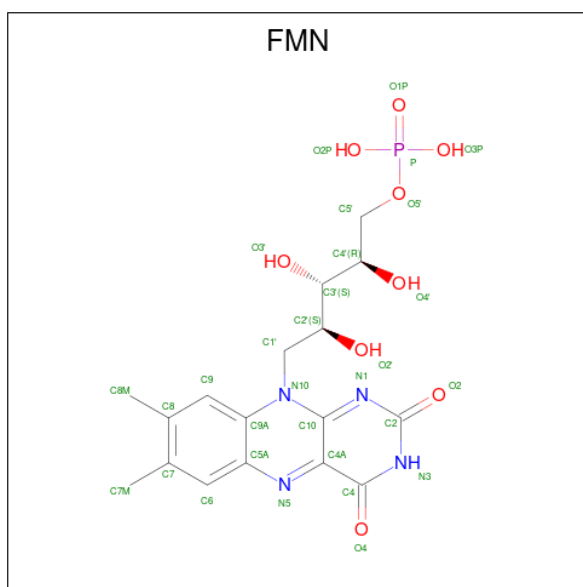
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
48	D	1	63	59	4	0

- Molecule 49 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).



Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
49	2	1	4	2	2	0
49	3	1	4	2	2	0

- Molecule 50 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C<sub>17</sub>H<sub>21</sub>N<sub>4</sub>O<sub>9</sub>P).

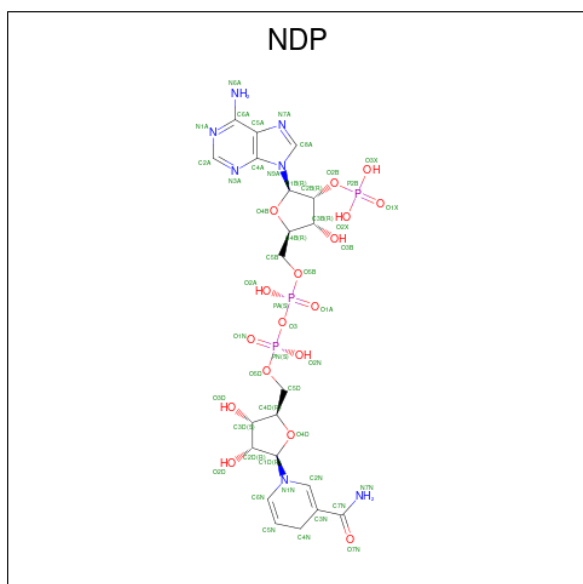


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
50	1	1	31	17	4	9	1	0

- Molecule 51 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
			Total	K	
51	3	1	1	1	0

- Molecule 52 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C<sub>21</sub>H<sub>30</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



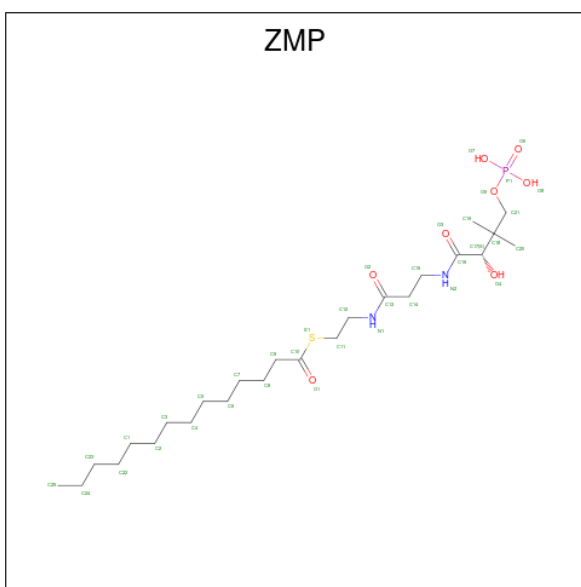


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
52	P	1	48	21	7	17	3	0

- Molecule 53 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
53	7	1	1	1	0

- Molecule 54 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonoxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (three-letter code: ZMP) (formula: C<sub>25</sub>H<sub>49</sub>N<sub>2</sub>O<sub>8</sub>PS).



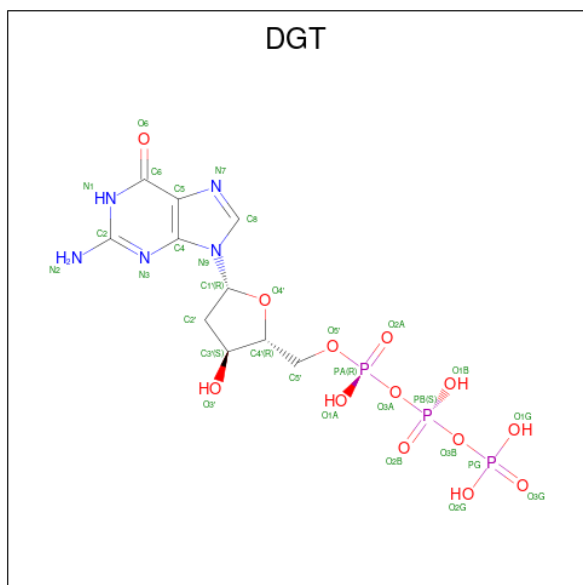
Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
54	W	1	34	23	2	7	1	1	0
54	n	1	32	21	2	7	1	1	0

- Molecule 55 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	
55	r	1	57	38	17	2	0
55	L	1	78	59	17	2	0
55	L	1	46	27	17	2	0
55	N	1	90	71	17	2	0
55	Y	1	94	75	17	2	0
55	Y	1	57	38	17	2	0
55	d	1	67	48	17	2	0
55	h	1	70	51	17	2	0
55	m	1	72	53	17	2	0

- Molecule 56 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (three-letter code: DGT) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



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

- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

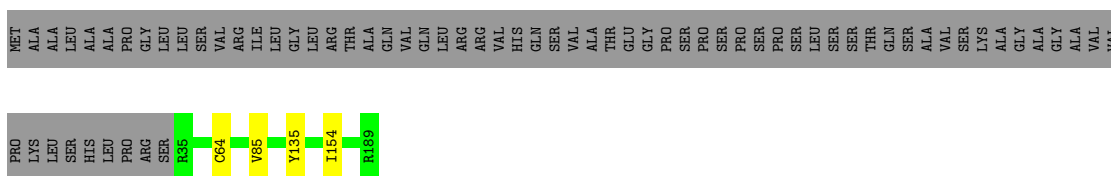
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
57	O	1	1	1	0

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


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

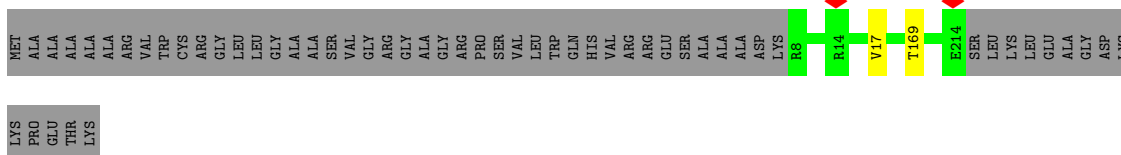
- Molecule 1: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain 6:  67% 31%



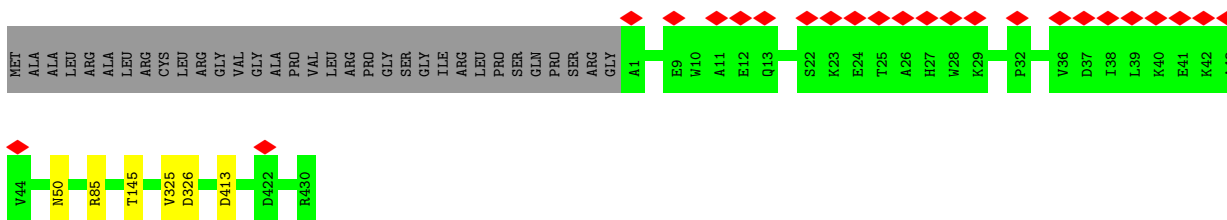
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

Chain C:  78% 21%




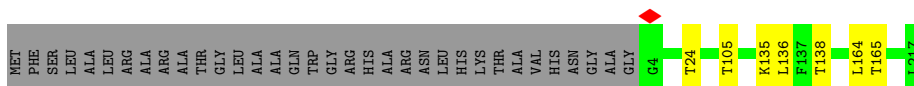
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

Chain D:  5% 92% 7%




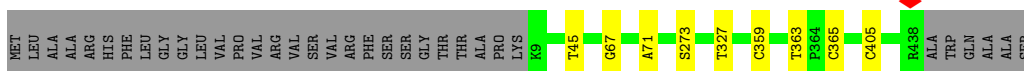
- Molecule 4: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain 2:  83% 14%



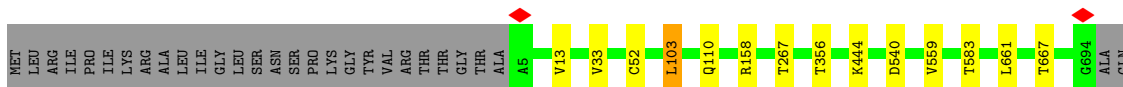
- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain 1:  91% 7%




- Molecule 6: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

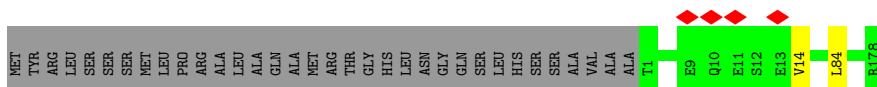
Chain 3:  93% 5%




ALA  
VAL  
GLU  
PRO  
SER  
ILE  
CYS

- Molecule 7: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain 9:  83% 16%



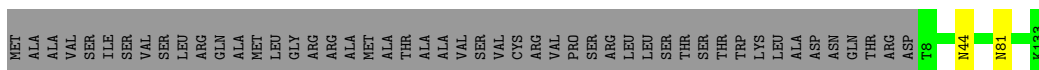
- Molecule 8: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain P:  89% 9%




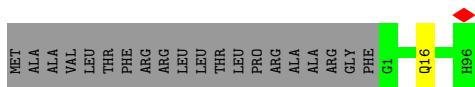
- Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain Q:  71% 28%

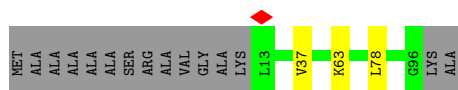
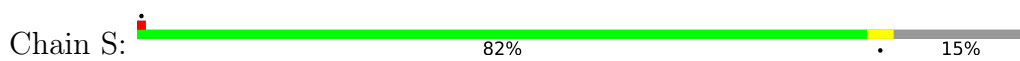


- Molecule 10: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

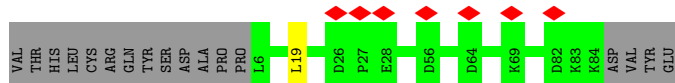
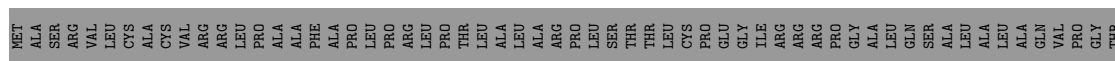
Chain 7:  82% 17%



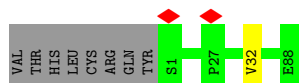
- Molecule 11: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



• Molecule 12: Acyl carrier protein, mitochondrial



• Molecule 12: Acyl carrier protein, mitochondrial



• Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



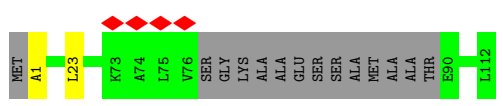
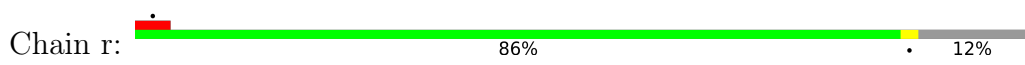
• Molecule 14: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



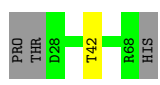
• Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



• Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7



• Molecule 17: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial



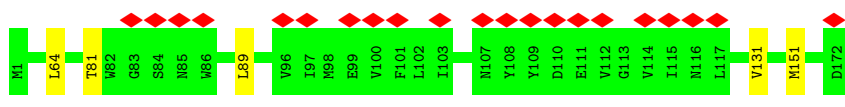
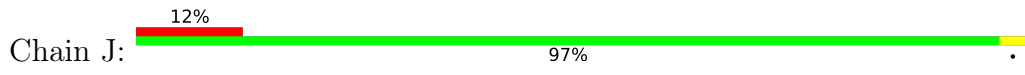
• Molecule 18: NADH-ubiquinone oxidoreductase chain 3



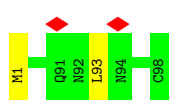
• Molecule 19: NADH-ubiquinone oxidoreductase chain 1



• Molecule 20: NADH-ubiquinone oxidoreductase chain 6



• Molecule 21: NADH-ubiquinone oxidoreductase chain 4L



• Molecule 22: NADH-ubiquinone oxidoreductase chain 5





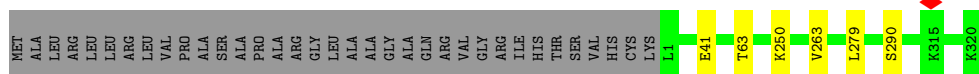
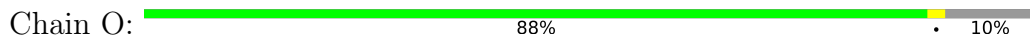
- Molecule 23: NADH-ubiquinone oxidoreductase chain 4



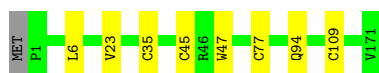
- Molecule 24: NADH-ubiquinone oxidoreductase chain 2



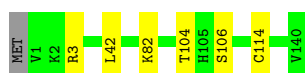
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial



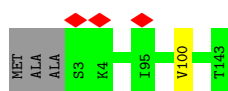
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



- Molecule 28: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



- Molecule 29: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

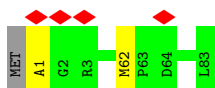


Chain a:  100%



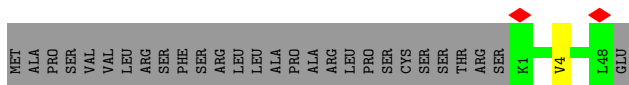
- Molecule 30: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain b:  96% 5%



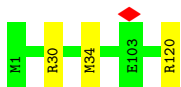
- Molecule 31: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

Chain c:  62% 37%



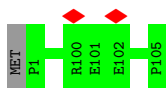
- Molecule 32: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain d:  98%




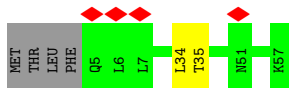
- Molecule 33: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain e:  99%



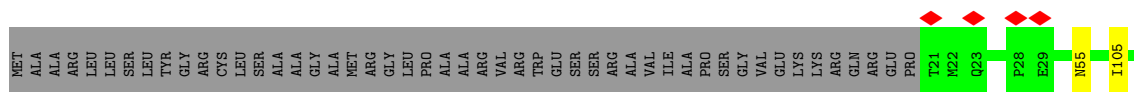
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

Chain f:  89% 7% 7%

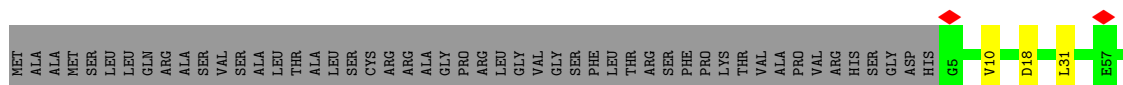


- Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

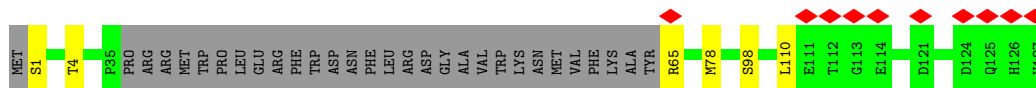
Chain g:  66% 33%



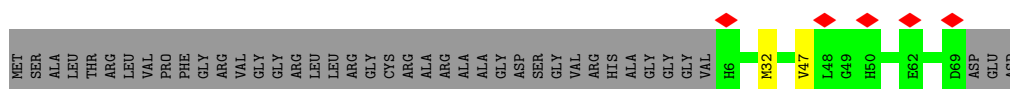
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



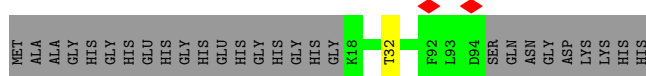
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



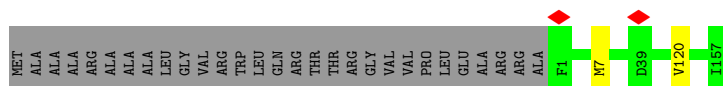
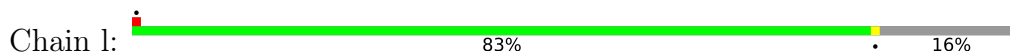
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

