



## Full wwPDB EM Validation Report ⓘ

Mar 18, 2025 – 04:20 pm GMT

PDB ID : 8QBY  
EMDB ID : EMD-18324  
Title : Respiratory complex I from *Paracoccus denitrificans* in MSP2N2 nanodiscs  
Authors : Ivanov, B.S.; Bridges, H.R.; Hirst, J.  
Deposited on : 2023-08-25  
Resolution : 2.30 Å (reported)  
Based on initial model : .

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.dev117  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.41

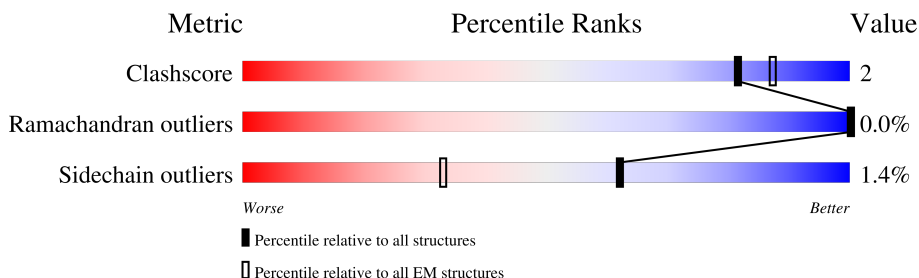
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.30 Å.

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



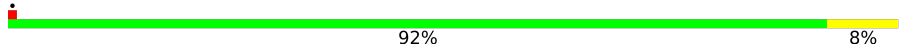
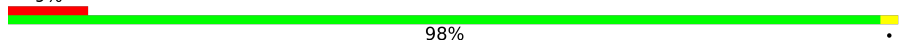
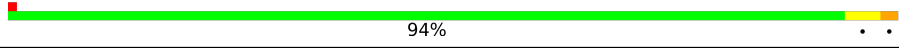
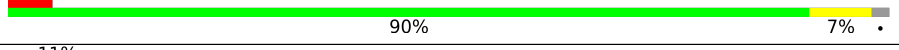

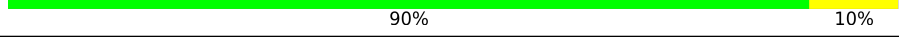
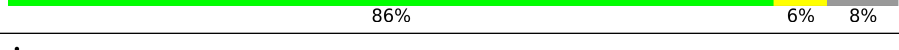
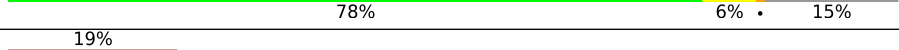
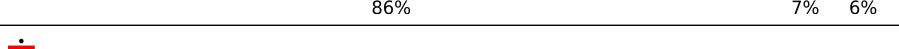
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	K	101	
2	G	674	
3	t	217	
4	I	163	
5	E	239	
6	N	499	
7	H	345	
8	F	431	

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Mol	Chain	Length	Quality of chain
9	D	412	
10	q	124	
11	A	121	
12	J	200	
13	R	62	
14	Q	103	
15	C	208	
16	B	175	
17	L	703	
18	M	513	

## 2 Entry composition

There are 31 unique types of molecules in this entry. The entry contains 42542 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-quinone oxidoreductase subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	K	101	Total	C	N	O	S	0	0
			763	508	123	127	5		

- Molecule 2 is a protein called NADH-quinone oxidoreductase.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	666	Total	C	N	O	S	0	0
			5073	3152	918	970	33		

- Molecule 3 is a protein called Protein-L-isoaspartate O-methyltransferase.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	t	216	Total	C	N	O	S	0	0
			1641	1033	294	305	9		

- Molecule 4 is a protein called NADH-quinone oxidoreductase subunit I.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	I	159	Total	C	N	O	S	0	0
			1294	820	227	236	11		

- Molecule 5 is a protein called NADH dehydrogenase subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	236	Total	C	N	O	S	0	0
			1814	1151	312	338	13		

- Molecule 6 is a protein called NADH-quinone oxidoreductase subunit N.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	N	479	Total	C	N	O	S	0	0
			3549	2337	564	616	32		

- Molecule 7 is a protein called NADH-quinone oxidoreductase subunit H.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	342	Total	C	N	O	S	0	0
			2730	1853	414	440	23		

- Molecule 8 is a protein called NADH-quinone oxidoreductase subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	F	421	Total	C	N	O	S	0	0
			3234	2023	582	598	31		

- Molecule 9 is a protein called NADH-quinone oxidoreductase subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	D	410	Total	C	N	O	S	0	0
			3268	2068	581	597	22		

- Molecule 10 is a protein called NADH:ubiquinone oxidoreductase 17.2 kD subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	q	124	Total	C	N	O	S	0	0
			1025	655	182	187	1		

- Molecule 11 is a protein called NADH-quinone oxidoreductase subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	A	121	Total	C	N	O	S	0	0
			968	658	141	163	6		

- Molecule 12 is a protein called NADH-quinone oxidoreductase chain 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	J	195	Total	C	N	O	S	0	0
			1498	996	241	249	12		

- Molecule 13 is a protein called Zinc finger CHCC-type domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	R	59	Total	C	N	O	S	0	0
			470	294	86	87	3		

- Molecule 14 is a protein called ETC complex I subunit conserved region.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Q	103	Total	C	N	O	S	0	0
			848	523	167	155	3		

- Molecule 15 is a protein called NADH-quinone oxidoreductase subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	C	191	Total	C	N	O	S	0	0
			1565	1005	271	287	2		

- Molecule 16 is a protein called NADH-quinone oxidoreductase subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	B	148	Total	C	N	O	S	0	0
			1161	734	207	207	13		

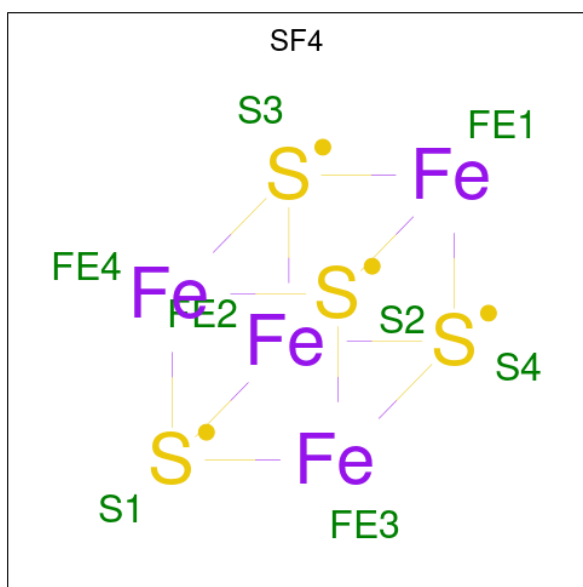
- Molecule 17 is a protein called NADH dehydrogenase subunit L.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	L	659	Total	C	N	O	S	0	0
			5198	3463	851	851	33		

- Molecule 18 is a protein called NADH dehydrogenase subunit M.

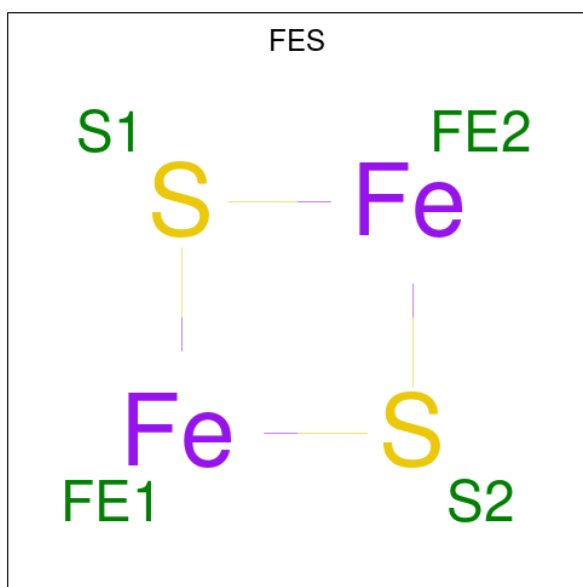
Mol	Chain	Residues	Atoms					AltConf	Trace
18	M	503	Total	C	N	O	S	0	0
			3913	2614	610	657	32		

- Molecule 19 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



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

- Molecule 20 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).



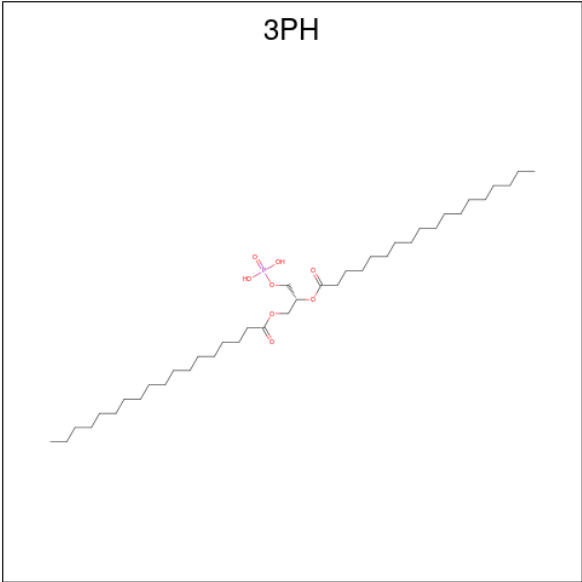
Mol	Chain	Residues	Atoms			AltConf
20	G	1	Total	Fe	S	0
			4	2	2	
20	E	1	Total	Fe	S	0
			4	2	2	

- Molecule 21 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
21	G	1	Total	Na	0
			1	1	

- Molecule 22 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (three-letter code: 3PH) (formula: C<sub>39</sub>H<sub>77</sub>O<sub>8</sub>P).





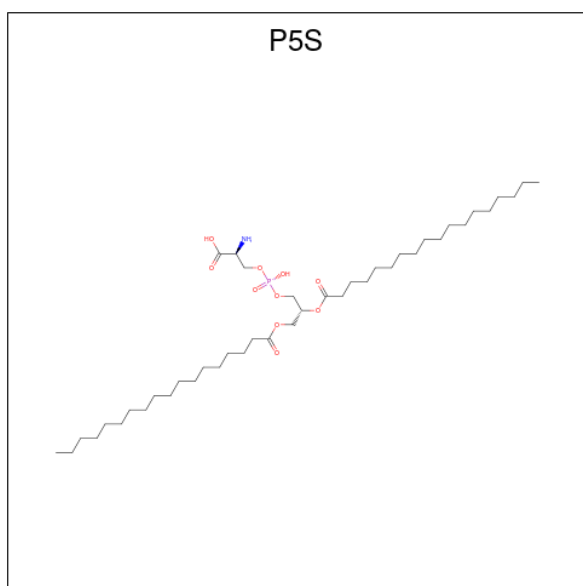
Mol	Chain	Residues	Atoms				AltConf
22	I	1	Total	C	O	P	0
			39	30	8	1	
22	N	1	Total	C	O	P	0
			46	37	8	1	
22	N	1	Total	C	O	P	0
			43	34	8	1	
22	H	1	Total	C	O	P	0
			36	27	8	1	
22	H	1	Total	C	O	P	0
			26	17	8	1	
22	H	1	Total	C	O	P	0
			30	21	8	1	
22	A	1	Total	C	O	P	0
			34	25	8	1	
22	J	1	Total	C	O	P	0
			32	23	8	1	
22	J	1	Total	C	O	P	0
			42	33	8	1	
22	L	1	Total	C	O	P	0
			47	38	8	1	
22	L	1	Total	C	O	P	0
			45	36	8	1	
22	L	1	Total	C	O	P	0
			36	27	8	1	
22	L	1	Total	C	O	P	0
			29	20	8	1	
22	M	1	Total	C	O	P	0
			31	22	8	1	

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Mol	Chain	Residues	Atoms				AltConf
22	M	1	Total	C	O	P	0
			33	24	8	1	
22	M	1	Total	C	O	P	0
			31	22	8	1	
22	M	1	Total	C	O	P	0
			33	24	8	1	

- Molecule 23 is O-[(R)-{[(2R)-2,3-bis(octadecanoyloxy)propyl]oxy}(hydroxy)phosphoryl]-L-serine (three-letter code: P5S) (formula: C<sub>42</sub>H<sub>82</sub>NO<sub>10</sub>P).

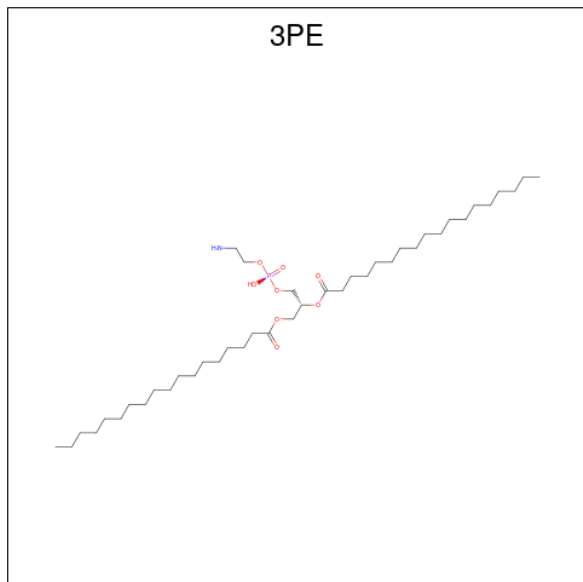


Mol	Chain	Residues	Atoms					AltConf
23	I	1	Total	C	N	O	P	0
			49	37	1	10	1	
23	L	1	Total	C	N	O	P	0
			40	28	1	10	1	

- Molecule 24 is CALCIUM ION (three-letter code: CA) (formula: Ca).

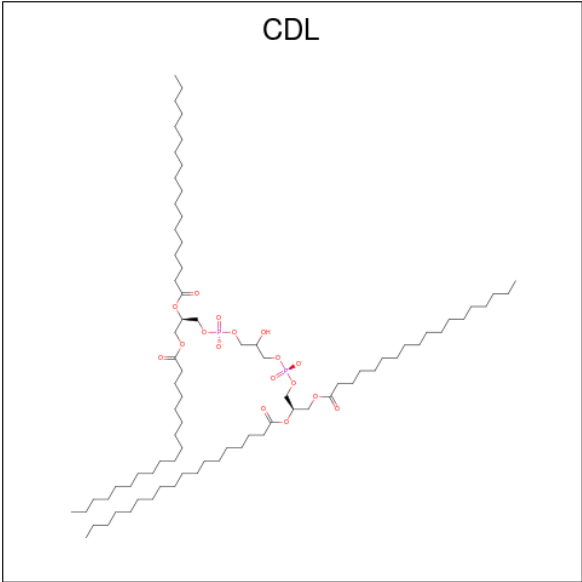
Mol	Chain	Residues	Atoms		AltConf
24	I	1	Total	Ca	0
			1	1	
24	N	1	Total	Ca	0
			1	1	
24	D	1	Total	Ca	0
			1	1	
24	M	1	Total	Ca	0
			1	1	

- Molecule 25 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula:  $C_{41}H_{82}NO_8P$ ).



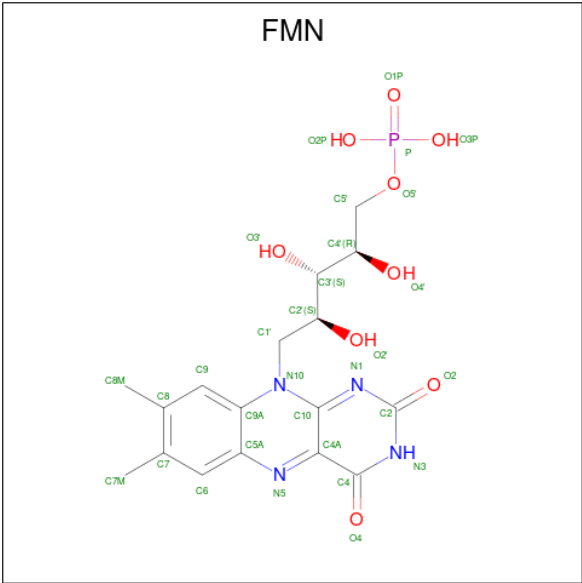
Mol	Chain	Residues	Atoms					AltConf
25	N	1	Total	C	N	O	P	0
			42	32	1	8	1	
25	N	1	Total	C	N	O	P	0
			48	38	1	8	1	
25	N	1	Total	C	N	O	P	0
			38	28	1	8	1	
25	H	1	Total	C	N	O	P	0
			43	33	1	8	1	
25	H	1	Total	C	N	O	P	0
			45	35	1	8	1	
25	q	1	Total	C	N	O	P	0
			36	26	1	8	1	
25	L	1	Total	C	N	O	P	0
			45	35	1	8	1	
25	M	1	Total	C	N	O	P	0
			42	32	1	8	1	
25	M	1	Total	C	N	O	P	0
			41	31	1	8	1	
25	M	1	Total	C	N	O	P	0
			29	19	1	8	1	

- Molecule 26 is CARDIOLIPIN (three-letter code: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ).



Mol	Chain	Residues	Atoms				AltConf
26	H	1	Total	C	O	P	0
			65	46	17	2	
26	M	1	Total	C	O	P	0
			65	46	17	2	

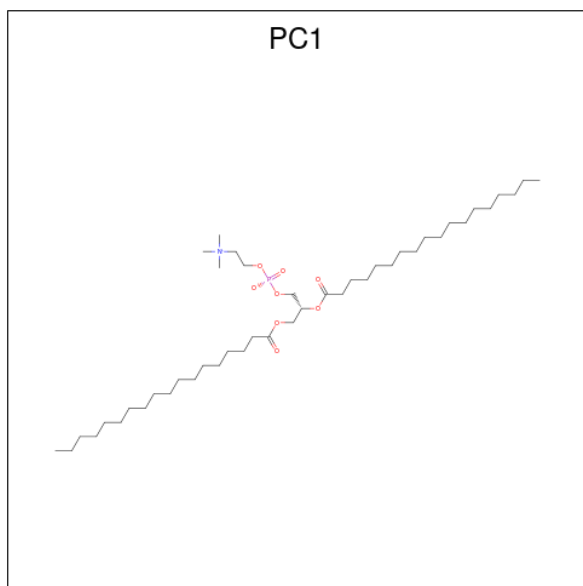
- Molecule 27 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C<sub>17</sub>H<sub>21</sub>N<sub>4</sub>O<sub>9</sub>P).



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

- Molecule 28 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code:

PC1) (formula:  $C_{44}H_{88}NO_8P$ ).

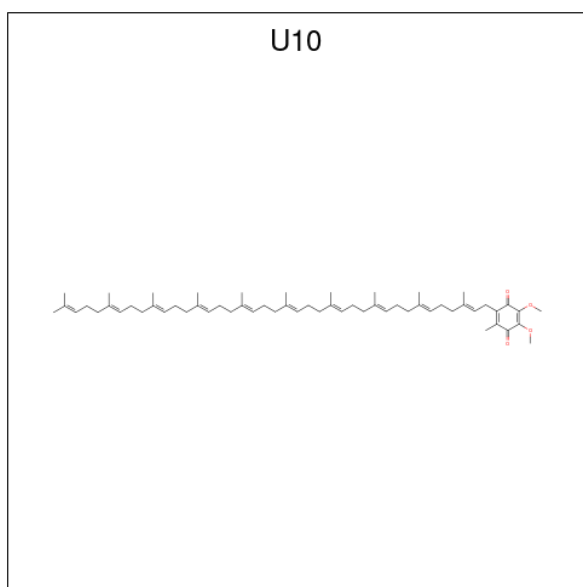


Mol	Chain	Residues	Atoms					AltConf
28	D	1	Total	C	N	O	P	0
			42	32	1	8	1	
28	J	1	Total	C	N	O	P	0
			45	35	1	8	1	

- Molecule 29 is ZINC ION (three-letter code: ZN) (formula:  $Zn$ ).

Mol	Chain	Residues	Atoms		AltConf
29	R	1	Total	Zn	0
			1	1	

- Molecule 30 is UBIQUINONE-10 (three-letter code: U10) (formula:  $C_{59}H_{90}O_4$ ).



Mol	Chain	Residues	Atoms			AltConf
30	B	1	Total	C	O	0
			29	25	4	

- Molecule 31 is water.

Mol	Chain	Residues	Atoms		AltConf
31	K	15	Total	O	0
			15	15	
31	G	220	Total	O	0
			220	220	
31	t	32	Total	O	0
			32	32	
31	I	75	Total	O	0
			75	75	
31	E	47	Total	O	0
			47	47	
31	N	61	Total	O	0
			61	61	
31	H	64	Total	O	0
			64	64	
31	F	70	Total	O	0
			70	70	
31	D	151	Total	O	0
			151	151	
31	q	22	Total	O	0
			22	22	
31	A	33	Total	O	0
			33	33	

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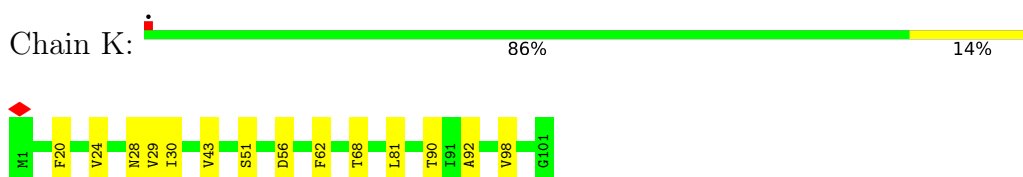
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Mol	Chain	Residues	Atoms		AltConf
31	J	35	Total 35	O 35	0
31	R	25	Total 25	O 25	0
31	Q	31	Total 31	O 31	0
31	C	73	Total 73	O 73	0
31	B	56	Total 56	O 56	0
31	L	16	Total 16	O 16	0
31	M	54	Total 54	O 54	0

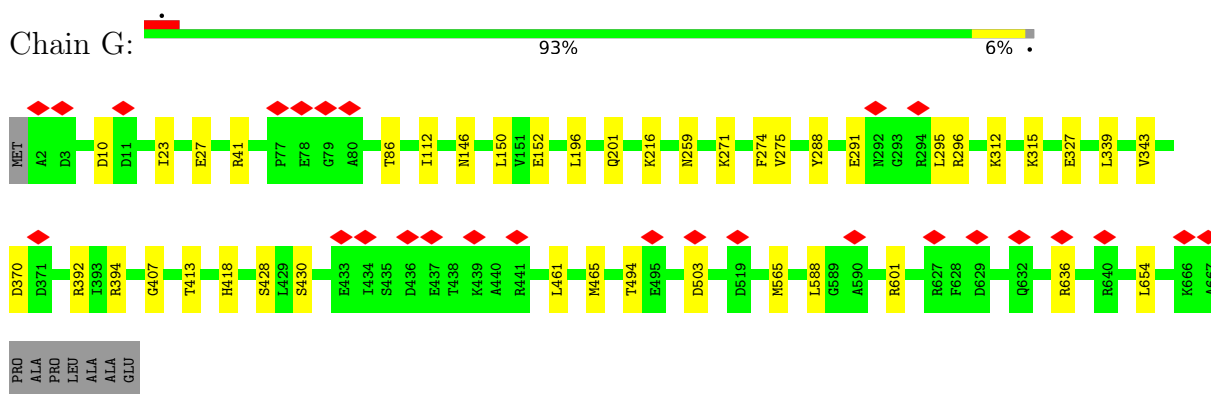
### 3 Residue-property plots [i](#)

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.

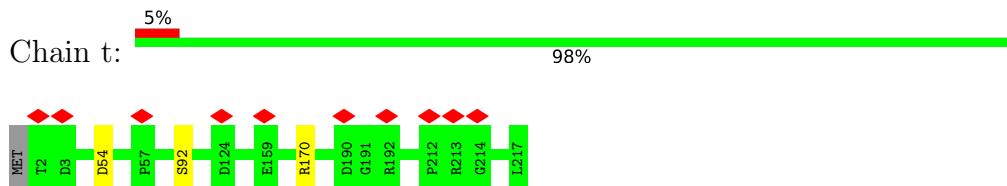
- Molecule 1: NADH-quinone oxidoreductase subunit K



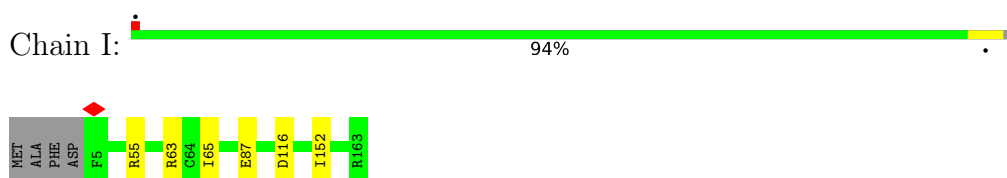
- Molecule 2: NADH-quinone oxidoreductase



- Molecule 3: Protein-L-isoaspartate O-methyltransferase




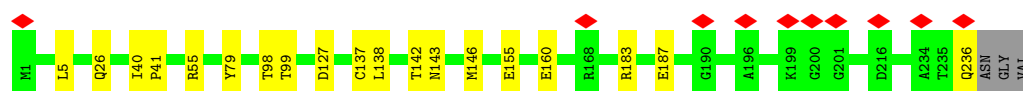
- Molecule 4: NADH-quinone oxidoreductase subunit I



- Molecule 5: NADH dehydrogenase subunit E

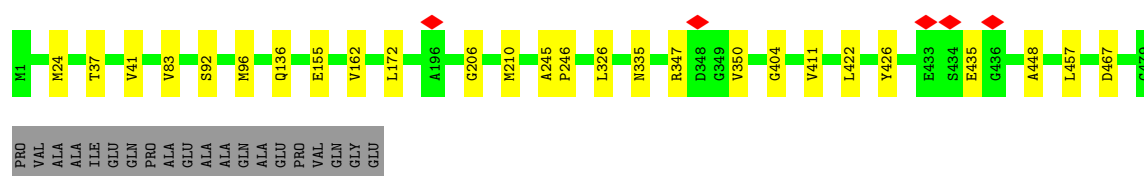


Chain E:  91% 8%



- Molecule 6: NADH-quinone oxidoreductase subunit N

Chain N:  91% 5%




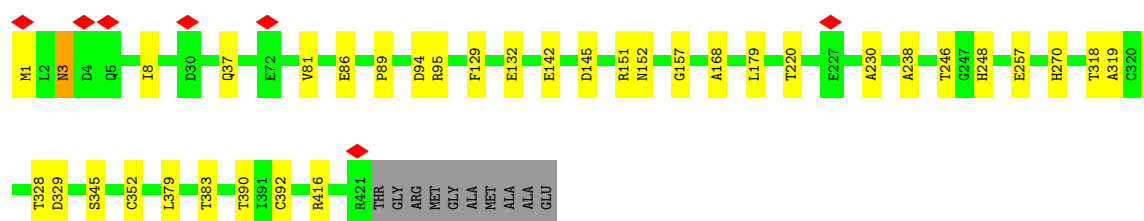
- Molecule 7: NADH-quinone oxidoreductase subunit H

Chain H:  95%

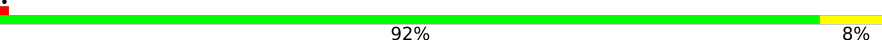


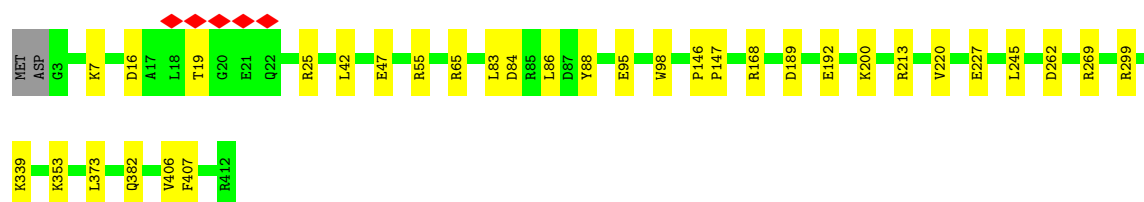
- Molecule 8: NADH-quinone oxidoreductase subunit F

Chain F:  89% 8%



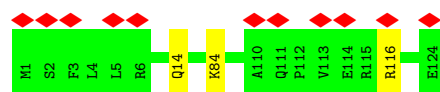
- Molecule 9: NADH-quinone oxidoreductase subunit D

Chain D:  92% 8%



- Molecule 10: NADH:ubiquinone oxidoreductase 17.2 kD subunit

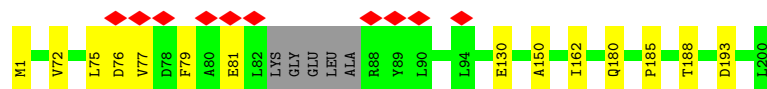
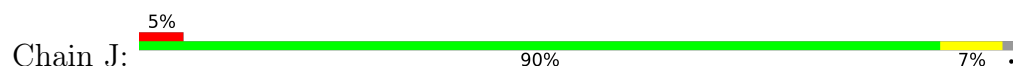
Chain q:  9% 98%



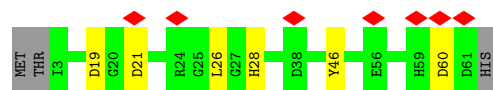
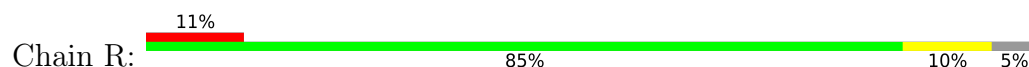
- Molecule 11: NADH-quinone oxidoreductase subunit A



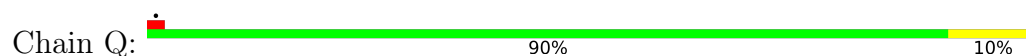
- Molecule 12: NADH-quinone oxidoreductase chain 10



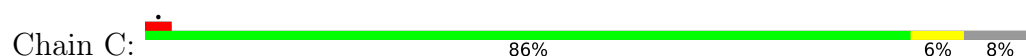
- Molecule 13: Zinc finger CHCC-type domain-containing protein



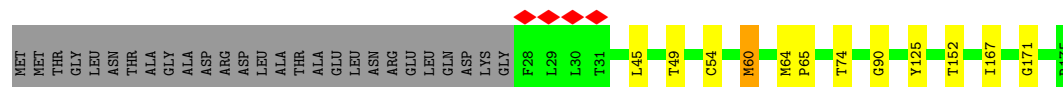
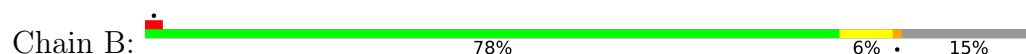
- Molecule 14: ETC complex I subunit conserved region



