wwPDB EM Validation Summary Report ⓘ

Sep 4, 2024 – 03:20 pm BST

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 wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

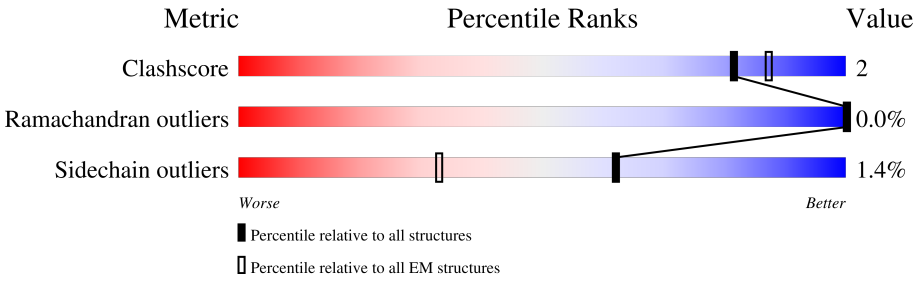
EMDB validation analysis	:	0.0.1.dev112
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.30 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 >=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 <=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	86% 14%
2	G	674	93% 6%
3	t	217	5% 98%
4	I	163	94%
5	E	239	91% 8%
6	N	499	91% 5%
7	H	345	95%
8	F	431	89% 8%

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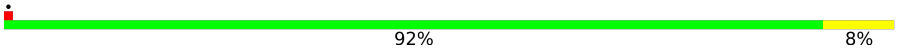
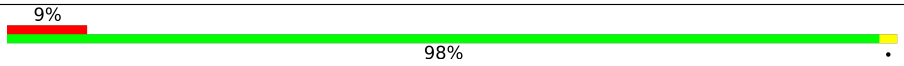
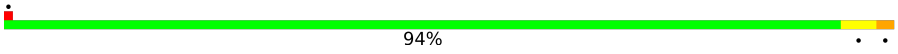
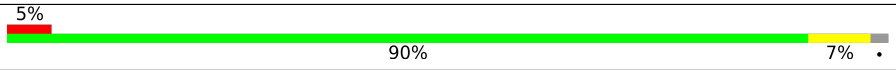
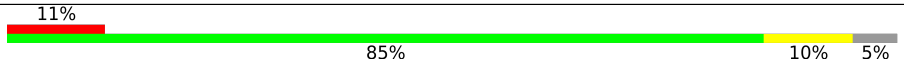
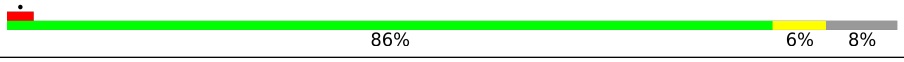
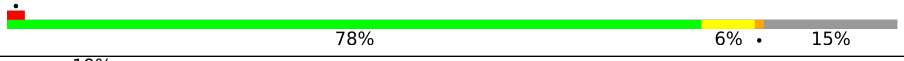
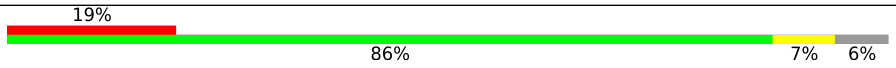
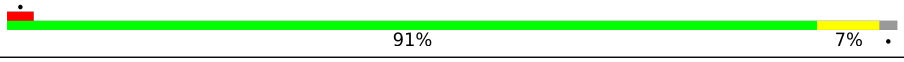
Mol	Chain	Length	Quality of chain
9	D	412	
10	q	124	
11	A	121	
12	J	200	
13	R	62	
14	Q	103	
15	C	208	
16	B	175	
17	L	703	
18	M	513	

2 Entry composition (i)

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
			Total	C	N	O	S		
1	K	101	763	508	123	127	5	0	0

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

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

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

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

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

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

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

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

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

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

- 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		

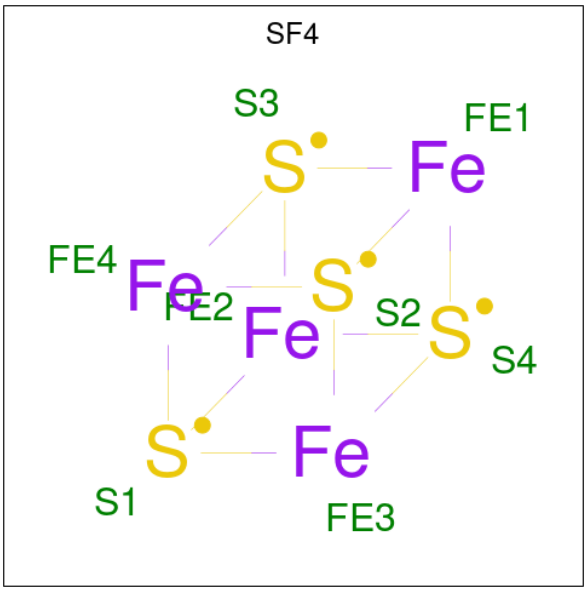
- Molecule 17 is a protein called NADH dehydrogenase subunit L.

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.

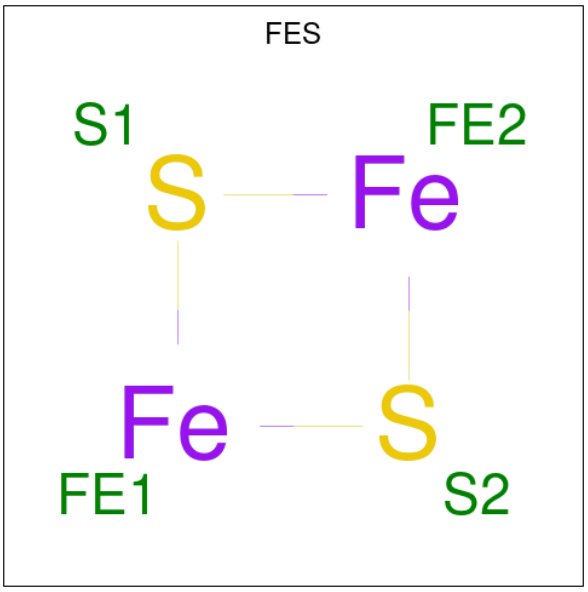
Mol	Chain	Residues	Atoms					AltConf	Trace
18	M	503	Total	C	N	O	S	0	0
			3913	2614	610	657	32		

- Molecule 19 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



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_2S_2).

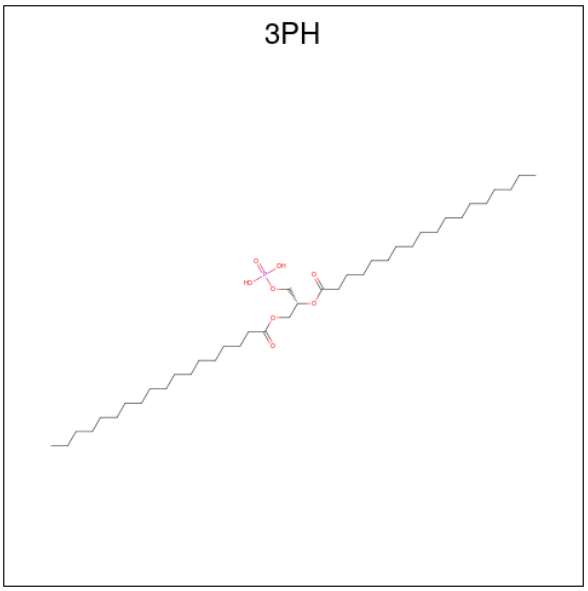


Mol	Chain	Residues	Atoms	AltConf
20	G	1	Total Fe S 4 2 2	0
20	E	1	Total Fe S 4 2 2	0

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

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

- Molecule 22 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (three-letter code: 3PH) (formula: $C_{39}H_{77}O_8P$).



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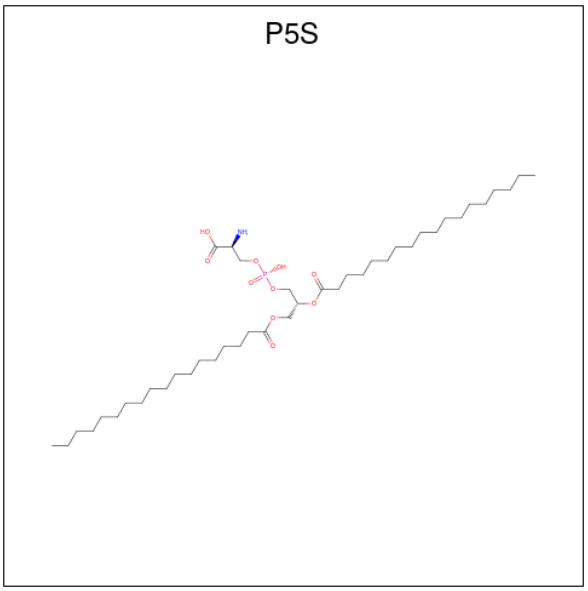
Mol	Chain	Residues	Atoms				AltConf
22	M	1	Total 33	C 24	O 8	P 1	0
22	M	1	Total 31	C 22	O 8	P 1	0
22	M	1	Total 33	C 24	O 8	P 1	0

- Molecule 23 is O-[(R)-{[(2R)-2,3-bis(octadecanoyloxy)propyl]oxy}(hydroxy)phosphoryl]-L-serine (three-letter code: P5S) (formula: $C_{42}H_{82}NO_{10}P$).

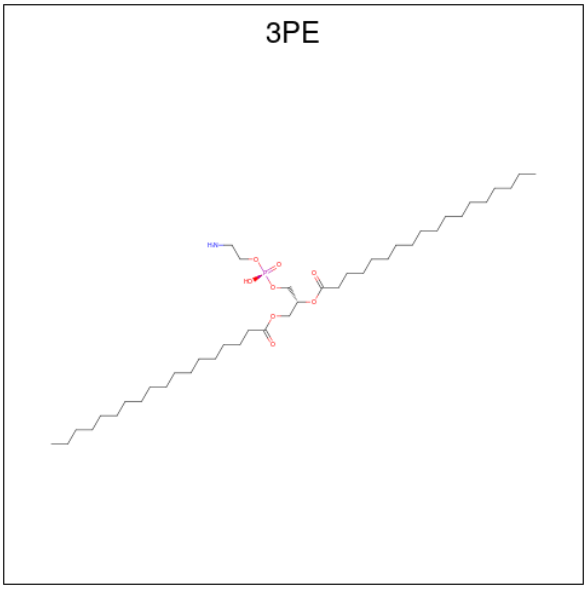


Mol	Chain	Residues	Atoms					AltConf
23	I	1	Total 49	C 37	N 1	O 10	P 1	0
23	L	1	Total 40	C 28	N 1	O 10	P 1	0

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

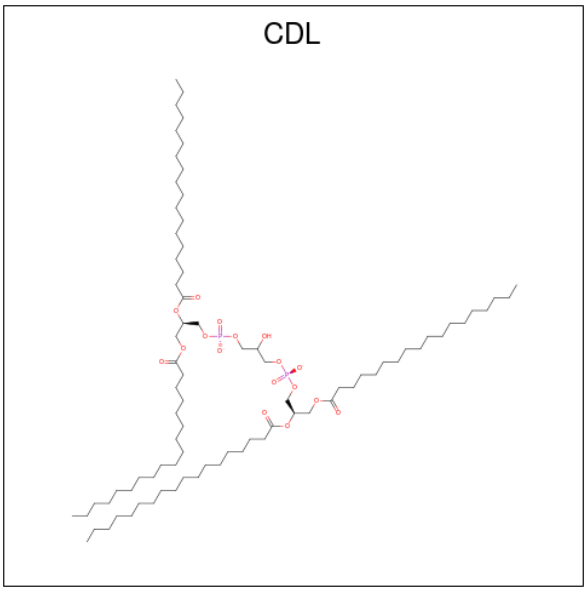
Mol	Chain	Residues	Atoms		AltConf
24	I	1	Total 1	Ca 1	0
24	N	1	Total 1	Ca 1	0
24	D	1	Total 1	Ca 1	0
24	M	1	Total 1	Ca 1	0

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



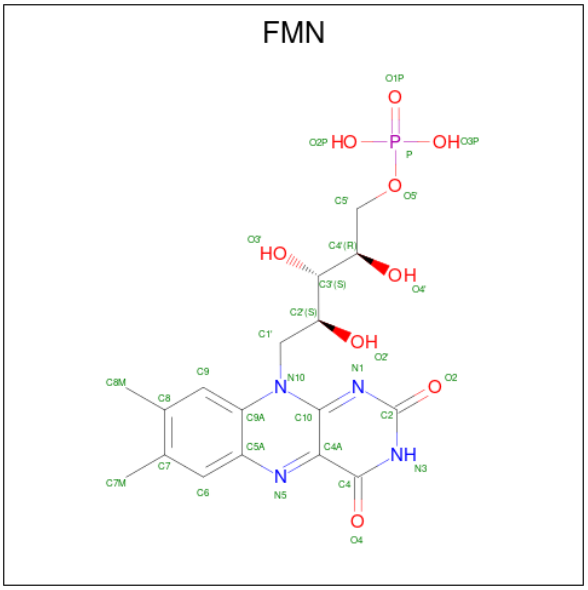
Mol	Chain	Residues	Atoms					AltConf
25	N	1	Total	C	N	O	P	0
			42	32	1	8	1	
25	N	1	Total	C	N	O	P	0
			48	38	1	8	1	
25	N	1	Total	C	N	O	P	0
			38	28	1	8	1	
25	H	1	Total	C	N	O	P	0
			43	33	1	8	1	
25	H	1	Total	C	N	O	P	0
			45	35	1	8	1	
25	q	1	Total	C	N	O	P	0
			36	26	1	8	1	
25	L	1	Total	C	N	O	P	0
			45	35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

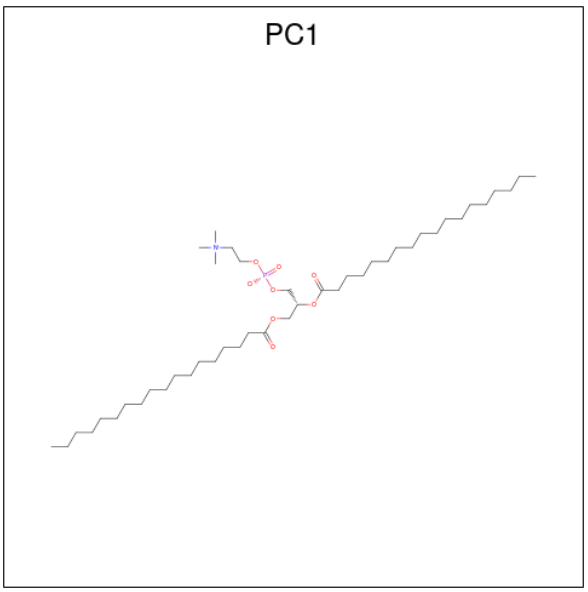
- Molecule 27 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



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: $C_{44}H_{88}NO_8P$).

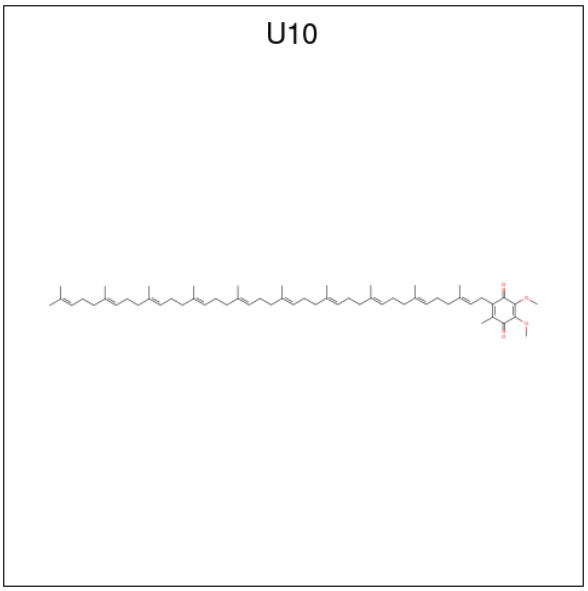


Mol	Chain	Residues	Atoms					AltConf
28	D	1	Total	C	N	O	P	0
			42	32	1	8	1	
28	J	1	Total	C	N	O	P	0
			45	35	1	8	1	

- 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 29 25 4	0

- Molecule 31 is water.

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

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

3 Residue-property plots (i)

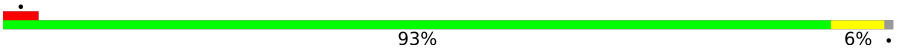
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

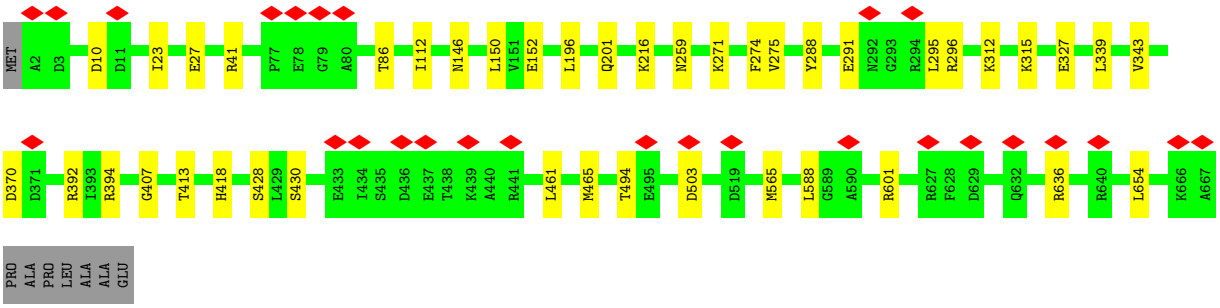
• Molecule 1: NADH-quinone oxidoreductase subunit K

Chain K:

• Molecule 2: NADH-quinone oxidoreductase

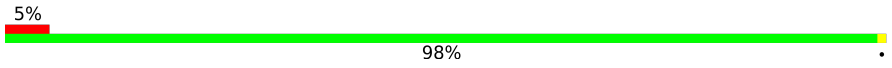
Chain G:

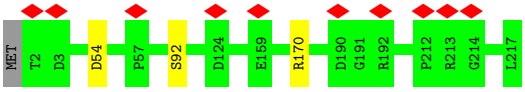




• Molecule 3: Protein-L-isoaspartate O-methyltransferase

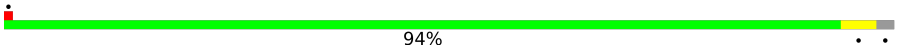
Chain t:

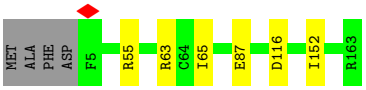




• Molecule 4: NADH-quinone oxidoreductase subunit I

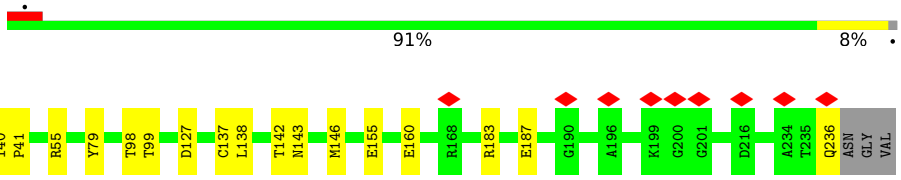
Chain I:





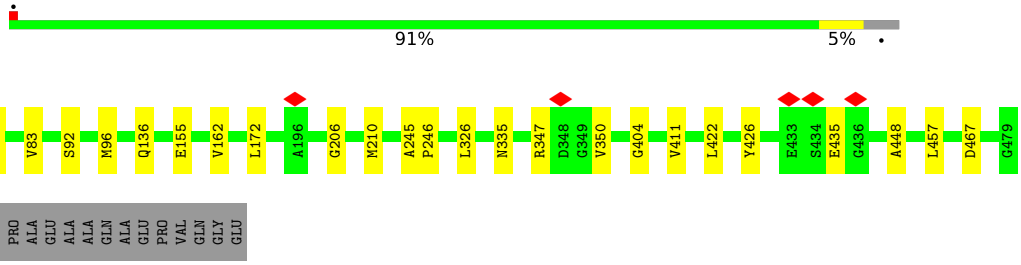
• Molecule 5: NADH dehydrogenase subunit E

Chain E:



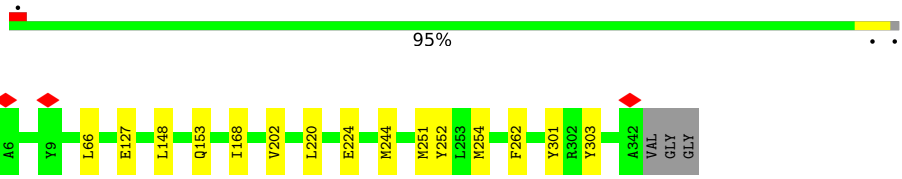
• Molecule 6: NADH-quinone oxidoreductase subunit N

Chain N:



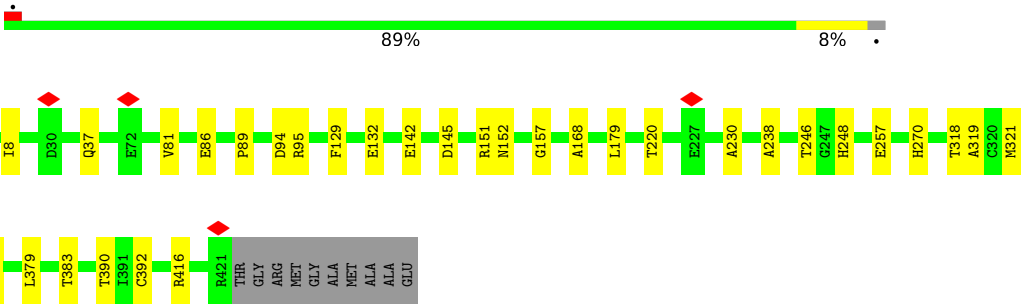
• Molecule 7: NADH-quinone oxidoreductase subunit H

Chain H:



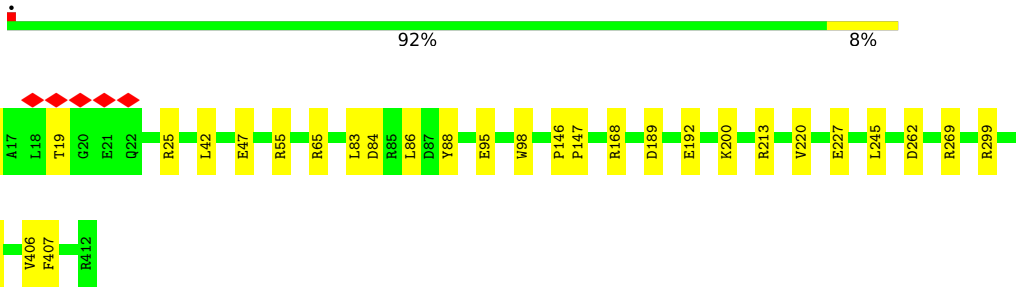
• Molecule 8: NADH-quinone oxidoreductase subunit F

