wwPDB EM Validation Summary Report (i)

Sep 7, 2026 – 11:44 pm BST

PDB ID	:	8B9Z / pdb_00008b9z
EMDB ID	:	EMD-15936
Title	:	Drosophila melanogaster complex I in the Active state (Dm1)
Authors	:	Agip, A.A.; Chung, I.; Sanchez-Martinez, A.; Whitworth, A.J.; Hirst, J.
Deposited on	:	2022-10-10
Resolution	:	3.28 Å(reported)
Based on initial model	:	6ZR2

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 (i) 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 (i)) were used in the production of this report:

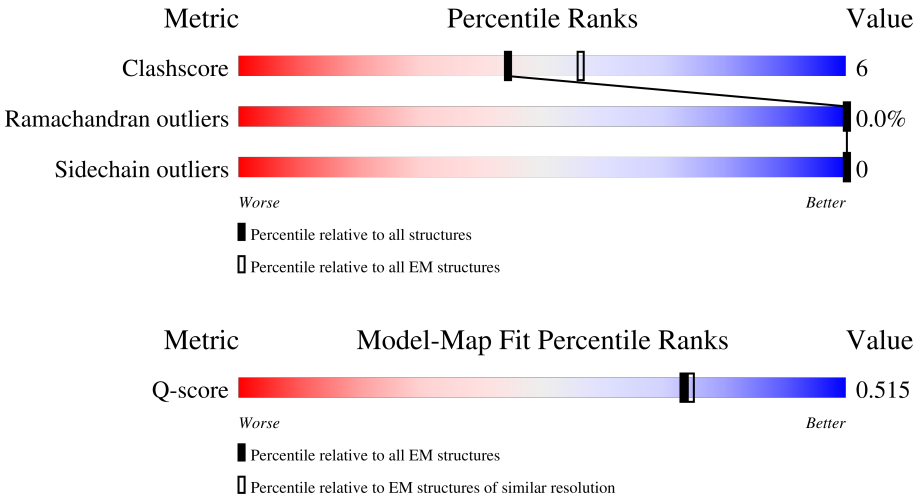
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.28 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14492 (2.78 - 3.78)

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	A	117	78% 22%
2	B	182	81% 18%
3	C	209	83% 17%
4	D	430	84% 16%

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Mol	Chain	Length	Quality of chain
5	E	214	78% 22%
6	F	441	82% 18%
7	G	731	82% 10% 7%
8	H	315	85% 14%
9	I	186	83% 17%
10	J	173	5% 74% 25%
11	K	96	5% 72% 28%
12	L	577	84% 16%
13	M	446	79% 21%
14	N	341	82% 18%
15	O	368	5% 85% 15%
16	P	377	88% 12%
17	Q	151	9% 86% 14%
18	R	89	89% 11%
19	T	85	33% 72% 19% 9%
19	U	85	12% 80% 20%
20	V	118	80% 20%
21	W	114	88% 12%
22	X	174	7% 89% 11%
23	Y	167	10% 87% 13%
24	Z	146	90% 10%
25	a	73	12% 82% 18%
26	b	66	6% 77% 23%
27	d	115	88% 12%
28	e	100	5% 84% 16%

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Mol	Chain	Length	Quality of chain
29	f	55	16% 87% 13%
30	g	108	12% 81% 19%
31	h	145	86% 14%
32	i	161	6% 83% 17%
33	j	66	8% 91% 9%
34	k	84	10% 92% 8%
35	l	146	10% 90% 10%
36	m	108	5% 89% 11%
37	n	134	9% 82% 18%
38	o	112	87% 13%
39	p	151	81% 19%
40	q	133	11% 92% 8%
41	r	103	7% 74% 13% 14%
42	s	62	24% 82% 18%

2 Entry composition (i)

There are 54 unique types of molecules in this entry. The entry contains 66970 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-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	117	956	652	141	156	7	0	0

- Molecule 2 is a protein called LD31474p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	182	1435	920	251	250	14	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	209	1726	1103	303	315	5	0	0

- Molecule 4 is a protein called Complex I-49kD.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	430	3434	2202	579	630	23	0	0

- Molecule 5 is a protein called NADH dehydrogenase (Ubiquinone) 24 kDa subunit, isoform A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	214	1679	1062	285	320	12	0	0

- Molecule 6 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	441	Total 3381	C 2136	N 602	O 617	S 26	0	0

- Molecule 7 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	677	Total 5146	C 3225	N 912	O 980	S 29	0	0

- Molecule 8 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	315	Total 2571	C 1764	N 367	O 418	S 22	0	0

- Molecule 9 is a protein called NADH dehydrogenase (ubiquinone) 23 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	186	Total 1485	C 935	N 251	O 287	S 12	0	0

- Molecule 10 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	173	Total 1397	C 946	N 201	O 233	S 17	0	0

- Molecule 11 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	96	Total 793	C 540	N 113	O 127	S 13	0	0

- Molecule 12 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	577	Total 4606	C 3092	N 680	O 774	S 60	0	0

- Molecule 13 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	446	Total 3617	C 2459	N 533	O 583	S 42	0	0

- Molecule 14 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	341	Total 2796	C 1893	N 411	O 458	S 34	0	0

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	368	Total 3007	C 1927	N 504	O 560	S 16	0	0

- Molecule 16 is a protein called NADH dehydrogenase (Ubiquinone) 39 kDa subunit, isoform A.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	377	Total 3032	C 1934	N 546	O 542	S 10	0	0

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	151	Total 1214	C 756	N 227	O 227	S 4	0	0

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	89	Total 716	C 453	N 130	O 129	S 4	0	0

- Molecule 19 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	77	Total 615	C 398	N 94	O 121	S 2	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	85	Total	C	N	O	S	0	0
			684	442	103	137	2		

- Molecule 20 is a protein called NADH dehydrogenase (Ubiquinone) 13 kDa B subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	V	118	Total	C	N	O	S	0	0
			922	588	162	168	4		

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	114	Total	C	N	O	S	0	0
			968	620	172	170	6		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	X	174	Total	C	N	O	S	0	0
			1383	867	240	266	10		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Y	167	Total	C	N	O	S	0	0
			1277	829	212	230	6		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Z	146	Total	C	N	O	S	0	0
			1201	787	203	209	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	a	73	Total	C	N	O	S	0	0
			601	386	101	108	6		

- Molecule 26 is a protein called RH45008p.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	b	66	Total	C	N	O	S	0	0
			519	327	95	96	1		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	d	115	Total	C	N	O	S	0	0
			907	590	159	157	1		

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	e	100	Total	C	N	O	S	0	0
			828	523	145	149	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
29	f	55	Total	C	N	O	S	0	0
			429	278	76	73	2		

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	g	108	Total	C	N	O	S	0	0
			883	567	142	173	1		

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	h	145	Total	C	N	O	S	0	0
			1234	795	213	223	3		

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	i	161	Total	C	N	O	S	0	0
			1302	829	242	226	5		

- Molecule 33 is a protein called GEO11417p1.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	j	66	Total	C	N	O	S	0	0
			541	352	96	92	1		

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	k	84	Total	C	N	O	S	0	0
			671	437	117	116	1		

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	l	146	Total	C	N	O	S	0	0
			1215	792	194	225	4		

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	m	108	Total	C	N	O	S	0	0
			892	571	163	157	1		

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	n	134	Total	C	N	O	S	0	0
			1152	735	218	196	3		

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	o	112	Total	C	N	O	S	0	0
			937	596	163	169	9		

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	p	151	Total	C	N	O	S	0	0
			1266	795	233	228	10		

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	q	133	Total	C	N	O	S	0	0
			1118	727	187	199	5		

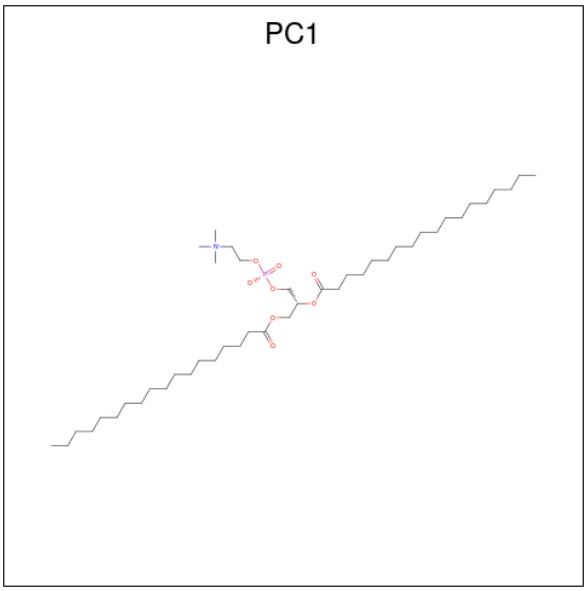
- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	r	89	Total	C	N	O	S	0	0
			724	457	136	130	1		

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

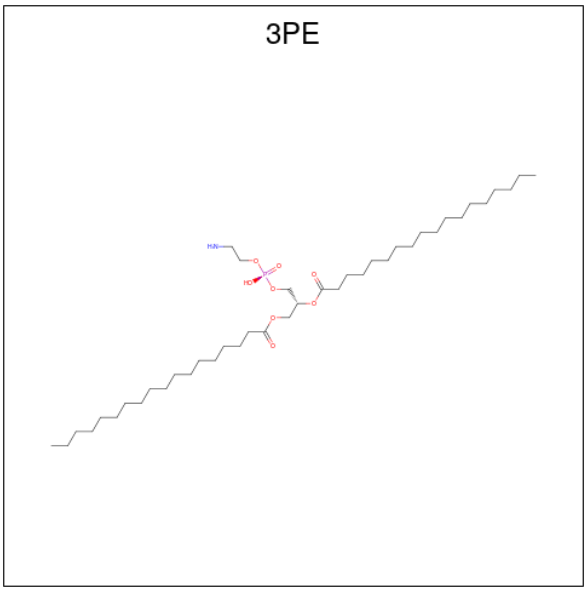
Mol	Chain	Residues	Atoms					AltConf	Trace
42	s	62	Total	C	N	O	S	0	0
			456	288	75	90	3		

- Molecule 43 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



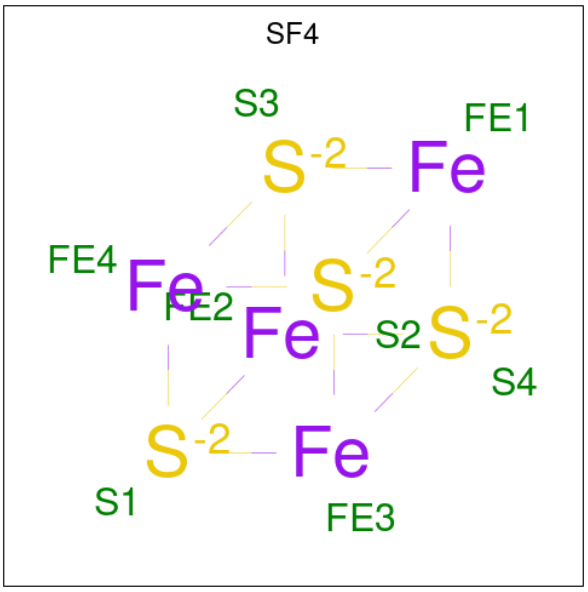
Mol	Chain	Residues	Atoms					AltConf
43	A	1	Total	C	N	O	P	0
			39	29	1	8	1	
43	J	1	Total	C	N	O	P	0
			44	34	1	8	1	
43	i	1	Total	C	N	O	P	0
			34	24	1	8	1	

- Molecule 44 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



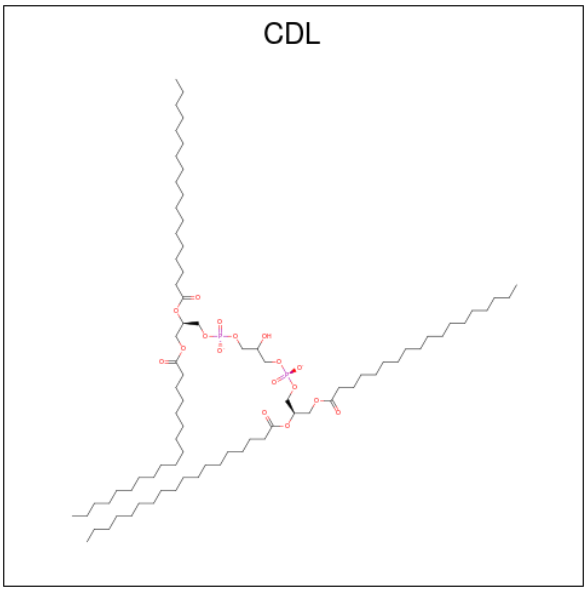
Mol	Chain	Residues	Atoms					AltConf
44	A	1	Total	C	N	O	P	0
			35	25	1	8	1	
44	A	1	Total	C	N	O	P	0
			44	34	1	8	1	
44	B	1	Total	C	N	O	P	0
			37	27	1	8	1	
44	H	1	Total	C	N	O	P	0
			47	37	1	8	1	
44	J	1	Total	C	N	O	P	0
			40	30	1	8	1	
44	J	1	Total	C	N	O	P	0
			24	14	1	8	1	
44	L	1	Total	C	N	O	P	0
			39	29	1	8	1	
44	L	1	Total	C	N	O	P	0
			44	34	1	8	1	
44	L	1	Total	C	N	O	P	0
			25	15	1	8	1	
44	M	1	Total	C	N	O	P	0
			35	25	1	8	1	
44	N	1	Total	C	N	O	P	0
			44	34	1	8	1	
44	X	1	Total	C	N	O	P	0
			30	20	1	8	1	
44	Y	1	Total	C	N	O	P	0
			44	34	1	8	1	
44	Y	1	Total	C	N	O	P	0
			30	20	1	8	1	
44	Y	1	Total	C	N	O	P	0
			33	23	1	8	1	
44	d	1	Total	C	N	O	P	0
			36	26	1	8	1	

- Molecule 45 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



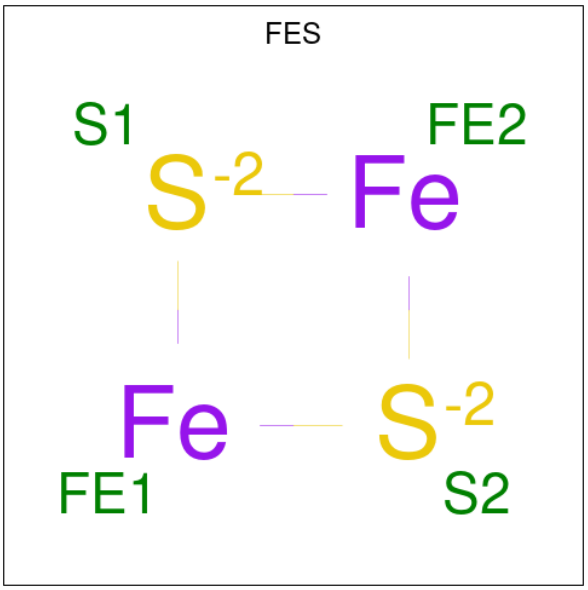
Mol	Chain	Residues	Atoms	AltConf
45	B	1	Total Fe S 8 4 4	0
45	F	1	Total Fe S 8 4 4	0
45	G	1	Total Fe S 8 4 4	0
45	G	1	Total Fe S 8 4 4	0
45	I	1	Total Fe S 8 4 4	0
45	I	1	Total Fe S 8 4 4	0

- Molecule 46 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



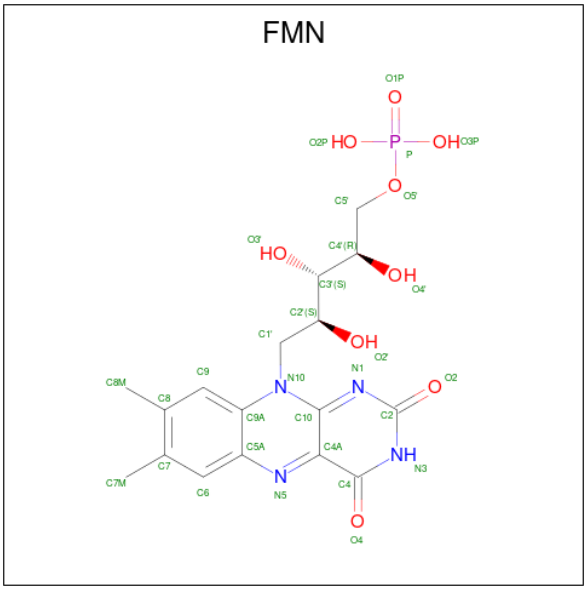
Mol	Chain	Residues	Atoms				AltConf
46	B	1	Total	C	O	P	0
			67	48	17	2	
46	P	1	Total	C	O	P	0
			54	35	17	2	
46	h	1	Total	C	O	P	0
			69	50	17	2	
46	h	1	Total	C	O	P	0
			60	41	17	2	

- Molecule 47 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



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

- Molecule 48 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).

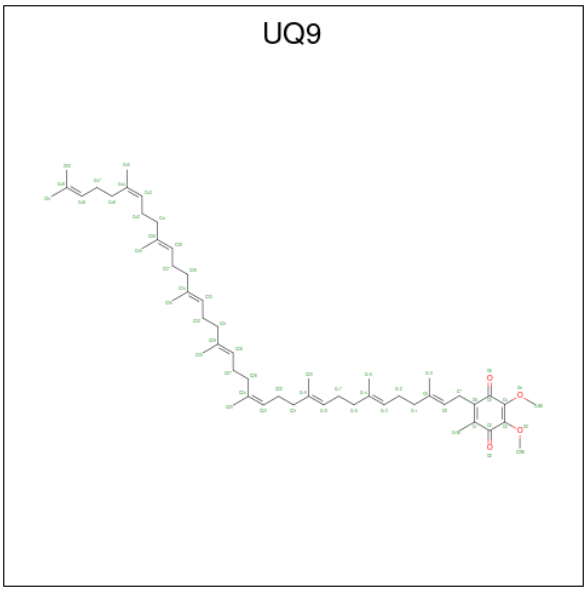


Mol	Chain	Residues	Atoms	AltConf
48	F	1	Total C N O P 31 17 4 9 1	0

- Molecule 49 is SODIUM ION (CCD ID: NA) (formula: Na).

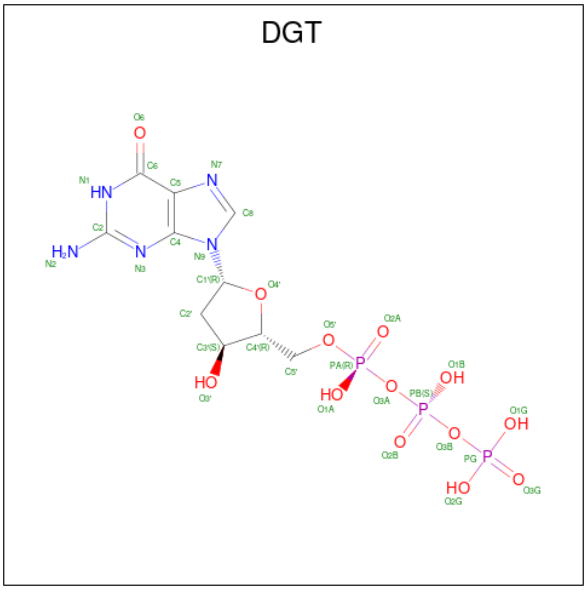
Mol	Chain	Residues	Atoms	AltConf
49	G	1	Total Na 1 1	0

- Molecule 50 is Ubiquinone-9 (CCD ID: UQ9) (formula: $C_{54}H_{82}O_4$) (labeled as "Ligand of Interest" by depositor).



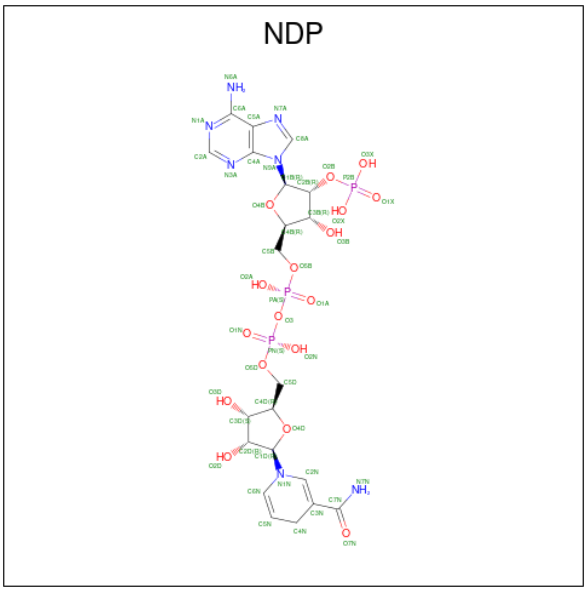
Mol	Chain	Residues	Atoms			AltConf
50	H	1	Total	C	O	0
			58	54	4	

- Molecule 51 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (CCD ID: DGT) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

- Molecule 52 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).

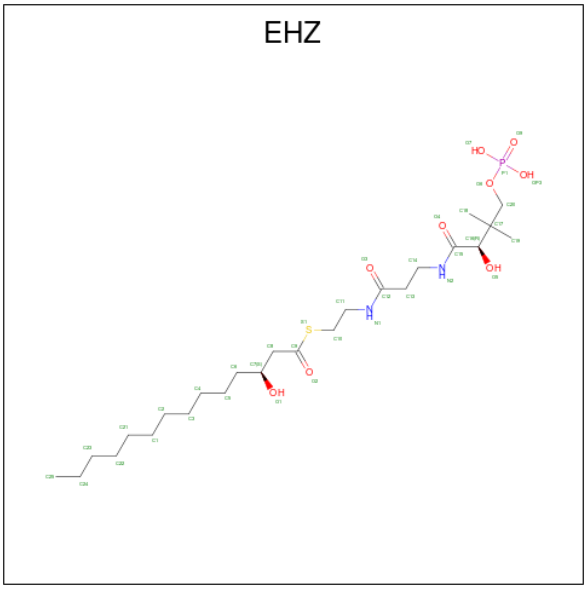


Mol	Chain	Residues	Atoms					AltConf
52	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 53 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 54 is {S}-[2-[3-[[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (CCD ID: EHZ) (formula: $C_{25}H_{49}N_2O_9PS$).



