Full wwPDB EM Validation Report ⓘ

Sep 8, 2026 – 11:41 pm BST

PDB ID	:	6RFR / pdb_00006rfr
EMDB ID	:	EMD-4873
Title	:	Cryo-EM structure of respiratory complex I from Yarrowia lipolytica at 3.2 A resolution
Authors	:	Parey, K.; Vonck, J.
Deposited on	:	2019-04-16
Resolution	:	3.20 Å(reported)
Based on initial model	:	6GCS

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:

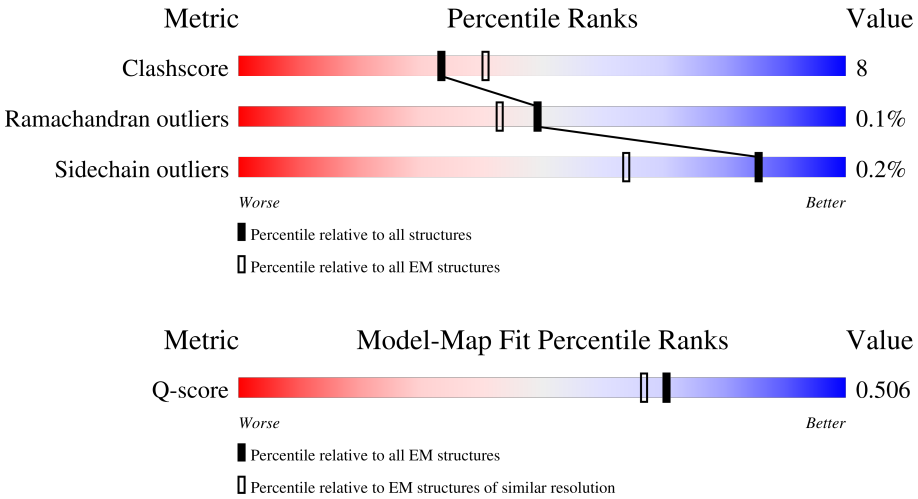
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data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

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15020 (2.70 - 3.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	728	95% 77% 17% 5%
2	B	488	93% 78% 15% 7%
3	C	466	94% 70% 23% 6%
4	D	87	99% 85% 14%

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Mol	Chain	Length	Quality of chain
5	E	375	93% 74% 19% 7%
6	F	144	84% 76% 8% 16%
7	G	281	85% 67% 17% 15%
8	H	243	89% 74% 15% 11%
9	I	229	83% 68% 15% 17%
10	J	198	90% 76% 15% 10%
11	K	210	84% 67% 16% 16%
12	L	89	100% 73% 27%
13	M	136	86% 70% 14% 14%
14	O	109	71% 67% 29%
15	P	124	99% 79% 20%
16	Q	132	64% 54% 11% 36%
17	R	109	97% 80% 17%
18	S	249	70% 58% 11% 30%
19	U	172	99% 87% 12%
20	W	123	98% 84% 15%
21	X	169	99% 81% 18%
22	Y	161	76% 66% 10% 24%
23	Z	182	99% 89% 10%
24	a	149	83% 74% 9% 17%
25	b	74	86% 70% 15% 14%
26	c	60	73% 63% 8% 27%
27	d	92	98% 75% 23%
28	e	67	78% 70% 6% 22%
29	f	87	92% 75% 15% 8%

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Mol	Chain	Length	Quality of chain
30	g	78	97% 82% 15%
31	h	138	99% 77% 22%
32	i	90	92% 80% 12% 8%
33	j	93	97% 85% 12%
34	n	120	95% 82% 12% 5%
35	1	341	100% 72% 28%
36	2	469	100% 75% 25%
37	3	128	99% 75% 24%
38	4	486	100% 72% 28%
39	5	655	100% 78% 21%
40	6	185	99% 78% 21%
41	8	99	83% 75% 7% 17%
42	9	89	97% 90% 7%

2 Entry composition (i)

There are 55 unique types of molecules in this entry. The entry contains 65934 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 Subunit NUAM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	692	5258	3263	926	1040	29	0	0

- Molecule 2 is a protein called Subunit NUBM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	456	3528	2229	621	654	24	0	0

- Molecule 3 is a protein called Subunit NUCM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	438	3472	2205	596	649	22	0	0

- Molecule 4 is a protein called Subunit NIMM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	86	681	432	127	119	3	0	0

- Molecule 5 is a protein called Subunit NUEM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	349	2798	1778	489	521	10	0	0

- Molecule 6 is a protein called Subunit NUFM of NADH:Ubiquinone Oxidoreductase (Com-

plex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	121	Total	C	N	O	S	0	0
			990	629	166	193	2		

- Molecule 7 is a protein called Subunit NUGM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	239	Total	C	N	O	S	0	0
			1978	1272	336	366	4		

- Molecule 8 is a protein called Subunit NUHM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	216	Total	C	N	O	S	0	0
			1688	1060	284	326	18		

- Molecule 9 is a protein called Subunit NUIM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	190	Total	C	N	O	S	0	0
			1519	966	254	289	10		

- Molecule 10 is a protein called Subunit NUJM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	179	Total	C	N	O	S	0	0
			1329	844	241	239	5		

- Molecule 11 is a protein called Subunit NUKM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	177	Total	C	N	O	S	0	0
			1395	885	246	249	15		

- Molecule 12 is a protein called Subunit NULM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	89	Total	C	N	O	S	0	0
			691	464	109	115	3		

- Molecule 13 is a protein called Subunit NUMM of protein NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	117	Total	C	N	O	S	0	0
			912	568	163	176	5		

- Molecule 14 is a protein called Acyl carrier protein ACPM1 of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms				AltConf	Trace
14	O	77	Total	C	N	O	0	0
			591	373	93	125		

- Molecule 15 is a protein called Subunit NB4M of protein NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	123	Total	C	N	O	S	0	0
			1036	667	182	185	2		

- Molecule 16 is a protein called Acyl carrier protein ACPM2 of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	85	Total	C	N	O	S	0	0
			648	405	103	138	2		

- Molecule 17 is a protein called Subunit NI2M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	106	Total	C	N	O	S	0	0
			884	562	168	151	3		

- Molecule 18 is a protein called Subunit NESM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	174	Total	C	N	O	S	0	0
			1430	920	245	263	2		

- Molecule 19 is a protein called Subunit NUPM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	171	Total	C	N	O	S	0	0
			1345	847	236	252	10		

- Molecule 20 is a protein called Subunit NB6M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
20	W	121	Total	C	N	O	S	0	0
			974	623	178	168	5		

- Molecule 21 is a protein called Subunit NUXM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
21	X	167	Total	C	N	O	S	0	0
			1296	839	221	232	4		

- Molecule 22 is a protein called Subunit NUYM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Y	123	Total	C	N	O	S	0	0
			1021	651	187	181	2		

- Molecule 23 is a protein called Subunit NUZM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Z	181	Total	C	N	O	S	0	0
			1389	893	240	255	1		

- Molecule 24 is a protein called Subunit NIAM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
24	a	124	Total	C	N	O	S	0	0
			1030	669	165	194	2		

- Molecule 25 is a protein called Subunit NEBM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms				AltConf	Trace
25	b	64	Total	C	N	O	0	0
			490	326	83	81		

- Molecule 26 is a protein called Subunit NB2M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms				AltConf	Trace
26	c	44	Total	C	N	O	0	0
			353	229	67	57		

- Molecule 27 is a protein called Subunit NIDM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
27	d	90	Total	C	N	O	S	0	0
			760	472	137	148	3		

- Molecule 28 is a protein called Subunit NUVM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
28	e	52	Total	C	N	O	S	0	0
			436	293	75	65	3		

- Molecule 29 is a protein called Subunit NI8M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
29	f	80	Total	C	N	O	S	0	0
			629	394	119	115	1		

- Molecule 30 is a protein called Subunit NI9M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms				AltConf	Trace
30	g	76	Total 617	C 405	N 112	O 100	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
g	71	GLY	GLN	conflict	UNP A0A1D8NJR0

- Molecule 31 is a protein called Subunit N7BM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
31	h	136	Total 1130	C 727	N 193	O 208	S 2	0	0

- Molecule 32 is a protein called Subunit NUUM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
32	i	83	Total 646	C 413	N 117	O 115	S 1	0	0

- Molecule 33 is a protein called Subunit NB5M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms				AltConf	Trace
33	j	90	Total 724	C 465	N 132	O 127	0	0

- Molecule 34 is a protein called Subunit NUNM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
34	n	114	Total 914	C 588	N 156	O 169	S 1	0	0

- Molecule 35 is a protein called Subunit NU1M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
35	1	340	Total 2714	C 1849	N 393	O 465	S 7	0	0

- Molecule 36 is a protein called Subunit NU2M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
36	2	469	Total	C	N	O	S	0	0
			3774	2557	550	655	12		

- Molecule 37 is a protein called Subunit NU3M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
37	3	127	Total	C	N	O	S	0	0
			1017	694	150	170	3		

- Molecule 38 is a protein called Subunit NU4M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
38	4	486	Total	C	N	O	S	0	0
			3855	2600	586	654	15		

- Molecule 39 is a protein called Subunit NU5M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
39	5	654	Total	C	N	O	S	0	0
			5197	3479	785	905	28		

- Molecule 40 is a protein called Subunit NU6M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
40	6	183	Total	C	N	O	S	0	0
			1443	979	207	249	8		

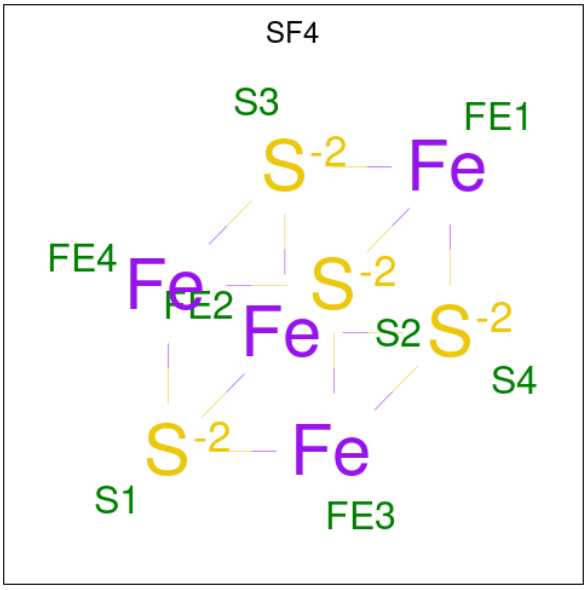
- Molecule 41 is a protein called Subunit NB8M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
41	8	82	Total	C	N	O	S	0	0
			672	426	122	116	8		

- Molecule 42 is a protein called Subunit NIPM of NADH:Ubiquinone Oxidoreductase (Complex I).

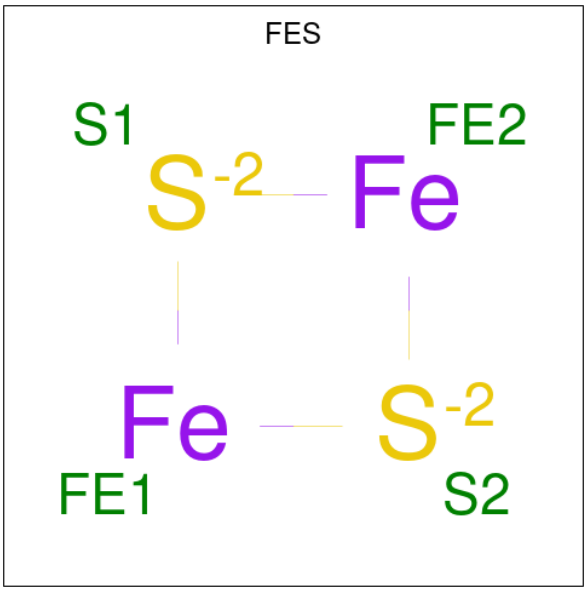
Mol	Chain	Residues	Atoms					AltConf	Trace
42	9	86	Total	C	N	O	S	0	0
			672	422	122	122	6		

- Molecule 43 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



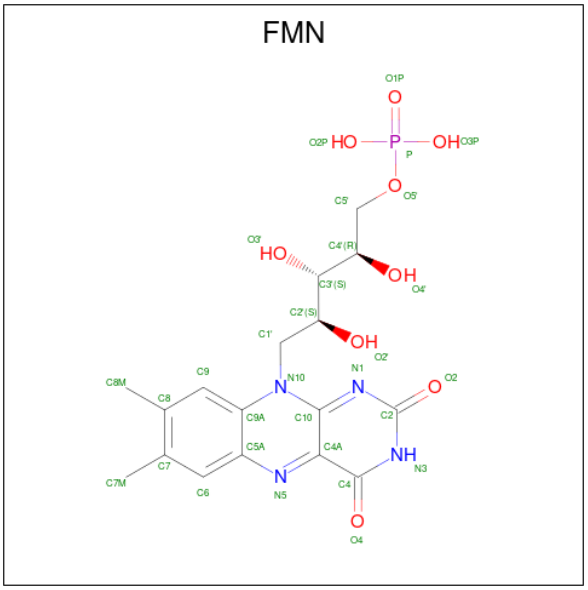
Mol	Chain	Residues	Atoms				AltConf
43	A	1	Total	Fe	S		0
			8	4	4		
43	A	1	Total	Fe	S		0
			8	4	4		
43	B	1	Total	Fe	S		0
			8	4	4		
43	I	1	Total	Fe	S		0
			8	4	4		
43	I	1	Total	Fe	S		0
			8	4	4		
43	K	1	Total	Fe	S		0
			8	4	4		

- Molecule 44 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			AltConf
44	A	1	Total	Fe	S	0
			4	2	2	
44	H	1	Total	Fe	S	0
			4	2	2	

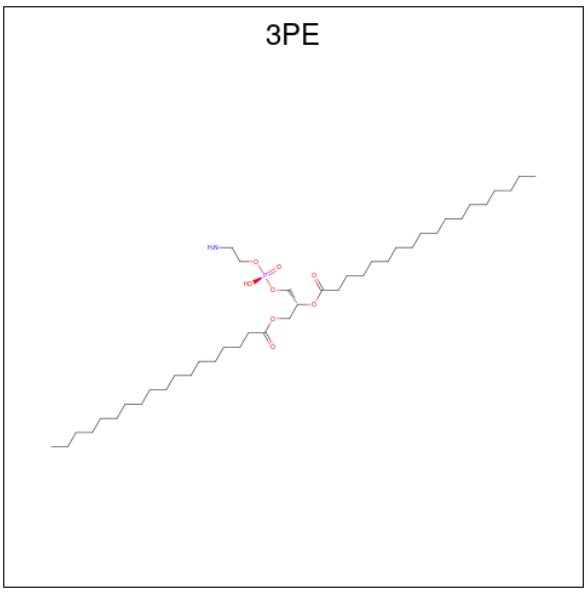
- Molecule 45 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



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

- Molecule 46 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula:

$C_{41}H_{82}NO_8P$).



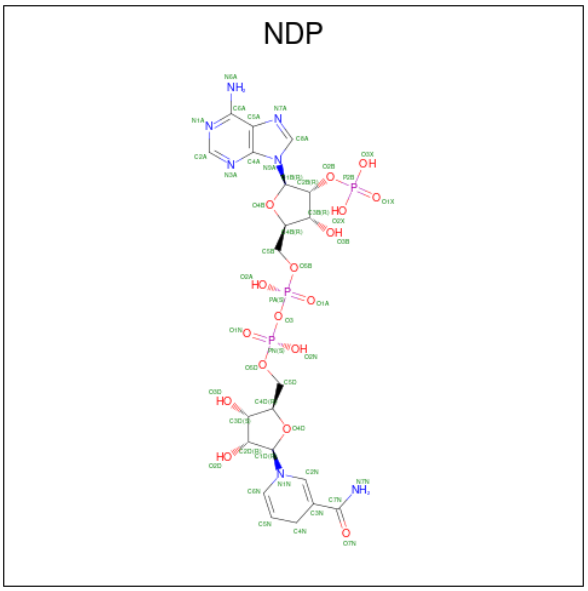
Mol	Chain	Residues	Atoms					AltConf
46	C	1	Total	C	N	O	P	0
			51	41	1	8	1	
46	E	1	Total	C	N	O	P	0
			36	26	1	8	1	
46	J	1	Total	C	N	O	P	0
			41	31	1	8	1	
46	J	1	Total	C	N	O	P	0
			44	34	1	8	1	
46	W	1	Total	C	N	O	P	0
			34	24	1	8	1	
46	b	1	Total	C	N	O	P	0
			42	32	1	8	1	
46	g	1	Total	C	N	O	P	0
			43	33	1	8	1	
46	1	1	Total	C	N	O	P	0
			36	26	1	8	1	
46	1	1	Total	C	N	O	P	0
			36	26	1	8	1	
46	4	1	Total	C	N	O	P	0
			42	32	1	8	1	
46	4	1	Total	C	N	O	P	0
			43	33	1	8	1	
46	4	1	Total	C	N	O	P	0
			42	32	1	8	1	
46	4	1	Total	C	N	O	P	0
			51	41	1	8	1	

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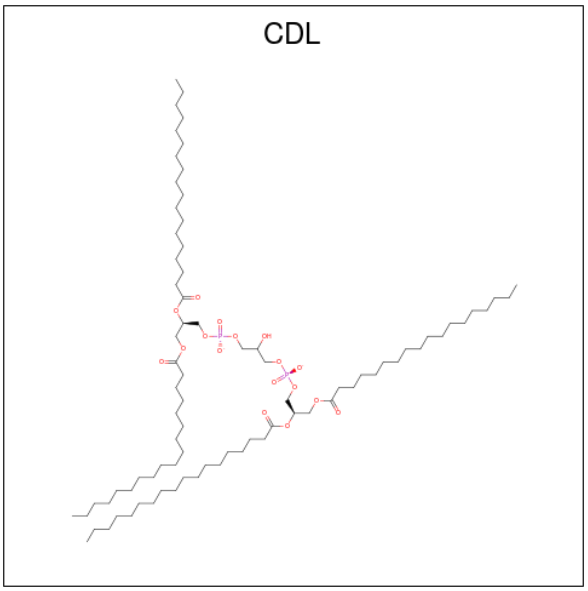
Mol	Chain	Residues	Atoms					AltConf
46	5	1	Total 42	C 32	N 1	O 8	P 1	0
46	5	1	Total 51	C 41	N 1	O 8	P 1	0

- Molecule 47 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



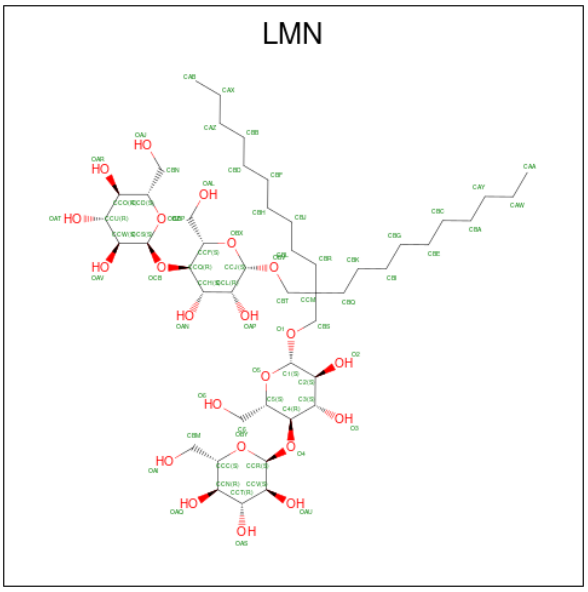
Mol	Chain	Residues	Atoms					AltConf
47	E	1	Total 48	C 21	N 7	O 17	P 3	0

- Molecule 48 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



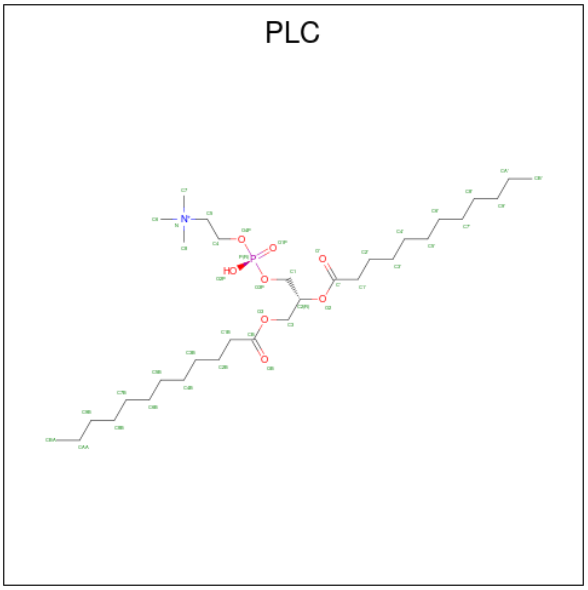
Mol	Chain	Residues	Atoms				AltConf
48	E	1	Total	C	O	P	0
			72	53	17	2	
48	X	1	Total	C	O	P	0
			86	67	17	2	
48	Z	1	Total	C	O	P	0
			76	57	17	2	
48	g	1	Total	C	O	P	0
			83	64	17	2	
48	j	1	Total	C	O	P	0
			78	59	17	2	
48	4	1	Total	C	O	P	0
			92	73	17	2	

- Molecule 49 is Lauryl Maltose Neopentyl Glycol (CCD ID: LMN) (formula: $C_{47}H_{88}O_{22}$).



Mol	Chain	Residues	Atoms			AltConf
49	J	1	Total	C	O	0
			69	47	22	
49	j	1	Total	C	O	0
			65	43	22	

- Molecule 50 is DIUNDECYL PHOSPHATIDYL CHOLINE (CCD ID: PLC) (formula: $C_{32}H_{65}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
50	K	1	Total	C	N	O	P	0
			39	29	1	8	1	
50	W	1	Total	C	N	O	P	0
			41	31	1	8	1	

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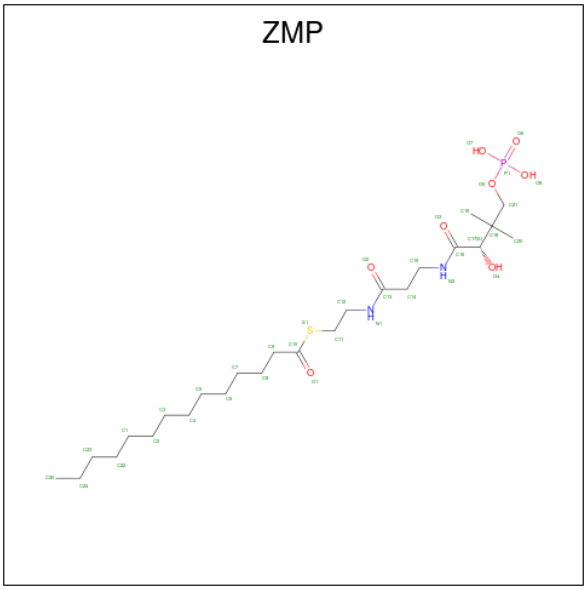
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Mol	Chain	Residues	Atoms					AltConf
50	W	1	Total	C	N	O	P	0
			42	32	1	8	1	
50	W	1	Total	C	N	O	P	0
			42	32	1	8	1	
50	n	1	Total	C	N	O	P	0
			42	32	1	8	1	
50	1	1	Total	C	N	O	P	0
			35	25	1	8	1	
50	5	1	Total	C	N	O	P	0
			31	21	1	8	1	

- Molecule 51 is ZINC ION (CCD ID: ZN) (formula: Zn).

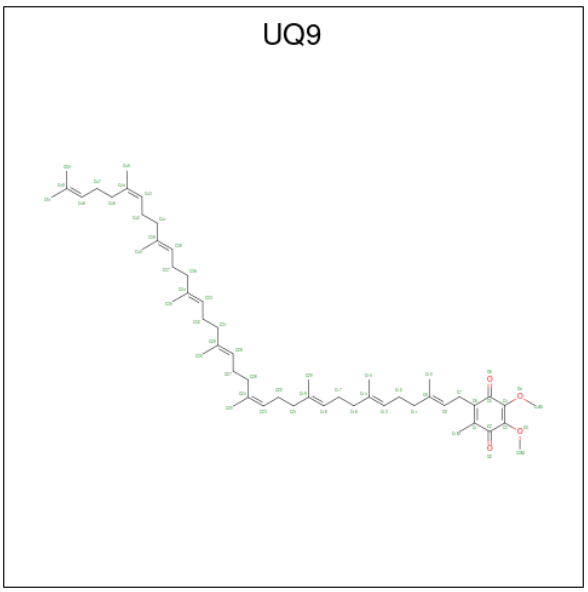
Mol	Chain	Residues	Atoms		AltConf
51	M	1	Total	Zn	0
			1	1	

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



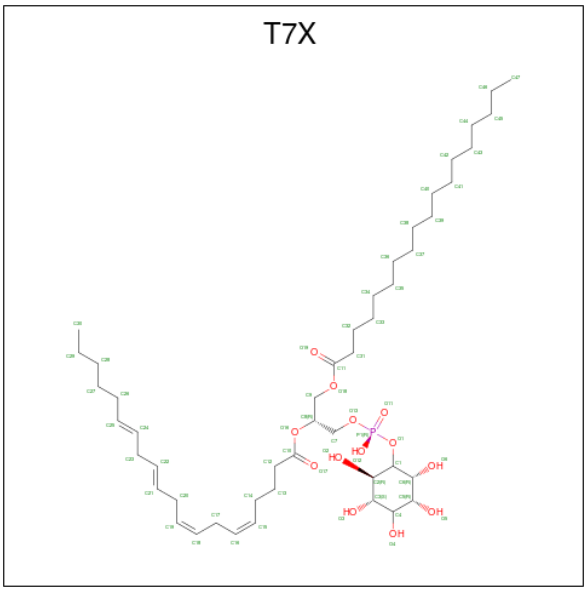
Mol	Chain	Residues	Atoms						AltConf
52	O	1	Total	C	N	O	P	S	0
			33	22	2	7	1	1	
52	Q	1	Total	C	N	O	P	S	0
			33	22	2	7	1	1	

- Molecule 53 is Ubiquinone-9 (CCD ID: UQ9) (formula: $C_{54}H_{82}O_4$).



Mol	Chain	Residues	Atoms			AltConf
53	1	1	Total	C	O	0
			35	31	4	

- Molecule 54 is Phosphatidylinositol (CCD ID: T7X) (formula: $C_{47}H_{83}O_{13}P$).



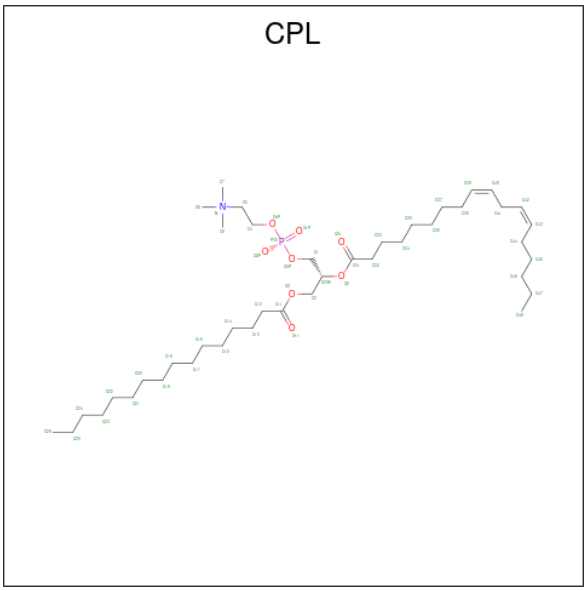
Mol	Chain	Residues	Atoms				AltConf
54	2	1	Total	C	O	P	0
			48	34	13	1	
54	2	1	Total	C	O	P	0
			52	38	13	1	

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Mol	Chain	Residues	Atoms				AltConf
54	3	1	Total	C	O	P	0
			49	35	13	1	
54	5	1	Total	C	O	P	0
			43	29	13	1	

- Molecule 55 is 1-PALMITOYL-2-LINOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: CPL) (formula: $C_{42}H_{80}NO_8P$).



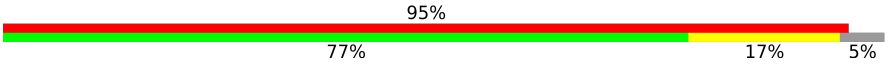
Mol	Chain	Residues	Atoms					AltConf
55	2	1	Total	C	N	O	P	0
			52	42	1	8	1	

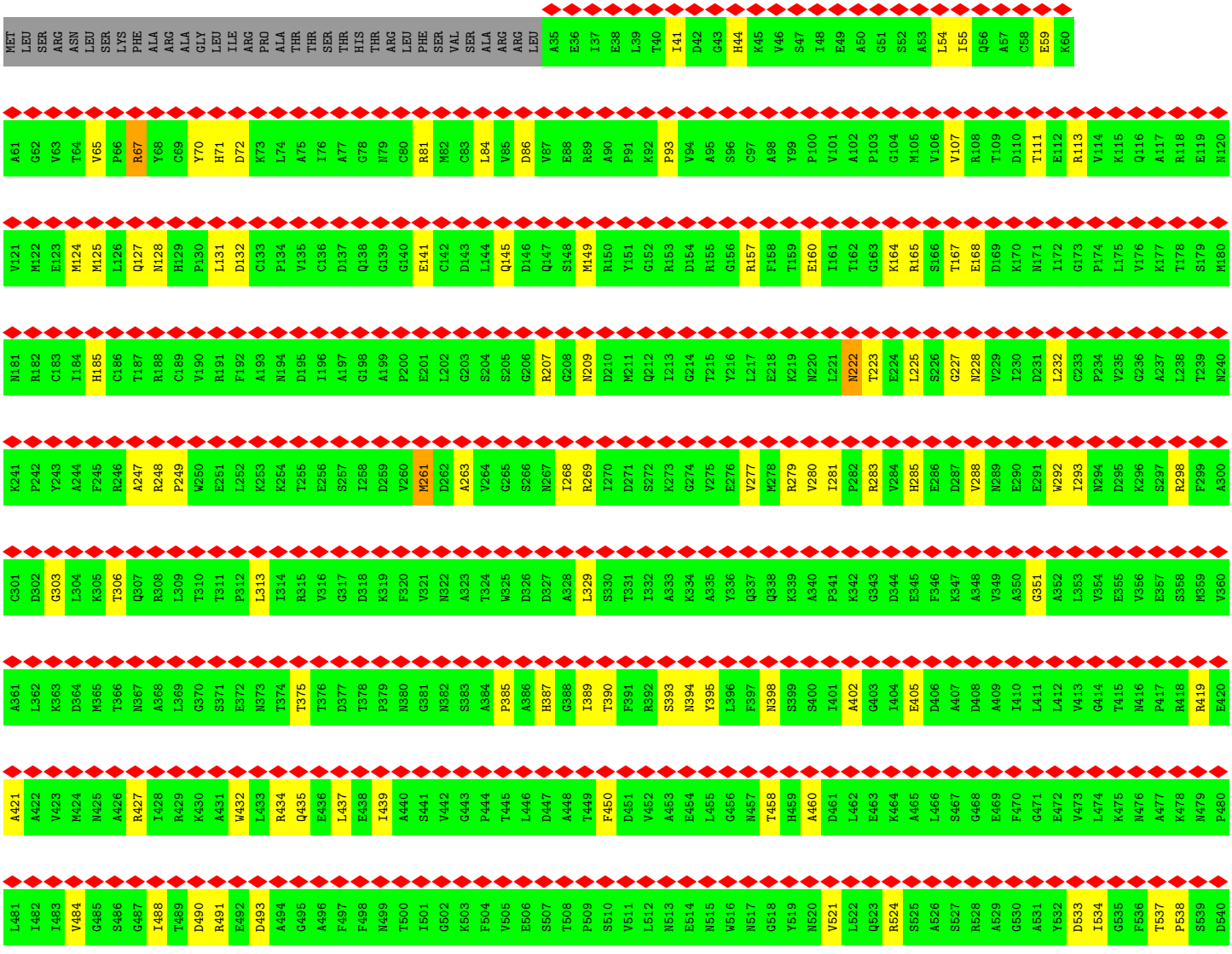
3 Residue-property plots (i)

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

- Molecule 1: Subunit NUAM of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain A:

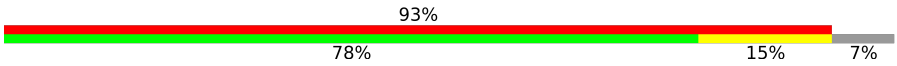


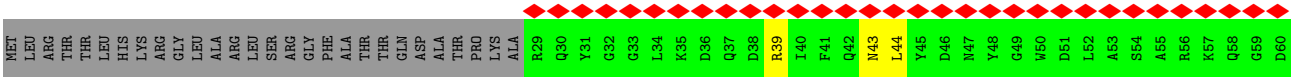


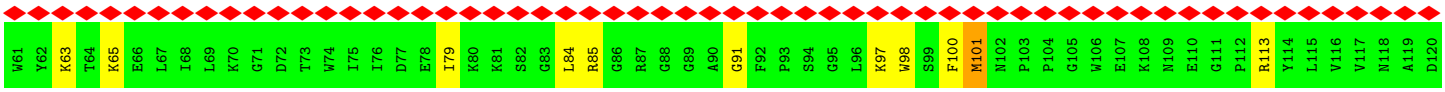


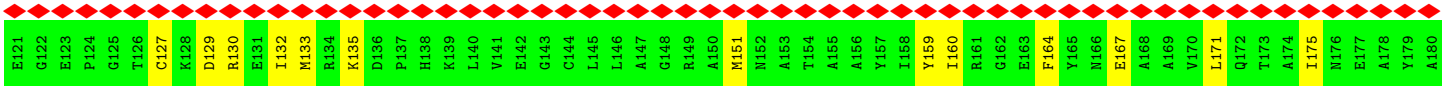
• Molecule 2: Subunit NUBM of NADH:Ubiquinone Oxidoreductase (Complex I)

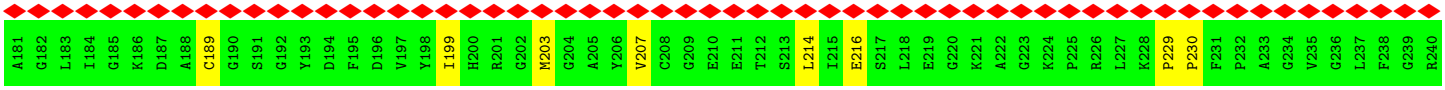
Chain B:

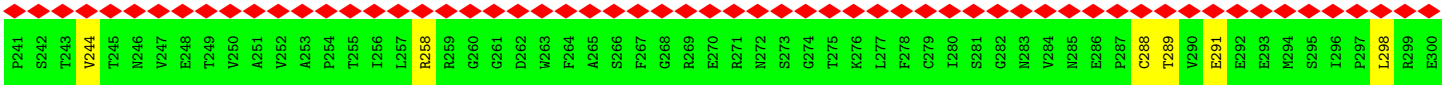


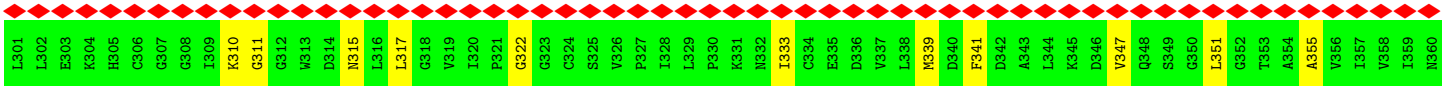


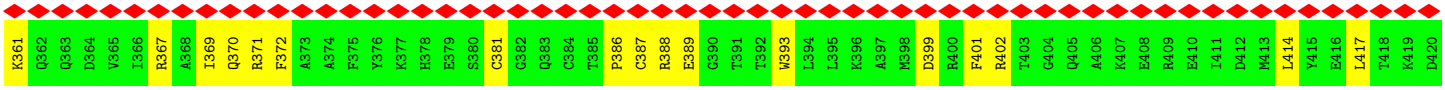


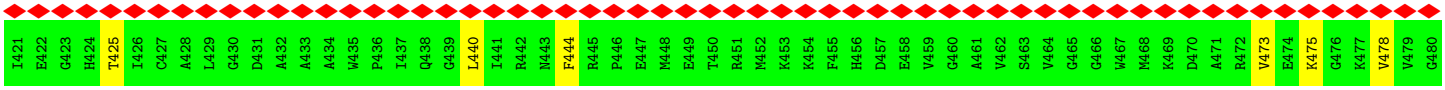


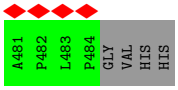






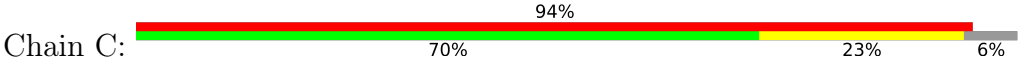


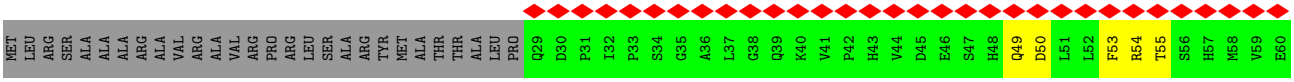


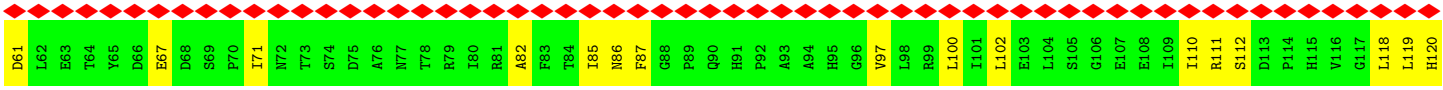


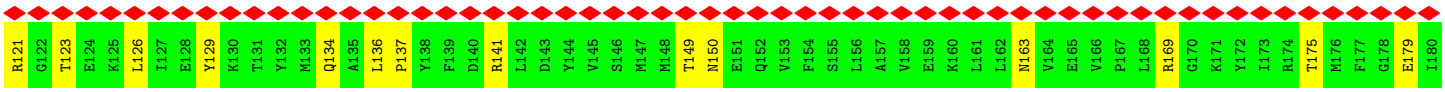
• Molecule 3: Subunit NUCM of NADH:Ubiquinone Oxidoreductase (Complex I)

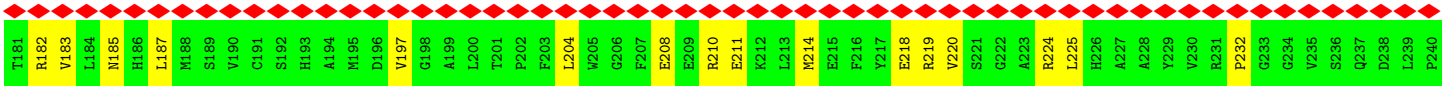
Chain C:

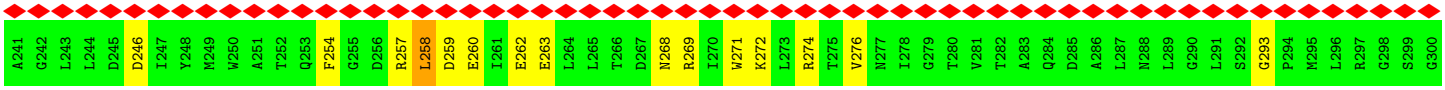


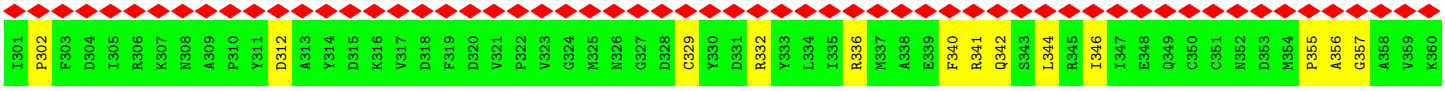


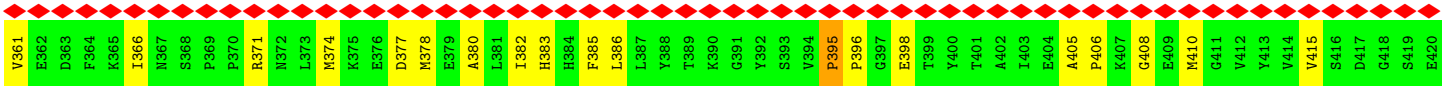


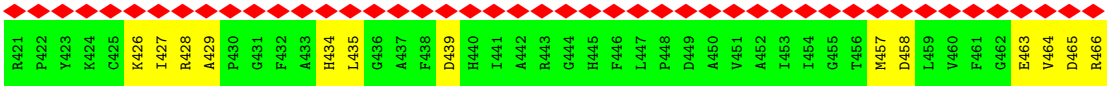






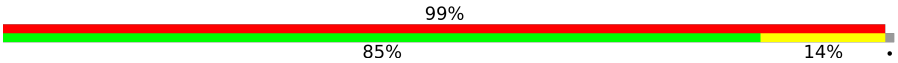


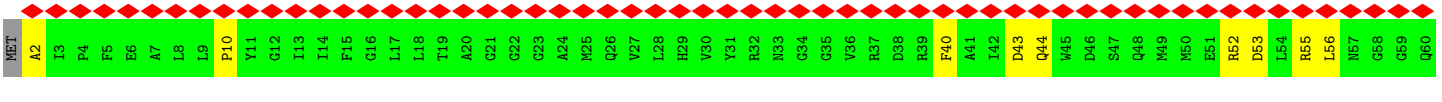


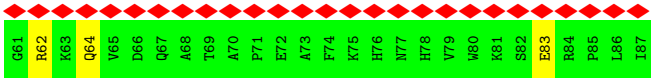


• Molecule 4: Subunit NIMM of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain D:

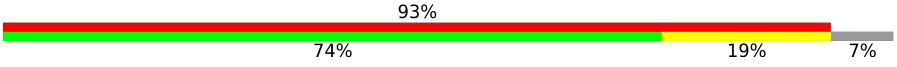


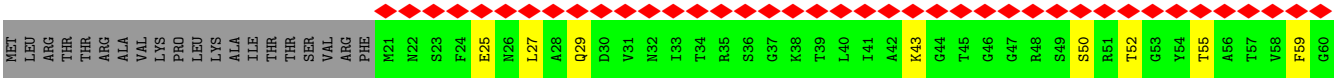


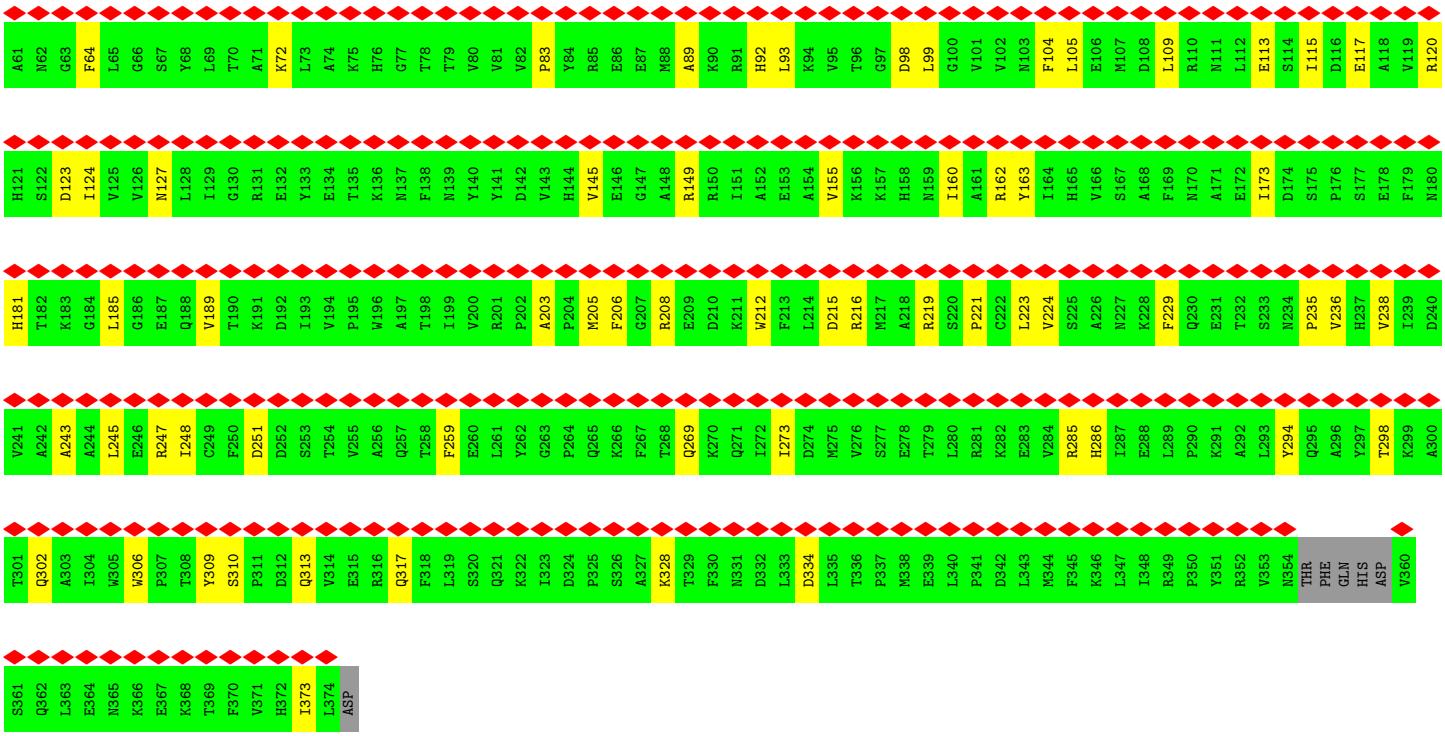


• Molecule 5: Subunit NUEM of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain E:



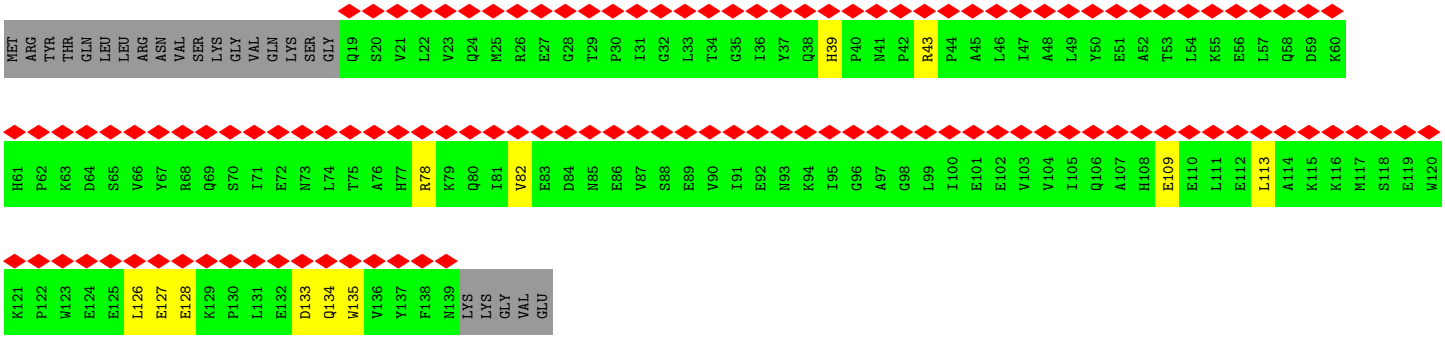




• Molecule 6: Subunit NUFM of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain F:

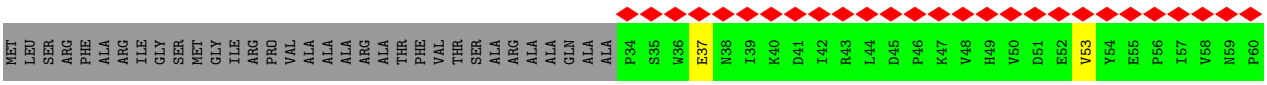


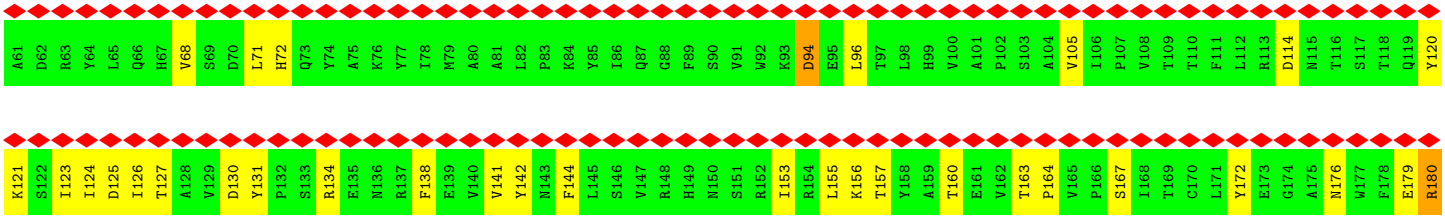


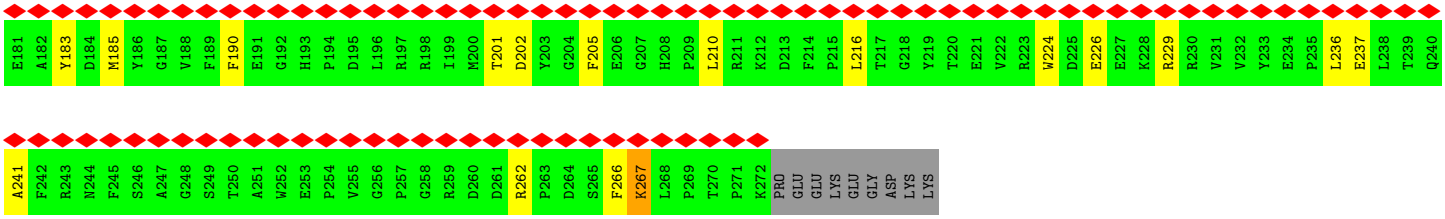
• Molecule 7: Subunit NUGM of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain G:

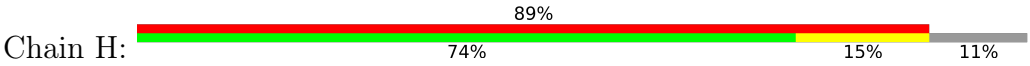


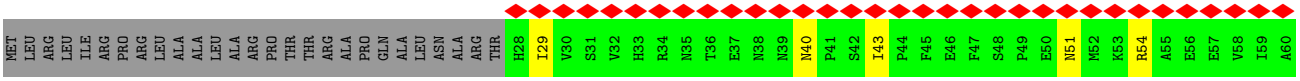


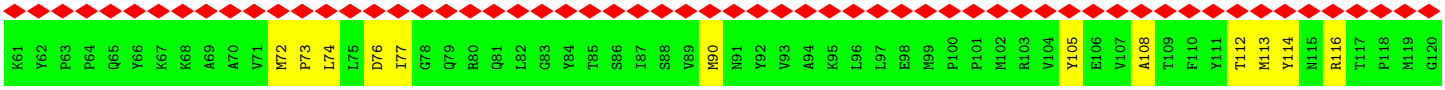


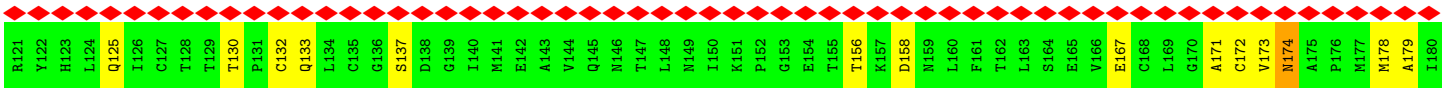


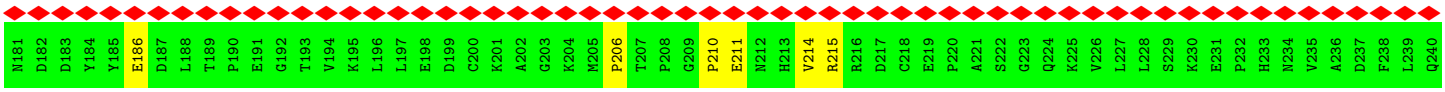
• Molecule 8: Subunit NUHM of NADH:Ubiquinone Oxidoreductase (Complex I)





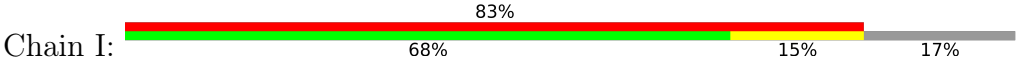


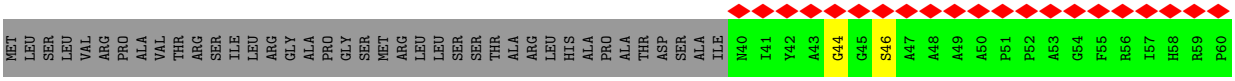


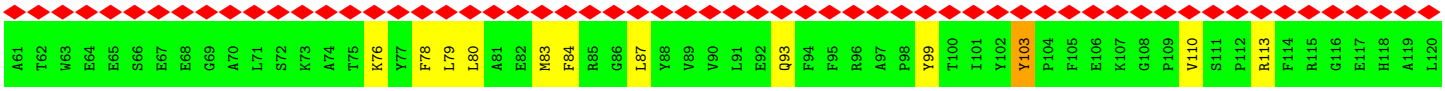


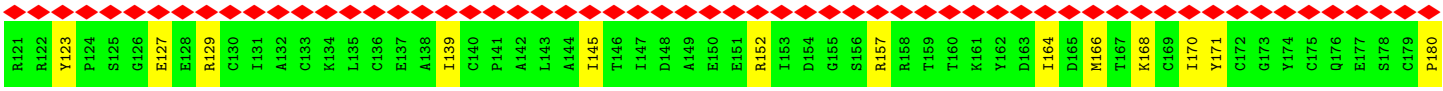


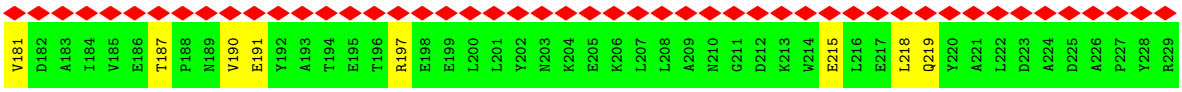
• Molecule 9: Subunit NUIM of NADH:Ubiquinone Oxidoreductase (Complex I)





