Full wwPDB EM Validation Report ⓘ

Aug 23, 2026 – 04:33 pm BST

PDB ID	:	7ZD6 / pdb_00007zd6
EMDB ID	:	EMD-14637
Title	:	Complex I from Ovis aries, at pH7.4, Open state
Authors	:	Sazanov, L.; Petrova, O.
Deposited on	:	2022-03-29
Resolution	:	3.16 Å(reported)
Based on initial model	:	6ZKE

This is a Full wwPDB EM Validation 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:

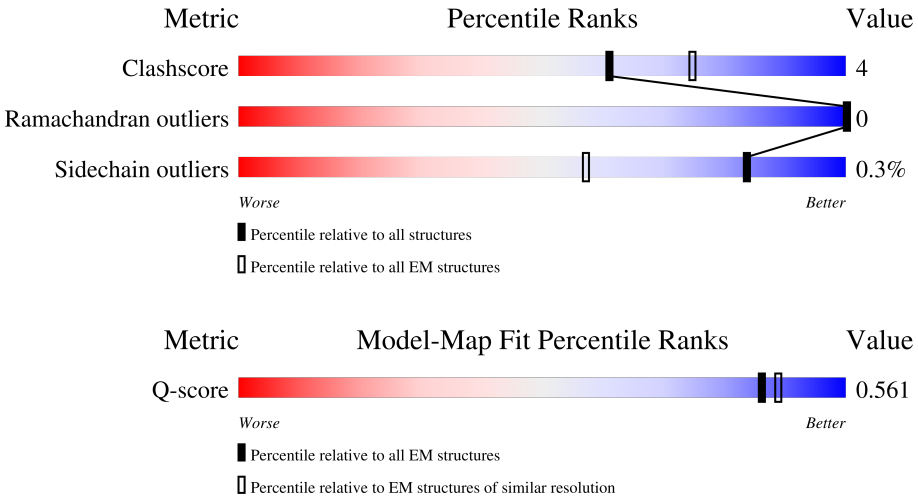
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data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

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

The reported resolution of this entry is 3.16 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.



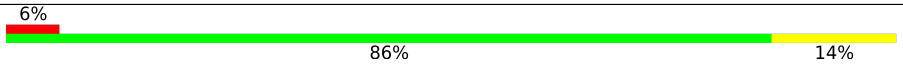
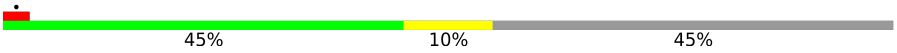
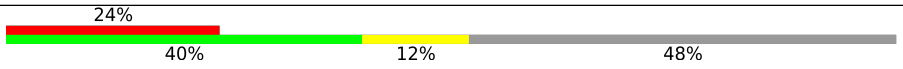
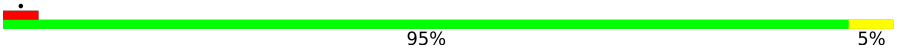
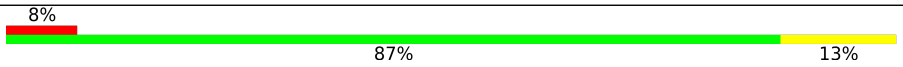
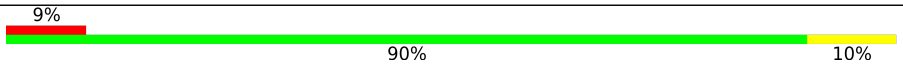
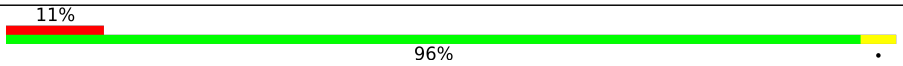
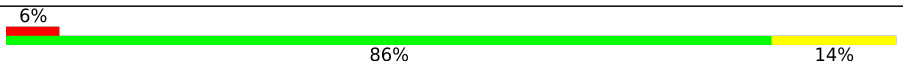
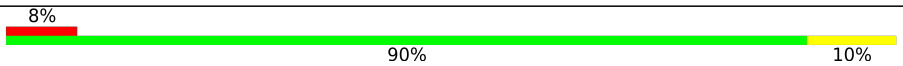
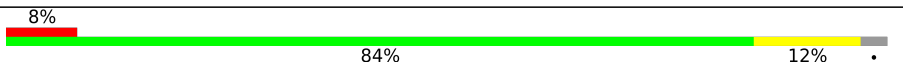
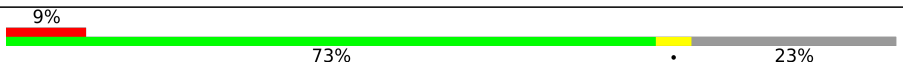
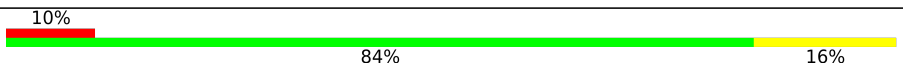
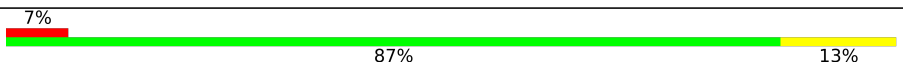
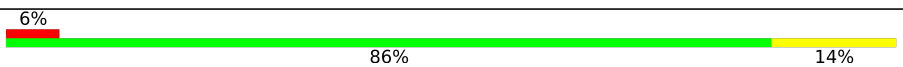
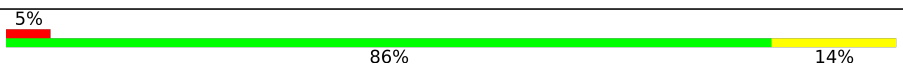
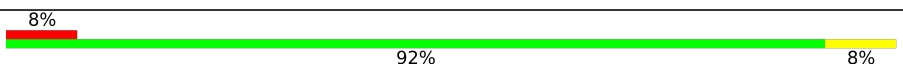
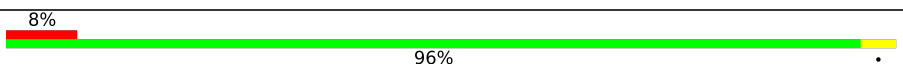
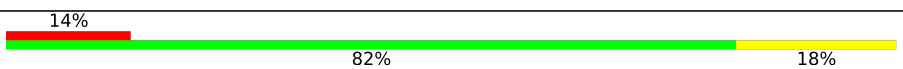
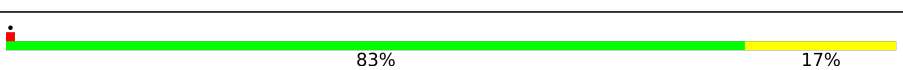
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14474 (2.66 - 3.66)

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	115	17%, 76%, 20%
2	H	318	83%, 16%
3	J	175	9%, 79%, 17%
4	K	98	86%, 14%

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Mol	Chain	Length	Quality of chain
5	L	606	
6	M	459	
7	N	347	
8	V	140	
9	W	139	
10	X	157	
10	j	157	
11	Y	171	
12	Z	171	
13	k	320	
14	l	105	
15	m	80	
16	n	79	
17	o	120	
18	p	128	
19	q	144	
20	r	128	
21	s	122	
22	t	177	
23	u	65	
24	v	155	
25	w	101	
26	x	49	
27	y	50	
28	z	70	

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Mol	Chain	Length	Quality of chain
29	1	430	5% 87% 13%
30	2	213	12% 87% 13%
31	3	688	5% 90% 10%
32	4	463	6% 79% 12% 9%
33	5	208	88% 12%
34	6	156	90% 10%
35	9	176	86% 14%
36	a	44	11% 93% 7%
37	b	95	13% 98%
38	c	126	87% 13%
39	d	380	8% 70% 8% 22%
40	e	86	10% 88% 12%
41	f	113	6% 92% 8%
42	g	114	11% 92% 8%
43	h	114	79% 5% 16%
44	i	145	6% 93% 7%

2 Entry composition (i)

There are 57 unique types of molecules in this entry. The entry contains 66748 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	110	880	593	128	153	6	0	0

- Molecule 2 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	H	314	2498	1685	380	414	19	0	0

- Molecule 3 is a protein called NADH-ubiquinone oxidoreductase chain 6.

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

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

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

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

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

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

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

- Molecule 7 is a protein called NADH-ubiquinone oxidoreductase chain 2.

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

- Molecule 8 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	V	140	Total	C	N	O	S	0	0
			1028	656	175	191	6		

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

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

- Molecule 10 is a protein called Acyl carrier protein.

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

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

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

- Molecule 12 is a protein called Complex I-PDSW.

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

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

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

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

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

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

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

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

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

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

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

- Molecule 18 is a protein called NADH:ubiquinone oxidoreductase subunit B4.

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

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

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

- Molecule 20 is a protein called Mitochondrial complex I, B17 subunit.

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

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

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

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

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

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

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

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

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

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

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

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

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

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

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

- Molecule 28 is a protein called Complex I-MWFE.

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

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	1	430	Total 3312	C 2086	N 593	O 613	S 20	0	0

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	2	213	Total 1655	C 1058	N 278	O 309	S 10	0	0

- Molecule 31 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	3	688	Total 5275	C 3301	N 922	O 1011	S 41	0	0

- Molecule 32 is a protein called Complex I-49kD.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	4	421	Total 3390	C 2165	N 581	O 619	S 25	0	0

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

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 NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	6	156	Total	C	N	O	S	0	0
			1247	795	225	213	14		

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	9	176	Total	C	N	O	S	0	0
			1414	889	243	270	12		

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

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

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

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

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

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

- Molecule 39 is a protein called NADH:ubiquinone oxidoreductase subunit A9.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	d	297	Total	C	N	O	S	0	0
			2372	1516	432	419	5		

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

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

- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

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

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

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

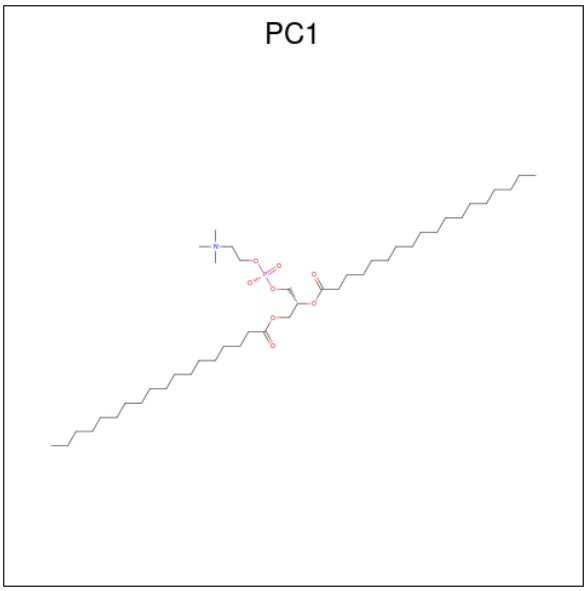
- Molecule 43 is a protein called Mitochondrial complex I, B14.5a subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	h	96	Total	C	N	O	S	0	0
			769	480	146	140	3		

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

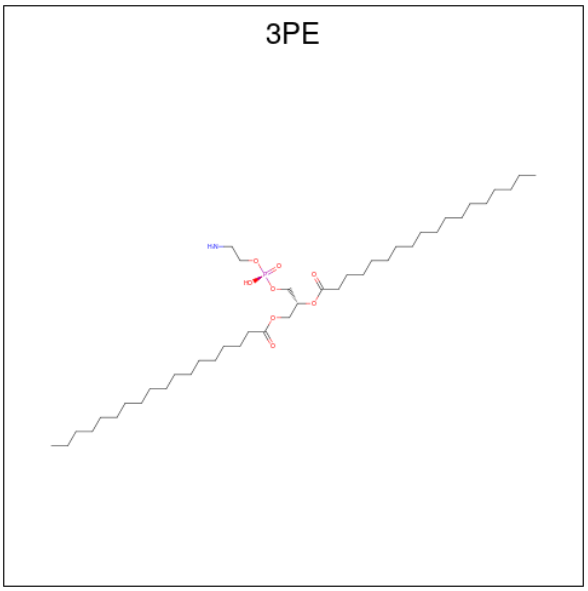
Mol	Chain	Residues	Atoms					AltConf	Trace
44	i	145	Total	C	N	O	S	0	0
			1209	778	216	210	5		

- Molecule 45 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



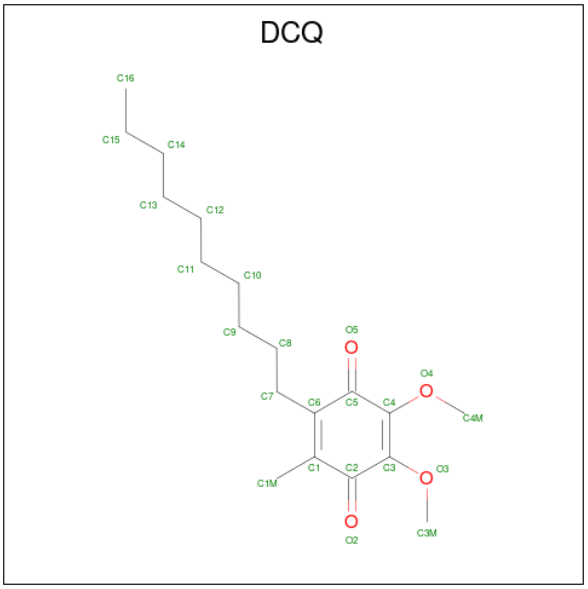
Mol	Chain	Residues	Atoms					AltConf
45	A	1	Total	C	N	O	P	0
			37	27	1	8	1	
45	A	1	Total	C	N	O	P	0
			46	36	1	8	1	
45	H	1	Total	C	N	O	P	0
			54	44	1	8	1	
45	L	1	Total	C	N	O	P	0
			54	44	1	8	1	
45	L	1	Total	C	N	O	P	0
			54	44	1	8	1	
45	M	1	Total	C	N	O	P	0
			54	44	1	8	1	

- Molecule 46 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



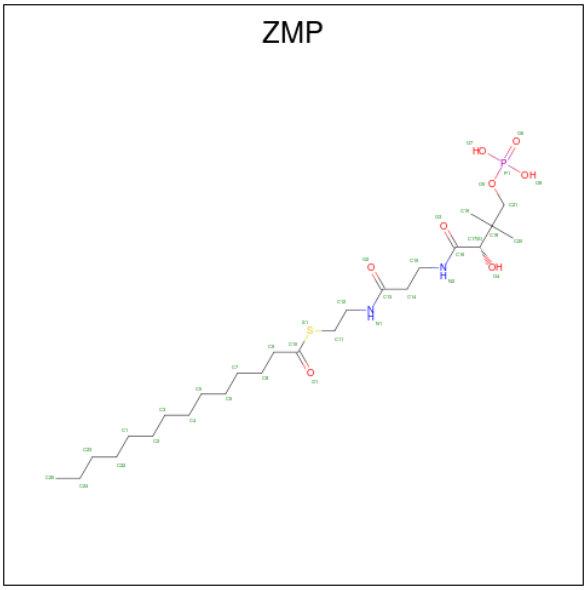
Mol	Chain	Residues	Atoms					AltConf
46	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
46	H	1	Total	C	N	O	P	0
			51	41	1	8	1	
46	H	1	Total	C	N	O	P	0
			51	41	1	8	1	
46	K	1	Total	C	N	O	P	0
			40	30	1	8	1	
46	L	1	Total	C	N	O	P	0
			51	41	1	8	1	
46	L	1	Total	C	N	O	P	0
			31	21	1	8	1	
46	M	1	Total	C	N	O	P	0
			44	34	1	8	1	
46	N	1	Total	C	N	O	P	0
			40	30	1	8	1	
46	N	1	Total	C	N	O	P	0
			51	41	1	8	1	
46	N	1	Total	C	N	O	P	0
			31	21	1	8	1	
46	V	1	Total	C	N	O	P	0
			35	25	1	8	1	
46	V	1	Total	C	N	O	P	0
			37	27	1	8	1	
46	V	1	Total	C	O	P		0
			27	18	8	1		
46	6	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 47 is 2-decyl-5,6-dimethoxy-3-methylcyclohexa-2,5-diene-1,4-dione (CCD ID: DCQ) (formula: $C_{19}H_{30}O_4$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
47	H	1	23	19	4	0

- Molecule 48 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (CCD ID: ZMP) (formula: $C_{25}H_{49}N_2O_8PS$).



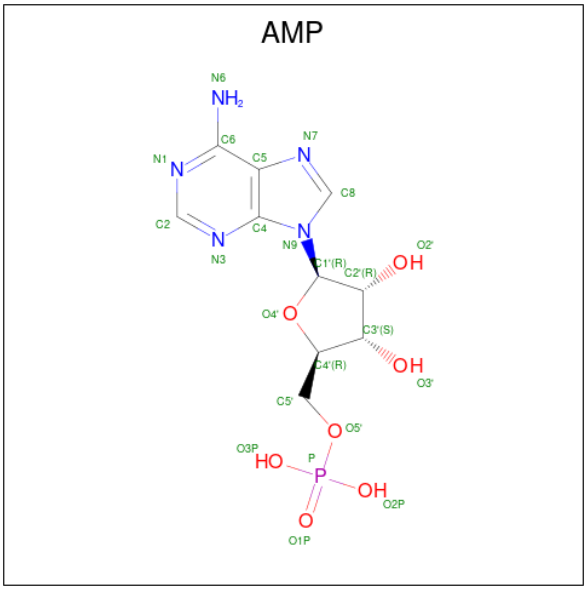
Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
48	X	1	31	20	2	7	1	1	0

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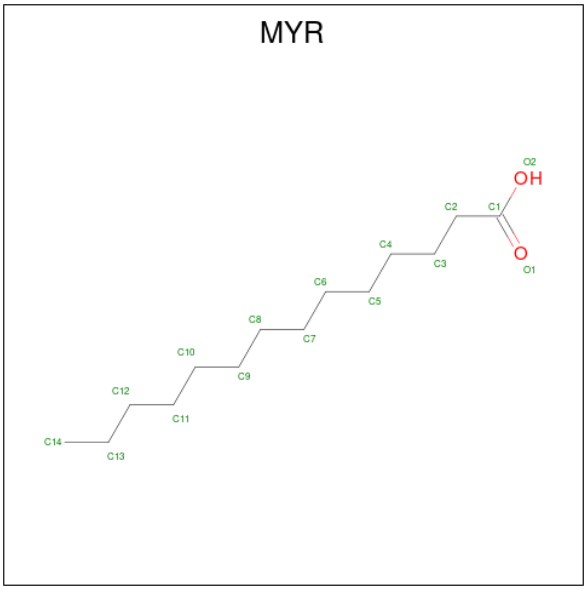
Mol	Chain	Residues	Atoms						AltConf
48	j	1	Total	C	N	O	P	S	0
			34	23	2	7	1	1	

- Molecule 49 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



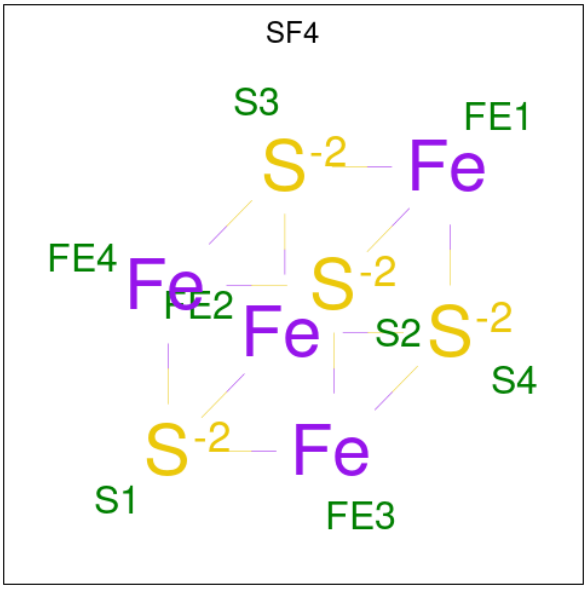
Mol	Chain	Residues	Atoms					AltConf
49	k	1	Total	C	N	O	P	0
			23	10	5	7	1	

- Molecule 50 is MYRISTIC ACID (CCD ID: MYR) (formula: $C_{14}H_{28}O_2$).



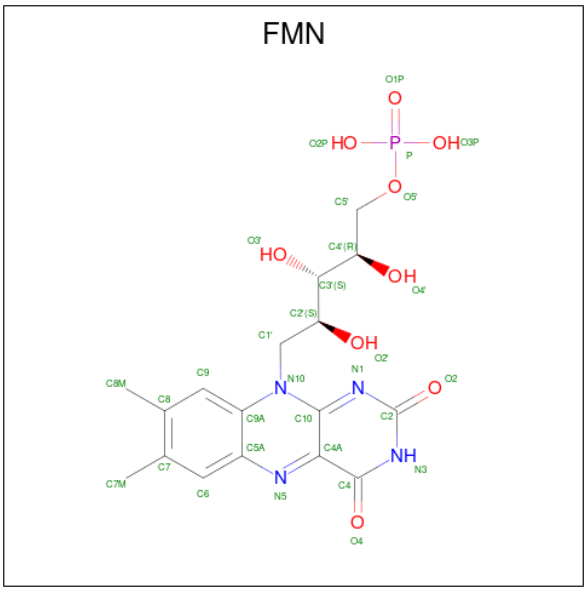
Mol	Chain	Residues	Atoms			AltConf
50	s	1	Total	C	O	0
			15	14	1	

- Molecule 51 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



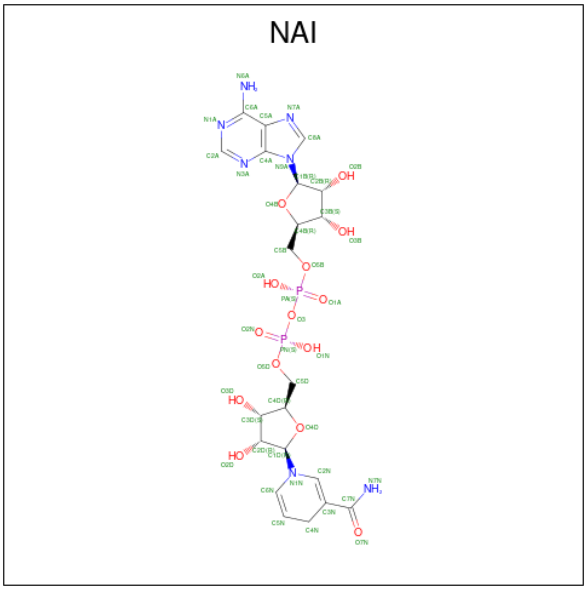
Mol	Chain	Residues	Atoms			AltConf
51	1	1	Total	Fe	S	0
			8	4	4	
51	3	1	Total	Fe	S	0
			8	4	4	
51	3	1	Total	Fe	S	0
			8	4	4	
51	6	1	Total	Fe	S	0
			8	4	4	
51	9	1	Total	Fe	S	0
			8	4	4	
51	9	1	Total	Fe	S	0
			8	4	4	

- Molecule 52 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



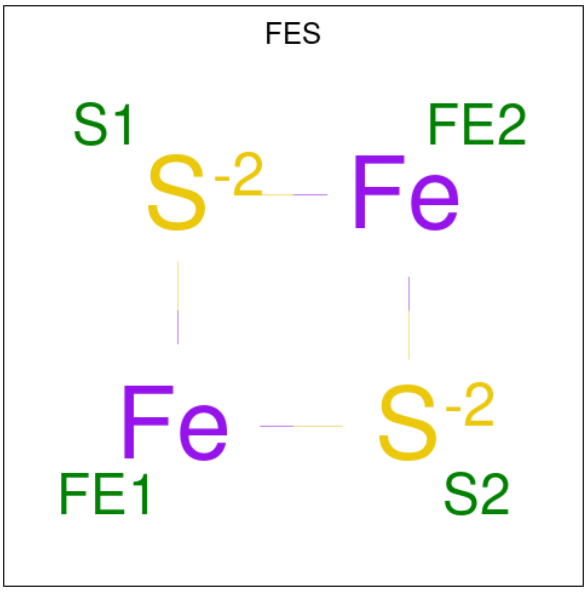
Mol	Chain	Residues	Atoms					AltConf
52	1	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 53 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms					AltConf
53	1	1	Total	C	N	O	P	0
			44	21	7	14	2	

- Molecule 54 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms	AltConf
54	2	1	Total Fe S 4 2 2	0
54	3	1	Total Fe S 4 2 2	0

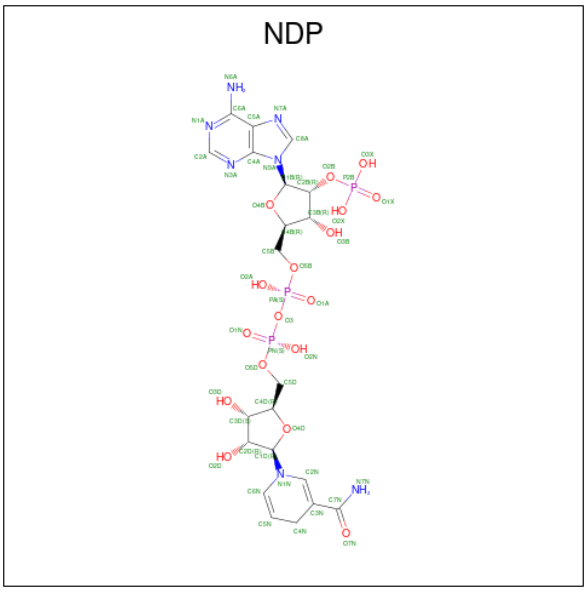
- Molecule 55 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	AltConf
55	3	1	Total K 1 1	0

- Molecule 56 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 57 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



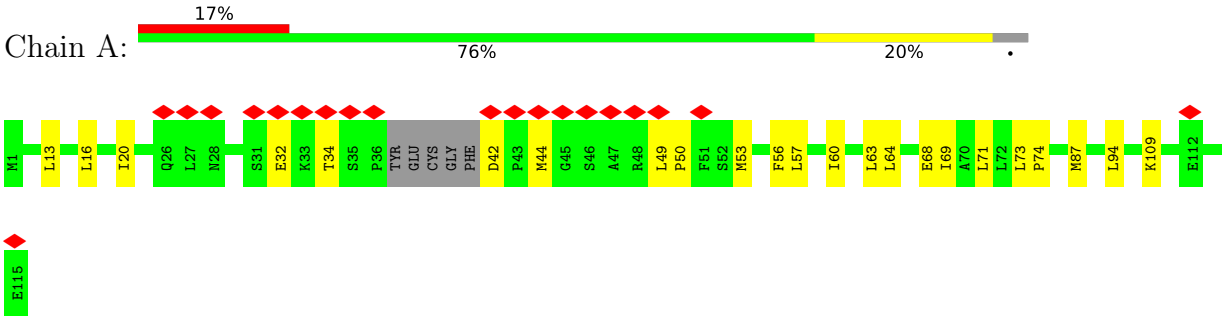
Mol	Chain	Residues	Atoms					AltConf
57	d	1	Total	C	N	O	P	0
			48	21	7	17	3	

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.

