



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 02:11 AM UTC

PDB ID : 6ZKP / pdb_00006zkp
EMDB ID : EMD-11257
Title : Native complex I, open1
Authors : Kampjut, D.; Sazanov, L.A.
Deposited on : 2020-06-30
Resolution : 3.20 Å(reported)
Based on initial model : 5LNK

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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
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) : 2.49

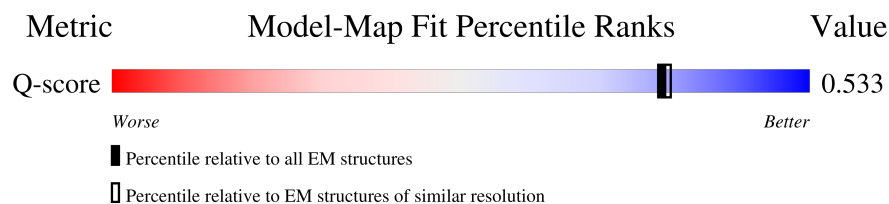
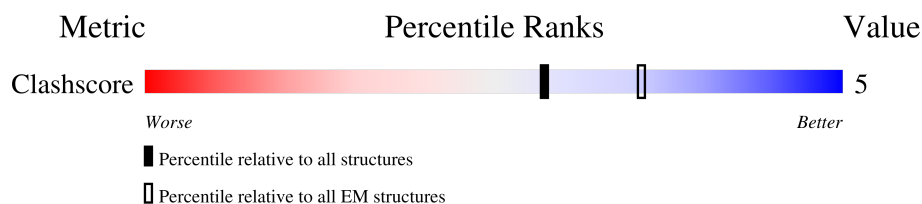
1 Overall quality at a glance

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	-
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 $\leq 5\%$. 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	1	464	 79% 14% 7%
2	2	246	 70% 16% 13%
3	3	727	 79% 16% 5%
4	4	463	 77% 14% 9%
5	5	266	 64% 14% 22%
6	6	223	 64% 6% 30%

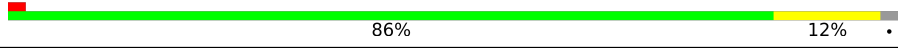
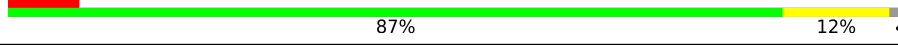
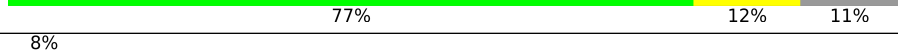
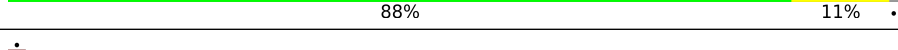
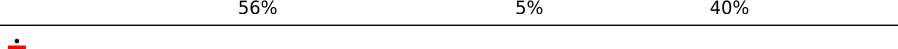
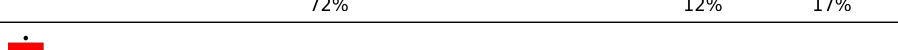
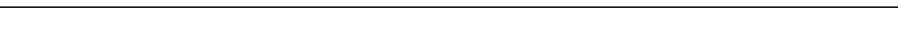
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Mol	Chain	Length	Quality of chain
7	9	217	
8	A	115	
9	H	318	
10	J	175	
11	K	98	
12	L	606	
13	M	459	
14	N	347	
15	V	141	
16	W	189	
17	X	157	
17	j	157	
18	Y	172	
19	Z	175	
20	a	109	
21	b	124	
22	c	170	
23	d	380	
24	e	99	
25	f	116	
26	g	140	
27	h	114	
28	i	145	
29	k	355	
30	l	106	

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Mol	Chain	Length	Quality of chain
31	m	84	
32	n	98	
33	o	122	
34	p	130	
35	q	144	
36	r	128	
37	s	137	
38	t	179	
39	u	108	
40	v	186	
41	w	154	
42	x	76	
43	y	58	
44	z	70	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
45	SF4	1	500	-	-	X	-
51	CDL	L	1004	X	-	-	-
51	CDL	N	403	X	-	-	-
51	CDL	V	204	X	-	-	-
51	CDL	y	201	X	-	-	-

2 Entry composition [i](#)

There are 56 unique types of molecules in this entry. The entry contains 67353 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

- Molecule 2 is a protein called Mitochondrial complex I, 24 kDa subunit.

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

- Molecule 3 is a protein called NADH:ubiquinone oxidoreductase core subunit S1.

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

- Molecule 4 is a protein called Mitochondrial complex I, 49 kDa subunit.

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

- Molecule 5 is a protein called NADH:ubiquinone oxidoreductase core subunit S3.

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

- Molecule 6 is a protein called Mitochondrial complex I, PSST subunit.

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

- Molecule 7 is a protein called Mitochondrial complex I, TYKY subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	9	176	Total	C	N	O	S	0	0
			1414	889	243	270	12		

- Molecule 8 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	A	110	Total	C	N	O	S	0	0
			880	593	128	153	6		

- Molecule 9 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	313	Total	C	N	O	S	0	0
			2489	1680	379	411	19		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	167	Total	C	N	O	S	0	0
			1273	856	182	222	13		

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

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

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

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

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

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

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

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

- Molecule 15 is a protein called Mitochondrial complex I, B14.7 subunit.

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

- Molecule 16 is a protein called NADH:ubiquinone oxidoreductase subunit B5.

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

- Molecule 17 is a protein called Acyl carrier protein.

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

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

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

- Molecule 19 is a protein called Mitochondrial complex I, PDSW subunit.

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

- Molecule 20 is a protein called Mitochondrial complex I, 10 kDa subunit.

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

- Molecule 21 is a protein called Mitochondrial complex I, 13 kDa subunit.

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

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

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

- Molecule 23 is a protein called NADH:ubiquinone oxidoreductase subunit A9.

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

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

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

- Molecule 25 is a protein called Mitochondrial complex I, B13 subunit.

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

- Molecule 26 is a protein called NADH:ubiquinone oxidoreductase subunit A6.

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

- Molecule 27 is a protein called Mitochondrial complex I, B14.5a subunit.

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

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

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

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

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

- Molecule 30 is a protein called NADH:ubiquinone oxidoreductase subunit S5.

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

- Molecule 31 is a protein called NADH:ubiquinone oxidoreductase subunit A3.

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

- Molecule 32 is a protein called NADH:ubiquinone oxidoreductase subunit B3.

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

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

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

- Molecule 34 is a protein called NADH:ubiquinone oxidoreductase subunit B4.

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

- Molecule 35 is a protein called Mitochondrial complex I, B16.6 subunit.

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

- Molecule 36 is a protein called Mitochondrial complex I, B17 subunit.

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

- Molecule 37 is a protein called NADH:ubiquinone oxidoreductase subunit B7.

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

- Molecule 38 is a protein called NADH:ubiquinone oxidoreductase subunit B9.

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

- Molecule 39 is a protein called NADH:ubiquinone oxidoreductase subunit B2.

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

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

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

- Molecule 41 is a protein called Mitochondrial complex I, ESSS subunit.

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

- Molecule 42 is a protein called Mitochondrial complex I, KFYI subunit.

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

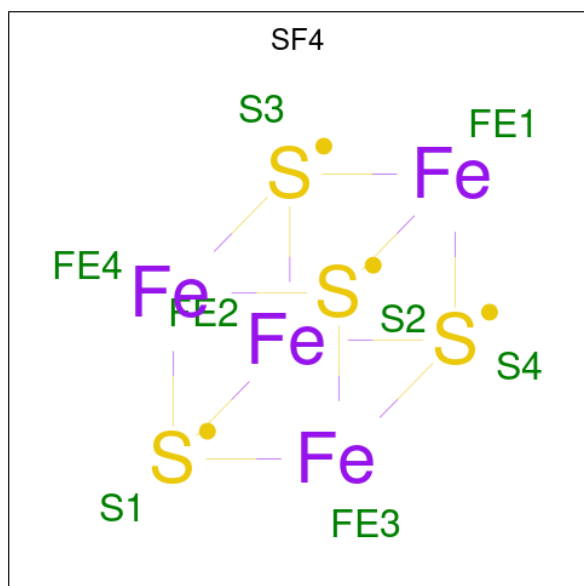
- Molecule 43 is a protein called Mitochondrial complex I, MNLL subunit.

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

- Molecule 44 is a protein called Mitochondrial complex I, MWFE subunit.

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

- Molecule 45 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



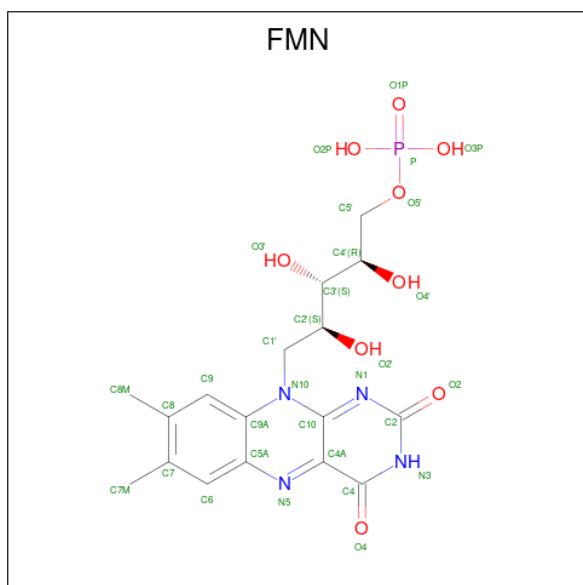
Mol	Chain	Residues	Atoms			AltConf
45	1	1	Total	Fe	S	0
			8	4	4	
45	3	1	Total	Fe	S	0
			8	4	4	
45	3	1	Total	Fe	S	0
			8	4	4	
45	6	1	Total	Fe	S	0
			8	4	4	

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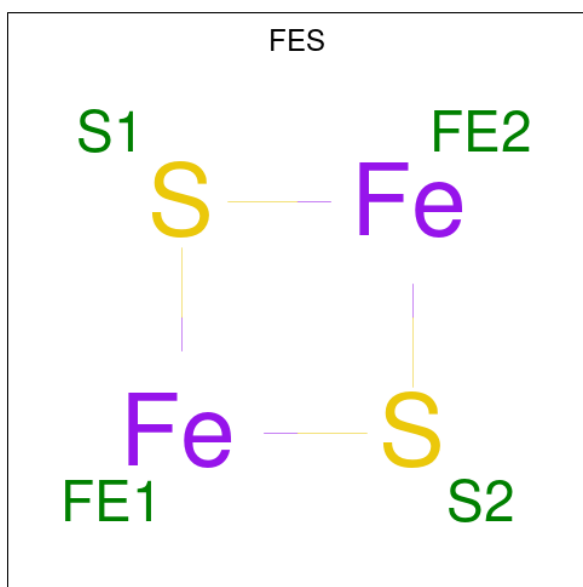
Mol	Chain	Residues	Atoms			AltConf
45	9	1	Total	Fe	S	0
			8	4	4	
45	9	1	Total	Fe	S	0
			8	4	4	

- Molecule 46 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



Mol	Chain	Residues	Atoms					AltConf
46	1	1	Total	C	N	O	P	0
			31	17	4	9	1	

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

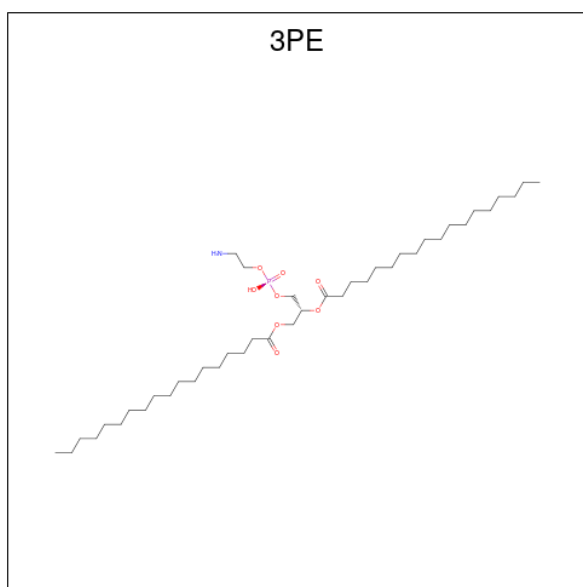


Mol	Chain	Residues	Atoms			AltConf
47	2	1	Total	Fe	S	0
			4	2	2	
47	3	1	Total	Fe	S	0
			4	2	2	

- Molecule 48 is POTASSIUM ION (CCD ID: K) (formula: K).

