wwPDB EM Validation Summary Report

Sep 8, 2026 – 02:48 am BST

PDB ID	:	9R03 / pdb_00009r03
EMDB ID	:	EMD-53477
Title	:	Complex I from Ovis aries in presence of D1 inhibitor, Open state
Authors	:	Sazanov, L.; Petrova, O.
Deposited on	:	2025-04-24
Resolution	:	3.20 Å(reported)
Based on initial model	:	6ZKI

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:

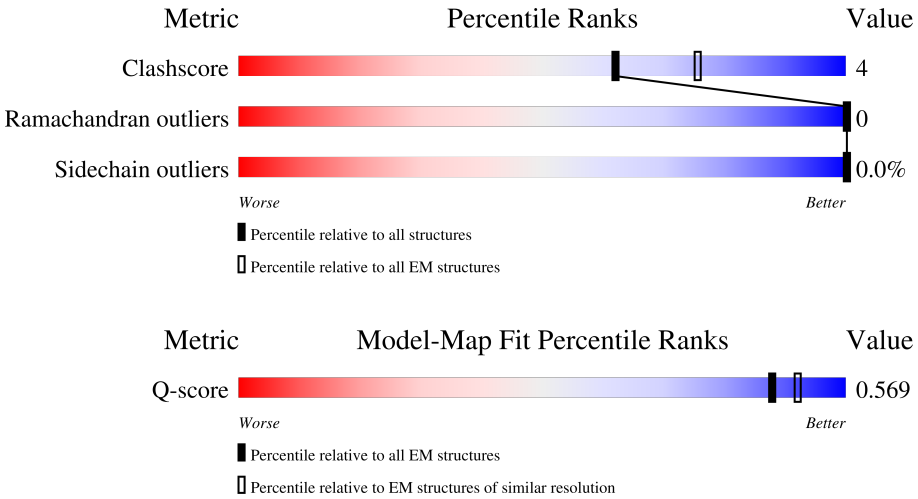
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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 3.20 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	15020 (2.70 - 3.70)

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	4	463	78% 13% 9%
2	A	115	81% 9% 10%
3	H	318	83% 14%
4	6	223	60% 10% 30%

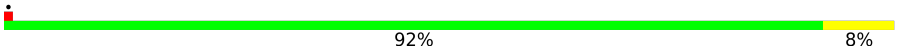
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Mol	Chain	Length	Quality of chain
5	J	175	80% 17%
6	K	98	89% 11%
7	L	606	87% 13%
8	M	459	84% 16%
9	N	347	87% 13%
10	V	141	96%
11	W	189	68% 5% 26%
12	X	87	5% 85% 15%
12	j	87	46% 70% 24% 6%
13	Y	171	86% 14%
14	Z	175	91% 7%
15	k	355	5% 79% 11% 10%
16	l	106	7% 85% 14%
17	m	84	6% 83% 12% 5%
18	n	98	5% 77% 19%
19	o	122	6% 94%
20	p	130	91% 8%
21	r	128	6% 69% 9% 23%
22	s	137	9% 77% 12% 11%
23	t	179	5% 93% 6%
24	u	108	50% 10% 40%
25	v	186	75% 9% 17%
26	w	154	6% 57% 8% 34%
27	x	76	63% 36%
28	y	58	9% 83% 14%

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Mol	Chain	Length	Quality of chain
29	z	70	
30	1	464	
31	2	246	
32	3	727	
33	5	266	
34	9	217	
35	a	109	
36	b	124	
37	c	170	
38	d	380	
39	e	99	
40	f	116	
41	g	140	
42	h	113	
43	i	145	
44	q	144	

2 Entry composition (i)

There are 58 unique types of molecules in this entry. The entry contains 66655 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	4	423	3409	2177	587	620	25	0	0

- Molecule 2 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	A	103	831	565	118	143	5	0	0

- Molecule 3 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	H	308	2453	1657	373	404	19	0	0

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	6	156	1247	795	225	213	14	0	0

- Molecule 5 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	J	169	1294	870	185	226	13	0	0

- Molecule 6 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	K	98	Total	C	N	O	S	0	0
			749	490	112	132	15		

- Molecule 7 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	L	606	Total	C	N	O	S	0	0
			4806	3187	746	829	44		

- Molecule 8 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	M	459	Total	C	N	O	S	0	0
			3647	2429	571	607	40		

- Molecule 9 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	N	347	Total	C	N	O	S	0	0
			2723	1808	416	459	40		

- Molecule 10 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	V	141	Total	C	N	O	S	0	0
			1028	656	175	191	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	0	ACE	-	acetylation	UNP A0A8V6VBD6

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	W	139	Total	C	N	O	S	0	0
			1155	761	194	198	2		

- Molecule 12 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	X	87	Total	C	N	O	S	0	0
			701	451	103	142	5		
12	j	82	Total	C	N	O	S	0	0
			660	425	98	132	5		

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Y	171	Total	C	N	O	S	0	0
			1403	889	253	251	10		

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Z	171	Total	C	N	O	S	0	0
			1441	905	266	262	8		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
15	k	320	Total	C	N	O	P	S	0	0
			2596	1659	432	494	1	10		

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	l	105	Total	C	N	O	S	0	0
			874	551	164	153	6		

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	m	80	Total	C	N	O	S	0	0
			626	411	103	110	2		

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	n	79	Total	C	N	O	S	0	0
			634	415	106	111	2		

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	o	120	Total	C	N	O	S	0	0
			1004	652	175	172	5		

- Molecule 20 is a protein called NADH:ubiquinone oxidoreductase subunit B4.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	p	128	Total	C	N	O	S	0	0
			1059	675	189	194	1		

- Molecule 21 is a protein called Mitochondrial complex I, B17 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	r	99	Total	C	N	O	S	0	0
			846	554	149	142	1		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	s	122	Total	C	N	O	S	0	0
			1047	653	199	186	9		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	t	177	Total	C	N	O	S	0	0
			1520	973	279	262	6		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	u	65	Total	C	N	O	S	0	0
			563	372	93	97	1		

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

8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	v	155	Total	C	N	O	S	0	0
			1307	846	213	239	9		

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	w	101	Total	C	N	O	S	0	0
			846	542	140	160	4		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	x	49	Total	C	N	O	0	0
			412	271	70	71		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
28	y	50	Total	C	N	O	0	0
			436	287	77	72		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
29	z	70	Total	C	N	O	S	0	0
			576	369	106	96	5		

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	1	430	Total	C	N	O	S	0	0
			3312	2086	593	613	20		

- Molecule 31 is a protein called Mitochondrial complex I, 24 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	2	213	Total	C	N	O	S	0	0
			1655	1058	278	309	10		

- Molecule 32 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	3	688	Total	C	N	O	S	0	0
			5275	3301	922	1011	41		

- Molecule 33 is a protein called NADH:ubiquinone oxidoreductase core subunit S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	5	208	Total	C	N	O	S	0	0
			1726	1112	296	315	3		

- Molecule 34 is a protein called Complex I-23kD.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	9	176	Total	C	N	O	S	0	0
			1414	889	243	270	12		

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	a	44	Total	C	N	O	S	0	0
			371	233	66	71	1		

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	b	95	Total	C	N	O	S	0	0
			737	451	139	144	3		

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	c	126	Total	C	N	O	S	0	0
			1024	646	182	193	3		

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	d	293	Total	C	N	O	S	0	0
			2345	1499	427	414	5		

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	e	86	Total	C	N	O	S	0	0
			691	434	129	126	2		

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	f	113	Total	C	N	O	S	0	0
			917	595	153	167	2		

- Molecule 41 is a protein called NADH:ubiquinone oxidoreductase subunit A6.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	g	114	Total	C	N	O	S	0	0
			969	619	180	166	4		

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	h	96	Total	C	N	O	S	0	0
			763	477	145	138	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
h	0	ACE	-	acetylation	UNP A0A6P3E9B7

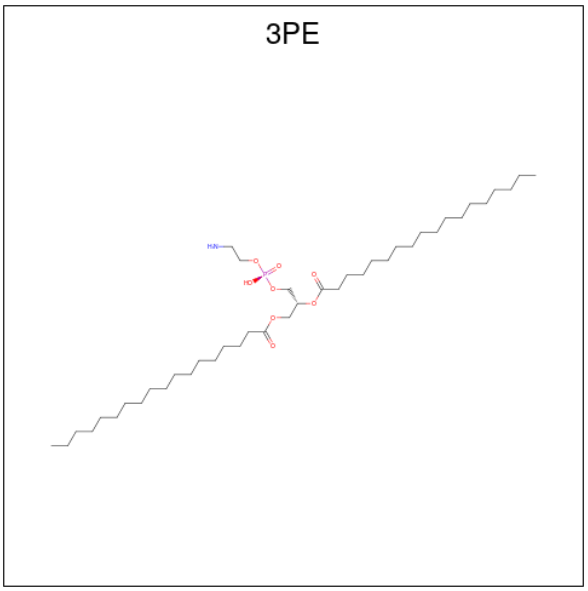
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	i	145	Total	C	N	O	S	0	0
			1209	778	216	210	5		

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	q	139	Total	C	N	O	S	0	0
			1142	733	200	200	9		

- Molecule 45 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



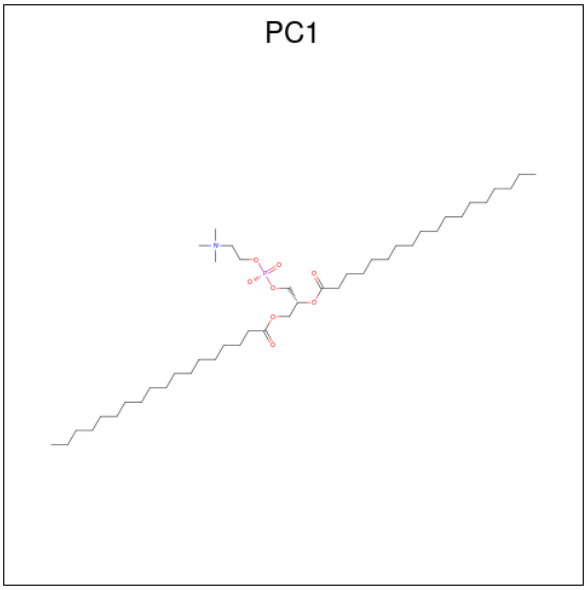
Mol	Chain	Residues	Atoms					AltConf
45	4	1	Total	C	N	O	P	0
			40	30	1	8	1	
45	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
45	H	1	Total	C	N	O	P	0
			51	41	1	8	1	
45	6	1	Total	C	N	O	P	0
			51	41	1	8	1	
45	K	1	Total	C	N	O	P	0
			40	30	1	8	1	
45	L	1	Total	C	N	O	P	0
			51	41	1	8	1	
45	L	1	Total	C	N	O	P	0
			31	21	1	8	1	

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Mol	Chain	Residues	Atoms	AltConf
45	M	1	Total C N O P 44 34 1 8 1	0
45	N	1	Total C N O P 51 41 1 8 1	0
45	V	1	Total C N O P 35 25 1 8 1	0
45	V	1	Total C N O P 37 27 1 8 1	0
45	o	1	Total C N O P 31 21 1 8 1	0
45	p	1	Total C O P 27 18 8 1	0
45	i	1	Total C N O P 51 41 1 8 1	0

- Molecule 46 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



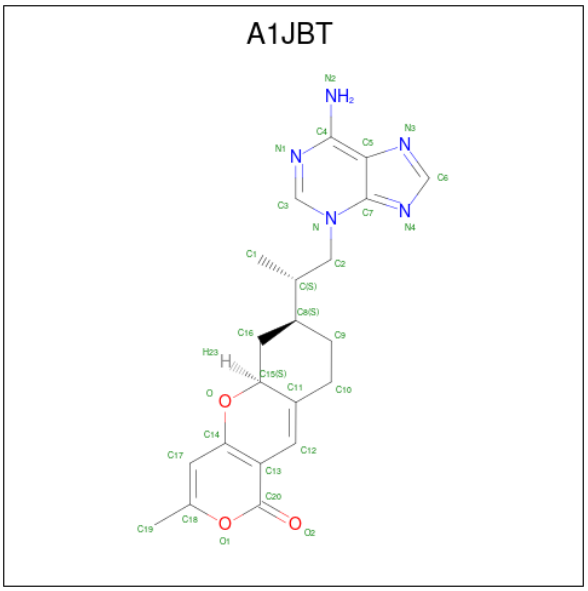
Mol	Chain	Residues	Atoms	AltConf
46	4	1	Total C N O P 54 44 1 8 1	0
46	A	1	Total C N O P 37 27 1 8 1	0
46	6	1	Total C N O P 46 36 1 8 1	0
46	L	1	Total C N O P 54 44 1 8 1	0

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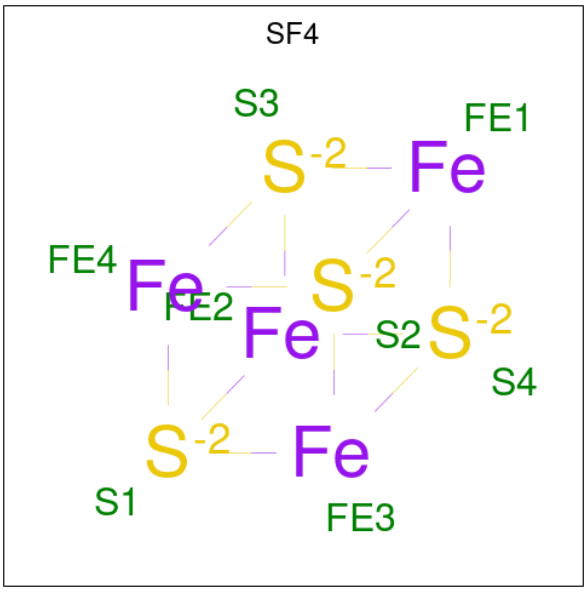
Mol	Chain	Residues	Atoms					AltConf
46	M	1	Total	C	N	O	P	0
			54	44	1	8	1	
46	M	1	Total	C	N	O	P	0
			54	44	1	8	1	

- Molecule 47 is (7 {S})-7-[(2 {S})-1-(6-azanylpurin-3-yl)propan-2-yl]-3-methyl-6,7,8,9-tetrahydro-5 {a} {H}-pyrano[4,3-b]chromen-1-one (CCD ID: A1JBT) (formula: $C_{21}H_{23}N_5O_3$) (labeled as "Ligand of Interest" by depositor).



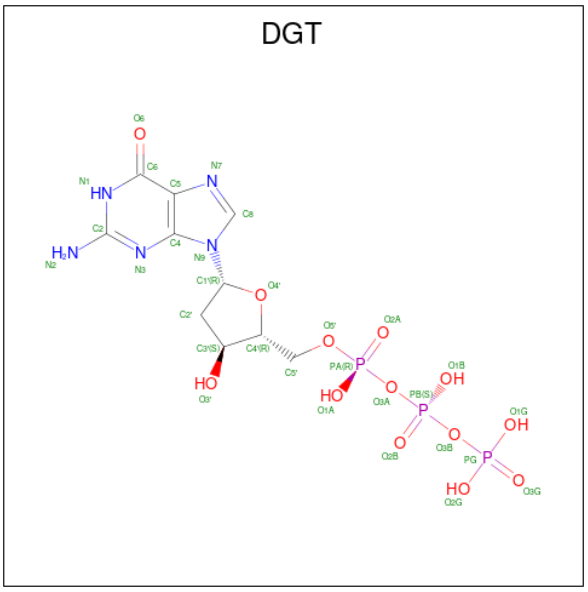
Mol	Chain	Residues	Atoms				AltConf
47	H	1	Total	C	N	O	0
			29	21	5	3	

- Molecule 48 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	AltConf
48	6	1	Total Fe S 8 4 4	0
48	1	1	Total Fe S 8 4 4	0
48	3	1	Total Fe S 8 4 4	0
48	3	1	Total Fe S 8 4 4	0
48	9	1	Total Fe S 8 4 4	0
48	9	1	Total Fe S 8 4 4	0

- Molecule 49 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (CCD ID: DGT) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

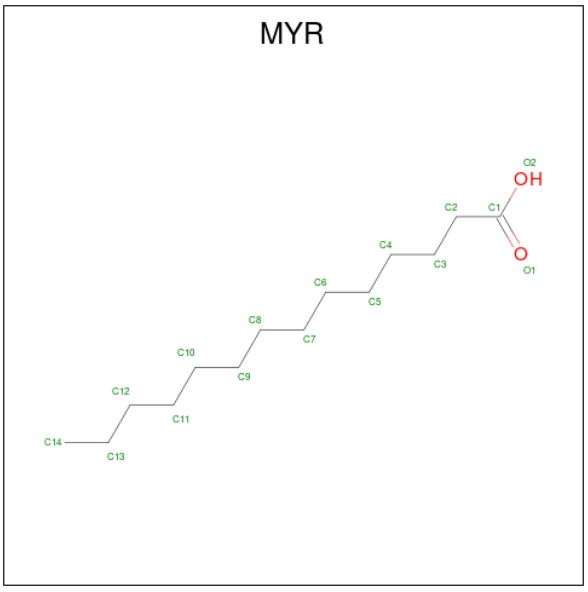


Mol	Chain	Residues	Atoms					AltConf
49	k	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 50 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

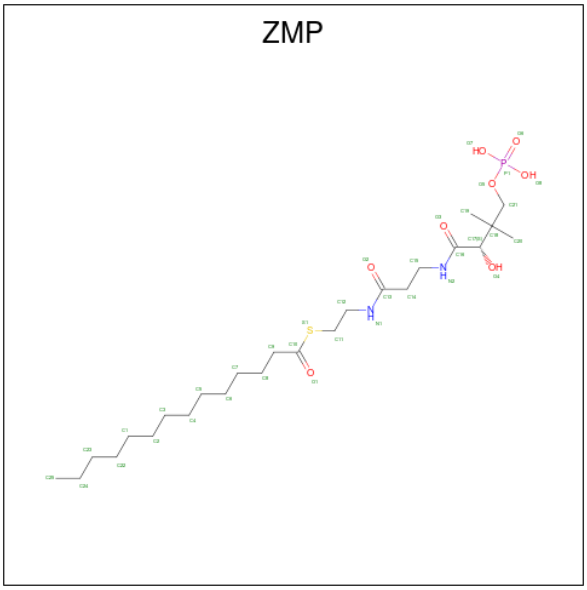
Mol	Chain	Residues	Atoms		AltConf
50	k	1	Total	Mg	0
			1	1	

- Molecule 51 is MYRISTIC ACID (CCD ID: MYR) (formula: $C_{14}H_{28}O_2$).



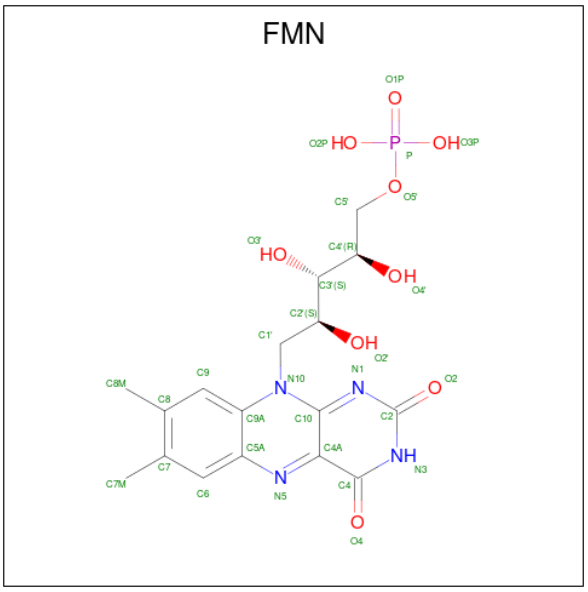
Mol	Chain	Residues	Atoms			AltConf
51	s	1	Total	C	O	0
			15	14	1	

- Molecule 52 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (CCD ID: ZMP) (formula: $C_{25}H_{49}N_2O_8PS$).