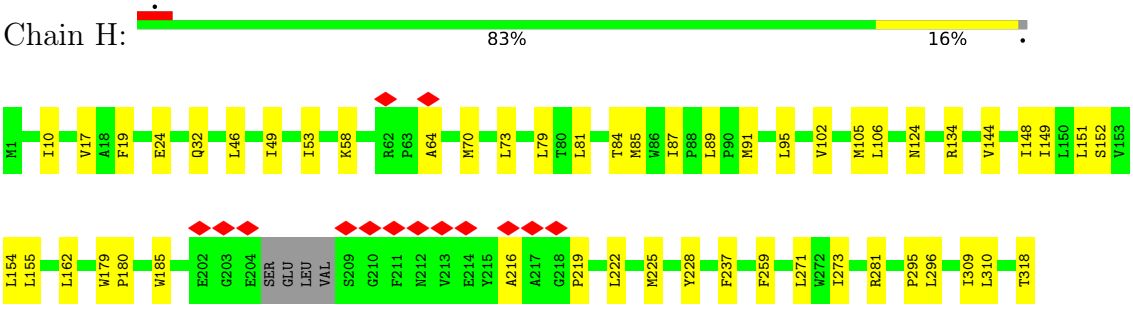
• Molecule 1: NADH-ubiquinone oxidoreductase chain 3

Chain A:



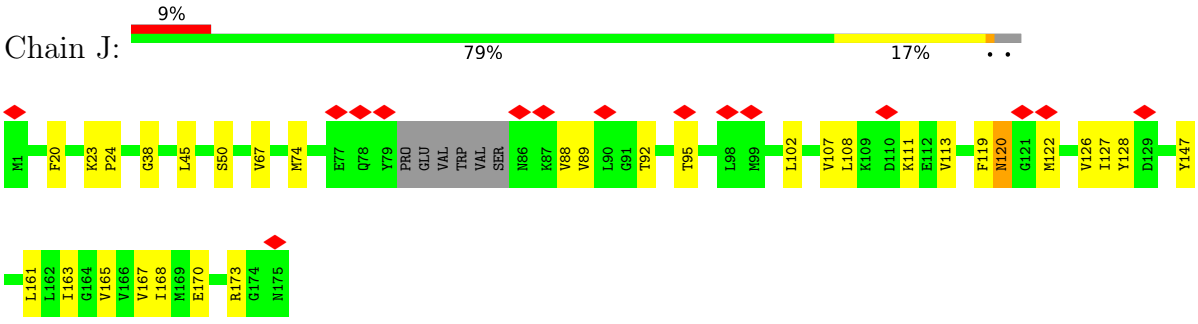
• Molecule 2: NADH-ubiquinone oxidoreductase chain 1

Chain H:



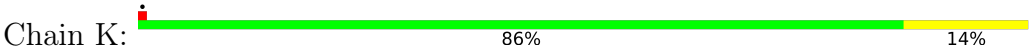
• Molecule 3: NADH-ubiquinone oxidoreductase chain 6

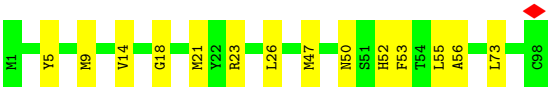
Chain J:



• Molecule 4: NADH-ubiquinone oxidoreductase chain 4L

Chain K:

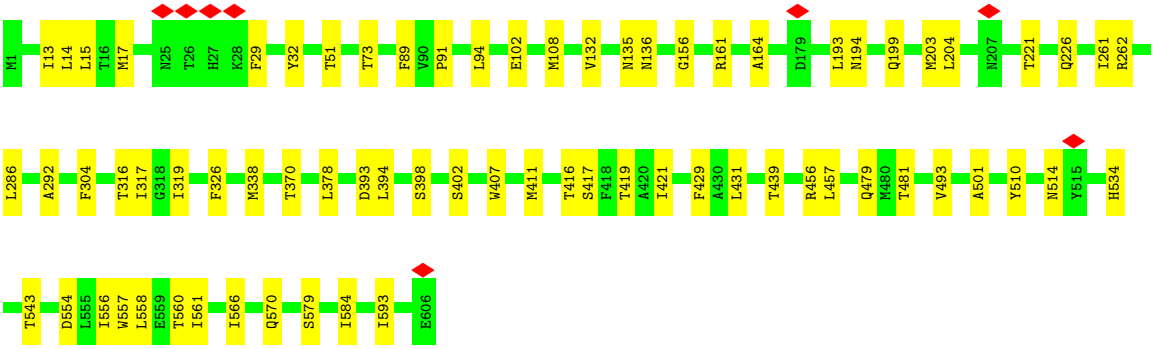




• Molecule 5: NADH-ubiquinone oxidoreductase chain 5

Chain L:

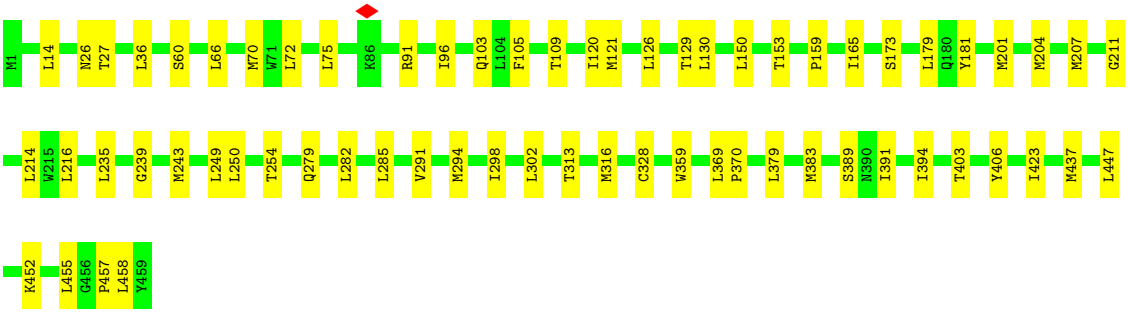




• Molecule 6: NADH-ubiquinone oxidoreductase chain 4

Chain M:

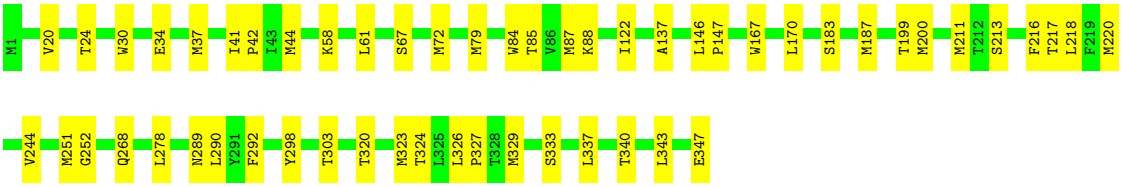




• Molecule 7: NADH-ubiquinone oxidoreductase chain 2

Chain N:

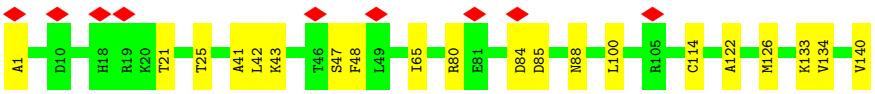




• Molecule 8: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

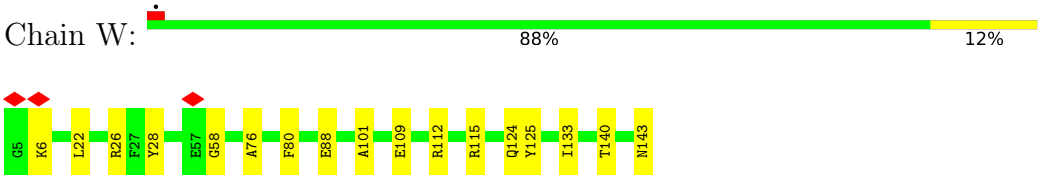
Chain V:





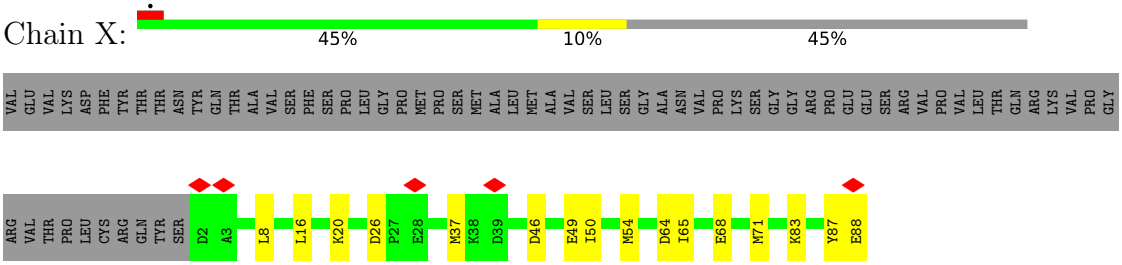
• Molecule 9: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain W:



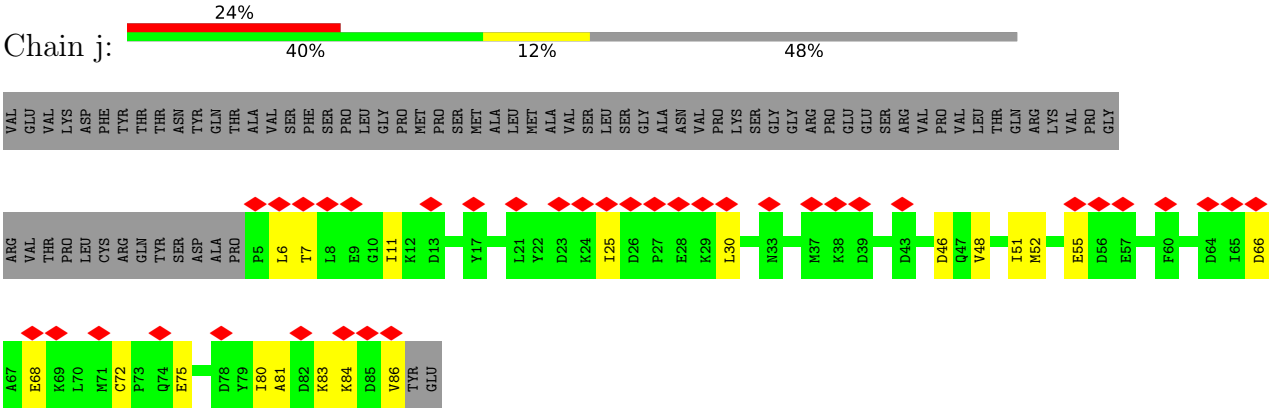
• Molecule 10: Acyl carrier protein

Chain X:



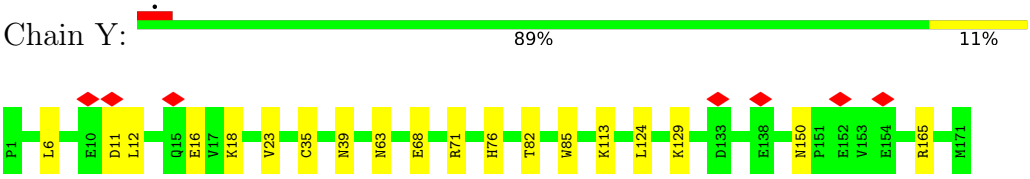
• Molecule 10: Acyl carrier protein

Chain j:



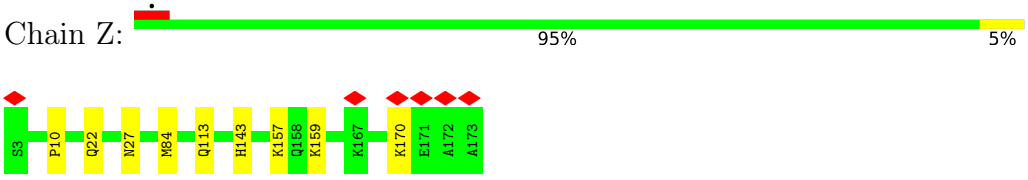
• Molecule 11: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain Y:



• Molecule 12: Complex I-PDSW

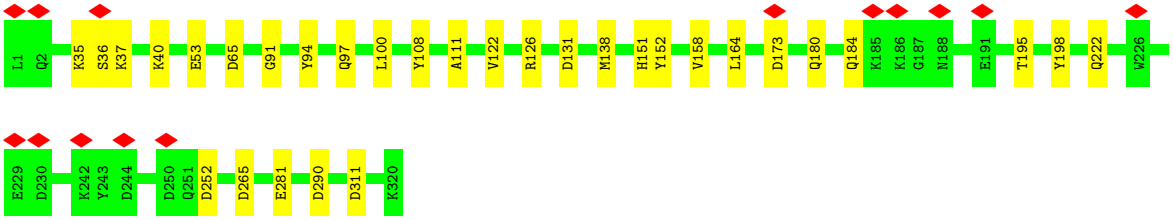
Chain Z:



• Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain k:

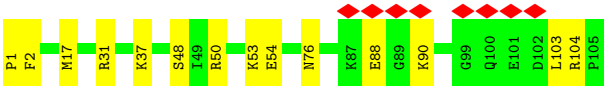




• Molecule 14: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

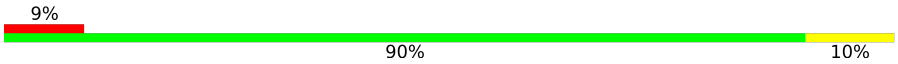
Chain l:

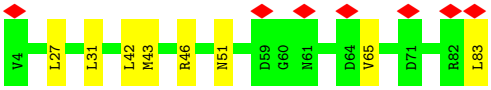




• Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

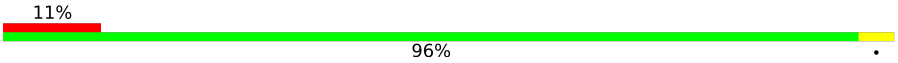
Chain m:

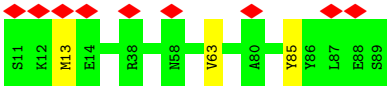




• Molecule 16: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain n:





• Molecule 17: NADH dehydrogenase [ubiquinone] 1 subunit C2

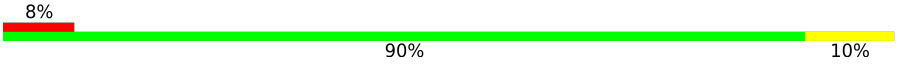
Chain o:

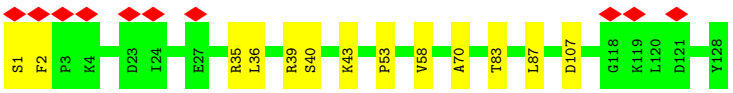




• Molecule 18: NADH:ubiquinone oxidoreductase subunit B4

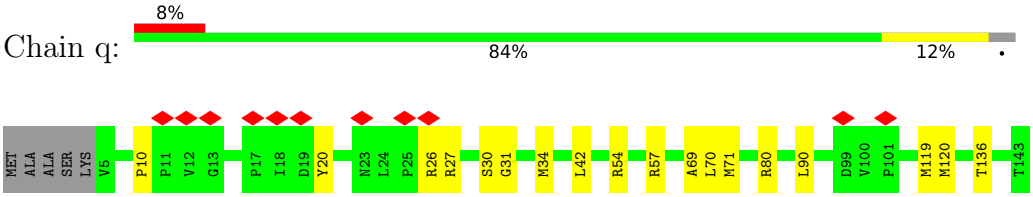
Chain p:





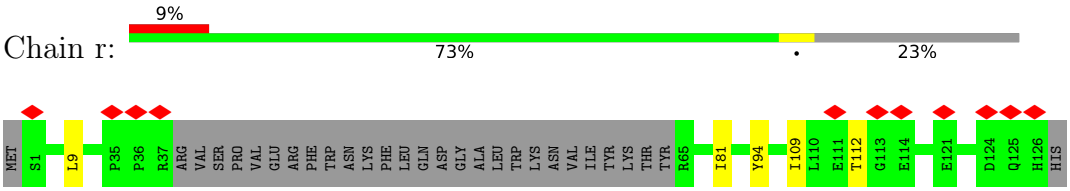
• Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain q:



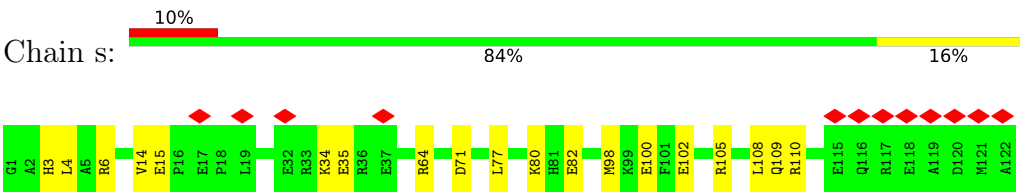
• Molecule 20: Mitochondrial complex I, B17 subunit

Chain r:



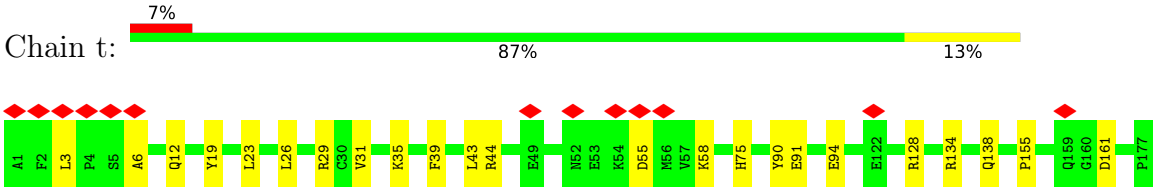
• Molecule 21: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain s:



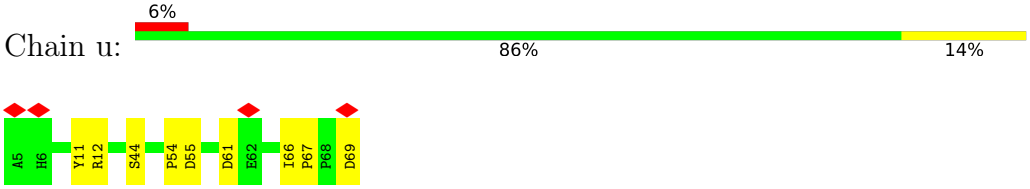
• Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

Chain t:



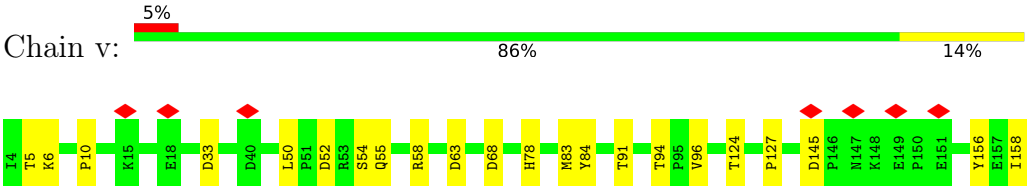
• Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

Chain u:



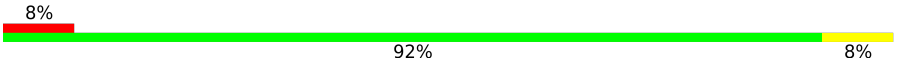
• Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

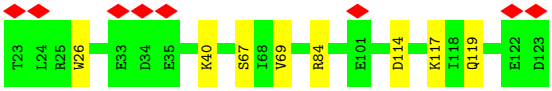
Chain v:



• Molecule 25: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

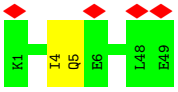
Chain w:



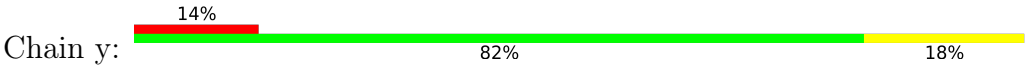


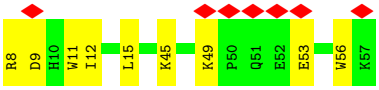
• Molecule 26: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



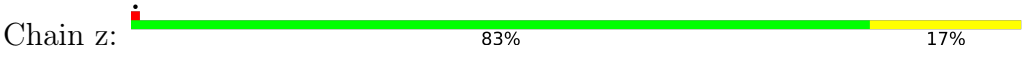


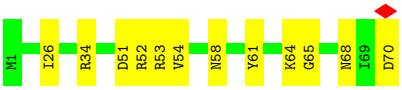
• Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



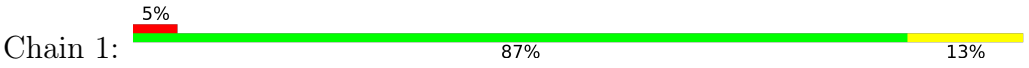


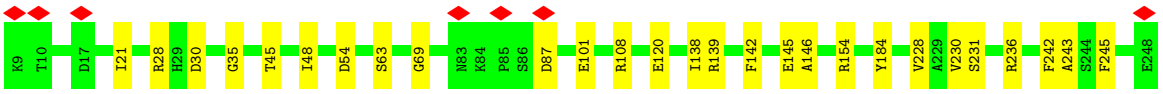
• Molecule 28: Complex I-MWFE

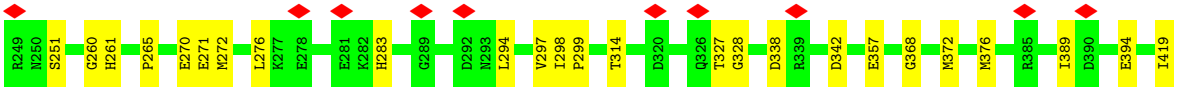


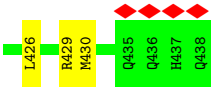


• Molecule 29: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

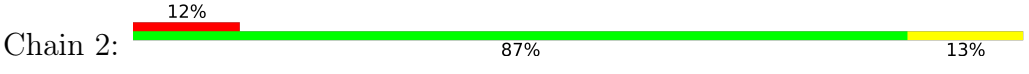


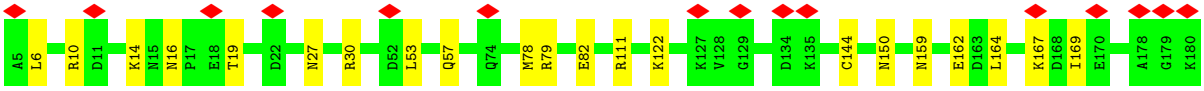






• Molecule 30: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

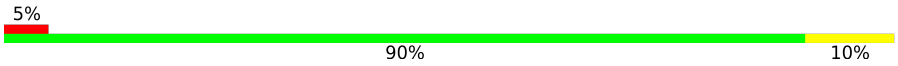


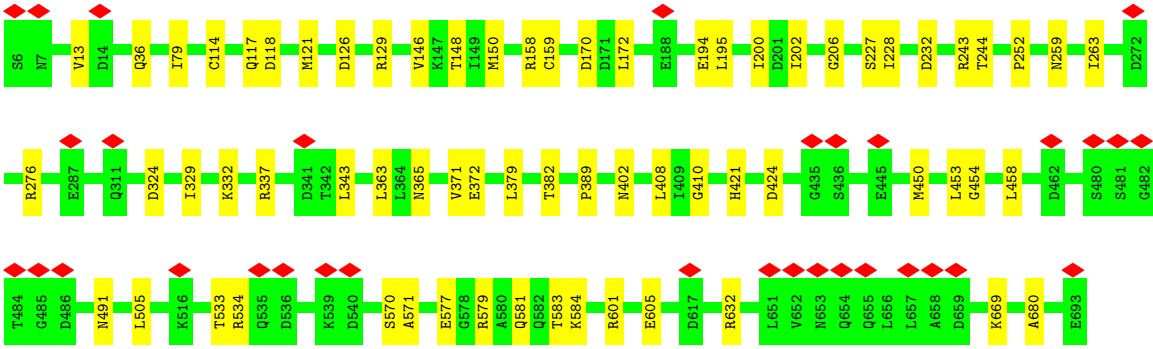




• Molecule 31: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain 3:

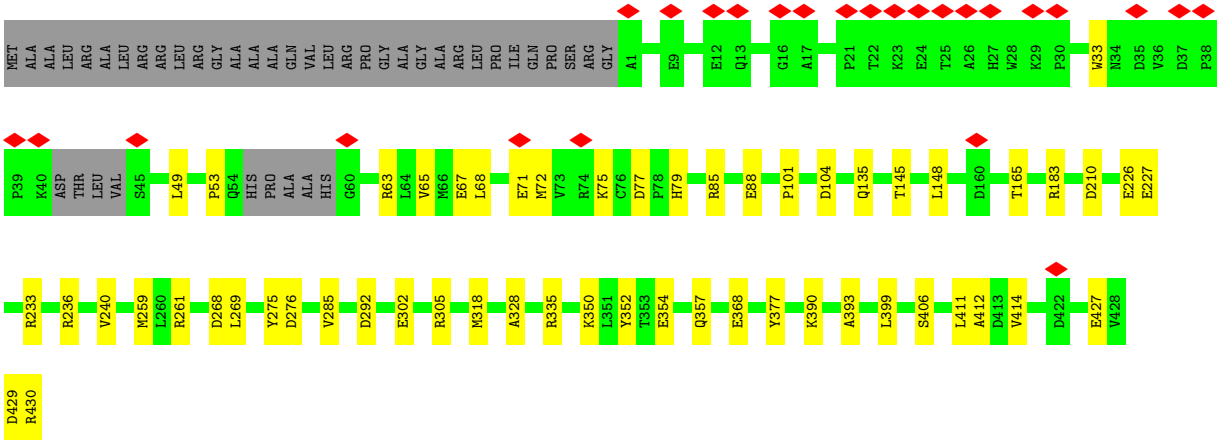




• Molecule 32: Complex I-49kD

Chain 4:

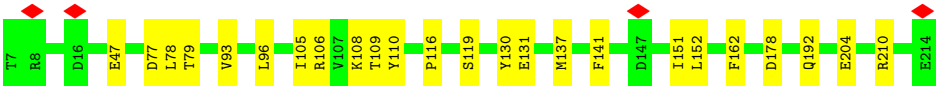




• Molecule 33: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

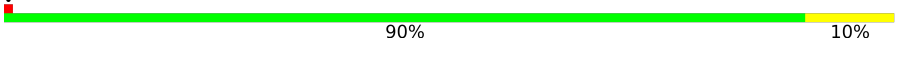
Chain 5:

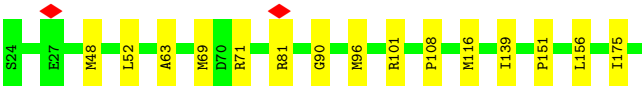




• Molecule 34: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain 6:

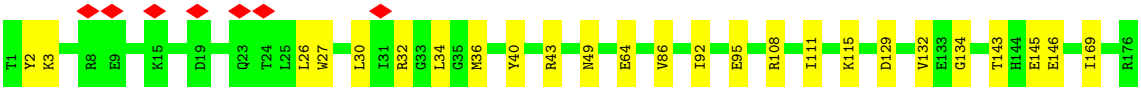




• Molecule 35: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

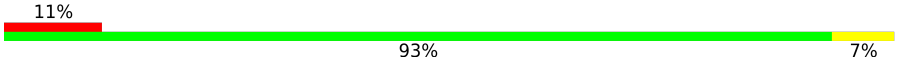
Chain 9:

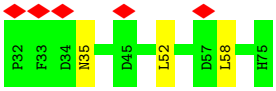




• Molecule 36: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

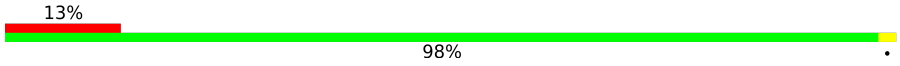
Chain a:

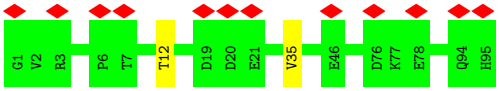




• Molecule 37: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain b:

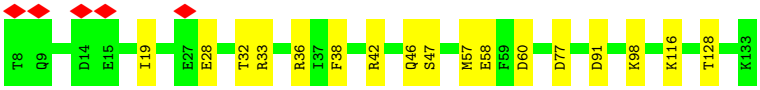




• Molecule 38: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain c:

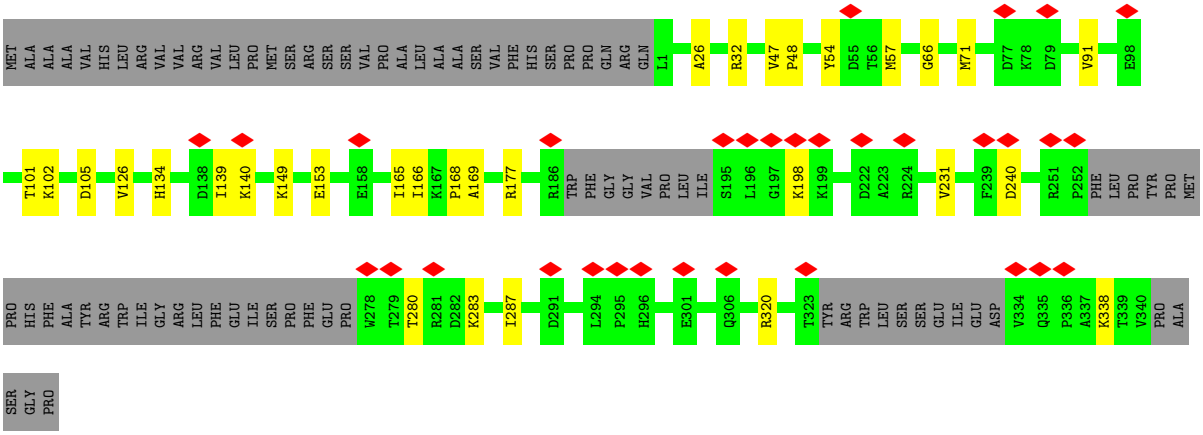




• Molecule 39: NADH:ubiquinone oxidoreductase subunit A9

Chain d:

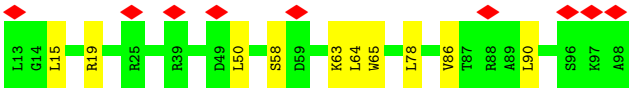




• Molecule 40: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

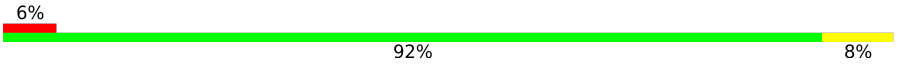
Chain e:

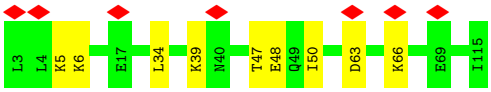




• Molecule 41: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

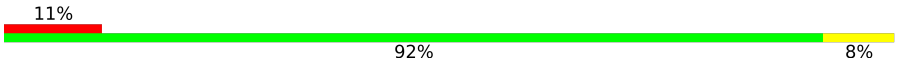
Chain f:

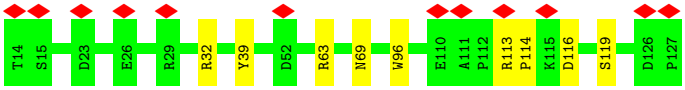




• Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain g:

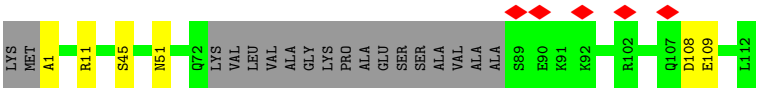




• Molecule 43: Mitochondrial complex I, B14.5a subunit

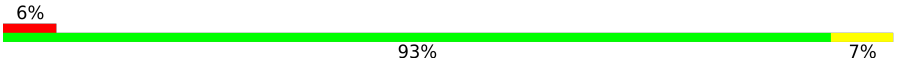
Chain h:

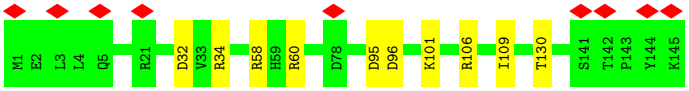




• Molecule 44: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain i:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	113712	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	0.556	Depositor
Minimum map value	-0.056	Depositor
Average map value	0.011	Depositor
Map value standard deviation	0.033	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	173.24, 193.98001, 291.58002	wwPDB
Map dimensions	239, 159, 142	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: FMN, AMP, ZMP, K, FME, SEP, NDP, AYA, FES, 2MR, NAI, ZN, SF4, DCQ, PC1, 3PE, MYR

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	0.24	0/902	0.53	0/1234
2	H	0.26	0/2572	0.47	0/3517
3	J	0.21	0/1324	0.41	0/1790
4	K	0.25	0/749	0.45	0/1014
5	L	0.24	0/4924	0.43	0/6698
6	M	0.26	0/3731	0.44	0/5085
7	N	0.26	0/2787	0.43	0/3795
8	V	0.17	0/1041	0.31	0/1412
9	W	0.21	0/1188	0.31	0/1607
10	X	0.20	0/713	0.41	0/963
10	j	0.22	0/670	0.51	0/902
11	Y	0.21	0/1440	0.37	0/1942
12	Z	0.20	0/1475	0.31	0/1989
13	k	0.20	0/2646	0.32	0/3579
14	l	0.21	0/896	0.42	0/1200
15	m	0.19	0/647	0.43	0/890
16	n	0.19	0/653	0.43	0/882
17	o	0.22	0/1035	0.33	0/1398
18	p	0.21	0/1085	0.38	0/1467
19	q	0.21	0/1171	0.40	1/1579 (0.1%)
20	r	0.22	0/874	0.36	0/1188
21	s	0.20	0/1072	0.39	0/1436
22	t	0.19	0/1573	0.37	0/2130
23	u	0.19	0/590	0.32	0/810
24	v	0.20	0/1361	0.36	0/1861
25	w	0.20	0/872	0.39	0/1185
26	x	0.19	0/425	0.35	0/576
27	y	0.23	0/449	0.40	0/605
28	z	0.26	0/591	0.51	0/795
29	1	0.19	0/3386	0.36	0/4575
30	2	0.18	0/1695	0.40	0/2306
31	3	0.20	0/5362	0.37	0/7266

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
32	4	0.23	0/3463	0.37	0/4687
33	5	0.22	0/1776	0.37	0/2417
34	6	0.23	0/1278	0.40	0/1728
35	9	0.24	0/1445	0.42	0/1956
36	a	0.15	0/383	0.34	0/518
37	b	0.18	0/749	0.29	0/1009
38	c	0.19	0/1047	0.31	0/1415
39	d	0.19	0/2424	0.34	0/3276
40	e	0.21	0/702	0.38	0/945
41	f	0.21	0/937	0.35	0/1271
42	g	0.22	0/993	0.35	0/1336
43	h	0.19	0/779	0.34	0/1053
44	i	0.20	0/1250	0.35	0/1698
All	All	0.22	0/67125	0.39	1/90985 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
31	3	0	1
32	4	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	q	71	MET	N-CA-C	5.29	121.50	109.81

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
31	3	259	ASN	Peptide
32	4	275	TYR	Peptide

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	880	0	920	20	0
2	H	2498	0	2609	38	0
3	J	1294	0	1317	27	0
4	K	749	0	793	16	0
5	L	4806	0	4945	49	0
6	M	3647	0	3849	42	0
7	N	2723	0	2930	36	0
8	V	1028	0	1036	9	0
9	W	1155	0	1177	13	0
10	X	701	0	692	11	0
10	j	660	0	662	13	0
11	Y	1403	0	1392	15	0
12	Z	1441	0	1419	8	0
13	k	2596	0	2559	21	0
14	l	874	0	869	16	0
15	m	626	0	635	6	0
16	n	634	0	616	2	0
17	o	1004	0	995	12	0
18	p	1059	0	1062	10	0
19	q	1142	0	1137	15	0
20	r	846	0	864	4	0
21	s	1047	0	1015	15	0
22	t	1520	0	1477	18	0
23	u	563	0	509	9	0
24	v	1307	0	1207	17	0
25	w	846	0	792	6	0
26	x	412	0	411	1	0
27	y	436	0	437	8	0
28	z	576	0	570	8	0
29	1	3312	0	3266	38	0
30	2	1655	0	1668	19	0
31	3	5275	0	5300	43	0
32	4	3390	0	3334	38	0
33	5	1726	0	1676	14	0
34	6	1247	0	1256	11	0
35	9	1414	0	1370	19	0
36	a	371	0	344	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	b	737	0	710	1	0
38	c	1024	0	1023	13	0
39	d	2372	0	2407	22	0
40	e	691	0	706	7	0
41	f	917	0	958	7	0
42	g	969	0	980	7	0
43	h	769	0	780	4	0
44	i	1209	0	1182	6	0
45	A	83	0	117	1	0
45	H	54	0	88	3	0
45	L	108	0	176	3	0
45	M	54	0	88	3	0
46	6	51	0	82	1	0
46	A	51	0	82	1	0
46	H	102	0	164	4	0
46	K	40	0	54	2	0
46	L	82	0	118	3	0
46	M	44	0	65	2	0
46	N	122	0	172	3	0
46	V	99	0	119	0	0
47	H	23	0	30	1	0
48	X	31	0	34	2	0
48	j	34	0	40	0	0
49	k	23	0	12	1	0
50	s	15	0	27	0	0
51	1	8	0	0	0	0
51	3	16	0	0	1	0
51	6	8	0	0	0	0
51	9	16	0	0	0	0
52	1	31	0	19	0	0
53	1	44	0	27	2	0
54	2	4	0	0	0	0
54	3	4	0	0	0	0
55	3	1	0	0	0	0
56	b	1	0	0	0	0
57	d	48	0	26	1	0
All	All	66748	0	67396	589	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.