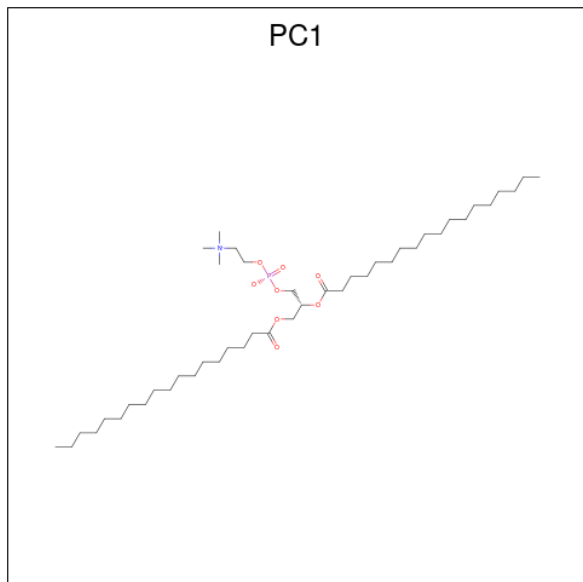
Mol	Chain	Residues	Atoms		AltConf
48	3	1	Total	K	0
			1	1	

- Molecule 49 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: C₄₁H₈₂NO₈P).



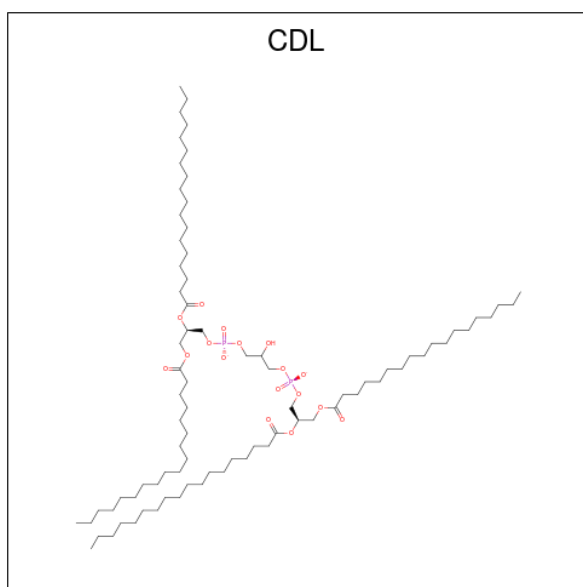
Mol	Chain	Residues	Atoms					AltConf
49	4	1	Total	C	N	O	P	0
			40	30	1	8	1	
49	6	1	Total	C	N	O	P	0
			51	41	1	8	1	
49	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
49	H	1	Total	C	N	O	P	0
			51	41	1	8	1	
49	J	1	Total	C	N	O	P	0
			40	30	1	8	1	
49	L	1	Total	C	N	O	P	0
			51	41	1	8	1	
49	L	1	Total	C	N	O	P	0
			31	21	1	8	1	
49	M	1	Total	C	N	O	P	0
			44	34	1	8	1	
49	N	1	Total	C	N	O	P	0
			51	41	1	8	1	
49	N	1	Total	C	N	O	P	0
			31	21	1	8	1	
49	V	1	Total	C	N	O	P	0
			35	25	1	8	1	
49	V	1	Total	C	N	O	P	0
			37	27	1	8	1	
49	i	1	Total	C	N	O	P	0
			51	41	1	8	1	
49	p	1	Total	C	O	P		0
			27	18	8	1		

- Molecule 50 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



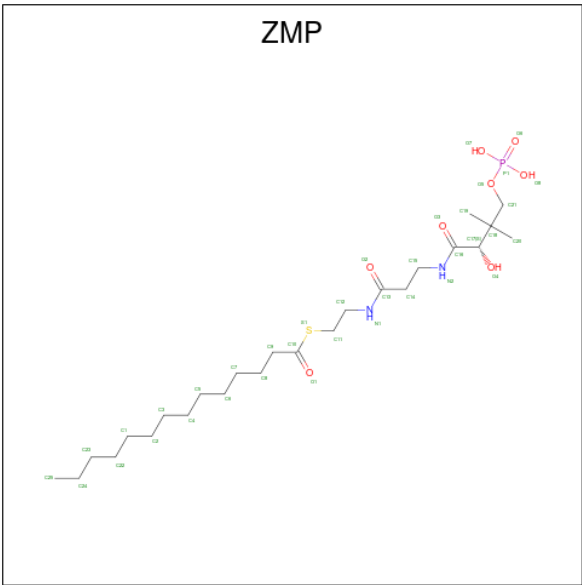
Mol	Chain	Residues	Atoms					AltConf
50	6	1	Total	C	N	O	P	0
			46	36	1	8	1	
50	9	1	Total	C	N	O	P	0
			54	44	1	8	1	
50	A	1	Total	C	N	O	P	0
			37	27	1	8	1	
50	L	1	Total	C	N	O	P	0
			54	44	1	8	1	
50	L	1	Total	C	N	O	P	0
			54	44	1	8	1	
50	M	1	Total	C	N	O	P	0
			54	44	1	8	1	

- Molecule 51 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
51	L	1	Total	C	O	P	0
			100	81	17	2	
51	N	1	Total	C	O	P	0
			75	56	17	2	
51	V	1	Total	C	O	P	0
			94	75	17	2	
51	V	1	Total	C	O	P	0
			85	66	17	2	
51	W	1	Total	C	O	P	0
			100	81	17	2	
51	h	1	Total	C	O	P	0
			58	39	17	2	
51	o	1	Total	C	O	P	0
			90	71	17	2	
51	y	1	Total	C	O	P	0
			100	81	17	2	

- Molecule 52 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (CCD ID: ZMP) (formula: C₂₅H₄₉N₂O₈PS).



Mol	Chain	Residues	Atoms					AltConf
52	X	1	Total	C	N	O	P	S
			31	20	2	7	1	1
52	g	1	Total	C	N	O	P	S
			34	23	2	7	1	1

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

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

- Molecule 54 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



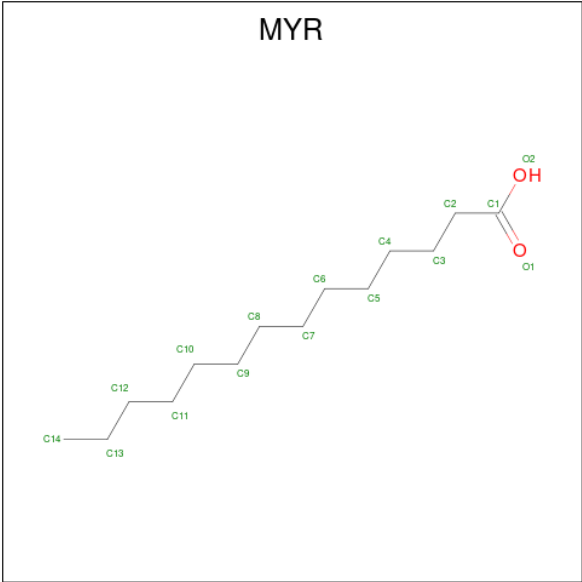
Mol	Chain	Residues	Atoms					AltConf
54	d	1	Total 48	C 21	N 7	O 17	P 3	0

- Molecule 55 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: $\text{C}_{10}\text{H}_{14}\text{N}_5\text{O}_7\text{P}$).



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

- Molecule 56 is MYRISTIC ACID (CCD ID: MYR) (formula: $C_{14}H_{28}O_2$).



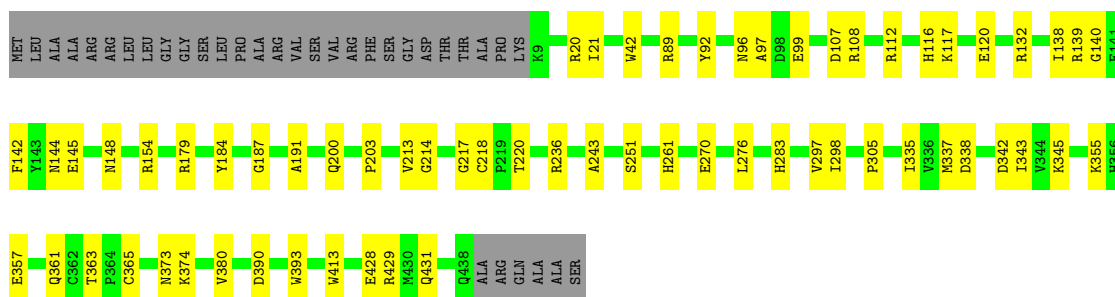
Mol	Chain	Residues	Atoms			AltConf
56	s	1	Total	C	O	0
			15	14	1	

3 Residue-property plots

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

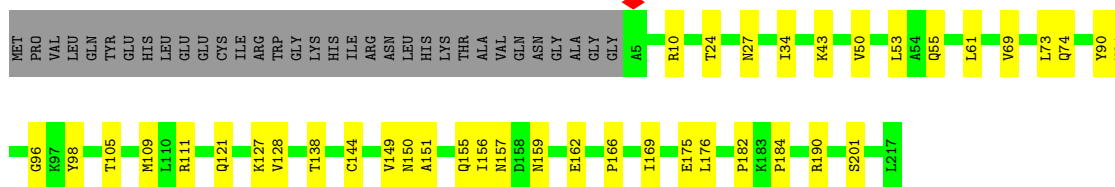
- Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain 1: 



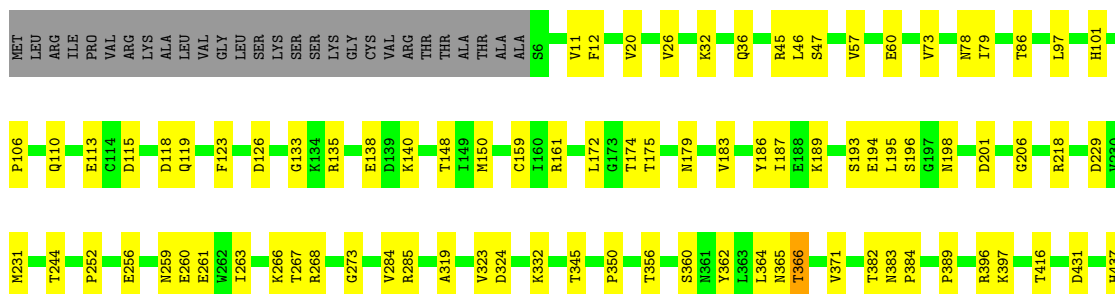
- Molecule 2: Mitochondrial complex I, 24 kDa subunit

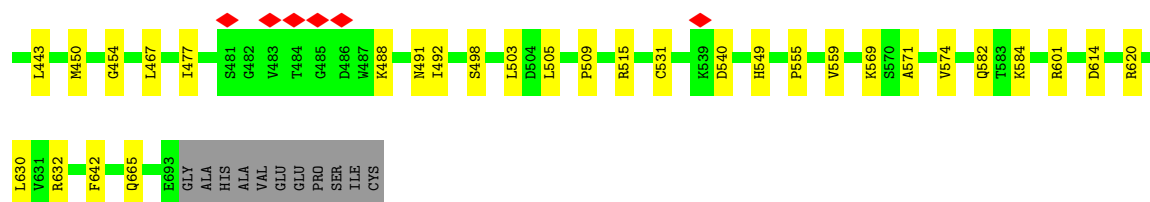
Chain 2: 



- Molecule 3: NADH:ubiquinone oxidoreductase core subunit S1

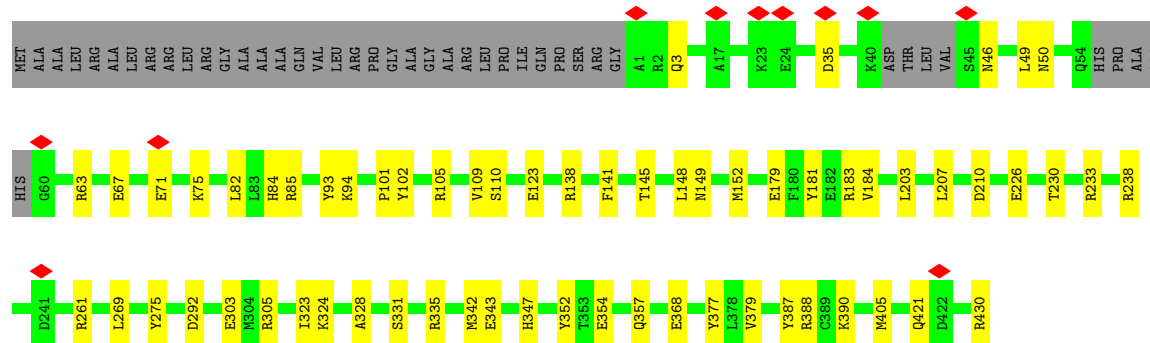
Chain 3: 