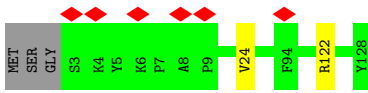


- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



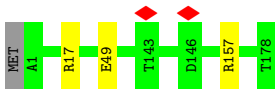
- Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

Chain m:  5% 96%




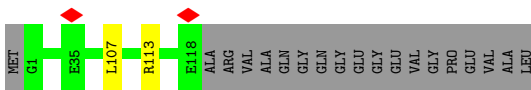
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

Chain n:  98%



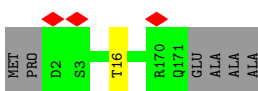
- Molecule 43: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain o:  85% 14%



- Molecule 44: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

Chain p:  96%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	95155	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 ( $e^-/\text{\AA}^2$ )	80	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.149	Depositor
Minimum map value	-0.018	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.018	Depositor
Map size (Å)	226.83998, 214.12, 203.51999	wwPDB
Map dimensions	214, 202, 192	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FES, AYA, MG, NDP, ZMP, SAC, K, FME, CDL, 3PE, 2MR, SF4, DGT, UQ, PC1, FMN, ZN

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	6	0.40	0/1272	0.55	0/1722
2	C	0.35	0/1771	0.55	0/2413
3	D	0.36	0/3540	0.54	0/4795
4	2	0.33	0/1700	0.54	0/2316
5	1	0.53	2/3396 (0.1%)	0.59	3/4586 (0.1%)
6	3	0.34	0/5392	0.54	2/7305 (0.0%)
7	9	0.36	0/1461	0.55	1/1974 (0.1%)
8	P	0.33	0/2823	0.55	0/3828
9	Q	0.31	0/1045	0.51	0/1411
10	7	0.34	0/773	0.52	0/1041
11	S	0.33	0/682	0.58	1/920 (0.1%)
12	T	0.27	0/646	0.54	0/869
12	U	0.32	0/718	0.52	0/970
13	V	0.30	0/937	0.46	0/1270
14	W	0.31	0/993	0.52	0/1335
15	q	0.34	0/1251	0.55	0/1702
16	r	0.32	0/806	0.53	0/1090
17	s	0.34	0/353	0.55	0/479
18	A	0.32	0/948	0.52	1/1295 (0.1%)
19	H	0.37	0/2607	0.54	1/3564 (0.0%)
20	J	0.35	0/1330	0.48	0/1810
21	K	0.32	0/738	0.50	0/1002
22	L	0.34	0/4913	0.52	0/6686
23	M	0.34	0/3709	0.53	0/5052
24	N	0.33	0/2755	0.52	1/3751 (0.0%)
25	O	0.34	0/2674	0.49	0/3626
26	X	0.31	0/1434	0.54	0/1937
27	Y	0.31	0/1061	0.47	0/1439
28	Z	0.32	0/1198	0.51	0/1616
29	a	0.33	0/585	0.54	0/788
30	b	0.30	0/666	0.45	0/914
31	c	0.29	0/409	0.45	0/555

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	d	0.33	0/1028	0.50	0/1387
33	e	0.30	0/900	0.49	0/1199
34	f	0.29	0/468	0.56	0/630
35	g	0.34	0/878	0.48	0/1196
36	h	0.33	0/1201	0.51	0/1626
37	i	0.30	0/846	0.53	0/1149
38	j	0.31	0/580	0.48	0/794
39	k	0.30	0/646	0.47	0/873
40	l	0.34	0/1379	0.48	0/1882
41	m	0.32	0/1079	0.53	0/1463
42	n	0.33	0/1596	0.51	0/2162
43	o	0.29	0/1039	0.50	0/1394
44	p	0.31	0/1471	0.51	0/1988
All	All	0.35	2/67697 (0.0%)	0.53	10/91804 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	1	67	GLY	C-N	-17.12	0.94	1.34
5	1	71	ALA	C-N	15.12	1.60	1.33

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	1	71	ALA	O-C-N	7.01	135.13	123.20
24	N	148	LEU	CA-CB-CG	6.43	130.08	115.30
5	1	71	ALA	CA-C-N	-6.17	103.87	116.20
5	1	71	ALA	C-N-CA	-5.93	109.85	122.30
19	H	233	LEU	CB-CG-CD1	-5.71	101.28	111.00

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

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	6	153/224 (68%)	146 (95%)	7 (5%)	0	100	100
2	C	205/263 (78%)	193 (94%)	12 (6%)	0	100	100
3	D	427/463 (92%)	398 (93%)	29 (7%)	0	100	100
4	2	212/248 (86%)	189 (89%)	23 (11%)	0	100	100
5	1	428/464 (92%)	399 (93%)	29 (7%)	0	100	100
6	3	688/727 (95%)	643 (94%)	45 (6%)	0	100	100
7	9	176/212 (83%)	173 (98%)	3 (2%)	0	100	100
8	P	340/377 (90%)	310 (91%)	30 (9%)	0	100	100
9	Q	124/175 (71%)	119 (96%)	5 (4%)	0	100	100
10	7	94/116 (81%)	88 (94%)	6 (6%)	0	100	100
11	S	82/99 (83%)	73 (89%)	9 (11%)	0	100	100
12	T	77/156 (49%)	73 (95%)	4 (5%)	0	100	100
12	U	86/156 (55%)	80 (93%)	6 (7%)	0	100	100
13	V	110/116 (95%)	107 (97%)	3 (3%)	0	100	100
14	W	112/131 (86%)	105 (94%)	7 (6%)	0	100	100
15	q	143/145 (99%)	127 (89%)	16 (11%)	0	100	100
16	r	95/113 (84%)	91 (96%)	4 (4%)	0	100	100
17	s	39/104 (38%)	38 (97%)	1 (3%)	0	100	100
18	A	113/115 (98%)	105 (93%)	8 (7%)	0	100	100
19	H	316/318 (99%)	299 (95%)	17 (5%)	0	100	100
20	J	170/172 (99%)	160 (94%)	10 (6%)	0	100	100
21	K	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
22	L	604/607 (100%)	558 (92%)	46 (8%)	0	100	100
23	M	457/459 (100%)	439 (96%)	18 (4%)	0	100	100
24	N	343/345 (99%)	330 (96%)	13 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	O	318/355 (90%)	295 (93%)	23 (7%)	0	100	100
26	X	169/172 (98%)	158 (94%)	11 (6%)	0	100	100
27	Y	138/141 (98%)	138 (100%)	0	0	100	100
28	Z	139/144 (96%)	134 (96%)	5 (4%)	0	100	100
29	a	68/70 (97%)	67 (98%)	1 (2%)	0	100	100
30	b	81/84 (96%)	77 (95%)	4 (5%)	0	100	100
31	c	46/76 (60%)	45 (98%)	1 (2%)	0	100	100
32	d	118/120 (98%)	113 (96%)	5 (4%)	0	100	100
33	e	103/106 (97%)	91 (88%)	12 (12%)	0	100	100
34	f	51/57 (90%)	42 (82%)	9 (18%)	0	100	100
35	g	99/151 (66%)	96 (97%)	3 (3%)	0	100	100
36	h	137/189 (72%)	129 (94%)	8 (6%)	0	100	100
37	i	94/128 (73%)	83 (88%)	11 (12%)	0	100	100
38	j	62/105 (59%)	58 (94%)	4 (6%)	0	100	100
39	k	75/104 (72%)	72 (96%)	3 (4%)	0	100	100
40	l	155/186 (83%)	147 (95%)	8 (5%)	0	100	100
41	m	124/129 (96%)	119 (96%)	5 (4%)	0	100	100
42	n	176/179 (98%)	167 (95%)	9 (5%)	0	100	100
43	o	116/137 (85%)	107 (92%)	9 (8%)	0	100	100
44	p	168/176 (96%)	161 (96%)	7 (4%)	0	100	100
All	All	8127/9212 (88%)	7635 (94%)	492 (6%)	0	100	100

There are no Ramachandran outliers to report.

### 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	6	131/185 (71%)	127 (97%)	4 (3%)	40	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	189/227 (83%)	187 (99%)	2 (1%)	73	90
3	D	370/394 (94%)	365 (99%)	5 (1%)	67	88
4	2	184/206 (89%)	177 (96%)	7 (4%)	33	69
5	1	345/370 (93%)	338 (98%)	7 (2%)	55	83
6	3	580/610 (95%)	567 (98%)	13 (2%)	52	81
7	9	152/178 (85%)	151 (99%)	1 (1%)	84	94
8	P	299/325 (92%)	292 (98%)	7 (2%)	50	80
9	Q	113/153 (74%)	111 (98%)	2 (2%)	59	85
10	7	81/96 (84%)	80 (99%)	1 (1%)	71	90
11	S	74/80 (92%)	72 (97%)	2 (3%)	44	77
12	T	73/135 (54%)	72 (99%)	1 (1%)	67	88
12	U	81/135 (60%)	80 (99%)	1 (1%)	71	90
13	V	100/102 (98%)	96 (96%)	4 (4%)	31	68
14	W	108/114 (95%)	105 (97%)	3 (3%)	43	77
15	q	131/131 (100%)	128 (98%)	3 (2%)	50	80
16	r	88/96 (92%)	87 (99%)	1 (1%)	73	90
17	s	40/95 (42%)	39 (98%)	1 (2%)	47	79
18	A	103/103 (100%)	100 (97%)	3 (3%)	42	76
19	H	279/279 (100%)	270 (97%)	9 (3%)	39	74
20	J	137/137 (100%)	132 (96%)	5 (4%)	35	70
21	K	87/87 (100%)	86 (99%)	1 (1%)	73	90
22	L	548/549 (100%)	534 (97%)	14 (3%)	46	78
23	M	414/414 (100%)	407 (98%)	7 (2%)	60	85
24	N	307/307 (100%)	297 (97%)	10 (3%)	38	73
25	O	284/309 (92%)	278 (98%)	6 (2%)	53	82
26	X	153/154 (99%)	145 (95%)	8 (5%)	23	59
27	Y	105/106 (99%)	99 (94%)	6 (6%)	20	56
28	Z	122/123 (99%)	121 (99%)	1 (1%)	81	93
29	a	60/60 (100%)	60 (100%)	0	100	100
30	b	72/73 (99%)	71 (99%)	1 (1%)	67	88
31	c	42/67 (63%)	41 (98%)	1 (2%)	49	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	d	107/107 (100%)	104 (97%)	3 (3%)	43	77
33	e	93/94 (99%)	93 (100%)	0	100	100
34	f	49/53 (92%)	47 (96%)	2 (4%)	30	67
35	g	92/129 (71%)	90 (98%)	2 (2%)	52	81
36	h	123/162 (76%)	119 (97%)	4 (3%)	38	73
37	i	92/119 (77%)	87 (95%)	5 (5%)	22	57
38	j	60/87 (69%)	58 (97%)	2 (3%)	38	73
39	k	60/78 (77%)	59 (98%)	1 (2%)	60	85
40	l	142/161 (88%)	140 (99%)	2 (1%)	67	88
41	m	112/114 (98%)	110 (98%)	2 (2%)	59	85
42	n	163/164 (99%)	160 (98%)	3 (2%)	59	85
43	o	109/121 (90%)	107 (98%)	2 (2%)	59	85
44	p	155/158 (98%)	154 (99%)	1 (1%)	86	95
All	All	7209/7947 (91%)	7043 (98%)	166 (2%)	53	80

5 of 166 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
25	O	250	LYS
35	g	105	ILE
12	U	32	VAL
27	Y	82	LYS
37	i	78	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
22	L	361	ASN
25	O	45	GLN
43	o	54	GLN
18	A	10	ASN
6	3	237	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

11 non-standard protein/DNA/RNA residues 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
16	AYA	r	1	16	6,7,8	1.34	1 (16%)	5,8,10	1.36	1 (20%)
22	FME	L	1	22	8,9,10	0.91	0	7,9,11	1.07	1 (14%)
3	2MR	D	85	3	10,12,13	1.99	1 (10%)	5,13,15	7.17	3 (60%)
18	FME	A	1	18	8,9,10	0.98	0	7,9,11	0.87	0
24	FME	N	1	24	8,9,10	0.95	0	7,9,11	0.88	0
21	FME	K	1	21	8,9,10	0.95	0	7,9,11	1.86	2 (28%)
19	FME	H	1	19	8,9,10	0.95	0	7,9,11	0.96	0
23	FME	M	1	23	8,9,10	0.98	0	7,9,11	0.69	0
30	AYA	b	1	30	6,7,8	1.25	1 (16%)	5,8,10	1.45	1 (20%)
20	FME	J	1	20	8,9,10	0.94	0	7,9,11	0.83	0
37	SAC	i	1	37	7,8,9	1.02	0	8,9,11	3.01	4 (50%)

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
16	AYA	r	1	16	-	0/4/6/8	-
22	FME	L	1	22	-	4/7/9/11	-
3	2MR	D	85	3	-	4/10/13/15	-
18	FME	A	1	18	-	1/7/9/11	-
24	FME	N	1	24	-	3/7/9/11	-
21	FME	K	1	21	-	4/7/9/11	-
19	FME	H	1	19	-	1/7/9/11	-
23	FME	M	1	23	-	2/7/9/11	-
30	AYA	b	1	30	-	1/4/6/8	-
20	FME	J	1	20	-	0/7/9/11	-
37	SAC	i	1	37	-	7/7/8/10	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	85	2MR	CZ-NE	5.66	1.46	1.34
16	r	1	AYA	CA-N	-2.74	1.43	1.46
30	b	1	AYA	CA-N	-2.32	1.44	1.46

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	85	2MR	NE-CZ-NH2	14.60	132.86	119.48
37	i	1	SAC	CA-N-C1A	6.04	134.29	123.15
3	D	85	2MR	CD-NE-CZ	4.51	131.85	123.41
3	D	85	2MR	CQ2-NH2-CZ	4.49	133.79	123.86
37	i	1	SAC	C2A-C1A-N	4.30	123.38	116.10

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	85	2MR	O-C-CA-CB
18	A	1	FME	N-CA-CB-CG
19	H	1	FME	N-CA-CB-CG
21	K	1	FME	O1-CN-N-CA
22	L	1	FME	CB-CA-N-CN