All (589) 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)
31:3:570:SER:HA	31:3:583:THR:O	1.76	0.86
1:A:69:ILE:HD11	2:H:148:ILE:HG12	1.70	0.72
32:4:269:LEU:HB2	32:4:368:GLU:HB2	1.76	0.66
21:s:110:ARG:HH12	23:u:69:ASP:HB2	1.60	0.66
24:v:50:LEU:HB2	24:v:78:HIS:HD2	1.59	0.66
35:9:43:ARG:HG2	43:h:11:ARG:HD2	1.77	0.66
42:g:32:ARG:NH1	10:j:68:GLU:OE2	2.31	0.64
11:Y:165:ARG:NH2	17:o:87:ASP:OD1	2.31	0.63
32:4:183:ARG:NH1	32:4:210:ASP:OD2	2.31	0.63
3:J:120:ASN:HD21	3:J:122:MET:HB2	1.63	0.63
17:o:3:THR:O	17:o:7:ALA:HB2	1.98	0.63
10:j:25:ILE:HD11	10:j:30:LEU:HD13	1.80	0.63
5:L:543:THR:HG23	24:v:83:MET:HE1	1.80	0.62
31:3:126:ASP:HB2	32:4:328:ALA:HB3	1.80	0.62
10:j:80:ILE:HD12	10:j:84:LYS:HZ1	1.65	0.62
26:x:4:ILE:HG23	26:x:5:GLN:HG2	1.82	0.61
1:A:68:GLU:HG2	3:J:161:LEU:HD13	1.82	0.61
30:2:159:ASN:HB3	30:2:184:PRO:HB3	1.82	0.61
32:4:67:GLU:HB3	32:4:75:LYS:HB2	1.82	0.60
29:1:30:ASP:HB3	29:1:35:GLY:HA3	1.84	0.60
2:H:58:LYS:HD2	34:6:108:PRO:HB2	1.83	0.60
21:s:102:GLU:OE2	21:s:105:ARG:NH2	2.34	0.60
31:3:148:THR:HG23	31:3:150:MET:HE3	1.82	0.60
31:3:228:ILE:HG13	31:3:581:GLN:HB3	1.84	0.60
46:A:202:3PE:H381	2:H:295:PRO:HB3	1.83	0.60
29:1:261:HIS:ND1	29:1:338:ASP:OD1	2.36	0.59
39:d:280:THR:HG23	39:d:283:LYS:H	1.67	0.59
28:z:52:ARG:NH1	28:z:58:ASN:OD1	2.32	0.59
44:i:32:ASP:OD2	44:i:34:ARG:NH1	2.36	0.59
34:6:116:MET:HG3	34:6:156:LEU:HD13	1.84	0.59
31:3:601:ARG:NH1	31:3:605:GLU:OE1	2.34	0.59
32:4:354:GLU:OE2	32:4:357:GLN:NE2	2.35	0.59
7:N:199:THR:HG21	7:N:347:GLU:HG2	1.83	0.59
5:L:221:THR:HG23	5:L:226:GLN:HB2	1.84	0.59
9:W:109:GLU:OE2	9:W:112:ARG:NH1	2.36	0.59
18:p:39:ARG:NH2	22:t:3:LEU:O	2.36	0.58
31:3:118:ASP:OD2	38:c:46:GLN:NE2	2.36	0.58
2:H:87:ILE:HG22	2:H:95:LEU:HD23	1.85	0.58
6:M:328:CYS:HB3	6:M:437:MET:HE1	1.84	0.58
9:W:58:GLY:O	27:y:49:LYS:NZ	2.37	0.58
15:m:43:MET:HA	15:m:46:ARG:HG2	1.84	0.58
33:5:151:ILE:HG23	33:5:152:LEU:HG	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:d:177:ARG:NH2	57:d:401:NDP:O2N	2.36	0.58
5:L:510:TYR:O	22:t:35:LYS:NZ	2.36	0.58
17:o:110:ARG:NH2	25:w:119:GLN:OE1	2.37	0.58
29:1:139:ARG:NH2	30:2:144:CYS:O	2.37	0.58
44:i:106:ARG:HB2	44:i:109:ILE:HG13	1.84	0.58
12:Z:159:LYS:NZ	17:o:112:VAL:O	2.36	0.57
2:H:149:ILE:HG21	2:H:185:TRP:HB2	1.86	0.57
6:M:391:ILE:HG23	6:M:394:ILE:HD12	1.87	0.57
31:3:243:ARG:HD2	31:3:244:THR:HG23	1.86	0.57
44:i:96:ASP:OD2	44:i:101:LYS:NZ	2.38	0.57
11:Y:12:LEU:O	14:l:104:ARG:NH2	2.37	0.57
41:f:34:LEU:HD21	41:f:47:THR:HB	1.87	0.57
3:J:127:ILE:HA	19:q:119:MET:HE2	1.85	0.57
2:H:64:ALA:O	2:H:124:ASN:ND2	2.38	0.56
6:M:36:LEU:HB2	25:w:69:VAL:HG22	1.87	0.56
32:4:227:GLU:OE2	35:9:32:ARG:NH1	2.35	0.56
10:X:46:ASP:OD1	22:t:44:ARG:NH2	2.38	0.56
5:L:14:LEU:HA	5:L:17:MET:HE3	1.87	0.56
34:6:71:ARG:NH2	35:9:49:ASN:OD1	2.38	0.56
31:3:424:ASP:N	31:3:424:ASP:OD1	2.38	0.56
42:g:116:ASP:OD1	42:g:119:SER:OG	2.23	0.56
5:L:286:LEU:HD13	5:L:411:MET:HE3	1.88	0.56
10:X:26:ASP:N	10:X:26:ASP:OD1	2.38	0.55
34:6:116:MET:HE2	34:6:151:PRO:HG2	1.88	0.55
1:A:60:ILE:HG21	3:J:168:ILE:HG21	1.89	0.55
30:2:27:ASN:OD1	30:2:57:GLN:NE2	2.39	0.55
17:o:46:ASN:OD1	17:o:51:ARG:NH1	2.40	0.55
33:5:178:ASP:OD2	39:d:32:ARG:NH1	2.40	0.55
6:M:129:THR:HG21	6:M:235:LEU:HD11	1.89	0.55
3:J:170:GLU:OE2	3:J:173:ARG:NH2	2.40	0.55
5:L:132:VAL:O	5:L:262:ARG:NH2	2.40	0.55
14:l:103:LEU:HB3	28:z:53:ARG:HD2	1.87	0.55
18:p:1:SER:OG	18:p:2:PHE:N	2.39	0.55
31:3:252:PRO:HG3	31:3:263:ILE:HG12	1.89	0.55
13:k:158:VAL:HG11	32:4:33:TRP:HB2	1.89	0.55
32:4:335:ARG:NH2	35:9:129:ASP:OD1	2.40	0.55
11:Y:63:ASN:OD1	19:q:80:ARG:NH2	2.36	0.55
24:v:54:SER:HA	24:v:84:TYR:HB3	1.88	0.55
31:3:194:GLU:HG3	31:3:389:PRO:HB3	1.89	0.55
29:1:342:ASP:OD1	29:1:429:ARG:NH2	2.40	0.54
38:c:42:ARG:NH1	38:c:46:GLN:O	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:102:GLU:OE1	5:L:456:ARG:NH2	2.40	0.54
6:M:211:GLY:HA3	46:M:501:3PE:H3G2	1.90	0.54
6:M:91:ARG:NH2	13:k:290:ASP:OD2	2.41	0.54
32:4:226:GLU:OE1	32:4:305:ARG:NH2	2.37	0.54
29:1:69:GLY:O	53:1:503:NAI:N7N	2.31	0.54
43:h:45:SER:O	43:h:51:ASN:ND2	2.39	0.54
4:K:73:LEU:HD21	7:N:41:ILE:HG13	1.89	0.54
8:V:47:SER:OG	8:V:48:PHE:N	2.41	0.53
8:V:140:VAL:O	9:W:115:ARG:NH1	2.41	0.53
18:p:35:ARG:NH1	24:v:33:ASP:OD2	2.41	0.53
25:w:114:ASP:HB3	25:w:117:LYS:HG2	1.89	0.53
28:z:64:LYS:HD3	28:z:68:ASN:HD21	1.74	0.53
30:2:79:ARG:NH2	31:3:170:ASP:OD1	2.40	0.53
34:6:63:ALA:HA	34:6:69:MET:HG2	1.89	0.53
7:N:200:MET:HE1	7:N:343:LEU:HD13	1.90	0.53
19:q:26:ARG:NH2	19:q:27:ARG:O	2.42	0.53
21:s:35:GLU:HA	24:v:156:TYR:HA	1.89	0.53
33:5:96:LEU:HB2	33:5:105:ILE:HG22	1.90	0.53
6:M:60:SER:HB2	6:M:457:PRO:HA	1.90	0.53
28:z:34:ARG:NH1	28:z:61:TYR:O	2.42	0.53
29:1:260:GLY:O	30:2:111:ARG:NH1	2.41	0.53
5:L:203:MET:HB2	12:Z:113:GLN:HG3	1.90	0.53
4:K:50:ASN:O	14:l:31:ARG:NH1	2.42	0.52
9:W:125:TYR:HB2	14:l:48:SER:HB3	1.90	0.52
21:s:110:ARG:NH1	23:u:67:PRO:O	2.43	0.52
27:y:12:ILE:HA	27:y:15:LEU:HD13	1.91	0.52
7:N:326:LEU:HA	7:N:329:MET:HE2	1.91	0.52
5:L:579:SER:OG	8:V:43:LYS:NZ	2.42	0.52
29:1:270:GLU:OE1	29:1:283:HIS:NE2	2.40	0.52
1:A:42:ASP:OD1	1:A:42:ASP:N	2.41	0.52
5:L:156:GLY:HA2	5:L:164:ALA:HB1	1.91	0.52
5:L:479:GLN:NE2	5:L:481:THR:O	2.42	0.52
13:k:53:GLU:OE2	13:k:126:ARG:NH1	2.43	0.52
22:t:134:ARG:HE	22:t:161:ASP:HB3	1.73	0.52
10:j:11:ILE:HG23	10:j:80:ILE:HD11	1.92	0.52
2:H:102:VAL:HG11	2:H:154:LEU:HD11	1.92	0.52
13:k:65:ASP:OD1	13:k:65:ASP:N	2.43	0.52
30:2:150:ASN:HB3	30:2:162:GLU:HB3	1.91	0.52
31:3:577:GLU:OE2	31:3:579:ARG:NH1	2.43	0.52
6:M:207:MET:HG3	6:M:294:MET:HB3	1.92	0.52
31:3:371:VAL:HG22	31:3:450:MET:HE1	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:4:68:LEU:HD11	32:4:411:LEU:HD13	1.91	0.52
33:5:192:GLN:OE1	35:9:115:LYS:NZ	2.42	0.52
7:N:298:TYR:O	7:N:303:THR:OG1	2.27	0.52
9:W:133:ILE:HD13	14:l:37:LYS:HG3	1.91	0.52
10:j:81:ALA:HB1	10:j:86:VAL:HG21	1.93	0.51
6:M:126:LEU:HD21	6:M:153:THR:HG21	1.93	0.51
6:M:389:SER:OG	18:p:107:ASP:OD2	2.27	0.51
31:3:584:LYS:HE3	38:c:36:ARG:HD2	1.93	0.51
15:m:51:ASN:OD1	15:m:51:ASN:N	2.42	0.51
7:N:34:GLU:OE2	7:N:67:SER:OG	2.22	0.51
38:c:19:ILE:HG12	38:c:98:LYS:HG2	1.92	0.51
1:A:44:MET:SD	1:A:44:MET:N	2.82	0.51
6:M:165:ILE:HG21	7:N:268:GLN:HA	1.92	0.51
3:J:120:ASN:OD1	14:l:76:ASN:ND2	2.44	0.51
32:4:145:THR:HA	32:4:148:LEU:HD12	1.93	0.51
19:q:10:PRO:HD3	32:4:318:MET:HB3	1.93	0.50
24:v:68:ASP:OD1	24:v:68:ASP:N	2.43	0.50
29:1:54:ASP:OD1	29:1:54:ASP:N	2.45	0.50
16:n:13:MET:HE1	23:u:11:TYR:HB2	1.93	0.50
31:3:372:GLU:O	31:3:402:ASN:ND2	2.44	0.50
5:L:421:ILE:HG23	5:L:501:ALA:HB2	1.94	0.50
12:Z:143:HIS:O	12:Z:157:LYS:NZ	2.39	0.50
23:u:55:ASP:OD1	23:u:55:ASP:N	2.42	0.50
8:V:80:ARG:NH2	8:V:85:ASP:OD2	2.44	0.50
32:4:63:ARG:HB3	32:4:79:HIS:HB2	1.93	0.50
5:L:15:LEU:HD11	5:L:94:LEU:HD21	1.94	0.50
22:t:138:GLN:NE2	22:t:155:PRO:O	2.44	0.50
32:4:88:GLU:OE2	32:4:430:ARG:NH1	2.45	0.50
42:g:39:TYR:HB3	10:j:52:MET:HE1	1.94	0.50
2:H:273:ILE:HD13	35:9:34:LEU:HD21	1.92	0.50
10:X:50:ILE:O	10:X:54:MET:HG2	2.11	0.50
3:J:92:THR:HA	3:J:95:THR:HG22	1.93	0.50
5:L:584:ILE:HG12	7:N:58:LYS:HE2	1.94	0.50
31:3:194:GLU:HG2	31:3:195:LEU:HG	1.93	0.50
31:3:533:THR:OG1	31:3:534:ARG:N	2.44	0.50
45:A:203:PC1:H3D1	2:H:53:ILE:HG23	1.92	0.49
3:J:167:VAL:HG22	7:N:42:PRO:HG2	1.92	0.49
7:N:327:PRO:HG3	17:o:45:ASP:HB2	1.94	0.49
6:M:216:LEU:HD23	6:M:291:VAL:HG22	1.94	0.49
31:3:232:ASP:OD1	31:3:232:ASP:N	2.43	0.49
2:H:179:TRP:HE1	19:q:42:LEU:HG	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:439:THR:HG23	23:u:12:ARG:HG3	1.95	0.49
11:Y:129:LYS:NZ	15:m:65:VAL:O	2.35	0.49
1:A:56:PHE:HB2	3:J:74:MET:HE1	1.93	0.49
4:K:47:MET:HE2	7:N:79:MET:HA	1.94	0.49
6:M:201:MET:HG3	45:M:502:PC1:H3E2	1.95	0.49
36:a:35:ASN:OD1	36:a:35:ASN:N	2.46	0.49
39:d:169:ALA:HB2	39:d:231:VAL:HG12	1.93	0.49
9:W:6:LYS:NZ	10:X:88:GLU:O	2.43	0.49
11:Y:18:LYS:NZ	14:l:104:ARG:O	2.45	0.49
32:4:406:SER:HB2	32:4:414:VAL:HG22	1.95	0.49
1:A:87:MET:HE1	2:H:309:ILE:HD11	1.94	0.49
3:J:23:LYS:NZ	4:K:21:MET:O	2.45	0.49
23:u:61:ASP:OD1	23:u:61:ASP:N	2.38	0.49
28:z:70:ASP:N	28:z:70:ASP:OD1	2.46	0.49
29:1:101:GLU:HB2	53:1:503:NAI:H42N	1.95	0.49
32:4:49:LEU:HD13	32:4:68:LEU:HD12	1.95	0.49
2:H:70:MET:HA	2:H:73:LEU:HB2	1.93	0.48
6:M:72:LEU:HA	6:M:75:LEU:HD12	1.95	0.48
22:t:29:ARG:HD2	22:t:75:HIS:CD2	2.48	0.48
1:A:13:LEU:HD22	2:H:10:ILE:HD12	1.95	0.48
23:u:61:ASP:HB2	23:u:66:ILE:HB	1.96	0.48
29:1:368:GLY:O	29:1:372:MET:HG3	2.12	0.48
32:4:377:TYR:HB3	32:4:390:LYS:HB3	1.95	0.48
1:A:34:THR:HA	39:d:320:ARG:HG3	1.94	0.48
7:N:252:GLY:HA3	7:N:290:LEU:HD13	1.95	0.48
11:Y:124:LEU:HD13	19:q:69:ALA:HB2	1.95	0.48
15:m:27:LEU:O	15:m:31:LEU:HB2	2.14	0.48
32:4:63:ARG:HH22	42:g:96:TRP:HA	1.79	0.48
38:c:28:GLU:O	38:c:32:THR:OG1	2.28	0.48
10:j:66:ASP:OD1	10:j:66:ASP:N	2.34	0.48
29:1:45:THR:HA	29:1:48:ILE:HD12	1.94	0.48
39:d:101:THR:OG1	39:d:102:LYS:N	2.46	0.48
21:s:4:LEU:HD11	24:v:124:THR:HA	1.94	0.48
29:1:389:ILE:HG23	29:1:419:ILE:HD12	1.95	0.48
7:N:44:MET:HE2	7:N:122:ILE:HG21	1.95	0.48
30:2:16:ASN:OD1	30:2:19:THR:OG1	2.27	0.48
10:X:16:LEU:O	10:X:20:LYS:HB2	2.13	0.48
13:k:180:GLN:O	13:k:184:GLN:HG2	2.14	0.48
15:m:83:LEU:HD13	19:q:54:ARG:HD3	1.96	0.48
31:3:632:ARG:HH12	40:e:58:SER:HB2	1.79	0.48
3:J:108:LEU:O	3:J:111:LYS:NZ	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:89:PHE:HB2	5:L:326:PHE:HZ	1.79	0.48
9:W:140:THR:O	9:W:143:ASN:ND2	2.47	0.48
32:4:352:TYR:HD1	35:9:86:VAL:HG21	1.79	0.48
2:H:46:LEU:HD13	2:H:49:ILE:HD13	1.96	0.48
8:V:65:ILE:HD11	8:V:100:LEU:HD23	1.95	0.48
13:k:111:ALA:HB1	13:k:122:VAL:HG11	1.95	0.48
13:k:173:ASP:OD2	13:k:222:GLN:NE2	2.47	0.48
31:3:121:MET:HG3	32:4:350:LYS:HG3	1.95	0.48
32:4:135:GLN:HB3	32:4:276:ASP:HB3	1.96	0.48
6:M:130:LEU:HD22	6:M:150:LEU:HD13	1.95	0.48
9:W:88:GLU:OE1	27:y:56:TRP:NE1	2.37	0.48
14:l:88:GLU:OE1	14:l:90:LYS:NZ	2.41	0.48
35:9:145:GLU:OE2	39:d:66:GLY:N	2.41	0.48
38:c:91:ASP:OD1	38:c:91:ASP:N	2.46	0.48
5:L:316:THR:HA	5:L:319:ILE:HG12	1.96	0.47
10:X:49:GLU:OE2	22:t:19:TYR:OH	2.30	0.47
35:9:27:TRP:HB3	35:9:30:LEU:HD12	1.96	0.47
17:o:1:MET:HG2	17:o:2:MET:HG3	1.96	0.47
17:o:52:PRO:HG2	17:o:56:ALA:HB2	1.97	0.47
23:u:44:SER:O	23:u:44:SER:OG	2.30	0.47
18:p:70:ALA:HB2	24:v:10:PRO:HG2	1.96	0.47
46:H:504:3PE:H221	46:6:202:3PE:H362	1.96	0.47
10:j:6:LEU:HG	10:j:7:THR:HG23	1.96	0.47
2:H:162:LEU:HD21	2:H:237:PHE:HE1	1.79	0.47
5:L:193:LEU:HG	5:L:204:LEU:HD12	1.97	0.47
46:M:501:3PE:H2A2	46:M:501:3PE:H371	1.97	0.47
3:J:23:LYS:HB2	4:K:23:ARG:HD3	1.96	0.47
4:K:53:PHE:HE2	7:N:84:TRP:HE1	1.62	0.47
6:M:452:LYS:HA	6:M:455:LEU:HD12	1.97	0.47
6:M:457:PRO:O	25:w:84:ARG:NH2	2.48	0.47
7:N:216:PHE:O	7:N:220:MET:HG3	2.15	0.47
24:v:145:ASP:N	24:v:145:ASP:OD1	2.47	0.47
29:1:142:PHE:HB3	29:1:145:GLU:HB2	1.97	0.47
32:4:261:ARG:NH1	32:4:268:ASP:OD1	2.48	0.47
39:d:140:LYS:HE2	39:d:140:LYS:HB2	1.78	0.47
2:H:273:ILE:HD11	45:H:503:PC1:H3A2	1.97	0.47
5:L:370:THR:HG23	5:L:431:LEU:HD13	1.97	0.47
5:L:558:LEU:HB3	6:M:214:LEU:HD21	1.97	0.47
11:Y:68:GLU:OE1	11:Y:71:ARG:NH1	2.47	0.47
31:3:158:ARG:HB3	31:3:202:ILE:HD12	1.97	0.47
35:9:92:ILE:HG12	35:9:111:ILE:HG12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:d:48:PRO:HA	39:d:71:MET:O	2.14	0.47
39:d:105:ASP:OD1	39:d:105:ASP:N	2.46	0.47
31:3:227:SER:OG	31:3:228:ILE:N	2.46	0.47
3:J:45:LEU:HD23	3:J:50:SER:HA	1.97	0.47
12:Z:10:PRO:O	20:r:94:TYR:OH	2.29	0.47
31:3:329:ILE:HD13	31:3:505:LEU:HD22	1.96	0.47
39:d:153:GLU:HG3	39:d:165:ILE:HD13	1.97	0.47
5:L:570:GLN:OE1	7:N:167:TRP:NE1	2.38	0.46
48:X:101:ZMP:H20A	22:t:12:GLN:HG3	1.97	0.46
32:4:393:ALA:HB1	32:4:427:GLU:HG3	1.97	0.46
38:c:60:ASP:N	38:c:60:ASP:OD1	2.47	0.46
3:J:23:LYS:O	4:K:23:ARG:NH1	2.48	0.46
3:J:88:VAL:O	3:J:92:THR:HG23	2.15	0.46
30:2:188:SER:OG	30:2:189:GLY:N	2.45	0.46
32:4:292:ASP:OD1	32:4:292:ASP:N	2.33	0.46
33:5:119:SER:OG	33:5:131:GLU:OE2	2.32	0.46
4:K:52:HIS:HB2	14:l:31:ARG:HG2	1.96	0.46
7:N:30:TRP:O	7:N:34:GLU:HG2	2.15	0.46
29:1:228:VAL:O	29:1:231:SER:OG	2.31	0.46
38:c:33:ARG:NH1	38:c:77:ASP:OD1	2.45	0.46
38:c:38:PHE:HE1	38:c:58:GLU:HG2	1.81	0.46
11:Y:11:ASP:OD1	11:Y:11:ASP:N	2.49	0.46
13:k:94:TYR:OH	13:k:151:HIS:ND1	2.39	0.46
1:A:109:LYS:HA	1:A:109:LYS:HD3	1.66	0.46
6:M:181:TYR:HB3	12:Z:84:MET:HE3	1.96	0.46
9:W:124:GLN:HB2	17:o:4:GLY:HA3	1.98	0.46
29:1:426:LEU:O	29:1:430:MET:HG2	2.15	0.46
31:3:324:ASP:HB3	31:3:571:ALA:HB1	1.97	0.46
2:H:318:THR:O	2:H:318:THR:OG1	2.33	0.46
4:K:23:ARG:HA	46:K:101:3PE:H11	1.96	0.46
5:L:29:PHE:HB3	5:L:32:TYR:HB2	1.97	0.46
5:L:566:ILE:HD13	45:M:502:PC1:H2I3	1.97	0.46
11:Y:150:ASN:OD1	14:l:50:ARG:NH1	2.49	0.46
21:s:98:MET:HE1	23:u:54:PRO:HD2	1.97	0.46
29:1:138:ILE:HG21	29:1:146:ALA:HB2	1.97	0.46
31:3:206:GLY:N	51:3:801:SF4:S2	2.80	0.46
5:L:514:ASN:OD1	5:L:514:ASN:N	2.48	0.46
7:N:337:LEU:O	7:N:340:THR:OG1	2.30	0.46
10:X:37:MET:HE3	10:X:71:MET:HE1	1.98	0.46
13:k:35:LYS:HE2	13:k:126:ARG:HG3	1.97	0.46
24:v:94:THR:OG1	24:v:96:VAL:O	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:4:101:PRO:HA	32:4:104:ASP:HB2	1.97	0.46
34:6:101:ARG:NH1	34:6:139:ILE:O	2.46	0.46
1:A:63:LEU:HB2	3:J:67:VAL:HG21	1.98	0.46
5:L:398:SER:O	5:L:402:SER:OG	2.25	0.46
19:q:20:TYR:OH	43:h:108:ASP:OD2	2.29	0.46
21:s:100:GLU:HG2	24:v:158:ILE:HG21	1.98	0.46
7:N:183:SER:O	7:N:187:MET:HG2	2.15	0.46
13:k:311:ASP:N	13:k:311:ASP:OD1	2.46	0.46
31:3:332:LYS:HG3	31:3:343:LEU:HD13	1.98	0.46
6:M:204:MET:HE1	6:M:302:LEU:HD11	1.98	0.45
19:q:30:SER:OG	19:q:31:GLY:N	2.49	0.45
6:M:313:THR:HA	6:M:316:MET:HE2	1.99	0.45
7:N:211:MET:HE3	7:N:251:MET:HG2	1.97	0.45
29:1:87:ASP:OD1	29:1:87:ASP:N	2.46	0.45
29:1:294:LEU:HD11	29:1:297:VAL:HG23	1.99	0.45
32:4:259:MET:HE3	32:4:259:MET:HB3	1.77	0.45
44:i:34:ARG:NH2	44:i:58:ARG:O	2.50	0.45
8:V:122:ALA:O	8:V:126:MET:HG3	2.16	0.45
13:k:97:GLN:HB2	13:k:138:MET:HE1	1.99	0.45
5:L:338:MET:HB2	5:L:457:LEU:HB3	1.98	0.45
10:X:8:LEU:HG	10:X:87:TYR:CE2	2.52	0.45
21:s:108:LEU:HD12	21:s:108:LEU:HA	1.87	0.45
10:j:51:ILE:O	10:j:55:GLU:HG3	2.17	0.45
2:H:81:LEU:HA	2:H:84:THR:HG22	1.99	0.45
2:H:152:SER:HA	2:H:155:LEU:HD12	1.98	0.45
6:M:423:ILE:HG12	18:p:58:VAL:HG22	1.99	0.45
21:s:3:HIS:CE1	24:v:127:PRO:HD3	2.51	0.45
31:3:114:CYS:HB3	31:3:117:GLN:HB2	1.98	0.45
3:J:107:VAL:HG22	3:J:113:VAL:HG11	1.99	0.45
5:L:292:ALA:HB2	5:L:304:PHE:HB3	1.99	0.45
6:M:66:LEU:O	6:M:70:MET:HG3	2.16	0.45
7:N:320:THR:OG1	13:k:265:ASP:OD1	2.35	0.45
31:3:159:CYS:HB3	31:3:172:LEU:HD13	1.99	0.45
37:b:12:THR:HG22	37:b:35:VAL:HG12	1.99	0.45
2:H:24:GLU:HA	2:H:271:LEU:HD13	1.99	0.45
5:L:407:TRP:O	5:L:411:MET:HG2	2.16	0.45
28:z:51:ASP:HA	28:z:54:VAL:HG12	1.98	0.45
2:H:91:MET:HG2	2:H:259:PHE:CZ	2.52	0.45
31:3:382:THR:HB	31:3:454:GLY:HA3	1.98	0.45
6:M:250:LEU:O	6:M:254:THR:OG1	2.34	0.44
13:k:37:LYS:HA	13:k:40:LYS:HE2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:s:64:ARG:HG2	21:s:82:GLU:HG2	1.99	0.44
29:1:120:GLU:OE2	29:1:236:ARG:NH2	2.50	0.44
31:3:453:LEU:HD21	31:3:458:LEU:HD21	1.98	0.44
42:g:116:ASP:OD1	42:g:116:ASP:N	2.50	0.44
5:L:15:LEU:HD23	5:L:15:LEU:HA	1.83	0.44
33:5:47:GLU:OE1	33:5:106:ARG:NH2	2.35	0.44
46:L:1004:3PE:H111	16:n:63:VAL:HG21	2.00	0.44
8:V:133:LYS:HE3	8:V:133:LYS:HB2	1.77	0.44
13:k:126:ARG:HH22	49:k:501:AMP:H5'2	1.82	0.44
14:l:50:ARG:NH2	14:l:54:GLU:OE2	2.49	0.44
2:H:17:VAL:HG11	2:H:225:MET:HG3	1.98	0.44
45:L:1003:PC1:H3F1	6:M:447:LEU:HD11	1.98	0.44
7:N:218:LEU:HD13	7:N:244:VAL:HG12	1.99	0.44
14:l:53:LYS:HB3	14:l:53:LYS:HE3	1.74	0.44
31:3:324:ASP:OD1	31:3:324:ASP:N	2.37	0.44
39:d:139:ILE:HG23	39:d:140:LYS:HG3	2.00	0.44
3:J:163:ILE:HD13	3:J:163:ILE:HA	1.82	0.44
29:1:394:GLU:OE1	31:3:129:ARG:NH1	2.50	0.44
5:L:13:ILE:HG13	20:r:81:ILE:HD11	1.99	0.44
32:4:302:GLU:HG2	35:9:3:LYS:HD2	1.98	0.44
3:J:122:MET:HE3	3:J:126:VAL:HG11	1.99	0.44
6:M:14:LEU:HD11	6:M:26:ASN:HB3	1.99	0.44
12:Z:22:GLN:HB2	21:s:71:ASP:HB3	2.00	0.44
18:p:43:LYS:NZ	24:v:63:ASP:O	2.50	0.44
40:e:19:ARG:HB2	40:e:65:TRP:HB2	1.99	0.44
41:f:6:LYS:HD3	41:f:6:LYS:HA	1.73	0.44
2:H:216:ALA:HB3	2:H:219:PRO:HD2	2.00	0.44
2:H:219:PRO:HA	2:H:222:LEU:HD12	2.00	0.44
5:L:534:HIS:HD2	46:L:1001:3PE:H332	1.82	0.44
5:L:554:ASP:HA	5:L:558:LEU:HB2	2.00	0.44
7:N:329:MET:HE3	7:N:329:MET:HB2	1.93	0.44
22:t:55:ASP:HB3	22:t:58:LYS:HB3	2.00	0.44
3:J:24:PRO:HB3	3:J:89:VAL:HG11	1.99	0.43
5:L:417:SER:HB3	5:L:493:VAL:HG13	2.00	0.43
7:N:213:SER:O	7:N:217:THR:OG1	2.33	0.43
11:Y:82:THR:HA	11:Y:85:TRP:CD1	2.52	0.43
22:t:91:GLU:HB2	22:t:94:GLU:HG3	1.99	0.43
29:1:63:SER:HB2	29:1:242:PHE:HB3	2.00	0.43
35:9:143:THR:HB	35:9:146:GLU:HG3	1.98	0.43
2:H:24:GLU:OE1	2:H:228:TYR:OH	2.18	0.43
5:L:108:MET:HE3	5:L:108:MET:HB3	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:286:LEU:HD13	5:L:411:MET:HB3	2.00	0.43
29:1:272:MET:HE3	29:1:272:MET:HB3	1.94	0.43
30:2:164:LEU:HD13	30:2:169:ILE:HD13	2.00	0.43
39:d:26:ALA:HB3	39:d:47:VAL:HG13	2.00	0.43
1:A:64:LEU:HD13	3:J:165:VAL:HG22	2.00	0.43
17:o:5:ARG:HA	17:o:8:ARG:HH12	1.82	0.43
30:2:78:MET:HE3	30:2:82:GLU:HG3	2.00	0.43
31:3:146:VAL:HG22	31:3:200:ILE:HD11	2.00	0.43
4:K:56:ALA:HA	14:l:17:MET:HE2	2.01	0.43
6:M:369:LEU:HD12	6:M:370:PRO:HD2	1.99	0.43
46:H:504:3PE:H282	46:H:504:3PE:H362	2.01	0.43
11:Y:6:LEU:HD12	19:q:90:LEU:HD13	1.99	0.43
33:5:116:PRO:HB3	33:5:141:PHE:HD2	1.83	0.43
11:Y:35:CYS:O	11:Y:39:ASN:ND2	2.51	0.43
24:v:5:THR:OG1	24:v:6:LYS:N	2.51	0.43
29:1:184:TYR:HB3	29:1:357:GLU:HB3	2.00	0.43
5:L:593:ILE:HD12	8:V:41:ALA:HB2	2.00	0.43
9:W:22:LEU:HB3	9:W:26:ARG:HH21	1.84	0.43
25:w:26:TRP:H	25:w:26:TRP:HE3	1.67	0.43
29:1:28:ARG:NH1	36:a:35:ASN:O	2.42	0.43
29:1:276:LEU:HD21	29:1:297:VAL:HG11	2.01	0.43
31:3:36:GLN:NE2	38:c:47:SER:O	2.52	0.43
31:3:410:GLY:O	31:3:421:HIS:NE2	2.49	0.43
42:g:113:ARG:HD3	42:g:114:PRO:HD2	2.00	0.43
10:j:72:CYS:SG	10:j:75:GLU:HG3	2.58	0.43
5:L:161:ARG:NH1	22:t:90:TYR:O	2.47	0.43
5:L:393:ASP:OD1	5:L:394:LEU:N	2.52	0.43
7:N:324:THR:HB	46:N:402:3PE:H261	2.01	0.43
29:1:21:ILE:HG21	29:1:230:VAL:HG12	2.00	0.43
29:1:314:THR:O	29:1:314:THR:OG1	2.33	0.43
31:3:276:ARG:NH1	31:3:680:ALA:O	2.51	0.43
31:3:337:ARG:HD3	31:3:337:ARG:HA	1.91	0.43
32:4:53:PRO:HB2	34:6:96:MET:HE1	2.00	0.43
38:c:36:ARG:O	38:c:57:MET:HA	2.18	0.43
27:y:11:TRP:CD1	27:y:11:TRP:H	2.37	0.43
29:1:108:ARG:NH2	30:2:162:GLU:OE2	2.51	0.43
33:5:137:MET:HB3	33:5:162:PHE:HB2	2.01	0.43
39:d:198:LYS:HD3	39:d:198:LYS:HA	1.76	0.43
6:M:120:ILE:HG22	6:M:121:MET:HE2	1.99	0.43
22:t:3:LEU:HD22	22:t:6:ALA:HB3	2.00	0.43
38:c:116:LYS:HD3	38:c:116:LYS:HA	1.90	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:i:60:ARG:HH22	44:i:95:ASP:HA	1.84	0.43
2:H:310:LEU:HD22	15:m:31:LEU:HB3	2.00	0.42
31:3:379:LEU:HB2	31:3:408:LEU:HD12	2.01	0.42
41:f:39:LYS:HE3	41:f:39:LYS:HB3	1.78	0.42
41:f:63:ASP:OD2	41:f:66:LYS:NZ	2.52	0.42
5:L:73:THR:HG21	5:L:194:ASN:HD21	1.85	0.42
6:M:279:GLN:HB2	6:M:285:LEU:HD12	2.02	0.42
48:X:101:ZMP:H5A	22:t:43:LEU:HD11	2.00	0.42
11:Y:76:HIS:HB3	11:Y:113:LYS:HD2	2.00	0.42
30:2:167:LYS:HB3	30:2:167:LYS:HE3	1.73	0.42
33:5:109:THR:OG1	33:5:110:TYR:N	2.52	0.42
2:H:85:MET:HE2	2:H:85:MET:HB3	1.95	0.42
6:M:201:MET:HA	6:M:201:MET:HE2	2.02	0.42
7:N:88:LYS:HE3	7:N:88:LYS:HB2	1.88	0.42
34:6:48:MET:HE3	34:6:48:MET:HB2	1.84	0.42
34:6:52:LEU:HB2	34:6:90:GLY:HA3	2.01	0.42
6:M:70:MET:HA	6:M:103:GLN:HE21	1.85	0.42
6:M:457:PRO:HD2	6:M:458:LEU:HD23	2.01	0.42
7:N:323:MET:HE3	7:N:323:MET:HB2	1.96	0.42
8:V:21:THR:O	8:V:25:THR:OG1	2.31	0.42
32:4:65:VAL:HB	32:4:77:ASP:HB3	2.01	0.42
39:d:134:HIS:HB2	39:d:149:LYS:HD3	2.01	0.42
39:d:338:LYS:HA	39:d:338:LYS:HD2	1.84	0.42
3:J:102:LEU:HD23	3:J:102:LEU:HA	1.89	0.42
6:M:105:PHE:O	6:M:109:THR:OG1	2.30	0.42
6:M:159:PRO:HB3	45:M:502:PC1:H361	2.00	0.42
7:N:24:THR:HG22	14:l:2:PHE:HZ	1.85	0.42
19:q:70:LEU:HD23	19:q:70:LEU:HA	1.89	0.42
29:1:243:ALA:HA	29:1:251:SER:HB3	2.01	0.42
34:6:81:ARG:H	34:6:81:ARG:HG2	1.42	0.42
29:1:376:MET:HE3	29:1:376:MET:HB3	1.74	0.42
35:9:3:LYS:NZ	43:h:109:GLU:OE1	2.50	0.42
35:9:95:GLU:HB2	35:9:108:ARG:HB3	2.00	0.42
5:L:534:HIS:CD2	46:L:1001:3PE:H332	2.55	0.42
22:t:26:LEU:HD21	22:t:39:PHE:HB3	2.01	0.42
27:y:45:LYS:HB3	27:y:45:LYS:HE2	1.81	0.42
40:e:64:LEU:HD12	40:e:78:LEU:HD11	2.02	0.42
1:A:16:LEU:O	1:A:20:ILE:HG12	2.19	0.42
46:H:502:3PE:H2G1	3:J:38:GLY:HA3	2.01	0.42
12:Z:27:ASN:OD1	12:Z:27:ASN:N	2.50	0.42
13:k:108:TYR:OH	13:k:164:LEU:O	2.24	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:r:109:ILE:HG22	20:r:112:THR:H	1.84	0.42
21:s:77:LEU:O	21:s:80:LYS:NZ	2.52	0.42
33:5:78:LEU:HB3	33:5:130:TYR:HB3	2.00	0.42
40:e:15:LEU:HD23	40:e:50:LEU:HD21	2.02	0.42
4:K:5:TYR:O	4:K:9:MET:HG2	2.20	0.42
5:L:135:ASN:ND2	5:L:199:GLN:OE1	2.51	0.42
39:d:91:VAL:HG23	39:d:126:VAL:HG11	2.01	0.42
1:A:74:PRO:HG2	3:J:147:TYR:HE1	1.85	0.42
3:J:23:LYS:NZ	4:K:18:GLY:O	2.35	0.42
3:J:113:VAL:HG13	3:J:119:PHE:HB2	2.01	0.42
5:L:416:THR:O	5:L:419:THR:OG1	2.30	0.42
29:1:430:MET:HE2	29:1:430:MET:HB3	1.97	0.42
40:e:90:LEU:HD12	40:e:90:LEU:HA	1.82	0.42
42:g:63:ARG:NH2	10:j:46:ASP:OD1	2.52	0.42
1:A:32:GLU:HB3	39:d:320:ARG:HH12	1.85	0.41
47:H:501:DCQ:H10	47:H:501:DCQ:H13A	1.92	0.41
5:L:136:ASN:HD21	45:L:1002:PC1:H2I1	1.85	0.41
6:M:207:MET:HG2	6:M:298:ILE:HG13	2.02	0.41
6:M:403:THR:HA	6:M:406:TYR:CE2	2.54	0.41
21:s:14:VAL:HG13	21:s:109:GLN:HG3	2.01	0.41
27:y:53:GLU:OE1	27:y:53:GLU:N	2.47	0.41
40:e:63:LYS:HE3	40:e:63:LYS:HB2	1.93	0.41
5:L:51:THR:HG21	5:L:91:PRO:HG2	2.03	0.41
7:N:170:LEU:HD23	7:N:170:LEU:HA	1.89	0.41
20:r:9:LEU:HD23	20:r:9:LEU:HA	1.92	0.41
30:2:6:LEU:HD13	30:2:10:ARG:HH12	1.85	0.41
30:2:30:ARG:HD3	36:a:52:LEU:HB3	2.02	0.41
1:A:53:MET:HG3	1:A:57:LEU:HD13	2.01	0.41
2:H:106:LEU:HD23	2:H:106:LEU:HA	1.90	0.41
4:K:55:LEU:HD23	4:K:55:LEU:HA	1.86	0.41
6:M:379:LEU:O	6:M:383:MET:HG2	2.20	0.41
10:X:64:ASP:O	10:X:68:GLU:HG2	2.21	0.41
12:Z:170:LYS:HB3	12:Z:170:LYS:HE2	1.98	0.41
13:k:37:LYS:HE2	13:k:37:LYS:HB2	1.87	0.41
13:k:252:ASP:OD1	13:k:252:ASP:N	2.51	0.41
24:v:6:LYS:HA	24:v:6:LYS:HD3	1.84	0.41
34:6:175:ILE:HD13	34:6:175:ILE:HA	1.91	0.41
19:q:57:ARG:HA	19:q:57:ARG:HD2	1.83	0.41
32:4:233:ARG:HA	32:4:236:ARG:HG2	2.01	0.41
38:c:128:THR:O	38:c:128:THR:OG1	2.36	0.41
2:H:281:ARG:HD3	32:4:412:ALA:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:27:THR:HG21	6:M:96:ILE:HG21	2.01	0.41
7:N:85:THR:HG22	7:N:87:MET:HG2	2.03	0.41
21:s:34:LYS:HE3	21:s:34:LYS:HB2	1.80	0.41
24:v:55:GLN:OE1	24:v:58:ARG:NH1	2.54	0.41
32:4:390:LYS:NZ	33:5:77:ASP:OD1	2.37	0.41
2:H:19:PHE:HZ	46:H:504:3PE:H3E1	1.85	0.41
6:M:179:LEU:HD13	6:M:249:LEU:HD21	2.03	0.41
46:N:402:3PE:H3I2	14:l:1:PRO:HG3	2.02	0.41
22:t:23:LEU:HD23	22:t:23:LEU:HA	1.81	0.41
29:1:245:PHE:HB3	29:1:271:GLU:HG3	2.03	0.41
30:2:181:ILE:HA	30:2:182:PRO:HD3	1.91	0.41
32:4:72:MET:HE3	32:4:72:MET:HB3	1.82	0.41
10:j:48:VAL:O	10:j:52:MET:HG3	2.20	0.41
1:A:71:LEU:HD23	1:A:71:LEU:HA	1.86	0.41
2:H:32:GLN:HG2	32:4:165:THR:HG22	2.02	0.41
2:H:89:LEU:HG	2:H:105:MET:HE1	2.01	0.41
7:N:211:MET:HG3	7:N:333:SER:HB2	2.03	0.41
13:k:91:GLY:HA3	13:k:281:GLU:HG3	2.02	0.41
28:z:26:ILE:HD13	28:z:26:ILE:HA	1.92	0.41
29:1:265:PRO:O	30:2:190:ARG:NH1	2.53	0.41
31:3:365:ASN:N	31:3:491:ASN:OD1	2.54	0.41
32:4:399:LEU:HD12	32:4:399:LEU:HA	1.94	0.41
32:4:429:ASP:OD1	32:4:429:ASP:N	2.52	0.41
33:5:77:ASP:OD2	33:5:79:THR:OG1	2.39	0.41
39:d:240:ASP:OD1	39:d:240:ASP:N	2.53	0.41
40:e:78:LEU:HD22	40:e:86:VAL:HG12	2.03	0.41
10:j:83:LYS:HD3	10:j:83:LYS:HA	1.73	0.41
1:A:94:LEU:HD23	1:A:94:LEU:HA	1.89	0.41
5:L:556:ILE:O	5:L:560:THR:OG1	2.24	0.41
6:M:173:SER:HB2	9:W:101:ALA:HB2	2.03	0.41
19:q:120:MET:HE2	19:q:120:MET:HB2	1.89	0.41
29:1:48:ILE:HG13	30:2:217:LEU:HD11	2.03	0.41
30:2:53:LEU:HD12	36:a:52:LEU:HG	2.02	0.41
5:L:557:TRP:O	5:L:561:ILE:HG12	2.21	0.41
7:N:289:ASN:HA	7:N:292:PHE:CE2	2.56	0.41
11:Y:23:VAL:HG21	28:z:65:GLY:HA2	2.02	0.41
17:o:109:TYR:HA	17:o:112:VAL:HG22	2.02	0.41
19:q:34:MET:HE3	35:9:26:LEU:HD12	2.02	0.41
27:y:8:ARG:HD2	27:y:8:ARG:HA	1.97	0.41
29:1:327:THR:OG1	29:1:328:GLY:N	2.54	0.41
29:1:338:ASP:OD1	29:1:338:ASP:N	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:d:287:ILE:HD13	39:d:287:ILE:HA	1.92	0.41
2:H:180:PRO:HB3	45:H:503:PC1:H261	2.03	0.41
5:L:429:PHE:HE1	22:t:31:VAL:HG21	1.85	0.41
7:N:146:LEU:HG	7:N:147:PRO:HD3	2.03	0.41
9:W:28:TYR:O	25:w:67:SER:OG	2.32	0.41
10:X:65:ILE:HD12	10:X:65:ILE:HA	1.86	0.41
10:X:83:LYS:HD3	10:X:83:LYS:HA	1.83	0.41
13:k:131:ASP:OD2	13:k:152:TYR:OH	2.36	0.41
13:k:195:THR:HG23	13:k:198:TYR:H	1.86	0.41
18:p:53:PRO:HB3	22:t:128:ARG:HD3	2.02	0.41
31:3:228:ILE:HB	31:3:583:THR:HG22	2.03	0.41
33:5:93:VAL:HG22	33:5:108:LYS:HG2	2.03	0.41
1:A:49:LEU:HD12	1:A:50:PRO:HD2	2.03	0.40
2:H:134:ARG:NH1	32:4:71:GLU:OE2	2.54	0.40
2:H:144:VAL:O	2:H:148:ILE:HG13	2.21	0.40
4:K:26:LEU:HD11	7:N:61:LEU:HD11	2.03	0.40
45:L:1002:PC1:H271	45:L:1003:PC1:H281	2.02	0.40
7:N:20:VAL:HG11	7:N:137:ALA:HB1	2.03	0.40
13:k:100:LEU:HD23	13:k:100:LEU:HA	1.95	0.40
18:p:36:LEU:O	18:p:40:SER:OG	2.36	0.40
18:p:83:THR:O	18:p:87:LEU:HB2	2.20	0.40
29:1:154:ARG:HA	36:a:58:LEU:HD21	2.04	0.40
29:1:298:ILE:HA	29:1:299:PRO:HD3	1.93	0.40
30:2:14:LYS:HA	30:2:14:LYS:HD2	1.80	0.40
35:9:64:GLU:O	35:9:134:GLY:N	2.47	0.40
41:f:47:THR:HA	41:f:50:ILE:HG12	2.03	0.40
3:J:128:TYR:HD2	19:q:136:THR:HB	1.86	0.40
4:K:73:LEU:HD11	7:N:41:ILE:HG21	2.04	0.40
6:M:239:GLY:O	6:M:243:MET:HG3	2.21	0.40
6:M:282:LEU:HD21	6:M:359:TRP:HH2	1.86	0.40
24:v:52:ASP:OD1	24:v:78:HIS:NE2	2.46	0.40
31:3:13:VAL:HG22	31:3:79:ILE:HD12	2.03	0.40
31:3:669:LYS:HB3	31:3:669:LYS:HE2	1.87	0.40
32:4:285:VAL:H	35:9:2:TYR:HA	1.85	0.40
33:5:204:GLU:OE1	33:5:210:ARG:NH2	2.52	0.40
4:K:14:VAL:HG22	46:K:101:3PE:H2B2	2.02	0.40
9:W:76:ALA:HA	9:W:80:PHE:HB2	2.03	0.40
22:t:58:LYS:HB2	22:t:58:LYS:HE3	1.69	0.40
27:y:9:ASP:OD1	27:y:9:ASP:N	2.49	0.40
35:9:132:VAL:HG11	35:9:169:ILE:HD11	2.02	0.40
39:d:54:TYR:HA	39:d:57:MET:HG2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:d:166:ILE:HG22	39:d:168:PRO:HD3	2.03	0.40
11:Y:16:GLU:OE2	14:l:104:ARG:NH1	2.53	0.40
17:o:31:LEU:HD12	17:o:31:LEU:HA	1.88	0.40
21:s:6:ARG:NH1	21:s:15:GLU:OE2	2.53	0.40
35:9:108:ARG:HB2	44:i:130:THR:HG23	2.03	0.40
41:f:34:LEU:HD23	41:f:48:GLU:HG3	2.04	0.40
1:A:73:LEU:HD23	2:H:151:LEU:HD12	2.04	0.40
2:H:79:LEU:HD11	2:H:222:LEU:HD22	2.04	0.40
2:H:296:LEU:HD13	45:H:503:PC1:H252	2.03	0.40
5:L:261:ILE:HG13	5:L:317:ILE:HD11	2.03	0.40
5:L:378:LEU:HD23	5:L:378:LEU:HA	1.91	0.40
46:N:402:3PE:H2E1	46:N:402:3PE:H3B2	2.03	0.40
31:3:363:LEU:HD23	31:3:363:LEU:HA	1.95	0.40
41:f:5:LYS:H	41:f:5:LYS:HG2	1.57	0.40