Chain F:



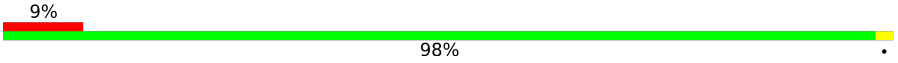
• Molecule 9: NADH-quinone oxidoreductase subunit D

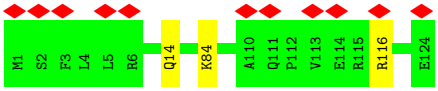
Chain D:



• Molecule 10: NADH:ubiquinone oxidoreductase 17.2 kD subunit

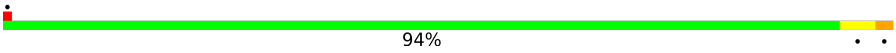
Chain q:

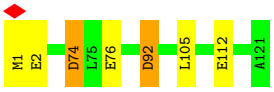




• Molecule 11: NADH-quinone oxidoreductase subunit A

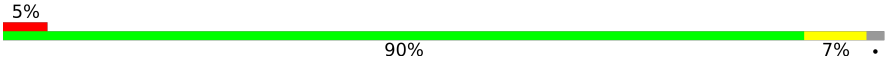
Chain A:

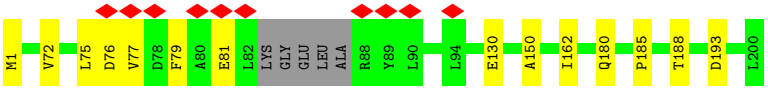




• Molecule 12: NADH-quinone oxidoreductase chain 10

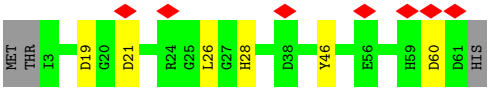
Chain J:





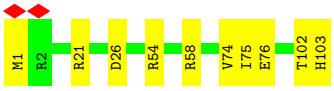
• Molecule 13: Zinc finger CHCC-type domain-containing protein

Chain R:



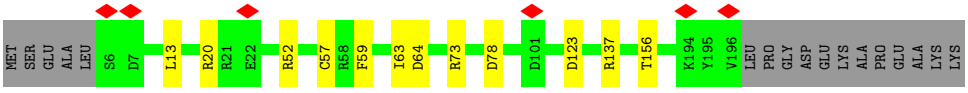
• Molecule 14: ETC complex I subunit conserved region

Chain Q:



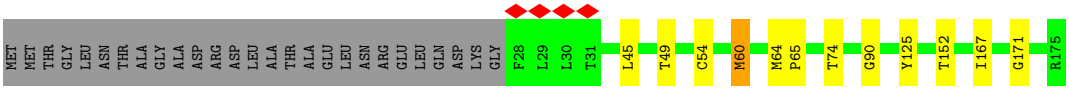
• Molecule 15: NADH-quinone oxidoreductase subunit C

Chain C:



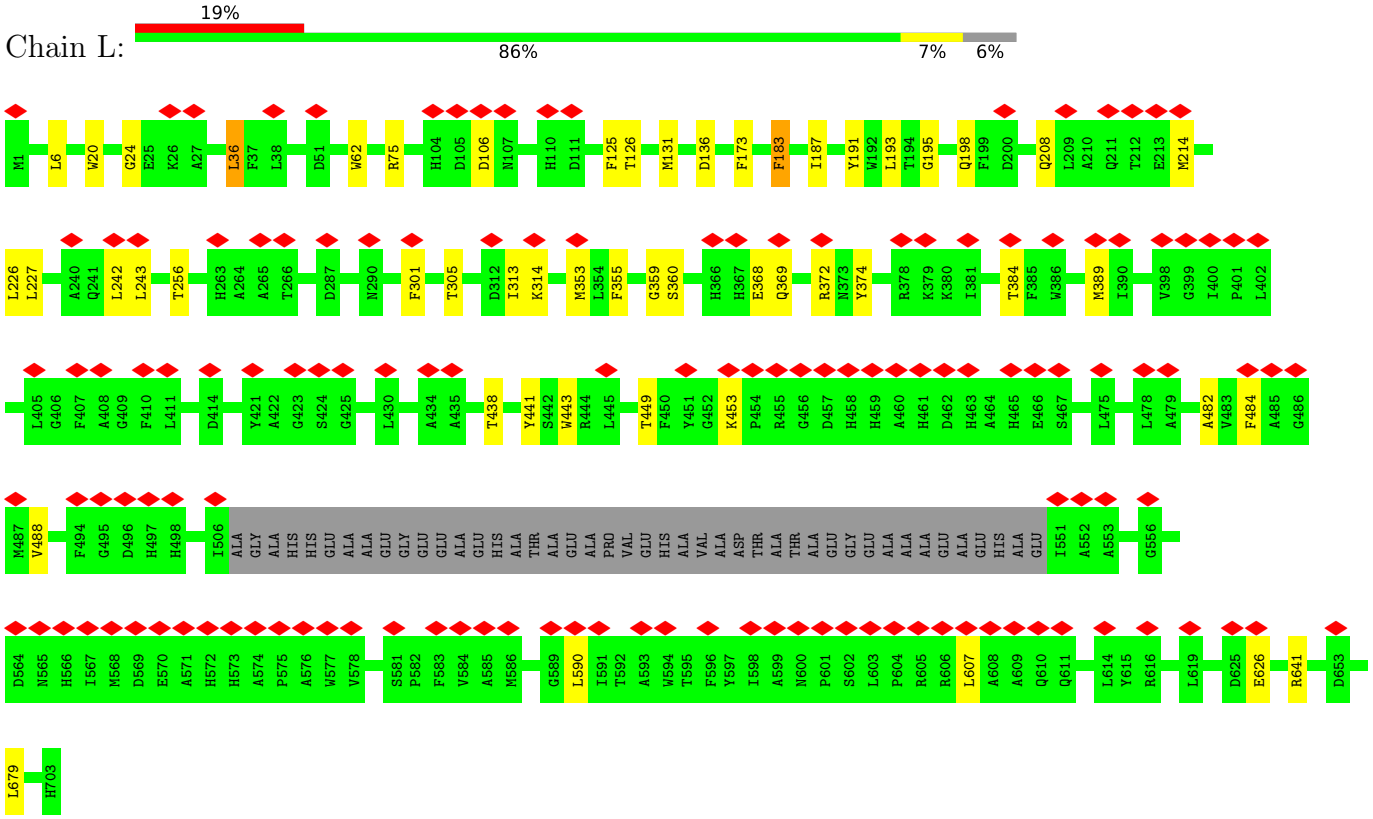
• Molecule 16: NADH-quinone oxidoreductase subunit B

Chain B:



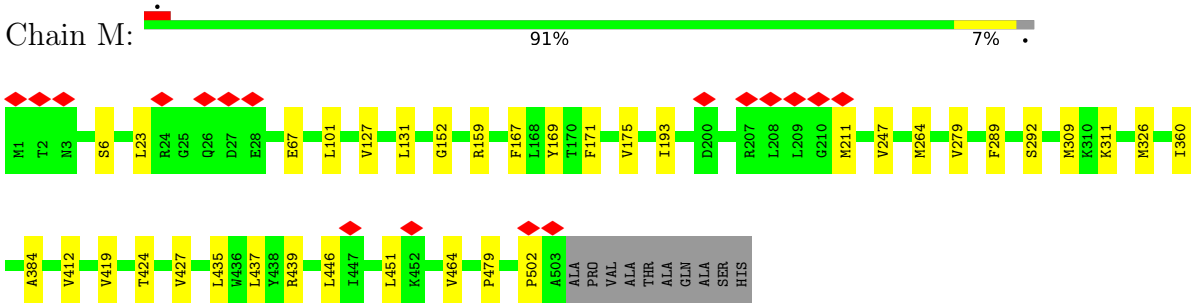
• Molecule 17: NADH dehydrogenase subunit L

Chain L:



• Molecule 18: NADH dehydrogenase subunit M

Chain M:



4 Experimental information (i)

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 ($e^-/Å^2$)	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

5.1 Standard geometry

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

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

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.

The worst 5 of 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

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	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
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 (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	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
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

5 of 59 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	D	339	LYS
17	L	641	ARG
12	J	193	ASP
17	L	453	LYS
17	L	208	GLN

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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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	N	502	-	45,45,47	0.65	1 (2%)	49,50,52	0.67	2 (4%)
22	3PH	L	802	-	44,44,47	0.64	1 (2%)	48,49,52	0.60	1 (2%)
25	3PE	q	201	-	35,35,50	0.61	0	38,40,55	0.74	2 (5%)
22	3PH	H	406	-	29,29,47	0.78	1 (3%)	33,34,52	0.83	2 (6%)
22	3PH	M	607	-	30,30,47	0.78	1 (3%)	34,35,52	0.71	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	FES	E	301	5	0,4,4	-	-	-		
19	SF4	G	802	2	0,12,12	-	-	-		
22	3PH	M	608	-	32,32,47	0.76	1 (3%)	36,37,52	0.69	1 (2%)
19	SF4	I	201	4	0,12,12	-	-	-		
25	3PE	N	503	-	47,47,50	0.53	0	50,52,55	0.56	2 (4%)
22	3PH	A	201	-	33,33,47	0.73	1 (3%)	37,38,52	0.90	2 (5%)
22	3PH	N	505	-	42,42,47	0.67	1 (2%)	46,47,52	0.58	0
28	PC1	J	301	-	44,44,53	0.54	0	50,52,61	0.52	1 (2%)
22	3PH	H	403	-	35,35,47	0.74	1 (2%)	39,40,52	0.72	1 (2%)
25	3PE	H	401	-	42,42,50	0.59	0	45,47,55	0.63	1 (2%)
22	3PH	L	801	-	46,46,47	0.65	1 (2%)	50,51,52	0.61	2 (4%)
22	3PH	J	302	-	31,31,47	0.76	1 (3%)	35,36,52	0.70	1 (2%)
23	P5S	I	204	-	47,48,53	0.57	0	51,55,60	0.75	2 (3%)
23	P5S	L	803	-	38,39,53	0.62	0	42,46,60	0.83	2 (4%)
19	SF4	G	801	2	0,12,12	-	-	-		
25	3PE	N	504	-	37,37,50	0.58	0	40,42,55	0.58	1 (2%)
22	3PH	L	805	-	35,35,47	0.73	1 (2%)	39,40,52	0.63	1 (2%)
25	3PE	M	602	-	41,41,50	0.58	0	44,46,55	0.55	1 (2%)
26	CDL	M	606	-	64,64,99	0.37	0	70,76,111	0.62	0
22	3PH	H	404	-	25,25,47	0.86	1 (4%)	29,30,52	0.81	1 (3%)
19	SF4	F	502	8	0,12,12	-	-	-		
22	3PH	J	303	-	41,41,47	0.67	1 (2%)	45,46,52	0.67	1 (2%)
22	3PH	I	203	-	38,38,47	0.69	1 (2%)	42,43,52	0.71	1 (2%)
25	3PE	H	405	-	44,44,50	0.57	0	47,49,55	0.56	1 (2%)
25	3PE	M	605	-	28,28,50	0.67	0	31,33,55	0.64	1 (3%)
25	3PE	N	501	-	41,41,50	0.56	0	44,46,55	0.58	1 (2%)
22	3PH	M	601	-	30,30,47	0.76	1 (3%)	34,35,52	0.77	3 (8%)
25	3PE	L	804	-	44,44,50	0.56	0	47,49,55	0.56	1 (2%)
19	SF4	I	202	4	0,12,12	-	-	-		
27	FMN	F	501	-	33,33,33	1.10	3 (9%)	48,50,50	1.28	7 (14%)
26	CDL	H	402	-	64,64,99	0.40	0	70,76,111	0.61	1 (1%)
20	FES	G	803	2	0,4,4	-	-	-		
28	PC1	D	501	-	41,41,53	0.57	0	47,49,61	0.53	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	-	-	-		
22	3PH	L	806	-	28,28,47	0.80	1 (3%)	32,33,52	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	U10	B	401	-	29,29,63	3.05	8 (27%)	35,38,79	2.36	11 (31%)
22	3PH	M	603	-	32,32,47	0.76	1 (3%)	36,37,52	0.71	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	N	502	-	-	17/47/47/49	-
22	3PH	L	802	-	-	17/46/46/49	-
25	3PE	q	201	-	-	21/39/39/54	-
22	3PH	H	406	-	-	16/31/31/49	-
22	3PH	M	607	-	-	11/32/32/49	-
20	FES	E	301	5	-	-	0/1/1/1
22	3PH	M	608	-	-	18/34/34/49	-
19	SF4	G	802	2	-	-	0/6/5/5
19	SF4	I	201	4	-	-	0/6/5/5
25	3PE	N	503	-	-	22/51/51/54	-
22	3PH	A	201	-	-	14/35/35/49	-
22	3PH	N	505	-	-	19/44/44/49	-
28	PC1	J	301	-	-	15/48/48/57	-
22	3PH	H	403	-	-	10/37/37/49	-
25	3PE	H	401	-	-	15/46/46/54	-
22	3PH	L	801	-	-	18/48/48/49	-
22	3PH	J	302	-	-	13/33/33/49	-
23	P5S	I	204	-	-	20/54/54/59	-
23	P5S	L	803	-	-	22/45/45/59	-
19	SF4	G	801	2	-	-	0/6/5/5
25	3PE	N	504	-	-	19/41/41/54	-
22	3PH	L	805	-	-	11/37/37/49	-
25	3PE	M	602	-	-	23/45/45/54	-
26	CDL	M	606	-	-	37/75/75/110	-
22	3PH	H	404	-	-	8/27/27/49	-
25	3PE	M	605	-	-	11/32/32/54	-
22	3PH	J	303	-	-	21/43/43/49	-
22	3PH	I	203	-	-	14/40/40/49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	3PE	H	405	-	-	23/48/48/54	-
19	SF4	F	502	8	-	-	0/6/5/5
25	3PE	N	501	-	-	12/45/45/54	-
22	3PH	M	601	-	-	14/32/32/49	-
25	3PE	L	804	-	-	19/48/48/54	-
19	SF4	I	202	4	-	-	0/6/5/5
27	FMN	F	501	-	-	4/18/18/18	0/3/3/3
26	CDL	H	402	-	-	43/75/75/110	-
20	FES	G	803	2	-	-	0/1/1/1
28	PC1	D	501	-	-	20/45/45/57	-
25	3PE	M	604	-	-	22/44/44/54	-
19	SF4	B	402	16	-	-	0/6/5/5
22	3PH	L	806	-	-	15/30/30/49	-
30	U10	B	401	-	-	11/23/47/87	0/1/1/1
22	3PH	M	603	-	-	5/34/34/49	-

The worst 5 of 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

The worst 5 of 59 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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

There are no chirality outliers.

5 of 600 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	N	502	3PH	O21-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
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

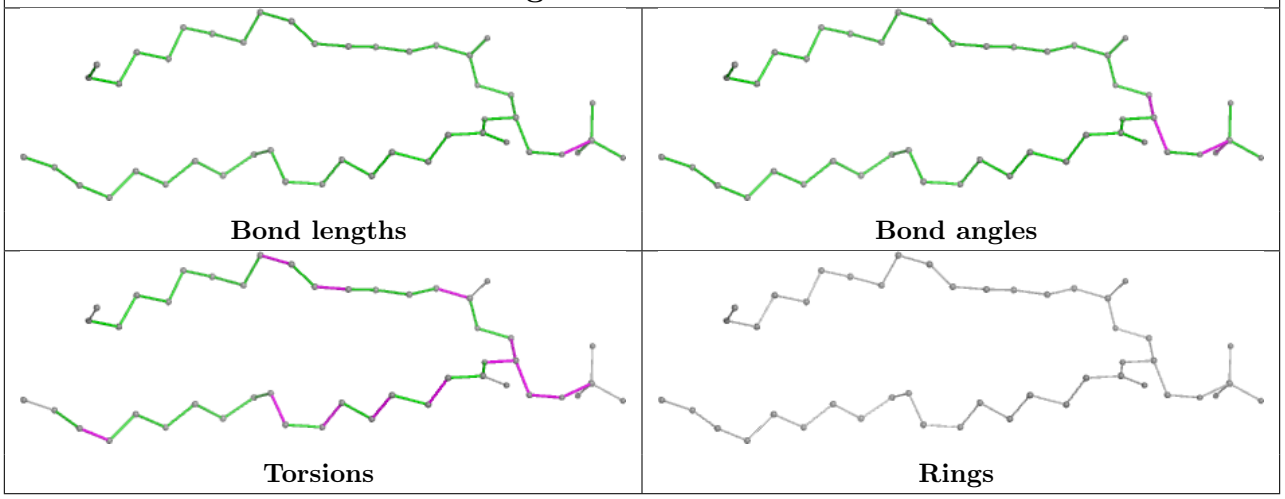
There are no ring outliers.

10 monomers are involved in 13 short contacts:

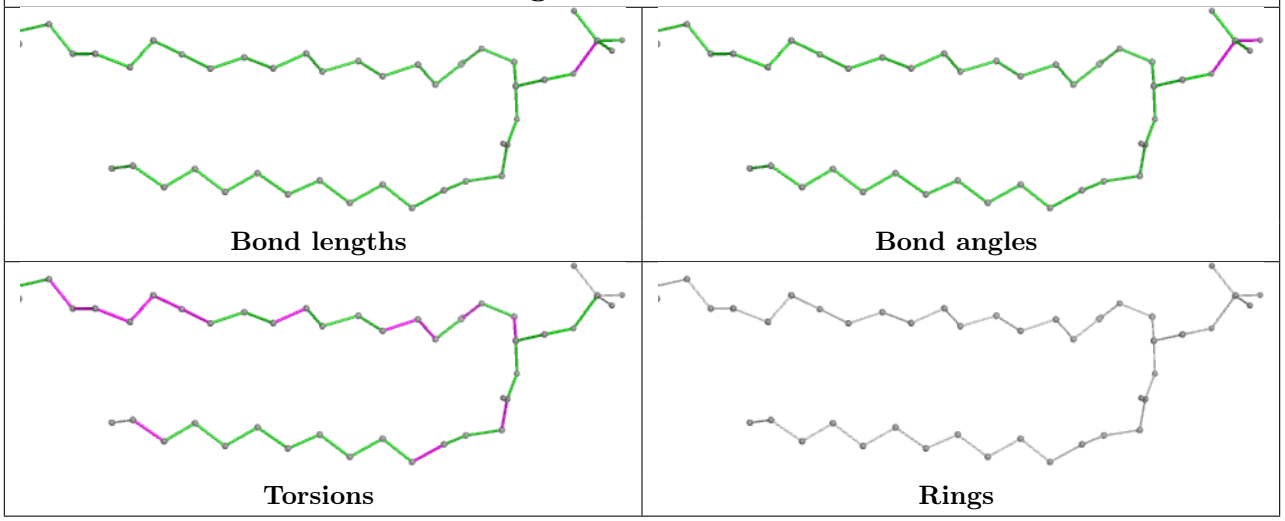
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	L	802	3PH	1	0
23	I	204	P5S	1	0
23	L	803	P5S	1	0
22	L	805	3PH	1	0
19	F	502	SF4	1	0
25	N	501	3PE	2	0
28	D	501	PC1	1	0
19	B	402	SF4	1	0
30	B	401	U10	3	0
22	M	603	3PH	1	0

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 then 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.