Mol	Chain	Residues	Atoms						AltConf
54	T	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	
54	U	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	

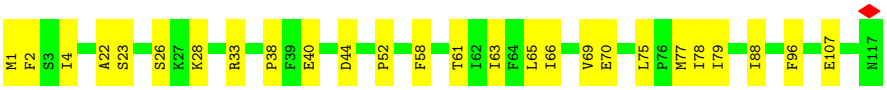
3 Residue-property plots (i)

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-ubiquinone oxidoreductase chain 3

Chain A:





• Molecule 2: LD31474p

Chain B:

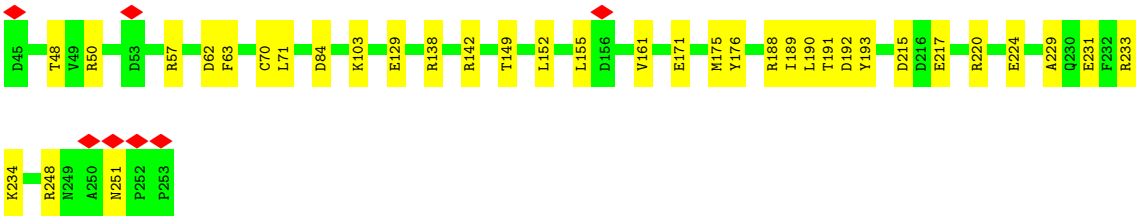




• Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

Chain C:

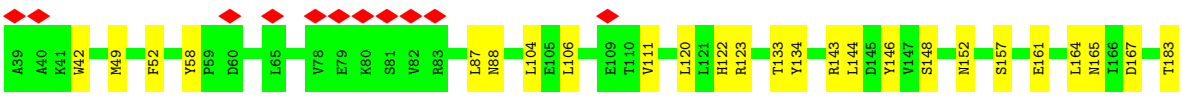


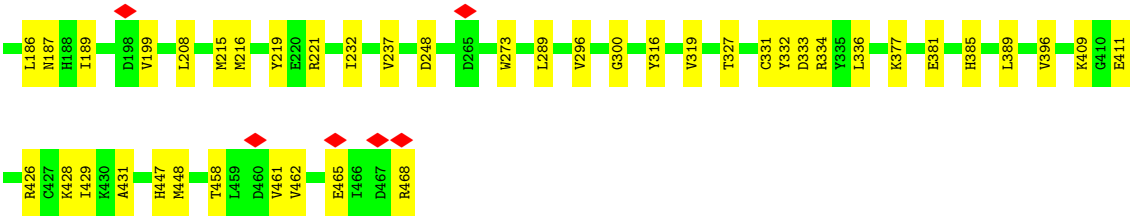


• Molecule 4: Complex I-49kD

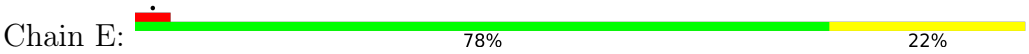
Chain D:

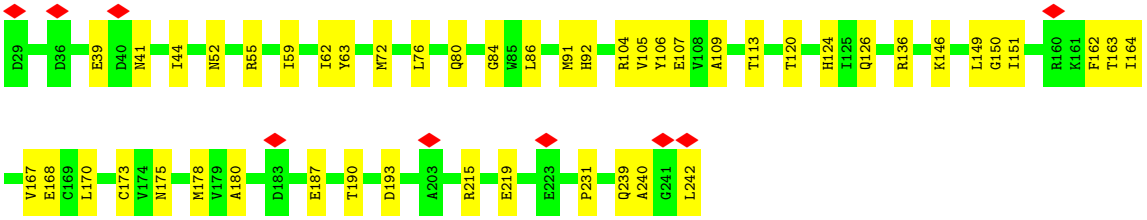




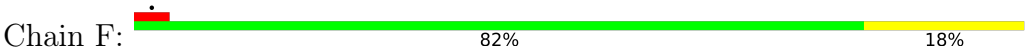


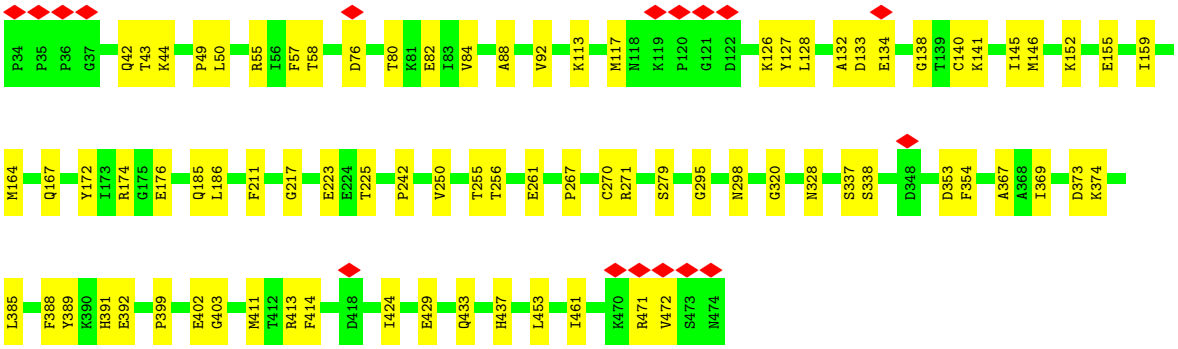
• Molecule 5: NADH dehydrogenase (Ubiquinone) 24 kDa subunit, isoform A



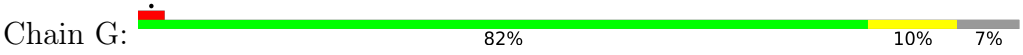


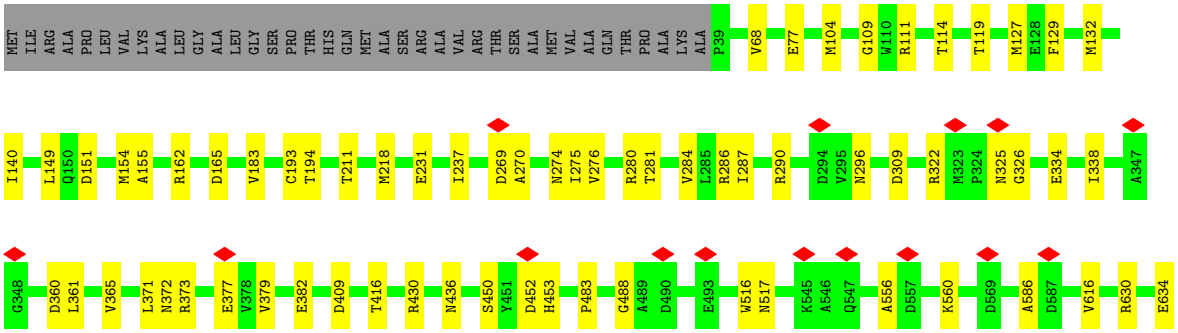
• Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

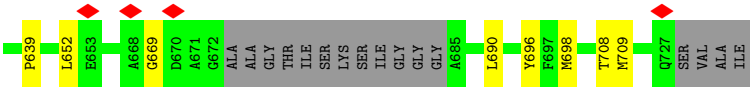




• Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial



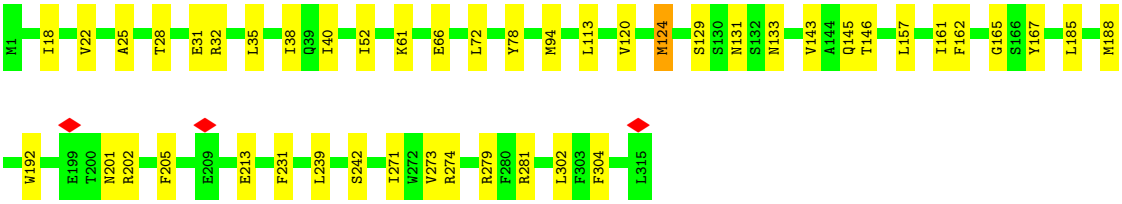




• Molecule 8: NADH-ubiquinone oxidoreductase chain 1

Chain H:

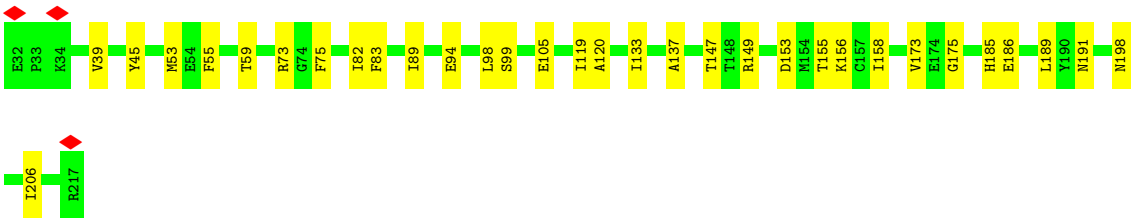




• Molecule 9: NADH dehydrogenase (ubiquinone) 23 kDa subunit

Chain I:

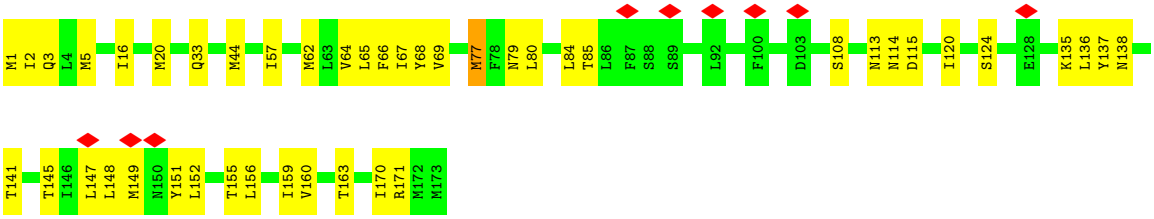




• Molecule 10: NADH-ubiquinone oxidoreductase chain 6

Chain J:

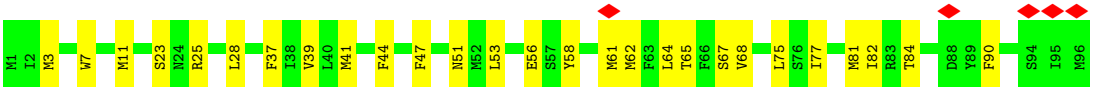




• Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

Chain K:

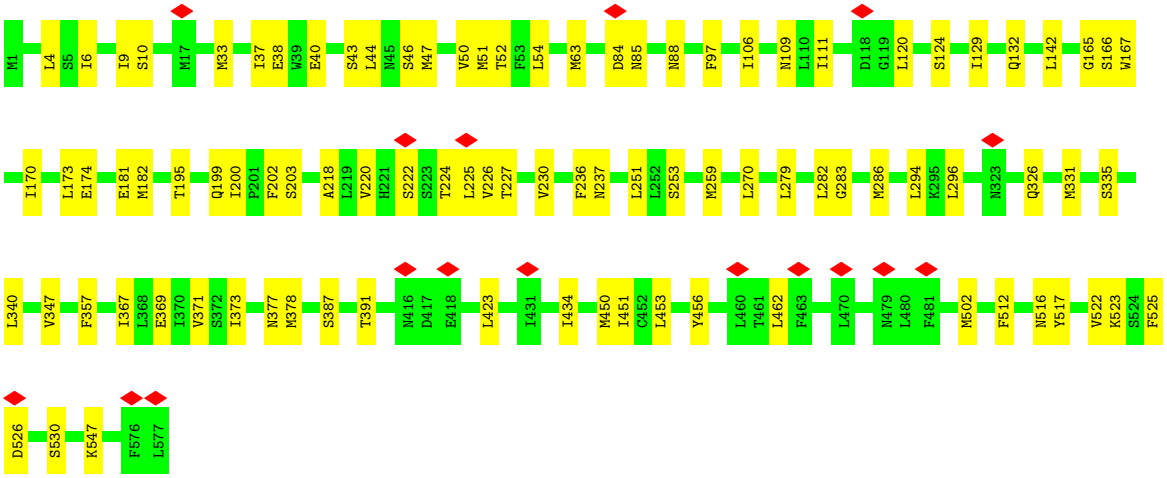




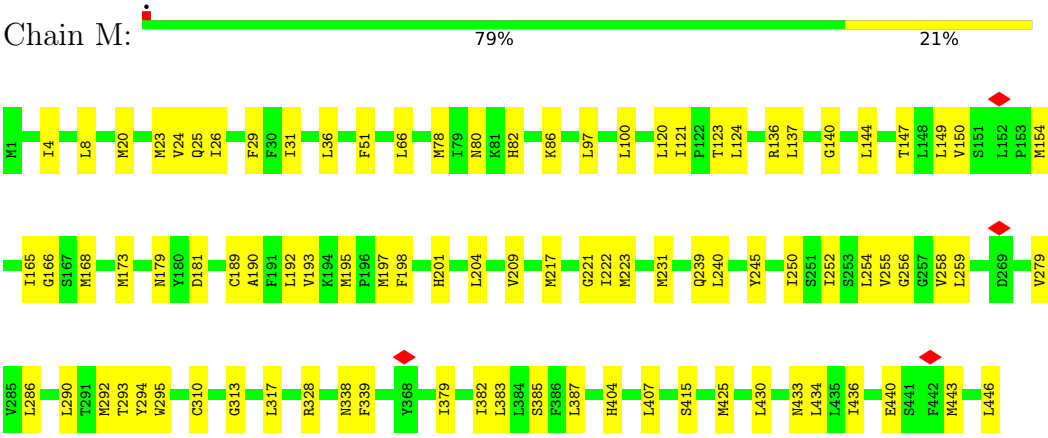
• Molecule 12: NADH-ubiquinone oxidoreductase chain 5

Chain L:

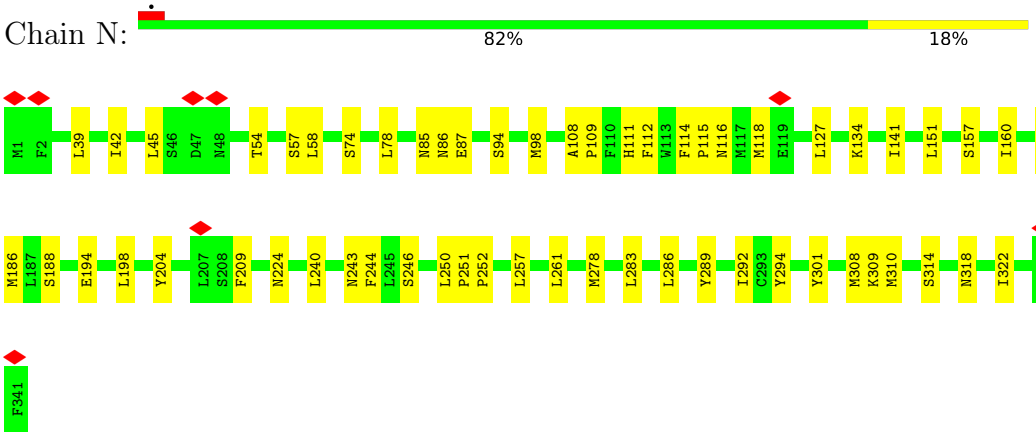




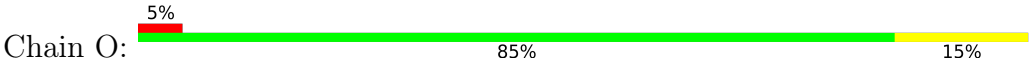
• Molecule 13: NADH-ubiquinone oxidoreductase chain 4

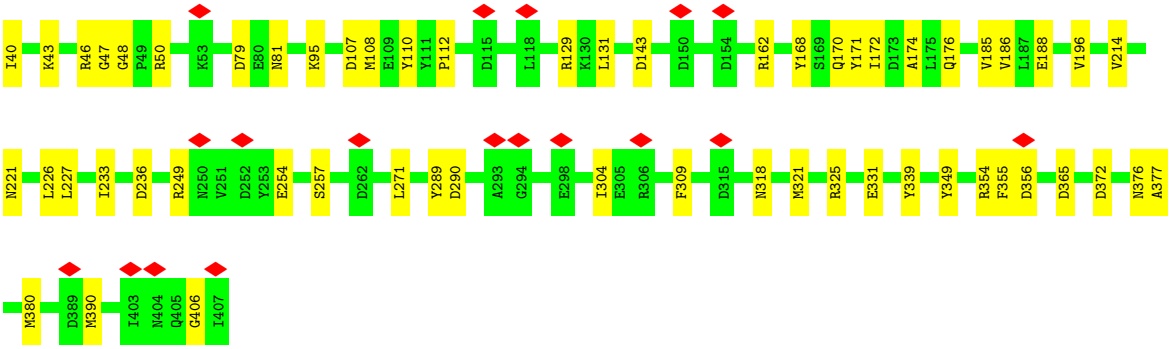


• Molecule 14: NADH-ubiquinone oxidoreductase chain 2

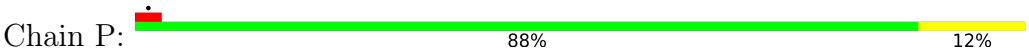


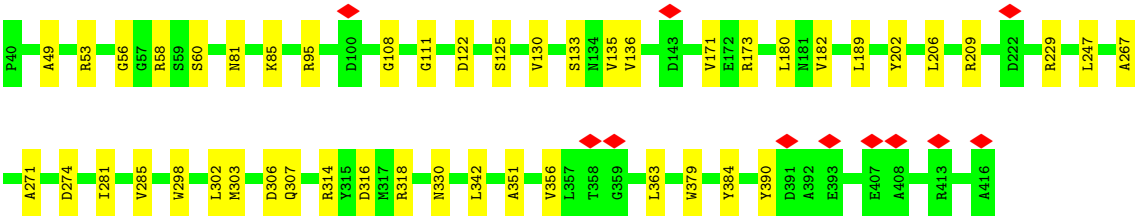
• Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial



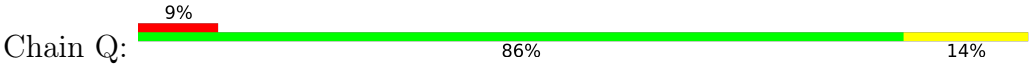


• Molecule 16: NADH dehydrogenase (Ubiquinone) 39 kDa subunit, isoform A



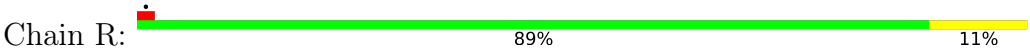


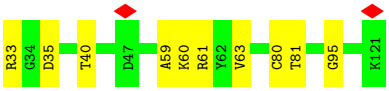
• Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial





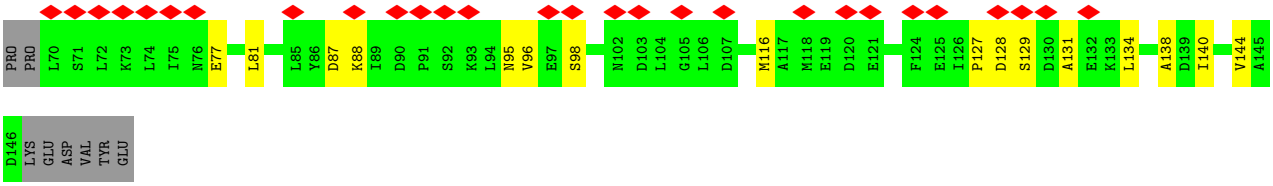
• Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial





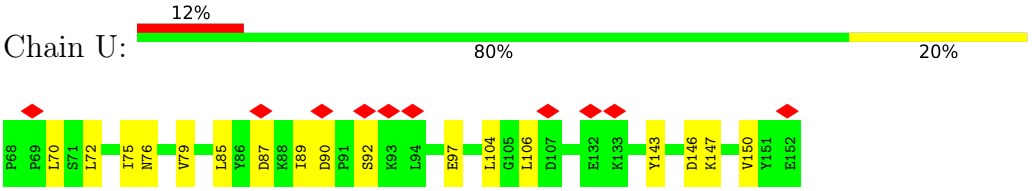
• Molecule 19: Acyl carrier protein, mitochondrial





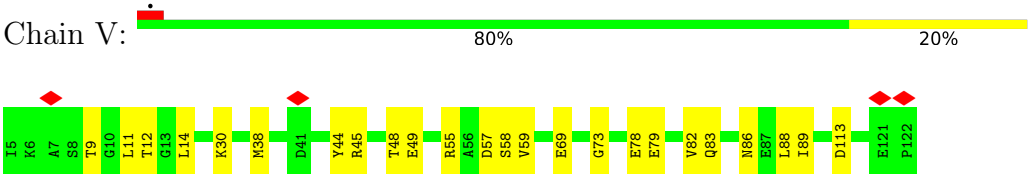
• Molecule 19: Acyl carrier protein, mitochondrial

Chain U:



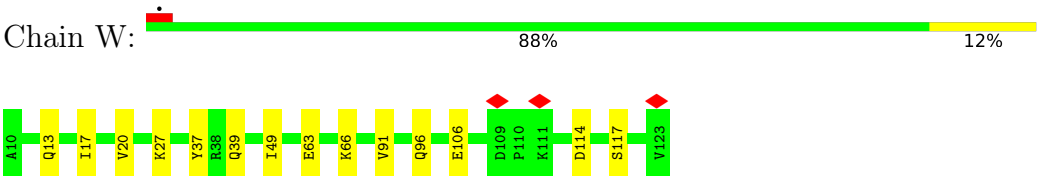
• Molecule 20: NADH dehydrogenase (Ubiquinone) 13 kDa B subunit

Chain V:



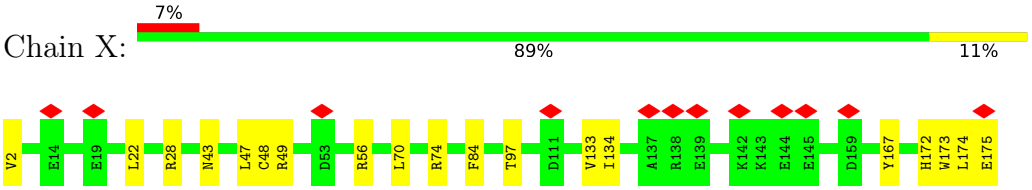
• Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain W:



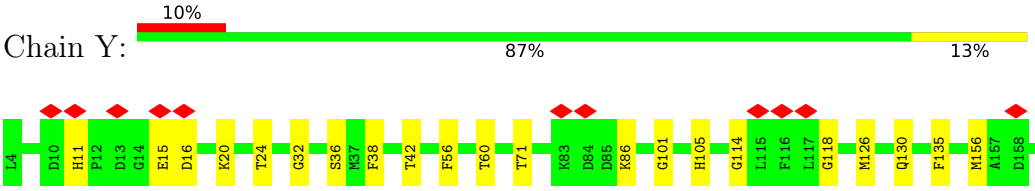
• Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain X:



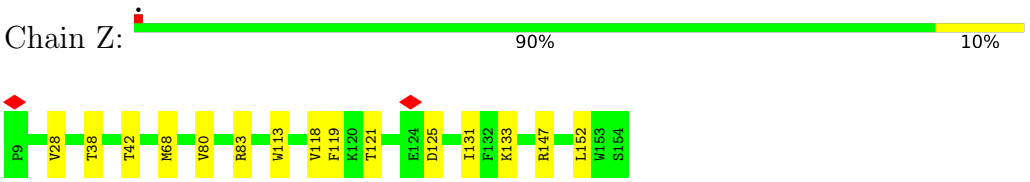
• Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain Y:



• Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

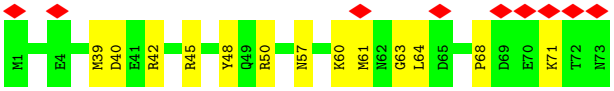
Chain Z:



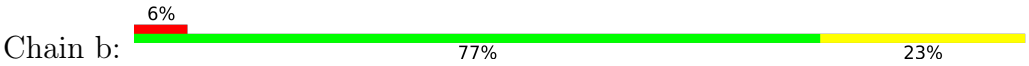
• Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

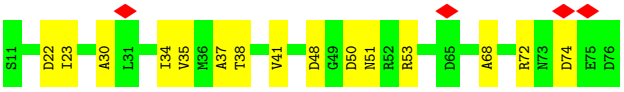
Chain a:



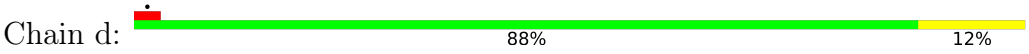


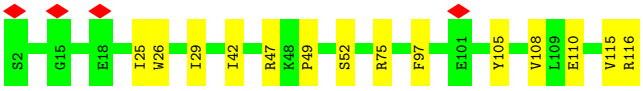
• Molecule 26: RH45008p



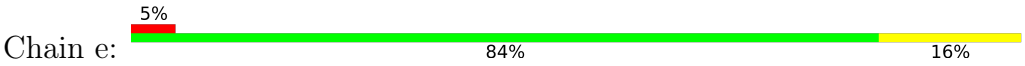


• Molecule 27: NADH dehydrogenase [ubiquinone] 1 subunit C2



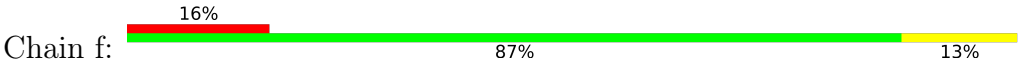


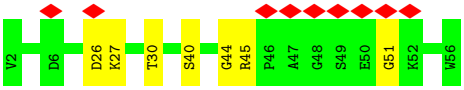
• Molecule 28: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



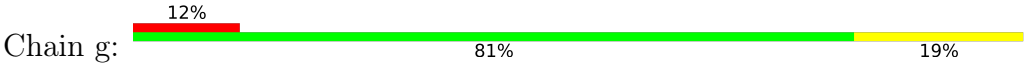


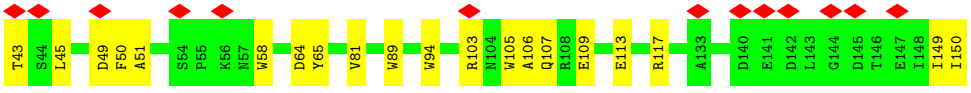
• Molecule 29: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



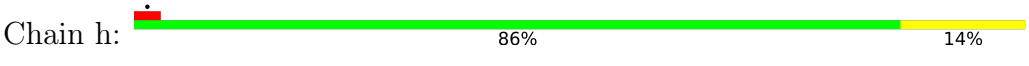


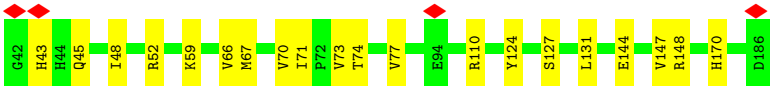
• Molecule 30: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial





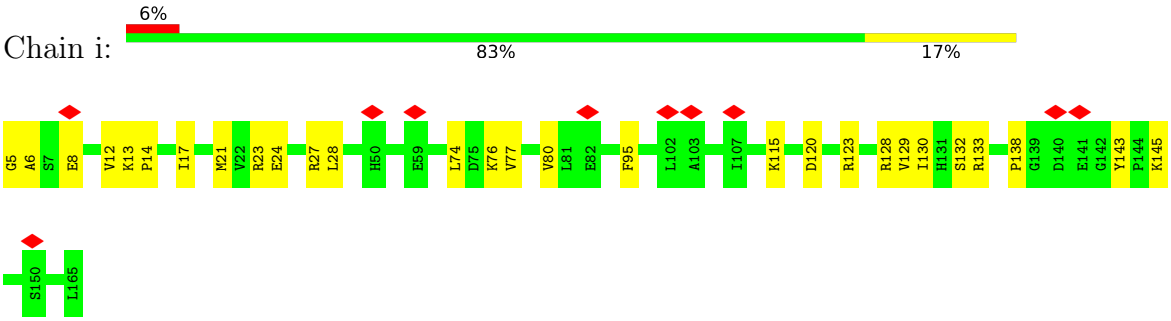
• Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial





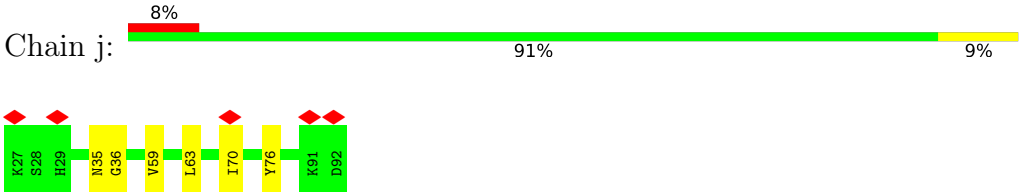
• Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain i:



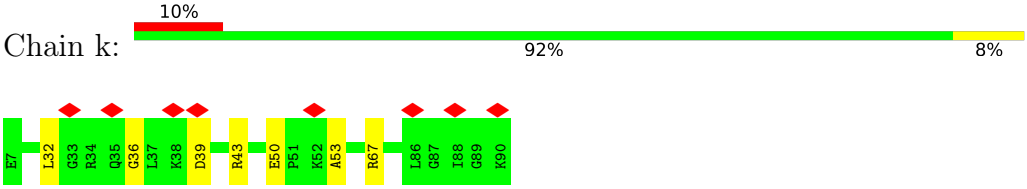
• Molecule 33: GEO11417p1

Chain j:



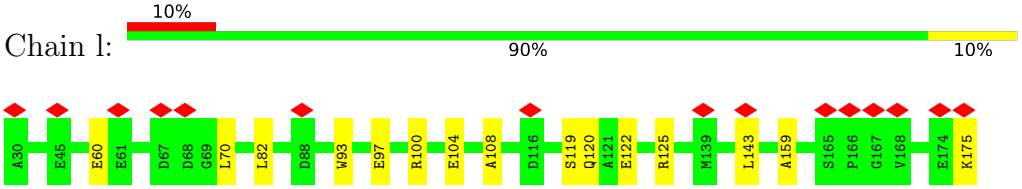
• Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain k:



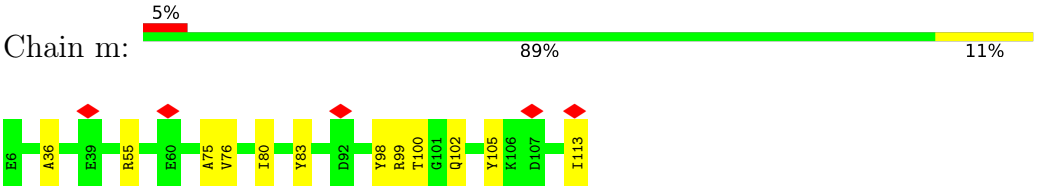
• Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain l:



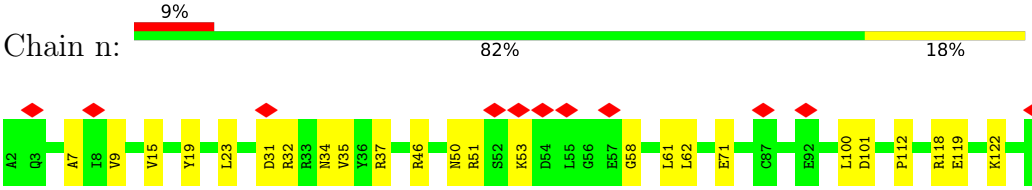
• Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

Chain m:



• Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

Chain n:



• Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain o:

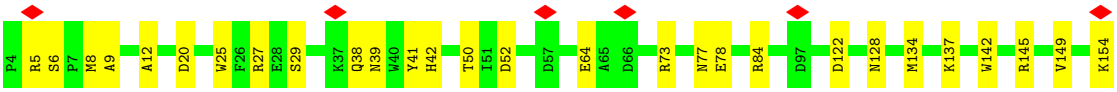




• Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

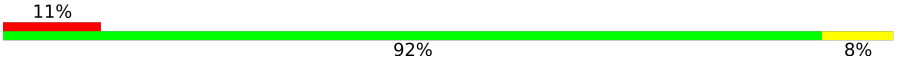
Chain p:

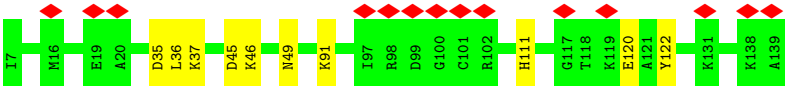




• Molecule 40: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain q:

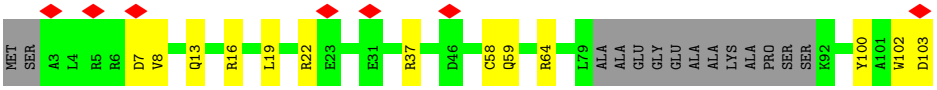




• Molecule 41: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

Chain r:

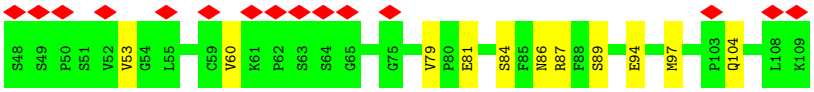




• Molecule 42: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

Chain s:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	37608	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 ($e^-/Å^2$)	41.88	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.103	Depositor
Minimum map value	-0.018	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.013	Depositor
Map size (Å)	471.59998, 471.59998, 471.59998	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.048, 1.048, 1.048	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: ZN, NA, DGT, 3PE, UQ9, PC1, EHZ, 2MR, FES, FMN, CDL, SF4, NDP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.30	0/979	0.46	0/1325
2	B	0.34	0/1473	0.42	1/1997 (0.1%)
3	C	0.31	0/1774	0.39	0/2412
4	D	0.30	0/3505	0.36	0/4751
5	E	0.27	0/1718	0.41	0/2328
6	F	0.27	0/3461	0.36	0/4678
7	G	0.27	0/5229	0.35	0/7088
8	H	0.30	0/2651	0.43	1/3593 (0.0%)
9	I	0.35	0/1518	0.39	0/2050
10	J	0.29	0/1424	0.44	1/1925 (0.1%)
11	K	0.28	0/814	0.39	0/1095
12	L	0.26	0/4726	0.34	0/6396
13	M	0.30	0/3723	0.35	0/5045
14	N	0.30	0/2875	0.39	0/3890
15	O	0.26	0/3082	0.35	0/4168
16	P	0.27	0/3108	0.37	0/4205
17	Q	0.28	0/1245	0.39	0/1687
18	R	0.28	0/733	0.34	0/987
19	T	0.16	0/624	0.31	0/843
19	U	0.21	0/696	0.30	0/940
20	V	0.24	0/942	0.34	0/1278
21	W	0.29	0/988	0.43	0/1329
22	X	0.23	0/1416	0.38	0/1911
23	Y	0.20	0/1314	0.32	0/1784
24	Z	0.25	0/1239	0.34	0/1682
25	a	0.25	0/614	0.37	0/827
26	b	0.22	0/528	0.34	0/714
27	d	0.24	0/935	0.33	0/1271
28	e	0.31	0/846	0.45	0/1128
29	f	0.23	0/440	0.34	0/590
30	g	0.28	0/908	0.35	0/1240
31	h	0.28	0/1269	0.36	0/1714

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	i	0.25	0/1338	0.39	0/1808
33	j	0.20	0/566	0.28	0/776
34	k	0.20	0/690	0.33	0/936
35	l	0.26	0/1264	0.36	0/1719
36	m	0.25	0/913	0.36	0/1222
37	n	0.25	0/1185	0.31	0/1597
38	o	0.22	0/960	0.39	0/1290
39	p	0.29	0/1299	0.34	0/1752
40	q	0.28	0/1157	0.38	0/1569
41	r	0.22	0/740	0.38	0/1003
42	s	0.21	0/469	0.41	0/637
All	All	0.27	0/67378	0.37	3/91180 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	H	124	MET	CB-CG-SD	-5.77	95.40	112.70
2	B	96	CYS	CA-CB-SG	5.46	126.95	114.40
10	J	77	MET	N-CA-C	5.12	117.59	109.50

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	A	956	0	1030	30	0
2	B	1435	0	1446	30	0
3	C	1726	0	1673	28	0
4	D	3434	0	3406	56	0
5	E	1679	0	1657	36	0
6	F	3381	0	3361	61	0
7	G	5146	0	5189	50	0
8	H	2571	0	2628	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	I	1485	0	1422	27	0
10	J	1397	0	1513	52	0
11	K	793	0	818	24	0
12	L	4606	0	4742	74	0
13	M	3617	0	3750	71	0
14	N	2796	0	2879	51	0
15	O	3007	0	2945	40	0
16	P	3032	0	3030	32	0
17	Q	1214	0	1186	17	0
18	R	716	0	700	6	0
19	T	615	0	625	10	0
19	U	684	0	687	12	0
20	V	922	0	946	15	0
21	W	968	0	991	14	0
22	X	1383	0	1328	15	0
23	Y	1277	0	1258	14	0
24	Z	1201	0	1211	14	0
25	a	601	0	603	9	0
26	b	519	0	517	11	0
27	d	907	0	896	14	0
28	e	828	0	809	14	0
29	f	429	0	436	4	0
30	g	883	0	834	25	0
31	h	1234	0	1198	17	0
32	i	1302	0	1295	28	0
33	j	541	0	508	7	0
34	k	671	0	671	6	0
35	l	1215	0	1125	14	0
36	m	892	0	885	16	0
37	n	1152	0	1124	19	0
38	o	937	0	922	12	0
39	p	1266	0	1217	27	0
40	q	1118	0	1071	8	0
41	r	724	0	727	11	0
42	s	456	0	440	12	0
43	A	39	0	52	0	0
43	J	44	0	62	0	0
43	i	34	0	42	1	0
44	A	79	0	106	1	0
44	B	37	0	48	0	0
44	H	47	0	71	0	0
44	J	64	0	76	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	L	108	0	144	1	0
44	M	35	0	44	0	0
44	N	44	0	62	0	0
44	X	30	0	34	0	0
44	Y	107	0	139	0	0
44	d	36	0	46	0	0
45	B	8	0	0	0	0
45	F	8	0	0	0	0
45	G	16	0	0	0	0
45	I	16	0	0	0	0
46	B	67	0	78	0	0
46	P	54	0	52	0	0
46	h	129	0	146	3	0
47	E	4	0	0	0	0
47	G	4	0	0	0	0
48	F	31	0	19	1	0
49	G	1	0	0	0	0
50	H	58	0	82	15	0
51	O	31	0	12	2	0
52	P	48	0	24	2	0
53	R	1	0	0	0	0
54	T	37	0	0	3	0
54	U	37	0	0	3	0
All	All	66970	0	67038	851	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 6.

The worst 5 of 851 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)
6:F:113:LYS:NZ	48:F:501:FMN:O1P	2.06	0.88
12:L:517:TYR:OH	36:m:75:ALA:O	1.93	0.87
4:D:448:MET:SD	8:H:281:ARG:NH2	2.49	0.86
54:U:201:EHZ:O5	37:n:51:ARG:NH1	2.10	0.84
31:h:124:TYR:OH	39:p:64:GLU:OE2	1.93	0.84

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
2	B	180/182 (99%)	172 (96%)	8 (4%)	0	100	100
3	C	207/209 (99%)	194 (94%)	13 (6%)	0	100	100
4	D	427/430 (99%)	410 (96%)	17 (4%)	0	100	100
5	E	212/214 (99%)	198 (93%)	14 (7%)	0	100	100
6	F	439/441 (100%)	422 (96%)	16 (4%)	1 (0%)	43	71
7	G	673/731 (92%)	649 (96%)	24 (4%)	0	100	100
8	H	313/315 (99%)	301 (96%)	12 (4%)	0	100	100
9	I	184/186 (99%)	177 (96%)	7 (4%)	0	100	100
10	J	171/173 (99%)	164 (96%)	7 (4%)	0	100	100
11	K	94/96 (98%)	91 (97%)	3 (3%)	0	100	100
12	L	575/577 (100%)	553 (96%)	22 (4%)	0	100	100
13	M	444/446 (100%)	428 (96%)	15 (3%)	1 (0%)	43	71
14	N	339/341 (99%)	328 (97%)	11 (3%)	0	100	100
15	O	366/368 (100%)	358 (98%)	8 (2%)	0	100	100
16	P	375/377 (100%)	361 (96%)	14 (4%)	0	100	100
17	Q	149/151 (99%)	139 (93%)	10 (7%)	0	100	100
18	R	87/89 (98%)	84 (97%)	3 (3%)	0	100	100
19	T	75/85 (88%)	73 (97%)	2 (3%)	0	100	100
19	U	83/85 (98%)	80 (96%)	3 (4%)	0	100	100
20	V	116/118 (98%)	114 (98%)	2 (2%)	0	100	100
21	W	112/114 (98%)	110 (98%)	2 (2%)	0	100	100
22	X	172/174 (99%)	162 (94%)	10 (6%)	0	100	100
23	Y	165/167 (99%)	159 (96%)	6 (4%)	0	100	100
24	Z	144/146 (99%)	140 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	a	71/73 (97%)	68 (96%)	3 (4%)	0	100	100
26	b	64/66 (97%)	63 (98%)	1 (2%)	0	100	100
27	d	113/115 (98%)	112 (99%)	1 (1%)	0	100	100
28	e	98/100 (98%)	94 (96%)	4 (4%)	0	100	100
29	f	53/55 (96%)	48 (91%)	5 (9%)	0	100	100
30	g	106/108 (98%)	101 (95%)	5 (5%)	0	100	100
31	h	143/145 (99%)	133 (93%)	10 (7%)	0	100	100
32	i	159/161 (99%)	152 (96%)	7 (4%)	0	100	100
33	j	64/66 (97%)	64 (100%)	0	0	100	100
34	k	82/84 (98%)	80 (98%)	2 (2%)	0	100	100
35	l	144/146 (99%)	139 (96%)	5 (4%)	0	100	100
36	m	106/108 (98%)	102 (96%)	4 (4%)	0	100	100
37	n	132/134 (98%)	131 (99%)	1 (1%)	0	100	100
38	o	110/112 (98%)	105 (96%)	5 (4%)	0	100	100
39	p	149/151 (99%)	146 (98%)	3 (2%)	0	100	100
40	q	131/133 (98%)	125 (95%)	6 (5%)	0	100	100
41	r	85/103 (82%)	82 (96%)	3 (4%)	0	100	100
42	s	60/62 (97%)	54 (90%)	6 (10%)	0	100	100
All	All	8087/8254 (98%)	7778 (96%)	307 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	M	51	PHE
6	F	49	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	110/110 (100%)	110 (100%)	0	100	100
2	B	152/152 (100%)	152 (100%)	0	100	100
3	C	187/187 (100%)	187 (100%)	0	100	100
4	D	367/367 (100%)	367 (100%)	0	100	100
5	E	185/185 (100%)	185 (100%)	0	100	100
6	F	353/353 (100%)	353 (100%)	0	100	100
7	G	546/582 (94%)	546 (100%)	0	100	100
8	H	282/282 (100%)	282 (100%)	0	100	100
9	I	159/159 (100%)	159 (100%)	0	100	100
10	J	166/166 (100%)	166 (100%)	0	100	100
11	K	91/91 (100%)	91 (100%)	0	100	100
12	L	518/518 (100%)	518 (100%)	0	100	100
13	M	404/404 (100%)	404 (100%)	0	100	100
14	N	317/317 (100%)	317 (100%)	0	100	100
15	O	324/324 (100%)	324 (100%)	0	100	100
16	P	319/319 (100%)	319 (100%)	0	100	100
17	Q	131/131 (100%)	131 (100%)	0	100	100
18	R	77/77 (100%)	77 (100%)	0	100	100
19	T	71/79 (90%)	71 (100%)	0	100	100
19	U	79/79 (100%)	79 (100%)	0	100	100
20	V	97/97 (100%)	97 (100%)	0	100	100
21	W	107/107 (100%)	107 (100%)	0	100	100
22	X	150/150 (100%)	150 (100%)	0	100	100
23	Y	128/128 (100%)	128 (100%)	0	100	100
24	Z	128/128 (100%)	128 (100%)	0	100	100
25	a	65/65 (100%)	65 (100%)	0	100	100
26	b	52/52 (100%)	52 (100%)	0	100	100
27	d	93/93 (100%)	93 (100%)	0	100	100
28	e	88/88 (100%)	88 (100%)	0	100	100
29	f	42/42 (100%)	42 (100%)	0	100	100
30	g	97/97 (100%)	97 (100%)	0	100	100
31	h	130/130 (100%)	130 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	i	133/133 (100%)	133 (100%)	0	100	100
33	j	57/57 (100%)	57 (100%)	0	100	100
34	k	69/69 (100%)	69 (100%)	0	100	100
35	l	122/122 (100%)	122 (100%)	0	100	100
36	m	89/89 (100%)	89 (100%)	0	100	100
37	n	117/117 (100%)	117 (100%)	0	100	100
38	o	101/101 (100%)	101 (100%)	0	100	100
39	p	135/135 (100%)	135 (100%)	0	100	100
40	q	115/115 (100%)	115 (100%)	0	100	100
41	r	78/86 (91%)	78 (100%)	0	100	100
42	s	50/50 (100%)	50 (100%)	0	100	100
All	All	7081/7133 (99%)	7081 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 56 such sidechains are listed below:

Mol	Chain	Res	Type
16	P	116	HIS
41	r	59	GLN
21	W	13	GLN
40	q	70	HIS
36	m	28	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\#\|Z\| > 2$
4	2MR	D	123	4	10,12,13	2.52	3 (30%)	5,13,15	3.08	1 (20%)

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
4	2MR	D	123	4	-	1/10/13/15	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	123	2MR	CZ-NE	5.43	1.45	1.34
4	D	123	2MR	CZ-NH2	5.36	1.45	1.33
4	D	123	2MR	O-C	2.02	1.28	1.19

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	123	2MR	NE-CZ-NH2	-6.55	113.48	119.48

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	123	2MR	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 39 ligands modelled in this entry, 2 are monoatomic - leaving 37 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	$\#\|Z\| > 2$
44	3PE	Y	301	-	43,43,50	0.92	4 (9%)	46,48,55	1.30	3 (6%)
50	UQ9	H	501	-	58,58,58	2.26	19 (32%)	70,73,73	1.55	11 (15%)
44	3PE	J	202	-	39,39,50	0.96	4 (10%)	42,44,55	1.17	2 (4%)
43	PC1	A	201	-	38,38,53	1.47	6 (15%)	44,46,61	1.04	2 (4%)
44	3PE	X	201	-	29,29,50	1.14	4 (13%)	32,34,55	1.23	3 (9%)
45	SF4	I	302	9	0,12,12	-	-	-		
47	FES	G	803	7	0,4,4	-	-	-		
45	SF4	B	301	2	0,12,12	-	-	-		
52	NDP	P	501	-	49,52,52	3.97	23 (46%)	66,80,80	2.07	15 (22%)
54	EHZ	T	201	19	29,36,37	1.68	6 (20%)	35,44,47	1.63	5 (14%)
46	CDL	B	303	-	66,66,99	1.10	6 (9%)	72,78,111	1.03	3 (4%)
44	3PE	N	401	-	43,43,50	0.93	2 (4%)	46,48,55	1.00	2 (4%)
46	CDL	h	201	-	68,68,99	1.07	7 (10%)	74,80,111	1.11	4 (5%)
45	SF4	I	301	9	0,12,12	-	-	-		
44	3PE	J	203	-	23,23,50	1.19	4 (17%)	26,28,55	1.23	2 (7%)
44	3PE	Y	303	-	32,32,50	1.06	4 (12%)	35,37,55	1.03	2 (5%)
44	3PE	d	201	-	35,35,50	1.01	4 (11%)	38,40,55	1.05	2 (5%)
44	3PE	B	302	-	36,36,50	1.02	3 (8%)	39,41,55	1.14	3 (7%)
46	CDL	P	502	-	53,53,99	1.21	7 (13%)	59,65,111	1.24	4 (6%)
45	SF4	F	502	6	0,12,12	-	-	-		
44	3PE	M	501	-	34,34,50	1.03	4 (11%)	37,39,55	1.10	2 (5%)
44	3PE	L	601	-	38,38,50	0.97	4 (10%)	41,43,55	1.04	2 (4%)
45	SF4	G	802	7	0,12,12	-	-	-		
44	3PE	L	603	-	24,24,50	1.18	4 (16%)	27,29,55	1.38	2 (7%)
44	3PE	A	202	-	34,34,50	1.02	4 (11%)	37,39,55	1.28	2 (5%)
44	3PE	L	602	-	43,43,50	0.92	4 (9%)	46,48,55	1.07	2 (4%)
47	FES	E	301	5	0,4,4	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
45	SF4	G	801	7	0,12,12	-	-	-		
51	DGT	O	501	-	29,33,33	3.21	13 (44%)	44,52,52	2.02	12 (27%)
54	EHZ	U	201	19	29,36,37	1.70	6 (20%)	35,44,47	1.73	7 (20%)
44	3PE	Y	302	-	29,29,50	1.10	4 (13%)	32,34,55	1.21	2 (6%)
44	3PE	A	203	-	43,43,50	0.91	4 (9%)	46,48,55	1.17	3 (6%)
43	PC1	i	201	-	33,33,53	1.53	6 (18%)	39,41,61	1.07	2 (5%)
44	3PE	H	502	-	46,46,50	0.88	4 (8%)	49,51,55	1.14	2 (4%)
46	CDL	h	202	-	59,59,99	1.13	7 (11%)	65,71,111	1.22	5 (7%)
48	FMN	F	501	-	33,33,33	2.63	10 (30%)	48,50,50	1.74	15 (31%)
43	PC1	J	201	-	43,43,53	1.38	6 (13%)	49,51,61	1.05	2 (4%)

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
44	3PE	Y	301	-	-	13/47/47/54	-
50	UQ9	H	501	-	-	14/57/81/81	0/1/1/1
44	3PE	J	202	-	-	19/43/43/54	-
43	PC1	A	201	-	-	15/42/42/57	-
44	3PE	X	201	-	-	21/33/33/54	-
45	SF4	I	302	9	-	-	0/6/5/5
47	FES	G	803	7	-	-	0/1/1/1
45	SF4	B	301	2	-	-	0/6/5/5
52	NDP	P	501	-	-	4/34/77/77	0/5/5/5
54	EHZ	T	201	19	-	13/42/44/45	-
46	CDL	B	303	-	-	44/77/77/110	-
44	3PE	N	401	-	-	19/47/47/54	-
46	CDL	h	201	-	-	40/79/79/110	-
45	SF4	I	301	9	-	-	0/6/5/5
44	3PE	J	203	-	-	13/27/27/54	-
44	3PE	Y	303	-	-	14/36/36/54	-
44	3PE	d	201	-	-	19/39/39/54	-
44	3PE	B	302	-	-	17/40/40/54	-
46	CDL	P	502	-	-	33/64/64/110	-
45	SF4	F	502	6	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
44	3PE	M	501	-	-	20/38/38/54	-
44	3PE	L	601	-	-	23/42/42/54	-
45	SF4	G	802	7	-	-	0/6/5/5
44	3PE	L	603	-	-	8/27/27/54	-
44	3PE	A	202	-	-	16/38/38/54	-
44	3PE	L	602	-	-	19/47/47/54	-
47	FES	E	301	5	-	-	0/1/1/1
45	SF4	G	801	7	-	-	0/6/5/5
51	DGT	O	501	-	-	4/22/34/34	0/3/3/3
54	EHZ	U	201	19	-	12/42/44/45	-
44	3PE	Y	302	-	-	12/33/33/54	-
44	3PE	A	203	-	-	15/47/47/54	-
43	PC1	i	201	-	-	17/37/37/57	-
44	3PE	H	502	-	-	16/50/50/54	-
46	CDL	h	202	-	-	34/70/70/110	-
48	FMN	F	501	-	-	8/18/18/18	0/3/3/3
43	PC1	J	201	-	-	14/47/47/57	-

The worst 5 of 183 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	P	501	NDP	C6N-C5N	12.12	1.55	1.33
50	H	501	UQ9	C6-C1	10.61	1.54	1.35
52	P	501	NDP	C2B-C1B	-8.71	1.30	1.53
52	P	501	NDP	C7N-N7N	8.24	1.55	1.33
51	O	501	DGT	C3'-C4'	-8.15	1.30	1.53

The worst 5 of 123 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	P	501	NDP	N6A-C6A-N1A	-5.64	106.00	118.35
52	P	501	NDP	C5A-C4A-N3A	-5.41	119.69	126.75
50	H	501	UQ9	C7-C6-C5	-5.30	112.09	118.48
54	T	201	EHZ	C8-C9-S1	5.29	120.17	113.63
52	P	501	NDP	N3A-C2A-N1A	-5.25	120.39	128.60

There are no chirality outliers.

5 of 516 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
43	A	201	PC1	C1-O11-P-O12
43	A	201	PC1	C1-O11-P-O14
43	J	201	PC1	O22-C21-O21-C2
43	i	201	PC1	C11-O13-P-O12
43	i	201	PC1	C11-O13-P-O14

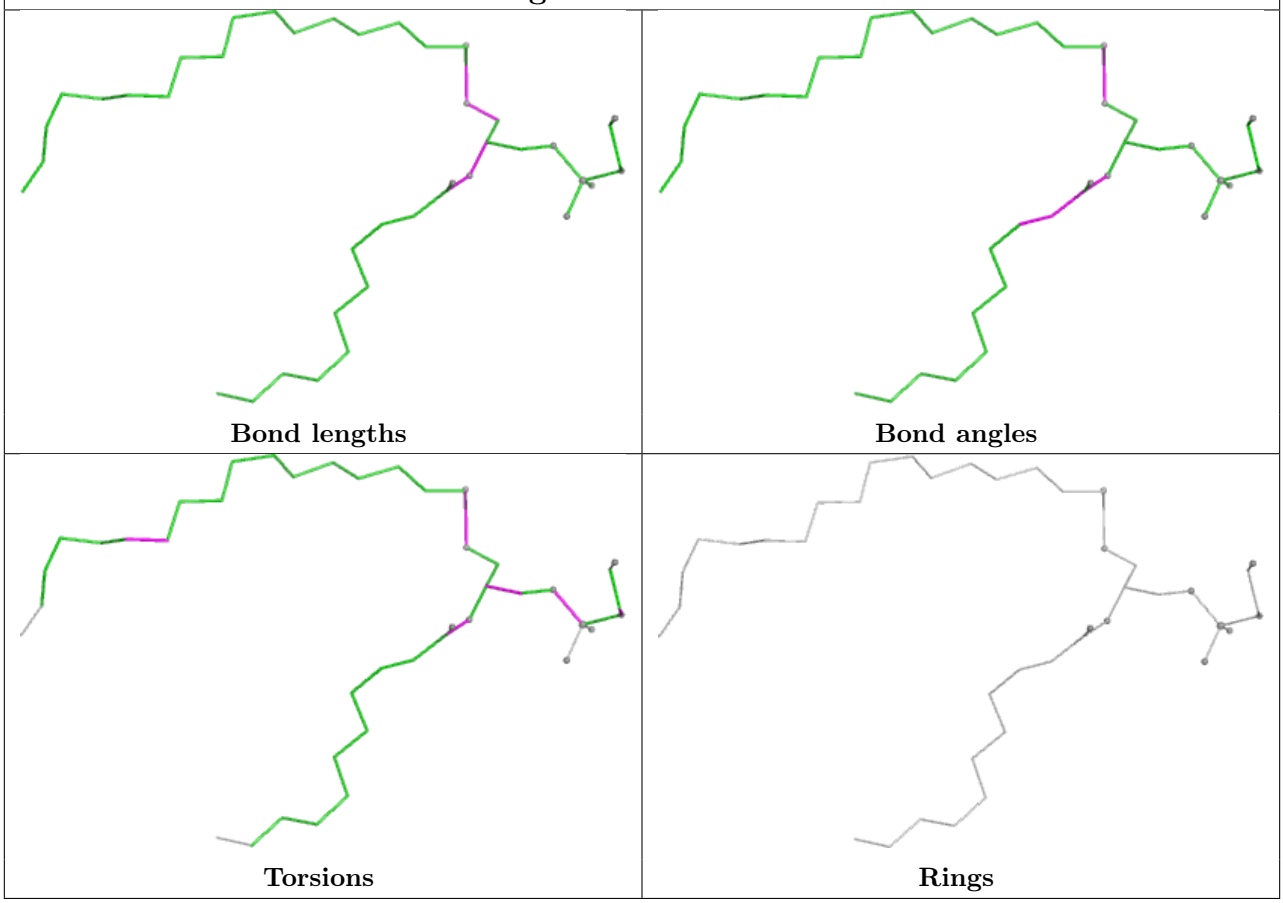
There are no ring outliers.