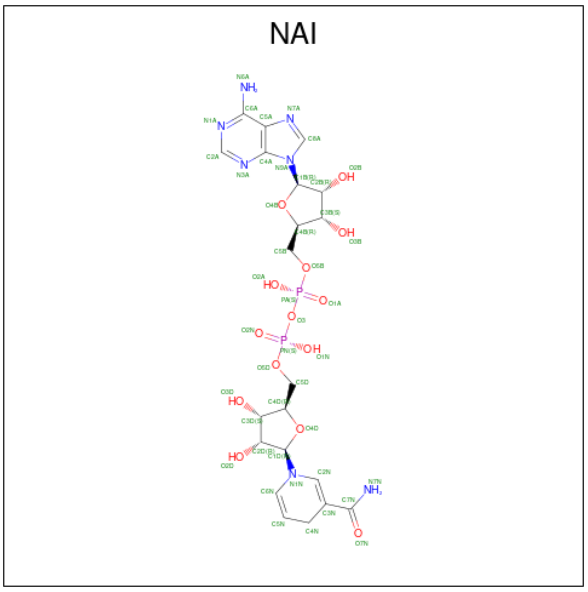
Mol	Chain	Residues	Atoms					AltConf
52	t	1	Total	C	N	O	P	S	0
			31	20	2	7	1	1	
52	j	1	Total	C	N	O	P	S	0
			34	23	2	7	1	1	

- Molecule 53 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



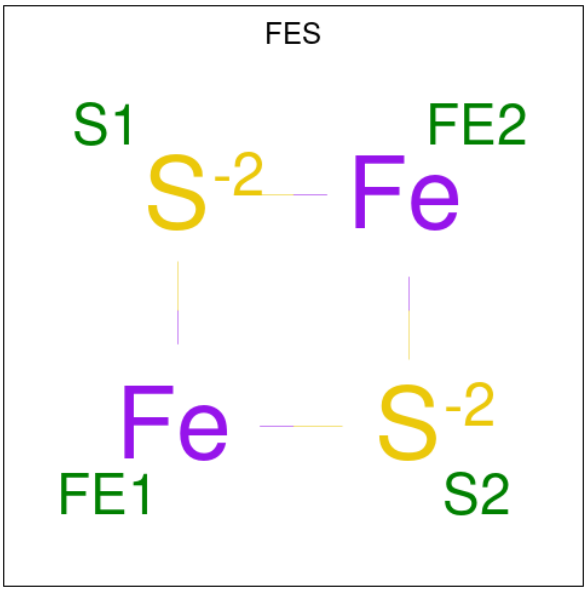
Mol	Chain	Residues	Atoms					AltConf
53	1	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 54 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms					AltConf
54	1	1	Total	C	N	O	P	0
			44	21	7	14	2	

- Molecule 55 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms	AltConf
55	2	1	Total Fe S 4 2 2	0
55	3	1	Total Fe S 4 2 2	0

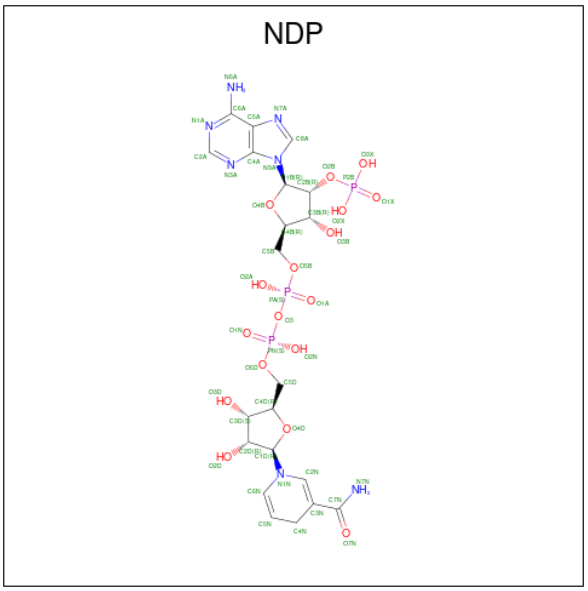
- Molecule 56 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	AltConf
56	3	1	Total K 1 1	0

- Molecule 57 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
57	b	1	Total Zn 1 1	0

- Molecule 58 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
58	d	1	Total	C	N	O	P	0
			48	21	7	17	3	

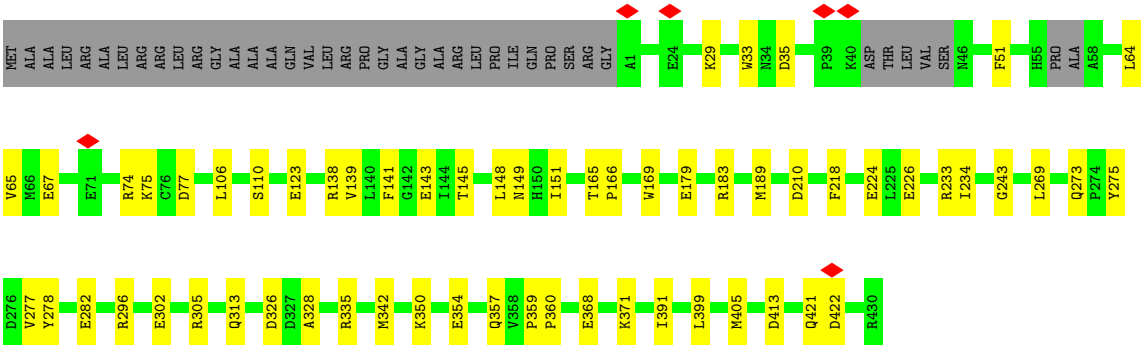
3 Residue-property plots (i)

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

• Molecule 1: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

Chain 4:

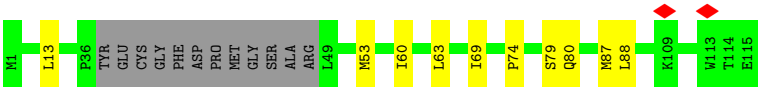




• Molecule 2: NADH-ubiquinone oxidoreductase chain 3

Chain A:

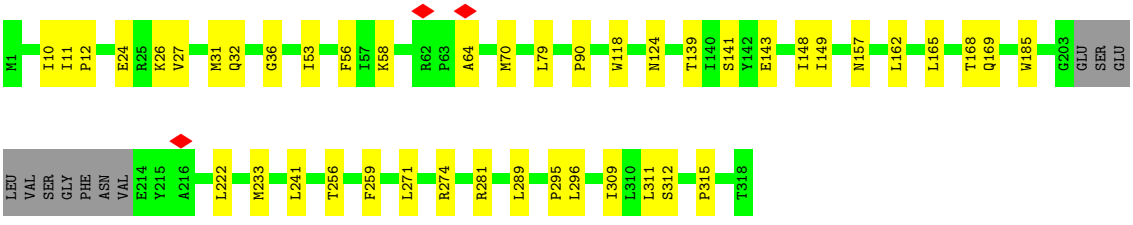




• Molecule 3: NADH-ubiquinone oxidoreductase chain 1

Chain H:

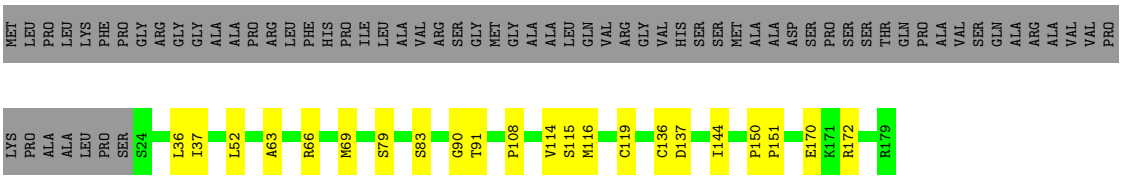




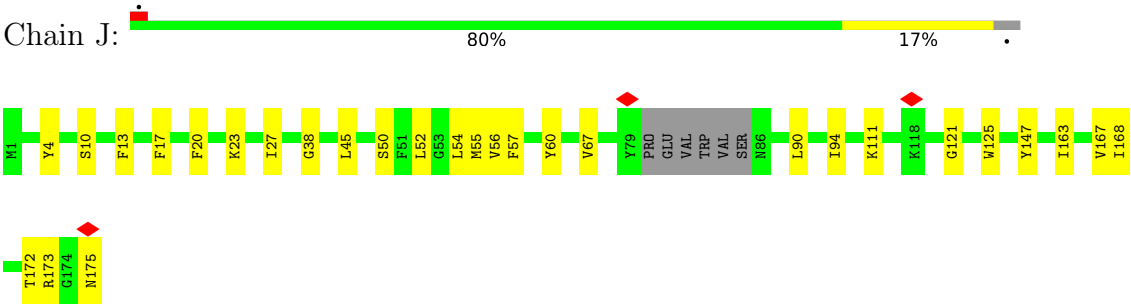
• Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain 6:

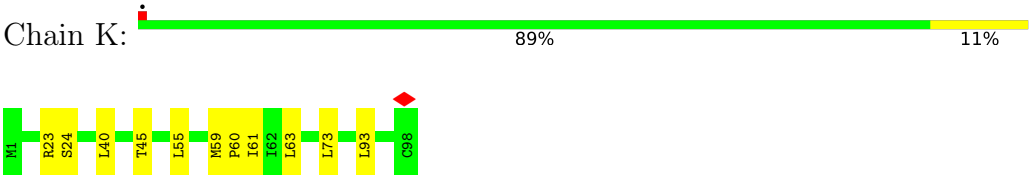




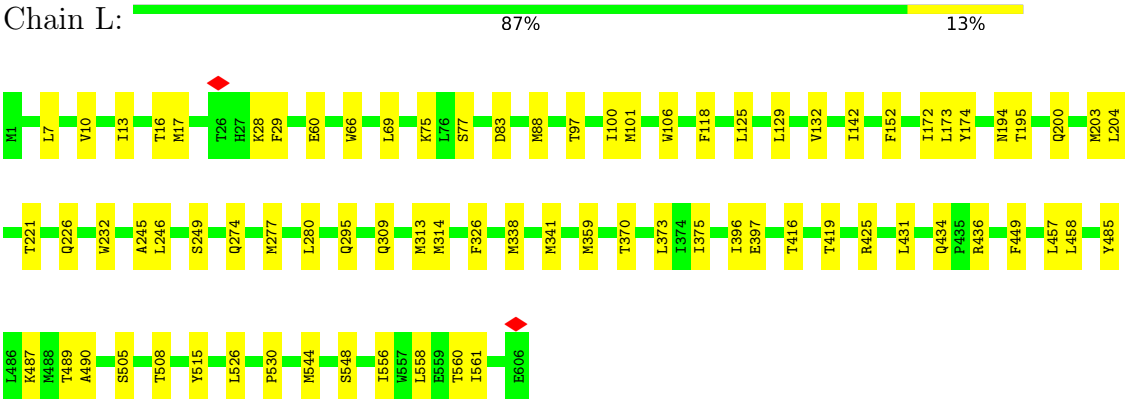
• Molecule 5: NADH-ubiquinone oxidoreductase chain 6



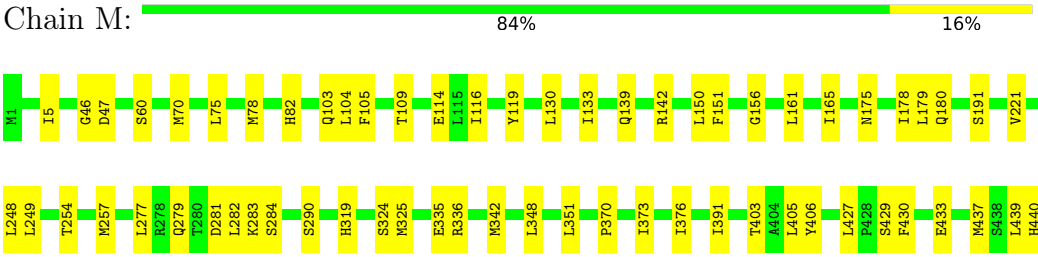
• Molecule 6: NADH-ubiquinone oxidoreductase chain 4L

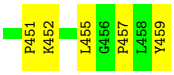


• Molecule 7: NADH-ubiquinone oxidoreductase chain 5



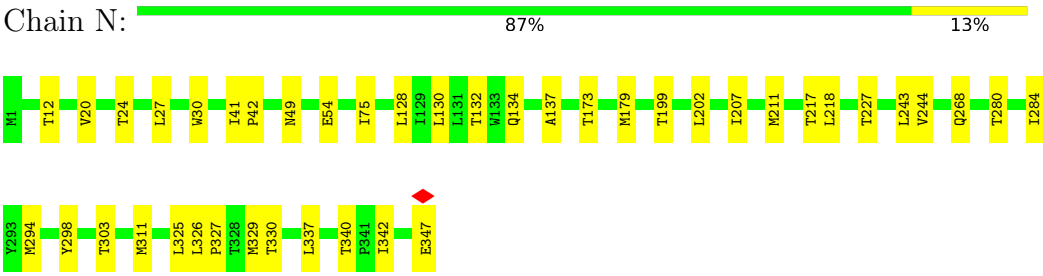
• Molecule 8: NADH-ubiquinone oxidoreductase chain 4





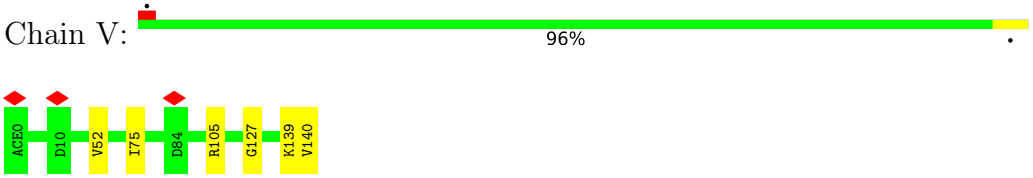
• Molecule 9: NADH-ubiquinone oxidoreductase chain 2

Chain N:



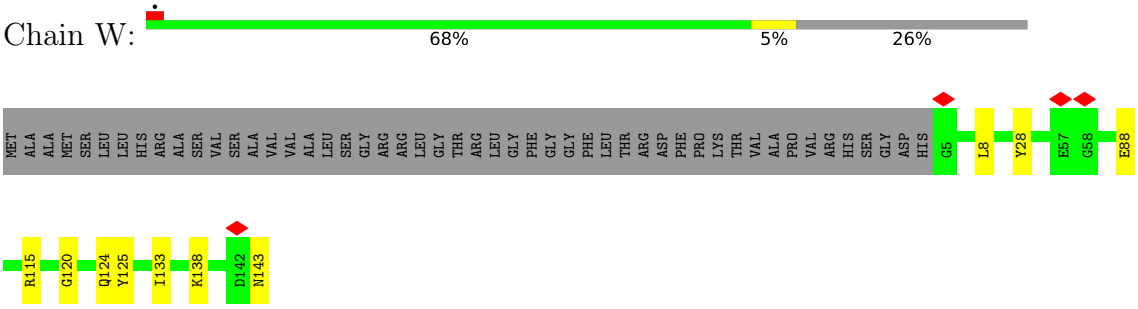
• Molecule 10: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain V:



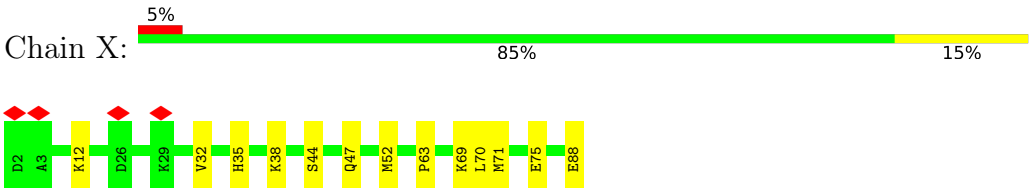
• Molecule 11: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain W:



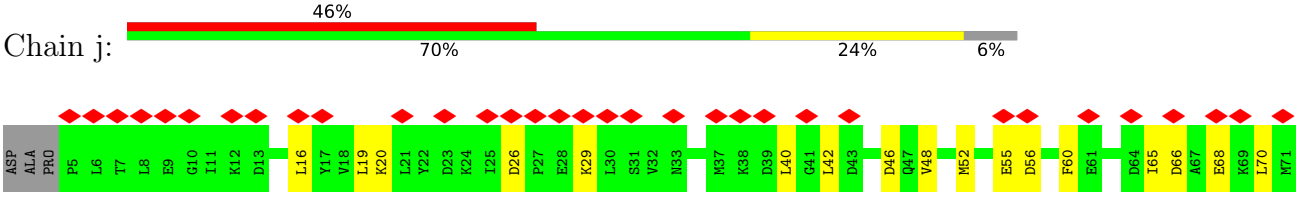
• Molecule 12: Acyl carrier protein

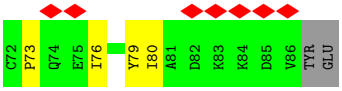
Chain X:



• Molecule 12: Acyl carrier protein

Chain j:

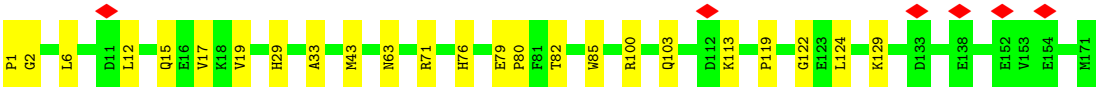




• Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

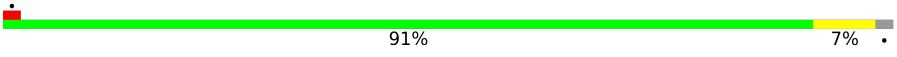
Chain Y:





• Molecule 14: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

Chain Z:

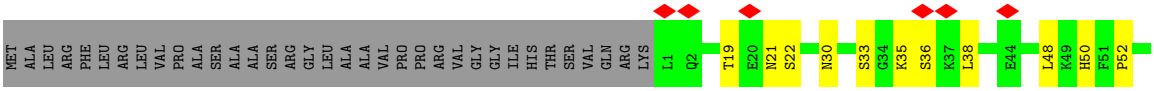


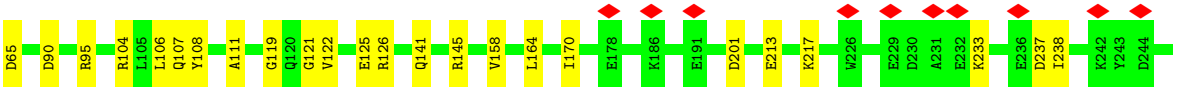


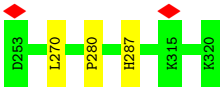
• Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain k:





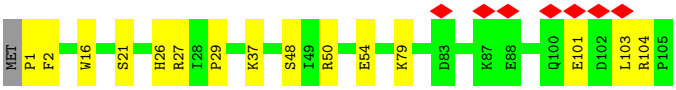




• Molecule 16: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain l:

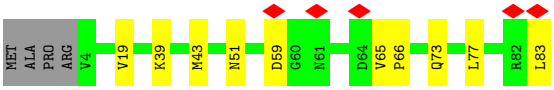




• Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain m:

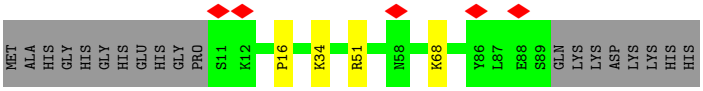




• Molecule 18: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

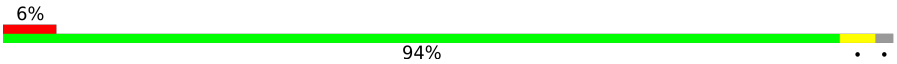
Chain n:

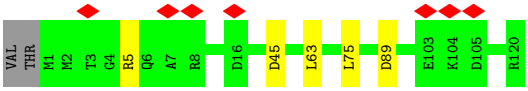




• Molecule 19: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain o:

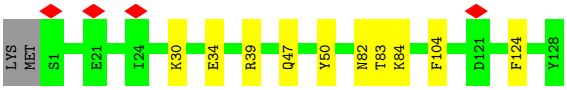




• Molecule 20: NADH:ubiquinone oxidoreductase subunit B4

Chain p:

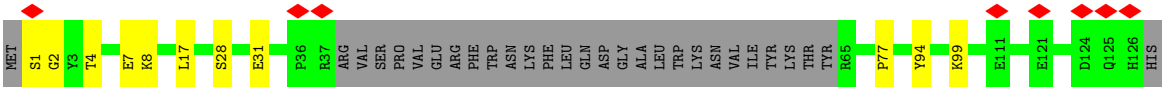




• Molecule 21: Mitochondrial complex I, B17 subunit

Chain r:

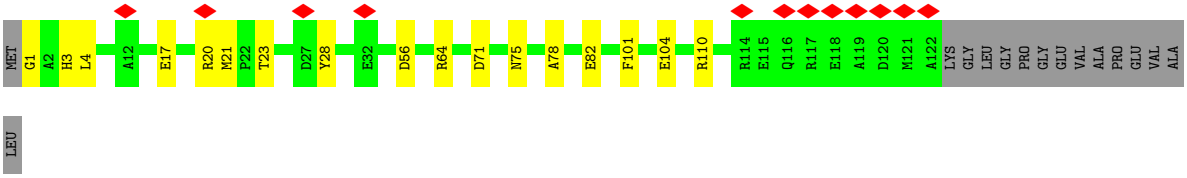




• Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

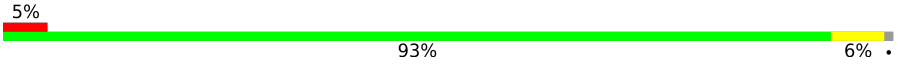
Chain s:

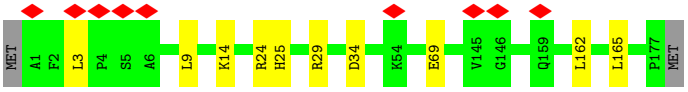




• Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

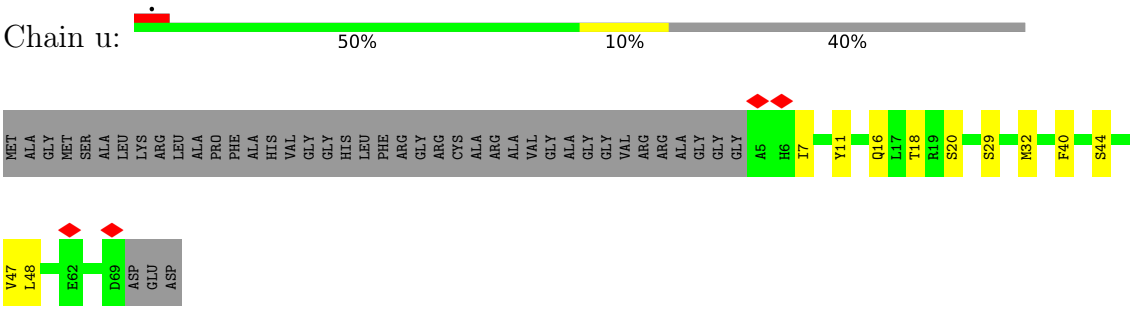
Chain t:





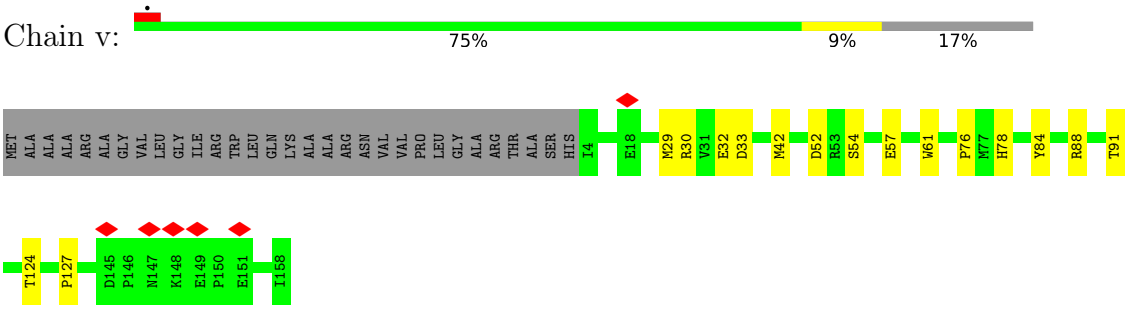
• Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

Chain u:



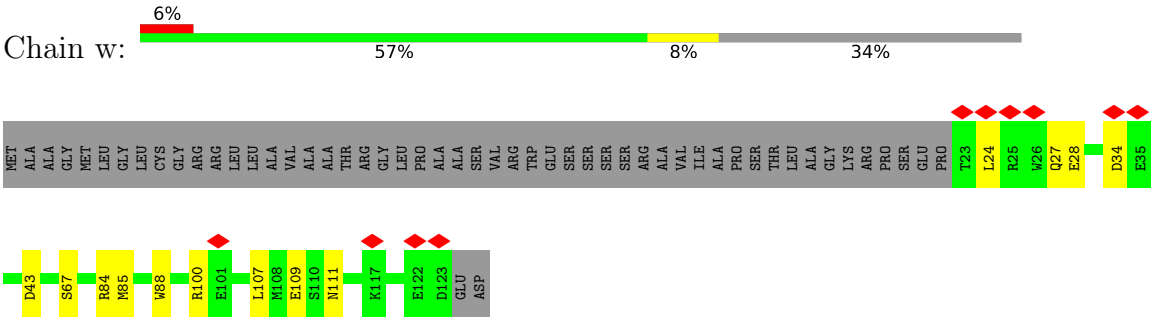
• Molecule 25: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain v:



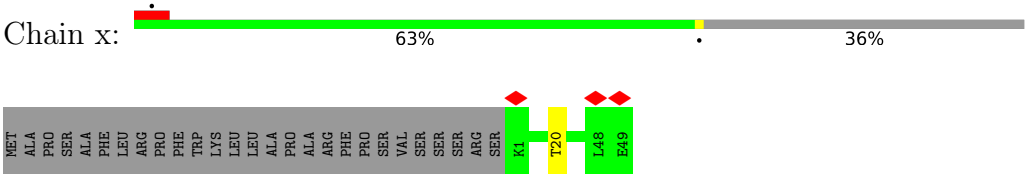
• Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain w:



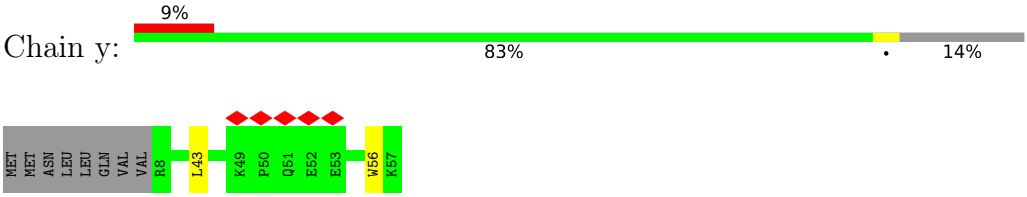
• Molecule 27: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

Chain x:



• Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

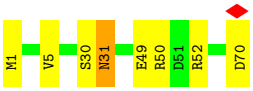
Chain y:



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

Chain z:

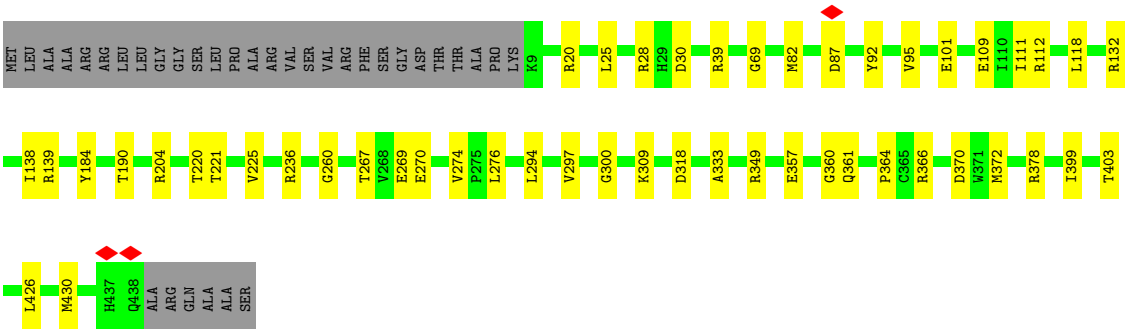




• Molecule 30: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain 1:

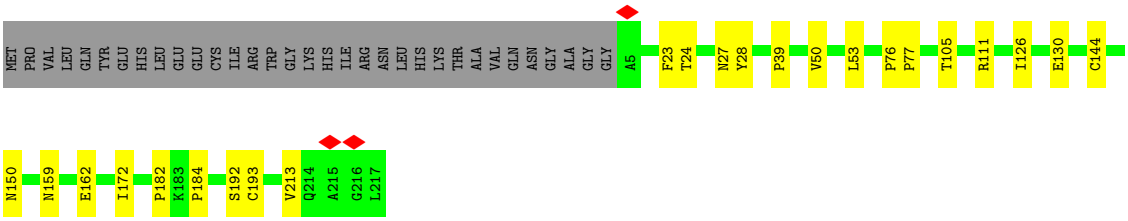




• Molecule 31: Mitochondrial complex I, 24 kDa subunit

Chain 2:

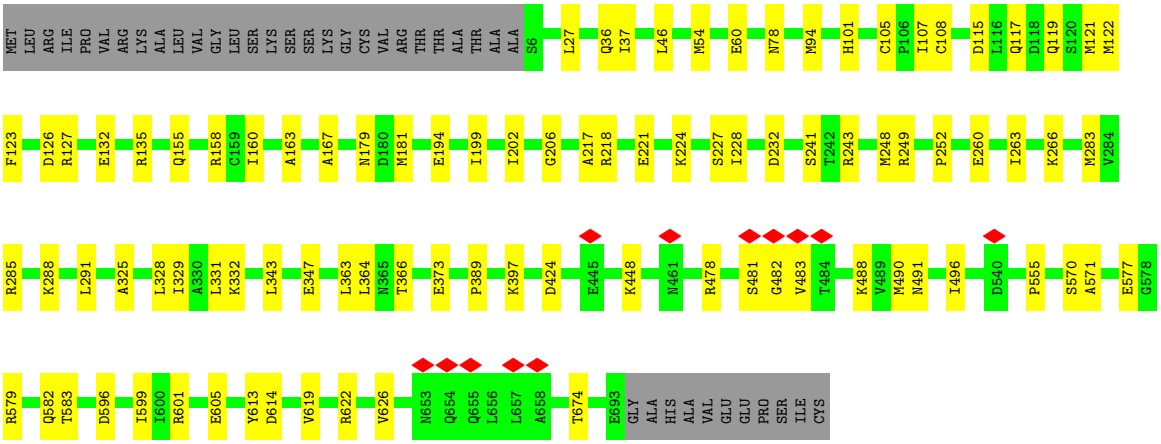




• Molecule 32: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain 3:



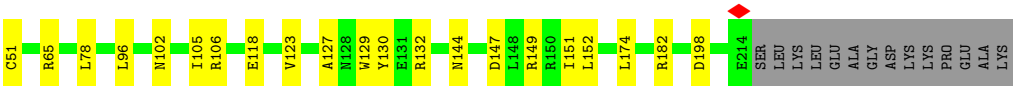


• Molecule 33: NADH:ubiquinone oxidoreductase core subunit S3

Chain 5:



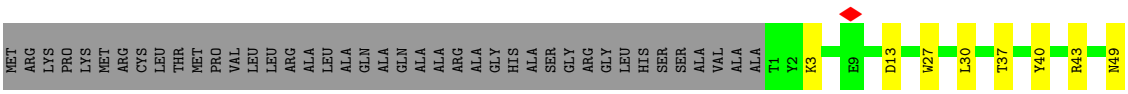


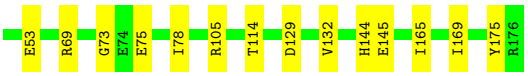


• Molecule 34: Complex I-23kD

Chain 9:







• Molecule 35: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

Chain a:



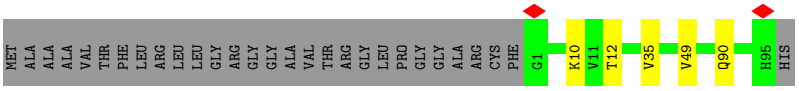




• Molecule 36: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain b:

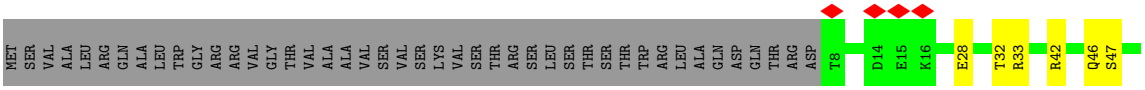


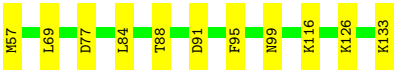


• Molecule 37: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain c:

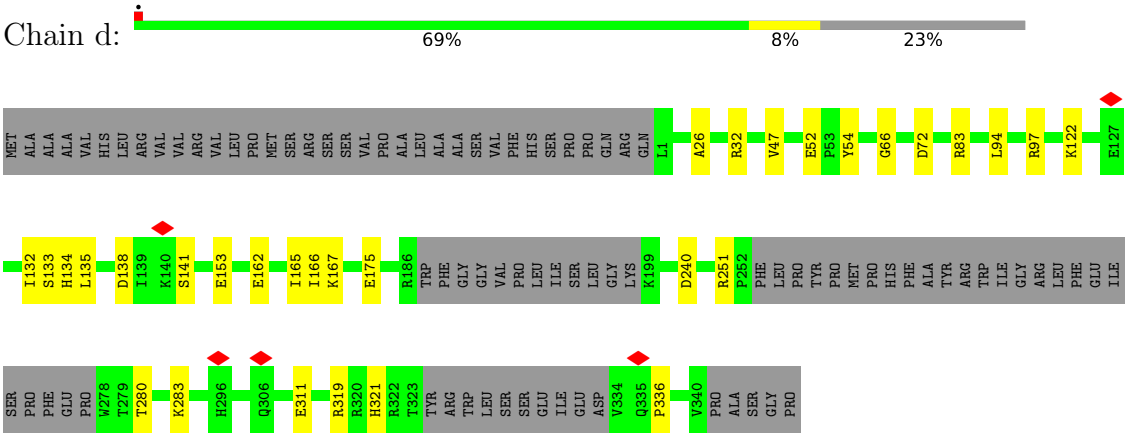






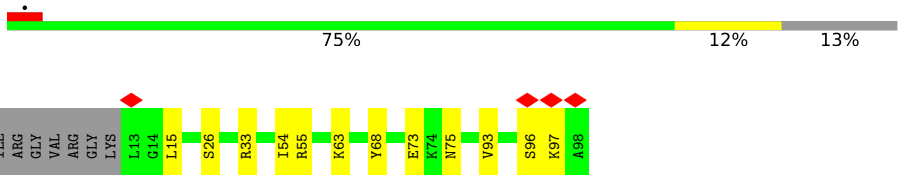
• Molecule 38: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain d:



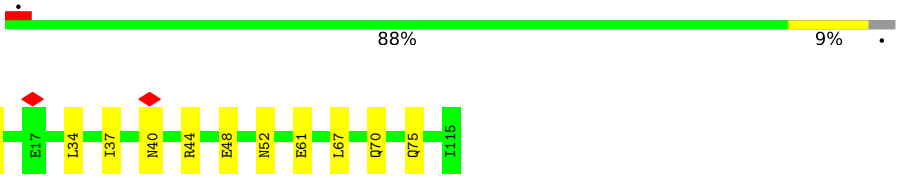
• Molecule 39: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain e:



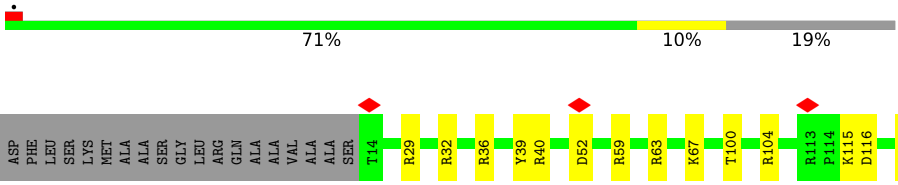
• Molecule 40: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

Chain f:



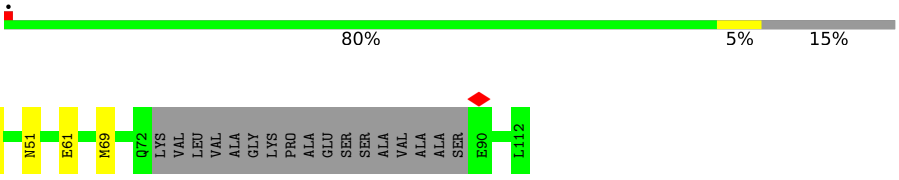
• Molecule 41: NADH:ubiquinone oxidoreductase subunit A6

Chain g:



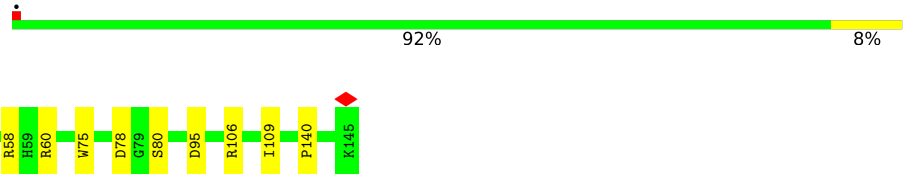
• Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

Chain h:



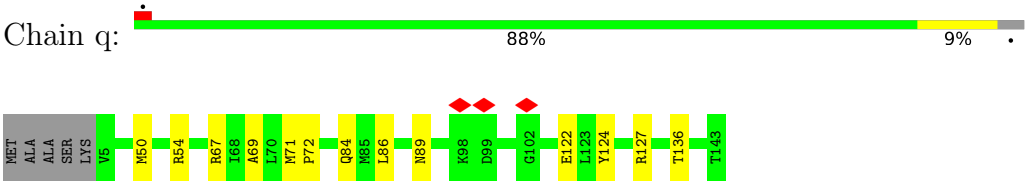
• Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain i:



• Molecule 44: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain q:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	76863	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	90	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	120000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.606	Depositor
Minimum map value	-0.066	Depositor
Average map value	0.013	Depositor
Map value standard deviation	0.036	Depositor
Recommended contour level	0.095	Depositor
Map size (Å)	170.8, 193.98001, 291.58002	wwPDB
Map dimensions	239, 159, 140	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.22, 1.22, 1.22	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: ZMP, NAI, SEP, FMN, NDP, ZN, DGT, MYR, MG, SF4, FME, 3PE, FES, PC1, A1JBT, 2MR, K, ACE

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	4	0.19	0/3484	0.41	0/4716
2	A	0.20	0/852	0.45	0/1167
3	H	0.22	0/2526	0.48	0/3455
4	6	0.18	0/1278	0.39	0/1728
5	J	0.18	0/1324	0.42	0/1790
6	K	0.22	0/749	0.46	0/1014
7	L	0.20	0/4924	0.44	0/6698
8	M	0.22	0/3731	0.46	0/5085
9	N	0.22	0/2787	0.45	0/3795
10	V	0.15	0/1047	0.31	0/1421
11	W	0.16	0/1188	0.33	0/1607
12	X	0.15	0/713	0.36	0/963
12	j	0.20	0/670	0.47	0/902
13	Y	0.15	0/1440	0.37	0/1942
14	Z	0.16	0/1475	0.32	0/1989
15	k	0.14	0/2646	0.32	0/3579
16	l	0.17	0/896	0.43	0/1200
17	m	0.17	0/647	0.42	0/890
18	n	0.16	0/653	0.39	0/882
19	o	0.15	0/1035	0.29	0/1398
20	p	0.15	0/1085	0.33	0/1467
21	r	0.15	0/874	0.36	0/1188
22	s	0.16	0/1072	0.39	0/1436
23	t	0.14	0/1573	0.33	0/2130
24	u	0.14	0/590	0.34	0/810
25	v	0.16	0/1361	0.36	0/1861
26	w	0.17	0/872	0.42	0/1185
27	x	0.15	0/425	0.33	0/576
28	y	0.15	0/449	0.37	0/605
29	z	0.16	0/591	0.37	0/795
30	1	0.16	0/3386	0.36	0/4575

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
31	2	0.16	0/1695	0.40	0/2306
32	3	0.16	0/5362	0.36	0/7266
33	5	0.17	0/1776	0.38	0/2417
34	9	0.19	0/1445	0.41	0/1956
35	a	0.13	0/383	0.28	0/518
36	b	0.17	0/749	0.35	0/1009
37	c	0.15	0/1047	0.34	0/1415
38	d	0.16	0/2397	0.34	0/3241
39	e	0.16	0/702	0.42	0/945
40	f	0.14	0/937	0.32	0/1271
41	g	0.16	0/993	0.32	0/1336
42	h	0.16	0/779	0.35	0/1054
43	i	0.15	0/1250	0.31	0/1698
44	q	0.17	0/1171	0.33	0/1579
All	All	0.18	0/67029	0.39	0/90860

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	4	3409	0	3347	43	0
2	A	831	0	874	9	0
3	H	2453	0	2571	36	0
4	6	1247	0	1256	14	0
5	J	1294	0	1317	25	0
6	K	749	0	793	12	0
7	L	4806	0	4945	51	0
8	M	3647	0	3849	46	0
9	N	2723	0	2930	32	0
10	V	1028	0	1036	6	0
11	W	1155	0	1177	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	X	701	0	693	10	0
12	j	660	0	663	17	0
13	Y	1403	0	1392	17	0
14	Z	1441	0	1419	10	0
15	k	2596	0	2559	24	0
16	l	874	0	869	15	0
17	m	626	0	635	8	0
18	n	634	0	616	4	0
19	o	1004	0	995	4	0
20	p	1059	0	1062	9	0
21	r	846	0	864	9	0
22	s	1047	0	1015	11	0
23	t	1520	0	1477	8	0
24	u	563	0	509	7	0
25	v	1307	0	1207	11	0
26	w	846	0	792	13	0
27	x	412	0	411	1	0
28	y	436	0	437	2	0
29	z	576	0	570	7	0
30	1	3312	0	3267	33	0
31	2	1655	0	1668	14	0
32	3	5275	0	5300	61	0
33	5	1726	0	1676	19	0
34	9	1414	0	1371	17	0
35	a	371	0	344	6	0
36	b	737	0	710	3	0
37	c	1024	0	1023	11	0
38	d	2345	0	2375	19	0
39	e	691	0	706	8	0
40	f	917	0	958	8	0
41	g	969	0	980	15	0
42	h	763	0	775	5	0
43	i	1209	0	1182	7	0
44	q	1142	0	1137	11	0
45	4	40	0	54	1	0
45	6	51	0	82	1	0
45	A	51	0	82	3	0
45	H	51	0	82	1	0
45	K	40	0	54	0	0
45	L	82	0	118	2	0
45	M	44	0	65	0	0
45	N	51	0	82	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	V	72	0	92	2	0
45	i	51	0	82	2	0
45	o	31	0	36	0	0
45	p	27	0	27	2	0
46	4	54	0	88	3	0
46	6	46	0	69	3	0
46	A	37	0	48	0	0
46	L	54	0	88	2	0
46	M	108	0	176	3	0
47	H	29	0	0	0	0
48	1	8	0	0	0	0
48	3	16	0	0	1	0
48	6	8	0	0	0	0
48	9	16	0	0	0	0
49	k	31	0	12	2	0
50	k	1	0	0	0	0
51	s	15	0	27	0	0
52	j	34	0	40	0	0
52	t	31	0	34	2	0
53	1	31	0	19	0	0
54	1	44	0	27	2	0
55	2	4	0	0	1	0
55	3	4	0	0	0	0
56	3	1	0	0	0	0
57	b	1	0	0	0	0
58	d	48	0	26	1	0
All	All	66655	0	67262	580	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 4.