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	106/115 (92%)	100 (94%)	6 (6%)	0	100	100
2	H	310/318 (98%)	303 (98%)	7 (2%)	0	100	100
3	J	165/175 (94%)	159 (96%)	6 (4%)	0	100	100
4	K	96/98 (98%)	94 (98%)	2 (2%)	0	100	100
5	L	604/606 (100%)	584 (97%)	20 (3%)	0	100	100
6	M	457/459 (100%)	451 (99%)	6 (1%)	0	100	100
7	N	345/347 (99%)	333 (96%)	12 (4%)	0	100	100
8	V	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
9	W	137/139 (99%)	136 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	X	85/157 (54%)	82 (96%)	3 (4%)	0	100	100
10	j	80/157 (51%)	79 (99%)	1 (1%)	0	100	100
11	Y	169/171 (99%)	167 (99%)	2 (1%)	0	100	100
12	Z	169/171 (99%)	166 (98%)	3 (2%)	0	100	100
13	k	317/320 (99%)	303 (96%)	14 (4%)	0	100	100
14	l	103/105 (98%)	95 (92%)	8 (8%)	0	100	100
15	m	78/80 (98%)	72 (92%)	6 (8%)	0	100	100
16	n	77/79 (98%)	74 (96%)	3 (4%)	0	100	100
17	o	118/120 (98%)	115 (98%)	3 (2%)	0	100	100
18	p	126/128 (98%)	121 (96%)	5 (4%)	0	100	100
19	q	137/144 (95%)	135 (98%)	2 (2%)	0	100	100
20	r	95/128 (74%)	92 (97%)	3 (3%)	0	100	100
21	s	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
22	t	175/177 (99%)	169 (97%)	6 (3%)	0	100	100
23	u	63/65 (97%)	60 (95%)	3 (5%)	0	100	100
24	v	153/155 (99%)	149 (97%)	4 (3%)	0	100	100
25	w	99/101 (98%)	95 (96%)	4 (4%)	0	100	100
26	x	47/49 (96%)	47 (100%)	0	0	100	100
27	y	48/50 (96%)	45 (94%)	3 (6%)	0	100	100
28	z	68/70 (97%)	68 (100%)	0	0	100	100
29	1	428/430 (100%)	420 (98%)	8 (2%)	0	100	100
30	2	211/213 (99%)	200 (95%)	11 (5%)	0	100	100
31	3	686/688 (100%)	665 (97%)	21 (3%)	0	100	100
32	4	414/463 (89%)	397 (96%)	17 (4%)	0	100	100
33	5	206/208 (99%)	195 (95%)	11 (5%)	0	100	100
34	6	154/156 (99%)	147 (96%)	7 (4%)	0	100	100
35	9	174/176 (99%)	169 (97%)	5 (3%)	0	100	100
36	a	42/44 (96%)	41 (98%)	1 (2%)	0	100	100
37	b	93/95 (98%)	91 (98%)	2 (2%)	0	100	100
38	c	124/126 (98%)	121 (98%)	3 (2%)	0	100	100
39	d	289/380 (76%)	282 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	e	84/86 (98%)	81 (96%)	3 (4%)	0	100	100
41	f	111/113 (98%)	108 (97%)	3 (3%)	0	100	100
42	g	112/114 (98%)	109 (97%)	3 (3%)	0	100	100
43	h	92/114 (81%)	87 (95%)	5 (5%)	0	100	100
44	i	143/145 (99%)	140 (98%)	3 (2%)	0	100	100
All	All	8048/8497 (95%)	7799 (97%)	249 (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	A	99/103 (96%)	99 (100%)	0	100	100
2	H	274/278 (99%)	274 (100%)	0	100	100
3	J	138/144 (96%)	136 (99%)	2 (1%)	59	73
4	K	86/86 (100%)	86 (100%)	0	100	100
5	L	538/538 (100%)	538 (100%)	0	100	100
6	M	411/411 (100%)	411 (100%)	0	100	100
7	N	315/315 (100%)	312 (99%)	3 (1%)	68	76
8	V	101/101 (100%)	96 (95%)	5 (5%)	22	50
9	W	122/122 (100%)	122 (100%)	0	100	100
10	X	80/141 (57%)	80 (100%)	0	100	100
10	j	76/141 (54%)	76 (100%)	0	100	100
11	Y	154/154 (100%)	154 (100%)	0	100	100
12	Z	155/155 (100%)	155 (100%)	0	100	100
13	k	283/283 (100%)	283 (100%)	0	100	100
14	l	94/94 (100%)	94 (100%)	0	100	100
15	m	69/69 (100%)	68 (99%)	1 (1%)	59	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
16	n	61/61 (100%)	60 (98%)	1 (2%)	55 71
17	o	107/107 (100%)	107 (100%)	0	100 100
18	p	114/114 (100%)	114 (100%)	0	100 100
19	q	119/122 (98%)	119 (100%)	0	100 100
20	r	95/122 (78%)	95 (100%)	0	100 100
21	s	110/110 (100%)	110 (100%)	0	100 100
22	t	159/159 (100%)	159 (100%)	0	100 100
23	u	59/59 (100%)	59 (100%)	0	100 100
24	v	140/140 (100%)	139 (99%)	1 (1%)	76 80
25	w	92/92 (100%)	91 (99%)	1 (1%)	65 75
26	x	44/44 (100%)	44 (100%)	0	100 100
27	y	46/46 (100%)	46 (100%)	0	100 100
28	z	59/59 (100%)	59 (100%)	0	100 100
29	1	344/344 (100%)	344 (100%)	0	100 100
30	2	183/183 (100%)	182 (100%)	1 (0%)	81 82
31	3	578/578 (100%)	578 (100%)	0	100 100
32	4	363/391 (93%)	362 (100%)	1 (0%)	86 85
33	5	189/189 (100%)	189 (100%)	0	100 100
34	6	132/132 (100%)	132 (100%)	0	100 100
35	9	151/151 (100%)	149 (99%)	2 (1%)	61 73
36	a	43/43 (100%)	43 (100%)	0	100 100
37	b	79/79 (100%)	79 (100%)	0	100 100
38	c	113/113 (100%)	113 (100%)	0	100 100
39	d	255/326 (78%)	255 (100%)	0	100 100
40	e	76/76 (100%)	76 (100%)	0	100 100
41	f	101/101 (100%)	101 (100%)	0	100 100
42	g	107/107 (100%)	106 (99%)	1 (1%)	70 77
43	h	84/96 (88%)	84 (100%)	0	100 100
44	i	131/131 (100%)	131 (100%)	0	100 100
All	All	7129/7410 (96%)	7110 (100%)	19 (0%)	84 85

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	J	20	PHE
3	J	120	ASN
7	N	37	MET
7	N	72	MET
7	N	278	LEU
8	V	42	LEU
8	V	84	ASP
8	V	88	ASN
8	V	114	CYS
8	V	134	VAL
15	m	42	LEU
16	n	85	TYR
24	v	91	THR
25	w	40	LYS
30	2	122	LYS
32	4	240	VAL
35	9	36	MET
35	9	40	TYR
42	g	69	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	247	HIS
3	J	120	ASN
4	K	25	HIS
4	K	50	ASN
5	L	65	ASN
5	L	192	ASN
5	L	248	HIS
5	L	296	ASN
5	L	434	GLN
5	L	446	ASN
6	M	338	HIS
6	M	415	GLN
6	M	422	HIS
7	N	48	HIS
7	N	120	GLN
7	N	144	GLN
7	N	174	GLN
7	N	204	ASN
7	N	232	HIS
10	X	35	HIS

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Mol	Chain	Res	Type
10	X	74	GLN
11	Y	139	ASN
12	Z	58	ASN
12	Z	148	HIS
13	k	50	HIS
13	k	200	GLN
13	k	251	GLN
14	l	20	GLN
14	l	76	ASN
14	l	81	GLN
16	n	32	GLN
20	r	25	GLN
20	r	88	HIS
20	r	126	HIS
22	t	74	GLN
22	t	77	GLN
24	v	56	GLN
24	v	66	HIS
25	w	36	ASN
26	x	34	GLN
26	x	46	ASN
27	y	39	ASN
28	z	44	GLN
29	1	264	ASN
30	2	101	GLN
30	2	112	ASN
31	3	293	HIS
31	3	621	ASN
31	3	644	GLN
32	4	306	GLN
32	4	409	HIS
33	5	19	HIS
35	9	170	GLN
36	a	55	ASN
37	b	94	GLN
38	c	43	ASN
41	f	70	GLN
42	g	25	ASN
43	h	46	HIS
44	i	91	HIS
44	i	112	ASN
10	j	33	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

7 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	$\#\|Z\| > 2$
4	FME	K	1	4	8,9,10	0.96	0	7,9,11	0.78	0
5	FME	L	1	5	8,9,10	0.95	0	7,9,11	0.88	0
6	FME	M	1	6	8,9,10	0.97	0	7,9,11	0.99	0
13	SEP	k	36	13	8,9,10	1.57	1 (12%)	8,12,14	1.65	2 (25%)
43	AYA	h	1	43	6,7,8	1.30	1 (16%)	5,8,10	1.37	1 (20%)
8	AYA	V	1	8	6,7,8	1.20	1 (16%)	5,8,10	1.92	2 (40%)
32	2MR	4	85	32	10,12,13	2.41	2 (20%)	5,13,15	1.03	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
4	FME	K	1	4	-	4/7/9/11	-
5	FME	L	1	5	-	3/7/9/11	-
6	FME	M	1	6	-	2/7/9/11	-
13	SEP	k	36	13	-	3/5/8/10	-
43	AYA	h	1	43	-	0/4/6/8	-
8	AYA	V	1	8	-	2/4/6/8	-
32	2MR	4	85	32	-	2/10/13/15	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	4	85	2MR	CZ-NE	5.18	1.45	1.34
32	4	85	2MR	CZ-NH2	4.91	1.44	1.33
13	k	36	SEP	P-O1P	3.39	1.61	1.50
43	h	1	AYA	CA-N	-2.61	1.43	1.46
8	V	1	AYA	CA-N	-2.21	1.44	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	V	1	AYA	CB-CA-N	3.19	113.16	109.61
13	k	36	SEP	OG-CB-CA	3.03	111.09	108.14
43	h	1	AYA	CB-CA-N	2.86	112.79	109.61
13	k	36	SEP	P-OG-CB	-2.84	110.48	118.30
8	V	1	AYA	CA-N-CT	2.43	125.06	121.52