12 monomers are involved in 33 short contacts:

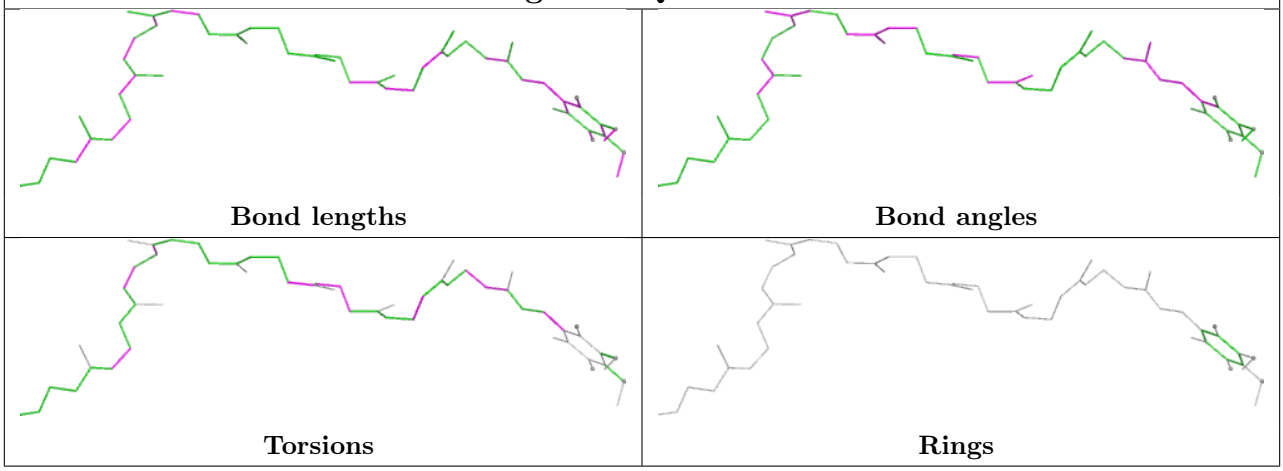
Mol	Chain	Res	Type	Clashes	Symm-Clashes
50	H	501	UQ9	15	0
52	P	501	NDP	2	0
54	T	201	EHZ	3	0
46	h	201	CDL	1	0
44	J	203	3PE	2	0
44	L	602	3PE	1	0
51	O	501	DGT	2	0
54	U	201	EHZ	3	0
44	A	203	3PE	1	0
43	i	201	PC1	1	0
46	h	202	CDL	2	0
48	F	501	FMN	1	0

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.