The worst 5 of 580 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)
32:3:570:SER:HA	32:3:583:THR:O	1.74	0.88
8:M:324:SER:HG	8:M:440:HIS:HE2	1.28	0.79
6:K:60:PRO:O	6:K:63:LEU:HB3	1.90	0.72
1:4:326:ASP:OD1	32:3:127:ARG:NH2	2.22	0.72
32:3:228:ILE:HB	32:3:583:THR:HG22	1.76	0.67

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	4	416/463 (90%)	403 (97%)	13 (3%)	0	100	100
2	A	99/115 (86%)	96 (97%)	3 (3%)	0	100	100
3	H	304/318 (96%)	299 (98%)	5 (2%)	0	100	100
4	6	154/223 (69%)	150 (97%)	4 (3%)	0	100	100
5	J	165/175 (94%)	153 (93%)	12 (7%)	0	100	100
6	K	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
7	L	604/606 (100%)	578 (96%)	26 (4%)	0	100	100
8	M	457/459 (100%)	451 (99%)	6 (1%)	0	100	100
9	N	345/347 (99%)	334 (97%)	11 (3%)	0	100	100
10	V	139/141 (99%)	139 (100%)	0	0	100	100
11	W	137/189 (72%)	136 (99%)	1 (1%)	0	100	100
12	X	85/87 (98%)	81 (95%)	4 (5%)	0	100	100
12	j	80/87 (92%)	76 (95%)	4 (5%)	0	100	100
13	Y	169/171 (99%)	165 (98%)	4 (2%)	0	100	100
14	Z	169/175 (97%)	168 (99%)	1 (1%)	0	100	100
15	k	317/355 (89%)	306 (96%)	11 (4%)	0	100	100
16	l	103/106 (97%)	98 (95%)	5 (5%)	0	100	100
17	m	78/84 (93%)	75 (96%)	3 (4%)	0	100	100
18	n	77/98 (79%)	75 (97%)	2 (3%)	0	100	100
19	o	118/122 (97%)	117 (99%)	1 (1%)	0	100	100
20	p	126/130 (97%)	122 (97%)	4 (3%)	0	100	100
21	r	95/128 (74%)	93 (98%)	2 (2%)	0	100	100
22	s	120/137 (88%)	117 (98%)	3 (2%)	0	100	100
23	t	175/179 (98%)	169 (97%)	6 (3%)	0	100	100
24	u	63/108 (58%)	61 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	v	153/186 (82%)	147 (96%)	6 (4%)	0	100	100
26	w	99/154 (64%)	94 (95%)	5 (5%)	0	100	100
27	x	47/76 (62%)	47 (100%)	0	0	100	100
28	y	48/58 (83%)	46 (96%)	2 (4%)	0	100	100
29	z	68/70 (97%)	67 (98%)	1 (2%)	0	100	100
30	1	428/464 (92%)	417 (97%)	11 (3%)	0	100	100
31	2	211/246 (86%)	198 (94%)	13 (6%)	0	100	100
32	3	686/727 (94%)	667 (97%)	19 (3%)	0	100	100
33	5	206/266 (77%)	199 (97%)	7 (3%)	0	100	100
34	9	174/217 (80%)	167 (96%)	7 (4%)	0	100	100
35	a	42/109 (38%)	42 (100%)	0	0	100	100
36	b	93/124 (75%)	92 (99%)	1 (1%)	0	100	100
37	c	124/170 (73%)	121 (98%)	3 (2%)	0	100	100
38	d	285/380 (75%)	278 (98%)	7 (2%)	0	100	100
39	e	84/99 (85%)	81 (96%)	3 (4%)	0	100	100
40	f	111/116 (96%)	109 (98%)	2 (2%)	0	100	100
41	g	112/140 (80%)	106 (95%)	6 (5%)	0	100	100
42	h	92/113 (81%)	90 (98%)	2 (2%)	0	100	100
43	i	143/145 (99%)	141 (99%)	2 (1%)	0	100	100
44	q	137/144 (95%)	134 (98%)	3 (2%)	0	100	100
All	All	8034/9105 (88%)	7798 (97%)	236 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	4	364/391 (93%)	364 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	94/103 (91%)	94 (100%)	0	100	100
3	H	269/278 (97%)	269 (100%)	0	100	100
4	6	132/181 (73%)	132 (100%)	0	100	100
5	J	138/144 (96%)	138 (100%)	0	100	100
6	K	86/86 (100%)	86 (100%)	0	100	100
7	L	538/538 (100%)	538 (100%)	0	100	100
8	M	411/411 (100%)	411 (100%)	0	100	100
9	N	315/315 (100%)	315 (100%)	0	100	100
10	V	101/101 (100%)	101 (100%)	0	100	100
11	W	122/160 (76%)	122 (100%)	0	100	100
12	X	80/80 (100%)	80 (100%)	0	100	100
12	j	76/80 (95%)	76 (100%)	0	100	100
13	Y	154/154 (100%)	154 (100%)	0	100	100
14	Z	155/157 (99%)	155 (100%)	0	100	100
15	k	283/309 (92%)	283 (100%)	0	100	100
16	l	94/95 (99%)	94 (100%)	0	100	100
17	m	69/72 (96%)	69 (100%)	0	100	100
18	n	61/76 (80%)	61 (100%)	0	100	100
19	o	107/109 (98%)	107 (100%)	0	100	100
20	p	114/116 (98%)	114 (100%)	0	100	100
21	r	95/122 (78%)	95 (100%)	0	100	100
22	s	110/120 (92%)	110 (100%)	0	100	100
23	t	159/161 (99%)	159 (100%)	0	100	100
24	u	59/84 (70%)	59 (100%)	0	100	100
25	v	140/160 (88%)	140 (100%)	0	100	100
26	w	92/130 (71%)	92 (100%)	0	100	100
27	x	44/67 (66%)	44 (100%)	0	100	100
28	y	46/54 (85%)	46 (100%)	0	100	100
29	z	59/59 (100%)	58 (98%)	1 (2%)	53	75
30	1	344/368 (94%)	344 (100%)	0	100	100
31	2	183/210 (87%)	183 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	3	578/608 (95%)	578 (100%)	0	100	100
33	5	189/230 (82%)	189 (100%)	0	100	100
34	9	151/179 (84%)	151 (100%)	0	100	100
35	a	43/93 (46%)	43 (100%)	0	100	100
36	b	79/97 (81%)	79 (100%)	0	100	100
37	c	113/150 (75%)	113 (100%)	0	100	100
38	d	252/326 (77%)	252 (100%)	0	100	100
39	e	76/82 (93%)	76 (100%)	0	100	100
40	f	101/102 (99%)	101 (100%)	0	100	100
41	g	107/124 (86%)	107 (100%)	0	100	100
42	h	83/94 (88%)	83 (100%)	0	100	100
43	i	131/131 (100%)	131 (100%)	0	100	100
44	q	119/122 (98%)	119 (100%)	0	100	100
All	All	7116/7829 (91%)	7115 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
29	z	31	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 65 such sidechains are listed below:

Mol	Chain	Res	Type
36	b	36	ASN
38	d	184	ASN
9	N	316	GLN
9	N	289	ASN
38	d	321	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

5 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	$\#\|Z\| > 2$
1	2MR	4	85	1	10,12,13	0.18	0	5,13,15	0.21	0
15	SEP	k	36	15	8,9,10	0.28	0	8,12,14	1.04	1 (12%)
6	FME	K	1	6	8,9,10	0.97	0	7,9,11	0.71	0
8	FME	M	1	8	8,9,10	0.93	0	7,9,11	0.90	0
7	FME	L	1	7	8,9,10	0.93	0	7,9,11	0.86	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
1	2MR	4	85	1	-	0/10/13/15	-
15	SEP	k	36	15	-	0/5/8/10	-
6	FME	K	1	6	-	4/7/9/11	-
8	FME	M	1	8	-	4/7/9/11	-
7	FME	L	1	7	-	1/7/9/11	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	k	36	SEP	P-OG-CB	2.69	125.72	118.30

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	K	1	FME	O1-CN-N-CA

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Mol	Chain	Res	Type	Atoms
7	L	1	FME	CA-CB-CG-SD
8	M	1	FME	CB-CA-N-CN
8	M	1	FME	C-CA-CB-CG
8	M	1	FME	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, 3 are monoatomic - leaving 36 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	$\#\|Z\| > 2$
45	3PE	4	501	-	39,39,50	0.33	0	42,44,55	0.34	0
49	DGT	k	401	50	29,33,33	0.30	0	44,52,52	0.34	0
48	SF4	3	802	32	0,12,12	-	-	-		
52	ZMP	t	201	-	24,30,36	0.78	1 (4%)	29,37,45	0.88	2 (6%)
46	PC1	4	502	-	53,53,53	0.30	0	59,61,61	0.45	0
45	3PE	L	1001	-	50,50,50	0.30	0	53,55,55	0.31	0
58	NDP	d	401	-	49,52,52	0.35	0	66,80,80	0.34	0
45	3PE	o	501	-	30,30,50	0.38	0	33,35,55	0.35	0
48	SF4	1	501	30	0,12,12	-	-	-		
46	PC1	6	202	-	45,45,53	0.32	0	51,53,61	0.31	0
45	3PE	L	1003	-	30,30,50	0.40	0	33,35,55	0.73	1 (3%)
45	3PE	p	201	-	26,26,50	0.48	0	30,31,55	0.53	1 (3%)
45	3PE	H	401	-	50,50,50	0.31	0	53,55,55	0.32	0
48	SF4	9	202	34	0,12,12	-	-	-		
46	PC1	A	201	-	36,36,53	0.37	0	42,44,61	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
55	FES	3	803	32	0,4,4	-	-	-		
45	3PE	N	401	-	50,50,50	0.32	0	53,55,55	0.47	0
48	SF4	6	201	4	0,12,12	-	-	-		
54	NAI	1	503	-	45,48,48	0.33	0	60,73,73	0.37	0
48	SF4	3	801	32	0,12,12	-	-	-		
45	3PE	K	101	-	39,39,50	0.34	0	42,44,55	0.36	0
45	3PE	V	201	-	34,34,50	0.36	0	37,39,55	0.31	0
55	FES	2	300	31	0,4,4	-	-	-		
45	3PE	6	203	-	50,50,50	0.31	0	53,55,55	0.29	0
45	3PE	M	501	-	43,43,50	0.32	0	46,48,55	0.33	0
51	MYR	s	201	22	14,14,15	0.20	0	13,13,15	0.17	0
52	ZMP	j	201	-	27,33,36	0.65	1 (3%)	32,40,45	1.09	3 (9%)
45	3PE	i	201	-	50,50,50	0.30	0	53,55,55	0.26	0
47	A1JBT	H	402	-	31,33,33	0.27	0	31,49,49	0.60	0
48	SF4	9	201	34	0,12,12	-	-	-		
46	PC1	L	1002	-	53,53,53	0.31	0	59,61,61	0.55	2 (3%)
46	PC1	M	503	-	53,53,53	0.29	0	59,61,61	0.34	0
45	3PE	V	202	-	36,36,50	0.35	0	39,41,55	0.32	0
46	PC1	M	502	-	53,53,53	0.29	0	59,61,61	0.29	0
53	FMN	1	502	-	33,33,33	0.28	0	48,50,50	0.42	0
45	3PE	A	202	-	50,50,50	0.30	0	53,55,55	0.30	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
45	3PE	4	501	-	-	8/43/43/54	-
49	DGT	k	401	50	-	1/22/34/34	0/3/3/3
48	SF4	3	802	32	-	-	0/6/5/5
52	ZMP	t	201	-	-	16/35/37/43	-
46	PC1	4	502	-	-	10/57/57/57	-
45	3PE	L	1001	-	-	13/54/54/54	-
58	NDP	d	401	-	-	6/34/77/77	0/5/5/5
45	3PE	o	501	-	-	6/34/34/54	-
48	SF4	1	501	30	-	-	0/6/5/5
46	PC1	6	202	-	-	9/49/49/57	-
45	3PE	L	1003	-	-	8/34/34/54	-
45	3PE	p	201	-	-	3/27/27/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	3PE	H	401	-	-	14/54/54/54	-
48	SF4	9	202	34	-	-	0/6/5/5
46	PC1	A	201	-	-	11/40/40/57	-
55	FES	3	803	32	-	-	0/1/1/1
45	3PE	N	401	-	-	11/54/54/54	-
48	SF4	6	201	4	-	-	0/6/5/5
54	NAI	1	503	-	-	5/29/72/72	0/5/5/5
48	SF4	3	801	32	-	-	0/6/5/5
45	3PE	K	101	-	-	6/43/43/54	-
45	3PE	V	201	-	-	6/38/38/54	-
55	FES	2	300	31	-	-	0/1/1/1
45	3PE	6	203	-	-	9/54/54/54	-
45	3PE	M	501	-	-	11/47/47/54	-
51	MYR	s	201	22	-	1/11/12/13	-
52	ZMP	j	201	-	-	4/38/40/43	-
45	3PE	i	201	-	-	9/54/54/54	-
47	A1JBT	H	402	-	-	6/8/29/29	0/5/5/5
48	SF4	9	201	34	-	-	0/6/5/5
46	PC1	L	1002	-	-	15/57/57/57	-
46	PC1	M	503	-	-	6/57/57/57	-
45	3PE	V	202	-	-	8/40/40/54	-
46	PC1	M	502	-	-	14/57/57/57	-
53	FMN	1	502	-	-	8/18/18/18	0/3/3/3
45	3PE	A	202	-	-	16/54/54/54	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	t	201	ZMP	C9-C10	2.58	1.53	1.50
52	j	201	ZMP	C9-C10	2.30	1.53	1.50

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	j	201	ZMP	O1-C10-C9	-2.63	120.88	123.99
52	t	201	ZMP	O1-C10-C9	-2.32	121.24	123.99
52	j	201	ZMP	C15-C14-C13	-2.26	108.60	112.36
46	L	1002	PC1	O21-C2-C1	2.23	116.48	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
46	L	1002	PC1	C2-O21-C21	2.23	123.27	117.79

There are no chirality outliers.

5 of 240 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	4	501	3PE	C1-O11-P-O12
45	4	501	3PE	C1-O11-P-O13
45	4	501	3PE	C1-O11-P-O14
45	4	501	3PE	C11-O13-P-O12
45	A	202	3PE	C1-O11-P-O12

There are no ring outliers.

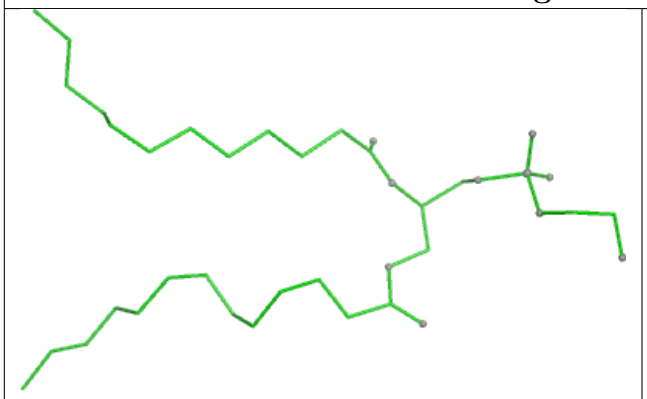
21 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	4	501	3PE	1	0
49	k	401	DGT	2	0
52	t	201	ZMP	2	0
46	4	502	PC1	3	0
45	L	1001	3PE	2	0
58	d	401	NDP	1	0
46	6	202	PC1	3	0
45	p	201	3PE	2	0
45	H	401	3PE	1	0
45	N	401	3PE	1	0
54	1	503	NAI	2	0
48	3	801	SF4	1	0
45	V	201	3PE	1	0
55	2	300	FES	1	0
45	6	203	3PE	1	0
45	i	201	3PE	2	0
46	L	1002	PC1	2	0
46	M	503	PC1	1	0
45	V	202	3PE	1	0
46	M	502	PC1	2	0
45	A	202	3PE	3	0

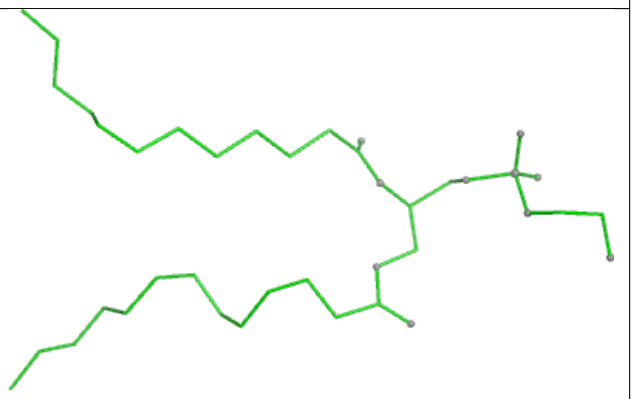
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