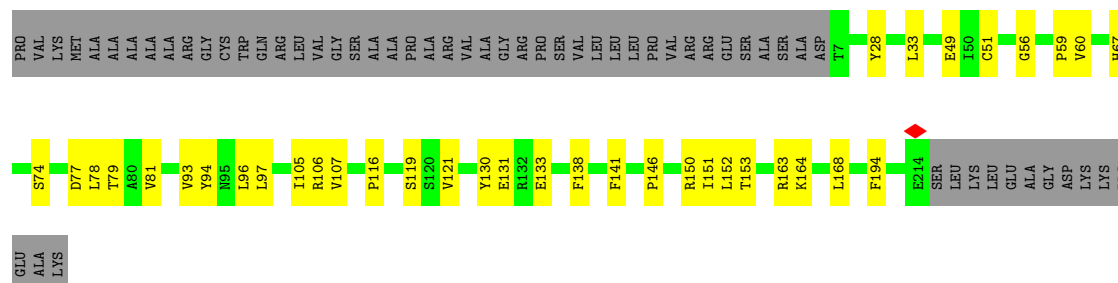
- Molecule 4: Mitochondrial complex I, 49 kDa subunit

Chain 4: 77% 14% 9%



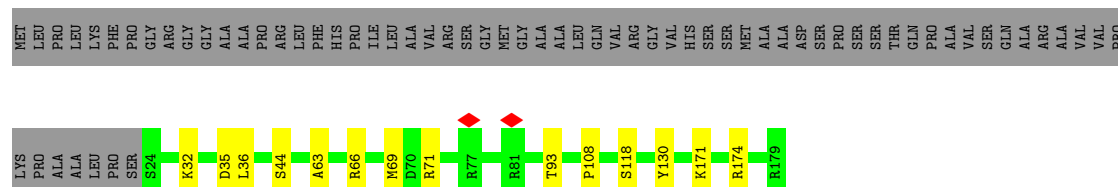
- Molecule 5: NADH:ubiquinone oxidoreductase core subunit S3

Chain 5: 64% 14% 22%



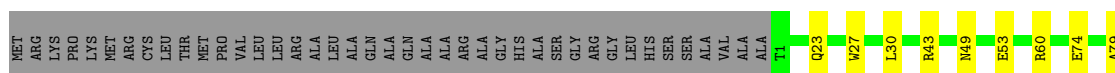
- Molecule 6: Mitochondrial complex I, PSST subunit

Chain 6: 64% 6% 30%

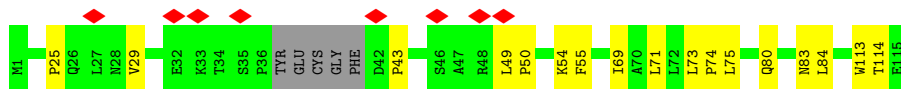
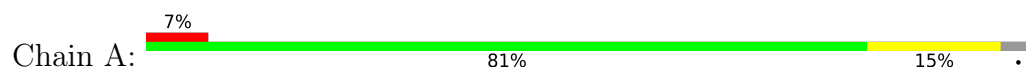


- Molecule 7: Mitochondrial complex I, TYKY subunit

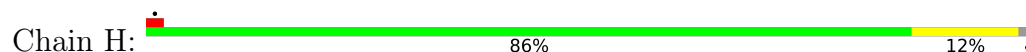
Chain 9: 66% 15% 19%



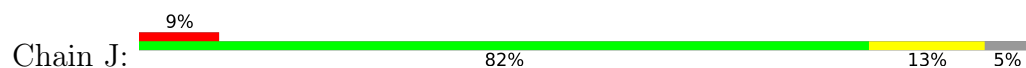
• Molecule 8: NADH-ubiquinone oxidoreductase chain 3



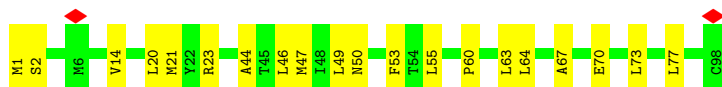
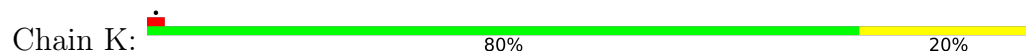
• Molecule 9: NADH-ubiquinone oxidoreductase chain 1



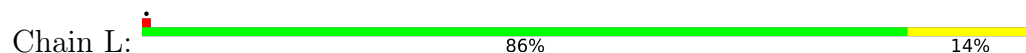
• Molecule 10: NADH-ubiquinone oxidoreductase chain 6

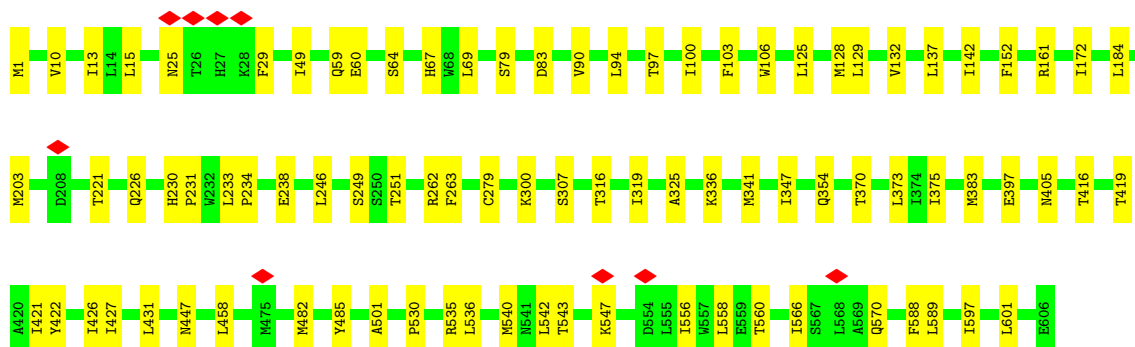


• Molecule 11: NADH-ubiquinone oxidoreductase chain 4L



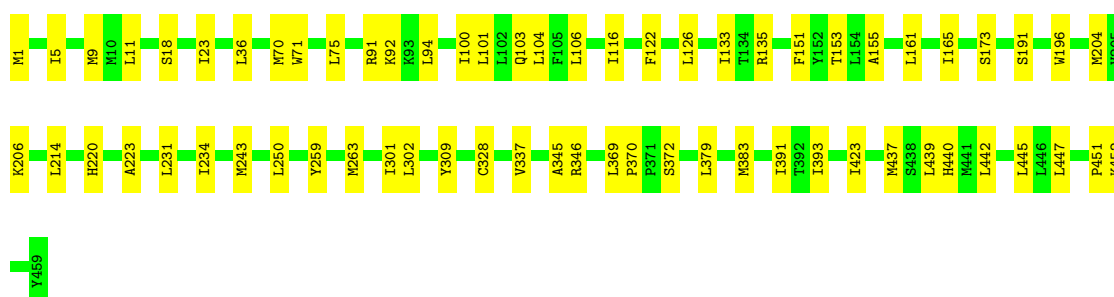
• Molecule 12: NADH-ubiquinone oxidoreductase chain 5





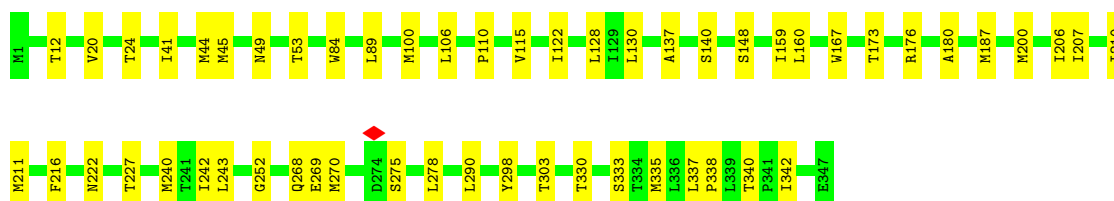
• Molecule 13: NADH-ubiquinone oxidoreductase chain 4

Chain M: 86% 14%



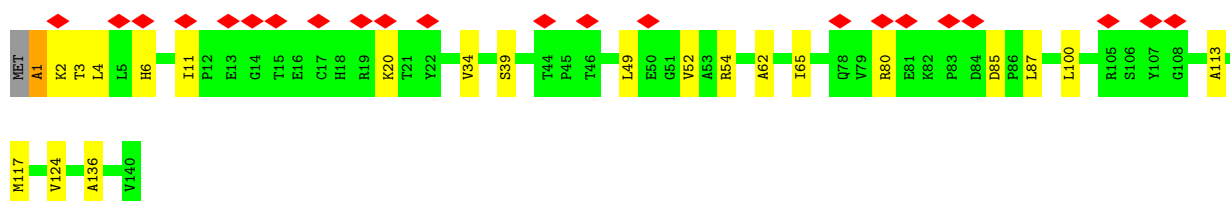
• Molecule 14: NADH-ubiquinone oxidoreductase chain 2

Chain N: 84% 16%



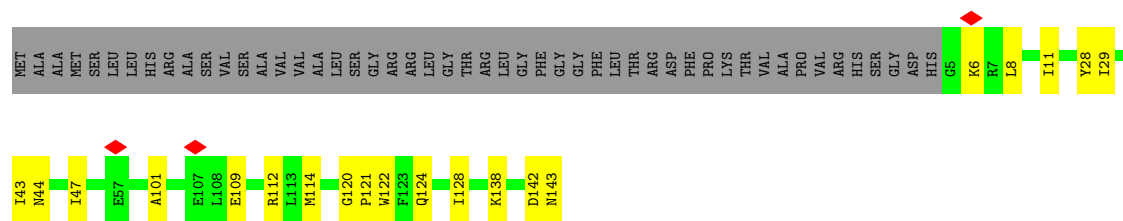
• Molecule 15: Mitochondrial complex I, B14.7 subunit

Chain V: 16% 84% 15% ..



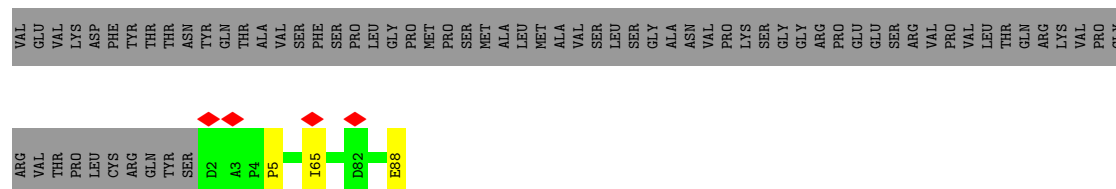
• Molecule 16: NADH:ubiquinone oxidoreductase subunit B5

Chain W: 63% 11% 26%



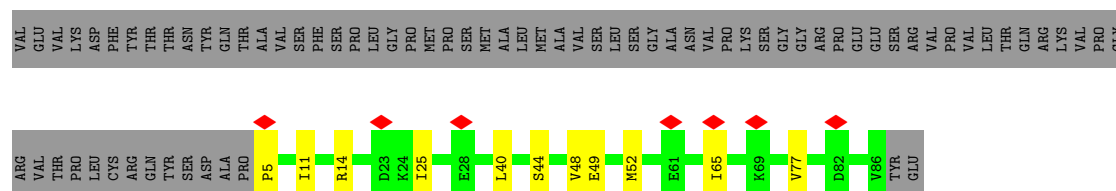
- Molecule 17: Acyl carrier protein

Chain X: 54% 45%



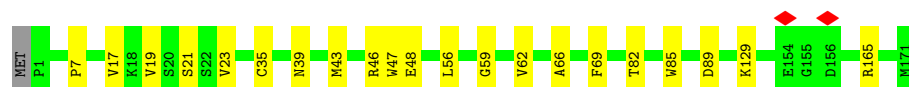
- Molecule 17: Acyl carrier protein

Chain j: 45% 7% 48%



- Molecule 18: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain Y: 87% 12%



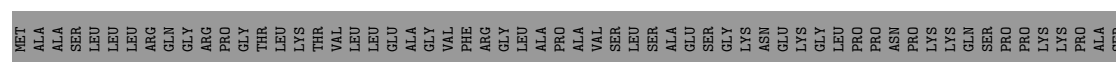
- Molecule 19: Mitochondrial complex I, PDSW subunit