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 45 ligands modelled in this entry, 3 are monoatomic - leaving 42 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$
50	FMN	1	501	-	33,33,33	0.38	0	48,50,50	0.57	2 (4%)
46	3PE	L	704	-	41,41,50	0.32	0	44,46,55	0.37	0
47	PC1	Z	402	-	46,46,53	0.32	0	52,54,61	0.32	0
54	ZMP	n	201	-	25,31,36	0.73	1 (4%)	30,38,45	0.92	1 (3%)
55	CDL	L	702	-	77,77,99	0.34	0	83,89,111	0.33	0
46	3PE	d	202	-	30,30,50	0.38	0	33,35,55	0.36	0
55	CDL	Y	403	-	56,56,99	0.39	0	62,68,111	0.46	1 (1%)
47	PC1	H	401	-	41,41,53	0.33	0	47,49,61	0.32	0
46	3PE	A	201	-	42,42,50	0.33	0	45,47,55	0.32	0
47	PC1	M	501	-	53,53,53	0.29	0	59,61,61	0.37	0
46	3PE	K	201	-	40,40,50	0.33	0	43,45,55	0.32	0
46	3PE	6	202	-	31,31,50	0.38	0	34,36,55	0.35	0
56	DGT	O	401	57	26,33,33	0.80	2 (7%)	32,52,52	0.47	0
54	ZMP	W	201	-	27,33,36	0.59	0	32,40,45	1.19	3 (9%)
55	CDL	L	703	-	45,45,99	0.43	0	51,57,111	0.34	0
52	NDP	P	501	-	45,52,52	0.57	0	53,80,80	0.63	1 (1%)
45	SF4	9	201	7	0,12,12	-	-	-	-	-
45	SF4	3	802	6	0,12,12	-	-	-	-	-
46	3PE	Z	401	-	50,50,50	0.31	0	53,55,55	0.47	0
55	CDL	r	201	-	56,56,99	0.40	0	62,68,111	0.58	1 (1%)
46	3PE	i	201	-	41,41,50	0.32	0	44,46,55	0.31	0
49	FES	3	803	6	0,4,4	-	-	-	-	-
55	CDL	N	401	-	89,89,99	0.31	0	95,101,111	0.41	0
46	3PE	L	701	-	50,50,50	0.31	0	53,55,55	0.46	0
47	PC1	9	203	-	53,53,53	0.30	0	59,61,61	0.43	0
45	SF4	6	201	1	0,12,12	-	-	-	-	-
45	SF4	9	202	7	0,12,12	-	-	-	-	-
47	PC1	6	203	-	42,42,53	0.34	0	48,50,61	0.48	0
48	UQ	D	501	-	63,63,63	0.26	0	76,79,79	0.53	1 (1%)
46	3PE	M	503	-	35,35,50	0.35	0	38,40,55	0.30	0
45	SF4	3	801	6	0,12,12	-	-	-	-	-
45	SF4	1	502	5	0,12,12	-	-	-	-	-
46	3PE	D	502	-	50,50,50	0.30	0	53,55,55	0.37	0
55	CDL	m	201	-	71,71,99	0.36	0	77,83,111	0.43	0
49	FES	2	301	4	0,4,4	-	-	-	-	-
55	CDL	d	201	-	66,66,99	0.36	0	72,78,111	0.36	0
46	3PE	h	202	-	50,50,50	0.31	0	53,55,55	0.27	0
46	3PE	m	202	-	29,29,50	0.39	0	32,34,55	0.33	0
55	CDL	h	201	-	69,69,99	0.35	0	75,81,111	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
46	3PE	M	502	-	50,50,50	0.30	0	53,55,55	0.32	0
55	CDL	Y	401	-	93,93,99	0.31	0	99,105,111	0.28	0
46	3PE	Y	402	-	27,27,50	0.40	0	30,32,55	0.38	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
50	FMN	1	501	-	-	6/18/18/18	0/3/3/3
46	3PE	L	704	-	-	8/45/45/54	-
47	PC1	Z	402	-	-	9/50/50/57	-
54	ZMP	n	201	-	-	20/36/38/43	-
55	CDL	L	702	-	-	19/88/88/110	-
46	3PE	d	202	-	-	7/34/34/54	-
55	CDL	Y	403	-	-	21/67/67/110	-
47	PC1	H	401	-	-	9/45/45/57	-
46	3PE	A	201	-	-	11/46/46/54	-
47	PC1	M	501	-	-	11/57/57/57	-
46	3PE	K	201	-	-	9/44/44/54	-
46	3PE	6	202	-	-	6/35/35/54	-
56	DGT	O	401	57	-	8/18/34/34	0/3/3/3
54	ZMP	W	201	-	-	10/38/40/43	-
55	CDL	L	703	-	-	10/56/56/110	-
52	NDP	P	501	-	-	4/30/77/77	0/5/5/5
45	SF4	9	201	7	-	-	0/6/5/5
45	SF4	3	802	6	-	-	0/6/5/5
46	3PE	Z	401	-	-	13/54/54/54	-
55	CDL	r	201	-	-	15/67/67/110	-
46	3PE	i	201	-	-	5/45/45/54	-
55	CDL	N	401	-	-	21/100/100/110	-
49	FES	3	803	6	-	-	0/1/1/1
46	3PE	L	701	-	-	10/54/54/54	-
47	PC1	9	203	-	-	14/57/57/57	-
45	SF4	6	201	1	-	-	0/6/5/5
47	PC1	6	203	-	-	9/46/46/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	UQ	D	501	-	-	20/63/87/87	0/1/1/1
45	SF4	9	202	7	-	-	0/6/5/5
46	3PE	M	503	-	-	6/39/39/54	-
45	SF4	3	801	6	-	-	0/6/5/5
45	SF4	1	502	5	-	-	0/6/5/5
46	3PE	D	502	-	-	14/54/54/54	-
55	CDL	m	201	-	-	18/82/82/110	-
55	CDL	d	201	-	-	26/77/77/110	-
49	FES	2	301	4	-	-	0/1/1/1
46	3PE	h	202	-	-	10/54/54/54	-
46	3PE	m	202	-	-	1/33/33/54	-
55	CDL	h	201	-	-	20/80/80/110	-
46	3PE	M	502	-	-	12/54/54/54	-
55	CDL	Y	401	-	-	16/104/104/110	-
46	3PE	Y	402	-	-	6/31/31/54	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	n	201	ZMP	C9-C10	2.36	1.53	1.50
56	O	401	DGT	C5-C6	-2.03	1.43	1.47
56	O	401	DGT	C5-C4	-2.01	1.38	1.43

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	W	201	ZMP	O1-C10-C9	-3.06	120.37	123.99
54	n	201	ZMP	O1-C10-C9	-2.52	121.01	123.99
54	W	201	ZMP	C15-C14-C13	-2.51	108.18	112.36
48	D	501	UQ	C7-C6-C1	-2.50	115.47	118.48
50	1	501	FMN	P-O5'-C5'	2.49	125.16	118.30

There are no chirality outliers.

5 of 404 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	6	202	3PE	C11-O13-P-O11
46	6	202	3PE	C11-O13-P-O14
46	6	202	3PE	O13-C11-C12-N

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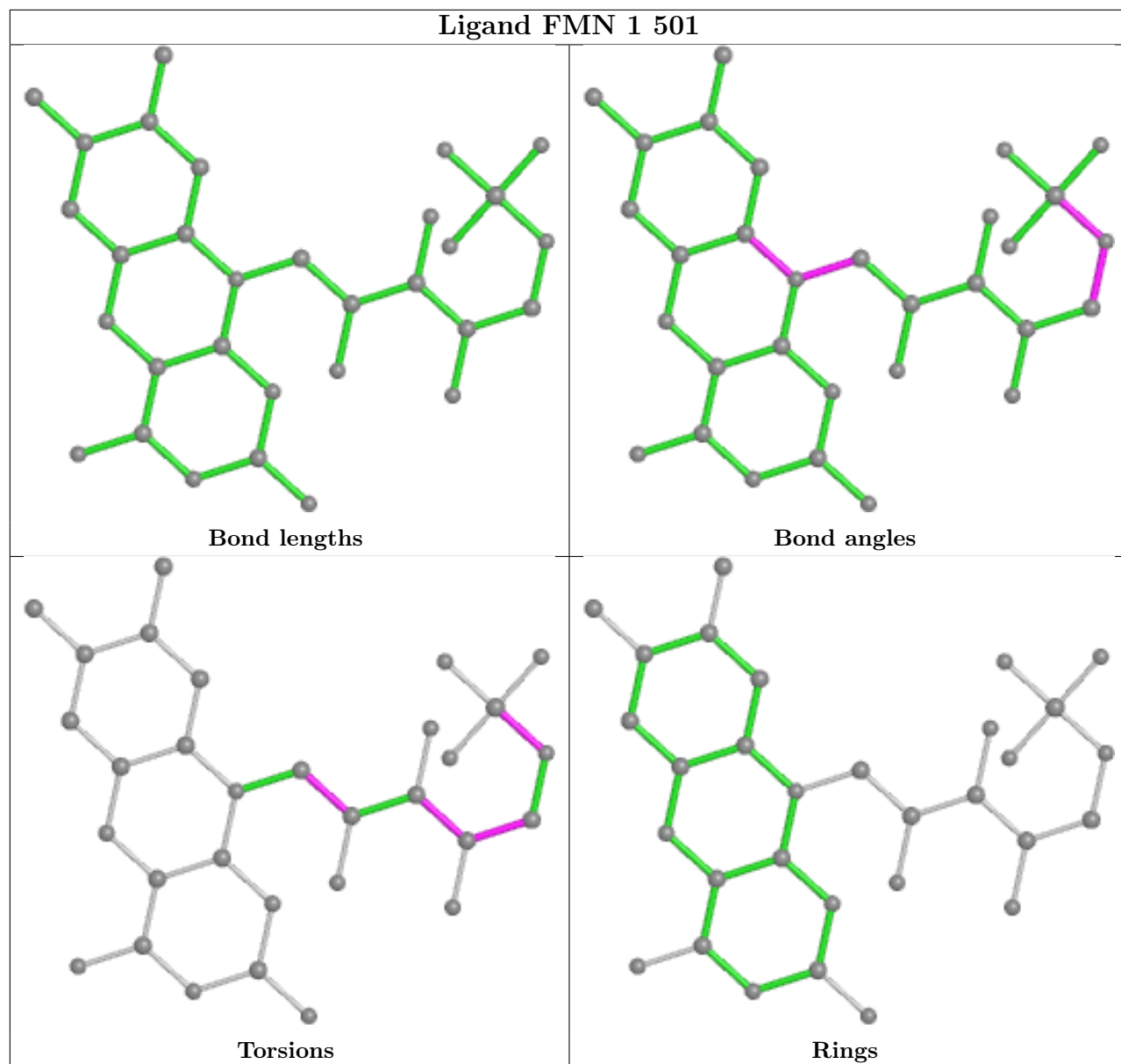
Mol	Chain	Res	Type	Atoms
46	D	502	3PE	C1-O11-P-O12
46	D	502	3PE	C1-O11-P-O13

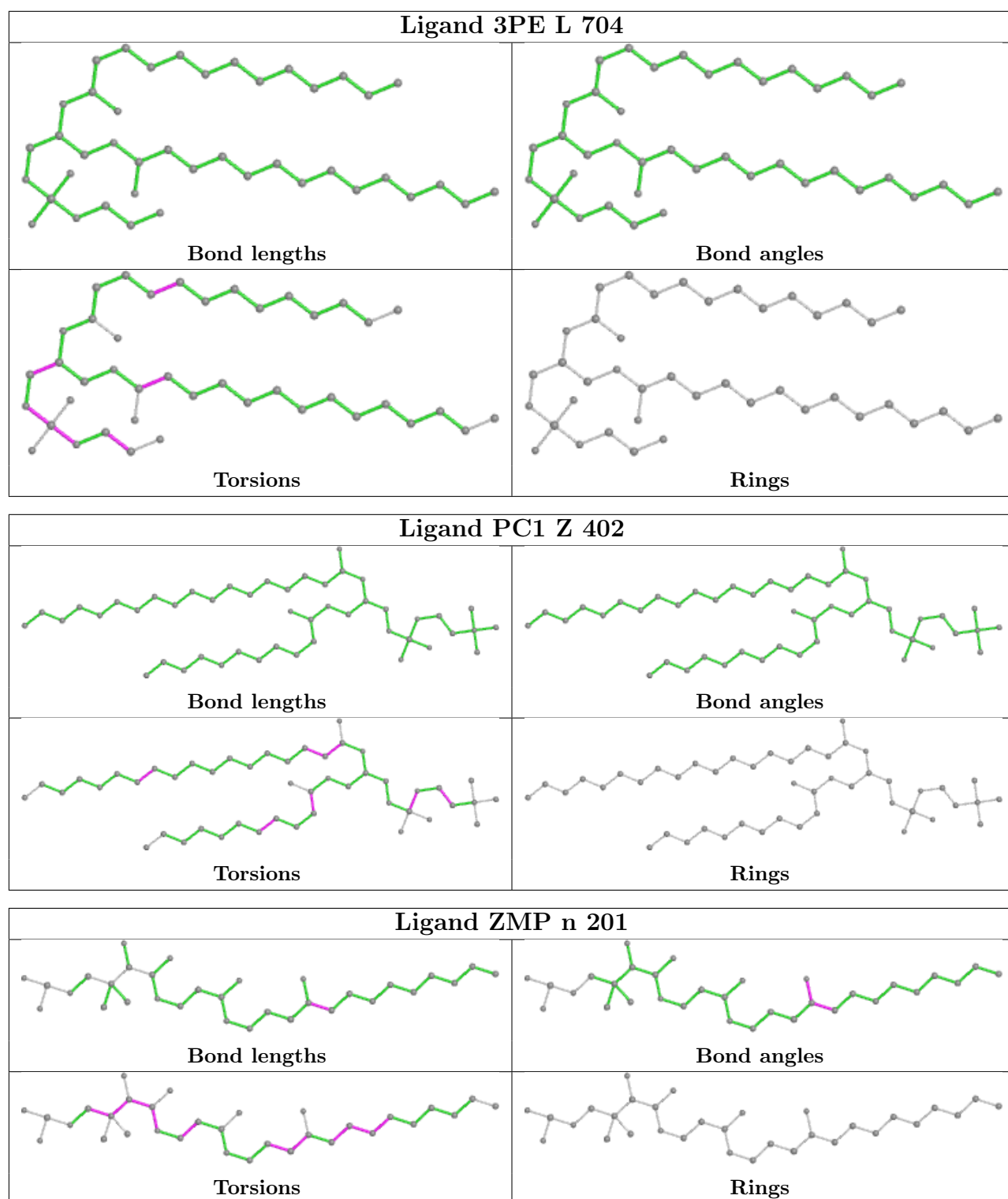
There are no ring outliers.

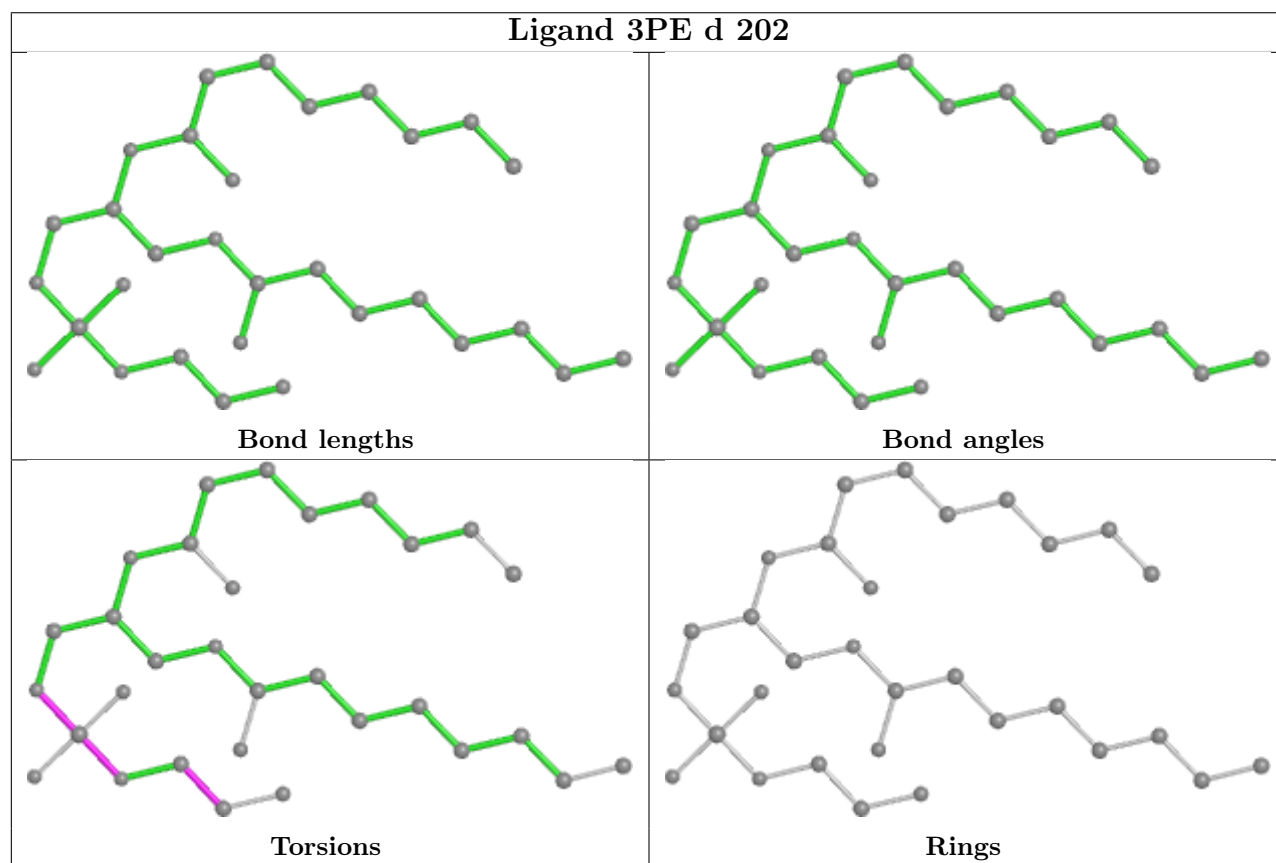
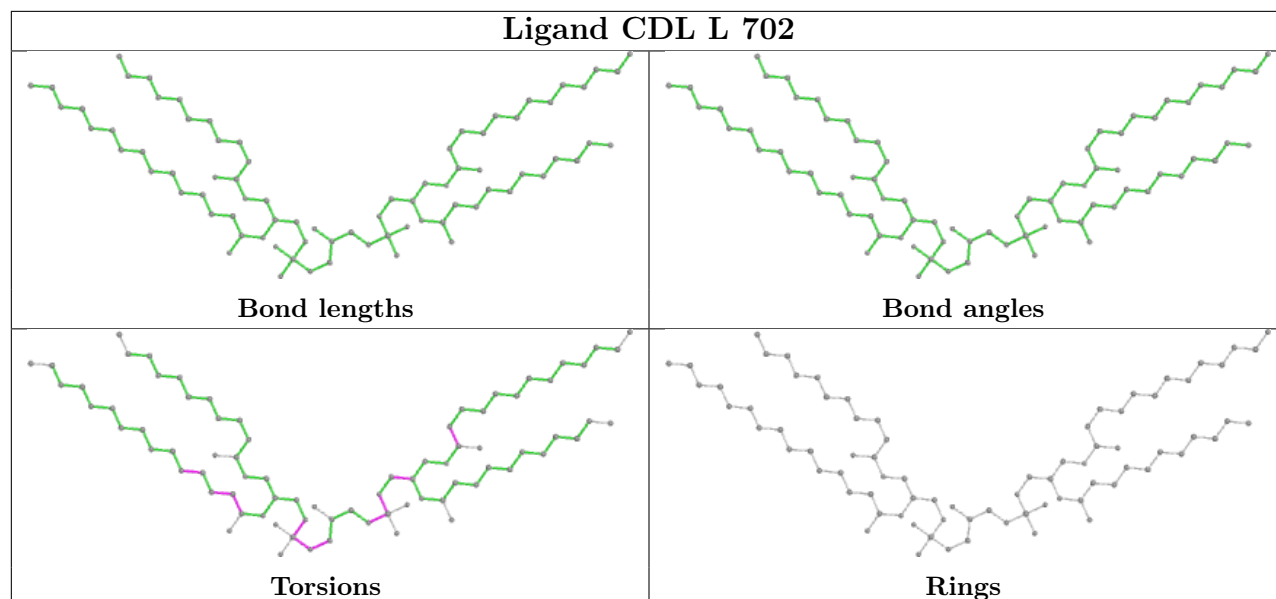
No monomer is involved in short contacts.