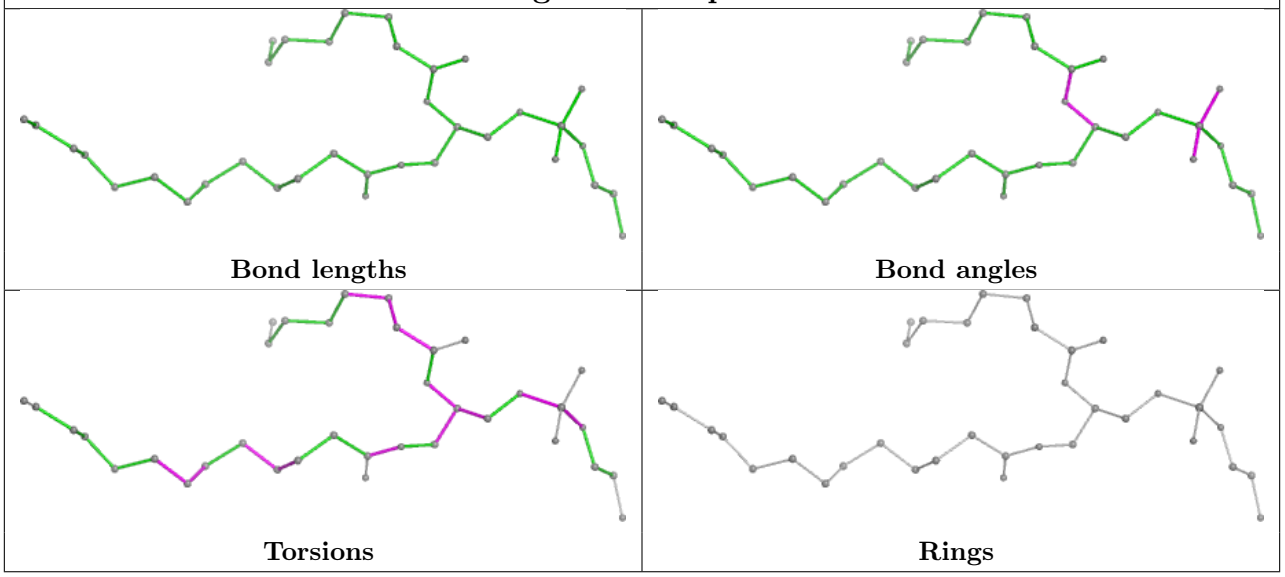
Ligand 3PH N 502



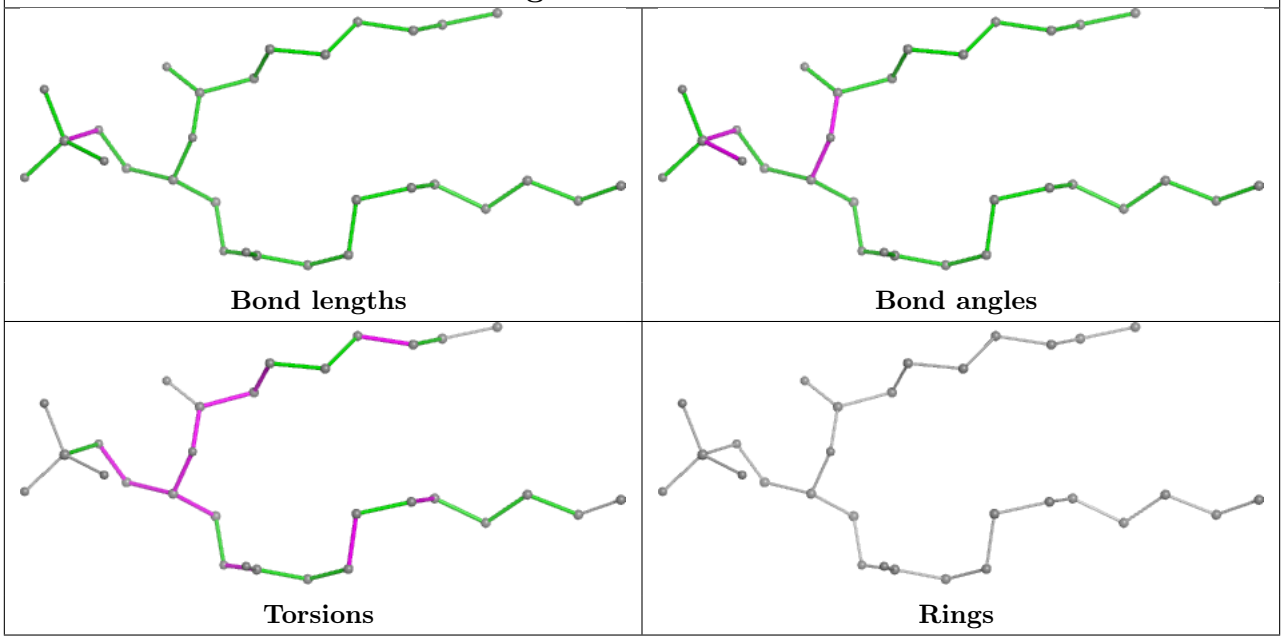
Ligand 3PH L 802



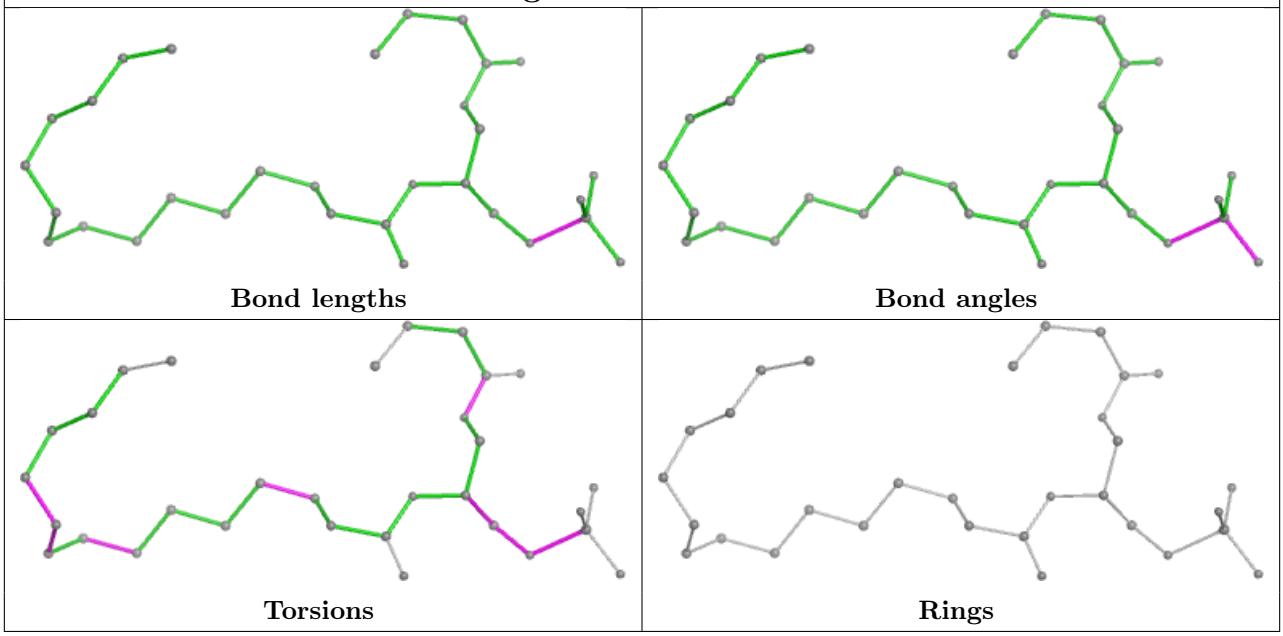
Ligand 3PE q 201



Ligand 3PH H 406



Ligand 3PH M 607



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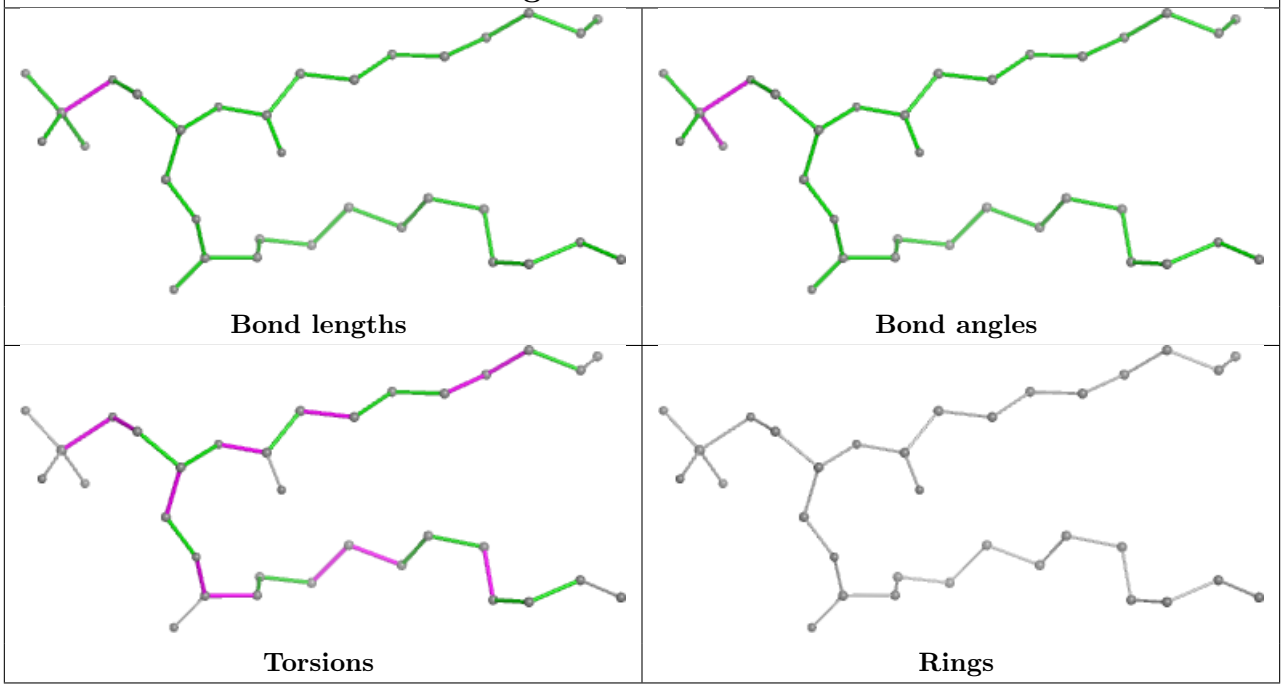

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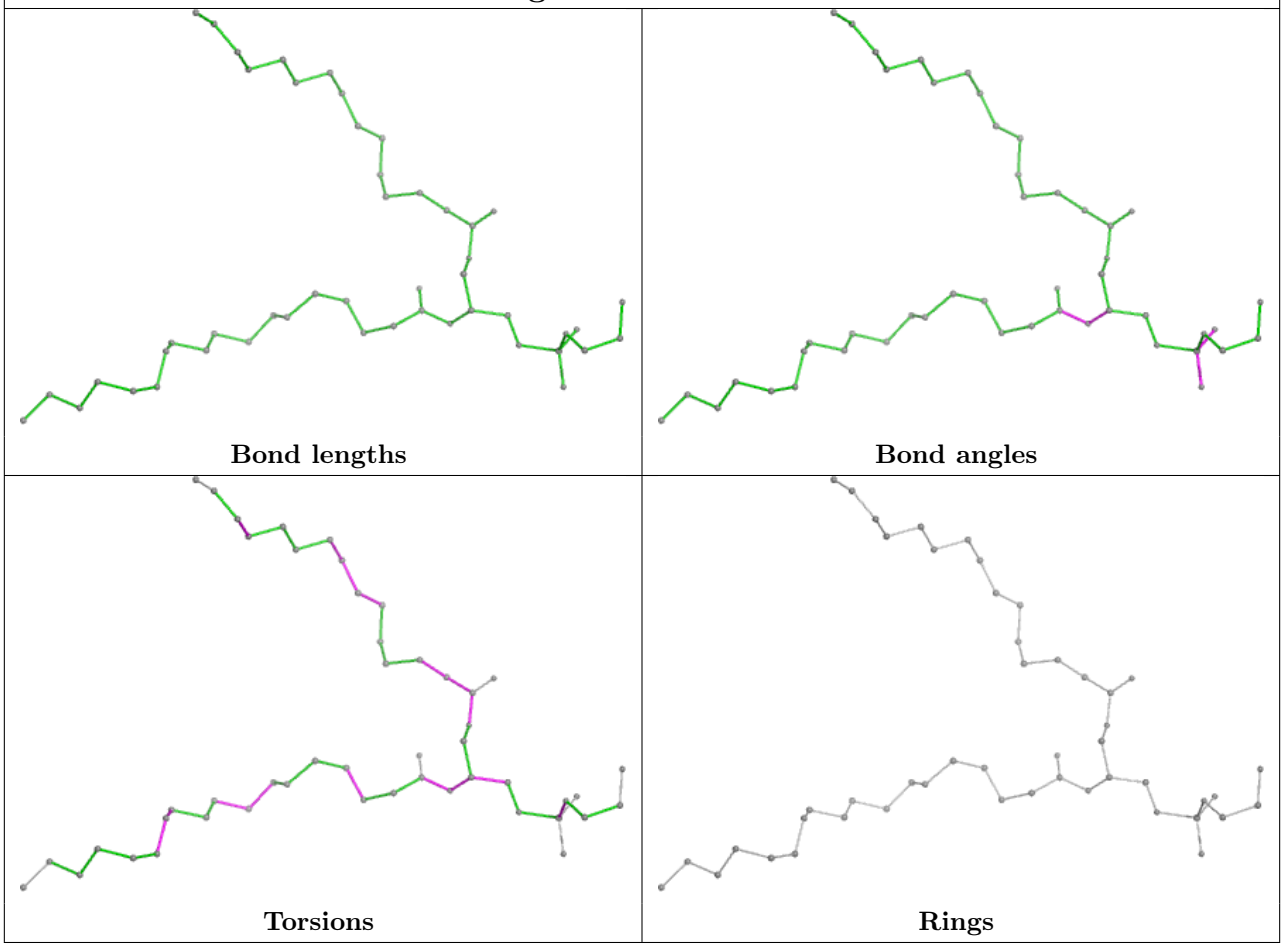
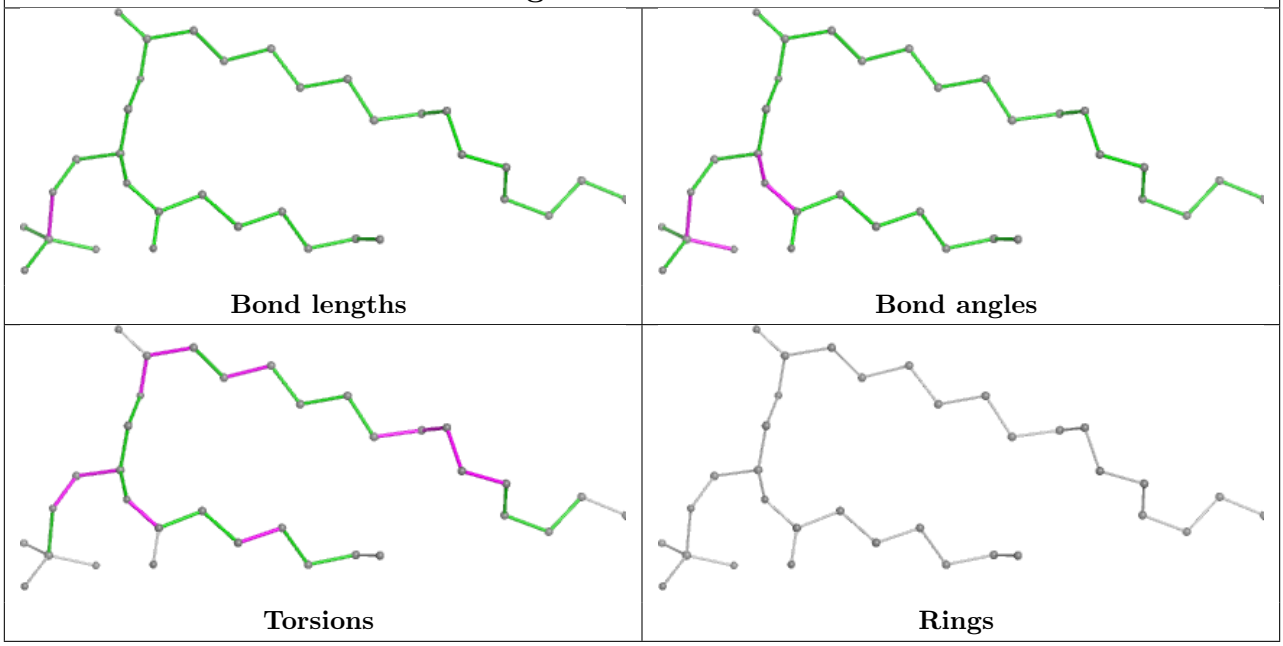
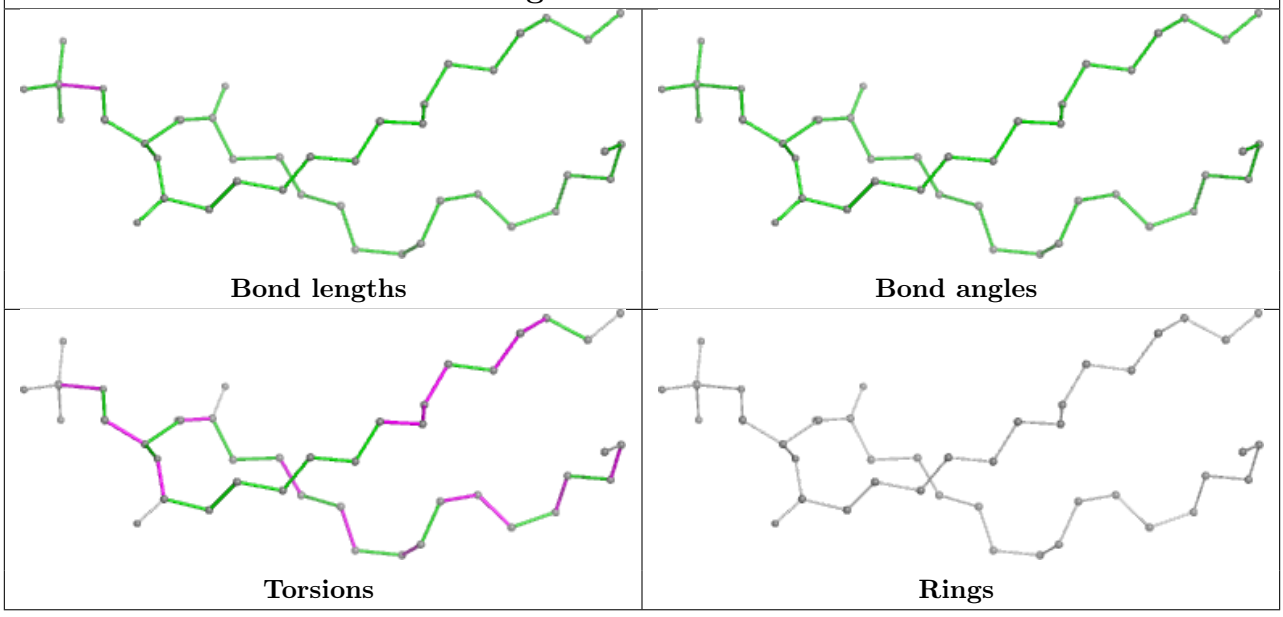