Chain Z: 89% 9%

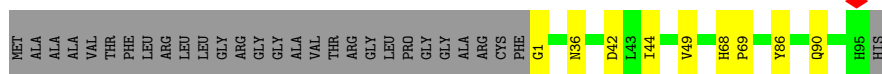


- Molecule 20: Mitochondrial complex I, 10 kDa subunit

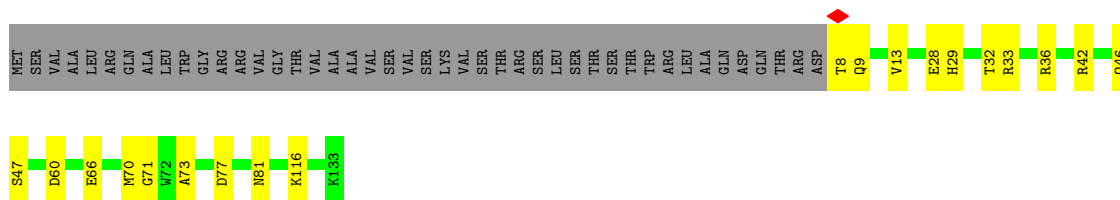
Chain a: 37% 60%



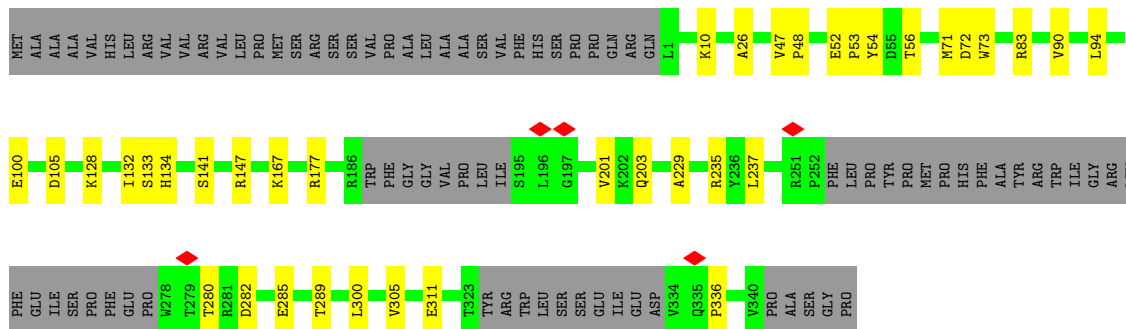
- Molecule 21: Mitochondrial complex I, 13 kDa subunit



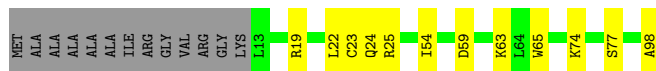
- Molecule 22: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



- Molecule 23: NADH:ubiquinone oxidoreductase subunit A9



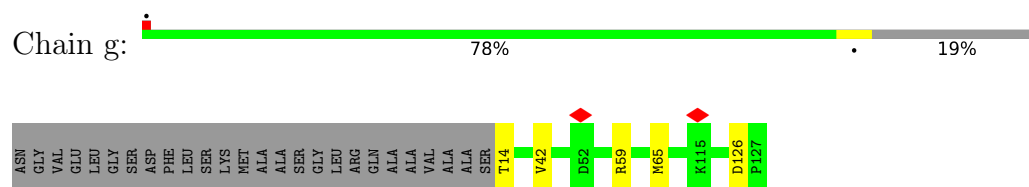
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



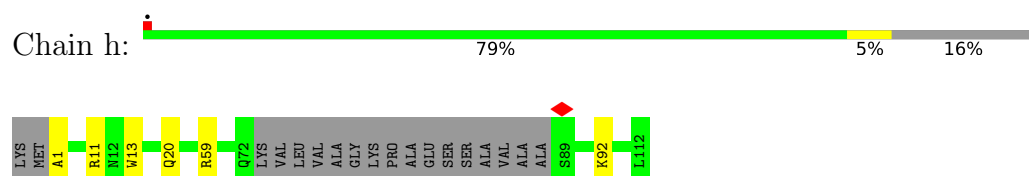
- Molecule 25: Mitochondrial complex I, B13 subunit



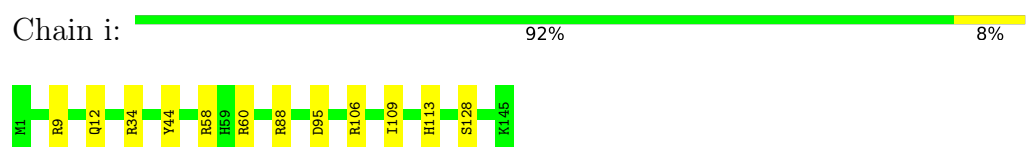
- Molecule 26: NADH:ubiquinone oxidoreductase subunit A6



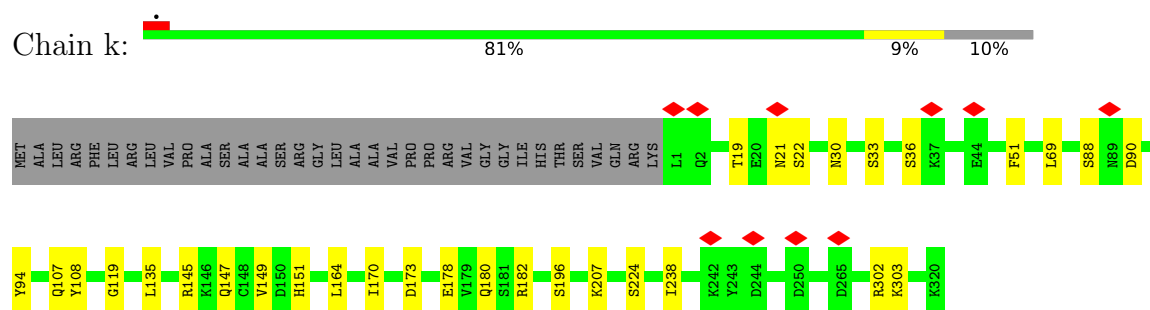
- Molecule 27: Mitochondrial complex I, B14.5a subunit



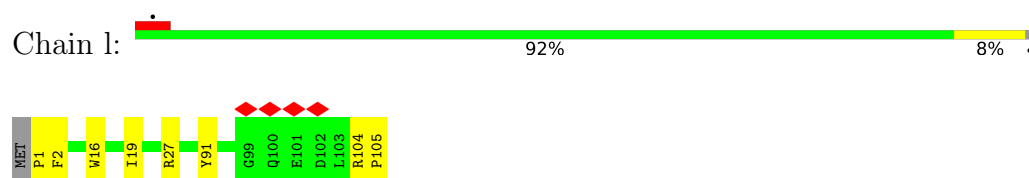
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



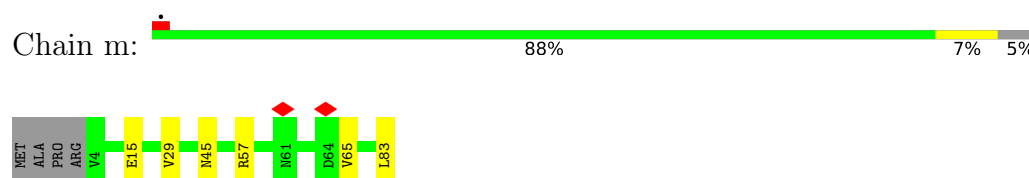
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial



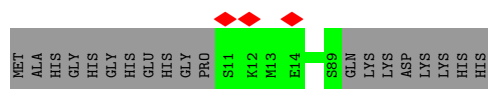
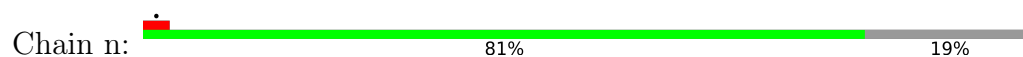
- Molecule 30: NADH:ubiquinone oxidoreductase subunit S5



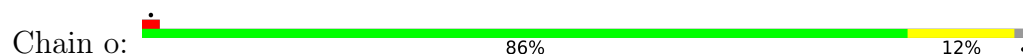
- Molecule 31: NADH:ubiquinone oxidoreductase subunit A3



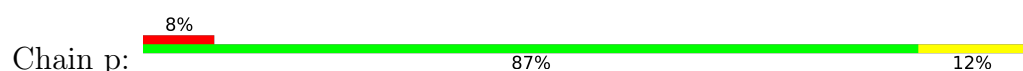
- Molecule 32: NADH:ubiquinone oxidoreductase subunit B3



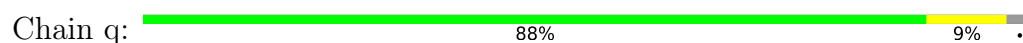
- Molecule 33: NADH dehydrogenase [ubiquinone] 1 subunit C2



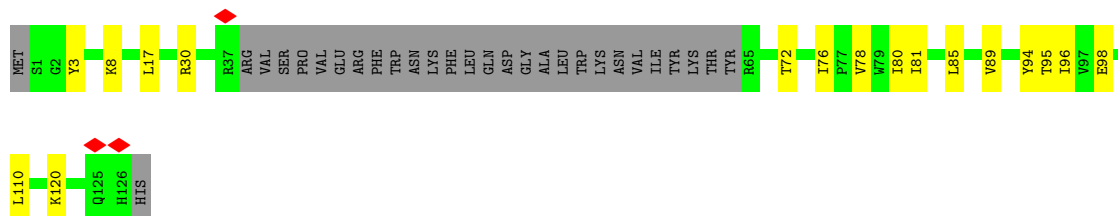
- Molecule 34: NADH:ubiquinone oxidoreductase subunit B4



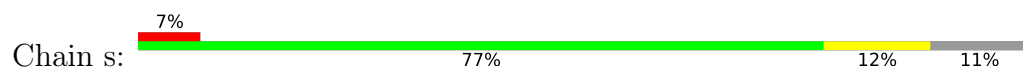
- Molecule 35: Mitochondrial complex I, B16.6 subunit



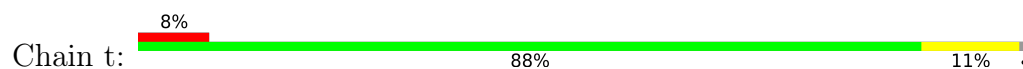
- Molecule 36: Mitochondrial complex I, B17 subunit



- Molecule 37: NADH:ubiquinone oxidoreductase subunit B7

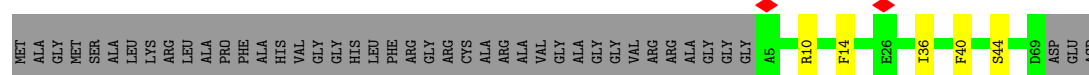


- Molecule 38: NADH:ubiquinone oxidoreductase subunit B9





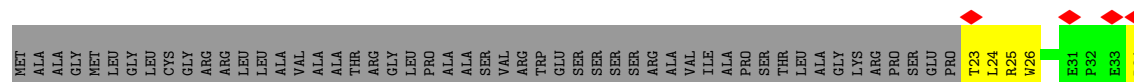
- Molecule 39: NADH:ubiquinone oxidoreductase subunit B2



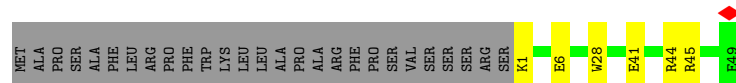
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



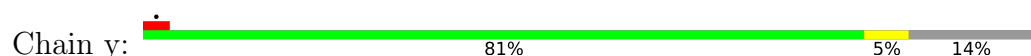
- Molecule 41: Mitochondrial complex I, ESSS subunit



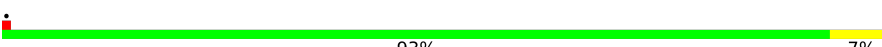
- Molecule 42: Mitochondrial complex I, KFYI subunit



- Molecule 43: Mitochondrial complex I, MNLL subunit



- Molecule 44: Mitochondrial complex I, MWFE subunit

Chain z:  93% 7%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	32982	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 ($e^-/\text{\AA}^2$)	100	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.336	Depositor
Minimum map value	-0.119	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	171.81, 193.39, 286.35	wwPDB
Map dimensions	345, 233, 207	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83000004	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, AYA, AMP, K, SEP, 2MR, CDL, FMN, MYR, SF4, FES, PC1, FME, NDP, 3PE, ZMP