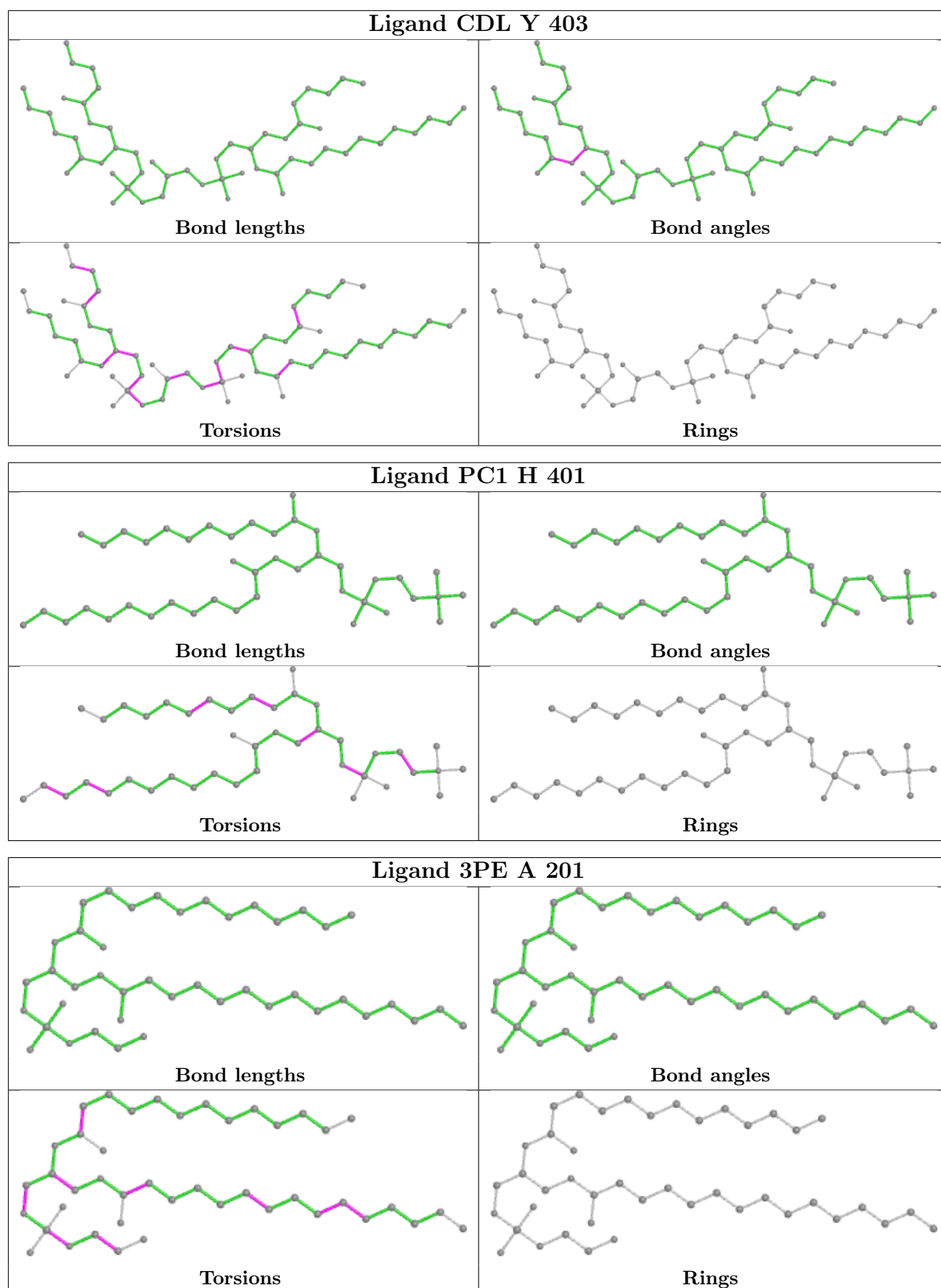
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

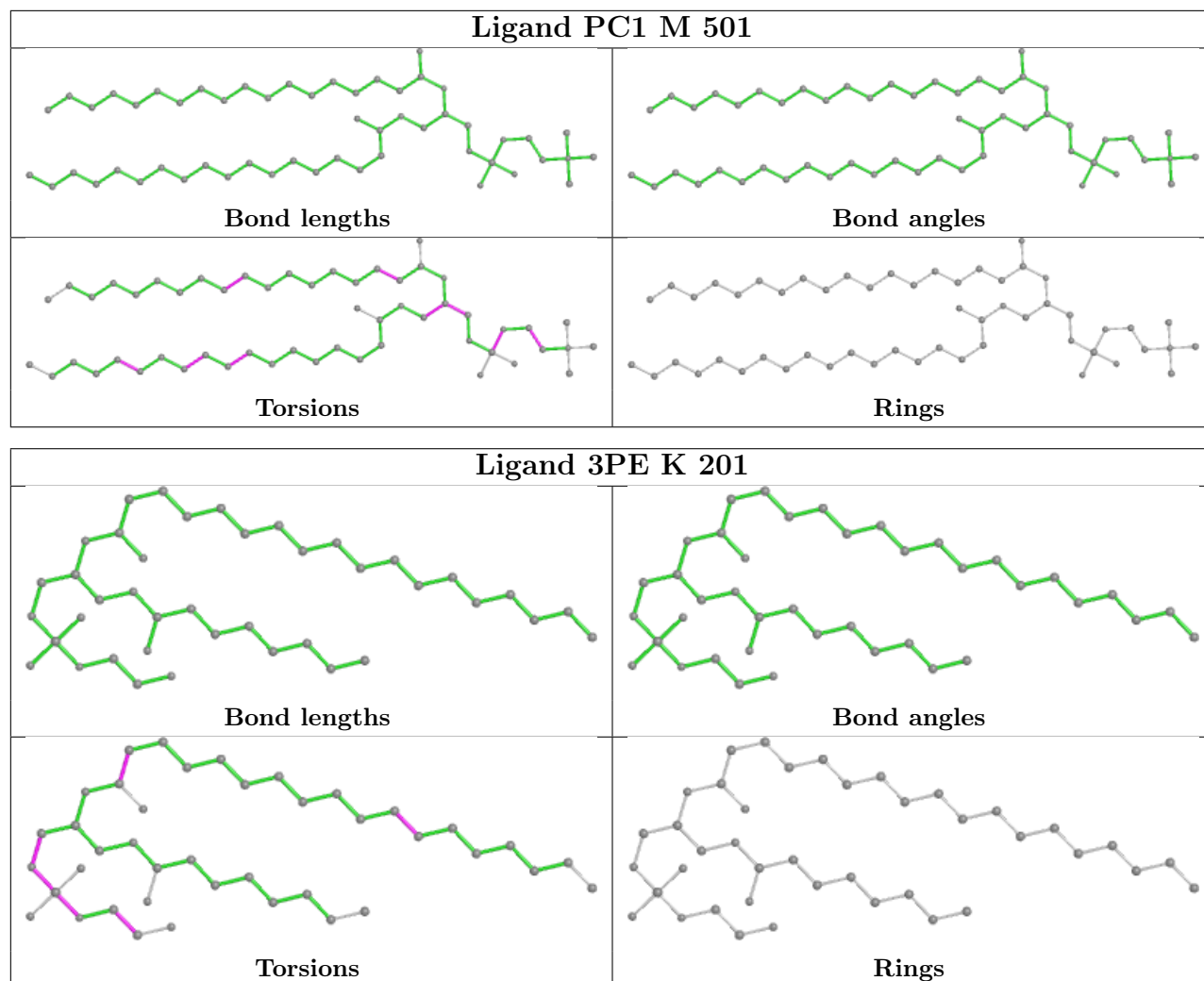


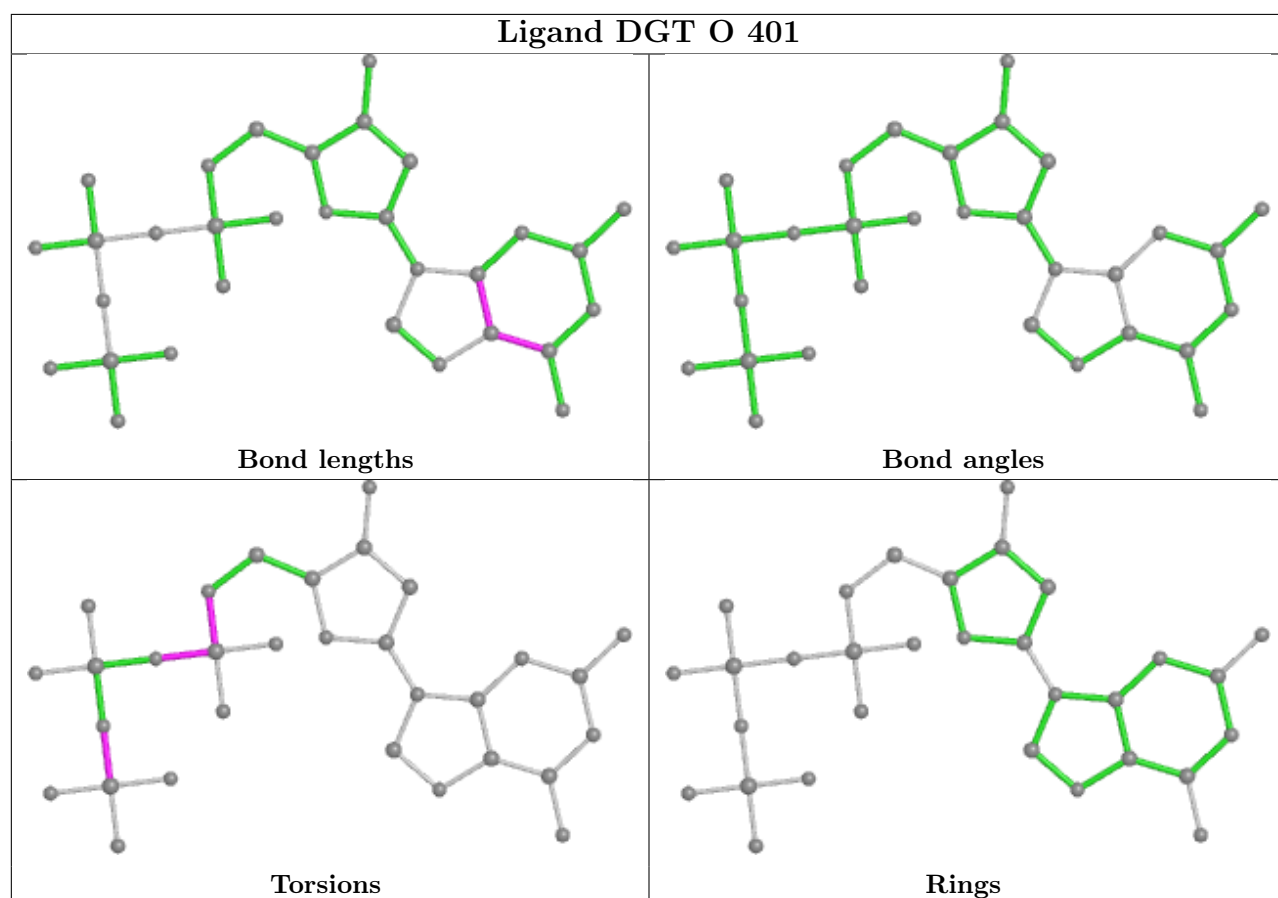
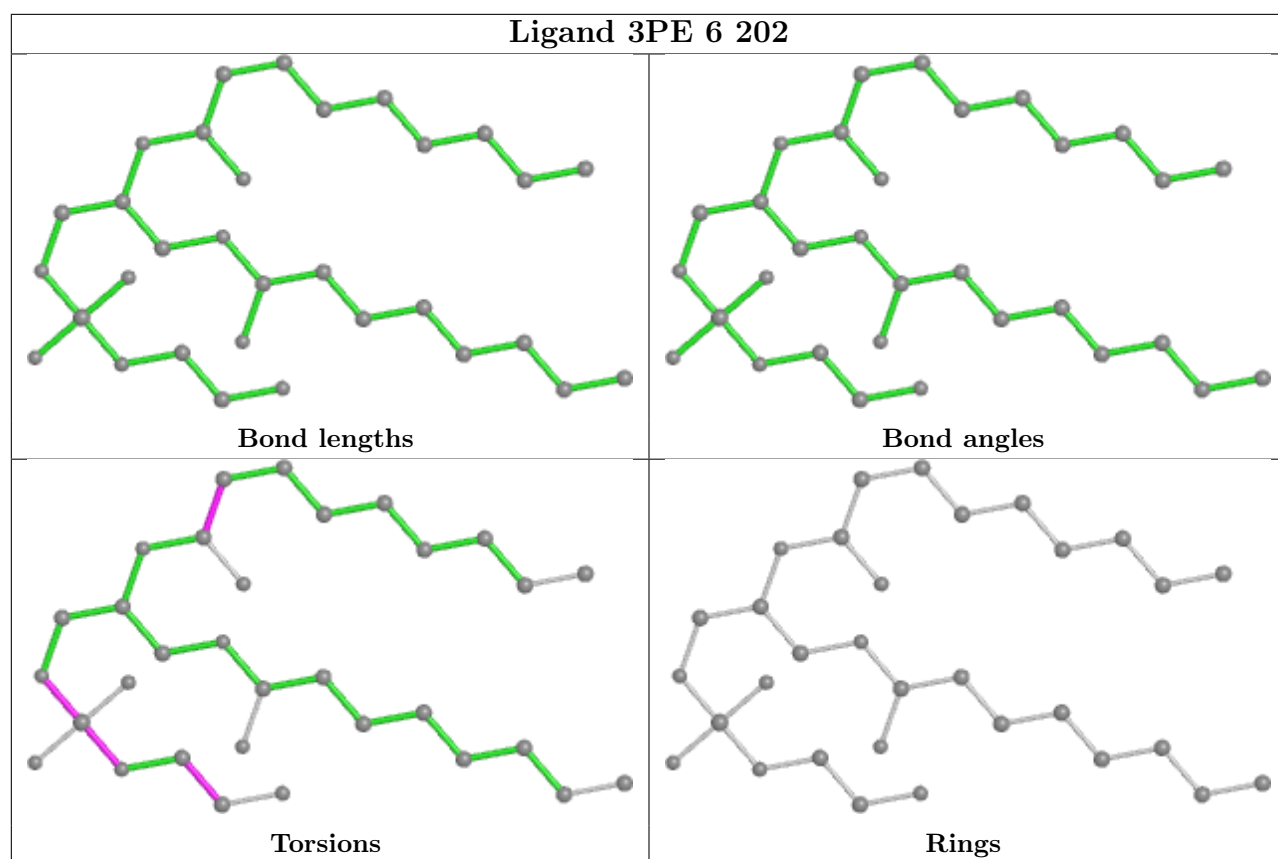