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	K	1	FME	O1-CN-N-CA
5	L	1	FME	CA-CB-CG-SD
6	M	1	FME	C-CA-CB-CG
6	M	1	FME	O-C-CA-CB
13	k	36	SEP	CB-OG-P-O1P
13	k	36	SEP	CB-OG-P-O2P
13	k	36	SEP	CB-OG-P-O3P
32	4	85	2MR	C-CA-CB-CG
8	V	1	AYA	OT-CT-N-CA
8	V	1	AYA	CM-CT-N-CA
4	K	1	FME	CA-CB-CG-SD
4	K	1	FME	CB-CG-SD-CE
5	L	1	FME	CB-CG-SD-CE
5	L	1	FME	N-CA-CB-CG
32	4	85	2MR	CA-CB-CG-CD
4	K	1	FME	CB-CA-N-CN

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 38 ligands modelled in this entry, 2 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	$\#\|Z\| > 2$
46	3PE	N	403	-	30,30,50	0.38	0	33,35,55	0.37	0
46	3PE	L	1001	-	50,50,50	0.30	0	53,55,55	0.31	0
48	ZMP	j	101	10	27,33,36	0.64	1 (3%)	32,40,45	1.06	2 (6%)
47	DCQ	H	501	-	23,23,23	0.18	0	26,29,29	0.53	0
46	3PE	A	202	-	50,50,50	0.31	0	53,55,55	0.30	0
46	3PE	V	201	-	34,34,50	0.36	0	37,39,55	0.30	0
46	3PE	M	501	-	43,43,50	0.32	0	46,48,55	0.30	0
46	3PE	V	203	-	26,26,50	0.48	0	30,31,55	0.52	1 (3%)
51	SF4	3	802	31	0,12,12	-	-	-		
48	ZMP	X	101	10	24,30,36	0.74	1 (4%)	29,37,45	1.01	1 (3%)
53	NAI	1	503	-	45,48,48	0.41	1 (2%)	60,73,73	1.65	3 (5%)
46	3PE	L	1004	-	30,30,50	0.41	0	33,35,55	0.66	1 (3%)
50	MYR	s	201	21	14,14,15	0.20	0	13,13,15	0.20	0
52	FMN	1	502	-	33,33,33	1.07	2 (6%)	48,50,50	1.26	7 (14%)
54	FES	2	300	30	0,4,4	-	-	-		
46	3PE	6	202	-	50,50,50	0.30	0	53,55,55	0.30	0
51	SF4	9	202	35	0,12,12	-	-	-		
45	PC1	L	1003	-	53,53,53	0.28	0	59,61,61	0.28	0
51	SF4	9	201	35	0,12,12	-	-	-		
49	AMP	k	501	-	25,25,25	1.38	4 (16%)	38,38,38	2.11	7 (18%)
51	SF4	3	801	31	0,12,12	-	-	-		
45	PC1	A	201	-	36,36,53	0.37	0	42,44,61	0.53	0
51	SF4	6	201	34	0,12,12	-	-	-		
45	PC1	M	502	-	53,53,53	0.30	0	59,61,61	0.32	0
46	3PE	H	502	-	50,50,50	0.31	0	53,55,55	0.34	0
57	NDP	d	401	-	49,52,52	0.38	0	66,80,80	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
46	3PE	K	101	-	39,39,50	0.34	0	42,44,55	0.34	0
46	3PE	V	202	-	36,36,50	0.35	0	39,41,55	0.31	0
46	3PE	H	504	-	50,50,50	0.30	0	53,55,55	0.28	0
45	PC1	L	1002	-	53,53,53	0.30	0	59,61,61	0.53	2 (3%)
46	3PE	N	402	-	50,50,50	0.32	0	53,55,55	0.49	0
51	SF4	1	501	29	0,12,12	-	-	-		
54	FES	3	803	31	0,4,4	-	-	-		
45	PC1	H	503	-	53,53,53	0.31	0	59,61,61	0.45	0
45	PC1	A	203	-	45,45,53	0.31	0	51,53,61	0.31	0
46	3PE	N	401	-	39,39,50	0.33	0	42,44,55	0.34	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
46	3PE	N	403	-	-	6/34/34/54	-
46	3PE	L	1001	-	-	10/54/54/54	-
48	ZMP	j	101	10	-	1/38/40/43	-
47	DCQ	H	501	-	-	3/14/38/38	0/1/1/1
46	3PE	A	202	-	-	14/54/54/54	-
46	3PE	V	201	-	-	6/38/38/54	-
46	3PE	M	501	-	-	11/47/47/54	-
46	3PE	V	203	-	-	1/27/27/54	-
51	SF4	3	802	31	-	-	0/6/5/5
48	ZMP	X	101	10	-	8/35/37/43	-
53	NAI	1	503	-	-	9/29/72/72	0/5/5/5
46	3PE	L	1004	-	-	7/34/34/54	-
50	MYR	s	201	21	-	2/11/12/13	-
52	FMN	1	502	-	-	5/18/18/18	0/3/3/3
54	FES	2	300	30	-	-	0/1/1/1
46	3PE	6	202	-	-	11/54/54/54	-
51	SF4	9	202	35	-	-	0/6/5/5
45	PC1	L	1003	-	-	6/57/57/57	-
51	SF4	9	201	35	-	-	0/6/5/5
49	AMP	k	501	-	-	4/10/26/26	0/3/3/3
51	SF4	3	801	31	-	-	0/6/5/5
45	PC1	A	201	-	-	9/40/40/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
51	SF4	6	201	34	-	-	0/6/5/5
45	PC1	M	502	-	-	17/57/57/57	-
46	3PE	H	502	-	-	13/54/54/54	-
57	NDP	d	401	-	-	3/34/77/77	0/5/5/5
46	3PE	K	101	-	-	11/43/43/54	-
46	3PE	V	202	-	-	11/40/40/54	-
46	3PE	H	504	-	-	7/54/54/54	-
45	PC1	L	1002	-	-	13/57/57/57	-
46	3PE	N	402	-	-	8/54/54/54	-
51	SF4	1	501	29	-	-	0/6/5/5
54	FES	3	803	31	-	-	0/1/1/1
45	PC1	H	503	-	-	10/57/57/57	-
45	PC1	A	203	-	-	13/49/49/57	-
46	3PE	N	401	-	-	10/43/43/54	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	k	501	AMP	C5-C4	4.59	1.47	1.39
52	1	502	FMN	C4A-N5	3.54	1.37	1.30
49	k	501	AMP	C5-C6	2.70	1.48	1.41
48	X	101	ZMP	C9-C10	2.34	1.53	1.50
49	k	501	AMP	C5-N7	-2.32	1.34	1.39
49	k	501	AMP	C8-N7	2.22	1.35	1.31
52	1	502	FMN	C10-N1	2.13	1.37	1.33
48	j	101	ZMP	C9-C10	2.07	1.53	1.50
53	1	503	NAI	PA-O5B	2.05	1.67	1.59

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	1	503	NAI	O5B-PA-O1A	-9.82	70.69	109.07
53	1	503	NAI	O2A-PA-O1A	-7.64	74.48	112.24
49	k	501	AMP	C5-C4-N3	-7.45	117.03	126.75
49	k	501	AMP	N3-C4-N9	5.89	136.78	127.08
49	k	501	AMP	C2-N3-C4	4.35	122.03	111.75
52	1	502	FMN	C4-N3-C2	-3.34	119.46	125.64
49	k	501	AMP	C4-C5-N7	-3.13	106.81	110.62
49	k	501	AMP	N3-C2-N1	-3.10	123.76	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	j	101	ZMP	O1-C10-C9	-3.03	120.41	123.99
52	1	502	FMN	C4A-C10-N10	2.89	120.71	116.48
52	1	502	FMN	C4A-C4-N3	2.71	120.08	113.19
49	k	501	AMP	C5-N7-C8	2.66	107.29	103.51
48	X	101	ZMP	O1-C10-C9	-2.64	120.88	123.99
52	1	502	FMN	O4-C4-C4A	-2.60	119.70	126.60
52	1	502	FMN	C4A-C10-N1	-2.37	119.23	124.73
45	L	1002	PC1	C2-O21-C21	2.30	123.44	117.79
53	1	503	NAI	O2A-PA-O5B	2.24	118.15	107.75
52	1	502	FMN	C10-C4A-N5	-2.20	120.19	124.86
46	V	203	3PE	O12-P-O14	2.17	119.17	110.68
49	k	501	AMP	C1'-N9-C8	-2.12	122.34	127.14
46	L	1004	3PE	C2-O21-C21	2.11	122.98	117.79
45	L	1002	PC1	O21-C2-C1	2.06	115.85	108.40
48	j	101	ZMP	C9-C10-S1	2.05	115.85	113.46
52	1	502	FMN	C4-C4A-C10	2.01	120.16	116.79

There are no chirality outliers.

All (229) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	A	203	PC1	C11-O13-P-O12
45	A	203	PC1	C1-O11-P-O14
45	H	503	PC1	C1-O11-P-O13
45	L	1002	PC1	C1-O11-P-O12
45	L	1002	PC1	C1-O11-P-O14
45	M	502	PC1	C11-O13-P-O12
45	M	502	PC1	C11-O13-P-O14
45	M	502	PC1	C11-O13-P-O11
45	M	502	PC1	C1-O11-P-O12
46	A	202	3PE	C1-O11-P-O12
46	A	202	3PE	C1-O11-P-O14
46	A	202	3PE	C11-O13-P-O12
46	H	502	3PE	C11-O13-P-O12
46	H	504	3PE	O13-C11-C12-N
46	K	101	3PE	C11-O13-P-O14
46	L	1001	3PE	C11-O13-P-O11
46	L	1001	3PE	C11-O13-P-O14
46	L	1004	3PE	C11-O13-P-O12
46	M	501	3PE	C11-O13-P-O14
46	N	401	3PE	C1-O11-P-O12
46	N	401	3PE	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
46	N	401	3PE	C1-O11-P-O14
46	N	401	3PE	C11-O13-P-O11
46	N	401	3PE	C11-O13-P-O12
46	N	401	3PE	C11-O13-P-O14
46	N	402	3PE	C11-O13-P-O11
46	N	402	3PE	C11-O13-P-O14
46	N	403	3PE	C11-O13-P-O11
46	N	403	3PE	C11-O13-P-O12
46	N	403	3PE	C11-O13-P-O14
46	N	403	3PE	O13-C11-C12-N
46	V	201	3PE	C1-O11-P-O12
46	V	201	3PE	C1-O11-P-O14
46	V	202	3PE	C1-O11-P-O14
46	V	202	3PE	C11-O13-P-O11
46	V	202	3PE	C11-O13-P-O12
46	V	202	3PE	C11-O13-P-O14
46	V	202	3PE	O13-C11-C12-N
46	6	202	3PE	C1-O11-P-O12
46	6	202	3PE	C1-O11-P-O14
46	6	202	3PE	C11-O13-P-O11
46	6	202	3PE	C11-O13-P-O12
46	6	202	3PE	C11-O13-P-O14
48	X	101	ZMP	C16-C17-C18-C21
48	X	101	ZMP	C17-C16-N2-C15
48	j	101	ZMP	S1-C11-C12-N1
50	s	201	MYR	C1-C2-C3-C4
52	1	502	FMN	N10-C1'-C2'-O2'
52	1	502	FMN	N10-C1'-C2'-C3'
52	1	502	FMN	C5'-O5'-P-O2P
52	1	502	FMN	C5'-O5'-P-O3P
53	1	503	NAI	C5D-O5D-PN-O3
53	1	503	NAI	C2D-C1D-N1N-C6N
57	d	401	NDP	C2B-O2B-P2B-O3X
48	X	101	ZMP	O3-C16-N2-C15
53	1	503	NAI	C2D-C1D-N1N-C2N
45	A	201	PC1	C11-O13-P-O11
45	A	203	PC1	C1-O11-P-O13
45	L	1002	PC1	C1-O11-P-O13
46	A	202	3PE	C1-O11-P-O13
46	H	502	3PE	C11-O13-P-O11
46	K	101	3PE	C1-O11-P-O13
46	L	1004	3PE	C11-O13-P-O11

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Mol	Chain	Res	Type	Atoms
46	V	201	3PE	C1-O11-P-O13
46	6	202	3PE	C1-O11-P-O13
45	M	502	PC1	C11-C12-N-C14
46	6	202	3PE	C36-C37-C38-C39
46	6	202	3PE	C3C-C3D-C3E-C3F
46	V	202	3PE	C2-C1-O11-P
45	A	203	PC1	C3B-C3C-C3D-C3E
46	N	402	3PE	C21-C22-C23-C24
45	A	203	PC1	C11-C12-N-C14
46	A	202	3PE	C2C-C2D-C2E-C2F
45	A	201	PC1	C11-C12-N-C13
46	V	203	3PE	C22-C23-C24-C25
46	A	202	3PE	C2E-C2F-C2G-C2H
45	A	203	PC1	C11-C12-N-C15
45	M	502	PC1	C11-C12-N-C15
45	M	502	PC1	C3A-C3B-C3C-C3D
47	H	501	DCQ	C11-C12-C13-C14
46	H	502	3PE	C1-O11-P-O13
46	V	202	3PE	C1-O11-P-O13
45	A	203	PC1	C11-C12-N-C13
45	M	502	PC1	C11-C12-N-C13
48	X	101	ZMP	O3-C16-C17-O4
52	1	502	FMN	C5'-O5'-P-O1P
45	A	201	PC1	C11-C12-N-C14
45	L	1002	PC1	C23-C24-C25-C26
46	N	401	3PE	C31-C32-C33-C34
45	A	201	PC1	C11-C12-N-C15
45	L	1002	PC1	O11-C1-C2-C3
45	M	502	PC1	O11-C1-C2-C3
46	A	202	3PE	O13-C11-C12-N
46	M	501	3PE	C38-C39-C3A-C3B
45	L	1002	PC1	C2-C1-O11-P
46	K	101	3PE	C11-O13-P-O11
45	M	502	PC1	C25-C26-C27-C28
47	H	501	DCQ	C11-C10-C9-C8
46	6	202	3PE	C33-C34-C35-C36
45	H	503	PC1	C2B-C2C-C2D-C2E
46	L	1001	3PE	C2-C1-O11-P
46	L	1004	3PE	C2-C1-O11-P
46	M	501	3PE	C2-C1-O11-P
45	L	1002	PC1	C3B-C3C-C3D-C3E
53	1	503	NAI	PN-O3-PA-O5B

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Mol	Chain	Res	Type	Atoms
46	M	501	3PE	O11-C1-C2-C3
45	A	201	PC1	O21-C21-C22-C23
45	L	1003	PC1	C39-C3A-C3B-C3C
46	K	101	3PE	C2-C1-O11-P
53	1	503	NAI	PA-O3-PN-O2N
46	V	202	3PE	C32-C33-C34-C35
46	A	202	3PE	C11-O13-P-O11
46	M	501	3PE	C11-O13-P-O11
46	V	201	3PE	C11-O13-P-O11
53	1	503	NAI	O4D-C1D-N1N-C6N
57	d	401	NDP	O4D-C1D-N1N-C6N
45	M	502	PC1	C2-C1-O11-P
46	H	502	3PE	C2-C1-O11-P
45	A	201	PC1	C11-O13-P-O14
45	A	203	PC1	C1-O11-P-O12
45	H	503	PC1	C1-O11-P-O12
46	A	202	3PE	C11-O13-P-O14
46	K	101	3PE	C1-O11-P-O14
46	L	1004	3PE	C11-O13-P-O14
46	V	202	3PE	C1-O11-P-O12
53	1	503	NAI	C5B-O5B-PA-O2A
46	N	401	3PE	O13-C11-C12-N
47	H	501	DCQ	C5-C4-O4-C4M
46	A	202	3PE	C12-C11-O13-P
46	H	502	3PE	C12-C11-O13-P
45	A	203	PC1	C22-C23-C24-C25
45	A	201	PC1	O11-C1-C2-O21
45	M	502	PC1	O11-C1-C2-O21
46	M	501	3PE	O11-C1-C2-O21
45	A	203	PC1	C23-C24-C25-C26
45	H	503	PC1	O13-C11-C12-N
45	L	1002	PC1	O13-C11-C12-N
46	M	501	3PE	C39-C3A-C3B-C3C
45	L	1002	PC1	C2A-C2B-C2C-C2D
46	H	502	3PE	C29-C2A-C2B-C2C
45	M	502	PC1	O31-C31-C32-C33
49	k	501	AMP	C5'-O5'-P-O1P
45	M	502	PC1	C39-C3A-C3B-C3C
45	L	1002	PC1	C3E-C3F-C3G-C3H
45	H	503	PC1	C11-O13-P-O11
45	L	1003	PC1	C11-O13-P-O11
46	H	504	3PE	C11-O13-P-O11

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Mol	Chain	Res	Type	Atoms
49	k	501	AMP	C4'-C5'-O5'-P
46	V	201	3PE	C33-C34-C35-C36
49	k	501	AMP	C2'-C1'-N9-C8
46	K	101	3PE	C34-C35-C36-C37
46	K	101	3PE	C21-C22-C23-C24
46	L	1001	3PE	C36-C37-C38-C39
46	6	202	3PE	C23-C24-C25-C26
46	H	502	3PE	C2F-C2G-C2H-C2I
45	H	503	PC1	C3A-C3B-C3C-C3D
48	X	101	ZMP	N2-C16-C17-C18
45	H	503	PC1	C3-C2-O21-C21
46	L	1001	3PE	C35-C36-C37-C38
45	A	201	PC1	C22-C23-C24-C25
53	1	503	NAI	O4D-C1D-N1N-C2N
46	A	202	3PE	C2-C1-O11-P
46	N	402	3PE	O11-C1-C2-O21
45	A	203	PC1	C3F-C3G-C3H-C3I
45	M	502	PC1	C36-C37-C38-C39
46	L	1001	3PE	C34-C35-C36-C37
46	M	501	3PE	C35-C36-C37-C38
45	L	1003	PC1	C37-C38-C39-C3A
45	H	503	PC1	C2C-C2D-C2E-C2F
46	H	502	3PE	C26-C27-C28-C29
46	6	202	3PE	C32-C33-C34-C35
48	X	101	ZMP	N2-C16-C17-O4
46	N	402	3PE	O31-C31-C32-C33
45	L	1003	PC1	C3E-C3F-C3G-C3H
45	L	1002	PC1	C1-C2-O21-C21
46	L	1004	3PE	C1-C2-O21-C21
46	L	1001	3PE	O31-C31-C32-C33
46	L	1004	3PE	O21-C21-C22-C23
50	s	201	MYR	C11-C10-C9-C8
46	H	502	3PE	O11-C1-C2-O21
46	N	401	3PE	O21-C21-C22-C23
45	H	503	PC1	C22-C23-C24-C25
46	N	403	3PE	C31-C32-C33-C34
48	X	101	ZMP	C16-C17-C18-C20
46	H	502	3PE	O11-C1-C2-C3
45	H	503	PC1	C35-C36-C37-C38
46	H	502	3PE	C28-C29-C2A-C2B
46	A	202	3PE	O21-C2-C3-O31
46	M	501	3PE	O31-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
46	V	202	3PE	O31-C31-C32-C33
46	A	202	3PE	O21-C21-C22-C23
45	A	201	PC1	O22-C21-C22-C23
46	L	1001	3PE	O32-C31-C32-C33
49	k	501	AMP	C2'-C1'-N9-C4
46	L	1004	3PE	O22-C21-C22-C23
46	N	402	3PE	O32-C31-C32-C33
46	L	1001	3PE	C3B-C3C-C3D-C3E
46	N	401	3PE	O22-C21-C22-C23
46	H	504	3PE	C36-C37-C38-C39
45	M	502	PC1	C1-O11-P-O13
46	M	501	3PE	O32-C31-C32-C33
45	A	203	PC1	C11-O13-P-O14
45	L	1002	PC1	C11-O13-P-O14
45	M	502	PC1	C1-O11-P-O14
46	H	502	3PE	C1-O11-P-O14
46	H	504	3PE	C1-O11-P-O12
46	H	504	3PE	C1-O11-P-O14
46	V	201	3PE	C11-O13-P-O12
53	1	503	NAI	C2N-C3N-C7N-N7N
57	d	401	NDP	O4B-C4B-C5B-O5B
46	K	101	3PE	O13-C11-C12-N
46	A	202	3PE	O22-C21-C22-C23
46	L	1001	3PE	C26-C27-C28-C29
45	L	1003	PC1	C12-C11-O13-P
46	H	504	3PE	C12-C11-O13-P
46	K	101	3PE	C12-C11-O13-P
46	N	402	3PE	C12-C11-O13-P
46	N	402	3PE	C3-C2-O21-C21
48	X	101	ZMP	O3-C16-C17-C18
46	H	502	3PE	C32-C33-C34-C35
46	H	504	3PE	O21-C21-C22-C23
46	K	101	3PE	O31-C31-C32-C33
45	L	1002	PC1	C37-C38-C39-C3A
46	K	101	3PE	O32-C31-C32-C33
45	A	203	PC1	C26-C27-C28-C29
46	M	501	3PE	C3C-C3D-C3E-C3F
46	N	403	3PE	O31-C31-C32-C33
46	V	202	3PE	O32-C31-C32-C33
45	L	1003	PC1	C26-C27-C28-C29

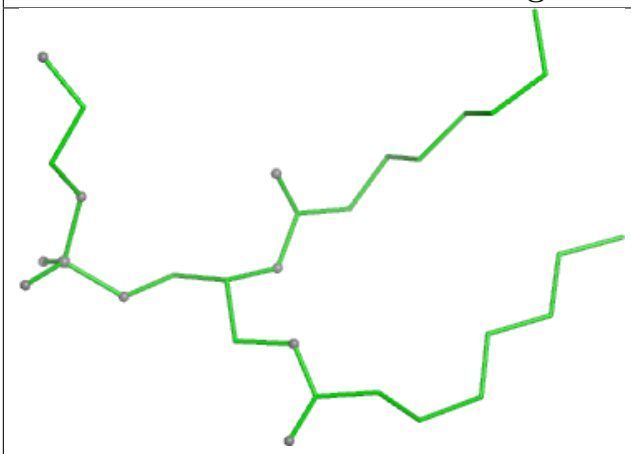
There are no ring outliers.

20 monomers are involved in 33 short contacts:

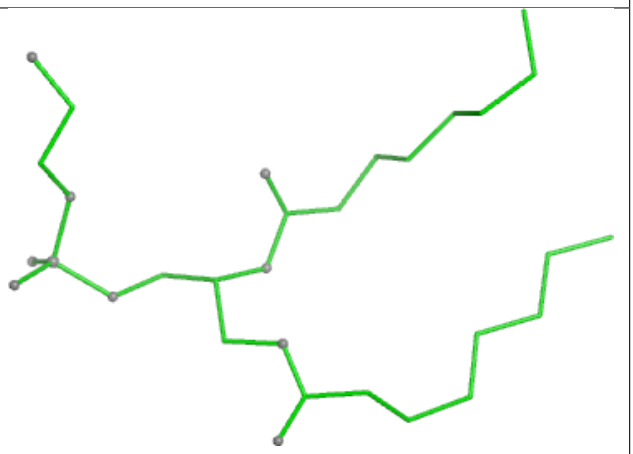
Mol	Chain	Res	Type	Clashes	Symm-Clashes
46	L	1001	3PE	2	0
47	H	501	DCQ	1	0
46	A	202	3PE	1	0
46	M	501	3PE	2	0
48	X	101	ZMP	2	0
53	1	503	NAI	2	0
46	L	1004	3PE	1	0
46	6	202	3PE	1	0
45	L	1003	PC1	2	0
49	k	501	AMP	1	0
51	3	801	SF4	1	0
45	M	502	PC1	3	0
46	H	502	3PE	1	0
57	d	401	NDP	1	0
46	K	101	3PE	2	0
46	H	504	3PE	3	0
45	L	1002	PC1	2	0
46	N	402	3PE	3	0
45	H	503	PC1	3	0
45	A	203	PC1	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.