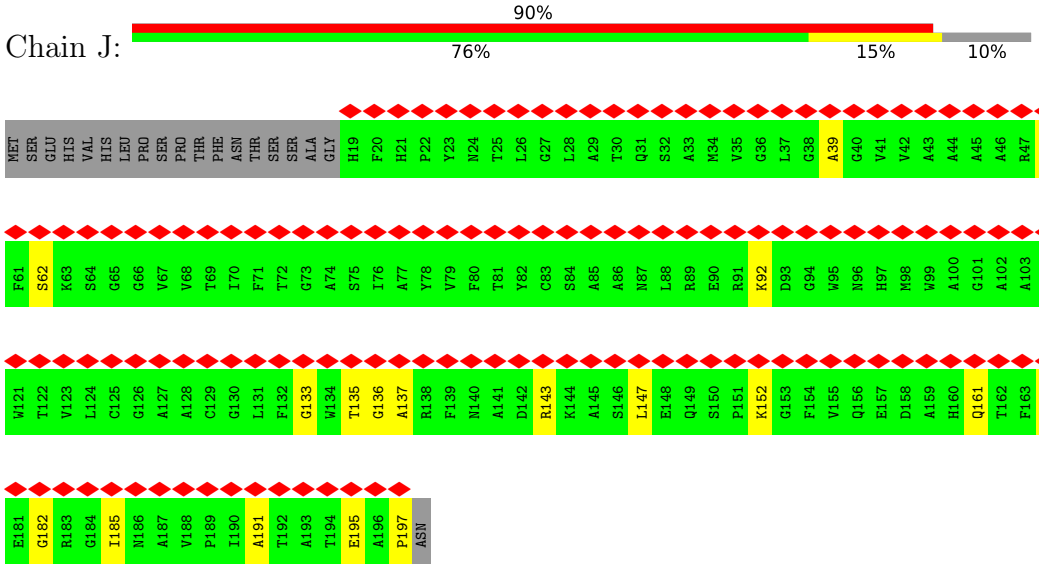






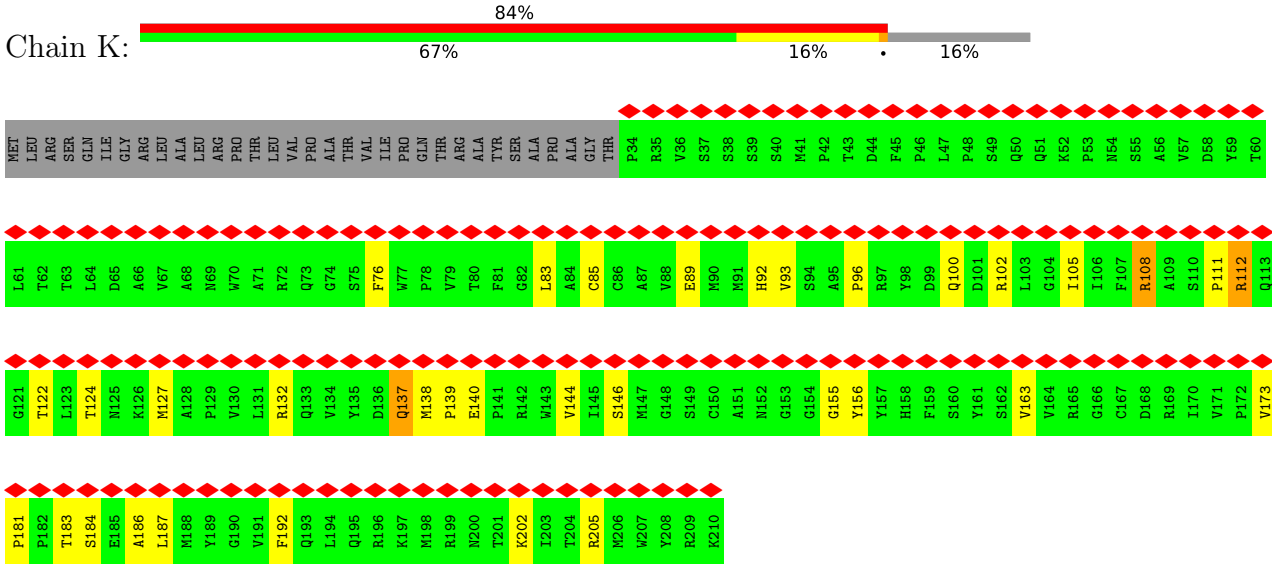
• Molecule 10: Subunit NUJM of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain J:



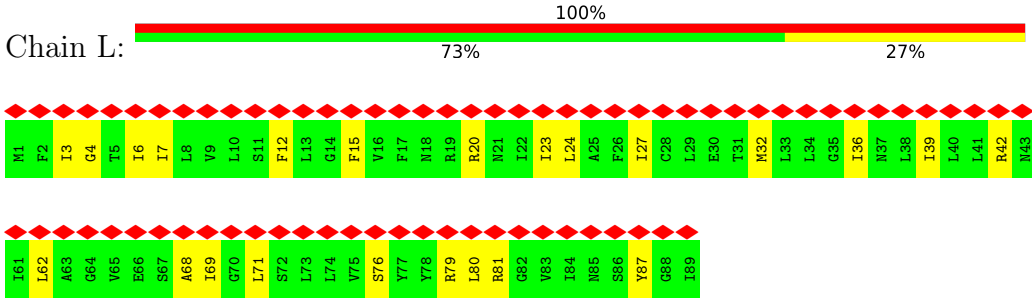
• Molecule 11: Subunit NUKM of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain K:



• Molecule 12: Subunit NULM of NADH:Ubiquinone Oxidoreductase (Complex I)

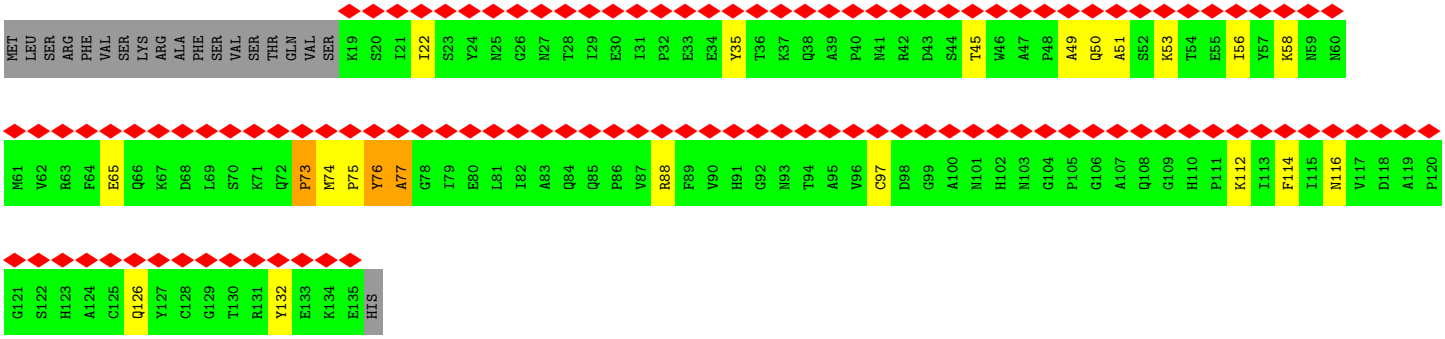
Chain L:



• Molecule 13: Subunit NUMM of protein NADH:Ubiquinone Oxidoreductase (Complex I)

Chain M:

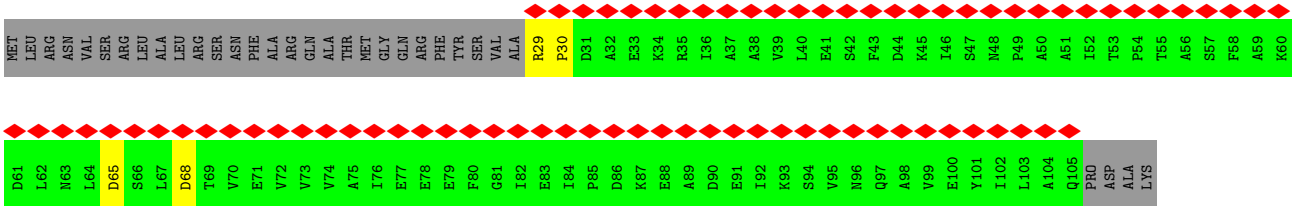




• Molecule 14: Acyl carrier protein ACPM1 of NADH:Ubiquinone Oxidoreductase (Complex I)

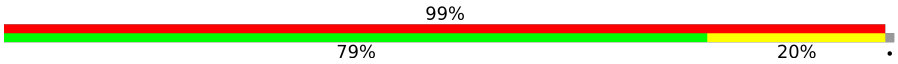
Chain O:

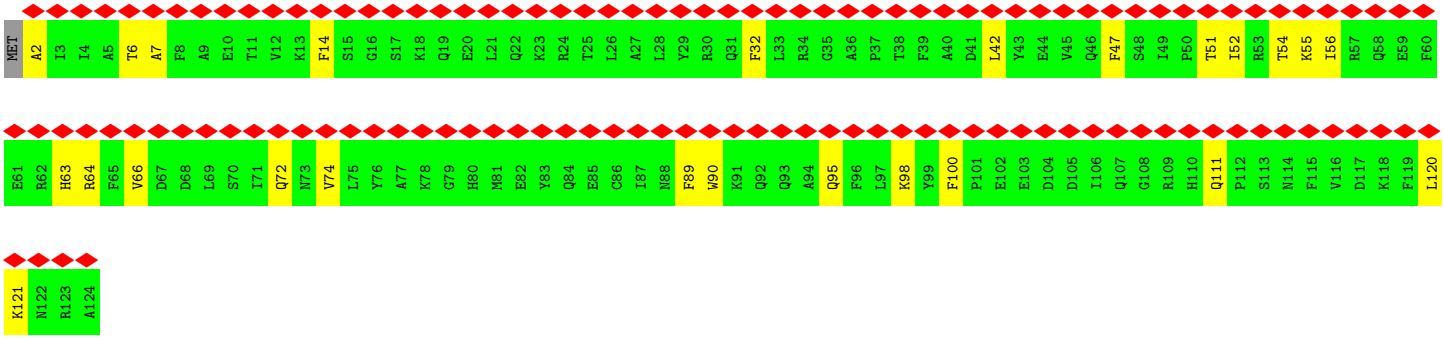




• Molecule 15: Subunit NB4M of protein NADH:Ubiquinone Oxidoreductase (Complex I)

Chain P:

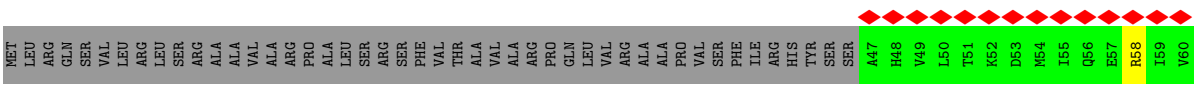


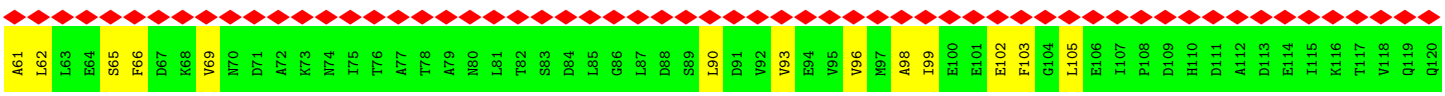


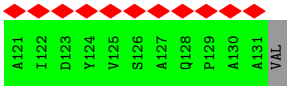
• Molecule 16: Acyl carrier protein ACPM2 of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain Q:



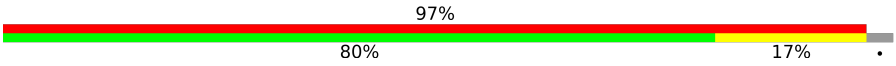


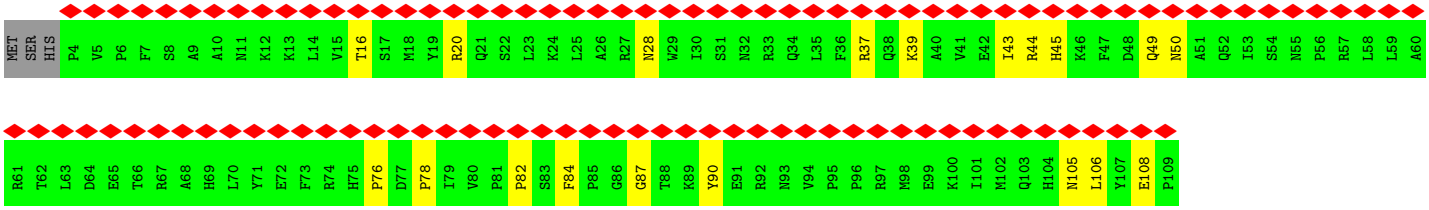




• Molecule 17: Subunit NI2M of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain R:

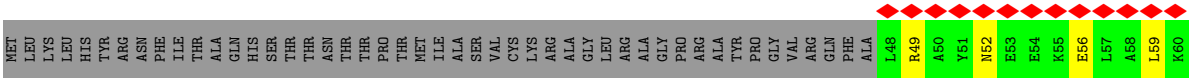


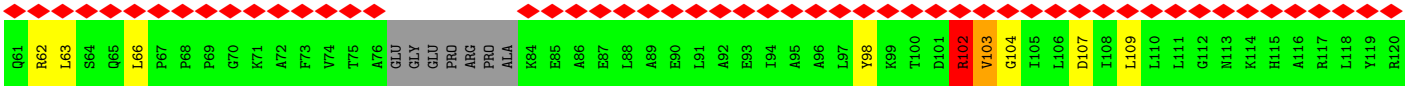


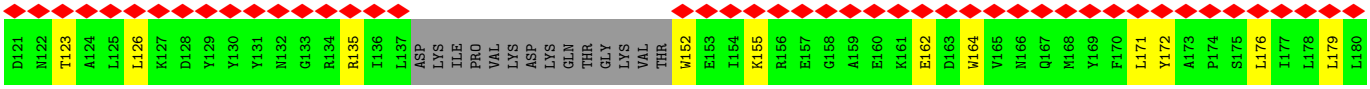
• Molecule 18: Subunit NESM of NADH:Ubiquinone Oxidoreductase (Complex I)

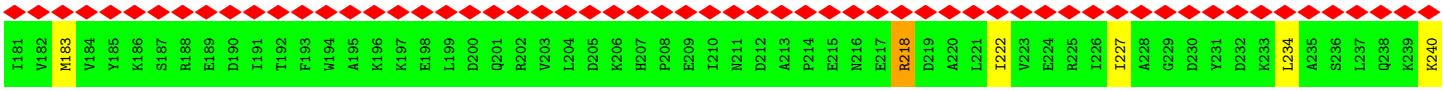
Chain S:

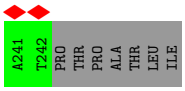






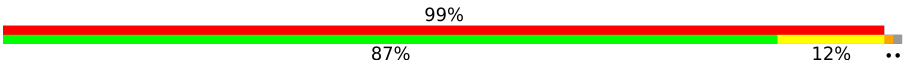


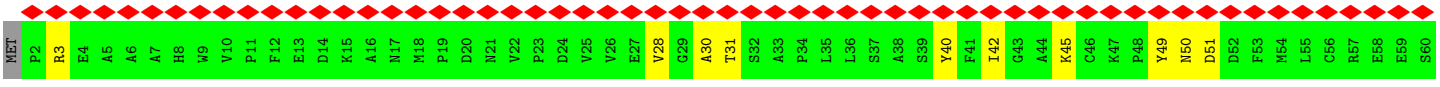


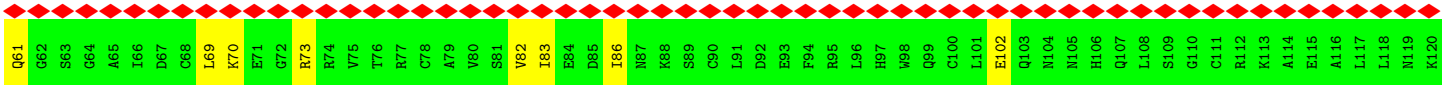


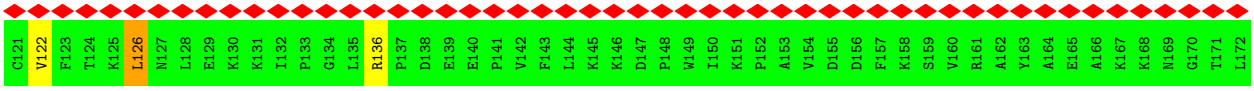
• Molecule 19: Subunit NUPM of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain U:



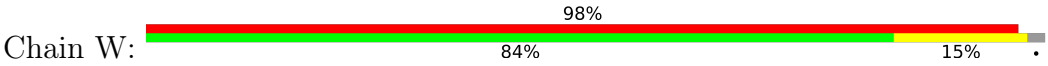


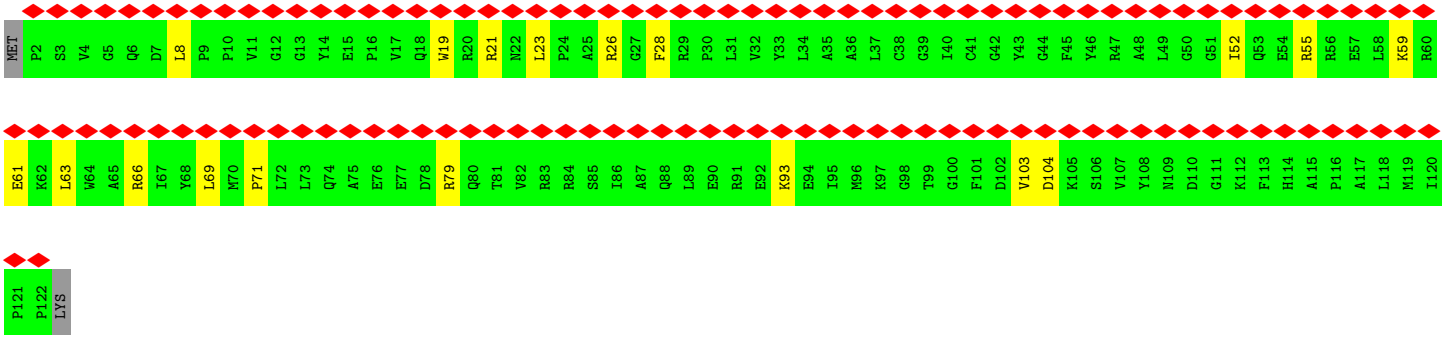




• Molecule 20: Subunit NB6M of NADH:Ubiquinone Oxidoreductase (Complex I)

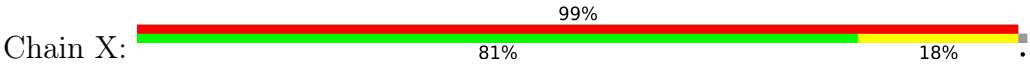
Chain W:

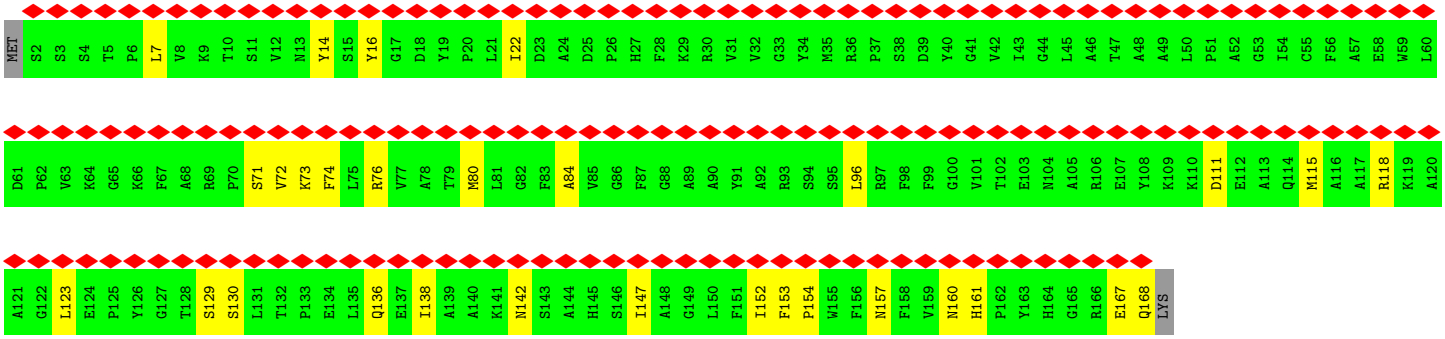




• Molecule 21: Subunit NUXM of NADH:Ubiquinone Oxidoreductase (Complex I)

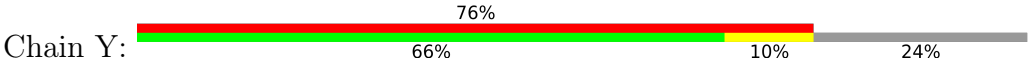
Chain X:

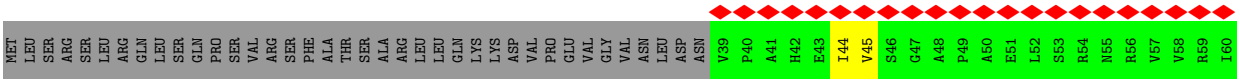


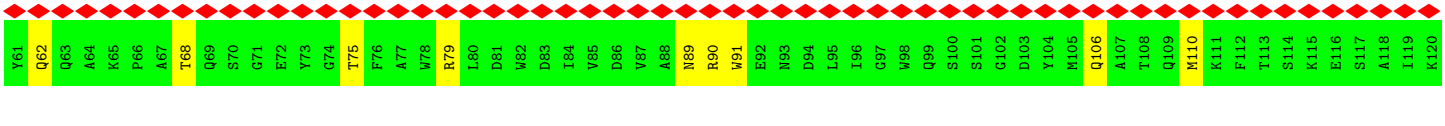


• Molecule 22: Subunit NUYM of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain Y:

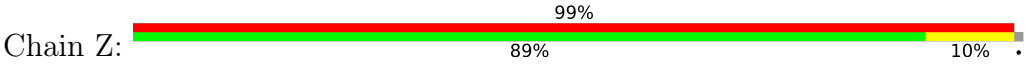


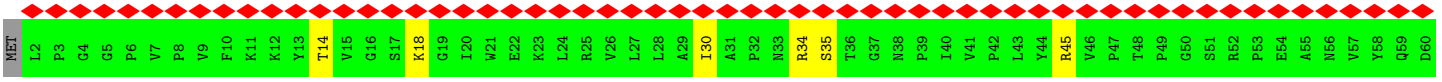


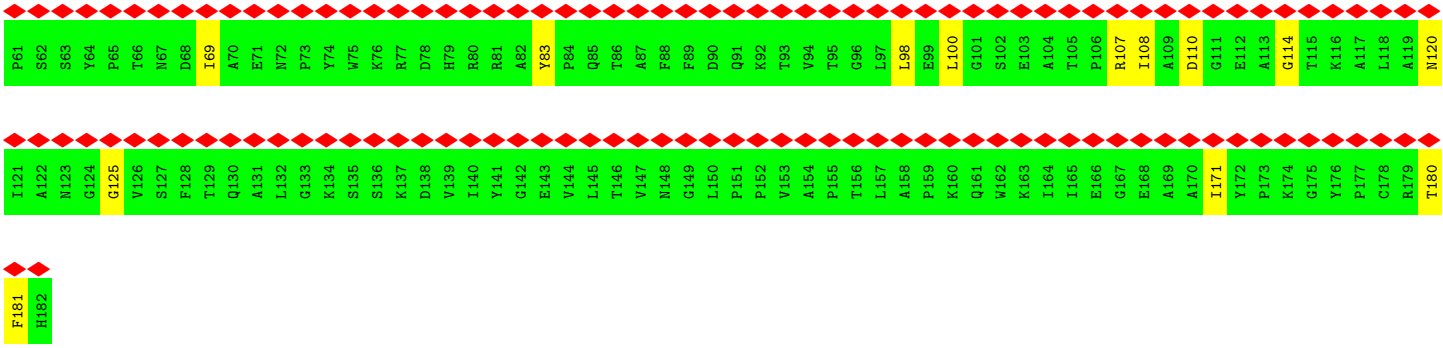


• Molecule 23: Subunit NUZM of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain Z:



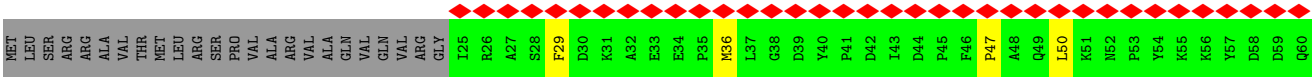


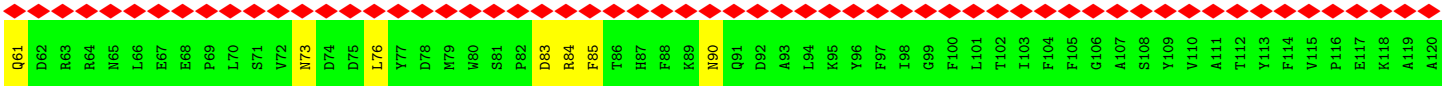


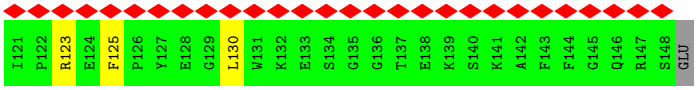
• Molecule 24: Subunit NIAM of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain a:





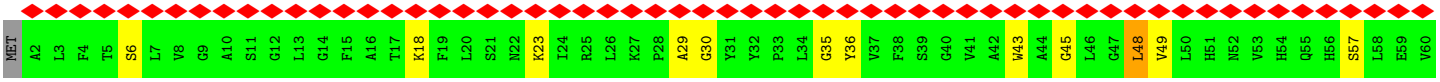


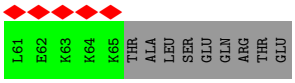


• Molecule 25: Subunit NEBM of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain b:



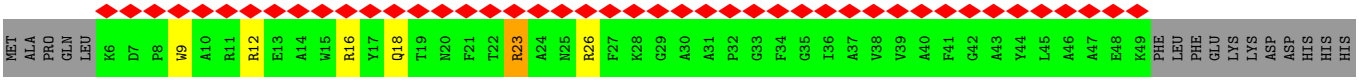




• Molecule 26: Subunit NB2M of NADH:Ubiquinone Oxidoreductase (Complex I)

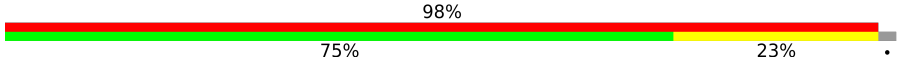
Chain c:

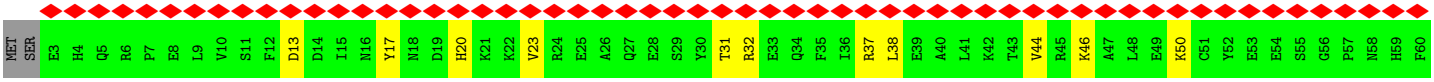


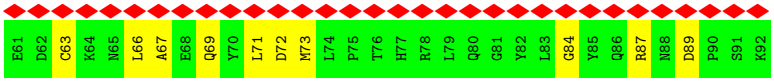


• Molecule 27: Subunit NIDM of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain d:



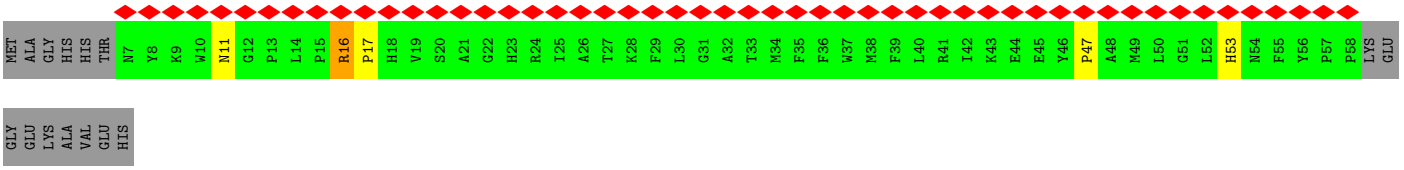




• Molecule 28: Subunit NUVM of NADH:Ubiquinone Oxidoreductase (Complex I)

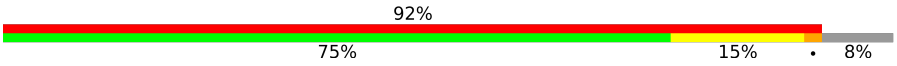
Chain e:

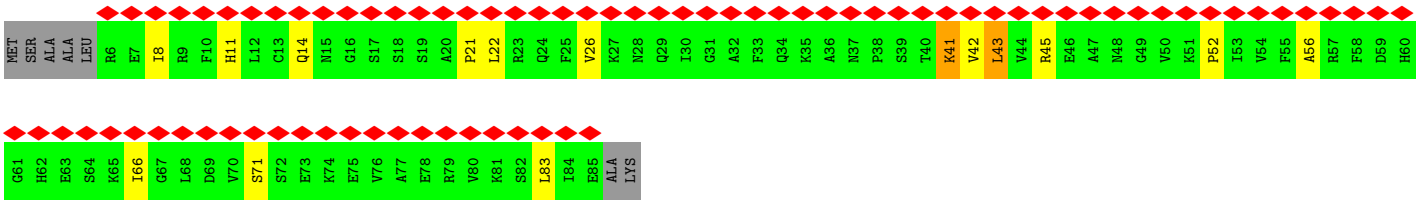




• Molecule 29: Subunit NI8M of NADH:Ubiquinone Oxidoreductase (Complex I)

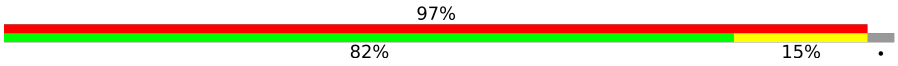
Chain f:





• Molecule 30: Subunit NI9M of NADH:Ubiquinone Oxidoreductase (Complex I)

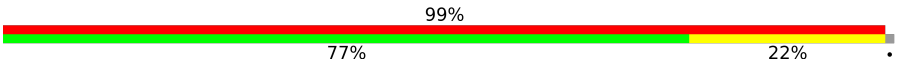
Chain g:

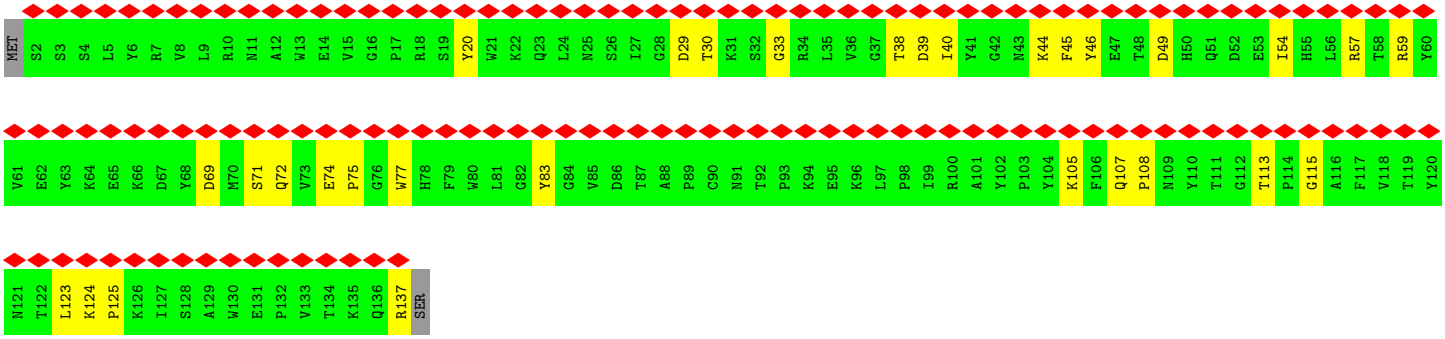




• Molecule 31: Subunit N7BM of NADH:Ubiquinone Oxidoreductase (Complex I)

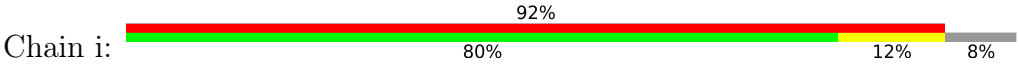
Chain h:

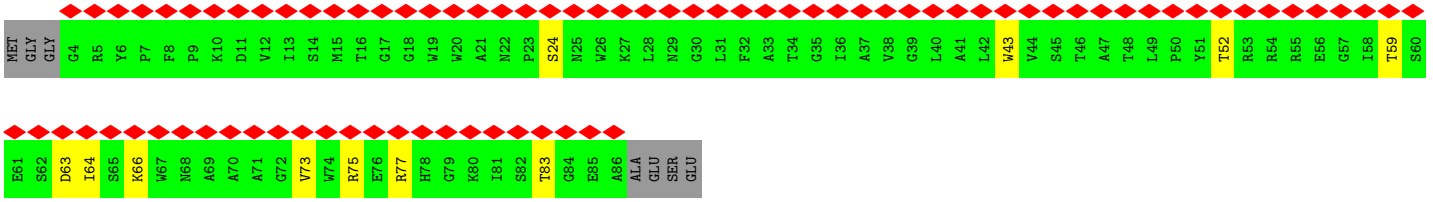




• Molecule 32: Subunit NUUM of NADH:Ubiquinone Oxidoreductase (Complex I)

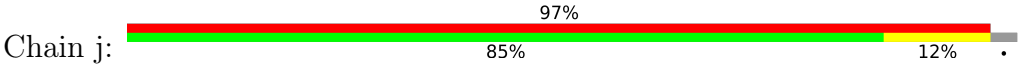
Chain i:

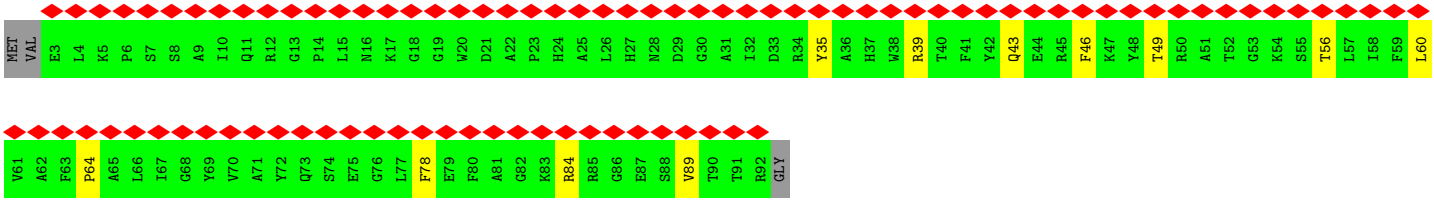




• Molecule 33: Subunit NB5M of NADH:Ubiquinone Oxidoreductase (Complex I)

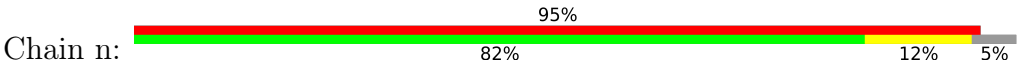
Chain j:

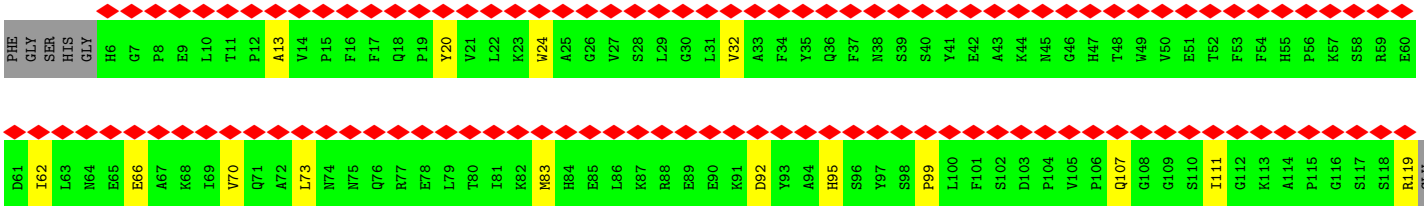




• Molecule 34: Subunit NUNM of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain n:

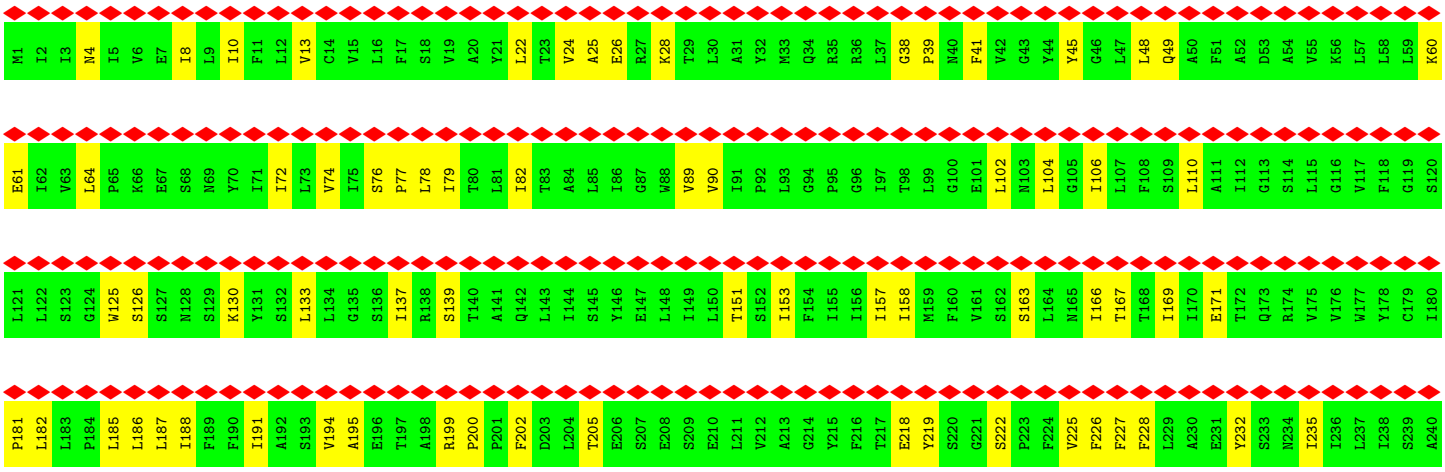




• Molecule 35: Subunit NU1M of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain 1:





F241 N242 G243 Y244 L245 L246 L247 G248 G249 Y250 L251 S252 F253 N254 Y255 S256 Y257 L258 F259 N260 I261 L262 F263 N264 D265 Y266 S267 Y268 V269 S270 F271 L272 F273 E274 G275 L276 I277 N278 S279 S280 A281 Y282 A283 I284 K285 L286 V287 F288 L289 M290 F291 S292 F293 I294 W295 V296 R297 A298 A299 F300

P301 R302 F303 T304 Y305 D306 N307 L308 I309 N310 F311 C312 W313 I314 I315 L316 L317 P318 L319 L320 F321 G322 I323 F324 L325 I326 I327 P328 S329 T330 L331 Y332 I333 F334 D335 S336 F337 P338 T339 L340 ILE

• Molecule 36: Subunit NU2M of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain 2: 100% 75% 25%

M1 L2 I3 L4 A5 I6 I7 S8 L9 I10 T11 F12 V13 S14 M15 S16 K17 L18 S19 D20 N21 R22 A23 I24 I25 R26 L27 I28 N29 I30 Y31 L32 I33 L34 V35 L36 V37 L38 D39 S40 F41 L42 Y43 L44 L45 F46 L47 N48 N49 Q50 T51 Y52 T53 V54 M55 G56 E57 L58 L59 I60

F61 N62 S63 F64 T65 F66 Y67 I68 D69 M70 L71 I72 Y73 F74 I75 M76 I77 V78 I79 S80 S81 L82 Y83 G84 Y85 N86 L87 Y88 N89 N90 N91 L92 Y93 K94 T95 L96 F97 E98 P99 K100 K101 E102 L103 I104 I105 L106 F107 L108 I109 N110 I111 L112 G113 A114 L115 L116 I117 V118 H119 S120

N121 D122 F123 I124 T125 L126 F127 V128 A129 I130 E131 L132 Q133 S134 Y135 S136 I137 Y138 L139 I140 T141 A142 I143 Y144 N145 S146 S147 Y148 K149 A150 S151 K152 A153 S154 M155 L156 Y157 F158 F159 M160 G161 G162 I163 L164 S165 I166 L167 I168 A169 Y170 S171 I172 N173 T174 Y175 Y176 S177 V178 L179 N180

S181 Y182 T183 L184 H185 S186 L187 D188 S189 L190 I191 I192 N193 T194 L195 D196 L197 N198 L199 I200 L201 I202 A203 L204 S205 L206 G207 L208 L209 F210 K211 I212 G213 I214 A215 P216 L217 H218 K219 W220 L221 I222 S223 I224 Y225 E226 N227 T228 P229 I230 L231 I232 T233 I234 Y235 I236 S237 L238 I239 P240

K241 I242 S243 I244 L245 S246 Y247 L248 V249 L250 S251 N252 I253 S254 I255 N256 S257 L258 V259 I260 S261 I262 L263 A264 I265 L266 T267 L268 L269 V270 G271 S272 V273 G274 G275 L276 L277 Q278 I279 K280 I281 K282 R283 L284 L285 A286 F287 S288 G289 L290 T291 N292 A293 G294 Y295 M296 M297 L298 L299 L300

L301 L302 N303 N304 N305 E306 F307 S308 Y309 L310 Y311 V312 I313 T314 Q315 Y316 S317 I318 S319 H320 L321 A322 I323 F324 M325 I326 I327 I328 F329 S330 I331 Y332 Y333 I334 N335 Y336 I337 N338 N339 Q340 Y341 N342 P343 I344 I345 Y346 V347 N348 Q349 L350 K351 G352 L353 I354 H355 D356 N357 A358 Y359 L360

Y361 L362 S363 M364 A365 I366 V367 Y368 F369 S370 F371 I372 G373 I374 P375 P376 L377 L378 G379 F380 F381 G382 K383 L384 N385 I386 L387 M388 S389 I390 L391 N392 N393 G394 Y395 Y396 F397 I398 S399 I400 V401 L402 I403 V404 A405 S406 L407 I408 S409 A410 L411 Y412 Y413 L414 Y415 L416 L417 N418 V419 S420

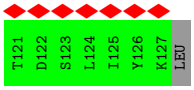
I421 Q422 D423 K424 N425 N426 I427 L428 I429 N430 S431 N432 E433 T434 V435 S436 S437 V438 L439 S440 Y441 I442 L443 S444 S445 L446 I447 I448 L449 I450 T451 F452 G453 F454 I455 Y456 N457 S458 L459 I460 I461 D462 I463 F464 N465 V466 Y467 F468 N469

• Molecule 37: Subunit NU3M of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain 3: 99% 75% 24%

M1 N2 T3 F4 I5 I6 F7 I8 I9 L10 I11 P12 I13 V14 G15 F16 A17 L18 L19 A20 V21 N22 I23 L24 L25 A26 V27 Y28 K29 P30 Y31 N32 E33 K34 L35 G36 A37 F38 E39 C40 G41 L42 T43 S44 F45 N46 Q47 T48 R49 L50 A51 F52 N53 A54 A55 F56 I57 L58 V59 A60

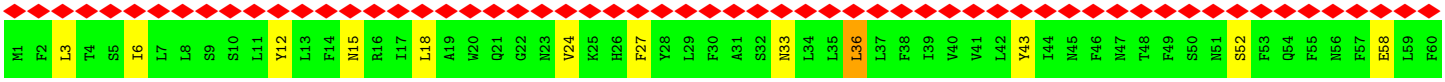
I61 L62 F63 L64 P65 F66 D67 L68 E69 T70 S71 T72 L73 L74 P75 Y76 V77 M78 S79 I80 Y81 L82 V83 S84 N85 Y86 G87 F88 T89 I90 V91 L92 L93 F94 L95 L96 I97 L98 I99 I100 G101 F102 V103 Y104 E105 I106 N107 T108 N109 A110 L111 K112 I113 N114 K115 H116 N117 K118 P119 N120

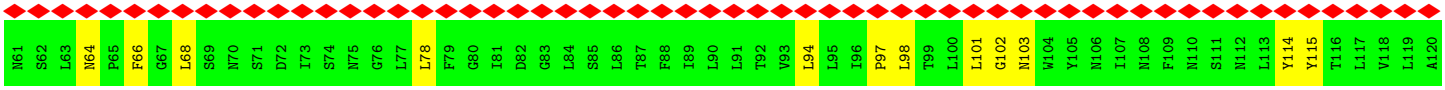


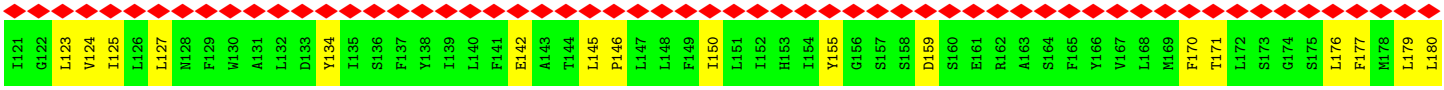
• Molecule 38: Subunit NU4M of NADH:Ubiquinone Oxidoreductase (Complex I)

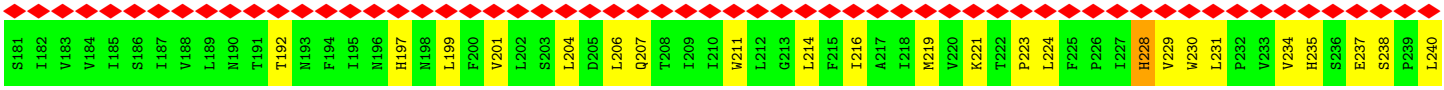
Chain 4:

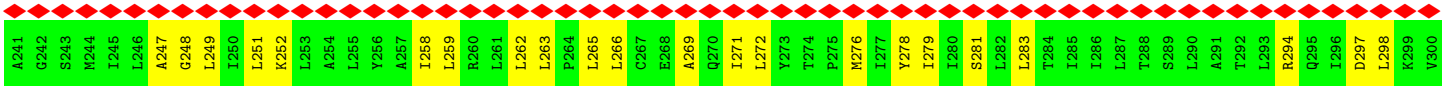


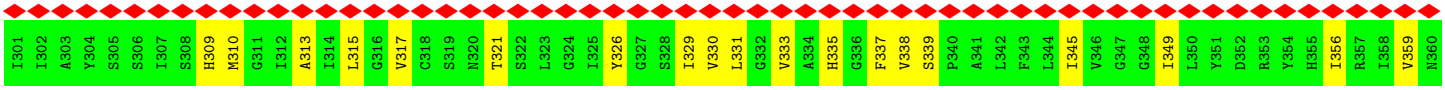


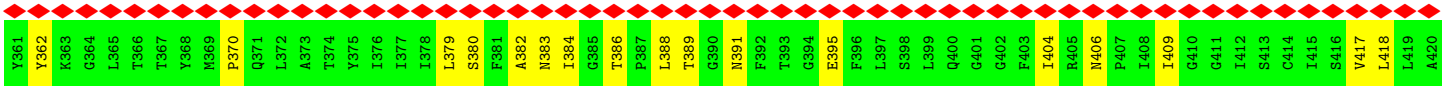


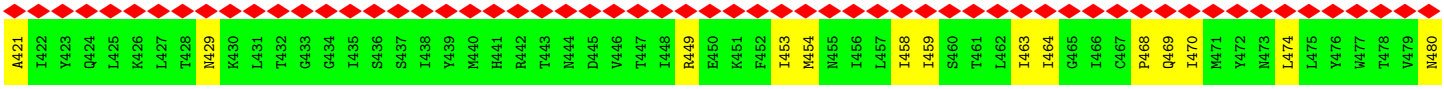


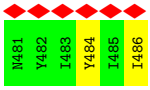








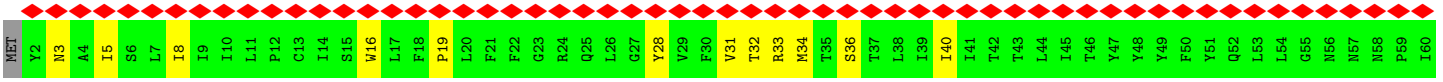


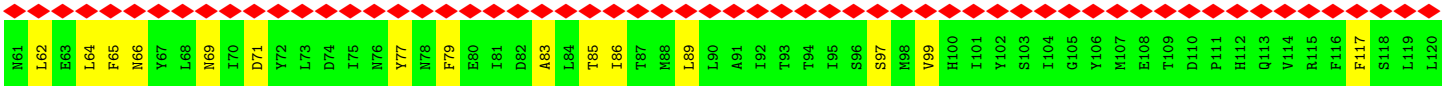


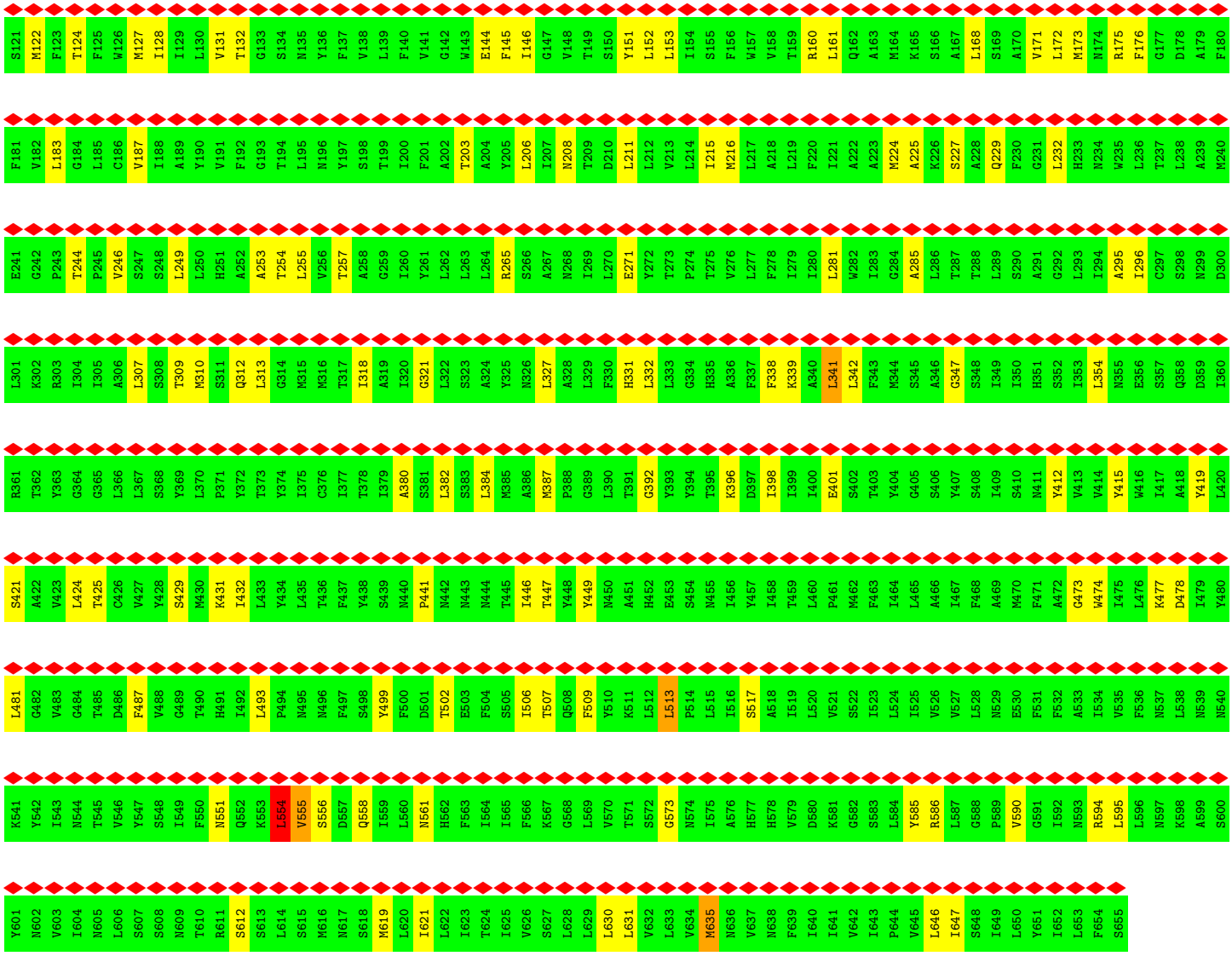
• Molecule 39: Subunit NU5M of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain 5:



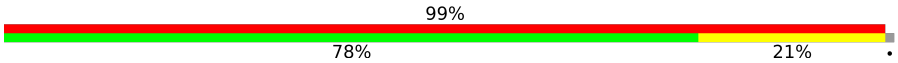






• Molecule 40: Subunit NU6M of NADH:Ubiquinone Oxidoreductase (Complex I)

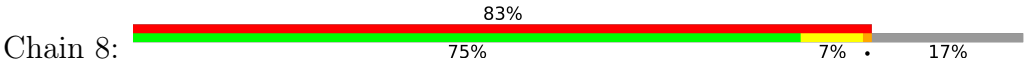
Chain 6:

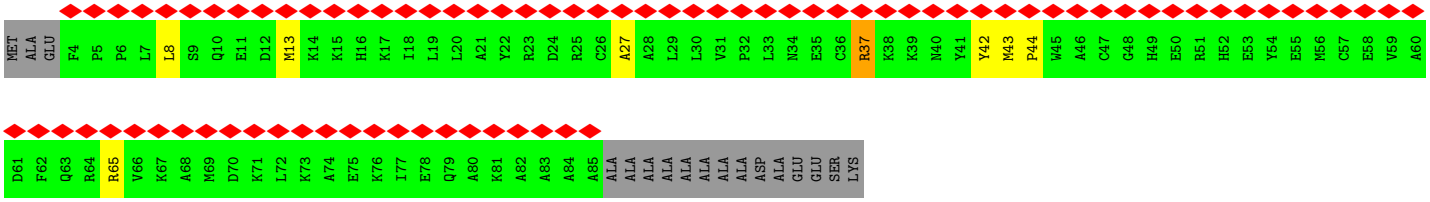




• Molecule 41: Subunit NB8M of NADH:Ubiquinone Oxidoreductase (Complex I)

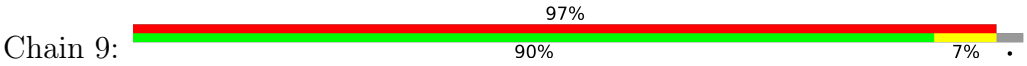
Chain 8:

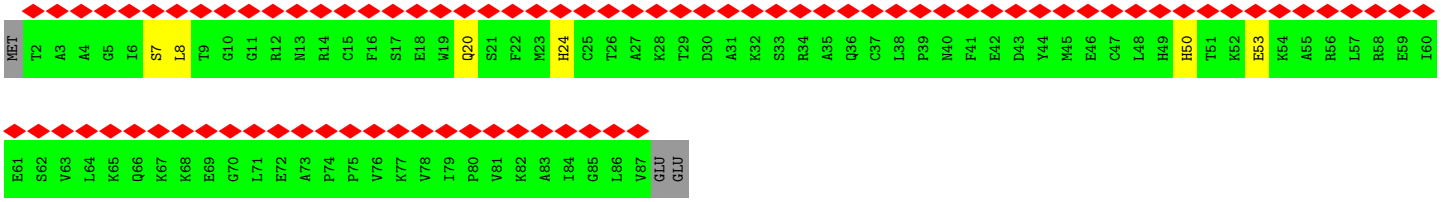




• Molecule 42: Subunit NIPM of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain 9:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	297066	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	-1500	Depositor
Maximum defocus (nm)	-2500	Depositor
Magnification	46425	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.276	Depositor
Minimum map value	-0.119	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	491.112, 491.112, 491.112	wwPDB
Map dimensions	456, 456, 456	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.077, 1.077, 1.077	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZMP, LMN, T7X, CPL, 3PE, NDP, CDL, ZN, FMN, PLC, SF4, FES, UQ9

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	0.46	0/5351	0.68	3/7262 (0.0%)
2	B	0.44	1/3605 (0.0%)	0.68	4/4865 (0.1%)
3	C	0.57	1/3554 (0.0%)	0.76	2/4817 (0.0%)
4	D	0.45	0/697	0.67	0/940
5	E	0.43	0/2858	0.74	0/3870
6	F	0.47	1/1011 (0.1%)	0.73	1/1371 (0.1%)
7	G	0.54	0/2040	0.79	1/2781 (0.0%)
8	H	0.39	0/1725	0.75	0/2343
9	I	0.56	0/1557	0.80	3/2110 (0.1%)
10	J	0.36	0/1362	0.66	1/1855 (0.1%)
11	K	0.54	0/1434	0.82	2/1950 (0.1%)
12	L	0.51	0/700	0.74	0/947
13	M	0.48	0/935	0.80	2/1268 (0.2%)
14	O	0.25	0/598	0.55	0/813
15	P	0.47	0/1061	0.73	2/1427 (0.1%)
16	Q	0.28	0/654	0.53	0/890
17	R	0.37	0/909	0.72	0/1229
18	S	0.34	0/1454	0.73	3/1960 (0.2%)
19	U	0.39	0/1374	0.71	2/1856 (0.1%)
20	W	0.41	0/998	0.64	1/1346 (0.1%)
21	X	0.41	0/1335	0.67	0/1811
22	Y	0.43	0/1051	0.62	0/1420
23	Z	0.38	0/1430	0.65	0/1955
24	a	0.33	0/1064	0.68	0/1439
25	b	0.37	0/503	0.60	1/679 (0.1%)
26	c	0.32	0/364	0.56	0/491
27	d	0.45	0/776	0.68	0/1043
28	e	0.32	0/456	0.70	1/619 (0.2%)
29	f	0.35	0/639	0.68	1/856 (0.1%)
30	g	0.34	0/643	0.54	0/880
31	h	0.47	0/1168	0.76	0/1589
32	i	0.36	0/666	0.55	0/907

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
33	j	0.39	0/745	0.59	0/1006
34	n	0.37	0/943	0.63	0/1279
35	1	0.53	0/2789	0.84	3/3808 (0.1%)
36	2	0.56	0/3854	0.80	5/5252 (0.1%)
37	3	0.45	0/1041	0.84	0/1419
38	4	0.51	0/3949	0.78	1/5392 (0.0%)
39	5	0.46	0/5327	0.75	5/7273 (0.1%)
40	6	0.46	0/1468	0.77	0/2003
41	8	0.31	0/686	0.65	0/918
42	9	0.37	0/684	0.61	0/918
All	All	0.46	3/65458 (0.0%)	0.73	44/88857 (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
1	A	0	3
3	C	0	1
8	H	0	2
10	J	0	1
11	K	0	1
18	S	0	1
26	c	0	2
31	h	0	1
32	i	0	1
33	j	0	1
35	1	0	1
36	2	0	1
38	4	0	1
39	5	0	3
41	8	0	1
All	All	0	21

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	395	PRO	CA-C	-7.50	1.47	1.51
2	B	101	MET	CA-CB	-7.09	1.41	1.53
6	F	39	HIS	CG-ND1	-6.67	1.30	1.38

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	M	76	TYR	N-CA-C	10.78	126.12	111.24
11	K	108	ARG	N-CA-C	-9.51	94.70	109.25
9	I	103	TYR	N-CA-C	9.16	125.22	112.75
11	K	137	GLN	N-CA-C	8.28	120.31	111.28
10	J	143	ARG	N-CA-C	8.19	120.28	111.36
13	M	75	PRO	N-CA-C	7.54	126.43	112.33
3	C	258	LEU	CB-CG-CD2	-6.87	90.09	110.70
36	2	215	ALA	N-CA-C	6.84	124.93	109.81
35	1	300	PHE	N-CA-C	6.67	120.08	108.82
18	S	103	VAL	N-CA-C	6.65	119.94	108.90
18	S	102	ARG	N-CA-C	6.19	118.03	111.28
36	2	277	LEU	CA-CB-CG	6.02	137.36	116.30
36	2	375	PRO	N-CA-C	5.98	117.99	110.70
9	I	103	TYR	CA-C-N	-5.87	113.70	120.04
9	I	103	TYR	C-N-CA	-5.87	113.70	120.04
2	B	100	PHE	CA-C-N	5.78	129.10	120.31
2	B	100	PHE	C-N-CA	5.78	129.10	120.31
39	5	635	MET	CB-CG-SD	-5.72	95.55	112.70
6	F	126	LEU	CA-CB-CG	5.69	136.22	116.30
1	A	659	TYR	CA-C-N	5.62	132.28	121.54
1	A	659	TYR	C-N-CA	5.62	132.28	121.54
7	G	180	ARG	NE-CZ-NH1	-5.60	115.90	121.50
18	S	218	ARG	N-CA-C	5.54	117.00	111.07
2	B	229	PRO	CA-C-N	-5.50	112.97	119.84
2	B	229	PRO	C-N-CA	-5.50	112.97	119.84
38	4	36	LEU	CB-CG-CD1	-5.50	94.21	110.70
39	5	338	PHE	CB-CA-C	-5.46	102.23	110.92
20	W	63	LEU	CA-CB-CG	5.41	135.24	116.30
3	C	395	PRO	O-C-N	-5.37	118.84	121.31
36	2	319	SER	CA-C-N	5.37	128.26	120.79
36	2	319	SER	C-N-CA	5.37	128.26	120.79
39	5	555	VAL	N-CA-C	5.28	120.33	109.34
15	P	121	LYS	CA-C-N	5.23	131.53	121.54
15	P	121	LYS	C-N-CA	5.23	131.53	121.54
19	U	126	LEU	CA-C-N	5.17	131.41	121.54
19	U	126	LEU	C-N-CA	5.17	131.41	121.54
28	e	16	ARG	N-CA-C	-5.17	103.27	109.83
25	b	48	LEU	CA-CB-CG	5.13	134.25	116.30
39	5	554	LEU	CA-C-N	5.13	131.20	121.97
39	5	554	LEU	C-N-CA	5.13	131.20	121.97
29	f	43	LEU	CA-CB-CG	5.12	134.21	116.30
1	A	261	MET	CA-CB-CG	5.10	124.31	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	1	297	ARG	NE-CZ-NH2	5.09	123.78	119.20
35	1	48	LEU	CA-CB-CG	5.02	133.86	116.30

There are no chirality outliers.