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	1	0.41	0/3386	0.59	0/4575
2	2	0.40	0/1695	0.61	0/2306
3	3	0.44	0/5362	0.59	2/7266 (0.0%)
4	4	0.46	0/3463	0.58	0/4687
5	5	0.45	0/1776	0.58	0/2417
6	6	0.48	0/1278	0.60	0/1728
7	9	0.53	0/1445	0.60	0/1956
8	A	0.37	0/902	0.68	0/1234
9	H	0.44	0/2563	0.65	0/3505
10	J	0.36	0/1302	0.61	0/1760
11	K	0.42	0/749	0.62	0/1014
12	L	0.35	0/4924	0.59	1/6698 (0.0%)
13	M	0.41	0/3731	0.61	0/5085
14	N	0.42	0/2787	0.60	0/3795
15	V	0.23	0/1041	0.47	0/1412
16	W	0.34	0/1188	0.51	0/1607
17	X	0.25	0/713	0.45	0/963
17	j	0.27	0/670	0.51	0/902
18	Y	0.35	0/1440	0.56	0/1942
19	Z	0.31	0/1475	0.50	0/1989
20	a	0.31	0/383	0.49	0/518
21	b	0.39	0/749	0.49	0/1009
22	c	0.43	0/1047	0.50	0/1415
23	d	0.36	0/2424	0.52	0/3276
24	e	0.34	0/702	0.53	0/945
25	f	0.34	0/937	0.52	0/1271
26	g	0.36	0/993	0.53	0/1336
27	h	0.39	0/779	0.56	0/1053
28	i	0.38	0/1250	0.49	0/1698
29	k	0.30	0/2646	0.47	0/3579
30	l	0.34	0/896	0.56	0/1200
31	m	0.31	0/647	0.50	0/890

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	n	0.24	0/653	0.44	0/882
33	o	0.33	0/1035	0.48	0/1398
34	p	0.28	0/1085	0.48	0/1467
35	q	0.35	0/1171	0.52	0/1579
36	r	0.32	0/874	0.51	0/1188
37	s	0.25	0/1072	0.50	0/1436
38	t	0.29	0/1573	0.55	0/2130
39	u	0.25	0/590	0.47	0/810
40	v	0.28	0/1361	0.51	2/1861 (0.1%)
41	w	0.32	0/872	0.57	0/1185
42	x	0.25	0/425	0.41	0/576
43	y	0.31	0/449	0.54	0/605
44	z	0.41	0/591	0.54	0/795
All	All	0.38	0/67094	0.56	5/90943 (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
3	3	0	2
4	4	0	1
8	A	0	2
35	q	0	1
All	All	0	6

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	366	THR	CA-C-N	6.03	133.05	121.54
3	3	366	THR	C-N-CA	6.03	133.05	121.54
12	L	230	HIS	N-CA-C	5.25	121.42	109.81
40	v	88	ARG	CA-C-N	5.04	128.06	120.69
40	v	88	ARG	C-N-CA	5.04	128.06	120.69

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	3	259	ASN	Peptide
3	3	366	THR	Peptide
4	4	275	TYR	Peptide
8	A	113	TRP	Peptide
8	A	29	VAL	Peptide
35	q	24	LEU	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	1	3312	0	3269	42	0
2	2	1655	0	1668	27	0
3	3	5275	0	5300	70	0
4	4	3390	0	3333	47	0
5	5	1726	0	1676	23	0
6	6	1247	0	1259	14	0
7	9	1414	0	1371	23	0
8	A	880	0	920	13	0
9	H	2489	0	2603	28	0
10	J	1273	0	1300	18	0
11	K	749	0	793	16	0
12	L	4806	0	4945	61	0
13	M	3647	0	3849	49	0
14	N	2723	0	2930	38	0
15	V	1028	0	1036	15	0
16	W	1155	0	1177	18	0
17	X	701	0	692	3	0
17	j	660	0	663	7	0
18	Y	1403	0	1392	15	0
19	Z	1441	0	1419	15	0
20	a	371	0	344	5	0
21	b	737	0	710	6	0
22	c	1024	0	1023	16	0
23	d	2372	0	2407	20	0
24	e	691	0	706	7	0
25	f	917	0	958	5	0
26	g	969	0	980	4	0
27	h	769	0	780	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	i	1209	0	1182	8	0
29	k	2596	0	2559	16	0
30	l	874	0	869	9	0
31	m	626	0	635	6	0
32	n	634	0	616	0	0
33	o	1004	0	995	12	0
34	p	1059	0	1062	15	0
35	q	1142	0	1137	11	0
36	r	846	0	864	13	0
37	s	1047	0	1015	12	0
38	t	1520	0	1477	18	0
39	u	563	0	509	3	0
40	v	1307	0	1207	17	0
41	w	846	0	792	13	0
42	x	412	0	411	4	0
43	y	436	0	437	2	0
44	z	576	0	570	5	0
45	1	8	0	0	3	0
45	3	16	0	0	1	0
45	6	8	0	0	1	0
45	9	16	0	0	0	0
46	1	31	0	19	2	0
47	2	4	0	0	1	0
47	3	4	0	0	0	0
48	3	1	0	0	0	0
49	4	40	0	54	1	0
49	6	51	0	82	4	0
49	A	51	0	82	2	0
49	H	51	0	82	1	0
49	J	40	0	54	3	0
49	L	82	0	118	2	0
49	M	44	0	65	1	0
49	N	82	0	118	2	0
49	V	72	0	92	2	0
49	i	51	0	82	0	0
49	p	27	0	27	0	0
50	6	46	0	69	1	0
50	9	54	0	88	2	0
50	A	37	0	48	2	0
50	L	108	0	176	7	0
50	M	54	0	88	4	0
51	L	100	0	156	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	N	75	0	97	5	0
51	V	179	0	261	8	0
51	W	100	0	156	4	0
51	h	58	0	60	0	0
51	o	90	0	133	6	0
51	y	100	0	156	5	0
52	X	31	0	34	2	0
52	g	34	0	40	2	0
53	b	1	0	0	0	0
54	d	48	0	26	1	0
55	k	23	0	12	0	0
56	s	15	0	27	0	0
All	All	67353	0	68342	645	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 5.