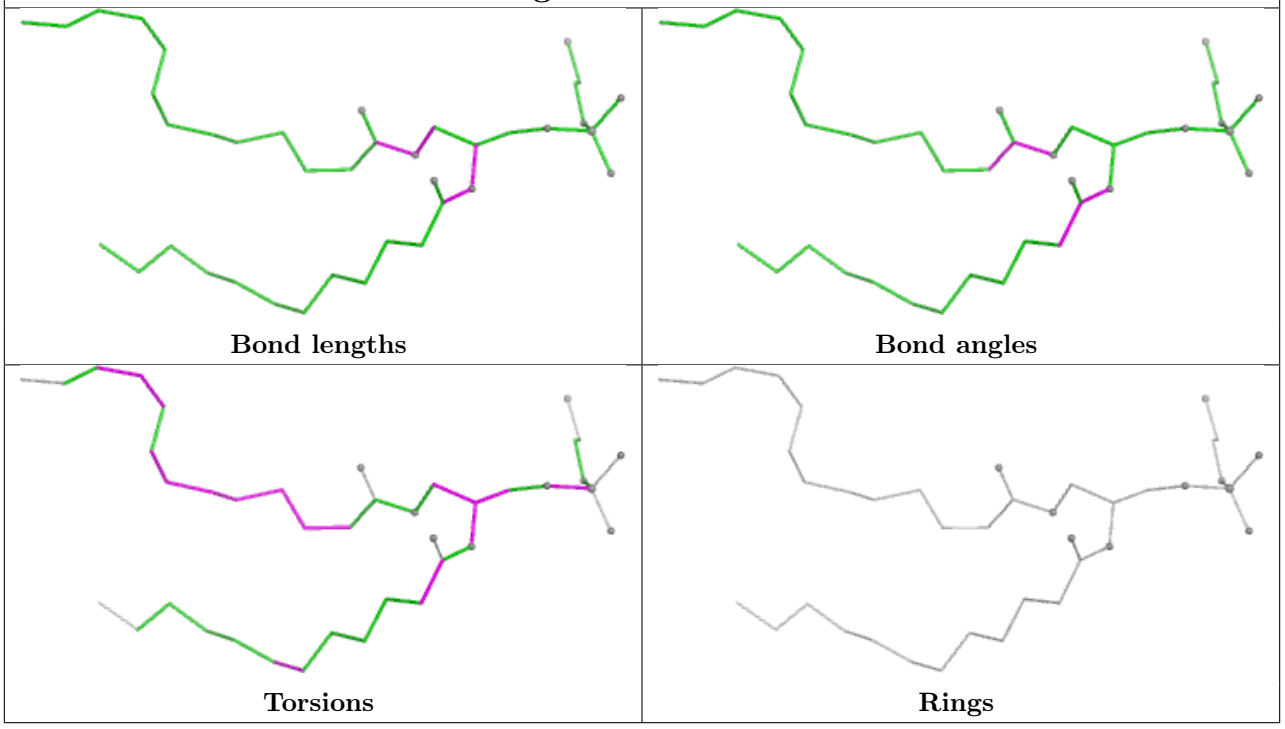
Ligand 3PE Y 301



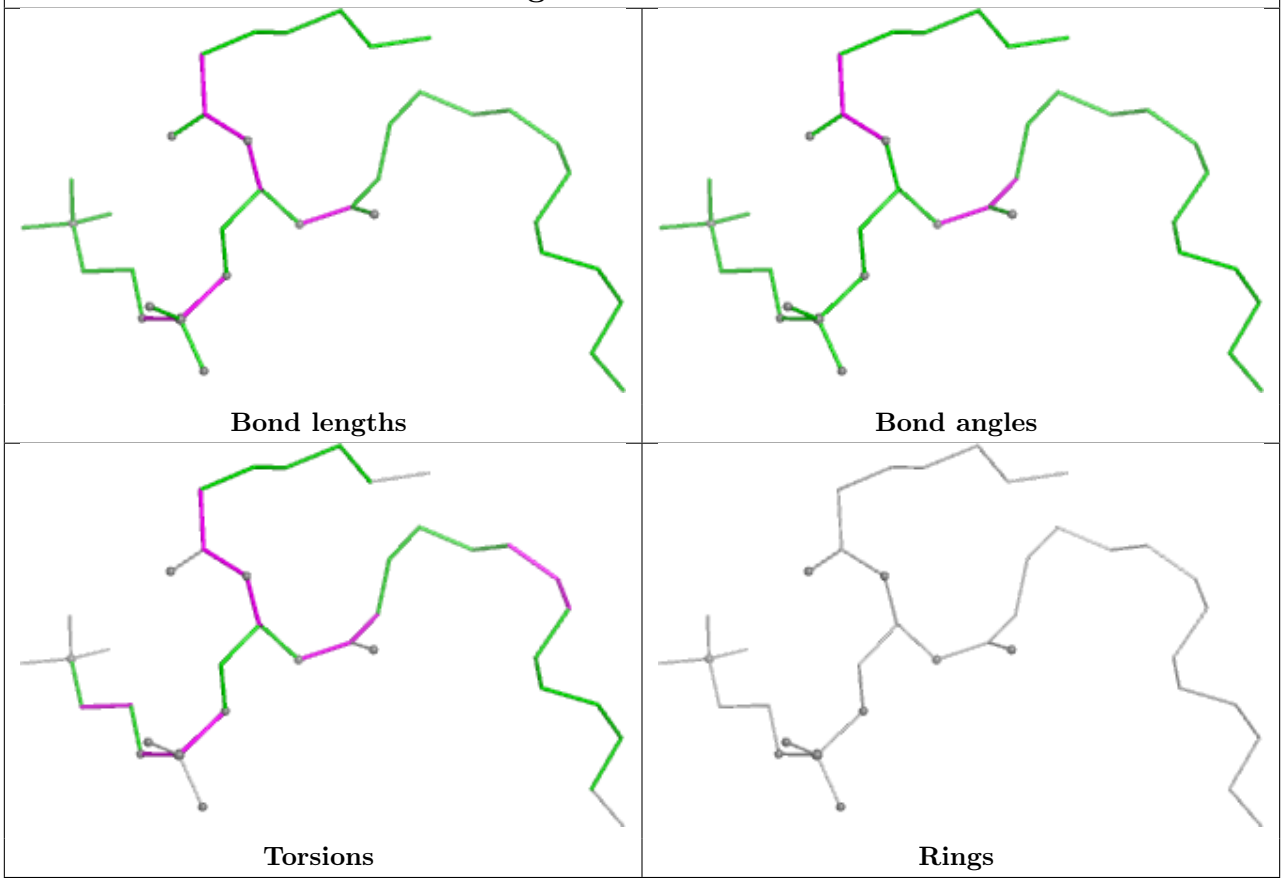
Ligand UQ9 H 501



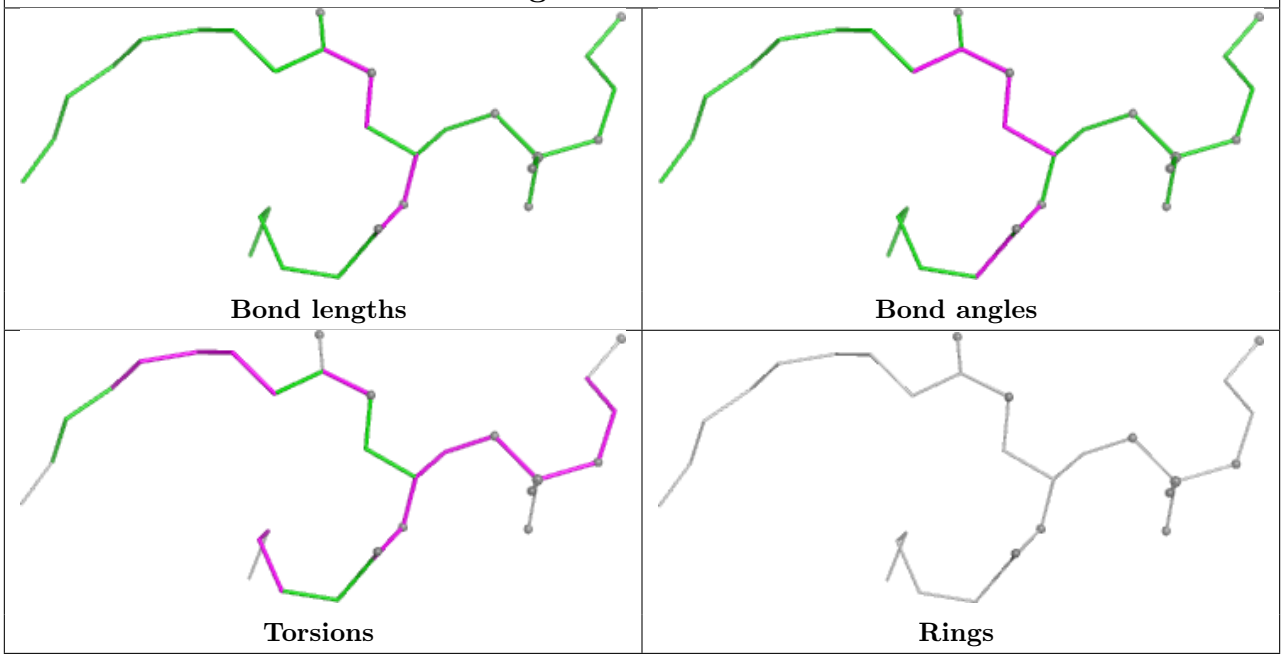
Ligand 3PE J 202



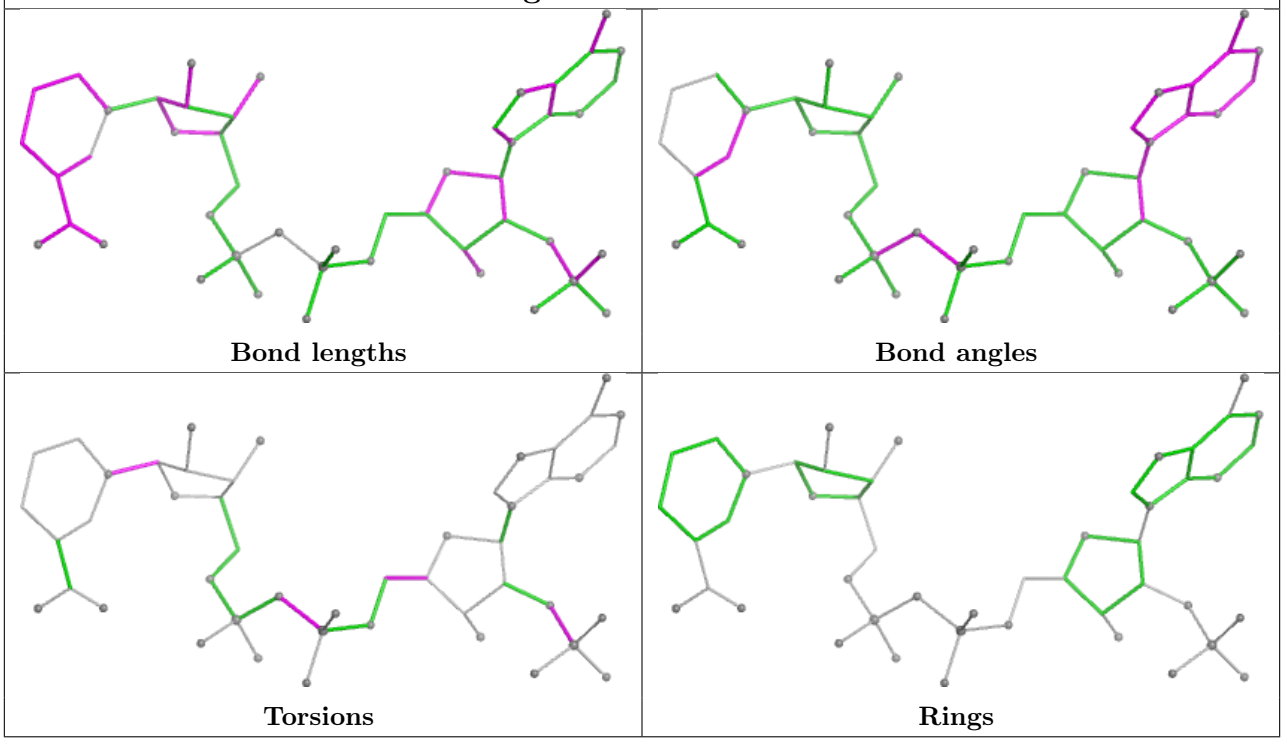
Ligand PC1 A 201



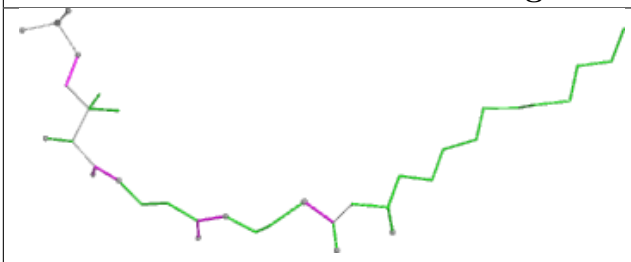
Ligand 3PE X 201



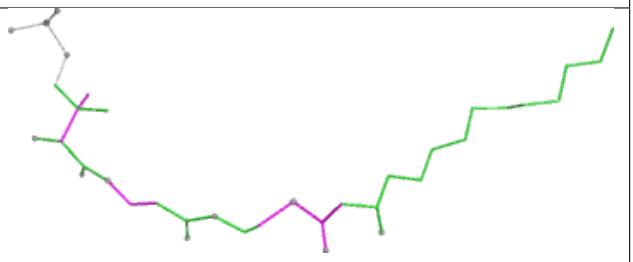
Ligand NDP P 501



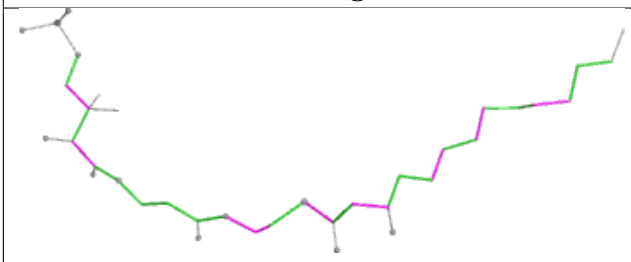
Ligand EHZ T 201



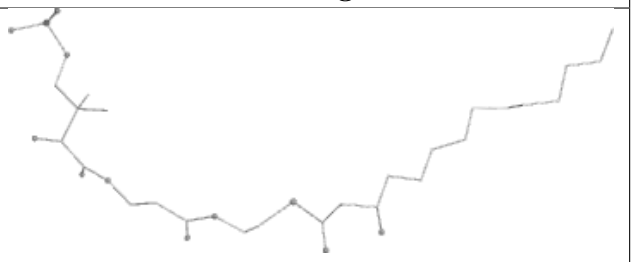
Bond lengths



Bond angles



Torsions

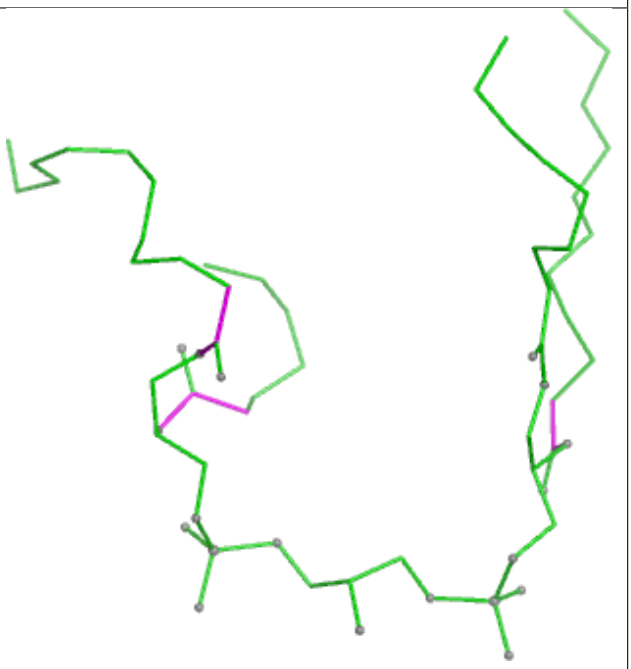


Rings

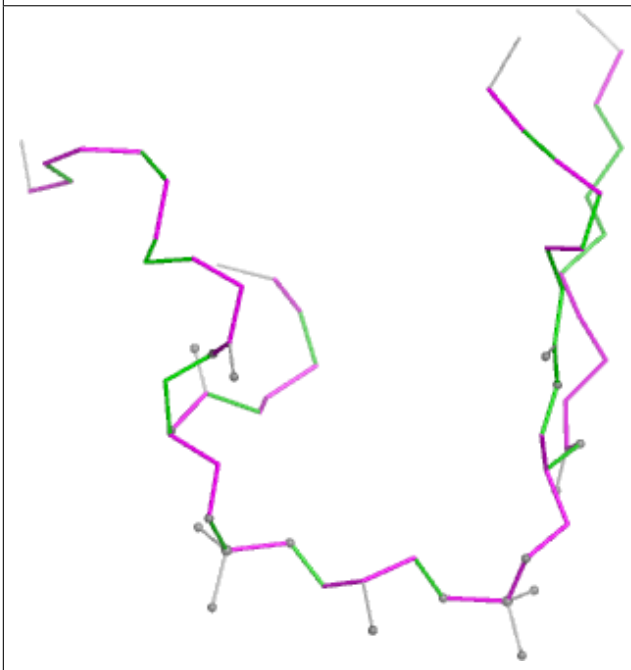
Ligand CDL B 303



Bond lengths



Bond angles

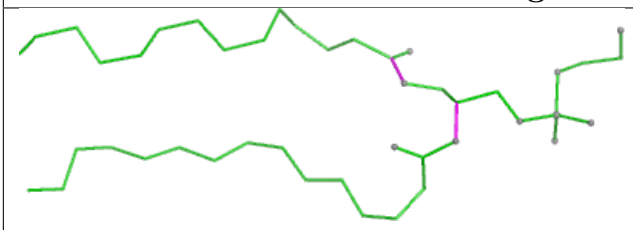


Torsions

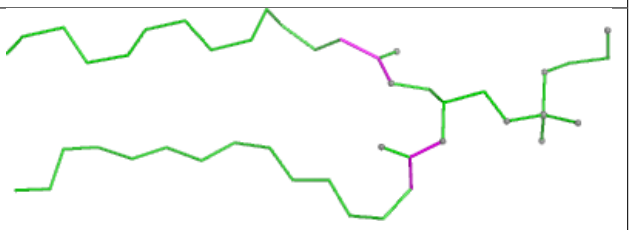


Rings

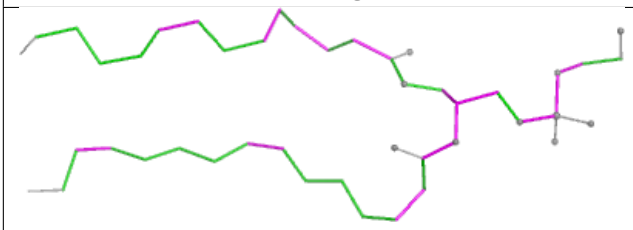
Ligand 3PE N 401



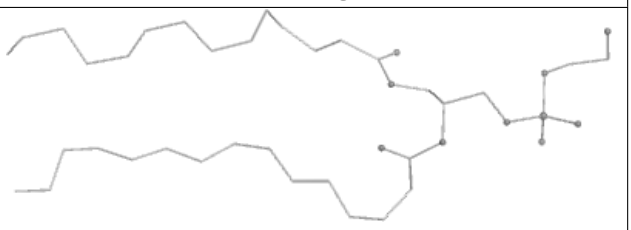
Bond lengths



Bond angles

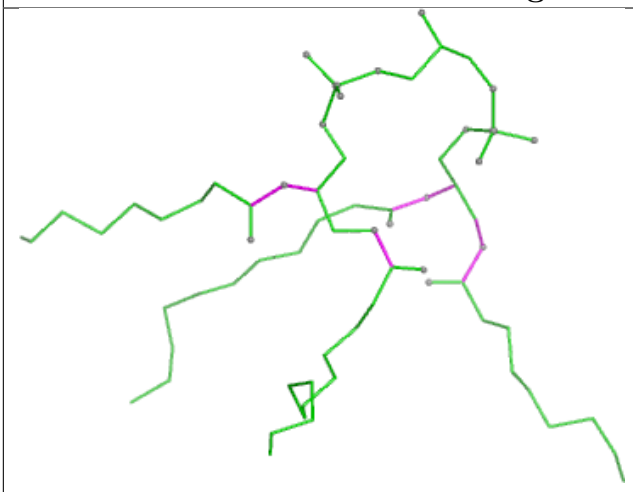


Torsions

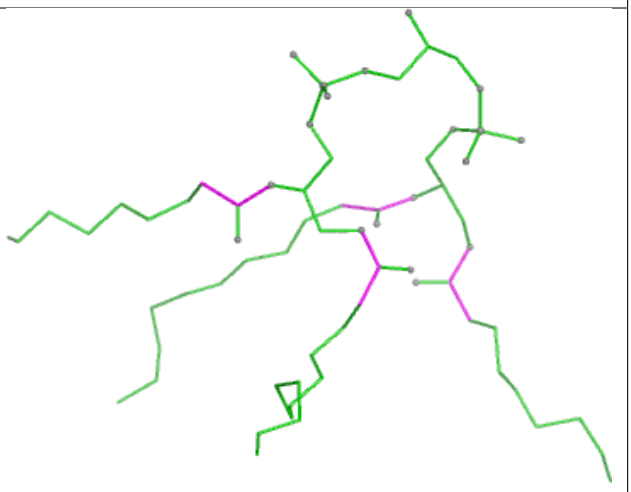


Rings

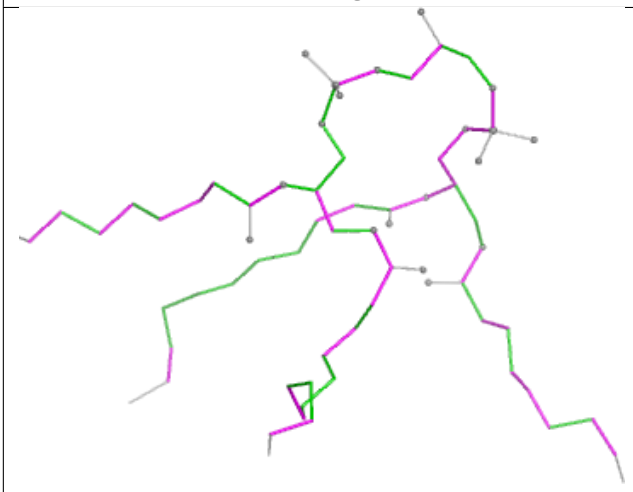
Ligand CDL h 201



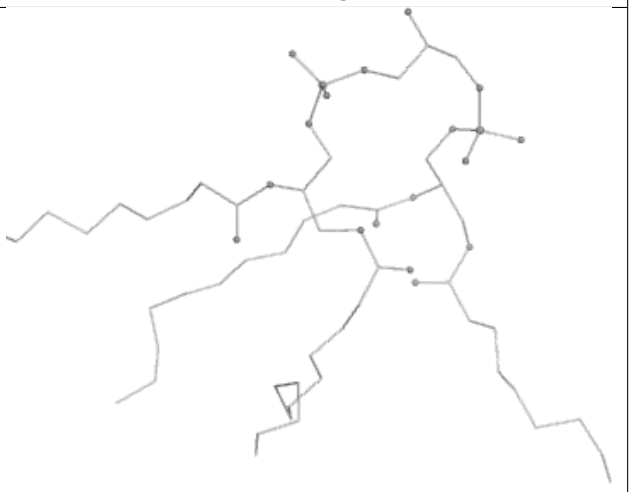
Bond lengths



Bond angles

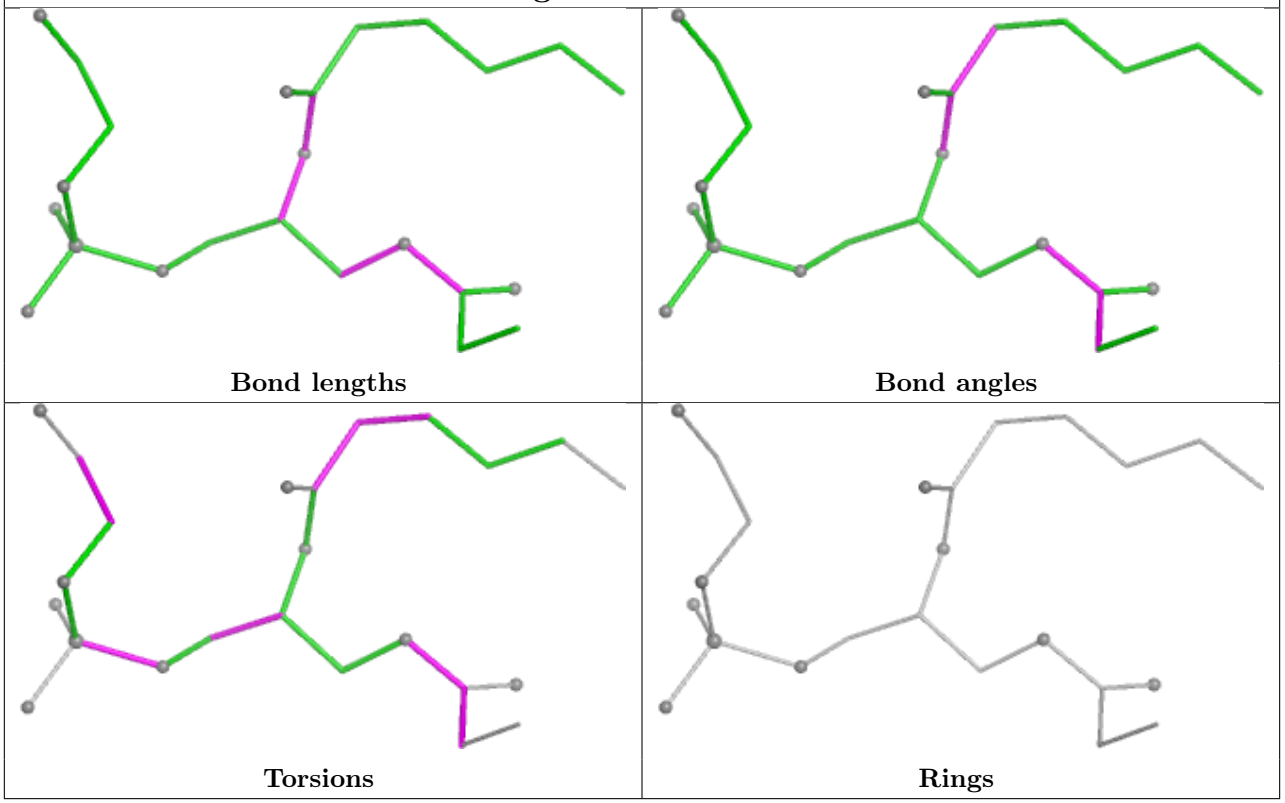


Torsions

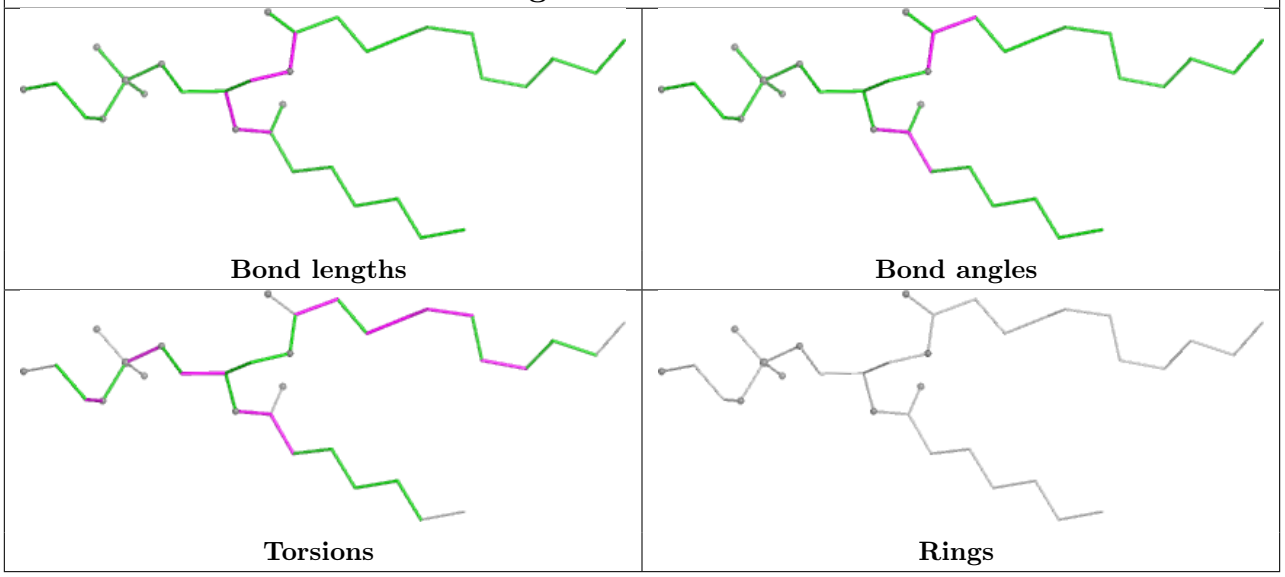


Rings

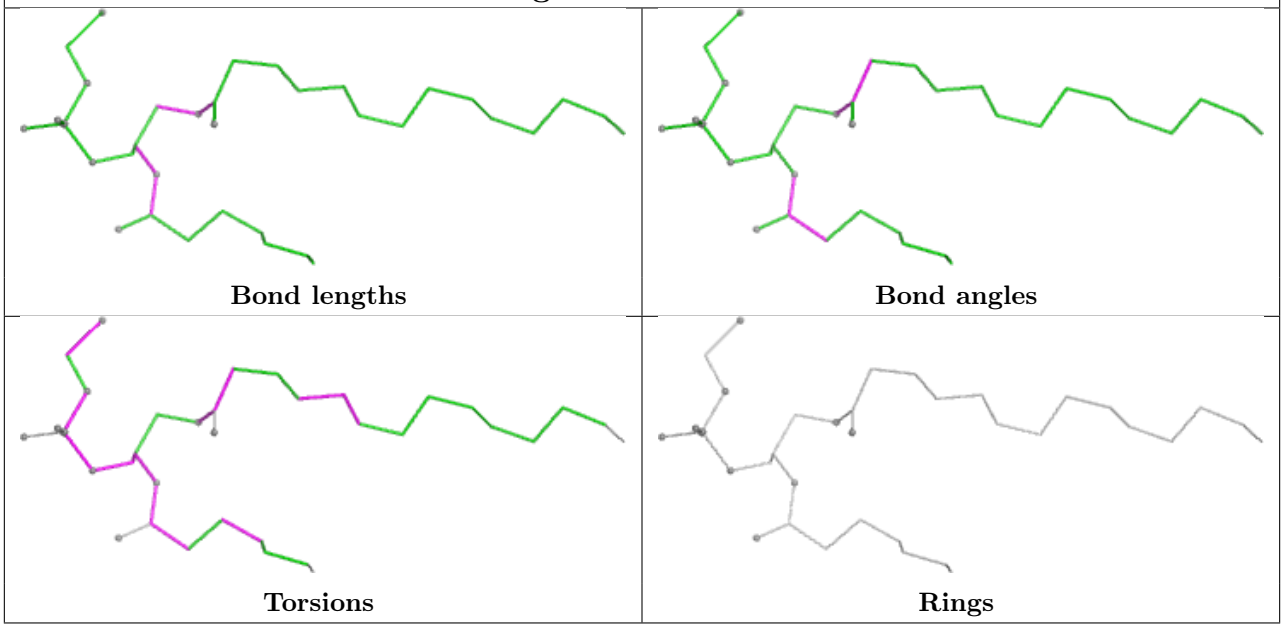
Ligand 3PE J 203



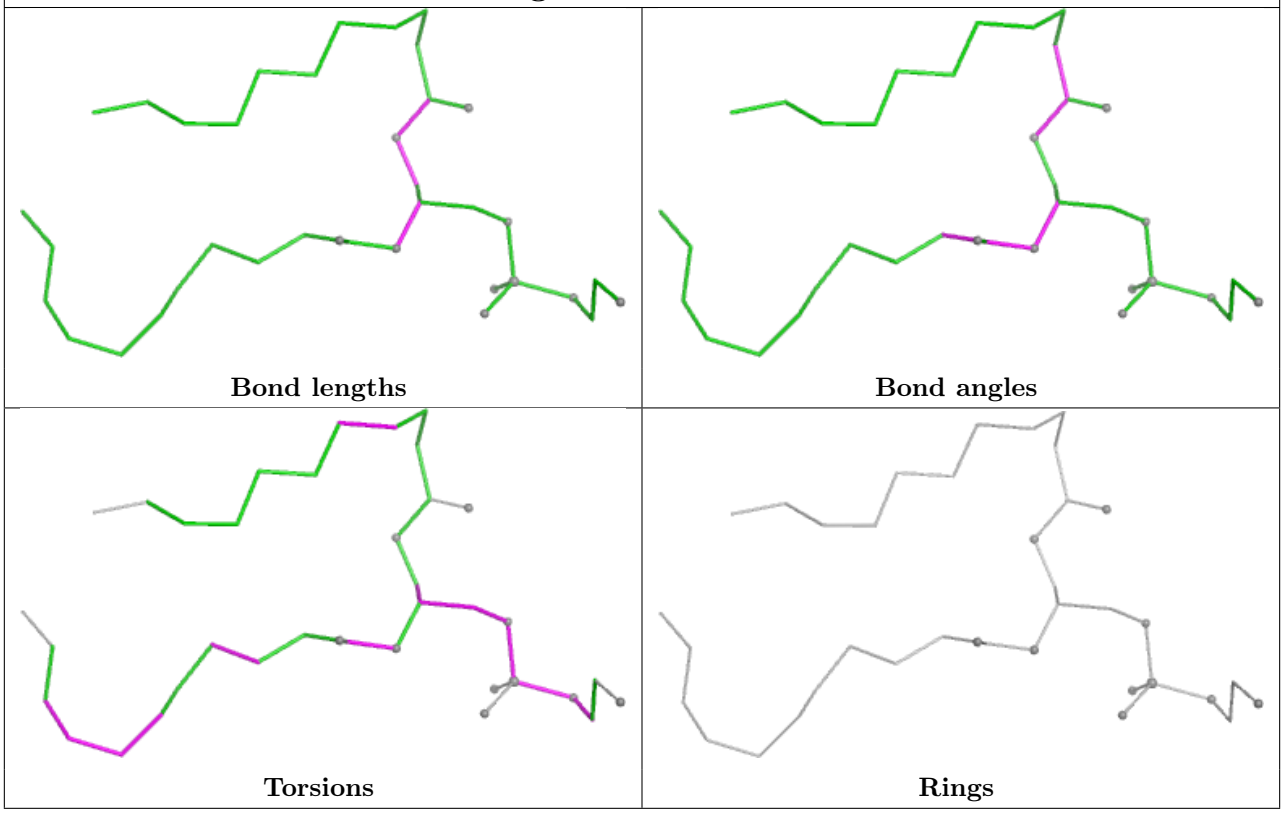
Ligand 3PE Y 303



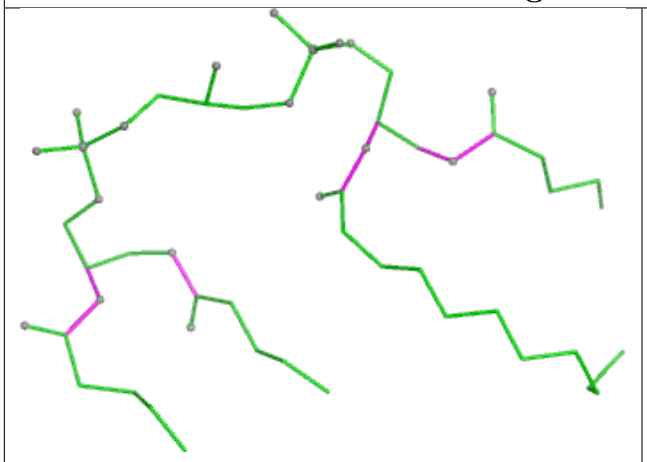
Ligand 3PE d 201



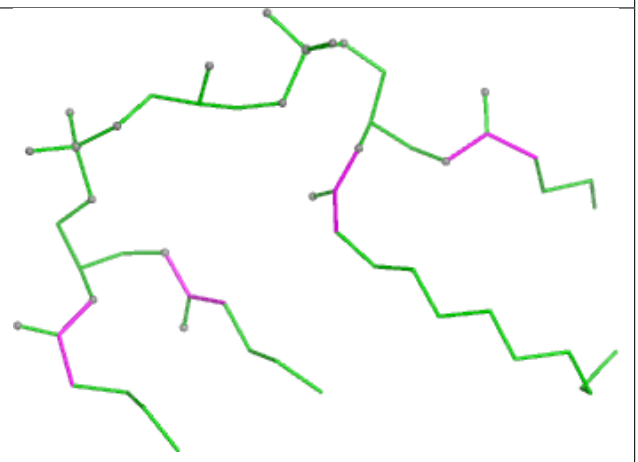
Ligand 3PE B 302



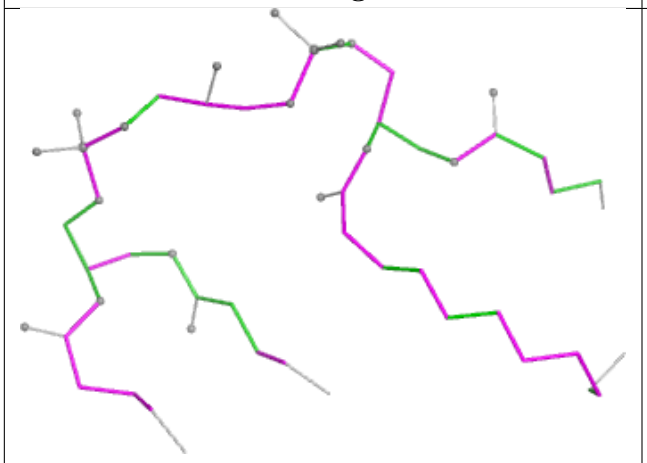
Ligand CDL P 502



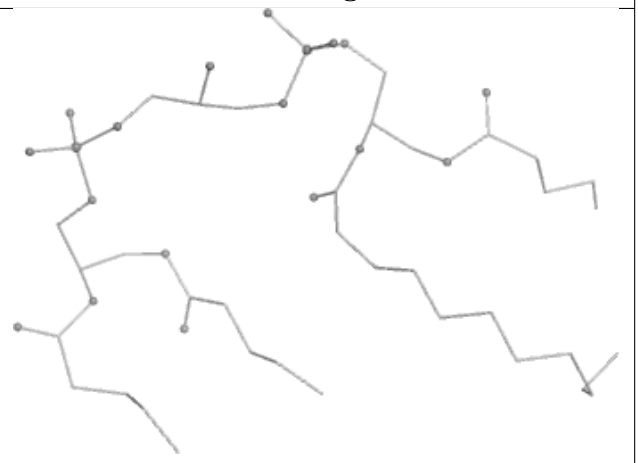
Bond lengths



Bond angles

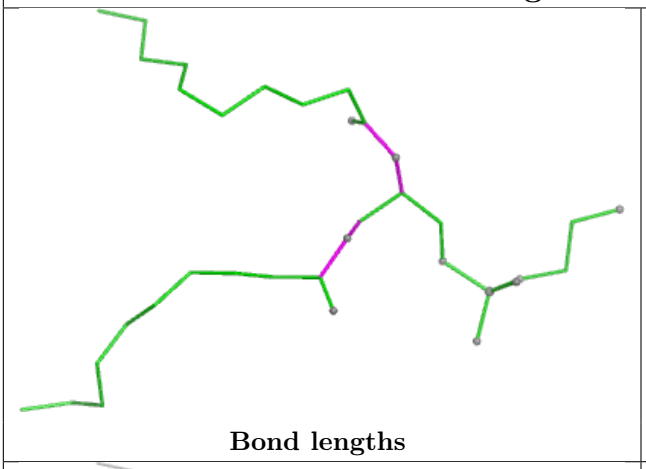


Torsions

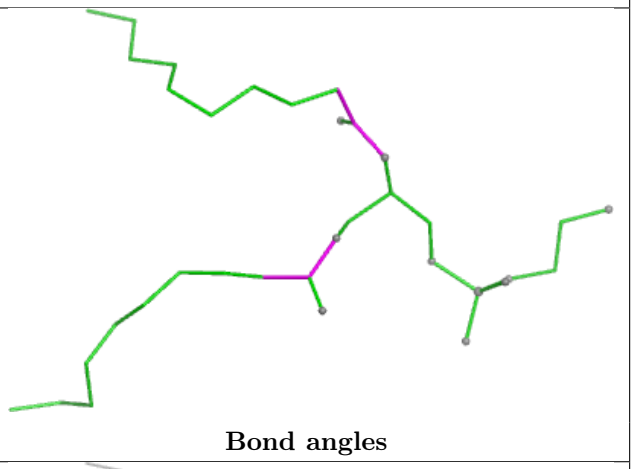


Rings

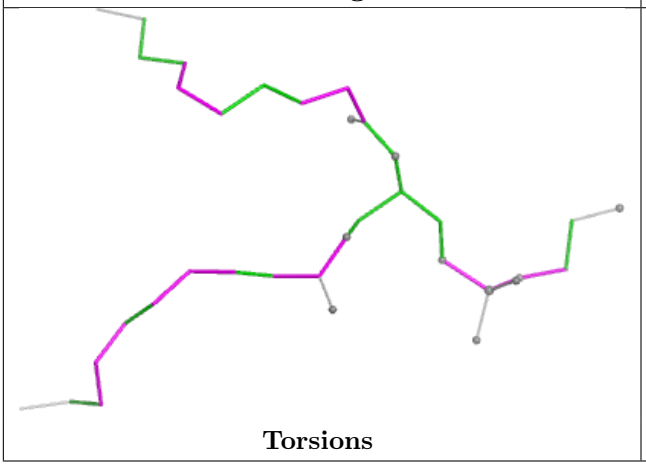
Ligand 3PE M 501



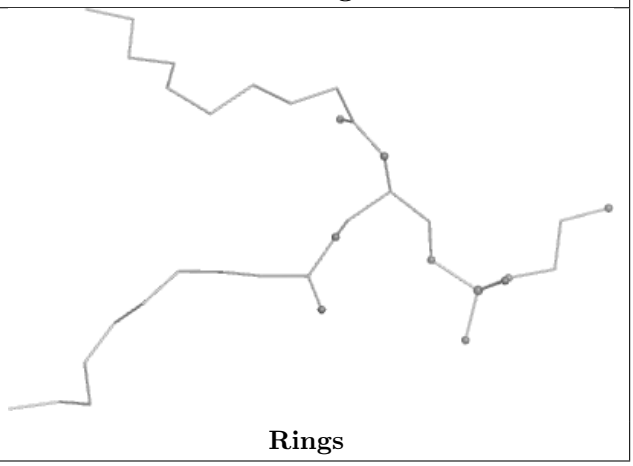
Bond lengths



Bond angles

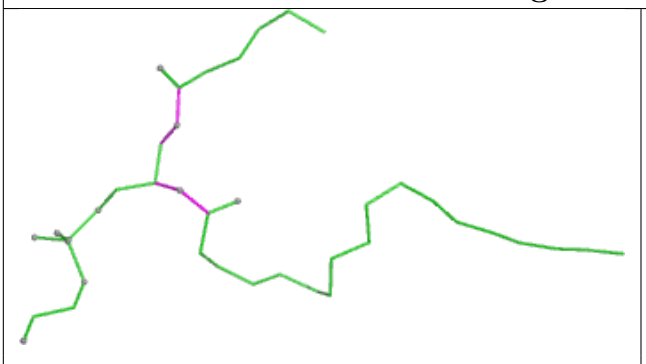