All (21) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
35	1	200	PRO	Peptide
36	2	214	ILE	Peptide
38	4	228	HIS	Peptide
39	5	227	SER	Peptide
39	5	253	ALA	Peptide
39	5	554	LEU	Peptide
41	8	37	ARG	Sidechain
1	A	222	ASN	Peptide
1	A	247	ALA	Peptide
1	A	67	ARG	Sidechain
3	C	86	ASN	Peptide
8	H	174	ASN	Peptide
8	H	29	ILE	Peptide
10	J	182	GLY	Peptide
11	K	112	ARG	Sidechain
18	S	102	ARG	Sidechain
26	c	18	GLN	Peptide
26	c	23	ARG	Sidechain
31	h	49	ASP	Peptide
32	i	75	ARG	Sidechain
33	j	78	PHE	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	5258	0	5159	96	0
2	B	3528	0	3489	49	0
3	C	3472	0	3403	93	0
4	D	681	0	671	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	2798	0	2788	48	0
6	F	990	0	977	7	0
7	G	1978	0	1908	50	0
8	H	1688	0	1660	23	0
9	I	1519	0	1460	37	0
10	J	1329	0	1311	22	0
11	K	1395	0	1375	38	0
12	L	691	0	754	30	0
13	M	912	0	869	26	0
14	O	591	0	585	7	0
15	P	1036	0	1018	23	0
16	Q	648	0	636	15	0
17	R	884	0	893	22	0
18	S	1430	0	1463	40	0
19	U	1345	0	1327	17	0
20	W	974	0	987	18	0
21	X	1296	0	1268	30	0
22	Y	1021	0	984	13	0
23	Z	1389	0	1395	16	0
24	a	1030	0	967	11	0
25	b	490	0	509	11	0
26	c	353	0	343	6	0
27	d	760	0	721	22	0
28	e	436	0	426	4	0
29	f	629	0	640	20	0
30	g	617	0	597	17	0
31	h	1130	0	1084	25	0
32	i	646	0	630	9	0
33	j	724	0	706	9	0
34	n	914	0	880	16	0
35	1	2714	0	2814	84	0
36	2	3774	0	4005	92	0
37	3	1017	0	1081	38	0
38	4	3855	0	4054	102	0
39	5	5197	0	5353	108	0
40	6	1443	0	1565	34	0
41	8	672	0	677	7	0
42	9	672	0	683	4	0
43	A	16	0	0	0	0
43	B	8	0	0	1	0
43	I	16	0	0	0	0
43	K	8	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	A	4	0	0	0	0
44	H	4	0	0	0	0
45	B	31	0	19	1	0
46	1	72	0	92	2	0
46	4	178	0	264	10	0
46	5	93	0	140	4	0
46	C	51	0	82	4	0
46	E	36	0	46	0	0
46	J	85	0	118	5	0
46	W	34	0	42	1	0
46	b	42	0	58	2	0
46	g	43	0	63	2	0
47	E	48	0	26	0	0
48	4	92	0	137	8	0
48	E	72	0	88	5	0
48	X	86	0	119	9	0
48	Z	76	0	96	2	0
48	g	83	0	116	6	0
48	j	78	0	103	3	0
49	J	69	0	88	5	0
49	j	65	0	77	2	0
50	1	35	0	44	1	0
50	5	31	0	36	1	0
50	K	39	0	55	5	0
50	W	125	0	187	7	0
50	n	42	0	64	3	0
51	M	1	0	0	0	0
52	O	33	0	38	3	0
52	Q	33	0	38	3	0
53	1	35	0	43	6	0
54	2	100	0	0	2	0
54	3	49	0	0	0	0
54	5	43	0	0	1	0
55	2	52	0	80	7	0
All	All	65934	0	66474	1104	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 8.

All (1104) 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)
37:3:69:GLU:HG3	37:3:98:LEU:CD1	1.53	1.36
19:U:61:GLN:HG3	34:n:119:ARG:HA	1.35	1.07
9:I:197:ARG:HG3	11:K:176:TYR:CE2	1.93	1.03
37:3:69:GLU:CG	37:3:98:LEU:CD1	2.37	1.02
37:3:69:GLU:CG	37:3:98:LEU:HD13	1.91	0.99
37:3:69:GLU:HG3	37:3:98:LEU:HD13	0.96	0.95
39:5:398:ILE:HD12	39:5:401:GLU:OE1	1.65	0.94
15:P:55:LYS:HE3	15:P:100:PHE:CE1	2.02	0.94
11:K:85:CYS:HB3	43:K:301:SF4:S1	2.10	0.91
31:h:54:ILE:CG1	31:h:57:ARG:HG3	2.00	0.90
3:C:410:MET:HE3	3:C:427:ILE:CG2	2.02	0.89
35:1:222:SER:H	37:3:22:ASN:ND2	1.70	0.89
21:X:167:GLU:N	21:X:167:GLU:OE1	2.08	0.86
37:3:69:GLU:HG3	37:3:98:LEU:HD11	1.59	0.85
5:E:373:ILE:HG21	12:L:79:ARG:NH2	1.95	0.82
35:1:222:SER:H	37:3:22:ASN:HD22	1.22	0.81
50:K:302:PLC:H81	35:1:41:PHE:CZ	2.15	0.81
31:h:54:ILE:HG13	31:h:57:ARG:CG	2.10	0.81
31:h:54:ILE:HG12	31:h:57:ARG:HG3	1.61	0.81
17:R:20:ARG:HB3	17:R:20:ARG:NH1	1.95	0.81
29:f:42:VAL:O	29:f:43:LEU:HD12	1.80	0.81
3:C:426:LYS:HE3	7:G:127:THR:HB	1.62	0.80
29:f:56:ALA:HB3	29:f:83:LEU:HD21	1.61	0.80
15:P:55:LYS:HE3	15:P:100:PHE:CD1	2.17	0.79
13:M:73:PRO:C	13:M:74:MET:HG2	2.09	0.78
7:G:201:THR:HG22	7:G:202:ASP:N	1.98	0.78
31:h:54:ILE:HG13	31:h:57:ARG:HG2	1.63	0.78
16:Q:90:LEU:HB3	17:R:44:ARG:HH22	1.46	0.78
4:D:53:ASP:HA	4:D:56:LEU:HD12	1.62	0.78
7:G:201:THR:HG21	7:G:205:PHE:CD2	2.19	0.77
5:E:221:PRO:O	5:E:285:ARG:HD2	1.85	0.77
9:I:197:ARG:HG3	11:K:176:TYR:HE2	1.45	0.76
29:f:56:ALA:HB3	29:f:83:LEU:CD2	2.15	0.76
38:4:159:ASP:HB3	38:4:237:GLU:HG2	1.68	0.76
31:h:54:ILE:CG1	31:h:57:ARG:CG	2.63	0.76
7:G:141:VAL:HG12	7:G:156:LYS:HG2	1.68	0.74
29:f:41:LYS:HB2	29:f:41:LYS:NZ	2.03	0.74
3:C:410:MET:HE3	3:C:427:ILE:HG21	1.69	0.74
18:S:102:ARG:NH1	18:S:126:LEU:HD11	2.02	0.74
1:A:67:ARG:HD2	1:A:70:TYR:HB3	1.70	0.74
39:5:398:ILE:CD1	39:5:401:GLU:OE1	2.36	0.73
38:4:335:HIS:CD2	38:4:339:SER:HB2	2.23	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:191:ALA:HB2	18:S:234:LEU:CD2	2.18	0.73
35:1:222:SER:N	37:3:22:ASN:HD22	1.86	0.73
18:S:234:LEU:HD13	27:d:37:ARG:HH21	1.52	0.72
35:1:41:PHE:HA	50:1:502:PLC:H81	1.70	0.71
11:K:108:ARG:HA	11:K:108:ARG:NH1	2.06	0.71
37:3:69:GLU:CG	37:3:98:LEU:HD11	2.17	0.71
13:M:35:TYR:CE1	13:M:74:MET:HE1	2.25	0.71
17:R:16:THR:O	17:R:20:ARG:HG3	1.91	0.71
36:2:403:ILE:HD12	38:4:176:LEU:HD12	1.73	0.71
3:C:123:THR:HG22	3:C:466:ARG:O	1.91	0.70
13:M:35:TYR:CD1	13:M:74:MET:HE1	2.25	0.70
28:e:16:ARG:HG3	28:e:17:PRO:HD2	1.74	0.69
2:B:371:ARG:HH22	8:H:167:GLU:HG2	1.57	0.69
15:P:55:LYS:CE	15:P:100:PHE:CE1	2.74	0.69
29:f:56:ALA:CB	29:f:83:LEU:CD2	2.71	0.69
32:i:73:VAL:O	32:i:77:ARG:HG2	1.92	0.69
11:K:137:GLN:HE22	37:3:38:PHE:HD1	1.40	0.69
10:J:169:ARG:HE	27:d:89:ASP:HB3	1.58	0.69
1:A:550:VAL:HB	1:A:569:VAL:HG12	1.75	0.69
14:O:29:ARG:N	14:O:30:PRO:HD2	2.08	0.69
1:A:434:ARG:HG3	1:A:435:GLN:HG3	1.76	0.68
5:E:373:ILE:HG13	12:L:79:ARG:HG3	1.76	0.68
38:4:281:SER:OG	38:4:315:LEU:HD23	1.95	0.67
18:S:102:ARG:HH12	18:S:126:LEU:HD11	1.57	0.67
1:A:389:ILE:HG22	29:f:43:LEU:HG	1.75	0.67
27:d:87:ARG:HE	38:4:201:VAL:HG22	1.60	0.67
9:I:166:MET:HE3	9:I:171:TYR:OH	1.95	0.66
21:X:129:SER:HB2	48:X:201:CDL:OA4	1.95	0.66
7:G:201:THR:HG22	7:G:202:ASP:H	1.58	0.66
2:B:129:ASP:HA	2:B:132:ILE:HG12	1.78	0.65
35:1:228:PHE:CE1	53:1:501:UQ9:H12A	2.31	0.65
5:E:373:ILE:HG21	12:L:79:ARG:CZ	2.26	0.65
1:A:263:ALA:HB3	1:A:421:ALA:HB2	1.79	0.64
10:J:195:GLU:HG2	10:J:197:PRO:HD2	1.79	0.64
36:2:299:LEU:O	36:2:305:ASN:ND2	2.29	0.64
38:4:313:ALA:HB2	38:4:331:LEU:HD22	1.78	0.64
39:5:85:THR:HG23	39:5:131:VAL:HG12	1.79	0.64
38:4:480:ASN:O	38:4:480:ASN:OD1	2.15	0.64
1:A:484:VAL:HB	1:A:521:VAL:HG12	1.80	0.64
18:S:102:ARG:NH2	18:S:123:THR:HG22	2.13	0.64
29:f:83:LEU:O	29:f:83:LEU:HD23	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:65:LYS:HG2	2:B:189:CYS:HB3	1.80	0.64
9:I:129:ARG:NH1	9:I:181:VAL:O	2.31	0.64
8:H:211:GLU:HG3	8:H:214:VAL:HG22	1.79	0.64
12:L:71:LEU:HD12	40:6:74:ILE:HG13	1.79	0.64
24:a:47:PRO:HB3	24:a:84:ARG:HH21	1.62	0.64
38:4:124:VAL:HG22	46:4:505:3PE:H2I3	1.80	0.63
3:C:426:LYS:HD2	7:G:127:THR:HG21	1.80	0.63
36:2:403:ILE:HG13	38:4:180:LEU:HD11	1.80	0.63
21:X:71:SER:OG	21:X:73:LYS:HG2	1.97	0.63
18:S:227:ILE:HG23	27:d:69:GLN:HE22	1.64	0.63
24:a:83:ASP:H	39:5:561:ASN:HD21	1.45	0.63
39:5:151:TYR:HB2	39:5:171:VAL:HG21	1.81	0.63
1:A:127:GLN:NE2	2:B:389:GLU:O	2.32	0.62
2:B:63:LYS:H	2:B:258:ARG:HH12	1.47	0.62
7:G:201:THR:CG2	7:G:202:ASP:H	2.12	0.62
18:S:102:ARG:NH1	18:S:126:LEU:CD1	2.61	0.62
3:C:410:MET:HE3	3:C:427:ILE:HG23	1.77	0.62
7:G:144:PHE:HB2	7:G:153:ILE:HG22	1.81	0.62
7:G:201:THR:CG2	7:G:202:ASP:N	2.62	0.62
17:R:28:ASN:HD22	17:R:78:PRO:HA	1.65	0.62
30:g:47:ARG:HH12	35:1:335:ASP:HB2	1.63	0.62
2:B:288:CYS:SG	2:B:289:THR:N	2.73	0.62
4:D:64:GLN:HA	19:U:31:THR:HG21	1.81	0.62
7:G:185:MET:HB3	7:G:210:LEU:HB2	1.80	0.62
18:S:103:VAL:CG2	18:S:104:GLY:N	2.63	0.62
3:C:263:GLU:OE2	23:Z:34:ARG:NH2	2.33	0.62
1:A:168:GLU:CA	13:M:116:ASN:HD22	2.12	0.61
39:5:509:PHE:O	39:5:513:LEU:HB2	1.99	0.61
4:D:52:ARG:HG3	4:D:55:ARG:HH21	1.65	0.61
14:O:29:ARG:HD2	14:O:29:ARG:O	2.00	0.61
36:2:229:PRO:HB3	36:2:341:TYR:HB3	1.82	0.61
3:C:259:ASP:OD1	3:C:341:ARG:NH2	2.34	0.61
38:4:370:PRO:HB3	46:5:802:3PE:H11	1.82	0.61
2:B:298:LEU:HB2	2:B:339:MET:HE3	1.83	0.61
1:A:389:ILE:HG13	1:A:537:THR:HG21	1.82	0.61
49:J:202:LMN:HBF	49:J:202:LMN:HAW	1.81	0.61
16:Q:90:LEU:HB3	17:R:44:ARG:NH2	2.16	0.61
21:X:129:SER:OG	21:X:136:GLN:NE2	2.34	0.61
38:4:197:HIS:HB2	38:4:265:LEU:HD23	1.83	0.61
1:A:145:GLN:HG2	3:C:386:LEU:HD11	1.82	0.61
8:H:125:GLN:HB2	8:H:179:ALA:HB3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:Y:79:ARG:HA	22:Y:110:MET:O	2.00	0.61
27:d:31:THR:HG23	38:4:480:ASN:ND2	2.15	0.61
39:5:32:THR:HG22	39:5:117:PHE:HE2	1.65	0.61
3:C:111:ARG:HH22	15:P:7:ALA:HB2	1.65	0.61
5:E:373:ILE:CG1	12:L:79:ARG:HG3	2.31	0.61
12:L:80:LEU:HD13	36:2:148:TYR:CD1	2.36	0.60
35:1:186:LEU:HA	35:1:246:LEU:HD21	1.81	0.60
1:A:268:ILE:O	1:A:283:ARG:NH1	2.31	0.60
37:3:6:ILE:O	37:3:10:LEU:HB2	2.01	0.60
38:4:98:LEU:HD12	38:4:453:ILE:HG23	1.82	0.60
32:i:63:ASP:O	32:i:66:LYS:HG2	2.01	0.60
38:4:150:ILE:HG13	46:4:502:3PE:H291	1.83	0.60
1:A:168:GLU:HB2	13:M:116:ASN:ND2	2.17	0.60
3:C:269:ARG:HH22	9:I:80:LEU:HG	1.66	0.60
7:G:176:ASN:HD21	15:P:2:ALA:HB3	1.65	0.60
39:5:3:ASN:OD1	39:5:5:ILE:HG22	2.01	0.60
2:B:333:ILE:HG21	2:B:347:VAL:HG11	1.83	0.60
15:P:55:LYS:CE	15:P:100:PHE:HE1	2.12	0.60
35:1:125:TRP:CD1	40:6:30:MET:SD	2.95	0.60
1:A:458:THR:HG22	1:A:460:ALA:H	1.67	0.60
39:5:151:TYR:HD2	39:5:152:LEU:HD12	1.66	0.60
18:S:103:VAL:HG22	18:S:104:GLY:N	2.15	0.60
19:U:61:GLN:HG3	34:n:119:ARG:CA	2.21	0.60
20:W:59:LYS:NZ	35:1:340:LEU:HD12	2.17	0.60
31:h:69:ASP:HB2	31:h:72:GLN:HG3	1.83	0.60
3:C:185:ASN:ND2	3:C:406:PRO:HB2	2.17	0.60
3:C:426:LYS:CE	7:G:127:THR:HB	2.30	0.60
31:h:105:LYS:HE3	31:h:107:GLN:HE22	1.67	0.60
35:1:28:LYS:HD2	35:1:38:GLY:HA3	1.83	0.60
36:2:455:ILE:HD13	38:4:66:PHE:HE1	1.67	0.60
1:A:569:VAL:HG23	1:A:583:ALA:HA	1.84	0.59
1:A:646:ARG:HE	1:A:657:VAL:HG13	1.66	0.59
11:K:111:PRO:O	11:K:138:MET:HG2	2.01	0.59
39:5:224:MET:HG3	39:5:229:GLN:HB2	1.83	0.59
39:5:341:LEU:HD12	39:5:380:ALA:HB2	1.84	0.59
1:A:185:HIS:HB2	2:B:388:ARG:HH12	1.65	0.59
7:G:202:ASP:HB3	7:G:205:PHE:HB2	1.84	0.59
50:K:302:PLC:C8	35:1:41:PHE:CZ	2.85	0.59
3:C:410:MET:CE	3:C:427:ILE:CG2	2.80	0.59
1:A:55:ILE:HD11	1:A:67:ARG:NH2	2.17	0.59
12:L:3:ILE:HB	40:6:13:ILE:HG12	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:1:171:GLU:OE2	35:1:250:TYR:OH	2.20	0.59
1:A:132:ASP:OD1	13:M:126:GLN:NE2	2.36	0.59
37:3:57:ILE:HD11	40:6:74:ILE:HD13	1.84	0.59
35:1:26:GLU:HG3	35:1:294:ILE:HG12	1.84	0.59
31:h:74:GLU:HB3	31:h:77:TRP:HD1	1.67	0.59
36:2:58:LEU:HD11	40:6:161:ILE:HD11	1.84	0.59
39:5:40:ILE:HD13	39:5:97:SER:HB2	1.84	0.59
4:D:10:PRO:HB2	35:1:25:ALA:HB2	1.84	0.59
35:1:218:GLU:OE1	37:3:37:ALA:HA	2.03	0.59
36:2:82:LEU:HD11	36:2:325:MET:HE2	1.83	0.59
38:4:294:ARG:HG3	39:5:573:GLY:HA2	1.84	0.59
34:n:66:GLU:OE2	38:4:52:SER:HB3	2.03	0.58
1:A:596:ALA:HA	1:A:609:SER:O	2.03	0.58
2:B:473:VAL:HG22	2:B:478:VAL:HG22	1.85	0.58
3:C:258:LEU:HD21	3:C:340:PHE:HB3	1.85	0.58
36:2:208:LEU:HD12	36:2:244:ILE:HG23	1.86	0.58
3:C:260:GLU:OE2	9:I:93:GLN:NE2	2.37	0.58
38:4:321:THR:HG21	38:4:404:ILE:HG13	1.85	0.58
14:O:29:ARG:HD2	14:O:29:ARG:C	2.29	0.58
16:Q:90:LEU:CB	17:R:44:ARG:HH22	2.16	0.58
40:6:52:LEU:HB3	40:6:55:PHE:HD2	1.69	0.58
39:5:590:VAL:HG12	39:5:594:ARG:HH12	1.67	0.58
9:I:123:TYR:HD2	9:I:127:GLU:HB3	1.69	0.58
46:J:203:3PE:H3A1	39:5:630:LEU:HD23	1.84	0.58
11:K:93:VAL:HG21	11:K:187:LEU:HD23	1.86	0.58
13:M:73:PRO:O	13:M:74:MET:CG	2.51	0.58
29:f:41:LYS:HB2	29:f:41:LYS:HZ2	1.67	0.58
36:2:22:ARG:NH1	36:2:86:ASN:OD1	2.35	0.58
36:2:212:ILE:HD11	36:2:244:ILE:HB	1.85	0.58
7:G:262:ARG:HH11	7:G:267:LYS:CB	2.17	0.58
31:h:20:TYR:OH	35:1:45:TYR:OH	2.22	0.58
30:g:47:ARG:NH1	35:1:335:ASP:HB2	2.18	0.58
35:1:4:ASN:HB2	37:3:3:THR:HB	1.86	0.58
5:E:64:PHE:HE2	5:E:238:VAL:HG21	1.69	0.57
18:S:183:MET:HE2	38:4:470:ILE:HG22	1.87	0.57
39:5:309:THR:OG1	39:5:339:LYS:HE2	2.04	0.57
1:A:405:GLU:OE2	1:A:434:ARG:NH1	2.37	0.57
1:A:419:ARG:HB3	1:A:694:ILE:HD11	1.87	0.57
39:5:296:ILE:HD11	39:5:424:LEU:HG	1.85	0.57
9:I:166:MET:CE	9:I:171:TYR:OH	2.51	0.57
23:Z:14:THR:HG21	23:Z:35:SER:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:a:123:ARG:HB3	41:8:65:ARG:HD3	1.86	0.57
39:5:66:ASN:HD21	39:5:69:ASN:HB2	1.67	0.57
33:j:56:THR:HG23	33:j:60:LEU:HD12	1.85	0.57
3:C:329:CYS:SG	3:C:332:ARG:NH2	2.77	0.57
36:2:284:LEU:HD11	36:2:412:TYR:HB2	1.85	0.57
11:K:108:ARG:HA	11:K:108:ARG:HH11	1.66	0.57
17:R:39:LYS:HE3	17:R:43:ILE:HD11	1.86	0.57
25:b:30:GLY:H	46:4:501:3PE:H112	1.70	0.57
34:n:73:LEU:HD11	38:4:78:LEU:HD11	1.86	0.57
35:1:199:ARG:HD3	35:1:235:ILE:HD11	1.86	0.57
38:4:219:MET:HG3	38:4:224:LEU:HB2	1.85	0.57
21:X:72:VAL:HG13	21:X:76:ARG:NH1	2.20	0.57
3:C:211:GLU:OE2	11:K:92:HIS:ND1	2.38	0.57
5:E:247:ARG:NH1	5:E:334:ASP:O	2.37	0.57
6:F:78:ARG:NH2	9:I:44:GLY:O	2.38	0.57
20:W:59:LYS:HZ1	35:1:340:LEU:HD12	1.69	0.57
1:A:111:THR:HG22	1:A:113:ARG:H	1.69	0.56
1:A:439:ILE:HG21	1:A:450:PHE:HE2	1.69	0.56
12:L:50:ILE:HG23	42:9:8:LEU:HA	1.87	0.56
48:X:201:CDL:H641	48:g:201:CDL:H241	1.87	0.56
29:f:8:ILE:O	29:f:42:VAL:HA	2.05	0.56
38:4:97:PRO:O	38:4:101:LEU:N	2.38	0.56
1:A:248:ARG:HH21	9:I:157:ARG:HH22	1.51	0.56
10:J:170:ARG:NH2	10:J:178:GLN:OE1	2.38	0.56
29:f:11:HIS:O	29:f:52:PRO:HA	2.06	0.56
38:4:94:LEU:HD11	38:4:337:PHE:HE1	1.71	0.56
38:4:134:TYR:H	38:4:192:THR:HB	1.69	0.56
9:I:44:GLY:H	9:I:46:SER:HB3	1.71	0.56
9:I:110:VAL:O	23:Z:45:ARG:NH2	2.38	0.56
1:A:565:ALA:HA	31:h:137:ARG:HD2	1.87	0.56
36:2:245:LEU:HD13	36:2:296:MET:HG3	1.88	0.56
38:4:24:VAL:O	38:4:27:PHE:N	2.38	0.56
52:O:201:ZMP:O6	15:P:64:ARG:CZ	2.53	0.56
36:2:127:PHE:O	36:2:131:GLU:HG2	2.06	0.56
36:2:456:TYR:HD1	36:2:459:LEU:HD12	1.70	0.56
38:4:395:GLU:OE2	38:4:417:VAL:HG22	2.05	0.56
38:4:429:ASN:HD21	39:5:168:LEU:HD22	1.70	0.56
21:X:130:SER:O	37:3:85:ASN:ND2	2.38	0.56
48:E:403:CDL:H592	46:1:503:3PE:H361	1.87	0.56
18:S:102:ARG:NH2	18:S:123:THR:CG2	2.69	0.56
1:A:432:TRP:HD1	1:A:437:LEU:HB3	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:X:201:CDL:H181	48:X:201:CDL:H541	1.88	0.56
35:1:102:LEU:HD12	35:1:104:LEU:H	1.70	0.56
10:J:191:ALA:CB	18:S:234:LEU:CD2	2.83	0.55
3:C:293:GLY:HA3	3:C:408:GLY:HA2	1.88	0.55
18:S:98:TYR:HB2	18:S:126:LEU:HB3	1.87	0.55
38:4:278:TYR:HB3	38:4:409:ILE:HG12	1.87	0.55
1:A:149:MET:SD	3:C:383:HIS:ND1	2.79	0.55
1:A:351:GLY:HA3	1:A:555:ALA:H	1.71	0.55
1:A:72:ASP:OD2	22:Y:137:ARG:HD3	2.07	0.55
12:L:27:ILE:HG21	40:6:33:ILE:HG13	1.89	0.55
12:L:68:ALA:HB2	37:3:64:LEU:HD22	1.87	0.55
13:M:73:PRO:C	13:M:74:MET:CG	2.78	0.55
41:8:8:LEU:HB2	41:8:13:MET:HE2	1.88	0.55
3:C:429:ALA:HB1	3:C:463:GLU:HB3	1.88	0.55
36:2:156:LEU:HD21	36:2:220:TRP:HB2	1.88	0.55
38:4:294:ARG:HG3	39:5:573:GLY:CA	2.37	0.55
39:5:16:TRP:CD1	39:5:122:MET:HB3	2.41	0.55
7:G:68:VAL:O	7:G:72:HIS:ND1	2.37	0.55
18:S:59:LEU:HA	18:S:62:ARG:HE	1.71	0.55
36:2:256:ASN:O	54:2:503:T7X:O6	2.25	0.55
39:5:354:LEU:HB3	39:5:447:THR:HG22	1.89	0.55
5:E:155:VAL:HG11	5:E:163:TYR:HB2	1.88	0.55
17:R:105:ASN:ND2	17:R:108:GLU:H	2.05	0.55
31:h:33:GLY:HA3	31:h:46:TYR:HB3	1.88	0.55
32:i:83:THR:HG21	39:5:206:LEU:HD22	1.88	0.55
38:4:379:LEU:HD11	38:4:458:ILE:HD11	1.89	0.55
2:B:44:LEU:O	2:B:44:LEU:HG	2.07	0.55
11:K:102:ARG:HA	35:1:39:PRO:HA	1.89	0.55
35:1:222:SER:HA	35:1:225:VAL:HG12	1.89	0.55
2:B:203:MET:HB3	8:H:113:MET:HB2	1.88	0.54
12:L:87:TYR:HD2	39:5:612:SER:HB3	1.72	0.54
18:S:103:VAL:HG22	18:S:104:GLY:O	2.07	0.54
35:1:39:PRO:HB2	35:1:49:GLN:HE21	1.72	0.54
5:E:212:TRP:HE3	5:E:216:ARG:HD2	1.71	0.54
36:2:292:ASN:HA	36:2:295:TYR:HD2	1.73	0.54
1:A:223:THR:HG23	1:A:225:LEU:H	1.72	0.54
21:X:84:ALA:HB1	36:2:4:LEU:HD21	1.89	0.54
38:4:265:LEU:HD12	38:4:266:LEU:HD22	1.88	0.54
5:E:72:LYS:HE2	5:E:243:ALA:HA	1.89	0.54
25:b:57:SER:HB2	36:2:466:VAL:HG21	1.89	0.54
31:h:123:LEU:HD12	31:h:123:LEU:C	2.32	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:97:VAL:HG13	3:C:118:LEU:HB2	1.90	0.54
3:C:374:MET:HE1	9:I:180:PRO:HB3	1.90	0.54
39:5:244:THR:HG21	39:5:347:GLY:HA3	1.89	0.54
1:A:55:ILE:HD11	1:A:67:ARG:HH21	1.73	0.54
3:C:120:HIS:HB2	3:C:465:ASP:HB2	1.90	0.54
38:4:389:THR:HG23	38:4:391:ASN:H	1.72	0.54
5:E:208:ARG:NH1	37:3:33:GLU:OE1	2.40	0.54
46:C:501:3PE:H391	35:1:319:LEU:HD21	1.88	0.54
33:j:35:TYR:OH	33:j:39:ARG:NH2	2.41	0.54
7:G:105:VAL:HG22	7:G:157:THR:HG21	1.90	0.54
21:X:157:ASN:HD21	21:X:161:HIS:HE1	1.55	0.54
35:1:8:ILE:HD11	37:3:7:PHE:HB2	1.89	0.54
36:2:212:ILE:HD12	36:2:241:LYS:HA	1.90	0.54
5:E:25:GLU:OE1	15:P:111:GLN:NE2	2.41	0.54
9:I:145:ILE:HD13	9:I:164:ILE:HG12	1.89	0.54
3:C:224:ARG:HH11	11:K:183:THR:HG23	1.73	0.53
7:G:226:GLU:O	7:G:229:ARG:NH1	2.37	0.53
12:L:80:LEU:HD13	36:2:148:TYR:HD1	1.74	0.53
39:5:446:ILE:HA	39:5:449:TYR:HD2	1.73	0.53
3:C:163:ASN:HD22	23:Z:83:TYR:HA	1.73	0.53
11:K:146:SER:HB2	11:K:173:VAL:HG11	1.91	0.53
23:Z:98:LEU:O	23:Z:107:ARG:NH2	2.41	0.53
38:4:251:LEU:HD23	38:4:310:MET:HG3	1.89	0.53
1:A:228:ASN:ND2	1:A:293:ILE:O	2.32	0.53
52:O:201:ZMP:H14	15:P:63:HIS:O	2.07	0.53
25:b:43:TRP:NE1	36:2:441:TYR:OH	2.35	0.53
36:2:252:ASN:HB2	36:2:255:ILE:HD11	1.89	0.53
36:2:374:ILE:HG22	36:2:376:PRO:HD2	1.90	0.53
39:5:5:ILE:HG23	39:5:62:LEU:HD23	1.89	0.53
2:B:43:ASN:ND2	2:B:135:LYS:O	2.42	0.53
9:I:215:GLU:O	9:I:219:GLN:HG2	2.09	0.53
13:M:73:PRO:O	13:M:74:MET:HG2	2.07	0.53
20:W:28:PHE:HA	50:W:403:PLC:H83	1.90	0.53
7:G:180:ARG:O	7:G:183:TYR:HB3	2.09	0.53
16:Q:102:GLU:HB2	26:c:12:ARG:HH22	1.74	0.53
38:4:58:GLU:HG2	38:4:78:LEU:HD23	1.91	0.53
3:C:149:THR:HG21	3:C:405:ALA:HA	1.89	0.53
6:F:43:ARG:NH2	6:F:82:VAL:O	2.41	0.53
50:n:1101:PLC:H31	39:5:65:PHE:HB3	1.91	0.53
35:1:242:ASN:HB3	35:1:289:LEU:HD21	1.91	0.53
36:2:29:ASN:ND2	36:2:81:SER:OG	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:i:24:SER:HB3	34:n:13:ALA:HB2	1.91	0.53
11:K:139:PRO:HB2	35:1:60:LYS:HE2	1.91	0.53
17:R:20:ARG:HB3	17:R:20:ARG:CZ	2.39	0.53
17:R:20:ARG:HB3	17:R:20:ARG:HH11	1.70	0.53
18:S:102:ARG:HD3	18:S:102:ARG:N	2.23	0.53
1:A:86:ASP:OD1	1:A:113:ARG:NH2	2.42	0.52
5:E:59:PHE:HB2	5:E:127:ASN:HA	1.90	0.52
18:S:103:VAL:HG21	18:S:107:ASP:HB2	1.91	0.52
35:1:284:ILE:HG12	35:1:288:PHE:CE2	2.44	0.52
1:A:145:GLN:HG3	3:C:382:ILE:HG23	1.92	0.52
1:A:313:LEU:HB2	1:A:586:VAL:HG22	1.91	0.52
3:C:141:ARG:HH21	9:I:170:ILE:HB	1.75	0.52
50:W:402:PLC:H2'2	50:W:402:PLC:H1A1	1.91	0.52
31:h:45:PHE:HE2	31:h:77:TRP:HB3	1.74	0.52
35:1:90:VAL:HG12	35:1:166:ILE:HD12	1.92	0.52
38:4:382:ALA:O	38:4:391:ASN:ND2	2.40	0.52
5:E:27:LEU:HD11	5:E:52:THR:HG23	1.90	0.52
13:M:76:TYR:O	13:M:77:ALA:C	2.53	0.52
18:S:109:LEU:HG	38:4:12:TYR:HE2	1.74	0.52
36:2:215:ALA:O	36:2:218:HIS:ND1	2.42	0.52
42:9:20:GLN:O	42:9:24:HIS:ND1	2.42	0.52
7:G:131:TYR:HB2	7:G:134:ARG:HE	1.74	0.52
36:2:144:TYR:HD2	36:2:229:PRO:HG3	1.74	0.52
11:K:100:GLN:HB2	11:K:105:ILE:HB	1.91	0.52
38:4:64:ASN:ND2	38:4:68:LEU:O	2.41	0.52
2:B:370:GLN:NE2	2:B:399:ASP:OD1	2.42	0.52
3:C:410:MET:CE	3:C:427:ILE:HG23	2.39	0.52
1:A:285:HIS:HD2	1:A:288:VAL:H	1.57	0.52
48:g:201:CDL:HB62	46:g:202:3PE:H251	1.91	0.52
46:C:501:3PE:H292	35:1:296:VAL:HG21	1.91	0.52
12:L:6:ILE:HG21	40:6:17:ILE:HG12	1.90	0.52
27:d:63:CYS:HB2	27:d:66:LEU:HB2	1.92	0.52
39:5:296:ILE:O	39:5:431:LYS:NZ	2.43	0.52
1:A:402:ALA:HA	1:A:427:ARG:HH12	1.74	0.52
19:U:40:TYR:OH	20:W:61:GLU:O	2.25	0.52
10:J:147:LEU:HG	10:J:152:LYS:NZ	2.24	0.52
11:K:112:ARG:HG3	35:1:218:GLU:HA	1.92	0.52
16:Q:65:SER:OG	28:e:11:ASN:ND2	2.43	0.52
19:U:51:ASP:OD2	30:g:67:ARG:NH2	2.43	0.52
1:A:534:ILE:HG13	1:A:652:ILE:HD13	1.91	0.51
2:B:160:ILE:HD11	2:B:171:LEU:HD23	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:62:LEU:HD11	36:2:128:VAL:HG22	1.91	0.51
27:d:31:THR:HG23	38:4:480:ASN:HD22	1.75	0.51
36:2:55:MET:HE2	40:6:160:PHE:HB2	1.92	0.51
38:4:123:LEU:HB3	46:4:505:3PE:H2E2	1.91	0.51
9:I:84:PHE:HA	9:I:87:LEU:HD12	1.92	0.51
36:2:140:ILE:HG22	36:2:232:ILE:HG23	1.93	0.51
2:B:79:ILE:HD11	2:B:84:LEU:HD22	1.91	0.51
5:E:155:VAL:HG13	5:E:160:ILE:HB	1.91	0.51
5:E:206:PHE:HD1	5:E:235:PRO:HB2	1.75	0.51
8:H:173:VAL:HG12	8:H:215:ARG:HH22	1.76	0.51
18:S:102:ARG:HH21	18:S:123:THR:CG2	2.23	0.51
36:2:5:ALA:O	36:2:9:LEU:HB2	2.10	0.51
39:5:342:LEU:HD12	39:5:380:ALA:HB1	1.93	0.51
1:A:55:ILE:HD11	1:A:65:VAL:HB	1.91	0.51
3:C:410:MET:CE	3:C:427:ILE:HG21	2.39	0.51
3:C:465:ASP:C	3:C:466:ARG:HG3	2.36	0.51
9:I:170:ILE:HG21	11:K:156:TYR:HD1	1.76	0.51
30:g:47:ARG:HG3	30:g:51:LEU:HD12	1.92	0.51
36:2:233:THR:HA	36:2:236:ILE:HG12	1.91	0.51
5:E:223:LEU:HD21	5:E:273:ILE:HD13	1.93	0.51
39:5:473:GLY:O	39:5:477:LYS:HB2	2.11	0.51
2:B:311:GLY:HA3	2:B:315:ASN:HD22	1.75	0.51
3:C:218:GLU:HB2	3:C:224:ARG:HG2	1.92	0.51
39:5:16:TRP:HH2	46:5:802:3PE:H391	1.75	0.51
39:5:153:LEU:HD22	39:5:246:VAL:HG22	1.93	0.51
38:4:335:HIS:HD2	38:4:339:SER:HB2	1.74	0.51
3:C:269:ARG:NH1	46:C:501:3PE:O32	2.44	0.51
5:E:89:ALA:O	5:E:92:HIS:ND1	2.42	0.51
17:R:20:ARG:HH11	17:R:20:ARG:CB	2.23	0.51
18:S:49:ARG:HG3	18:S:104:GLY:N	2.26	0.51
27:d:71:LEU:HB3	33:j:84:ARG:HH12	1.76	0.51
35:1:110:LEU:HD21	35:1:151:THR:HG23	1.92	0.51
5:E:145:VAL:HG21	5:E:185:LEU:HG	1.92	0.51
50:K:302:PLC:H82	35:1:41:PHE:CE2	2.45	0.51
18:S:56:GLU:OE2	18:S:102:ARG:HG2	2.11	0.51
20:W:26:ARG:NH2	23:Z:30:ILE:O	2.43	0.51
32:i:52:THR:HG22	39:5:62:LEU:HB3	1.92	0.51
35:1:321:PHE:HA	35:1:324:PHE:HD2	1.75	0.51
1:A:165:ARG:NH1	1:A:167:THR:OG1	2.44	0.51
1:A:222:ASN:HB3	1:A:723:LYS:HE3	1.93	0.51
2:B:310:LYS:O	2:B:315:ASN:ND2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:5:64:LEU:HB2	39:5:77:TYR:HB2	1.92	0.51
1:A:395:TYR:OH	1:A:533:ASP:OD1	2.27	0.50
20:W:66:ARG:NH2	40:6:141:ILE:O	2.39	0.50
7:G:167:SER:HB3	7:G:190:PHE:HB3	1.93	0.50
19:U:50:ASN:HB3	20:W:71:PRO:HG2	1.93	0.50
21:X:80:MET:HB3	48:g:201:CDL:H172	1.91	0.50
46:b:201:3PE:H232	46:4:502:3PE:H322	1.94	0.50
1:A:595:LYS:NZ	1:A:622:ASP:OD2	2.40	0.50
2:B:322:GLY:N	2:B:355:ALA:O	2.44	0.50
3:C:129:TYR:HE2	7:G:216:LEU:HB2	1.76	0.50
7:G:68:VAL:HG22	7:G:94:ASP:H	1.75	0.50
38:4:214:LEU:HB3	38:4:262:LEU:HD11	1.93	0.50
38:4:384:ILE:HG12	38:4:421:ALA:HA	1.92	0.50
10:J:147:LEU:HD13	10:J:164:TRP:CE3	2.46	0.50
26:c:16:ARG:HG2	39:5:441:PRO:HG2	1.93	0.50
31:h:29:ASP:OD1	31:h:30:THR:N	2.44	0.50
33:j:64:PRO:HG3	38:4:283:LEU:HD11	1.94	0.50
38:4:207:GLN:HB3	38:4:269:ALA:HB2	1.92	0.50
1:A:390:THR:O	1:A:394:ASN:ND2	2.45	0.50
3:C:257:ARG:NH1	23:Z:35:SER:O	2.43	0.50
11:K:144:VAL:HG13	11:K:173:VAL:HA	1.92	0.50
20:W:59:LYS:HG2	35:1:339:THR:HG21	1.94	0.50
25:b:23:LYS:HB3	36:2:359:TYR:HD2	1.77	0.50
3:C:428:ARG:HD2	7:G:125:ASP:HB2	1.93	0.50
7:G:126:ILE:HG22	7:G:142:TYR:HA	1.94	0.50
35:1:222:SER:N	37:3:22:ASN:ND2	2.47	0.50
2:B:164:PHE:HB3	2:B:167:GLU:HB2	1.92	0.50
8:H:73:PRO:O	8:H:76:ASP:HB3	2.11	0.50
35:1:247:LEU:HD23	35:1:285:LYS:HD2	1.94	0.50
3:C:269:ARG:HH21	9:I:83:MET:HG3	1.75	0.50
9:I:127:GLU:OE2	9:I:152:ARG:NH2	2.43	0.50
19:U:70:LYS:HG3	19:U:73:ARG:HH12	1.77	0.50
19:U:83:ILE:HA	19:U:86:ILE:HG22	1.94	0.50
38:4:464:ILE:HD11	48:4:503:CDL:H632	1.93	0.50
13:M:35:TYR:HD1	13:M:74:MET:HE1	1.76	0.49
15:P:66:VAL:O	15:P:72:GLN:NE2	2.45	0.49
35:1:157:ILE:HG21	35:1:245:LEU:HB2	1.94	0.49
39:5:208:ASN:HB3	39:5:211:LEU:HD13	1.94	0.49
3:C:54:ARG:HG2	3:C:55:THR:HG23	1.92	0.49
9:I:170:ILE:HG21	11:K:156:TYR:CD1	2.47	0.49
10:J:56:ASN:HA	40:6:91:ILE:HG23	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:191:ALA:HB2	18:S:234:LEU:HD22	1.95	0.49
20:W:52:ILE:HG12	20:W:55:ARG:HH22	1.76	0.49
35:1:182:LEU:HD23	35:1:185:LEU:HD22	1.94	0.49
38:4:386:THR:HG22	39:5:145:PHE:HE1	1.76	0.49
1:A:41:ILE:HG12	1:A:107:VAL:HB	1.95	0.49
3:C:434:HIS:HB3	3:C:457:MET:HB2	1.92	0.49
8:H:51:ASN:OD1	8:H:54:ARG:NH2	2.46	0.49
11:K:139:PRO:HB3	35:1:61:GLU:HG2	1.94	0.49
38:4:388:LEU:HD12	39:5:145:PHE:HE2	1.77	0.49
7:G:241:ALA:CB	22:Y:90:ARG:HH11	2.25	0.49
36:2:10:ILE:HG22	36:2:105:ILE:HG12	1.94	0.49
38:4:145:LEU:HD21	38:4:171:THR:HG21	1.93	0.49
38:4:235:HIS:NE2	38:4:247:ALA:HB2	2.27	0.49
1:A:699:MET:HB3	1:A:705:ARG:HG2	1.94	0.49
18:S:63:LEU:HA	18:S:66:LEU:HD12	1.94	0.49
30:g:60:GLN:HB3	34:n:111:ILE:HG13	1.95	0.49
36:2:110:ASN:ND2	36:2:235:TYR:HE2	2.11	0.49
36:2:316:TYR:O	36:2:320:HIS:HB2	2.11	0.49
38:4:294:ARG:NH1	39:5:573:GLY:HA3	2.26	0.49
1:A:389:ILE:HG22	29:f:43:LEU:CG	2.42	0.49
1:A:490:ASP:OD2	1:A:524:ARG:NH1	2.46	0.49
5:E:203:ALA:HB3	5:E:236:VAL:HG23	1.93	0.49
9:I:187:THR:HG22	9:I:218:LEU:HD21	1.94	0.49
36:2:238:LEU:HD12	36:2:320:HIS:ND1	2.28	0.49
38:4:146:PRO:HG2	46:4:502:3PE:H2F1	1.94	0.49
39:5:225:ALA:HA	39:5:232:LEU:HD11	1.94	0.49
3:C:179:GLU:HG3	3:C:346:ILE:HG21	1.95	0.49
10:J:175:THR:HG22	10:J:185:ILE:HD11	1.93	0.49
48:X:201:CDL:H241	48:g:201:CDL:H801	1.93	0.49
25:b:45:GLY:HA2	25:b:48:LEU:HD23	1.94	0.49
1:A:277:VAL:HG21	1:A:593:THR:HG21	1.94	0.49
2:B:440:LEU:HD12	2:B:444:PHE:HB2	1.95	0.49
3:C:97:VAL:HG23	11:K:83:LEU:HB2	1.93	0.49
3:C:118:LEU:HB3	11:K:127:MET:HE3	1.95	0.49
7:G:72:HIS:HB3	7:G:266:PHE:HD2	1.78	0.49
10:J:168:HIS:HB3	27:d:17:TYR:HD2	1.78	0.49
1:A:375:THR:HA	1:A:538:PRO:HD3	1.95	0.48
27:d:20:HIS:HB2	34:n:70:VAL:HG11	1.94	0.48
35:1:106:ILE:HD11	35:1:169:ILE:HD11	1.95	0.48
36:2:353:LEU:HD11	36:2:360:LEU:HD23	1.95	0.48
38:4:98:LEU:O	38:4:102:GLY:N	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:216:GLU:OE1	22:Y:161:LYS:NZ	2.47	0.48
3:C:82:ALA:HB2	3:C:110:ILE:HD11	1.95	0.48
3:C:336:ARG:NH2	3:C:458:ASP:OD2	2.45	0.48
18:S:227:ILE:HG12	27:d:44:VAL:HG22	1.95	0.48
19:U:136:ARG:HH22	30:g:53:PRO:HG2	1.78	0.48
36:2:264:ALA:HB1	36:2:298:LEU:HD12	1.95	0.48
38:4:43:TYR:HE1	38:4:474:LEU:HD21	1.78	0.48
1:A:128:ASN:ND2	2:B:389:GLU:OE1	2.46	0.48
7:G:202:ASP:OD1	15:P:95:GLN:NE2	2.46	0.48
35:1:89:VAL:HB	35:1:90:VAL:HG23	1.95	0.48
37:3:58:LEU:HD21	37:3:110:ALA:HB1	1.95	0.48
12:L:69:ILE:HD11	40:6:172:GLY:HA2	1.96	0.48
30:g:44:THR:HG22	35:1:333:ILE:HA	1.95	0.48
35:1:153:ILE:HD11	35:1:188:ILE:HD12	1.95	0.48
1:A:207:ARG:NH2	8:H:112:THR:OG1	2.46	0.48
5:E:309:TYR:OH	5:E:317:GLN:NE2	2.46	0.48
13:M:49:ALA:HA	31:h:124:LYS:CD	2.44	0.48
14:O:29:ARG:C	14:O:29:ARG:CD	2.87	0.48
21:X:111:ASP:OD1	21:X:111:ASP:O	2.32	0.48
23:Z:171:ILE:HG12	23:Z:180:THR:HB	1.95	0.48
29:f:56:ALA:HB2	29:f:83:LEU:CD2	2.44	0.48
35:1:188:ILE:HA	35:1:191:ILE:HG12	1.95	0.48
38:4:379:LEU:HD21	38:4:454:MET:HE1	1.95	0.48
6:F:127:GLU:HG3	6:F:128:GLU:HG3	1.95	0.48
13:M:22:ILE:O	13:M:58:LYS:NZ	2.41	0.48
16:Q:96:VAL:HA	16:Q:99:ILE:HG22	1.94	0.48
18:S:52:ASN:O	18:S:56:GLU:HG2	2.13	0.48
21:X:129:SER:HB3	21:X:160:ASN:HB2	1.94	0.48
27:d:23:VAL:HG11	38:4:199:LEU:HD21	1.95	0.48
35:1:185:LEU:HD12	35:1:188:ILE:HD11	1.95	0.48
38:4:101:LEU:O	38:4:449:ARG:NH1	2.40	0.48
13:M:97:CYS:O	13:M:112:LYS:HA	2.13	0.48
37:3:68:LEU:O	37:3:72:THR:OG1	2.27	0.48
2:B:127:CYS:SG	8:H:172:CYS:N	2.85	0.48
3:C:268:ASN:HB3	3:C:271:TRP:HB3	1.95	0.48
24:a:36:MET:SD	24:a:36:MET:N	2.87	0.48
35:1:74:VAL:O	35:1:78:LEU:HD13	2.14	0.48
36:2:9:LEU:HD21	36:2:104:ILE:HG23	1.95	0.48
2:B:85:ARG:NE	2:B:91:GLY:O	2.40	0.48
12:L:62:LEU:HD13	36:2:131:GLU:HG3	1.94	0.48
17:R:37:ARG:HH21	26:c:9:TRP:HB2	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:X:73:LYS:HG3	21:X:74:PHE:CD1	2.49	0.48
48:g:201:CDL:H542	48:g:201:CDL:H741	1.96	0.48
35:1:137:ILE:HG13	40:6:77:LEU:HD23	1.94	0.48
36:2:354:ILE:HD12	36:2:421:ILE:HG22	1.95	0.48
3:C:377:ASP:HB3	3:C:380:ALA:HB3	1.96	0.48
24:a:76:LEU:O	24:a:84:ARG:NH1	2.45	0.48
25:b:6:SER:HA	38:4:66:PHE:HD2	1.78	0.48
37:3:103:VAL:HA	37:3:106:ILE:HG22	1.95	0.48
38:4:103:ASN:HD21	38:4:240:LEU:HB3	1.79	0.48
38:4:223:PRO:HB3	38:4:228:HIS:HA	1.95	0.48
16:Q:61:ALA:O	28:e:11:ASN:ND2	2.46	0.47
16:Q:66:PHE:HD2	16:Q:69:VAL:HG13	1.79	0.47
21:X:138:ILE:HG21	40:6:156:THR:HB	1.96	0.47
40:6:77:LEU:HD12	40:6:78:LEU:HD12	1.95	0.47
2:B:175:ILE:HD12	2:B:199:ILE:HD11	1.96	0.47
6:F:134:GLN:HG3	6:F:135:TRP:CD1	2.49	0.47
10:J:39:ALA:HB2	46:J:203:3PE:H392	1.95	0.47
35:1:125:TRP:CG	40:6:30:MET:SD	3.07	0.47
35:1:130:LYS:HE3	37:3:49:ARG:NH1	2.29	0.47
39:5:28:TYR:HA	39:5:31:VAL:HG12	1.96	0.47
1:A:41:ILE:O	1:A:44:HIS:HB2	2.14	0.47
2:B:475:LYS:HB2	13:M:88:ARG:HG2	1.95	0.47
50:W:402:PLC:H1'1	50:W:402:PLC:H2	1.68	0.47
48:j:102:CDL:H511	39:5:595:LEU:HD12	1.97	0.47
40:6:158:ASN:HB3	40:6:161:ILE:HD12	1.96	0.47
3:C:257:ARG:HH22	23:Z:35:SER:HB2	1.78	0.47
5:E:124:ILE:HG22	5:E:162:ARG:HB2	1.96	0.47
7:G:201:THR:HG21	7:G:205:PHE:CG	2.50	0.47
27:d:46:LYS:HE3	27:d:50:LYS:HE3	1.95	0.47
2:B:133:MET:HE3	2:B:171:LEU:HD22	1.96	0.47
18:S:102:ARG:HH21	18:S:123:THR:HG22	1.79	0.47
21:X:22:ILE:HG23	21:X:111:ASP:OD2	2.15	0.47
34:n:92:ASP:HB2	34:n:95:HIS:HD2	1.80	0.47
35:1:39:PRO:CB	35:1:49:GLN:HE21	2.26	0.47
36:2:46:PHE:HB3	36:2:63:SER:HB2	1.95	0.47
36:2:460:ILE:HG21	55:2:502:CPL:H142	1.96	0.47
45:B:502:FMN:O4'	45:B:502:FMN:O2'	2.25	0.47
5:E:29:GLN:HG2	15:P:120:LEU:HB3	1.97	0.47
17:R:106:LEU:HD12	18:S:135:ARG:HG3	1.97	0.47
31:h:39:ASP:OD1	31:h:40:ILE:N	2.47	0.47
1:A:81:ARG:HA	1:A:81:ARG:HD3	1.66	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:664:PRO:O	29:f:14:GLN:NE2	2.46	0.47
8:H:132:CYS:HB3	8:H:137:SER:HB3	1.96	0.47
8:H:156:THR:HG22	8:H:158:ASP:H	1.78	0.47
9:I:168:LYS:HA	11:K:155:GLY:HA2	1.95	0.47
38:4:276:MET:HA	38:4:279:ILE:HD12	1.97	0.47
38:4:335:HIS:HA	38:4:338:VAL:HG12	1.97	0.47
5:E:43:LYS:HD3	22:Y:91:TRP:CD1	2.50	0.47
48:E:403:CDL:H552	35:1:64:LEU:HD11	1.96	0.47
8:H:108:ALA:O	8:H:116:ARG:NH2	2.48	0.47
12:L:69:ILE:HD12	36:2:139:LEU:HD11	1.97	0.47
26:c:23:ARG:HA	26:c:26:ARG:HE	1.79	0.47
30:g:26:LEU:HD22	46:g:202:3PE:H332	1.96	0.47
33:j:49:THR:HB	49:j:101:LMN:H5	1.97	0.47
39:5:327:LEU:HD23	39:5:481:LEU:HD21	1.97	0.47
5:E:245:LEU:HA	5:E:248:ILE:HD12	1.97	0.47
7:G:144:PHE:HE1	7:G:172:TYR:HE2	1.61	0.47
15:P:6:THR:HG21	15:P:90:TRP:HH2	1.80	0.47
16:Q:62:LEU:HD11	26:c:12:ARG:NH1	2.30	0.47
35:1:22:LEU:HD23	35:1:232:TYR:HB3	1.97	0.47
1:A:491:ARG:HG2	1:A:493:ASP:H	1.80	0.47
2:B:101:MET:O	2:B:113:ARG:NH1	2.48	0.47
3:C:435:LEU:HD23	3:C:464:VAL:HG11	1.97	0.47
7:G:224:TRP:CZ3	11:K:132:ARG:HG2	2.50	0.47
29:f:21:PRO:HG3	29:f:71:SER:HA	1.97	0.47
33:j:43:GLN:HG3	39:5:590:VAL:HG21	1.97	0.47
36:2:86:ASN:O	36:2:436:SER:OG	2.26	0.47
1:A:141:GLU:OE2	1:A:279:ARG:NH2	2.36	0.46
8:H:72:MET:O	8:H:114:TYR:OH	2.33	0.46
15:P:47:PHE:HE1	15:P:52:ILE:HG13	1.80	0.46
20:W:93:LYS:HA	20:W:103:VAL:HG21	1.97	0.46
1:A:696:ASN:HD21	1:A:699:MET:HB2	1.80	0.46
2:B:207:VAL:HG11	2:B:381:CYS:HB3	1.96	0.46
3:C:87:PHE:HB2	3:C:100:LEU:HB3	1.97	0.46
3:C:121:ARG:HD3	11:K:122:THR:HG21	1.96	0.46
3:C:356:ALA:HB2	20:W:8:LEU:HD11	1.97	0.46
9:I:80:LEU:HD13	35:1:187:LEU:HD21	1.98	0.46
53:1:501:UQ9:H10	53:1:501:UQ9:H7A	1.71	0.46
36:2:215:ALA:HA	36:2:218:HIS:HB3	1.96	0.46
38:4:326:TYR:OH	38:4:468:PRO:O	2.32	0.46
39:5:183:LEU:O	39:5:187:VAL:HG23	2.15	0.46
39:5:630:LEU:HD11	40:6:103:VAL:HG21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:ARG:HD3	23:Z:69:ILE:O	2.16	0.46
2:B:230:PRO:HG3	22:Y:144:TYR:HD2	1.81	0.46
7:G:262:ARG:HH11	7:G:267:LYS:HB3	1.79	0.46
10:J:161:GLN:NE2	10:J:165:GLU:O	2.41	0.46
13:M:49:ALA:HA	31:h:124:LYS:HD3	1.98	0.46
52:O:201:ZMP:H14A	15:P:72:GLN:HG2	1.97	0.46
55:2:502:CPL:H182	55:2:502:CPL:H211	1.78	0.46
2:B:97:LYS:NZ	2:B:244:VAL:O	2.39	0.46
3:C:361:VAL:HG11	3:C:366:ILE:HD11	1.97	0.46
11:K:76:PHE:HD2	11:K:105:ILE:HG12	1.79	0.46
35:1:10:ILE:HA	35:1:13:VAL:HG12	1.97	0.46
36:2:26:ARG:HG2	36:2:85:TYR:HE1	1.81	0.46
1:A:268:ILE:HG22	1:A:293:ILE:HD11	1.97	0.46
13:M:35:TYR:HE1	13:M:74:MET:HE1	1.78	0.46
14:O:65:ASP:H	14:O:68:ASP:HB2	1.79	0.46
39:5:66:ASN:ND2	39:5:69:ASN:HB2	2.31	0.46
3:C:302:PRO:HB3	23:Z:181:PHE:CD2	2.51	0.46
9:I:103:TYR:HD2	11:K:192:PHE:HE2	1.64	0.46
21:X:16:TYR:HE1	34:n:99:PRO:HG2	1.80	0.46
21:X:152:ILE:HD11	36:2:119:HIS:CD2	2.51	0.46
24:a:90:ASN:OD1	39:5:558:GLN:NE2	2.37	0.46
25:b:29:ALA:O	25:b:36:TYR:OH	2.29	0.46
39:5:144:GLU:OE1	39:5:175:ARG:NH2	2.49	0.46
42:9:7:SER:OG	42:9:8:LEU:N	2.49	0.46
21:X:167:GLU:HG2	21:X:168:GLN:HG3	1.98	0.46
29:f:43:LEU:HD23	29:f:45:ARG:NH1	2.31	0.46
36:2:368:VAL:HA	36:2:371:PHE:HD2	1.80	0.46
38:4:114:TYR:HB2	38:4:155:TYR:HE2	1.80	0.46
1:A:168:GLU:HB2	13:M:116:ASN:HD22	1.78	0.46
5:E:113:GLU:O	5:E:117:GLU:HB2	2.15	0.46
9:I:79:LEU:HB3	50:W:401:PLC:H3'2	1.97	0.46
13:M:45:THR:HB	13:M:50:GLN:HB3	1.97	0.46
21:X:76:ARG:HD2	30:g:9:TRP:CZ3	2.51	0.46
19:U:28:VAL:HG12	19:U:30:ALA:H	1.81	0.46
29:f:56:ALA:CB	29:f:83:LEU:HD21	2.34	0.46
35:1:194:VAL:HG13	35:1:199:ARG:HB2	1.97	0.46
37:3:49:ARG:HA	37:3:49:ARG:HD3	1.48	0.46
37:3:69:GLU:HG2	37:3:98:LEU:HD11	1.97	0.46
39:5:173:MET:HB3	39:5:232:LEU:HD13	1.98	0.46
1:A:709:THR:O	1:A:713:SER:HB2	2.16	0.46
4:D:43:ASP:OD1	4:D:44:GLN:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:74:LEU:HD23	8:H:77:ILE:HD12	1.97	0.46
15:P:32:PHE:HB3	15:P:56:ILE:HD13	1.98	0.46
16:Q:58:ARG:NH2	16:Q:102:GLU:O	2.49	0.46
24:a:29:PHE:HD2	24:a:73:ASN:HD22	1.63	0.46
35:1:228:PHE:CZ	53:1:501:UQ9:C13	2.99	0.46
36:2:85:TYR:HB2	36:2:439:LEU:HD12	1.97	0.46
39:5:412:TYR:O	39:5:415:TYR:HB3	2.16	0.46
3:C:220:VAL:O	9:I:113:ARG:NH1	2.48	0.45
5:E:83:PRO:HA	5:E:105:LEU:O	2.16	0.45
5:E:109:LEU:HA	5:E:115:ILE:HD11	1.97	0.45
27:d:84:GLY:HA3	38:4:486:ILE:HA	1.96	0.45
39:5:215:ILE:HG22	39:5:216:MET:HE2	1.98	0.45
40:6:32:SER:HA	40:6:35:TYR:HD2	1.80	0.45
3:C:357:GLY:HA2	7:G:53:VAL:HG11	1.98	0.45
10:J:136:GLY:HA2	49:J:202:LMN:H3	1.97	0.45
11:K:140:GLU:HG2	37:3:29:LYS:HD2	1.98	0.45
22:Y:90:ARG:HH12	22:Y:106:GLN:CD	2.24	0.45
25:b:49:VAL:HG21	55:2:502:CPL:H483	1.98	0.45
5:E:229:PHE:HB3	5:E:269:GLN:HB2	1.99	0.45
50:K:302:PLC:C8	35:1:41:PHE:CE2	2.99	0.45
18:S:103:VAL:CG2	18:S:107:ASP:HB2	2.45	0.45
18:S:240:LYS:HB2	27:d:13:ASP:OD2	2.16	0.45
50:n:1101:PLC:H9'2	38:4:463:ILE:HG12	1.99	0.45
35:1:77:PRO:HB3	35:1:226:PHE:HB2	1.98	0.45
42:9:50:HIS:ND1	42:9:53:GLU:OE1	2.49	0.45
1:A:627:ARG:NE	1:A:639:TYR:O	2.40	0.45
3:C:126:LEU:HD23	7:G:216:LEU:HD11	1.98	0.45
3:C:175:THR:OG1	3:C:312:ASP:O	2.33	0.45
3:C:428:ARG:NE	7:G:124:ILE:O	2.42	0.45
7:G:262:ARG:HH11	7:G:267:LYS:HB2	1.81	0.45
9:I:171:TYR:N	9:I:171:TYR:CD1	2.84	0.45
10:J:49:SER:HB2	39:5:619:MET:HE1	1.98	0.45
12:L:76:SER:HB2	40:6:179:ILE:HG21	1.98	0.45
21:X:76:ARG:HD2	30:g:9:TRP:CE3	2.51	0.45
28:e:47:PRO:HB2	28:e:53:HIS:HE1	1.81	0.45
30:g:39:ALA:HA	30:g:43:LEU:HD23	1.98	0.45
36:2:233:THR:HG21	36:2:282:LYS:NZ	2.31	0.45
1:A:269:ARG:HB3	1:A:281:ILE:HG23	1.98	0.45
2:B:341:PHE:HE1	2:B:351:LEU:HD12	1.81	0.45
3:C:97:VAL:HG22	11:K:127:MET:HE1	1.97	0.45
8:H:90:MET:HE3	8:H:108:ALA:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:1:219:TYR:HE2	35:1:227:PHE:HE2	1.65	0.45
38:4:127:LEU:HD12	46:4:505:3PE:H2I2	1.97	0.45
39:5:28:TYR:O	39:5:32:THR:HG23	2.17	0.45
2:B:369:ILE:HA	2:B:372:PHE:HD2	1.82	0.45
5:E:306:TRP:HZ2	48:E:403:CDL:H142	1.82	0.45
46:b:201:3PE:H352	46:4:501:3PE:H251	1.98	0.45
35:1:82:ILE:HG22	37:3:11:ILE:HG22	1.98	0.45
39:5:271:GLU:HB3	39:5:493:LEU:HG	1.98	0.45
12:L:12:PHE:HA	12:L:32:MET:HE2	1.99	0.45
15:P:55:LYS:HE2	15:P:100:PHE:HE1	1.80	0.45
18:S:172:TYR:CD1	38:4:36:LEU:HD11	2.52	0.45
31:h:113:THR:HG22	31:h:115:GLY:H	1.81	0.45
16:Q:105:LEU:HA	17:R:84:PHE:HE2	1.81	0.45
18:S:162:GLU:OE1	18:S:164:TRP:NE1	2.38	0.45
18:S:176:LEU:HG	48:4:503:CDL:H582	1.99	0.45
50:W:402:PLC:H7'1	50:W:402:PLC:H8A1	1.98	0.45
31:h:69:ASP:HB3	31:h:71:SER:H	1.82	0.45
33:j:89:VAL:HG11	39:5:211:LEU:HD11	1.99	0.45
39:5:631:LEU:O	39:5:635:MET:HB2	2.17	0.45
48:E:403:CDL:H731	37:3:24:LEU:HD21	1.99	0.45
8:H:174:ASN:HB3	8:H:186:GLU:HB3	1.98	0.45
15:P:42:LEU:HD21	15:P:89:PHE:HB2	1.99	0.45
17:R:45:HIS:O	17:R:49:GLN:HG2	2.17	0.45
50:W:403:PLC:H4A2	46:W:404:3PE:H382	1.99	0.45
32:i:52:THR:HG21	39:5:3:ASN:HD21	1.80	0.45
36:2:311:TYR:HD1	55:2:502:CPL:H141	1.81	0.45
5:E:120:ARG:NH1	13:M:65:GLU:OE2	2.49	0.45
8:H:130:THR:HA	8:H:133:GLN:HB3	1.98	0.45
10:J:48:ASN:HD21	10:J:60:THR:HA	1.81	0.45
18:S:102:ARG:HH12	18:S:126:LEU:CD1	2.26	0.45
29:f:66:ILE:HG22	29:f:83:LEU:HD13	1.99	0.45
31:h:45:PHE:CE2	31:h:77:TRP:HB3	2.52	0.45
41:8:37:ARG:HB3	41:8:42:TYR:CE1	2.52	0.45
2:B:130:ARG:NE	2:B:167:GLU:OE2	2.51	0.44
4:D:62:ARG:NH1	19:U:102:GLU:O	2.50	0.44
4:D:83:GLU:OE1	19:U:3:ARG:NH1	2.43	0.44
7:G:72:HIS:HB3	7:G:266:PHE:CD2	2.51	0.44
12:L:7:ILE:HD11	40:6:16:ALA:HB1	1.99	0.44
12:L:15:PHE:HE2	36:2:163:ILE:HD11	1.82	0.44
14:O:29:ARG:N	14:O:30:PRO:CD	2.80	0.44
38:4:418:LEU:HD12	39:5:176:PHE:HA	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:5:79:PHE:HD1	39:5:132:THR:HG23	1.82	0.44
1:A:269:ARG:O	1:A:280:VAL:HA	2.17	0.44
3:C:121:ARG:HH21	11:K:122:THR:HG21	1.81	0.44
18:S:49:ARG:HG3	18:S:104:GLY:CA	2.48	0.44
29:f:41:LYS:NZ	29:f:41:LYS:CB	2.74	0.44
35:1:199:ARG:HA	35:1:199:ARG:HD2	1.79	0.44
35:1:318:PRO:HG3	37:3:102:PHE:HE2	1.80	0.44
37:3:94:PHE:CD1	40:6:166:ALA:HB2	2.52	0.44
1:A:723:LYS:HE2	1:A:723:LYS:HB3	1.68	0.44
3:C:225:LEU:HD23	11:K:181:PRO:HB3	2.00	0.44
12:L:32:MET:O	12:L:36:ILE:HD12	2.17	0.44
38:4:15:ASN:HA	38:4:18:LEU:HD12	1.99	0.44
48:4:503:CDL:H311	48:4:503:CDL:HA62	1.87	0.44
1:A:131:LEU:HD12	13:M:112:LYS:O	2.18	0.44
1:A:393:SER:HA	1:A:398:ASN:HD21	1.81	0.44
1:A:577:ASP:OD2	1:A:705:ARG:NH2	2.42	0.44
3:C:183:VAL:O	3:C:187:LEU:HB2	2.16	0.44
3:C:371:ARG:HA	3:C:374:MET:HG3	1.98	0.44
5:E:205:MET:HB3	5:E:238:VAL:HG22	2.00	0.44
21:X:111:ASP:OD1	21:X:115:MET:HG2	2.17	0.44
35:1:323:ILE:HA	35:1:326:ILE:HG22	1.98	0.44
37:3:76:TYR:CG	37:3:91:VAL:HG21	2.53	0.44
1:A:248:ARG:HD3	1:A:249:PRO:HD2	2.00	0.44
3:C:341:ARG:HD2	20:W:19:TRP:O	2.17	0.44
5:E:224:VAL:HG13	5:E:294:TYR:HE1	1.81	0.44
9:I:103:TYR:O	9:I:103:TYR:CD1	2.71	0.44
10:J:59:THR:HA	10:J:62:SER:HB3	1.99	0.44
11:K:93:VAL:HG12	11:K:100:GLN:HB3	1.99	0.44
52:Q:201:ZMP:S1	17:R:50:ASN:ND2	2.91	0.44
21:X:14:TYR:CE2	34:n:99:PRO:HB3	2.53	0.44
37:3:6:ILE:O	37:3:10:LEU:CB	2.64	0.44
39:5:392:GLY:O	39:5:396:LYS:HB3	2.17	0.44
2:B:159:TYR:CG	2:B:214:LEU:HD11	2.53	0.44
9:I:76:LYS:HE2	50:W:401:PLC:O2P	2.18	0.44
11:K:124:THR:HA	11:K:163:VAL:HA	1.98	0.44
18:S:234:LEU:HD22	27:d:37:ARG:NH2	2.31	0.44
35:1:191:ILE:HD12	35:1:311:PHE:HZ	1.83	0.44
36:2:377:LEU:HD11	46:4:502:3PE:H2F2	2.00	0.44
38:4:229:VAL:HG13	39:5:585:TYR:HE1	1.83	0.44
39:5:339:LYS:HZ2	39:5:342:LEU:HD22	1.81	0.44
1:A:145:GLN:HE22	3:C:385:PHE:HD2	1.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:432:TRP:HB2	1:A:437:LEU:HD23	1.99	0.44
2:B:203:MET:HA	8:H:113:MET:SD	2.58	0.44
17:R:90:TYR:O	39:5:160:ARG:NH1	2.49	0.44
18:S:102:ARG:HD3	18:S:102:ARG:H	1.81	0.44
31:h:54:ILE:HD11	31:h:57:ARG:HH21	1.83	0.44
38:4:258:ILE:HG23	38:4:317:VAL:HG11	2.00	0.44
39:5:281:LEU:HB2	39:5:321:GLY:HA3	2.00	0.44
2:B:387:CYS:HB3	43:B:501:SF4:S4	2.57	0.44
3:C:129:TYR:HD2	7:G:216:LEU:HD22	1.83	0.44
3:C:344:LEU:HD22	20:W:19:TRP:HB3	2.00	0.44
5:E:149:ARG:HE	5:E:189:VAL:HG11	1.82	0.44
5:E:162:ARG:NH1	5:E:251:ASP:O	2.51	0.44
9:I:103:TYR:OH	9:I:191:GLU:HG2	2.17	0.44
10:J:133:GLY:HA2	10:J:137:ALA:HB2	1.99	0.44
17:R:76:PRO:HB2	39:5:551:ASN:ND2	2.33	0.44
23:Z:100:LEU:HA	23:Z:108:ILE:HD11	1.99	0.44
2:B:386:PRO:HG2	2:B:425:THR:HG22	2.00	0.44
3:C:254:PHE:HD2	3:C:344:LEU:HD12	1.82	0.44
9:I:190:VAL:HB	11:K:186:ALA:HB2	2.00	0.44
19:U:42:ILE:HD11	20:W:69:LEU:HD23	2.00	0.44
22:Y:44:ILE:HG13	22:Y:45:VAL:HG13	1.98	0.44
23:Z:110:ASP:O	23:Z:114:GLY:N	2.51	0.44
31:h:59:ARG:HB2	31:h:83:TYR:HE1	1.83	0.44
39:5:99:VAL:HG11	39:5:249:LEU:HG	1.99	0.44
39:5:312:GLN:HB3	39:5:331:HIS:HE1	1.82	0.44
7:G:130:ASP:HB3	7:G:138:PHE:CE1	2.53	0.43
46:J:203:3PE:H2A1	36:2:266:LEU:HG	2.01	0.43
18:S:176:LEU:HD23	48:4:503:CDL:H522	2.00	0.43
29:f:41:LYS:HB2	29:f:41:LYS:HZ3	1.79	0.43
38:4:103:ASN:O	38:4:115:TYR:OH	2.21	0.43
16:Q:98:ALA:HB1	26:c:12:ARG:NH1	2.33	0.43
20:W:93:LYS:NZ	20:W:104:ASP:OD1	2.48	0.43
21:X:153:PHE:HB2	48:X:201:CDL:H431	1.99	0.43
36:2:70:MET:HG2	55:2:502:CPL:H411	2.00	0.43
36:2:132:LEU:HD13	40:6:168:VAL:HG22	2.00	0.43
3:C:378:MET:HE3	3:C:382:ILE:HG13	2.00	0.43
19:U:45:LYS:HD3	19:U:82:VAL:HG22	2.00	0.43
21:X:142:ASN:HA	36:2:55:MET:HA	2.01	0.43
34:n:20:TYR:O	34:n:24:TRP:HD1	2.01	0.43
53:1:501:UQ9:H12	53:1:501:UQ9:H15	1.89	0.43
36:2:352:GLY:HA3	36:2:424:LYS:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:4:259:LEU:HD11	38:4:329:ILE:HD11	2.01	0.43
39:5:554:LEU:C	39:5:556:SER:H	2.26	0.43
40:6:122:LEU:O	40:6:125:ALA:HB3	2.18	0.43
5:E:373:ILE:HG21	12:L:79:ARG:HH22	1.79	0.43
7:G:120:TYR:HB3	7:G:144:PHE:HB3	1.99	0.43
17:R:20:ARG:NH1	17:R:20:ARG:CB	2.73	0.43
17:R:82:PRO:HA	17:R:87:GLY:HA3	2.01	0.43
18:S:218:ARG:O	18:S:222:ILE:HG13	2.17	0.43
23:Z:120:ASN:O	23:Z:125:GLY:N	2.47	0.43
35:1:76:SER:HA	35:1:79:ILE:HG12	1.99	0.43
35:1:228:PHE:HZ	53:1:501:UQ9:H10A	1.83	0.43
1:A:385:PRO:O	1:A:387:HIS:ND1	2.52	0.43
1:A:432:TRP:CH2	22:Y:156:LYS:HB2	2.54	0.43
5:E:64:PHE:CE2	5:E:238:VAL:HG21	2.50	0.43
46:J:203:3PE:H2C2	36:2:266:LEU:HD23	2.00	0.43
25:b:18:LYS:HE3	25:b:35:GLY:HA3	2.00	0.43
27:d:69:GLN:HG2	27:d:73:MET:HE2	1.98	0.43
53:1:501:UQ9:H22	53:1:501:UQ9:H25	1.76	0.43
36:2:233:THR:HG21	36:2:282:LYS:HZ3	1.83	0.43
48:4:503:CDL:H422	48:4:503:CDL:H452	1.80	0.43
39:5:429:SER:HA	39:5:432:ILE:HG12	1.99	0.43
41:8:43:MET:HA	41:8:44:PRO:HD3	1.87	0.43
1:A:84:LEU:HB3	1:A:93:PRO:HB2	2.01	0.43
3:C:136:LEU:HD13	3:C:232:PRO:HD3	1.99	0.43
3:C:398:GLU:HG2	3:C:415:VAL:HG22	1.99	0.43
5:E:55:THR:O	5:E:123:ASP:N	2.49	0.43
15:P:6:THR:HG21	15:P:90:TRP:CH2	2.53	0.43
19:U:122:VAL:HG13	19:U:126:LEU:HB3	2.00	0.43
21:X:76:ARG:CD	30:g:9:TRP:CE3	3.01	0.43
31:h:38:THR:HG22	31:h:44:LYS:HG2	2.00	0.43
38:4:204:LEU:HD21	38:4:272:LEU:HD11	1.99	0.43
39:5:8:ILE:HG21	39:5:89:LEU:HD21	2.00	0.43
39:5:499:TYR:HA	39:5:502:THR:HG22	2.01	0.43
7:G:37:GLU:OE2	23:Z:18:LYS:HE2	2.19	0.43
7:G:71:LEU:HD11	7:G:96:LEU:HB2	2.01	0.43
16:Q:93:VAL:HG13	17:R:20:ARG:HG2	1.99	0.43
22:Y:62:GLN:NE2	22:Y:75:THR:O	2.42	0.43
36:2:100:LYS:HG2	36:2:144:TYR:HE1	1.84	0.43
38:4:380:SER:O	38:4:384:ILE:HD12	2.19	0.43
1:A:55:ILE:CD1	1:A:65:VAL:HB	2.49	0.43
6:F:113:LEU:HD13	7:G:114:ASP:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:U:69:LEU:HD11	20:W:79:ARG:HG2	2.01	0.43
39:5:382:LEU:HD22	39:5:387:MET:HG3	2.00	0.43
2:B:393:TRP:CD1	2:B:417:LEU:HD22	2.54	0.43
6:F:109:GLU:OE2	7:G:121:LYS:NZ	2.51	0.43
6:F:133:ASP:OD1	6:F:134:GLN:N	2.52	0.43
24:a:47:PRO:HG2	24:a:50:LEU:HB2	2.01	0.43
30:g:47:ARG:NE	35:1:333:ILE:O	2.51	0.43
35:1:195:ALA:HB2	35:1:202:PHE:HD2	1.83	0.43
36:2:363:SER:HB2	36:2:447:ILE:HD11	2.00	0.43
39:5:419:TYR:OH	39:5:517:SER:OG	2.31	0.43
1:A:168:GLU:CB	13:M:116:ASN:HD22	2.30	0.43
2:B:133:MET:HE2	2:B:133:MET:HB3	1.88	0.43
46:J:203:3PE:H2B2	39:5:646:LEU:HD22	2.01	0.43
11:K:111:PRO:HG2	11:K:137:GLN:HE21	1.83	0.43
35:1:181:PRO:HB2	35:1:182:LEU:HD12	2.00	0.43
40:6:106:ILE:O	40:6:110:MET:HG2	2.19	0.43
3:C:208:GLU:HG3	9:I:99:TYR:CE2	2.54	0.42
48:E:403:CDL:H752	46:1:503:3PE:H371	2.01	0.42
7:G:164:PRO:HB3	15:P:14:PHE:HE2	1.84	0.42
11:K:202:LYS:HB2	11:K:205:ARG:HB2	2.00	0.42
12:L:15:PHE:CE2	36:2:163:ILE:HD11	2.54	0.42
13:M:53:LYS:HA	13:M:56:ILE:HD12	2.00	0.42
21:X:157:ASN:HD21	21:X:161:HIS:CE1	2.37	0.42
35:1:284:ILE:HG12	35:1:288:PHE:CZ	2.53	0.42
15:P:51:THR:HA	15:P:54:THR:HG22	2.00	0.42
38:4:177:PHE:HB2	38:4:216:ILE:HD11	2.02	0.42
38:4:248:GLY:O	38:4:252:LYS:HD3	2.19	0.42
39:5:124:THR:O	39:5:128:ILE:HG12	2.19	0.42
1:A:232:LEU:HD13	1:A:292:TRP:HH2	1.84	0.42
2:B:317:LEU:HB2	2:B:361:LYS:HA	1.99	0.42
3:C:67:GLU:HB3	36:2:148:TYR:HD2	1.84	0.42
10:J:135:THR:HG22	49:J:202:LMN:HBH	2.01	0.42
21:X:154:PRO:HB3	48:X:201:CDL:H671	2.01	0.42
35:1:106:ILE:HD13	35:1:158:ILE:HD11	2.00	0.42
37:3:7:PHE:CE2	37:3:11:ILE:HD11	2.54	0.42
38:4:459:ILE:HG21	48:4:503:CDL:H551	2.01	0.42
39:5:257:THR:HG23	39:5:332:LEU:HD21	2.02	0.42
39:5:285:ALA:HA	39:5:318:ILE:HD11	2.00	0.42
40:6:142:GLU:HG3	40:6:144:THR:HG23	2.00	0.42
3:C:50:ASP:HB2	3:C:53:PHE:HD2	1.83	0.42
5:E:43:LYS:O	5:E:50:SER:OG	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:123:ILE:HD12	7:G:123:ILE:HA	1.86	0.42
40:6:26:ALA:HB3	40:6:32:SER:HB3	2.00	0.42
1:A:627:ARG:HA	1:A:637:LEU:HD12	2.02	0.42
5:E:310:SER:HB2	5:E:313:GLN:HB2	2.01	0.42
12:L:20:ARG:HH12	40:6:27:LYS:HA	1.85	0.42
12:L:39:ILE:O	12:L:42:ARG:HG2	2.19	0.42
21:X:7:LEU:O	34:n:107:GLN:NE2	2.40	0.42
36:2:365:ALA:HA	36:2:417:LEU:HD21	2.00	0.42
38:4:211:TRP:HD1	38:4:266:LEU:HG	1.84	0.42
39:5:421:SER:O	39:5:425:THR:N	2.48	0.42
3:C:61:ASP:HB3	36:2:283:ARG:CZ	2.50	0.42
3:C:272:LYS:O	3:C:276:VAL:HG23	2.20	0.42
5:E:173:ILE:O	5:E:181:HIS:ND1	2.46	0.42
5:E:206:PHE:CD1	5:E:235:PRO:HB2	2.54	0.42
9:I:110:VAL:H	23:Z:45:ARG:HH22	1.67	0.42
11:K:138:MET:HA	11:K:139:PRO:HD3	1.86	0.42
24:a:85:PHE:HD2	39:5:558:GLN:HB2	1.85	0.42
34:n:62:ILE:O	34:n:66:GLU:HG2	2.18	0.42
36:2:212:ILE:HG23	36:2:241:LYS:HG2	2.01	0.42
37:3:93:LEU:O	37:3:97:ILE:HG12	2.19	0.42
38:4:345:ILE:HD13	38:4:349:ILE:HD12	2.01	0.42
39:5:32:THR:HG22	39:5:117:PHE:CE2	2.50	0.42
39:5:172:LEU:HD23	46:5:804:3PE:H322	2.02	0.42
39:5:506:ILE:HG22	39:5:507:THR:O	2.20	0.42
1:A:54:LEU:HD11	1:A:107:VAL:HG21	2.02	0.42
1:A:55:ILE:O	1:A:59:GLU:HG3	2.19	0.42
3:C:262:GLU:OE2	20:W:21:ARG:NE	2.53	0.42
7:G:236:LEU:HD22	7:G:237:GLU:H	1.85	0.42
12:L:24:LEU:HA	12:L:27:ILE:HG12	2.02	0.42
16:Q:90:LEU:HD21	52:Q:201:ZMP:H20A	2.01	0.42
48:X:201:CDL:H561	37:3:93:LEU:HD21	2.02	0.42
35:1:287:VAL:HA	35:1:290:MET:HG2	2.00	0.42
36:2:375:PRO:HG2	38:4:142:GLU:HB2	2.02	0.42
39:5:32:THR:OG1	39:5:33:ARG:N	2.53	0.42
3:C:197:VAL:HG13	3:C:274:ARG:HH11	1.85	0.42
3:C:342:GLN:O	3:C:346:ILE:HG12	2.20	0.42
4:D:2:ALA:HB2	48:Z:201:CDL:HB21	2.01	0.42
48:X:201:CDL:H412	40:6:163:LEU:HD21	2.01	0.42
24:a:125:PHE:HB3	24:a:130:LEU:HD13	2.01	0.42
36:2:299:LEU:HA	36:2:302:LEU:HD23	2.02	0.42
38:4:356:ILE:O	38:4:362:TYR:OH	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:8:13:MET:HE1	41:8:27:ALA:HB3	2.02	0.42
1:A:165:ARG:HD3	1:A:209:ASN:HB3	2.00	0.42
1:A:303:GLY:HA2	1:A:306:THR:HG22	2.01	0.42
3:C:219:ARG:NH2	3:C:246:ASP:OD2	2.53	0.42
36:2:302:LEU:HD21	36:2:390:ILE:HD13	2.02	0.42
36:2:449:LEU:HD22	55:2:502:CPL:H202	2.02	0.42
39:5:127:MET:HE3	39:5:254:THR:HB	2.01	0.42
54:5:801:T7X:O11	54:5:801:T7X:O2	2.37	0.42
2:B:98:TRP:HA	2:B:151:MET:HE3	2.02	0.42
8:H:40:ASN:HB2	8:H:43:ILE:HG22	2.01	0.42
10:J:179:LEU:HD13	38:4:271:ILE:HD12	2.02	0.42
32:i:63:ASP:HA	32:i:66:LYS:HG2	2.02	0.42
35:1:72:ILE:HG22	35:1:126:SER:HB3	2.02	0.42
36:2:199:LEU:HG	40:6:111:ILE:HD11	2.02	0.42
36:2:374:ILE:HA	36:2:375:PRO:HD3	1.89	0.42
39:5:307:LEU:HA	39:5:307:LEU:HD13	1.82	0.42
39:5:635:MET:HB2	39:5:635:MET:HE3	1.92	0.42
1:A:227:GLY:O	1:A:298:ARG:NE	2.53	0.41
2:B:367:ARG:HD2	2:B:402:ARG:HH11	1.84	0.41
3:C:134:GLN:HE21	9:I:139:ILE:HA	1.85	0.41
15:P:89:PHE:CE2	37:3:44:SER:HA	2.55	0.41
18:S:152:TRP:HD1	18:S:155:LYS:HG3	1.84	0.41
19:U:49:TYR:OH	30:g:73:THR:O	2.31	0.41
32:i:43:TRP:HH2	34:n:32:VAL:HG11	1.85	0.41
35:1:79:ILE:HA	35:1:82:ILE:HG12	2.02	0.41
38:4:125:ILE:HD13	38:4:249:LEU:HD13	2.01	0.41
39:5:36:SER:O	39:5:40:ILE:HG12	2.20	0.41
39:5:83:ALA:HA	39:5:86:ILE:HG22	2.01	0.41
39:5:146:ILE:HD12	39:5:255:LEU:HD12	2.02	0.41
39:5:310:MET:HA	39:5:313:LEU:HD13	2.02	0.41
1:A:125:MET:HE3	1:A:125:MET:HB2	1.95	0.41
1:A:261:MET:HE1	1:A:703:ILE:HB	2.03	0.41
1:A:329:LEU:HG	1:A:629:VAL:HG22	2.02	0.41
3:C:112:SER:HB3	3:C:439:ASP:HB3	2.02	0.41
3:C:182:ARG:HG3	3:C:406:PRO:HG3	2.01	0.41
5:E:298:THR:O	5:E:302:GLN:HG2	2.20	0.41
34:n:24:TRP:CH2	38:4:459:ILE:HD11	2.55	0.41
36:2:62:ASN:HD21	36:2:250:LEU:HD11	1.84	0.41
55:2:502:CPL:H40	55:2:502:CPL:H372	1.80	0.41
38:4:330:VAL:HA	38:4:333:VAL:HG12	2.02	0.41
1:A:160:GLU:HG2	2:B:393:TRP:CZ3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:618:GLY:O	1:A:620:ARG:NH1	2.53	0.41
2:B:39:ARG:NH1	2:B:291:GLU:O	2.53	0.41
5:E:98:ASP:OD1	5:E:99:LEU:N	2.53	0.41
27:d:71:LEU:HD11	39:5:203:THR:HB	2.01	0.41
30:g:9:TRP:HE1	48:g:201:CDL:HA31	1.85	0.41
48:j:102:CDL:H652	39:5:647:ILE:HG12	2.01	0.41
36:2:3:ILE:O	36:2:7:ILE:HG12	2.20	0.41
50:5:803:PLC:H72	50:5:803:PLC:H12	2.02	0.41
3:C:119:LEU:O	3:C:121:ARG:HG3	2.19	0.41
46:C:501:3PE:H291	35:1:191:ILE:HG22	2.02	0.41
7:G:241:ALA:HB1	22:Y:90:ARG:NH1	2.35	0.41
8:H:90:MET:HE2	8:H:105:TYR:HD1	1.85	0.41
8:H:186:GLU:N	8:H:210:PRO:O	2.47	0.41
21:X:147:ILE:HD12	21:X:147:ILE:HA	1.86	0.41
25:b:23:LYS:HB3	36:2:359:TYR:CD2	2.54	0.41
27:d:67:ALA:HB1	39:5:203:THR:HG22	2.01	0.41
46:4:505:3PE:H3F2	46:4:505:3PE:H3C1	1.95	0.41
39:5:265:ARG:HD2	39:5:265:ARG:HA	1.79	0.41
46:5:802:3PE:H392	46:5:802:3PE:H2A1	2.02	0.41
3:C:49:GLN:HB2	3:C:71:ILE:HD11	2.03	0.41
27:d:72:ASP:OD1	33:j:84:ARG:NH2	2.52	0.41
50:n:1101:PLC:H9'1	48:4:503:CDL:H762	2.02	0.41
36:2:316:TYR:O	36:2:320:HIS:CB	2.68	0.41
38:4:231:LEU:HD22	38:4:235:HIS:HE1	1.84	0.41
38:4:298:LEU:HD13	38:4:359:VAL:HG22	2.01	0.41
1:A:164:LYS:H	13:M:114:PHE:HE2	1.69	0.41
5:E:259:PHE:CD1	5:E:328:LYS:HB2	2.56	0.41
7:G:142:TYR:HB2	7:G:155:LEU:HB3	2.02	0.41
12:L:4:GLY:HA3	12:L:39:ILE:HG13	2.01	0.41
18:S:171:LEU:HD23	38:4:33:ASN:HB3	2.02	0.41
38:4:223:PRO:HG2	38:4:231:LEU:HG	2.02	0.41
38:4:297:ASP:OD1	38:4:298:LEU:N	2.48	0.41
40:6:177:ILE:O	40:6:181:MET:HG2	2.21	0.41
1:A:124:MET:HB3	1:A:124:MET:HE3	1.81	0.41
1:A:484:VAL:HG13	1:A:488:ILE:HD11	2.02	0.41
52:Q:201:ZMP:H4	17:R:43:ILE:HD12	2.01	0.41
34:n:83:MET:HE2	36:2:465:ASN:HB3	2.02	0.41
35:1:163:SER:HA	37:3:78:MET:HE1	2.02	0.41
35:1:314:ILE:HG23	37:3:106:ILE:HD11	2.01	0.41
36:2:217:LEU:HD13	39:5:621:ILE:HG22	2.01	0.41
39:5:478:ASP:HB2	41:8:44:PRO:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:126:ILE:HD11	7:G:179:GLU:HG2	2.03	0.41
20:W:23:LEU:HD23	20:W:23:LEU:HA	1.83	0.41
35:1:133:LEU:O	35:1:137:ILE:HG12	2.21	0.41
39:5:295:ALA:HB2	39:5:307:LEU:HB3	2.03	0.41
1:A:71:HIS:O	22:Y:142:LYS:NZ	2.54	0.41
1:A:141:GLU:HB3	22:Y:68:THR:HG21	2.03	0.41
2:B:317:LEU:HD22	2:B:361:LYS:HA	2.03	0.41
3:C:210:ARG:O	3:C:214:MET:HG2	2.20	0.41
5:E:93:LEU:HB2	5:E:104:PHE:HZ	1.86	0.41
50:K:302:PLC:H8A1	50:K:302:PLC:HEA3	1.89	0.41
13:M:51:ALA:HB2	31:h:124:LYS:N	2.36	0.41
48:X:201:CDL:H172	48:X:201:CDL:H201	1.88	0.41
49:j:101:LMN:HBKA	49:j:101:LMN:HBS	1.86	0.41
48:j:102:CDL:HB32	39:5:594:ARG:HB3	2.02	0.41
35:1:139:SER:HB3	35:1:205:THR:HG21	2.03	0.41
36:2:364:MET:HE2	36:2:416:LEU:HB3	2.03	0.41
38:4:36:LEU:HD21	38:4:94:LEU:HA	2.02	0.41
38:4:309:HIS:NE2	38:4:383:ASN:OD1	2.53	0.41
5:E:215:ASP:OD1	5:E:219:ARG:NH1	2.52	0.41
49:J:202:LMN:HBQ	49:J:202:LMN:HBLA	2.01	0.41
11:K:89:GLU:OE2	11:K:184:SER:N	2.53	0.41
12:L:23:ILE:HG12	40:6:75:ILE:HD11	2.03	0.41
12:L:80:LEU:HD12	12:L:81:ARG:NH1	2.36	0.41
48:Z:201:CDL:H152	48:Z:201:CDL:H182	1.87	0.41
27:d:38:LEU:HD21	39:5:71:ASP:HA	2.03	0.41
36:2:297:MET:HE2	36:2:297:MET:HB3	1.75	0.41
38:4:469:GLN:CD	39:5:69:ASN:H	2.29	0.41
39:5:380:ALA:O	39:5:384:LEU:HB2	2.21	0.41
9:I:78:PHE:HZ	30:g:25:HIS:HA	1.86	0.40
10:J:147:LEU:HG	10:J:152:LYS:HZ1	1.86	0.40
13:M:88:ARG:HB2	13:M:132:TYR:CD1	2.57	0.40
15:P:95:GLN:HA	15:P:98:LYS:HG3	2.02	0.40
21:X:96:LEU:HD11	36:2:41:PHE:HD2	1.84	0.40
36:2:102:GLU:OE2	40:6:183:HIS:NE2	2.54	0.40
36:2:258:LEU:N	54:2:503:T7X:O11	2.49	0.40
39:5:19:PRO:HD3	39:5:34:MET:HE1	2.02	0.40
7:G:160:THR:HB	7:G:163:THR:HG22	2.03	0.40
10:J:92:LYS:HE3	49:J:202:LMN:HCC	2.04	0.40
14:O:29:ARG:HB3	14:O:30:PRO:CD	2.51	0.40
30:g:39:ALA:O	30:g:43:LEU:HB2	2.20	0.40
31:h:124:LYS:HB2	31:h:125:PRO:HD2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:i:59:THR:HG23	32:i:64:ILE:HD11	2.03	0.40
36:2:117:ILE:HG22	36:2:247:TYR:HB2	2.04	0.40
36:2:122:ASP:OD1	36:2:123:PHE:N	2.54	0.40
36:2:352:GLY:HA3	36:2:424:LYS:HD3	2.02	0.40
38:4:3:LEU:HD23	38:4:6:ILE:HD12	2.02	0.40
1:A:650:ALA:HB2	1:A:657:VAL:HG21	2.03	0.40
2:B:130:ARG:NH2	8:H:171:ALA:HB2	2.37	0.40
2:B:401:PHE:CE2	2:B:414:LEU:HD22	2.56	0.40
16:Q:58:ARG:HH22	16:Q:103:PHE:HA	1.86	0.40
24:a:61:GLN:HE21	39:5:161:LEU:HD23	1.85	0.40
25:b:6:SER:HA	38:4:66:PHE:CD2	2.56	0.40
27:d:32:ARG:HH21	27:d:32:ARG:HD2	1.70	0.40
35:1:24:VAL:HG22	35:1:49:GLN:HB3	2.04	0.40
36:2:34:LEU:HD23	36:2:34:LEU:HA	1.83	0.40
38:4:234:VAL:O	38:4:238:SER:HB2	2.21	0.40
39:5:83:ALA:HB1	39:5:487:PHE:CE2	2.57	0.40
39:5:474:TRP:O	41:8:44:PRO:HG2	2.21	0.40
40:6:61:MET:HE3	40:6:61:MET:HB2	1.79	0.40
3:C:169:ARG:NH2	3:C:355:PRO:O	2.51	0.40
3:C:204:LEU:HD23	11:K:96:PRO:HG3	2.03	0.40
4:D:40:PHE:HB2	35:1:167:THR:HG21	2.04	0.40
5:E:229:PHE:HE2	5:E:286:HIS:HD2	1.69	0.40
8:H:178:MET:HB2	8:H:178:MET:HE2	1.83	0.40
21:X:118:ARG:NH1	21:X:123:LEU:HD13	2.36	0.40
33:j:46:PHE:O	39:5:586:ARG:NH2	2.55	0.40
38:4:170:PHE:CD2	38:4:230:TRP:HB3	2.56	0.40
48:4:503:CDL:H631	48:4:503:CDL:H602	1.83	0.40
1:A:248:ARG:NH2	9:I:157:ARG:HH12	2.19	0.40
3:C:85:ILE:HD11	3:C:102:LEU:HD12	2.03	0.40
3:C:137:PRO:O	3:C:141:ARG:HG2	2.22	0.40
3:C:150:ASN:ND2	3:C:410:MET:SD	2.94	0.40
3:C:395:PRO:HA	3:C:396:PRO:HD3	1.90	0.40
29:f:22:LEU:O	29:f:26:VAL:HG23	2.21	0.40
36:2:384:LEU:HD13	38:4:179:LEU:HD11	2.04	0.40
38:4:259:LEU:HD23	38:4:263:LEU:HD12	2.04	0.40
38:4:271:ILE:HD11	38:4:484:TYR:HD2	1.85	0.40
38:4:406:ASN:HB3	38:4:409:ILE:HG22	2.02	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	690/728 (95%)	638 (92%)	52 (8%)	0	100	100
2	B	454/488 (93%)	425 (94%)	29 (6%)	0	100	100
3	C	436/466 (94%)	402 (92%)	34 (8%)	0	100	100
4	D	84/87 (97%)	80 (95%)	4 (5%)	0	100	100
5	E	345/375 (92%)	323 (94%)	22 (6%)	0	100	100
6	F	119/144 (83%)	111 (93%)	8 (7%)	0	100	100
7	G	237/281 (84%)	222 (94%)	14 (6%)	1 (0%)	30	62
8	H	214/243 (88%)	191 (89%)	22 (10%)	1 (0%)	24	59
9	I	188/229 (82%)	178 (95%)	10 (5%)	0	100	100
10	J	177/198 (89%)	171 (97%)	6 (3%)	0	100	100
11	K	175/210 (83%)	161 (92%)	14 (8%)	0	100	100
12	L	87/89 (98%)	85 (98%)	2 (2%)	0	100	100
13	M	115/136 (85%)	106 (92%)	7 (6%)	2 (2%)	7	35
14	O	75/109 (69%)	71 (95%)	4 (5%)	0	100	100
15	P	121/124 (98%)	113 (93%)	8 (7%)	0	100	100
16	Q	83/132 (63%)	80 (96%)	3 (4%)	0	100	100
17	R	104/109 (95%)	98 (94%)	6 (6%)	0	100	100
18	S	168/249 (68%)	164 (98%)	4 (2%)	0	100	100
19	U	169/172 (98%)	157 (93%)	12 (7%)	0	100	100
20	W	119/123 (97%)	116 (98%)	3 (2%)	0	100	100
21	X	165/169 (98%)	160 (97%)	5 (3%)	0	100	100
22	Y	121/161 (75%)	113 (93%)	7 (6%)	1 (1%)	16	50
23	Z	179/182 (98%)	165 (92%)	14 (8%)	0	100	100
24	a	122/149 (82%)	111 (91%)	11 (9%)	0	100	100
25	b	62/74 (84%)	61 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	c	42/60 (70%)	37 (88%)	5 (12%)	0	100	100
27	d	88/92 (96%)	86 (98%)	2 (2%)	0	100	100
28	e	50/67 (75%)	48 (96%)	2 (4%)	0	100	100
29	f	78/87 (90%)	75 (96%)	3 (4%)	0	100	100
30	g	74/78 (95%)	66 (89%)	8 (11%)	0	100	100
31	h	134/138 (97%)	127 (95%)	6 (4%)	1 (1%)	18	52
32	i	81/90 (90%)	76 (94%)	5 (6%)	0	100	100
33	j	88/93 (95%)	83 (94%)	5 (6%)	0	100	100
34	n	112/120 (93%)	103 (92%)	9 (8%)	0	100	100
35	1	338/341 (99%)	318 (94%)	20 (6%)	0	100	100
36	2	467/469 (100%)	435 (93%)	30 (6%)	2 (0%)	30	62
37	3	125/128 (98%)	114 (91%)	11 (9%)	0	100	100
38	4	484/486 (100%)	466 (96%)	18 (4%)	0	100	100
39	5	652/655 (100%)	617 (95%)	34 (5%)	1 (0%)	43	73
40	6	181/185 (98%)	170 (94%)	11 (6%)	0	100	100
41	8	80/99 (81%)	76 (95%)	4 (5%)	0	100	100
42	9	84/89 (94%)	81 (96%)	3 (4%)	0	100	100
All	All	7967/8704 (92%)	7480 (94%)	478 (6%)	9 (0%)	49	79