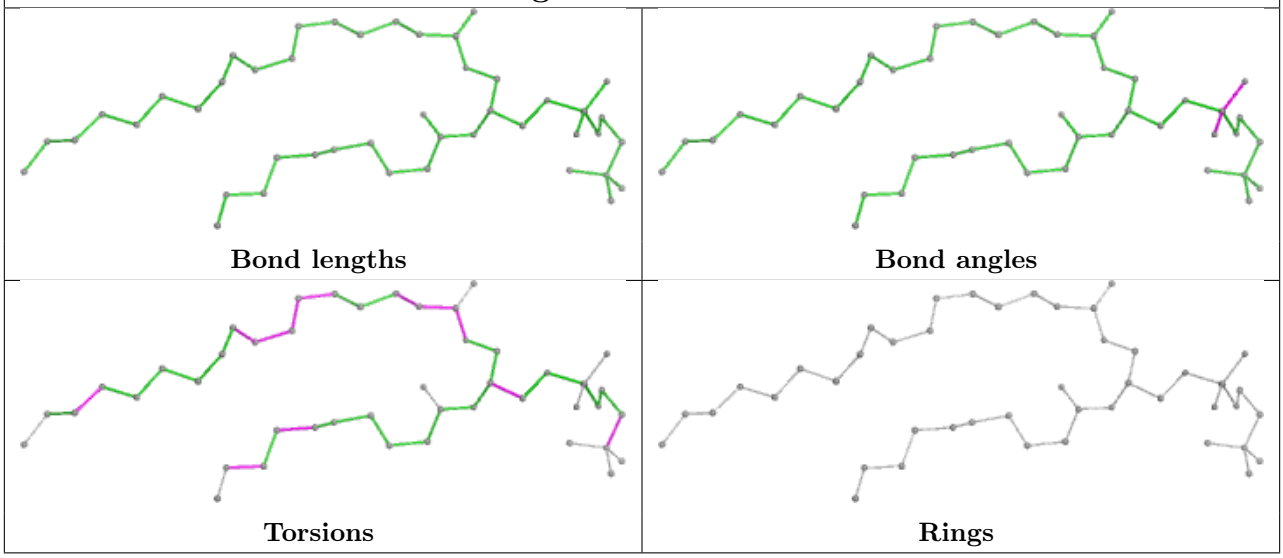
Ligand 3PH A 201



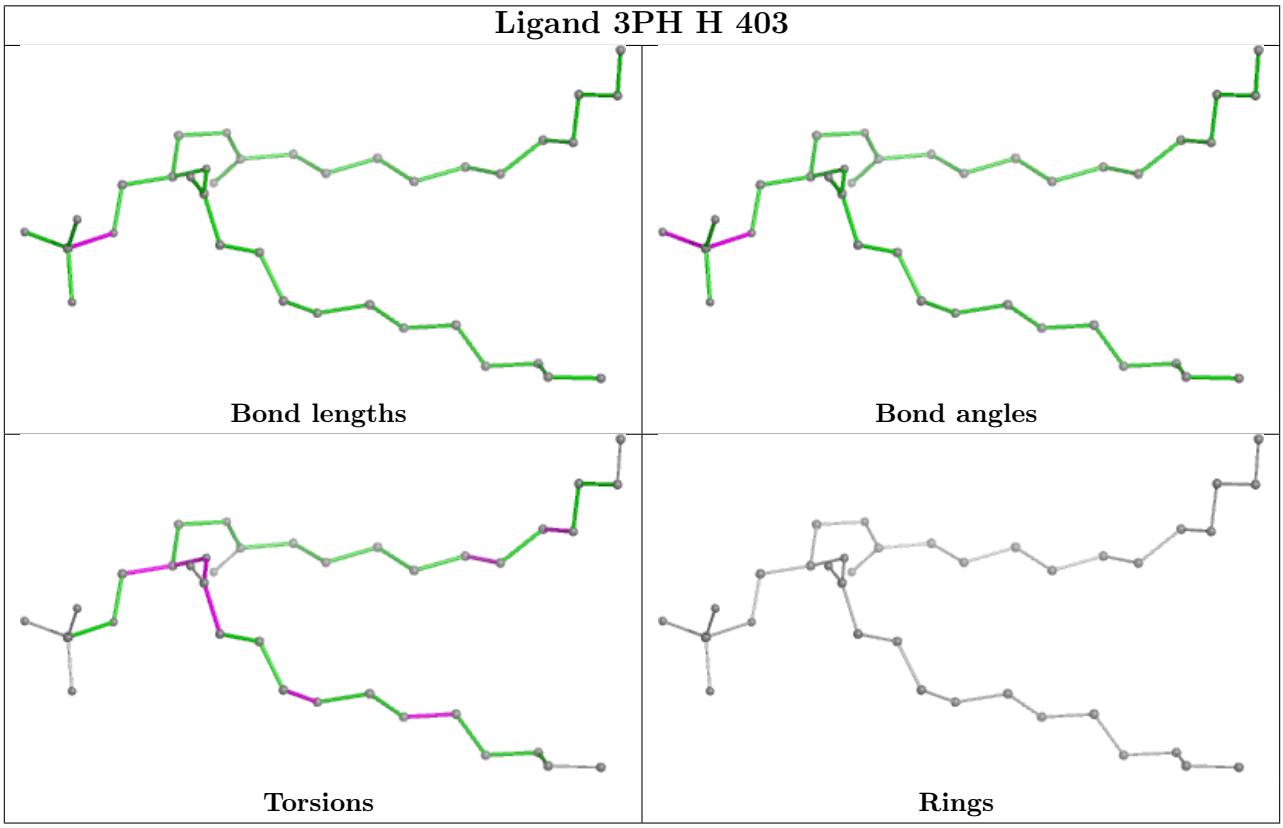
Ligand 3PH N 505



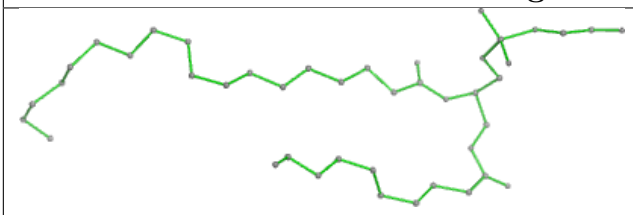
Ligand PC1 J 301



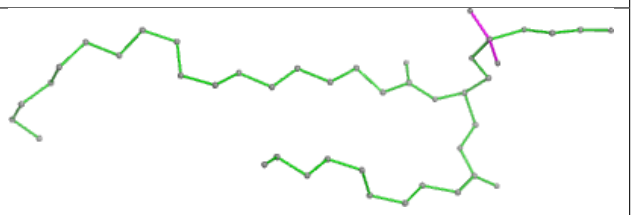
Ligand 3PH H 403



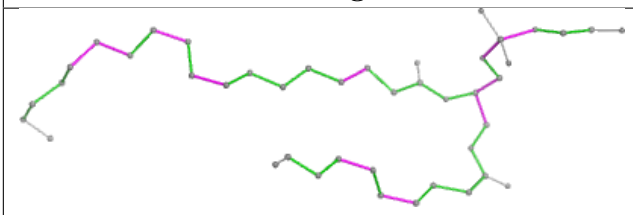
Ligand 3PE H 401



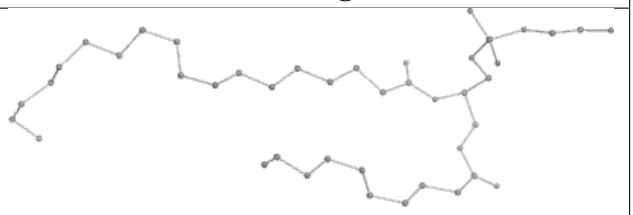
Bond lengths



Bond angles

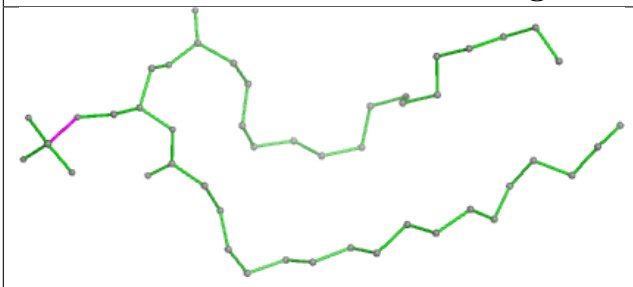


Torsions

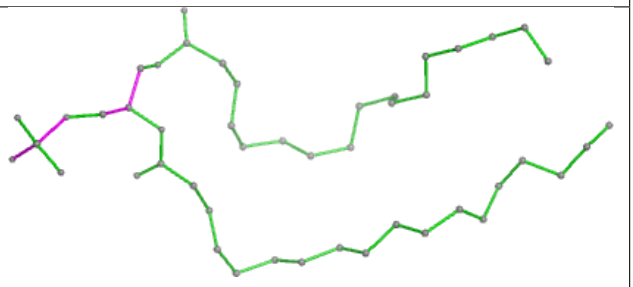


Rings

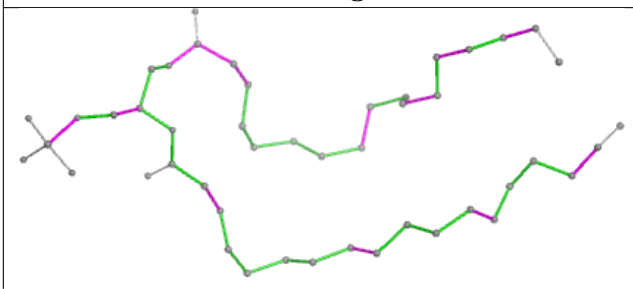
Ligand 3PH L 801



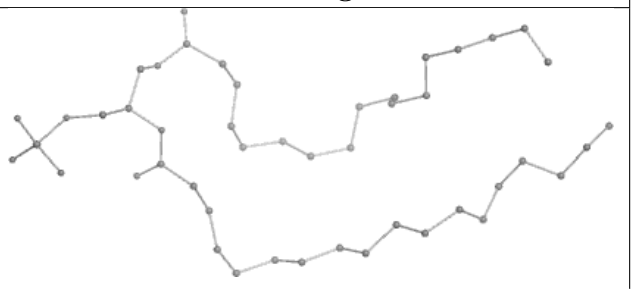
Bond lengths



Bond angles

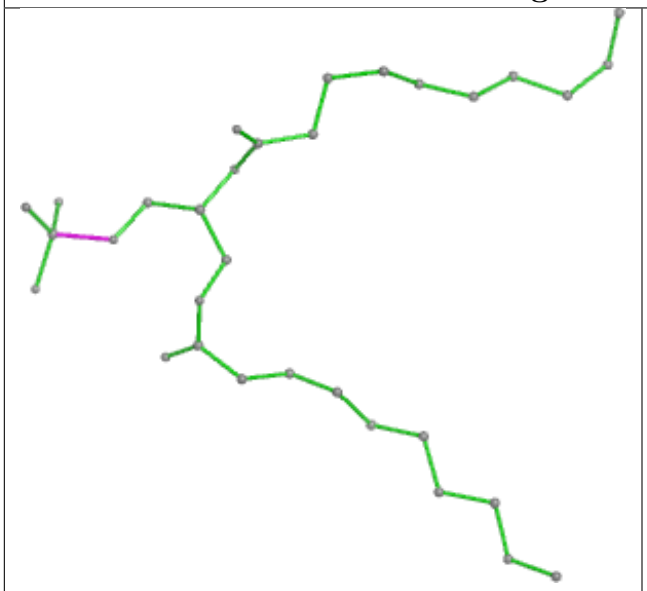


Torsions

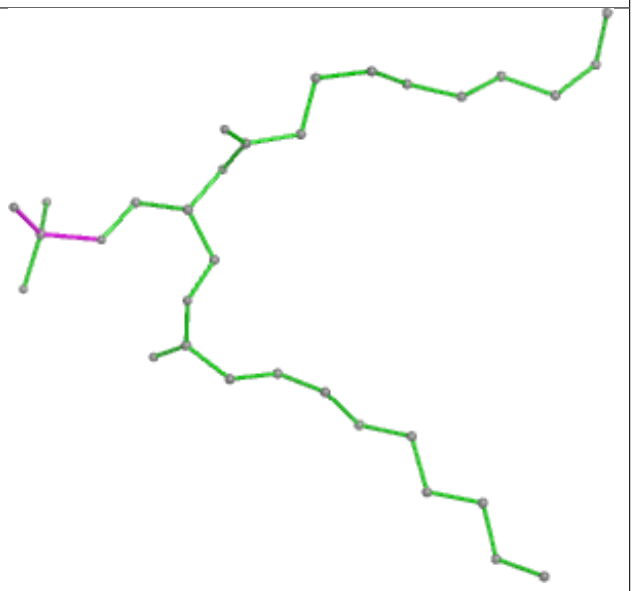


Rings

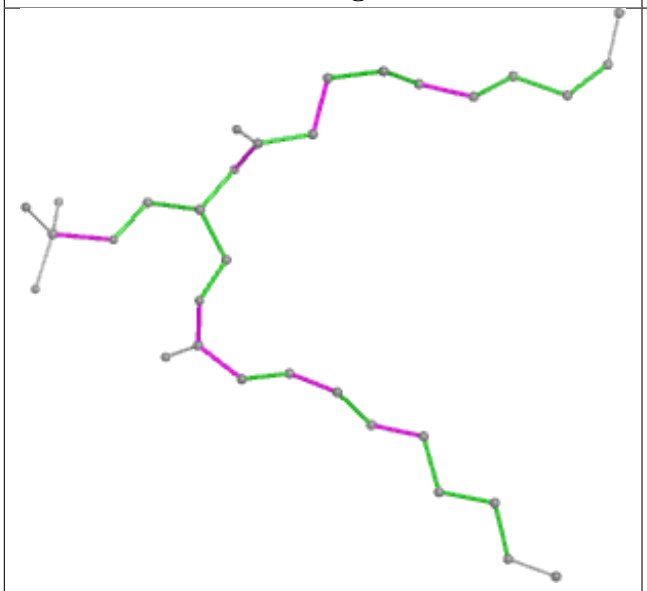
Ligand 3PH J 302



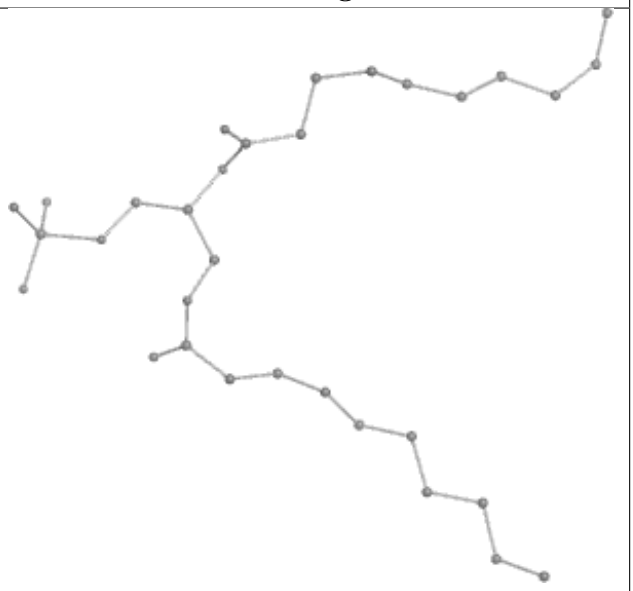
Bond lengths



Bond angles

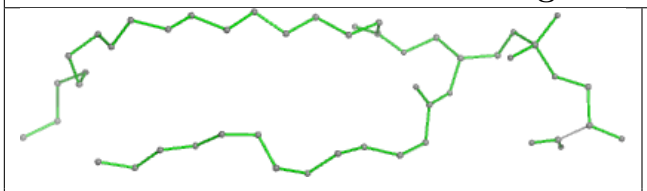


Torsions

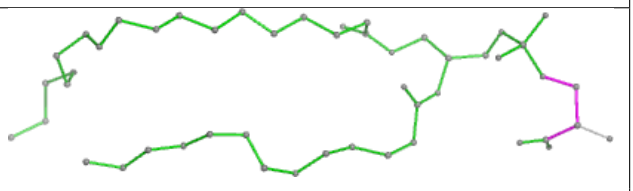


Rings

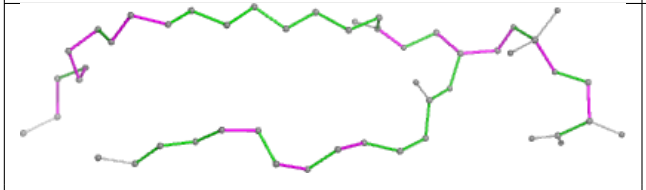
Ligand P5S I 204



Bond lengths



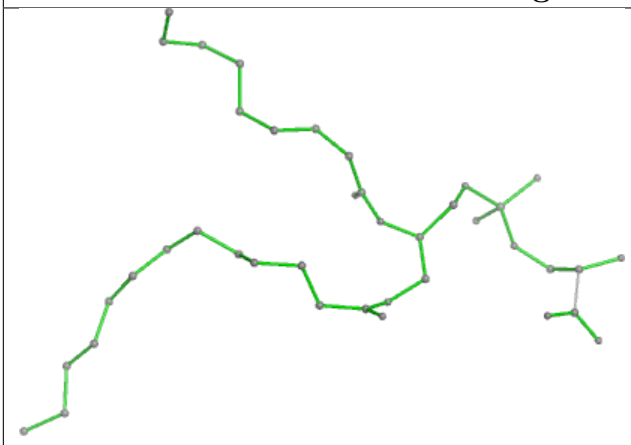
Bond angles



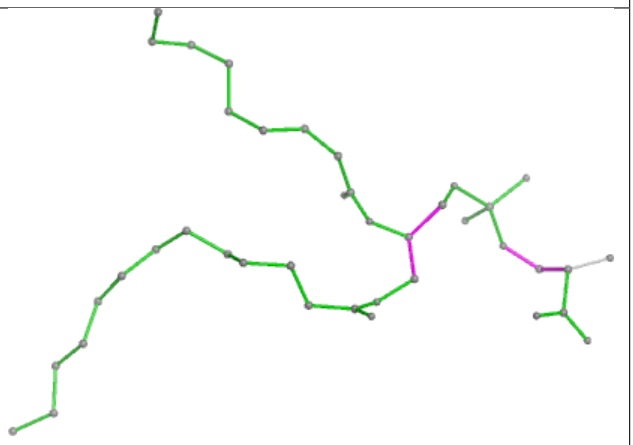
Torsions

Rings

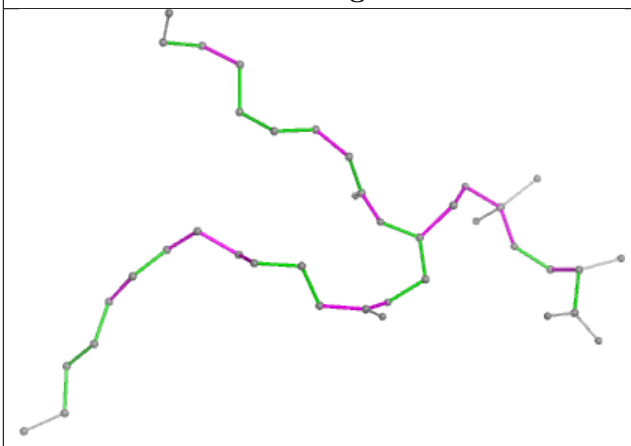
Ligand P5S L 803



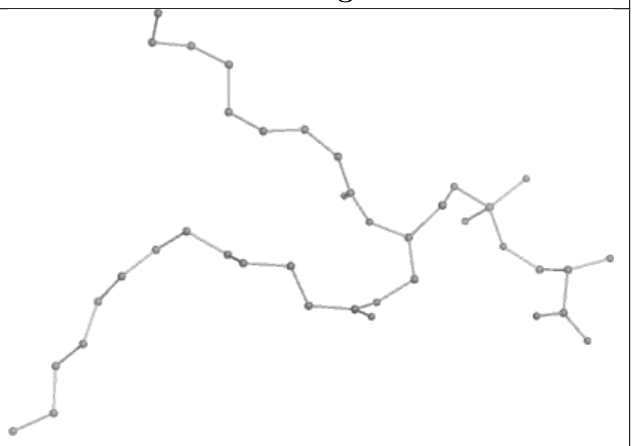
Bond lengths



Bond angles

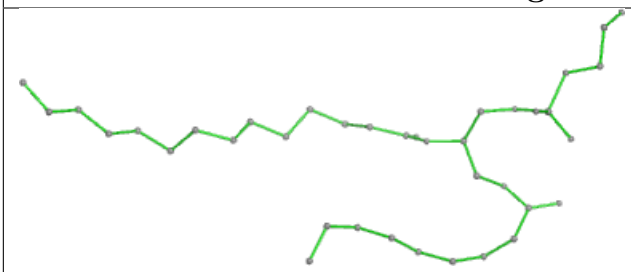


Torsions

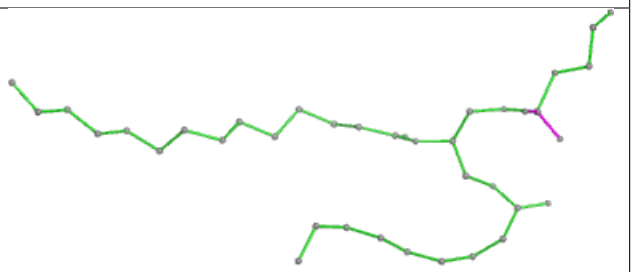


Rings

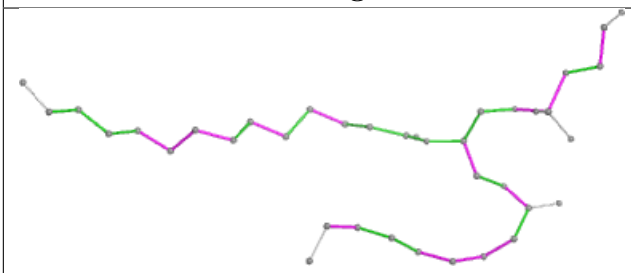
Ligand 3PE N 504



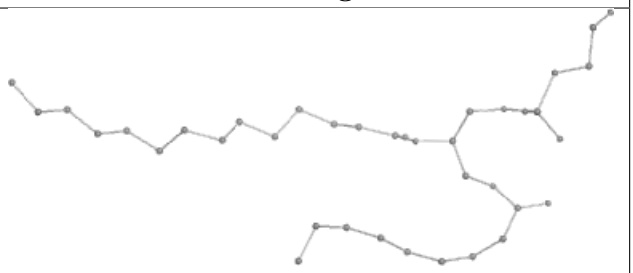