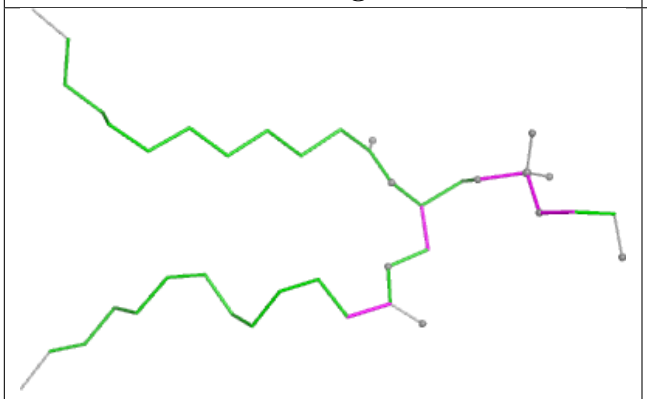
Ligand 3PE 4 501



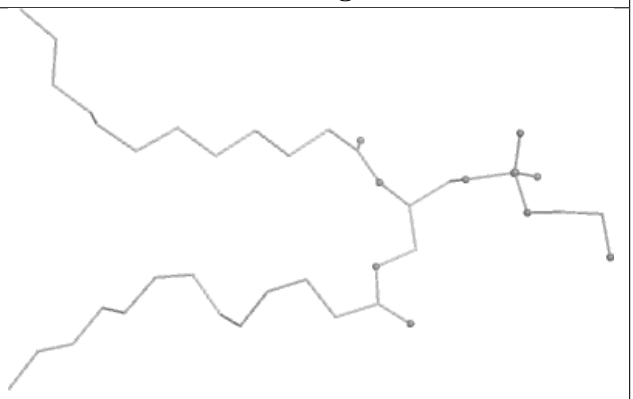
Bond lengths



Bond angles

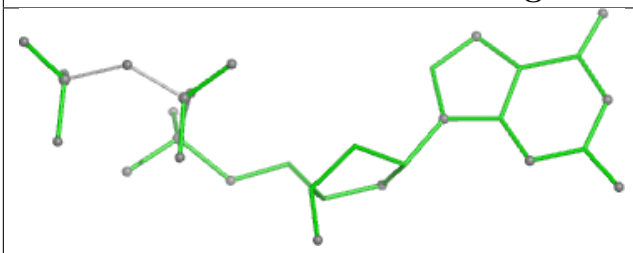


Torsions

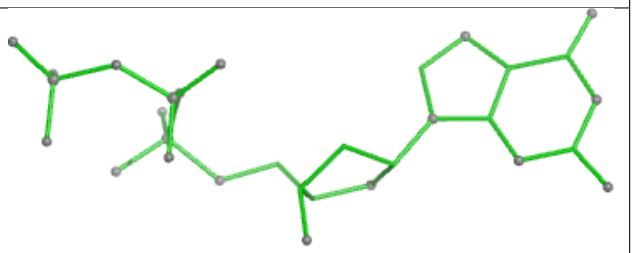


Rings

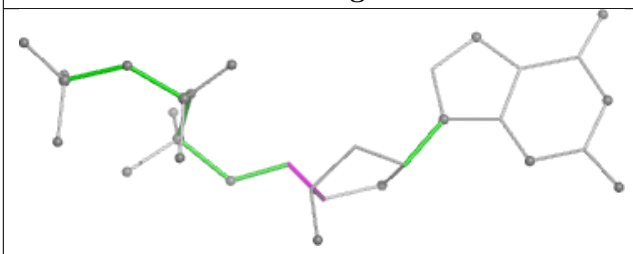
Ligand DGT k 401



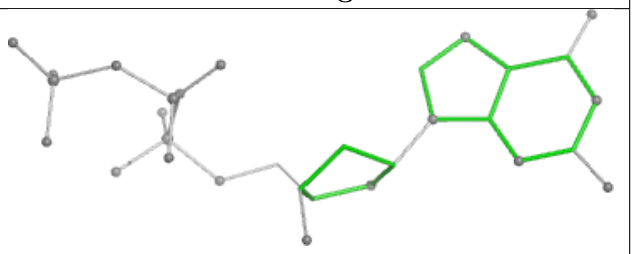
Bond lengths



Bond angles

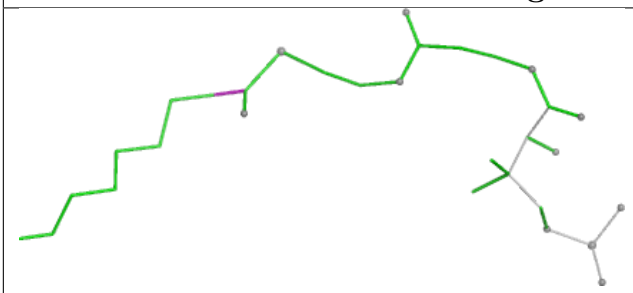


Torsions

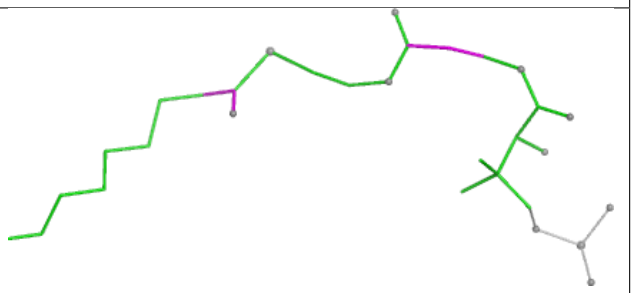


Rings

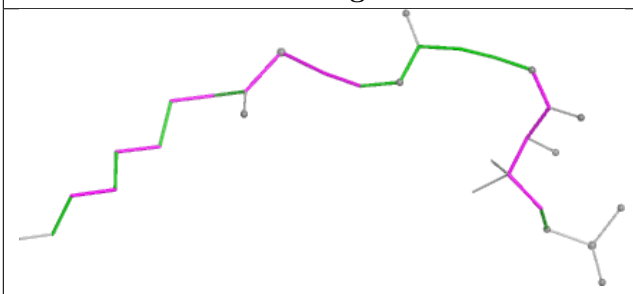
Ligand ZMP t 201



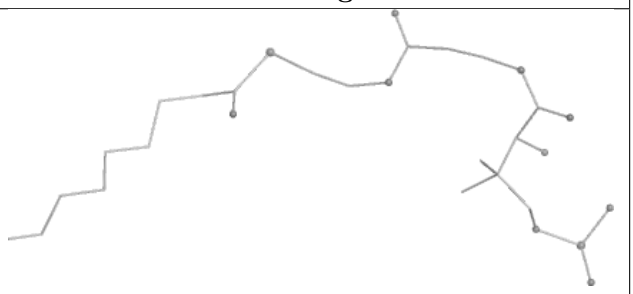
Bond lengths



Bond angles

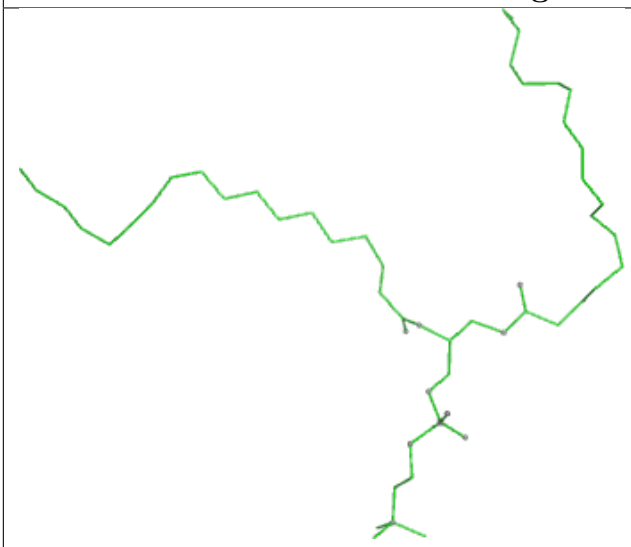


Torsions



Rings

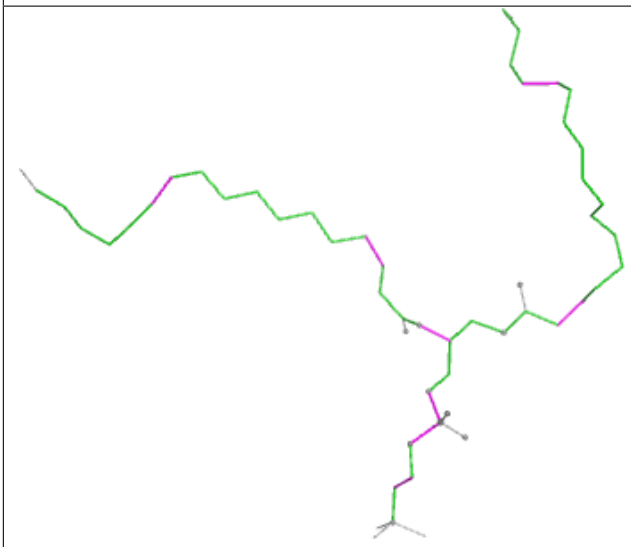
Ligand PC1 4 502



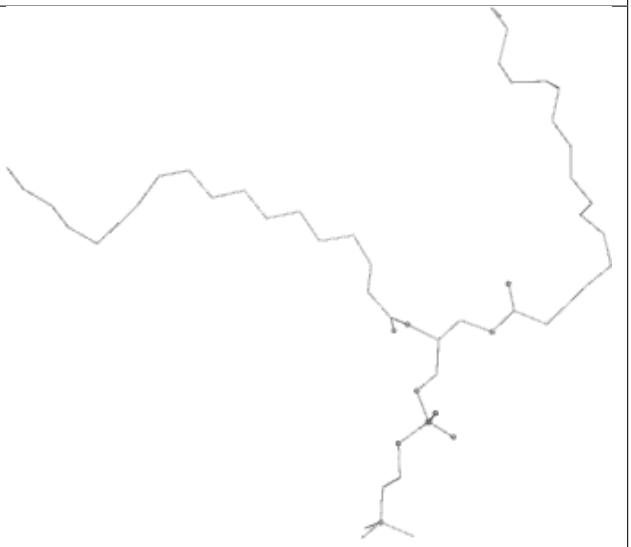
Bond lengths



Bond angles

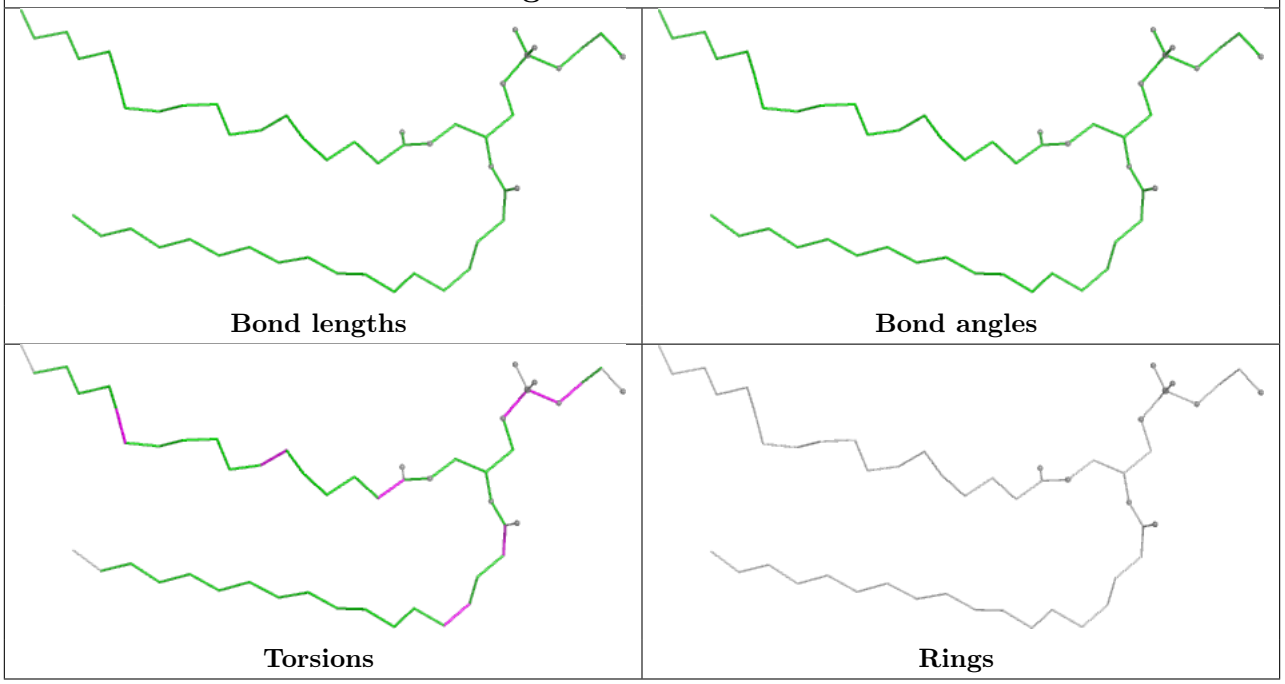


Torsions

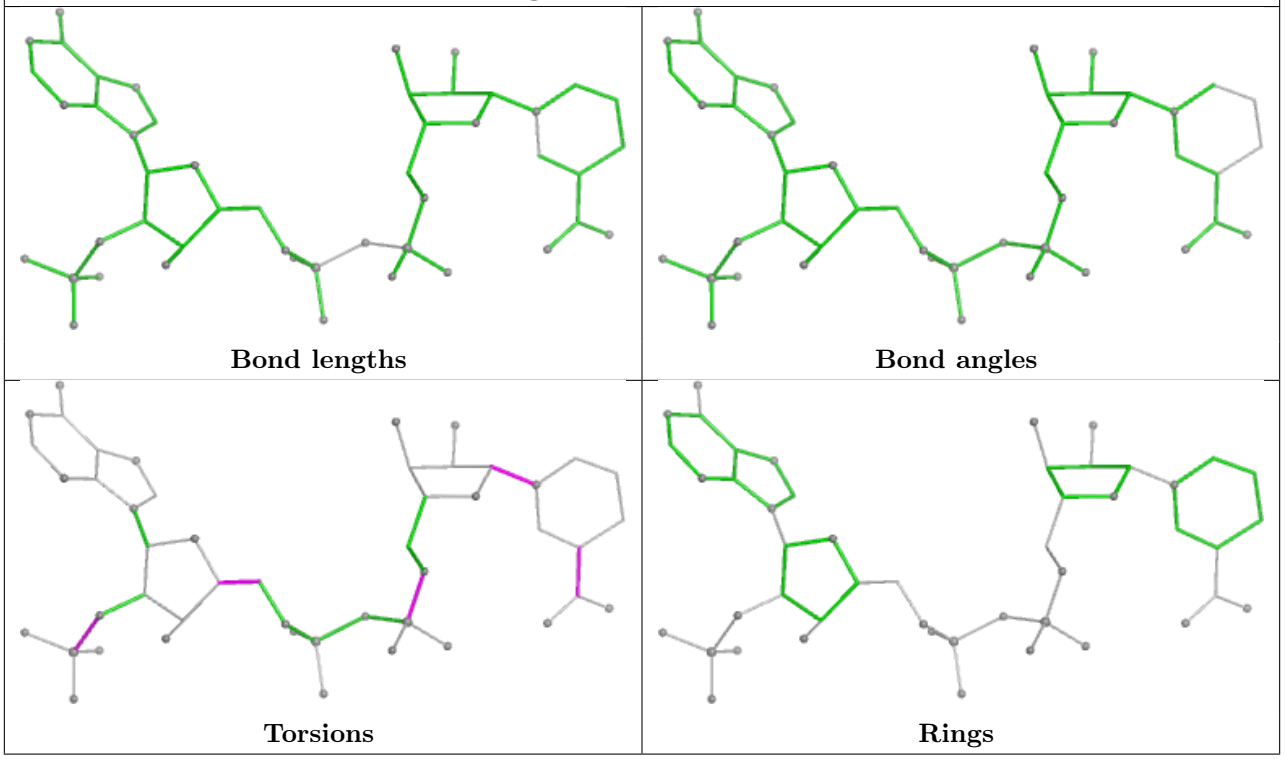


Rings

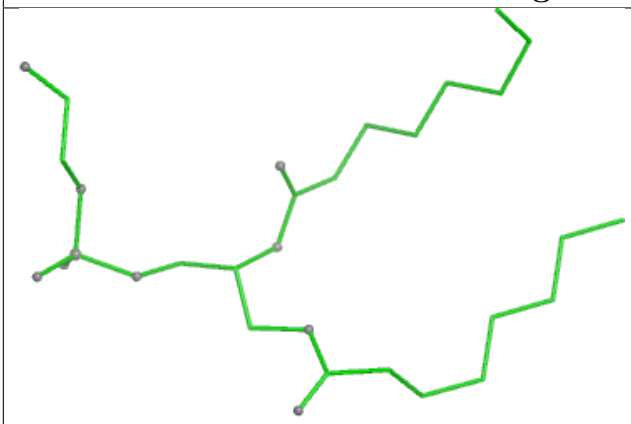
Ligand 3PE L 1001



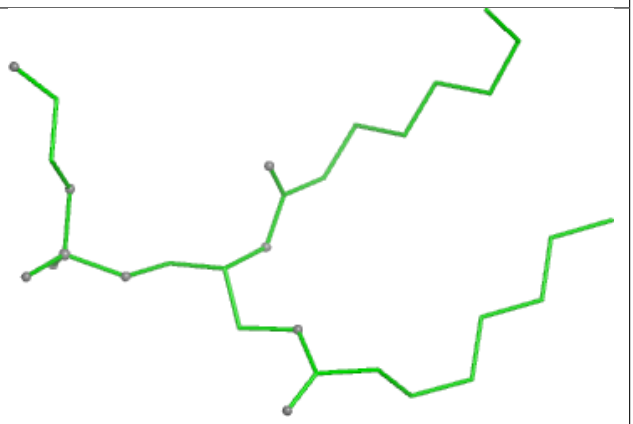
Ligand NDP d 401



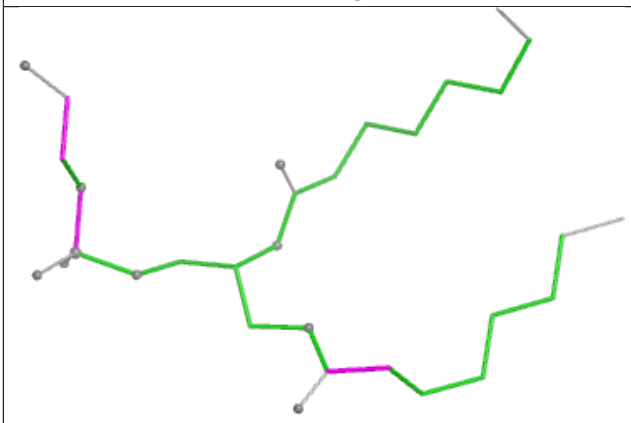
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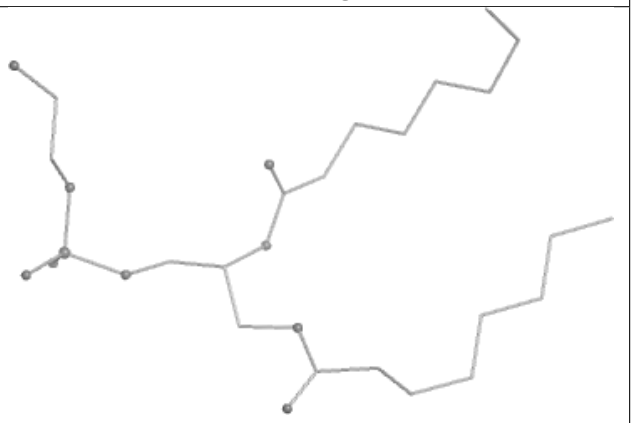
Bond lengths



Bond angles

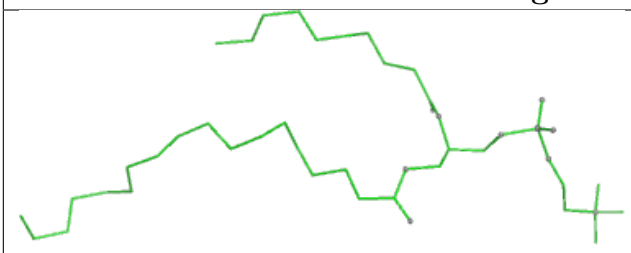


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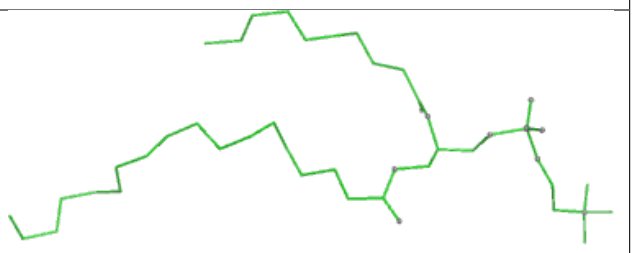