All (645) 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)
16:W:124:GLN:HB2	33:o:4:GLY:HA3	1.76	0.68
44:z:34:ARG:NH2	44:z:61:TYR:O	2.28	0.67
3:3:118:ASP:OD2	22:c:46:GLN:NE2	2.28	0.66
41:w:100:ARG:HB2	41:w:105:LEU:HB2	1.77	0.66
6:6:108:PRO:HB2	9:H:58:LYS:HD2	1.78	0.66
24:e:19:ARG:HB2	24:e:65:TRP:HB2	1.78	0.66
7:9:43:ARG:HG2	27:h:11:ARG:HD2	1.77	0.65
14:N:106:LEU:HD22	14:N:187:MET:HE2	1.79	0.64
14:N:45:MET:HE3	14:N:53:THR:HG22	1.80	0.64
18:Y:165:ARG:NH1	33:o:87:ASP:OD1	2.30	0.64
8:A:84:LEU:HD11	31:m:45:ASN:HD22	1.63	0.63
4:4:354:GLU:OE2	4:4:357:GLN:NE2	2.32	0.63
4:4:50:ASN:HD21	4:4:63:ARG:HH21	1.45	0.62
12:L:370:THR:HG23	12:L:431:LEU:HD13	1.80	0.62
14:N:243:LEU:HD22	14:N:330:THR:HG21	1.82	0.62
4:4:405:MET:SD	4:4:421:GLN:NE2	2.72	0.62
13:M:23:ILE:HD11	13:M:92:LYS:HD2	1.82	0.61
12:L:570:GLN:OE1	14:N:167:TRP:NE1	2.33	0.61
1:1:132:ARG:NH2	20:a:64:PRO:O	2.33	0.61
35:q:81:ARG:NH1	35:q:85:MET:SD	2.74	0.61
2:2:10:ARG:NH2	3:3:138:GLU:OE2	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:100:ILE:HG21	12:L:246:LEU:HB2	1.82	0.61
4:4:269:LEU:HB2	4:4:368:GLU:HB2	1.82	0.60
3:3:364:LEU:HD12	3:3:491:ASN:HB3	1.83	0.60
9:H:26:LYS:HB3	44:z:5:VAL:HG12	1.83	0.60
30:l:104:ARG:NH1	35:q:84:GLN:OE1	2.34	0.60
16:W:6:LYS:HE2	17:X:5:PRO:HG3	1.84	0.60
3:3:515:ARG:NH2	3:3:531:CYS:O	2.34	0.60
13:M:328:CYS:HB3	13:M:437:MET:HE1	1.83	0.60
23:d:167:LYS:HB2	23:d:229:ALA:HA	1.83	0.59
1:1:96:ASN:ND2	46:1:501:FMN:O4'	2.35	0.59
4:4:145:THR:HG1	4:4:181:TYR:HH	1.48	0.59
24:e:23:CYS:SG	24:e:24:GLN:N	2.75	0.59
3:3:632:ARG:HH12	24:e:59:ASP:H	1.51	0.59
19:Z:67:PHE:HD1	43:y:43:LEU:HD21	1.68	0.59
38:t:142:GLU:OE2	38:t:157:ARG:NH2	2.36	0.59
5:5:33:LEU:HD13	5:5:60:VAL:HG22	1.83	0.58
18:Y:43:MET:HE3	18:Y:47:TRP:HZ3	1.67	0.58
1:1:20:ARG:HH12	2:2:201:SER:HB2	1.68	0.58
11:K:67:ALA:O	11:K:70:GLU:HB3	2.04	0.58
36:r:3:TYR:HB2	36:r:8:LYS:HG3	1.83	0.58
5:5:151:ILE:HG23	5:5:152:LEU:HG	1.86	0.58
51:V:203:CDL:H391	51:V:203:CDL:H571	1.84	0.58
4:4:430:ARG:NH2	5:5:133:GLU:OE2	2.36	0.58
12:L:161:ARG:HA	38:t:91:GLU:HG3	1.86	0.58
9:H:64:ALA:O	9:H:124:ASN:ND2	2.37	0.58
37:s:6:ARG:NH1	37:s:15:GLU:OE2	2.37	0.58
2:2:74:GLN:O	20:a:74:ARG:NH2	2.37	0.58
3:3:252:PRO:HG3	3:3:263:ILE:HG12	1.86	0.57
4:4:335:ARG:NH2	7:9:129:ASP:OD1	2.37	0.57
12:L:103:PHE:HB2	12:L:341:MET:HE3	1.85	0.57
12:L:547:LYS:NZ	40:v:44:TYR:OH	2.37	0.57
28:i:34:ARG:NH2	28:i:58:ARG:O	2.36	0.57
14:N:159:ILE:HG21	14:N:278:LEU:HD11	1.85	0.57
11:K:21:MET:HG2	12:L:589:LEU:HD23	1.85	0.57
4:4:352:TYR:HD1	7:9:86:VAL:HG21	1.69	0.57
22:c:42:ARG:NH1	22:c:46:GLN:O	2.38	0.57
3:3:383:ASN:ND2	3:3:665:GLN:O	2.34	0.57
11:K:46:LEU:O	11:K:50:ASN:HB2	2.03	0.57
18:Y:89:ASP:OD2	44:z:34:ARG:NH1	2.38	0.57
2:2:150:ASN:HB3	2:2:162:GLU:HB3	1.86	0.56
3:3:574:VAL:HG21	3:3:630:LEU:HD22	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:233:ARG:NH2	7:9:23:GLN:O	2.37	0.56
1:1:108:ARG:NH2	2:2:162:GLU:OE2	2.38	0.56
11:K:73:LEU:HD11	14:N:41:ILE:HG13	1.87	0.56
14:N:211:MET:HG2	14:N:333:SER:HB2	1.86	0.56
25:f:71:LEU:HD13	25:f:79:VAL:HG11	1.87	0.56
39:u:10:ARG:NH1	39:u:14:PHE:O	2.38	0.56
23:d:10:LYS:NZ	26:g:126:ASP:OD2	2.38	0.56
3:3:360:SER:O	3:3:365:ASN:ND2	2.30	0.56
1:1:345:LYS:NZ	2:2:109:MET:SD	2.78	0.56
3:3:45:ARG:NH2	3:3:256:GLU:OE2	2.34	0.56
6:6:44:SER:O	9:H:54:LYS:NZ	2.38	0.56
9:H:10:ILE:HA	9:H:13:ILE:HD12	1.88	0.56
9:H:141:SER:HB3	9:H:289:LEU:HD22	1.87	0.55
49:J:201:3PE:H2B2	11:K:14:VAL:HG22	1.89	0.55
34:p:47:GLN:HA	34:p:50:TYR:HB3	1.88	0.55
1:1:142:PHE:HB3	1:1:145:GLU:HB2	1.88	0.55
4:4:261:ARG:NH2	4:4:303:GLU:OE2	2.39	0.55
6:6:71:ARG:HA	9:H:37:PRO:HA	1.89	0.55
10:J:163:ILE:HG21	14:N:12:THR:HG21	1.88	0.55
12:L:83:ASP:OD2	12:L:262:ARG:NH1	2.38	0.55
12:L:221:THR:HG23	12:L:226:GLN:HB2	1.86	0.55
12:L:421:ILE:HG12	12:L:501:ALA:HB2	1.88	0.55
18:Y:35:CYS:O	18:Y:39:ASN:ND2	2.40	0.55
2:2:105:THR:OG1	47:2:300:FES:S2	2.64	0.55
4:4:110:SER:OG	4:4:149:ASN:ND2	2.40	0.55
15:V:1:AYA:HA	15:V:4:LEU:HD23	1.87	0.55
3:3:106:PRO:O	3:3:218:ARG:NH2	2.40	0.55
5:5:150:ARG:NH1	5:5:153:THR:OG1	2.39	0.55
12:L:542:LEU:HB2	40:v:83:MET:HE3	1.88	0.55
29:k:173:ASP:HB2	29:k:224:SER:HA	1.87	0.55
41:w:92:GLU:OE2	41:w:95:ARG:NH2	2.37	0.55
52:X:101:ZMP:O6	38:t:12:GLN:NE2	2.39	0.55
19:Z:136:LYS:NZ	19:Z:140:ASP:OD2	2.39	0.55
2:2:159:ASN:HB3	2:2:184:PRO:HB3	1.88	0.55
8:A:80:GLN:NE2	9:H:315:PRO:O	2.39	0.55
14:N:338:PRO:HG3	51:y:201:CDL:H792	1.88	0.55
5:5:119:SER:OG	5:5:131:GLU:OE2	2.25	0.55
23:d:26:ALA:HB3	23:d:47:VAL:HG13	1.89	0.55
2:2:121:GLN:HE21	2:2:128:VAL:HG23	1.71	0.54
1:1:120:GLU:OE2	1:1:236:ARG:NH1	2.37	0.54
40:v:52:ASP:OD1	40:v:78:HIS:NE2	2.31	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:111:ARG:HD3	2:2:151:ALA:HB3	1.90	0.54
3:3:148:THR:HG23	3:3:150:MET:HE3	1.88	0.54
33:o:66:THR:OG1	42:x:28:TRP:NE1	2.41	0.54
50:M:502:PC1:H2A2	50:M:502:PC1:H381	1.90	0.54
3:3:101:HIS:HD2	4:4:342:MET:HE2	1.73	0.54
16:W:43:ILE:HG12	16:W:47:ILE:HD12	1.88	0.54
34:p:47:GLN:HG3	38:t:165:LEU:HD13	1.89	0.54
34:p:70:ALA:HB2	40:v:10:PRO:HG2	1.89	0.54
12:L:67:HIS:HB3	50:L:1002:PC1:H111	1.90	0.54
2:2:175:GLU:HG3	2:2:182:PRO:HG3	1.89	0.54
3:3:36:GLN:NE2	22:c:47:SER:O	2.40	0.54
21:b:1:GLY:N	21:b:42:ASP:OD2	2.41	0.54
38:t:29:ARG:HD2	38:t:75:HIS:CD2	2.43	0.54
3:3:194:GLU:HG3	3:3:389:PRO:HB3	1.90	0.54
16:W:138:LYS:HA	30:l:27:ARG:HB3	1.89	0.54
2:2:149:VAL:O	2:2:190:ARG:NH2	2.40	0.53
4:4:179:GLU:OE2	6:6:66:ARG:NH1	2.31	0.53
5:5:96:LEU:HB2	5:5:105:ILE:HG22	1.91	0.53
13:M:126:LEU:HD21	13:M:153:THR:HG21	1.89	0.53
27:h:13:TRP:O	35:q:27:ARG:NH2	2.36	0.53
42:x:1:LYS:NZ	42:x:6:GLU:OE1	2.38	0.53
3:3:126:ASP:HB2	4:4:328:ALA:HB3	1.89	0.53
3:3:193:SER:H	3:3:196:SER:HB3	1.73	0.53
17:j:48:VAL:HG12	17:j:52:MET:HE2	1.90	0.53
4:4:238:ARG:NH1	9:H:279:ARG:O	2.41	0.53
29:k:170:ILE:HD11	29:k:238:ILE:HD11	1.89	0.53
7:9:145:GLU:HA	7:9:148:LEU:HD13	1.89	0.53
14:N:115:VAL:HG12	14:N:180:ALA:HB1	1.91	0.53
22:c:28:GLU:O	22:c:32:THR:OG1	2.24	0.53
28:i:60:ARG:HH22	28:i:95:ASP:HA	1.72	0.53
14:N:252:GLY:HA3	14:N:290:LEU:HD13	1.89	0.53
15:V:2:LYS:O	15:V:6:HIS:ND1	2.33	0.53
36:r:17:LEU:HD11	38:t:162:LEU:HD22	1.91	0.53
3:3:323:VAL:H	3:3:498:SER:HB3	1.72	0.53
4:4:183:ARG:NH1	4:4:210:ASP:OD2	2.33	0.53
30:l:91:TYR:OH	35:q:92:GLU:OE1	2.25	0.52
3:3:201:ASP:OD2	3:3:268:ARG:NH2	2.38	0.52
3:3:382:THR:HG23	3:3:384:PRO:HD3	1.91	0.52
4:4:388:ARG:HG2	5:5:81:VAL:HG22	1.91	0.52
12:L:316:THR:HA	12:L:319:ILE:HG12	1.91	0.52
16:W:120:GLY:O	16:W:124:GLN:NE2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Z:5:ASP:OD2	41:w:98:LYS:NZ	2.37	0.52
4:4:71:GLU:OE2	9:H:134:ARG:NH1	2.43	0.52
29:k:180:GLN:NE2	29:k:196:SER:OG	2.39	0.52
4:4:35:ASP:O	14:N:49:ASN:ND2	2.43	0.52
13:M:133:ILE:HD11	13:M:231:LEU:HD11	1.90	0.52
37:s:30:PHE:HB3	37:s:33:ARG:HB2	1.92	0.52
3:3:443:LEU:HD13	3:3:477:ILE:HD11	1.92	0.52
4:4:3:GLN:NE2	13:M:135:ARG:O	2.42	0.52
14:N:335:MET:HG2	51:o:201:CDL:H661	1.92	0.52
16:W:44:ASN:HB3	51:W:201:CDL:HA31	1.92	0.52
5:5:121:VAL:HG21	5:5:146:PRO:HD3	1.93	0.52
10:J:40:GLY:HA2	10:J:43:ILE:HD12	1.92	0.52
18:Y:66:ALA:O	18:Y:69:PHE:HB3	2.10	0.52
14:N:207:ILE:HG22	14:N:211:MET:HE2	1.92	0.51
13:M:101:LEU:HD21	51:o:201:CDL:H841	1.92	0.51
50:L:1003:PC1:H291	51:L:1004:CDL:H431	1.92	0.51
25:f:34:LEU:HD12	25:f:37:ILE:HD12	1.92	0.51
1:1:361:GLN:N	45:1:500:SF4:S4	2.81	0.51
9:H:24:GLU:OE2	9:H:274:ARG:NH1	2.44	0.51
12:L:427:ILE:HG23	12:L:431:LEU:HD12	1.92	0.51
23:d:141:SER:O	23:d:147:ARG:NH1	2.40	0.51
1:1:89:ARG:NH1	1:1:217:GLY:O	2.44	0.51
51:L:1004:CDL:H562	51:L:1004:CDL:H642	1.92	0.51
13:M:423:ILE:HG12	34:p:58:VAL:HG22	1.93	0.51
1:1:261:HIS:ND1	1:1:338:ASP:OD1	2.43	0.51
51:L:1004:CDL:H621	13:M:372:SER:HB3	1.92	0.51
14:N:270:MET:O	14:N:275:SER:OG	2.28	0.51
38:t:100:GLU:OE1	38:t:121:ARG:NH1	2.44	0.51