Bond lengths



Bond angles

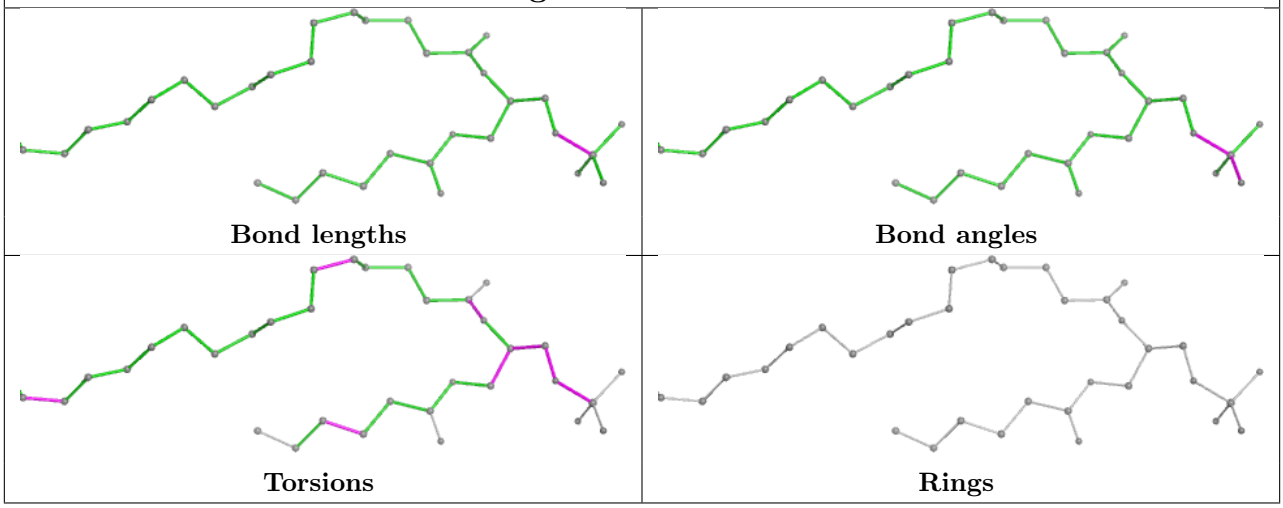


Torsions

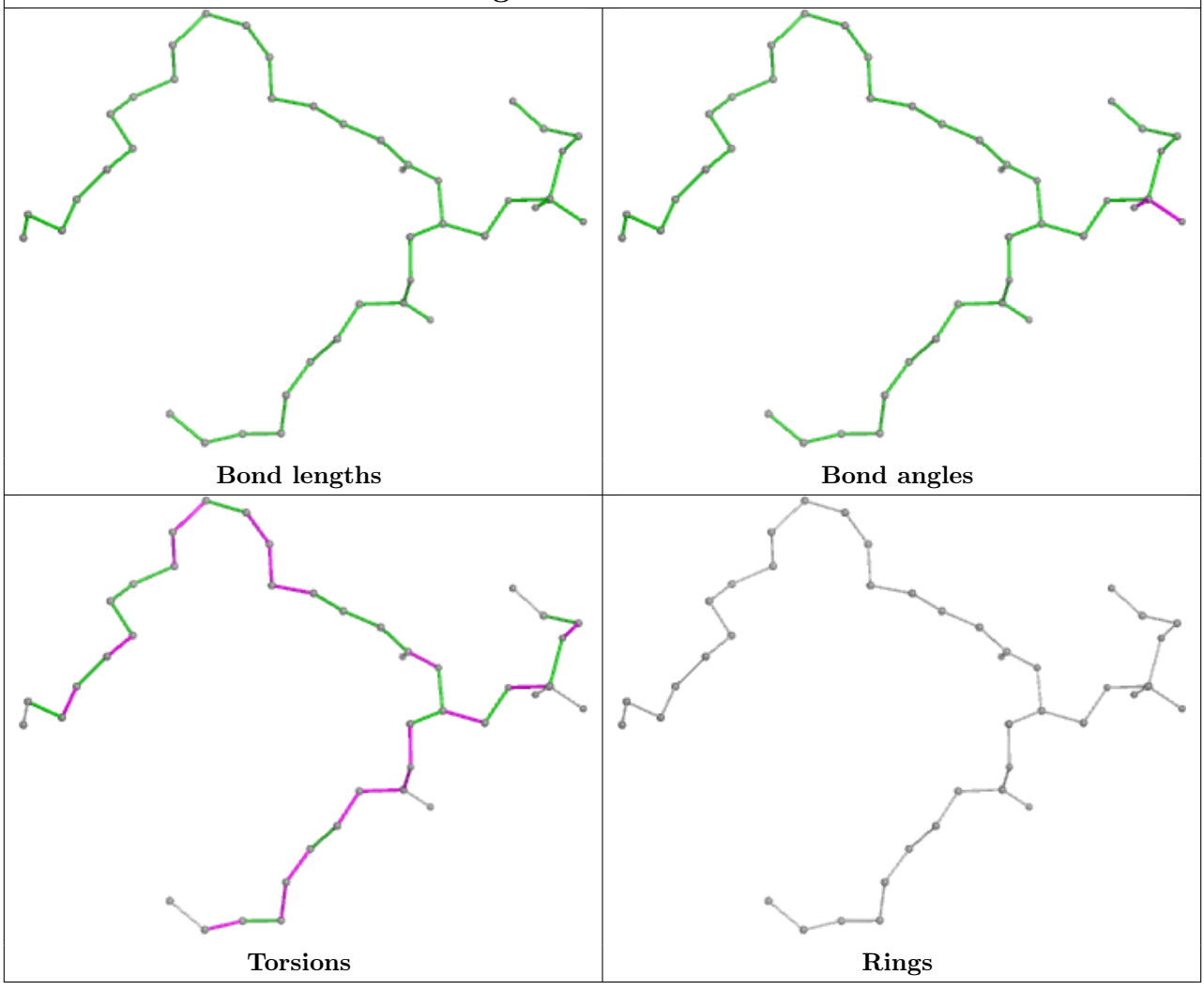


Rings

Ligand 3PH L 805

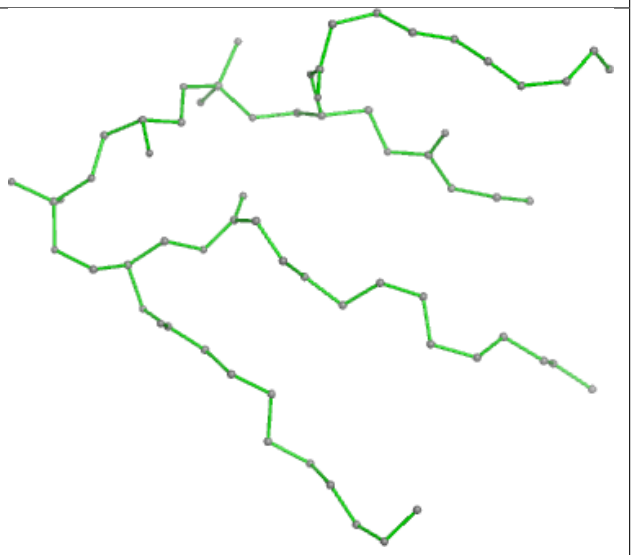


Ligand 3PE M 602

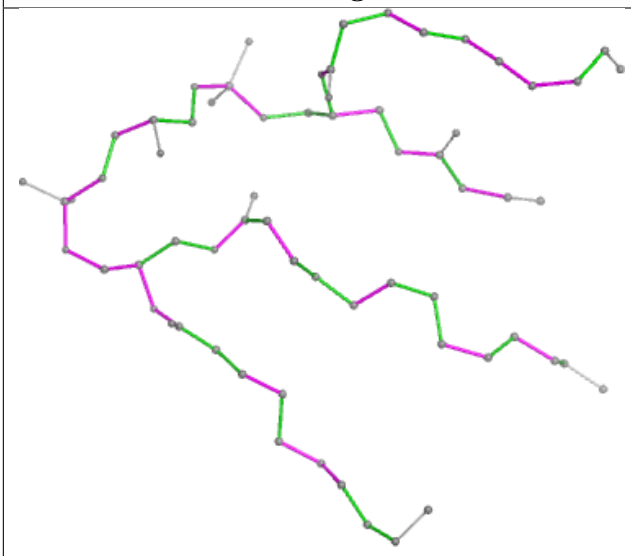


Ligand CDL M 606

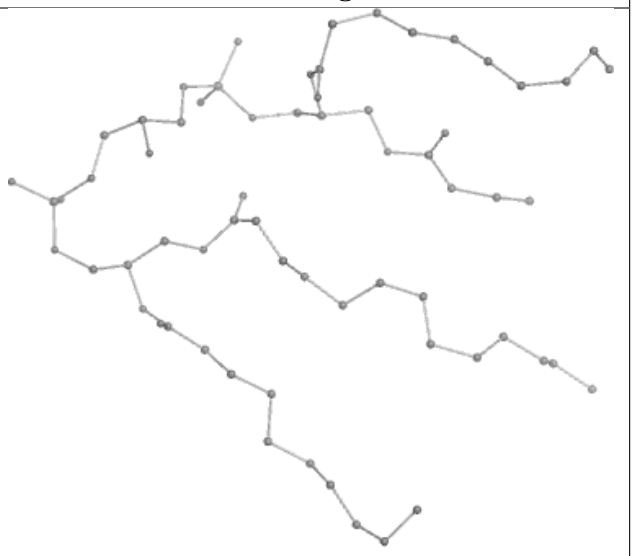
Bond lengths



Bond angles

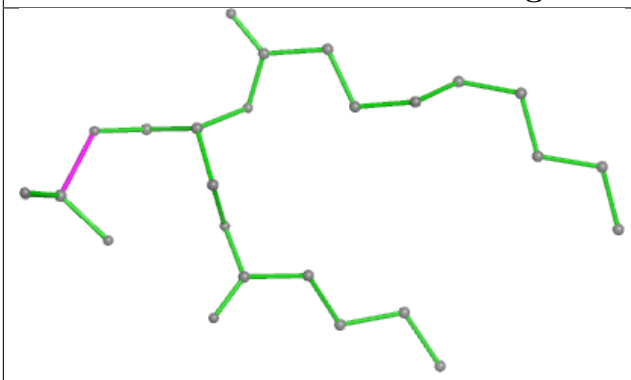


Torsions

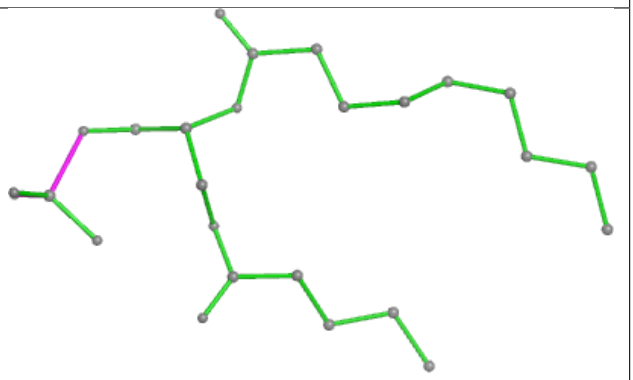


Rings

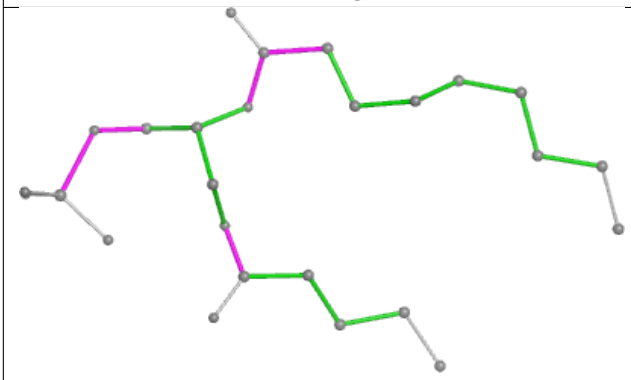
Ligand 3PH H 404



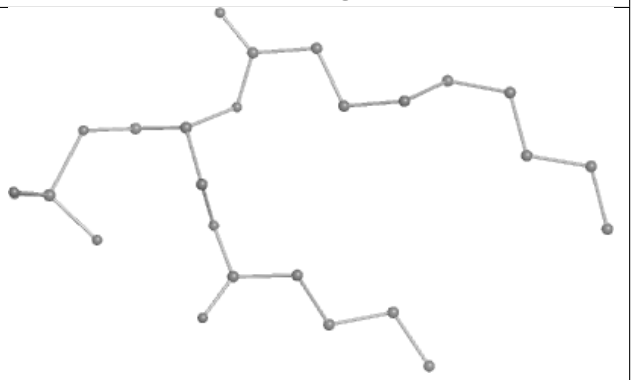
Bond lengths



Bond angles

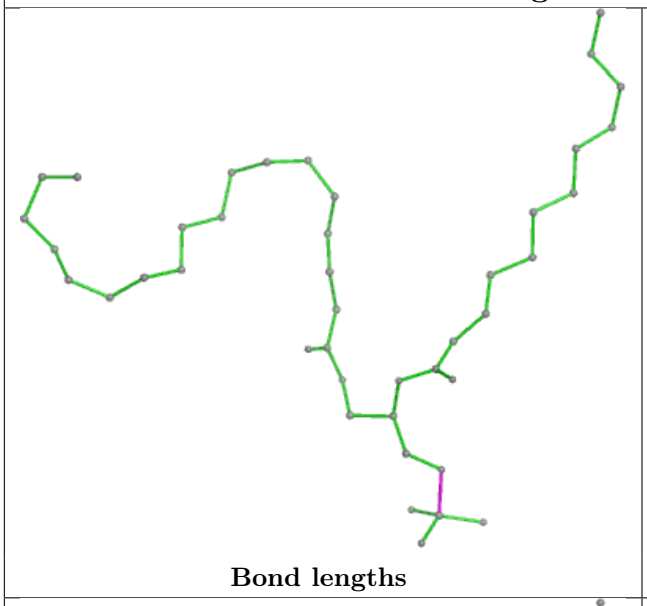


Torsions

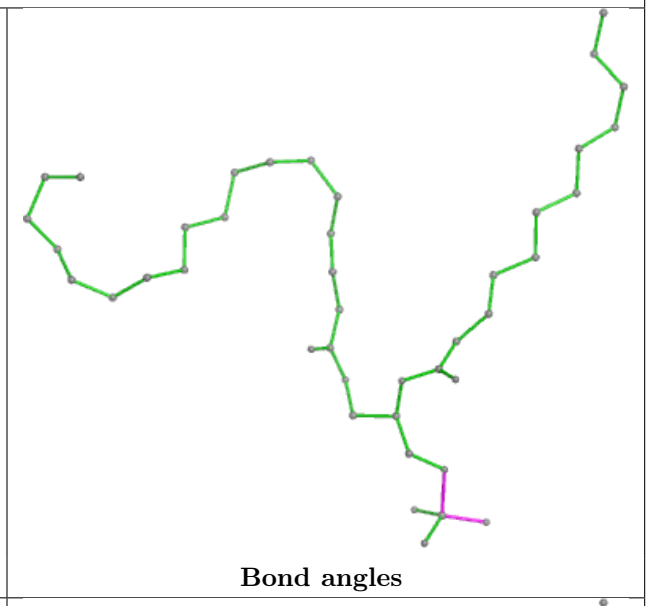


Rings

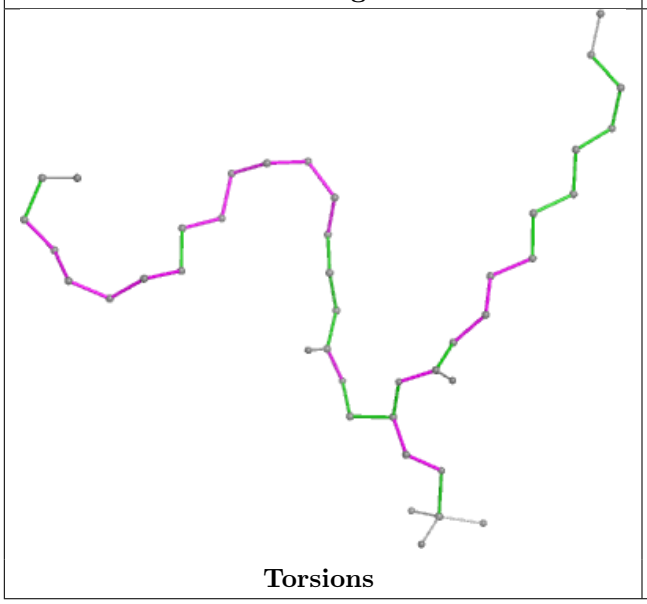
Ligand 3PH J 303



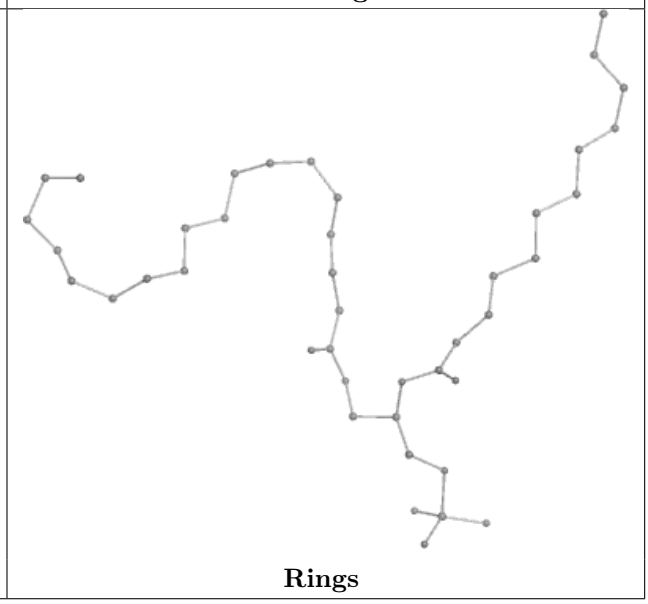
Bond lengths



Bond angles

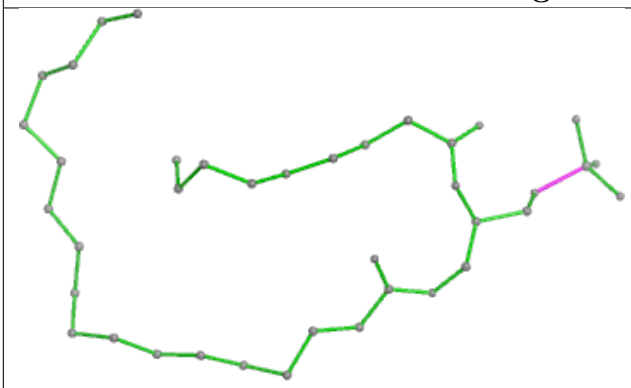


Torsions

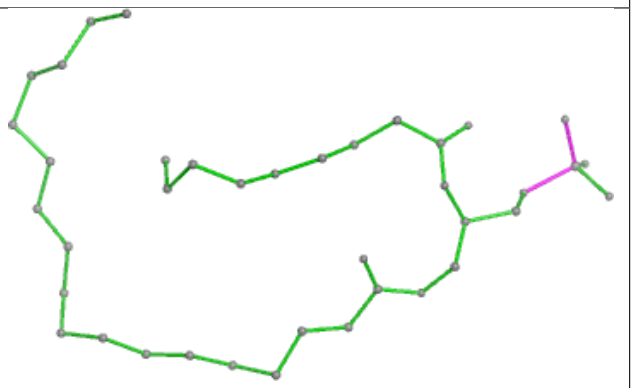


Rings

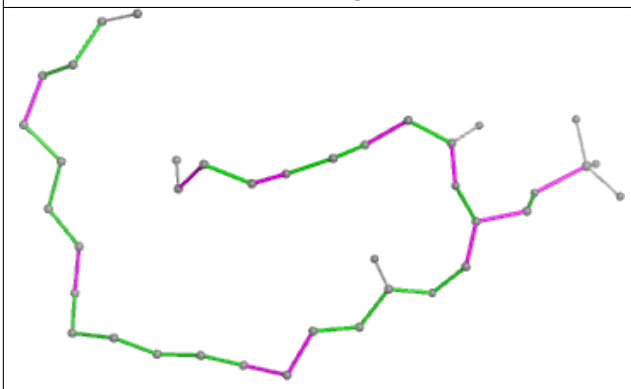
Ligand 3PH I 203



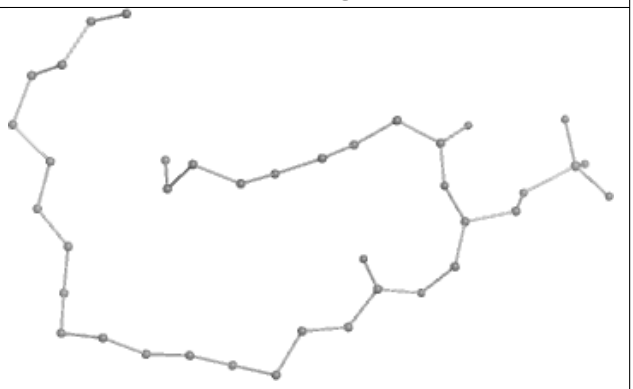
Bond lengths



Bond angles

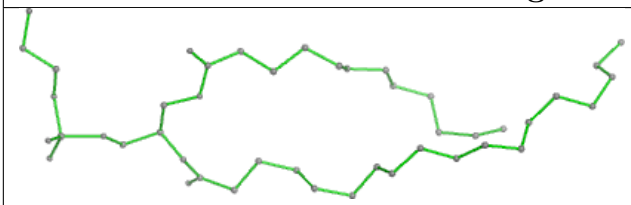


Torsions

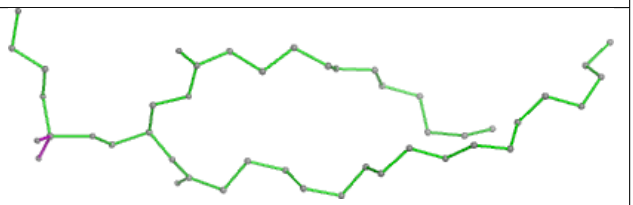


Rings

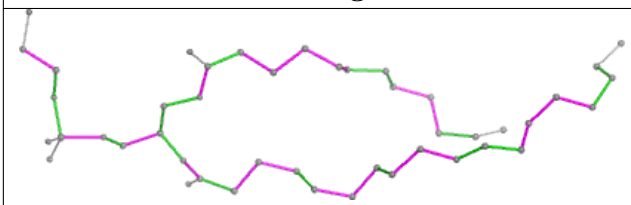
Ligand 3PE H 405



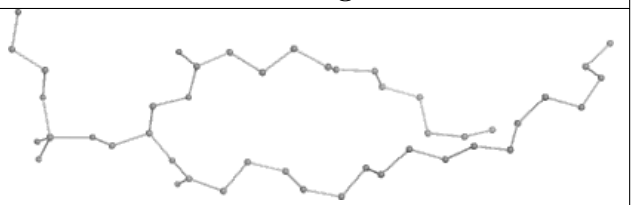
Bond lengths



Bond angles

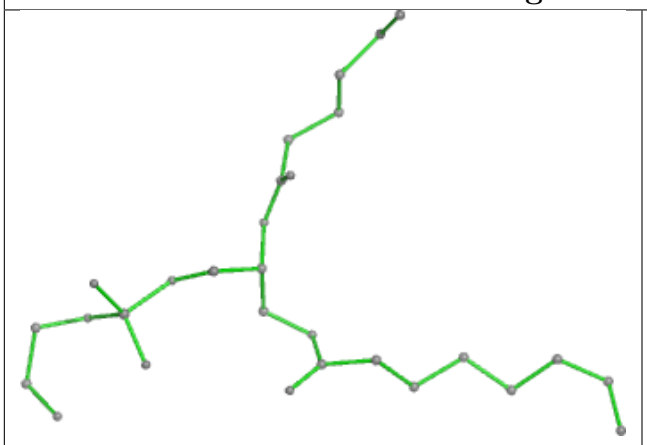


Torsions

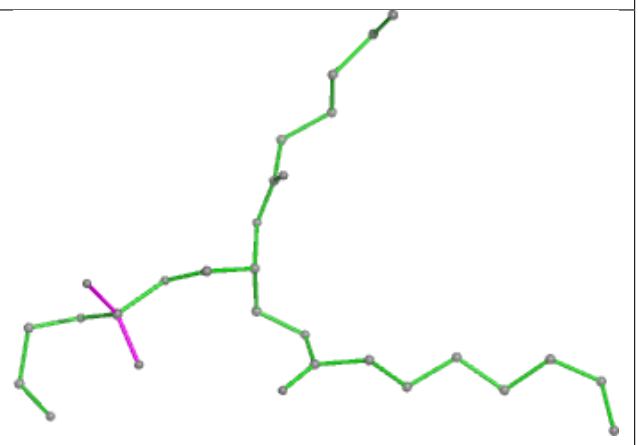


Rings

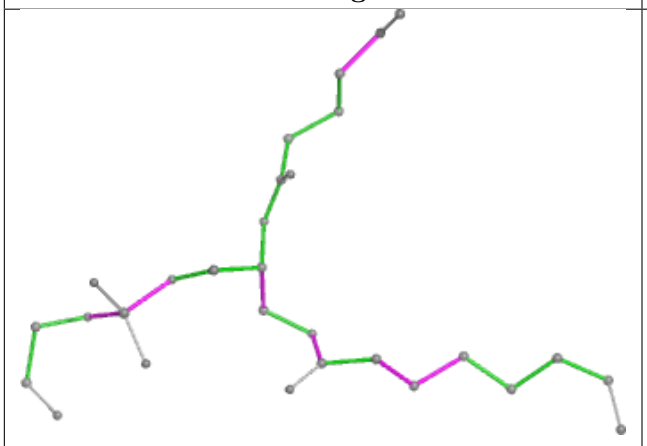
Ligand 3PE M 605



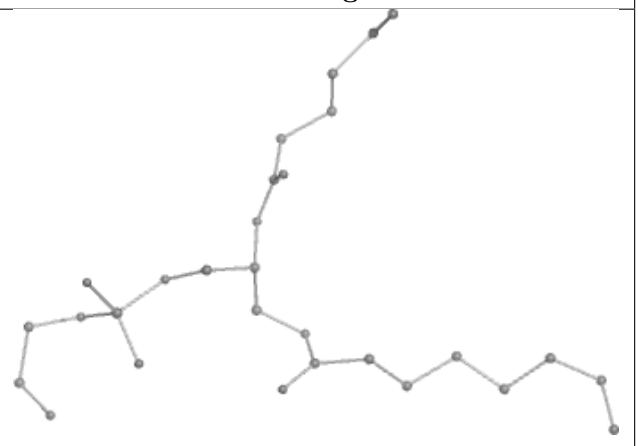