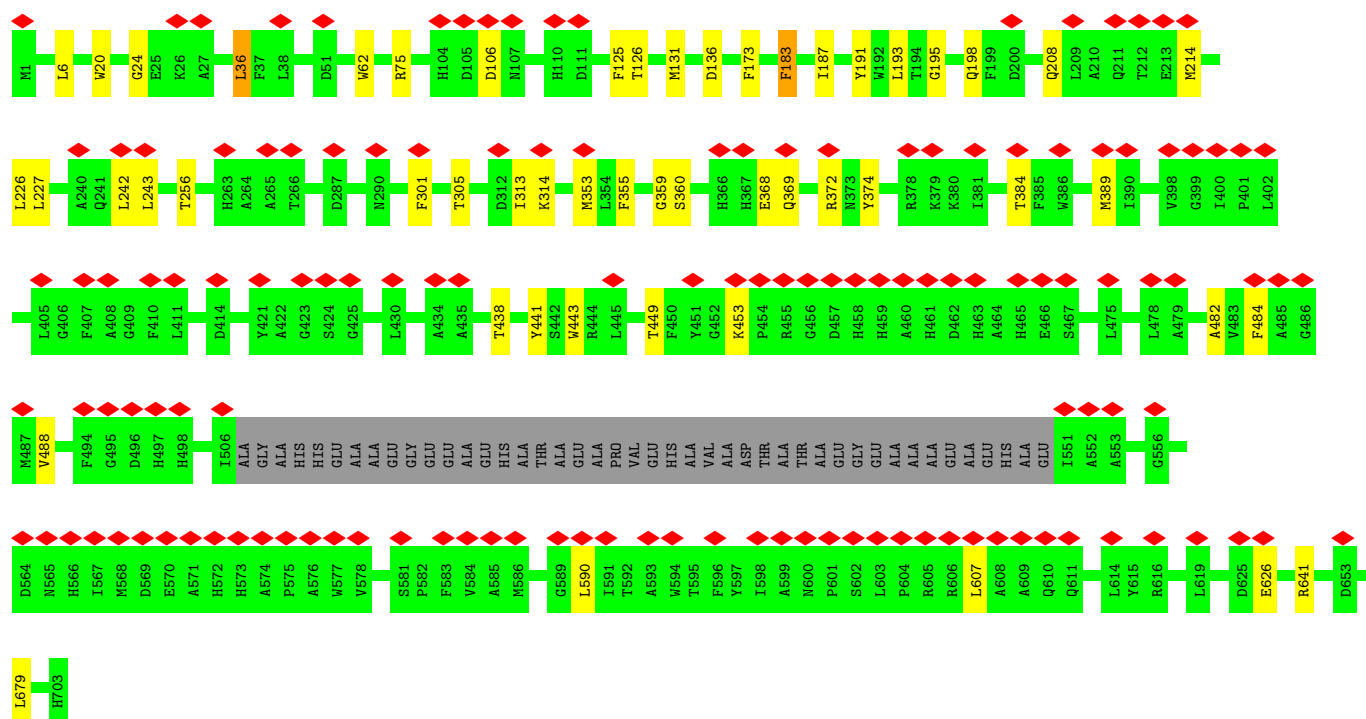
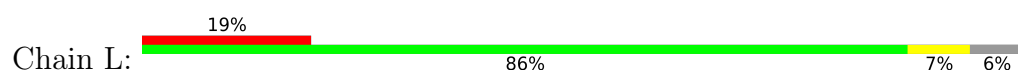
- Molecule 15: NADH-quinone oxidoreductase subunit C



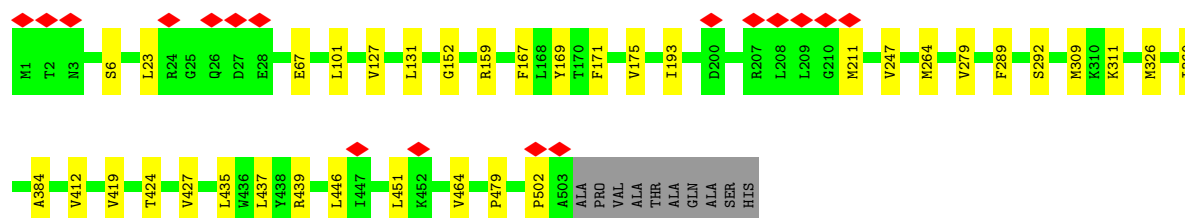
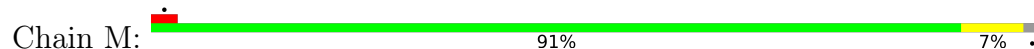
- Molecule 16: NADH-quinone oxidoreductase subunit B



- Molecule 17: NADH dehydrogenase subunit L



- Molecule 18: NADH dehydrogenase subunit M



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	146603	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 ( $e^-/\text{\AA}^2$ )	40.0	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.111	Depositor
Minimum map value	-0.043	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.019	Depositor
Map size (Å)	476.8, 476.8, 476.8	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.745, 0.745, 0.745	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, FME, CDL, P5S, 3PE, 3PH, U10, SF4, 2MR, NA, FES, ZN, PC1, FMN

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	K	0.30	0/774	0.47	0/1050
2	G	0.33	0/5161	0.55	0/6989
3	t	0.31	0/1668	0.55	0/2266
4	I	0.41	0/1328	0.56	0/1794
5	E	0.32	0/1857	0.49	0/2526
6	N	0.33	0/3626	0.48	0/4923
7	H	0.36	0/2823	0.46	0/3847
8	F	0.33	0/3301	0.53	0/4446
9	D	0.35	0/3330	0.55	0/4509
10	q	0.34	0/1066	0.51	0/1456
11	A	0.36	0/987	0.44	0/1345
12	J	0.33	0/1527	0.48	0/2075
13	R	0.34	0/484	0.54	0/660
14	Q	0.36	0/871	0.60	0/1181
15	C	0.37	0/1603	0.55	0/2179
16	B	0.42	0/1188	0.59	0/1613
17	L	0.30	0/5372	0.46	0/7314
18	M	0.32	0/4018	0.47	0/5470
All	All	0.34	0/40984	0.51	0/55643

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	K	763	0	817	8	0
2	G	5073	0	5042	23	0
3	t	1641	0	1643	0	0
4	I	1294	0	1241	7	0
5	E	1814	0	1790	13	0
6	N	3549	0	3649	18	0
7	H	2730	0	2756	7	0
8	F	3234	0	3181	23	0
9	D	3268	0	3213	17	0
10	q	1025	0	949	0	0
11	A	968	0	970	5	0
12	J	1498	0	1583	10	0
13	R	470	0	436	3	0
14	Q	848	0	812	5	0
15	C	1565	0	1535	7	0
16	B	1161	0	1159	8	0
17	L	5198	0	5164	27	0
18	M	3913	0	4025	24	0
19	B	8	0	0	1	0
19	F	8	0	0	1	0
19	G	16	0	0	0	0
19	I	16	0	0	0	0
20	E	4	0	0	0	0
20	G	4	0	0	0	0
21	G	1	0	0	0	0
22	A	34	0	41	0	0
22	H	92	0	103	0	0
22	I	39	0	54	0	0
22	J	74	0	97	0	0
22	L	157	0	215	2	0
22	M	128	0	148	1	0
22	N	89	0	127	0	0
23	I	49	0	67	1	0
23	L	40	0	46	1	0
24	D	1	0	0	0	0
24	I	1	0	0	0	0
24	M	1	0	0	0	0
24	N	1	0	0	0	0
25	H	88	0	130	0	0
25	L	45	0	64	0	0
25	M	112	0	149	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	N	128	0	184	2	0
25	q	36	0	46	0	0
26	H	65	0	74	0	0
26	M	65	0	74	0	0
27	F	31	0	19	0	0
28	D	42	0	58	1	0
28	J	45	0	64	0	0
29	R	1	0	0	0	0
30	B	29	0	33	3	0
31	A	33	0	0	1	0
31	B	56	0	0	0	0
31	C	73	0	0	1	0
31	D	151	0	0	1	0
31	E	47	0	0	1	0
31	F	70	0	0	3	0
31	G	220	0	0	1	0
31	H	64	0	0	2	0
31	I	75	0	0	2	0
31	J	35	0	0	0	0
31	K	15	0	0	0	0
31	L	16	0	0	0	0
31	M	54	0	0	0	0
31	N	61	0	0	1	0
31	Q	31	0	0	0	0
31	R	25	0	0	0	0
31	q	22	0	0	0	0
31	t	32	0	0	0	0
All	All	42542	0	41758	187	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (187) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:J:81:GLU:OE1	12:J:81:GLU:N	2.10	0.85
18:M:6:SER:OG	18:M:67:GLU:OE2	1.94	0.84
9:D:47:GLU:OE1	9:D:55:ARG:NH1	2.14	0.81
17:L:368:GLU:O	17:L:374:TYR:OH	2.02	0.76
2:G:150:LEU:HD12	2:G:201:GLN:HE21	1.51	0.75
9:D:192:GLU:OE1	9:D:299:ARG:NH1	2.19	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:F:246:THR:OG1	8:F:321:MET:O	2.06	0.73
2:G:394:ARG:NH1	2:G:413:THR:O	2.22	0.73
4:I:87:GLU:N	4:I:87:GLU:OE2	2.21	0.72
23:I:204:P5S:O13	31:I:301:HOH:O	2.09	0.70
1:K:98:VAL:HG22	6:N:155:GLU:OE1	1.92	0.69
6:N:326:LEU:HD21	6:N:467:ASP:HA	1.75	0.68
9:D:88:TYR:CG	16:B:54:CYS:HB3	2.29	0.68
6:N:448:ALA:HB2	25:N:501:3PE:H2I3	1.77	0.66
11:A:112:GLU:HG2	12:J:162:ILE:HD11	1.77	0.66
8:F:329:ASP:OD1	8:F:416:ARG:NH2	2.29	0.65
11:A:74:ASP:OD2	31:A:301:HOH:O	2.14	0.65
5:E:98:THR:HG22	5:E:99:THR:H	1.62	0.65
12:J:76:ASP:OD1	12:J:77:VAL:N	2.31	0.64
4:I:55:ARG:NH2	31:I:304:HOH:O	2.32	0.63
22:L:802:3PH:O13	18:M:439:ARG:NH2	2.31	0.63
8:F:3:ASN:N	8:F:3:ASN:OD1	2.32	0.63
1:K:90:THR:HG22	1:K:92:ALA:H	1.63	0.62
30:B:401:U10:H102	30:B:401:U10:O5	2.00	0.62
17:L:626:GLU:N	17:L:626:GLU:OE1	2.32	0.61
18:M:326:MET:HB3	18:M:412:VAL:HG21	1.83	0.60
2:G:112:ILE:HG23	4:I:65:ILE:HD12	1.83	0.59
17:L:36:LEU:HD11	17:L:126:THR:HG21	1.84	0.59
14:Q:58:ARG:NH1	14:Q:76:GLU:OE2	2.36	0.58
1:K:51:SER:OG	1:K:56:ASP:O	2.15	0.58
8:F:86:GLU:OE2	8:F:94:ASP:N	2.34	0.58
2:G:146:ASN:ND2	31:G:910:HOH:O	2.35	0.58
8:F:95:ARG:NH1	31:F:602:HOH:O	2.35	0.58
7:H:168:ILE:HD11	7:H:262:PHE:CE1	2.39	0.58
2:G:271:LYS:O	2:G:275:VAL:HG13	2.03	0.57
12:J:75:LEU:HD11	12:J:79:PHE:CE2	2.39	0.57
18:M:171:PHE:O	18:M:175:VAL:HG13	2.05	0.56
15:C:52:ARG:NH2	31:C:302:HOH:O	2.39	0.56
17:L:214:MET:CE	17:L:226:LEU:HD23	2.35	0.56
2:G:112:ILE:CG2	4:I:65:ILE:HD12	2.35	0.56
17:L:173:PHE:CD1	18:M:435:LEU:HD11	2.41	0.55
31:H:561:HOH:O	30:B:401:U10:H1M2	2.06	0.55
2:G:291:GLU:OE2	2:G:296:ARG:NH2	2.37	0.54
2:G:10:ASP:OD2	2:G:86:THR:OG1	2.23	0.54
30:B:401:U10:H4M2	30:B:401:U10:O3	2.07	0.54
17:L:484:PHE:O	17:L:488:VAL:HG23	2.08	0.54
12:J:77:VAL:HG22	12:J:77:VAL:O	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:202:VAL:HG22	7:H:262:PHE:CD1	2.44	0.53
1:K:28:ASN:OD1	1:K:30:ILE:N	2.43	0.52
18:M:446:LEU:HD11	18:M:451:LEU:HB2	1.90	0.52
6:N:162:VAL:HG11	17:L:679:LEU:HD21	1.90	0.52
8:F:257:GLU:OE2	8:F:270:HIS:NE2	2.42	0.52
8:F:345:SER:HB2	8:F:352:CYS:SG	2.50	0.52
7:H:244:MET:HA	7:H:244:MET:HE2	1.92	0.51
17:L:214:MET:HE3	17:L:226:LEU:HD23	1.92	0.51
7:H:220:LEU:HD21	7:H:301:TYR:O	2.10	0.51
17:L:20:TRP:O	17:L:24:GLY:N	2.42	0.50
11:A:76:GLU:HB3	11:A:105:LEU:HD12	1.94	0.50
5:E:143:ASN:HB3	5:E:155:GLU:HB3	1.92	0.50
16:B:167:ILE:O	16:B:171:GLY:N	2.44	0.50
18:M:127:VAL:HG11	18:M:264:MET:HG2	1.93	0.50
18:M:289:PHE:HB3	18:M:419:VAL:HG21	1.93	0.50
5:E:236:GLN:O	8:F:151:ARG:NH2	2.45	0.49
18:M:152:GLY:O	18:M:159:ARG:NE	2.42	0.49
4:I:63:ARG:NH2	13:R:26:LEU:O	2.45	0.49
8:F:152:ASN:OD1	8:F:157:GLY:N	2.40	0.49
17:L:6:LEU:HD11	17:L:131:MET:HG2	1.94	0.49
6:N:37:THR:O	6:N:41:VAL:HG23	2.13	0.49
6:N:404:GLY:N	31:N:609:HOH:O	2.44	0.49
4:I:55:ARG:HD3	4:I:152:ILE:HG21	1.95	0.48
9:D:227:GLU:HG3	9:D:245:LEU:HD11	1.95	0.48
22:L:805:3PH:H251	18:M:384:ALA:HB3	1.94	0.48
6:N:411:VAL:HB	18:M:175:VAL:HB	1.95	0.48
8:F:248:HIS:CE1	8:F:328:THR:HG22	2.48	0.48
14:Q:1:MET:SD	14:Q:1:MET:N	2.83	0.48
18:M:247:VAL:HG21	18:M:311:LYS:HG3	1.96	0.48
17:L:353:MET:HE1	17:L:482:ALA:HB3	1.96	0.48
15:C:13:LEU:HD11	15:C:57:CYS:HB3	1.96	0.47
8:F:81:VAL:HG11	8:F:179:LEU:HD22	1.95	0.47
2:G:461:LEU:O	2:G:465:MET:HG3	2.15	0.47
17:L:256:THR:HG21	17:L:359:GLY:CA	2.45	0.47
18:M:131:LEU:HA	18:M:193:ILE:HD12	1.95	0.47
18:M:424:THR:O	18:M:427:VAL:HG22	2.14	0.47
6:N:24:MET:HA	6:N:24:MET:CE	2.44	0.47
8:F:230:ALA:HA	8:F:238:ALA:HB1	1.97	0.47
12:J:185:PRO:HA	12:J:188:THR:HG22	1.95	0.47
15:C:123:ASP:OD1	15:C:137:ARG:NH1	2.46	0.47
15:C:156:THR:HG22	15:C:156:THR:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:F:248:HIS:HE1	8:F:328:THR:HG22	1.81	0.46
9:D:146:PRO:N	9:D:147:PRO:HD2	2.30	0.46
18:M:309:MET:SD	18:M:360:ILE:HD11	2.55	0.46
1:K:43:VAL:HG11	6:N:172:LEU:HB3	1.97	0.46
17:L:183:PHE:CE1	17:L:187:ILE:HD11	2.50	0.46
14:Q:58:ARG:NE	14:Q:74:VAL:HG11	2.30	0.46
5:E:142:THR:O	5:E:183:ARG:NH2	2.40	0.46
15:C:73:ARG:NH1	15:C:78:ASP:OD2	2.45	0.46
16:B:90:GLY:HA2	19:B:402:SF4:S3	2.56	0.46
9:D:42:LEU:HB2	9:D:407:PHE:CZ	2.51	0.45
6:N:245:ALA:HB3	6:N:246:PRO:HD3	1.96	0.45
17:L:607:LEU:HD22	23:L:803:P5S:H21A	1.98	0.45
8:F:142:GLU:OE1	31:F:601:HOH:O	2.21	0.45
9:D:168:ARG:HD3	16:B:152:THR:HG22	1.98	0.45
9:D:189:ASP:OD1	9:D:299:ARG:NH2	2.50	0.45
5:E:137:CYS:SG	8:F:89:PRO:O	2.75	0.45
7:H:224:GLU:H	7:H:224:GLU:CD	2.21	0.45
12:J:75:LEU:HD11	12:J:79:PHE:CD2	2.51	0.45
5:E:26:GLN:OE1	31:E:401:HOH:O	2.21	0.45
7:H:148:LEU:HD21	12:J:72:VAL:HG21	1.99	0.44
16:B:60:MET:O	16:B:64:MET:HG2	2.17	0.44
17:L:193:LEU:HD11	17:L:214:MET:HE2	1.99	0.44
17:L:242:LEU:O	17:L:243:LEU:HB2	2.17	0.44
6:N:83:VAL:HG12	25:N:501:3PE:H2A1	1.99	0.44
8:F:8:ILE:HG12	8:F:220:THR:HG21	1.99	0.44
9:D:213:ARG:HD3	28:D:501:PC1:O12	2.16	0.44
5:E:138:LEU:HD12	5:E:146:MET:SD	2.58	0.44
1:K:20:PHE:CE1	1:K:24:VAL:HG11	2.53	0.44
11:A:92:ASP:OD2	11:A:92:ASP:N	2.51	0.44
6:N:422:LEU:HD11	18:M:167:PHE:CD1	2.52	0.44
18:M:247:VAL:HG21	18:M:311:LYS:CG	2.48	0.44
18:M:279:VAL:HG22	18:M:502:PRO:HD3	2.00	0.44
7:H:254:MET:HE3	31:H:511:HOH:O	2.17	0.44
17:L:443:TRP:CD1	17:L:590:LEU:HD13	2.53	0.44
16:B:45:LEU:O	16:B:74:THR:HA	2.18	0.44
9:D:86:LEU:HD11	9:D:373:LEU:HD13	1.99	0.43
2:G:196:LEU:HB2	2:G:201:GLN:OE1	2.18	0.43
6:N:92:SER:O	6:N:96:MET:HG3	2.18	0.43
9:D:220:VAL:HG11	12:J:180:GLN:HA	2.00	0.43
17:L:374:TYR:HD2	17:L:449:THR:HG22	1.83	0.43
1:K:29:VAL:HG11	1:K:81:LEU:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:503:ASP:OD2	2:G:503:ASP:O	2.36	0.43
17:L:301:PHE:O	17:L:305:THR:HG23	2.19	0.43
2:G:288:TYR:HB3	2:G:295:LEU:HD22	2.01	0.42
9:D:7:LYS:HB3	9:D:7:LYS:NZ	2.34	0.42
11:A:1:FME:SD	11:A:2:GLU:N	2.93	0.42
15:C:57:CYS:HB2	15:C:59:PHE:CE2	2.54	0.42
18:M:292:SER:CB	18:M:326:MET:HG3	2.49	0.42
6:N:347:ARG:O	6:N:350:VAL:HG12	2.19	0.42
14:Q:102:THR:O	14:Q:103:HIS:HB2	2.20	0.42
2:G:41:ARG:NH2	2:G:259:ASN:OD1	2.51	0.42
18:M:292:SER:HB2	18:M:326:MET:HG3	2.01	0.42
2:G:23:ILE:O	2:G:27:GLU:HG3	2.20	0.42
8:F:37:GLN:NE2	31:F:615:HOH:O	2.53	0.42
2:G:327:GLU:OE2	2:G:601:ARG:NE	2.49	0.42
5:E:5:LEU:HD12	5:E:55:ARG:CZ	2.49	0.42
5:E:187:GLU:OE1	5:E:187:GLU:N	2.48	0.42
9:D:16:ASP:HB2	9:D:19:THR:HG23	2.01	0.42
9:D:83:LEU:HG	9:D:98:TRP:HB2	2.02	0.42
15:C:63:ILE:O	15:C:64:ASP:HB3	2.19	0.42
17:L:193:LEU:HD12	17:L:227:LEU:HD11	2.01	0.42
8:F:390:THR:HB	19:F:502:SF4:S4	2.60	0.42
9:D:84:ASP:OD1	9:D:95:GLU:OE2	2.37	0.42
18:M:446:LEU:HD11	18:M:451:LEU:CB	2.48	0.42
17:L:136:ASP:OD1	17:L:198:GLN:NE2	2.52	0.42
17:L:360:SER:HB3	17:L:384:THR:HG21	2.02	0.42
2:G:327:GLU:OE2	2:G:601:ARG:NH2	2.50	0.41
8:F:129:PHE:HB3	8:F:132:GLU:HB2	2.00	0.41
17:L:313:ILE:HG23	17:L:314:LYS:N	2.35	0.41
1:K:68:THR:HG21	12:J:150:ALA:HB1	2.01	0.41
5:E:98:THR:HG21	8:F:89:PRO:HB3	2.02	0.41
17:L:438:THR:HA	17:L:441:TYR:CE2	2.55	0.41
6:N:467:ASP:N	6:N:467:ASP:OD1	2.52	0.41
5:E:79:TYR:HB3	8:F:168:ALA:HB3	2.03	0.41
8:F:379:LEU:O	8:F:383:THR:HG23	2.20	0.41
6:N:206:GLY:O	6:N:210:MET:HG3	2.21	0.41
2:G:343:VAL:O	2:G:494:THR:HG23	2.21	0.41
13:R:19:ASP:HA	13:R:28:HIS:CE1	2.56	0.41
2:G:274:PHE:HB3	2:G:654:LEU:HD23	2.03	0.41
2:G:370:ASP:OD2	2:G:392:ARG:NH1	2.54	0.41
2:G:407:GLY:O	2:G:418:HIS:NE2	2.42	0.41
5:E:40:ILE:HB	5:E:41:PRO:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:160:GLU:H	5:E:160:GLU:CD	2.24	0.41
9:D:353:LYS:HE2	9:D:406:VAL:HG23	2.03	0.41
16:B:49:THR:O	16:B:49:THR:HG22	2.20	0.41
17:L:374:TYR:HB3	17:L:449:THR:HA	2.03	0.41
17:L:62:TRP:O	18:M:479:PRO:HG2	2.21	0.41
6:N:457:LEU:HD11	22:M:603:3PH:H3C1	2.02	0.40
2:G:152:GLU:HB2	2:G:216:LYS:HG3	2.02	0.40
2:G:339:LEU:HD11	2:G:588:LEU:HD13	2.03	0.40
16:B:64:MET:HB3	16:B:65:PRO:CD	2.51	0.40
18:M:101:LEU:HD23	18:M:464:VAL:HG22	2.02	0.40
2:G:565:MET:HE2	14:Q:75:ILE:HD11	2.03	0.40
4:I:65:ILE:HD13	13:R:46:TYR:CD1	2.56	0.40
6:N:435:GLU:OE1	6:N:435:GLU:N	2.52	0.40
9:D:382:GLN:NE2	31:D:622:HOH:O	2.54	0.40
18:M:309:MET:HG3	18:M:437:LEU:HD11	2.03	0.40
8:F:318:THR:O	8:F:319:ALA:HB3	2.21	0.40
17:L:191:TYR:O	17:L:195:GLY:N	2.51	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	99/101 (98%)	97 (98%)	2 (2%)	0	100	100
2	G	664/674 (98%)	651 (98%)	13 (2%)	0	100	100
3	t	214/217 (99%)	210 (98%)	4 (2%)	0	100	100
4	I	157/163 (96%)	153 (98%)	4 (2%)	0	100	100
5	E	234/239 (98%)	225 (96%)	9 (4%)	0	100	100
6	N	477/499 (96%)	469 (98%)	8 (2%)	0	100	100
7	H	340/345 (99%)	330 (97%)	10 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	F	419/431 (97%)	413 (99%)	6 (1%)	0	100	100
9	D	407/412 (99%)	396 (97%)	11 (3%)	0	100	100
10	q	122/124 (98%)	119 (98%)	2 (2%)	1 (1%)	16	20
11	A	119/121 (98%)	116 (98%)	3 (2%)	0	100	100
12	J	191/200 (96%)	189 (99%)	2 (1%)	0	100	100
13	R	57/62 (92%)	56 (98%)	1 (2%)	0	100	100
14	Q	101/103 (98%)	101 (100%)	0	0	100	100
15	C	189/208 (91%)	184 (97%)	5 (3%)	0	100	100
16	B	146/175 (83%)	140 (96%)	6 (4%)	0	100	100
17	L	655/703 (93%)	630 (96%)	25 (4%)	0	100	100
18	M	501/513 (98%)	495 (99%)	6 (1%)	0	100	100
All	All	5092/5290 (96%)	4974 (98%)	117 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	q	14	GLN

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	81/81 (100%)	80 (99%)	1 (1%)	67	81
2	G	530/535 (99%)	525 (99%)	5 (1%)	75	87
3	t	167/168 (99%)	164 (98%)	3 (2%)	54	71
4	I	134/137 (98%)	133 (99%)	1 (1%)	81	90
5	E	188/190 (99%)	187 (100%)	1 (0%)	86	93
6	N	356/369 (96%)	353 (99%)	3 (1%)	79	89
7	H	278/279 (100%)	272 (98%)	6 (2%)	47	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	F	330/335 (98%)	326 (99%)	4 (1%)	67	81
9	D	340/342 (99%)	335 (98%)	5 (2%)	60	76
10	q	105/105 (100%)	103 (98%)	2 (2%)	52	69
11	A	97/97 (100%)	95 (98%)	2 (2%)	48	66
12	J	157/160 (98%)	154 (98%)	3 (2%)	52	69
13	R	49/52 (94%)	47 (96%)	2 (4%)	26	39
14	Q	87/87 (100%)	84 (97%)	3 (3%)	32	47
15	C	170/183 (93%)	169 (99%)	1 (1%)	84	92
16	B	125/145 (86%)	123 (98%)	2 (2%)	58	74
17	L	520/544 (96%)	508 (98%)	12 (2%)	45	63
18	M	411/417 (99%)	408 (99%)	3 (1%)	81	90
All	All	4125/4226 (98%)	4066 (99%)	59 (1%)	62	77

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	62	PHE
2	G	312	LYS
2	G	315	LYS
2	G	428	SER
2	G	430	SER
2	G	636	ARG
3	t	54	ASP
3	t	92	SER
3	t	170	ARG
4	I	116	ASP
5	E	127	ASP
6	N	136	GLN
6	N	335	ASN
6	N	426	TYR
7	H	66	LEU
7	H	127	GLU
7	H	153	GLN
7	H	251	MET
7	H	252	TYR
7	H	303	TYR
8	F	1	MET
8	F	3	ASN

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Mol	Chain	Res	Type
8	F	145	ASP
8	F	392	CYS
9	D	25	ARG
9	D	200	LYS
9	D	262	ASP
9	D	269	ARG
9	D	339	LYS
10	q	84	LYS
10	q	116	ARG
11	A	74	ASP
11	A	92	ASP
12	J	1	MET
12	J	130	GLU
12	J	193	ASP
13	R	21	ASP
13	R	60	ASP
14	Q	21	ARG
14	Q	26	ASP
14	Q	54	ARG
15	C	20	ARG
16	B	60	MET
16	B	125	TYR
17	L	36	LEU
17	L	75	ARG
17	L	106	ASP
17	L	125	PHE
17	L	183	PHE
17	L	208	GLN
17	L	355	PHE
17	L	369	GLN
17	L	372	ARG
17	L	389	MET
17	L	453	LYS
17	L	641	ARG
18	M	23	LEU
18	M	169	TYR
18	M	211	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	G	201	GLN

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Mol	Chain	Res	Type
9	D	270	ASN
17	L	505	HIS
18	M	499	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 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
9	2MR	D	65	9	10,12,13	2.30	3 (30%)	5,13,15	0.98	0
11	FME	A	1	11	8,9,10	0.94	0	7,9,11	0.92	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
9	2MR	D	65	9	-	0/10/13/15	-
11	FME	A	1	11	-	2/7/9/11	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	65	2MR	CZ-NH2	4.79	1.44	1.33
9	D	65	2MR	CZ-NE	4.56	1.44	1.34
9	D	65	2MR	CQ1-NH1	-2.21	1.41	1.46



There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	1	FME	O1-CN-N-CA
11	A	1	FME	CB-CA-N-CN

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	1	FME	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 49 ligands modelled in this entry, 6 are monoatomic - leaving 43 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
22	3PH	H	406	-	29,29,47	0.78	1 (3%)	33,34,52	0.83	2 (6%)
22	3PH	I	203	-	38,38,47	0.69	1 (2%)	42,43,52	0.71	1 (2%)
19	SF4	G	802	2	0,12,12	-	-	-	-	-
22	3PH	H	403	-	35,35,47	0.74	1 (2%)	39,40,52	0.72	1 (2%)
22	3PH	M	607	-	30,30,47	0.78	1 (3%)	34,35,52	0.71	1 (2%)
19	SF4	G	801	2	0,12,12	-	-	-	-	-
22	3PH	N	505	-	42,42,47	0.67	1 (2%)	46,47,52	0.58	0
19	SF4	I	202	4	0,12,12	-	-	-	-	-
23	P5S	I	204	-	47,48,53	0.57	0	51,55,60	0.75	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	3PH	M	603	-	32,32,47	0.76	1 (3%)	36,37,52	0.71	1 (2%)
25	3PE	N	503	-	47,47,50	0.53	0	50,52,55	0.56	2 (4%)
25	3PE	H	405	-	44,44,50	0.57	0	47,49,55	0.56	1 (2%)
20	FES	G	803	2	0,4,4	-	-	-		
19	SF4	I	201	4	0,12,12	-	-	-		
22	3PH	H	404	-	25,25,47	0.86	1 (4%)	29,30,52	0.81	1 (3%)
26	CDL	H	402	-	64,64,99	0.40	0	70,76,111	0.61	1 (1%)
19	SF4	F	502	8	0,12,12	-	-	-		
26	CDL	M	606	-	64,64,99	0.37	0	70,76,111	0.62	0
20	FES	E	301	5	0,4,4	-	-	-		
30	U10	B	401	-	29,29,63	3.05	8 (27%)	35,38,79	2.36	11 (31%)
22	3PH	M	608	-	32,32,47	0.76	1 (3%)	36,37,52	0.69	1 (2%)
22	3PH	J	303	-	41,41,47	0.67	1 (2%)	45,46,52	0.67	1 (2%)
28	PC1	J	301	-	44,44,53	0.54	0	50,52,61	0.52	1 (2%)
25	3PE	M	604	-	40,40,50	0.57	0	43,45,55	0.74	2 (4%)
19	SF4	B	402	16	0,12,12	-	-	-		
25	3PE	M	605	-	28,28,50	0.67	0	31,33,55	0.64	1 (3%)
25	3PE	L	804	-	44,44,50	0.56	0	47,49,55	0.56	1 (2%)
28	PC1	D	501	-	41,41,53	0.57	0	47,49,61	0.53	1 (2%)
25	3PE	N	501	-	41,41,50	0.56	0	44,46,55	0.58	1 (2%)
22	3PH	L	801	-	46,46,47	0.65	1 (2%)	50,51,52	0.61	2 (4%)
23	P5S	L	803	-	38,39,53	0.62	0	42,46,60	0.83	2 (4%)
22	3PH	L	802	-	44,44,47	0.64	1 (2%)	48,49,52	0.60	1 (2%)
22	3PH	A	201	-	33,33,47	0.73	1 (3%)	37,38,52	0.90	2 (5%)
22	3PH	N	502	-	45,45,47	0.65	1 (2%)	49,50,52	0.67	2 (4%)
25	3PE	H	401	-	42,42,50	0.59	0	45,47,55	0.63	1 (2%)
22	3PH	M	601	-	30,30,47	0.76	1 (3%)	34,35,52	0.77	3 (8%)
22	3PH	L	805	-	35,35,47	0.73	1 (2%)	39,40,52	0.63	1 (2%)
25	3PE	q	201	-	35,35,50	0.61	0	38,40,55	0.74	2 (5%)
22	3PH	L	806	-	28,28,47	0.80	1 (3%)	32,33,52	0.71	0
22	3PH	J	302	-	31,31,47	0.76	1 (3%)	35,36,52	0.70	1 (2%)
27	FMN	F	501	-	33,33,33	1.10	3 (9%)	48,50,50	1.28	7 (14%)
25	3PE	M	602	-	41,41,50	0.58	0	44,46,55	0.55	1 (2%)
25	3PE	N	504	-	37,37,50	0.58	0	40,42,55	0.58	1 (2%)