Torsions

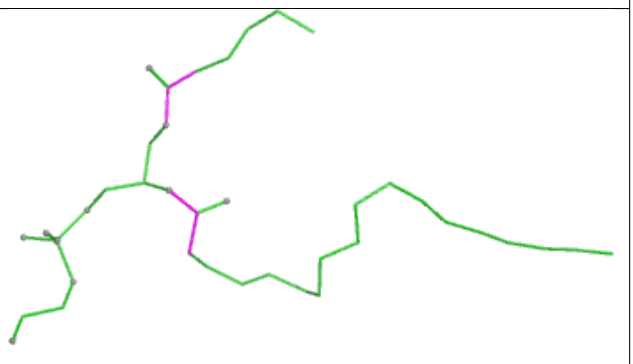


Rings

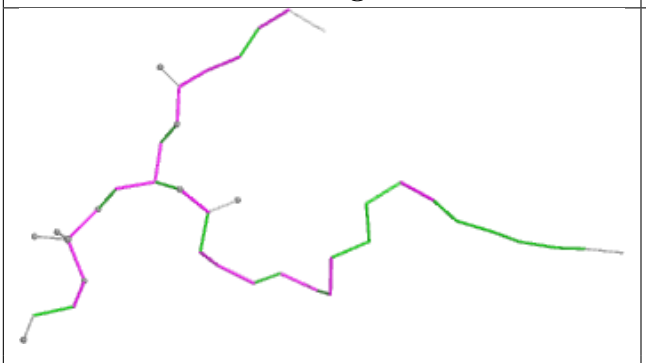
Ligand 3PE L 601



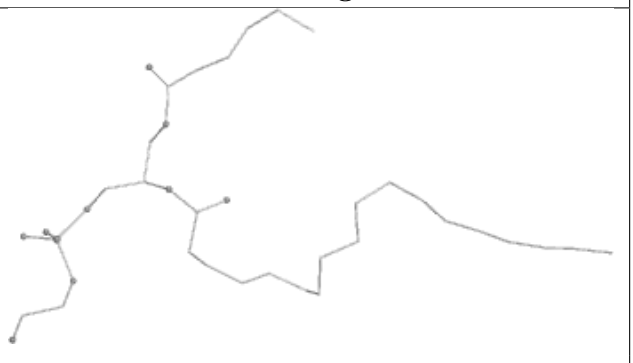
Bond lengths



Bond angles

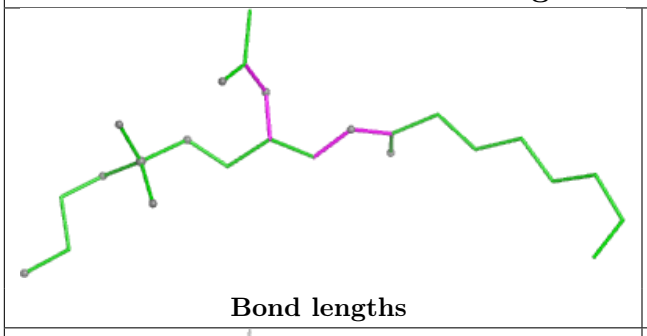


Torsions

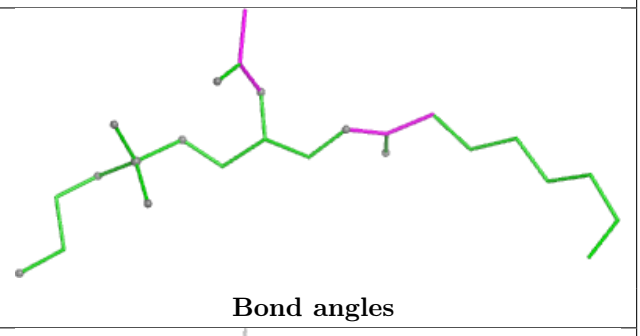


Rings

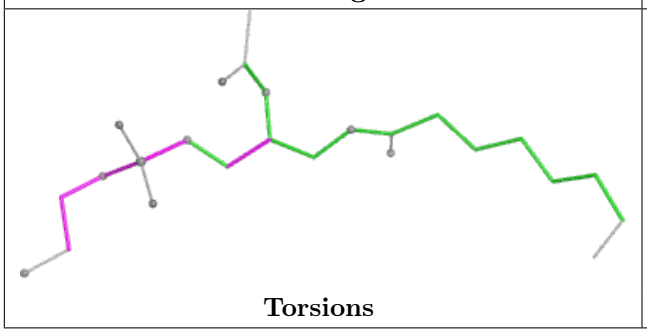
Ligand 3PE L 603



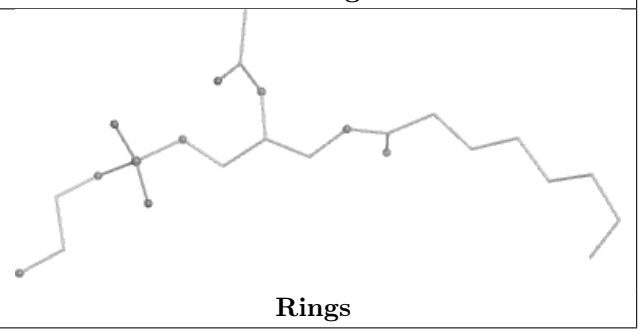
Bond lengths



Bond angles

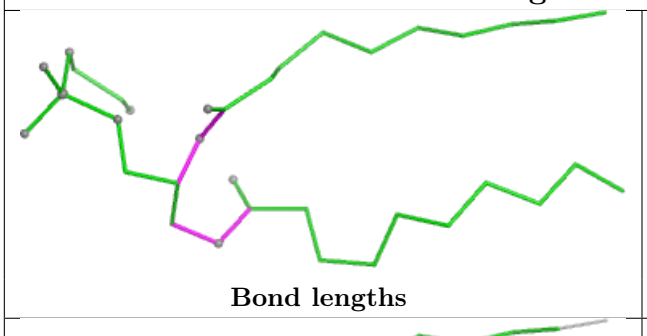


Torsions

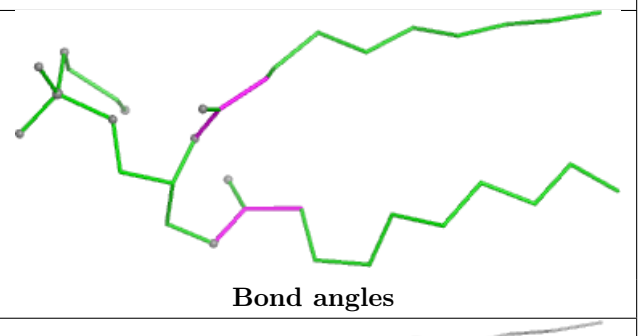


Rings

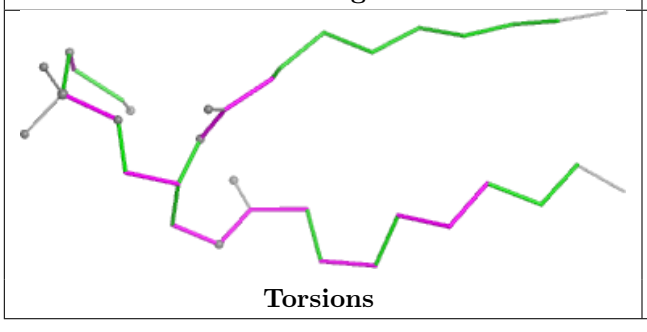
Ligand 3PE A 202



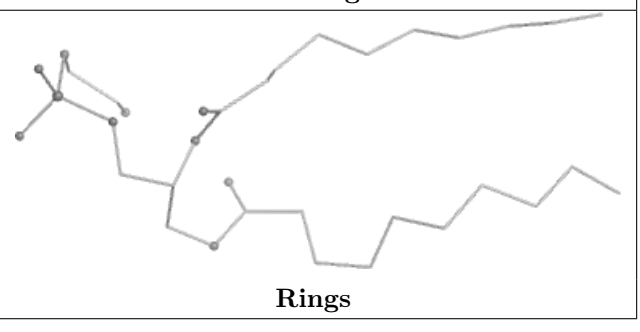
Bond lengths



Bond angles

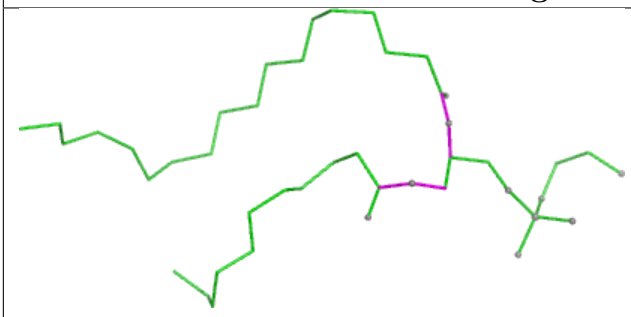


Torsions

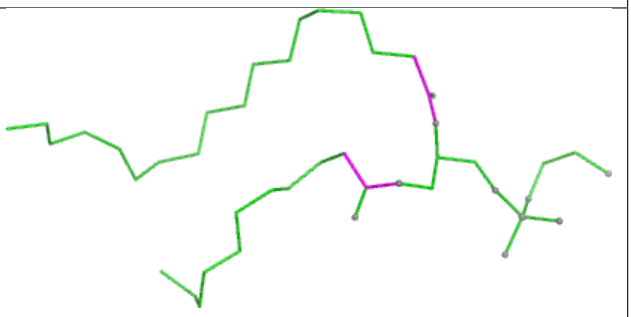


Rings

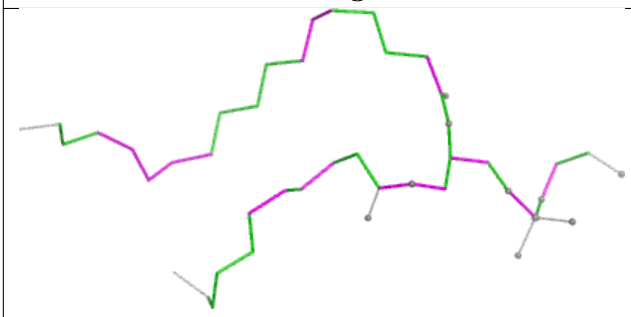
Ligand 3PE L 602



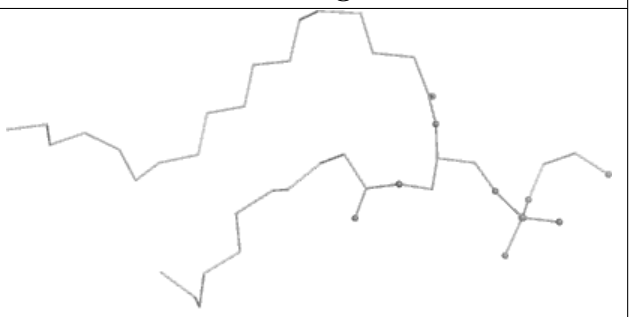
Bond lengths



Bond angles

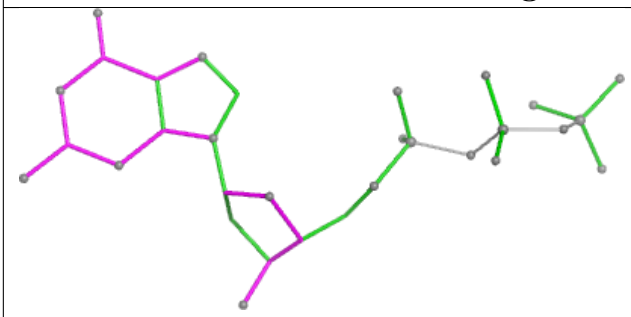


Torsions

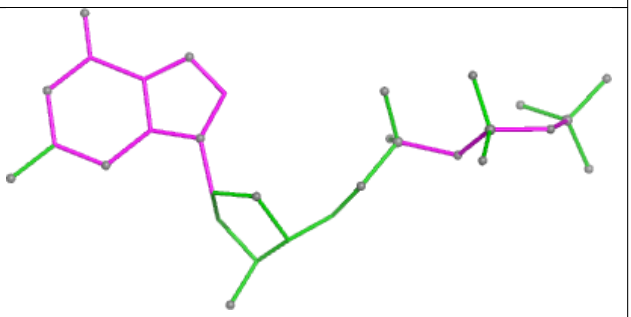


Rings

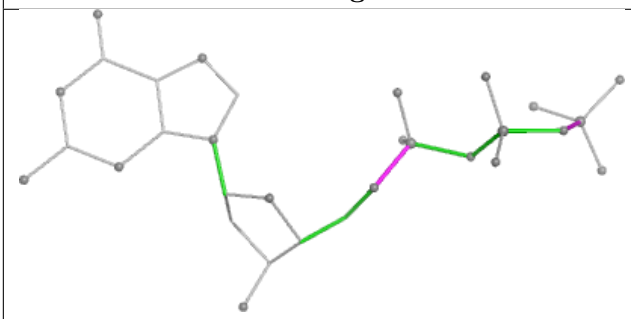
Ligand DGT O 501



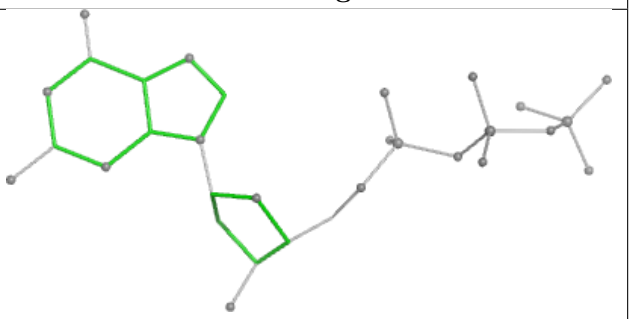
Bond lengths



Bond angles

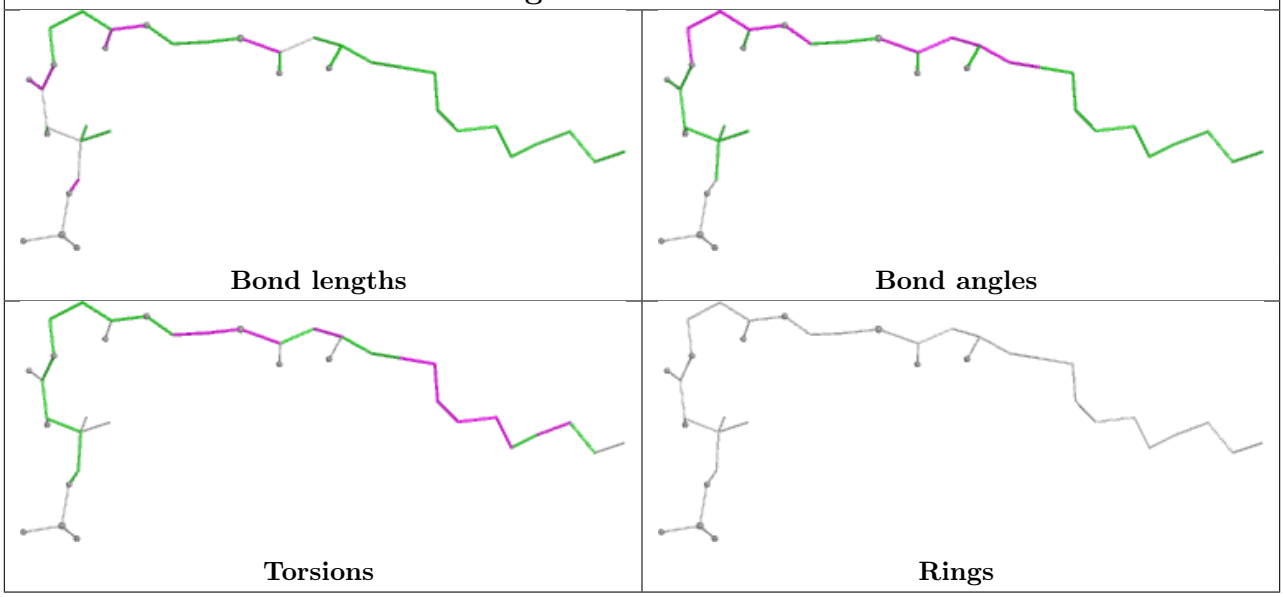


Torsions

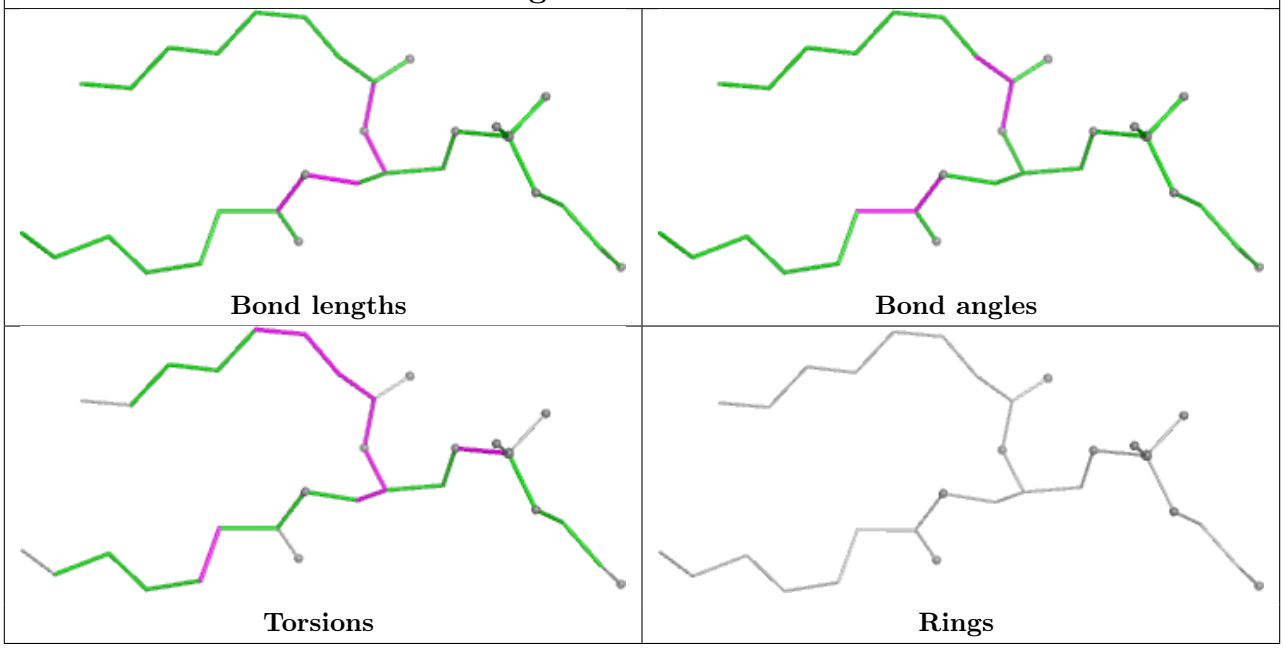


Rings

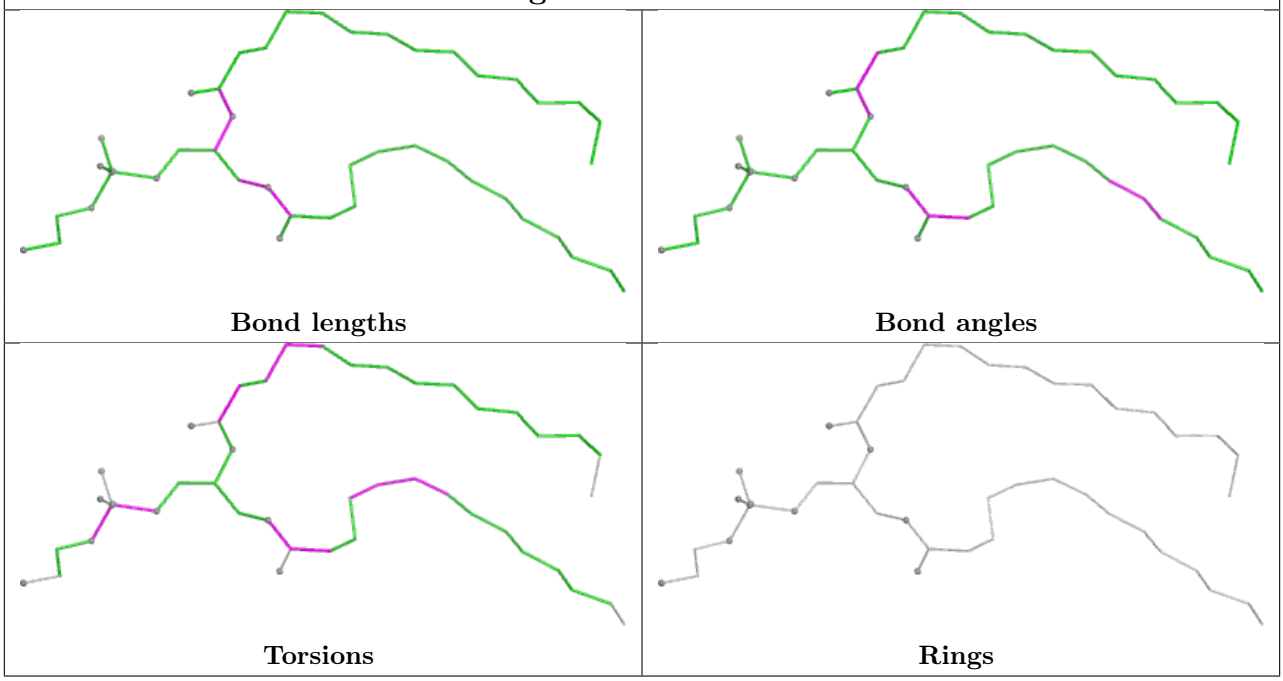
Ligand EHZ U 201



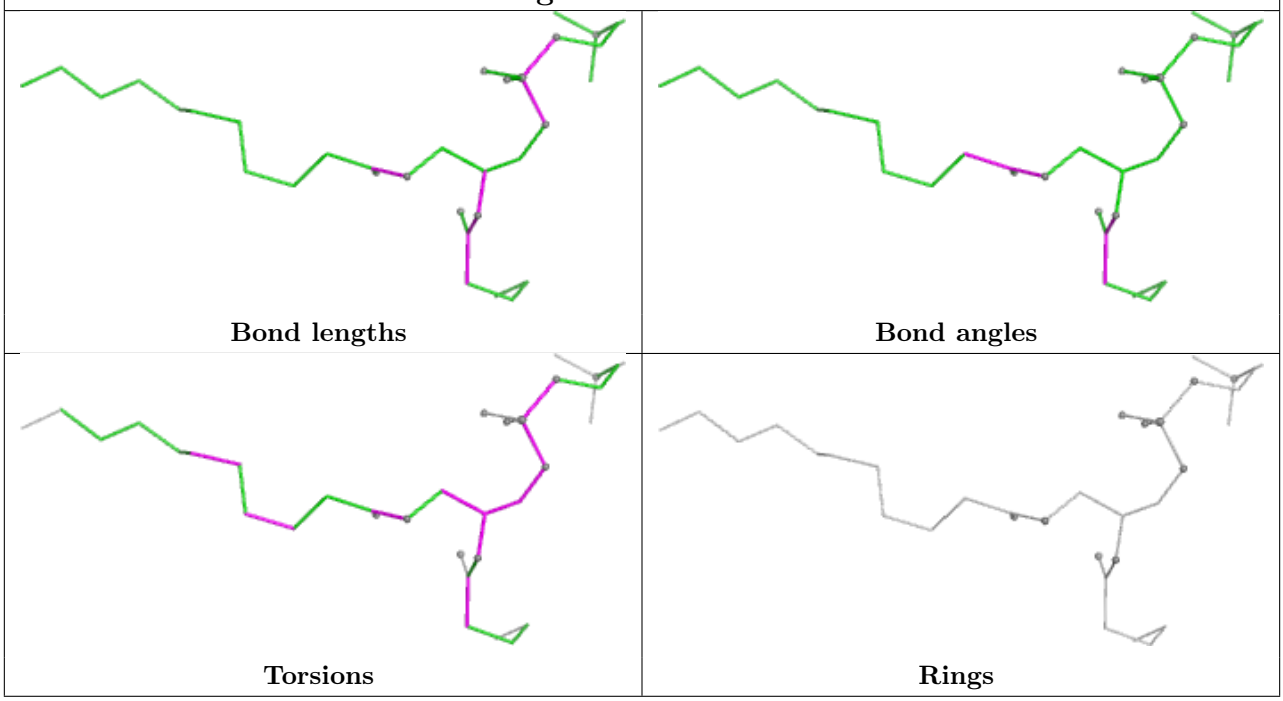
Ligand 3PE Y 302



Ligand 3PE A 203



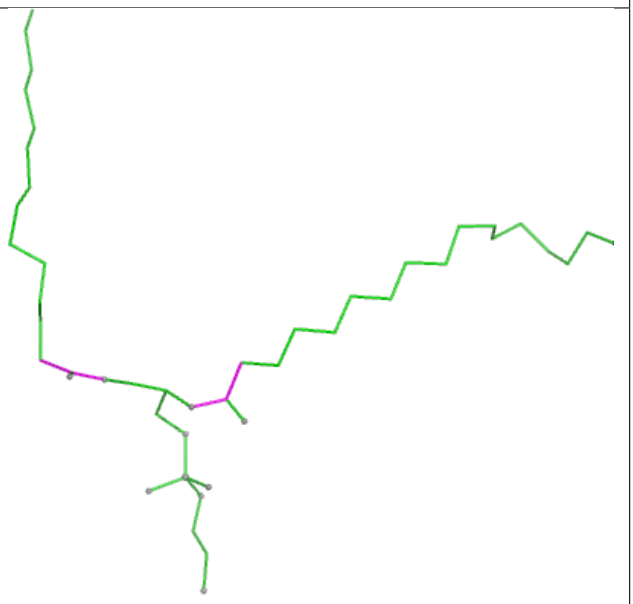
Ligand PC1 i 201



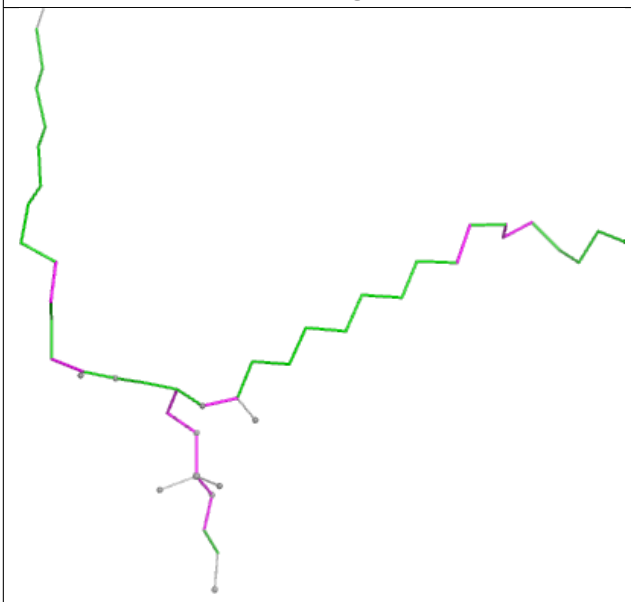
Ligand 3PE H 502



Bond lengths



Bond angles

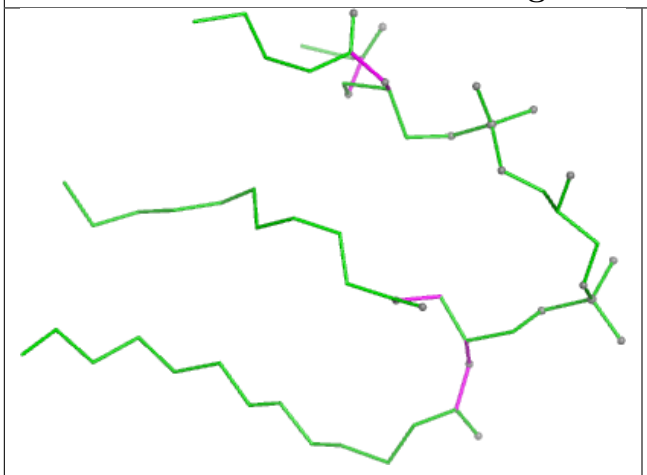


Torsions

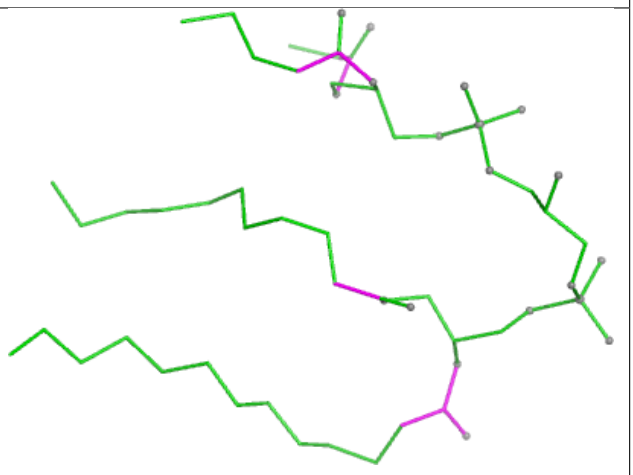


Rings

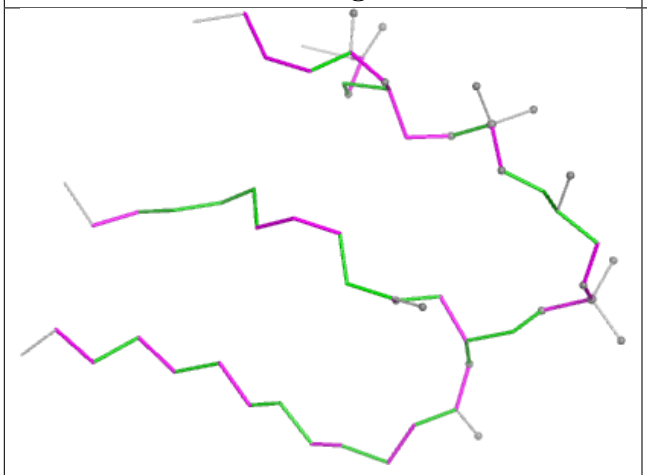
Ligand CDL h 202



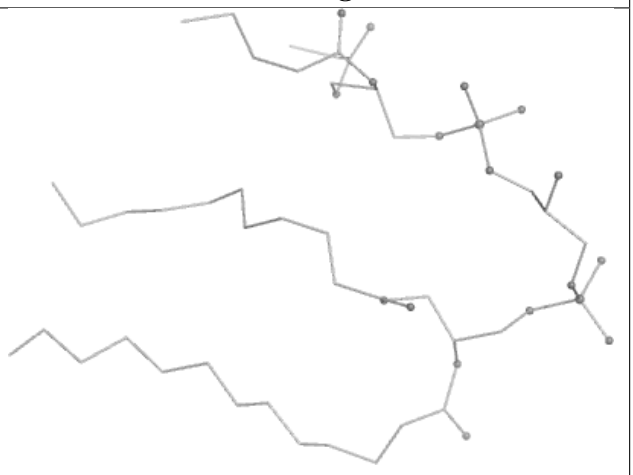
Bond lengths



Bond angles

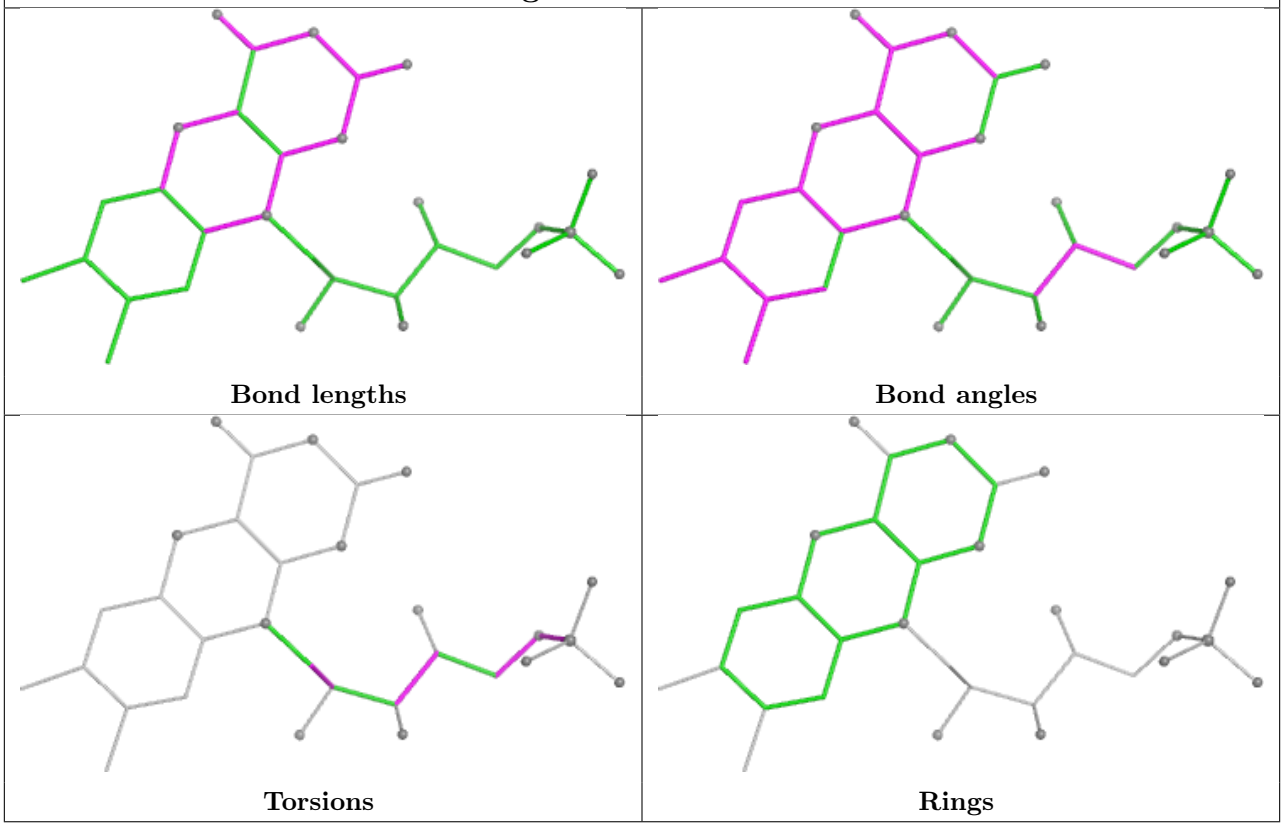


Torsions

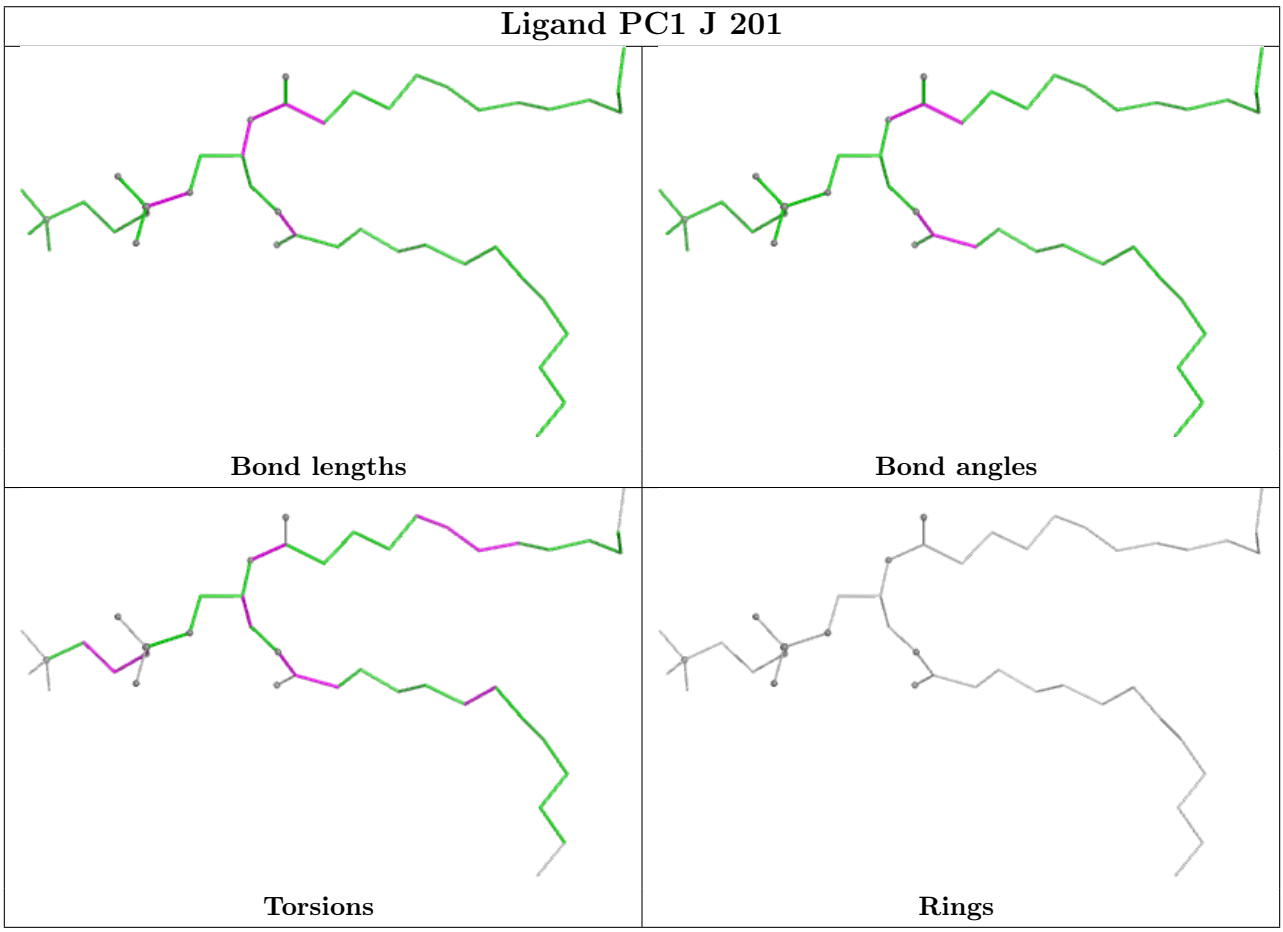


Rings

Ligand FMN F 501