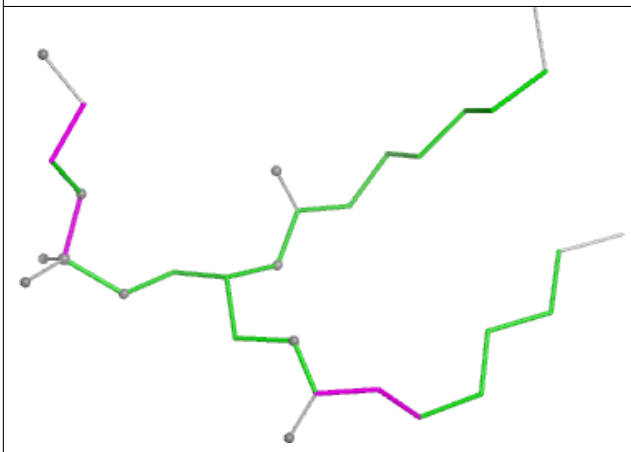
Ligand 3PE N 403



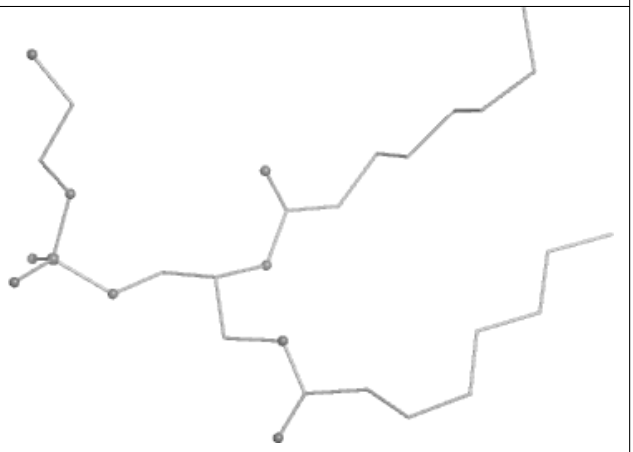
Bond lengths



Bond angles

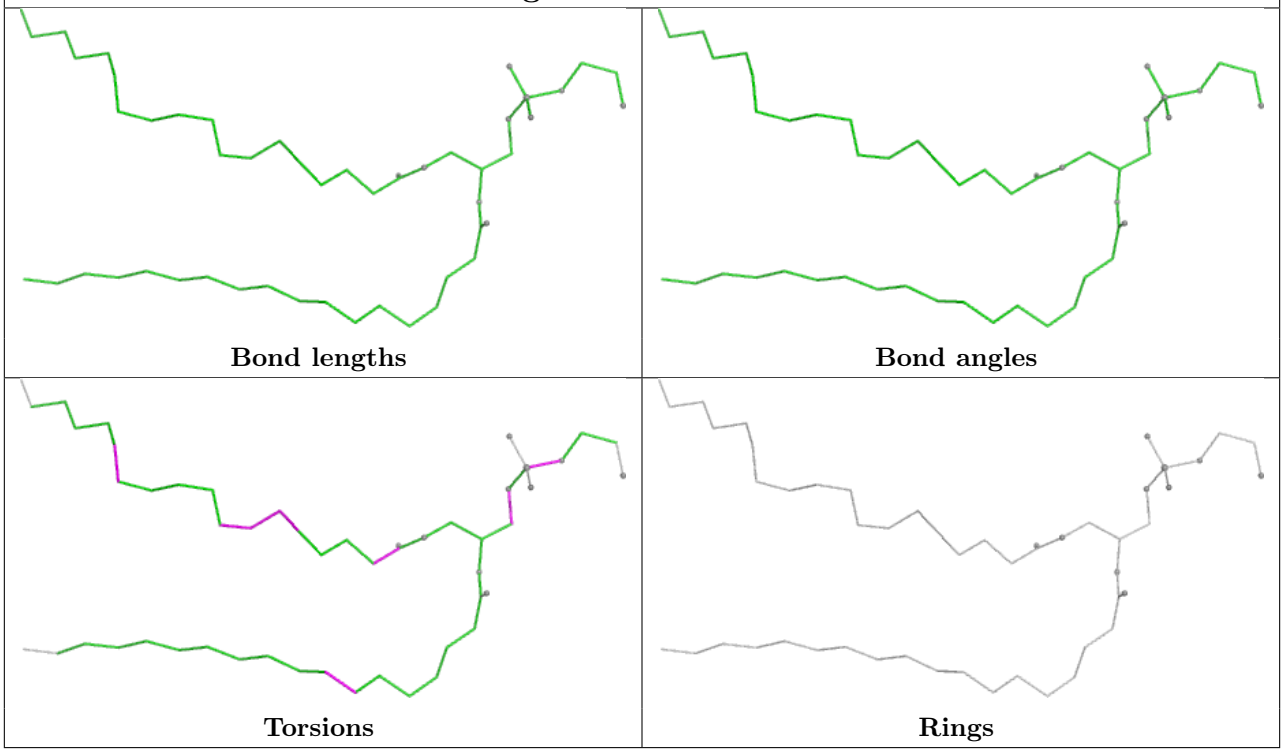


Torsions

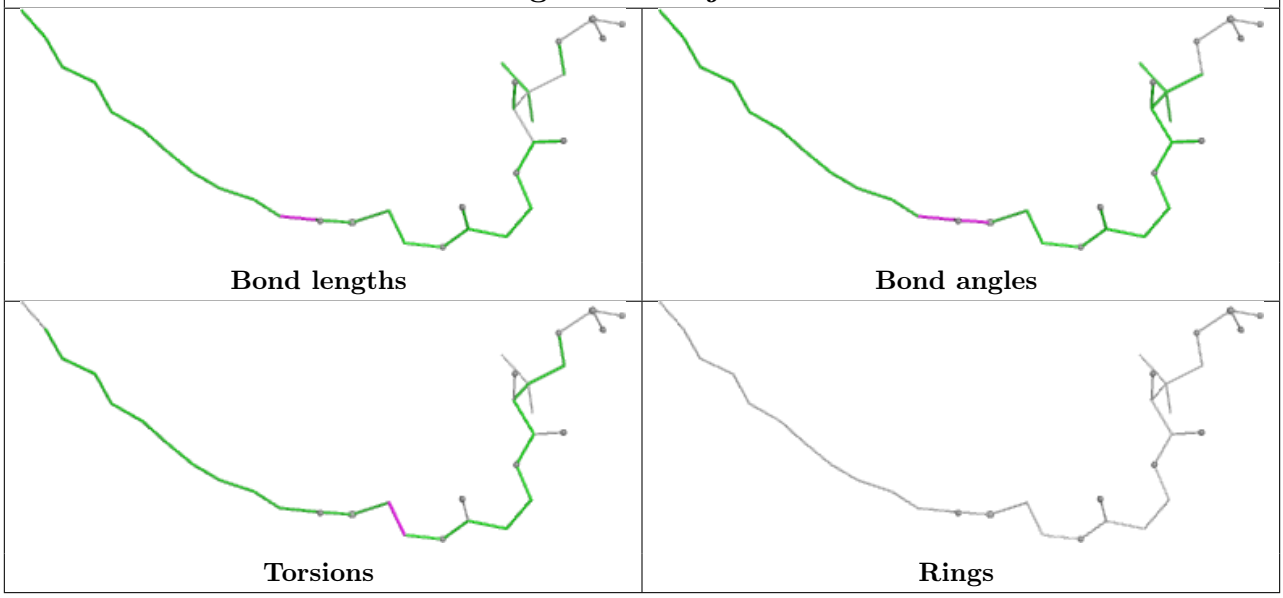


Rings

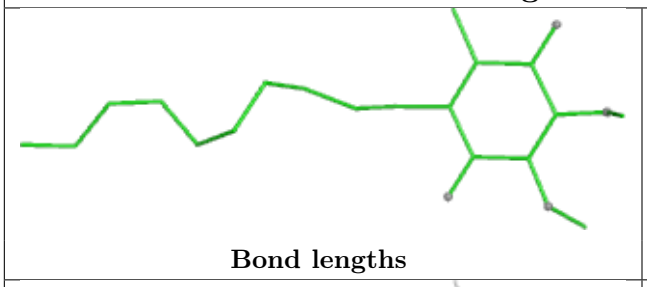
Ligand 3PE L 1001



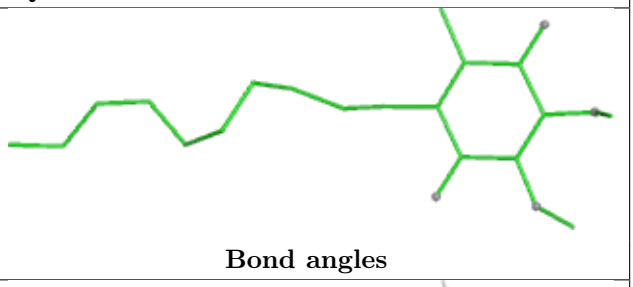
Ligand ZMP j 101



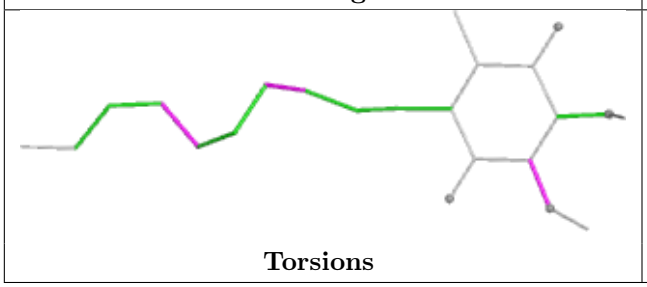
Ligand DCQ H 501



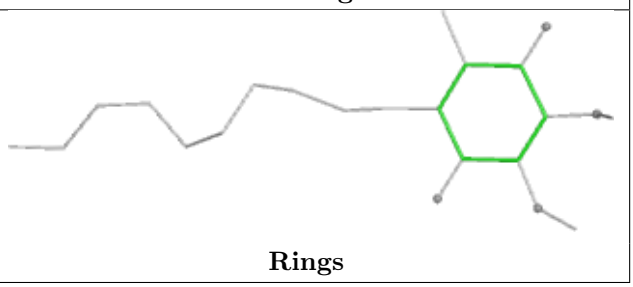
Bond lengths



Bond angles

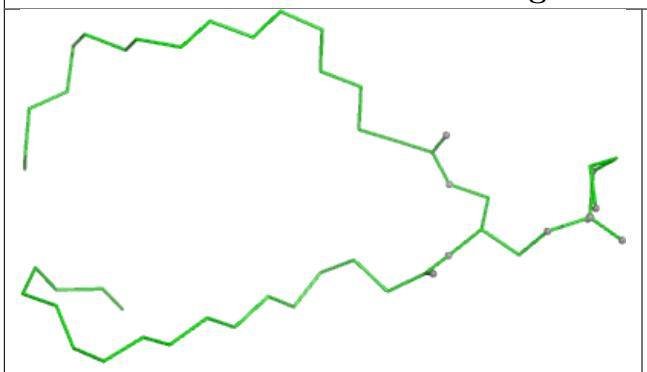


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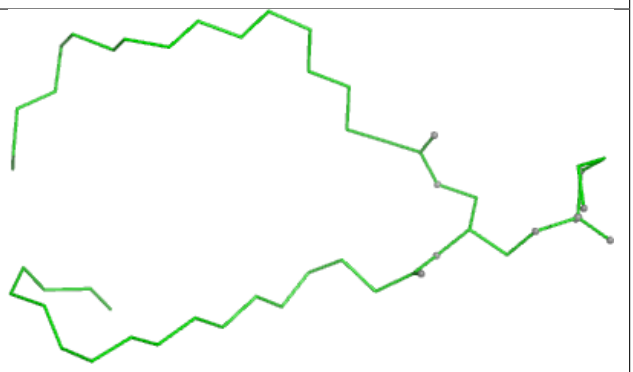


Rings

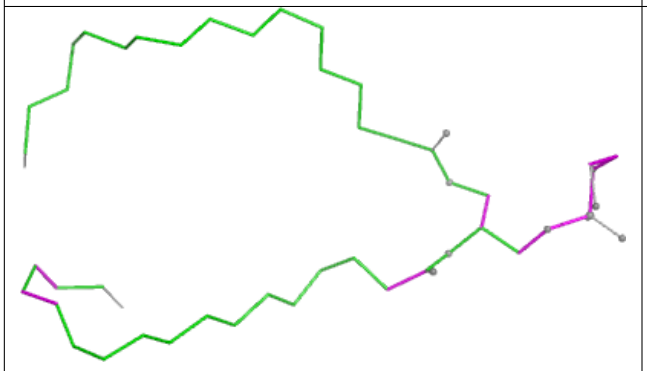
Ligand 3PE A 202



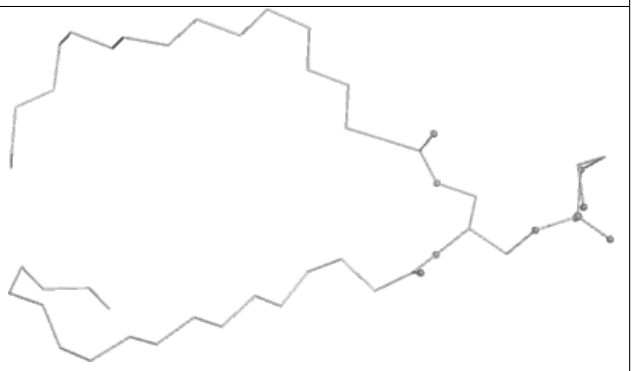
Bond lengths



Bond angles

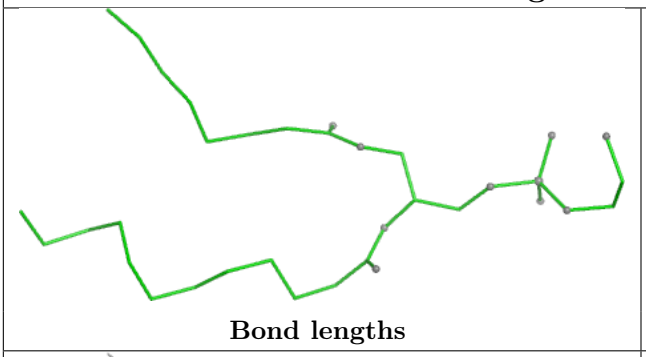


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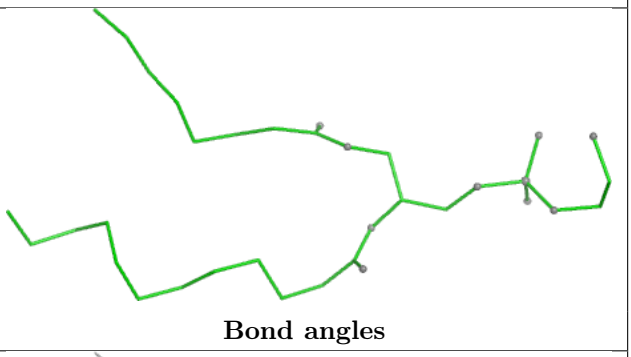


Rings

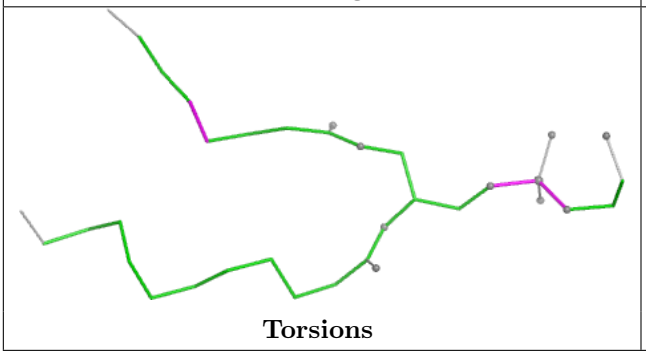
Ligand 3PE V 201



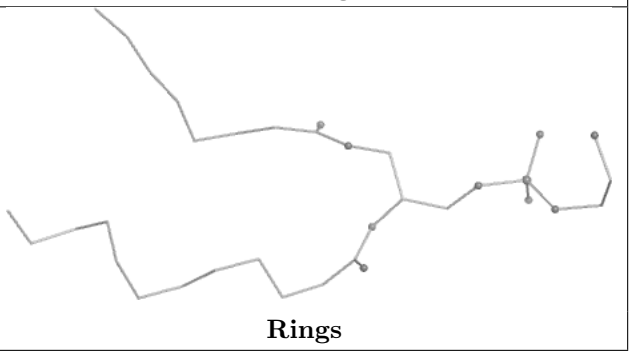
Bond lengths



Bond angles

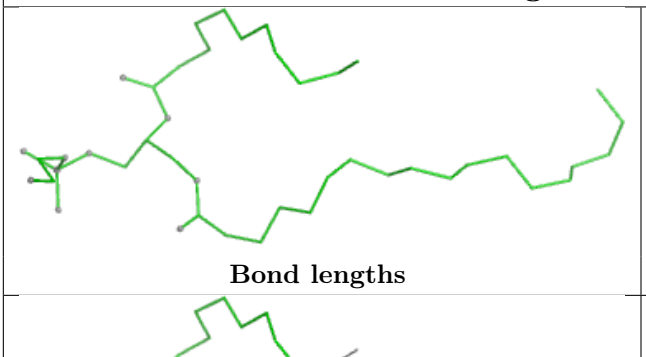


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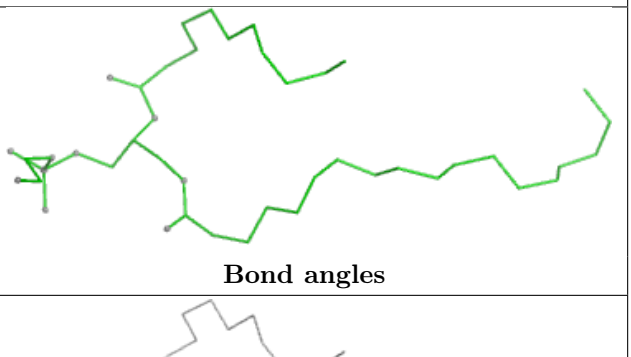


Rings

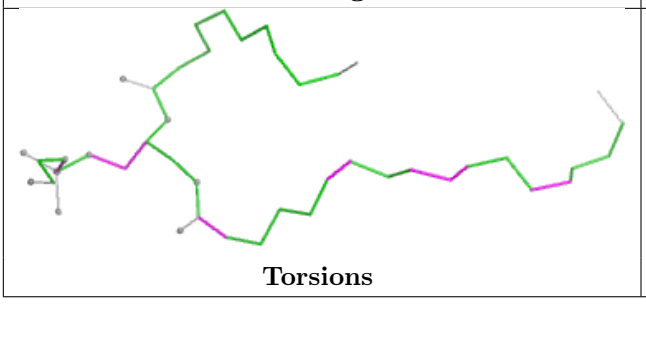
Ligand 3PE M 501



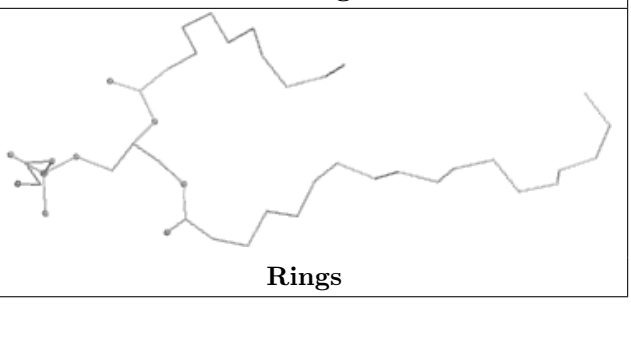
Bond lengths



Bond angles

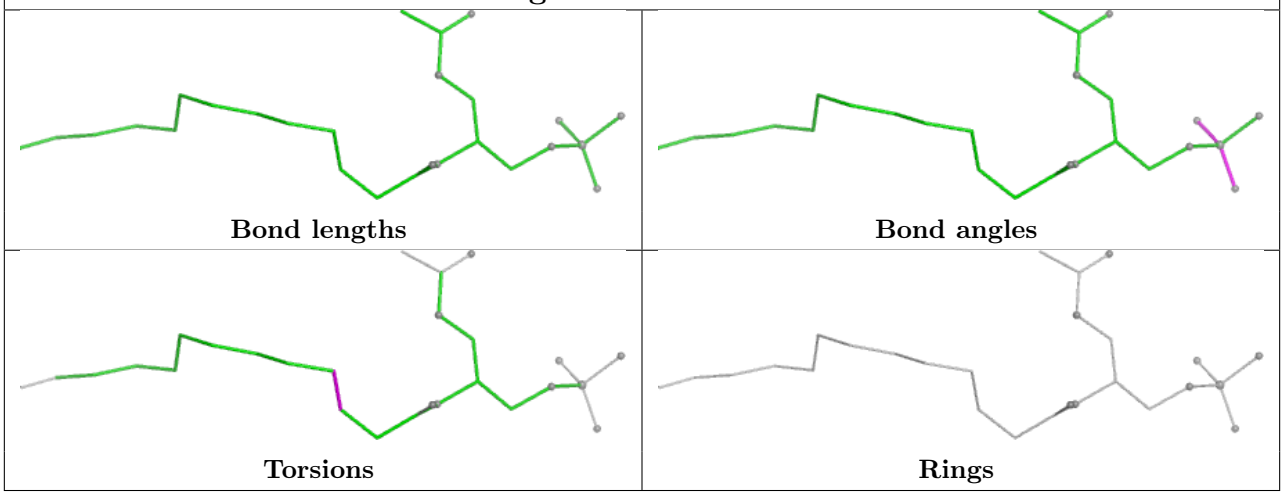


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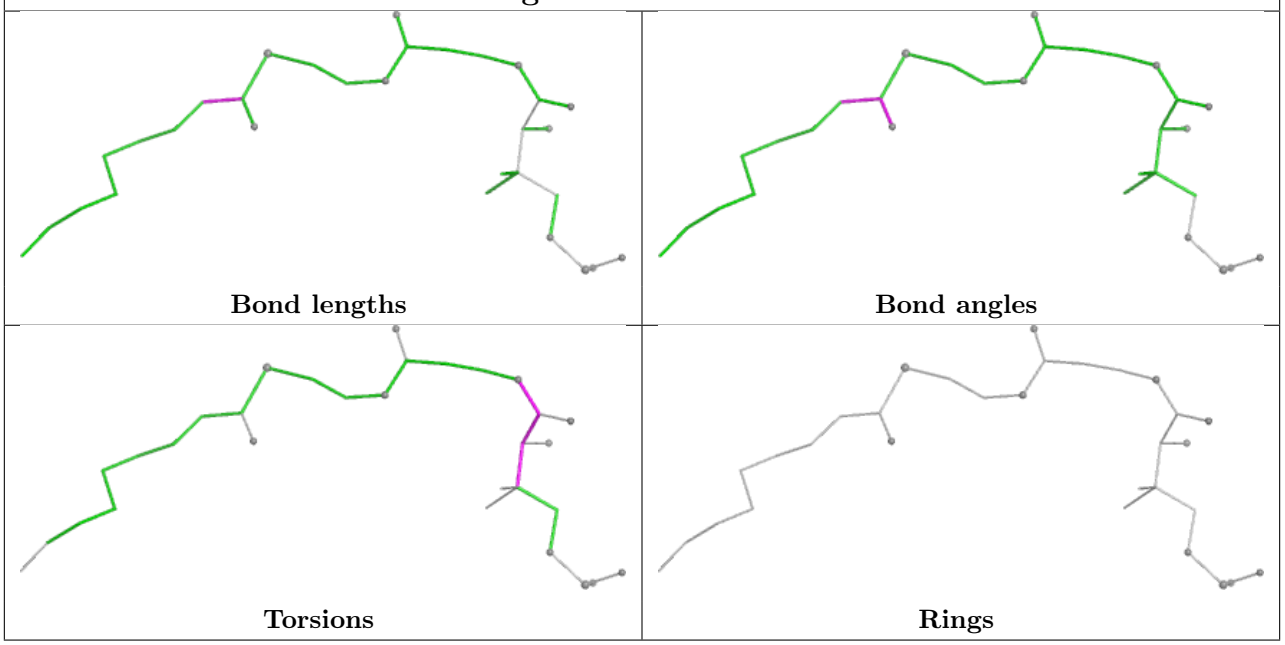


Rings

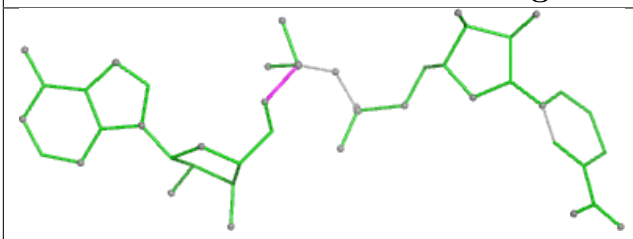
Ligand 3PE V 203



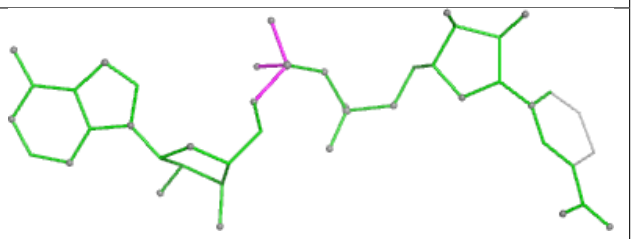
Ligand ZMP X 101



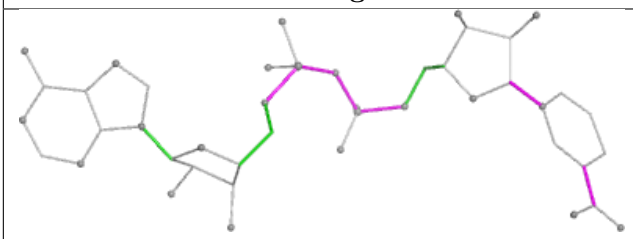
Ligand NAI 1 503



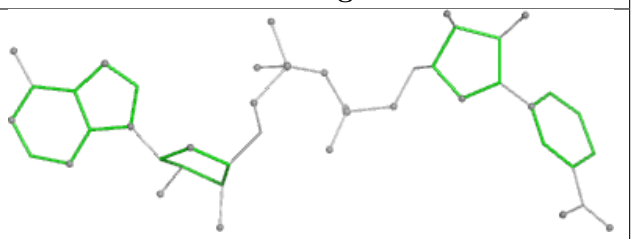
Bond lengths



Bond angles

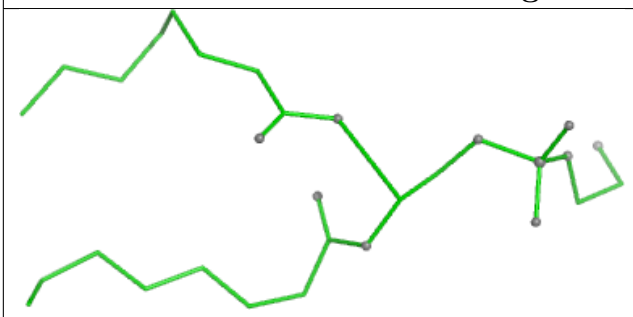


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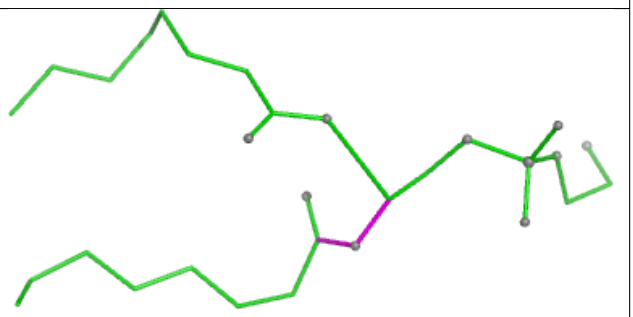


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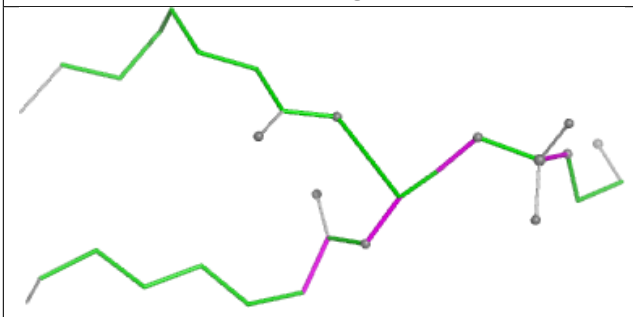
Ligand 3PE L 1004



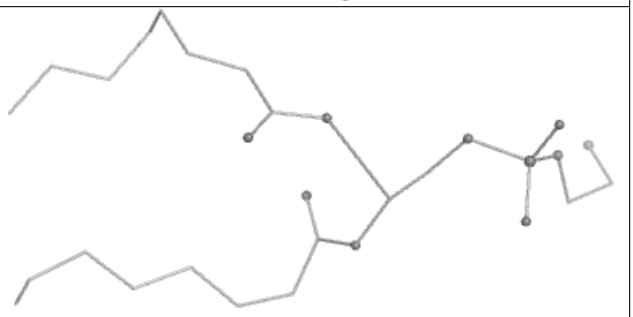
Bond lengths



Bond angles

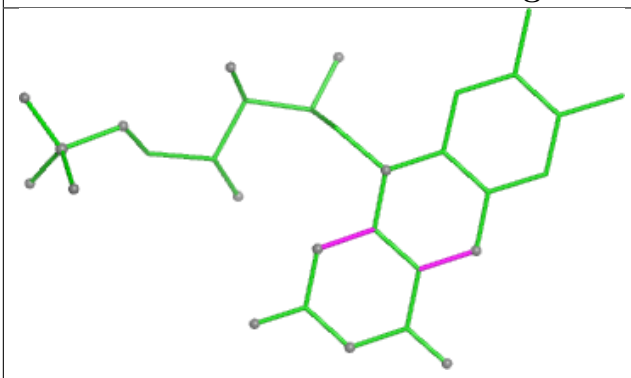


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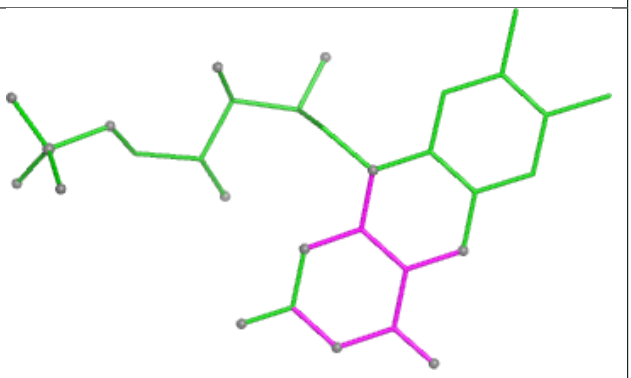


Rings

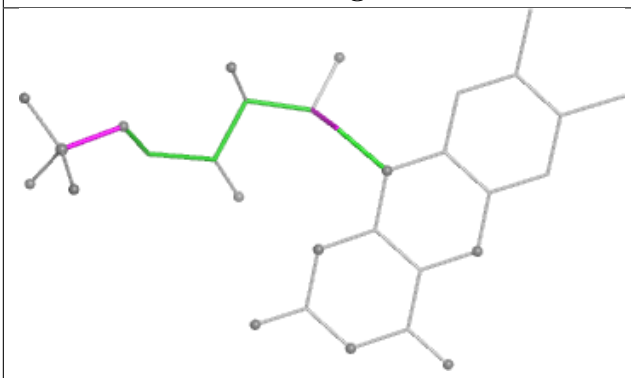
Ligand FMN 1 502



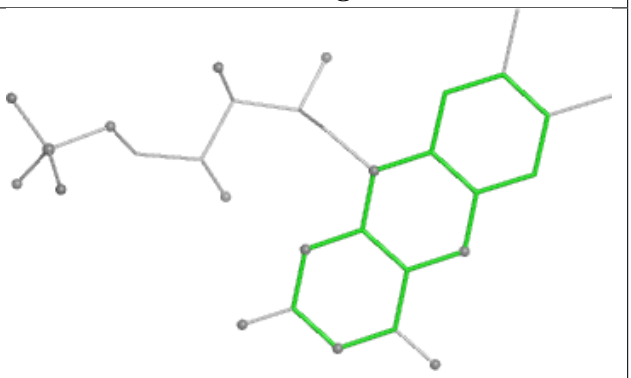
Bond lengths



Bond angles

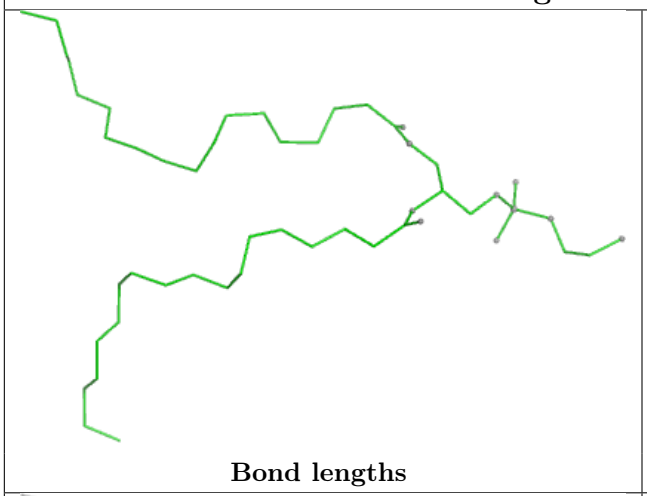


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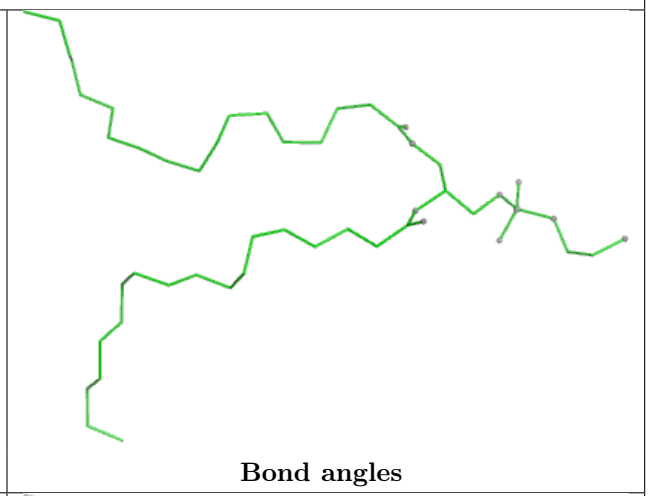


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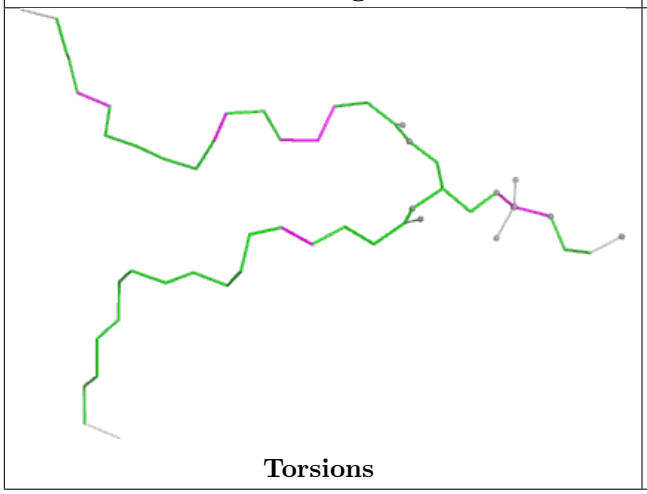
Ligand 3PE 6 202