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
39	5	555	VAL
13	M	77	ALA
31	h	108	PRO
22	Y	89	ASN
36	2	188	ASP
7	G	94	ASP
8	H	206	PRO
36	2	340	GLN
13	M	73	PRO

5.3.2 Protein sidechains (i)

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

entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	565/595 (95%)	565 (100%)	0	100	100
2	B	364/389 (94%)	364 (100%)	0	100	100
3	C	374/394 (95%)	374 (100%)	0	100	100
4	D	68/69 (99%)	68 (100%)	0	100	100
5	E	305/329 (93%)	305 (100%)	0	100	100
6	F	109/129 (84%)	109 (100%)	0	100	100
7	G	216/245 (88%)	215 (100%)	1 (0%)	81	85
8	H	191/212 (90%)	191 (100%)	0	100	100
9	I	156/187 (83%)	156 (100%)	0	100	100
10	J	130/147 (88%)	130 (100%)	0	100	100
11	K	154/180 (86%)	154 (100%)	0	100	100
12	L	77/77 (100%)	77 (100%)	0	100	100
13	M	97/115 (84%)	97 (100%)	0	100	100
14	O	65/91 (71%)	65 (100%)	0	100	100
15	P	109/110 (99%)	108 (99%)	1 (1%)	70	81
16	Q	72/111 (65%)	72 (100%)	0	100	100
17	R	97/100 (97%)	97 (100%)	0	100	100
18	S	149/211 (71%)	148 (99%)	1 (1%)	76	83
19	U	147/148 (99%)	147 (100%)	0	100	100
20	W	100/102 (98%)	100 (100%)	0	100	100
21	X	131/133 (98%)	131 (100%)	0	100	100
22	Y	105/140 (75%)	105 (100%)	0	100	100
23	Z	147/148 (99%)	147 (100%)	0	100	100
24	a	108/129 (84%)	108 (100%)	0	100	100
25	b	50/59 (85%)	50 (100%)	0	100	100
26	c	30/45 (67%)	30 (100%)	0	100	100
27	d	83/85 (98%)	83 (100%)	0	100	100
28	e	44/55 (80%)	44 (100%)	0	100	100
29	f	69/73 (94%)	68 (99%)	1 (1%)	59	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
30	g	62/64 (97%)	62 (100%)	0	100 100
31	h	121/123 (98%)	120 (99%)	1 (1%)	73 82
32	i	64/68 (94%)	64 (100%)	0	100 100
33	j	71/73 (97%)	71 (100%)	0	100 100
34	n	98/102 (96%)	98 (100%)	0	100 100
35	1	301/302 (100%)	301 (100%)	0	100 100
36	2	433/433 (100%)	432 (100%)	1 (0%)	87 89
37	3	113/114 (99%)	113 (100%)	0	100 100
38	4	434/434 (100%)	432 (100%)	2 (0%)	81 85
39	5	579/580 (100%)	577 (100%)	2 (0%)	86 88
40	6	165/167 (99%)	164 (99%)	1 (1%)	78 84
41	8	69/76 (91%)	69 (100%)	0	100 100
42	9	73/76 (96%)	73 (100%)	0	100 100
All	All	6895/7420 (93%)	6884 (100%)	11 (0%)	85 89

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	G	267	LYS
15	P	74	VAL
18	S	179	LEU
29	f	41	LYS
31	h	75	PRO
36	2	266	LEU
38	4	206	LEU
38	4	221	LYS
39	5	341	LEU
39	5	513	LEU
40	6	96	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (94) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	267	ASN
1	A	285	HIS
1	A	398	ASN

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Mol	Chain	Res	Type
1	A	499	ASN
2	B	42	GLN
2	B	138	HIS
2	B	315	ASN
3	C	120	HIS
3	C	134	GLN
3	C	268	ASN
3	C	367	ASN
3	C	440	HIS
5	E	137	ASN
5	E	286	HIS
5	E	295	GLN
5	E	317	GLN
6	F	39	HIS
6	F	77	HIS
6	F	106	GLN
7	G	143	ASN
8	H	125	GLN
8	H	174	ASN
9	I	40	ASN
10	J	48	ASN
11	K	100	GLN
11	K	125	ASN
11	K	137	GLN
11	K	158	HIS
13	M	25	ASN
13	M	93	ASN
13	M	116	ASN
13	M	123	HIS
15	P	80	HIS
15	P	122	ASN
17	R	45	HIS
17	R	49	GLN
17	R	50	ASN
17	R	105	ASN
18	S	122	ASN
18	S	201	GLN
21	X	142	ASN
21	X	161	HIS
21	X	168	GLN
22	Y	109	GLN
22	Y	135	HIS

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Mol	Chain	Res	Type
23	Z	38	ASN
23	Z	79	HIS
27	d	20	HIS
27	d	34	GLN
27	d	65	ASN
27	d	69	GLN
28	e	7	ASN
28	e	11	ASN
28	e	53	HIS
29	f	11	HIS
29	f	34	GLN
29	f	60	HIS
31	h	51	GLN
31	h	78	HIS
31	h	107	GLN
34	n	45	ASN
34	n	95	HIS
35	1	49	GLN
36	2	29	ASN
36	2	50	GLN
36	2	90	ASN
36	2	110	ASN
36	2	173	ASN
36	2	304	ASN
36	2	340	GLN
36	2	425	ASN
37	3	22	ASN
37	3	53	ASN
38	4	33	ASN
38	4	56	ASN
38	4	193	ASN
38	4	196	ASN
38	4	335	HIS
38	4	355	HIS
38	4	424	GLN
38	4	444	ASN
38	4	469	GLN
39	5	25	GLN
39	5	66	ASN
39	5	78	ASN
39	5	331	HIS
39	5	450	ASN

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Mol	Chain	Res	Type
39	5	491	HIS
39	5	495	ASN
39	5	638	ASN
40	6	81	ASN
40	6	128	ASN
40	6	152	ASN
42	9	13	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 49 ligands modelled in this entry, 1 is monoatomic - leaving 48 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	4	505	-	50,50,50	0.85	3 (6%)	53,55,55	1.22	2 (3%)
46	3PE	5	802	-	41,41,50	0.98	4 (9%)	44,46,55	1.31	3 (6%)
50	PLC	K	302	-	38,38,41	1.35	5 (13%)	44,46,49	1.05	2 (4%)
50	PLC	1	502	-	34,34,41	1.46	6 (17%)	40,42,49	1.22	2 (5%)
44	FES	H	301	8	0,4,4	-	-	-		
46	3PE	5	804	-	50,50,50	0.89	3 (6%)	53,55,55	1.04	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
49	LMN	j	101	-	68,68,72	1.58	13 (19%)	92,94,98	1.63	15 (16%)
50	PLC	n	1101	-	41,41,41	1.30	5 (12%)	47,49,49	1.09	2 (4%)
55	CPL	2	502	-	51,51,51	0.98	4 (7%)	57,59,59	0.93	3 (5%)
46	3PE	4	501	-	41,41,50	0.93	4 (9%)	44,46,55	1.11	2 (4%)
46	3PE	1	503	-	35,35,50	1.01	4 (11%)	38,40,55	1.20	2 (5%)
46	3PE	g	202	-	42,42,50	0.94	4 (9%)	45,47,55	1.23	2 (4%)
54	T7X	5	801	-	43,43,61	1.06	4 (9%)	53,55,73	1.65	10 (18%)
43	SF4	A	802	1	0,12,12	-	-	-		
52	ZMP	Q	201	16	26,32,36	1.86	6 (23%)	31,39,45	1.84	4 (12%)
53	UQ9	1	501	-	35,35,58	2.48	15 (42%)	42,45,73	1.53	11 (26%)
43	SF4	B	501	2	0,12,12	-	-	-		
43	SF4	K	301	11	0,12,12	-	-	-		
50	PLC	5	803	-	30,30,41	1.47	4 (13%)	36,38,49	1.12	2 (5%)
50	PLC	W	402	-	41,41,41	1.30	5 (12%)	47,49,49	1.22	3 (6%)
54	T7X	2	501	-	48,48,61	0.93	2 (4%)	57,60,73	1.41	8 (14%)
48	CDL	4	503	-	91,91,99	0.92	7 (7%)	97,103,111	1.22	6 (6%)
48	CDL	j	102	-	77,77,99	0.99	7 (9%)	83,89,111	1.14	5 (6%)
52	ZMP	O	201	14	26,32,36	1.86	6 (23%)	31,39,45	1.93	7 (22%)
50	PLC	W	401	-	40,40,41	1.31	4 (10%)	46,48,49	1.14	3 (6%)
43	SF4	I	301	9	0,12,12	-	-	-		
50	PLC	W	403	-	41,41,41	1.30	4 (9%)	47,49,49	1.07	3 (6%)
54	T7X	2	503	-	52,52,61	0.90	4 (7%)	62,64,73	1.29	5 (8%)
54	T7X	3	201	-	49,49,61	0.93	4 (8%)	59,61,73	1.33	7 (11%)
46	3PE	W	404	-	33,33,50	1.03	4 (12%)	36,38,55	1.12	2 (5%)
47	NDP	E	401	-	49,52,52	3.67	20 (40%)	66,80,80	2.19	15 (22%)
46	3PE	4	504	-	41,41,50	0.93	4 (9%)	44,46,55	1.08	2 (4%)
48	CDL	Z	201	-	75,75,99	0.99	7 (9%)	81,87,111	1.10	4 (4%)
46	3PE	J	201	-	40,40,50	0.95	4 (10%)	43,45,55	1.22	3 (6%)
48	CDL	E	403	-	71,71,99	1.04	6 (8%)	77,83,111	1.17	4 (5%)
46	3PE	b	201	-	41,41,50	0.93	4 (9%)	44,46,55	1.20	2 (4%)
46	3PE	E	402	-	35,35,50	1.03	4 (11%)	38,40,55	1.18	2 (5%)
46	3PE	J	203	-	43,43,50	0.93	4 (9%)	46,48,55	1.17	2 (4%)
43	SF4	I	302	9	0,12,12	-	-	-		
48	CDL	g	201	-	82,82,99	0.95	6 (7%)	88,94,111	1.24	5 (5%)
44	FES	A	803	1	0,4,4	-	-	-		
46	3PE	C	501	-	50,50,50	0.89	4 (8%)	53,55,55	1.26	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
46	3PE	1	504	-	35,35,50	1.01	4 (11%)	38,40,55	1.14	2 (5%)
46	3PE	4	502	-	42,42,50	0.93	4 (9%)	45,47,55	1.14	2 (4%)
48	CDL	X	201	-	85,85,99	0.92	8 (9%)	91,97,111	1.24	5 (5%)
45	FMN	B	502	-	33,33,33	2.81	11 (33%)	48,50,50	1.62	11 (22%)
49	LMN	J	202	-	72,72,72	1.52	9 (12%)	96,98,98	1.72	19 (19%)
43	SF4	A	801	1	0,12,12	-	-	-		