37:s:102:GLU:OE2	37:s:105:ARG:NH2	2.38	0.51
3:3:396:ARG:NH1	3:3:416:THR:O	2.44	0.51
9:H:303:TRP:O	9:H:307:LEU:HB2	2.10	0.51
2:2:156:ILE:HD13	2:2:176:LEU:HD11	1.92	0.51
6:6:171:LYS:HG2	6:6:174:ARG:HH11	1.76	0.51
12:L:279:CYS:SG	12:L:405:ASN:ND2	2.84	0.51
12:L:589:LEU:HD11	49:V:201:3PE:H232	1.93	0.51
19:Z:139:GLN:NE2	34:p:122:ARG:O	2.43	0.51
19:Z:19:PRO:HD3	36:r:110:LEU:HD11	1.91	0.50
19:Z:161:ARG:NH2	41:w:110:SER:O	2.44	0.50
29:k:145:ARG:NH1	29:k:147:GLN:OE1	2.44	0.50
1:1:21:ILE:O	1:1:117:LYS:NZ	2.42	0.50
4:4:123:GLU:OE2	4:4:138:ARG:NH2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:71:LEU:O	10:J:147:TYR:OH	2.28	0.50
3:3:582:GLN:OE1	3:3:620:ARG:NH1	2.41	0.50
4:4:233:ARG:NH1	50:9:401:PC1:O12	2.44	0.50
5:5:77:ASP:OD2	5:5:79:THR:OG1	2.28	0.50
7:9:106:THR:O	7:9:151:LYS:NZ	2.44	0.50
7:9:132:VAL:HG21	7:9:165:ILE:HG21	1.93	0.50
24:e:74:LYS:NZ	24:e:98:ALA:O	2.45	0.50
51:y:201:CDL:H872	51:y:201:CDL:H641	1.93	0.50
8:A:83:ASN:ND2	50:A:201:PC1:O14	2.40	0.50
15:V:1:AYA:HM2	15:V:3:THR:HG22	1.93	0.50
3:3:46:LEU:O	22:c:116:LYS:NZ	2.41	0.50
3:3:601:ARG:NH2	3:3:614:ASP:OD1	2.43	0.50
12:L:543:THR:HG23	40:v:83:MET:HE1	1.94	0.50
49:M:501:3PE:H221	15:V:87:LEU:HB2	1.93	0.50
16:W:138:LYS:HB2	16:W:143:ASN:HD21	1.76	0.50
36:r:72:THR:HA	36:r:76:ILE:HD12	1.93	0.50
3:3:273:GLY:O	3:3:549:HIS:NE2	2.37	0.50
8:A:74:PRO:HG2	10:J:147:TYR:HE2	1.77	0.50
9:H:114:TYR:OH	10:J:61:LEU:O	2.26	0.50
12:L:128:MET:HG2	12:L:251:THR:HG22	1.94	0.50
1:1:390:ASP:O	1:1:393:TRP:HB3	2.11	0.50
3:3:244:THR:HB	22:c:73:ALA:HB2	1.94	0.50
12:L:535:ARG:NH1	40:v:90:ASP:O	2.45	0.50
14:N:242:ILE:HG21	51:o:201:CDL:H562	1.93	0.50
15:V:113:ALA:O	15:V:117:MET:HB2	2.11	0.50
12:L:90:VAL:HG22	12:L:129:LEU:HD22	1.93	0.50
50:L:1003:PC1:H3F1	13:M:447:LEU:HD11	1.94	0.50
18:Y:129:LYS:NZ	31:m:65:VAL:O	2.39	0.50
38:t:137:LYS:HA	38:t:140:GLN:HG2	1.94	0.50
6:6:118:SER:N	45:6:201:SF4:S4	2.85	0.49
51:L:1004:CDL:H561	51:L:1004:CDL:H762	1.93	0.49
43:y:8:ARG:HG3	43:y:10:HIS:H	1.76	0.49
1:1:139:ARG:NH2	2:2:144:CYS:O	2.30	0.49
7:9:108:ARG:NH2	28:i:128:SER:OG	2.45	0.49
12:L:25:ASN:HD22	12:L:29:PHE:HE2	1.59	0.49
14:N:200:MET:HG3	14:N:269:GLU:HG3	1.94	0.49
8:A:25:PRO:HB2	9:H:60:PRO:HD3	1.94	0.49
12:L:142:ILE:HG12	13:M:370:PRO:HB2	1.94	0.49
23:d:72:ASP:O	23:d:83:ARG:NH2	2.45	0.49
36:r:85:LEU:HD22	36:r:96:ILE:HD11	1.94	0.49
3:3:324:ASP:OD1	3:3:324:ASP:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:226:GLU:OE1	4:4:305:ARG:NH2	2.39	0.49
12:L:203:MET:HB2	19:Z:113:GLN:HG3	1.94	0.49
16:W:109:GLU:OE2	16:W:112:ARG:NH2	2.35	0.49
31:m:83:LEU:HD13	35:q:54:ARG:HD3	1.94	0.49
51:y:201:CDL:H311	51:y:201:CDL:H562	1.94	0.49
1:1:342:ASP:OD1	1:1:429:ARG:NH2	2.40	0.49
12:L:558:LEU:HB3	13:M:214:LEU:HD21	1.95	0.49
38:t:29:ARG:HD2	38:t:75:HIS:HD2	1.77	0.49
1:1:184:TYR:HB3	1:1:357:GLU:HB3	1.95	0.49
2:2:96:GLY:H	2:2:138:THR:HG1	1.58	0.49
3:3:206:GLY:N	45:3:801:SF4:S2	2.81	0.49
33:o:34:ILE:HG22	33:o:68:PHE:HB3	1.94	0.49
12:L:97:THR:HG21	12:L:125:LEU:HD22	1.94	0.48
4:4:46:ASN:ND2	4:4:67:GLU:OE2	2.45	0.48
12:L:536:LEU:HG	12:L:540:MET:HE2	1.95	0.48
14:N:337:LEU:O	14:N:340:THR:OG1	2.27	0.48
51:N:403:CDL:H112	33:o:63:LEU:HD23	1.93	0.48
26:g:42:VAL:HG11	26:g:59:ARG:HG3	1.95	0.48
29:k:51:PHE:HB3	29:k:107:GLN:HE21	1.78	0.48
3:3:260:GLU:OE2	3:3:397:LYS:NZ	2.30	0.48
5:5:28:TYR:OH	5:5:67:HIS:NE2	2.37	0.48
14:N:24:THR:HG22	30:l:2:PHE:HZ	1.77	0.48
14:N:342:ILE:HD11	33:o:75:LEU:HB3	1.95	0.48
4:4:377:TYR:HB3	4:4:390:LYS:HB3	1.95	0.48
12:L:601:LEU:O	15:V:1:AYA:N	2.46	0.48
1:1:355:LYS:HD3	1:1:373:ASN:HD22	1.78	0.48
8:A:54:LYS:HE2	8:A:114:THR:HG23	1.95	0.48
15:V:65:ILE:HD11	15:V:100:LEU:HD23	1.95	0.48
3:3:60:GLU:HG2	3:3:78:ASN:HB3	1.95	0.48
3:3:187:ILE:HG13	3:3:189:LYS:HB2	1.95	0.48
12:L:556:ILE:O	12:L:560:THR:N	2.46	0.48
22:c:13:VAL:O	26:g:14:THR:OG1	2.31	0.48
12:L:485:TYR:OH	37:s:1:GLY:N	2.47	0.48
49:N:401:3PE:H3I2	30:l:1:PRO:HG2	1.96	0.48
29:k:22:SER:OG	29:k:119:GLY:O	2.29	0.48
34:p:12:SER:OG	40:v:57:GLU:OE2	2.29	0.48
5:5:138:PHE:O	5:5:163:ARG:NE	2.47	0.48
6:6:63:ALA:HB2	6:6:69:MET:HE3	1.96	0.48
9:H:79:LEU:HD11	9:H:222:LEU:HD22	1.96	0.48
13:M:5:ILE:HG23	13:M:104:LEU:HD11	1.96	0.48
6:6:32:LYS:HG3	49:6:203:3PE:H3H1	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:9:162:GLU:HB3	28:i:109:ILE:HG12	1.96	0.48
17:X:65:ILE:HD13	38:t:3:LEU:HD22	1.96	0.48
23:d:94:LEU:HD23	23:d:132:ILE:HG13	1.95	0.48
2:2:43:LYS:HE2	2:2:73:LEU:HA	1.96	0.47
12:L:383:MET:HE2	39:u:36:ILE:HD13	1.96	0.47
12:L:10:VAL:HG21	36:r:78:VAL:HG22	1.95	0.47
15:V:39:SER:OG	15:V:54:ARG:NH2	2.46	0.47
9:H:14:LEU:HD22	9:H:225:MET:HE2	1.96	0.47
1:1:380:VAL:O	1:1:429:ARG:NH1	2.41	0.47
5:5:49:GLU:OE2	5:5:106:ARG:NH1	2.46	0.47
49:J:201:3PE:H11	11:K:23:ARG:HG2	1.96	0.47
12:L:129:LEU:HA	12:L:132:VAL:HG22	1.95	0.47
49:V:201:3PE:H291	49:V:201:3PE:H342	1.97	0.47
16:W:142:ASP:OD1	18:Y:46:ARG:NH1	2.40	0.47
30:l:105:PRO:HD3	35:q:81:ARG:HD3	1.96	0.47
12:L:233:LEU:HD23	12:L:307:SER:HB3	1.96	0.47
13:M:204:MET:HE1	13:M:302:LEU:HD11	1.96	0.47
1:1:112:ARG:HB2	1:1:145:GLU:HG3	1.97	0.47
1:1:428:GLU:HA	1:1:431:GLN:HG2	1.97	0.47
3:3:12:PHE:HB2	3:3:78:ASN:HA	1.96	0.47
49:4:501:3PE:H382	13:M:151:PHE:HB3	1.97	0.47
13:M:94:LEU:HD21	51:o:201:CDL:H551	1.97	0.47
14:N:110:PRO:HD3	14:N:160:LEU:HD23	1.97	0.47
16:W:8:LEU:HD21	17:X:88:GLU:HB2	1.97	0.47
18:Y:7:PRO:HG3	18:Y:56:LEU:HD11	1.97	0.47
12:L:59:GLN:NE2	36:r:98:GLU:OE2	2.45	0.47
50:L:1002:PC1:H341	51:W:201:CDL:H512	1.97	0.47
14:N:206:ILE:HG23	49:N:401:3PE:H2I2	1.96	0.47
4:4:145:THR:HA	4:4:148:LEU:HD12	1.96	0.47
7:9:155:LEU:HB3	21:b:36:ASN:HD22	1.80	0.47
9:H:102:VAL:HG21	9:H:154:LEU:HD21	1.97	0.47
14:N:122:ILE:O	14:N:176:ARG:NH1	2.48	0.47
29:k:30:ASN:N	29:k:33:SER:OG	2.48	0.47
3:3:356:THR:HG21	3:3:503:LEU:HD22	1.96	0.47
6:6:36:LEU:HD22	49:6:203:3PE:H3A1	1.95	0.47
12:L:161:ARG:NE	12:L:238:GLU:OE2	2.47	0.47
51:N:403:CDL:OA7	51:N:403:CDL:O1	2.33	0.47
3:3:47:SER:O	3:3:161:ARG:NH1	2.47	0.46
51:N:403:CDL:HB4	51:N:403:CDL:H732	1.97	0.46
1:1:374:LYS:NZ	3:3:133:GLY:O	2.47	0.46
7:9:74:GLU:HB2	21:b:44:ILE:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:4:TYR:O	10:J:7:PHE:HB3	2.16	0.46
19:Z:159:LYS:HE2	41:w:118:ILE:HG23	1.97	0.46
3:3:261:GLU:OE1	22:c:42:ARG:NH2	2.48	0.46
12:L:106:TRP:CD1	12:L:447:ASN:HD22	2.33	0.46
29:k:108:TYR:OH	29:k:164:LEU:O	2.27	0.46
1:1:96:ASN:ND2	46:1:501:FMN:HO4'	2.14	0.46
3:3:285:ARG:NH2	3:3:555:PRO:O	2.49	0.46
4:4:49:LEU:HD22	8:A:43:PRO:HB2	1.97	0.46
9:H:46:LEU:HD13	9:H:49:ILE:HD13	1.96	0.46
12:L:597:ILE:HD13	15:V:34:VAL:HG13	1.98	0.46
3:3:362:TYR:HA	3:3:492:ILE:HD12	1.98	0.46
3:3:371:VAL:HG22	3:3:450:MET:HE1	1.97	0.46
10:J:23:LYS:O	11:K:23:ARG:NH1	2.49	0.46
23:d:300:LEU:HB3	23:d:305:VAL:HB	1.98	0.46
34:p:39:ARG:NE	38:t:151:GLU:OE2	2.36	0.46
34:p:42:LEU:HD11	40:v:28:ASN:HB3	1.96	0.46
3:3:332:LYS:NZ	3:3:505:LEU:O	2.45	0.46
15:V:124:VAL:HG11	51:V:203:CDL:H862	1.97	0.46
22:c:29:HIS:HD2	22:c:33:ARG:HH11	1.62	0.46
23:d:52:GLU:HG3	23:d:54:TYR:H	1.80	0.46
12:L:416:THR:O	12:L:419:THR:OG1	2.32	0.46
4:4:343:GLU:O	4:4:347:HIS:ND1	2.30	0.46
50:L:1003:PC1:H2B1	50:L:1003:PC1:H282	1.83	0.46
13:M:173:SER:HB2	16:W:101:ALA:HB2	1.97	0.46
15:V:62:ALA:HB2	51:V:203:CDL:H722	1.98	0.46
51:N:403:CDL:H171	51:N:403:CDL:H142	1.74	0.46
3:3:26:VAL:HG13	3:3:79:ILE:HD13	1.97	0.45
4:4:335:ARG:NH2	7:9:126:CYS:O	2.43	0.45
5:5:79:THR:HB	5:5:93:VAL:HB	1.99	0.45
7:9:108:ARG:NH1	22:c:70:MET:O	2.43	0.45
14:N:160:LEU:HD21	51:V:203:CDL:H191	1.96	0.45
36:r:30:ARG:NH1	38:t:116:ASP:OD1	2.45	0.45
1:1:276:LEU:HD21	1:1:297:VAL:HG11	1.97	0.45
3:3:503:LEU:HD21	3:3:509:PRO:HB3	1.99	0.45
14:N:275:SER:HB3	15:V:136:ALA:HB3	1.99	0.45
19:Z:10:PRO:O	36:r:94:TYR:OH	2.31	0.45
35:q:92:GLU:HA	35:q:95:THR:HG22	1.99	0.45