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
22	3PH	H	406	-	-	16/31/31/49	-
22	3PH	I	203	-	-	14/40/40/49	-
22	3PH	H	403	-	-	10/37/37/49	-
19	SF4	G	802	2	-	-	0/6/5/5
22	3PH	M	607	-	-	11/32/32/49	-
19	SF4	G	801	2	-	-	0/6/5/5
22	3PH	N	505	-	-	19/44/44/49	-
19	SF4	I	202	4	-	-	0/6/5/5
23	P5S	I	204	-	-	20/54/54/59	-
22	3PH	M	603	-	-	5/34/34/49	-
25	3PE	N	503	-	-	22/51/51/54	-
25	3PE	H	405	-	-	23/48/48/54	-
20	FES	G	803	2	-	-	0/1/1/1
19	SF4	I	201	4	-	-	0/6/5/5
22	3PH	H	404	-	-	8/27/27/49	-
26	CDL	H	402	-	-	43/75/75/110	-
26	CDL	M	606	-	-	37/75/75/110	-
19	SF4	F	502	8	-	-	0/6/5/5
20	FES	E	301	5	-	-	0/1/1/1
30	U10	B	401	-	-	11/23/47/87	0/1/1/1
22	3PH	M	608	-	-	18/34/34/49	-
22	3PH	J	303	-	-	21/43/43/49	-
28	PC1	J	301	-	-	15/48/48/57	-
25	3PE	M	604	-	-	22/44/44/54	-
19	SF4	B	402	16	-	-	0/6/5/5
25	3PE	M	605	-	-	11/32/32/54	-
25	3PE	L	804	-	-	19/48/48/54	-
28	PC1	D	501	-	-	20/45/45/57	-
25	3PE	N	501	-	-	12/45/45/54	-
22	3PH	L	801	-	-	18/48/48/49	-
23	P5S	L	803	-	-	22/45/45/59	-
22	3PH	L	802	-	-	17/46/46/49	-
22	3PH	A	201	-	-	14/35/35/49	-
22	3PH	N	502	-	-	17/47/47/49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	3PE	H	401	-	-	15/46/46/54	-
22	3PH	M	601	-	-	14/32/32/49	-
22	3PH	L	805	-	-	11/37/37/49	-
25	3PE	q	201	-	-	21/39/39/54	-
22	3PH	L	806	-	-	15/30/30/49	-
22	3PH	J	302	-	-	13/33/33/49	-
27	FMN	F	501	-	-	4/18/18/18	0/3/3/3
25	3PE	M	602	-	-	23/45/45/54	-
25	3PE	N	504	-	-	19/41/41/54	-

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	B	401	U10	C13-C14	8.68	1.53	1.33
30	B	401	U10	C8-C9	8.44	1.53	1.33
30	B	401	U10	C18-C19	8.29	1.52	1.33
22	H	403	3PH	P-O11	3.43	1.71	1.60
22	L	801	3PH	P-O11	3.39	1.71	1.60
22	M	608	3PH	P-O11	3.39	1.71	1.60
22	M	603	3PH	P-O11	3.37	1.71	1.60
22	N	505	3PH	P-O11	3.34	1.71	1.60
22	L	805	3PH	P-O11	3.34	1.71	1.60
27	F	501	FMN	C4A-N5	3.34	1.37	1.30
22	L	806	3PH	P-O11	3.34	1.71	1.60
22	M	607	3PH	P-O11	3.30	1.70	1.60
22	N	502	3PH	P-O11	3.28	1.70	1.60
22	J	302	3PH	P-O11	3.28	1.70	1.60
22	H	404	3PH	P-O11	3.27	1.70	1.60
22	J	303	3PH	P-O11	3.24	1.70	1.60
22	I	203	3PH	P-O11	3.21	1.70	1.60
22	H	406	3PH	P-O11	3.19	1.70	1.60
22	A	201	3PH	P-O11	3.19	1.70	1.60
22	M	601	3PH	P-O11	3.19	1.70	1.60
22	L	802	3PH	P-O11	3.17	1.70	1.60
30	B	401	U10	C6-C5	2.51	1.53	1.46
30	B	401	U10	O5-C5	-2.35	1.18	1.23
30	B	401	U10	O3-C3M	-2.14	1.40	1.45
27	F	501	FMN	C10-N1	2.10	1.37	1.33
30	B	401	U10	O4-C4M	-2.09	1.40	1.45
30	B	401	U10	O2-C2	-2.07	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	F	501	FMN	C4A-C10	-2.04	1.38	1.44

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	B	401	U10	C7-C8-C9	-6.93	115.25	126.79
30	B	401	U10	C17-C18-C19	-6.04	113.12	127.66
30	B	401	U10	C12-C13-C14	-4.56	116.68	127.66
30	B	401	U10	C7-C6-C5	4.07	123.38	118.48
30	B	401	U10	C20-C19-C18	-3.59	114.46	123.68
30	B	401	U10	C10-C9-C8	-3.47	114.77	123.68
25	M	604	3PE	C2-O21-C21	3.40	126.17	117.79
27	F	501	FMN	C4-N3-C2	-3.32	119.51	125.64
23	L	803	P5S	OG-CB-CA	3.16	110.81	108.06
27	F	501	FMN	O4-C4-C4A	-2.75	119.29	126.60
27	F	501	FMN	C4A-C4-N3	2.72	120.09	113.19
27	F	501	FMN	C4A-C10-N10	2.67	120.38	116.48
30	B	401	U10	C21-C19-C18	-2.66	113.93	120.50
22	A	201	3PH	C2-O21-C21	2.60	124.19	117.79
22	N	502	3PH	O13-P-O11	-2.56	99.93	106.73
25	q	201	3PE	C2-O21-C21	2.52	123.99	117.79
30	B	401	U10	C16-C14-C13	-2.51	116.03	121.12
22	A	201	3PH	O13-P-O11	-2.39	100.37	106.73
27	F	501	FMN	C4A-C10-N1	-2.39	119.18	124.73
22	J	303	3PH	O13-P-O11	-2.38	100.41	106.73
22	L	802	3PH	O13-P-O11	-2.37	100.42	106.73
28	J	301	PC1	O12-P-O14	2.37	123.94	112.24
25	N	501	3PE	O12-P-O14	2.37	123.93	112.24
25	N	504	3PE	O12-P-O14	2.36	123.93	112.24
28	D	501	PC1	O12-P-O14	2.36	123.92	112.24
25	M	602	3PE	O12-P-O14	2.36	123.89	112.24
22	I	203	3PH	O13-P-O11	-2.35	100.47	106.73
25	H	405	3PE	O12-P-O14	2.33	123.77	112.24
25	N	503	3PE	C2-O21-C21	2.32	123.51	117.79
25	M	605	3PE	O12-P-O14	2.32	123.72	112.24
30	B	401	U10	C11-C9-C8	-2.28	116.49	121.12
23	I	204	P5S	OG-CB-CA	2.28	110.05	108.06
22	M	601	3PH	O13-P-O11	-2.28	100.66	106.73
25	H	401	3PE	O12-P-O14	2.28	123.52	112.24
25	N	503	3PE	O12-P-O14	2.28	123.50	112.24
22	H	406	3PH	C2-O21-C21	2.27	123.39	117.79
25	q	201	3PE	O12-P-O14	2.27	123.47	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	L	801	3PH	O13-P-O11	-2.27	100.69	106.73
25	L	804	3PE	O12-P-O14	2.26	123.42	112.24
22	H	404	3PH	O13-P-O11	-2.25	100.75	106.73
22	M	608	3PH	O13-P-O11	-2.24	100.77	106.73
22	M	607	3PH	O13-P-O11	-2.23	100.79	106.73
25	M	604	3PE	O12-P-O14	2.22	123.20	112.24
30	B	401	U10	C6-C1-C2	2.21	120.93	119.18
23	L	803	P5S	C3-C2-C1	2.20	116.98	111.79
26	H	402	CDL	CB2-C1-CA2	-2.18	106.37	112.79
27	F	501	FMN	C10-C4A-N5	-2.17	120.25	124.86
22	L	805	3PH	O13-P-O11	-2.14	101.04	106.73
22	J	302	3PH	O13-P-O11	-2.13	101.07	106.73
27	F	501	FMN	C4-C4A-C10	2.10	120.31	116.79
22	N	502	3PH	C3-C2-C1	2.09	116.73	111.79
22	M	601	3PH	C3-C2-C1	2.07	116.69	111.79
22	M	601	3PH	O14-P-O13	2.05	115.45	107.64
22	L	801	3PH	C3-C2-C1	2.03	116.59	111.79
22	H	406	3PH	O13-P-O11	-2.02	101.35	106.73
30	B	401	U10	C15-C14-C13	-2.01	118.51	123.68
22	M	603	3PH	O13-P-O11	-2.01	101.39	106.73
23	I	204	P5S	CB-CA-C	-2.01	107.02	110.93
22	H	403	3PH	O13-P-O11	-2.00	101.41	106.73

There are no chirality outliers.

All (600) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	N	502	3PH	O21-C2-C3-O31
22	N	505	3PH	C22-C21-O21-C2
22	H	403	3PH	O22-C21-O21-C2
22	H	403	3PH	C22-C21-O21-C2
22	H	404	3PH	C1-O11-P-O13
22	H	404	3PH	C1-O11-P-O14
22	H	406	3PH	O22-C21-O21-C2
22	A	201	3PH	O11-C1-C2-O21
22	A	201	3PH	O22-C21-O21-C2
22	A	201	3PH	C22-C21-O21-C2
22	J	302	3PH	C1-O11-P-O13
22	J	302	3PH	C1-O11-P-O14
22	J	303	3PH	C22-C21-O21-C2
22	L	801	3PH	C1-O11-P-O13
22	L	801	3PH	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
22	L	806	3PH	C1-O11-P-O13
22	L	806	3PH	C1-O11-P-O14
22	L	806	3PH	C1-O11-P-O12
22	M	607	3PH	C1-O11-P-O13
22	M	607	3PH	C1-O11-P-O14
22	M	608	3PH	C1-O11-P-O13
22	M	608	3PH	C1-O11-P-O14
22	M	608	3PH	C1-O11-P-O12
23	I	204	P5S	C-CA-CB-OG
23	I	204	P5S	N-CA-CB-OG
23	I	204	P5S	CB-OG-P12-O15
23	L	803	P5S	C-CA-CB-OG
23	L	803	P5S	N-CA-CB-OG
23	L	803	P5S	CB-OG-P12-O13
23	L	803	P5S	C3-O16-P12-OG
23	L	803	P5S	C3-O16-P12-O13
23	L	803	P5S	C3-O16-P12-O15
25	N	503	3PE	C11-O13-P-O11
25	N	503	3PE	C11-O13-P-O12
25	N	503	3PE	C11-O13-P-O14
25	N	503	3PE	C3-C2-O21-C21
25	N	503	3PE	C22-C21-O21-C2
25	N	504	3PE	C1-O11-P-O14
25	N	504	3PE	C11-O13-P-O14
25	N	504	3PE	O13-C11-C12-N
25	H	401	3PE	C11-O13-P-O12
25	H	405	3PE	O13-C11-C12-N
25	q	201	3PE	C1-O11-P-O14
25	q	201	3PE	C11-O13-P-O14
25	L	804	3PE	C1-O11-P-O12
25	M	602	3PE	C1-O11-P-O14
25	M	602	3PE	O11-C1-C2-O21
25	M	604	3PE	C1-O11-P-O13
25	M	604	3PE	C11-O13-P-O12
25	M	604	3PE	C11-O13-P-O14
25	M	604	3PE	O13-C11-C12-N
25	M	604	3PE	C22-C21-O21-C2
25	M	605	3PE	C11-O13-P-O11
26	H	402	CDL	O1-C1-CA2-OA2
26	H	402	CDL	CA2-OA2-PA1-OA3
26	H	402	CDL	CB2-OB2-PB2-OB3
26	H	402	CDL	CB3-OB5-PB2-OB3

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Mol	Chain	Res	Type	Atoms
26	H	402	CDL	CB3-OB5-PB2-OB4
26	H	402	CDL	C51-CB5-OB6-CB4
26	M	606	CDL	CA2-OA2-PA1-OA3
26	M	606	CDL	CA3-OA5-PA1-OA4
26	M	606	CDL	CA4-CA3-OA5-PA1
26	M	606	CDL	CB2-OB2-PB2-OB3
26	M	606	CDL	CB2-OB2-PB2-OB4
27	F	501	FMN	C5'-O5'-P-O2P
28	D	501	PC1	C1-O11-P-O14
28	D	501	PC1	O13-C11-C12-N
30	B	401	U10	C1-C6-C7-C8
30	B	401	U10	C5-C6-C7-C8
30	B	401	U10	C7-C8-C9-C10
30	B	401	U10	C12-C13-C14-C16
25	N	504	3PE	O32-C31-O31-C3
25	M	602	3PE	O32-C31-O31-C3
26	M	606	CDL	OA9-CA7-OA8-CA6
28	D	501	PC1	O32-C31-O31-C3
25	N	504	3PE	C32-C31-O31-C3
26	M	606	CDL	C31-CA7-OA8-CA6
22	N	505	3PH	O32-C31-O31-C3
22	H	404	3PH	O32-C31-O31-C3
22	M	607	3PH	O32-C31-O31-C3
23	I	204	P5S	O18-C17-O19-C1
25	M	604	3PE	O32-C31-O31-C3
26	H	402	CDL	OB9-CB7-OB8-CB6
22	J	303	3PH	O22-C21-O21-C2
25	M	602	3PE	O22-C21-O21-C2
25	M	604	3PE	O22-C21-O21-C2
26	H	402	CDL	OB7-CB5-OB6-CB4
23	I	204	P5S	C20-C17-O19-C1
25	M	602	3PE	C32-C31-O31-C3
28	D	501	PC1	C32-C31-O31-C3
22	H	406	3PH	C22-C21-O21-C2
25	M	602	3PE	C22-C21-O21-C2
22	N	505	3PH	C32-C31-O31-C3
22	H	404	3PH	C32-C31-O31-C3
22	L	802	3PH	C32-C31-O31-C3
22	L	806	3PH	C32-C31-O31-C3
22	M	607	3PH	C32-C31-O31-C3
22	M	608	3PH	C32-C31-O31-C3
25	M	604	3PE	C32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
26	H	402	CDL	C71-CB7-OB8-CB6
30	B	401	U10	C17-C18-C19-C20
22	N	505	3PH	O22-C21-O21-C2
25	N	503	3PE	O22-C21-O21-C2
30	B	401	U10	C7-C8-C9-C11
22	H	406	3PH	O32-C31-O31-C3
22	A	201	3PH	O32-C31-O31-C3
22	J	302	3PH	O32-C31-O31-C3
22	L	801	3PH	O32-C31-O31-C3
26	M	606	CDL	O1-C1-CA2-OA2
22	A	201	3PH	C32-C31-O31-C3
22	M	601	3PH	C32-C31-O31-C3
22	L	802	3PH	O32-C31-O31-C3
22	L	806	3PH	O32-C31-O31-C3
22	M	608	3PH	O32-C31-O31-C3
22	M	601	3PH	O32-C31-O31-C3
22	H	406	3PH	C32-C31-O31-C3
22	J	302	3PH	C32-C31-O31-C3
22	L	801	3PH	C32-C31-O31-C3
22	H	406	3PH	C2-C1-O11-P
30	B	401	U10	C9-C11-C12-C13
25	N	503	3PE	C32-C31-O31-C3
26	M	606	CDL	CA7-C31-C32-C33
25	N	503	3PE	O32-C31-O31-C3
22	L	801	3PH	C21-C22-C23-C24
22	I	203	3PH	C21-C22-C23-C24
23	L	803	P5S	C38-C39-C40-C41
25	N	504	3PE	C31-C32-C33-C34
25	M	602	3PE	C31-C32-C33-C34
28	D	501	PC1	C21-C22-C23-C24
28	J	301	PC1	C34-C35-C36-C37
22	L	805	3PH	C22-C21-O21-C2
25	H	401	3PE	C27-C28-C29-C2A
26	H	402	CDL	C31-CA7-OA8-CA6
23	L	803	P5S	C39-C38-O37-C2
23	I	204	P5S	CB-OG-P12-O16
25	N	501	3PE	C11-O13-P-O11
25	N	504	3PE	C1-O11-P-O13
25	H	401	3PE	C11-O13-P-O11
25	q	201	3PE	C11-O13-P-O11
25	M	604	3PE	C11-O13-P-O11
26	H	402	CDL	CB2-OB2-PB2-OB5

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Mol	Chain	Res	Type	Atoms
26	H	402	CDL	CB3-OB5-PB2-OB2
26	M	606	CDL	CA3-OA5-PA1-OA2
26	M	606	CDL	CB2-OB2-PB2-OB5
26	M	606	CDL	CB3-OB5-PB2-OB2
28	D	501	PC1	C1-O11-P-O13
28	J	301	PC1	C32-C31-O31-C3
25	N	503	3PE	C31-C32-C33-C34
26	M	606	CDL	CB2-C1-CA2-OA2
22	L	805	3PH	O22-C21-O21-C2
22	L	801	3PH	C31-C32-C33-C34
22	I	203	3PH	C32-C33-C34-C35
22	L	806	3PH	C22-C21-O21-C2
25	N	501	3PE	C28-C29-C2A-C2B
25	M	602	3PE	C25-C26-C27-C28
23	I	204	P5S	C27-C28-C29-C30
25	H	405	3PE	C2B-C2C-C2D-C2E
22	L	806	3PH	O22-C21-O21-C2
23	L	803	P5S	O47-C38-O37-C2
26	H	402	CDL	CA5-C11-C12-C13
22	J	303	3PH	C37-C38-C39-C3A
28	J	301	PC1	C37-C38-C39-C3A
22	N	505	3PH	C27-C28-C29-C2A
26	H	402	CDL	O1-C1-CB2-OB2
25	L	804	3PE	C34-C35-C36-C37
22	M	607	3PH	C26-C27-C28-C29
26	H	402	CDL	C39-C40-C41-C42
23	I	204	P5S	C31-C32-C33-C34
26	H	402	CDL	C33-C34-C35-C36
25	M	605	3PE	C31-C32-C33-C34
22	J	303	3PH	C35-C36-C37-C38
26	H	402	CDL	C31-C32-C33-C34
26	H	402	CDL	C77-C78-C79-C80
22	H	403	3PH	C37-C38-C39-C3A
22	J	303	3PH	C3E-C3F-C3G-C3H
28	J	301	PC1	C25-C26-C27-C28
25	q	201	3PE	C33-C34-C35-C36
25	M	604	3PE	C27-C28-C29-C2A
26	H	402	CDL	C12-C13-C14-C15
25	M	602	3PE	C24-C25-C26-C27
26	H	402	CDL	C71-C72-C73-C74
22	M	608	3PH	C25-C26-C27-C28
25	L	804	3PE	C32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
25	N	503	3PE	C22-C23-C24-C25
26	M	606	CDL	C11-C12-C13-C14
23	L	803	P5S	C23-C24-C25-C26
26	M	606	CDL	C55-C56-C57-C58
26	H	402	CDL	OA9-CA7-OA8-CA6
22	N	505	3PH	C2A-C2B-C2C-C2D
22	H	403	3PH	C23-C24-C25-C26
25	N	503	3PE	C3B-C3C-C3D-C3E
26	H	402	CDL	C11-C12-C13-C14
28	D	501	PC1	C35-C36-C37-C38
22	N	505	3PH	C36-C37-C38-C39
25	L	804	3PE	C22-C23-C24-C25
22	H	404	3PH	C22-C21-O21-C2
22	J	302	3PH	C22-C21-O21-C2
26	M	606	CDL	C11-CA5-OA6-CA4
25	M	602	3PE	C2-C3-O31-C31
26	H	402	CDL	C37-C38-C39-C40
22	N	502	3PH	C27-C28-C29-C2A
22	L	806	3PH	C34-C35-C36-C37
22	M	608	3PH	C37-C38-C39-C3A
26	M	606	CDL	CB7-C71-C72-C73
28	J	301	PC1	O32-C31-O31-C3
25	M	604	3PE	C37-C38-C39-C3A
25	q	201	3PE	C21-C22-C23-C24
22	J	303	3PH	C3C-C3D-C3E-C3F
22	A	201	3PH	C39-C3A-C3B-C3C
28	D	501	PC1	C11-C12-N-C13
22	N	505	3PH	C26-C27-C28-C29
25	N	503	3PE	C27-C28-C29-C2A
25	H	401	3PE	C33-C34-C35-C36
25	q	201	3PE	C32-C33-C34-C35
25	q	201	3PE	C35-C36-C37-C38
22	I	203	3PH	C22-C21-O21-C2
26	M	606	CDL	C51-CB5-OB6-CB4
25	H	401	3PE	C35-C36-C37-C38
25	H	405	3PE	C21-C22-C23-C24
23	I	204	P5S	C40-C41-C42-C43
30	B	401	U10	C12-C11-C9-C8
25	L	804	3PE	O32-C31-O31-C3
22	H	404	3PH	O22-C21-O21-C2
26	M	606	CDL	OA7-CA5-OA6-CA4
26	H	402	CDL	CB7-C71-C72-C73

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Mol	Chain	Res	Type	Atoms
28	D	501	PC1	C31-C32-C33-C34
23	L	803	P5S	C20-C17-O19-C1
22	L	801	3PH	C3A-C3B-C3C-C3D
26	M	606	CDL	C13-C14-C15-C16
25	M	604	3PE	C36-C37-C38-C39
22	L	805	3PH	C24-C25-C26-C27
28	D	501	PC1	C28-C29-C2A-C2B
22	L	801	3PH	C37-C38-C39-C3A
25	H	405	3PE	C2D-C2E-C2F-C2G
26	H	402	CDL	C72-C73-C74-C75
22	M	603	3PH	C21-C22-C23-C24
23	L	803	P5S	C22-C23-C24-C25
25	L	804	3PE	C26-C27-C28-C29
26	M	606	CDL	OB7-CB5-OB6-CB4
22	N	502	3PH	C25-C26-C27-C28
22	L	802	3PH	C39-C3A-C3B-C3C
22	M	601	3PH	O21-C2-C3-O31
25	H	401	3PE	O21-C2-C3-O31
26	H	402	CDL	OA6-CA4-CA6-OA8
22	M	601	3PH	C37-C38-C39-C3A
28	D	501	PC1	C11-C12-N-C15
22	J	302	3PH	C32-C33-C34-C35
22	M	601	3PH	C33-C34-C35-C36
22	J	303	3PH	C23-C24-C25-C26
25	N	504	3PE	C32-C33-C34-C35
28	D	501	PC1	C22-C23-C24-C25
22	I	203	3PH	C39-C3A-C3B-C3C
22	J	303	3PH	C36-C37-C38-C39
22	I	203	3PH	O22-C21-O21-C2
22	J	302	3PH	O22-C21-O21-C2
22	I	203	3PH	C24-C25-C26-C27
22	N	505	3PH	C3B-C3C-C3D-C3E
22	H	406	3PH	C32-C33-C34-C35
22	J	303	3PH	C3A-C3B-C3C-C3D
22	M	607	3PH	C29-C2A-C2B-C2C
23	I	204	P5S	C29-C30-C31-C32
25	H	405	3PE	C25-C26-C27-C28
22	M	607	3PH	C2-C1-O11-P
22	N	505	3PH	C28-C29-C2A-C2B
25	H	405	3PE	C2C-C2D-C2E-C2F
25	M	605	3PE	C32-C33-C34-C35
23	L	803	P5S	C1-C2-C3-O16

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Mol	Chain	Res	Type	Atoms
25	M	604	3PE	O11-C1-C2-C3
22	J	302	3PH	C34-C35-C36-C37
25	L	804	3PE	C27-C28-C29-C2A
22	L	802	3PH	C23-C24-C25-C26
22	J	303	3PH	C3B-C3C-C3D-C3E
26	M	606	CDL	C38-C39-C40-C41
26	H	402	CDL	CA2-C1-CB2-OB2
25	H	401	3PE	C2C-C2D-C2E-C2F
23	I	204	P5S	C44-C45-C46-C48
25	M	602	3PE	C34-C35-C36-C37
25	N	503	3PE	C35-C36-C37-C38
22	H	406	3PH	C1-C2-C3-O31
22	L	806	3PH	C1-C2-C3-O31
22	M	601	3PH	C1-C2-C3-O31
22	H	406	3PH	C34-C35-C36-C37
25	H	401	3PE	C29-C2A-C2B-C2C
22	L	802	3PH	C31-C32-C33-C34
23	L	803	P5S	O18-C17-O19-C1
26	H	402	CDL	C38-C39-C40-C41
22	J	303	3PH	C33-C34-C35-C36
22	L	801	3PH	C2B-C2C-C2D-C2E
25	H	405	3PE	C22-C21-O21-C2
22	N	502	3PH	C21-C22-C23-C24
25	M	605	3PE	C32-C31-O31-C3
22	I	203	3PH	C26-C27-C28-C29
26	H	402	CDL	CB6-CB4-OB6-CB5
26	M	606	CDL	C54-C55-C56-C57
23	I	204	P5S	C26-C27-C28-C29
22	N	502	3PH	C1-O11-P-O12
22	N	502	3PH	C2-C1-O11-P
22	L	801	3PH	C1-O11-P-O12
22	L	805	3PH	C1-O11-P-O12
23	I	204	P5S	C33-C34-C35-C36
25	q	201	3PE	C32-C31-O31-C3
22	H	406	3PH	O11-C1-C2-O21
28	D	501	PC1	C11-C12-N-C14
22	A	201	3PH	C22-C23-C24-C25
22	M	601	3PH	C34-C35-C36-C37
22	J	302	3PH	C21-C22-C23-C24
25	L	804	3PE	O31-C31-C32-C33
26	M	606	CDL	C33-C34-C35-C36
25	H	405	3PE	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
25	N	501	3PE	C2C-C2D-C2E-C2F
22	N	502	3PH	C34-C35-C36-C37
28	J	301	PC1	C36-C37-C38-C39
22	A	201	3PH	C38-C39-C3A-C3B
26	M	606	CDL	C36-C37-C38-C39
22	I	203	3PH	O11-C1-C2-C3
22	N	502	3PH	O11-C1-C2-C3
22	H	403	3PH	O11-C1-C2-C3
22	A	201	3PH	O11-C1-C2-C3
22	J	303	3PH	O11-C1-C2-C3
22	L	801	3PH	O11-C1-C2-C3
22	M	601	3PH	O11-C1-C2-C3
22	M	607	3PH	O11-C1-C2-C3
23	I	204	P5S	C1-C2-C3-O16
25	N	503	3PE	O11-C1-C2-C3
25	q	201	3PE	O11-C1-C2-C3
26	H	402	CDL	OA5-CA3-CA4-CA6
26	M	606	CDL	OA5-CA3-CA4-CA6
22	M	607	3PH	C28-C29-C2A-C2B
22	M	608	3PH	C33-C34-C35-C36
26	M	606	CDL	C71-CB7-OB8-CB6
22	J	302	3PH	C24-C25-C26-C27
23	L	803	P5S	C2-C3-O16-P12
28	D	501	PC1	C29-C2A-C2B-C2C
25	H	405	3PE	C22-C23-C24-C25
22	I	203	3PH	C1-C2-C3-O31
22	L	802	3PH	C1-C2-C3-O31
22	M	608	3PH	C1-C2-C3-O31
25	H	401	3PE	C1-C2-C3-O31
25	M	605	3PE	C1-C2-C3-O31
28	D	501	PC1	C37-C38-C39-C3A
25	M	602	3PE	C33-C34-C35-C36
22	L	806	3PH	C22-C23-C24-C25
26	H	402	CDL	C11-CA5-OA6-CA4
22	L	802	3PH	C2C-C2D-C2E-C2F
25	q	201	3PE	C22-C23-C24-C25
25	H	401	3PE	C1-O11-P-O13
25	N	501	3PE	C2F-C2G-C2H-C2I
25	M	602	3PE	C36-C37-C38-C39
22	J	303	3PH	O11-C1-C2-O21
22	L	805	3PH	O11-C1-C2-O21
22	M	607	3PH	O11-C1-C2-O21

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Mol	Chain	Res	Type	Atoms
23	L	803	P5S	O37-C2-C3-O16
26	H	402	CDL	OA5-CA3-CA4-OA6
22	A	201	3PH	C36-C37-C38-C39
26	H	402	CDL	C40-C41-C42-C43
25	M	605	3PE	O32-C31-O31-C3
25	H	405	3PE	C33-C34-C35-C36
25	q	201	3PE	C36-C37-C38-C39
22	I	203	3PH	O21-C2-C3-O31
22	L	805	3PH	O21-C2-C3-O31
23	I	204	P5S	O19-C1-C2-O37
25	q	201	3PE	O21-C2-C3-O31
25	M	605	3PE	O21-C2-C3-O31
22	A	201	3PH	C37-C38-C39-C3A
26	H	402	CDL	CB2-C1-CA2-OA2
22	L	802	3PH	C3D-C3E-C3F-C3G
25	H	405	3PE	O22-C21-O21-C2
26	H	402	CDL	OA7-CA5-OA6-CA4
22	H	404	3PH	C2-C1-O11-P
22	A	201	3PH	C2-C1-O11-P
22	L	805	3PH	C2-C1-O11-P
22	L	806	3PH	C2-C1-O11-P
25	M	604	3PE	C2-C1-O11-P
25	q	201	3PE	O32-C31-O31-C3
22	L	801	3PH	C2F-C2G-C2H-C2I
26	H	402	CDL	C75-C76-C77-C78
22	N	505	3PH	O11-C1-C2-C3
25	M	602	3PE	O11-C1-C2-C3
22	L	805	3PH	C32-C33-C34-C35
22	H	406	3PH	C24-C25-C26-C27
25	N	503	3PE	C2B-C2C-C2D-C2E
27	F	501	FMN	C5'-O5'-P-O3P
25	H	405	3PE	C32-C31-O31-C3
22	L	805	3PH	C2E-C2F-C2G-C2H
23	L	803	P5S	C25-C26-C27-C28
22	H	403	3PH	C1-C2-O21-C21
22	H	406	3PH	C1-C2-O21-C21
25	q	201	3PE	C1-C2-O21-C21
25	M	604	3PE	C1-C2-O21-C21
26	M	606	CDL	CA6-CA4-OA6-CA5
25	H	405	3PE	C31-C32-C33-C34
22	I	203	3PH	C33-C34-C35-C36
22	N	505	3PH	C2B-C2C-C2D-C2E