Rings

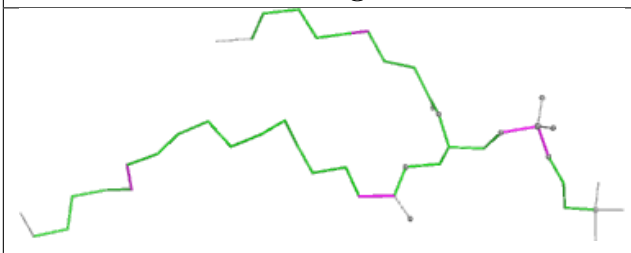
Ligand PC1 6 202



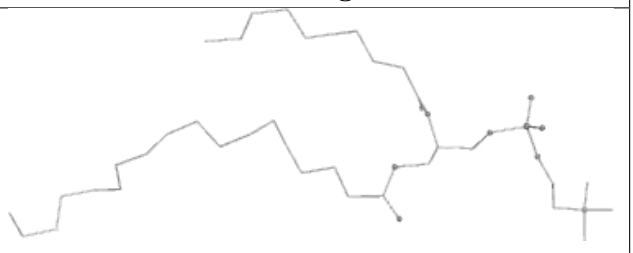
Bond lengths



Bond angles

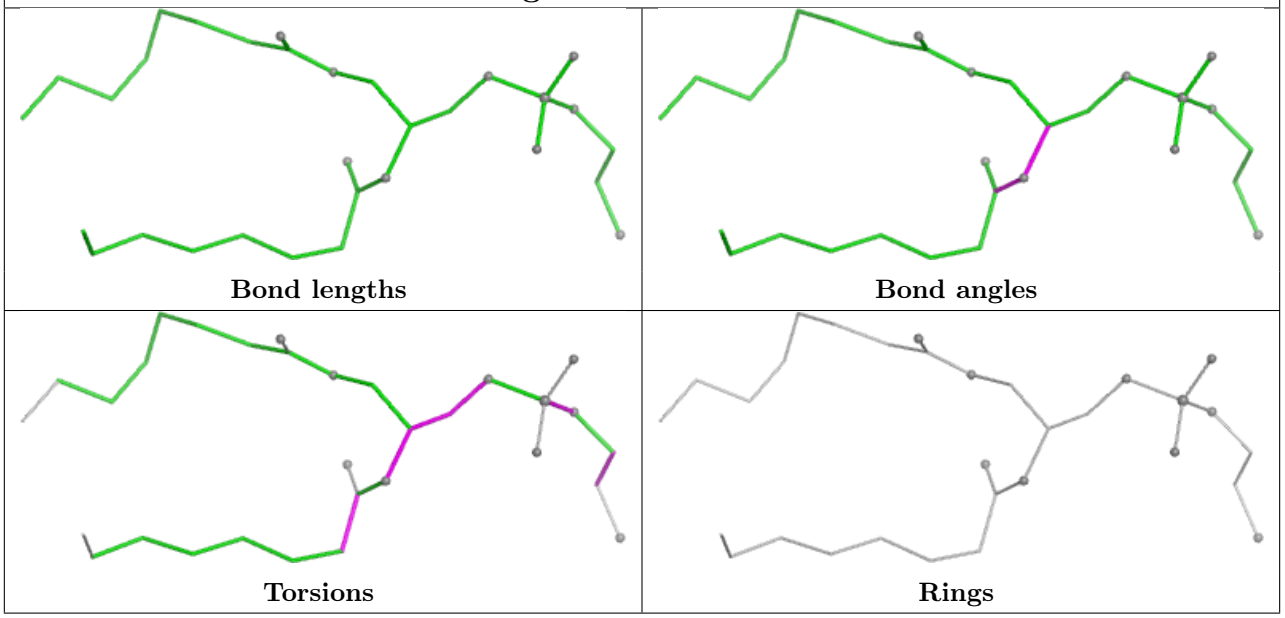


Torsions

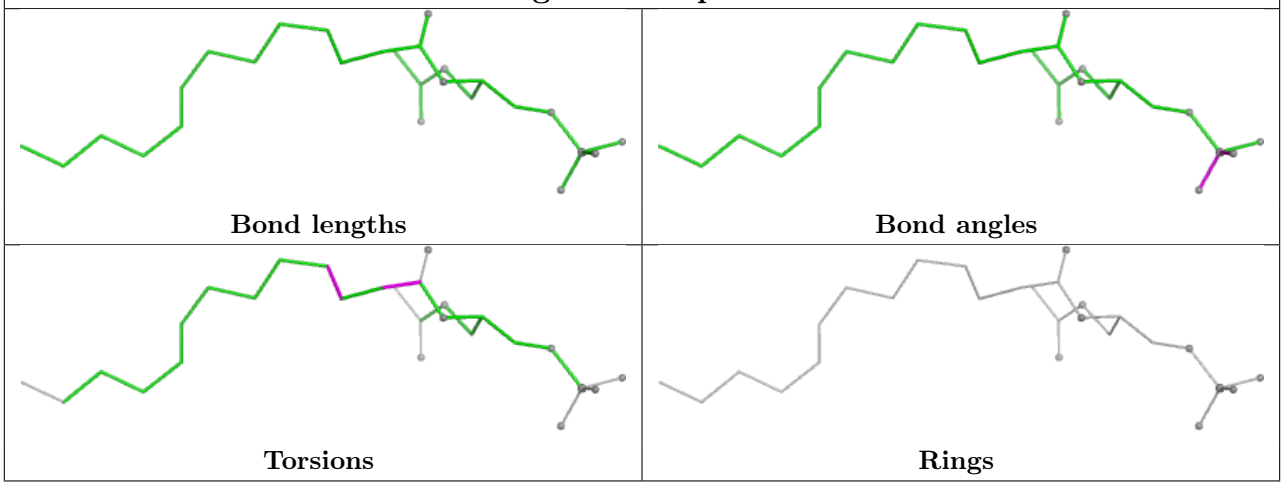


Rings

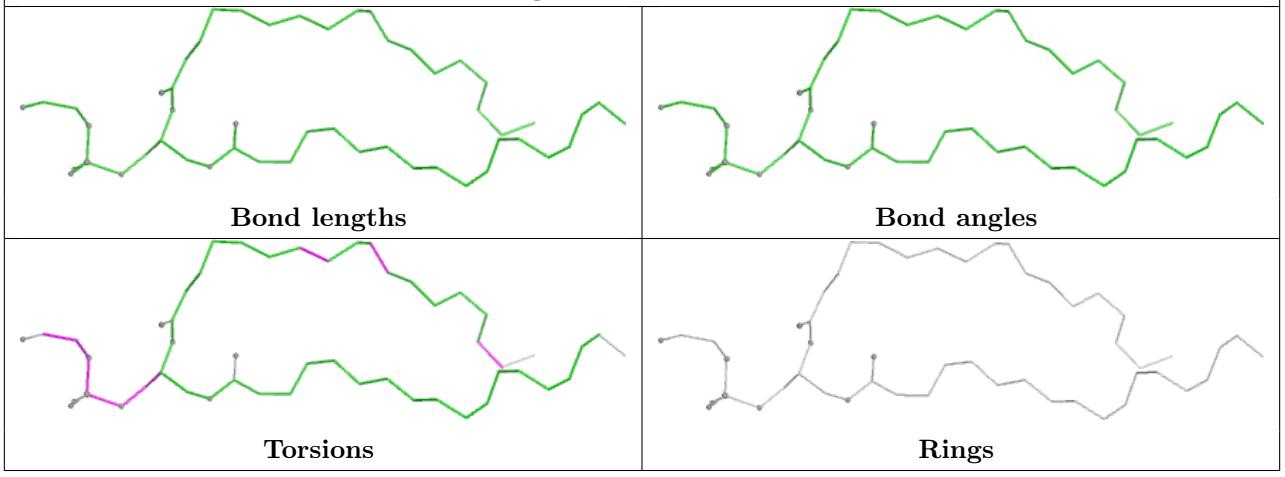
Ligand 3PE L 1003



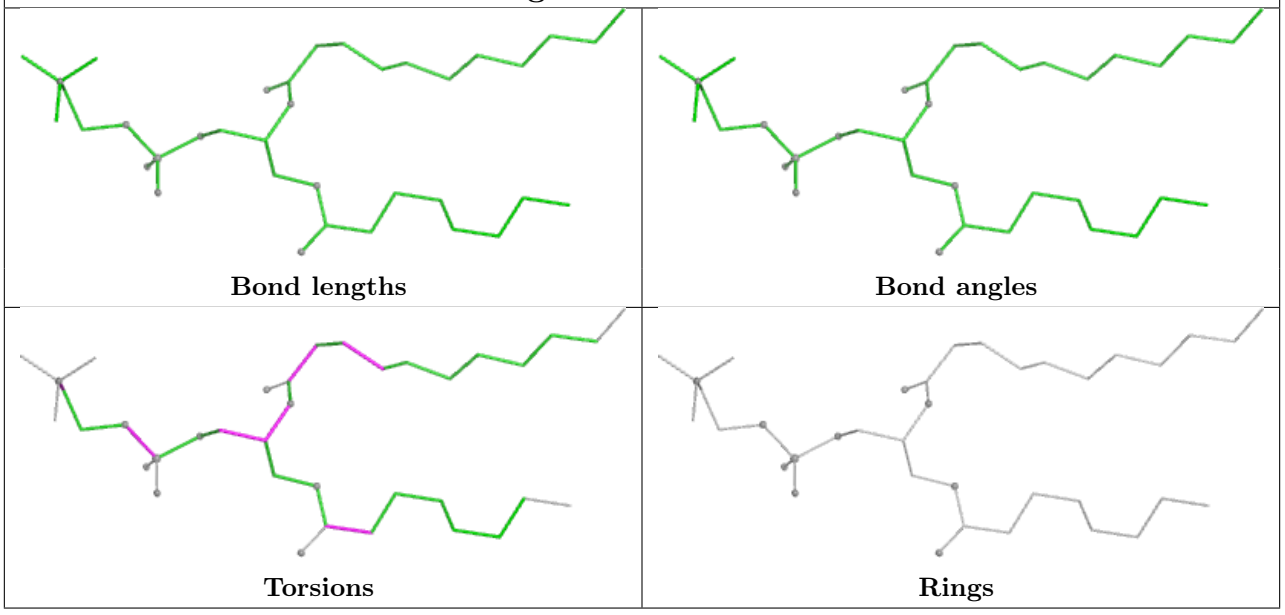
Ligand 3PE p 201



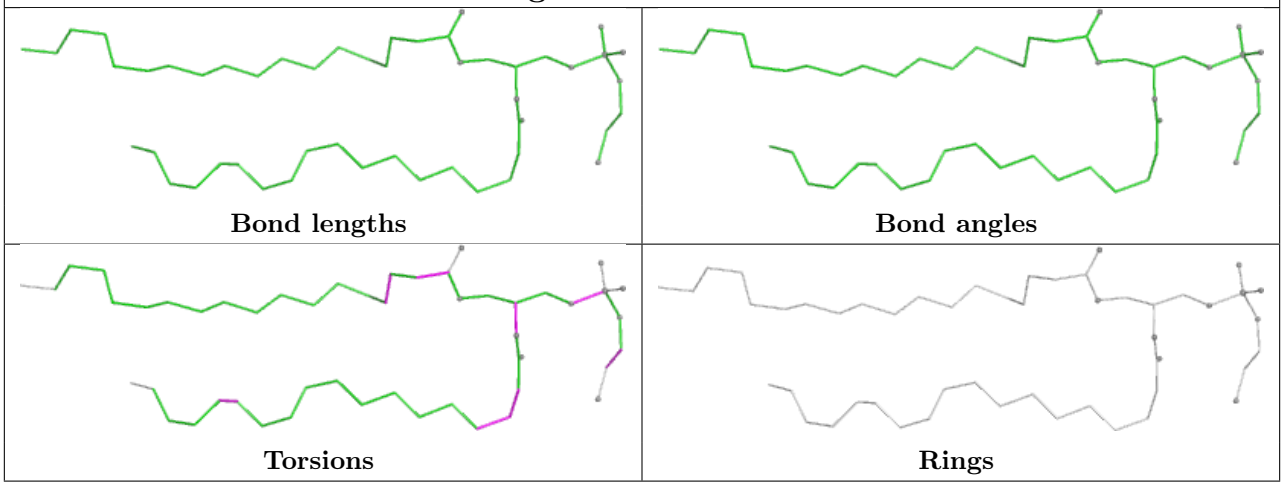
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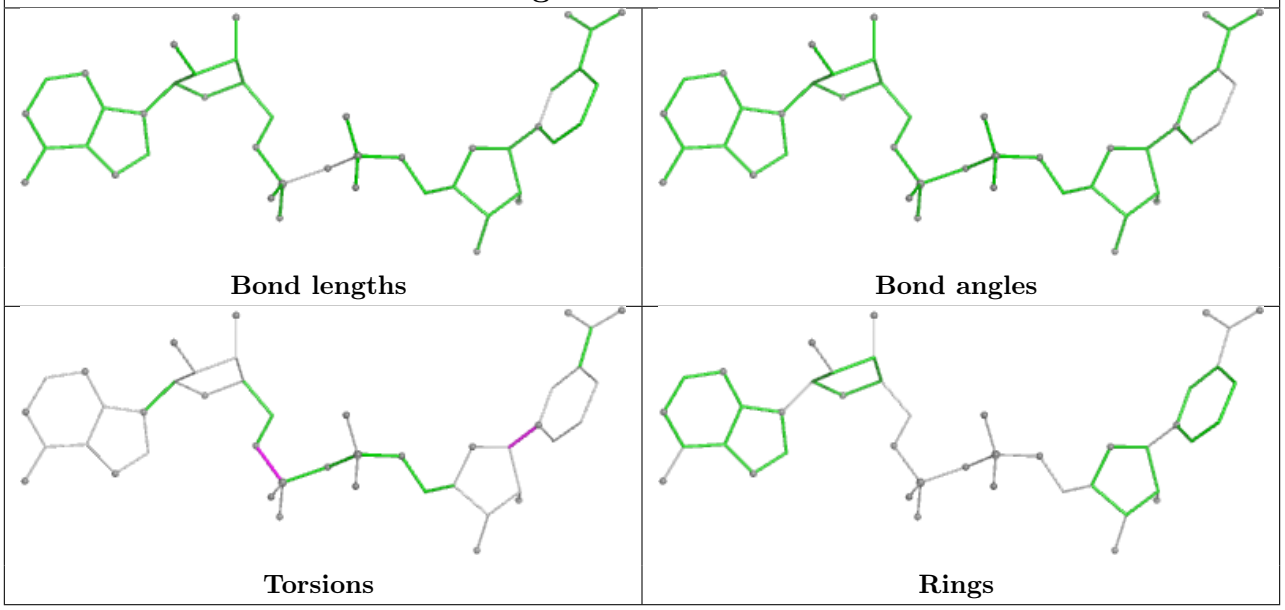
Ligand PC1 A 201



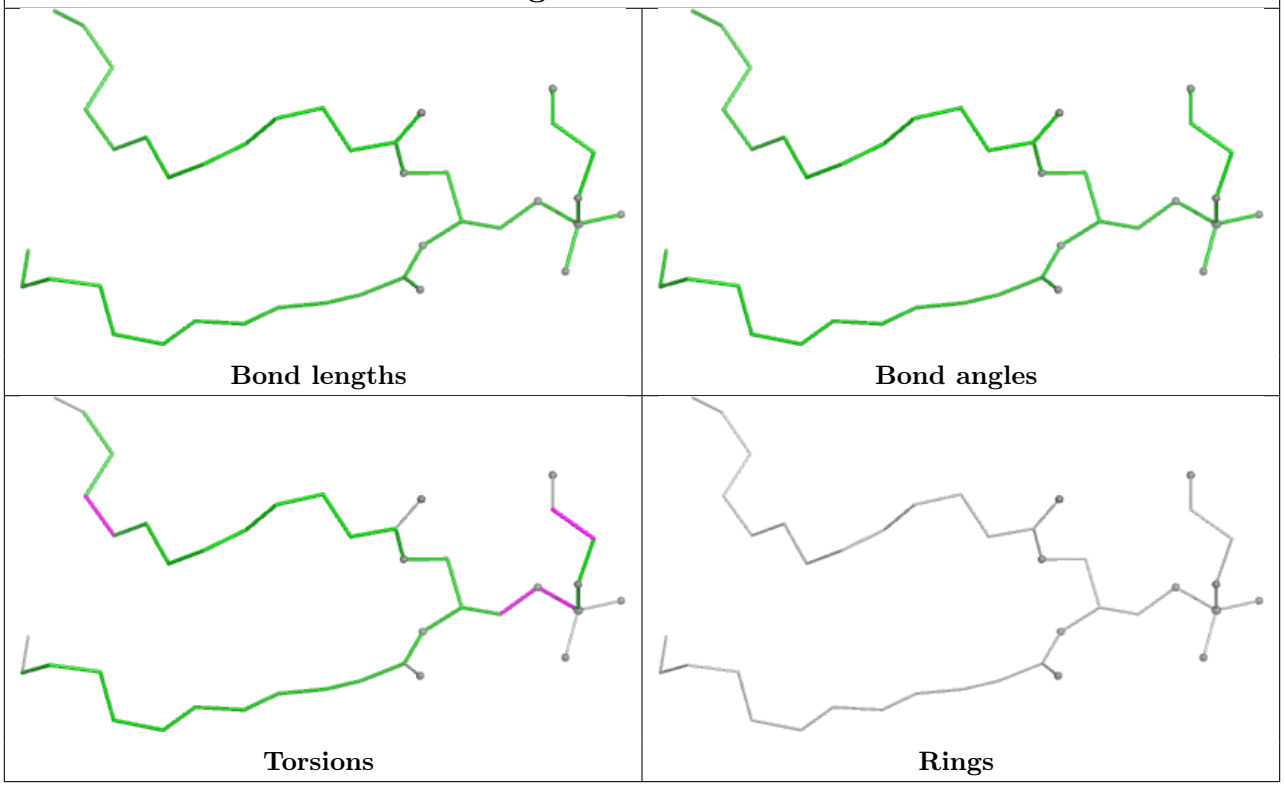
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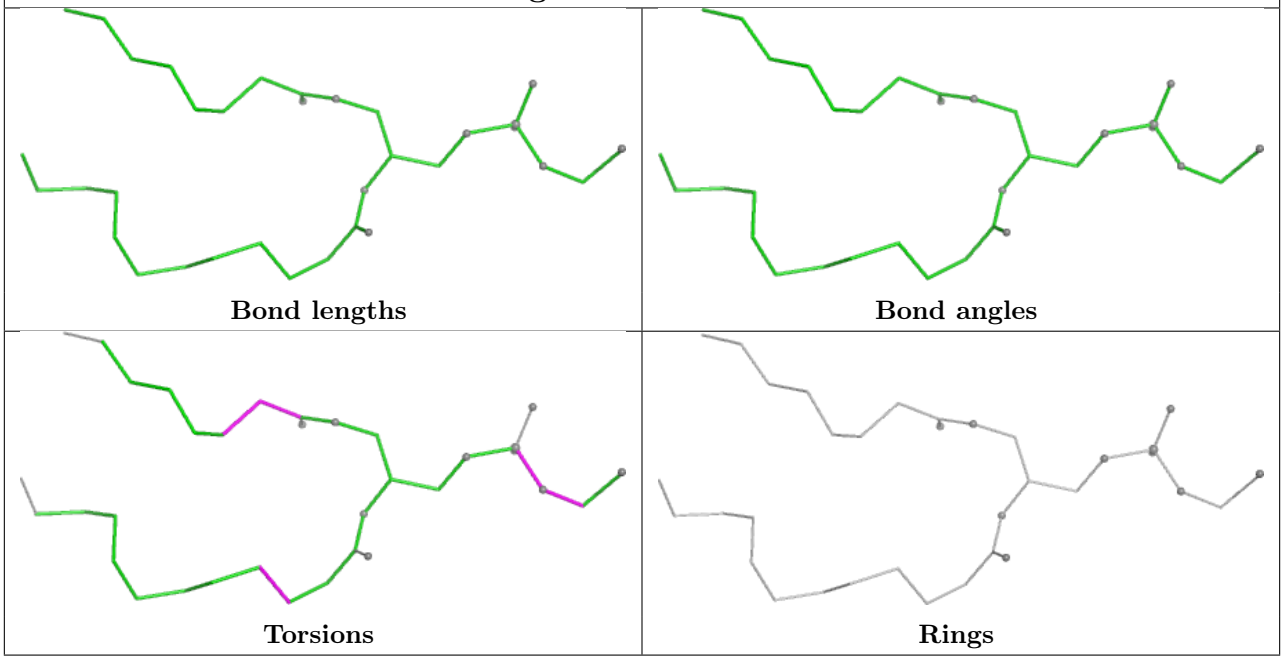
Ligand NAI 1 503