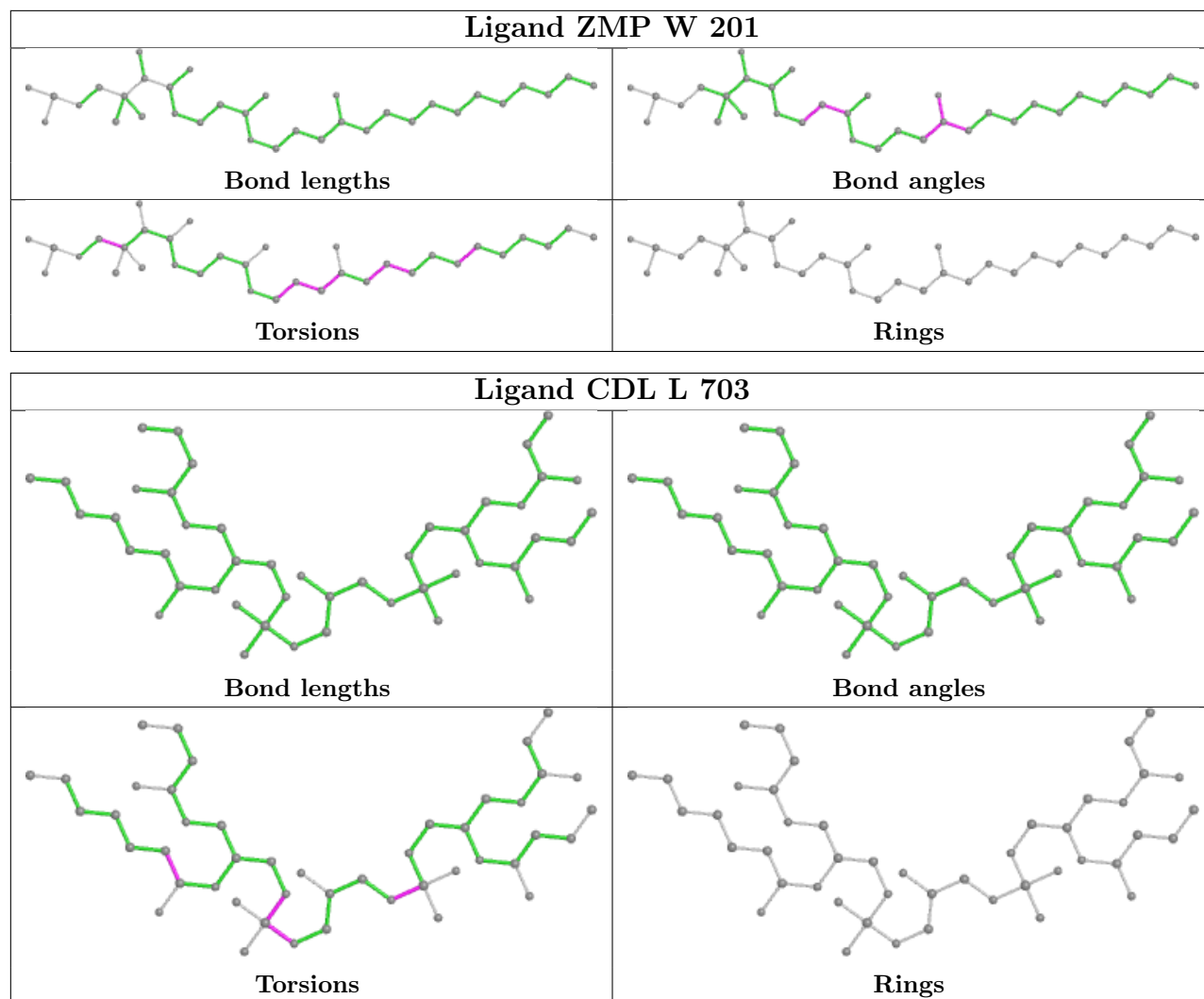


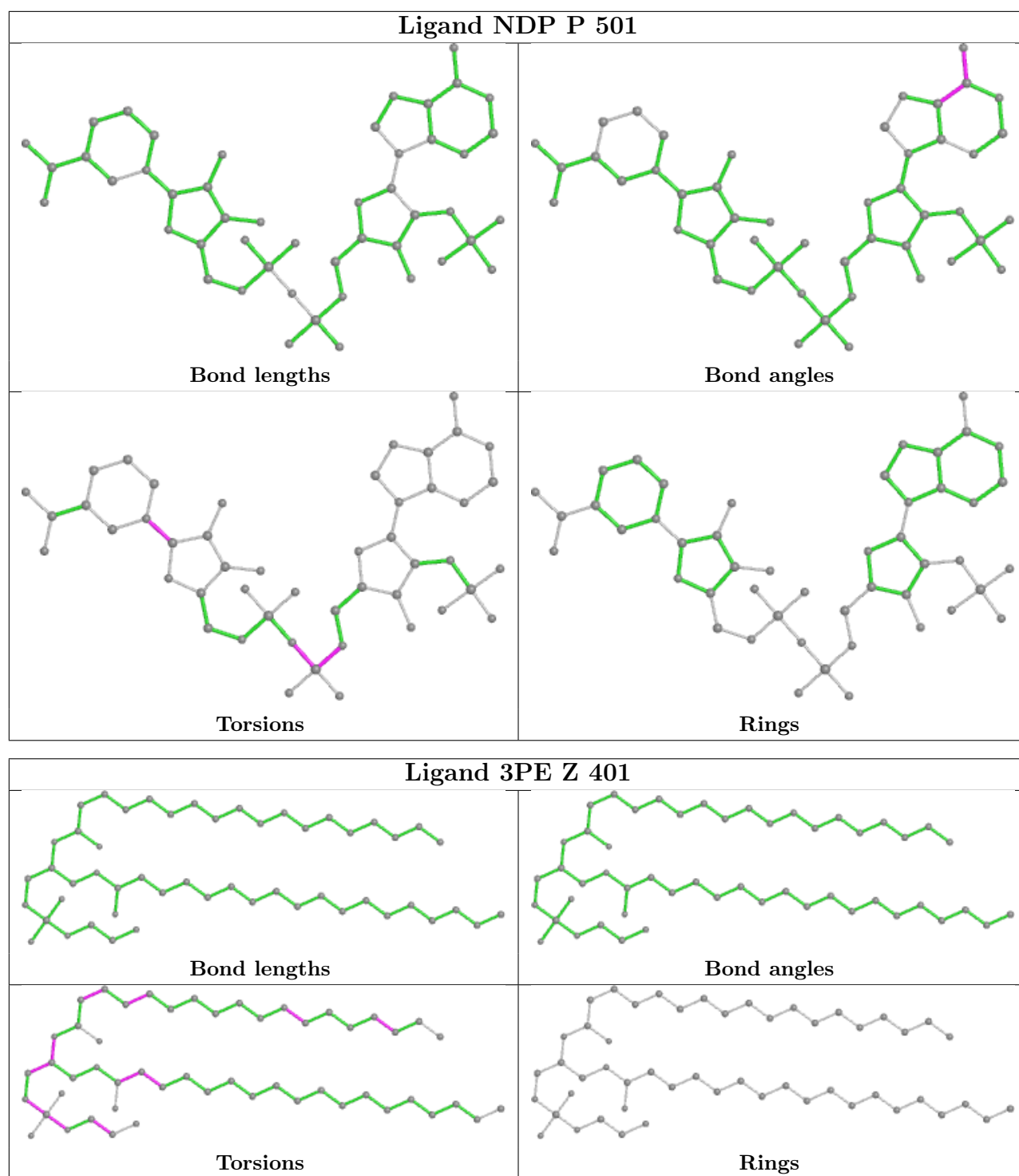




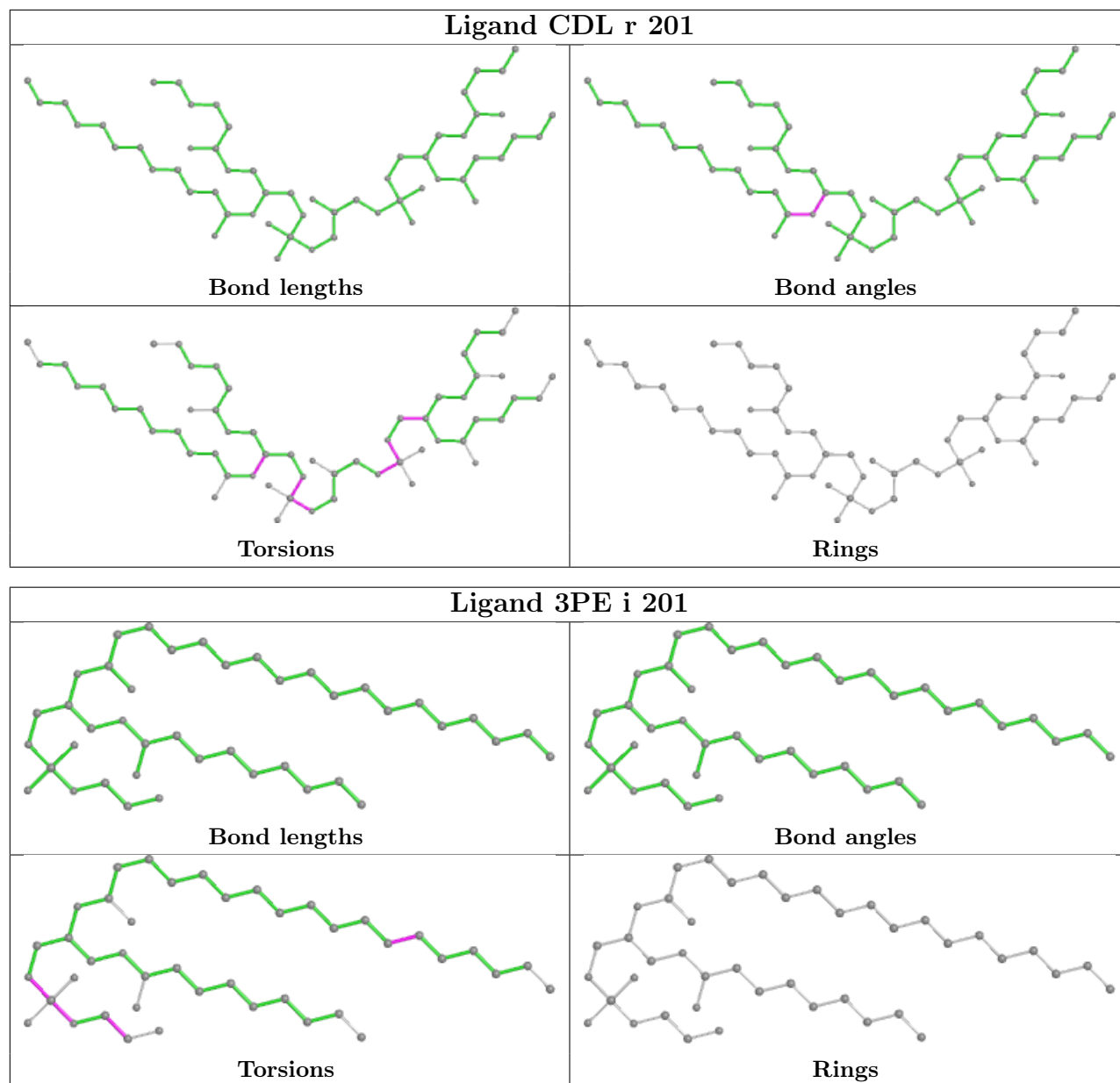


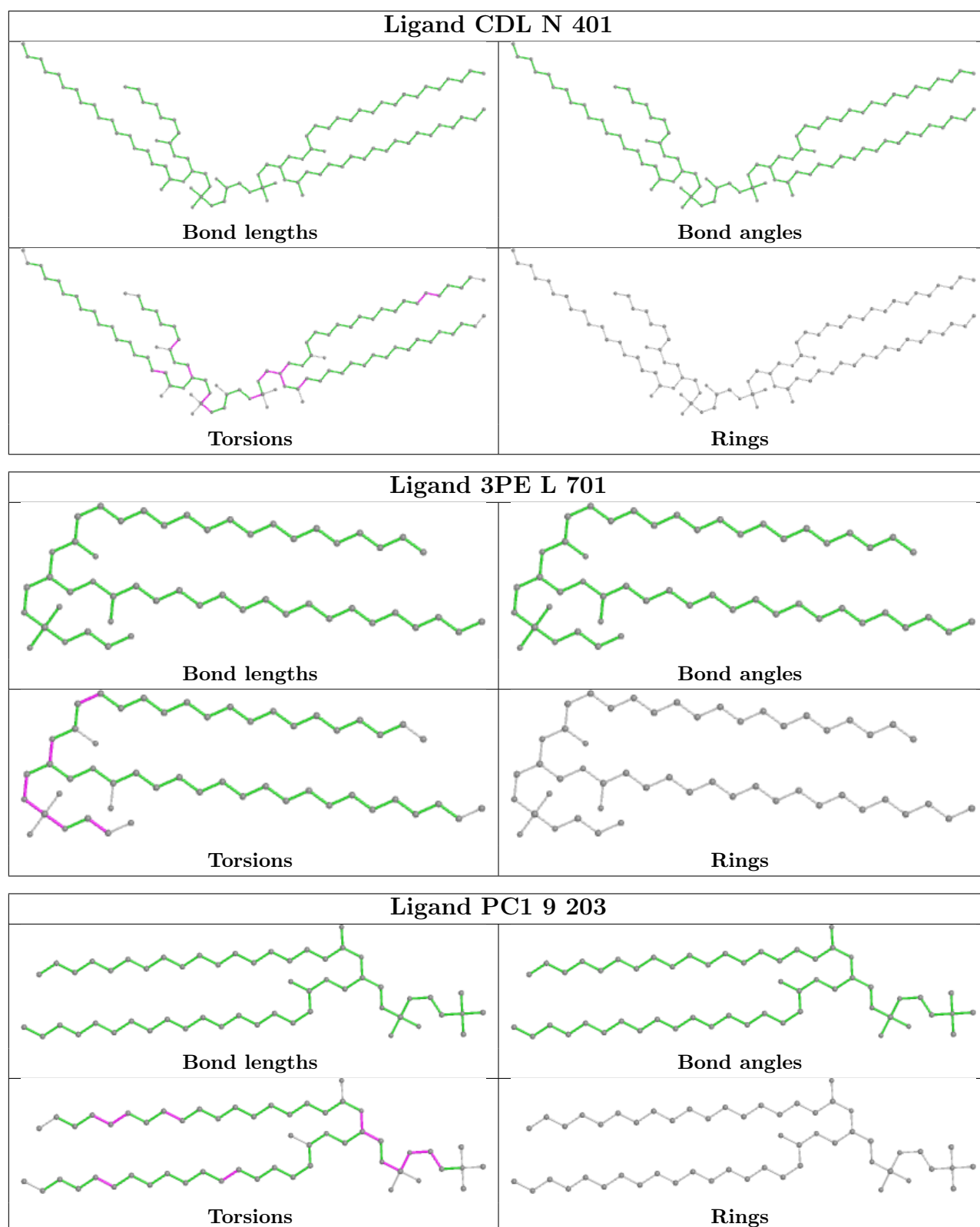


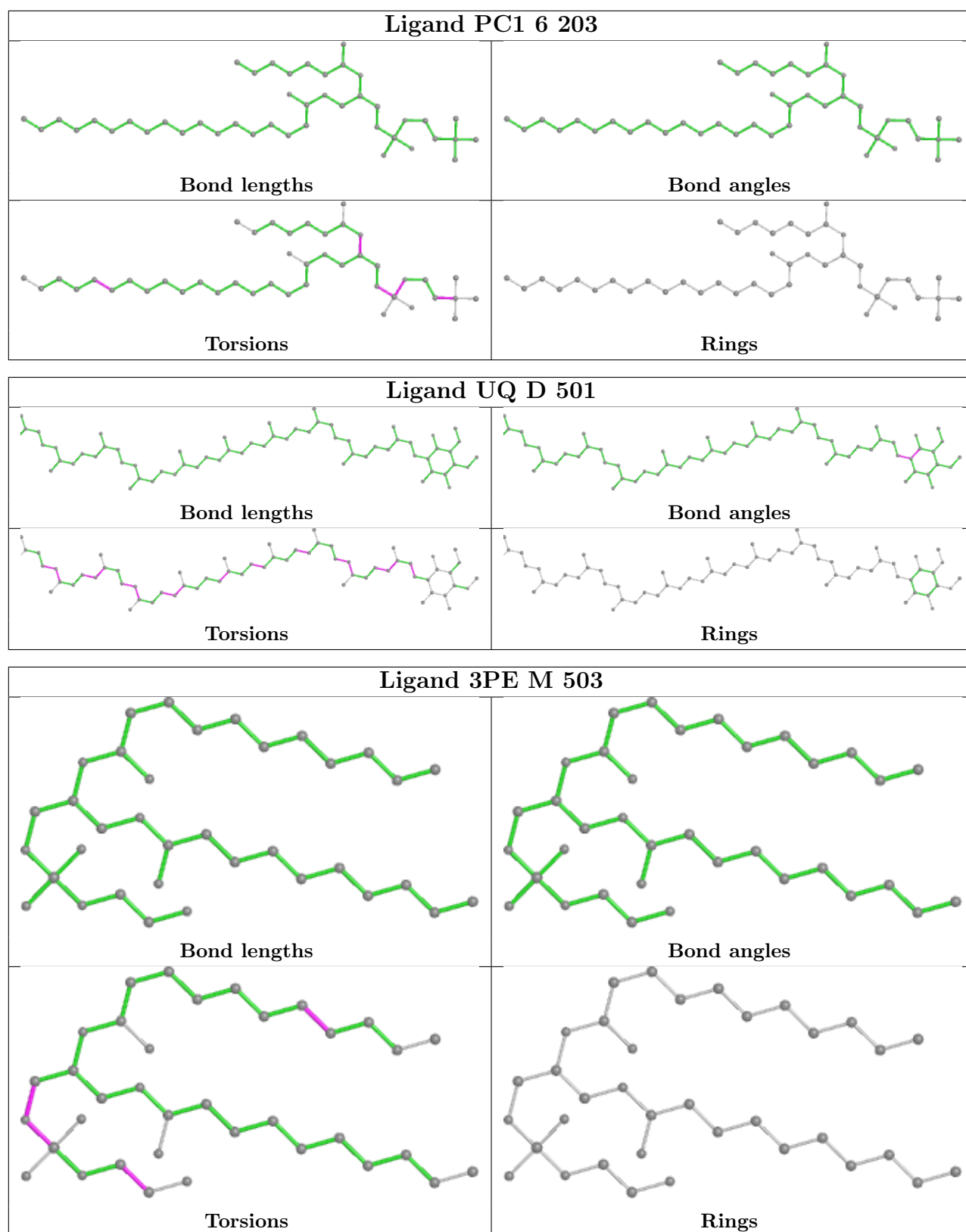