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Mol	Chain	Res	Type	Atoms
22	N	502	3PH	C1-C2-C3-O31
23	I	204	P5S	C2-C3-O16-P12
22	L	801	3PH	O11-C1-C2-O21
22	M	601	3PH	O11-C1-C2-O21
23	I	204	P5S	O37-C2-C3-O16
25	N	503	3PE	O11-C1-C2-O21
28	J	301	PC1	O11-C1-C2-O21
25	N	504	3PE	C28-C29-C2A-C2B
25	H	405	3PE	C38-C39-C3A-C3B
22	H	406	3PH	O21-C2-C3-O31
22	L	802	3PH	O21-C2-C3-O31
25	N	504	3PE	O21-C2-C3-O31
26	M	606	CDL	OB9-CB7-OB8-CB6
25	M	602	3PE	C23-C24-C25-C26
22	L	802	3PH	C3C-C3D-C3E-C3F
26	H	402	CDL	C74-C75-C76-C77
23	L	803	P5S	CB-OG-P12-O16
25	N	504	3PE	C11-O13-P-O11
26	H	402	CDL	CA2-OA2-PA1-OA5
22	M	601	3PH	C2-C1-O11-P
22	M	608	3PH	C2-C1-O11-P
26	H	402	CDL	C1-CA2-OA2-PA1
25	N	501	3PE	C11-O13-P-O14
25	N	504	3PE	C1-O11-P-O12
25	H	405	3PE	C1-O11-P-O14
25	q	201	3PE	C11-O13-P-O12
25	M	604	3PE	C1-O11-P-O12
25	M	605	3PE	C11-O13-P-O12
26	M	606	CDL	CA3-OA5-PA1-OA3
26	M	606	CDL	CB3-OB5-PB2-OB4
28	D	501	PC1	C1-O11-P-O12
22	M	608	3PH	C24-C25-C26-C27
22	H	406	3PH	O11-C1-C2-C3
25	H	401	3PE	O11-C1-C2-C3
25	H	405	3PE	O11-C1-C2-C3
28	J	301	PC1	O11-C1-C2-C3
28	D	501	PC1	C34-C35-C36-C37
22	L	802	3PH	C3E-C3F-C3G-C3H
28	J	301	PC1	C3D-C3E-C3F-C3G
25	M	602	3PE	C12-C11-O13-P
30	B	401	U10	C18-C19-C21-C22
26	M	606	CDL	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
28	D	501	PC1	C2A-C2B-C2C-C2D
25	N	503	3PE	C2A-C2B-C2C-C2D
22	H	406	3PH	C21-C22-C23-C24
22	M	608	3PH	C21-C22-C23-C24
25	H	405	3PE	C27-C28-C29-C2A
22	I	203	3PH	O11-C1-C2-O21
22	N	505	3PH	O11-C1-C2-O21
25	H	405	3PE	O11-C1-C2-O21
25	q	201	3PE	O11-C1-C2-O21
25	M	604	3PE	O11-C1-C2-O21
26	M	606	CDL	OA5-CA3-CA4-OA6
22	J	303	3PH	C21-C22-C23-C24
25	N	504	3PE	C33-C34-C35-C36
25	N	504	3PE	C1-C2-C3-O31
25	q	201	3PE	C1-C2-C3-O31
26	H	402	CDL	CA3-CA4-CA6-OA8
26	M	606	CDL	CB3-CB4-CB6-OB8
25	H	405	3PE	O32-C31-O31-C3
22	L	806	3PH	O21-C2-C3-O31
22	N	502	3PH	C36-C37-C38-C39
22	L	801	3PH	C3E-C3F-C3G-C3H
22	N	505	3PH	C39-C3A-C3B-C3C
22	J	303	3PH	C34-C35-C36-C37
22	L	806	3PH	C21-C22-C23-C24
25	N	504	3PE	C26-C27-C28-C29
25	N	501	3PE	C36-C37-C38-C39
22	N	502	3PH	C2E-C2F-C2G-C2H
25	H	405	3PE	C37-C38-C39-C3A
25	L	804	3PE	C25-C26-C27-C28
22	M	601	3PH	O22-C21-O21-C2
22	M	601	3PH	C22-C21-O21-C2
25	N	504	3PE	C24-C25-C26-C27
22	H	404	3PH	O21-C21-C22-C23
22	N	505	3PH	C34-C35-C36-C37
25	M	602	3PE	C28-C29-C2A-C2B
22	L	805	3PH	O11-C1-C2-C3
22	M	601	3PH	O31-C31-C32-C33
22	N	505	3PH	C1-O11-P-O12
27	F	501	FMN	C4'-C5'-O5'-P
27	F	501	FMN	C5'-O5'-P-O1P
22	N	502	3PH	O11-C1-C2-O21
22	H	403	3PH	O11-C1-C2-O21

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Mol	Chain	Res	Type	Atoms
23	L	803	P5S	C42-C43-C44-C45
22	M	608	3PH	O21-C2-C3-O31
25	M	602	3PE	C1-O11-P-O13
25	M	605	3PE	C1-O11-P-O13
26	M	606	CDL	CA2-OA2-PA1-OA5
22	L	801	3PH	C27-C28-C29-C2A
30	B	401	U10	C5-C4-O4-C4M
22	N	502	3PH	C23-C24-C25-C26
25	N	504	3PE	C27-C28-C29-C2A
22	J	303	3PH	C2-C1-O11-P
25	L	804	3PE	C31-C32-C33-C34
22	L	802	3PH	C32-C33-C34-C35
22	M	603	3PH	C39-C3A-C3B-C3C
25	N	504	3PE	C36-C37-C38-C39
22	N	505	3PH	C32-C33-C34-C35
23	L	803	P5S	C21-C22-C23-C24
25	N	503	3PE	C37-C38-C39-C3A
25	N	504	3PE	C22-C23-C24-C25
25	M	602	3PE	C27-C28-C29-C2A
25	H	405	3PE	C28-C29-C2A-C2B
22	M	608	3PH	O22-C21-O21-C2
25	M	602	3PE	C2E-C2F-C2G-C2H
22	J	303	3PH	C38-C39-C3A-C3B
25	H	405	3PE	C34-C35-C36-C37
22	L	801	3PH	C3C-C3D-C3E-C3F
25	N	501	3PE	C34-C35-C36-C37
25	N	501	3PE	C26-C27-C28-C29
25	L	804	3PE	C35-C36-C37-C38
23	I	204	P5S	O19-C1-C2-C3
25	H	401	3PE	C22-C23-C24-C25
22	H	403	3PH	C35-C36-C37-C38
22	H	403	3PH	C26-C27-C28-C29
22	M	601	3PH	C24-C25-C26-C27
25	q	201	3PE	C1-O11-P-O13
25	L	804	3PE	C1-O11-P-O13
28	J	301	PC1	C31-C32-C33-C34
25	N	501	3PE	C25-C26-C27-C28
28	D	501	PC1	C26-C27-C28-C29
25	H	401	3PE	O11-C1-C2-O21
25	M	604	3PE	C34-C35-C36-C37
25	M	604	3PE	C28-C29-C2A-C2B
25	L	804	3PE	C2D-C2E-C2F-C2G

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Mol	Chain	Res	Type	Atoms
22	M	603	3PH	O21-C21-C22-C23
30	B	401	U10	C12-C11-C9-C10
25	L	804	3PE	C39-C3A-C3B-C3C
25	L	804	3PE	O32-C31-C32-C33
22	A	201	3PH	O31-C31-C32-C33
25	M	604	3PE	O21-C21-C22-C23
25	M	602	3PE	O31-C31-C32-C33
22	H	406	3PH	O21-C21-C22-C23
22	J	302	3PH	O31-C31-C32-C33
22	N	505	3PH	C3D-C3E-C3F-C3G
22	M	608	3PH	C22-C21-O21-C2
22	I	203	3PH	C1-O11-P-O14
22	N	502	3PH	C1-O11-P-O14
22	L	805	3PH	C1-O11-P-O13
25	L	804	3PE	C2A-C2B-C2C-C2D
28	J	301	PC1	C27-C28-C29-C2A
25	q	201	3PE	O21-C21-C22-C23
22	L	806	3PH	C24-C25-C26-C27
22	M	608	3PH	C34-C35-C36-C37
22	I	203	3PH	C3D-C3E-C3F-C3G
28	D	501	PC1	C27-C28-C29-C2A
25	N	503	3PE	C26-C27-C28-C29
22	J	303	3PH	C22-C23-C24-C25
22	L	802	3PH	O21-C21-C22-C23
25	H	401	3PE	C2B-C2C-C2D-C2E
22	N	502	3PH	O31-C31-C32-C33
26	H	402	CDL	C12-C11-CA5-OA6
26	M	606	CDL	C53-C54-C55-C56
22	J	302	3PH	C1-O11-P-O12
25	L	804	3PE	O11-C1-C2-O21
22	A	201	3PH	C32-C33-C34-C35
23	I	204	P5S	C30-C31-C32-C33
25	N	503	3PE	C36-C37-C38-C39
26	M	606	CDL	C51-C52-C53-C54
25	N	503	3PE	O31-C31-C32-C33
22	M	608	3PH	O31-C31-C32-C33
23	L	803	P5S	O19-C17-C20-C21
22	J	303	3PH	C3D-C3E-C3F-C3G
25	H	405	3PE	C32-C33-C34-C35
25	M	605	3PE	C23-C24-C25-C26
22	H	406	3PH	O22-C21-C22-C23
25	M	602	3PE	O32-C31-C32-C33

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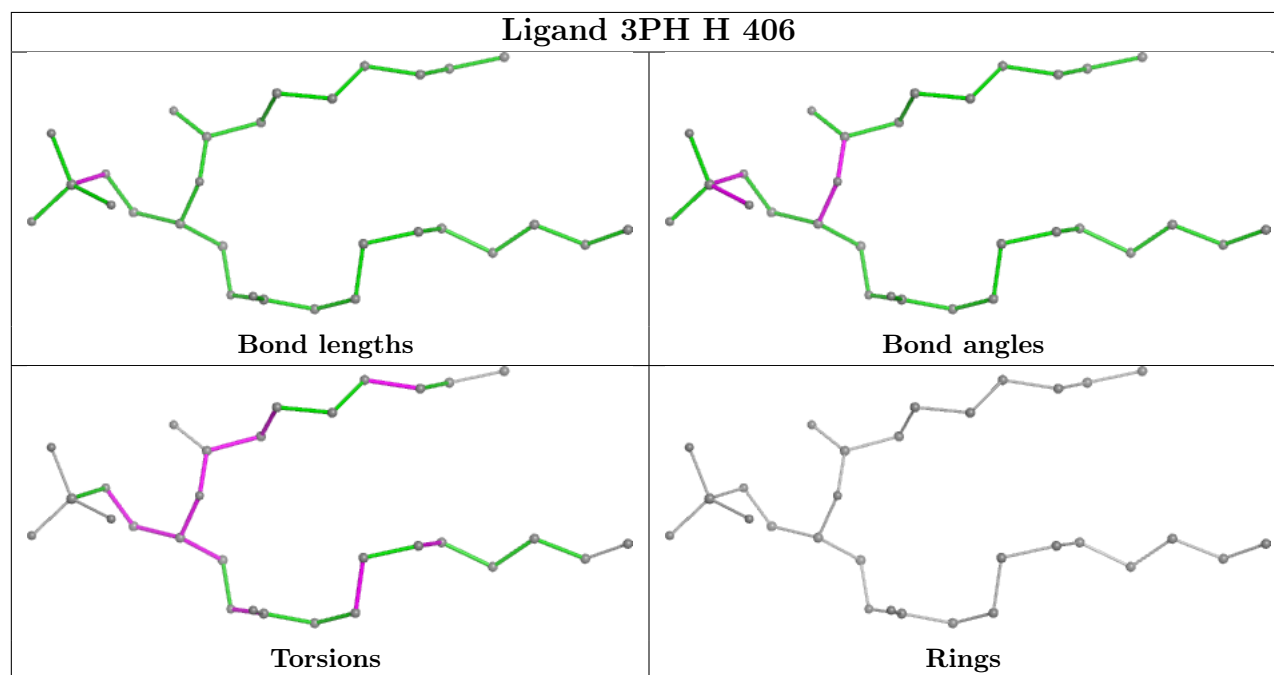
Mol	Chain	Res	Type	Atoms
22	L	802	3PH	C36-C37-C38-C39
22	L	801	3PH	O31-C31-C32-C33
25	N	501	3PE	C32-C33-C34-C35
22	J	303	3PH	C32-C31-O31-C3
23	I	204	P5S	C42-C43-C44-C45
25	N	501	3PE	C2E-C2F-C2G-C2H
22	J	302	3PH	O32-C31-C32-C33
26	H	402	CDL	C12-C11-CA5-OA7
28	J	301	PC1	O31-C31-C32-C33
22	L	802	3PH	C3A-C3B-C3C-C3D
26	H	402	CDL	CA4-CA3-OA5-PA1
22	N	505	3PH	C38-C39-C3A-C3B
25	L	804	3PE	C2C-C2D-C2E-C2F
22	N	502	3PH	O32-C31-C32-C33
25	q	201	3PE	O22-C21-C22-C23
25	H	401	3PE	C1-O11-P-O14
25	q	201	3PE	C1-O11-P-O12
25	L	804	3PE	C1-O11-P-O14
25	M	605	3PE	C1-O11-P-O14
22	M	608	3PH	O32-C31-C32-C33
22	L	802	3PH	C3B-C3C-C3D-C3E
25	M	604	3PE	C33-C34-C35-C36
25	M	602	3PE	C2C-C2D-C2E-C2F
22	J	303	3PH	O32-C31-O31-C3
28	J	301	PC1	C35-C36-C37-C38
22	M	607	3PH	C22-C23-C24-C25
22	L	802	3PH	O22-C21-C22-C23
22	N	502	3PH	C1-C2-O21-C21
22	M	603	3PH	O31-C31-C32-C33
25	N	503	3PE	O32-C31-C32-C33
28	J	301	PC1	O32-C31-C32-C33
22	L	801	3PH	O32-C31-C32-C33
23	L	803	P5S	O18-C17-C20-C21
25	M	604	3PE	C32-C33-C34-C35
22	M	603	3PH	O32-C31-C32-C33
25	N	501	3PE	O21-C21-C22-C23
22	L	806	3PH	C26-C27-C28-C29
28	J	301	PC1	C11-C12-N-C14
22	H	403	3PH	O21-C21-C22-C23

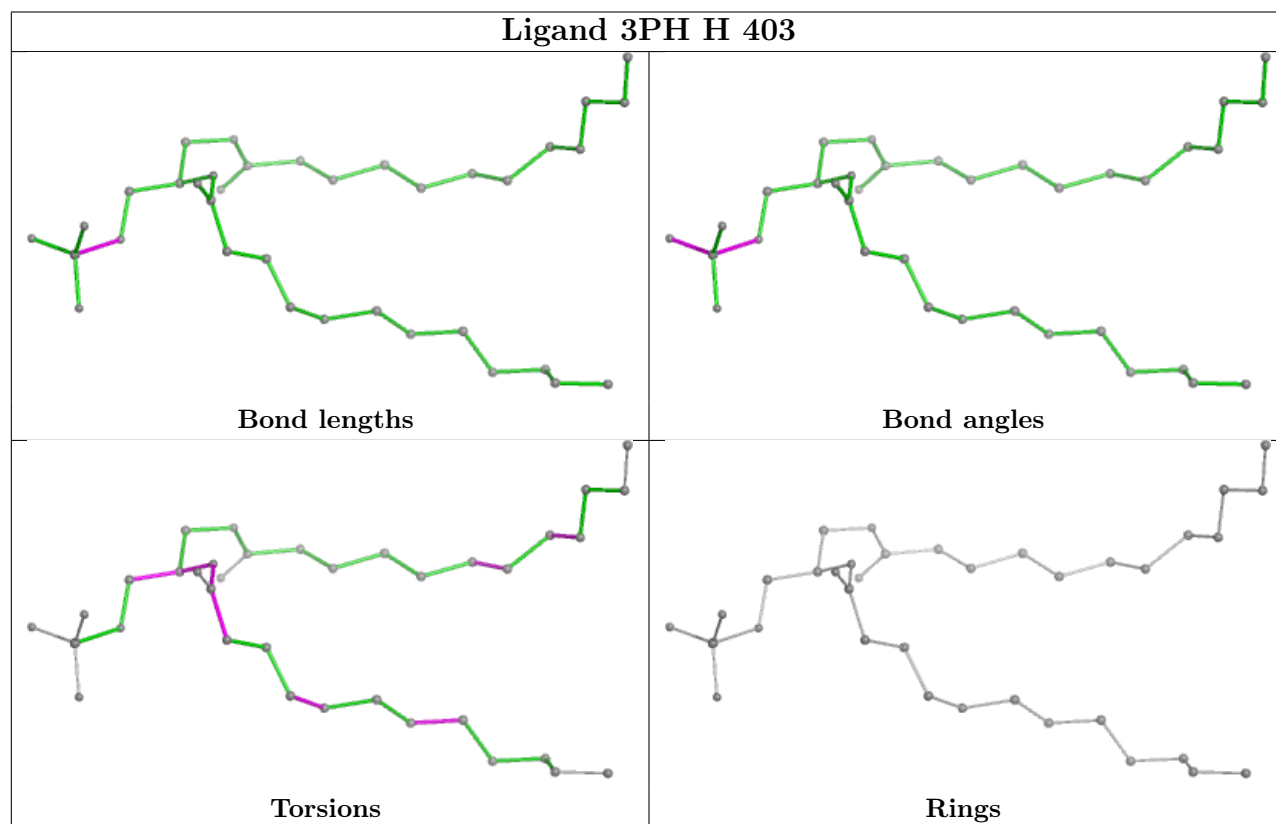
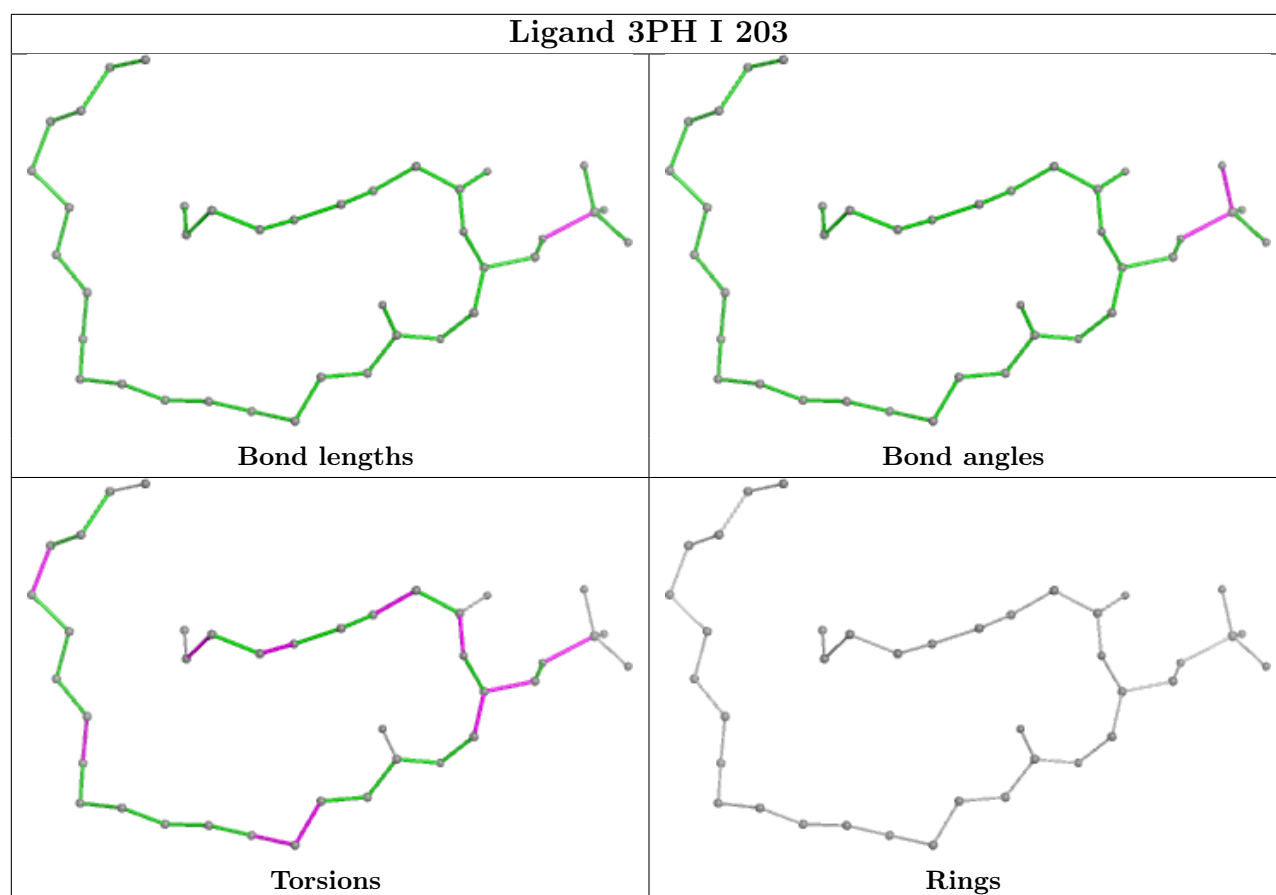
There are no ring outliers.

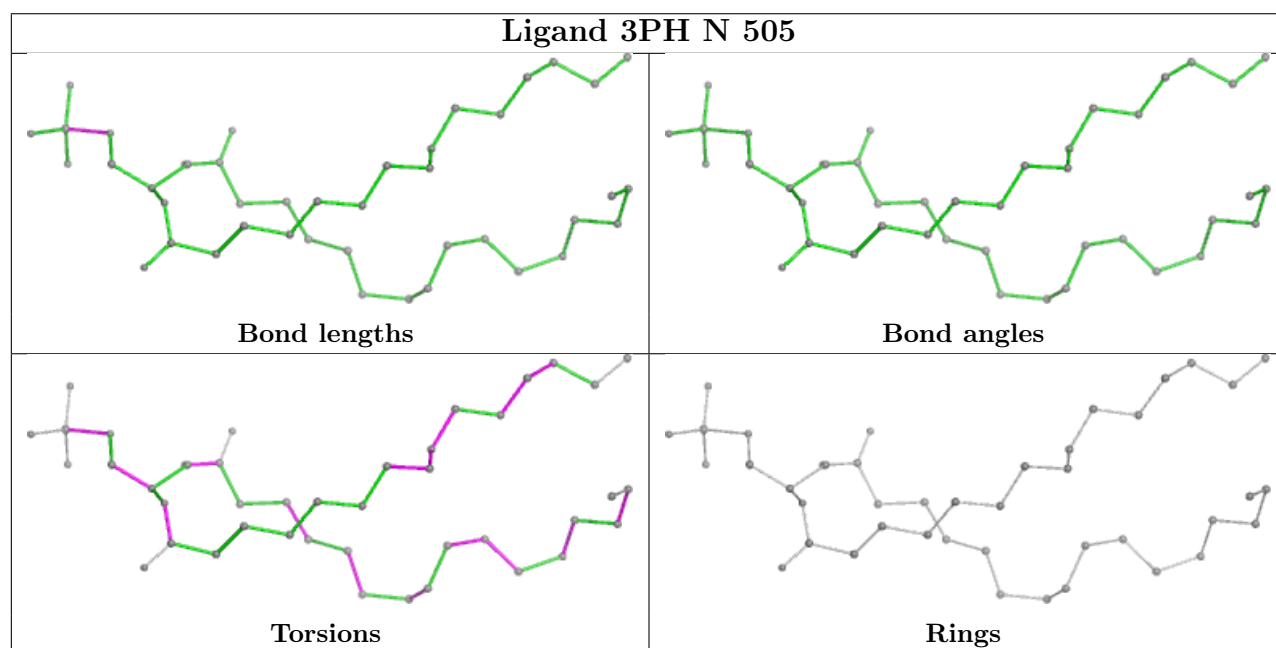
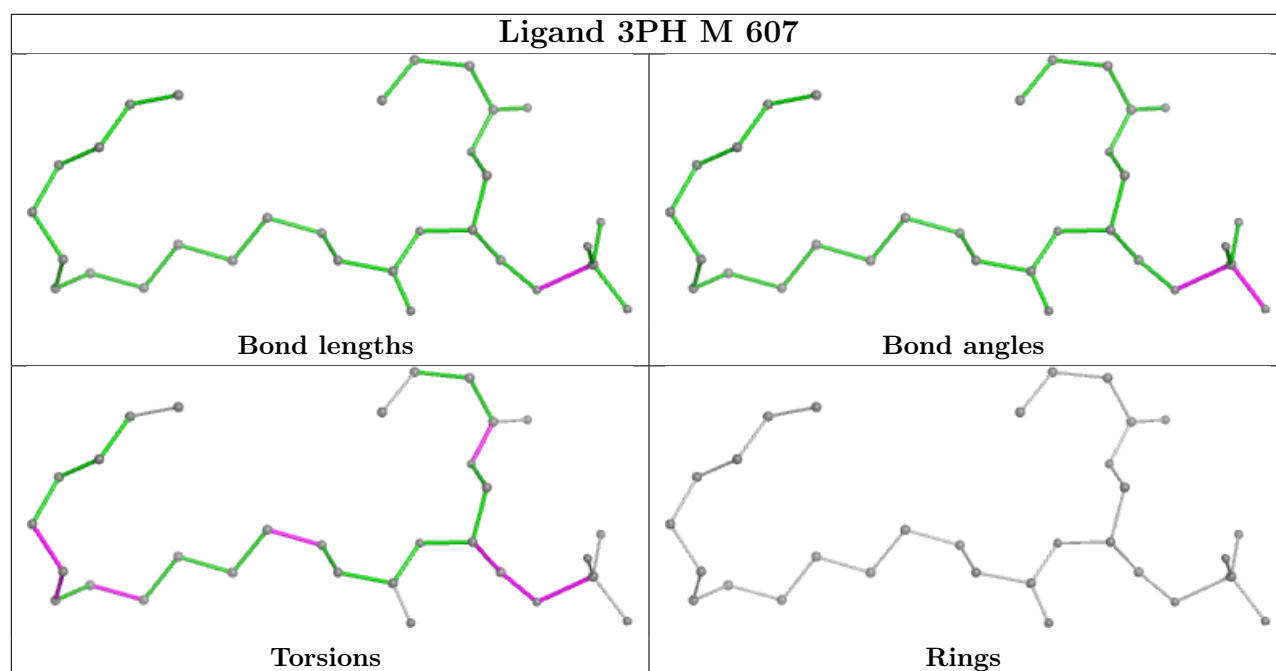
10 monomers are involved in 13 short contacts:

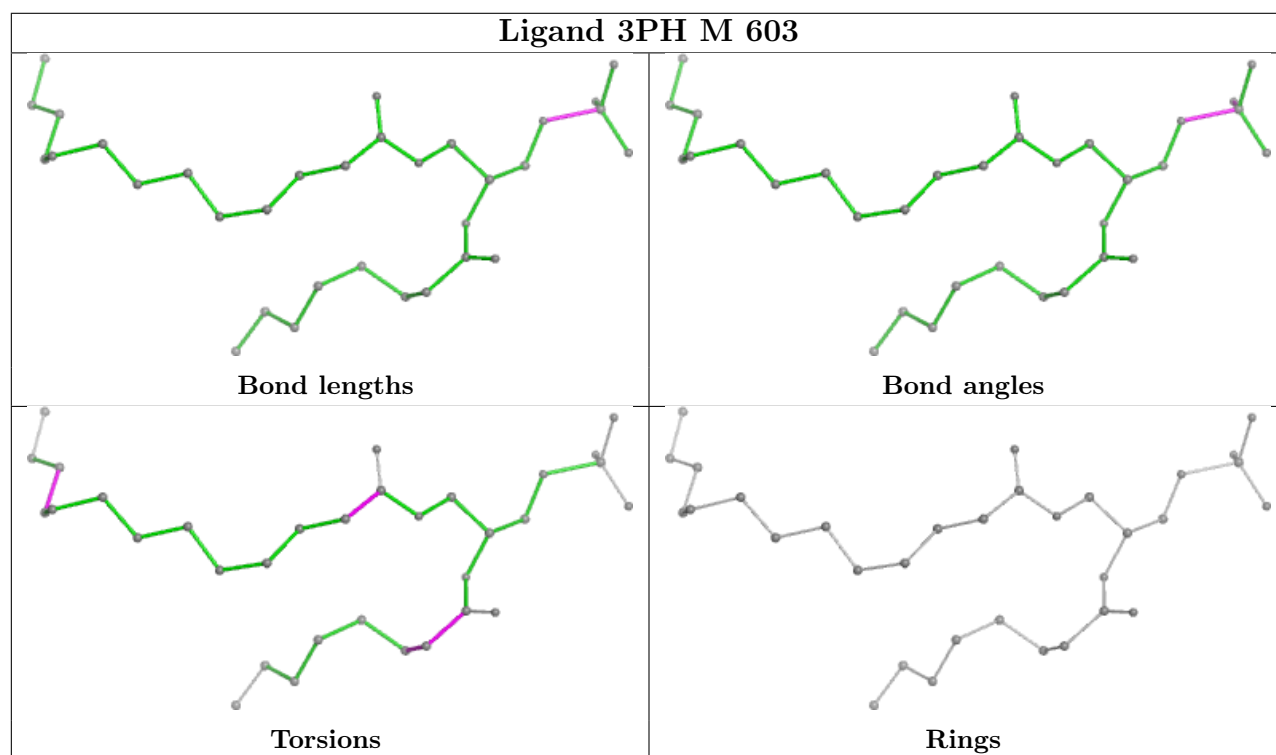
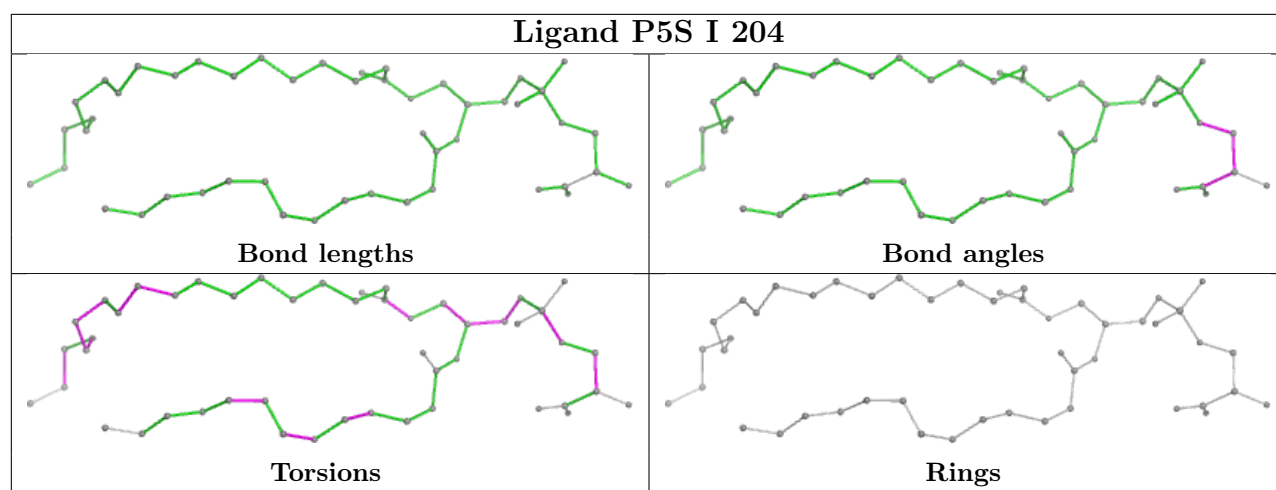
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	I	204	P5S	1	0
22	M	603	3PH	1	0
19	F	502	SF4	1	0
30	B	401	U10	3	0
19	B	402	SF4	1	0
28	D	501	PC1	1	0
25	N	501	3PE	2	0
23	L	803	P5S	1	0
22	L	802	3PH	1	0
22	L	805	3PH	1	0