Bond lengths



Bond angles

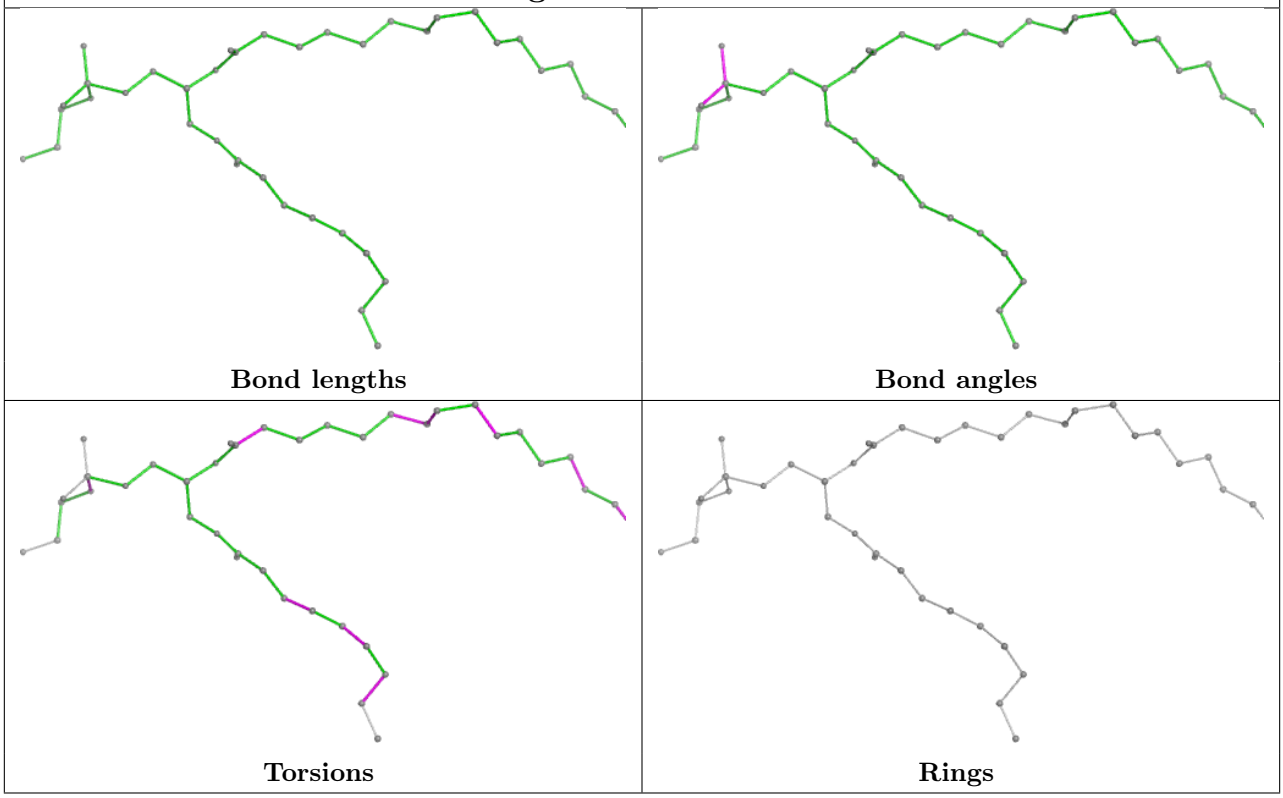


Torsions

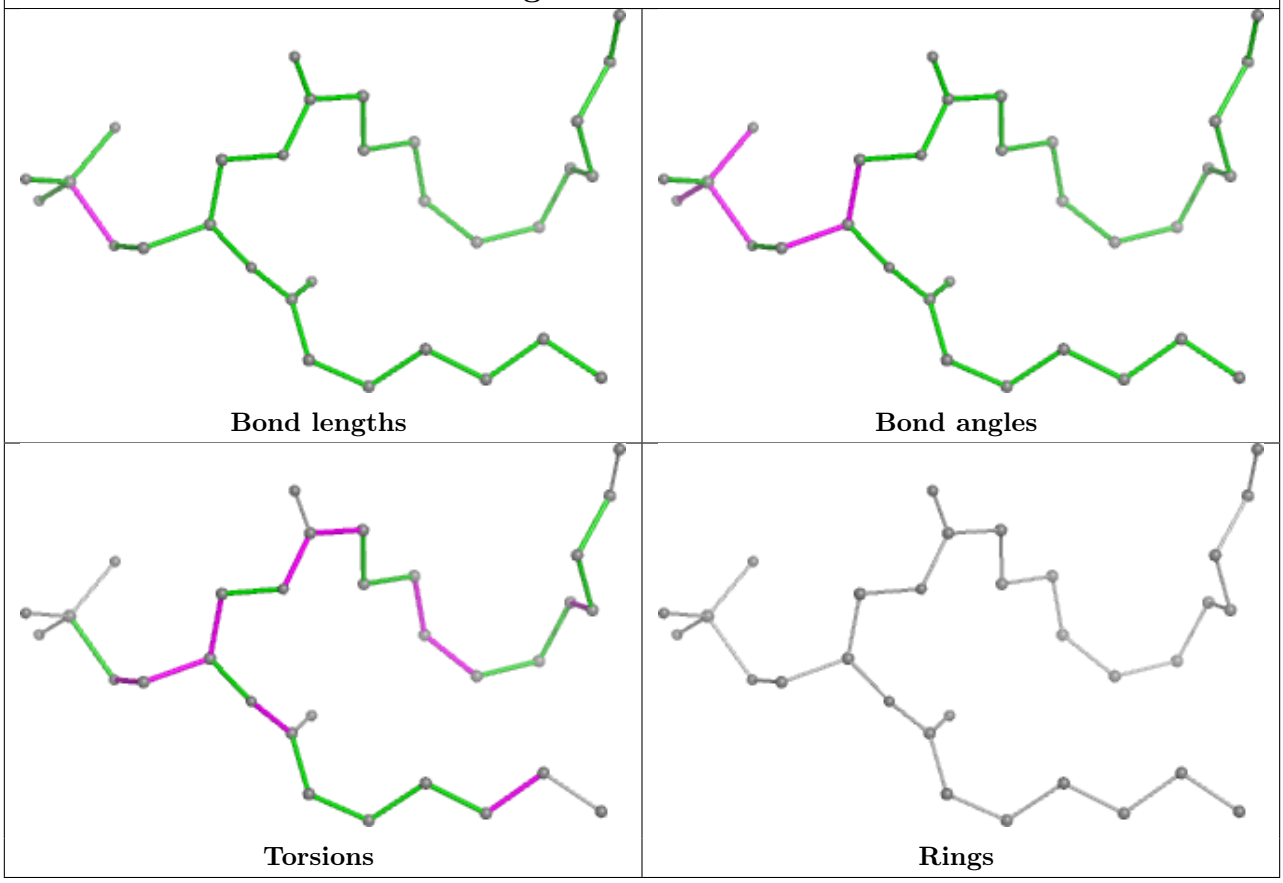


Rings

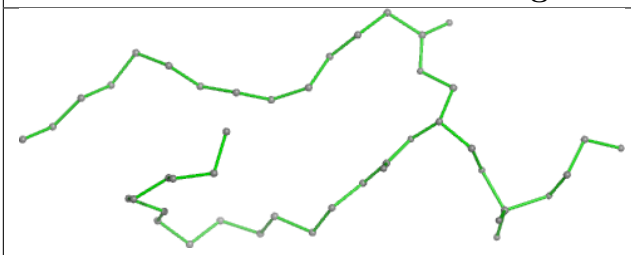
Ligand 3PE N 501



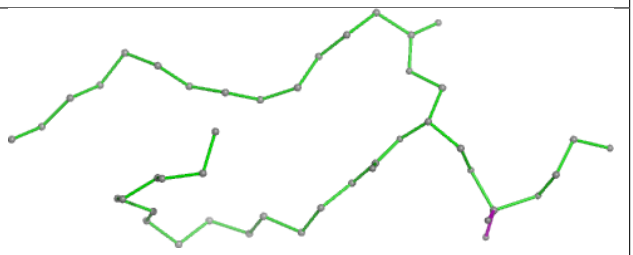
Ligand 3PH M 601



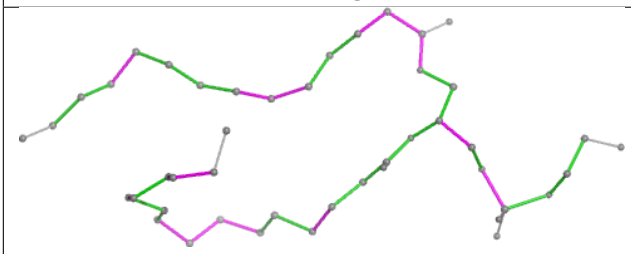
Ligand 3PE L 804



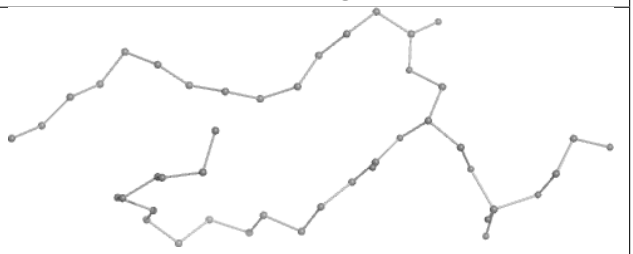
Bond lengths



Bond angles

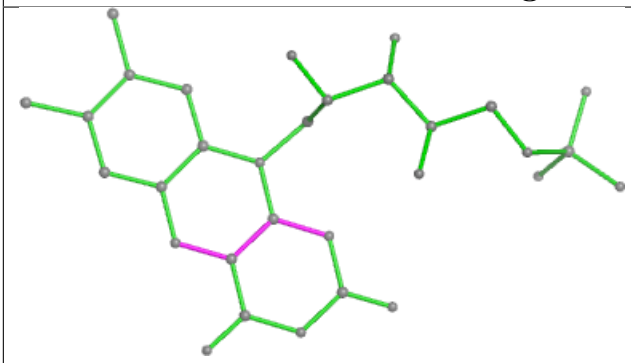


Torsions

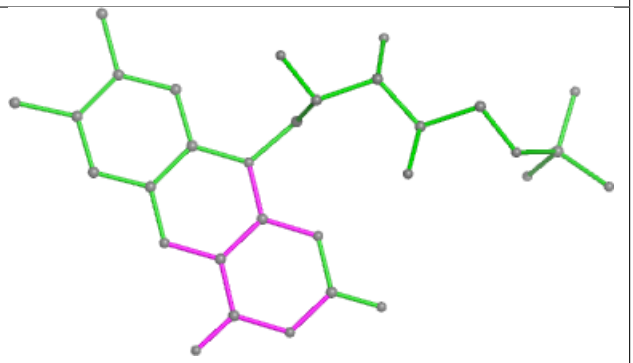


Rings

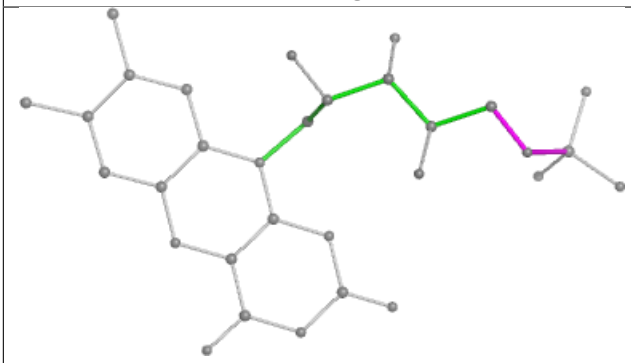
Ligand FMN F 501



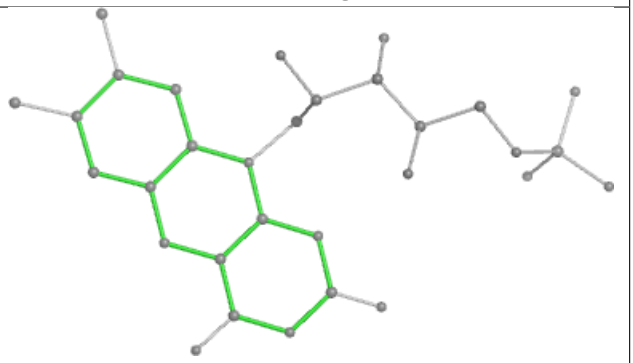
Bond lengths



Bond angles

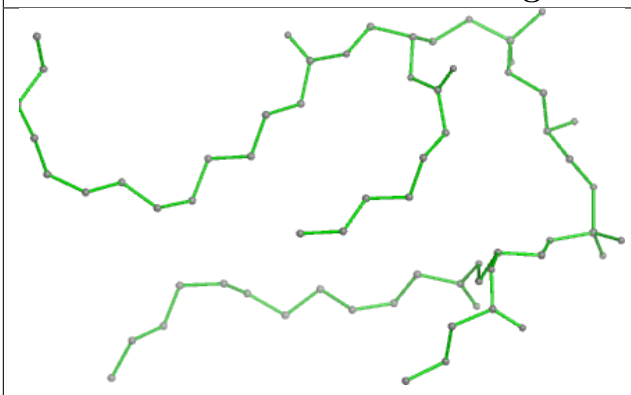


Torsions

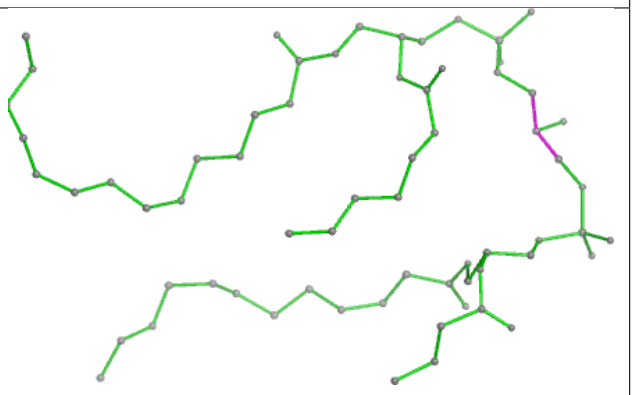


Rings

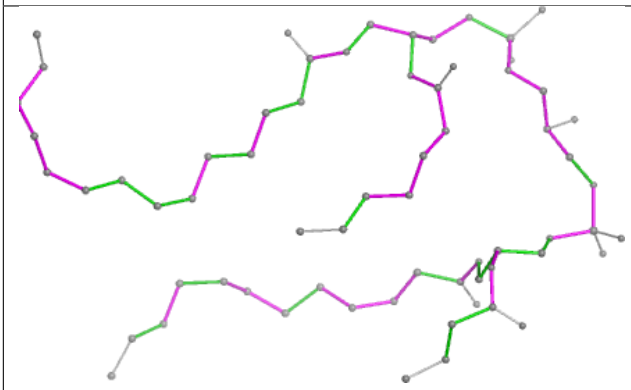
Ligand CDL H 402



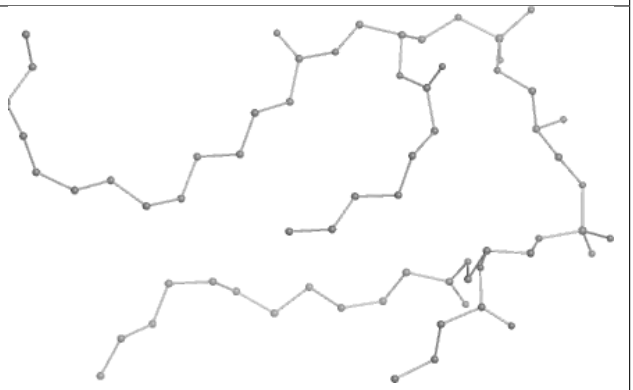
Bond lengths



Bond angles

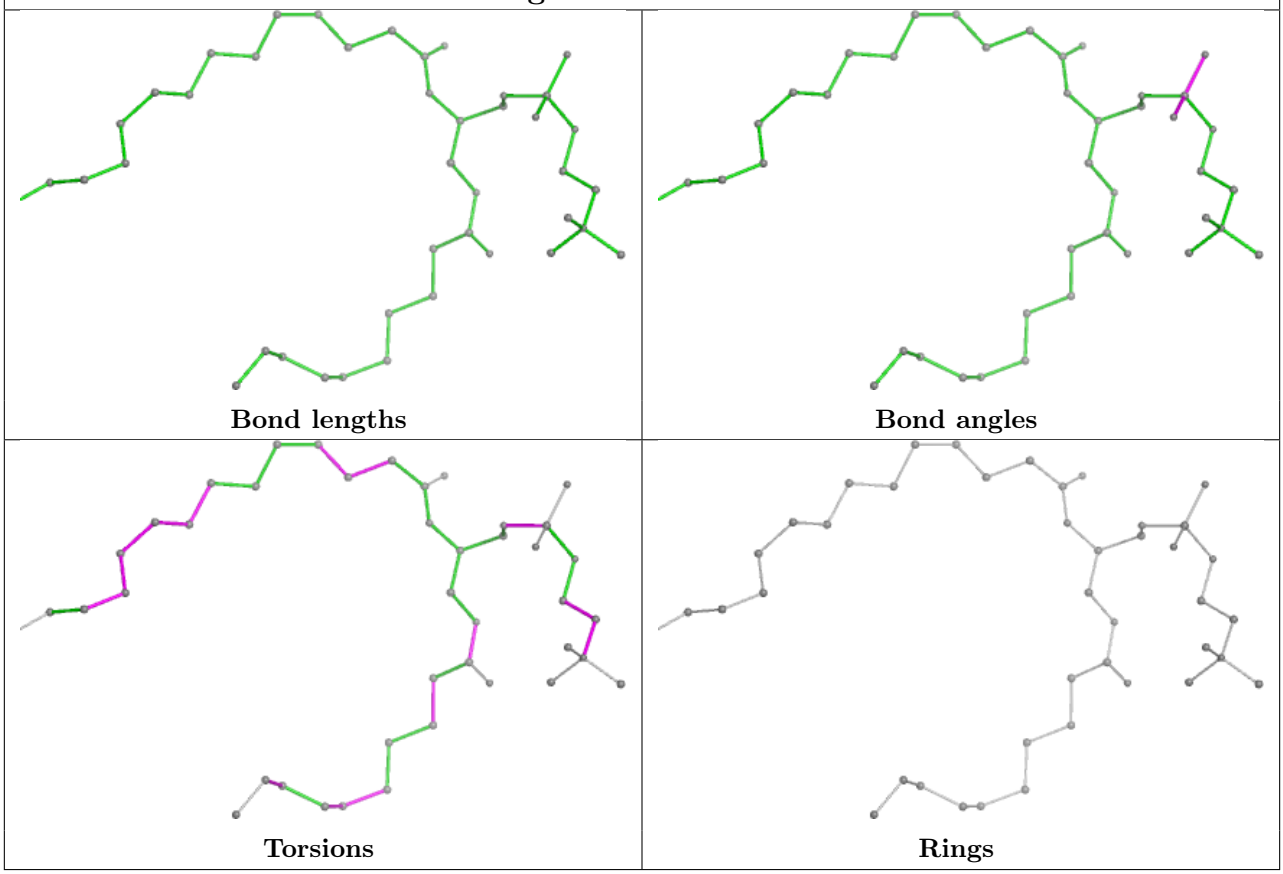


Torsions

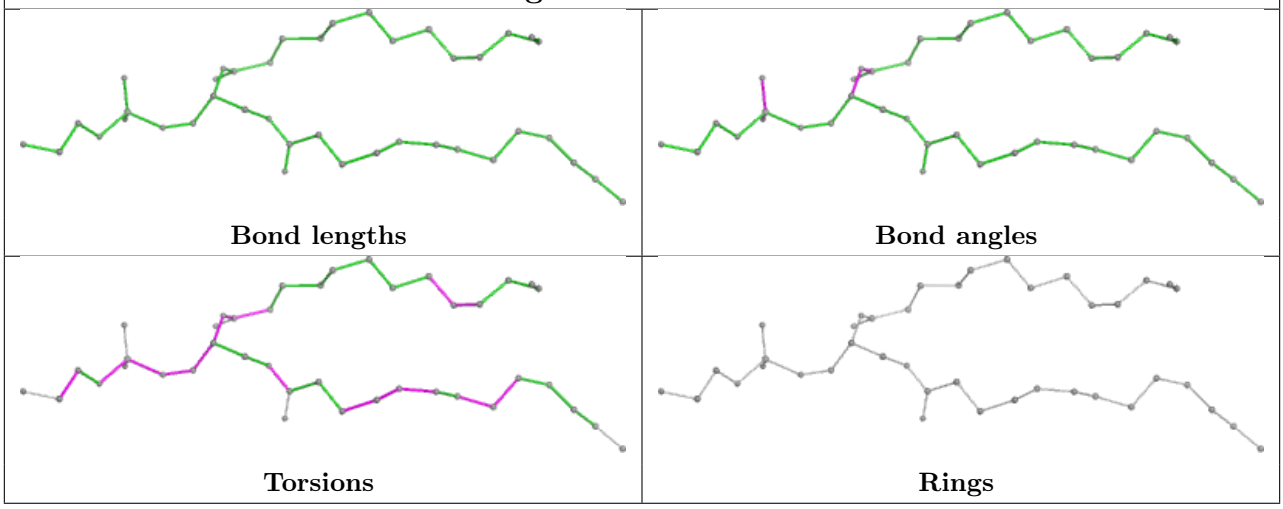


Rings

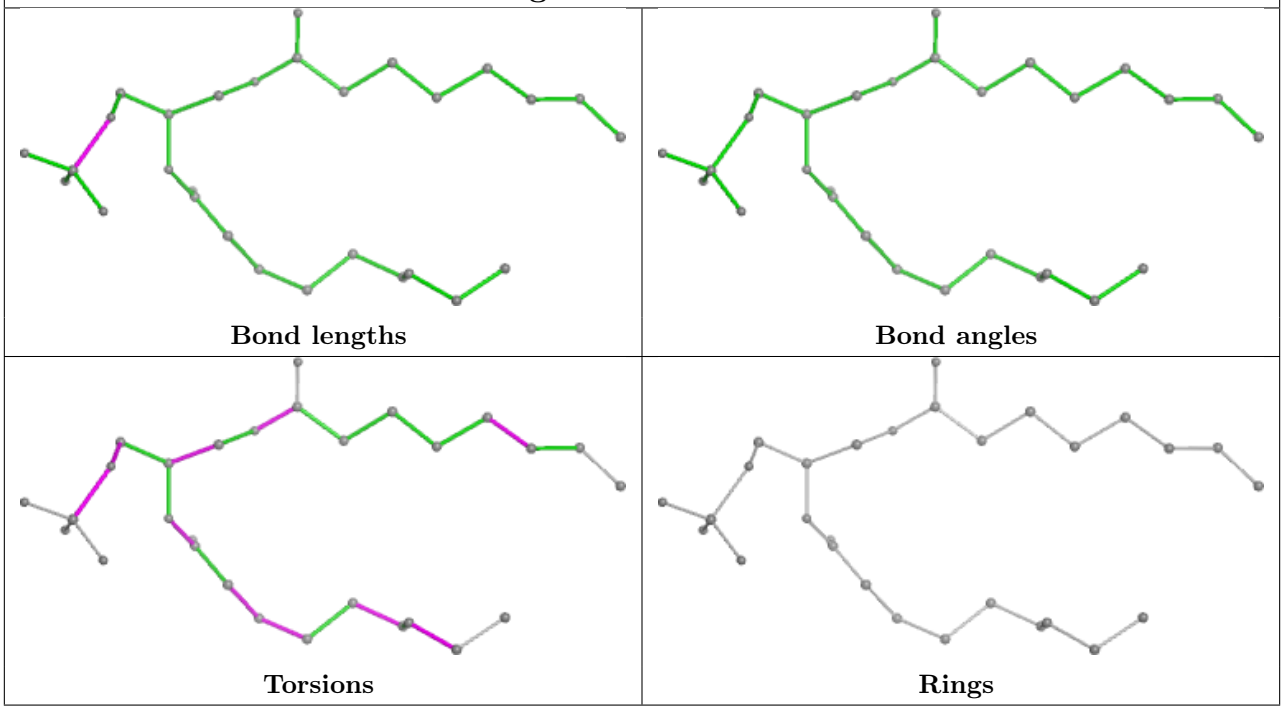
Ligand PC1 D 501



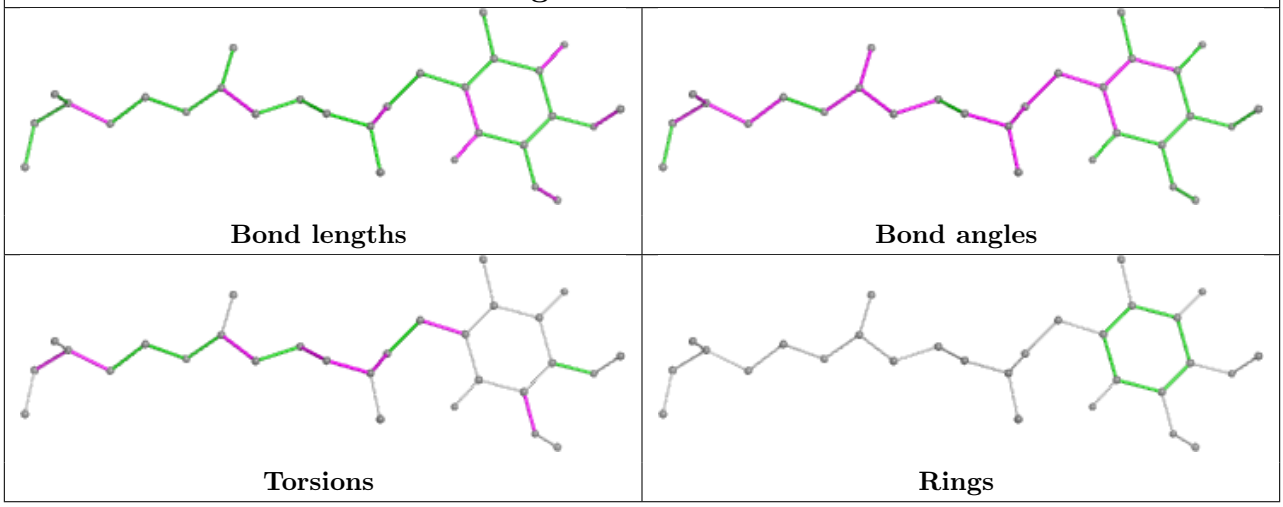
Ligand 3PE M 604



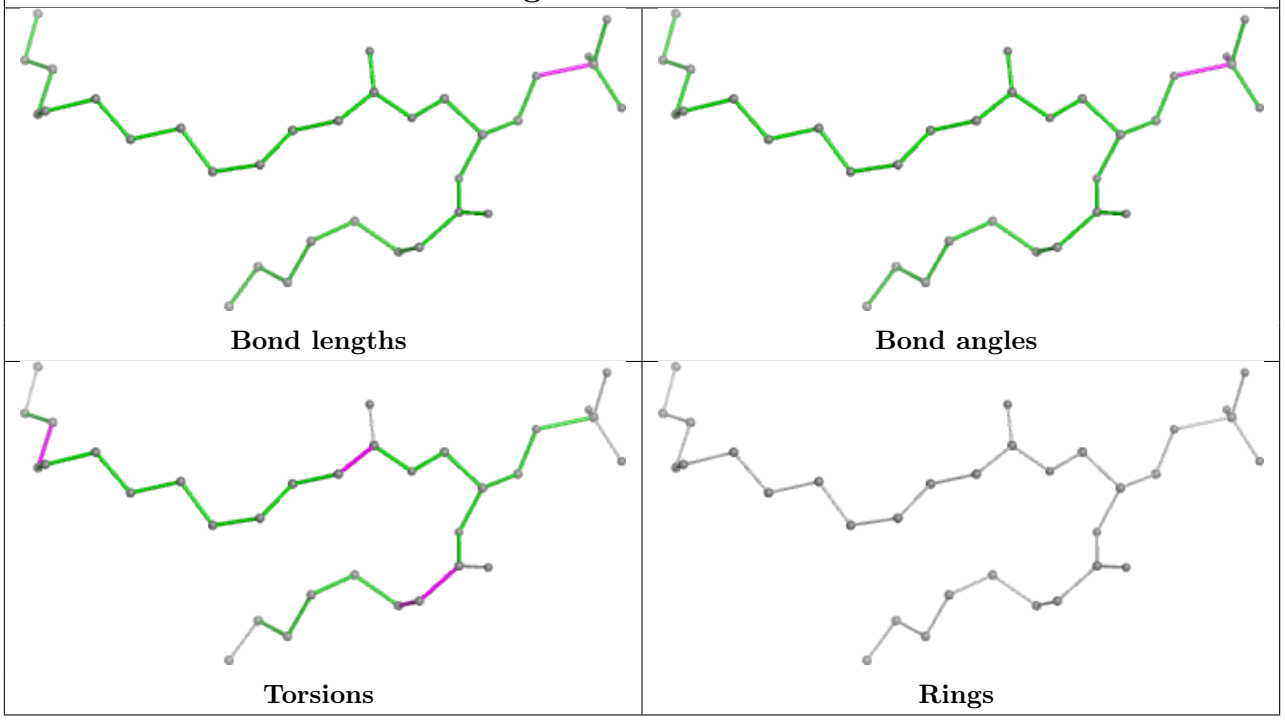
Ligand 3PH L 806



Ligand U10 B 401



Ligand 3PH M 603



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.

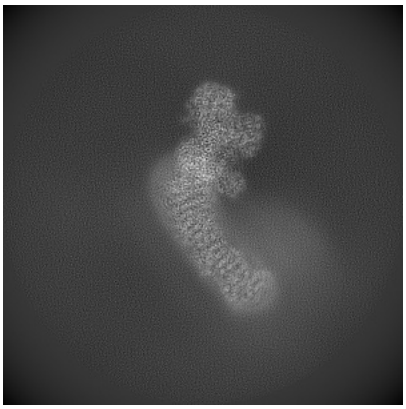
6 Map visualisation

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.

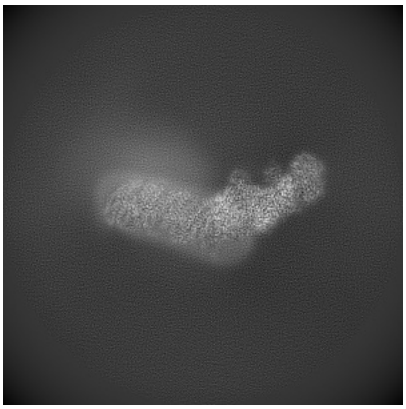
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