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	4	505	-	-	22/54/54/54	-
46	3PE	5	802	-	-	19/45/45/54	-
50	PLC	K	302	-	-	15/42/42/45	-
50	PLC	1	502	-	-	12/38/38/45	-
44	FES	H	301	8	-	-	0/1/1/1
46	3PE	5	804	-	-	12/54/54/54	-
49	LMN	j	101	-	-	21/46/126/130	0/4/4/4
50	PLC	n	1101	-	-	11/45/45/45	-
55	CPL	2	502	-	-	31/55/55/55	-
46	3PE	4	501	-	-	18/45/45/54	-
46	3PE	1	503	-	-	21/39/39/54	-
46	3PE	g	202	-	-	18/46/46/54	-
54	T7X	5	801	-	-	15/38/62/80	0/1/1/1
43	SF4	A	802	1	-	-	0/6/5/5
52	ZMP	Q	201	16	-	10/37/39/43	-
53	UQ9	1	501	-	-	7/30/54/81	0/1/1/1
43	SF4	B	501	2	-	-	0/6/5/5
43	SF4	K	301	11	-	-	0/6/5/5
50	PLC	5	803	-	-	15/34/34/45	-
50	PLC	W	402	-	-	24/45/45/45	-
48	CDL	4	503	-	-	48/102/102/110	-
48	CDL	j	102	-	-	32/88/88/110	-
52	ZMP	O	201	14	-	5/37/39/43	-
50	PLC	W	401	-	-	19/44/44/45	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
43	SF4	I	301	9	-	-	0/6/5/5
50	PLC	W	403	-	-	18/45/45/45	-
54	T7X	2	503	-	-	12/47/71/80	0/1/1/1
54	T7X	3	201	-	-	21/44/68/80	0/1/1/1
46	3PE	W	404	-	-	15/37/37/54	-
47	NDP	E	401	-	-	13/34/77/77	0/5/5/5
46	3PE	4	504	-	-	23/45/45/54	-
48	CDL	Z	201	-	-	43/86/86/110	-
46	3PE	J	201	-	-	13/44/44/54	-
48	CDL	E	403	-	-	35/82/82/110	-
46	3PE	b	201	-	-	21/45/45/54	-
46	3PE	J	203	-	-	21/47/47/54	-
46	3PE	E	402	-	-	14/39/39/54	-
48	CDL	g	201	-	-	39/93/93/110	-
43	SF4	I	302	9	-	-	0/6/5/5
46	3PE	C	501	-	-	28/54/54/54	-
46	3PE	4	502	-	-	21/46/46/54	-
46	3PE	1	504	-	-	21/39/39/54	-
54	T7X	2	501	-	-	16/43/67/80	0/1/1/1
44	FES	A	803	1	-	-	0/1/1/1
48	CDL	X	201	-	-	34/96/96/110	-
45	FMN	B	502	-	-	10/18/18/18	0/3/3/3
49	LMN	J	202	-	-	22/50/130/130	0/4/4/4
43	SF4	A	801	1	-	-	0/6/5/5

All (230) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	E	401	NDP	C6N-C5N	12.21	1.55	1.33
53	1	501	UQ9	C6-C1	9.39	1.52	1.35
47	E	401	NDP	C2B-C1B	-7.96	1.32	1.53
45	B	502	FMN	C4A-N5	7.65	1.45	1.30
47	E	401	NDP	O4B-C1B	7.57	1.59	1.42
47	E	401	NDP	O4D-C1D	7.48	1.59	1.42
47	E	401	NDP	C2D-C1D	-7.37	1.29	1.53
47	E	401	NDP	O4D-C4D	-7.14	1.29	1.45
47	E	401	NDP	O4B-C4B	-6.51	1.30	1.45
45	B	502	FMN	C10-N1	6.36	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	Q	201	ZMP	C16-N2	5.70	1.46	1.33
49	J	202	LMN	O1-C1	-5.39	1.31	1.40
52	O	201	ZMP	C16-N2	5.38	1.45	1.33
52	O	201	ZMP	C13-N1	5.30	1.45	1.33
52	Q	201	ZMP	C13-N1	5.25	1.45	1.33
49	j	101	LMN	O1-C1	-5.10	1.31	1.40
49	j	101	LMN	O5-C1	5.09	1.54	1.41
49	J	202	LMN	O5-C1	5.06	1.54	1.41
45	B	502	FMN	C2-N1	5.02	1.48	1.36
45	B	502	FMN	C5A-N5	5.02	1.49	1.39
47	E	401	NDP	C2N-C3N	4.96	1.48	1.34
45	B	502	FMN	C9A-N10	4.78	1.49	1.41
47	E	401	NDP	C6A-N6A	4.40	1.45	1.34
45	B	502	FMN	C2-N3	4.37	1.49	1.39
47	E	401	NDP	O2D-C2D	4.24	1.53	1.43
53	1	501	UQ9	C4-C3	4.01	1.52	1.36
47	E	401	NDP	P2B-O2B	3.98	1.66	1.59
50	W	403	PLC	O2-C'	3.74	1.44	1.34
47	E	401	NDP	C4N-C3N	3.74	1.57	1.49
45	B	502	FMN	C10-N10	3.72	1.45	1.37
50	1	502	PLC	O2-C'	3.56	1.44	1.34
47	E	401	NDP	C7N-N7N	3.45	1.42	1.33
50	W	401	PLC	O2-C'	3.42	1.43	1.34
50	n	1101	PLC	O2-C'	3.41	1.43	1.34
50	W	402	PLC	O2-C'	3.37	1.43	1.34
50	K	302	PLC	O2-C'	3.37	1.43	1.34
50	1	502	PLC	O3-CB	3.37	1.43	1.33
45	B	502	FMN	C4-N3	3.36	1.45	1.38
50	5	803	PLC	O2-C'	3.28	1.43	1.34
50	n	1101	PLC	O3-CB	3.28	1.42	1.33
50	W	401	PLC	O3-CB	3.24	1.42	1.33
50	W	403	PLC	O3-CB	3.21	1.42	1.33
50	5	803	PLC	O3-CB	3.15	1.42	1.33
47	E	401	NDP	C5A-C4A	-3.14	1.33	1.39
50	K	302	PLC	O3-CB	3.12	1.42	1.33
50	W	402	PLC	O3-CB	3.06	1.42	1.33
45	B	502	FMN	O2-C2	-3.04	1.18	1.24
49	J	202	LMN	OBY-CCR	3.00	1.49	1.41
48	g	201	CDL	OA6-CA4	-2.97	1.39	1.46
49	j	101	LMN	OBZ-CCS	2.94	1.49	1.41
49	J	202	LMN	O4-C4	2.94	1.51	1.43
48	j	102	CDL	OA6-CA4	-2.92	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	1	501	UQ9	C11-C9	2.91	1.57	1.51
53	1	501	UQ9	C16-C14	2.89	1.57	1.51
49	J	202	LMN	CBT-CCM	2.87	1.60	1.53
53	1	501	UQ9	C21-C19	2.81	1.57	1.51
47	E	401	NDP	C6N-N1N	2.81	1.44	1.37
45	B	502	FMN	O4-C4	-2.80	1.18	1.23
46	C	501	3PE	O31-C3	-2.80	1.38	1.45
49	j	101	LMN	CBT-CCM	2.79	1.59	1.53
49	j	101	LMN	CBS-CCM	2.79	1.59	1.53
48	j	102	CDL	OB6-CB4	-2.78	1.39	1.46
49	j	101	LMN	OBY-CCR	2.77	1.48	1.41
46	5	804	3PE	O21-C2	-2.76	1.39	1.46
48	4	503	CDL	OB6-CB4	-2.76	1.39	1.46
52	O	201	ZMP	O5-C21	-2.75	1.38	1.44
46	J	203	3PE	O21-C2	-2.74	1.39	1.46
49	J	202	LMN	OBZ-CCS	2.69	1.48	1.41
46	J	201	3PE	O21-C2	-2.67	1.39	1.46
48	Z	201	CDL	OB6-CB4	-2.67	1.39	1.46
49	J	202	LMN	OBY-CCC	2.66	1.50	1.44
48	E	403	CDL	OA8-CA7	2.63	1.41	1.33
48	X	201	CDL	OB6-CB4	-2.60	1.40	1.46
46	4	505	3PE	O21-C2	-2.60	1.40	1.46
48	E	403	CDL	OA6-CA4	-2.60	1.40	1.46
46	C	501	3PE	O21-C2	-2.59	1.40	1.46
46	4	501	3PE	O21-C2	-2.58	1.40	1.46
54	3	201	T7X	O16-C8	-2.58	1.40	1.46
46	5	802	3PE	O21-C2	-2.57	1.40	1.46
50	5	803	PLC	O2-C2	-2.56	1.40	1.46
54	2	503	T7X	O16-C8	-2.56	1.40	1.46
53	1	501	UQ9	O5-C5	-2.56	1.17	1.23
48	g	201	CDL	OA8-CA7	2.56	1.40	1.33
50	W	402	PLC	O2-C2	-2.56	1.40	1.46
48	4	503	CDL	OA8-CA7	2.56	1.40	1.33
52	Q	201	ZMP	C9-C10	2.55	1.53	1.50
46	5	802	3PE	O31-C3	-2.54	1.39	1.45
48	4	503	CDL	OA6-CA4	-2.54	1.40	1.46
55	2	502	CPL	O2-C2	-2.54	1.40	1.46
47	E	401	NDP	C4N-C5N	2.54	1.55	1.48
53	1	501	UQ9	O4-C4M	-2.54	1.39	1.45
54	2	503	T7X	O18-C11	2.54	1.40	1.33
48	g	201	CDL	OB8-CB7	2.52	1.40	1.33
46	E	402	3PE	O21-C2	-2.52	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	E	403	CDL	OB6-CB4	-2.51	1.40	1.46
46	g	202	3PE	O21-C2	-2.51	1.40	1.46
48	Z	201	CDL	OA6-CA4	-2.51	1.40	1.46
49	j	101	LMN	OBX-CCJ	2.51	1.48	1.41
48	g	201	CDL	OB6-CB4	-2.50	1.40	1.46
53	1	501	UQ9	C26-C24	2.50	1.56	1.51
46	4	504	3PE	O21-C2	-2.49	1.40	1.46
54	5	801	T7X	O16-C10	2.49	1.41	1.34
48	E	403	CDL	OB8-CB7	2.48	1.40	1.33
46	W	404	3PE	O31-C31	2.46	1.40	1.33
48	j	102	CDL	OB8-CB7	2.46	1.40	1.33
46	1	503	3PE	O21-C2	-2.46	1.40	1.46
49	j	101	LMN	CBR-CCM	2.45	1.58	1.54
47	E	401	NDP	C5A-N7A	-2.44	1.34	1.39
46	b	201	3PE	O21-C2	-2.44	1.40	1.46
54	5	801	T7X	O18-C9	-2.44	1.39	1.45
46	J	203	3PE	O31-C31	2.44	1.40	1.33
46	4	502	3PE	O31-C3	-2.41	1.39	1.45
46	4	502	3PE	O21-C2	-2.41	1.40	1.46
53	1	501	UQ9	C7-C8	2.40	1.54	1.50
53	1	501	UQ9	C6-C5	2.40	1.53	1.46
52	O	201	ZMP	C10-S1	2.39	1.81	1.76
46	W	404	3PE	O21-C2	-2.39	1.40	1.46
50	W	401	PLC	O2-C2	-2.39	1.40	1.46
53	1	501	UQ9	O2-C2	-2.39	1.18	1.23
54	2	501	T7X	O16-C10	2.37	1.41	1.34
50	K	302	PLC	O2-C2	-2.37	1.40	1.46
48	j	102	CDL	OA8-CA7	2.37	1.40	1.33
49	j	101	LMN	O4-C4	2.37	1.50	1.43
46	1	504	3PE	O31-C31	2.37	1.40	1.33
46	1	504	3PE	O21-C2	-2.37	1.40	1.46
54	2	501	T7X	O18-C11	2.37	1.40	1.33
47	E	401	NDP	O3B-C3B	-2.37	1.37	1.43
48	Z	201	CDL	OB8-CB6	-2.36	1.39	1.45
53	1	501	UQ9	O3-C3M	-2.36	1.39	1.45
55	2	502	CPL	O3-C3	-2.36	1.39	1.45
52	O	201	ZMP	O2-C13	-2.35	1.18	1.23
47	E	401	NDP	C5D-C4D	2.34	1.58	1.51
54	5	801	T7X	O18-C11	2.34	1.40	1.33
53	1	501	UQ9	C22-C23	2.34	1.58	1.50
46	5	804	3PE	O31-C31	2.34	1.40	1.33
50	1	502	PLC	O2-C2	-2.33	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	4	502	3PE	O31-C31	2.33	1.40	1.33
46	5	802	3PE	O31-C31	2.33	1.40	1.33
50	K	302	PLC	P-O3P	2.33	1.68	1.59
46	E	402	3PE	O31-C3	-2.32	1.39	1.45
48	X	201	CDL	OA8-CA6	-2.32	1.39	1.45
46	4	504	3PE	O31-C31	2.31	1.40	1.33
54	3	201	T7X	O18-C11	2.31	1.40	1.33
52	Q	201	ZMP	O2-C13	-2.30	1.18	1.23
48	4	503	CDL	OB8-CB7	2.30	1.40	1.33
48	X	201	CDL	OA6-CA5	2.29	1.40	1.34
52	O	201	ZMP	O3-C16	-2.29	1.18	1.23
48	Z	201	CDL	OA8-CA7	2.29	1.40	1.33
46	b	201	3PE	O31-C31	2.28	1.40	1.33
46	4	502	3PE	O21-C21	2.28	1.40	1.34
48	X	201	CDL	OB8-CB7	2.28	1.40	1.33
48	X	201	CDL	OB8-CB6	-2.28	1.40	1.45
46	g	202	3PE	O31-C31	2.27	1.40	1.33
48	X	201	CDL	OA6-CA4	-2.27	1.40	1.46
50	W	403	PLC	P-O4P	2.27	1.68	1.59
53	1	501	UQ9	C7-C6	2.27	1.55	1.51
46	1	503	3PE	O21-C21	2.26	1.40	1.34
53	1	501	UQ9	C12-C13	2.26	1.57	1.50
52	Q	201	ZMP	C10-S1	2.26	1.81	1.76
48	E	403	CDL	OB6-CB5	2.25	1.40	1.34
49	J	202	LMN	CBQ-CCM	2.25	1.58	1.54
46	5	804	3PE	O31-C3	-2.25	1.40	1.45
46	4	501	3PE	O31-C31	2.25	1.39	1.33
46	5	802	3PE	O21-C21	2.24	1.40	1.34
48	j	102	CDL	OA8-CA6	-2.24	1.40	1.45
50	1	502	PLC	P-O3P	2.24	1.68	1.59
54	3	201	T7X	O18-C9	-2.23	1.40	1.45
46	1	503	3PE	O31-C31	2.23	1.39	1.33
46	4	504	3PE	O31-C3	-2.23	1.40	1.45
46	b	201	3PE	O31-C3	-2.23	1.40	1.45
47	E	401	NDP	C8A-N9A	-2.23	1.33	1.37
46	4	501	3PE	O31-C3	-2.23	1.40	1.45
45	B	502	FMN	C7M-C7	2.23	1.55	1.51
46	4	505	3PE	O31-C31	2.22	1.39	1.33
52	Q	201	ZMP	O3-C16	-2.22	1.19	1.23
48	E	403	CDL	OA6-CA5	2.22	1.40	1.34
46	4	505	3PE	O31-C3	-2.22	1.40	1.45
46	1	504	3PE	O31-C3	-2.22	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	Z	201	CDL	OB8-CB7	2.21	1.39	1.33
48	4	503	CDL	OB8-CB6	-2.21	1.40	1.45
50	n	1101	PLC	O2-C2	-2.21	1.41	1.46
46	J	201	3PE	O31-C31	2.21	1.39	1.33
55	2	502	CPL	O3-C11	2.20	1.39	1.33
48	X	201	CDL	OA8-CA7	2.20	1.39	1.33
55	2	502	CPL	O2-C31	2.20	1.40	1.34
46	1	504	3PE	O21-C21	2.20	1.40	1.34
48	g	201	CDL	OB6-CB5	2.18	1.40	1.34
49	j	101	LMN	CBQ-CCM	2.17	1.58	1.54
46	g	202	3PE	O31-C3	-2.17	1.40	1.45
46	W	404	3PE	O21-C21	2.17	1.40	1.34
50	1	502	PLC	C8-N	-2.17	1.43	1.50
46	E	402	3PE	O31-C31	2.17	1.39	1.33
46	b	201	3PE	O21-C21	2.17	1.40	1.34
50	5	803	PLC	P-O3P	2.16	1.68	1.59
46	J	203	3PE	O21-C21	2.16	1.40	1.34
46	J	201	3PE	O31-C3	-2.15	1.40	1.45
46	1	503	3PE	O31-C3	-2.14	1.40	1.45
48	Z	201	CDL	OA8-CA6	-2.14	1.40	1.45
46	4	504	3PE	O21-C21	2.13	1.40	1.34
48	4	503	CDL	OA6-CA5	2.13	1.40	1.34
46	E	402	3PE	O21-C21	2.12	1.40	1.34
50	n	1101	PLC	P-O3P	2.11	1.67	1.59
54	2	503	T7X	O16-C10	2.11	1.40	1.34
54	5	801	T7X	P1-O1	2.10	1.66	1.60
46	W	404	3PE	O31-C3	-2.08	1.40	1.45
48	j	102	CDL	OB6-CB5	2.08	1.40	1.34
49	J	202	LMN	CBS-CCM	2.08	1.58	1.53
46	C	501	3PE	O31-C31	2.07	1.39	1.33
50	W	402	PLC	P-O4P	2.07	1.67	1.59
48	j	102	CDL	OB8-CB6	-2.07	1.40	1.45
49	j	101	LMN	OAN-CCH	2.07	1.47	1.43
48	g	201	CDL	OA8-CA6	-2.06	1.40	1.45
50	W	402	PLC	P-O3P	2.06	1.67	1.59
50	n	1101	PLC	P-O4P	2.06	1.67	1.59
48	Z	201	CDL	OA6-CA5	2.05	1.40	1.34
50	K	302	PLC	P-O4P	2.05	1.67	1.59
54	3	201	T7X	O16-C10	2.04	1.40	1.34
46	J	201	3PE	O21-C21	2.04	1.40	1.34
46	4	501	3PE	O21-C21	2.04	1.40	1.34
48	4	503	CDL	OA8-CA6	-2.04	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	W	403	PLC	P-O3P	2.03	1.67	1.59
46	J	203	3PE	O31-C3	-2.03	1.40	1.45
46	g	202	3PE	O21-C21	2.03	1.40	1.34
48	X	201	CDL	OB6-CB5	2.02	1.40	1.34
50	W	401	PLC	P-O3P	2.02	1.67	1.59
50	1	502	PLC	P-O4P	2.02	1.67	1.59
46	C	501	3PE	O21-C21	2.02	1.40	1.34
49	j	101	LMN	OCB-CCQ	2.02	1.49	1.43
54	2	503	T7X	O18-C9	-2.01	1.40	1.45
49	j	101	LMN	OBY-CCC	2.00	1.49	1.44

All (194) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	Q	201	ZMP	C9-C10-S1	6.79	121.36	113.46
52	O	201	ZMP	C9-C10-S1	6.29	120.78	113.46
49	j	101	LMN	CBR-CBL-CBJ	6.23	131.75	113.19
47	E	401	NDP	C4A-N9A-C1B	-6.22	111.77	126.59
47	E	401	NDP	N6A-C6A-N1A	-6.19	104.79	118.35
54	5	801	T7X	O16-C10-C12	6.12	124.70	111.50
47	E	401	NDP	C1B-N9A-C8A	5.71	140.04	127.14
47	E	401	NDP	N3A-C2A-N1A	-5.66	119.75	128.60
50	W	402	PLC	O2-C'-C1'	5.46	123.28	111.50
47	E	401	NDP	C5A-C6A-N6A	5.35	135.07	123.43
47	E	401	NDP	C5A-C4A-N3A	-5.23	119.93	126.75
49	J	202	LMN	CBR-CBL-CBJ	5.16	128.57	113.19
50	1	502	PLC	O2-C'-C1'	4.99	122.26	111.50
46	g	202	3PE	O21-C21-C22	4.89	122.05	111.50
49	j	101	LMN	OCB-CCQ-CCH	4.68	119.73	107.28
46	4	505	3PE	O21-C21-C22	4.65	121.52	111.50
46	5	802	3PE	O21-C21-C22	4.56	121.33	111.50
46	1	503	3PE	O21-C21-C22	4.55	121.32	111.50
48	4	503	CDL	OB6-CB5-C51	4.52	121.25	111.50
46	J	203	3PE	O21-C21-C22	4.35	120.89	111.50
48	g	201	CDL	OB6-CB5-C51	4.34	120.86	111.50
48	X	201	CDL	OB6-CB5-C51	4.34	120.85	111.50
49	J	202	LMN	CCL-CCH-CCQ	4.32	119.55	109.68
48	Z	201	CDL	OB6-CB5-C51	4.29	120.75	111.50
47	E	401	NDP	N9A-C8A-N7A	-4.29	108.05	113.91
49	J	202	LMN	O3-C3-C2	-4.26	100.50	110.35
54	2	501	T7X	O16-C10-C12	4.23	120.61	111.50
50	5	803	PLC	O2-C'-C1'	4.19	120.53	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	K	302	PLC	O2-C'-C1'	4.12	120.38	111.50
46	E	402	3PE	O21-C21-C22	4.11	120.36	111.50
46	1	504	3PE	O21-C21-C22	4.10	120.33	111.50
49	J	202	LMN	OBZ-CCD-CCO	4.05	117.04	109.69
49	j	101	LMN	CCJ-CCL-CCH	4.04	118.41	110.00
49	J	202	LMN	CCW-CCU-CCO	4.04	117.87	110.82
48	4	503	CDL	OA6-CA5-C11	4.03	120.18	111.50
48	Z	201	CDL	OA6-CA5-C11	3.98	120.08	111.50
46	4	502	3PE	O21-C21-C22	3.93	119.97	111.50
46	C	501	3PE	O21-C21-C22	3.92	119.95	111.50
54	2	503	T7X	O16-C10-C12	3.92	119.94	111.50
54	2	503	T7X	C6-C1-C2	3.91	116.50	110.85
46	b	201	3PE	O21-C21-C22	3.86	119.81	111.50
52	O	201	ZMP	O1-C10-C9	-3.84	119.45	123.99
49	J	202	LMN	CCU-CCO-CCD	3.84	117.09	110.24
49	J	202	LMN	C2-C3-C4	3.84	118.44	109.68
46	J	201	3PE	O21-C21-C22	3.83	119.75	111.50
45	B	502	FMN	C4-N3-C2	-3.82	118.59	125.64
46	W	404	3PE	O21-C21-C22	3.81	119.70	111.50
50	n	1101	PLC	O2-C'-C1'	3.80	119.70	111.50
48	g	201	CDL	OA6-CA5-C11	3.80	119.69	111.50
55	2	502	CPL	O2-C31-C32	3.77	119.62	111.50
48	E	403	CDL	OA6-CA5-C11	3.76	119.60	111.50
48	E	403	CDL	OB6-CB5-C51	3.75	119.59	111.50
46	4	501	3PE	O21-C21-C22	3.74	119.55	111.50
46	C	501	3PE	O31-C31-C32	3.73	123.62	111.91
46	5	802	3PE	C3-C2-C1	-3.68	103.08	111.79
54	3	201	T7X	C6-C1-C2	3.68	116.15	110.85
49	j	101	LMN	CCW-CCU-CCO	3.65	117.20	110.82
52	Q	201	ZMP	O1-C10-S1	-3.65	117.87	122.61
54	3	201	T7X	O16-C10-C12	3.62	119.30	111.50
45	B	502	FMN	C7M-C7-C6	-3.61	112.82	119.49
49	J	202	LMN	O4-CCR-CCV	3.60	117.42	108.10
50	W	401	PLC	O2-C'-C1'	3.60	119.25	111.50
46	4	504	3PE	O21-C21-C22	3.59	119.24	111.50
49	J	202	LMN	CCJ-CCL-CCH	3.57	117.44	110.00
47	E	401	NDP	C2A-N3A-C4A	3.57	120.18	111.75
46	5	804	3PE	O21-C21-C22	3.56	119.17	111.50
48	j	102	CDL	OB6-CB5-C51	3.56	119.17	111.50
52	O	201	ZMP	C11-C12-N1	-3.55	104.95	112.42
54	5	801	T7X	O1-C1-C2	3.54	116.91	108.66
48	j	102	CDL	OA6-CA5-C11	3.50	119.05	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	2	501	T7X	C6-C1-C2	3.49	115.89	110.85
54	2	501	T7X	O18-C11-C31	3.40	122.57	111.91
48	4	503	CDL	OB8-CB7-C71	3.39	122.53	111.91
48	X	201	CDL	OA6-CA5-C11	3.32	118.66	111.50
53	1	501	UQ9	C12-C13-C14	-3.32	119.66	127.66
49	j	101	LMN	OBX-CCJ-CCL	3.30	117.33	110.35
49	J	202	LMN	CCV-CCT-CCN	3.29	116.56	110.82
45	B	502	FMN	C7M-C7-C8	3.29	127.47	120.74
46	J	201	3PE	O31-C31-C32	3.29	122.22	111.91
45	B	502	FMN	O4-C4-C4A	-3.25	117.99	126.60
47	E	401	NDP	C2B-C1B-N9A	-3.21	108.13	113.53
49	j	101	LMN	C2-C3-C4	3.19	116.95	109.68
54	3	201	T7X	C12-C13-C14	-3.18	107.56	113.23
48	g	201	CDL	OB8-CB7-C71	3.16	121.84	111.91
47	E	401	NDP	N3A-C4A-N9A	3.13	132.24	127.08
48	E	403	CDL	OB8-CB7-C71	3.11	121.68	111.91
54	3	201	T7X	C3-C2-C1	3.08	116.71	109.68
53	1	501	UQ9	C25-C24-C26	3.05	120.40	115.27
54	2	501	T7X	C5-C6-C1	3.04	116.62	109.68
48	E	403	CDL	OA8-CA7-C31	3.02	121.38	111.91
52	O	201	ZMP	C15-N2-C16	-3.01	117.21	122.59
46	g	202	3PE	O31-C31-C32	3.01	121.36	111.91
54	5	801	T7X	O18-C11-C31	3.01	121.34	111.91
50	W	403	PLC	O3-CB-C1B	2.95	121.16	111.91
54	3	201	T7X	C5-C6-C1	2.94	116.40	109.68
47	E	401	NDP	C5A-N7A-C8A	2.90	107.64	103.51
45	B	502	FMN	C5'-C4'-C3'	-2.87	106.66	112.20
50	1	502	PLC	O3-CB-C1B	2.86	120.89	111.91
48	4	503	CDL	OA8-CA7-C31	2.86	120.87	111.91
54	2	503	T7X	C5-C6-C1	2.85	116.19	109.68
49	j	101	LMN	CCJ-OBX-CCF	2.83	119.24	113.69
54	2	503	T7X	C3-C2-C1	2.81	116.10	109.68
53	1	501	UQ9	C7-C8-C9	-2.80	122.13	126.79
53	1	501	UQ9	C20-C19-C21	2.79	119.96	115.27
48	X	201	CDL	OA8-CA7-C31	2.79	120.65	111.91
46	5	802	3PE	O31-C31-C32	2.78	120.62	111.91
49	J	202	LMN	CCR-O4-C4	-2.77	111.11	117.96
54	2	501	T7X	C6-C5-C4	2.77	115.65	110.82
54	5	801	T7X	C6-C5-C4	2.76	115.64	110.82
45	B	502	FMN	C4A-C4-N3	2.76	120.19	113.19
49	j	101	LMN	O1-C1-C2	2.75	112.60	108.30
49	j	101	LMN	OAN-CCH-CCL	-2.75	103.98	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	n	1101	PLC	O3-CB-C1B	2.75	120.55	111.91
50	W	401	PLC	C3-C2-C1	-2.75	105.28	111.79
46	J	203	3PE	O31-C31-C32	2.74	120.50	111.91
54	3	201	T7X	O18-C11-C31	2.74	120.50	111.91
52	Q	201	ZMP	O1-C10-C9	-2.73	120.77	123.99
45	B	502	FMN	C5A-C9A-N10	2.73	120.77	117.95
53	1	501	UQ9	C1M-C1-C6	-2.71	119.97	124.40
54	2	501	T7X	C3-C2-C1	2.71	115.86	109.68
45	B	502	FMN	C9A-C5A-N5	-2.70	119.49	122.43
49	J	202	LMN	C1-C2-C3	2.68	115.58	110.00
49	J	202	LMN	O4-C4-C3	2.67	114.38	107.28
49	j	101	LMN	CCS-CCW-CCU	2.67	115.55	110.00
46	W	404	3PE	O31-C31-C32	2.66	120.25	111.91
50	K	302	PLC	O3-CB-C1B	2.64	120.19	111.91
50	W	401	PLC	O3-CB-C1B	2.64	120.18	111.91
53	1	501	UQ9	C27-C26-C24	-2.61	110.35	114.62
48	j	102	CDL	CB2-C1-CA2	-2.60	105.13	112.79
45	B	502	FMN	C4-C4A-C10	2.58	121.13	116.79
46	4	505	3PE	O31-C31-C32	2.58	120.00	111.91
48	Z	201	CDL	OA8-CA7-C31	2.57	119.98	111.91
50	W	403	PLC	O2-C'-C1'	2.57	117.04	111.50
48	X	201	CDL	OB8-CB7-C71	2.55	119.92	111.91
48	j	102	CDL	OB8-CB7-C71	2.54	119.89	111.91
46	1	504	3PE	O31-C31-C32	2.54	119.88	111.91
49	j	101	LMN	O5-C1-C2	-2.54	104.97	110.35
52	O	201	ZMP	C17-C16-N2	2.52	121.60	116.58
49	J	202	LMN	CCS-OCB-CCQ	-2.51	111.76	117.96
54	3	201	T7X	C6-C5-C4	2.51	115.20	110.82
46	1	503	3PE	O31-C31-C32	2.50	119.75	111.91
47	E	401	NDP	C5B-C4B-C3B	-2.48	105.87	115.18
46	b	201	3PE	O31-C31-C32	2.48	119.68	111.91
48	g	201	CDL	OA8-CA7-C31	2.44	119.55	111.91
50	W	402	PLC	O3-CB-C1B	2.43	119.54	111.91
48	Z	201	CDL	OB8-CB7-C71	2.43	119.54	111.91
54	5	801	T7X	P1-O1-C1	2.43	128.24	119.41
46	5	804	3PE	O31-C31-C32	2.43	119.52	111.91
46	4	501	3PE	O31-C31-C32	2.43	119.52	111.91
50	5	803	PLC	O3-CB-C1B	2.42	119.50	111.91
46	4	504	3PE	O31-C31-C32	2.41	119.48	111.91
54	5	801	T7X	O18-C9-C8	2.40	115.42	108.43
54	2	503	T7X	O18-C11-C31	2.38	119.38	111.91
54	5	801	T7X	O16-C8-C7	2.36	116.96	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	j	101	LMN	OBZ-CCS-CCW	2.36	115.34	110.35
53	1	501	UQ9	C17-C18-C19	-2.36	121.98	127.66
49	j	101	LMN	CCL-CCH-CCQ	2.33	115.00	109.68
47	E	401	NDP	PN-O3-PA	-2.32	124.86	132.83
49	j	101	LMN	CCS-OBZ-CCD	2.31	118.23	113.69
48	g	201	CDL	CA4-OA6-CA5	-2.31	112.11	117.79
54	2	501	T7X	C8-O16-C10	2.31	123.47	117.79
46	4	502	3PE	O31-C31-C32	2.30	119.14	111.91
45	B	502	FMN	C4A-C10-N1	-2.30	119.40	124.73
49	J	202	LMN	OBY-CCC-CCN	2.28	113.84	109.69
47	E	401	NDP	C4A-N9A-C8A	2.27	108.19	105.73
53	1	501	UQ9	C22-C23-C24	-2.25	122.25	127.66
50	W	403	PLC	C2-O2-C'	2.24	123.32	117.79
54	5	801	T7X	C13-C12-C10	-2.23	105.50	113.62
53	1	501	UQ9	C15-C14-C16	2.23	119.03	115.27
49	J	202	LMN	O4-C4-C5	-2.23	103.34	109.45
46	E	402	3PE	O31-C31-C32	2.23	118.90	111.91
55	2	502	CPL	O3-C11-C12	2.19	118.79	111.91
52	O	201	ZMP	O1-C10-S1	-2.19	119.77	122.61
48	X	201	CDL	CB6-CB4-CB3	-2.17	106.65	111.79
46	J	201	3PE	C2-O21-C21	-2.16	112.46	117.79
48	j	102	CDL	OA8-CA7-C31	2.15	118.64	111.91
50	W	402	PLC	O2-C'-O'	-2.13	118.55	123.70
54	5	801	T7X	C3-C2-C1	2.13	114.55	109.68
47	E	401	NDP	C6A-C5A-C4A	2.13	120.04	117.18
49	J	202	LMN	CCS-OBZ-CCD	2.10	117.81	113.69
46	C	501	3PE	C33-C32-C31	-2.10	105.99	113.62
49	J	202	LMN	CBL-CBR-CCM	-2.09	110.42	117.16
53	1	501	UQ9	C21-C22-C23	-2.09	105.00	111.88
48	4	503	CDL	OB8-CB7-OB9	-2.07	118.37	123.59
53	1	501	UQ9	C10-C9-C11	2.07	118.75	115.27
55	2	502	CPL	C14-C13-C12	-2.05	105.81	113.19
45	B	502	FMN	C9-C9A-N10	-2.04	119.07	121.84
54	5	801	T7X	O16-C10-O17	-2.04	118.76	123.70
52	Q	201	ZMP	C14-C15-N2	-2.04	107.78	111.90
48	4	503	CDL	OB6-CB5-OB7	-2.03	118.80	123.70
52	O	201	ZMP	O3-C16-N2	-2.02	118.65	122.99
49	J	202	LMN	OCB-CCS-CCW	2.02	113.34	108.10
54	2	501	T7X	C12-C13-C14	-2.02	109.63	113.23
49	j	101	LMN	O5-C5-C4	2.02	114.01	109.75

There are no chirality outliers.

All (815) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	B	502	FMN	N10-C1'-C2'-O2'
45	B	502	FMN	N10-C1'-C2'-C3'
45	B	502	FMN	C1'-C2'-C3'-O3'
45	B	502	FMN	C1'-C2'-C3'-C4'
45	B	502	FMN	O2'-C2'-C3'-O3'
45	B	502	FMN	O2'-C2'-C3'-C4'
45	B	502	FMN	O3'-C3'-C4'-C5'
46	C	501	3PE	C1-O11-P-O12
46	C	501	3PE	C1-O11-P-O13
46	C	501	3PE	C1-O11-P-O14
46	C	501	3PE	O13-C11-C12-N
46	E	402	3PE	C1-O11-P-O14
46	E	402	3PE	O13-C11-C12-N
46	J	201	3PE	C1-O11-P-O14
46	J	201	3PE	O13-C11-C12-N
46	J	203	3PE	C22-C21-O21-C2
46	W	404	3PE	C1-O11-P-O12
46	W	404	3PE	C1-O11-P-O14
46	W	404	3PE	C11-O13-P-O14
46	W	404	3PE	O13-C11-C12-N
46	b	201	3PE	C1-O11-P-O14
46	b	201	3PE	O11-C1-C2-O21
46	g	202	3PE	C1-O11-P-O14
46	g	202	3PE	C22-C21-O21-C2
46	1	503	3PE	C1-O11-P-O12
46	1	503	3PE	C1-O11-P-O13
46	1	503	3PE	C1-O11-P-O14
46	1	503	3PE	O22-C21-O21-C2
46	1	503	3PE	C22-C21-O21-C2
46	1	504	3PE	C1-O11-P-O12
46	1	504	3PE	C1-O11-P-O14
46	4	501	3PE	C1-O11-P-O12
46	4	501	3PE	C1-O11-P-O13
46	4	501	3PE	C1-O11-P-O14
46	4	502	3PE	C1-O11-P-O12
46	4	502	3PE	C1-O11-P-O14
46	4	504	3PE	C1-O11-P-O12
46	4	504	3PE	C1-O11-P-O14
46	5	802	3PE	C1-O11-P-O12
46	5	802	3PE	C1-O11-P-O13
46	5	804	3PE	C1-O11-P-O14
46	5	804	3PE	O13-C11-C12-N

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Mol	Chain	Res	Type	Atoms
47	E	401	NDP	C4B-C5B-O5B-PA
47	E	401	NDP	O4B-C4B-C5B-O5B
47	E	401	NDP	C3B-C4B-C5B-O5B
47	E	401	NDP	C2B-O2B-P2B-O1X
47	E	401	NDP	C2B-O2B-P2B-O3X
48	E	403	CDL	CA2-OA2-PA1-OA3
48	E	403	CDL	CA2-OA2-PA1-OA5
48	E	403	CDL	C11-CA5-OA6-CA4
48	E	403	CDL	CB3-OB5-PB2-OB3
48	E	403	CDL	CB3-OB5-PB2-OB4
48	X	201	CDL	CB3-OB5-PB2-OB3
48	X	201	CDL	CB3-OB5-PB2-OB4
48	Z	201	CDL	CA3-OA5-PA1-OA3
48	Z	201	CDL	CA3-OA5-PA1-OA4
48	g	201	CDL	CB2-C1-CA2-OA2
48	g	201	CDL	C11-CA5-OA6-CA4
48	g	201	CDL	CB3-OB5-PB2-OB3
48	j	102	CDL	O1-C1-CA2-OA2
48	j	102	CDL	CA2-OA2-PA1-OA3
48	j	102	CDL	C11-CA5-OA6-CA4
48	4	503	CDL	C1-CA2-OA2-PA1
48	4	503	CDL	CA2-OA2-PA1-OA4
48	4	503	CDL	CA3-OA5-PA1-OA3
48	4	503	CDL	CA3-OA5-PA1-OA4
48	4	503	CDL	CB2-OB2-PB2-OB3
48	4	503	CDL	CB2-OB2-PB2-OB4
48	4	503	CDL	CB3-OB5-PB2-OB3
48	4	503	CDL	CB3-OB5-PB2-OB4
48	4	503	CDL	OB7-CB5-OB6-CB4
49	J	202	LMN	C2-C1-O1-CBS
49	J	202	LMN	O5-C1-O1-CBS
49	J	202	LMN	OBX-CCJ-OBV-CBT
49	j	101	LMN	OBY-CCR-O4-C4
49	j	101	LMN	O1-CBS-CCM-CBQ
49	j	101	LMN	O1-CBS-CCM-CBR
49	j	101	LMN	OBX-CCJ-OBV-CBT
50	K	302	PLC	C1-O3P-P-O1P
50	W	401	PLC	C1-O3P-P-O1P
50	W	401	PLC	C4-O4P-P-O1P
50	W	401	PLC	C4-O4P-P-O3P
50	W	402	PLC	O4P-C4-C5-N
50	W	402	PLC	C1'-C'-O2-C2

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Mol	Chain	Res	Type	Atoms
50	W	402	PLC	O'-C'-O2-C2
50	W	402	PLC	C1-O3P-P-O2P
50	n	1101	PLC	C1-O3P-P-O1P
50	n	1101	PLC	C1-O3P-P-O2P
50	1	502	PLC	O4P-C4-C5-N
50	1	502	PLC	C1'-C'-O2-C2
50	1	502	PLC	O'-C'-O2-C2
50	1	502	PLC	C4-O4P-P-O2P
50	5	803	PLC	O3P-C1-C2-O2
50	5	803	PLC	O4P-C4-C5-N
50	5	803	PLC	C1'-C'-O2-C2
50	5	803	PLC	O'-C'-O2-C2
52	Q	201	ZMP	C12-C11-S1-C10
53	1	501	UQ9	C20-C19-C21-C22
53	1	501	UQ9	C18-C19-C21-C22
53	1	501	UQ9	C15-C14-C16-C17
53	1	501	UQ9	C13-C14-C16-C17
54	2	501	T7X	C7-O13-P1-O11
54	2	501	T7X	C7-O13-P1-O12
54	2	501	T7X	C12-C10-O16-C8
54	2	501	T7X	C15-C16-C17-C18
54	2	503	T7X	C7-O13-P1-O12
54	3	201	T7X	C7-O13-P1-O11
54	3	201	T7X	C7-O13-P1-O12
54	5	801	T7X	C2-C1-O1-P1
54	5	801	T7X	C6-C1-O1-P1
54	5	801	T7X	C7-O13-P1-O12
55	2	502	CPL	O2-C2-C3-O3
55	2	502	CPL	O4P-C4-C5-N
55	2	502	CPL	C40-C41-C42-C43
55	2	502	CPL	C1-O3P-P-O1P
55	2	502	CPL	C4-O4P-P-O1P
55	2	502	CPL	C4-O4P-P-O2P
49	j	101	LMN	CCH-CCQ-OCB-CCS
48	4	503	CDL	OA9-CA7-OA8-CA6
54	2	503	T7X	O19-C11-O18-C9
54	5	801	T7X	O19-C11-O18-C9
48	4	503	CDL	C31-CA7-OA8-CA6
54	2	503	T7X	C31-C11-O18-C9
54	5	801	T7X	C31-C11-O18-C9
49	j	101	LMN	OAL-CBP-CCF-CCQ
46	1	503	3PE	O32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
46	4	501	3PE	O32-C31-O31-C3
48	Z	201	CDL	OA9-CA7-OA8-CA6
48	j	102	CDL	OA9-CA7-OA8-CA6
48	4	503	CDL	OB9-CB7-OB8-CB6
54	3	201	T7X	O19-C11-O18-C9
46	J	203	3PE	O22-C21-O21-C2
46	g	202	3PE	O22-C21-O21-C2
48	E	403	CDL	OA7-CA5-OA6-CA4
48	g	201	CDL	OA7-CA5-OA6-CA4
48	j	102	CDL	OA7-CA5-OA6-CA4
54	2	501	T7X	O17-C10-O16-C8
54	5	801	T7X	O17-C10-O16-C8
46	C	501	3PE	C32-C31-O31-C3
46	1	503	3PE	C32-C31-O31-C3
46	4	501	3PE	C32-C31-O31-C3
48	X	201	CDL	C71-CB7-OB8-CB6
48	Z	201	CDL	C31-CA7-OA8-CA6
48	4	503	CDL	C71-CB7-OB8-CB6
50	W	402	PLC	C1B-CB-O3-C3
54	3	201	T7X	C31-C11-O18-C9
48	4	503	CDL	C51-CB5-OB6-CB4
54	5	801	T7X	C12-C10-O16-C8
49	j	101	LMN	O1-CBS-CCM-CBT
49	j	101	LMN	OAL-CBP-CCF-OBX
48	j	102	CDL	C31-CA7-OA8-CA6
46	C	501	3PE	O32-C31-O31-C3
50	W	402	PLC	OB-CB-O3-C3
46	C	501	3PE	C27-C28-C29-C2A
48	X	201	CDL	OB9-CB7-OB8-CB6
46	5	802	3PE	C22-C21-O21-C2
50	K	302	PLC	C1'-C'-O2-C2
49	J	202	LMN	OAL-CBP-CCF-OBX
47	E	401	NDP	O4D-C4D-C5D-O5D
49	J	202	LMN	OAL-CBP-CCF-CCQ
47	E	401	NDP	C3B-C2B-O2B-P2B
48	E	403	CDL	CB2-C1-CA2-OA2
48	j	102	CDL	CB2-C1-CA2-OA2
46	5	802	3PE	O22-C21-O21-C2
49	j	101	LMN	C4-C5-C6-O6
46	W	404	3PE	C32-C31-O31-C3
46	W	404	3PE	C31-C32-C33-C34
49	J	202	LMN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
49	j	101	LMN	O5-C5-C6-O6
48	E	403	CDL	O1-C1-CA2-OA2
46	g	202	3PE	C21-C22-C23-C24
53	1	501	UQ9	C24-C26-C27-C28
46	W	404	3PE	O32-C31-O31-C3
50	K	302	PLC	O'-C'-O2-C2
48	Z	201	CDL	C11-CA5-OA6-CA4
48	4	503	CDL	C11-CA5-OA6-CA4
46	1	504	3PE	C21-C22-C23-C24
49	J	202	LMN	CBI-CBK-CBQ-CCM
46	b	201	3PE	C31-C32-C33-C34
48	Z	201	CDL	CA5-C11-C12-C13
45	B	502	FMN	O3'-C3'-C4'-O4'
46	J	203	3PE	C31-C32-C33-C34
46	4	501	3PE	C21-C22-C23-C24
50	K	302	PLC	CB-C1B-C2B-C3B
50	W	403	PLC	CB-C1B-C2B-C3B
50	5	803	PLC	CB-C1B-C2B-C3B
54	2	501	T7X	C10-C12-C13-C14
54	2	501	T7X	C11-C31-C32-C33
54	3	201	T7X	C11-C31-C32-C33
49	J	202	LMN	OAI-CBM-CCC-OBY
49	J	202	LMN	C5-C4-O4-CCR
48	X	201	CDL	OA7-CA5-OA6-CA4
48	4	503	CDL	OA7-CA5-OA6-CA4
49	J	202	LMN	CAW-CAY-CBA-CBC
46	1	503	3PE	C31-C32-C33-C34
48	Z	201	CDL	CB5-C51-C52-C53
48	4	503	CDL	CB5-C51-C52-C53
48	X	201	CDL	C11-CA5-OA6-CA4
49	J	202	LMN	C3-C4-O4-CCR
53	1	501	UQ9	C9-C11-C12-C13
48	g	201	CDL	O1-C1-CA2-OA2
48	g	201	CDL	CA5-C11-C12-C13
54	3	201	T7X	C10-C12-C13-C14
45	B	502	FMN	C2'-C3'-C4'-C5'
46	E	402	3PE	C1-O11-P-O13
46	J	203	3PE	C1-O11-P-O13
46	W	404	3PE	C11-O13-P-O11
46	g	202	3PE	C1-O11-P-O13
46	1	504	3PE	C1-O11-P-O13
46	4	502	3PE	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
46	4	504	3PE	C1-O11-P-O13
46	5	804	3PE	C1-O11-P-O13
48	E	403	CDL	CB3-OB5-PB2-OB2
48	X	201	CDL	CB3-OB5-PB2-OB2
48	Z	201	CDL	CA3-OA5-PA1-OA2
48	g	201	CDL	CB3-OB5-PB2-OB2
48	j	102	CDL	CA2-OA2-PA1-OA5
48	j	102	CDL	CB3-OB5-PB2-OB2
48	4	503	CDL	CA2-OA2-PA1-OA5
48	4	503	CDL	CA3-OA5-PA1-OA2
48	4	503	CDL	CB2-OB2-PB2-OB5
48	4	503	CDL	CB3-OB5-PB2-OB2
50	K	302	PLC	C1-O3P-P-O4P
50	W	402	PLC	C1-O3P-P-O4P
50	W	402	PLC	C4-O4P-P-O3P
50	n	1101	PLC	C1-O3P-P-O4P
50	1	502	PLC	C1-O3P-P-O4P
50	1	502	PLC	C4-O4P-P-O3P
54	2	501	T7X	C7-O13-P1-O1
54	2	503	T7X	C7-O13-P1-O1
54	3	201	T7X	C7-O13-P1-O1
54	5	801	T7X	C7-O13-P1-O1
55	2	502	CPL	C1-O3P-P-O4P
55	2	502	CPL	C4-O4P-P-O3P
55	2	502	CPL	C12-C11-O3-C3
50	W	401	PLC	C'-C1'-C2'-C3'
49	j	101	LMN	OAI-CBM-CCC-OBY
48	Z	201	CDL	OA7-CA5-OA6-CA4
50	5	803	PLC	C'-C1'-C2'-C3'
46	J	201	3PE	C22-C21-O21-C2
47	E	401	NDP	C3D-C4D-C5D-O5D
46	C	501	3PE	C24-C25-C26-C27
46	g	202	3PE	C2D-C2E-C2F-C2G
48	g	201	CDL	C51-C52-C53-C54
49	j	101	LMN	CBH-CBJ-CBL-CBR
50	W	403	PLC	C6'-C7'-C8'-C9'
46	4	505	3PE	C36-C37-C38-C39
46	5	804	3PE	C39-C3A-C3B-C3C
46	J	201	3PE	O22-C21-O21-C2
45	B	502	FMN	C2'-C3'-C4'-O4'
48	4	503	CDL	C38-C39-C40-C41
55	2	502	CPL	C44-C45-C46-C47

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Mol	Chain	Res	Type	Atoms
46	4	504	3PE	C32-C33-C34-C35
48	Z	201	CDL	C37-C38-C39-C40
48	j	102	CDL	C16-C17-C18-C19
54	2	503	T7X	C33-C34-C35-C36
46	g	202	3PE	C24-C25-C26-C27
48	Z	201	CDL	C32-C33-C34-C35
54	2	501	T7X	C32-C33-C34-C35
46	C	501	3PE	C31-C32-C33-C34
46	C	501	3PE	C21-C22-C23-C24
48	Z	201	CDL	C33-C34-C35-C36
48	g	201	CDL	C78-C79-C80-C81
48	j	102	CDL	C76-C77-C78-C79
50	W	403	PLC	C1B-C2B-C3B-C4B
54	2	503	T7X	C32-C33-C34-C35
55	2	502	CPL	O11-C11-O3-C3
46	1	503	3PE	C24-C25-C26-C27
49	J	202	LMN	CBD-CBF-CBH-CBJ
50	W	403	PLC	C5'-C6'-C7'-C8'
48	X	201	CDL	C57-C58-C59-C60
50	1	502	PLC	C2B-C3B-C4B-C5B
50	5	803	PLC	C1B-C2B-C3B-C4B
54	3	201	T7X	C32-C33-C34-C35
46	4	505	3PE	C33-C34-C35-C36
54	3	201	T7X	O17-C10-O16-C8
46	4	505	3PE	C22-C21-O21-C2
54	3	201	T7X	C12-C10-O16-C8
48	g	201	CDL	C74-C75-C76-C77
54	5	801	T7X	C35-C36-C37-C38
46	J	203	3PE	C21-C22-C23-C24
55	2	502	CPL	C11-C12-C13-C14
46	C	501	3PE	C39-C3A-C3B-C3C
46	J	203	3PE	C29-C2A-C2B-C2C
46	b	201	3PE	C34-C35-C36-C37
46	4	505	3PE	C37-C38-C39-C3A
48	4	503	CDL	C33-C34-C35-C36
48	4	503	CDL	C35-C36-C37-C38
50	W	402	PLC	C1B-C2B-C3B-C4B
46	4	502	3PE	C26-C27-C28-C29
48	g	201	CDL	C23-C24-C25-C26
46	4	501	3PE	O13-C11-C12-N
46	C	501	3PE	C26-C27-C28-C29
46	J	203	3PE	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
46	4	504	3PE	C36-C37-C38-C39
46	4	505	3PE	C2B-C2C-C2D-C2E
48	g	201	CDL	C72-C73-C74-C75
54	2	503	T7X	C35-C36-C37-C38
49	J	202	LMN	C4-C5-C6-O6
46	4	501	3PE	C33-C34-C35-C36
46	4	501	3PE	C3A-C3B-C3C-C3D
48	4	503	CDL	C59-C60-C61-C62
52	O	201	ZMP	S1-C11-C12-N1
46	4	501	3PE	C23-C24-C25-C26
50	W	403	PLC	C6B-C7B-C8B-C9B
46	4	505	3PE	C38-C39-C3A-C3B
54	3	201	T7X	C33-C34-C35-C36
50	K	302	PLC	C'-C1'-C2'-C3'
55	2	502	CPL	C32-C31-O2-C2
50	W	402	PLC	C2'-C3'-C4'-C5'
48	4	503	CDL	CA7-C31-C32-C33
46	1	503	3PE	C23-C24-C25-C26
49	j	101	LMN	CBF-CBH-CBJ-CBL
48	g	201	CDL	C11-C12-C13-C14
50	W	401	PLC	C4B-C5B-C6B-C7B
46	5	802	3PE	C21-C22-C23-C24
46	4	504	3PE	C33-C34-C35-C36
48	4	503	CDL	C36-C37-C38-C39
49	j	101	LMN	CAW-CAY-CBA-CBC
46	4	505	3PE	O22-C21-O21-C2
55	2	502	CPL	O31-C31-O2-C2
50	K	302	PLC	C6B-C7B-C8B-C9B
48	j	102	CDL	C55-C56-C57-C58
50	K	302	PLC	C3B-C4B-C5B-C6B
50	W	401	PLC	C1B-C2B-C3B-C4B
54	3	201	T7X	C22-C23-C24-C25
46	J	201	3PE	C32-C33-C34-C35
48	4	503	CDL	C54-C55-C56-C57
48	g	201	CDL	C12-C13-C14-C15
48	g	201	CDL	C76-C77-C78-C79
48	E	403	CDL	C31-C32-C33-C34
48	X	201	CDL	C13-C14-C15-C16
48	X	201	CDL	C54-C55-C56-C57
49	j	101	LMN	CAY-CBA-CBC-CBE
48	Z	201	CDL	C71-CB7-OB8-CB6
48	j	102	CDL	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
48	j	102	CDL	C74-C75-C76-C77
50	W	402	PLC	C2B-C3B-C4B-C5B
46	E	402	3PE	C32-C33-C34-C35
46	C	501	3PE	C37-C38-C39-C3A
46	4	505	3PE	C31-C32-C33-C34
50	1	502	PLC	CB-C1B-C2B-C3B
46	J	203	3PE	C32-C33-C34-C35
48	g	201	CDL	C22-C23-C24-C25
49	J	202	LMN	CBB-CBD-CBF-CBH
52	Q	201	ZMP	C13-C14-C15-N2
46	J	203	3PE	C38-C39-C3A-C3B
48	Z	201	CDL	C31-C32-C33-C34
48	4	503	CDL	C15-C16-C17-C18
48	X	201	CDL	OA5-CA3-CA4-OA6
55	2	502	CPL	O3P-C1-C2-O2
50	W	402	PLC	C5B-C6B-C7B-C8B
46	4	502	3PE	C2D-C2E-C2F-C2G
46	5	802	3PE	C38-C39-C3A-C3B
48	X	201	CDL	C72-C73-C74-C75
46	b	201	3PE	O21-C2-C3-O31
46	4	504	3PE	O21-C2-C3-O31
49	j	101	LMN	CBG-CBI-CBK-CBQ
50	W	403	PLC	C4'-C5'-C6'-C7'
46	4	501	3PE	C37-C38-C39-C3A
55	2	502	CPL	C36-C37-C38-C39
46	b	201	3PE	C33-C34-C35-C36
48	Z	201	CDL	C38-C39-C40-C41
50	n	1101	PLC	C1B-C2B-C3B-C4B
46	W	404	3PE	C34-C35-C36-C37
46	5	804	3PE	O22-C21-O21-C2
46	5	804	3PE	C22-C21-O21-C2
46	C	501	3PE	C2B-C2C-C2D-C2E
46	W	404	3PE	C1-O11-P-O13
48	E	403	CDL	C31-CA7-OA8-CA6
46	b	201	3PE	O11-C1-C2-C3
46	g	202	3PE	O11-C1-C2-C3
48	g	201	CDL	OB5-CB3-CB4-CB6
50	5	803	PLC	O3P-C1-C2-C3
55	2	502	CPL	O3P-C1-C2-C3
49	J	202	LMN	CBG-CBI-CBK-CBQ
55	2	502	CPL	C15-C16-C17-C18
46	4	504	3PE	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
46	4	501	3PE	C22-C21-O21-C2
48	Z	201	CDL	OB9-CB7-OB8-CB6
46	J	203	3PE	C34-C35-C36-C37
46	E	402	3PE	C1-C2-C3-O31
46	b	201	3PE	C1-C2-C3-O31
46	1	504	3PE	C1-C2-C3-O31
48	j	102	CDL	CB3-CB4-CB6-OB8
50	K	302	PLC	C2'-C3'-C4'-C5'
50	W	402	PLC	C1-C2-C3-O3
55	2	502	CPL	C1-C2-C3-O3
48	X	201	CDL	C64-C65-C66-C67
48	Z	201	CDL	C34-C35-C36-C37
48	j	102	CDL	C31-C32-C33-C34
46	J	203	3PE	C39-C3A-C3B-C3C
46	4	505	3PE	C2F-C2G-C2H-C2I
49	J	202	LMN	CBF-CBH-CBJ-CBL
50	W	401	PLC	C7'-C8'-C9'-CA'
49	j	101	LMN	CBJ-CBL-CBR-CCM
48	X	201	CDL	CA5-C11-C12-C13
46	4	501	3PE	C32-C33-C34-C35
48	g	201	CDL	C79-C80-C81-C82
48	X	201	CDL	C63-C64-C65-C66
54	5	801	T7X	C33-C34-C35-C36
46	1	503	3PE	C37-C38-C39-C3A
48	g	201	CDL	C16-C17-C18-C19
48	g	201	CDL	CB7-C71-C72-C73
48	E	403	CDL	C71-CB7-OB8-CB6
48	Z	201	CDL	C19-C20-C21-C22
46	J	203	3PE	C27-C28-C29-C2A
48	Z	201	CDL	C12-C13-C14-C15
49	j	101	LMN	CBA-CBC-CBE-CBG
46	b	201	3PE	C22-C23-C24-C25
50	W	402	PLC	CB-C1B-C2B-C3B
48	4	503	CDL	C19-C20-C21-C22
49	j	101	LMN	CAA-CAW-CAY-CBA
48	j	102	CDL	CA7-C31-C32-C33
46	J	203	3PE	O21-C2-C3-O31
46	1	504	3PE	O21-C2-C3-O31
46	4	502	3PE	O21-C2-C3-O31
48	j	102	CDL	OB6-CB4-CB6-OB8
46	C	501	3PE	C3C-C3D-C3E-C3F
48	X	201	CDL	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
55	2	502	CPL	C21-C22-C23-C24
48	Z	201	CDL	CA7-C31-C32-C33
55	2	502	CPL	C37-C38-C39-C40
48	E	403	CDL	OA9-CA7-OA8-CA6
48	Z	201	CDL	C35-C36-C37-C38
48	Z	201	CDL	CA4-CA6-OA8-CA7
46	4	502	3PE	C22-C21-O21-C2
50	W	401	PLC	C1'-C'-O2-C2
46	4	502	3PE	C29-C2A-C2B-C2C
46	1	503	3PE	C35-C36-C37-C38
48	j	102	CDL	C54-C55-C56-C57
50	W	403	PLC	C1'-C2'-C3'-C4'
50	K	302	PLC	C7B-C8B-C9B-CAA
50	W	403	PLC	C4B-C5B-C6B-C7B
52	Q	201	ZMP	C1-C2-C3-C4
48	g	201	CDL	C75-C76-C77-C78
46	4	502	3PE	O11-C1-C2-C3
46	5	804	3PE	C3C-C3D-C3E-C3F
46	J	203	3PE	O13-C11-C12-N
46	J	203	3PE	C25-C26-C27-C28
48	Z	201	CDL	C72-C73-C74-C75
48	g	201	CDL	C40-C41-C42-C43
50	W	401	PLC	C5B-C6B-C7B-C8B
50	n	1101	PLC	C4'-C5'-C6'-C7'
46	1	503	3PE	C32-C33-C34-C35
50	1	502	PLC	C3B-C4B-C5B-C6B
47	E	401	NDP	C1B-C2B-O2B-P2B
48	g	201	CDL	C14-C15-C16-C17
48	E	403	CDL	C51-C52-C53-C54
48	E	403	CDL	C53-C54-C55-C56
46	C	501	3PE	C29-C2A-C2B-C2C
46	4	501	3PE	C3D-C3E-C3F-C3G
48	X	201	CDL	C21-C22-C23-C24
46	J	203	3PE	C1-C2-C3-O31
46	4	504	3PE	C1-C2-C3-O31
46	5	802	3PE	C1-C2-C3-O31
48	E	403	CDL	CA3-CA4-CA6-OA8
48	X	201	CDL	CB3-CB4-CB6-OB8
50	K	302	PLC	C1-C2-C3-O3
50	n	1101	PLC	C1-C2-C3-O3
54	3	201	T7X	C7-C8-C9-O18
46	1	504	3PE	C27-C28-C29-C2A