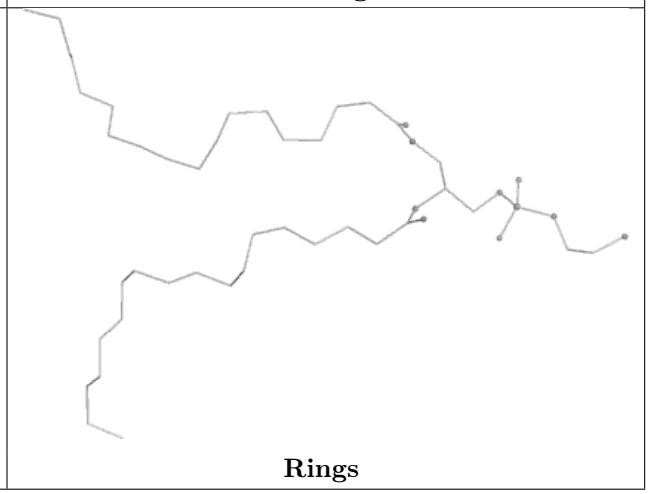
Bond lengths



Bond angles

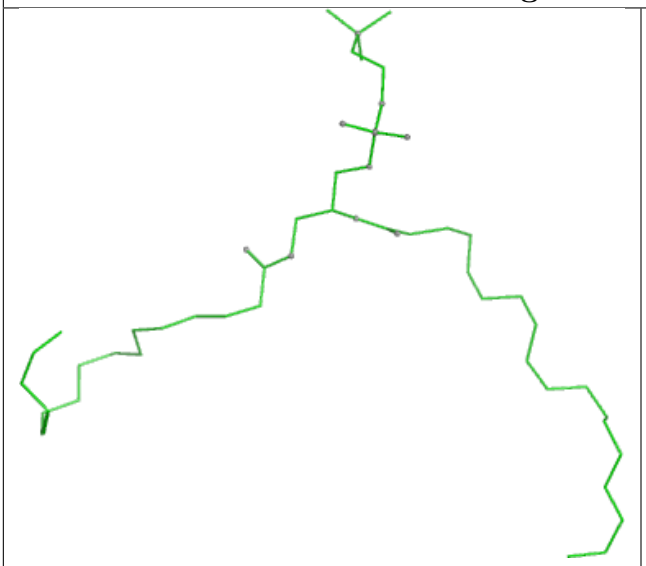


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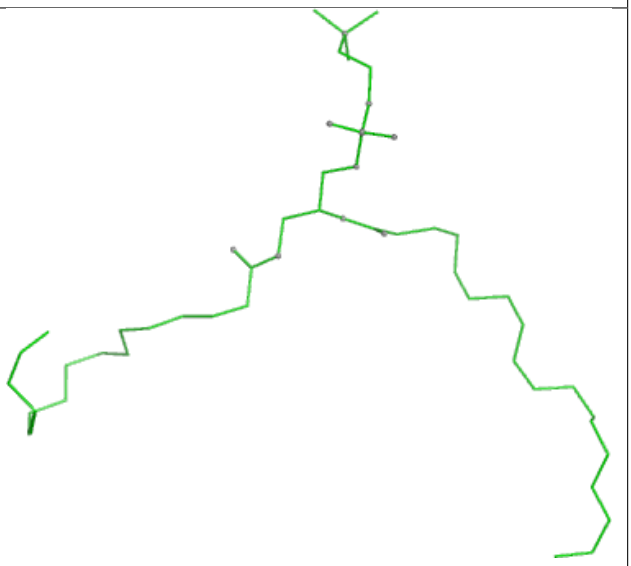


Rings

Ligand PC1 L 1003



Bond lengths



Bond angles

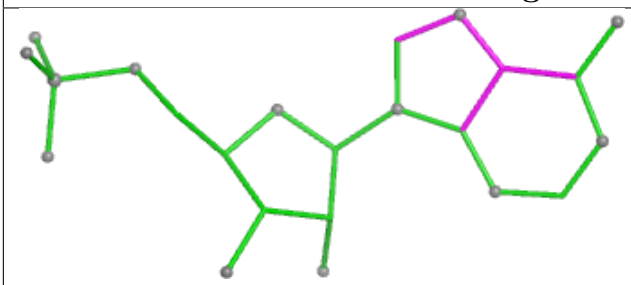


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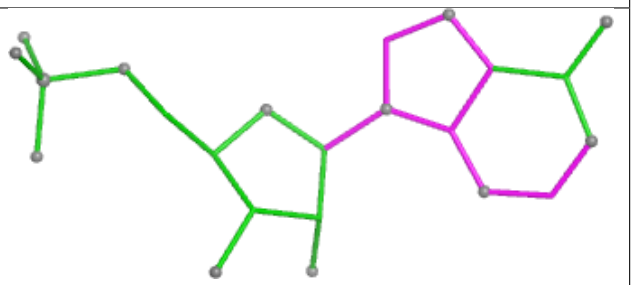


Rings

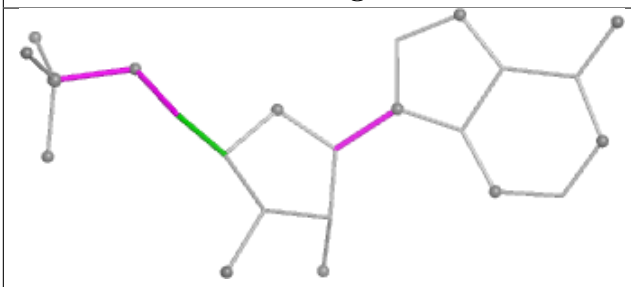
Ligand AMP k 501



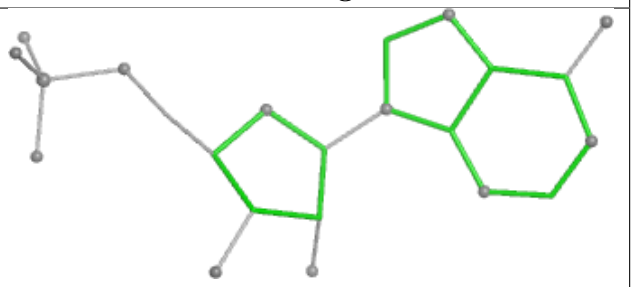
Bond lengths



Bond angles

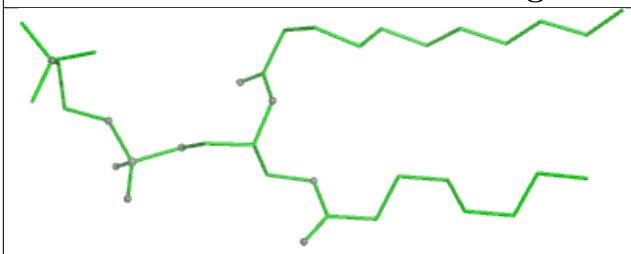


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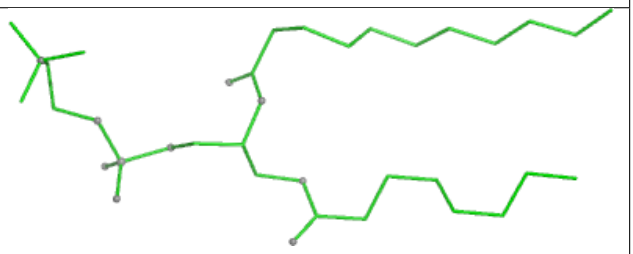


Rings

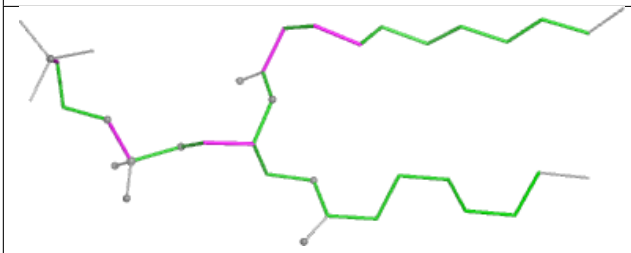
Ligand PC1 A 201



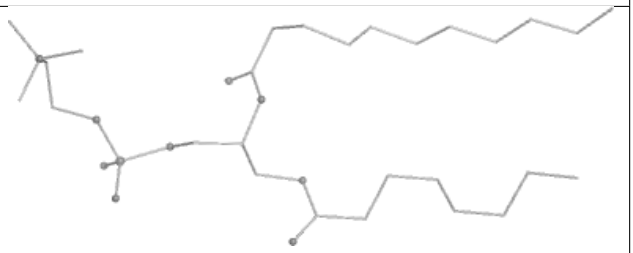
Bond lengths



Bond angles

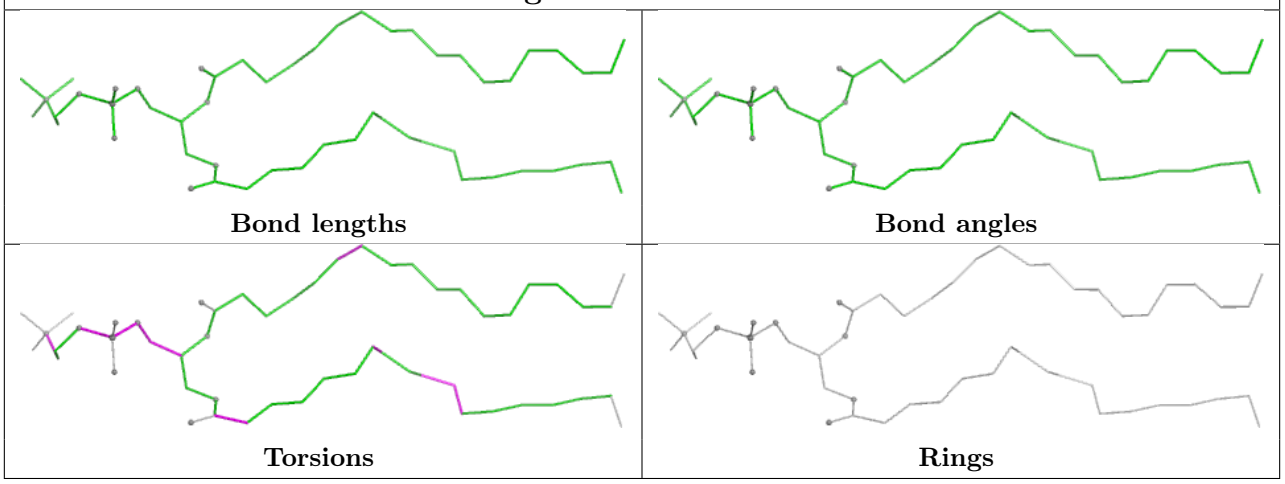


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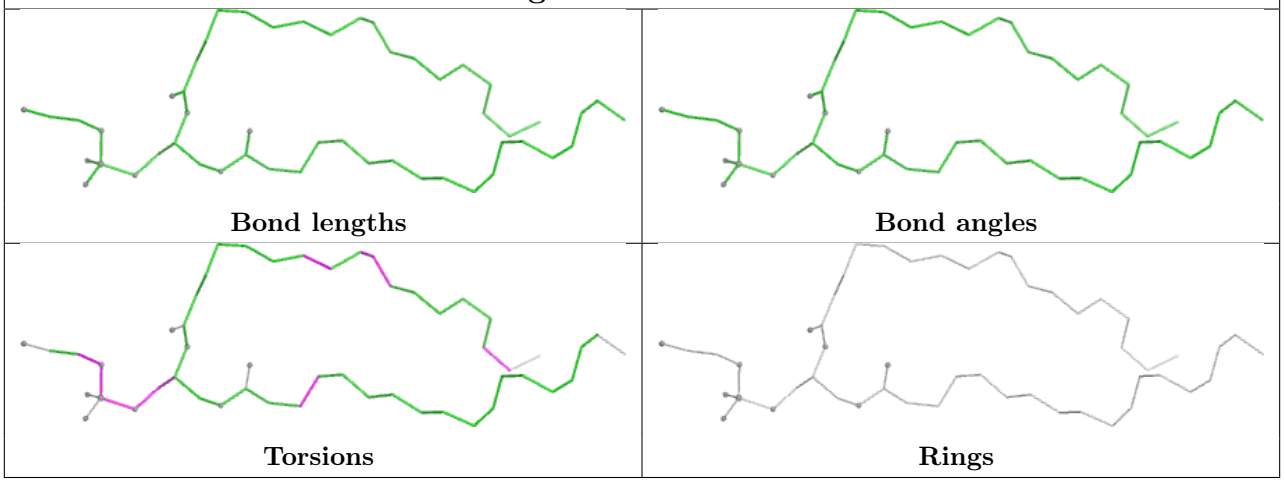


Rings

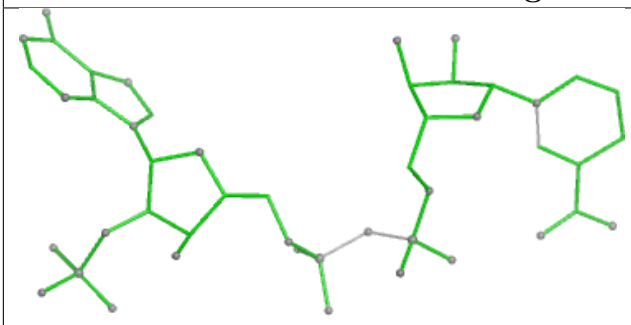
Ligand PC1 M 502



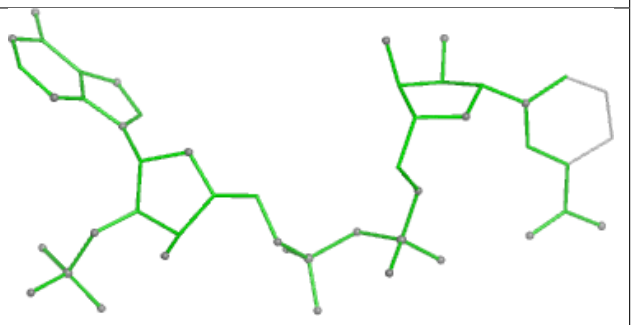
Ligand 3PE H 502



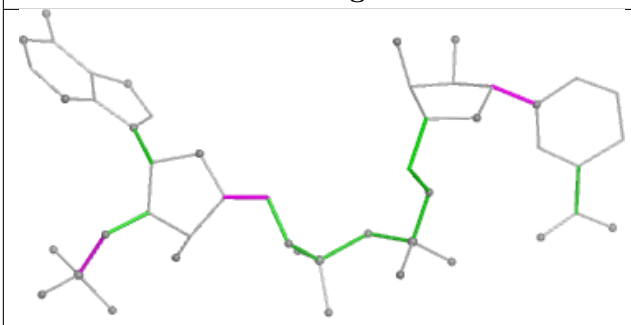
Ligand NDP d 401



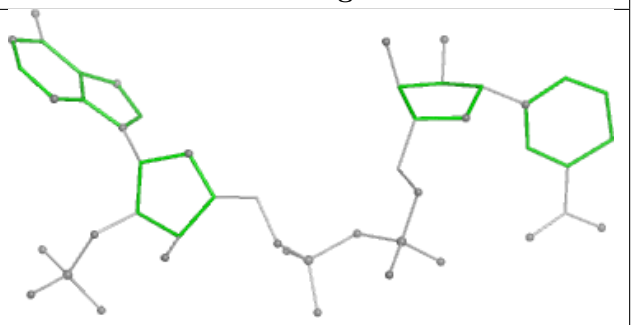
Bond lengths



Bond angles

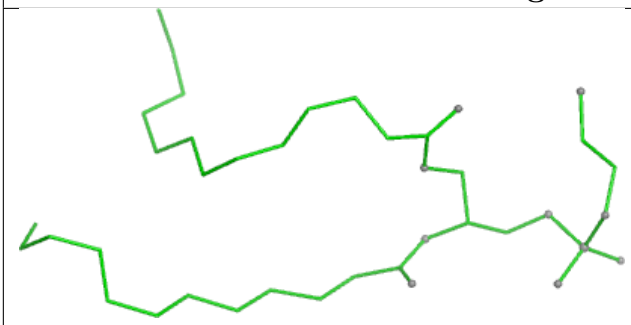


Torsions

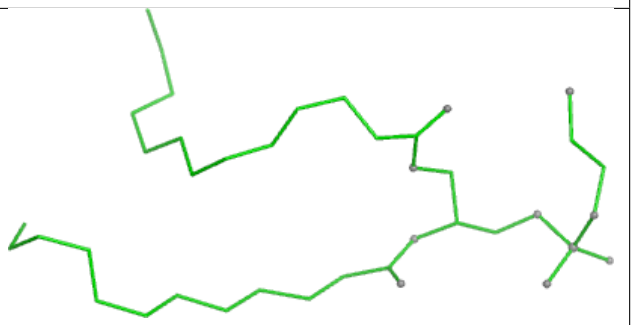


Rings

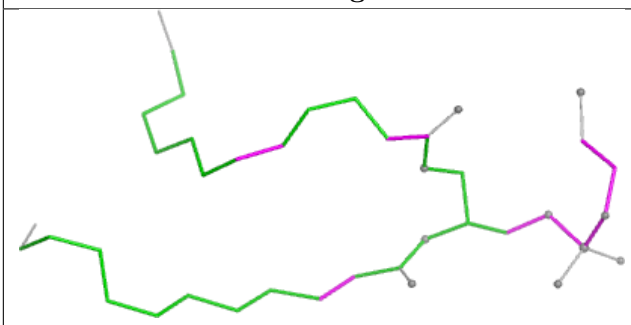
Ligand 3PE K 101



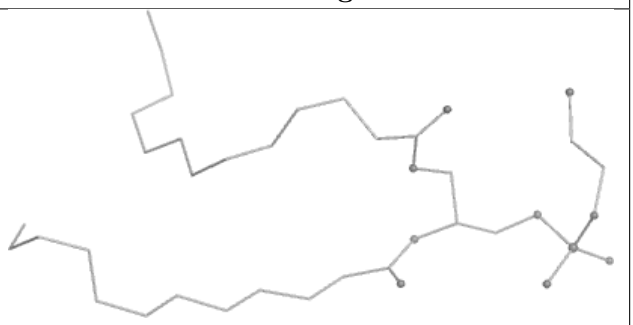
Bond lengths



Bond angles

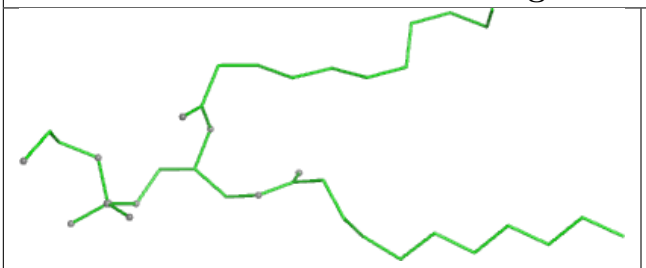


Torsions

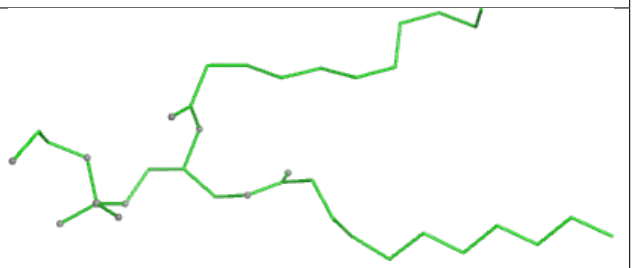


Rings

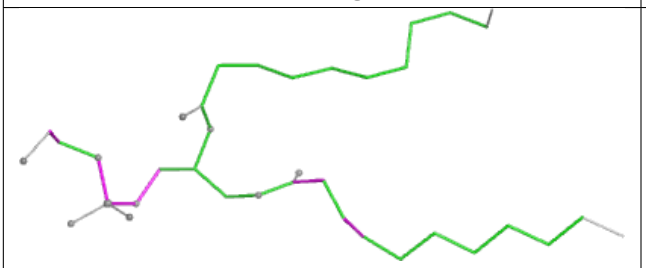
Ligand 3PE V 202



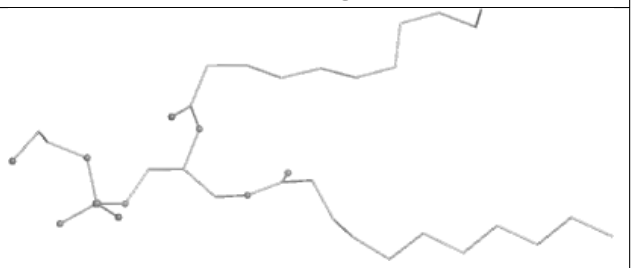
Bond lengths



Bond angles

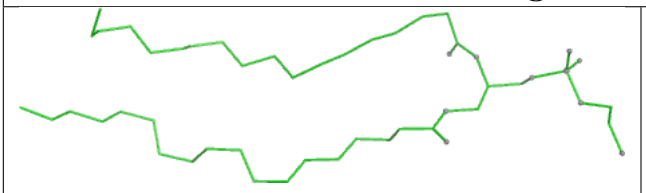


Torsions

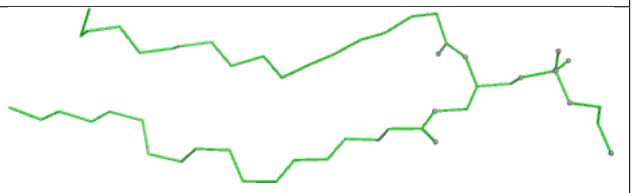


Rings

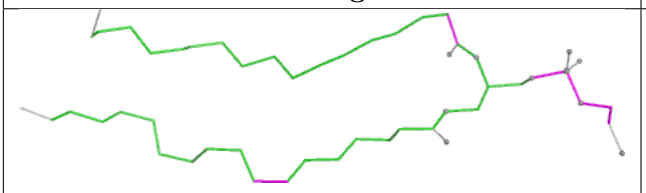
Ligand 3PE H 504



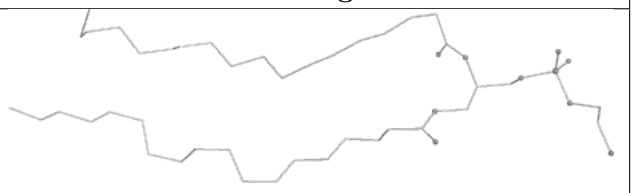
Bond lengths



Bond angles

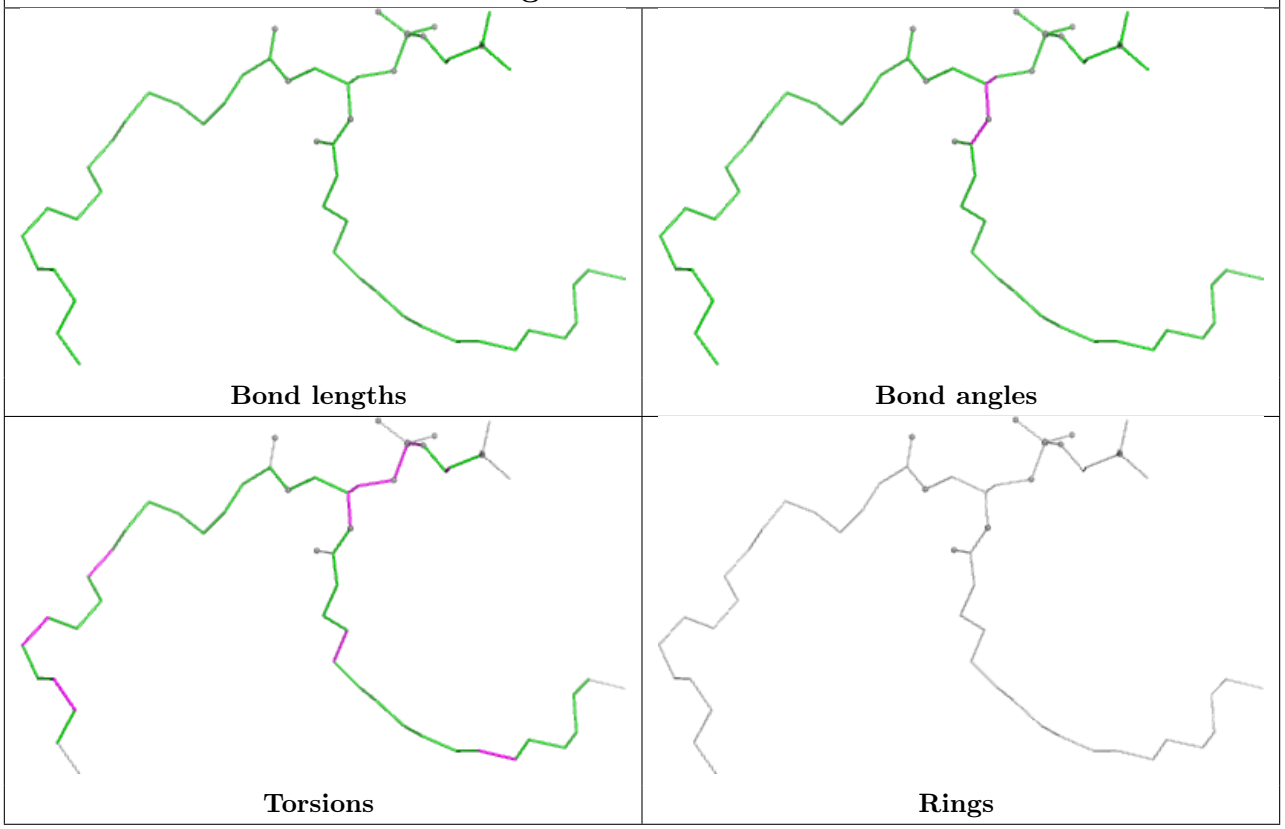


Torsions

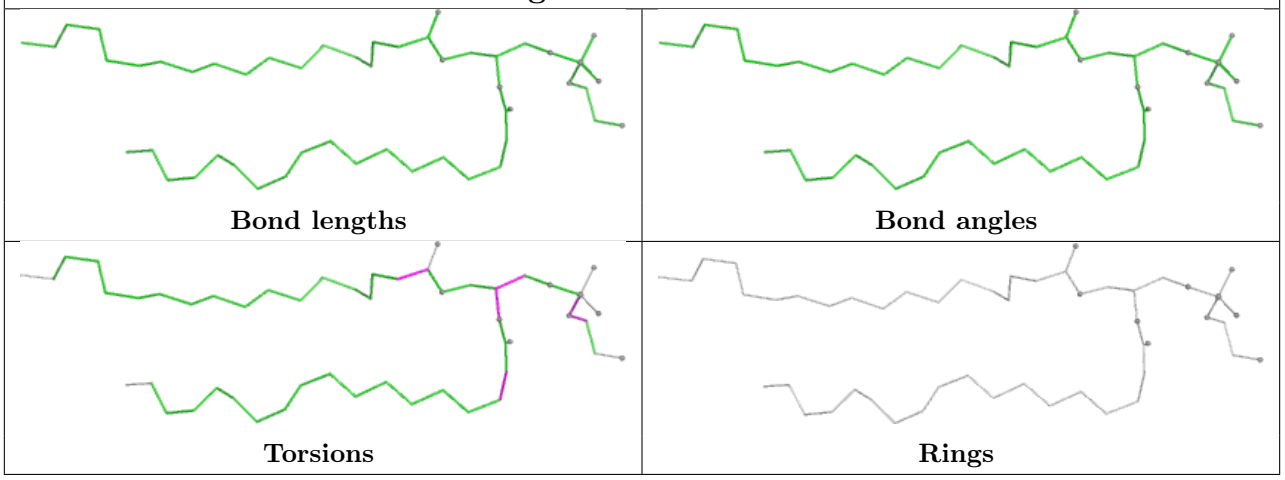


Rings

Ligand PC1 L 1002



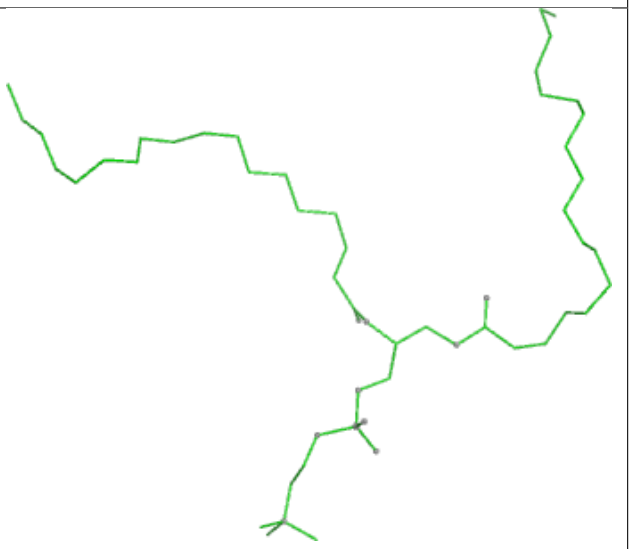
Ligand 3PE N 402



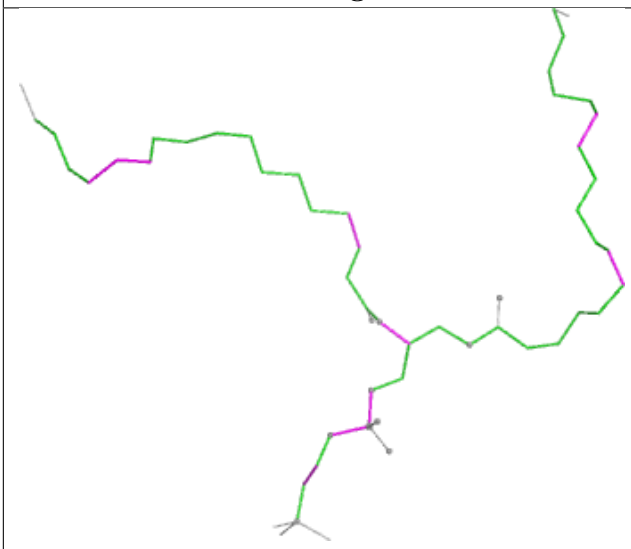
Ligand PC1 H 503



Bond lengths



Bond angles

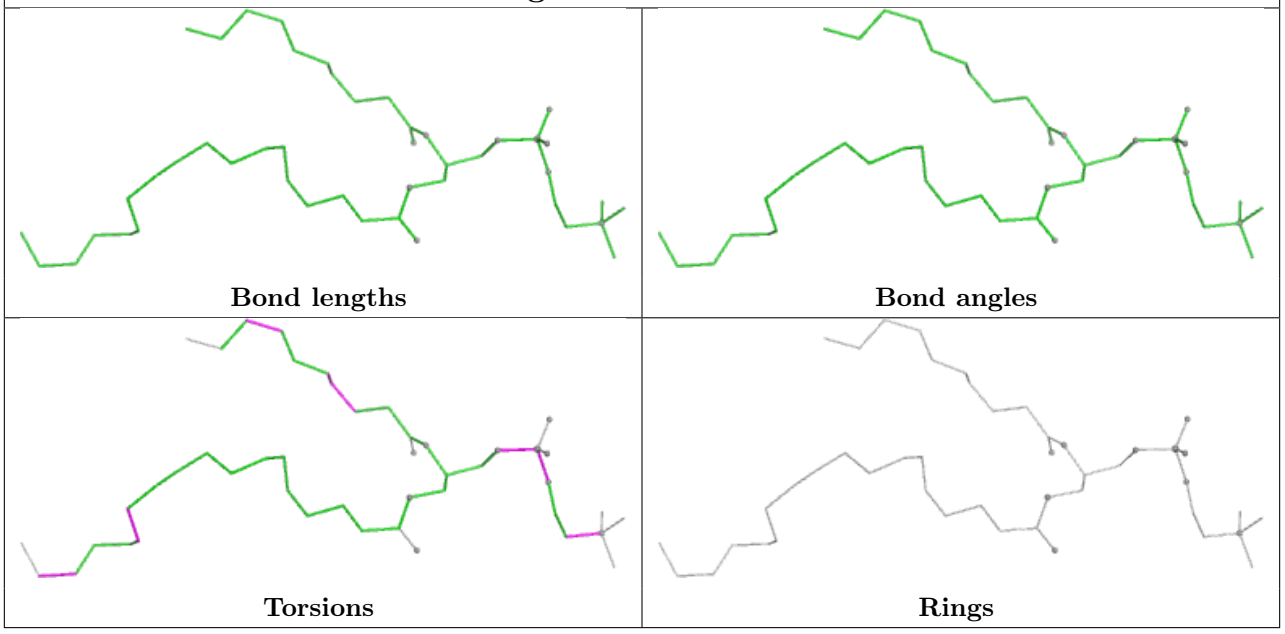


Torsions

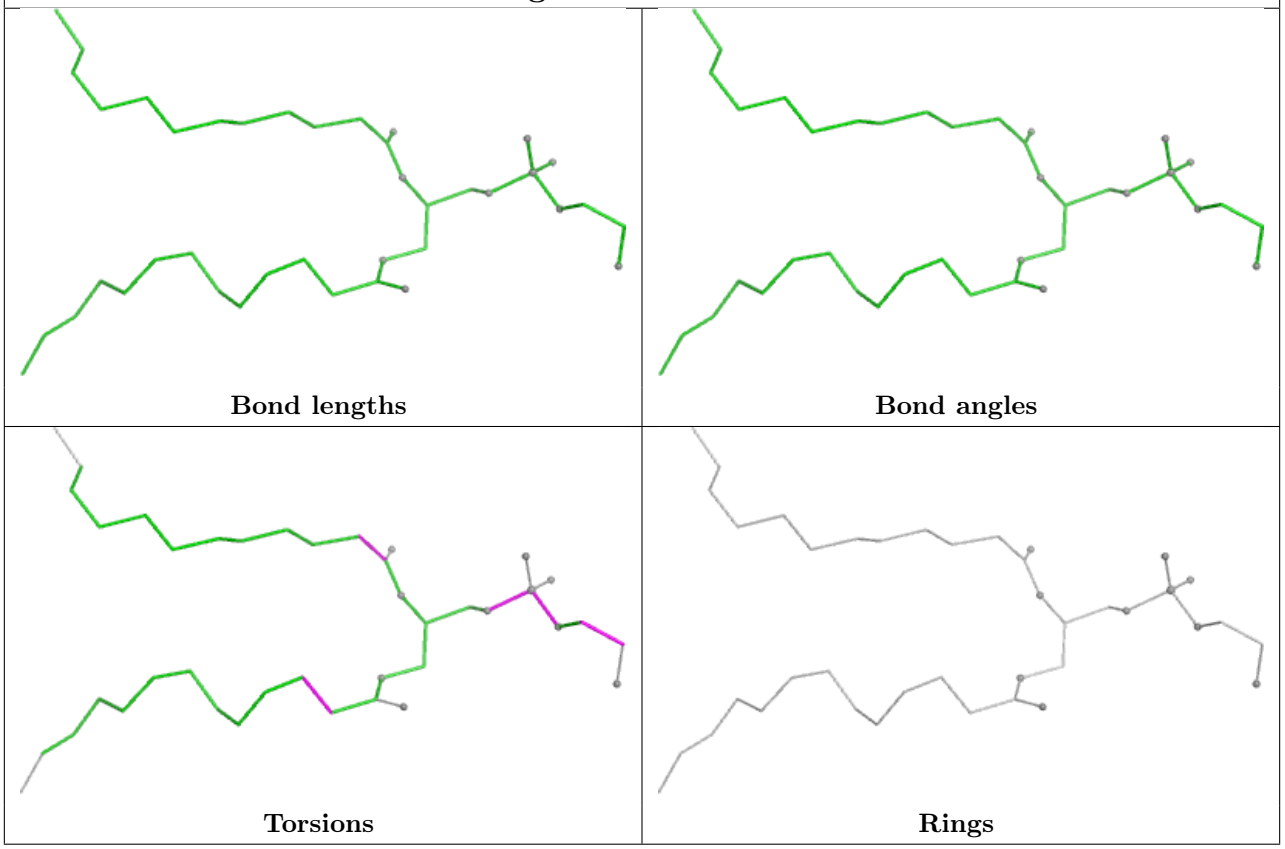


Rings

Ligand PC1 A 203



Ligand 3PE N 401



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.