Ligand PC1 J 201



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.

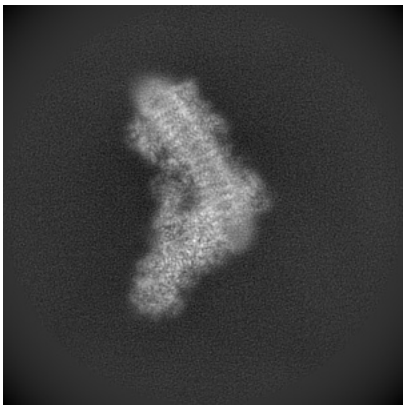
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-15936. These allow visual inspection of the internal detail of the map and identification of artifacts.

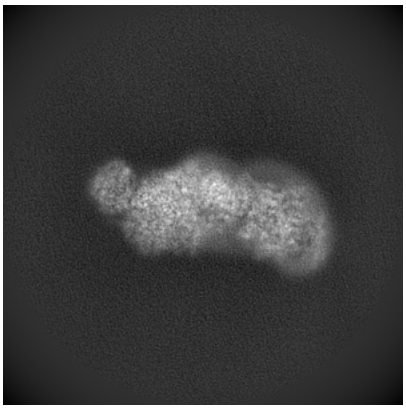
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

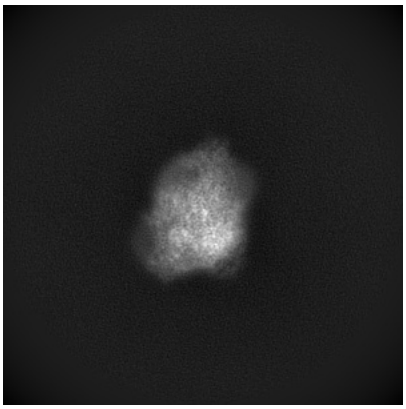
6.1.1 Primary map



X

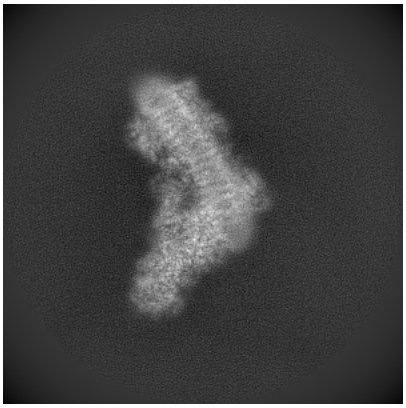


Y

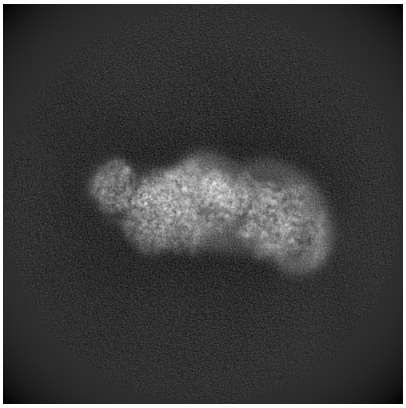


Z

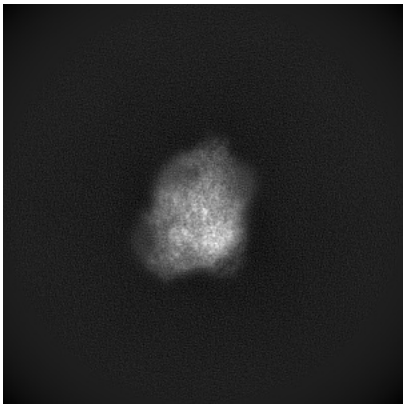
6.1.2 Raw map



X



Y

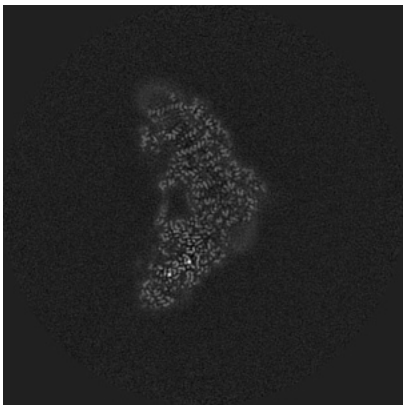


Z

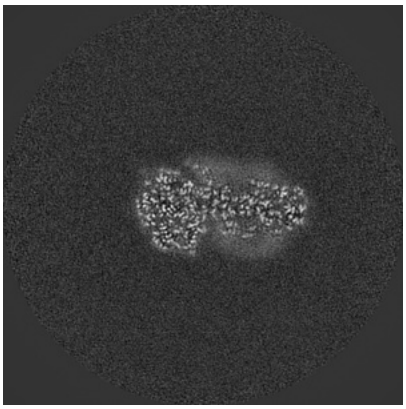
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

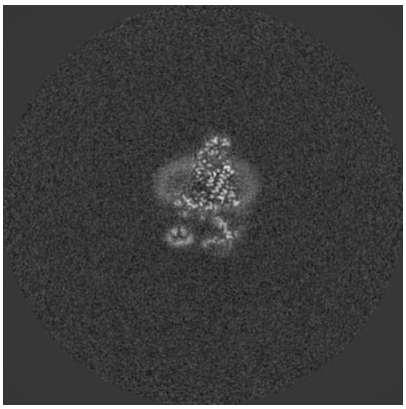
6.2.1 Primary map



X Index: 225

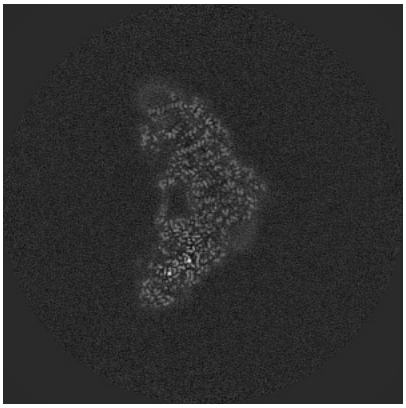


Y Index: 225

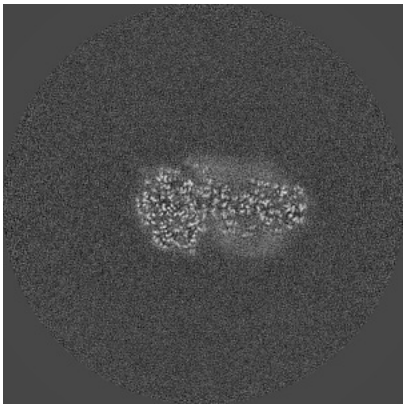


Z Index: 225

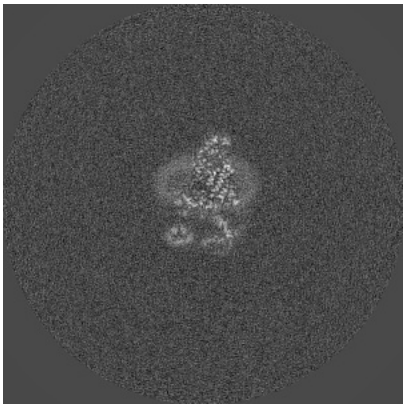
6.2.2 Raw map



X Index: 225



Y Index: 225

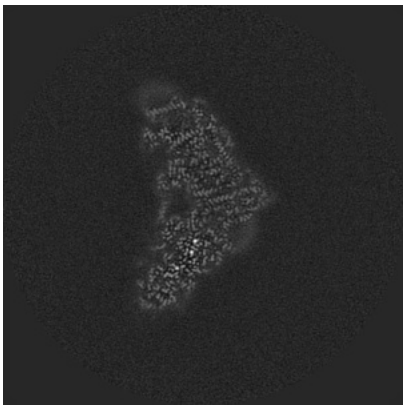


Z Index: 225

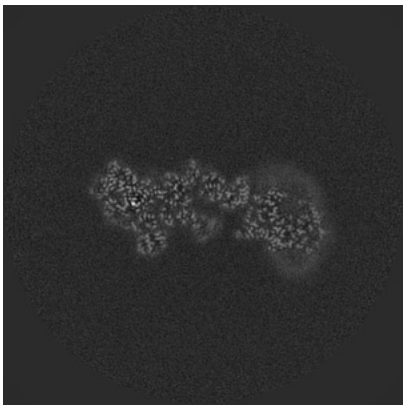
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

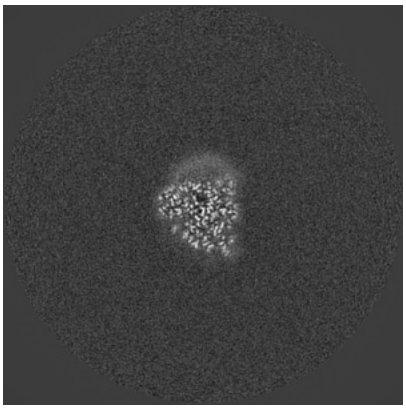
6.3.1 Primary map



X Index: 228

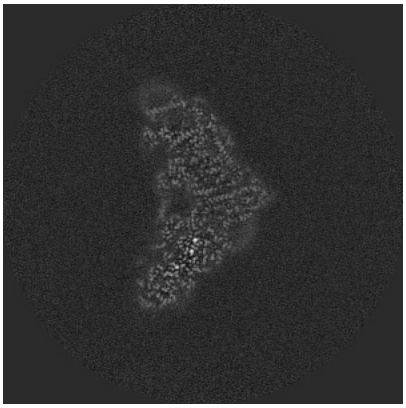


Y Index: 188

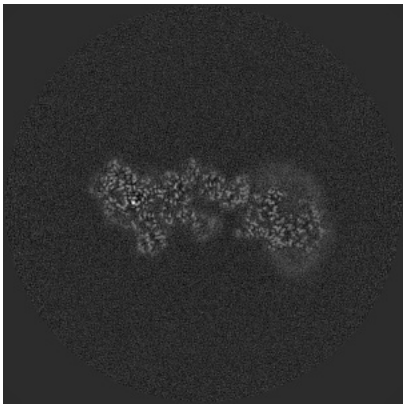


Z Index: 188

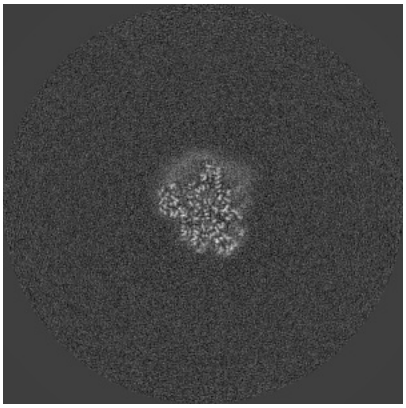
6.3.2 Raw map



X Index: 228



Y Index: 188

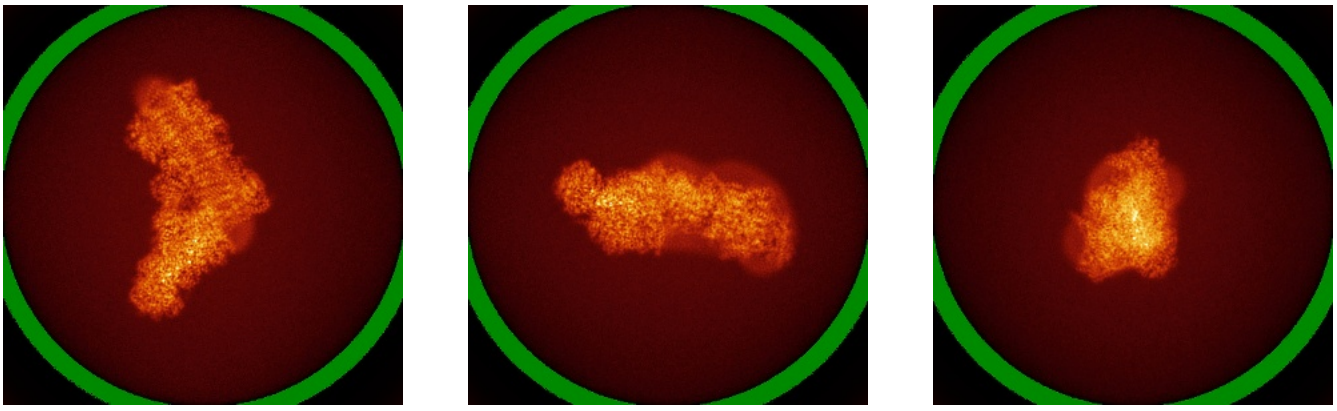


Z Index: 206

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

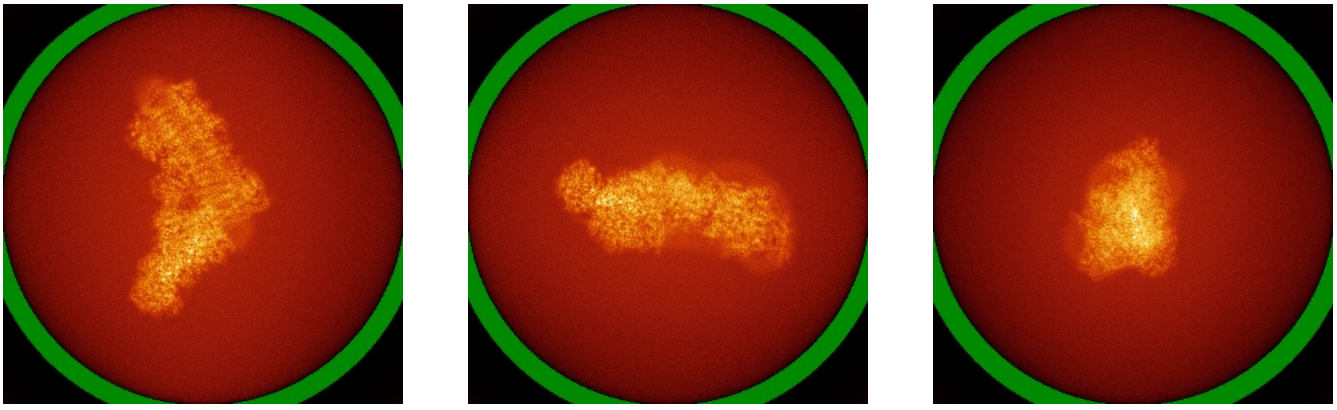
6.4 Orthogonal standard-deviation projections (False-color) (i)

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)

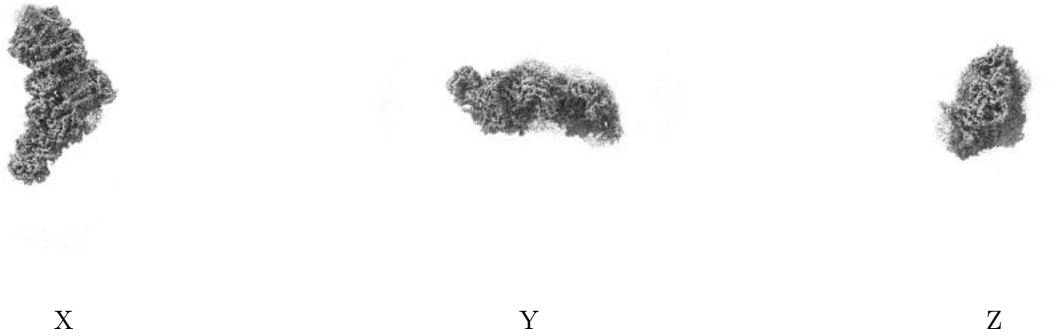
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.013. 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.