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

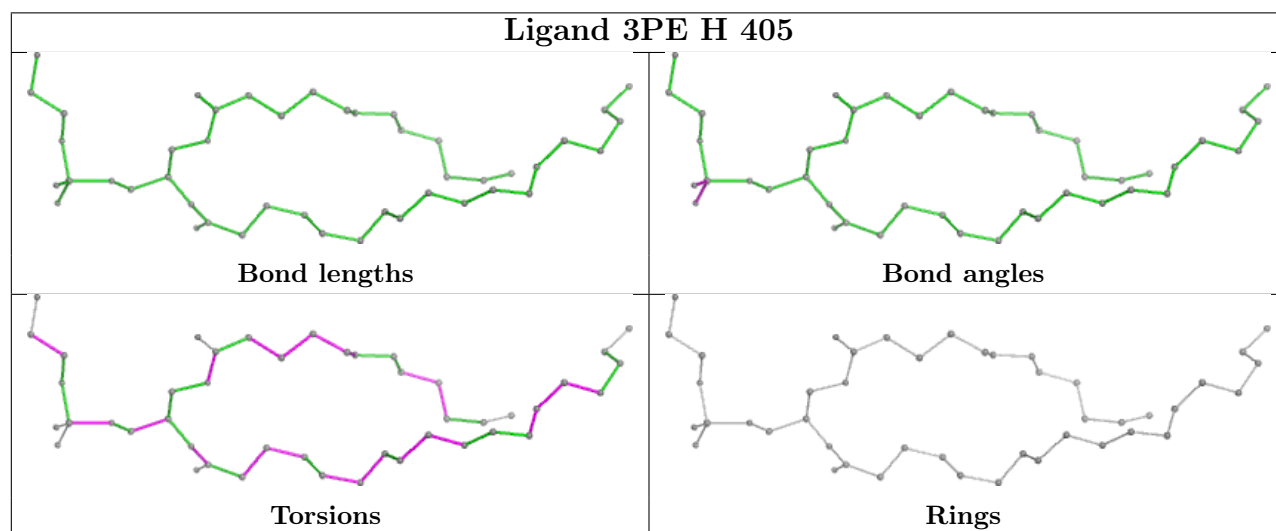
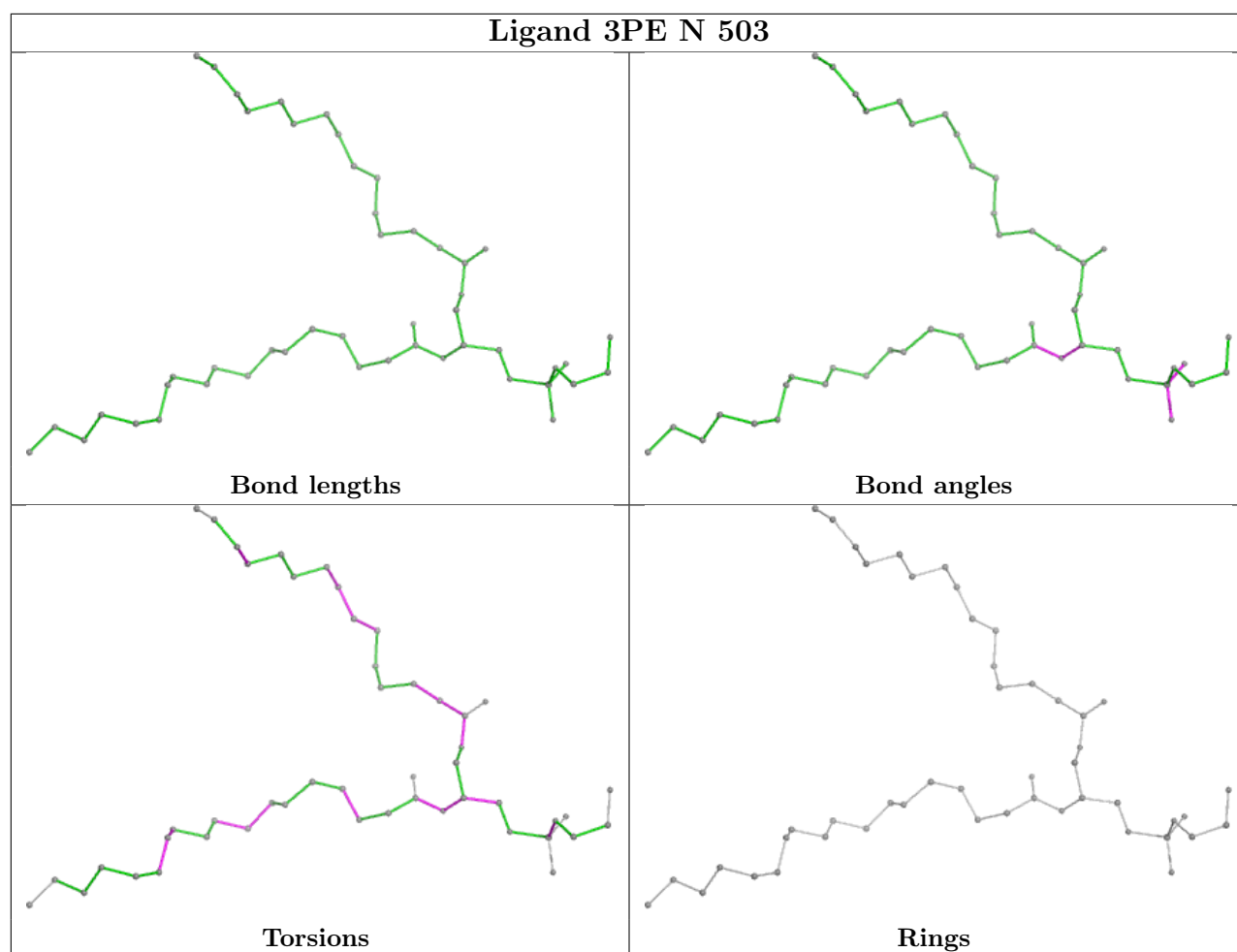


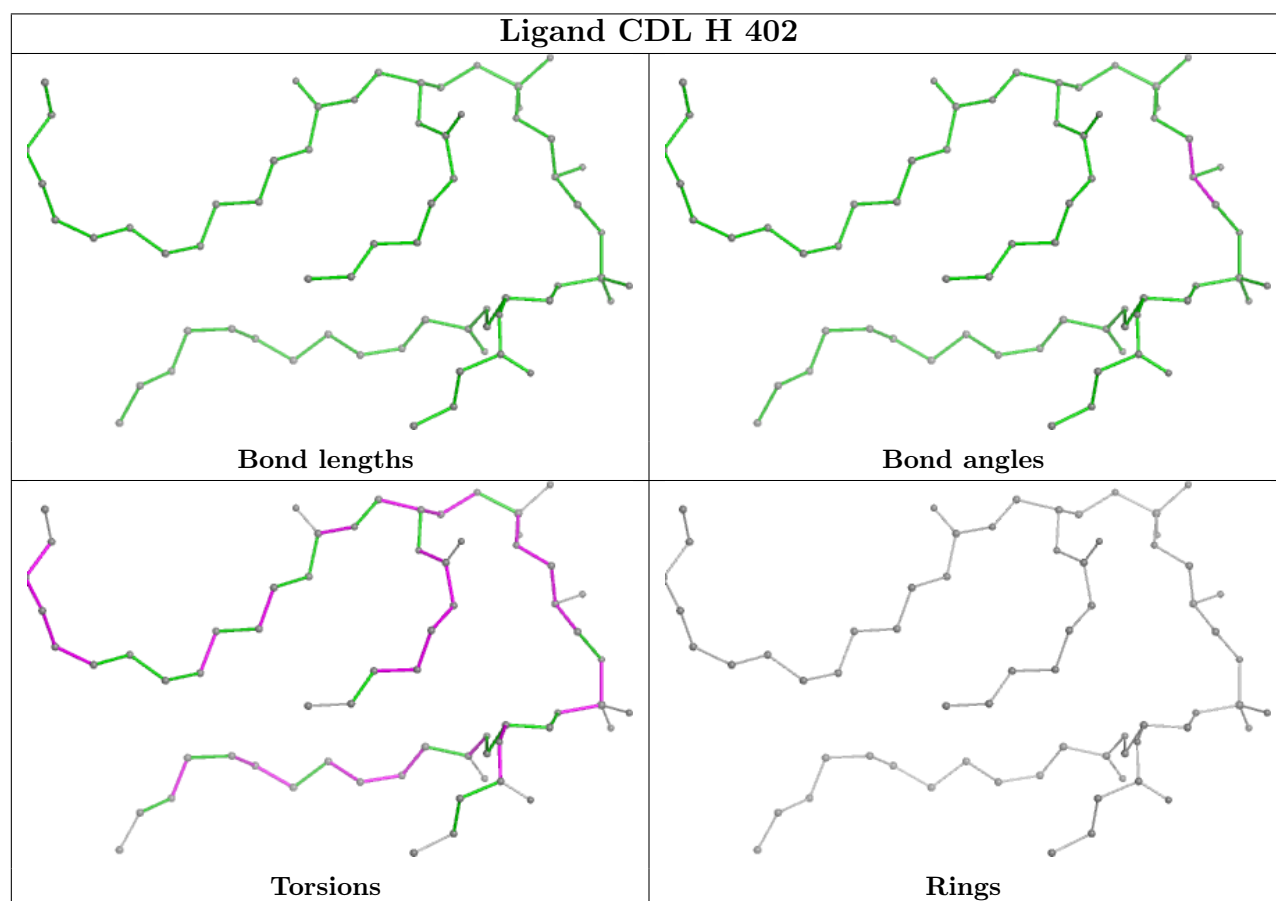
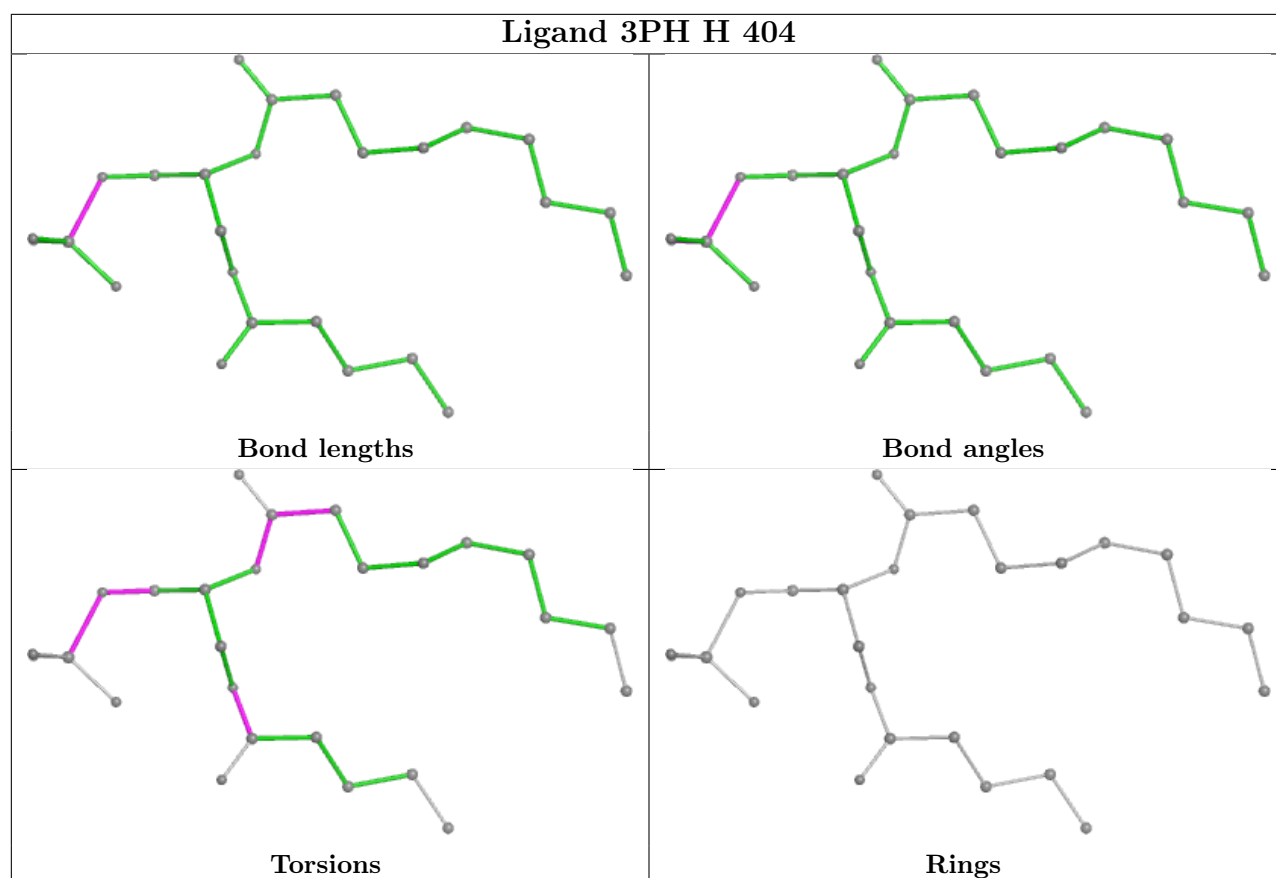


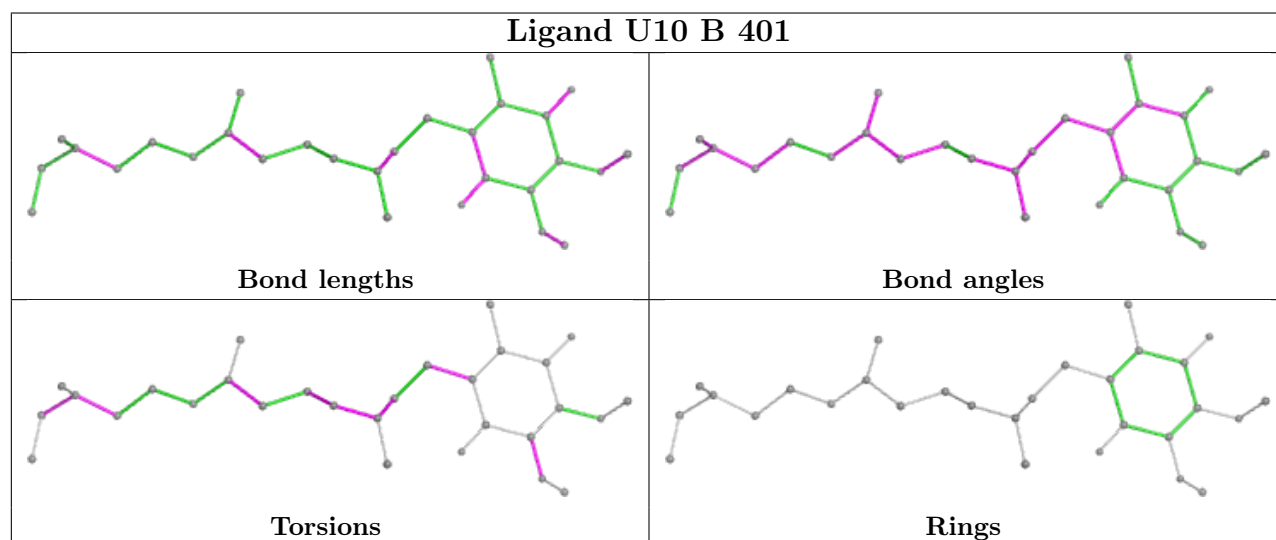
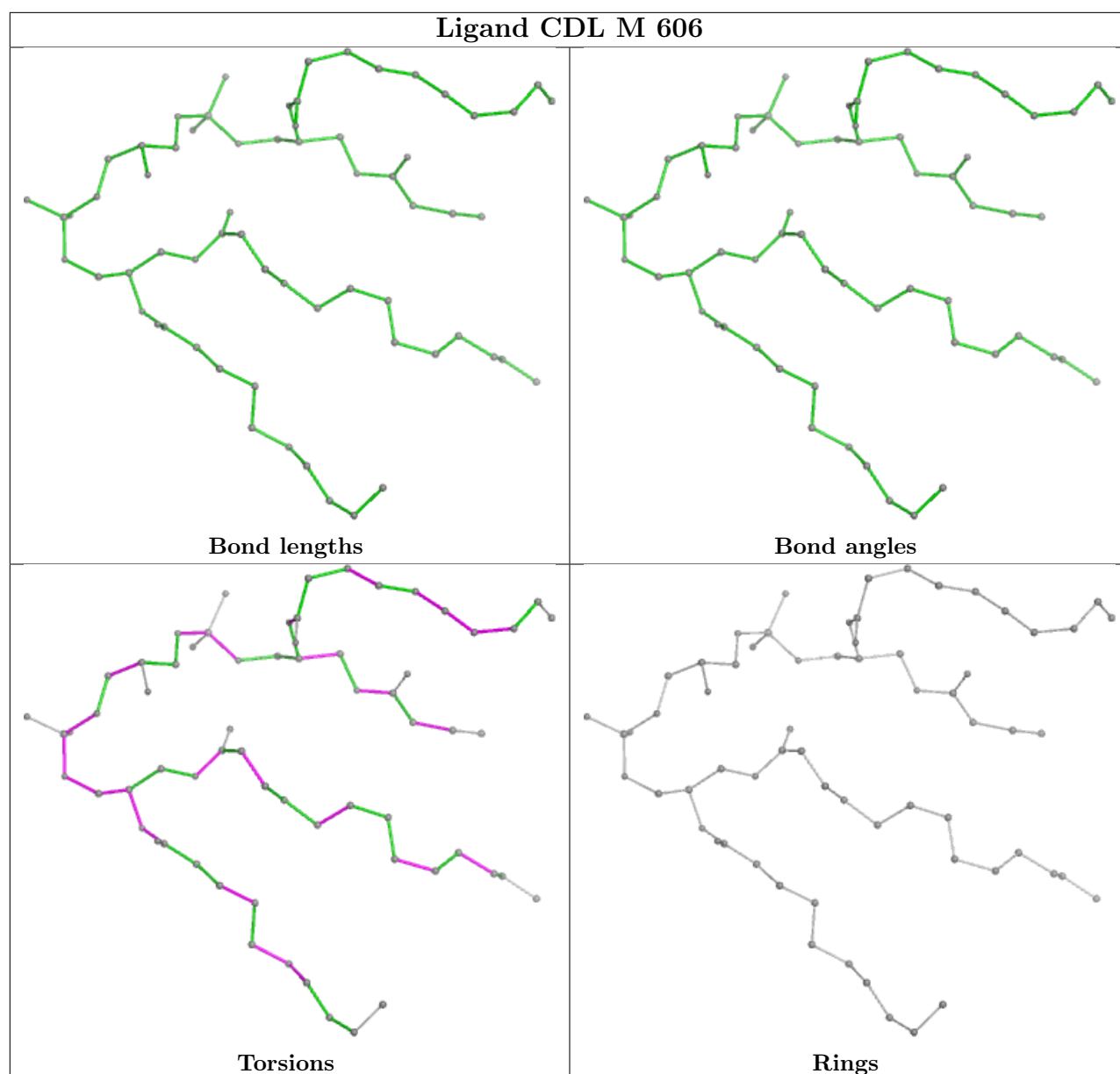