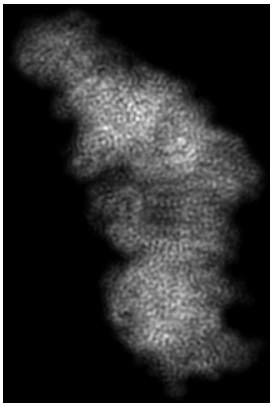
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-14637. These allow visual inspection of the internal detail of the map and identification of artifacts.

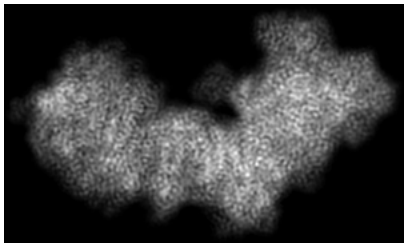
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

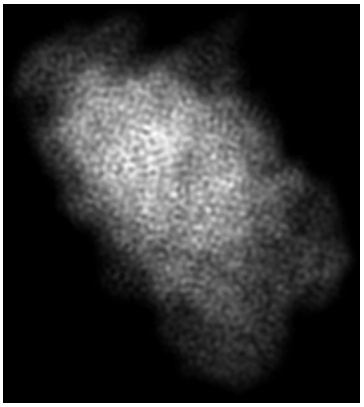
6.1.1 Primary map



X



Y

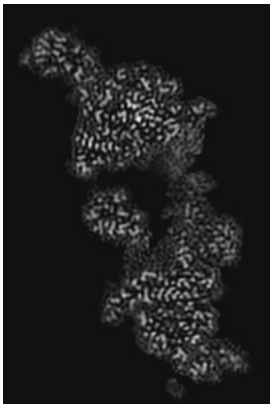


Z

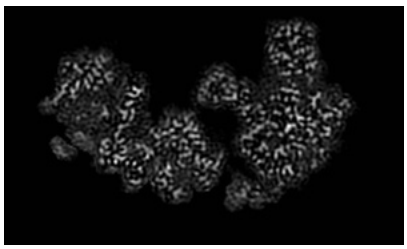
The images above show the map projected in three orthogonal directions.

6.2 Central slices

6.2.1 Primary map



X Index: 71



Y Index: 79



Z Index: 119

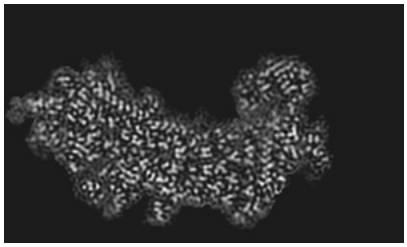
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

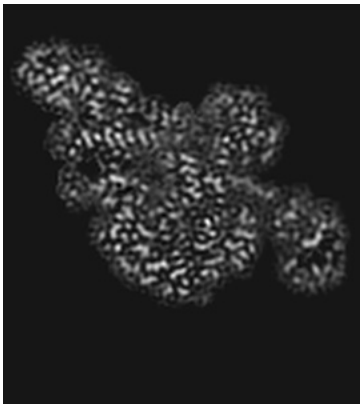
6.3.1 Primary map



X Index: 58



Y Index: 106

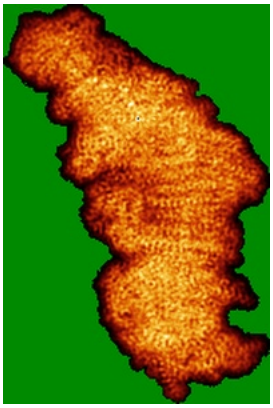


Z Index: 158

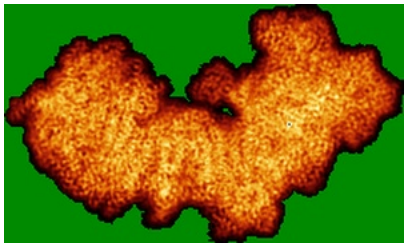
The images above show the largest variance slices of the map in three orthogonal directions.

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

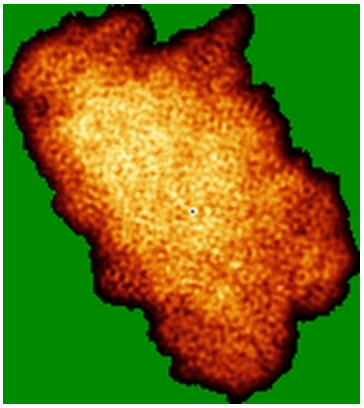
6.4.1 Primary map



X



Y

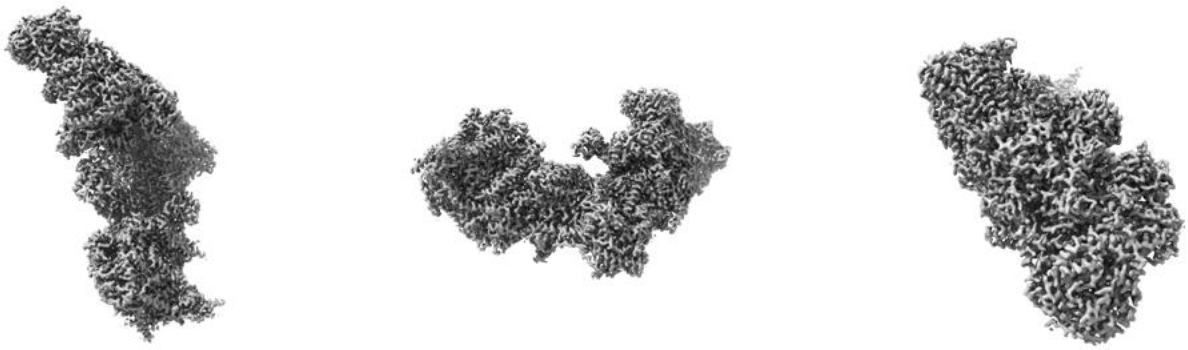


Z

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 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

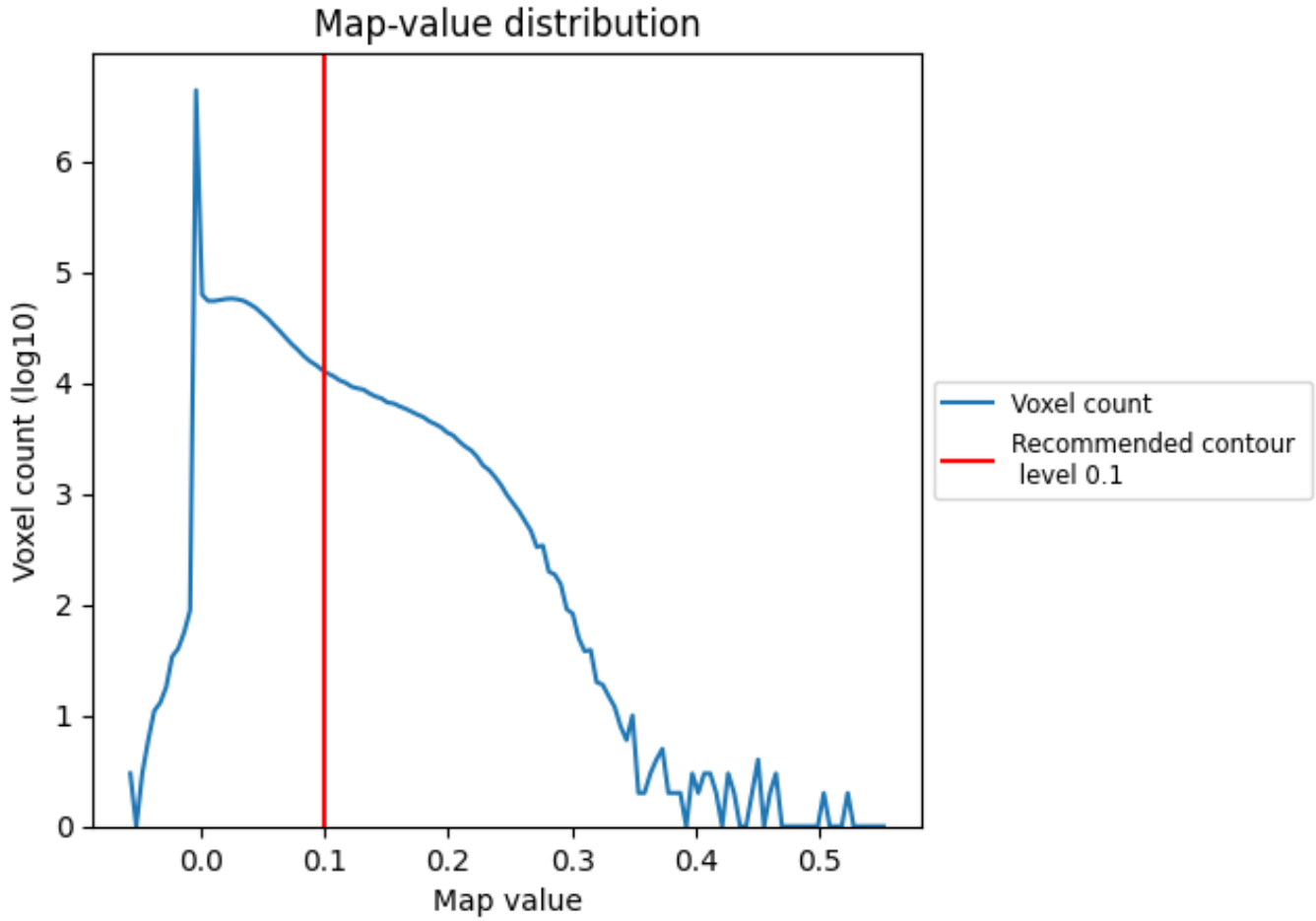
6.6 Mask visualisation (i)

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

7 Map analysis

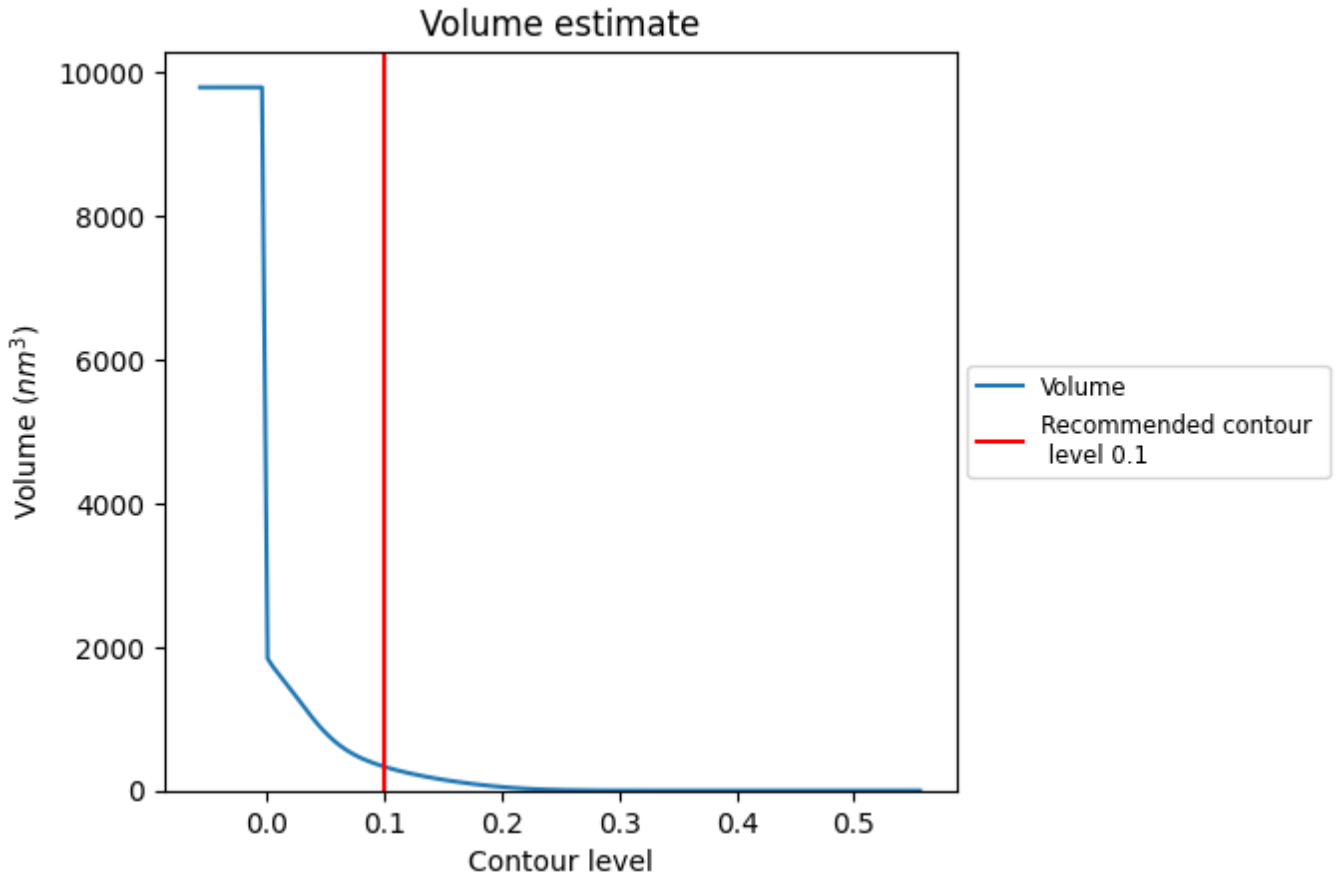
This section contains the results of statistical analysis of the map.

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



The volume at the recommended contour level is 334 nm^3; this corresponds to an approximate mass of 302 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.

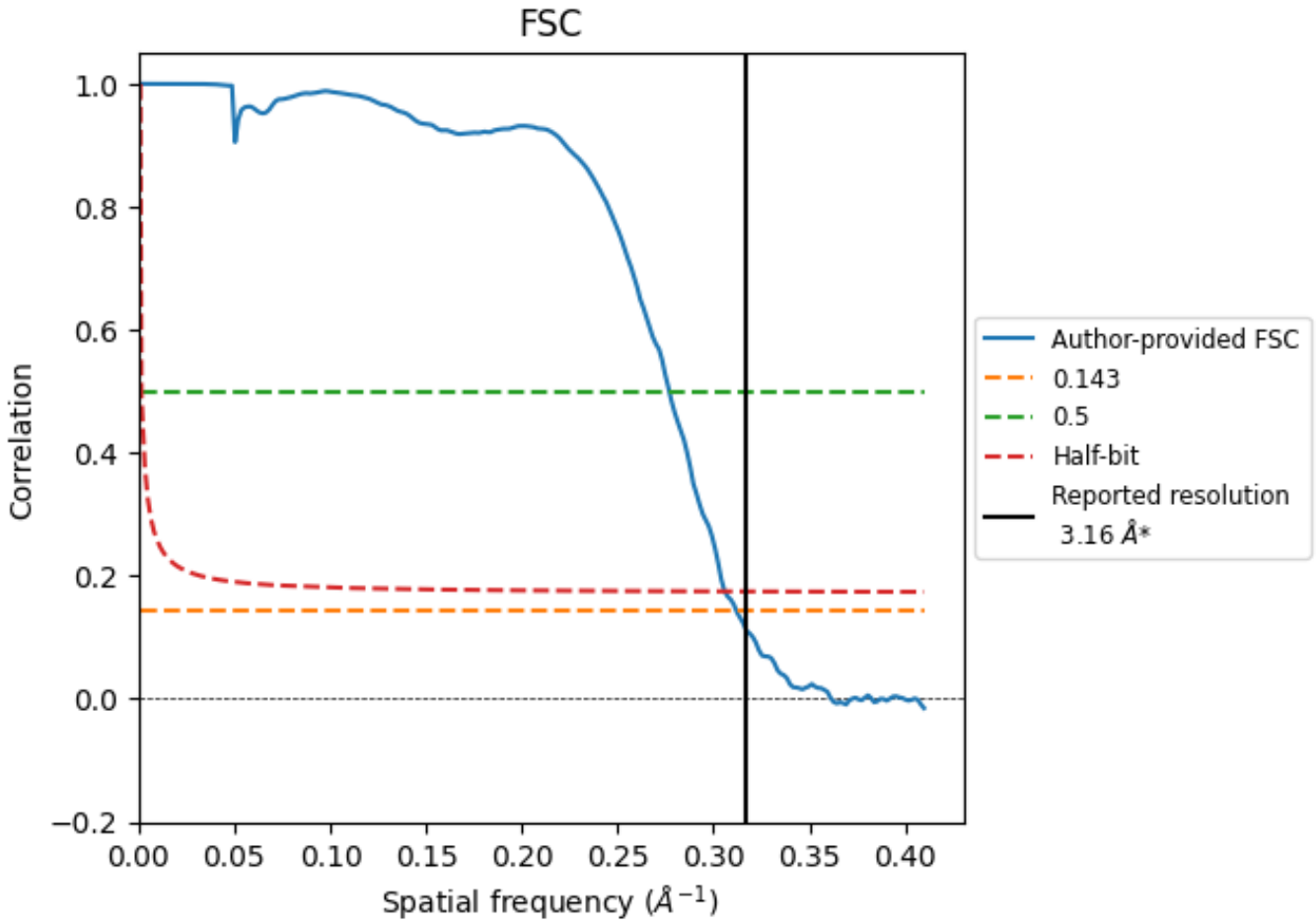
7.3 Rotationally averaged power spectrum

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

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 0.316 Å^{-1}

8.2 Resolution estimates (i)

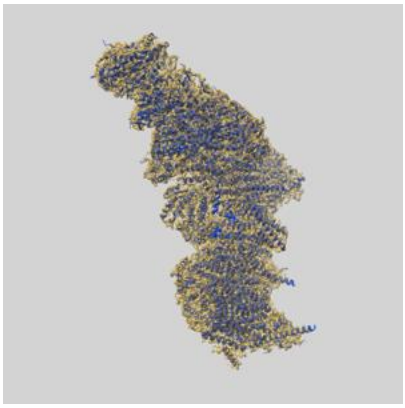
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.16	-	-
Author-provided FSC curve	3.21	3.61	3.27
Unmasked-calculated*	-	-	-

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

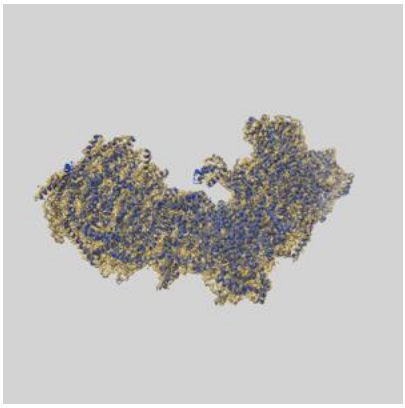
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-14637 and PDB model 7ZD6. Per-residue inclusion information can be found in section 3 on page 20.

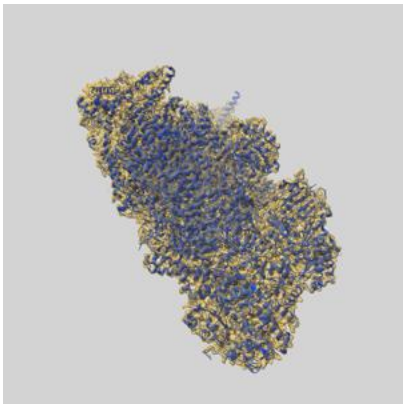
9.1 Map-model overlay



X



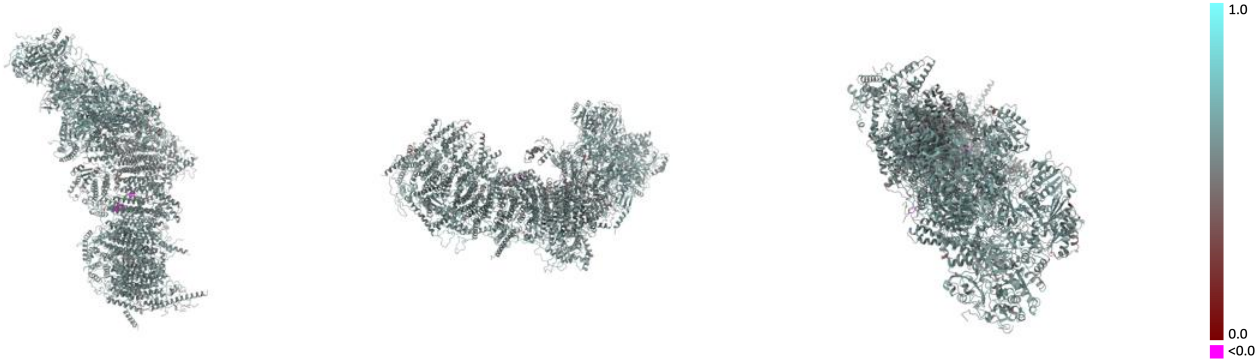
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1 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.

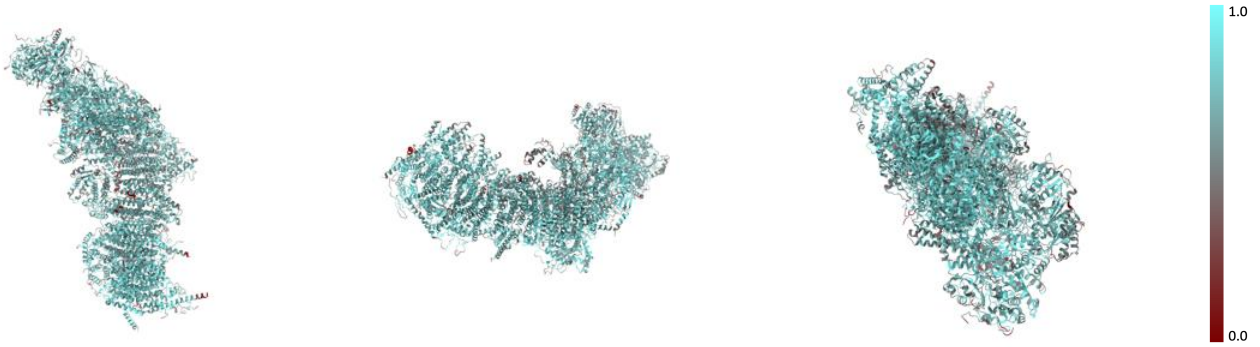
9.2 Q-score mapped to coordinate model (i)



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.

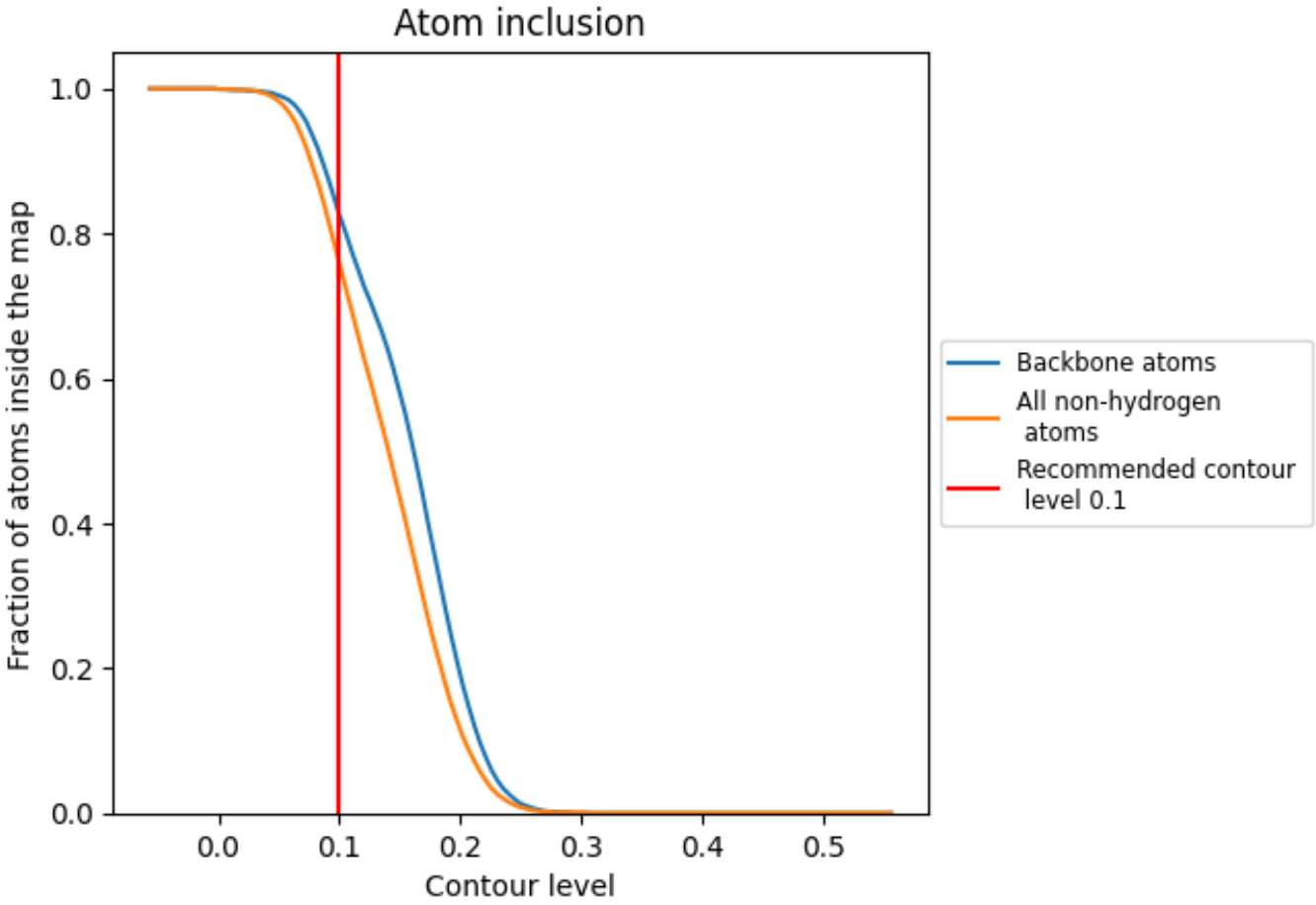
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.1).

9.4 Atom inclusion (i)



At the recommended contour level, 83% of all backbone atoms, 76% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7580	0.5610
1	0.7280	0.5640
2	0.6840	0.5530
3	0.7360	0.5710
4	0.7770	0.5600
5	0.8300	0.5920
6	0.8430	0.5840
9	0.8320	0.5790
A	0.6210	0.5020
H	0.7790	0.5480
J	0.7190	0.5370
K	0.7820	0.5550
L	0.8080	0.5620
M	0.8440	0.5770
N	0.8230	0.5710
V	0.6550	0.5350
W	0.8180	0.5770
X	0.7050	0.5400
Y	0.7610	0.5590
Z	0.7650	0.5610
a	0.6740	0.5640
b	0.7150	0.5840
c	0.7420	0.5820
d	0.6960	0.5560
e	0.6730	0.5650
f	0.7050	0.5680
g	0.7190	0.5650
h	0.7430	0.5770
i	0.7850	0.5880
j	0.4690	0.4970
k	0.7610	0.5610
l	0.7420	0.5500
m	0.7280	0.5400
n	0.7180	0.5310
o	0.8030	0.5680



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
p	0.7580	0.5610
q	0.7310	0.5450
r	0.7260	0.5520
s	0.7200	0.5350
t	0.7560	0.5590
u	0.7900	0.5480
v	0.7970	0.5680
w	0.7370	0.5520
x	0.7070	0.5430
y	0.7140	0.5540
z	0.8140	0.5520