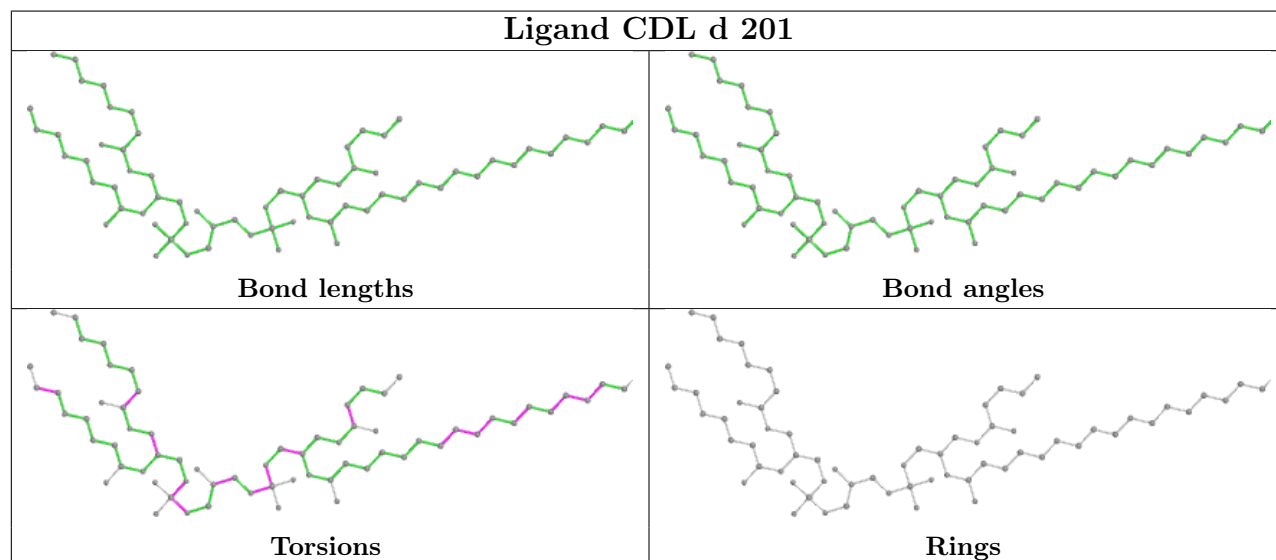
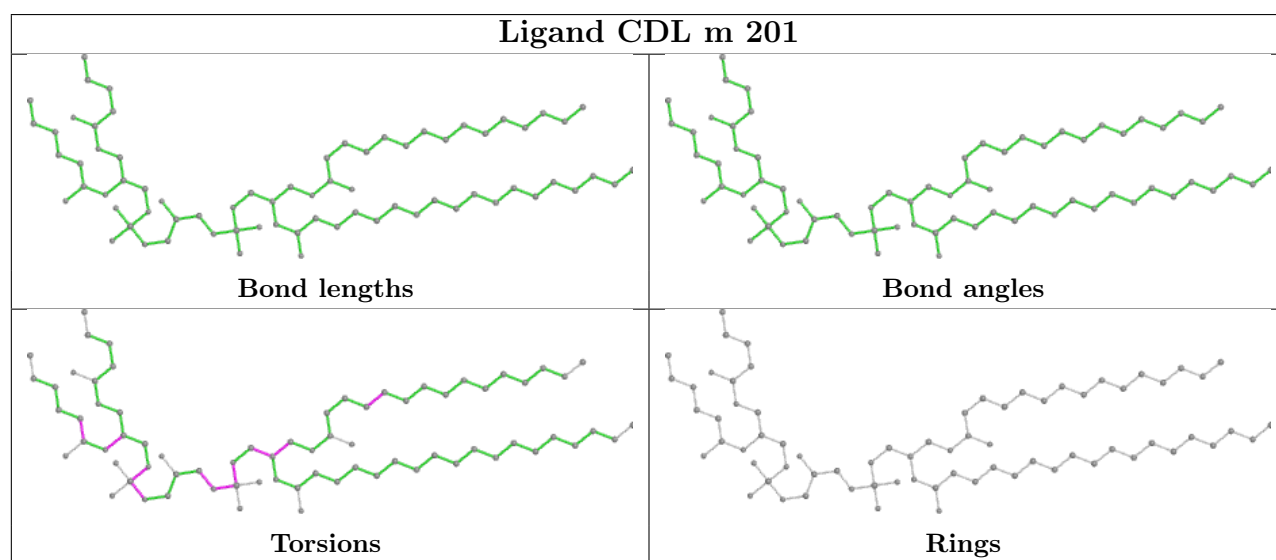
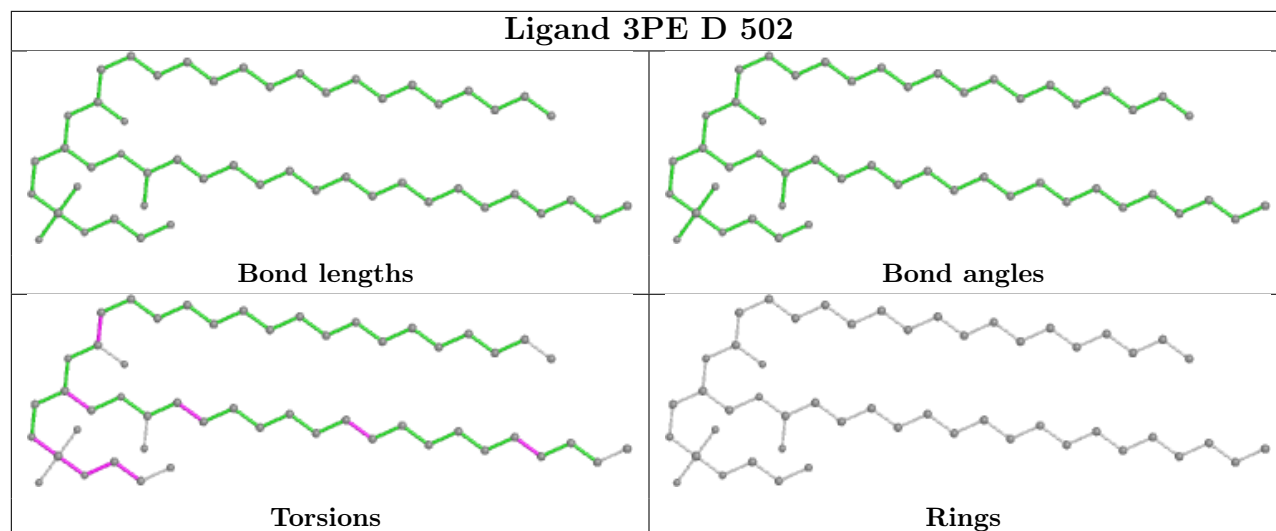


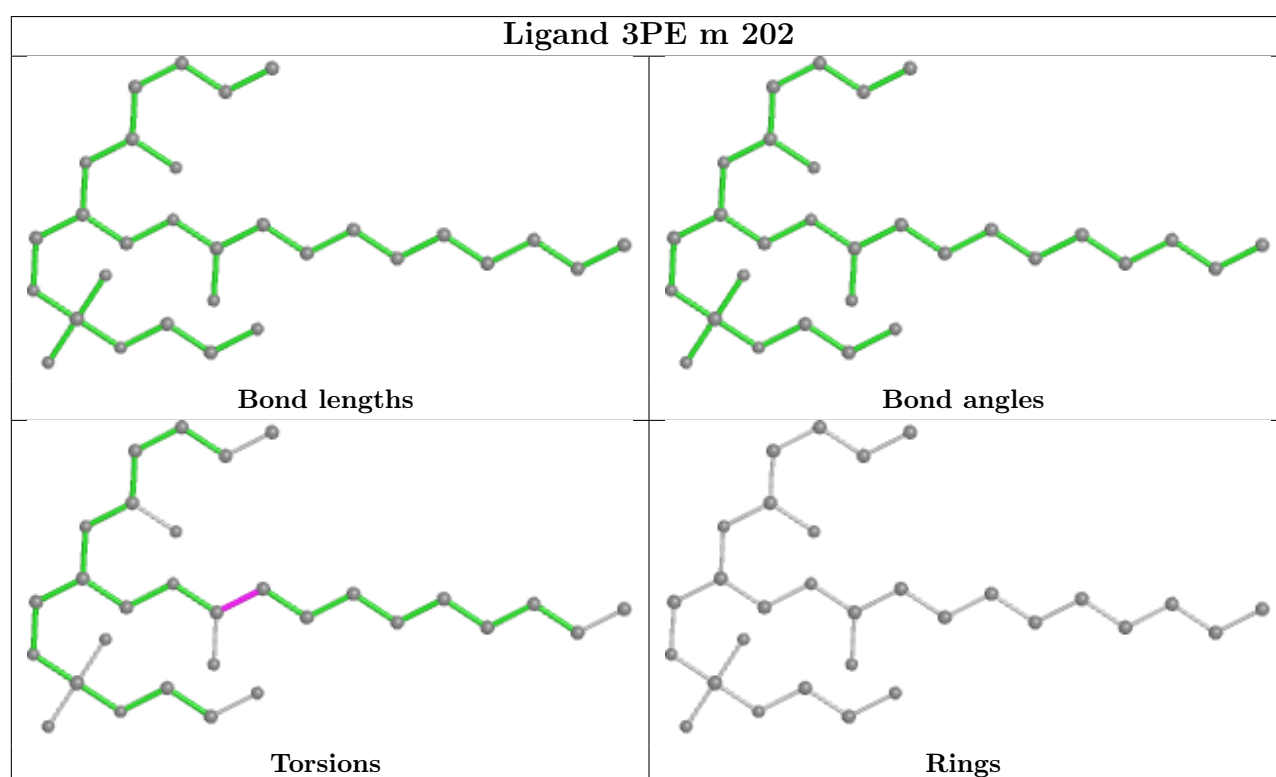
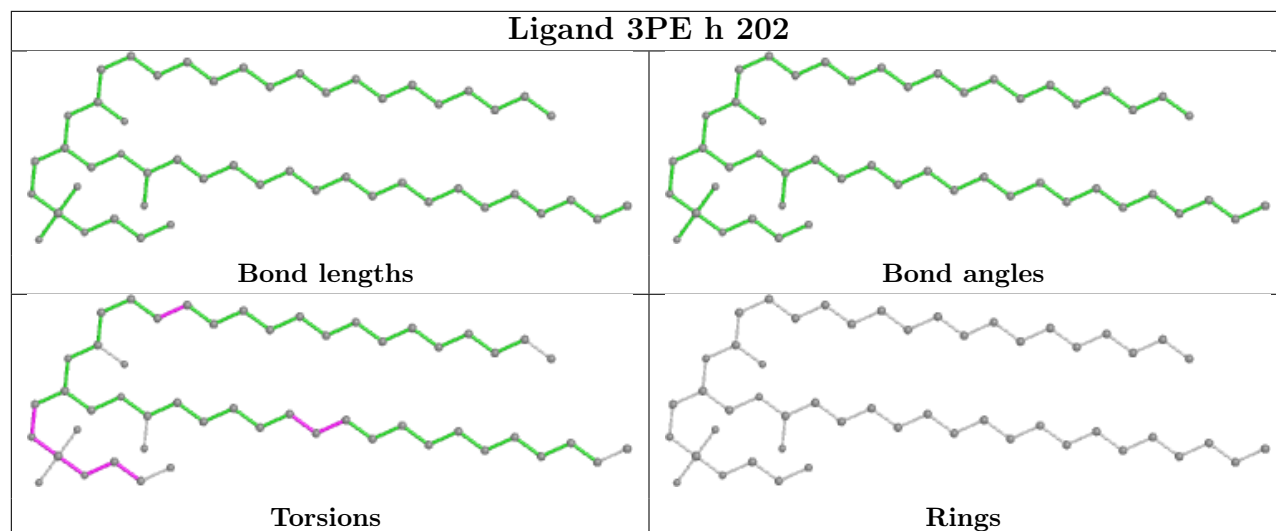