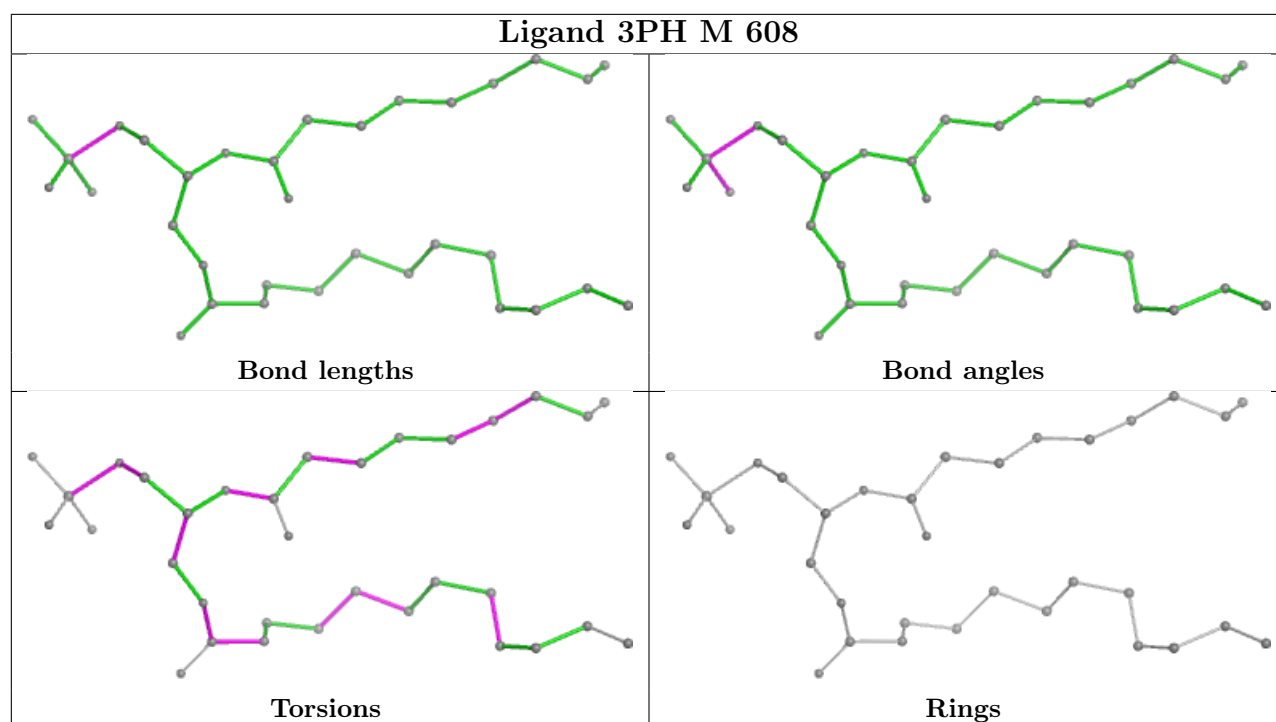


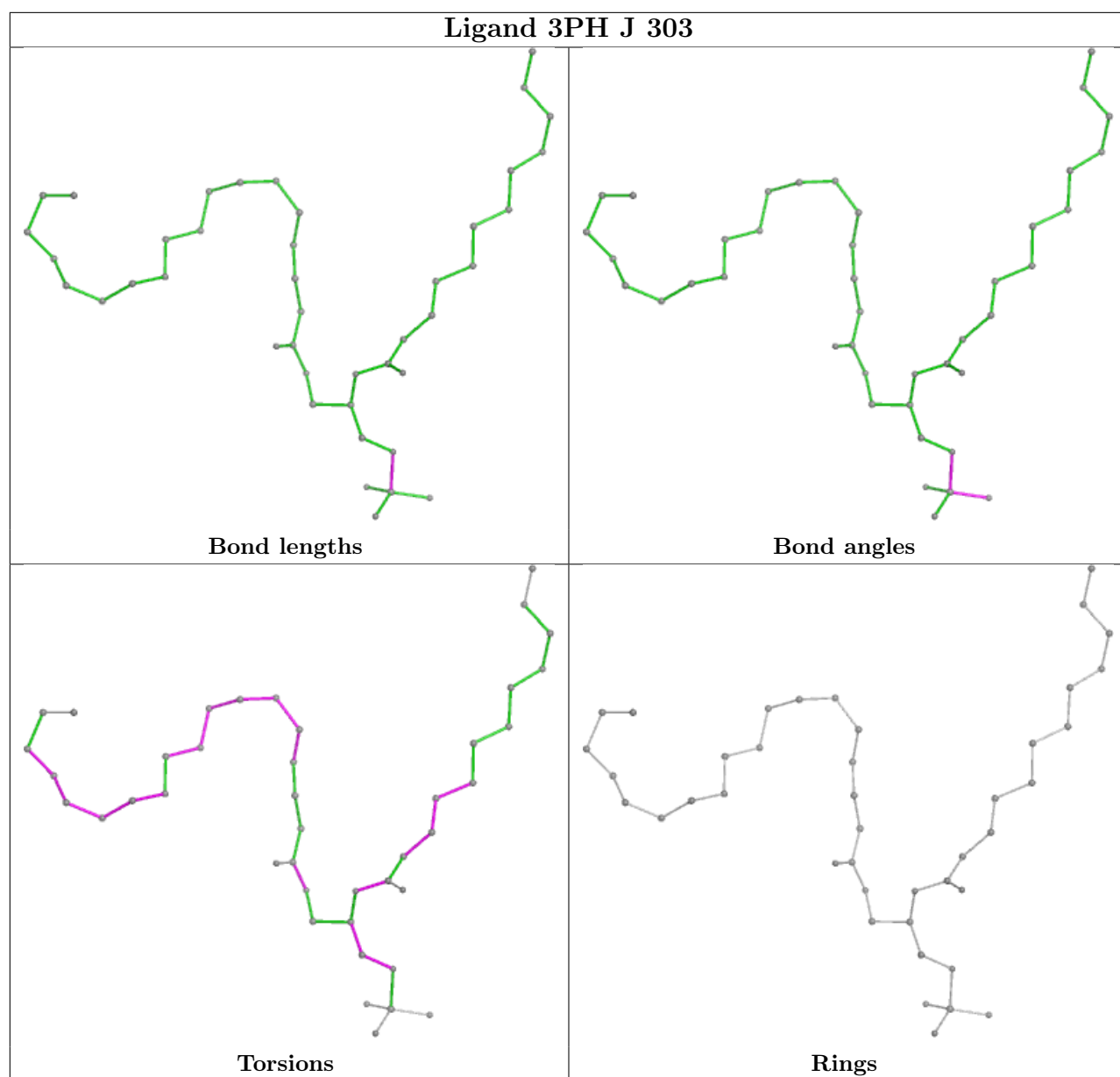


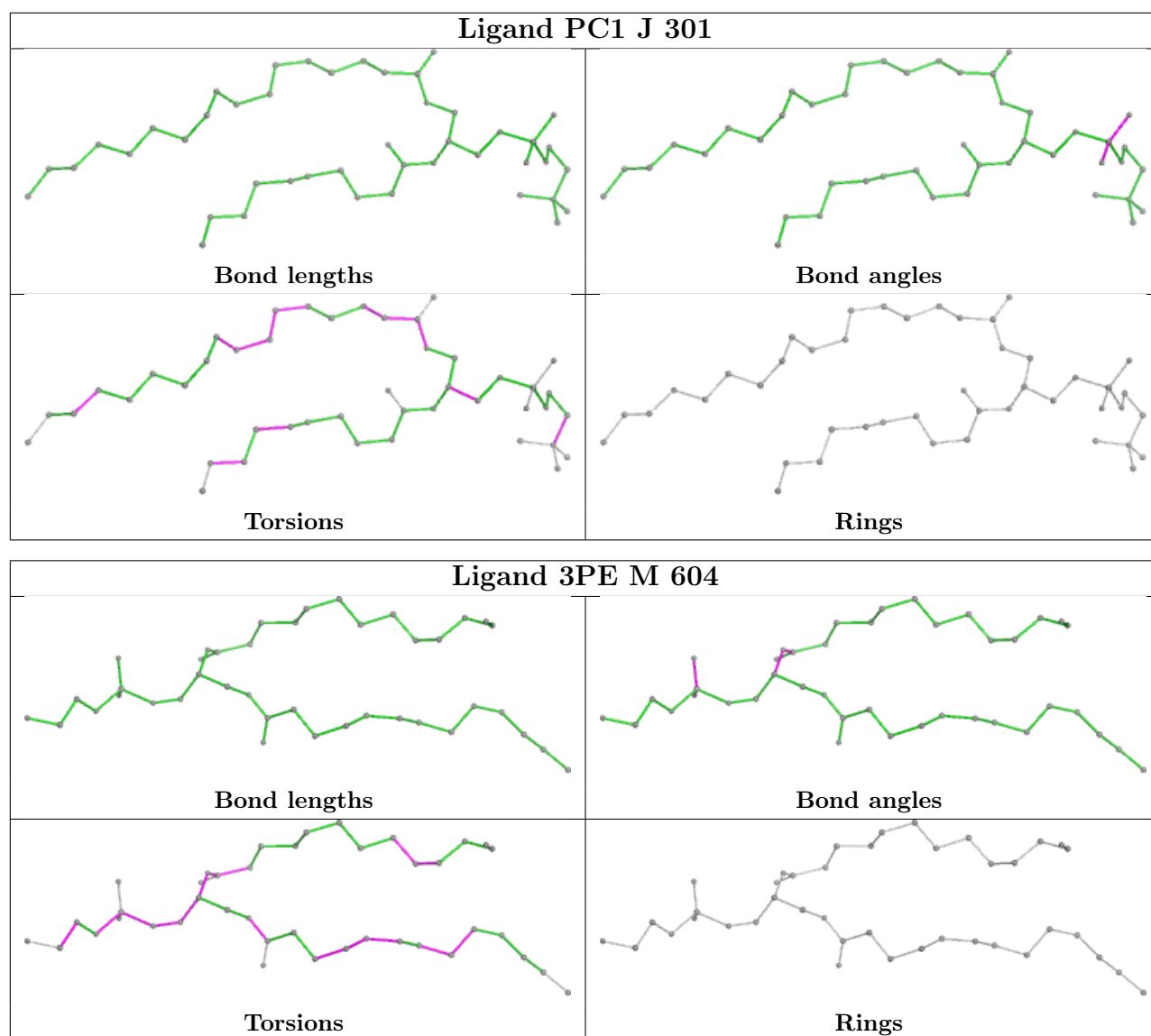


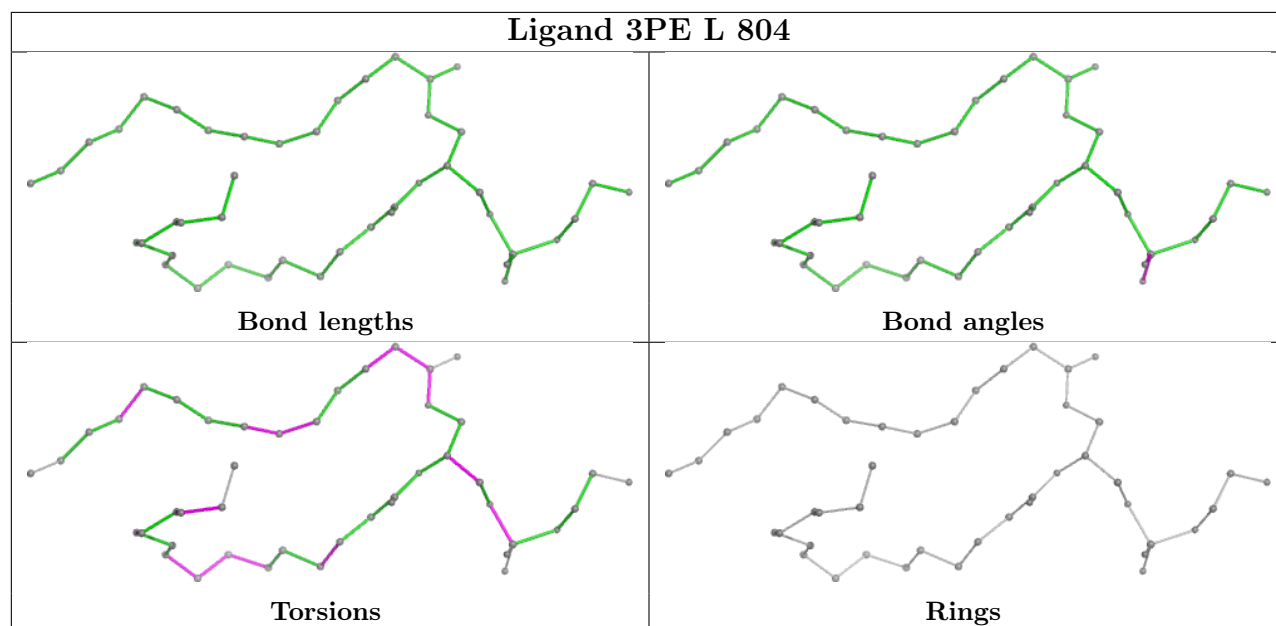
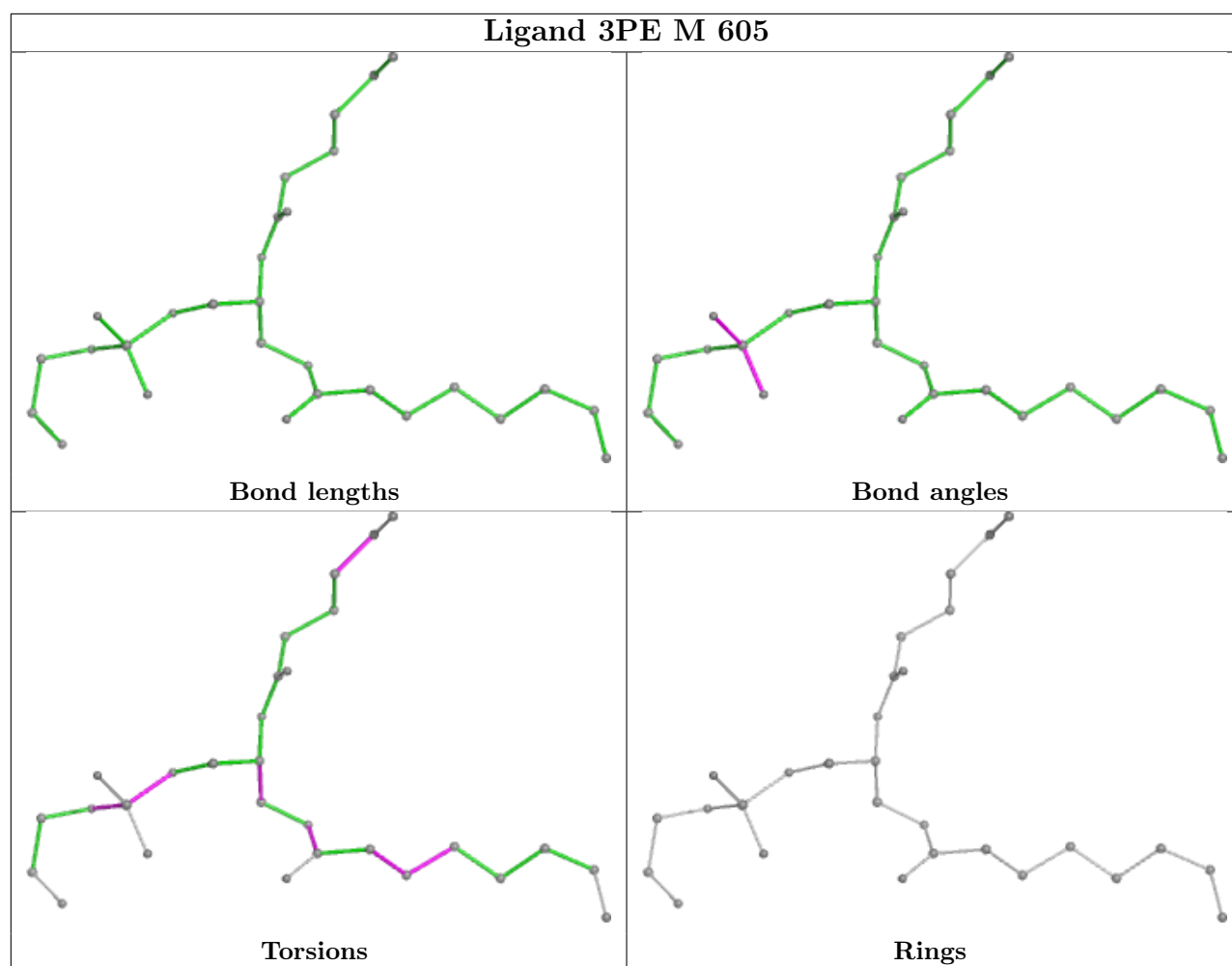


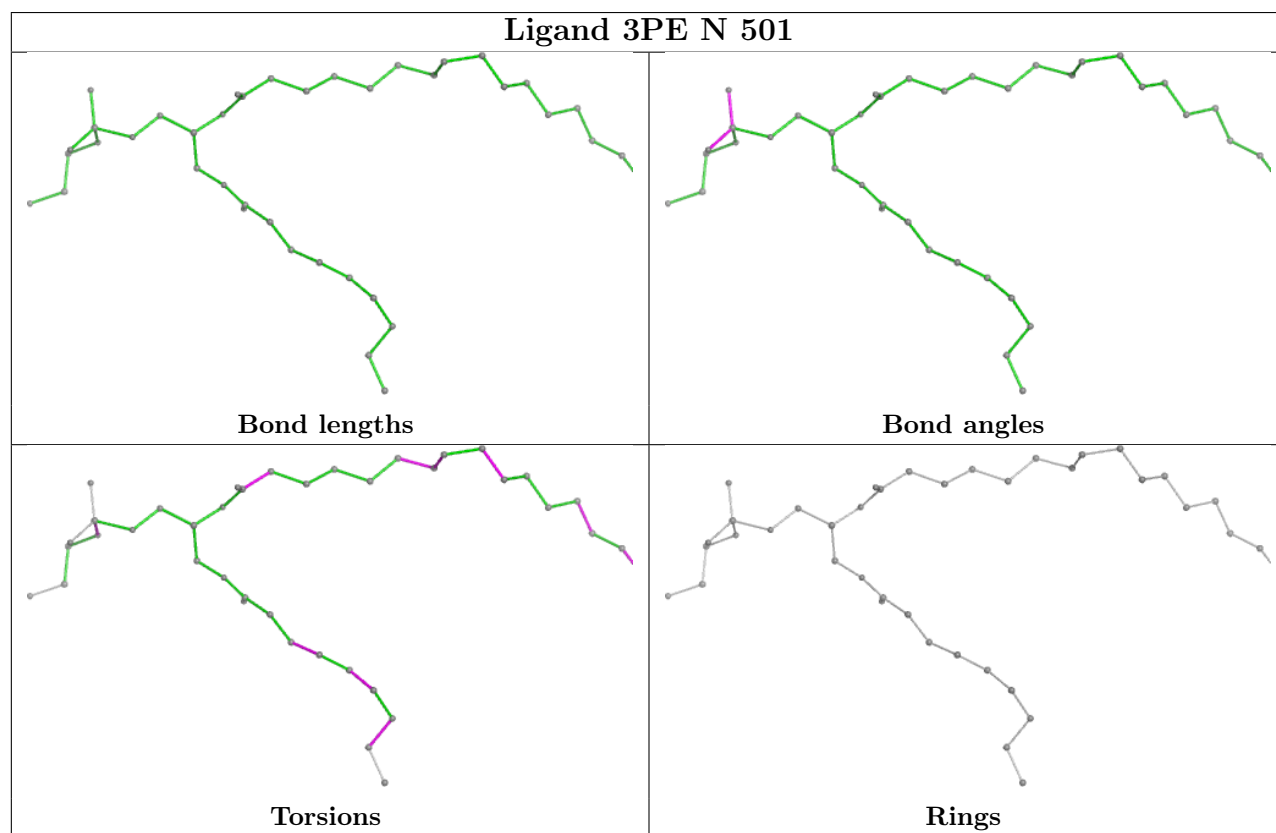
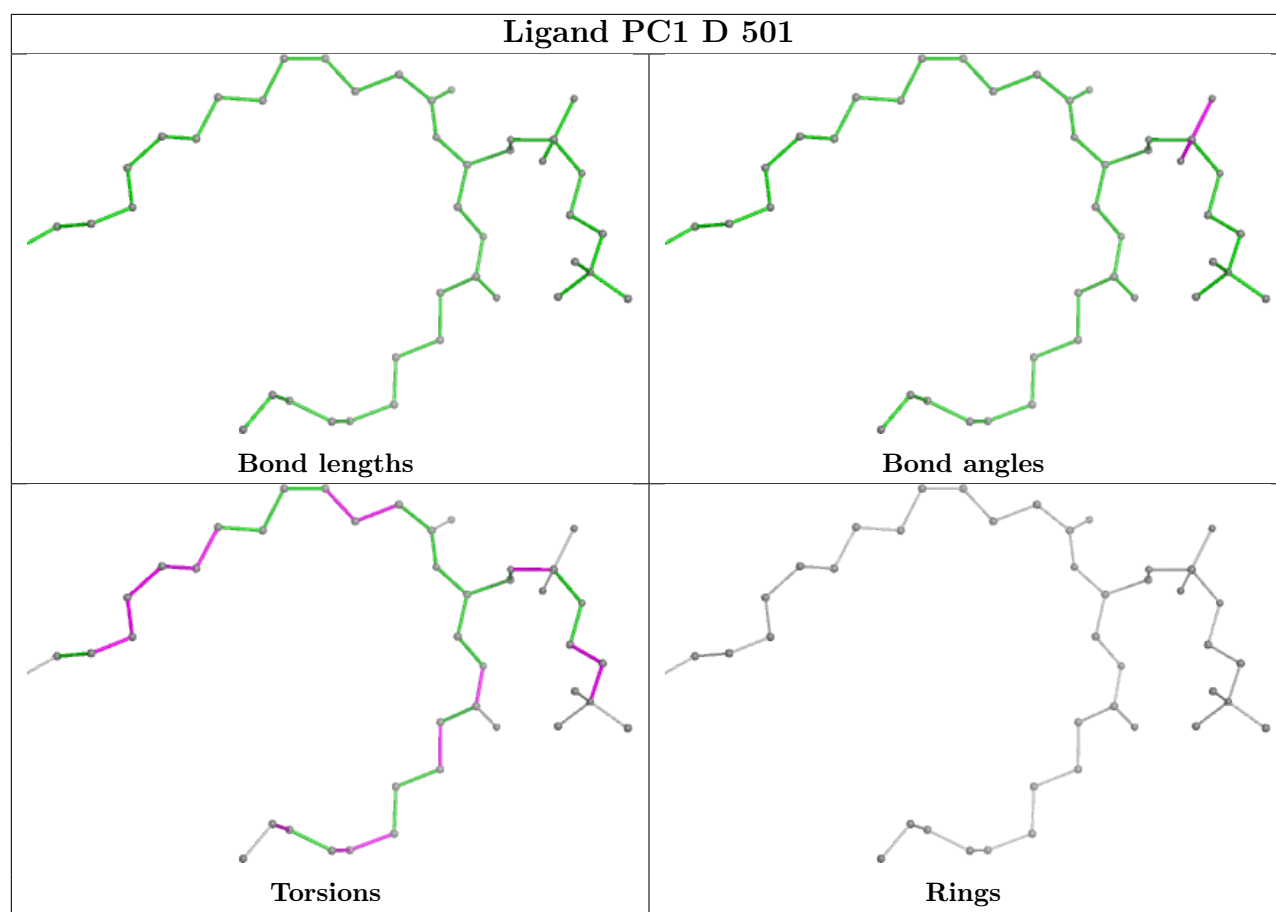




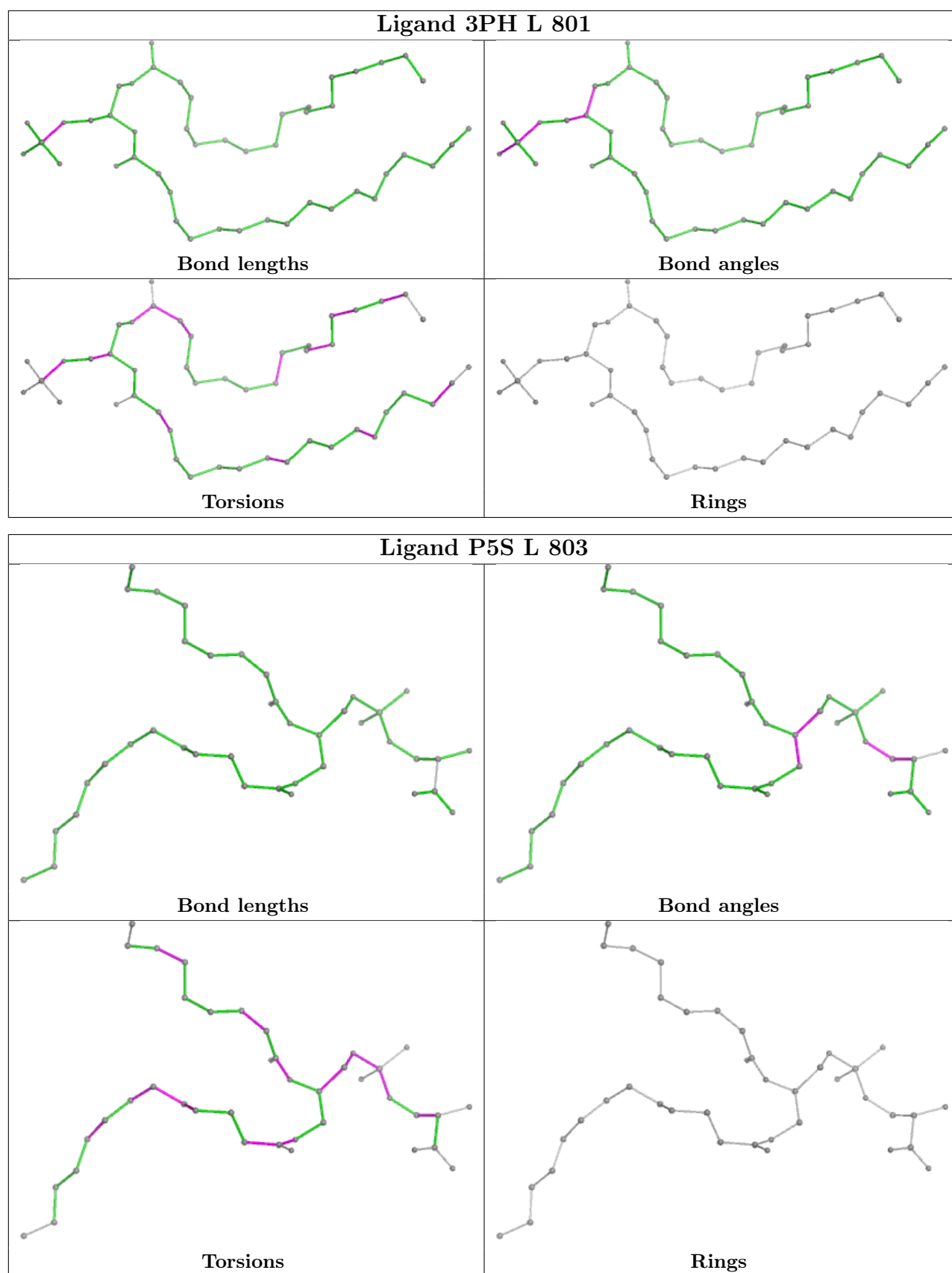


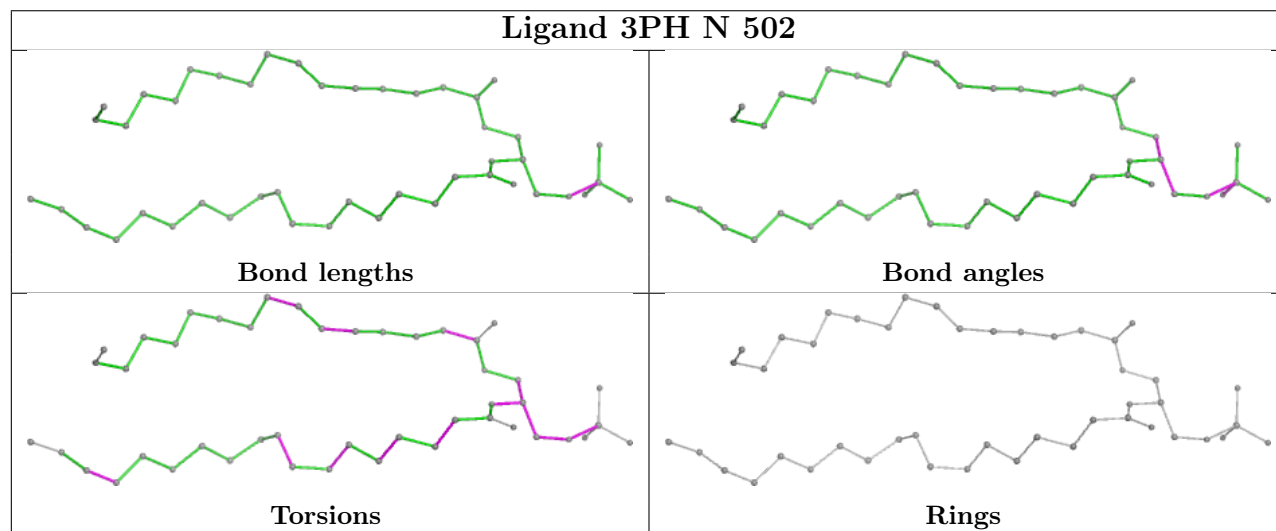
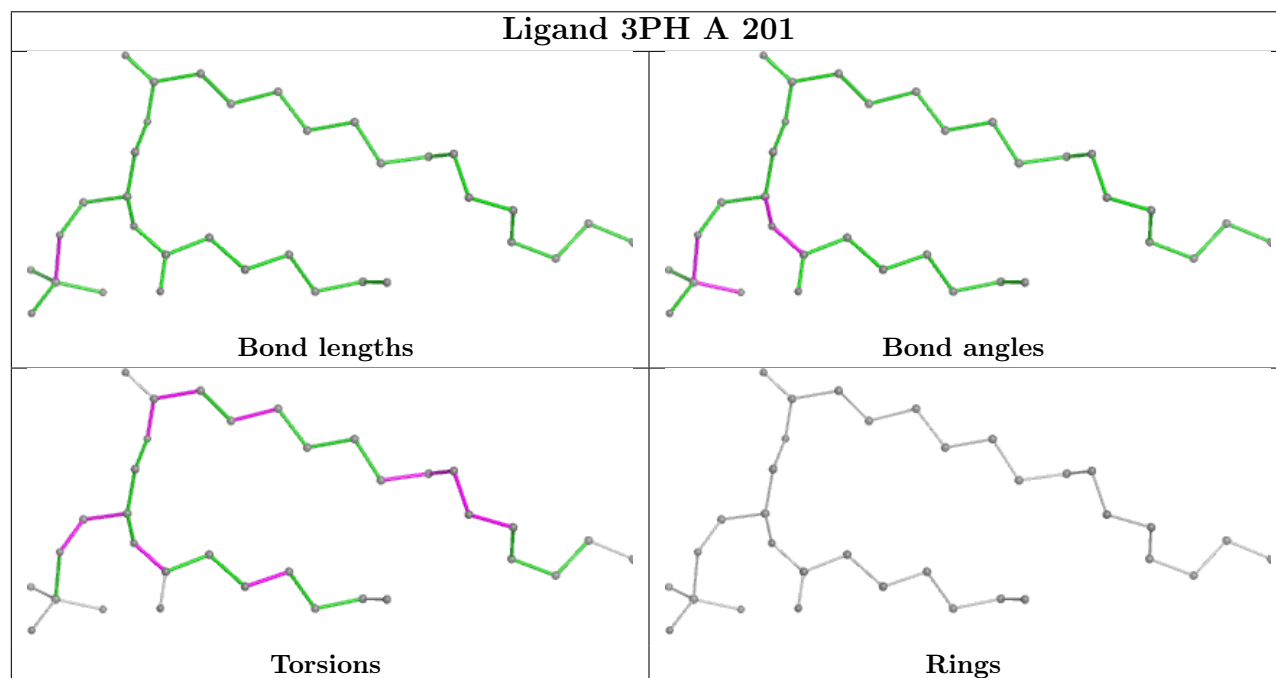
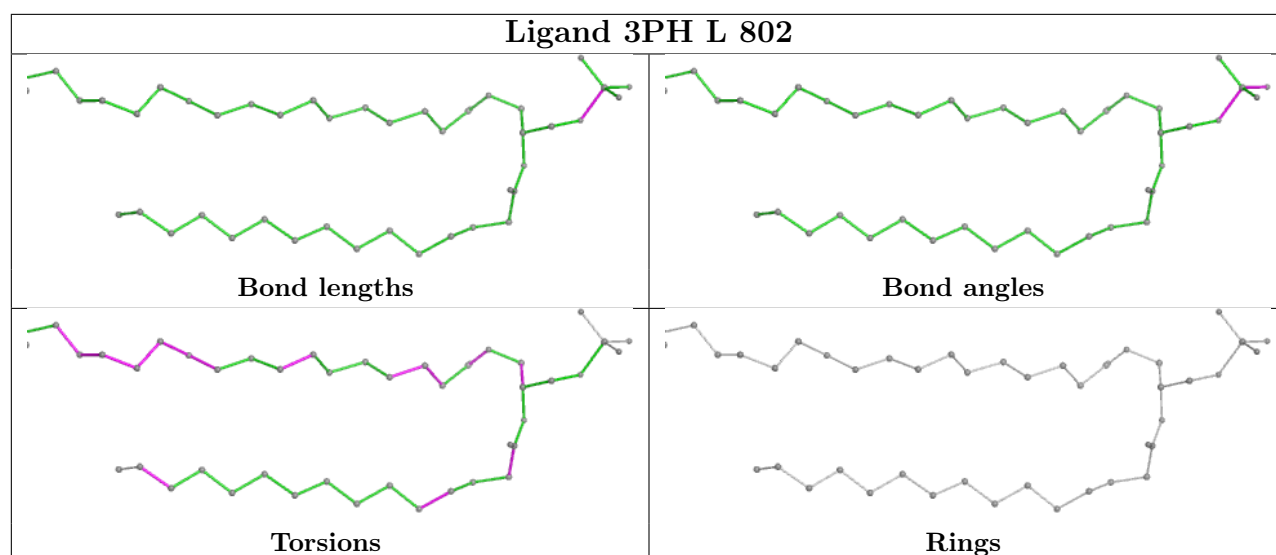


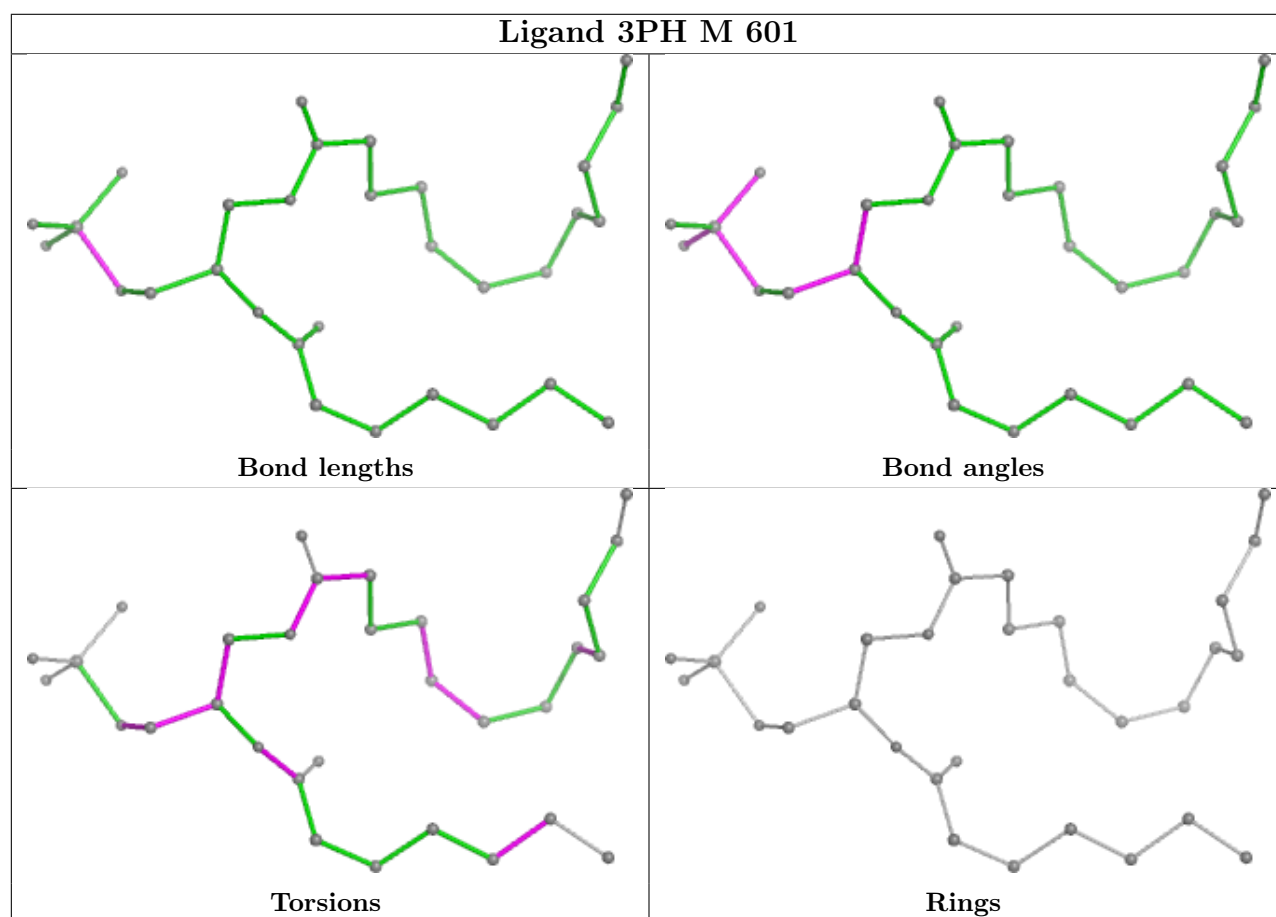
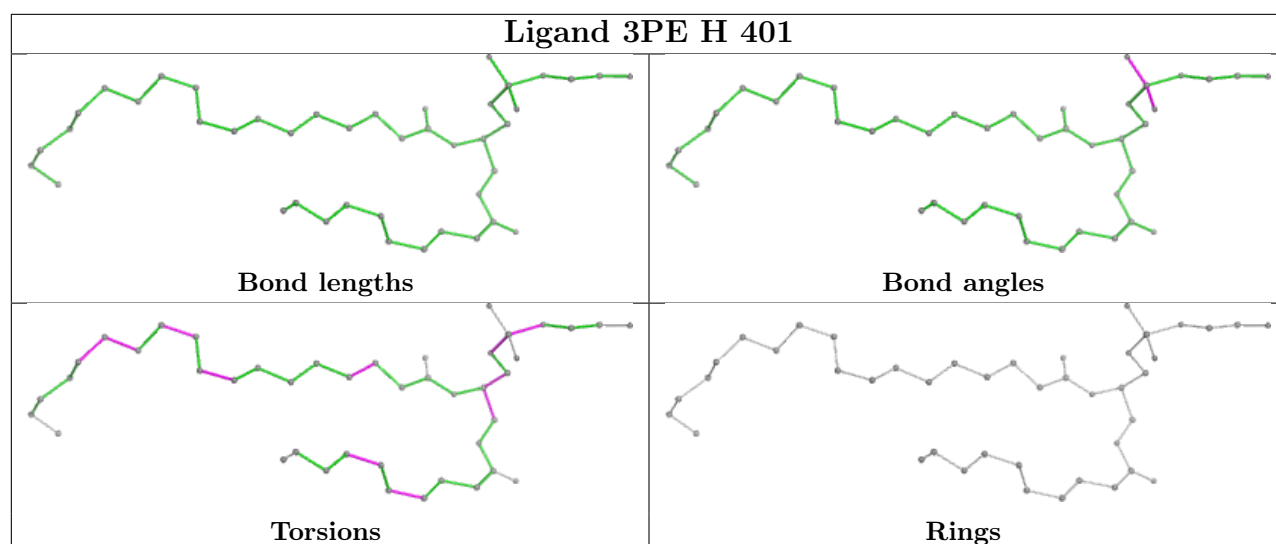