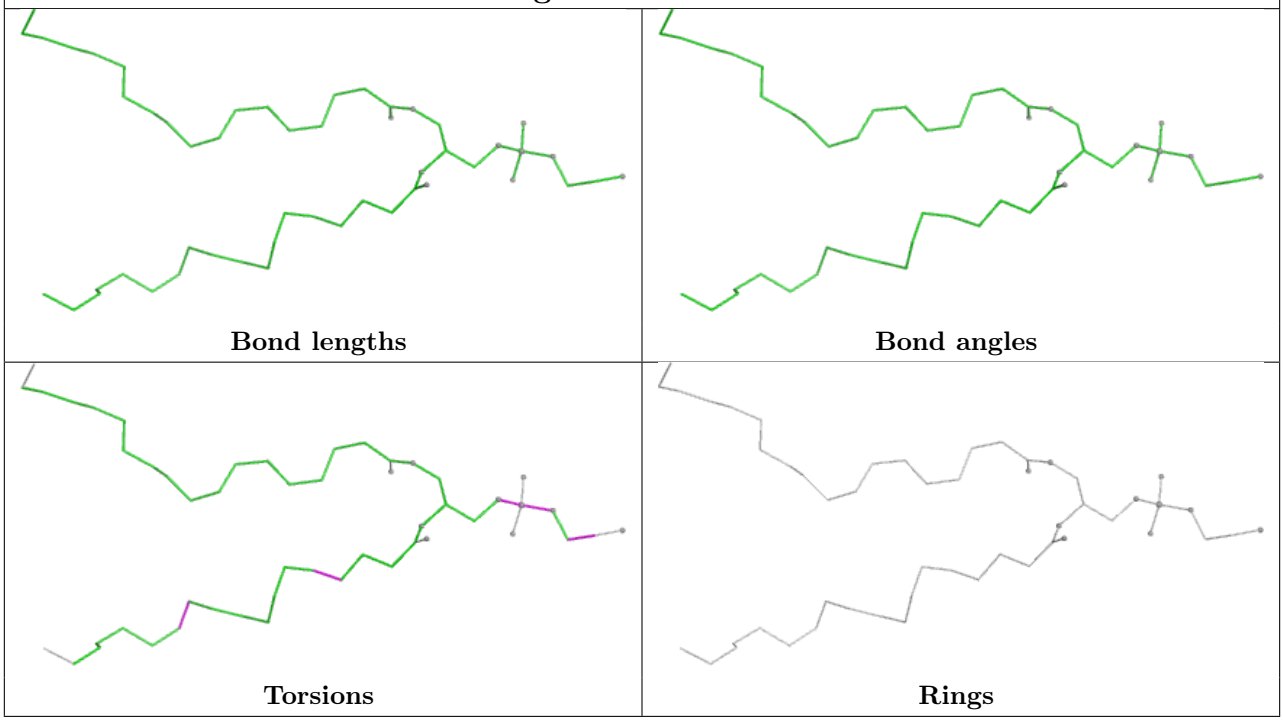
Ligand 3PE K 101



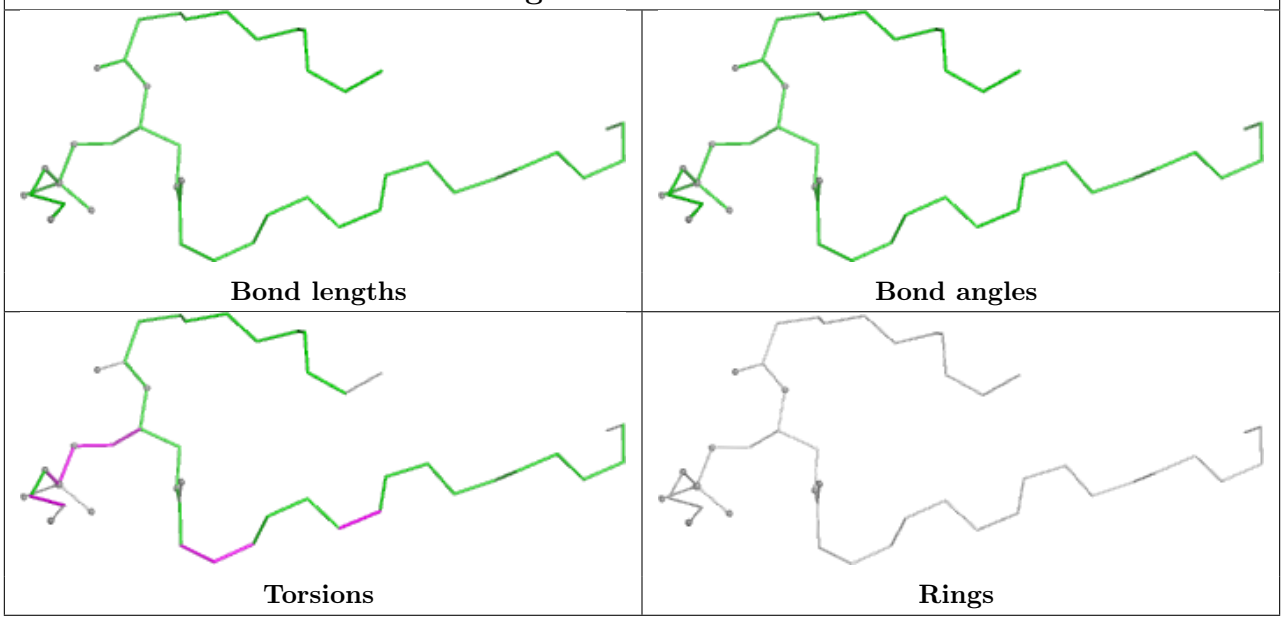
Ligand 3PE V 201



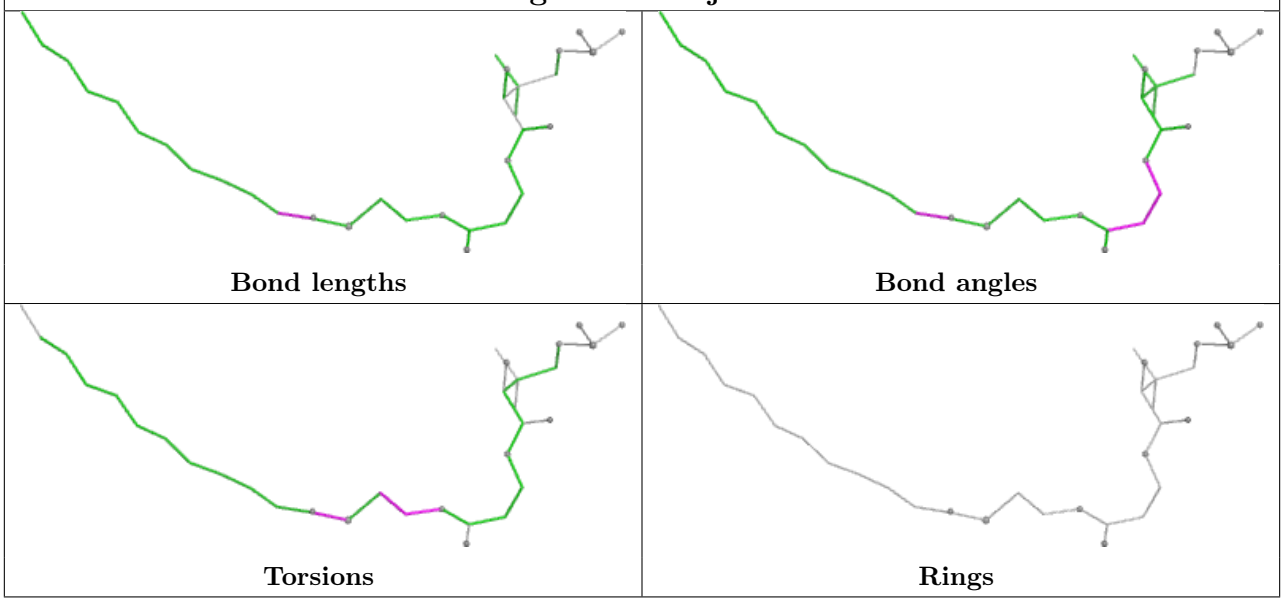
Ligand 3PE 6 203



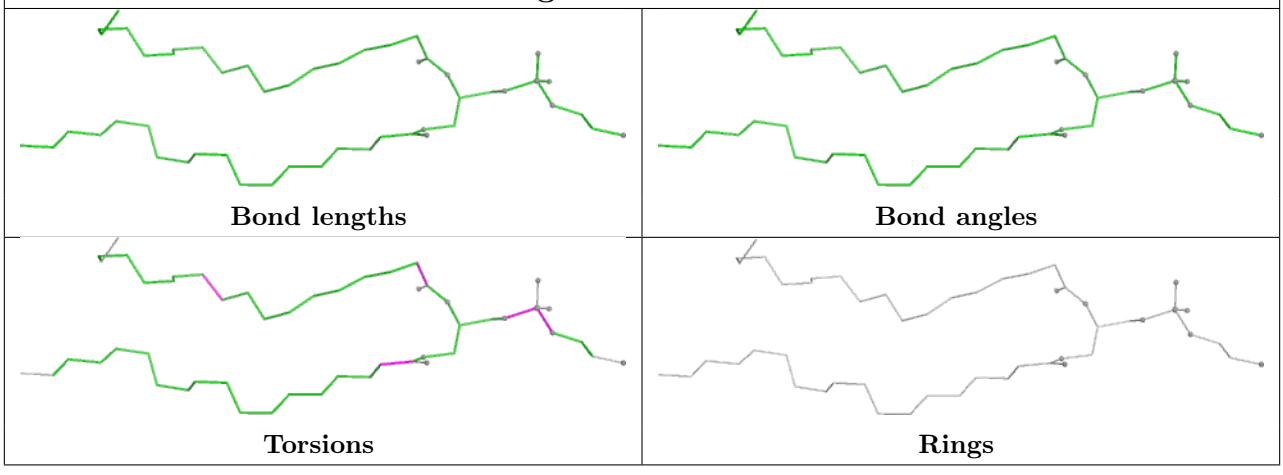
Ligand 3PE M 501



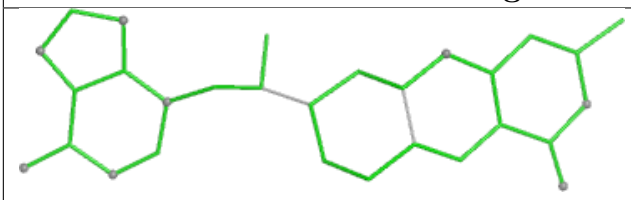
Ligand ZMP j 201



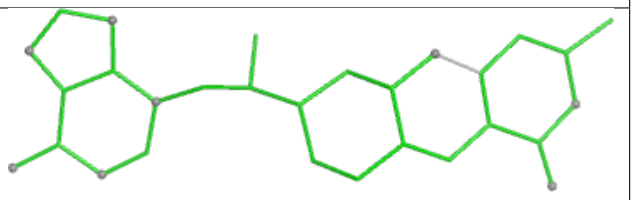
Ligand 3PE i 201



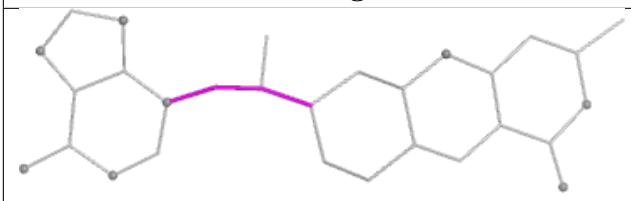
Ligand A1JBT H 402



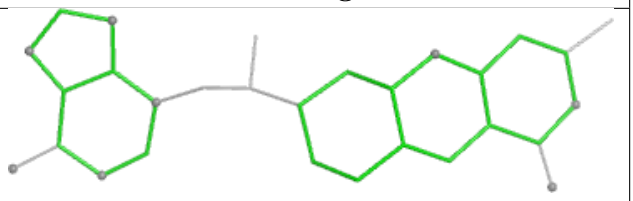
Bond lengths



Bond angles

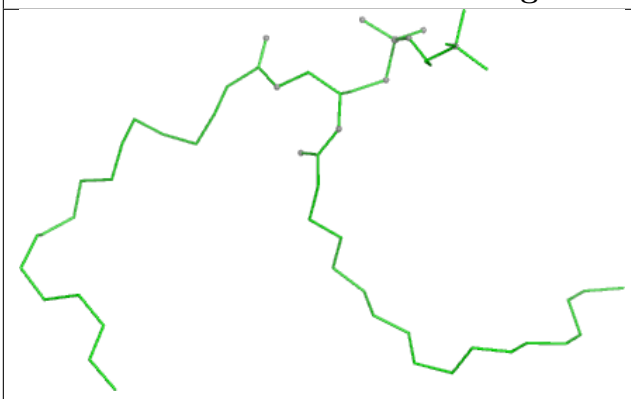


Torsions

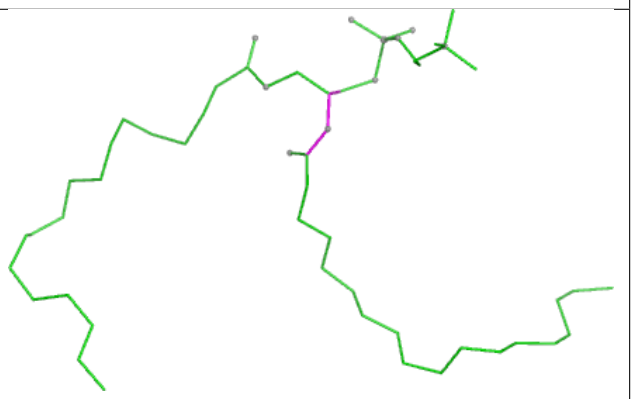


Rings

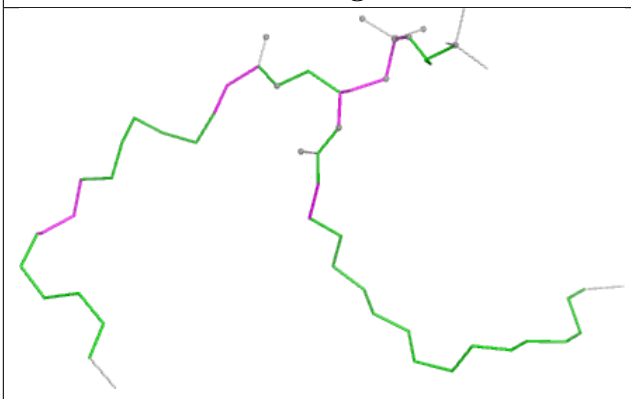
Ligand PC1 L 1002



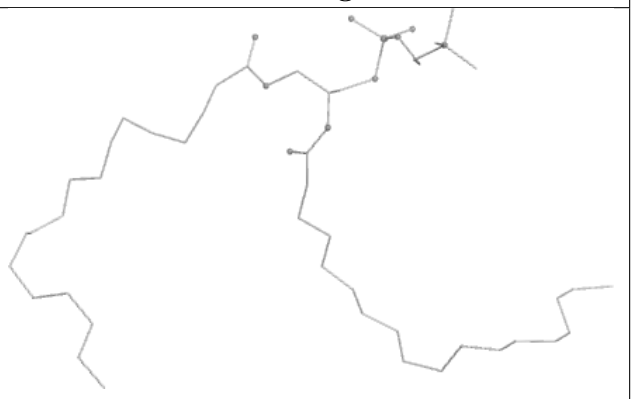
Bond lengths



Bond angles

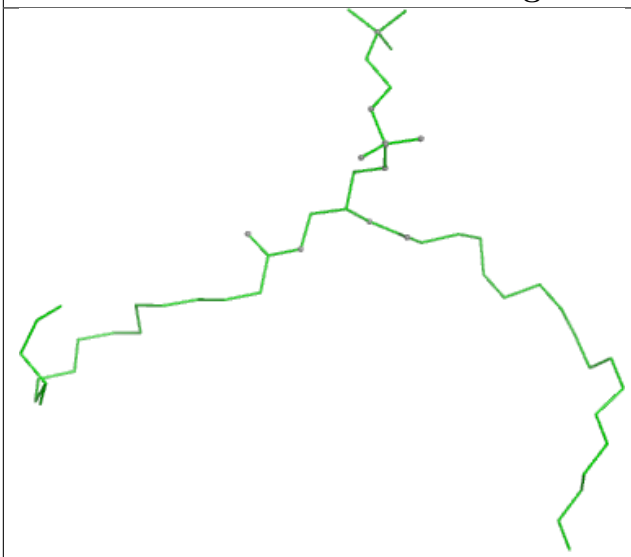


Torsions

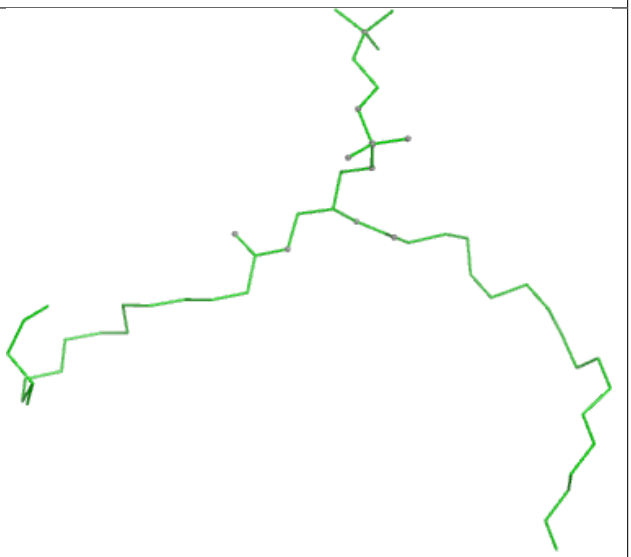


Rings

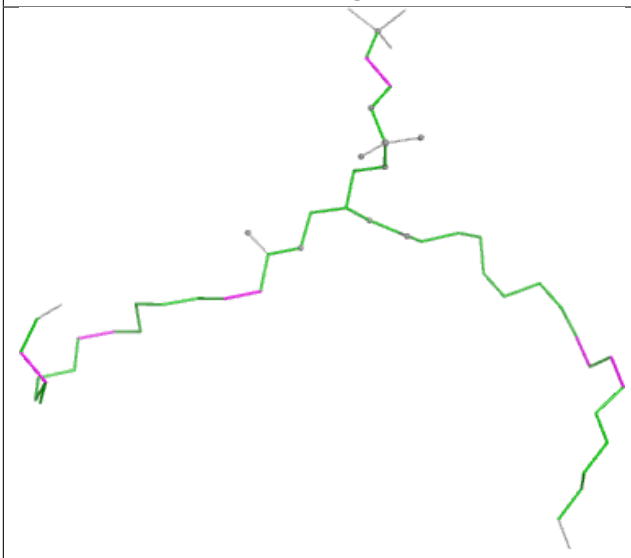
Ligand PC1 M 503



Bond lengths



Bond angles

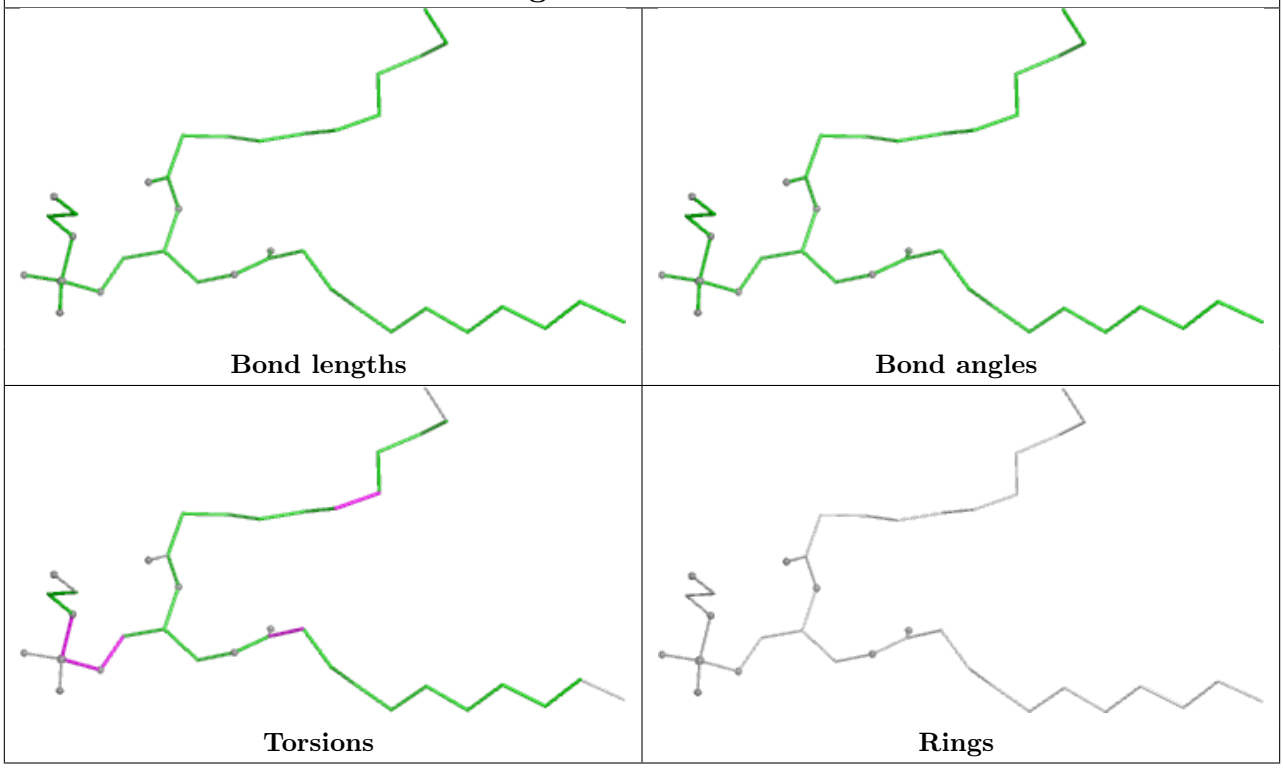


Torsions

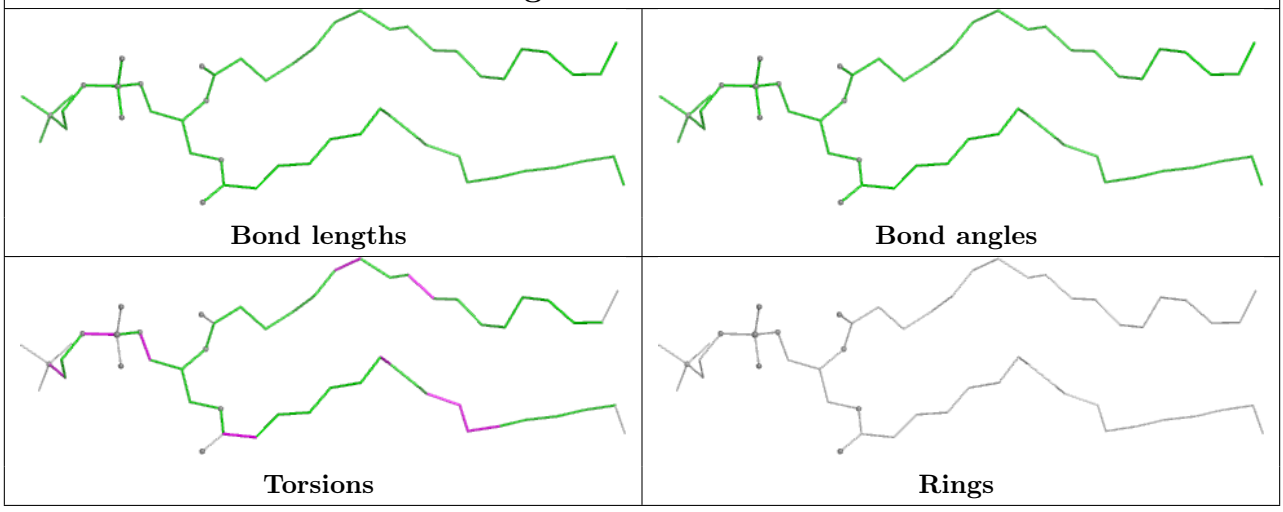


Rings

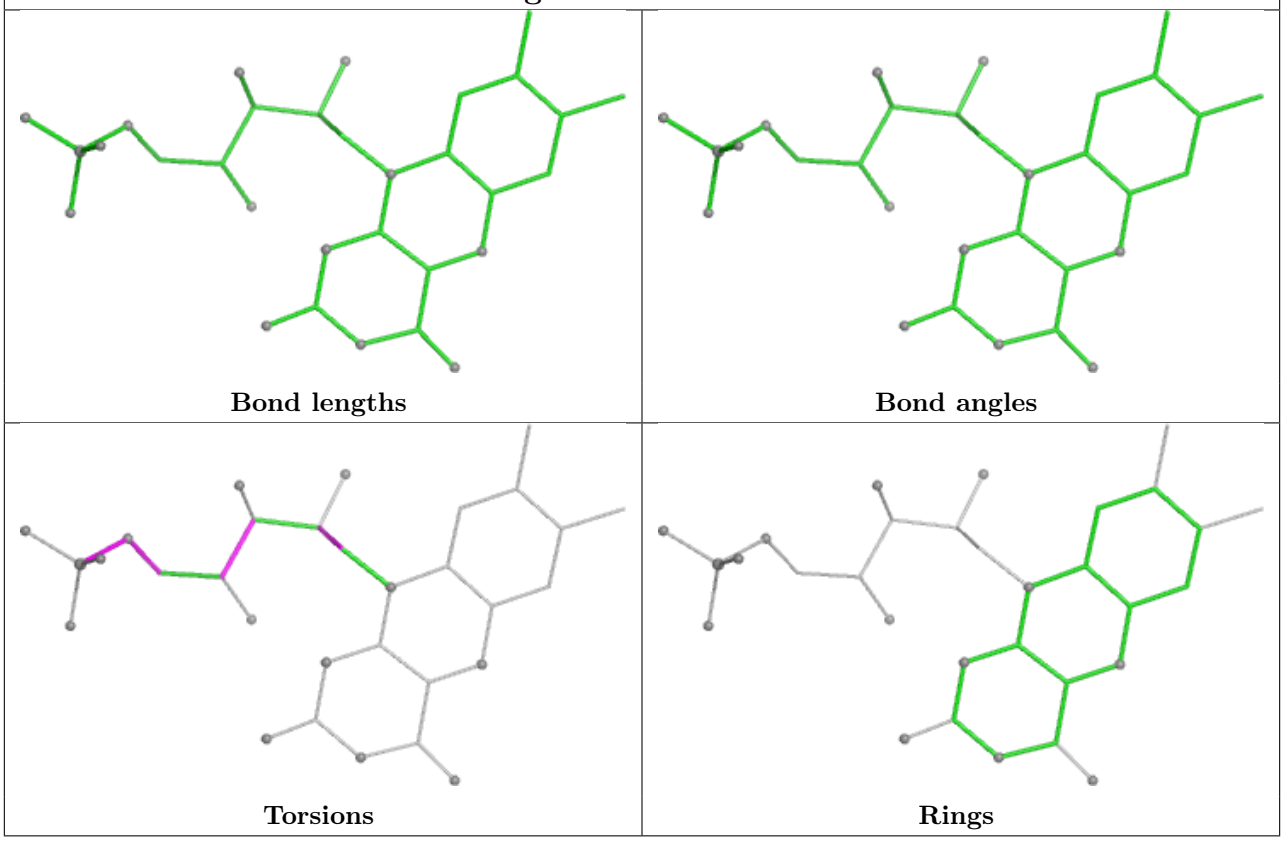
Ligand 3PE V 202



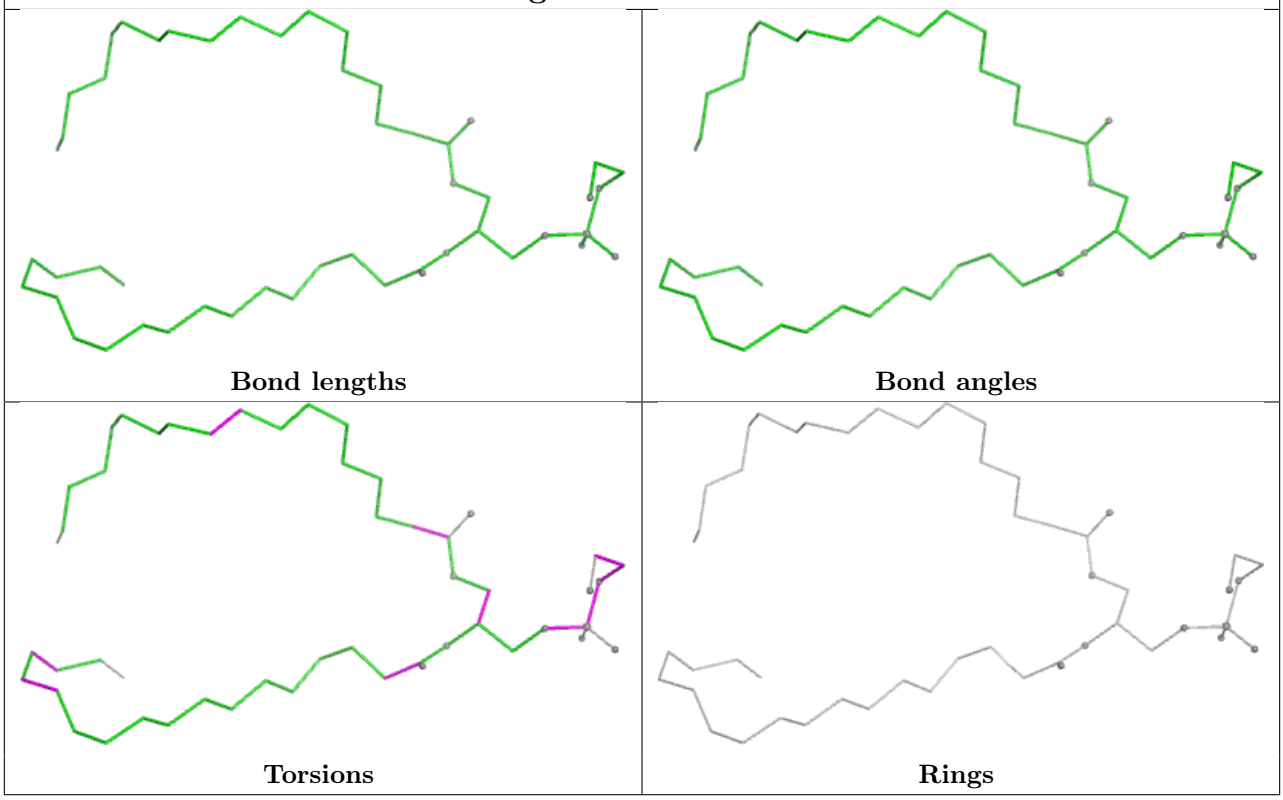
Ligand PC1 M 502



Ligand FMN 1 502



Ligand 3PE A 202



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.

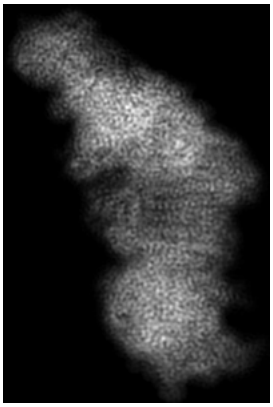
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-53477. These allow visual inspection of the internal detail of the map and identification of artifacts.

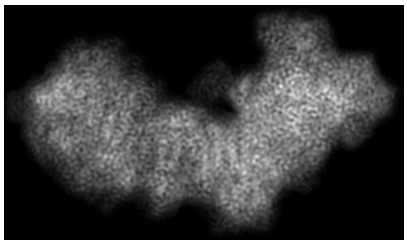
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

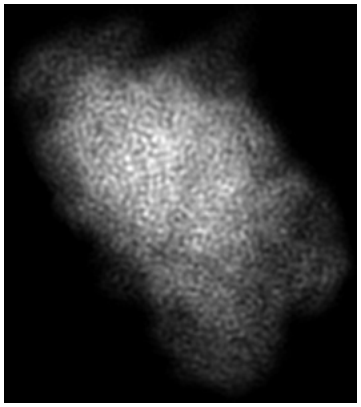
6.1.1 Primary map



X



Y

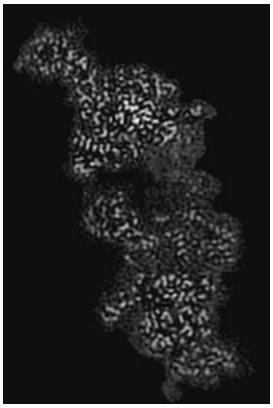


Z

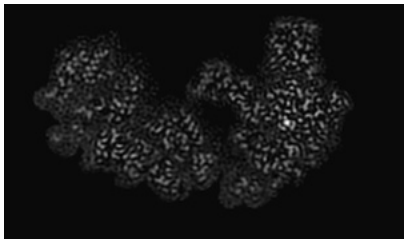
The images above show the map projected in three orthogonal directions.