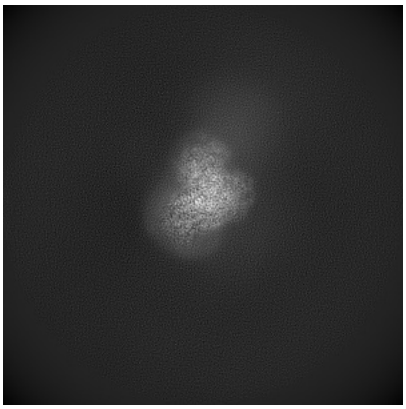
6.1.1 Primary map



X

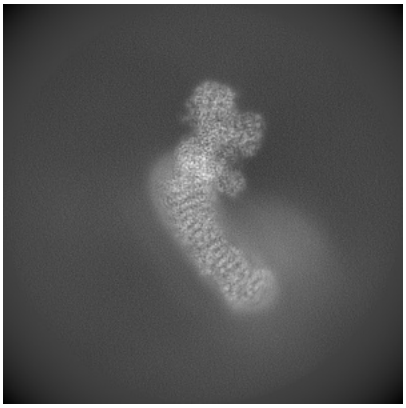


Y

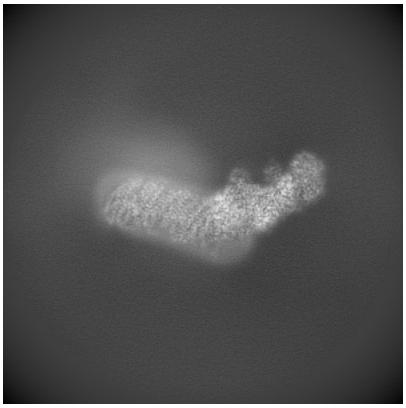


Z

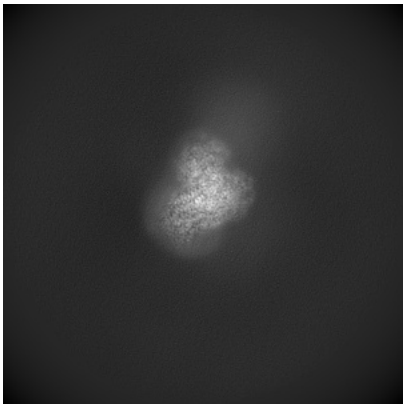
6.1.2 Raw map



X



Y

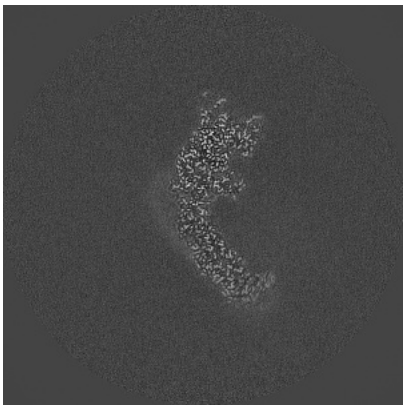


Z

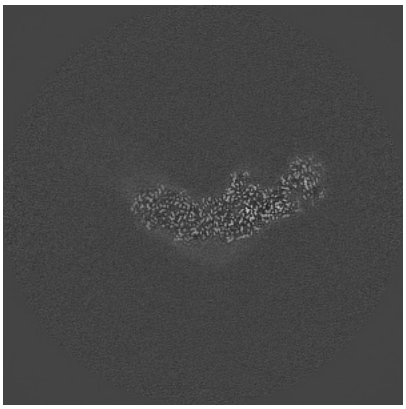
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

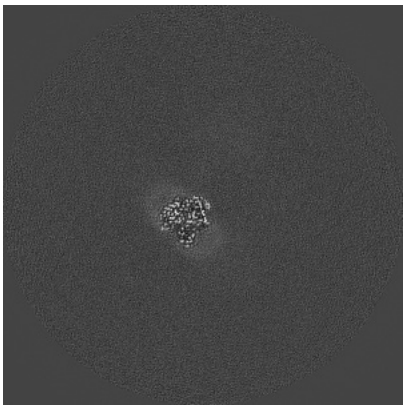
6.2.1 Primary map



X Index: 320

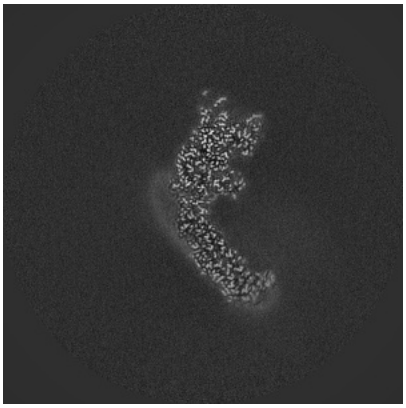


Y Index: 320

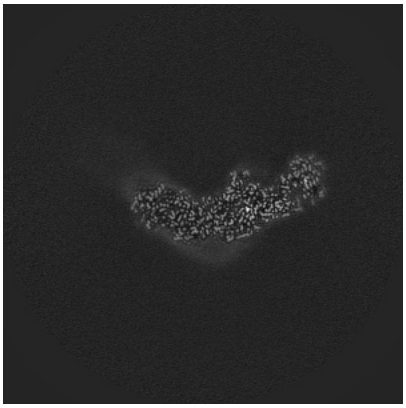


Z Index: 320

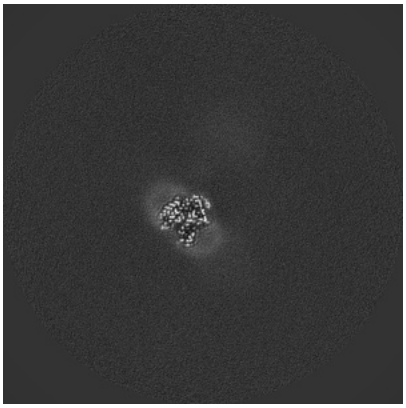
6.2.2 Raw map



X Index: 320



Y Index: 320

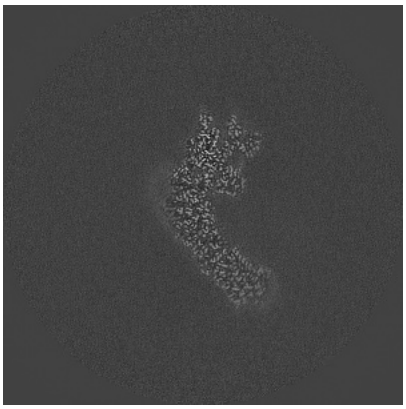


Z Index: 320

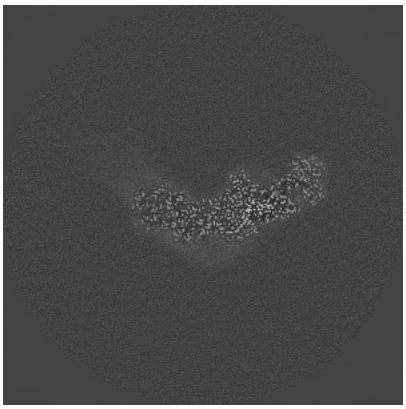
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

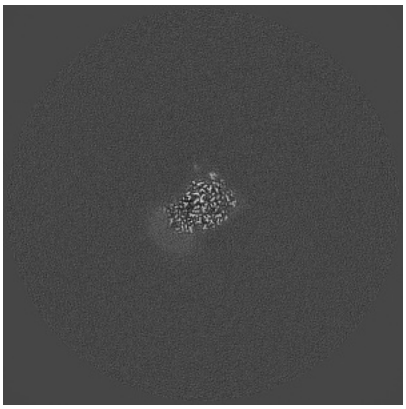
6.3.1 Primary map



X Index: 308

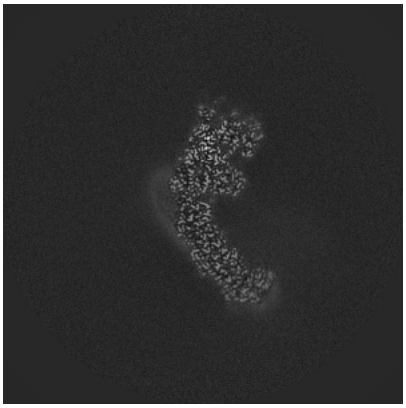


Y Index: 322

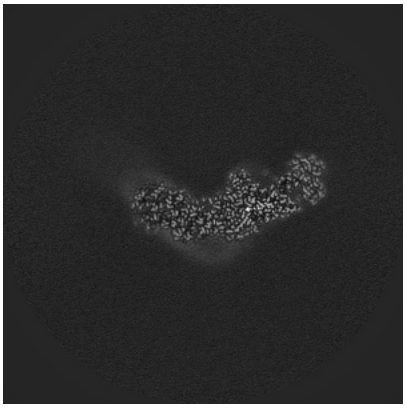


Z Index: 386

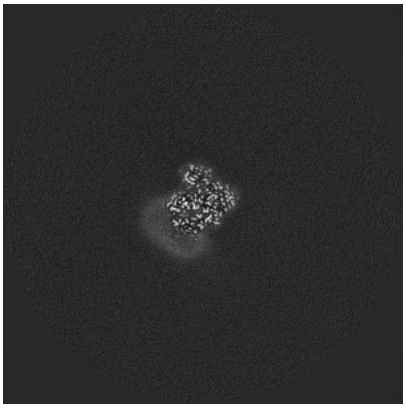
6.3.2 Raw map



X Index: 315



Y Index: 322

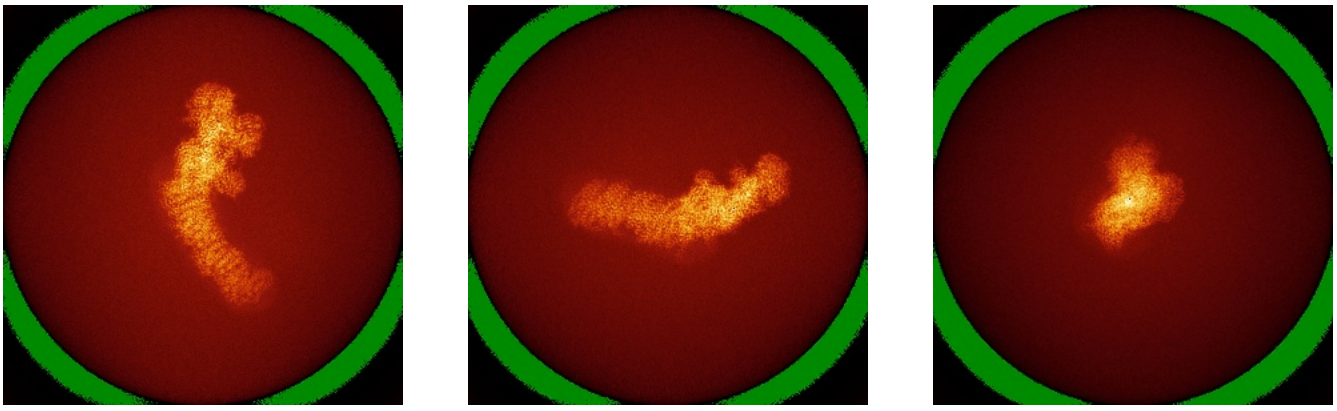


Z Index: 366

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

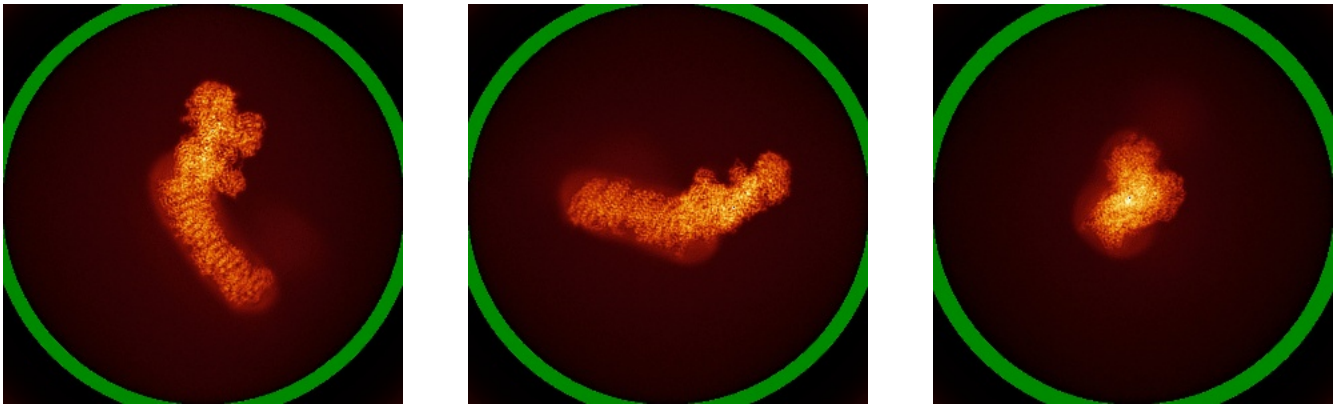
6.4 Orthogonal standard-deviation projections (False-color) (i)

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.

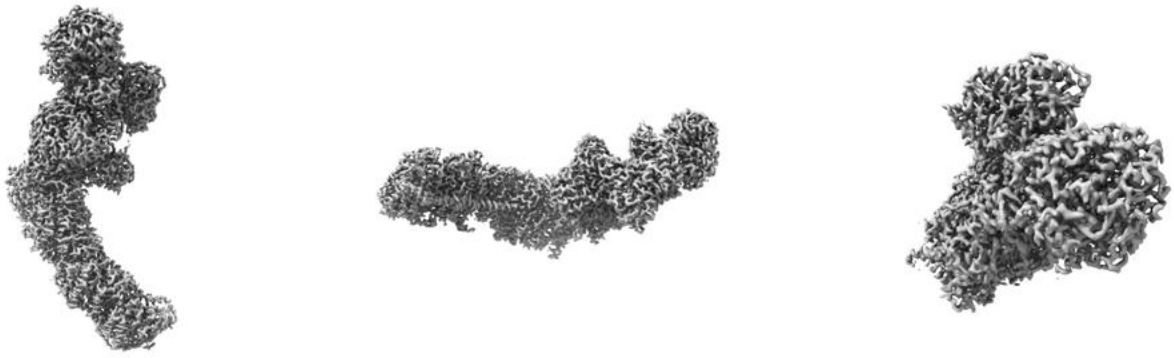
6.5 Orthogonal surface views (i)

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.