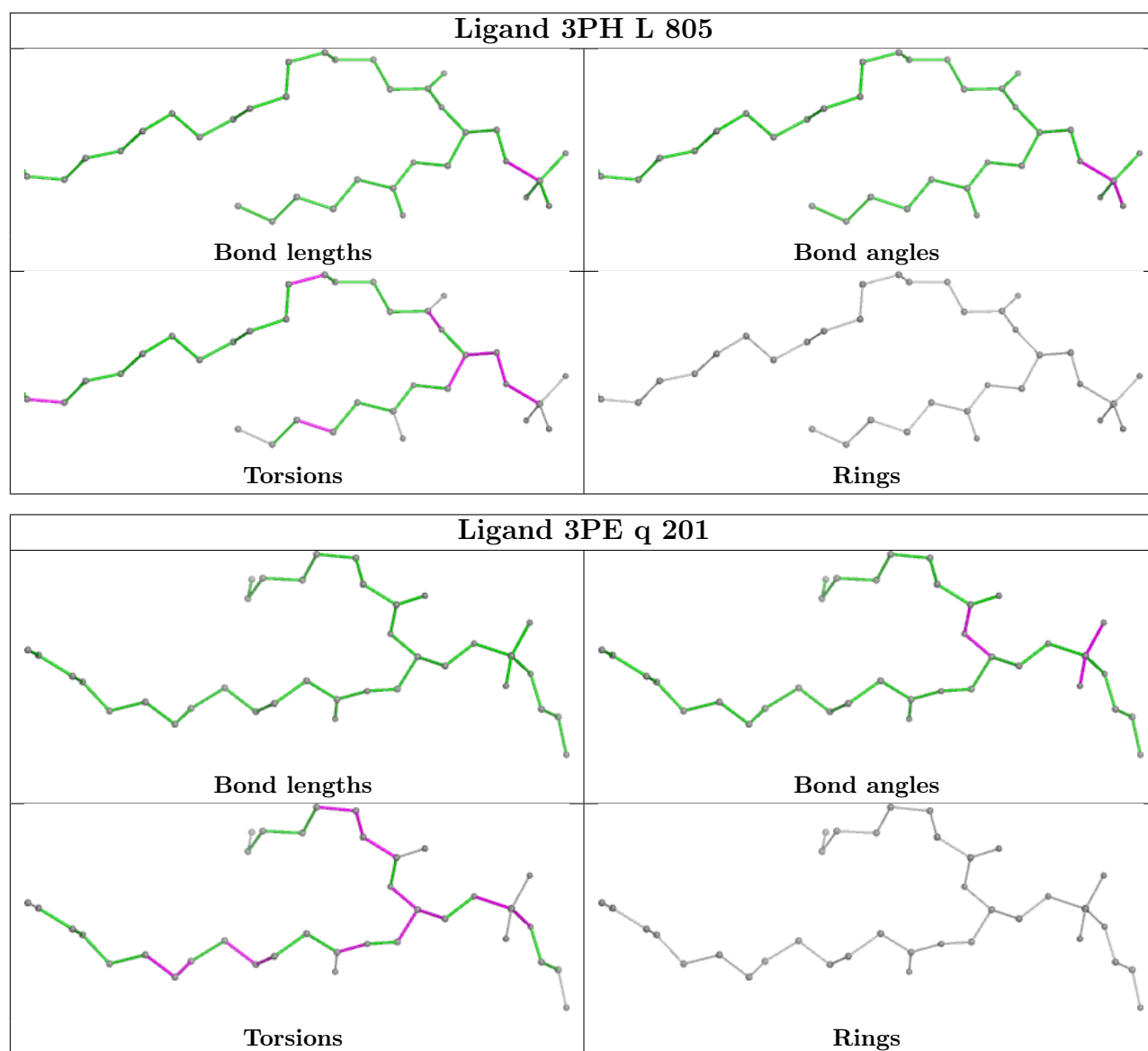


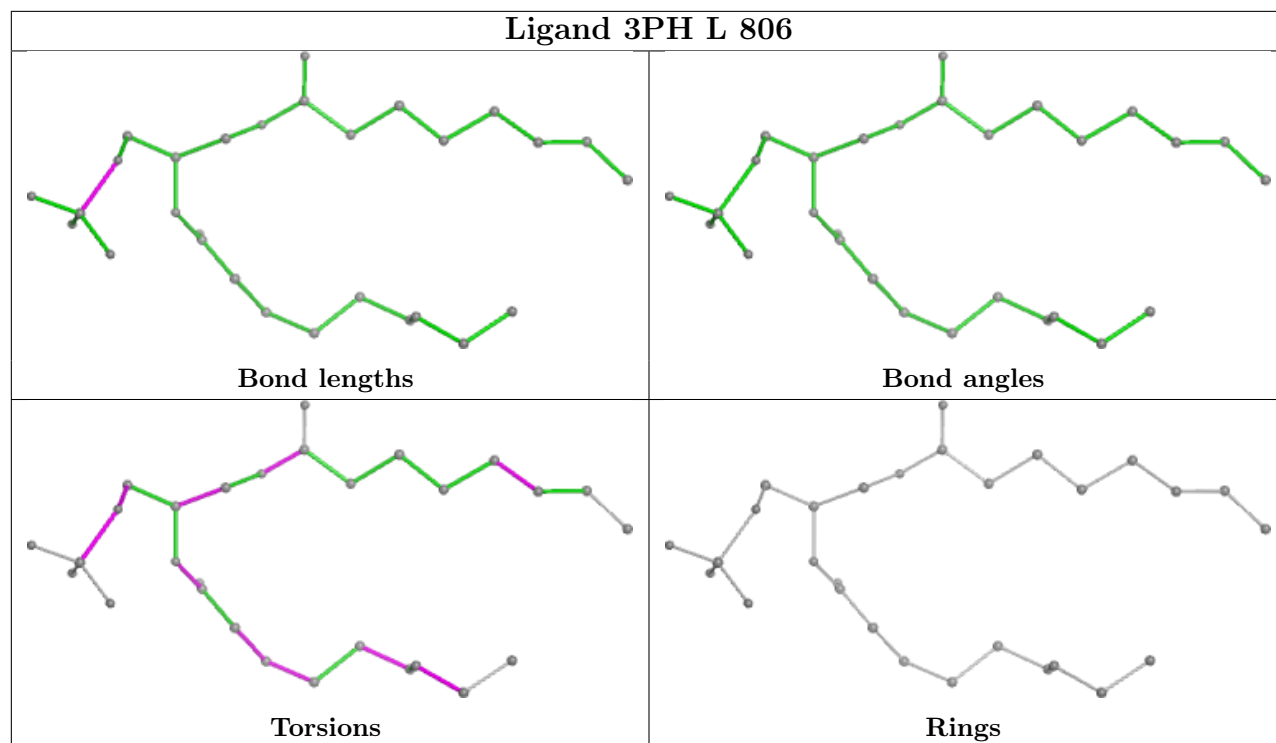


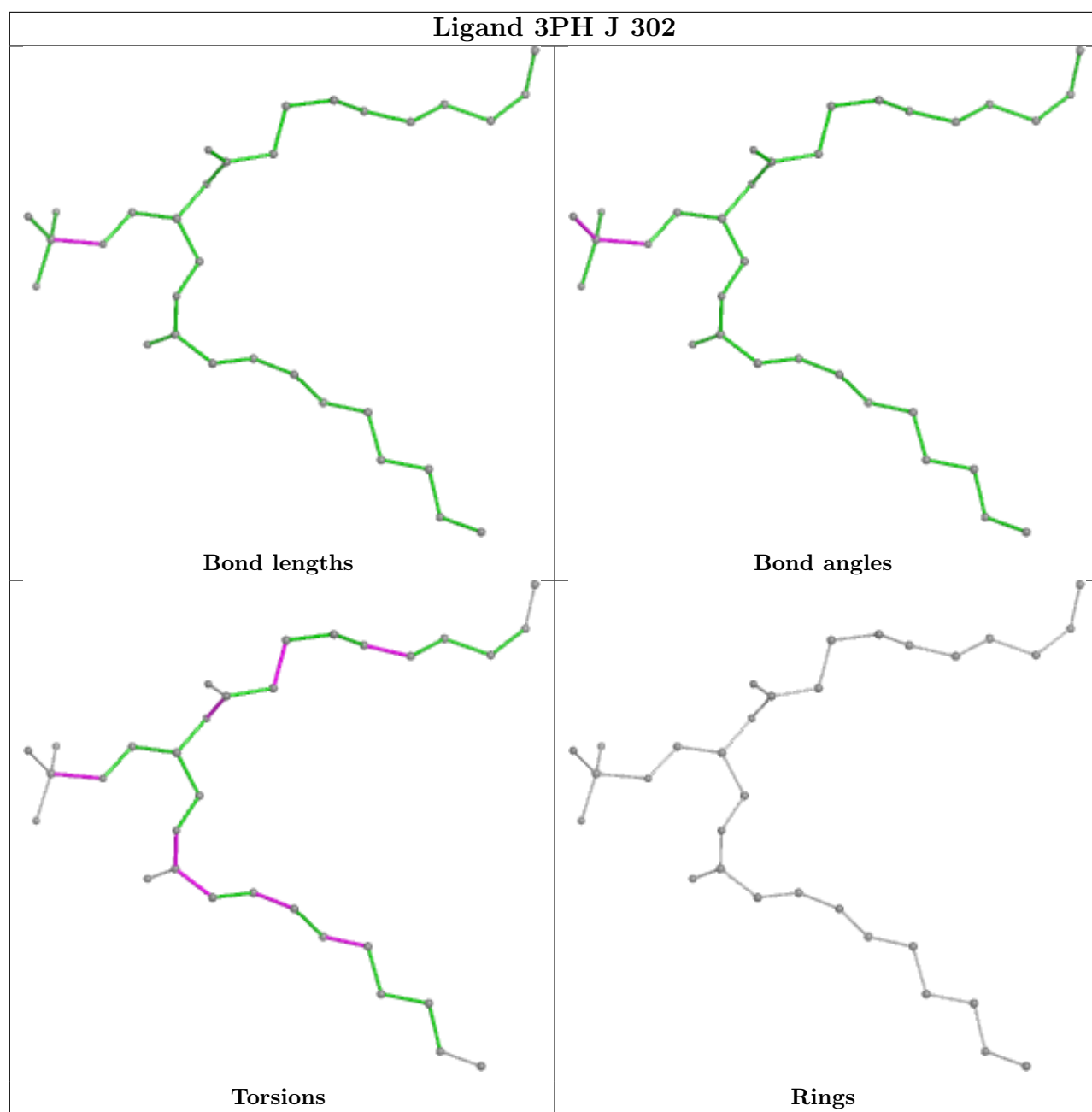


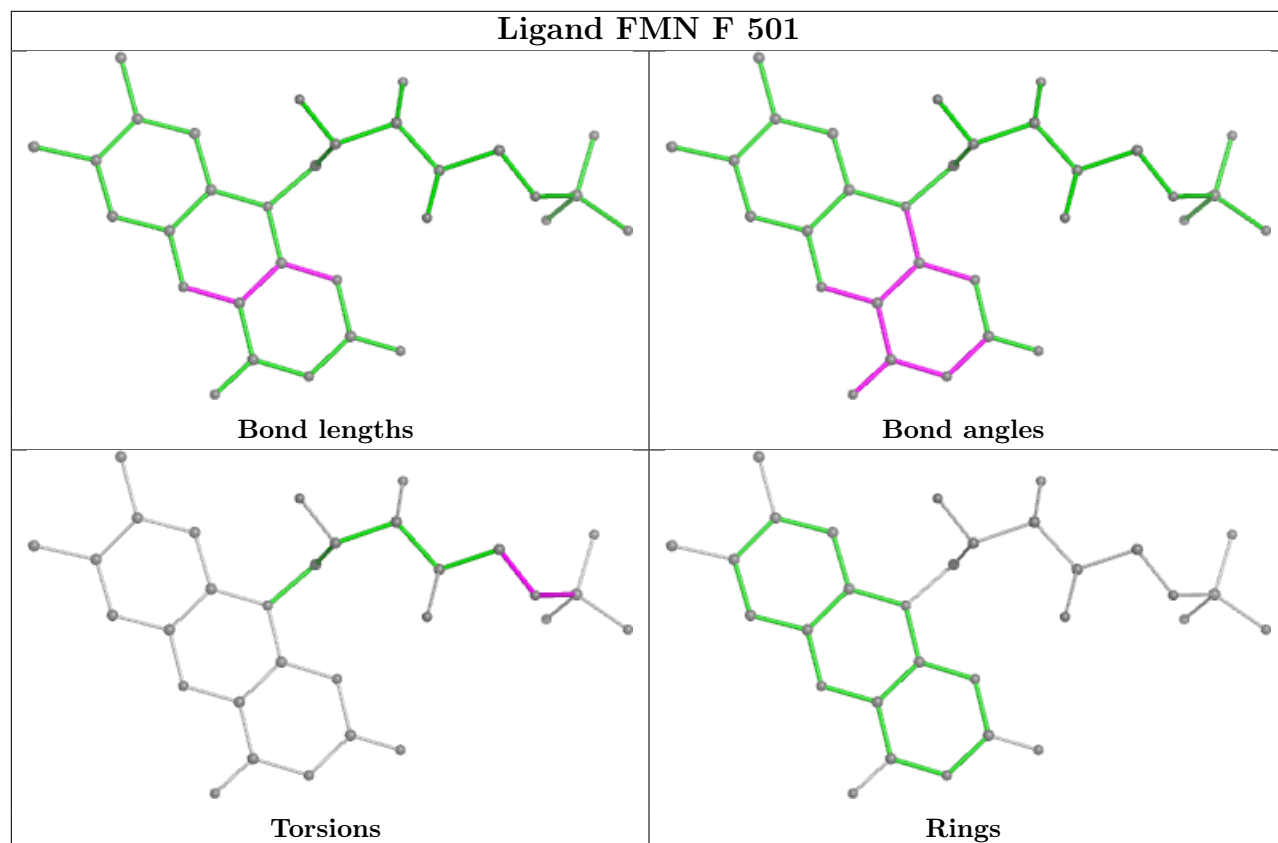


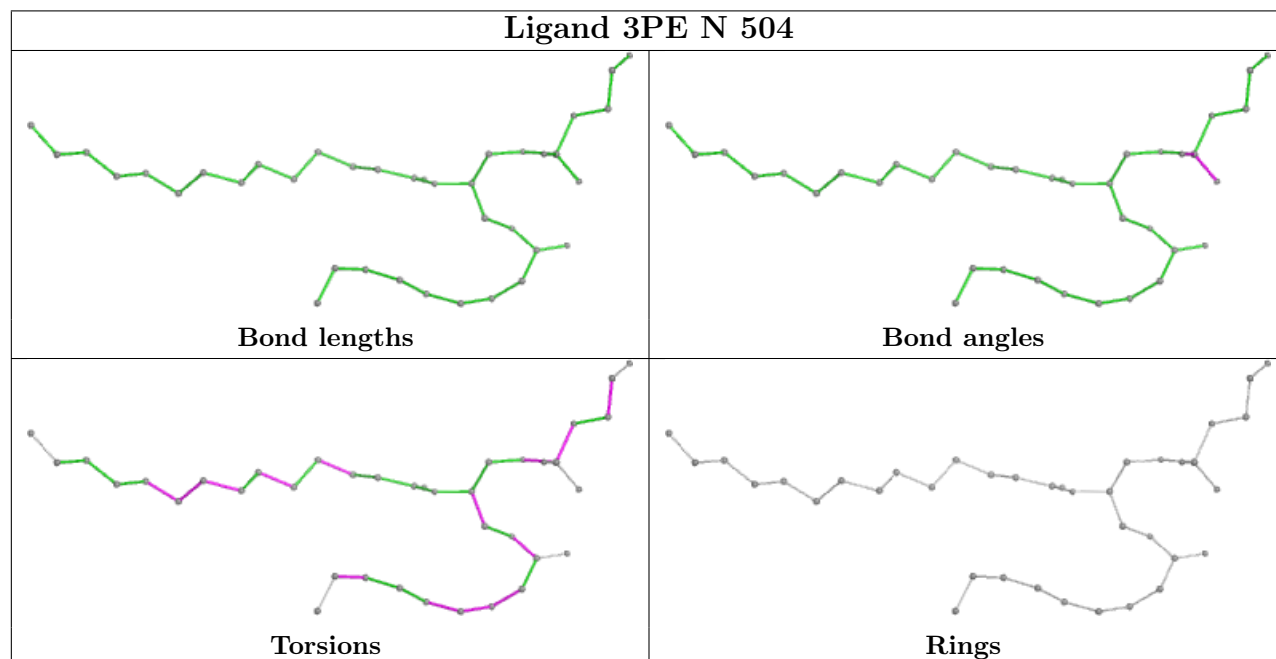
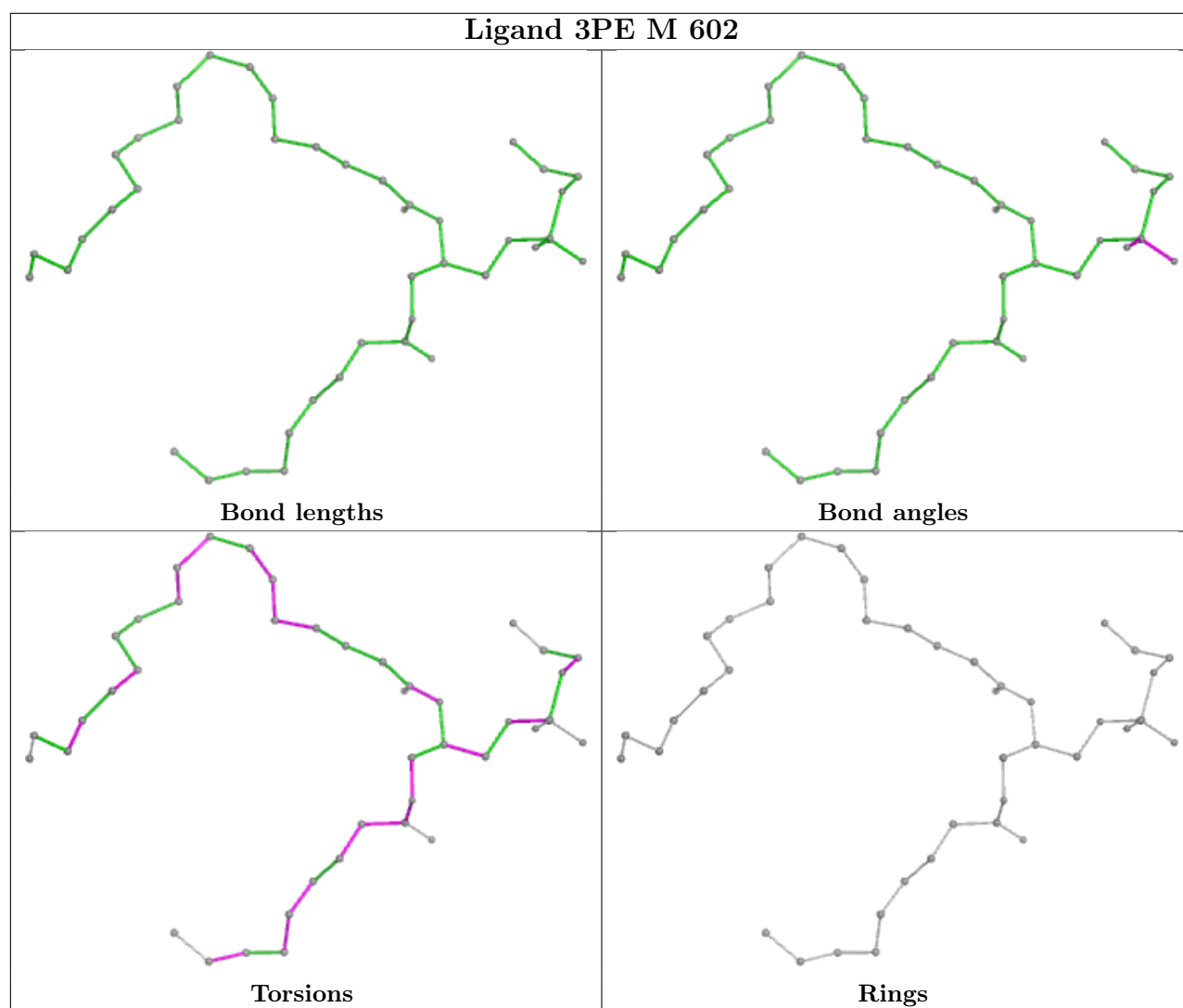














## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

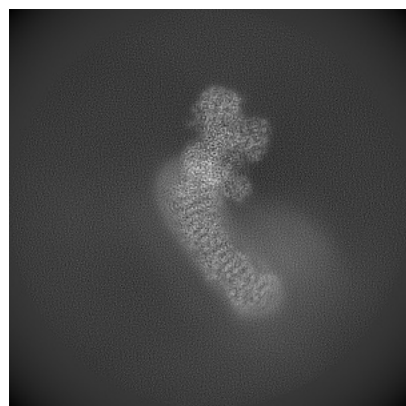
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18324. These allow visual inspection of the internal detail of the map and identification of artifacts.

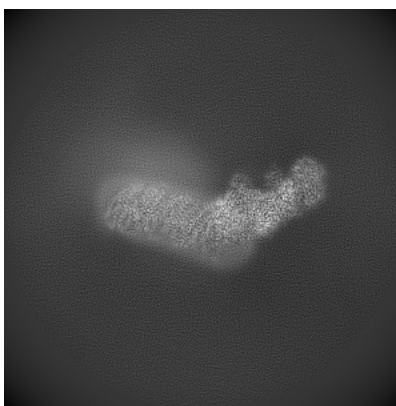
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

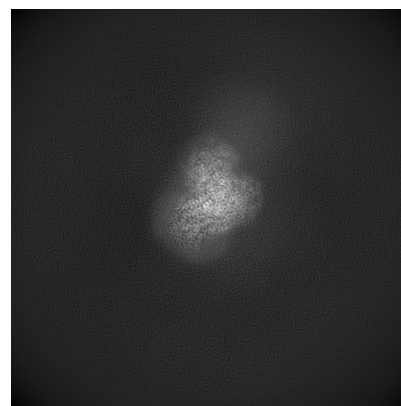
#### 6.1.1 Primary map



X

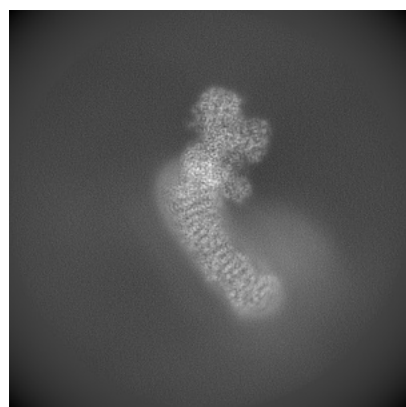


Y

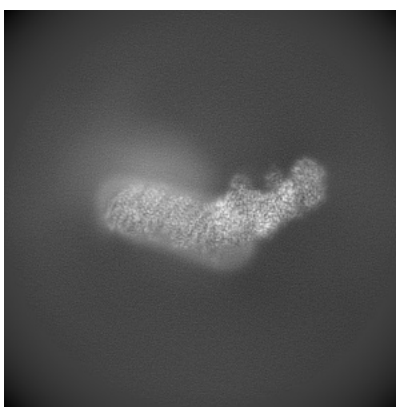


Z

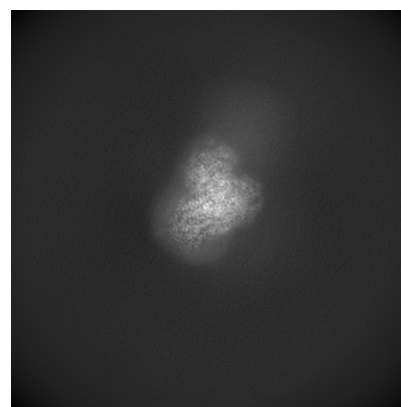
#### 6.1.2 Raw map



X



Y

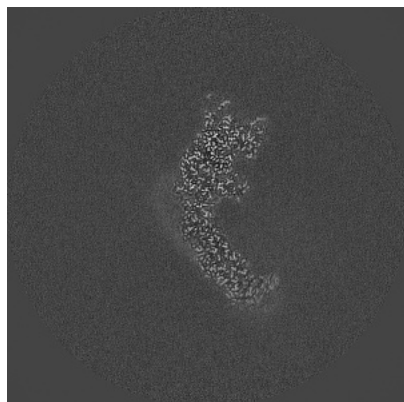


Z

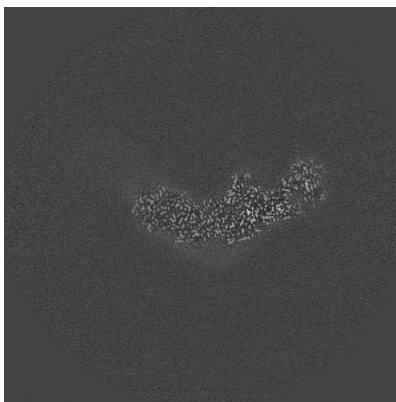
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

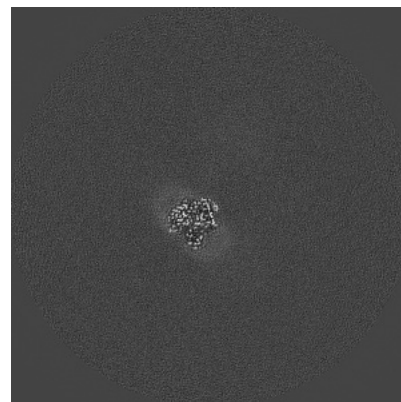
### 6.2.1 Primary map



X Index: 320

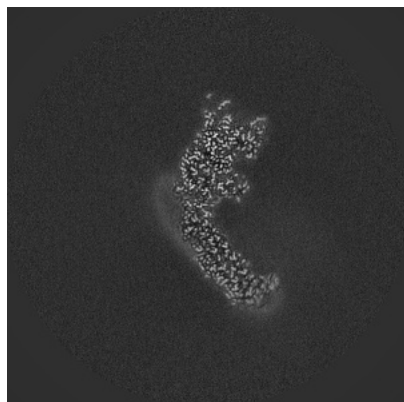


Y Index: 320

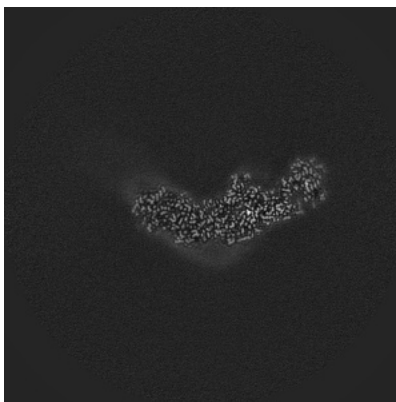


Z Index: 320

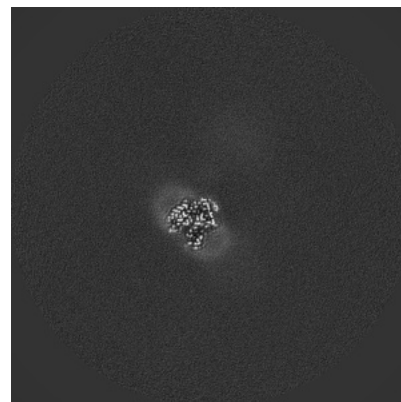
### 6.2.2 Raw map



X Index: 320



Y Index: 320

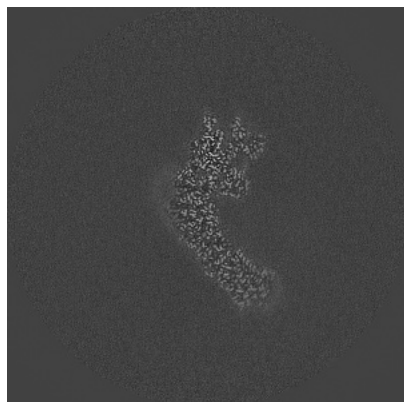


Z Index: 320

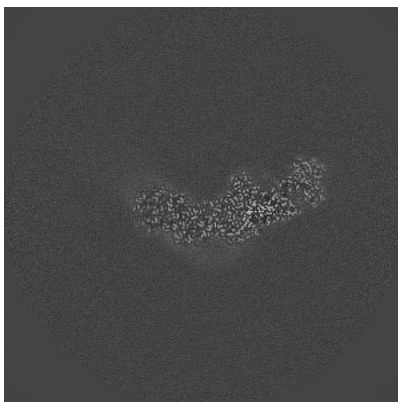
The images above show central slices of the map in three orthogonal directions.

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

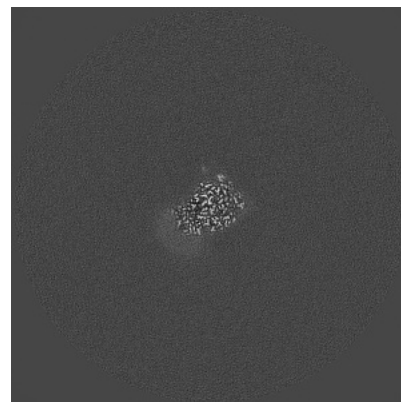
### 6.3.1 Primary map



X Index: 308

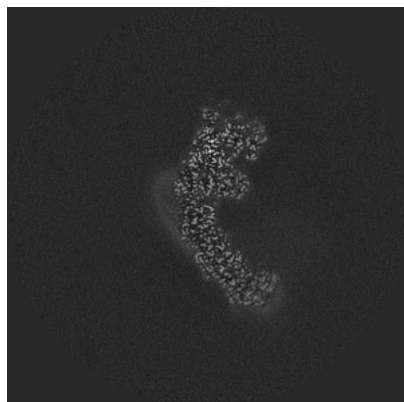


Y Index: 322

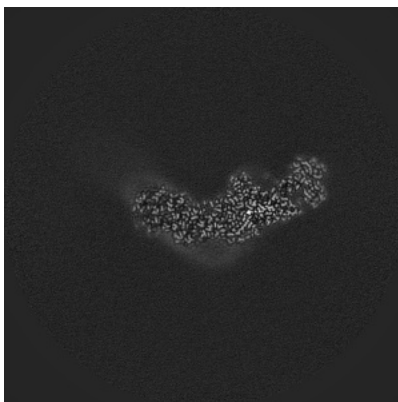


Z Index: 386

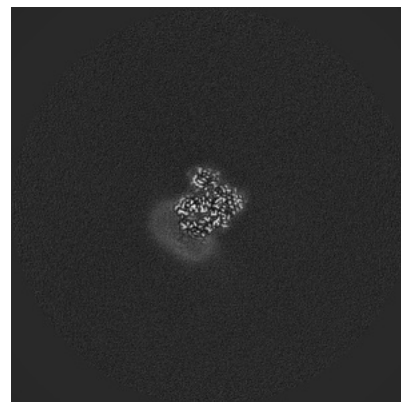
### 6.3.2 Raw map



X Index: 315



Y Index: 322

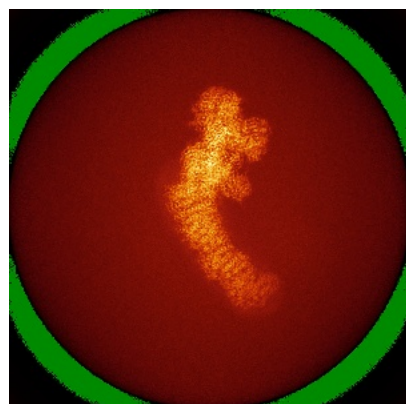


Z Index: 366

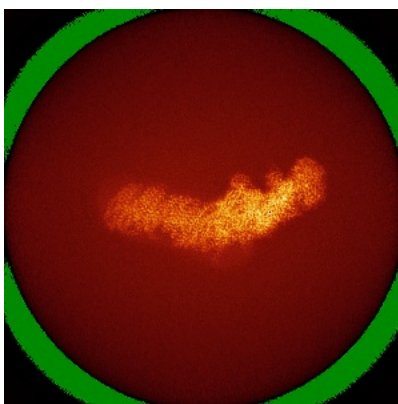
The images above show the largest variance slices of the map in three orthogonal directions.