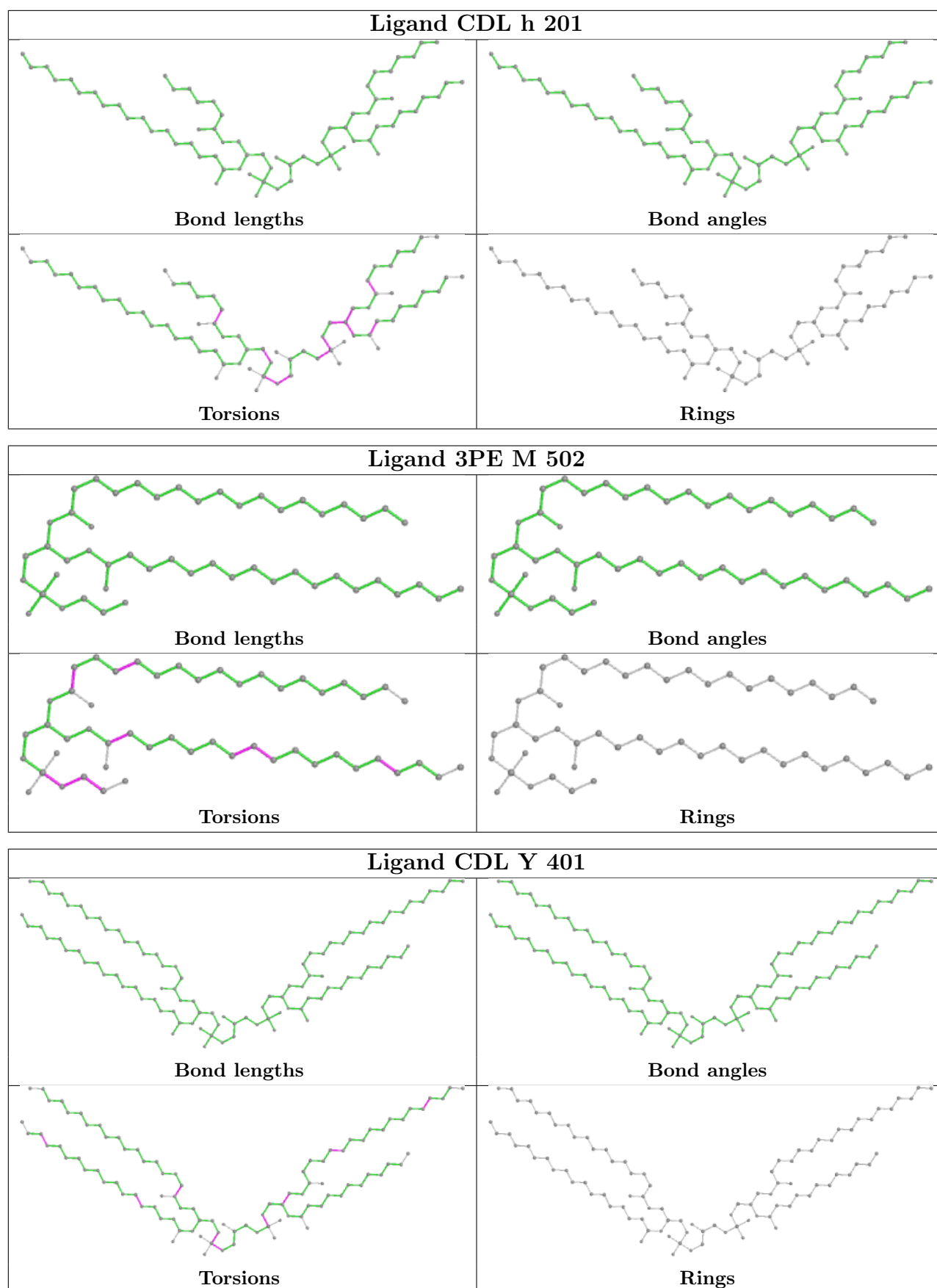


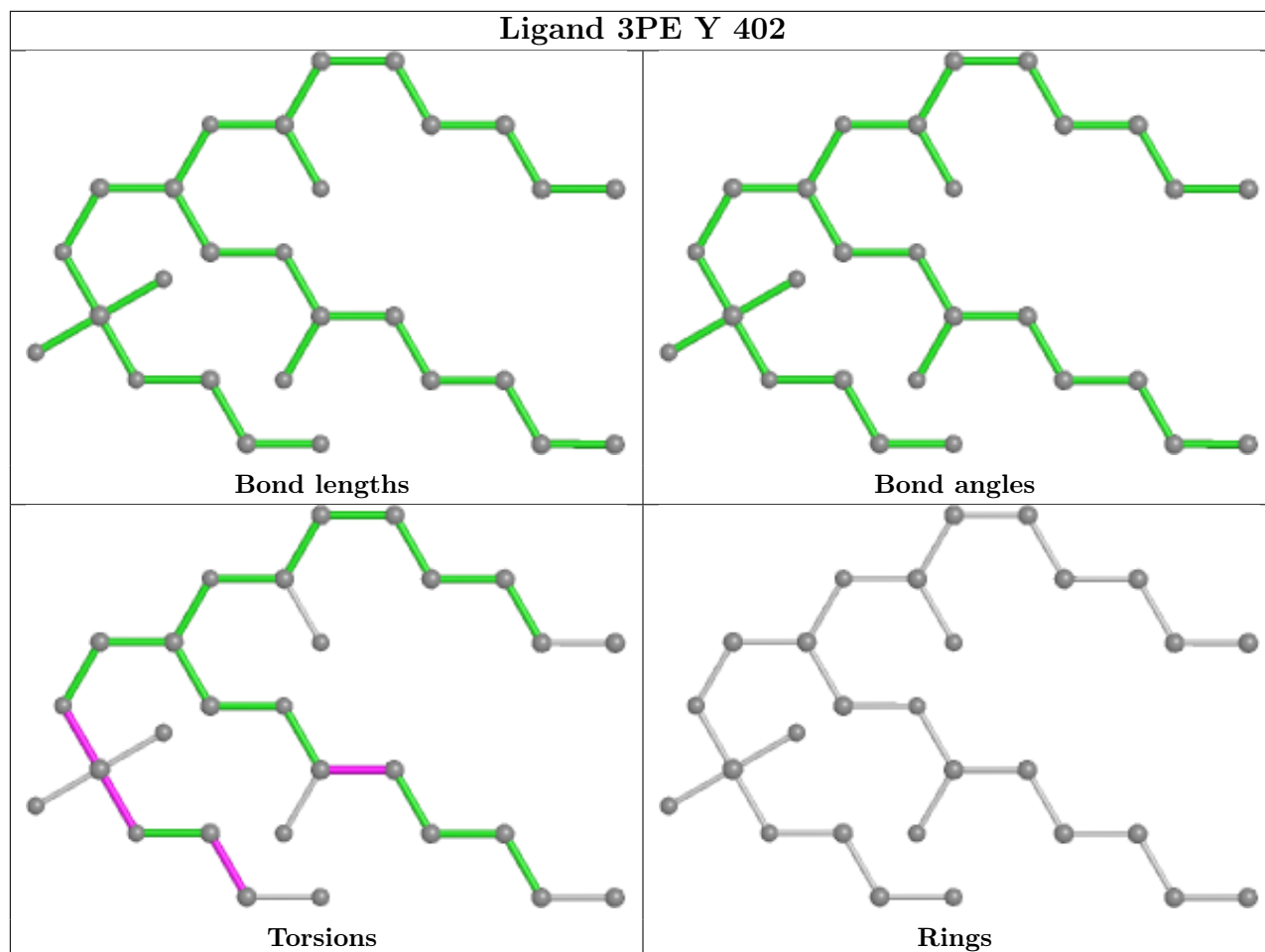












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
5	1	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	67:GLY	C	68:ARG	N	0.94

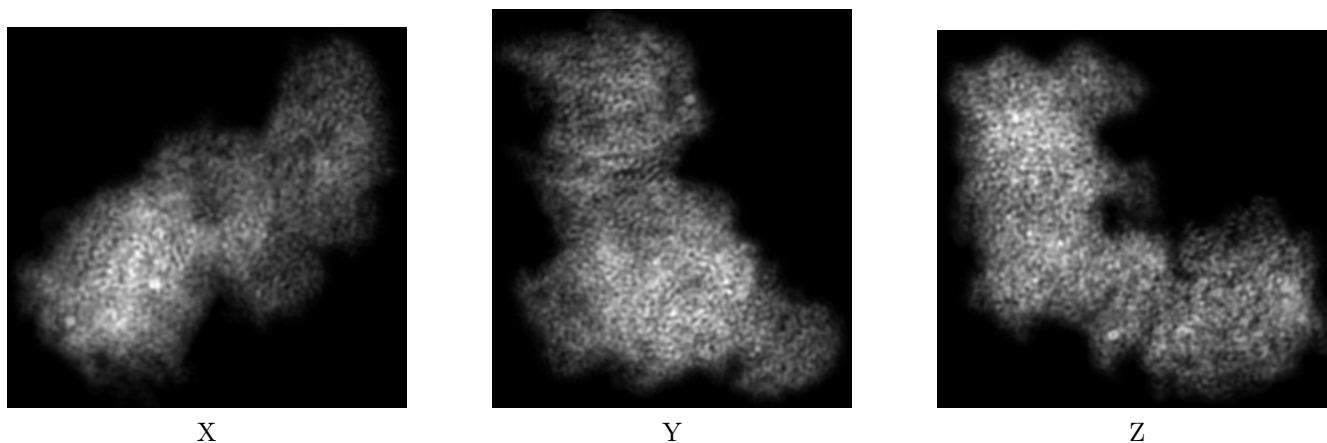
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19145. 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](#)

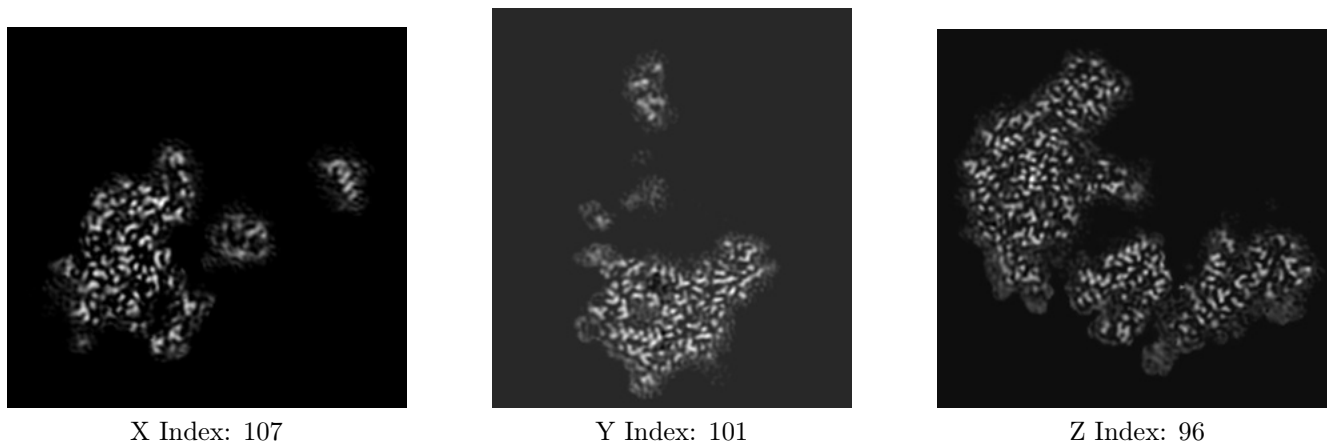
#### 6.1.1 Primary map



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

### 6.2 Central slices [i](#)

#### 6.2.1 Primary map

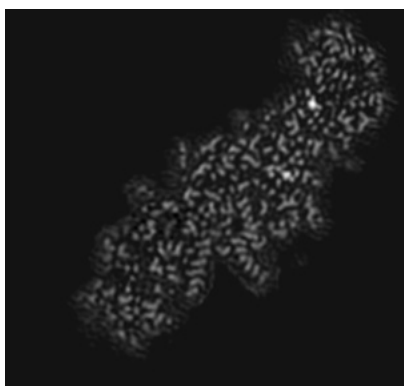




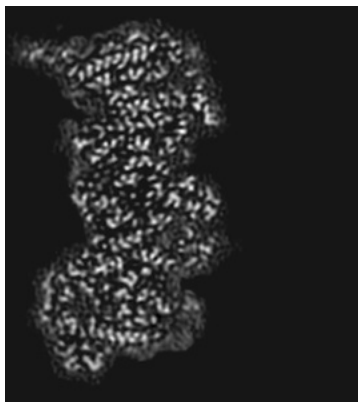
The images above show central slices of the map in three orthogonal directions.

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

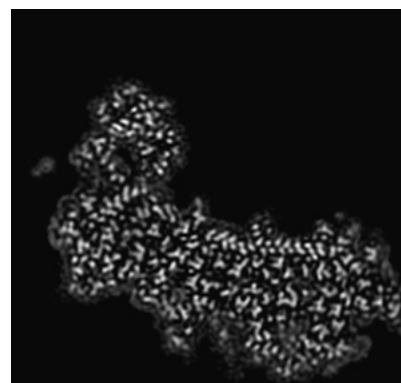
### 6.3.1 Primary map



X Index: 41



Y Index: 63

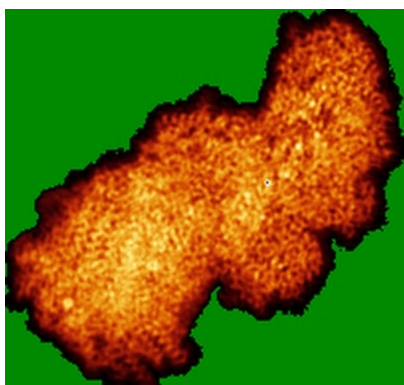


Z Index: 63

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

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

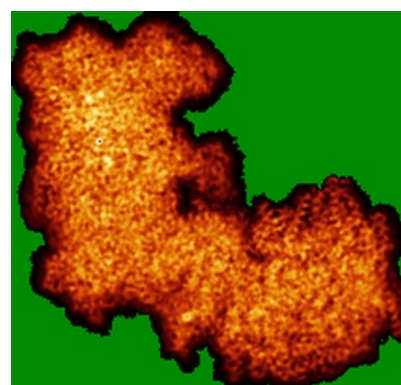
### 6.4.1 Primary map



X



Y

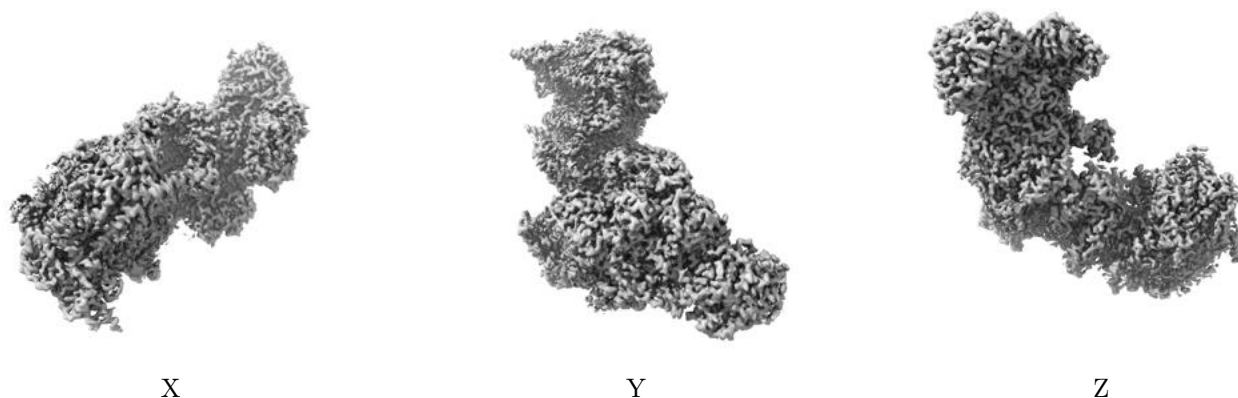


Z

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.

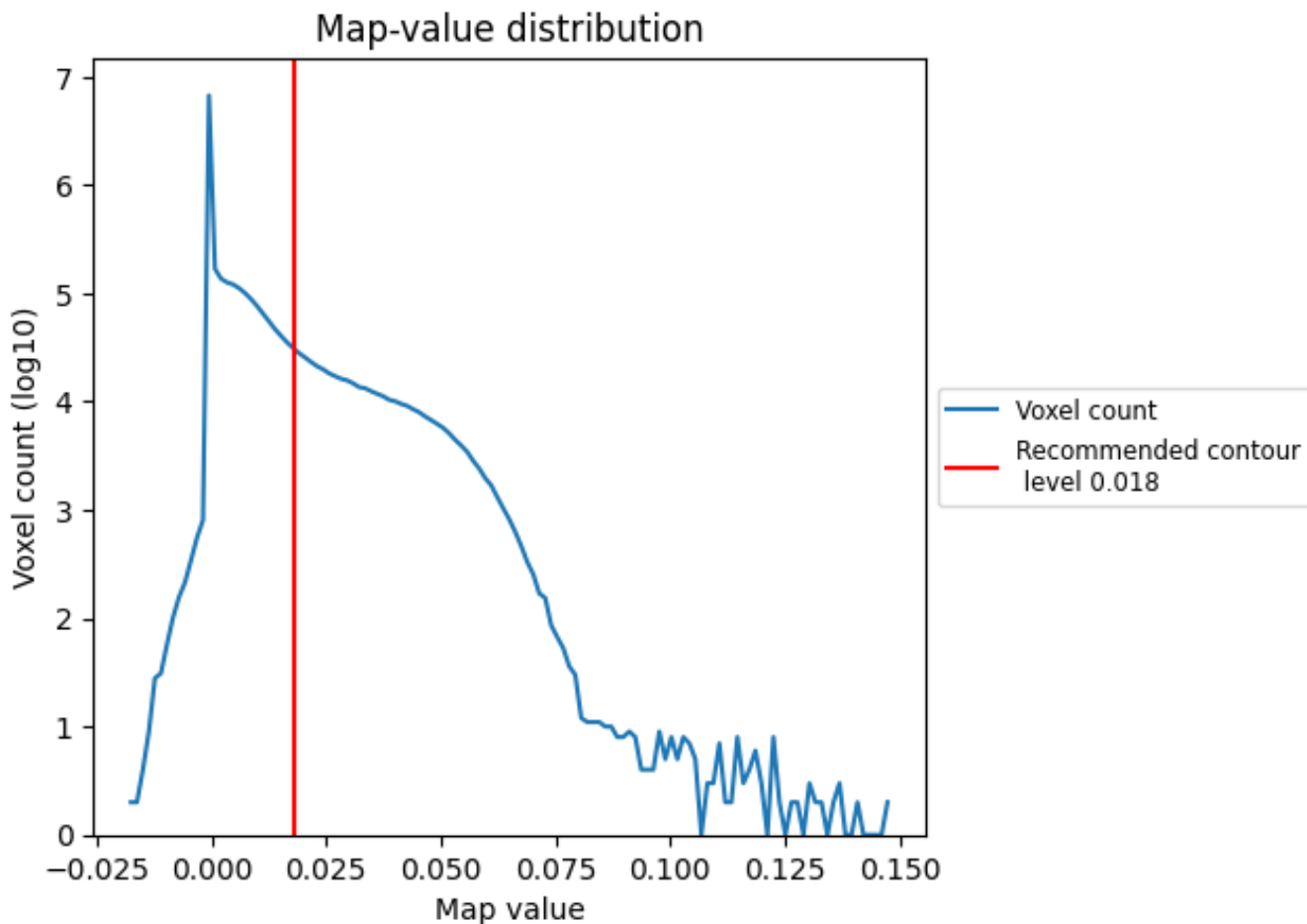
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

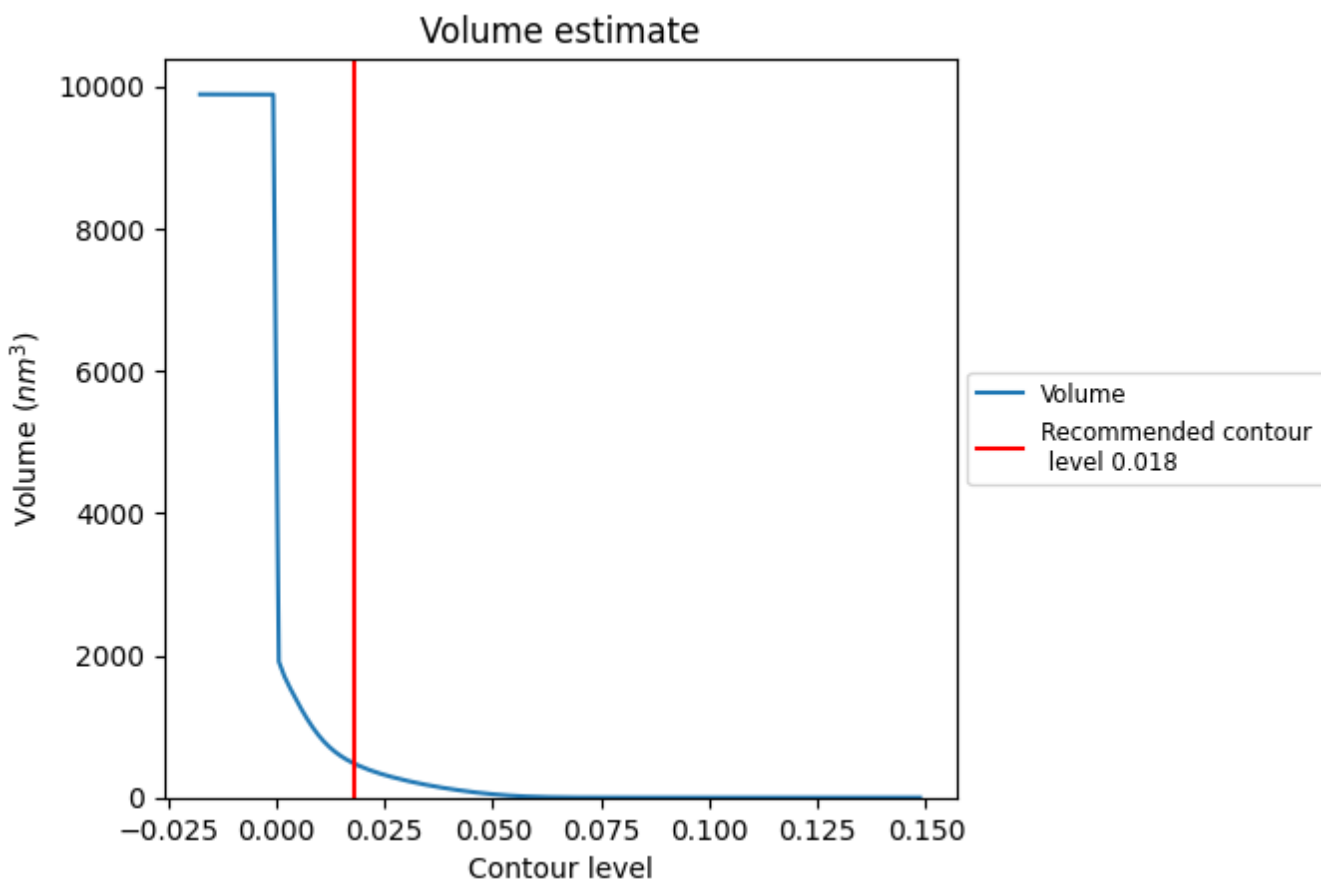
This section contains the results of statistical analysis of the map.