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Mol	Chain	Res	Type	Atoms
49	j	101	LMN	CBC-CBE-CBG-CBI
46	g	202	3PE	C29-C2A-C2B-C2C
52	Q	201	ZMP	C5-C6-C7-C8
46	4	505	3PE	C3E-C3F-C3G-C3H
46	1	504	3PE	C24-C25-C26-C27
48	g	201	CDL	C33-C34-C35-C36
46	J	201	3PE	C1-O11-P-O13
46	b	201	3PE	C1-O11-P-O13
46	b	201	3PE	C11-O13-P-O11
46	4	505	3PE	C11-O13-P-O11
54	2	501	T7X	C16-C17-C18-C19
54	5	801	T7X	C15-C16-C17-C18
46	b	201	3PE	C26-C27-C28-C29
46	1	504	3PE	O11-C1-C2-O21
48	g	201	CDL	OB5-CB3-CB4-OB6
46	5	802	3PE	C29-C2A-C2B-C2C
46	J	201	3PE	O31-C31-C32-C33
46	1	504	3PE	O21-C21-C22-C23
48	E	403	CDL	OB9-CB7-OB8-CB6
50	W	402	PLC	O2-C2-C3-O3
54	2	501	T7X	O16-C8-C9-O18
48	Z	201	CDL	CA2-C1-CB2-OB2
48	4	503	CDL	CB2-C1-CA2-OA2
46	4	502	3PE	C23-C24-C25-C26
46	4	501	3PE	O22-C21-O21-C2
50	W	401	PLC	O'-C'-O2-C2
48	E	403	CDL	C72-C73-C74-C75
48	X	201	CDL	C39-C40-C41-C42
46	b	201	3PE	C25-C26-C27-C28
46	1	504	3PE	C25-C26-C27-C28
46	5	804	3PE	C32-C33-C34-C35
48	X	201	CDL	C1-CB2-OB2-PB2
48	g	201	CDL	C1-CB2-OB2-PB2
48	E	403	CDL	C55-C56-C57-C58
52	O	201	ZMP	O1-C10-S1-C11
52	Q	201	ZMP	O1-C10-S1-C11
55	2	502	CPL	C13-C14-C15-C16
46	J	203	3PE	C24-C25-C26-C27
46	4	501	3PE	C36-C37-C38-C39
48	Z	201	CDL	C13-C14-C15-C16
55	2	502	CPL	C31-C32-C33-C34
46	4	504	3PE	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
46	W	404	3PE	O11-C1-C2-C3
46	1	504	3PE	O11-C1-C2-C3
48	X	201	CDL	OA5-CA3-CA4-CA6
48	4	503	CDL	O1-C1-CA2-OA2
52	O	201	ZMP	C22-C1-C2-C3
54	2	503	T7X	C12-C13-C14-C15
46	4	502	3PE	O22-C21-O21-C2
48	g	201	CDL	C31-CA7-OA8-CA6
46	b	201	3PE	C24-C25-C26-C27
50	n	1101	PLC	C8B-C9B-CAA-CBA
50	W	401	PLC	C1'-C2'-C3'-C4'
48	X	201	CDL	CA6-CA4-OA6-CA5
50	W	403	PLC	C1-C2-O2-C'
52	O	201	ZMP	C9-C10-S1-C11
52	Q	201	ZMP	C9-C10-S1-C11
54	2	501	T7X	C7-C8-O16-C10
48	4	503	CDL	C51-C52-C53-C54
50	W	401	PLC	O2-C'-C1'-C2'
46	E	402	3PE	C21-C22-C23-C24
46	4	502	3PE	C1-C2-C3-O31
48	E	403	CDL	CB3-CB4-CB6-OB8
48	X	201	CDL	CA4-CA3-OA5-PA1
48	j	102	CDL	C1-CA2-OA2-PA1
48	4	503	CDL	CB3-CB4-CB6-OB8
46	4	505	3PE	C2E-C2F-C2G-C2H
50	W	402	PLC	C1'-C2'-C3'-C4'
46	W	404	3PE	O11-C1-C2-O21
46	g	202	3PE	O11-C1-C2-O21
50	1	502	PLC	O3P-C1-C2-O2
48	E	403	CDL	C35-C36-C37-C38
52	Q	201	ZMP	C6-C7-C8-C9
48	j	102	CDL	C32-C33-C34-C35
48	g	201	CDL	OA9-CA7-OA8-CA6
50	W	401	PLC	C6B-C7B-C8B-C9B
46	E	402	3PE	O21-C2-C3-O31
48	E	403	CDL	OA6-CA4-CA6-OA8
48	X	201	CDL	OB6-CB4-CB6-OB8
48	4	503	CDL	OB6-CB4-CB6-OB8
50	n	1101	PLC	O2-C2-C3-O3
50	W	402	PLC	C6'-C7'-C8'-C9'
46	4	502	3PE	C25-C26-C27-C28
48	4	503	CDL	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
50	W	403	PLC	O'-C'-O2-C2
48	4	503	CDL	C37-C38-C39-C40
48	g	201	CDL	C41-C42-C43-C44
55	2	502	CPL	C35-C36-C37-C38
48	4	503	CDL	C76-C77-C78-C79
48	4	503	CDL	C44-C45-C46-C47
46	4	501	3PE	C11-O13-P-O11
46	4	502	3PE	C11-O13-P-O11
48	g	201	CDL	CB2-OB2-PB2-OB5
50	W	401	PLC	C1-O3P-P-O4P
48	Z	201	CDL	C1-CA2-OA2-PA1
54	5	801	T7X	C8-C7-O13-P1
46	g	202	3PE	C37-C38-C39-C3A
46	E	402	3PE	C1-O11-P-O12
46	E	402	3PE	C11-O13-P-O14
46	J	203	3PE	C1-O11-P-O14
46	b	201	3PE	C1-O11-P-O12
46	4	501	3PE	C11-O13-P-O14
46	4	505	3PE	C1-O11-P-O12
46	5	802	3PE	C1-O11-P-O14
46	5	804	3PE	C1-O11-P-O12
48	g	201	CDL	CB3-OB5-PB2-OB4
48	j	102	CDL	CB2-OB2-PB2-OB3
48	j	102	CDL	CB3-OB5-PB2-OB4
48	4	503	CDL	CA2-OA2-PA1-OA3
50	K	302	PLC	C1-O3P-P-O2P
50	W	402	PLC	C1-O3P-P-O1P
50	W	402	PLC	C4-O4P-P-O2P
50	1	502	PLC	C1-O3P-P-O1P
50	5	803	PLC	C1-O3P-P-O1P
50	5	803	PLC	C1-O3P-P-O2P
50	5	803	PLC	C4-O4P-P-O1P
54	2	503	T7X	C7-O13-P1-O11
50	1	502	PLC	O3P-C1-C2-C3
48	E	403	CDL	C56-C57-C58-C59
49	J	202	LMN	OAI-CBM-CCC-CCN
46	4	504	3PE	C38-C39-C3A-C3B
46	5	804	3PE	C34-C35-C36-C37
46	b	201	3PE	C29-C2A-C2B-C2C
46	4	502	3PE	C33-C34-C35-C36
48	E	403	CDL	C13-C14-C15-C16
48	g	201	CDL	C42-C43-C44-C45

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Mol	Chain	Res	Type	Atoms
48	j	102	CDL	C52-C53-C54-C55
46	4	502	3PE	O11-C1-C2-O21
48	E	403	CDL	OA5-CA3-CA4-OA6
46	E	402	3PE	C33-C34-C35-C36
48	j	102	CDL	C73-C74-C75-C76
46	4	505	3PE	C26-C27-C28-C29
46	C	501	3PE	C2D-C2E-C2F-C2G
50	W	401	PLC	C4-C5-N-C8
48	g	201	CDL	C38-C39-C40-C41
50	W	403	PLC	O4P-C4-C5-N
50	n	1101	PLC	O4P-C4-C5-N
50	n	1101	PLC	C6'-C7'-C8'-C9'
46	5	802	3PE	O21-C2-C3-O31
48	E	403	CDL	OB6-CB4-CB6-OB8
50	K	302	PLC	O2-C2-C3-O3
54	3	201	T7X	O16-C8-C9-O18
48	g	201	CDL	CB5-C51-C52-C53
46	b	201	3PE	C2-C1-O11-P
50	W	403	PLC	C5B-C6B-C7B-C8B
48	g	201	CDL	C15-C16-C17-C18
48	E	403	CDL	C57-C58-C59-C60
46	1	504	3PE	C35-C36-C37-C38
50	W	401	PLC	C4-C5-N-C7
46	C	501	3PE	C28-C29-C2A-C2B
55	2	502	CPL	C19-C20-C21-C22
55	2	502	CPL	C22-C23-C24-C25
46	J	203	3PE	C36-C37-C38-C39
48	Z	201	CDL	C18-C19-C20-C21
48	4	503	CDL	CA6-CA4-OA6-CA5
54	5	801	T7X	C9-C8-O16-C10
48	E	403	CDL	OA5-CA3-CA4-CA6
48	4	503	CDL	C71-C72-C73-C74
46	J	201	3PE	C22-C23-C24-C25
48	X	201	CDL	C18-C19-C20-C21
50	W	401	PLC	C4-C5-N-C6
48	X	201	CDL	C59-C60-C61-C62
46	1	504	3PE	C34-C35-C36-C37
50	W	401	PLC	C5'-C6'-C7'-C8'
50	W	403	PLC	C1'-C'-O2-C2
48	j	102	CDL	C33-C34-C35-C36
46	C	501	3PE	C11-O13-P-O11
46	1	504	3PE	C11-O13-P-O11

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Mol	Chain	Res	Type	Atoms
48	Z	201	CDL	CA2-OA2-PA1-OA5
48	Z	201	CDL	CB3-OB5-PB2-OB2
50	W	403	PLC	C1-O3P-P-O4P
46	g	202	3PE	C27-C28-C29-C2A
46	g	202	3PE	C2C-C2D-C2E-C2F
46	5	802	3PE	C32-C33-C34-C35
48	4	503	CDL	C32-C33-C34-C35
49	J	202	LMN	OBY-CCR-O4-C4
50	5	803	PLC	C1-C2-C3-O3
47	E	401	NDP	O4D-C1D-N1N-C6N
47	E	401	NDP	PN-O3-PA-O2A
49	J	202	LMN	CBE-CBG-CBI-CBK
46	E	402	3PE	C3A-C3B-C3C-C3D
46	4	505	3PE	C32-C31-O31-C3
46	4	502	3PE	C2-C1-O11-P
48	Z	201	CDL	CA4-CA3-OA5-PA1
49	J	202	LMN	CAZ-CBB-CBD-CBF
46	g	202	3PE	C28-C29-C2A-C2B
46	5	802	3PE	C32-C31-O31-C3
46	1	503	3PE	C21-C22-C23-C24
47	E	401	NDP	C2D-C1D-N1N-C6N
48	E	403	CDL	C52-C53-C54-C55
46	4	505	3PE	C3B-C3C-C3D-C3E
46	4	502	3PE	O13-C11-C12-N
46	5	802	3PE	O13-C11-C12-N
48	Z	201	CDL	C55-C56-C57-C58
46	5	802	3PE	O32-C31-O31-C3
46	b	201	3PE	C2B-C2C-C2D-C2E
54	2	503	T7X	C25-C26-C27-C28
46	W	404	3PE	O21-C2-C3-O31
46	g	202	3PE	O21-C2-C3-O31
48	E	403	CDL	C11-C12-C13-C14
54	2	501	T7X	C34-C35-C36-C37
54	3	201	T7X	C36-C37-C38-C39
46	1	503	3PE	C2-C1-O11-P
46	4	504	3PE	C3B-C3C-C3D-C3E
50	K	302	PLC	C1'-C2'-C3'-C4'
46	4	504	3PE	C22-C23-C24-C25
46	5	802	3PE	C3A-C3B-C3C-C3D
46	1	503	3PE	C28-C29-C2A-C2B
48	E	403	CDL	C61-C62-C63-C64
52	Q	201	ZMP	C19-C18-C21-O5

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Mol	Chain	Res	Type	Atoms
46	1	503	3PE	C34-C35-C36-C37
46	4	505	3PE	O32-C31-O31-C3
54	3	201	T7X	C9-C8-O16-C10
48	j	102	CDL	C58-C59-C60-C61
48	j	102	CDL	C17-C18-C19-C20
50	5	803	PLC	C1-O3P-P-O4P
54	2	501	T7X	C22-C23-C24-C25
54	3	201	T7X	C15-C16-C17-C18
54	3	201	T7X	C16-C17-C18-C19
54	3	201	T7X	C19-C20-C21-C22
46	4	504	3PE	C27-C28-C29-C2A
48	j	102	CDL	C72-C73-C74-C75
55	2	502	CPL	C2-C1-O3P-P
48	g	201	CDL	OA5-CA3-CA4-OA6
46	C	501	3PE	C3D-C3E-C3F-C3G
46	1	503	3PE	C25-C26-C27-C28
48	g	201	CDL	C31-C32-C33-C34
54	2	503	T7X	C10-C12-C13-C14
52	O	201	ZMP	C12-C11-S1-C10
48	X	201	CDL	C60-C61-C62-C63
55	2	502	CPL	C45-C46-C47-C48
46	C	501	3PE	C2E-C2F-C2G-C2H
46	5	802	3PE	C36-C37-C38-C39
46	4	502	3PE	C37-C38-C39-C3A
46	4	505	3PE	O31-C31-C32-C33
48	Z	201	CDL	O1-C1-CA2-OA2
46	W	404	3PE	C32-C33-C34-C35
46	1	503	3PE	C26-C27-C28-C29
46	E	402	3PE	C37-C38-C39-C3A
52	Q	201	ZMP	C2-C3-C4-C5
46	g	202	3PE	C2E-C2F-C2G-C2H
46	5	802	3PE	C23-C24-C25-C26
46	5	804	3PE	C35-C36-C37-C38
46	J	201	3PE	O11-C1-C2-O21
46	4	504	3PE	O11-C1-C2-O21
46	4	504	3PE	C3D-C3E-C3F-C3G
48	X	201	CDL	C52-C53-C54-C55
48	Z	201	CDL	OA5-CA3-CA4-CA6
46	4	504	3PE	C3A-C3B-C3C-C3D
50	W	402	PLC	C4'-C5'-C6'-C7'
48	X	201	CDL	OB7-CB5-OB6-CB4
46	E	402	3PE	C38-C39-C3A-C3B

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Mol	Chain	Res	Type	Atoms
46	5	802	3PE	O21-C21-C22-C23
50	5	803	PLC	O2-C'-C1'-C2'
46	b	201	3PE	O21-C21-C22-C23
54	2	503	T7X	C24-C25-C26-C27
48	X	201	CDL	C15-C16-C17-C18
49	J	202	LMN	CAA-CAW-CAY-CBA
46	C	501	3PE	O31-C31-C32-C33
46	4	505	3PE	O21-C21-C22-C23
54	2	501	T7X	O16-C10-C12-C13
48	j	102	CDL	C53-C54-C55-C56
46	1	504	3PE	O31-C31-C32-C33
55	2	502	CPL	C42-C43-C44-C45
46	W	404	3PE	C1-C2-C3-O31
48	4	503	CDL	CA3-CA4-CA6-OA8
48	4	503	CDL	C1-CB2-OB2-PB2
55	2	502	CPL	O2-C31-C32-C33
46	1	504	3PE	C26-C27-C28-C29
46	4	504	3PE	O31-C31-C32-C33
46	1	504	3PE	O22-C21-C22-C23
46	J	201	3PE	O32-C31-C32-C33
50	W	402	PLC	C2B-C1B-CB-O3
49	J	202	LMN	OAJ-CBN-CCD-OBZ
48	4	503	CDL	C41-C42-C43-C44
46	4	504	3PE	O21-C21-C22-C23
46	C	501	3PE	C3E-C3F-C3G-C3H
48	E	403	CDL	C36-C37-C38-C39
46	C	501	3PE	O21-C21-C22-C23
50	W	403	PLC	C2B-C1B-CB-O3
48	j	102	CDL	C18-C19-C20-C21
52	Q	201	ZMP	O4-C17-C18-C19
46	J	201	3PE	O21-C21-C22-C23
54	5	801	T7X	O18-C11-C31-C32
50	W	401	PLC	C8B-C9B-CAA-CBA
50	W	402	PLC	C3B-C4B-C5B-C6B
47	E	401	NDP	PN-O3-PA-O1A
46	E	402	3PE	C35-C36-C37-C38
53	1	501	UQ9	C5-C4-O4-C4M
48	X	201	CDL	C51-CB5-OB6-CB4
46	C	501	3PE	O32-C31-C32-C33
50	5	803	PLC	O'-C'-C1'-C2'
55	2	502	CPL	O31-C31-C32-C33
48	Z	201	CDL	C32-C31-CA7-OA8

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Mol	Chain	Res	Type	Atoms
48	Z	201	CDL	C52-C51-CB5-OB6
54	2	501	T7X	O17-C10-C12-C13
49	j	101	LMN	OAJ-CBN-CCD-OBZ
46	1	504	3PE	O32-C31-C32-C33
46	C	501	3PE	O22-C21-C22-C23
46	b	201	3PE	C2A-C2B-C2C-C2D
46	5	804	3PE	C24-C25-C26-C27
46	5	802	3PE	O22-C21-C22-C23
46	1	503	3PE	O21-C21-C22-C23
50	K	302	PLC	C1B-C2B-C3B-C4B
50	W	402	PLC	C2B-C1B-CB-OB
46	C	501	3PE	C11-O13-P-O14
46	J	203	3PE	C11-O13-P-O14
46	g	202	3PE	C11-O13-P-O14
46	1	504	3PE	C11-O13-P-O14
46	4	505	3PE	C11-O13-P-O12
48	E	403	CDL	CB2-OB2-PB2-OB3
48	X	201	CDL	CA2-OA2-PA1-OA4
48	Z	201	CDL	CA2-OA2-PA1-OA3
48	j	102	CDL	CB3-OB5-PB2-OB3
50	n	1101	PLC	C3'-C4'-C5'-C6'
46	4	504	3PE	O32-C31-C32-C33
48	Z	201	CDL	C52-C51-CB5-OB7
46	J	201	3PE	O11-C1-C2-C3
46	4	502	3PE	C22-C23-C24-C25
46	1	504	3PE	O13-C11-C12-N
46	4	504	3PE	O13-C11-C12-N
46	4	504	3PE	O22-C21-C22-C23
48	E	403	CDL	C38-C39-C40-C41
46	b	201	3PE	O22-C21-C22-C23
46	J	203	3PE	O31-C31-C32-C33
46	J	201	3PE	O22-C21-C22-C23
46	4	505	3PE	O22-C21-C22-C23
54	5	801	T7X	O19-C11-C31-C32
48	X	201	CDL	C14-C15-C16-C17
54	3	201	T7X	C7-C8-O16-C10
50	W	403	PLC	OB-CB-O3-C3
46	1	503	3PE	O22-C21-C22-C23
54	3	201	T7X	C13-C14-C15-C16
48	g	201	CDL	C32-C31-CA7-OA8
48	4	503	CDL	C14-C15-C16-C17
46	g	202	3PE	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
46	C	501	3PE	C2C-C2D-C2E-C2F
48	4	503	CDL	C56-C57-C58-C59
50	W	403	PLC	C2B-C1B-CB-OB
48	Z	201	CDL	C15-C16-C17-C18
48	Z	201	CDL	OA5-CA3-CA4-OA6
50	W	403	PLC	O3P-C1-C2-O2
48	E	403	CDL	C32-C31-CA7-OA8
48	Z	201	CDL	C72-C71-CB7-OB8
46	4	504	3PE	C21-C22-C23-C24
48	Z	201	CDL	C72-C71-CB7-OB9
48	g	201	CDL	C32-C31-CA7-OA9
48	Z	201	CDL	C32-C31-CA7-OA9
46	4	505	3PE	C3C-C3D-C3E-C3F
48	X	201	CDL	C12-C11-CA5-OA6
50	W	402	PLC	O2-C'-C1'-C2'
46	4	502	3PE	C2C-C2D-C2E-C2F
48	Z	201	CDL	C17-C18-C19-C20

There are no ring outliers.

35 monomers are involved in 103 short contacts:

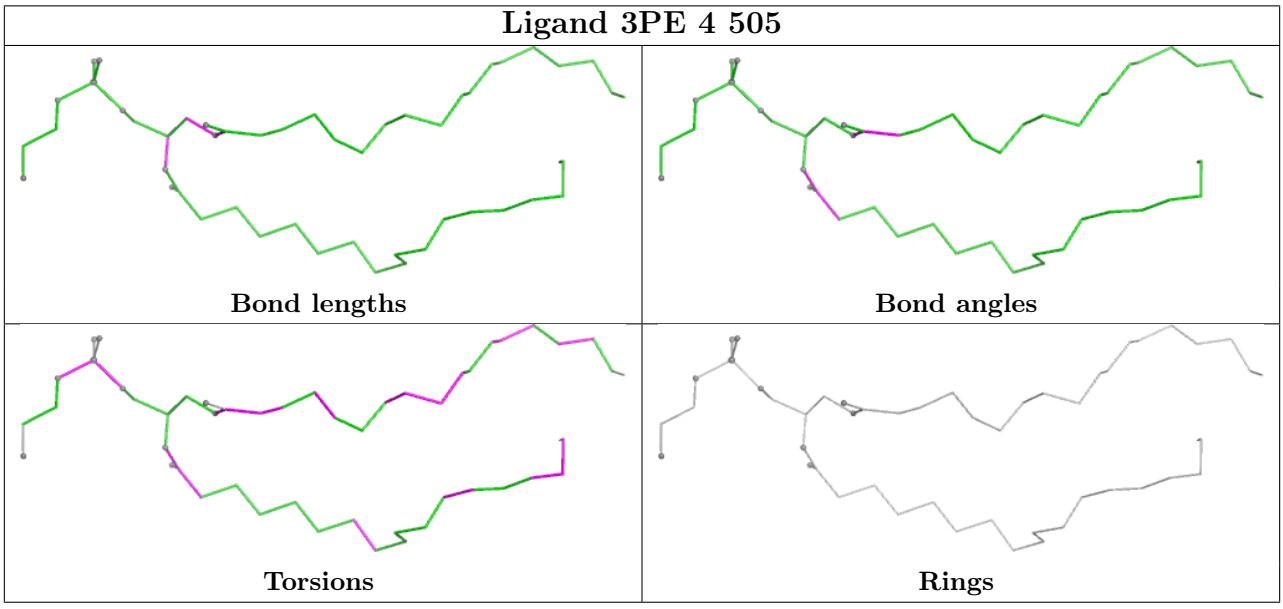
Mol	Chain	Res	Type	Clashes	Symm-Clashes
46	4	505	3PE	4	0
46	5	802	3PE	3	0
50	K	302	PLC	5	0
50	1	502	PLC	1	0
46	5	804	3PE	1	0
49	j	101	LMN	2	0
50	n	1101	PLC	3	0
55	2	502	CPL	7	0
46	4	501	3PE	2	0
46	1	503	3PE	2	0
46	g	202	3PE	2	0
54	5	801	T7X	1	0
52	Q	201	ZMP	3	0
53	1	501	UQ9	6	0
43	B	501	SF4	1	0
43	K	301	SF4	1	0
50	5	803	PLC	1	0
50	W	402	PLC	3	0
48	4	503	CDL	8	0
48	j	102	CDL	3	0

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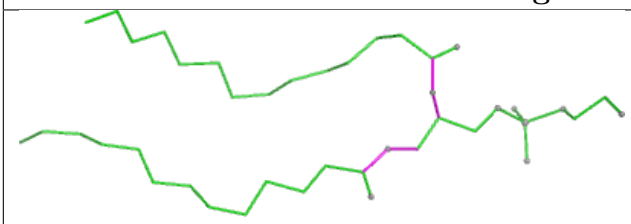
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
52	O	201	ZMP	3	0
50	W	401	PLC	2	0
50	W	403	PLC	2	0
54	2	503	T7X	2	0
46	W	404	3PE	1	0
48	Z	201	CDL	2	0
48	E	403	CDL	5	0
46	b	201	3PE	2	0
46	J	203	3PE	5	0
48	g	201	CDL	6	0
46	C	501	3PE	4	0
46	4	502	3PE	4	0
48	X	201	CDL	9	0
45	B	502	FMN	1	0
49	J	202	LMN	5	0

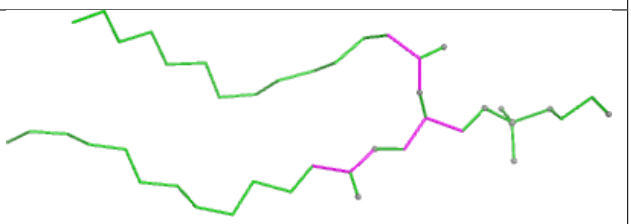
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



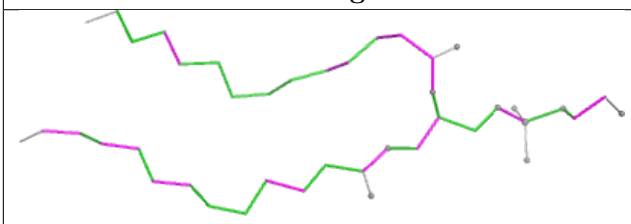
Ligand 3PE 5 802



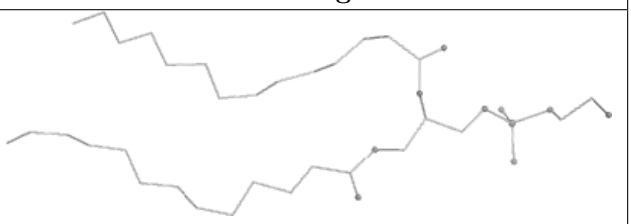
Bond lengths



Bond angles

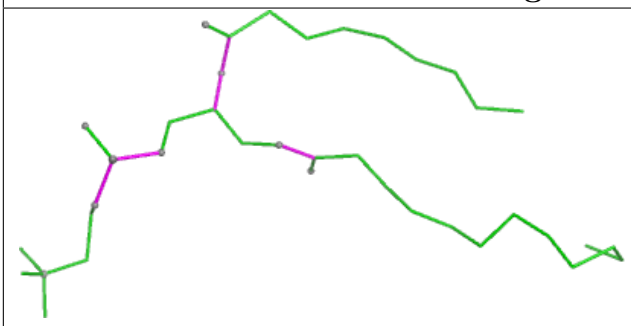


Torsions

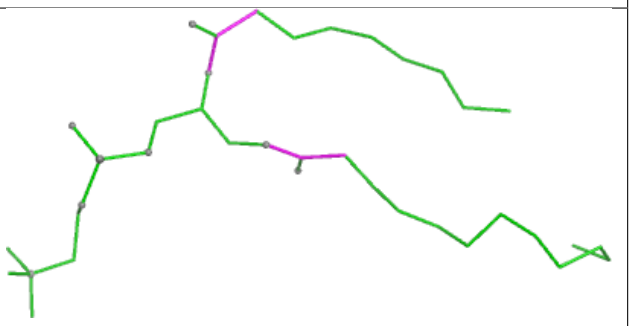


Rings

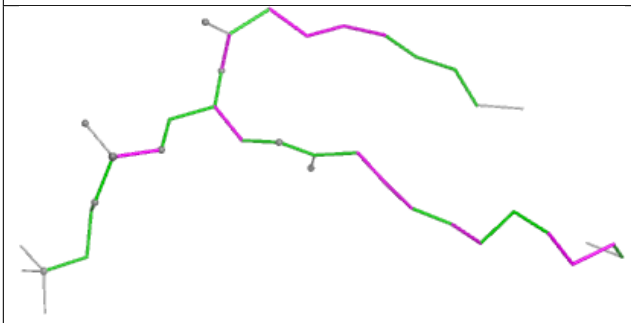
Ligand PLC K 302



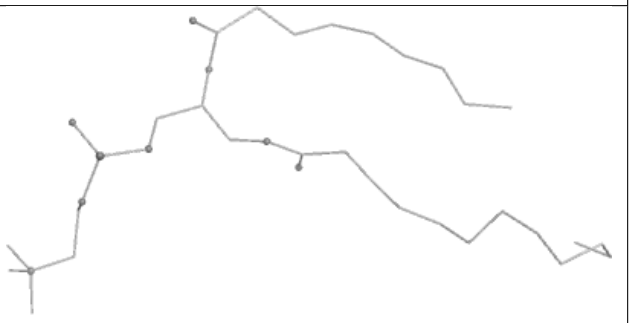
Bond lengths



Bond angles

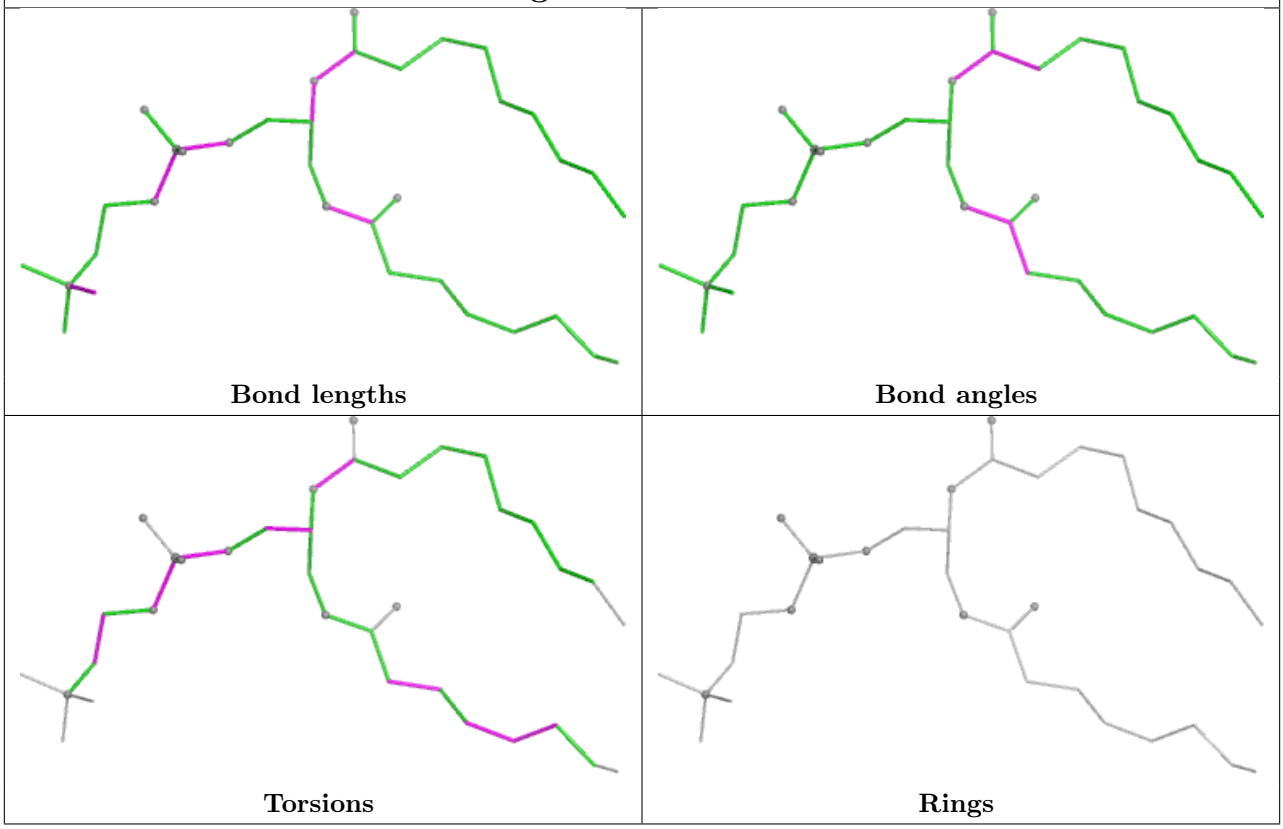


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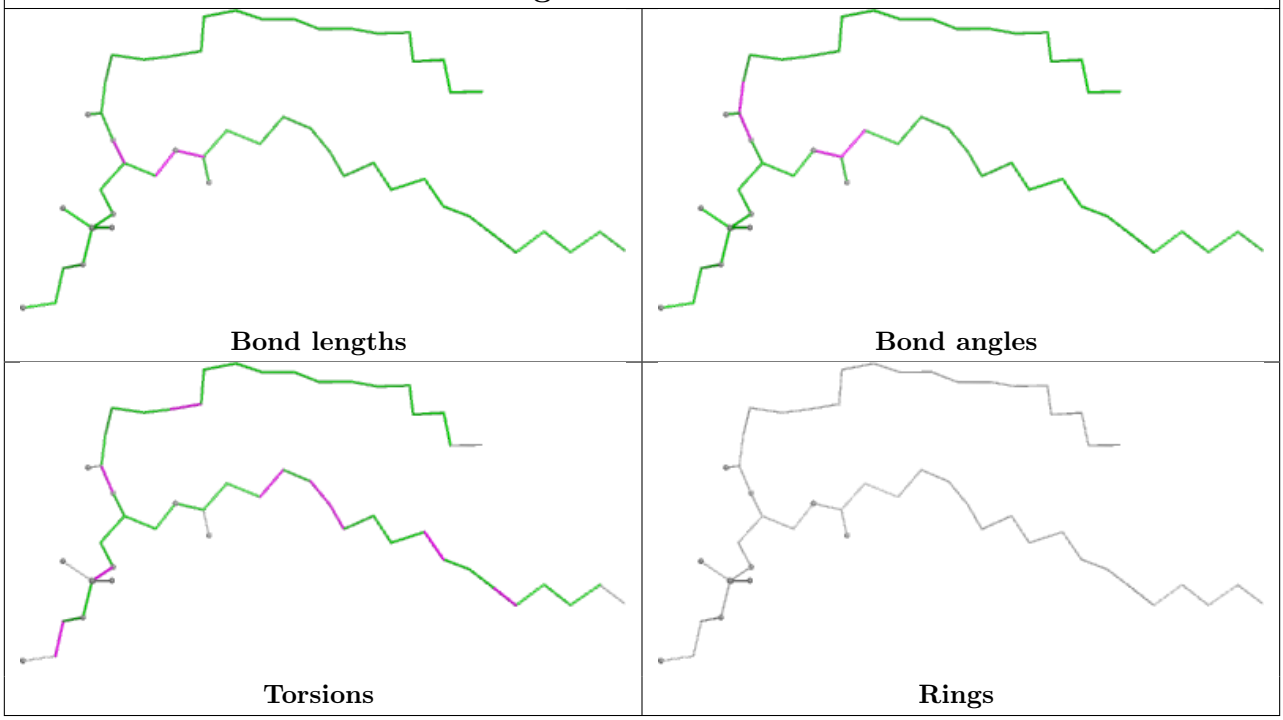


Rings

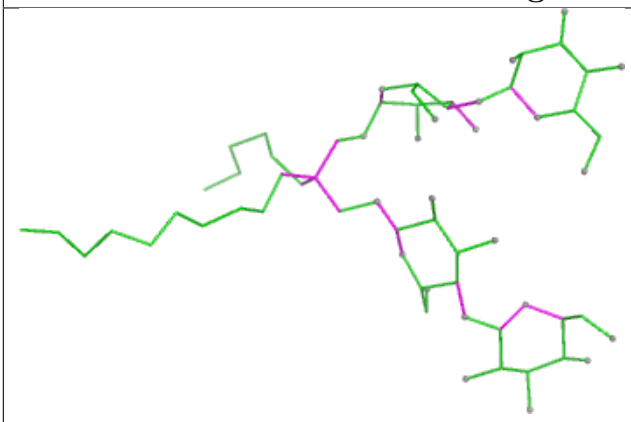
Ligand PLC 1 502



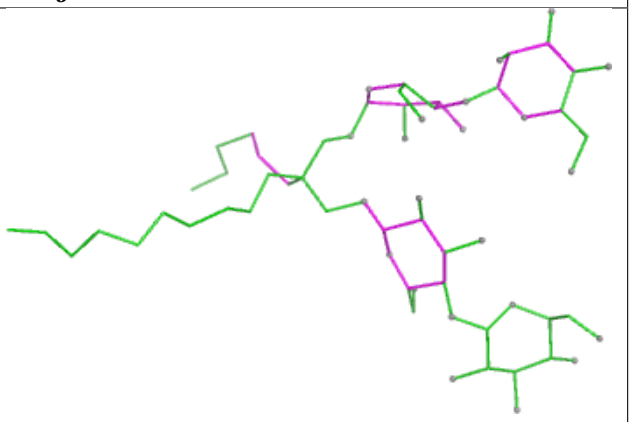
Ligand 3PE 5 804



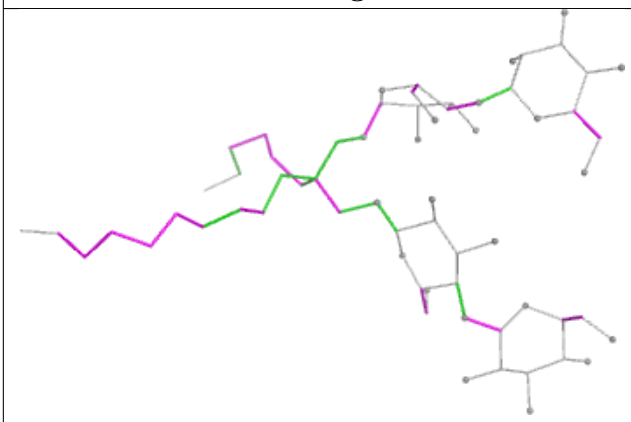
Ligand LMN j 101



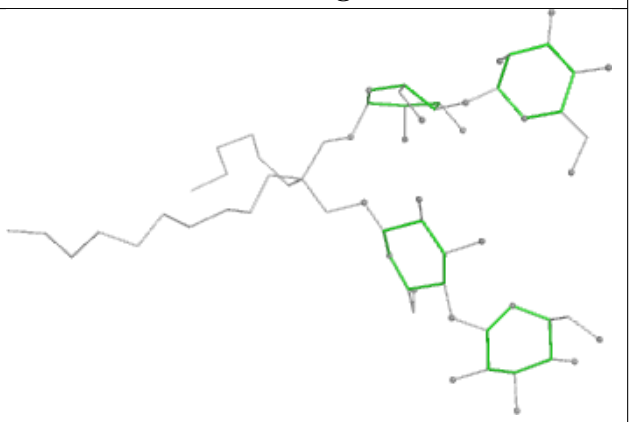
Bond lengths



Bond angles

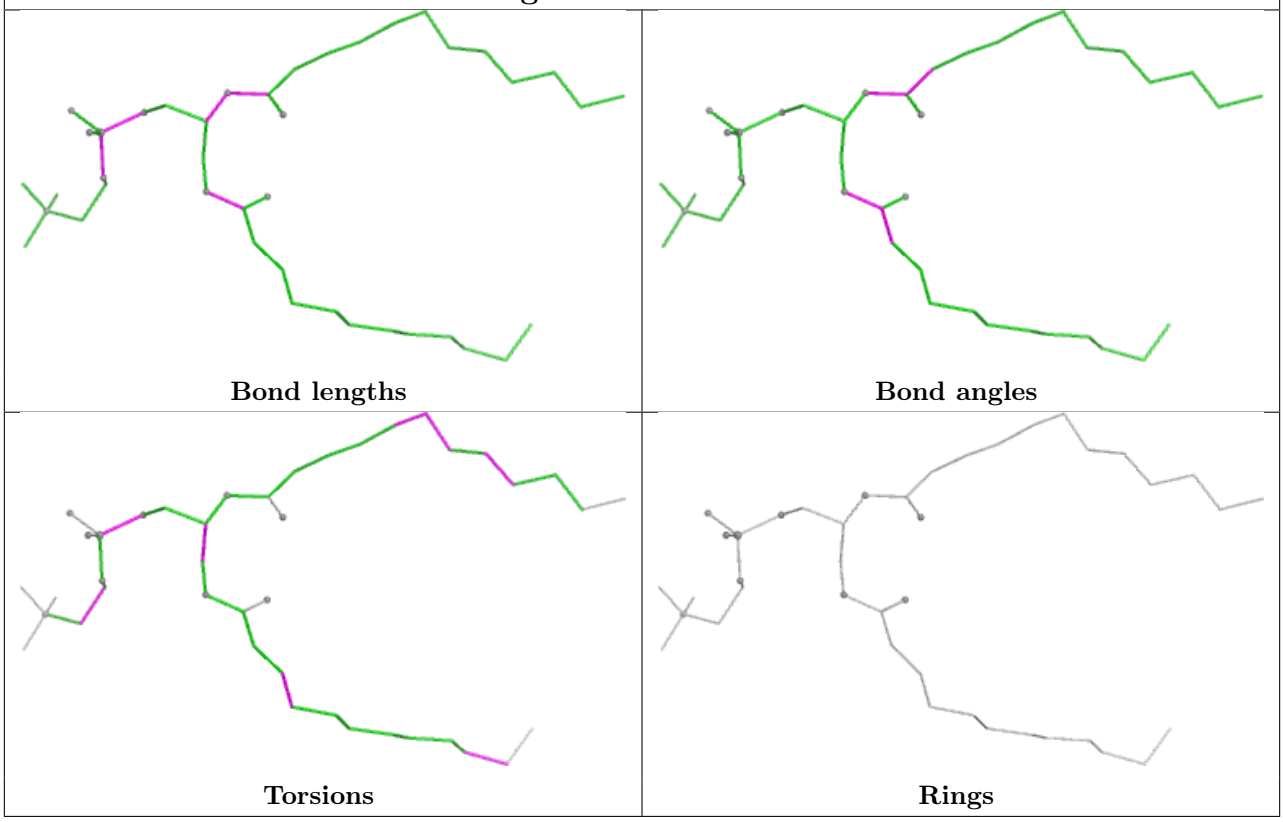


Torsions



Rings

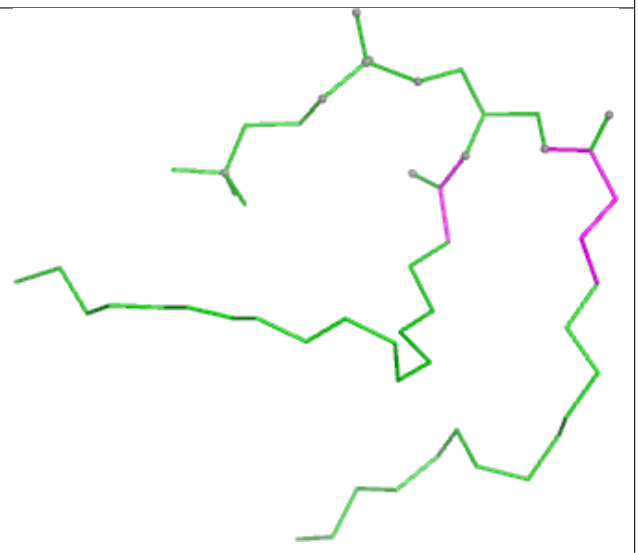
Ligand PLC n 1101



Ligand CPL 2 502



Bond lengths



Bond angles

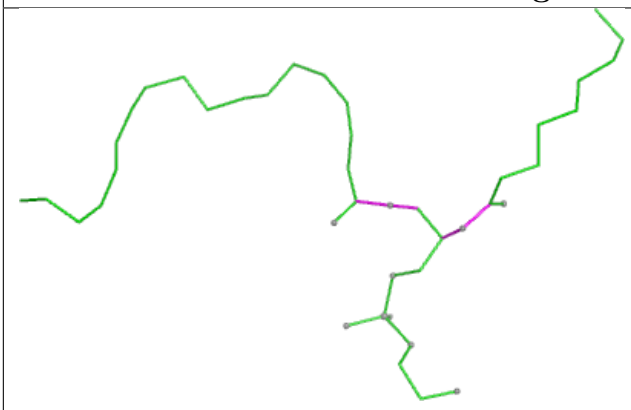


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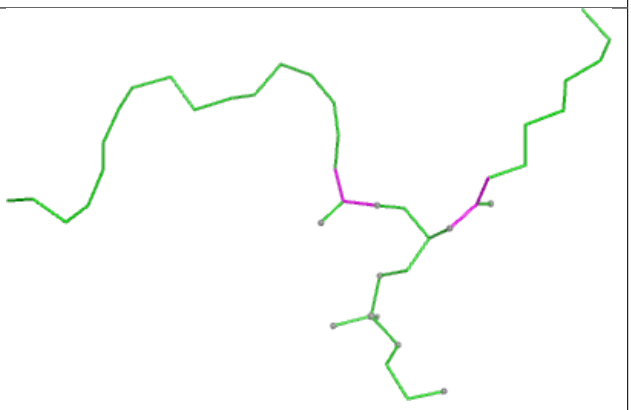


Rings

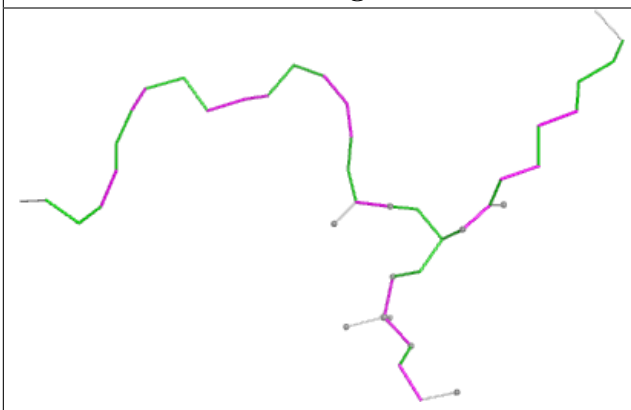
Ligand 3PE 4 501



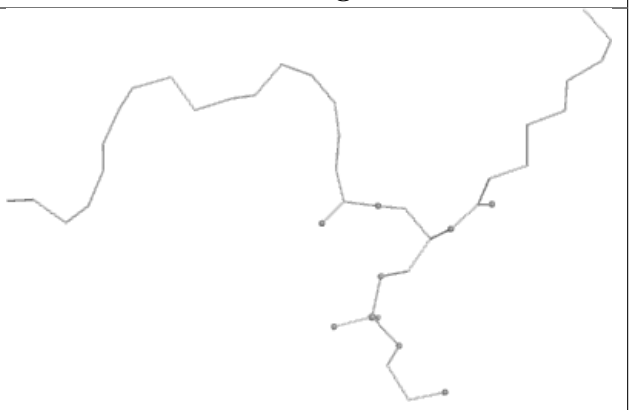
Bond lengths



Bond angles

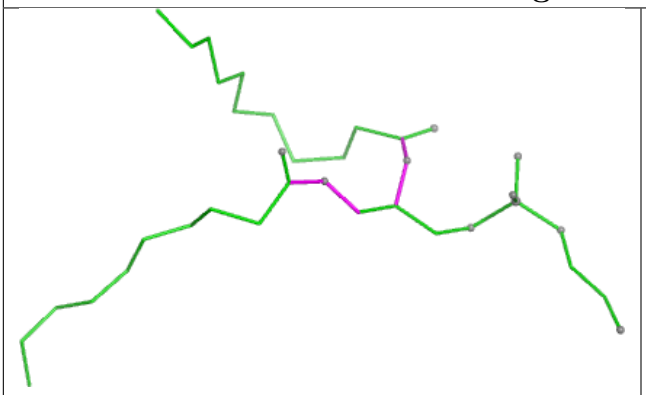


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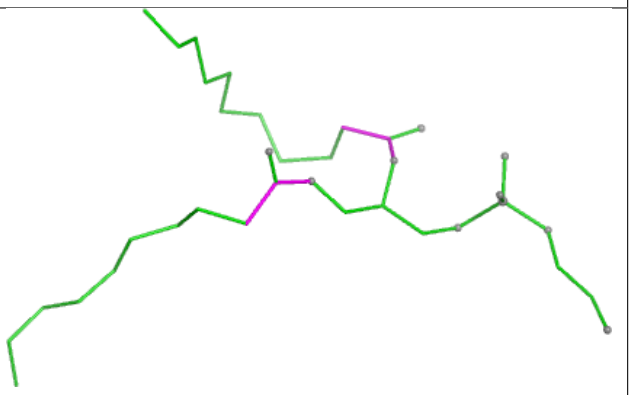


Rings

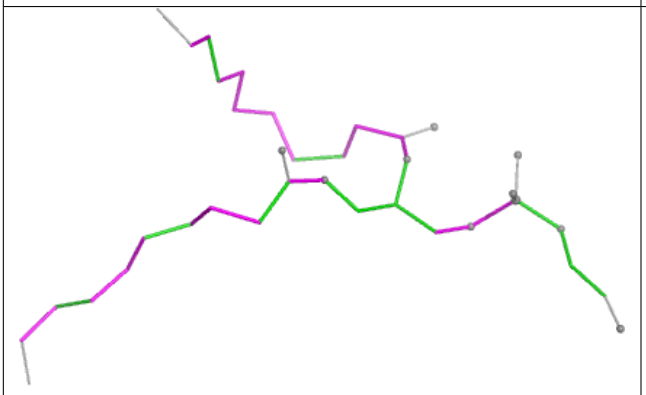
Ligand 3PE 1 503



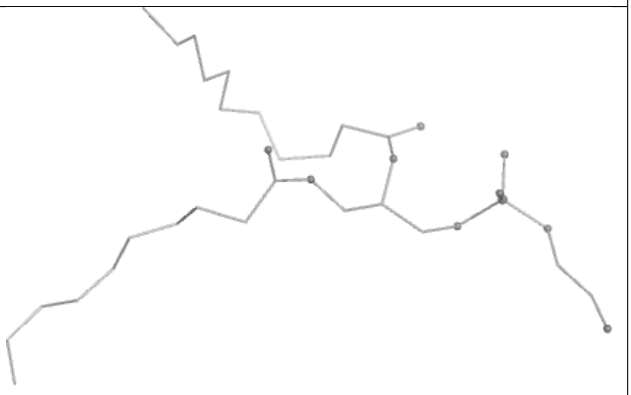
Bond lengths



Bond angles

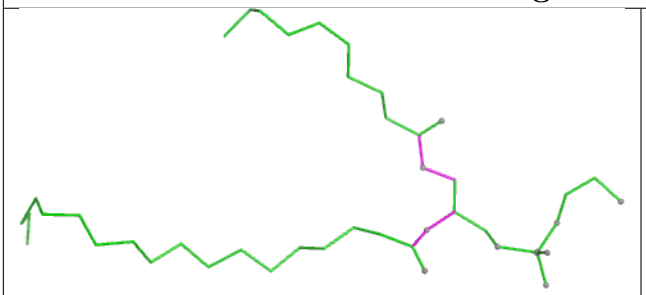


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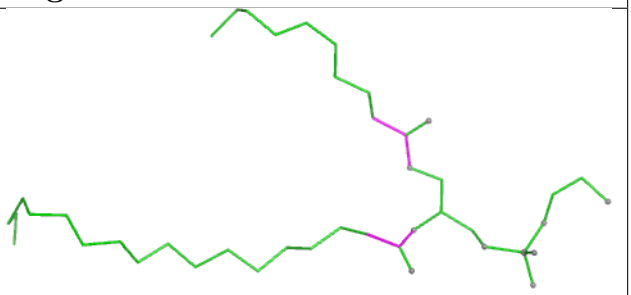