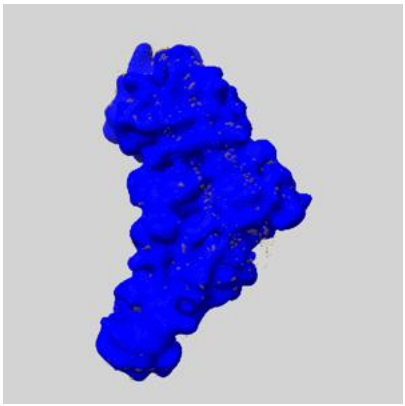
6.6 Mask visualisation

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

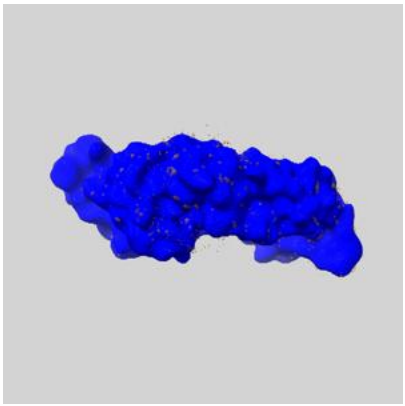
A mask typically either:

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

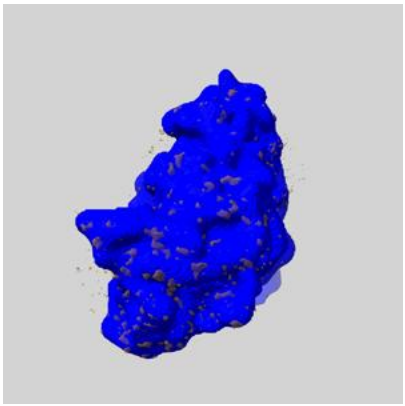
6.6.1 emd_15936_msk_1.map



X



Y

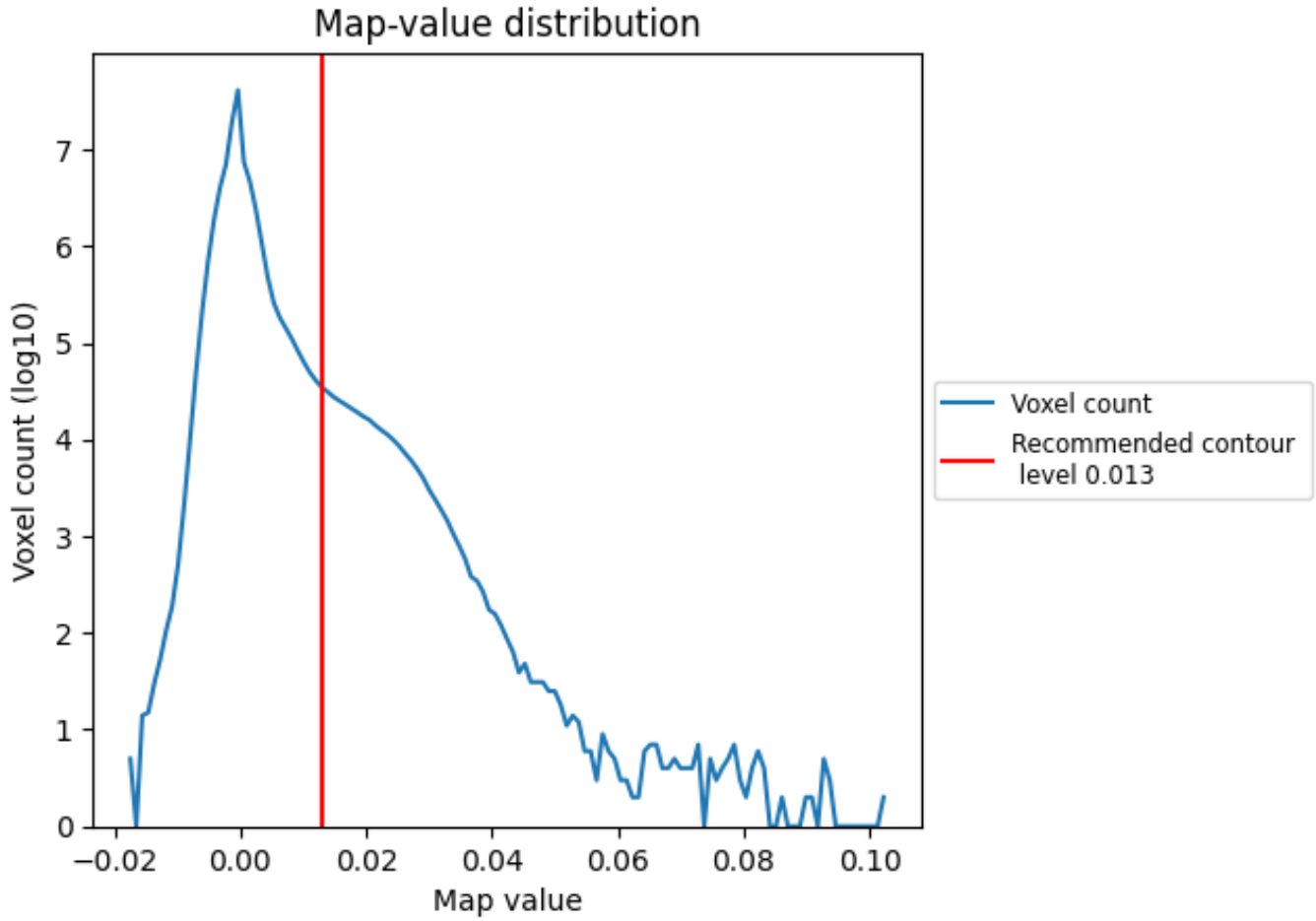


Z

7 Map analysis

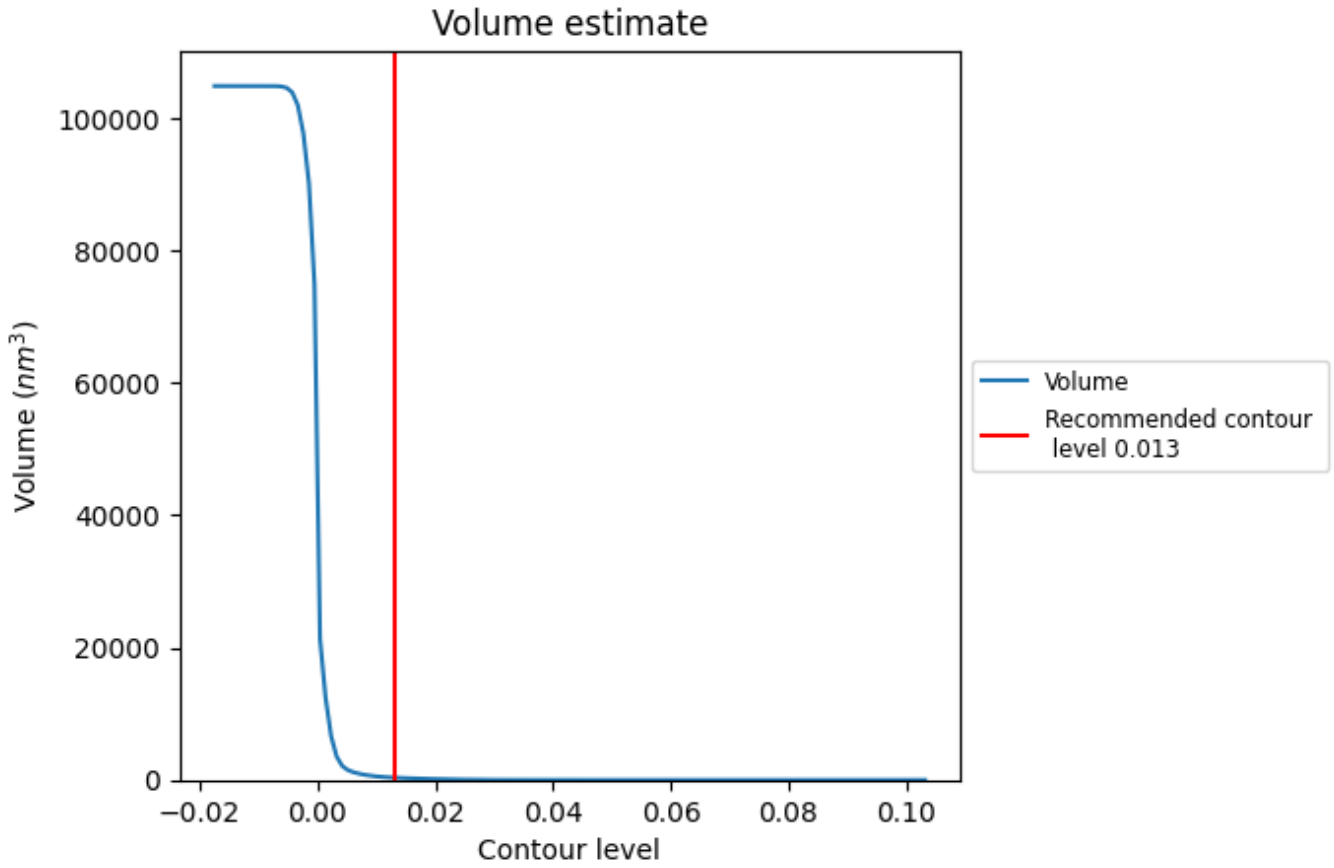
This section contains the results of statistical analysis of the map.

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.

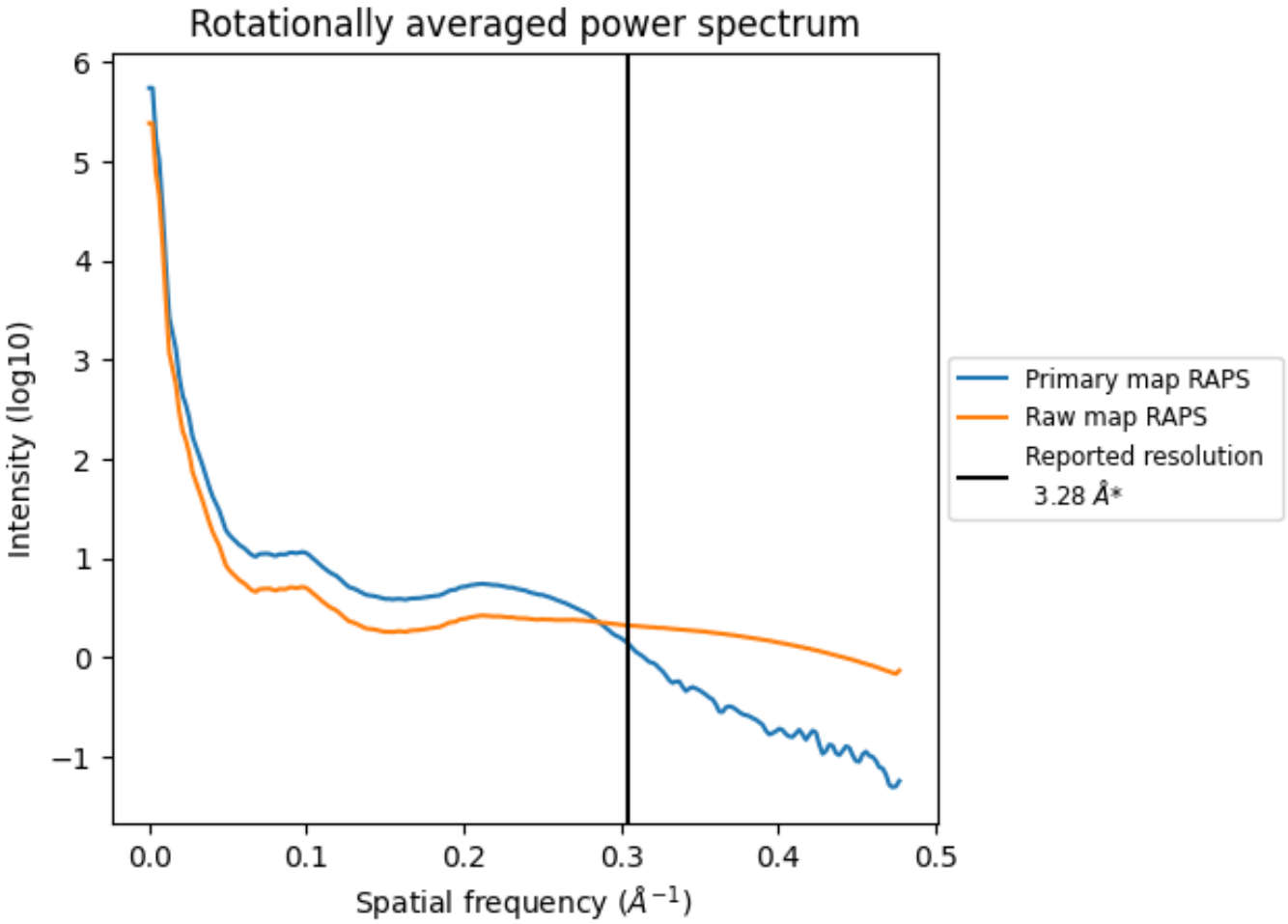
7.2 Volume estimate



The volume at the recommended contour level is 349 nm^3; this corresponds to an approximate mass of 315 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)

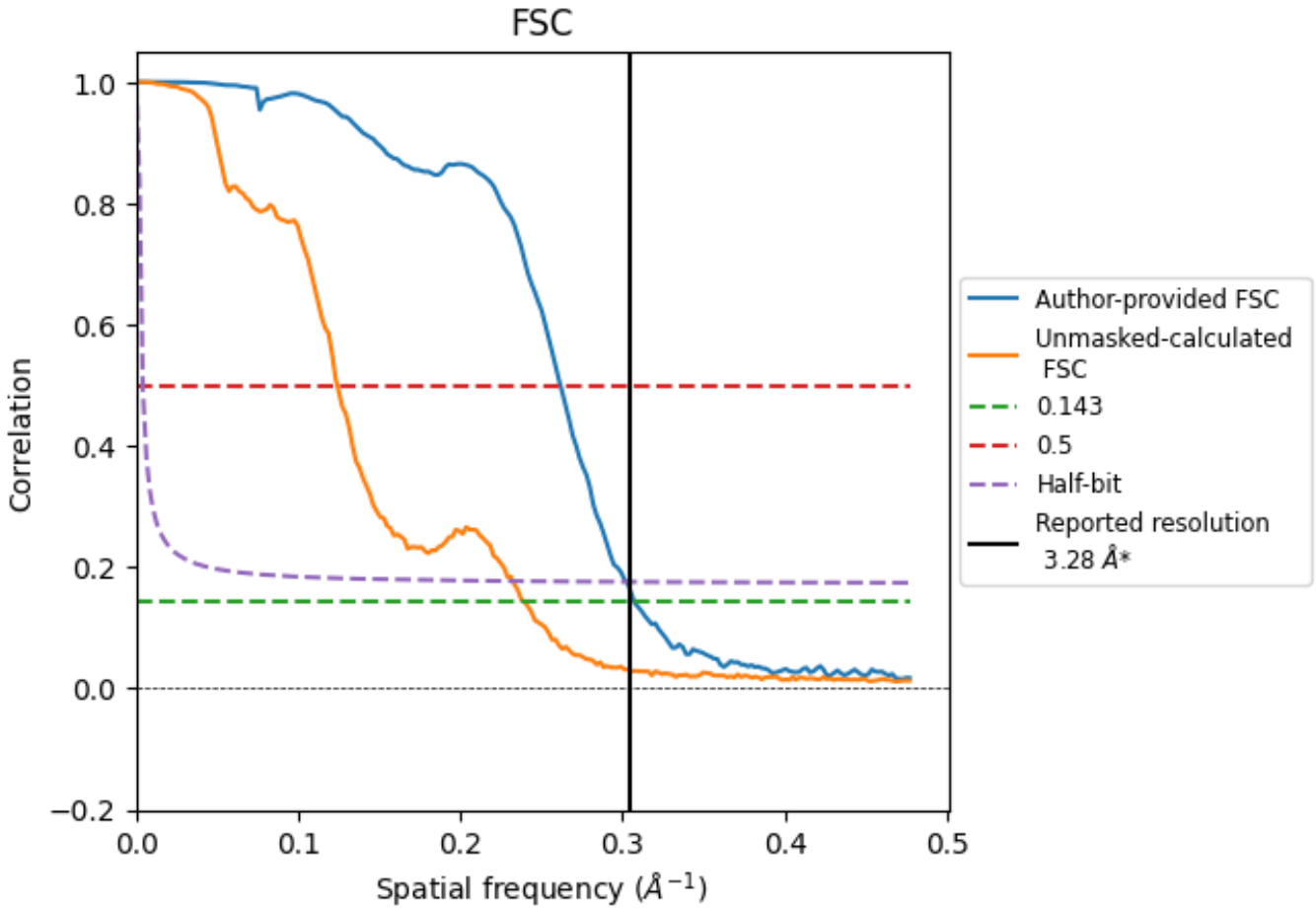


*Reported resolution corresponds to spatial frequency of 0.305 Å^{-1}

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 0.305 Å^{-1}

8.2 Resolution estimates (i)

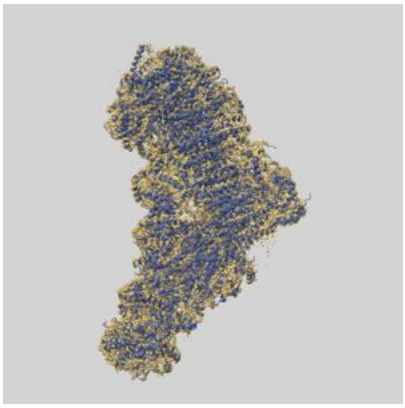
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.28	-	-
Author-provided FSC curve	3.26	3.82	3.31
Unmasked-calculated*	4.18	8.06	4.30

*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 4.18 differs from the reported value 3.28 by more than 10 %

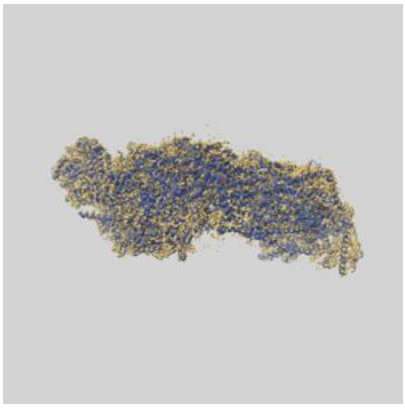
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-15936 and PDB model 8B9Z. Per-residue inclusion information can be found in section 3 on page 20.

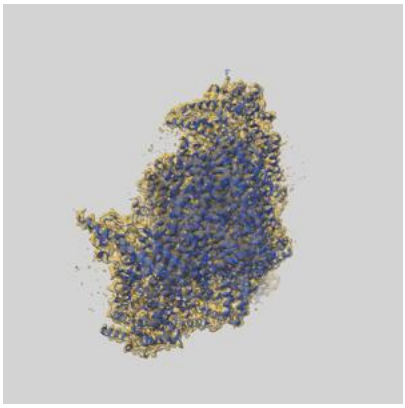
9.1 Map-model overlay



X



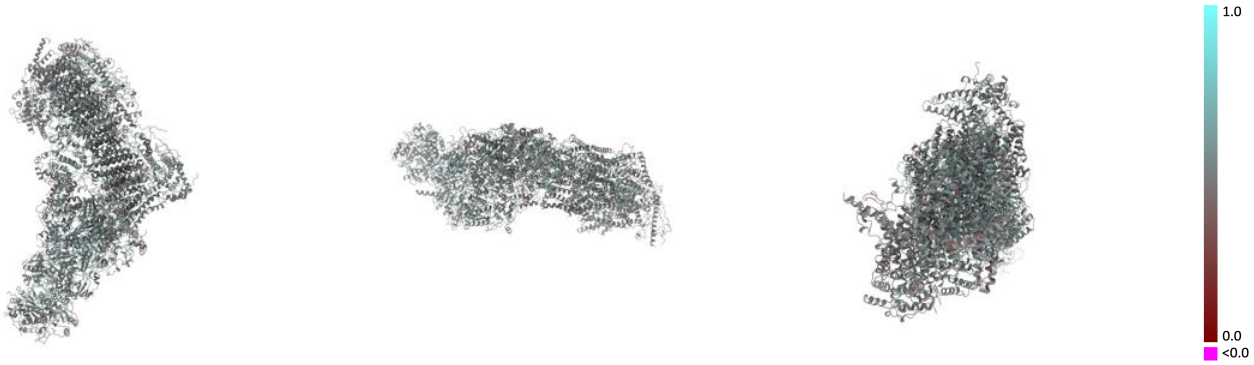
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.013 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.

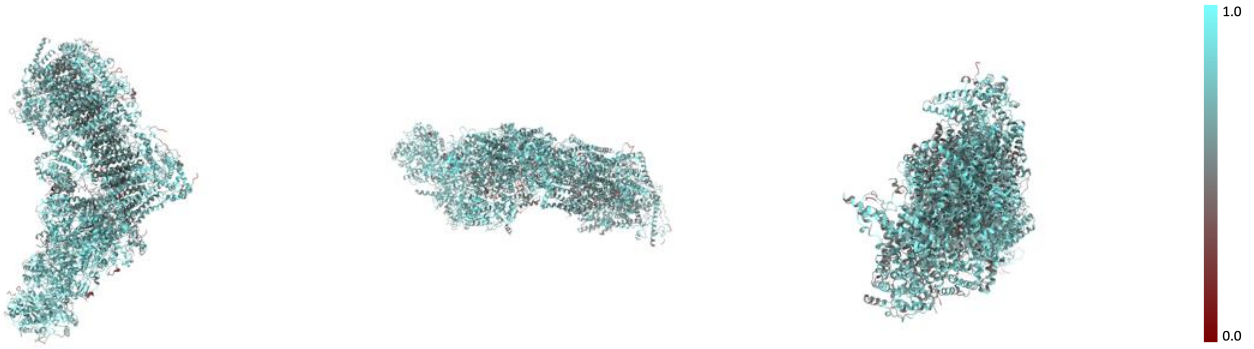
9.2 Q-score mapped to coordinate model (i)



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.

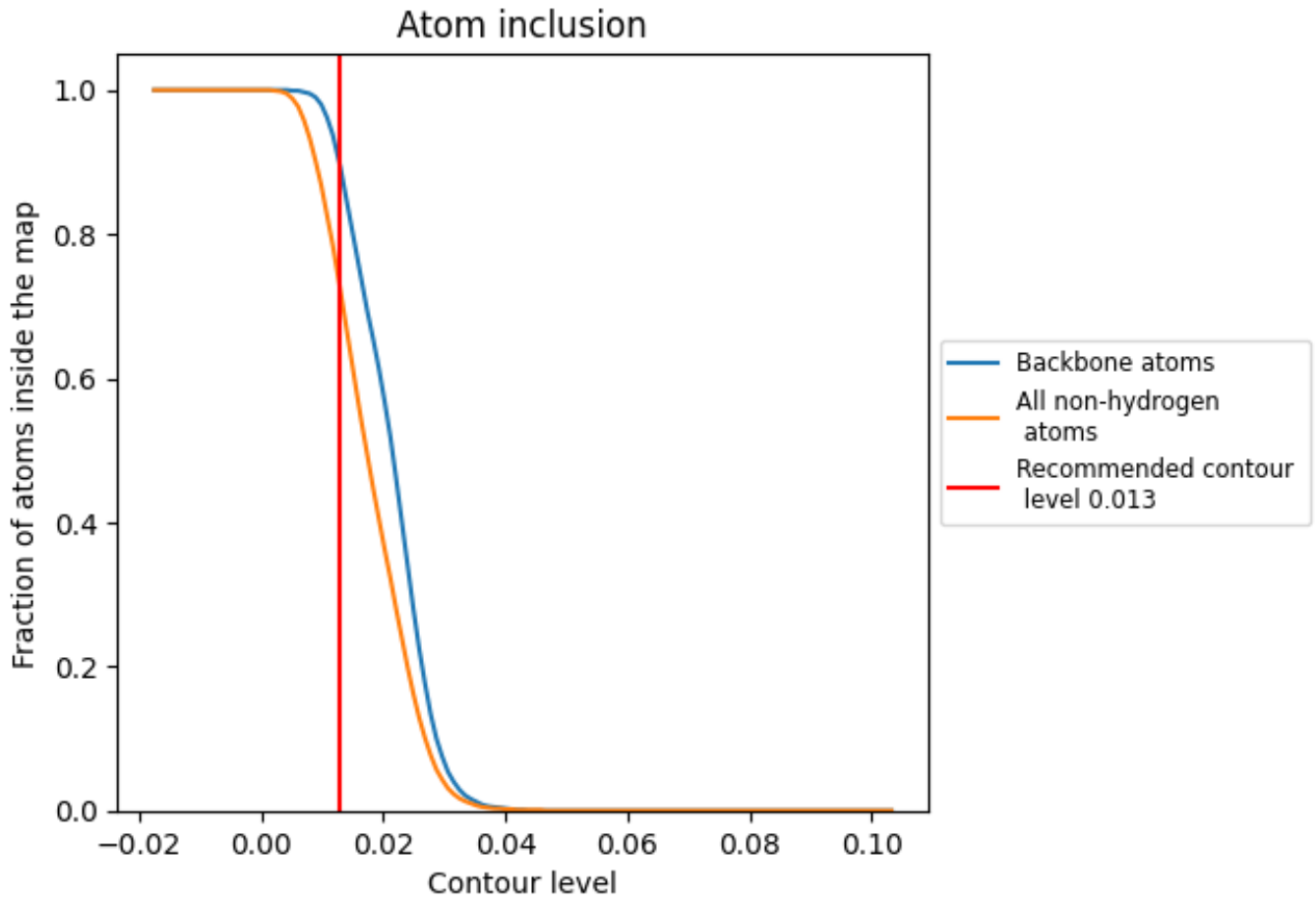
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.013).

9.4 Atom inclusion (i)



At the recommended contour level, 89% of all backbone atoms, 72% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.013) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7210	0.5150
A	0.6370	0.5070
B	0.7580	0.5360
C	0.7910	0.5430
D	0.7580	0.5340
E	0.7410	0.5090
F	0.7750	0.5210
G	0.7620	0.5290
H	0.6990	0.5190
I	0.8060	0.5410
J	0.6320	0.5060
K	0.6500	0.5100
L	0.6770	0.5060
M	0.7080	0.5290
N	0.6920	0.5220
O	0.7460	0.5180
P	0.7660	0.5250
Q	0.7360	0.5250
R	0.8060	0.5420
T	0.4810	0.4040
U	0.5990	0.4740
V	0.7170	0.5110
W	0.7360	0.5150
X	0.7160	0.5070
Y	0.6030	0.4900
Z	0.7700	0.5180
a	0.7060	0.5020
b	0.7210	0.4920
d	0.7070	0.5110
e	0.7370	0.5140
f	0.6240	0.4940
g	0.6810	0.5110
h	0.7140	0.5220
i	0.7060	0.4950
j	0.6630	0.4720



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Chain	Atom inclusion	Q-score
k	0.6540	0.4750
l	0.7290	0.5140
m	0.7390	0.5050
n	0.7270	0.5010
o	0.6990	0.4750
p	0.7620	0.5100
q	0.7580	0.5210
r	0.7170	0.5220
s	0.6090	0.4830