6.2 Central slices

6.2.1 Primary map



X Index: 70



Y Index: 79

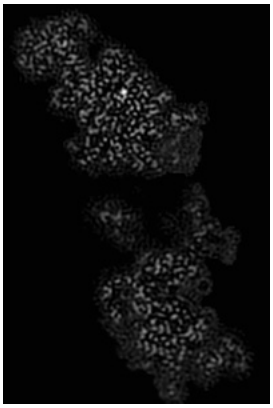


Z Index: 119

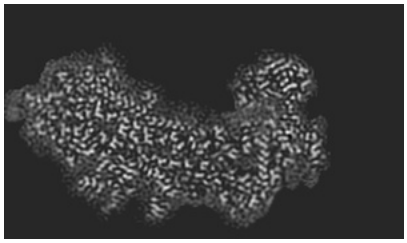
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

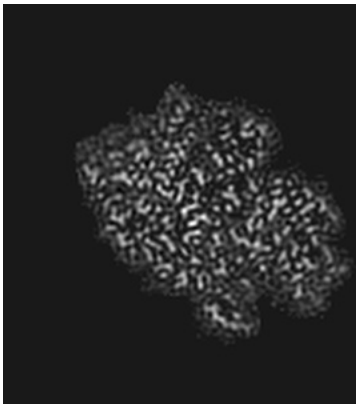
6.3.1 Primary map



X Index: 78



Y Index: 104

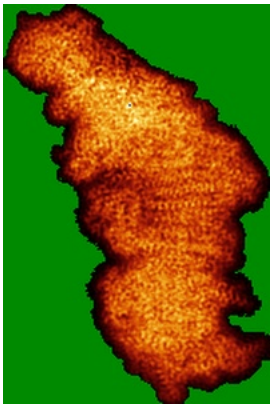


Z Index: 174

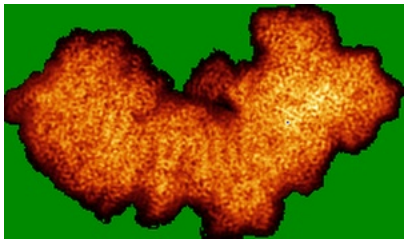
The images above show the largest variance slices of the map in three orthogonal directions.

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

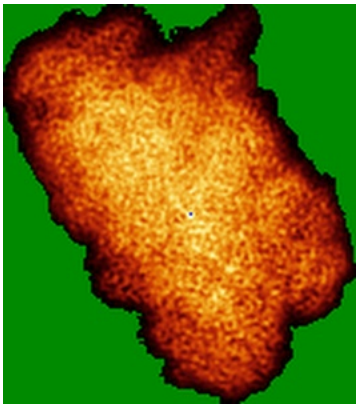
6.4.1 Primary map



X



Y

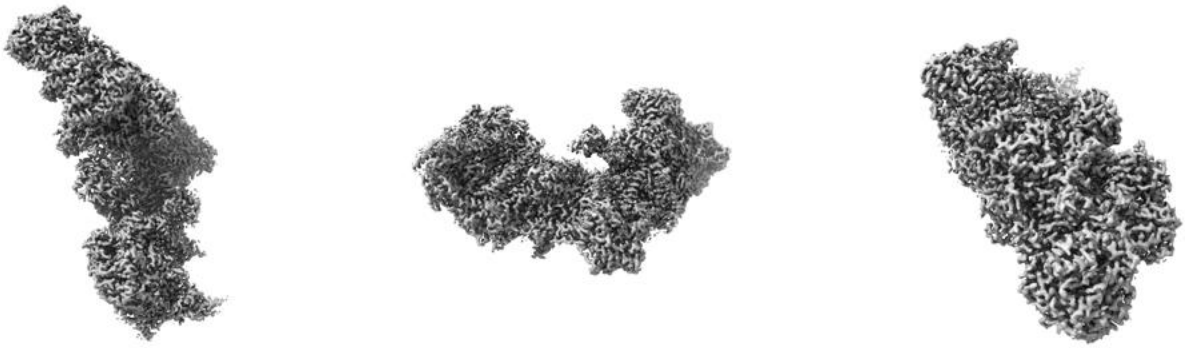


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.095. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

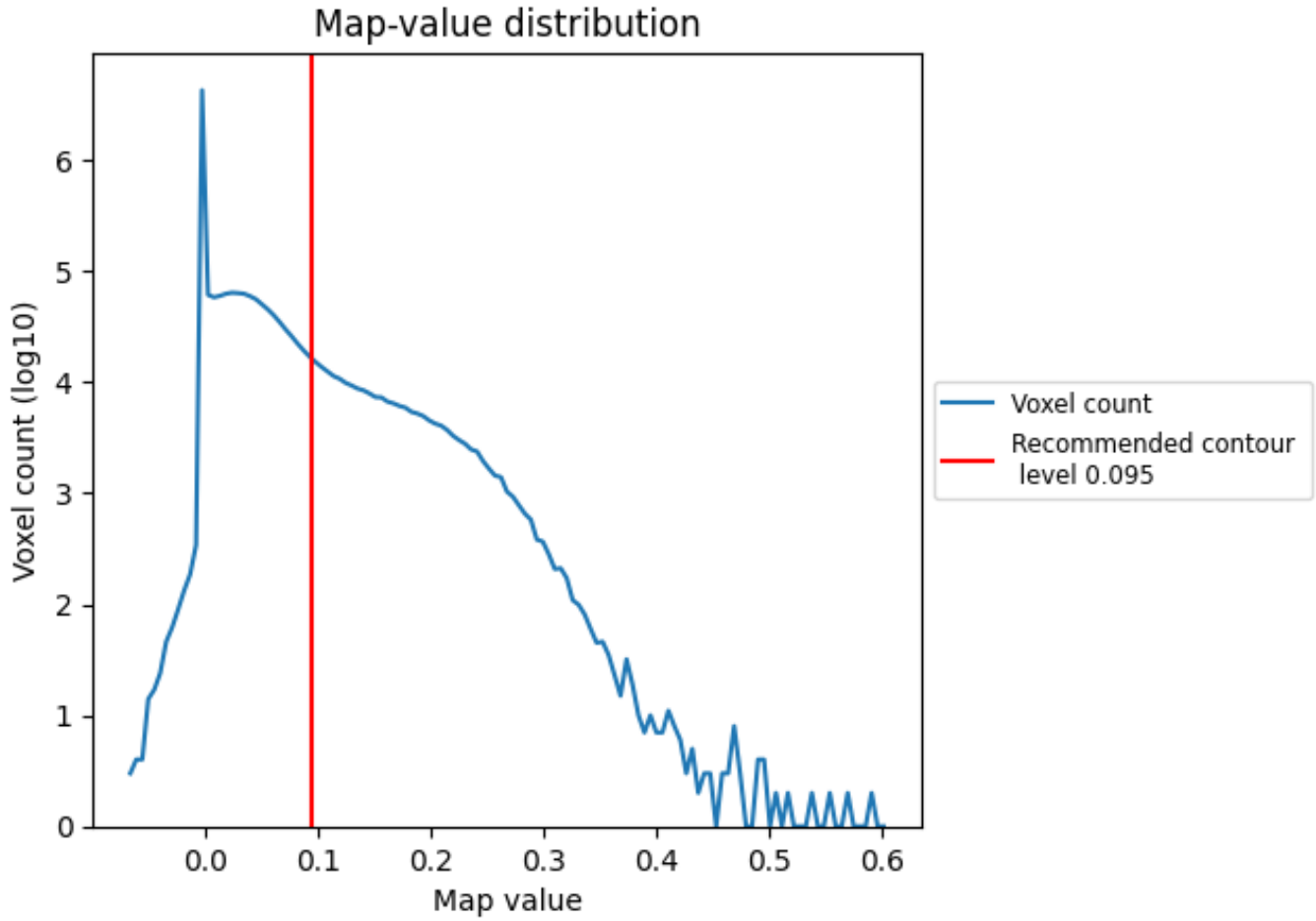
6.6 Mask visualisation (i)

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

7 Map analysis

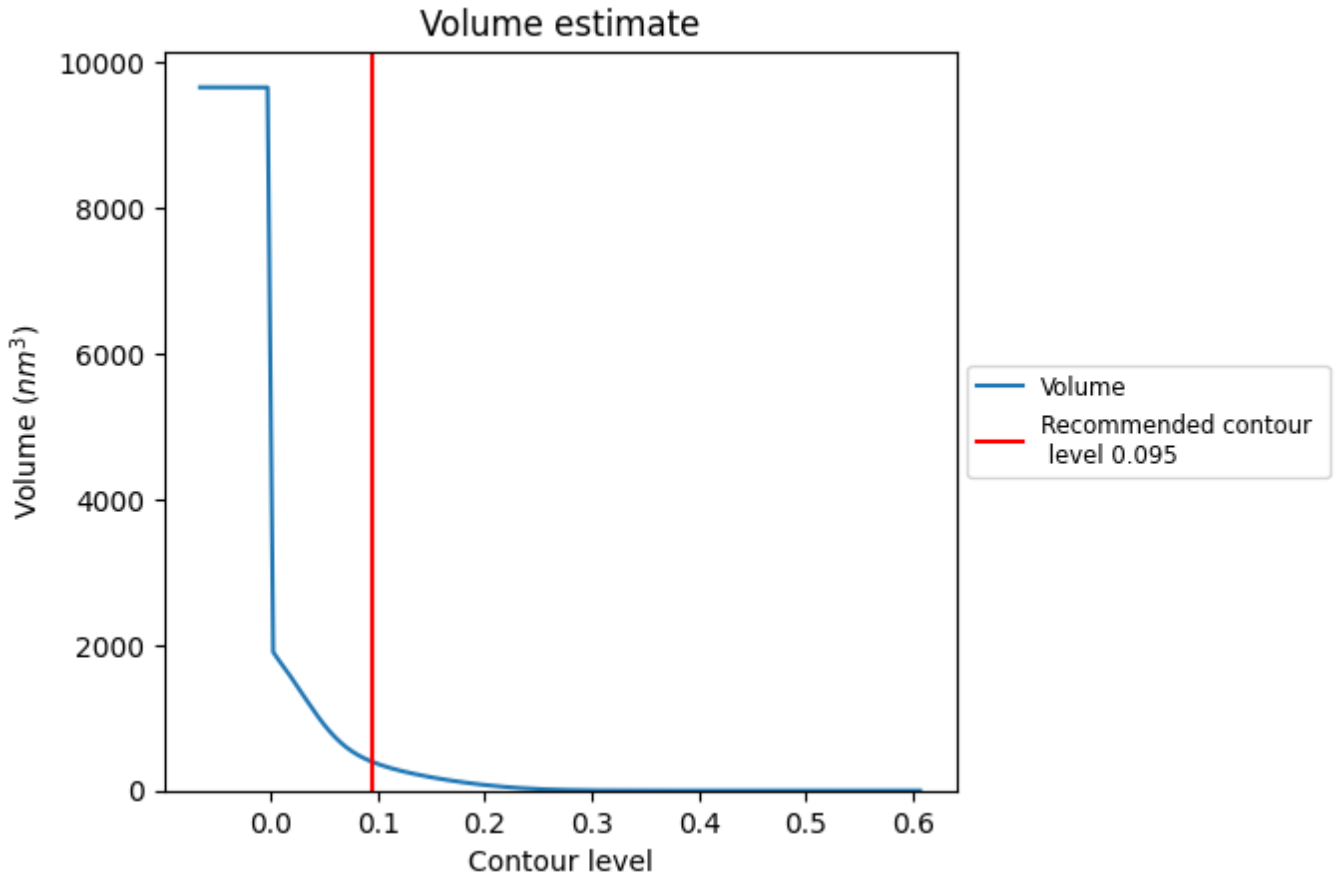
This section contains the results of statistical analysis of the map.

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 394 nm^3; this corresponds to an approximate mass of 356 kDa.

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

7.3 Rotationally averaged power spectrum (i)

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

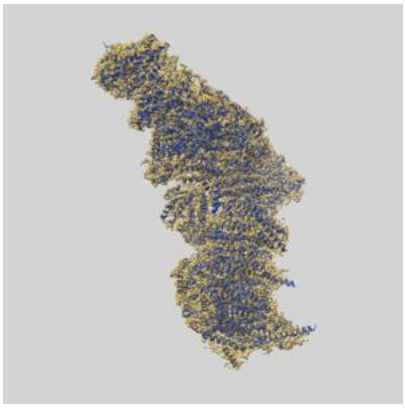
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

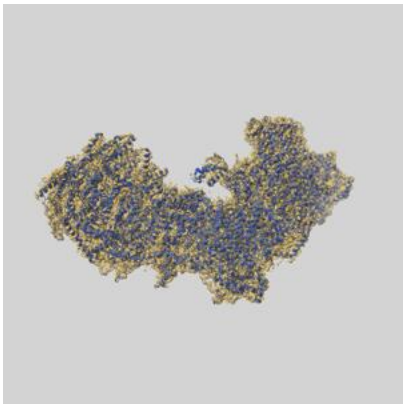
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-53477 and PDB model 9R03. Per-residue inclusion information can be found in section 3 on page 21.

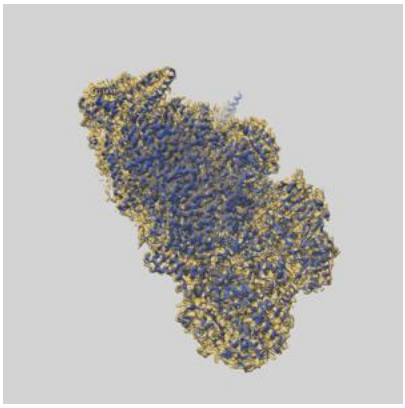
9.1 Map-model overlay



X



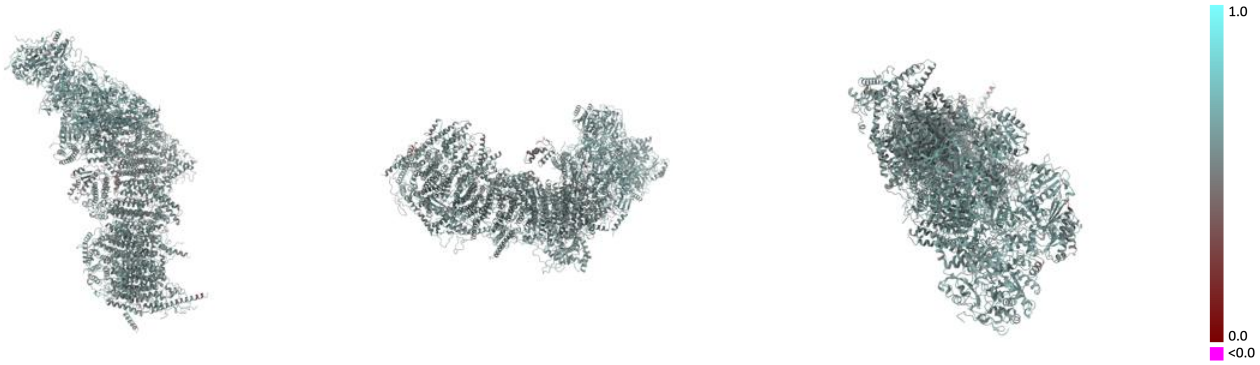
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.095 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.

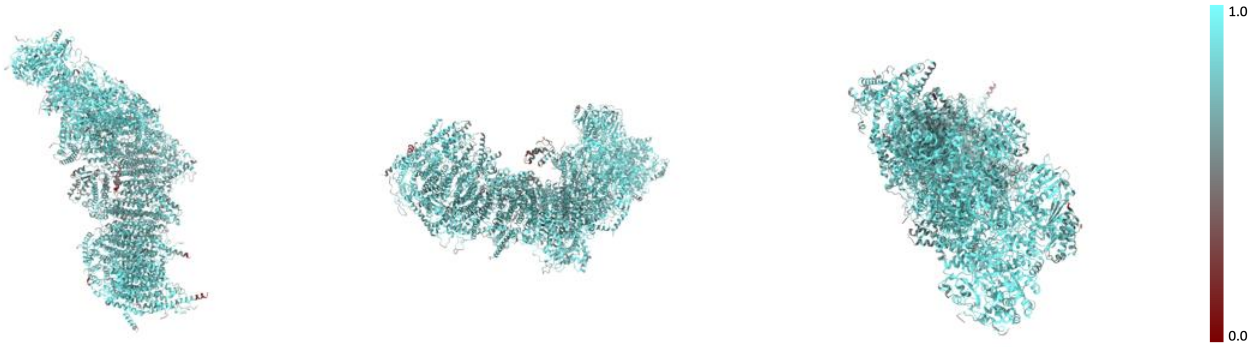
9.2 Q-score mapped to coordinate model (i)



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.

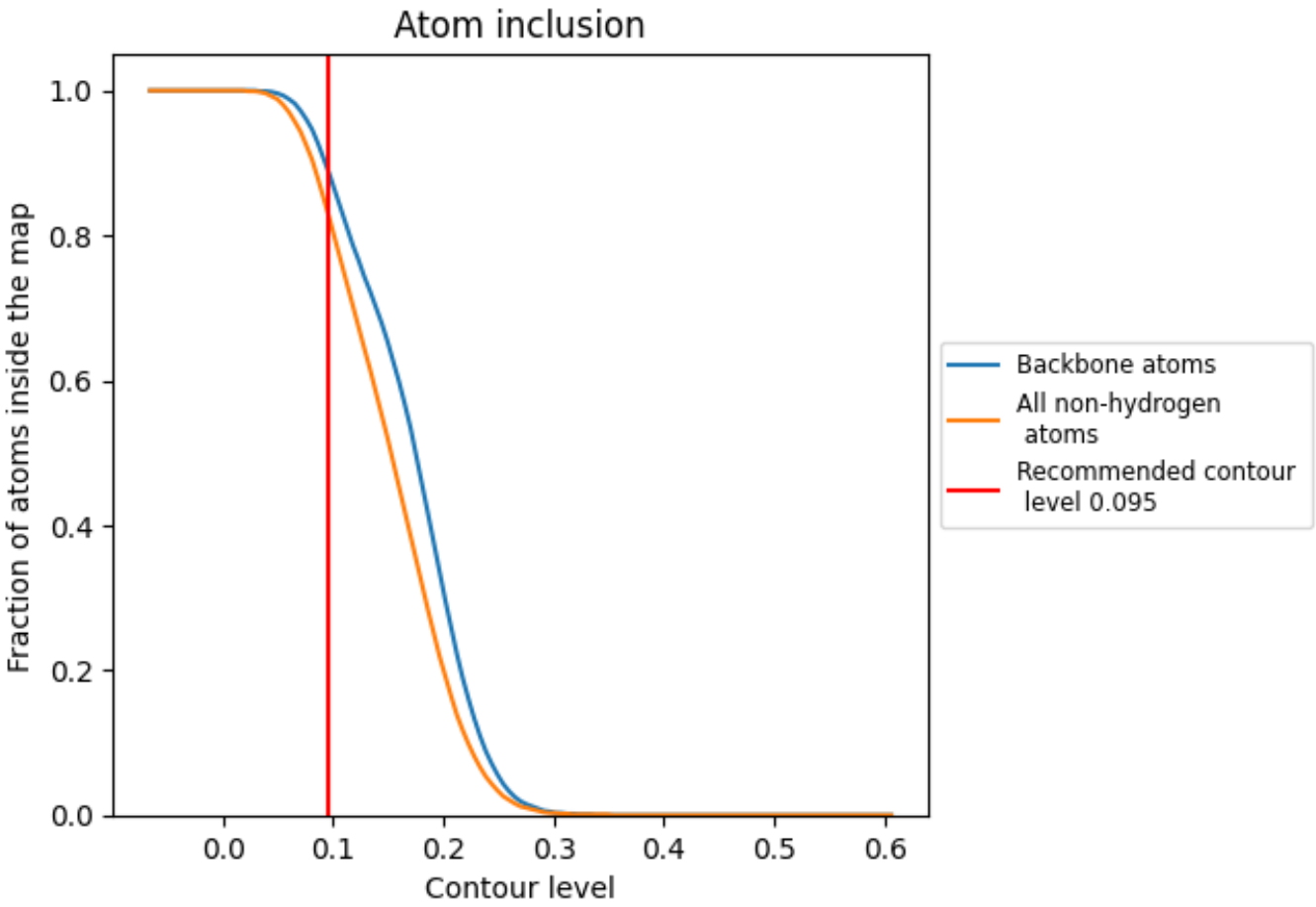
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.095).

9.4 Atom inclusion (i)



At the recommended contour level, 89% of all backbone atoms, 83% 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 (0.095) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8340	0.5690
1	0.8920	0.5810
2	0.8490	0.5700
3	0.8780	0.5890
4	0.8790	0.5840
5	0.9110	0.6030
6	0.9150	0.5880
9	0.9370	0.5980
A	0.7380	0.5380
H	0.8410	0.5530
J	0.7810	0.5400
K	0.8310	0.5630
L	0.8670	0.5620
M	0.8780	0.5780
N	0.8510	0.5700
V	0.7310	0.5450
W	0.8590	0.5770
X	0.7710	0.5410
Y	0.7820	0.5590
Z	0.8020	0.5600
a	0.8540	0.5700
b	0.8650	0.5980
c	0.8780	0.6000
d	0.8400	0.5790
e	0.7870	0.5670
f	0.7400	0.5630
g	0.8050	0.5770
h	0.8410	0.5910
i	0.8630	0.5950
j	0.4890	0.4820
k	0.7360	0.5510
l	0.7920	0.5560
m	0.7570	0.5450
n	0.7780	0.5430
o	0.8060	0.5650



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
p	0.7940	0.5600
q	0.8390	0.5630
r	0.7690	0.5480
s	0.7790	0.5380
t	0.8210	0.5640
u	0.8210	0.5490
v	0.8210	0.5630
w	0.7770	0.5490
x	0.7490	0.5450
y	0.7590	0.5500
z	0.8450	0.5660