Rings

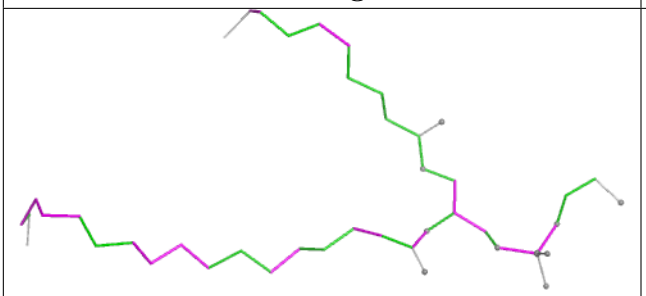
Ligand 3PE g 202



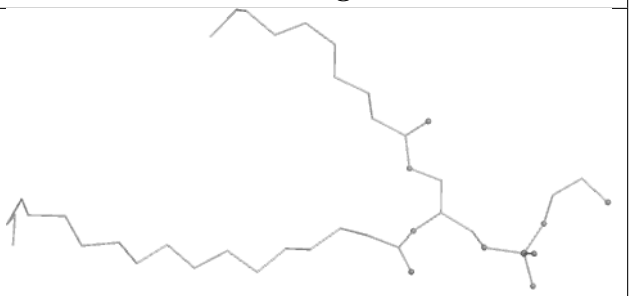
Bond lengths



Bond angles

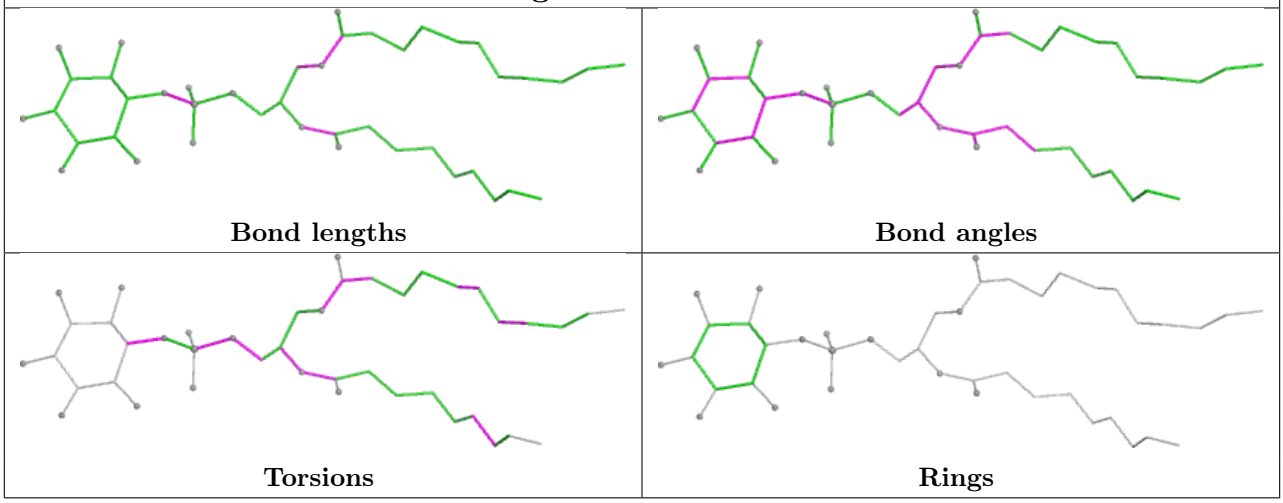


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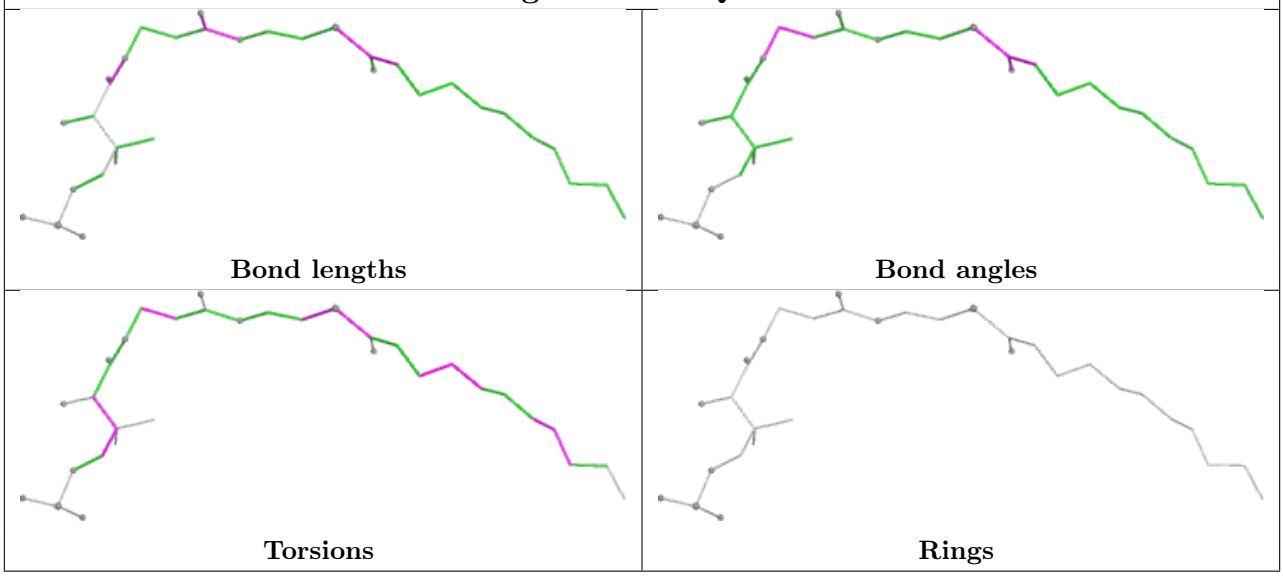


Rings

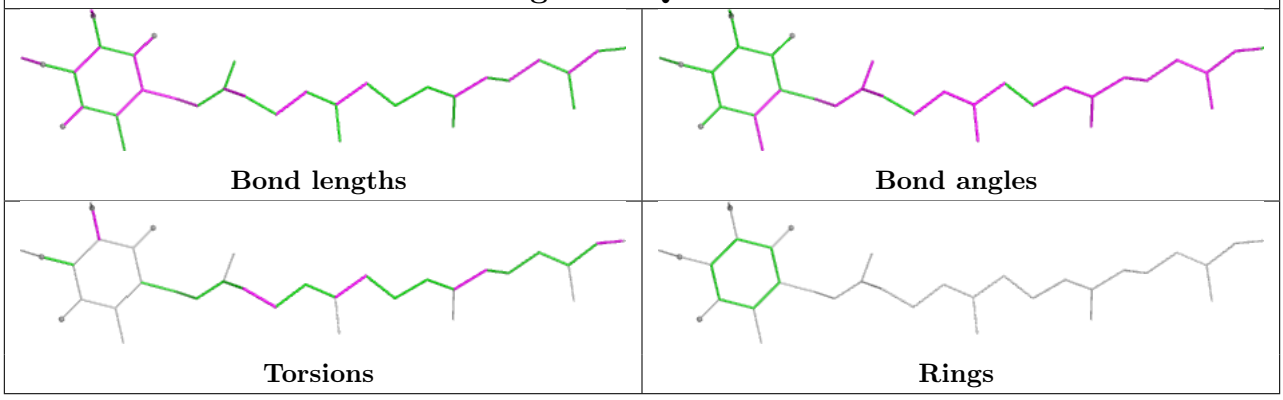
Ligand T7X 5 801



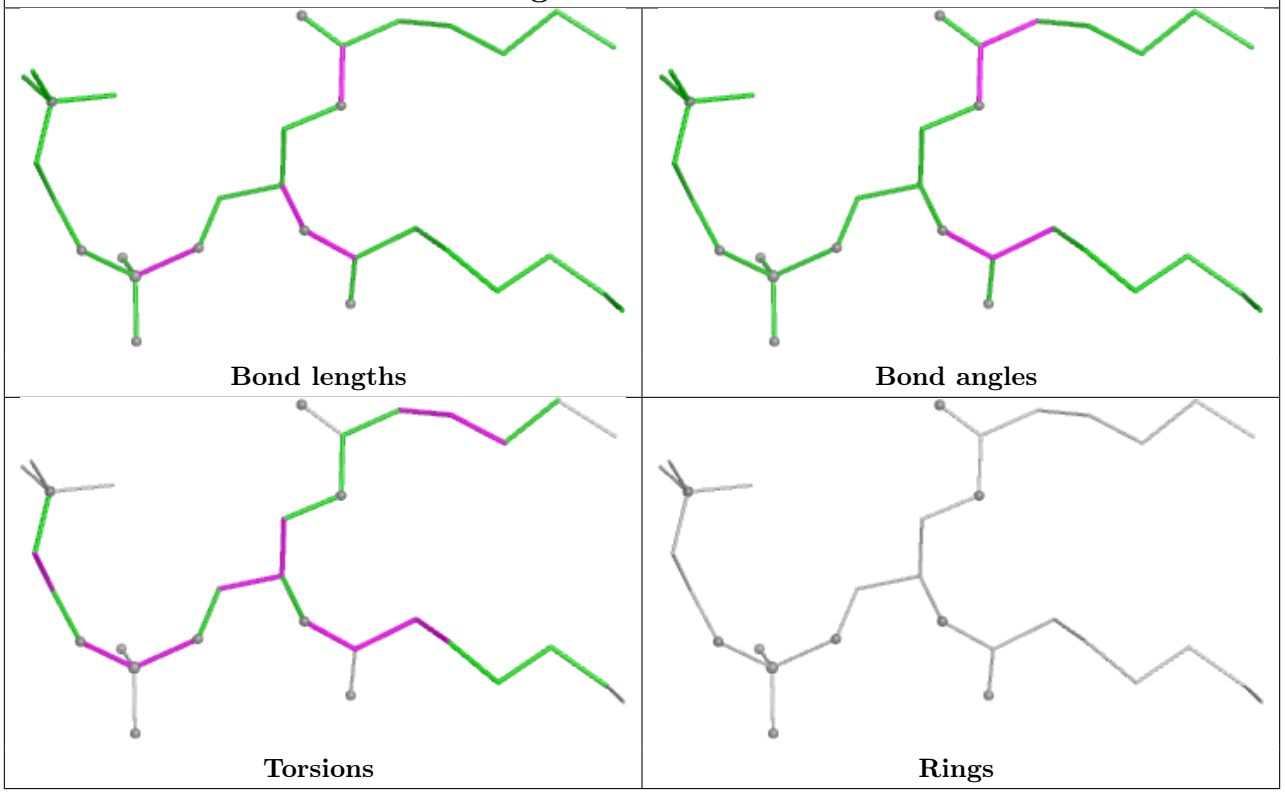
Ligand ZMP Q 201



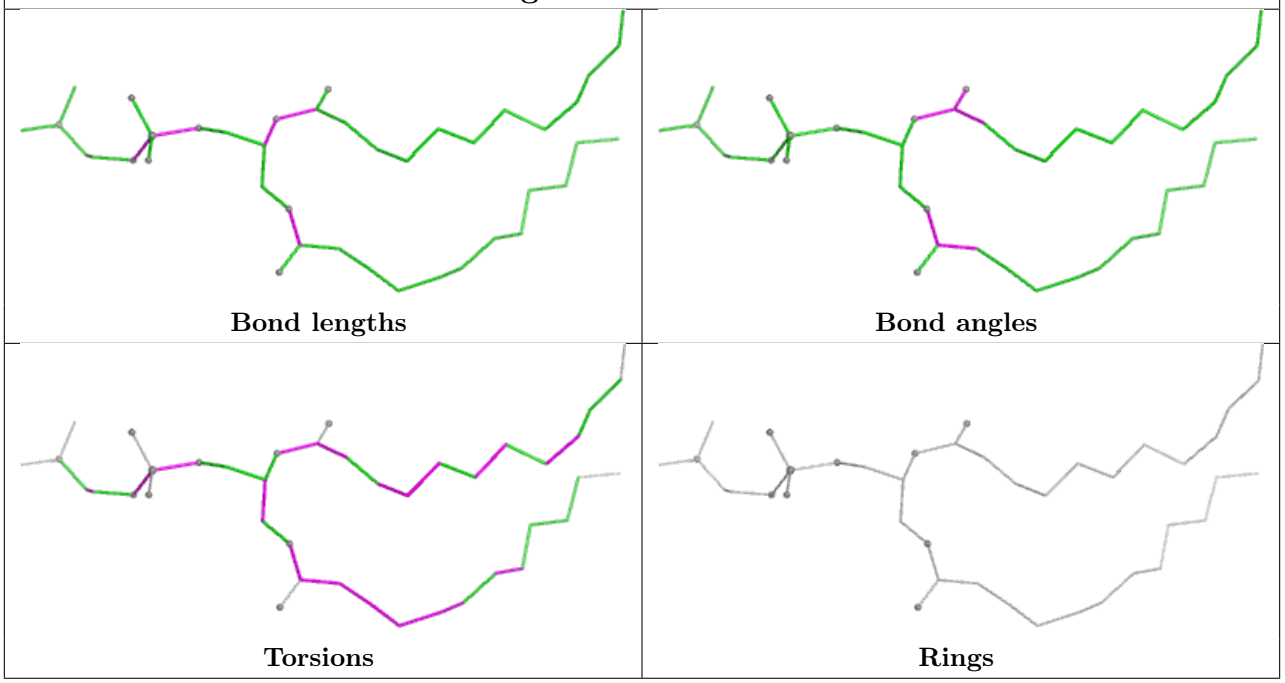
Ligand UQ9 1 501



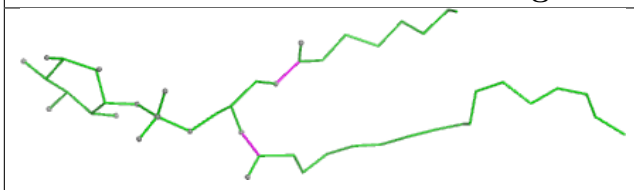
Ligand PLC 5 803



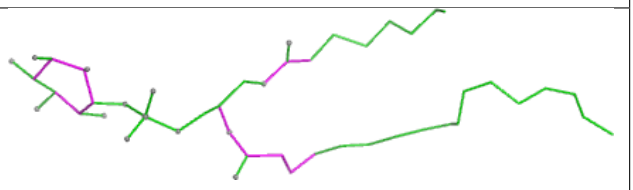
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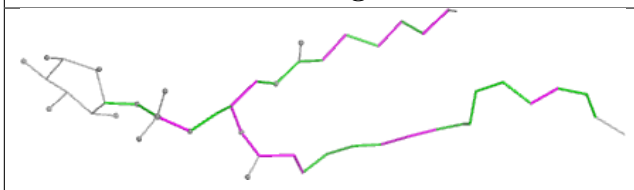
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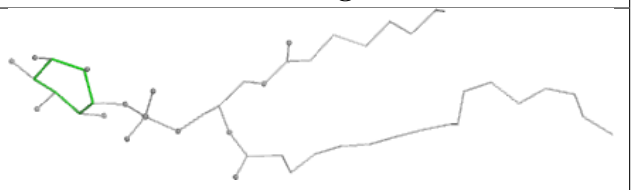
Bond lengths



Bond angles

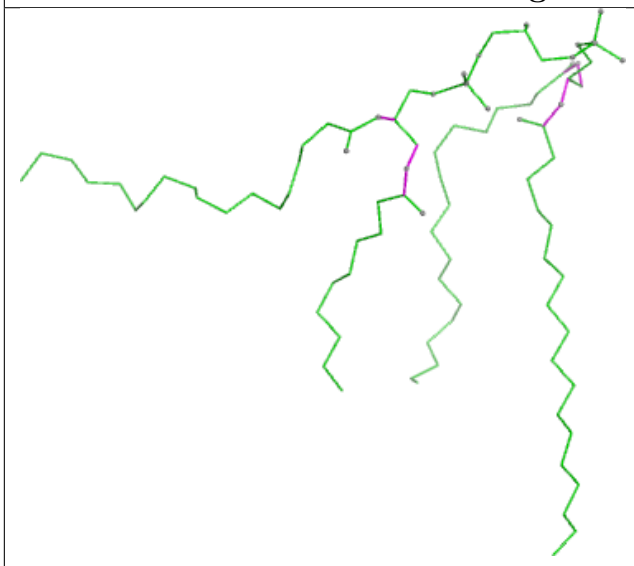


Torsions

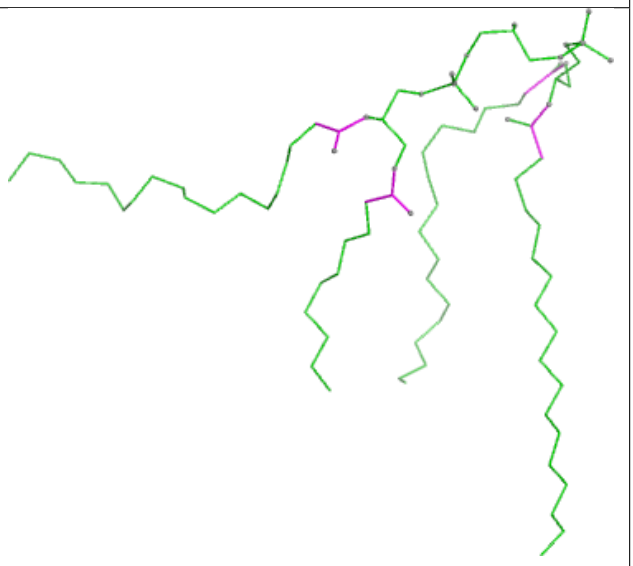


Rings

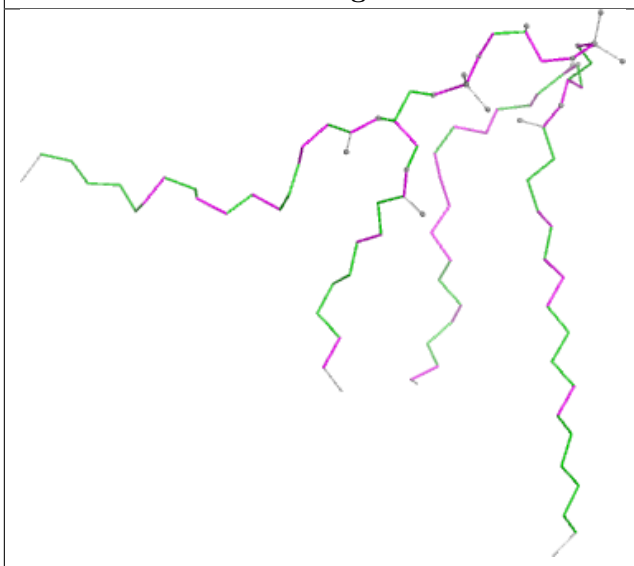
Ligand CDL 4 503



Bond lengths



Bond angles

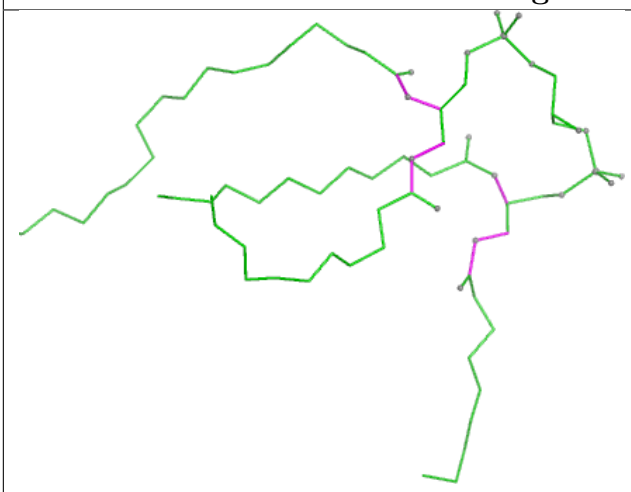


Torsions



Rings

Ligand CDL j 102



Bond lengths



Bond angles



Torsions

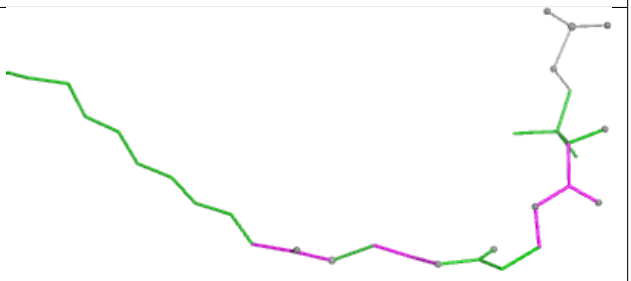


Rings

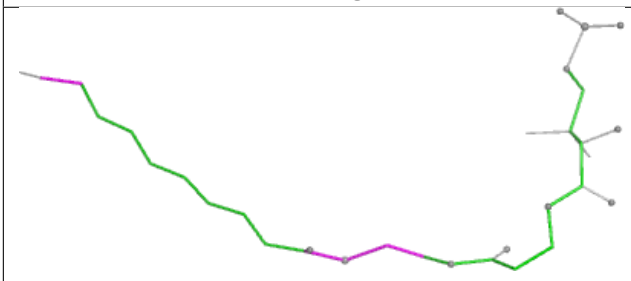
Ligand ZMP O 201



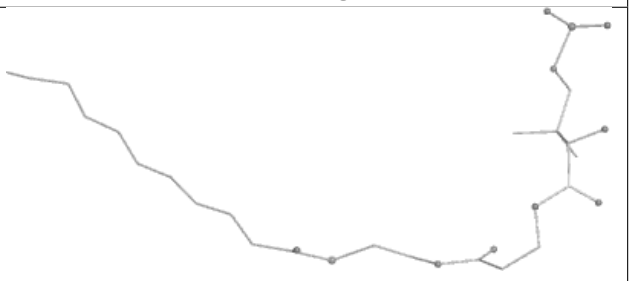
Bond lengths



Bond angles

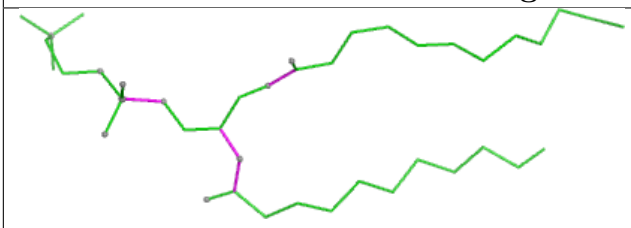


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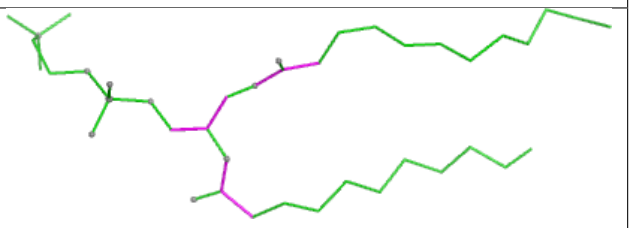


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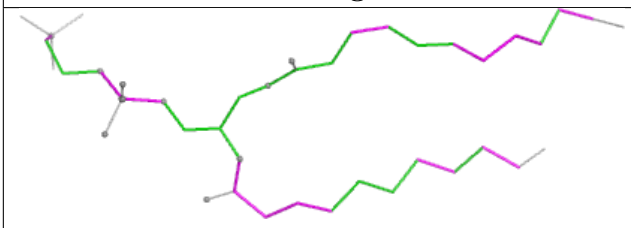
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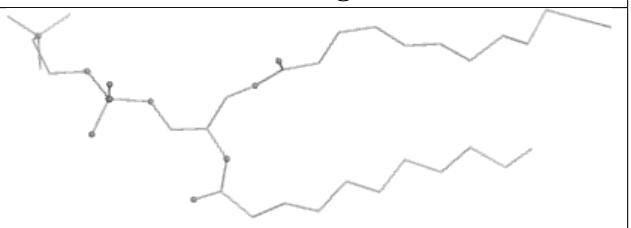
Bond lengths



Bond angles

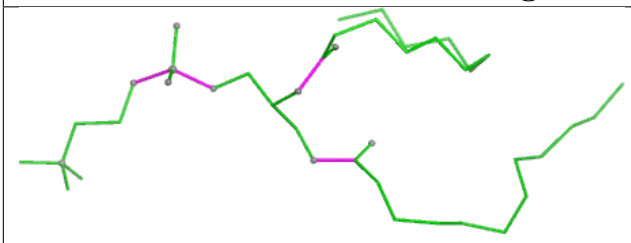


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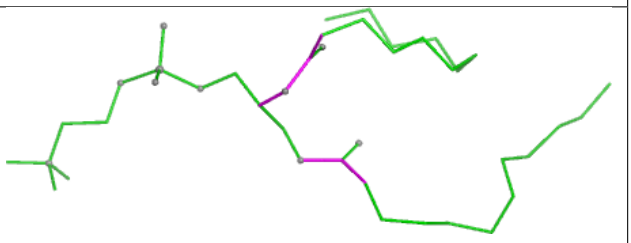


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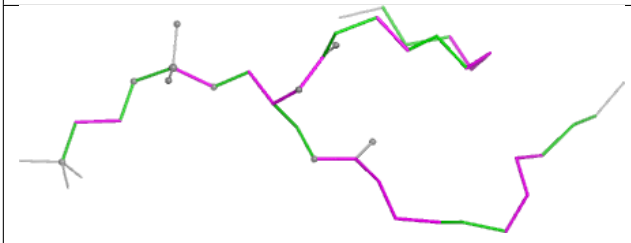
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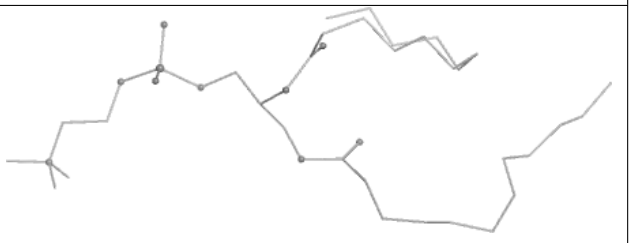
Bond lengths



Bond angles

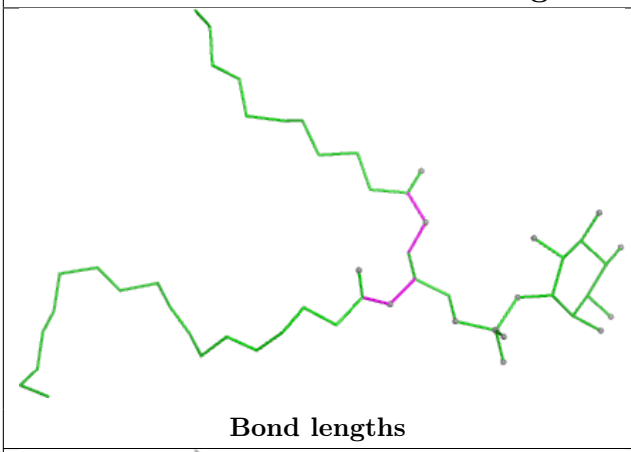


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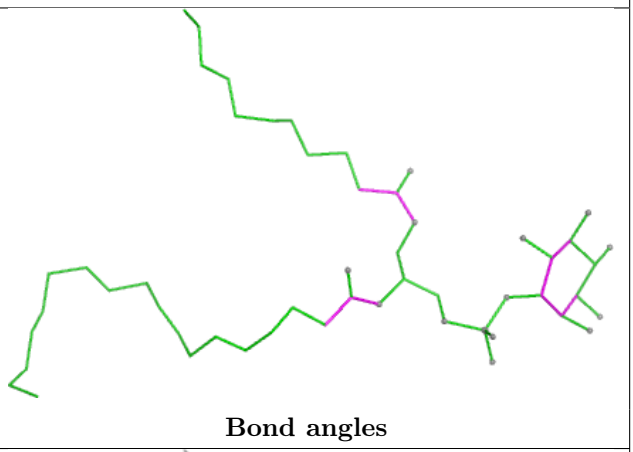


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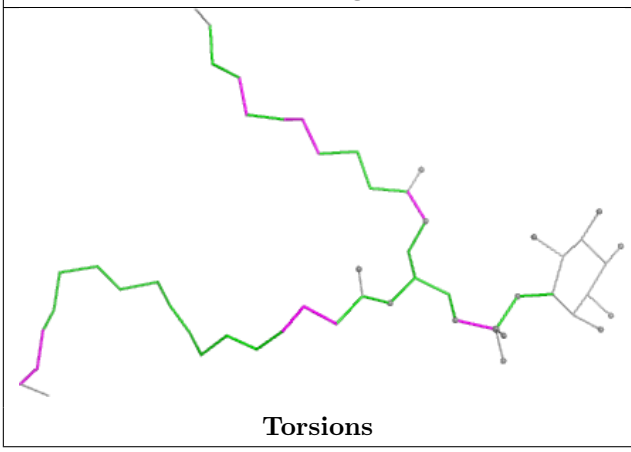
Ligand T7X 2 503



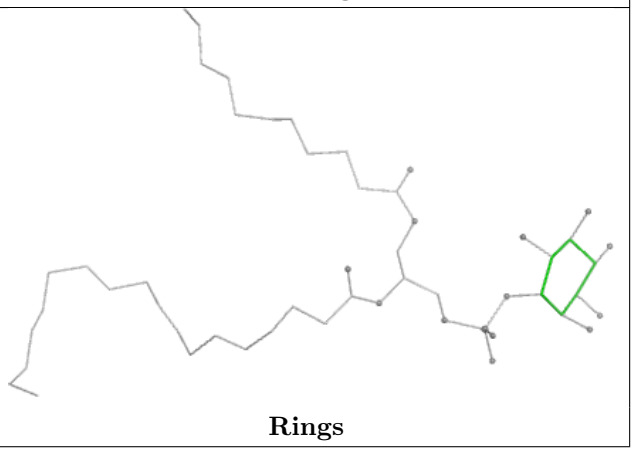
Bond lengths



Bond angles

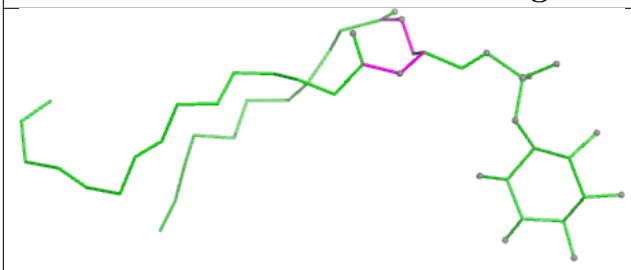


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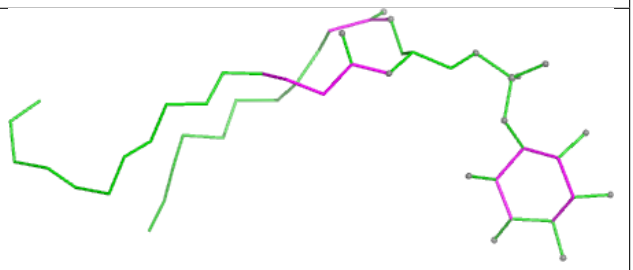


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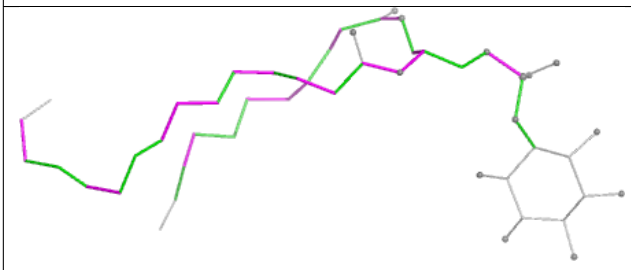
Ligand T7X 3 201



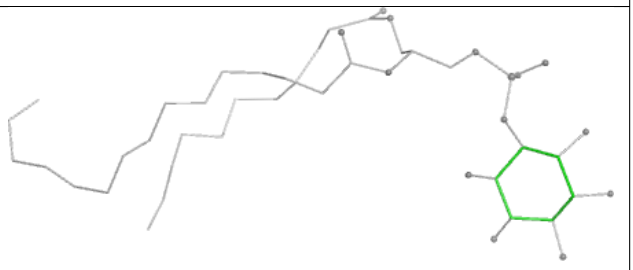
Bond lengths



Bond angles

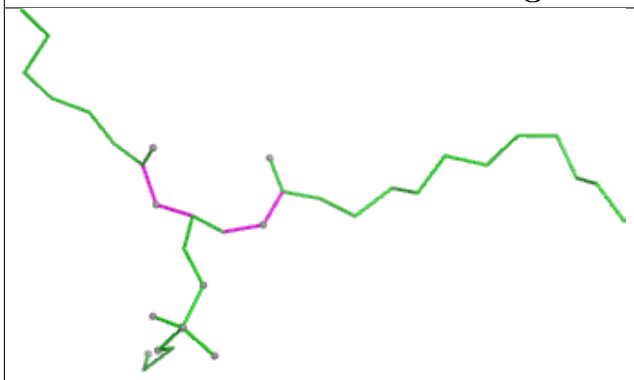


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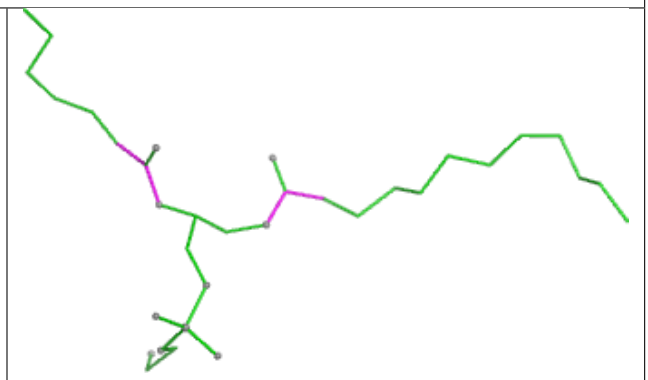


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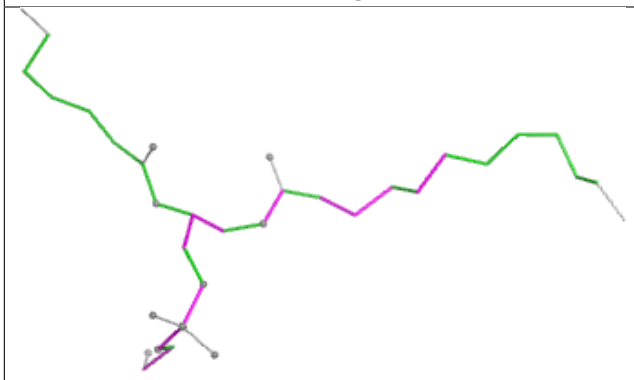
Ligand 3PE W 404



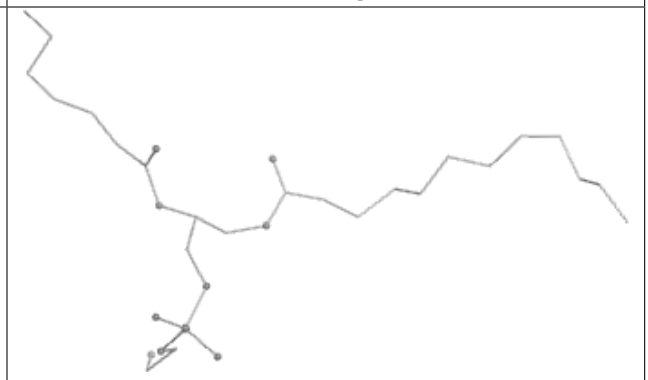
Bond lengths



Bond angles

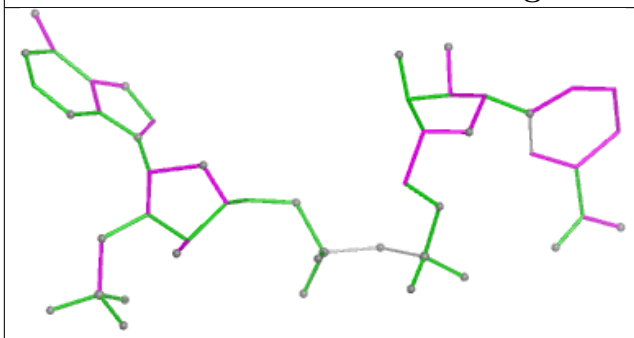


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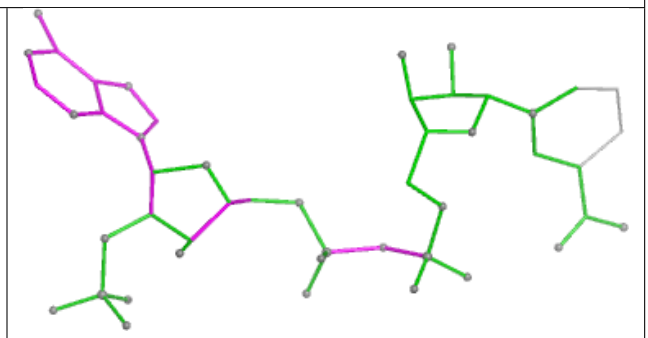


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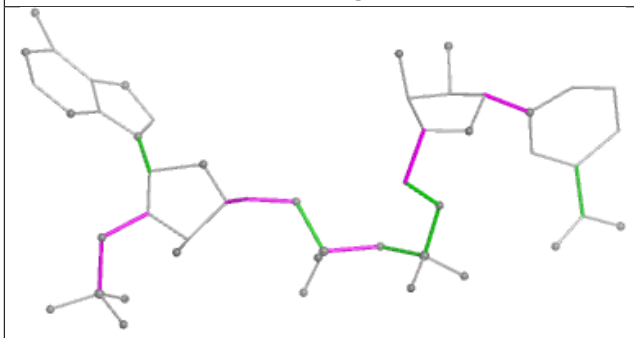
Ligand NDP E 401



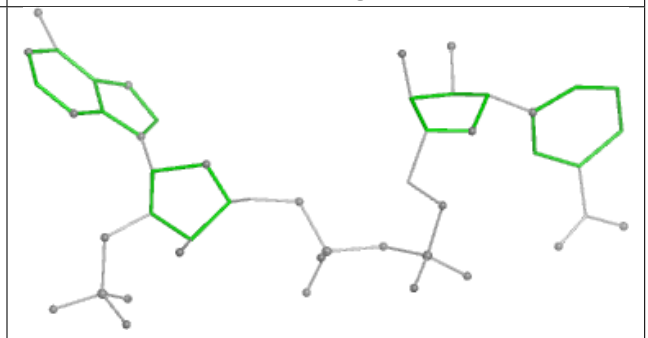
Bond lengths



Bond angles

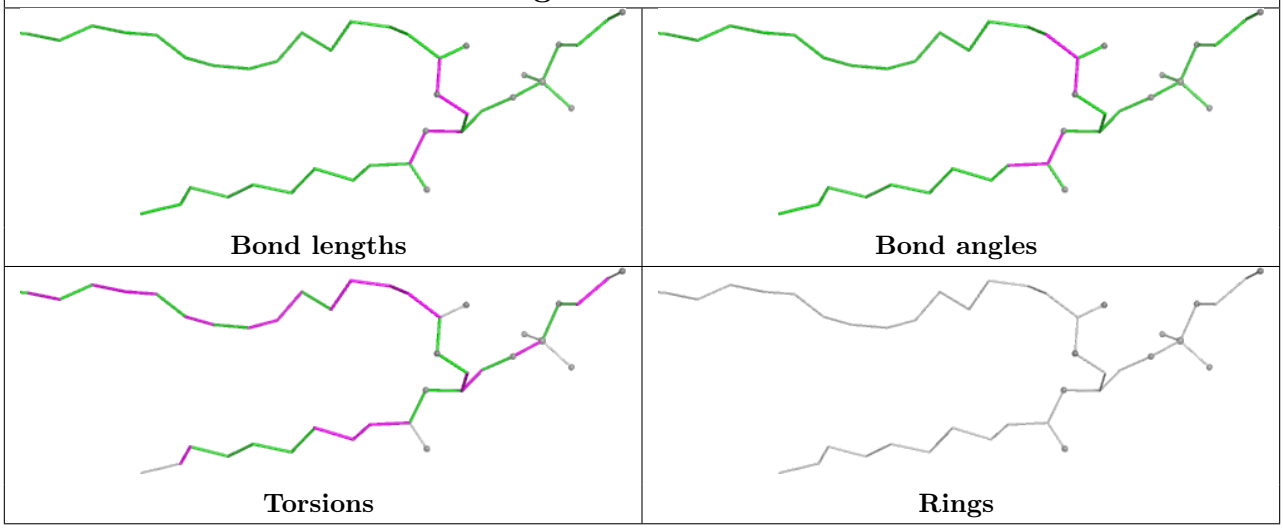


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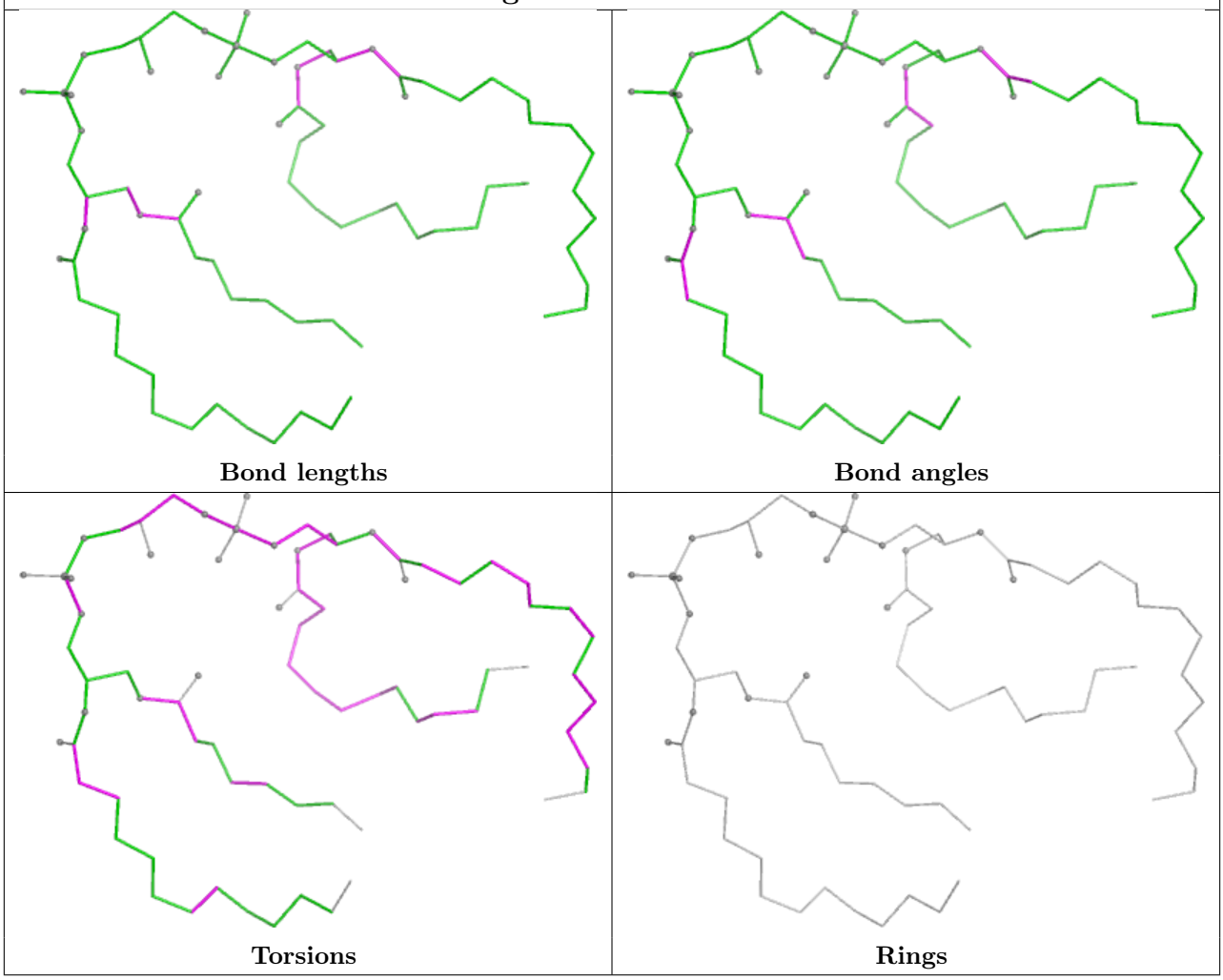


Rings

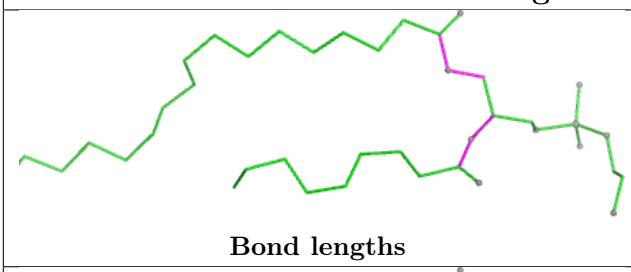
Ligand 3PE 4 504



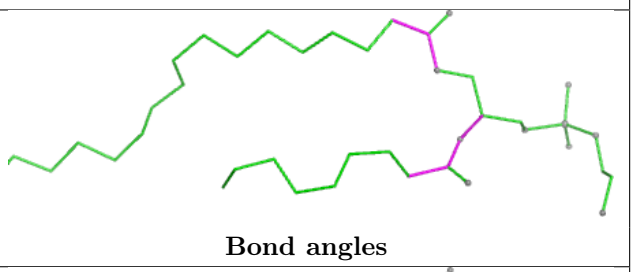
Ligand CDL Z 201



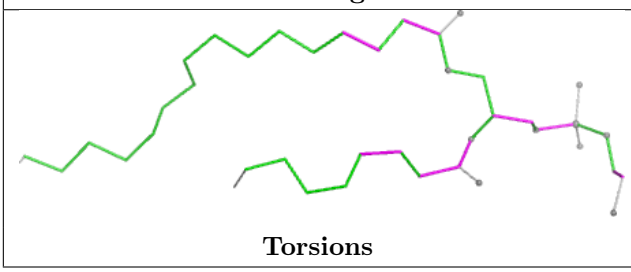
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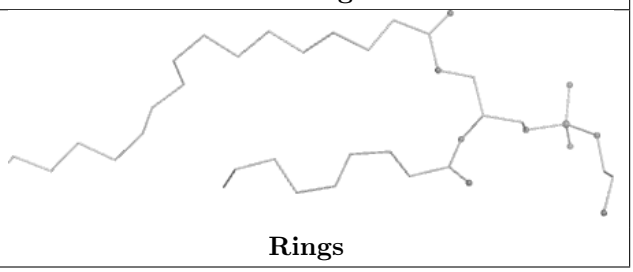
Bond lengths



Bond angles

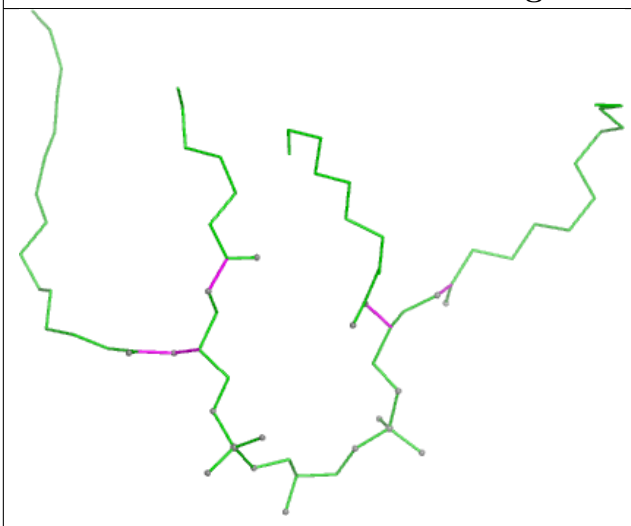


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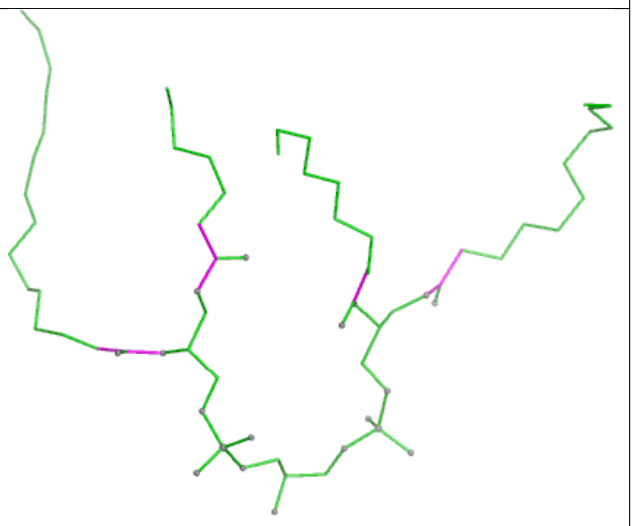


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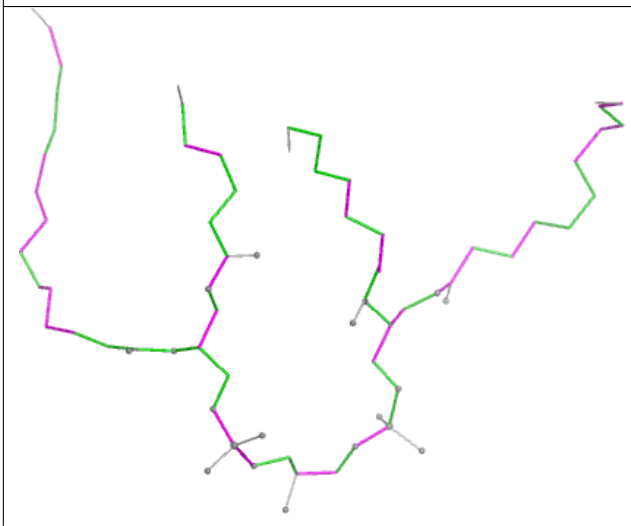
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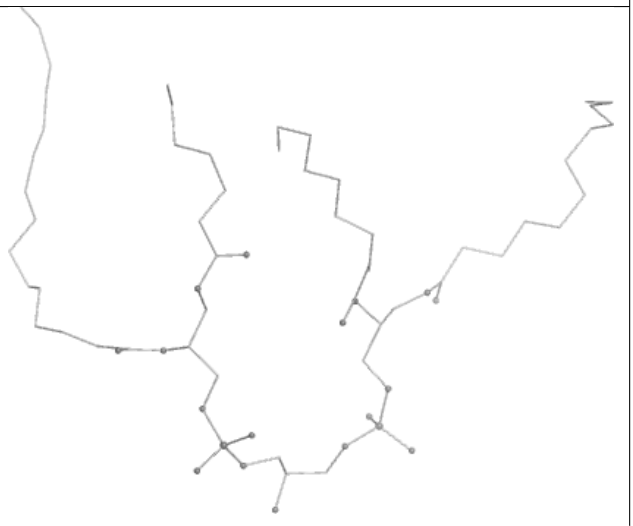
Bond lengths



Bond angles

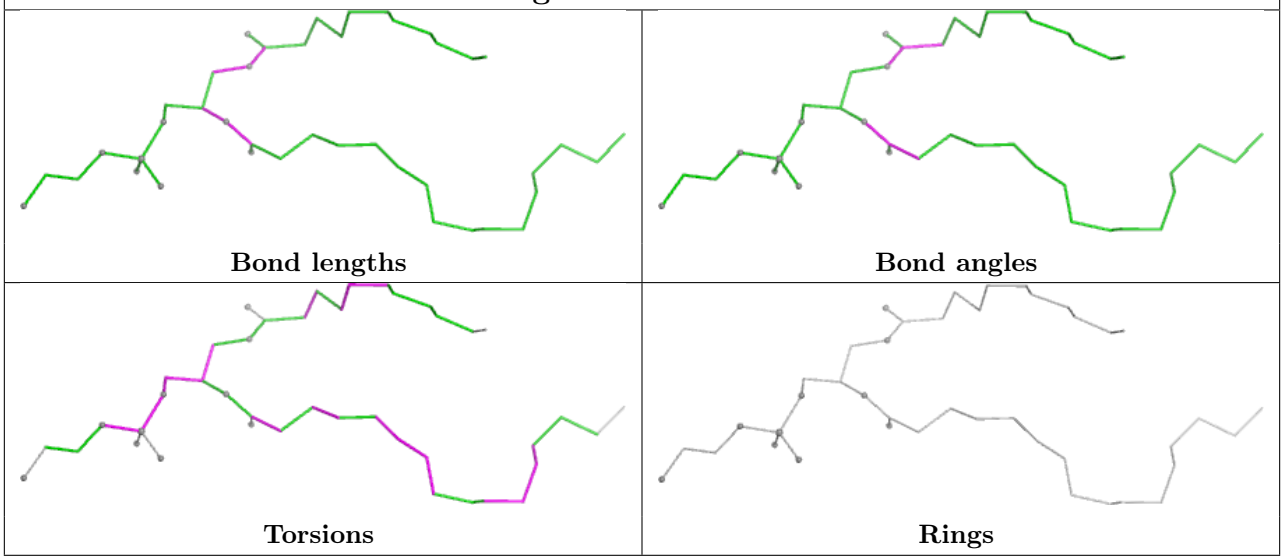


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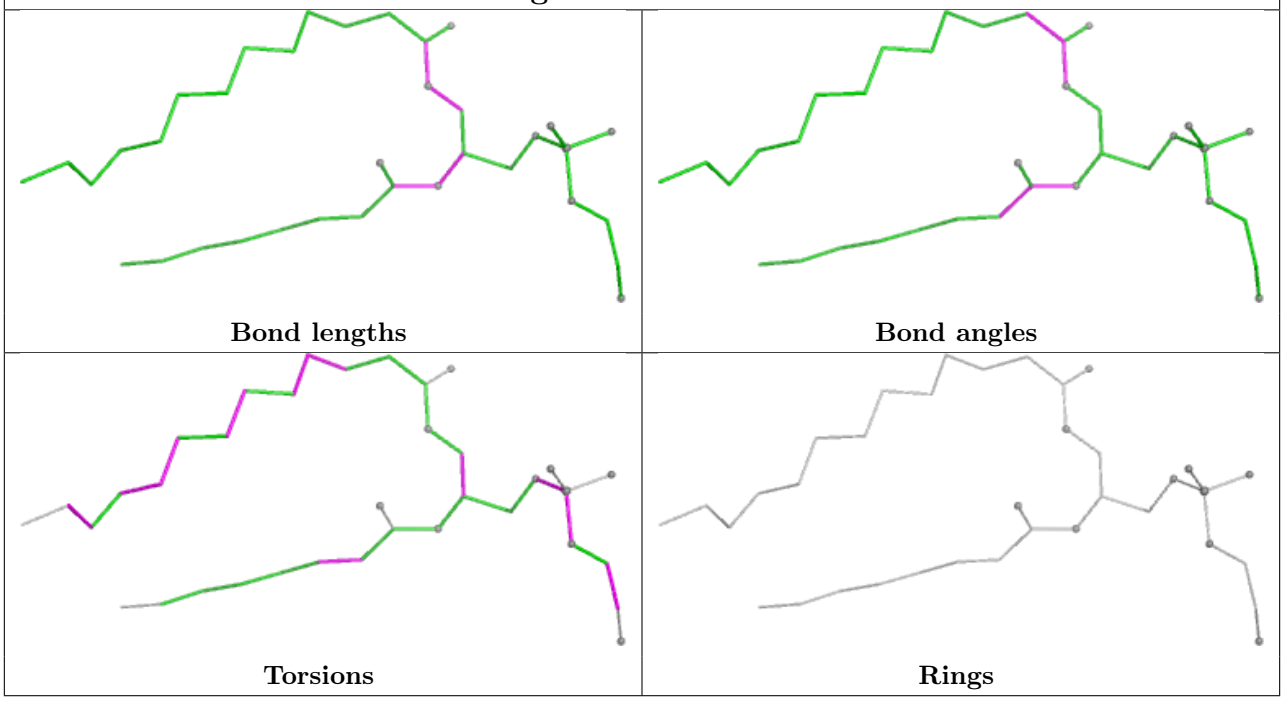