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

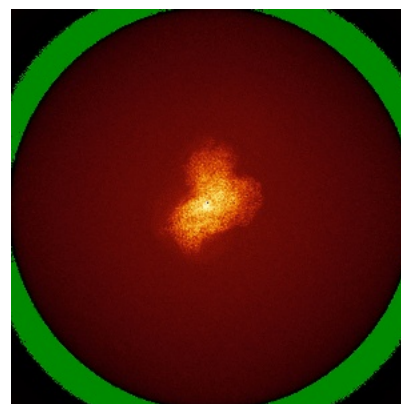
### 6.4.1 Primary map



X



Y

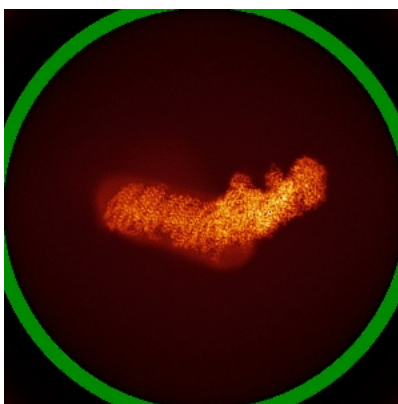


Z

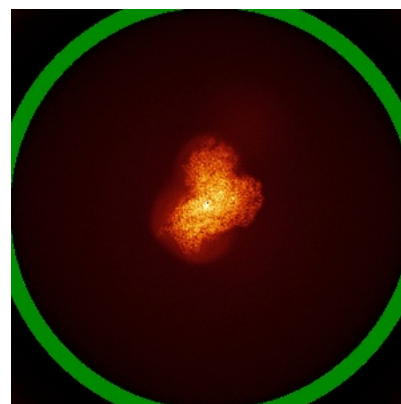
### 6.4.2 Raw map



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



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.019. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

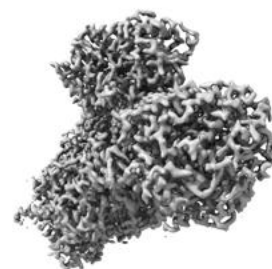
### 6.5.2 Raw map



X



Y



Z

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.

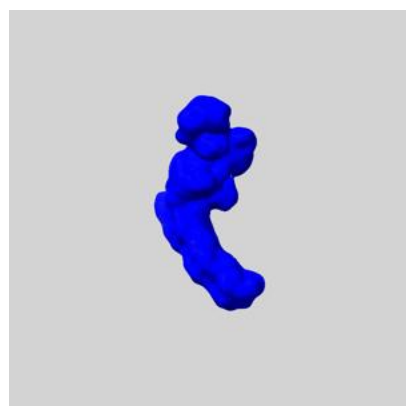
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

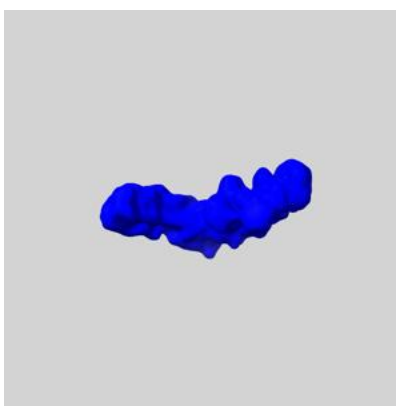
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

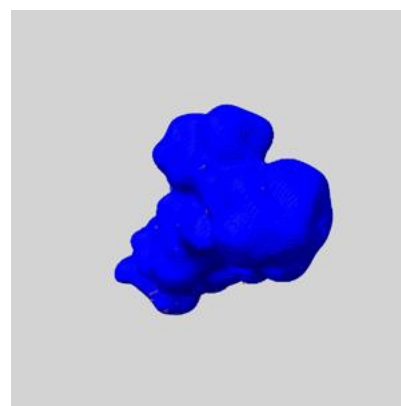
### 6.6.1 emd\_18324\_msk\_1.map [i](#)



X



Y

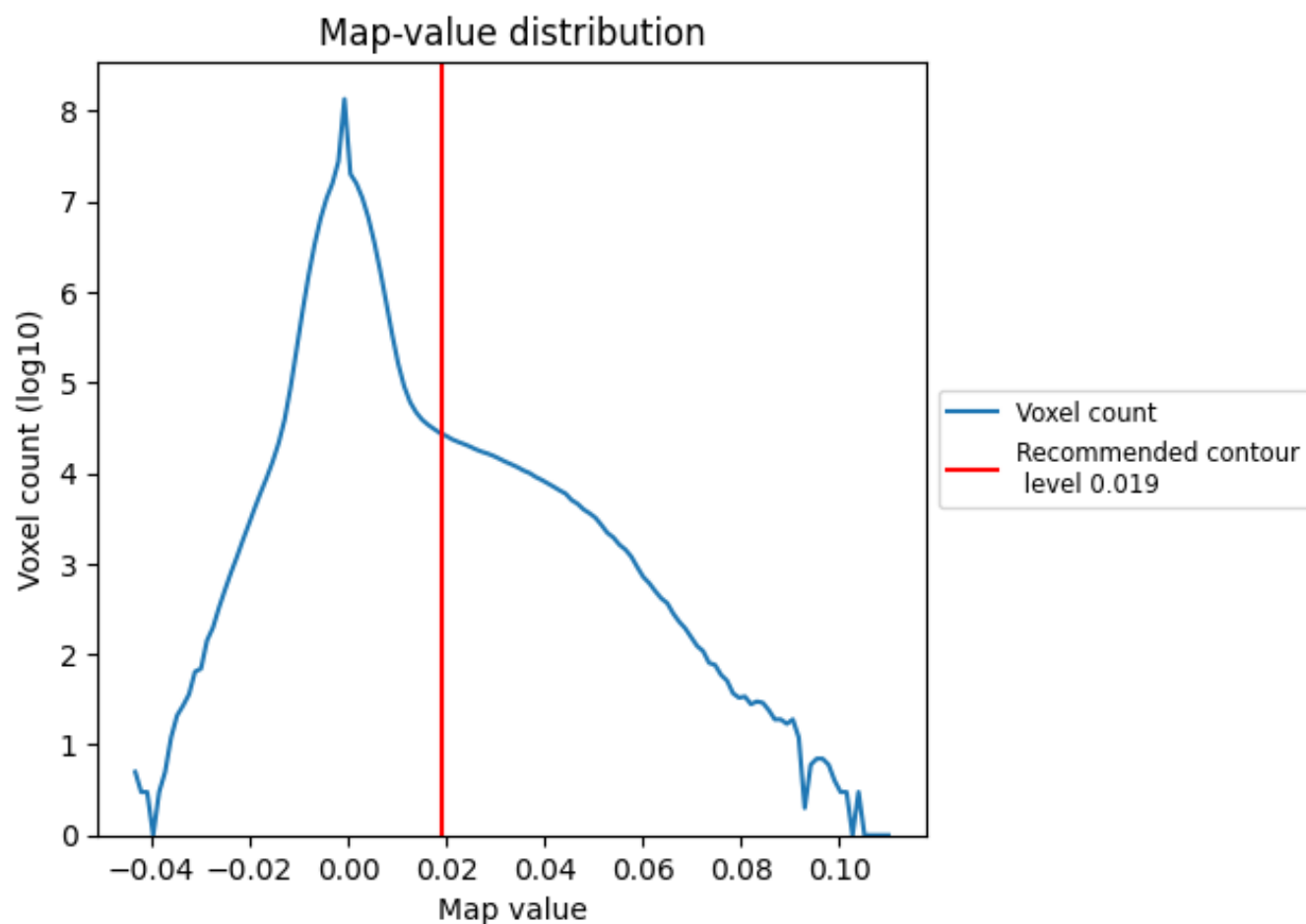


Z

## 7 Map analysis [i](#)

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

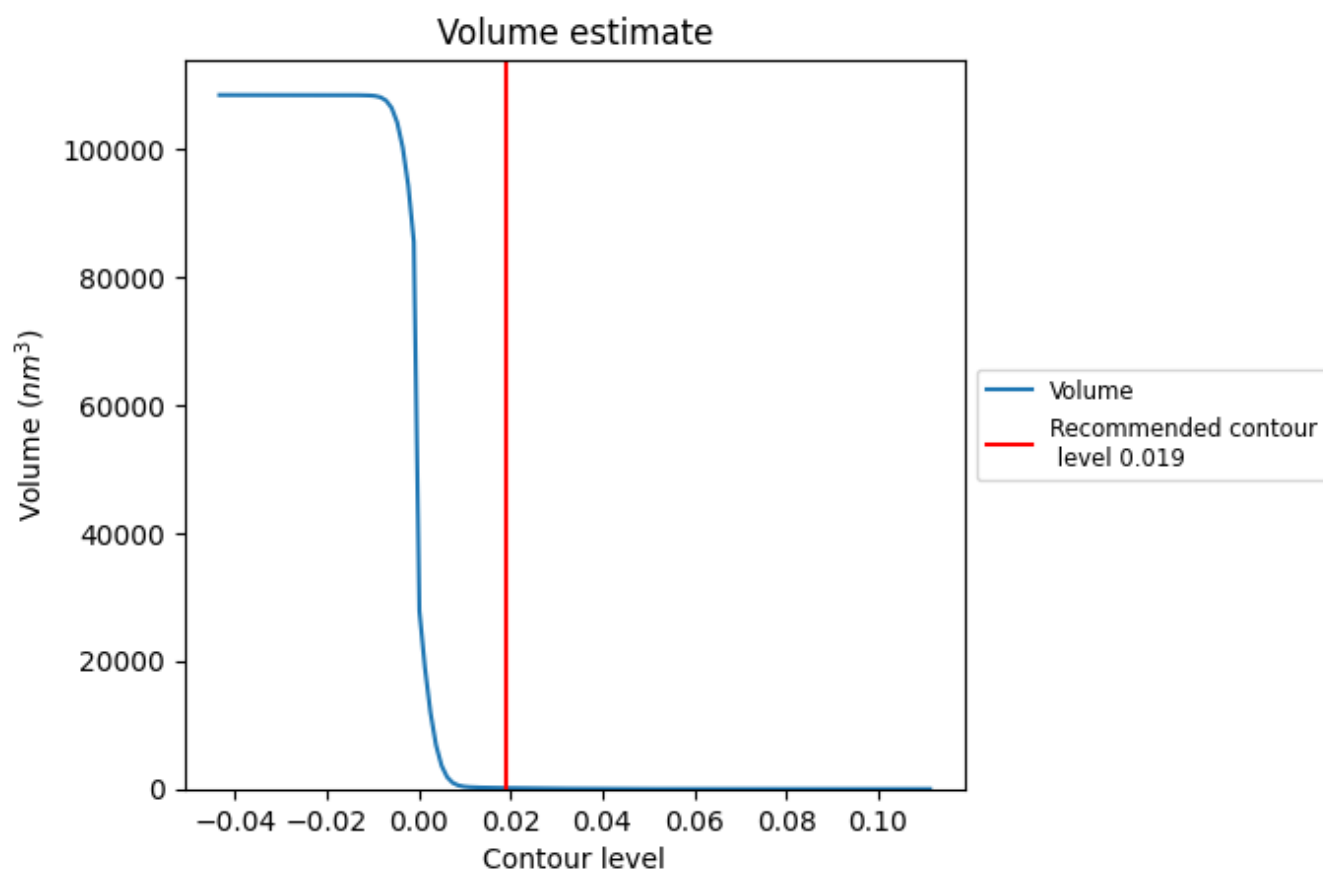
### 7.1 Map-value distribution [i](#)



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.



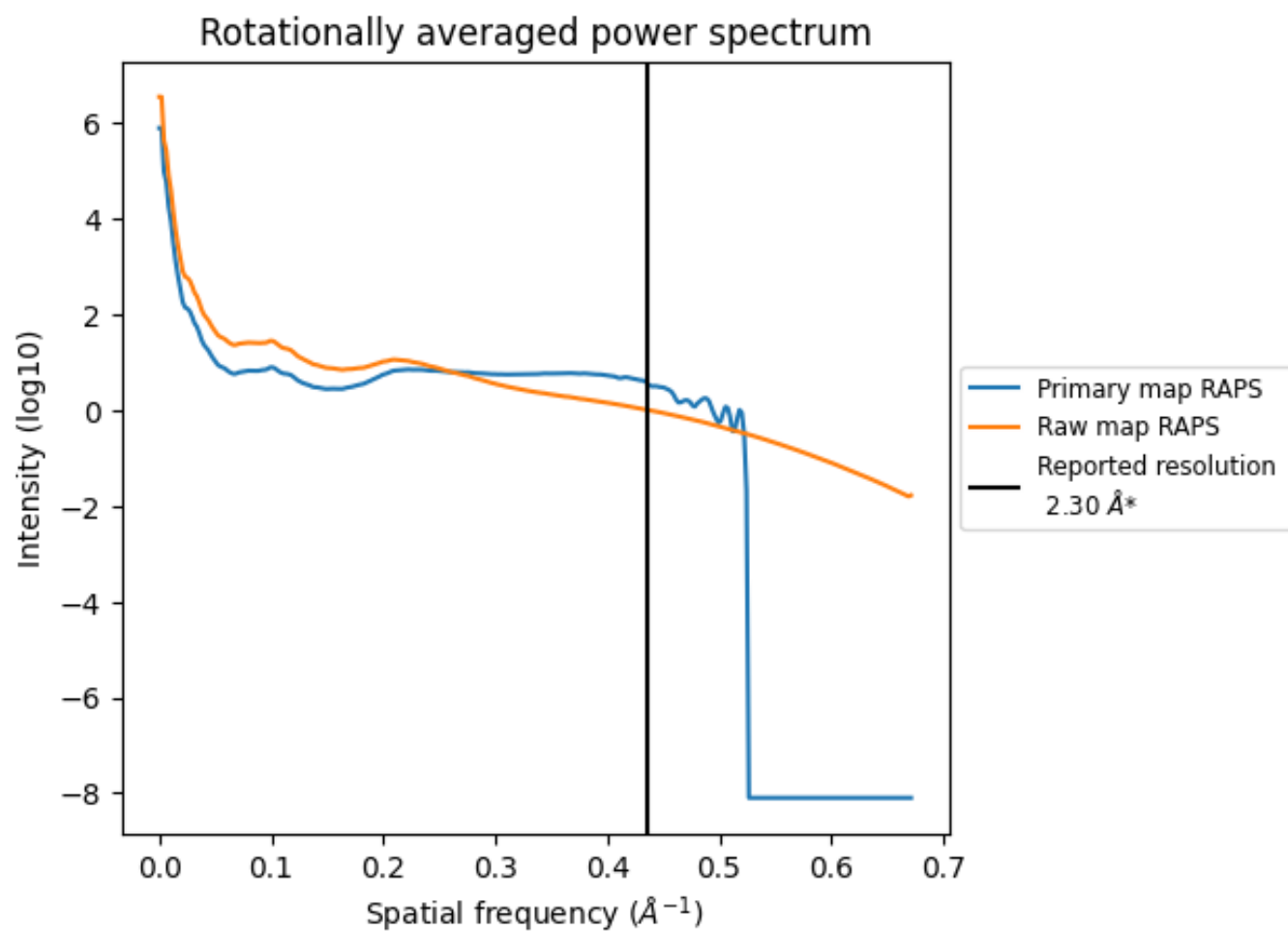
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 147  $\text{nm}^3$ ; this corresponds to an approximate mass of 133 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ

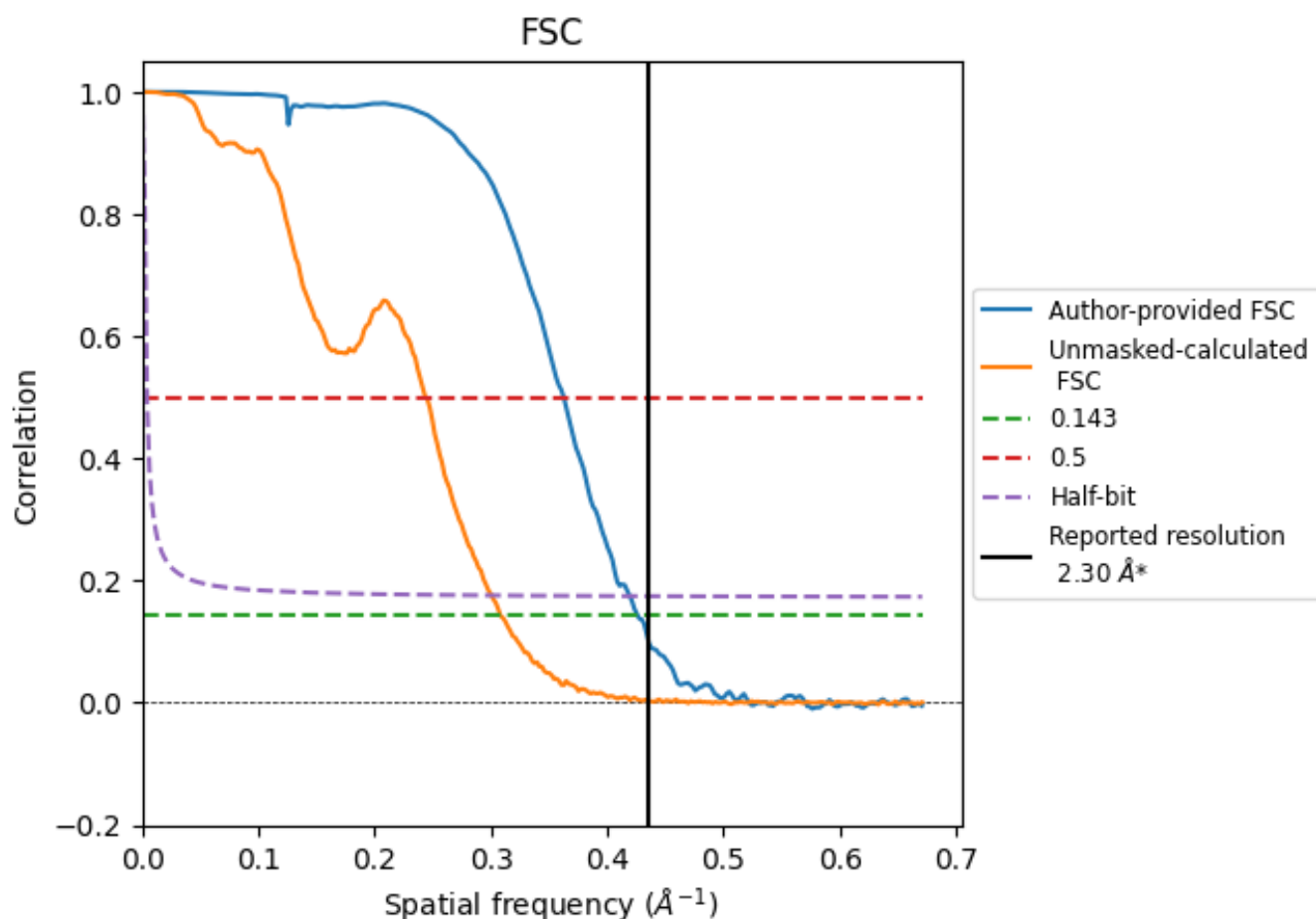


\*Reported resolution corresponds to spatial frequency of 0.435 Å<sup>-1</sup>

## 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 0.435  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

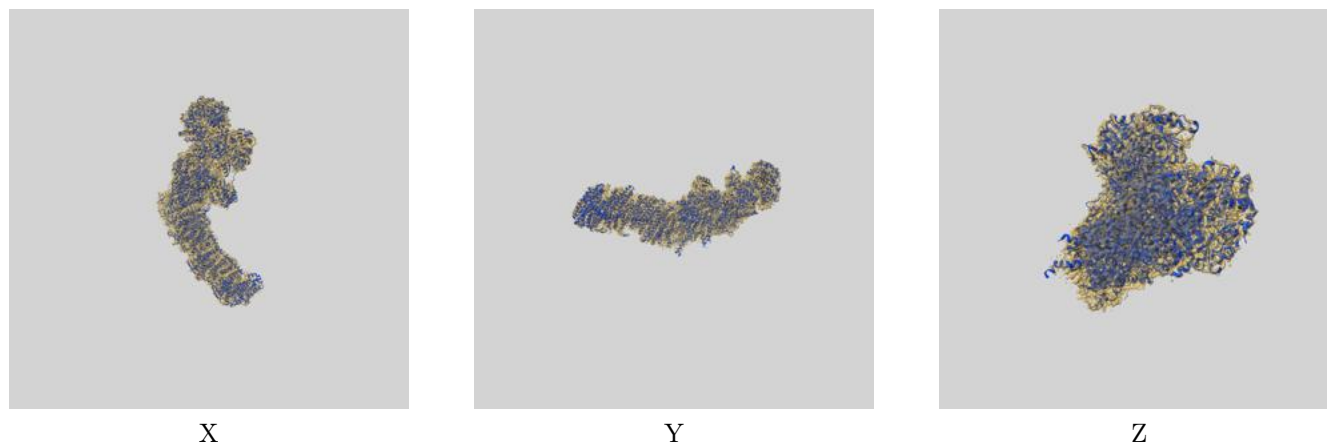
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.30	-	-
Author-provided FSC curve	2.35	2.76	2.38
Unmasked-calculated*	3.24	4.10	3.33

\*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 3.24 differs from the reported value 2.3 by more than 10 %

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

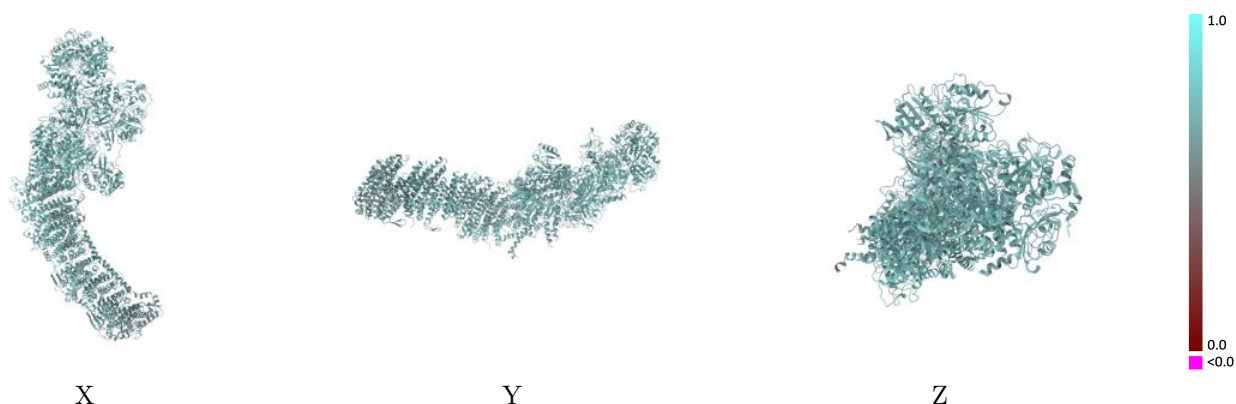
This section contains information regarding the fit between EMDB map EMD-18324 and PDB model 8QBY. Per-residue inclusion information can be found in section [3](#) on page [16](#).

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



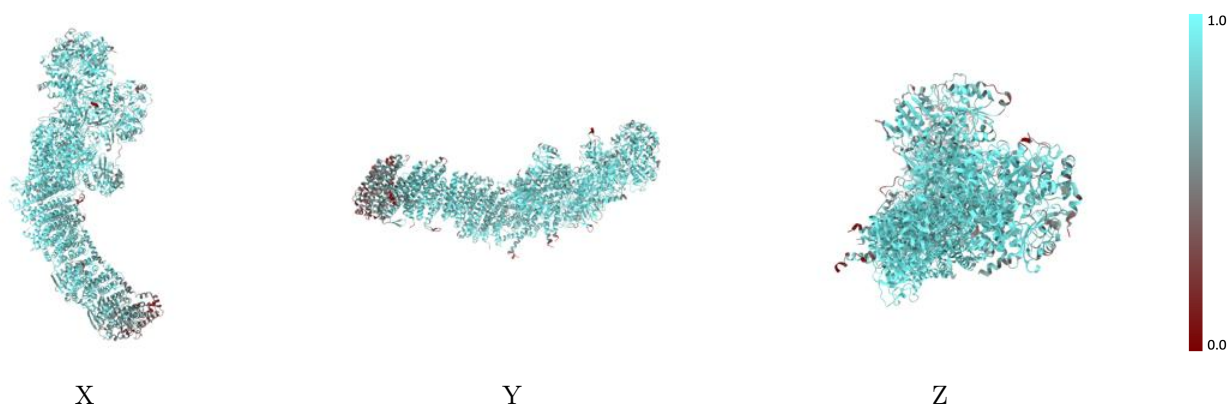
The images above show the 3D surface view of the map at the recommended contour level 0.019 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



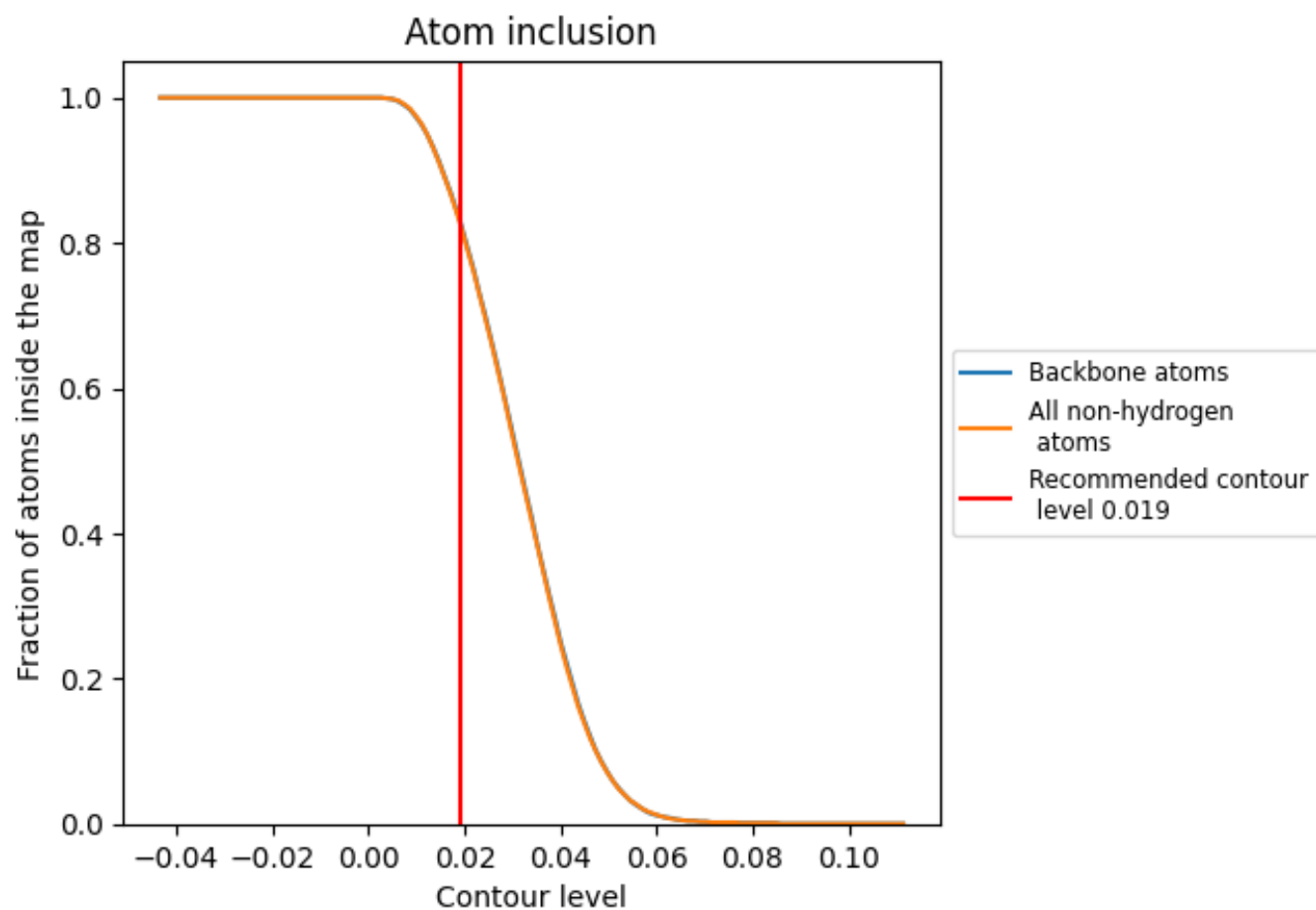
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.019).

## 9.4 Atom inclusion ⓘ



At the recommended contour level, 83% of all backbone atoms, 83% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.019) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.8290</div>	<div><div></div>0.6830</div>
A	<div><div></div>0.8900</div>	<div><div></div>0.7060</div>
B	<div><div></div>0.9250</div>	<div><div></div>0.7130</div>
C	<div><div></div>0.9090</div>	<div><div></div>0.7030</div>
D	<div><div></div>0.9370</div>	<div><div></div>0.7160</div>
E	<div><div></div>0.8330</div>	<div><div></div>0.6720</div>
F	<div><div></div>0.8510</div>	<div><div></div>0.6760</div>
G	<div><div></div>0.8630</div>	<div><div></div>0.6890</div>
H	<div><div></div>0.8860</div>	<div><div></div>0.7000</div>
I	<div><div></div>0.9180</div>	<div><div></div>0.7100</div>
J	<div><div></div>0.8270</div>	<div><div></div>0.6890</div>
K	<div><div></div>0.9030</div>	<div><div></div>0.7070</div>
L	<div><div></div>0.6060</div>	<div><div></div>0.6250</div>
M	<div><div></div>0.8050</div>	<div><div></div>0.6740</div>
N	<div><div></div>0.9000</div>	<div><div></div>0.7020</div>
Q	<div><div></div>0.8790</div>	<div><div></div>0.6900</div>
R	<div><div></div>0.8230</div>	<div><div></div>0.6690</div>
q	<div><div></div>0.7920</div>	<div><div></div>0.6830</div>
t	<div><div></div>0.8160</div>	<div><div></div>0.6770</div>

1.0

0.0

<0.0