### 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 479 nm<sup>3</sup>; this corresponds to an approximate mass of 433 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.

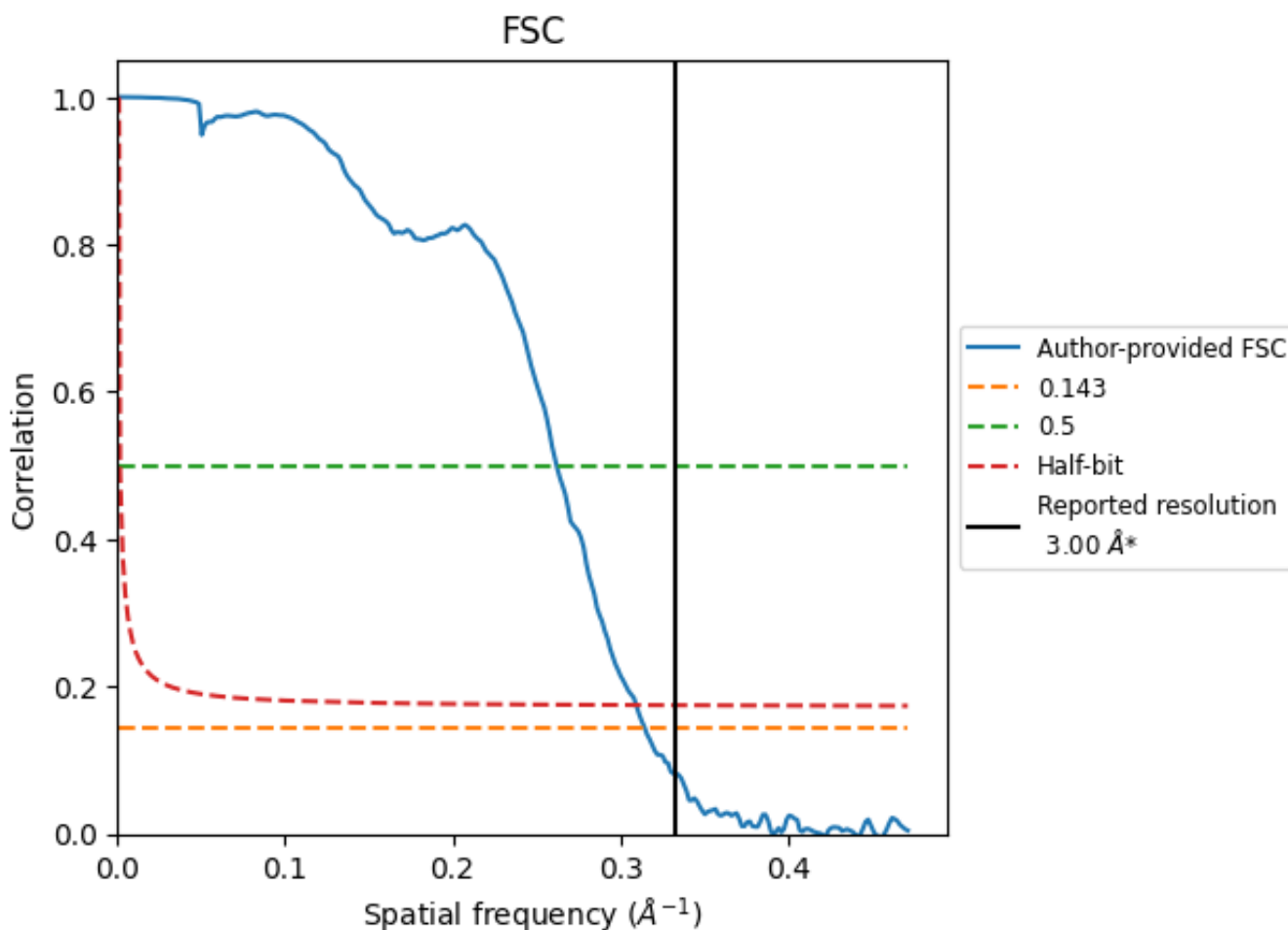
## 7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

## 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 0.333 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

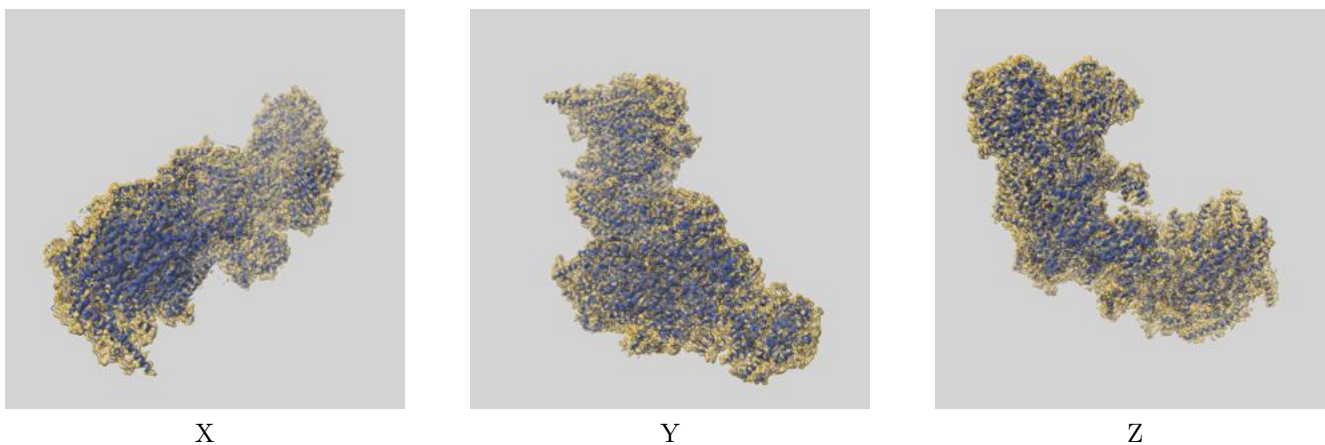
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.18	3.82	3.23
Unmasked-calculated*	-	-	-

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

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

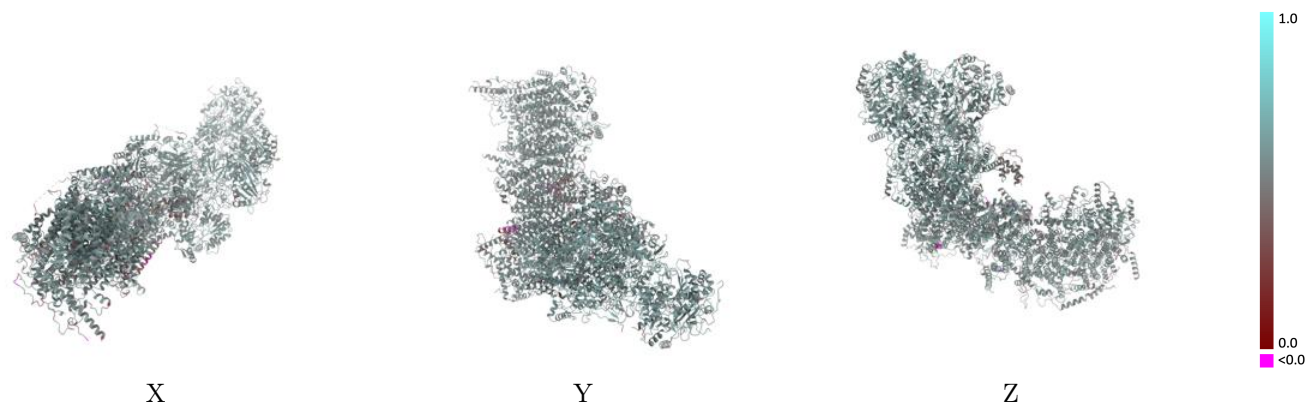
This section contains information regarding the fit between EMDB map EMD-19145 and PDB model 8RGP. Per-residue inclusion information can be found in section 3 on page 20.

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



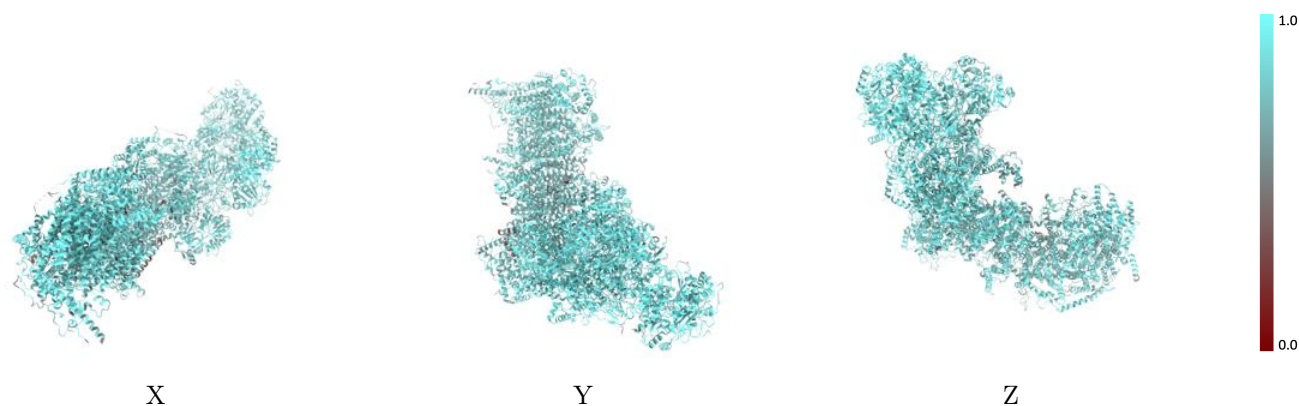
The images above show the 3D surface view of the map at the recommended contour level 0.018 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

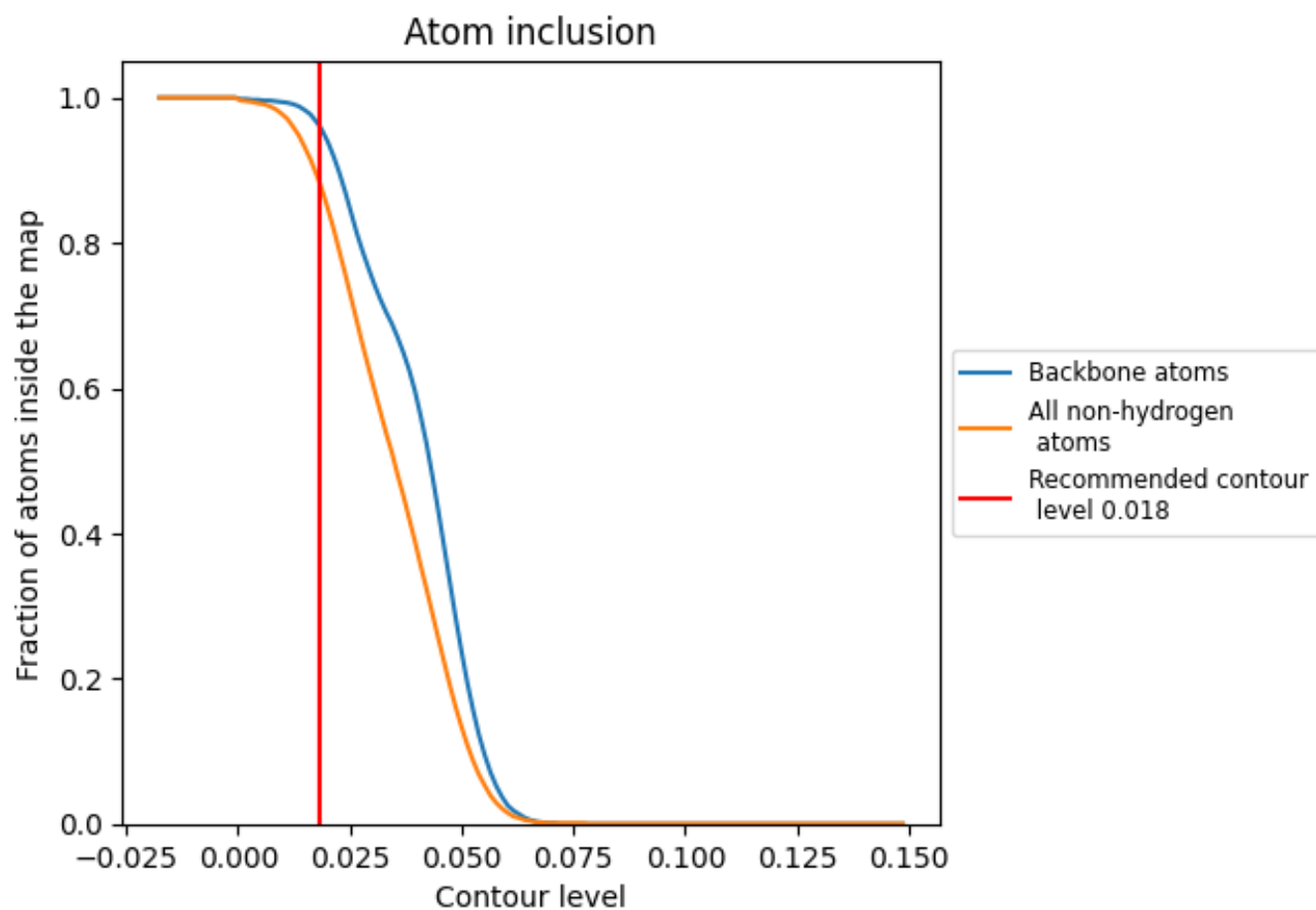
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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, 96% of all backbone atoms, 89% 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	 0.8870	 0.5450
1	 0.9190	 0.5650
2	 0.9040	 0.5490
3	 0.9090	 0.5620
6	 0.9440	 0.5730
7	 0.9140	 0.5630
9	 0.9340	 0.5780
A	 0.8790	 0.5470
C	 0.9390	 0.5860
D	 0.8860	 0.5460
H	 0.9090	 0.5490
J	 0.7760	 0.4630
K	 0.8710	 0.5380
L	 0.8910	 0.5450
M	 0.9020	 0.5640
N	 0.9020	 0.5550
O	 0.8970	 0.5430
P	 0.8910	 0.5610
Q	 0.8940	 0.5730
S	 0.8880	 0.5410
T	 0.7260	 0.4370
U	 0.8540	 0.5220
V	 0.9020	 0.5580
W	 0.8960	 0.5610
X	 0.8850	 0.5310
Y	 0.7650	 0.4720
Z	 0.8700	 0.5390
a	 0.9200	 0.5490
b	 0.8840	 0.5260
c	 0.8420	 0.5180
d	 0.8610	 0.5440
e	 0.8700	 0.5280
f	 0.8130	 0.4970
g	 0.8480	 0.5230
h	 0.8830	 0.5480



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Chain	Atom inclusion	Q-score
i	 0.8180	 0.5000
j	 0.8520	 0.4990
k	 0.8830	 0.5320
l	 0.8810	 0.5450
m	 0.7870	 0.5130
n	 0.9030	 0.5420
o	 0.8570	 0.5160
p	 0.8830	 0.5310
q	 0.9230	 0.5600
r	 0.8890	 0.5540
s	 0.9370	 0.5740