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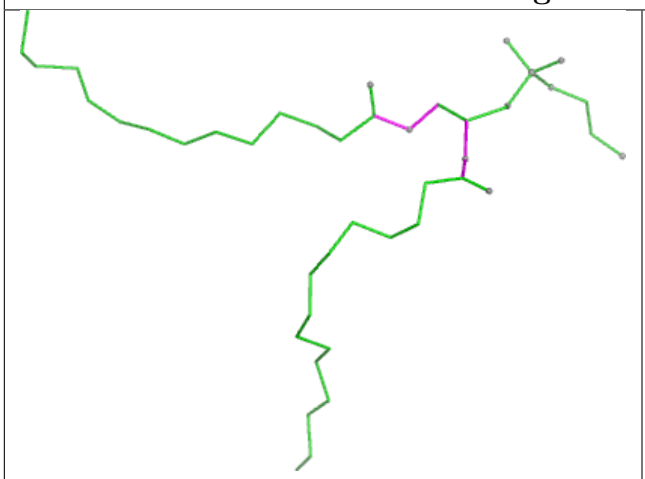
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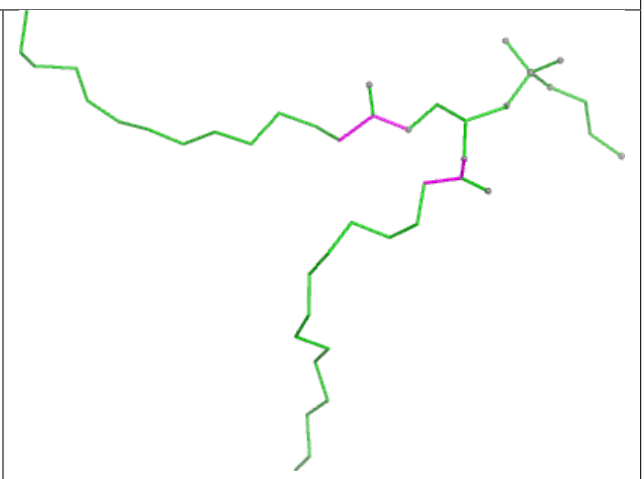
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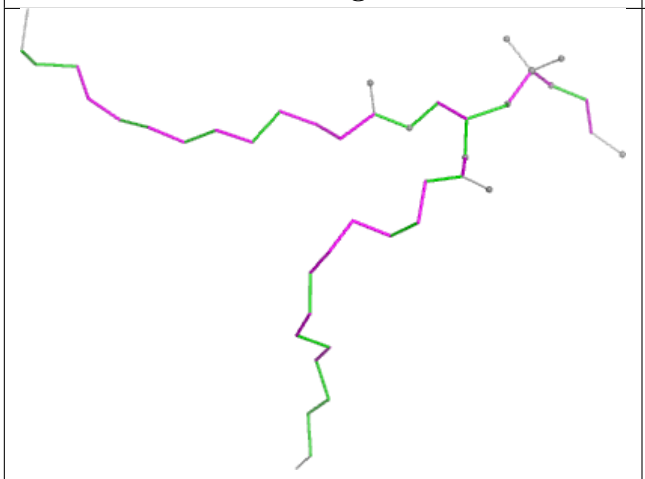
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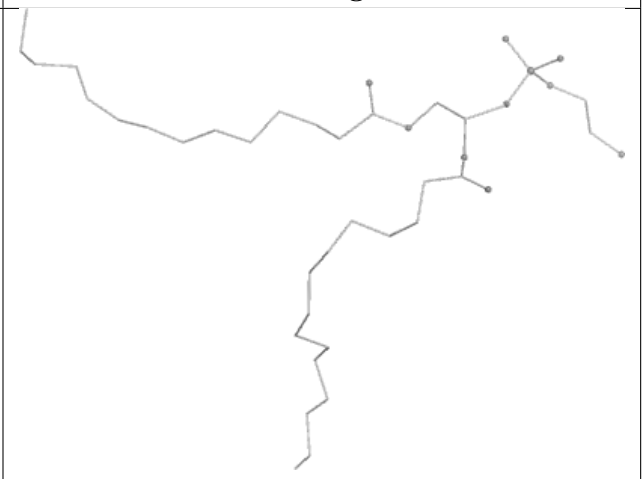
Bond lengths



Bond angles

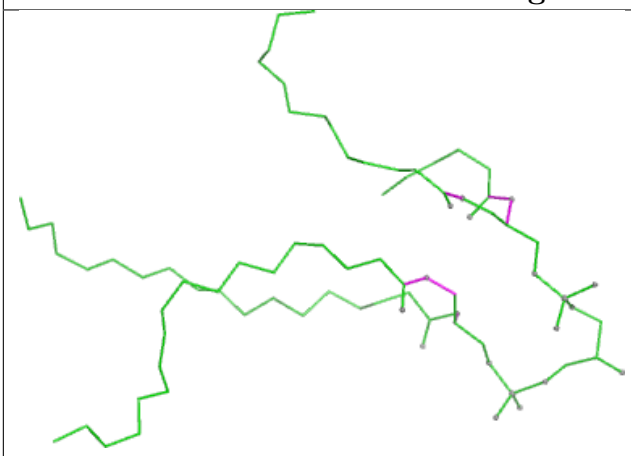


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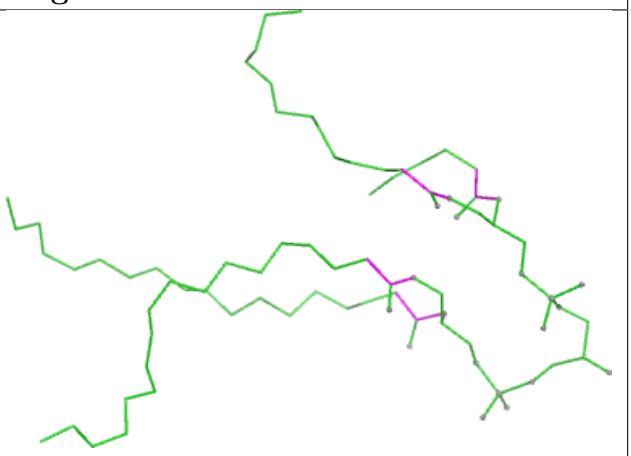


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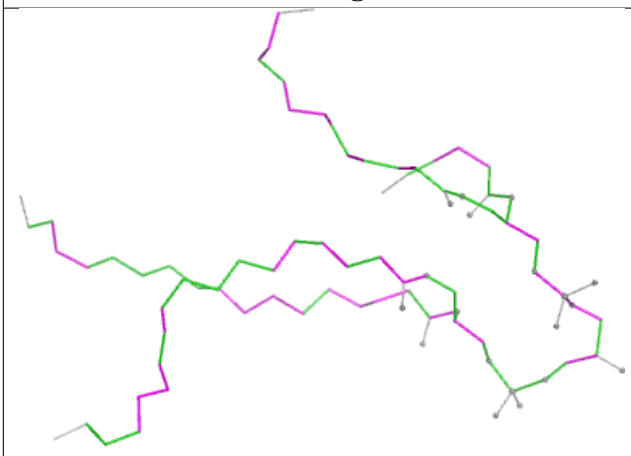
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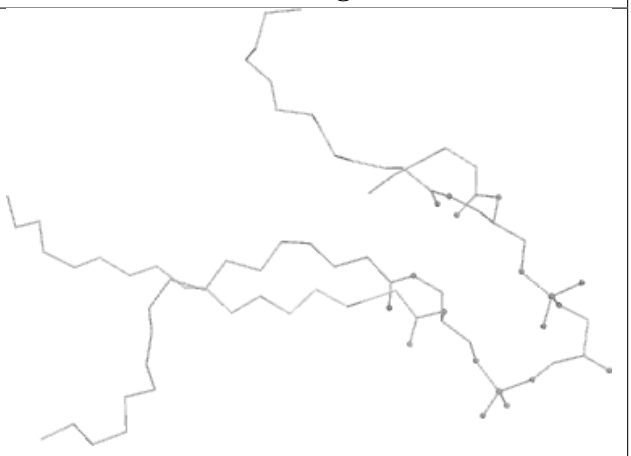
Bond lengths



Bond angles



Torsions

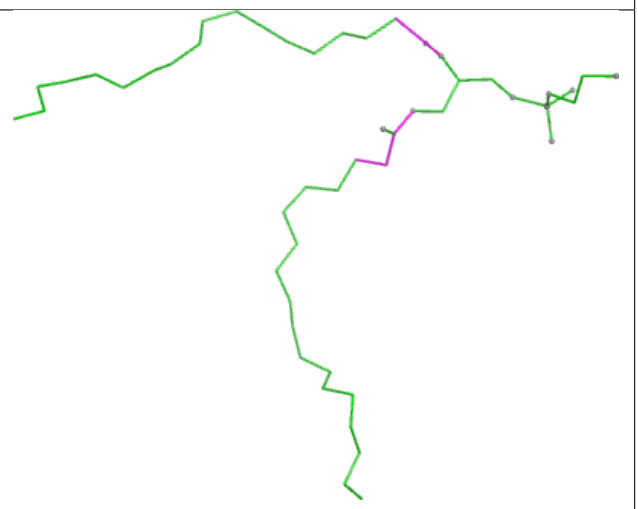


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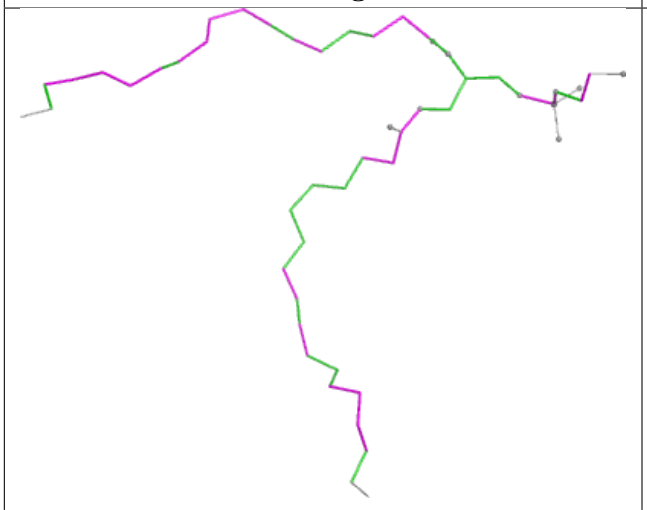
Ligand 3PE C 501



Bond lengths



Bond angles

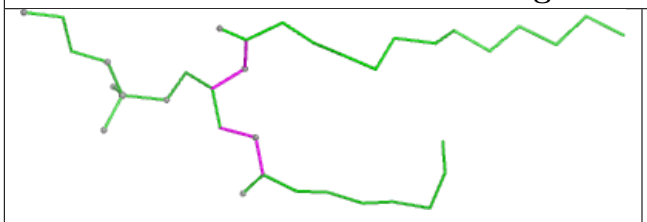


Torsions



Rings

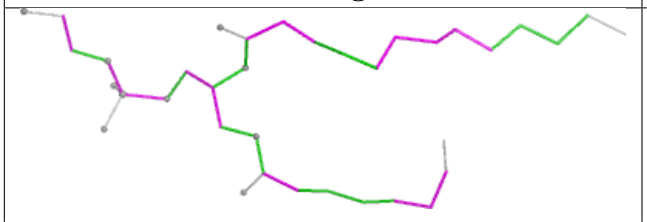
Ligand 3PE 1 504



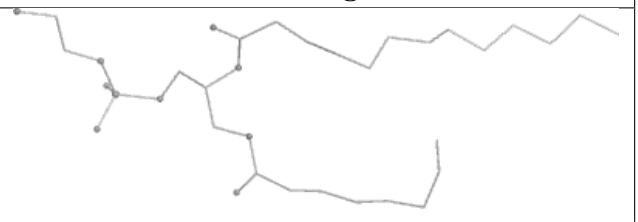
Bond lengths



Bond angles

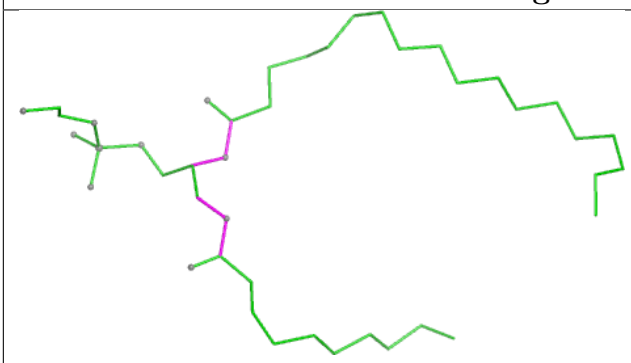


Torsions

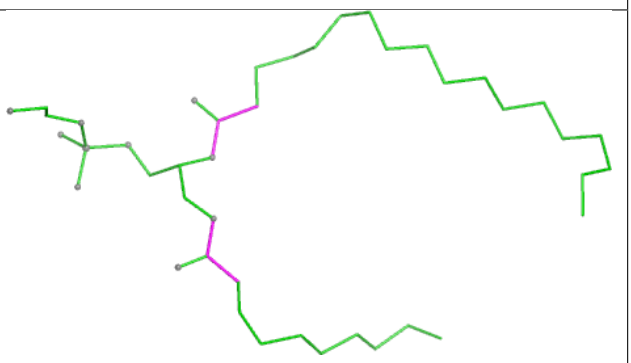


Rings

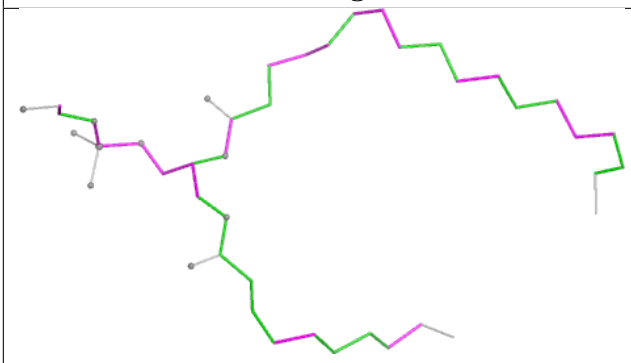
Ligand 3PE 4 502



Bond lengths



Bond angles

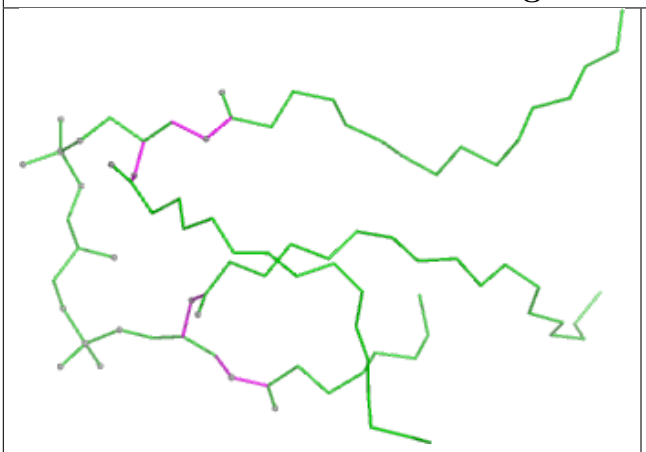


Torsions

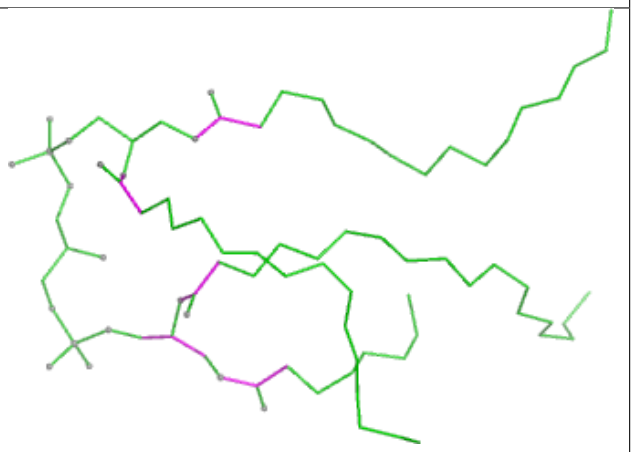


Rings

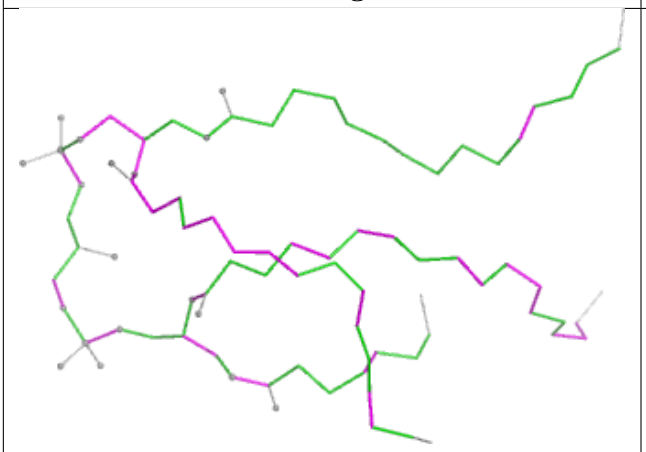
Ligand CDL X 201



Bond lengths



Bond angles

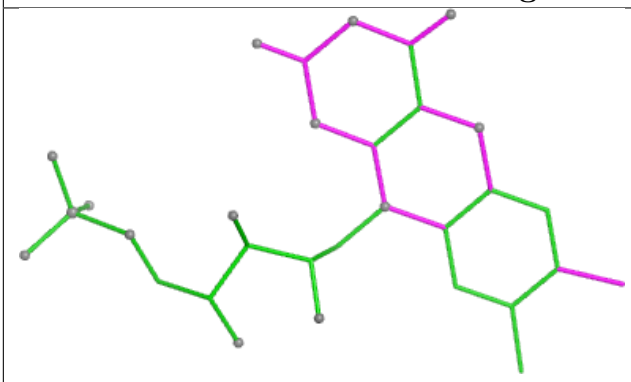


Torsions

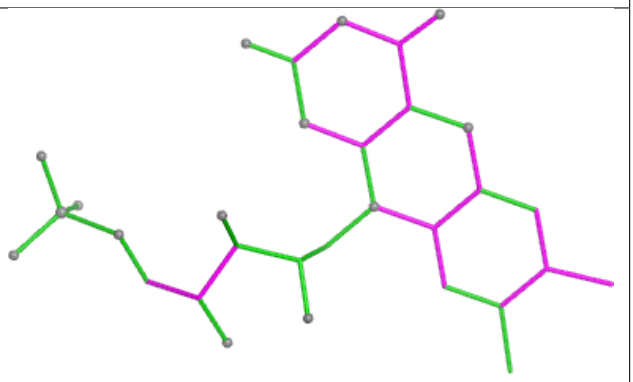


Rings

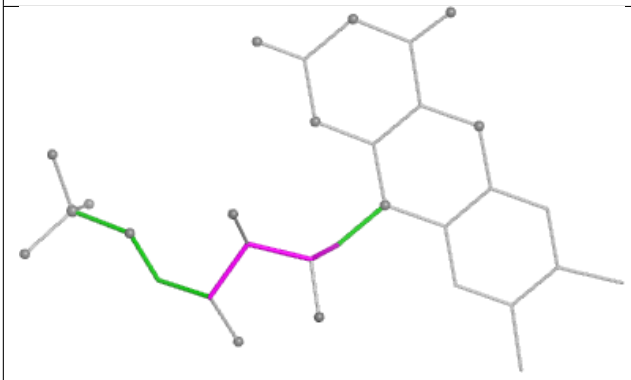
Ligand FMN B 502



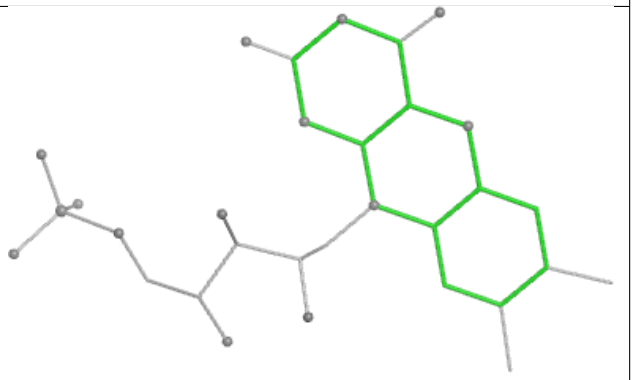
Bond lengths



Bond angles

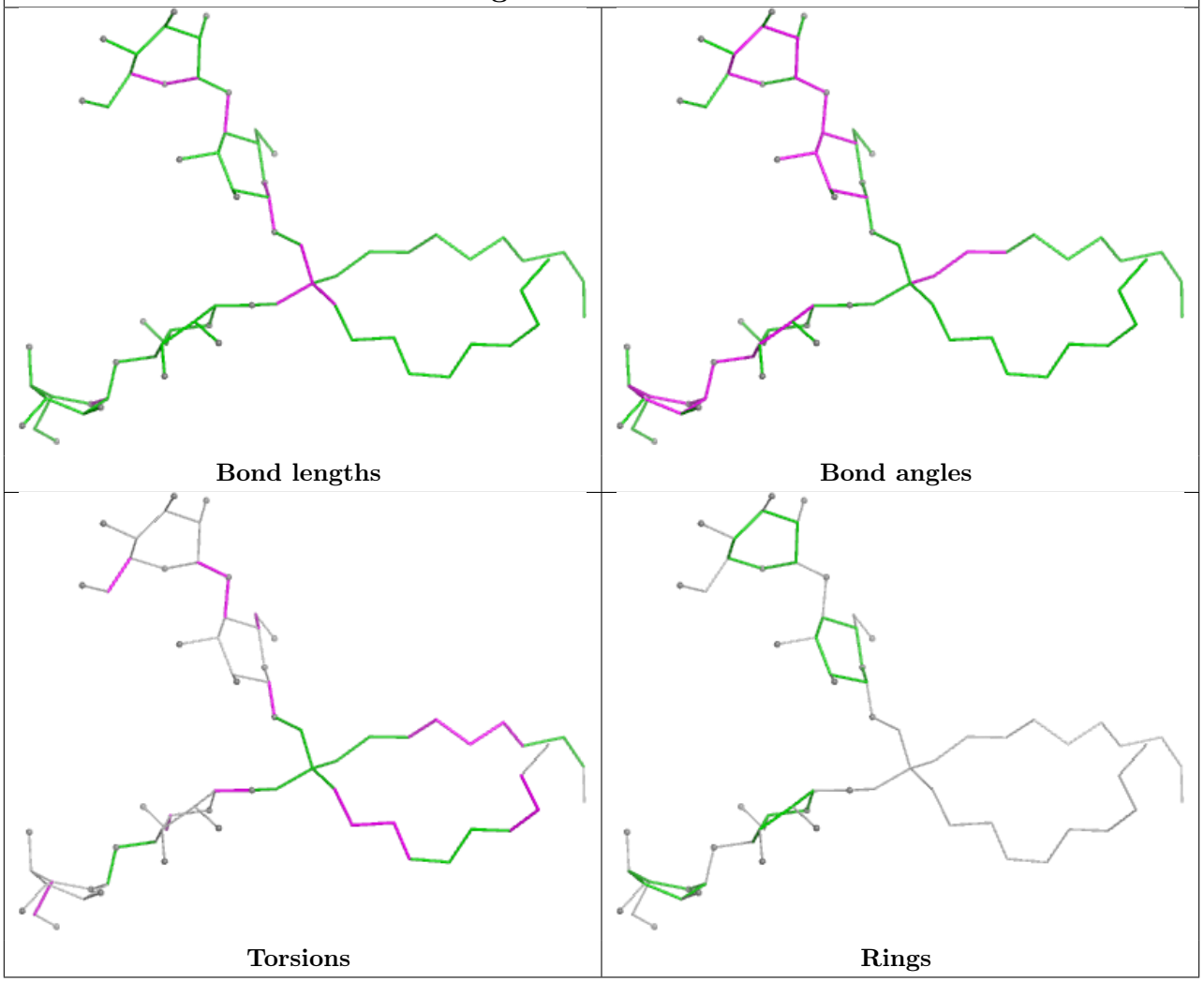


Torsions



Rings

Ligand LMN J 202



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

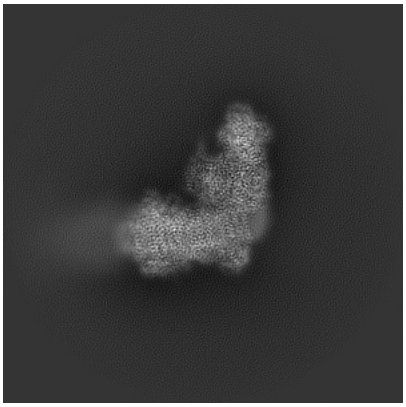
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-4873. These allow visual inspection of the internal detail of the map and identification of artifacts.

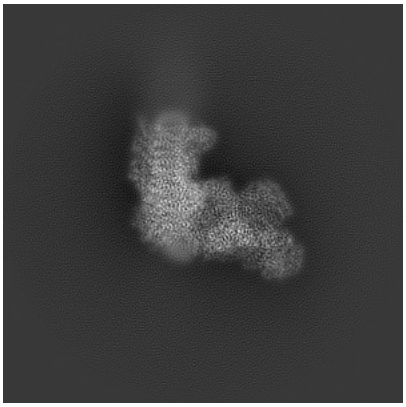
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

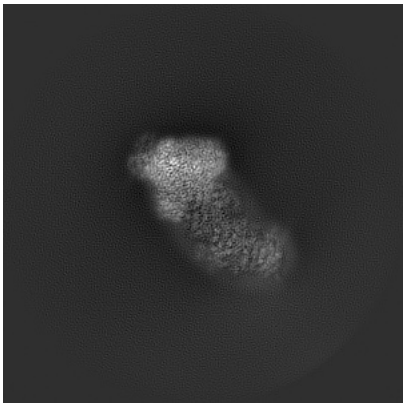
6.1.1 Primary map



X



Y

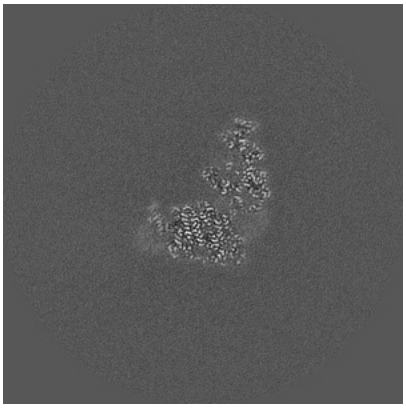


Z

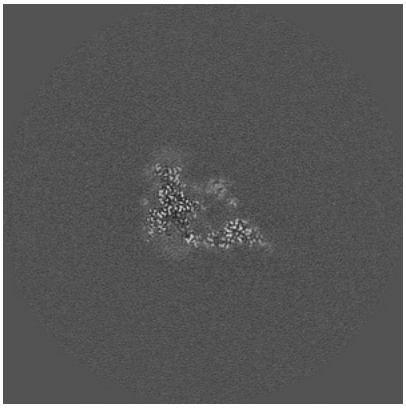
The images above show the map projected in three orthogonal directions.

6.2 Central slices

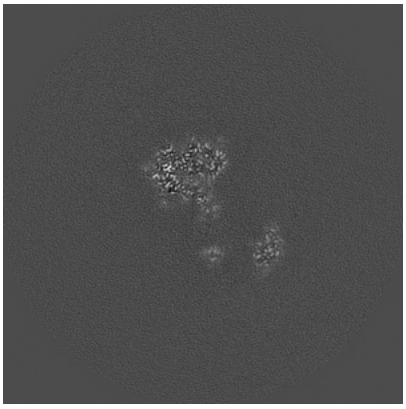
6.2.1 Primary map



X Index: 228



Y Index: 228

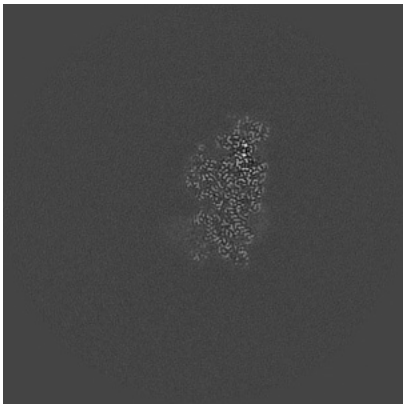


Z Index: 228

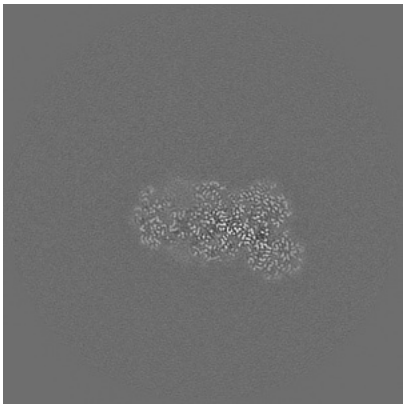
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

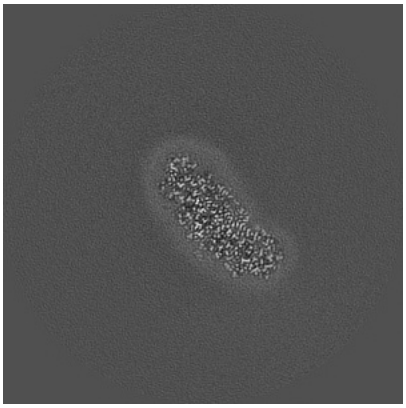
6.3.1 Primary map



X Index: 192



Y Index: 270

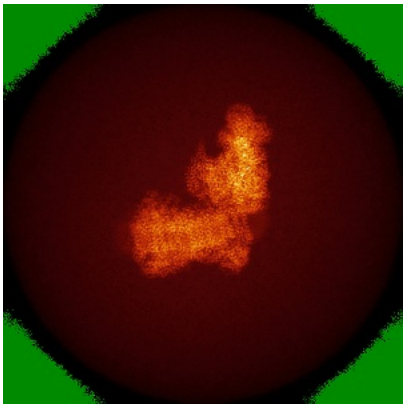


Z Index: 201

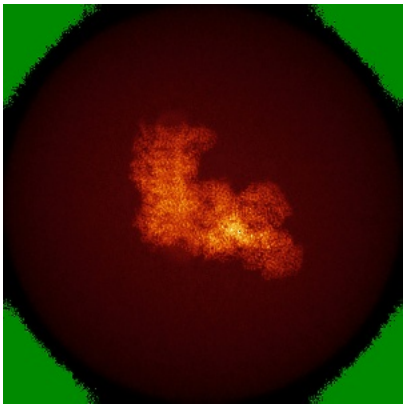
The images above show the largest variance slices of the map in three orthogonal directions.

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

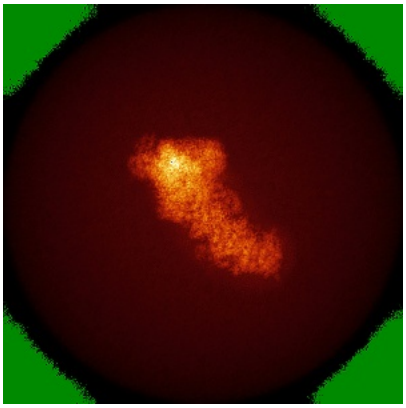
6.4.1 Primary map



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



The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

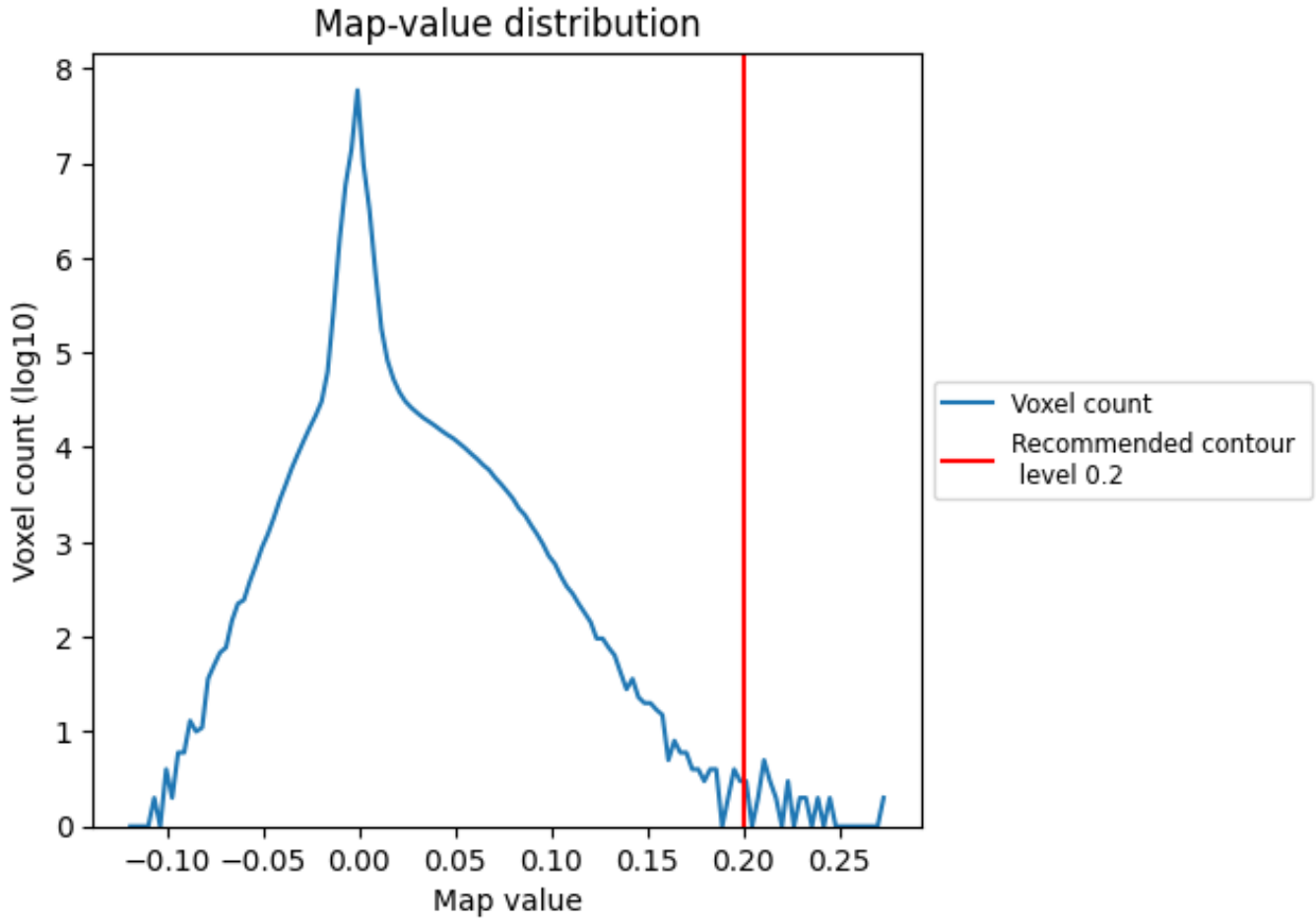
6.6 Mask visualisation (i)

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

7 Map analysis

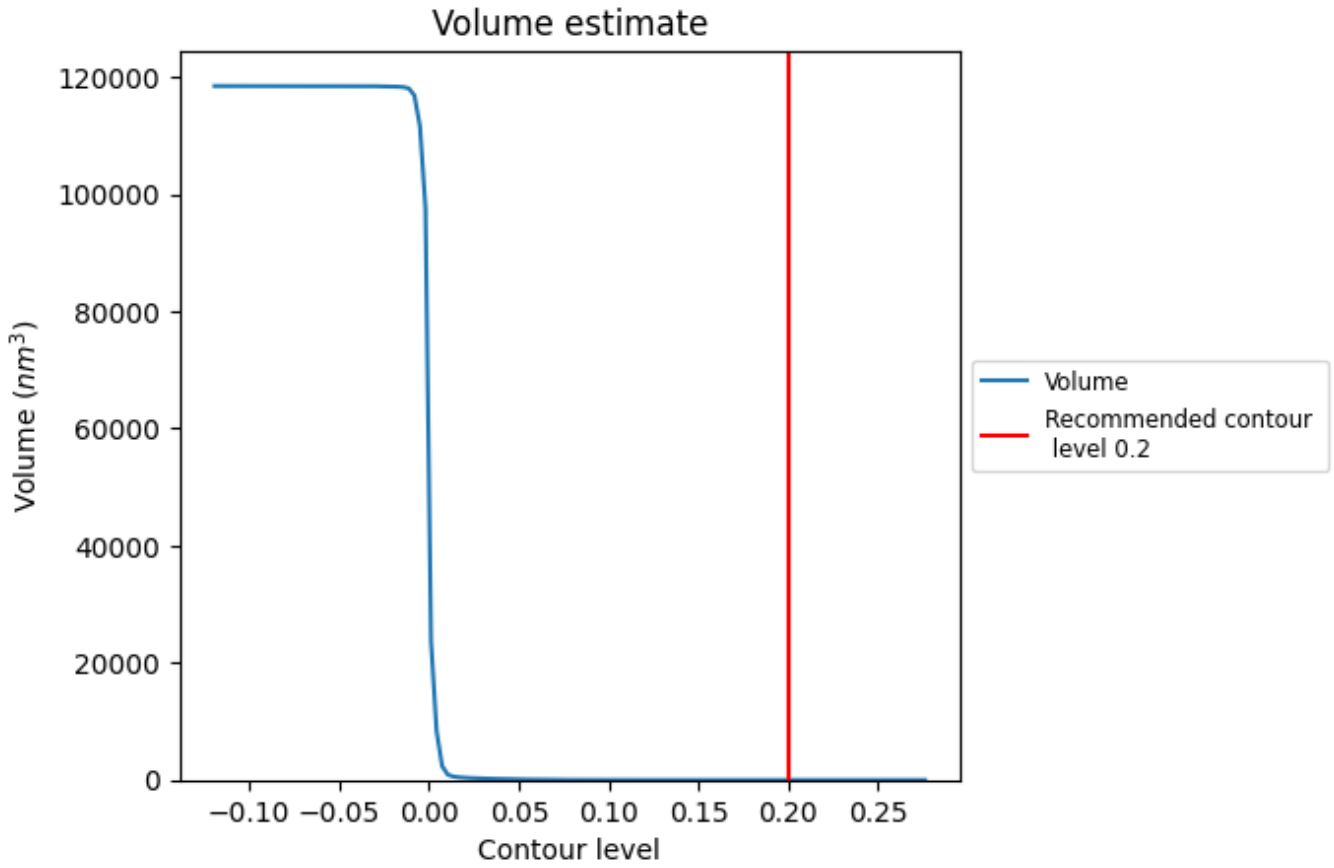
This section contains the results of statistical analysis of the map.

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.

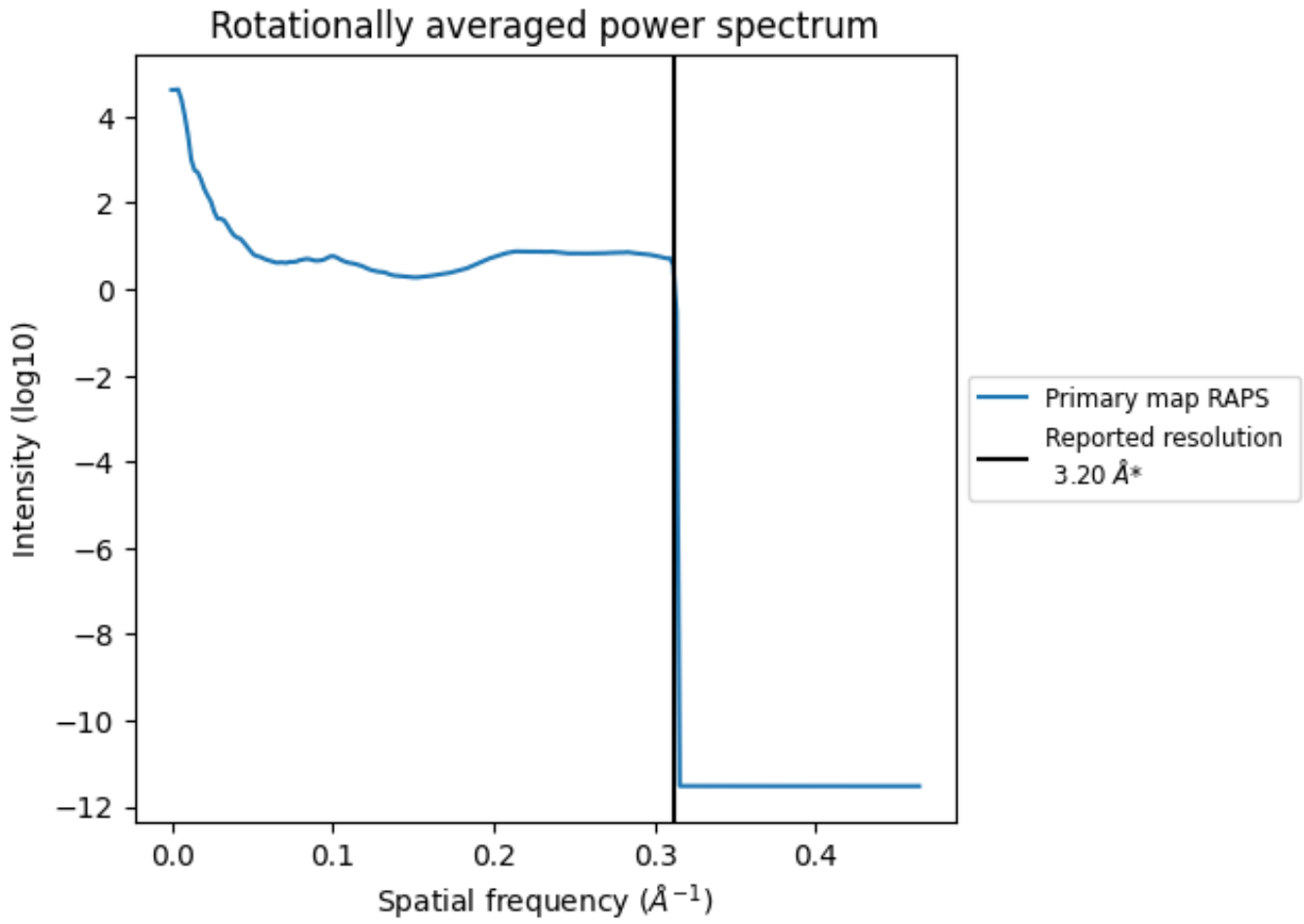
7.2 Volume estimate



The volume at the recommended contour level is 0 nm^3; this corresponds to an approximate mass of 0 kDa.

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

7.3 Rotationally averaged power spectrum (i)

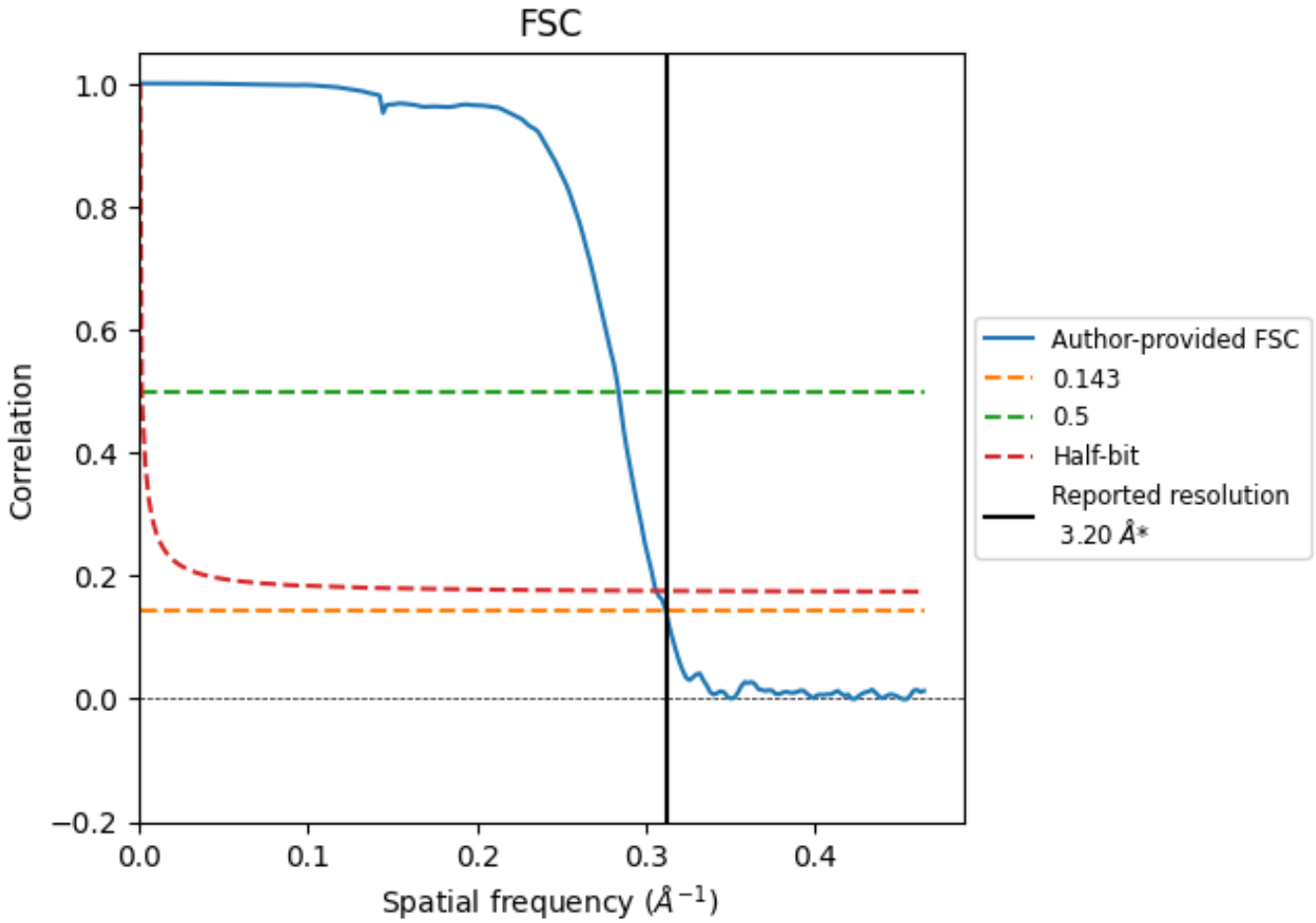


*Reported resolution corresponds to spatial frequency of 0.312 $Å^{-1}$

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8.2 Resolution estimates (i)

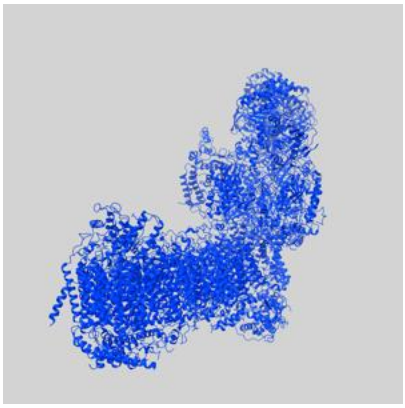
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.21	3.52	3.27
Unmasked-calculated*	-	-	-

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

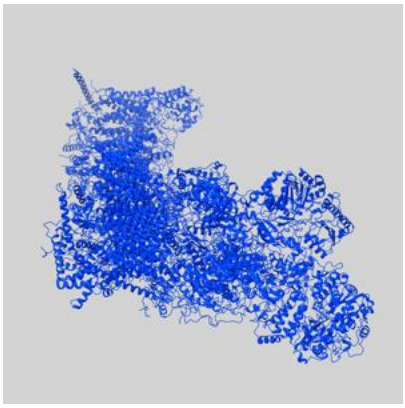
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-4873 and PDB model 6RFR. Per-residue inclusion information can be found in section 3 on page 21.

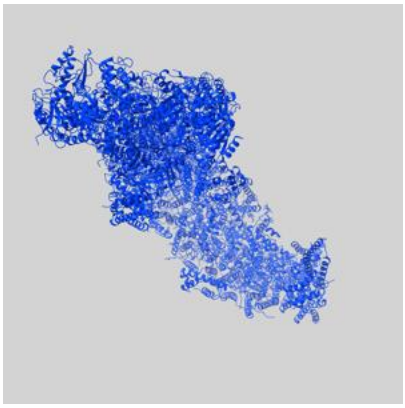
9.1 Map-model overlay



X



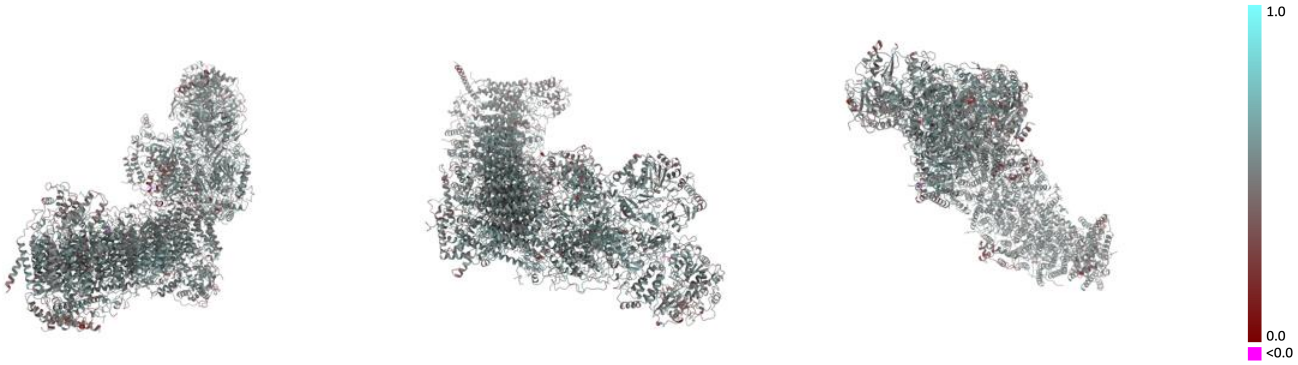
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.2 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.

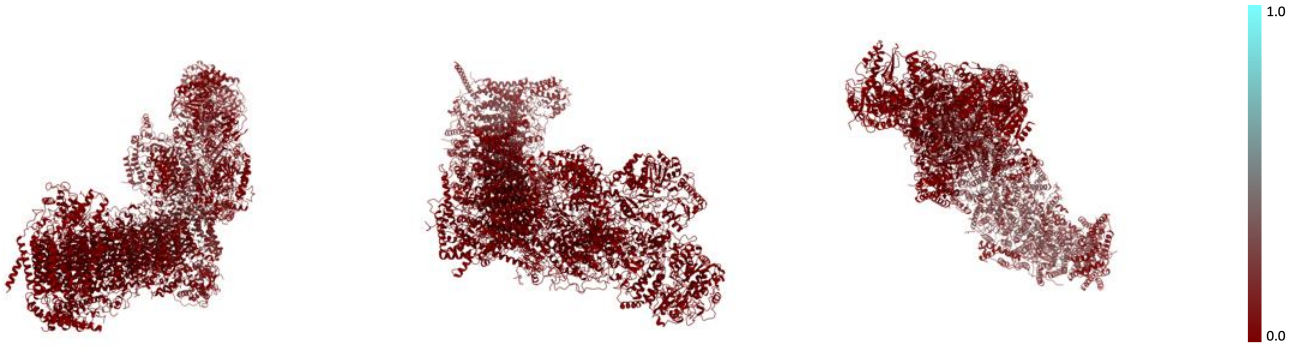
9.2 Q-score mapped to coordinate model (i)



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.

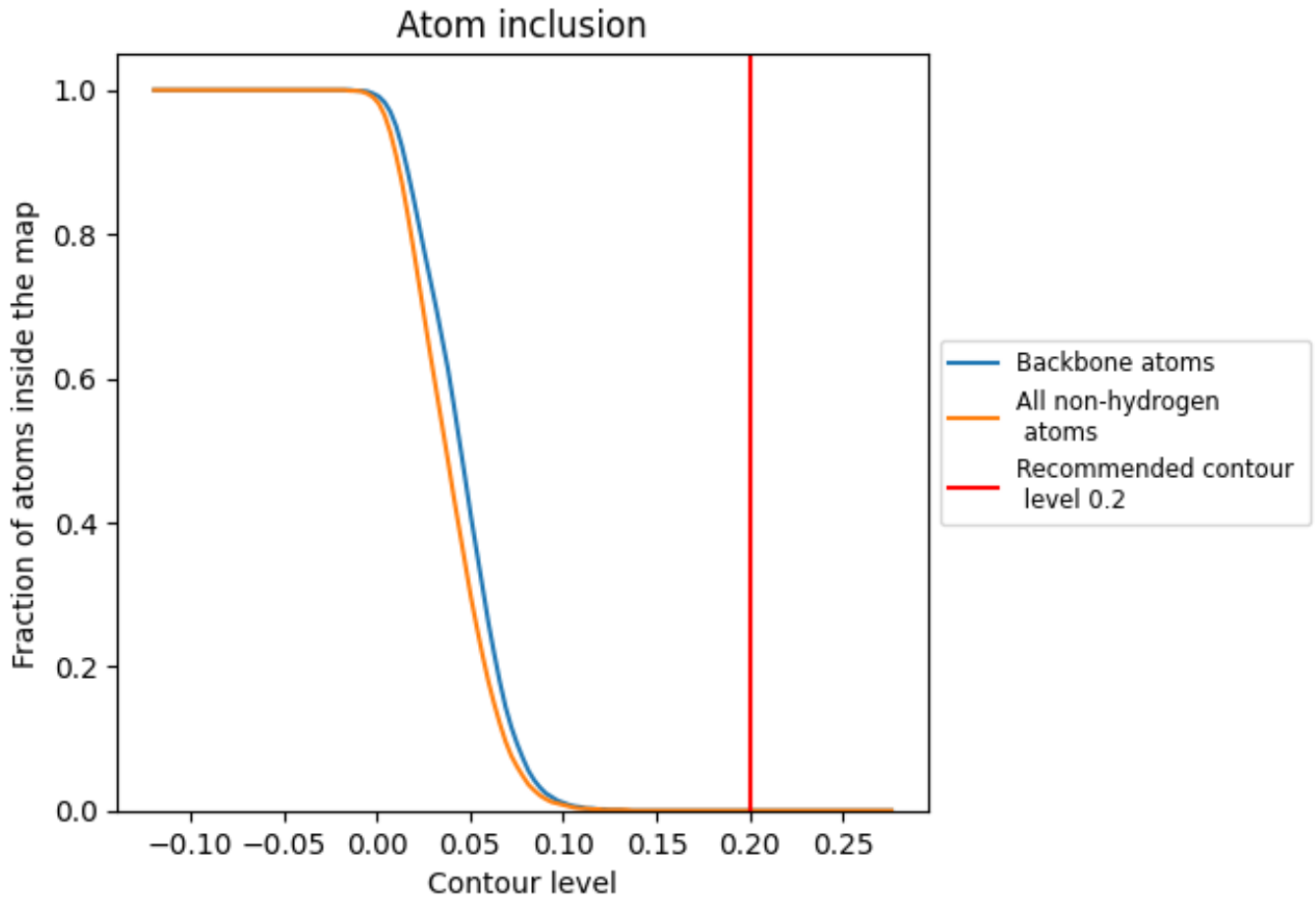
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.2).

9.4 Atom inclusion (i)



At the recommended contour level, 0% of all backbone atoms, 0% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.0000	0.5060
1	0.0000	0.5000
2	0.0000	0.5410
3	0.0000	0.4980
4	0.0000	0.5330
5	0.0000	0.5210
6	0.0000	0.5030
8	0.0000	0.4320
9	0.0000	0.4790
A	0.0000	0.5060
B	0.0000	0.4840
C	0.0000	0.5180
D	0.0000	0.5050
E	0.0000	0.5020
F	0.0000	0.4840
G	0.0000	0.5340
H	0.0000	0.4710
I	0.0000	0.5340
J	0.0000	0.5130
K	0.0000	0.5340
L	0.0000	0.5220
M	0.0000	0.5370
O	0.0000	0.3900
P	0.0000	0.4880
Q	0.0000	0.4330
R	0.0000	0.4790
S	0.0000	0.4330
U	0.0000	0.4950
W	0.0000	0.5190
X	0.0000	0.5230
Y	0.0000	0.5260
Z	0.0000	0.5060
a	0.0000	0.4790
b	0.0000	0.5370
c	0.0000	0.4460



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
d	0.0000	0.5100
e	0.0000	0.4850
f	0.0000	0.4570
g	0.0000	0.5260
h	0.0000	0.5130
i	0.0000	0.5030
j	0.0000	0.4910
n	0.0000	0.5010