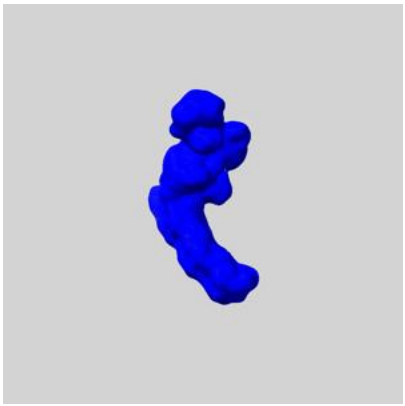
6.6 Mask visualisation (i)

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

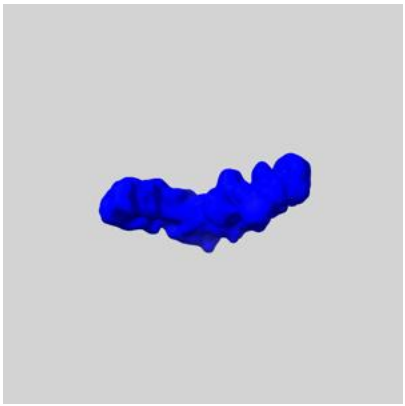
A mask typically either:

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

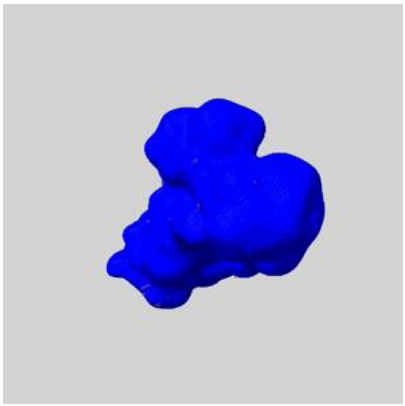
6.6.1 emd_18324_msk_1.map (i)



X



Y

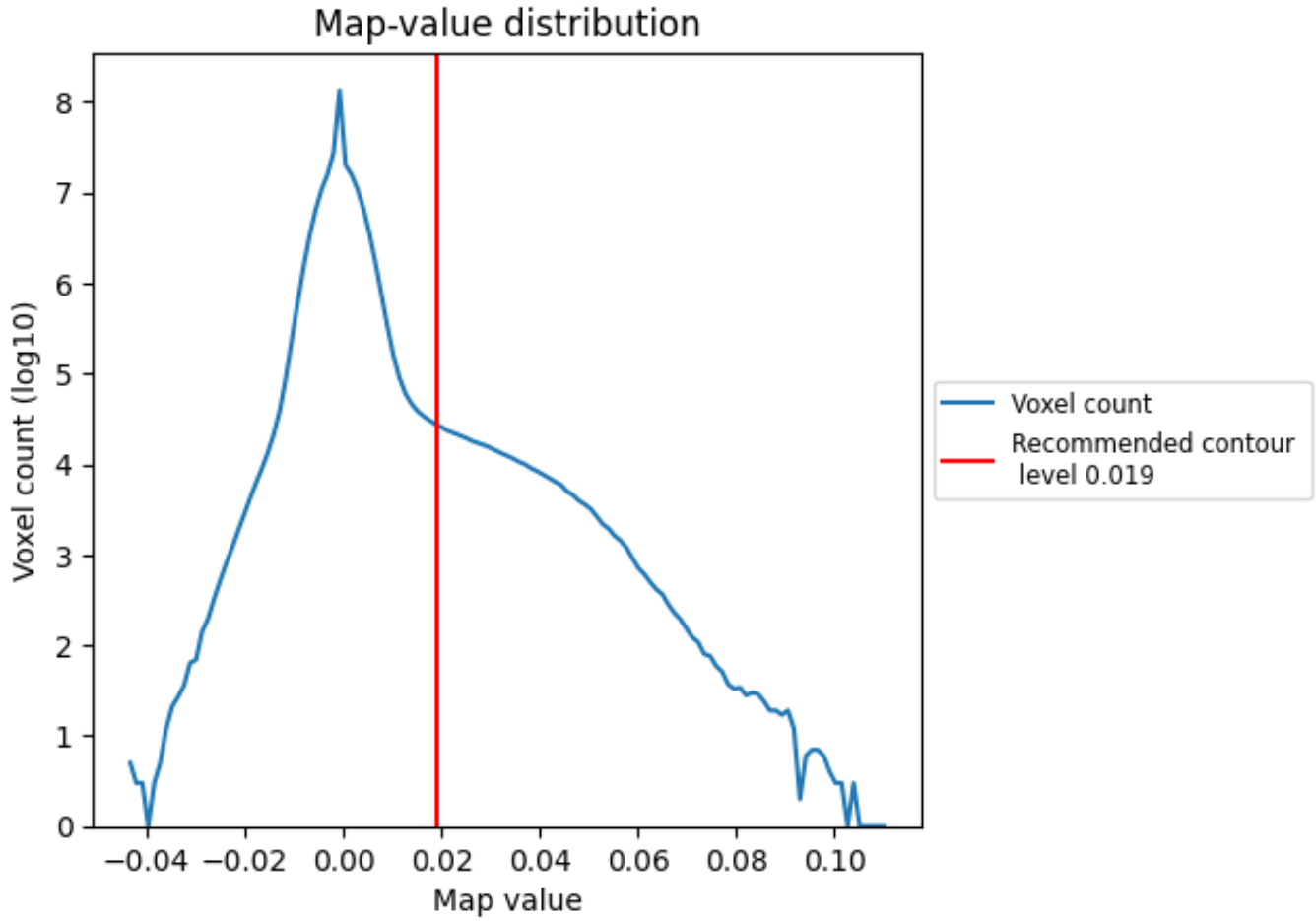


Z

7 Map analysis

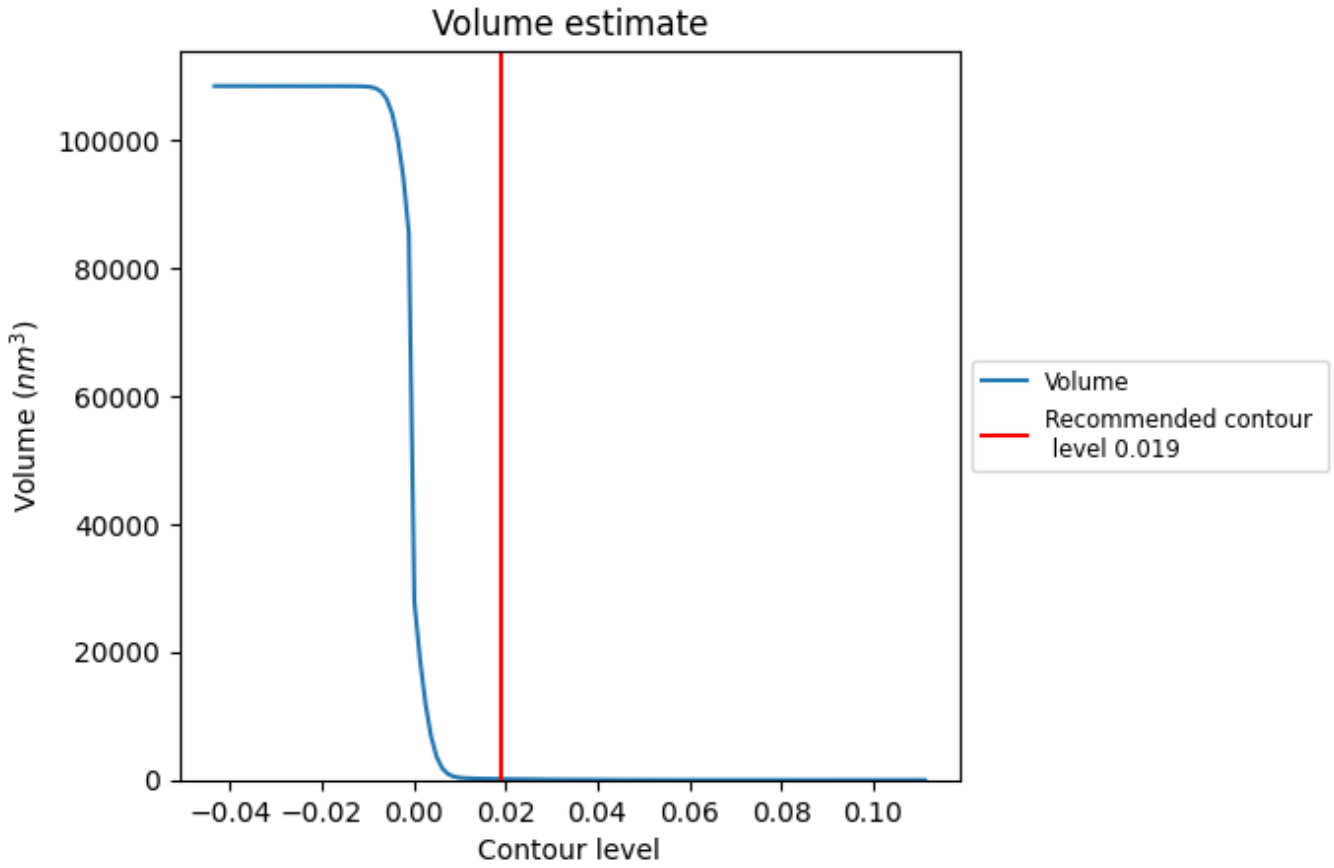
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

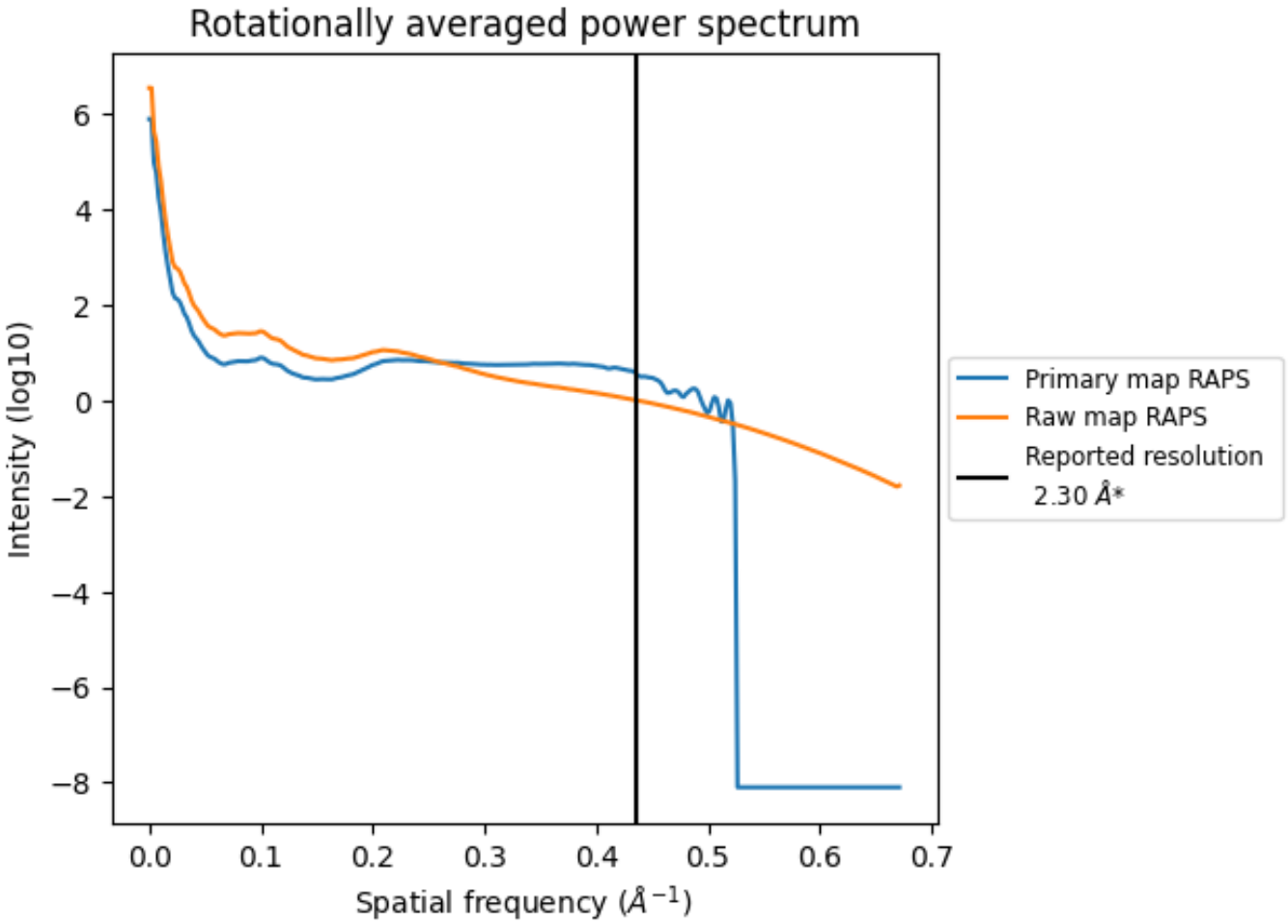
7.2 Volume estimate (i)



The volume at the recommended contour level is 147 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 (i)

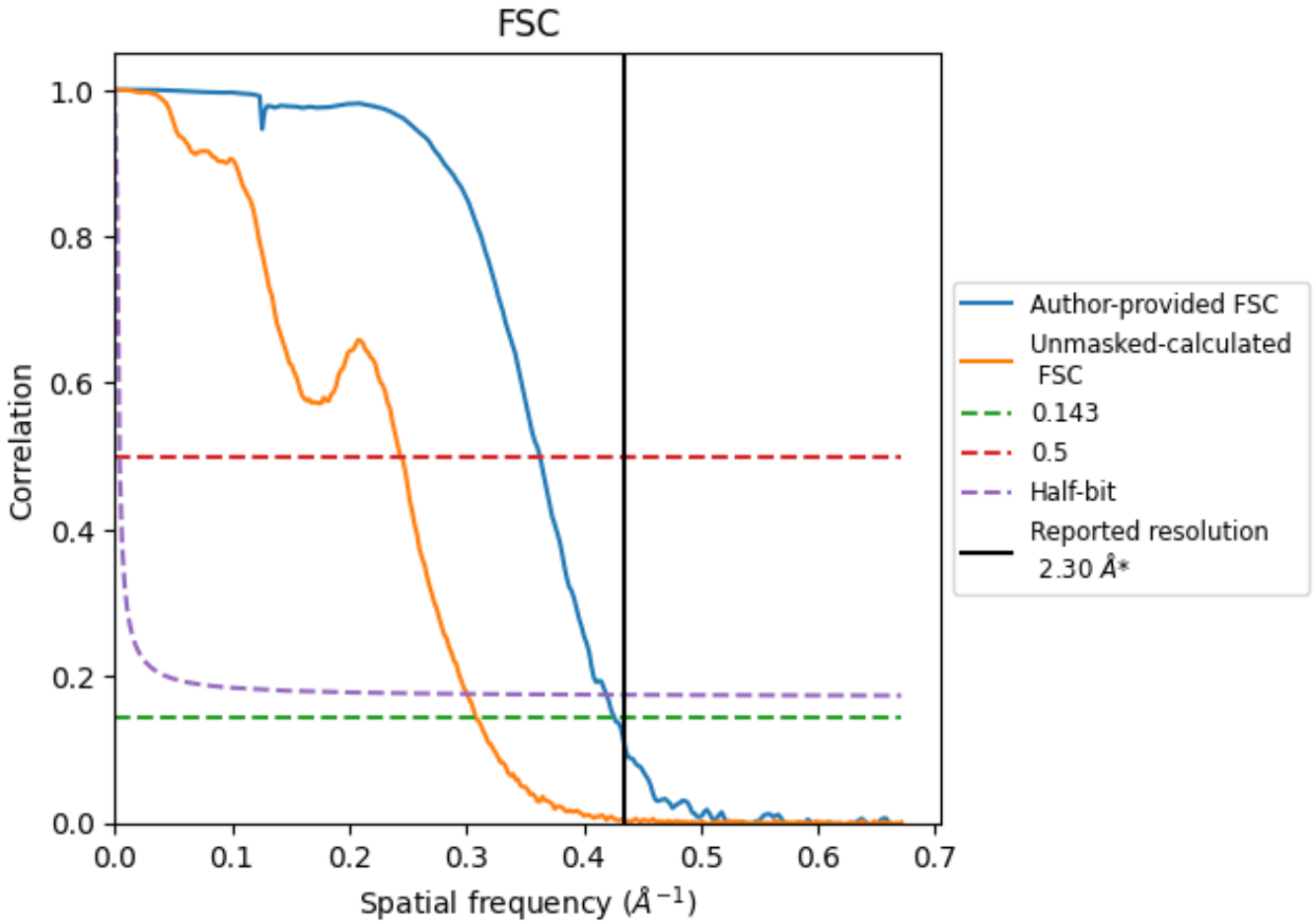


*Reported resolution corresponds to spatial frequency of 0.435 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.435 Å^{-1}

8.2 Resolution estimates (i)

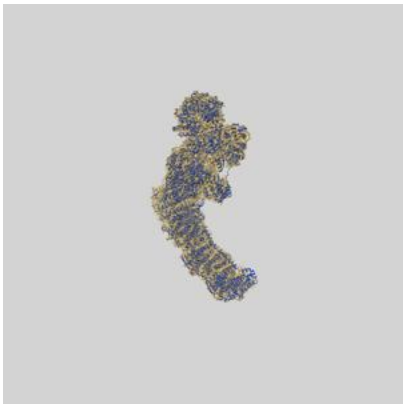
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.30	-	-
Author-provided FSC curve	2.35	2.76	2.38
Unmasked-calculated*	3.24	4.10	3.33

*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 %

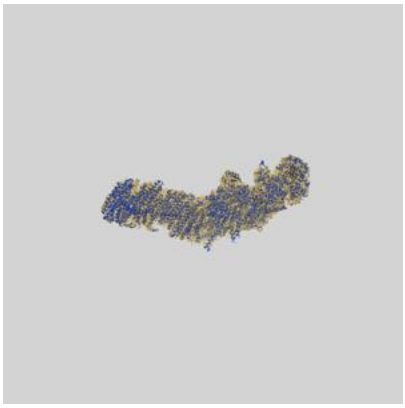
9 Map-model fit

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.

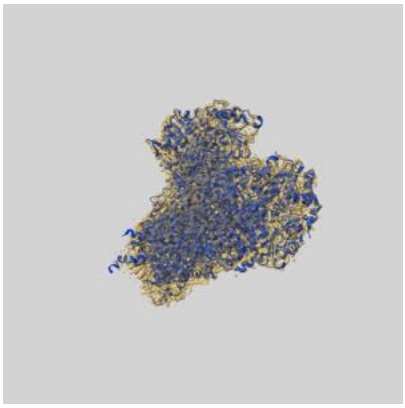
9.1 Map-model overlay



X



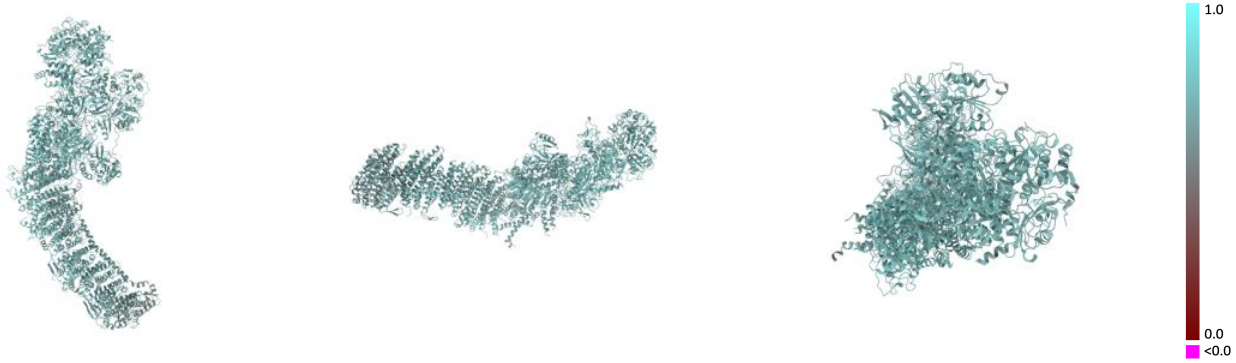
Y



Z

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.

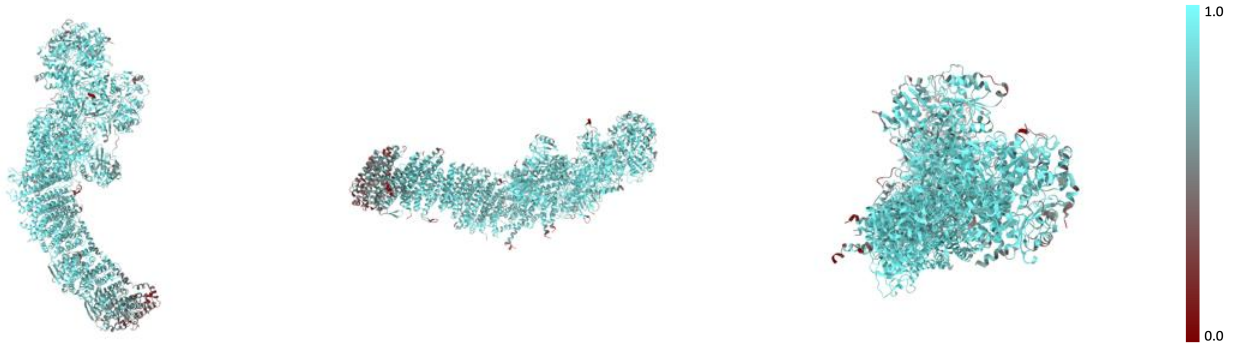
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

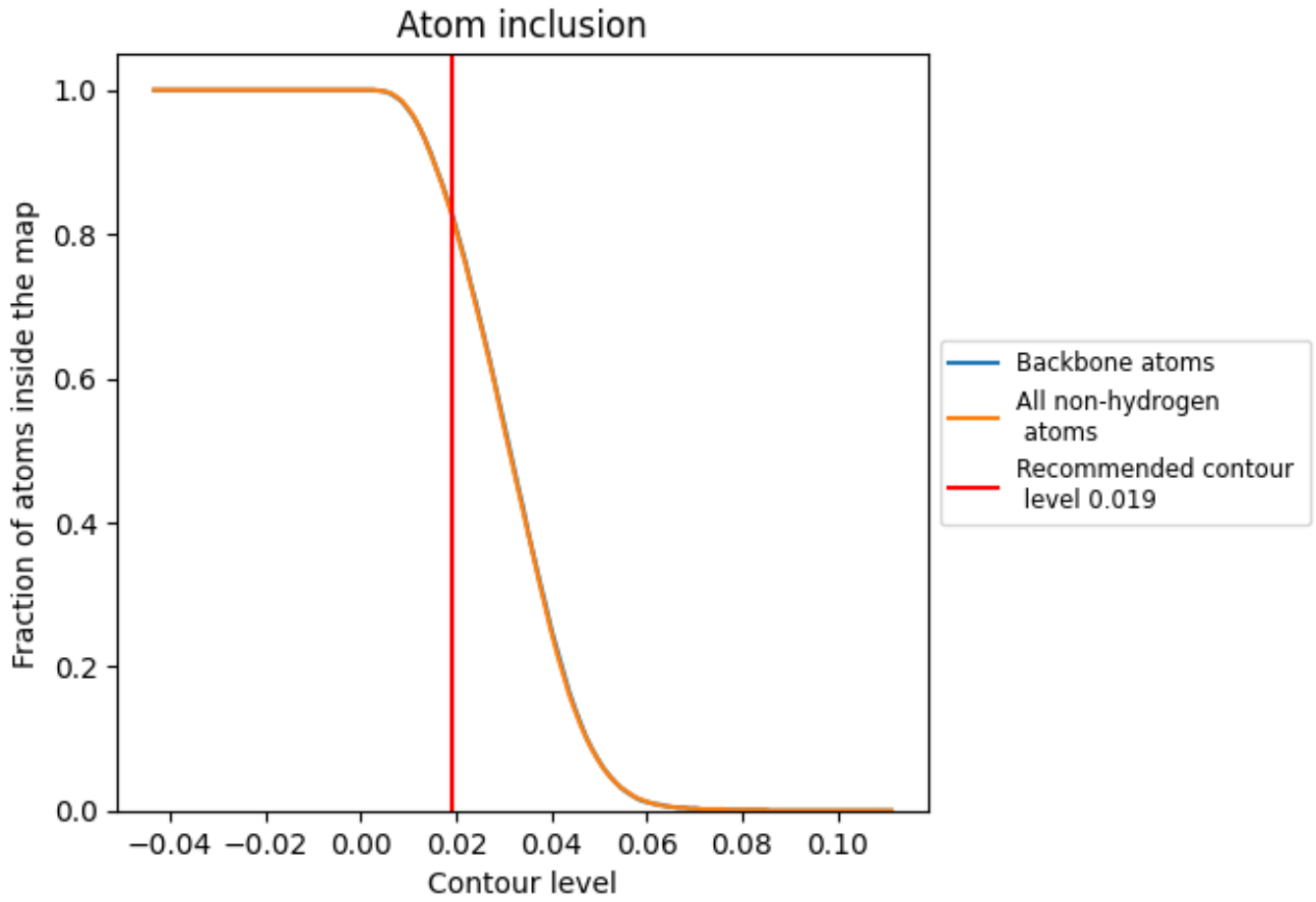
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (i)



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

9.5 Map-model fit summary

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

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