40:v:80:ASP:HB3	40:v:83:MET:HB3	1.98	0.45
3:3:231:MET:HB3	3:3:266:LYS:HD2	1.98	0.45
13:M:106:LEU:HD13	13:M:234:ILE:HG21	1.98	0.45
1:1:96:ASN:ND2	1:1:187:GLY:O	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:82:LEU:O	6:6:93:THR:OG1	2.29	0.45
13:M:391:ILE:HB	34:p:104:PHE:HE1	1.81	0.45
16:W:11:ILE:HG12	38:t:103:LEU:HD11	1.97	0.45
28:i:106:ARG:HB2	28:i:109:ILE:HG13	1.98	0.45
35:q:94:ALA:HA	35:q:105:VAL:HG11	1.99	0.45
37:s:4:LEU:HD11	40:v:124:THR:HA	1.98	0.45
38:t:169:ILE:O	38:t:172:ARG:NH1	2.45	0.45
6:6:35:ASP:HB3	49:6:203:3PE:H331	1.98	0.45
49:A:202:3PE:N	31:m:15:GLU:OE2	2.49	0.45
29:k:94:TYR:OH	29:k:151:HIS:ND1	2.39	0.45
51:o:201:CDL:H652	51:o:201:CDL:H842	1.99	0.45
9:H:149:ILE:HG21	9:H:185:TRP:HB2	1.98	0.45
51:L:1004:CDL:H182	13:M:442:LEU:HD13	1.98	0.45
15:V:80:ARG:NH1	15:V:85:ASP:OD2	2.43	0.45
16:W:114:MET:HE2	16:W:121:PRO:HD2	1.98	0.45
15:V:11:ILE:HB	15:V:20:LYS:HD3	1.99	0.45
2:2:55:GLN:NE2	2:2:91:ASN:OD1	2.50	0.45
2:2:121:GLN:HG2	2:2:127:LYS:HA	1.98	0.45
3:3:319:ALA:HB3	3:3:345:THR:HG22	1.98	0.45
5:5:78:LEU:HB3	5:5:130:TYR:HB3	1.99	0.45
23:d:280:THR:HG23	23:d:282:ASP:H	1.81	0.45
28:i:44:TYR:OH	28:i:113:HIS:N	2.45	0.45
3:3:110:GLN:NE2	3:3:113:GLU:O	2.50	0.45
50:9:401:PC1:H242	9:H:183:MET:HE2	1.99	0.45
9:H:24:GLU:HA	9:H:271:LEU:HD13	1.99	0.45
13:M:259:TYR:HB3	34:p:101:TYR:HE1	1.82	0.45
14:N:210:ILE:HG22	14:N:333:SER:HB3	1.98	0.45
40:v:145:ASP:N	40:v:145:ASP:OD1	2.49	0.45
4:4:203:LEU:HD22	4:4:207:LEU:HD23	1.98	0.45
7:9:143:THR:HB	7:9:146:GLU:HG3	1.98	0.45
12:L:69:LEU:HD13	13:M:451:PRO:HG2	1.99	0.45
12:L:161:ARG:NH2	38:t:90:TYR:O	2.46	0.45
22:c:33:ARG:NH2	22:c:77:ASP:OD2	2.47	0.45
1:1:365:CYS:HB3	45:1:500:SF4:S3	2.57	0.44
51:L:1004:CDL:H851	51:W:201:CDL:H671	1.98	0.44
29:k:178:GLU:OE2	29:k:182:ARG:NE	2.50	0.44
4:4:141:PHE:O	4:4:145:THR:OG1	2.34	0.44
18:Y:82:THR:HA	18:Y:85:TRP:CD1	2.53	0.44
36:r:120:LYS:HB3	37:s:39:VAL:HG13	1.99	0.44
41:w:23:THR:OG1	41:w:24:LEU:N	2.49	0.44
1:1:243:ALA:HA	1:1:251:SER:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:24:THR:OG1	2:2:27:ASN:OD1	2.35	0.44
12:L:64:SER:HA	12:L:79:SER:HA	2.00	0.44
13:M:155:ALA:HB1	50:M:502:PC1:H2H2	1.99	0.44
23:d:285:GLU:O	23:d:289:THR:OG1	2.34	0.44
34:p:24:ILE:H	34:p:24:ILE:HG13	1.66	0.44
1:1:298:ILE:HB	1:1:335:ILE:HB	2.00	0.44
3:3:584:LYS:HE3	22:c:36:ARG:HE	1.83	0.44
13:M:346:ARG:NE	40:v:68:ASP:OD2	2.46	0.44
1:1:144:ASN:O	1:1:148:ASN:HB2	2.17	0.44
3:3:11:VAL:HG11	3:3:73:VAL:HB	2.00	0.44
27:h:11:ARG:NH2	27:h:20:GLN:OE1	2.50	0.44
33:o:45:ASP:OD2	33:o:51:ARG:NH2	2.50	0.44
3:3:159:CYS:HB3	3:3:172:LEU:HD13	2.00	0.44
29:k:88:SER:OG	29:k:90:ASP:OD1	2.34	0.44
39:u:40:PHE:O	39:u:44:SER:OG	2.31	0.44
3:3:324:ASP:HB3	3:3:571:ALA:HB1	1.99	0.44
4:4:379:VAL:HB	4:4:388:ARG:HB3	1.99	0.44
16:W:44:ASN:ND2	51:W:201:CDL:OB4	2.43	0.44
19:Z:140:ASP:O	19:Z:161:ARG:NH1	2.51	0.44
21:b:49:VAL:HG22	21:b:90:GLN:HG3	1.98	0.44
10:J:139:GLU:HG3	11:K:49:LEU:HD21	1.99	0.44
14:N:89:LEU:N	14:N:148:SER:OG	2.47	0.44
52:X:101:ZMP:H15	52:X:101:ZMP:H17	1.62	0.44
37:s:33:ARG:NH1	37:s:103:ARG:HH22	2.15	0.44
3:3:140:LYS:HD3	3:3:150:MET:HG3	2.00	0.44
5:5:116:PRO:HB3	5:5:141:PHE:HD2	1.83	0.44
10:J:170:GLU:OE1	10:J:173:ARG:NH2	2.50	0.44
13:M:301:ILE:HA	13:M:309:TYR:HE1	1.83	0.44
18:Y:39:ASN:HB3	35:q:72:PRO:HG2	2.00	0.44
22:c:8:THR:OG1	22:c:9:GLN:N	2.49	0.44
1:1:200:GLN:NE2	3:3:174:THR:O	2.42	0.43
3:3:115:ASP:O	3:3:119:GLN:HG2	2.17	0.43
3:3:119:GLN:HB2	3:3:123:PHE:HD2	1.82	0.43
8:A:49:LEU:HD12	8:A:50:PRO:HD2	1.99	0.43
14:N:298:TYR:O	14:N:303:THR:OG1	2.32	0.43
4:4:93:TYR:HE2	5:5:168:LEU:HB2	1.83	0.43
18:Y:17:VAL:HG12	18:Y:19:VAL:HG22	1.98	0.43
17:j:11:ILE:HG22	17:j:77:VAL:HG23	2.00	0.43
29:k:19:THR:HG23	29:k:21:ASN:H	1.82	0.43
36:r:89:VAL:O	36:r:95:THR:OG1	2.32	0.43
4:4:93:TYR:HD2	5:5:168:LEU:HD22	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:152:PHE:HB2	12:L:172:ILE:HD11	2.01	0.43
13:M:70:MET:HA	13:M:103:GLN:HE21	1.83	0.43
13:M:337:VAL:HG11	13:M:345:ALA:HB2	2.00	0.43
14:N:173:THR:O	14:N:227:THR:OG1	2.34	0.43
16:W:122:TRP:CD1	33:o:2:MET:HG2	2.53	0.43
1:1:365:CYS:HB2	45:1:500:SF4:S3	2.55	0.43
2:2:53:LEU:HD12	20:a:52:LEU:HD13	2.01	0.43
3:3:198:ASN:OD1	3:3:268:ARG:NH2	2.47	0.43
4:4:226:GLU:HG3	4:4:230:THR:OG1	2.18	0.43
5:5:51:CYS:HB3	25:f:111:TRP:CE2	2.54	0.43
8:A:69:ILE:HD11	9:H:144:VAL:HG13	2.00	0.43
12:L:397:GLU:HB3	12:L:482:MET:HE1	2.01	0.43
51:L:1004:CDL:H541	51:L:1004:CDL:H512	1.78	0.43
21:b:68:HIS:ND1	21:b:69:PRO:O	2.49	0.43
1:1:214:GLY:N	1:1:218:CYS:O	2.49	0.43
12:L:13:ILE:HG13	36:r:81:ILE:HD11	2.01	0.43
51:L:1004:CDL:H391	51:L:1004:CDL:H171	2.00	0.43
13:M:122:PHE:HZ	13:M:206:LYS:HG3	1.83	0.43
29:k:173:ASP:OD1	29:k:207:LYS:NZ	2.50	0.43
2:2:155:GLN:HA	2:2:159:ASN:O	2.18	0.43
7:9:83:CYS:SG	7:9:109:TYR:OH	2.75	0.43
7:9:164:GLU:HG3	28:i:88:ARG:HG3	2.01	0.43
17:j:49:GLU:HA	17:j:52:MET:HE3	1.99	0.43
38:t:107:HIS:NE2	41:w:43:ASP:OD1	2.43	0.43
3:3:229:ASP:OD2	3:3:267:THR:OG1	2.31	0.43
12:L:184:LEU:HD13	13:M:393:ILE:HG21	2.00	0.43
1:1:92:TYR:O	1:1:220:THR:HA	2.18	0.43
3:3:194:GLU:HG2	3:3:195:LEU:HG	2.01	0.43
3:3:488:LYS:HD2	3:3:642:PHE:HE2	1.83	0.43
13:M:18:SER:HB2	13:M:23:ILE:HG22	2.00	0.43
25:f:49:GLN:HE22	27:h:92:LYS:HA	1.84	0.43
17:j:25:ILE:HG23	17:j:40:LEU:HD22	2.01	0.43
40:v:5:THR:OG1	40:v:6:LYS:N	2.48	0.43
9:H:162:LEU:HD21	9:H:237:PHE:HE1	1.83	0.43
9:H:233:MET:HB3	9:H:233:MET:HE3	1.86	0.43
11:K:60:PRO:HA	11:K:63:LEU:HB3	2.00	0.43
14:N:100:MET:HE1	51:V:203:CDL:H272	2.00	0.43
14:N:222:ASN:HD21	14:N:240:MET:HB3	1.83	0.43
19:Z:81:VAL:HA	19:Z:84:MET:HG2	2.01	0.43
19:Z:145:LEU:HD22	19:Z:153:LYS:HB3	2.00	0.43
29:k:69:LEU:HD21	29:k:302:ARG:HH21	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:363:THR:HG21	3:3:97:LEU:HG	1.99	0.43
3:3:569:LYS:HG3	3:3:571:ALA:HB2	2.00	0.43
13:M:11:LEU:HB3	13:M:100:ILE:HD13	2.00	0.43
16:W:28:TYR:O	41:w:67:SER:OG	2.28	0.43
37:s:21:MET:HE1	37:s:101:PHE:HA	2.01	0.43
11:K:44:ALA:HA	11:K:47:MET:HE3	1.99	0.42
12:L:60:GLU:HG2	12:L:83:ASP:HA	2.01	0.42
12:L:161:ARG:HH22	38:t:90:TYR:HB3	1.84	0.42
13:M:116:ILE:HD11	13:M:161:LEU:HD12	2.00	0.42
23:d:53:PRO:O	23:d:56:THR:OG1	2.36	0.42
34:p:39:ARG:NH2	38:t:3:LEU:O	2.40	0.42
1:1:270:GLU:OE1	1:1:283:HIS:NE2	2.51	0.42
2:2:98:TYR:HA	2:2:157:ASN:HD21	1.83	0.42
11:K:60:PRO:O	11:K:64:LEU:N	2.49	0.42
12:L:137:LEU:HD21	12:L:263:PHE:HZ	1.85	0.42
1:1:140:GLY:O	1:1:179:ARG:NH2	2.48	0.42
2:2:50:VAL:HG12	2:2:69:VAL:HG22	2.01	0.42
7:9:79:ALA:HB3	7:9:104:ARG:HG2	2.02	0.42
13:M:220:HIS:NE2	13:M:231:LEU:HB3	2.33	0.42
23:d:48:PRO:HA	23:d:71:MET:O	2.19	0.42
34:p:87:LEU:O	34:p:91:LEU:HB2	2.18	0.42
37:s:33:ARG:NE	40:v:157:GLU:O	2.36	0.42
41:w:34:ASP:OD1	41:w:34:ASP:N	2.52	0.42
50:A:201:PC1:H132	50:A:201:PC1:H111	1.89	0.42
19:Z:144:ASP:OD2	34:p:122:ARG:NH1	2.53	0.42
40:v:71:LEU:HD21	40:v:77:MET:HG2	2.01	0.42
50:6:202:PC1:H3D1	9:H:53:ILE:HG23	2.01	0.42
50:L:1002:PC1:H341	50:L:1002:PC1:H372	1.82	0.42
14:N:44:MET:HE2	14:N:130:LEU:HD12	2.02	0.42
18:Y:23:VAL:HG21	44:z:65:GLY:HA2	2.01	0.42
17:j:5:PRO:HD3	17:j:14:ARG:HH22	1.84	0.42
51:o:201:CDL:CA7	51:o:201:CDL:H531	2.50	0.42
37:s:7:ARG:HH21	37:s:17:GLU:HG3	1.84	0.42
1:1:154:ARG:HA	20:a:58:LEU:HD21	2.02	0.42
1:1:191:ALA:HB2	1:1:203:PRO:HG3	2.01	0.42
4:4:101:PRO:O	4:4:105:ARG:NH1	2.49	0.42
3:3:57:VAL:HA	3:3:86:THR:HG23	2.00	0.42
10:J:126:VAL:HG23	10:J:127:ILE:HG23	2.02	0.42
11:K:1:FME:HB3	11:K:2:SER:H	1.67	0.42
11:K:20:LEU:HD13	12:L:588:PHE:HD1	1.84	0.42
12:L:15:LEU:HD11	12:L:94:LEU:HD21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:231:PRO:HB3	12:L:530:PRO:HG3	2.02	0.42
12:L:375:ILE:HD12	12:L:458:LEU:HD11	2.01	0.42
13:M:36:LEU:HB2	41:w:69:VAL:HG22	2.01	0.42
52:g:201:ZMP:O6	17:j:44:SER:OG	2.37	0.42
17:j:65:ILE:H	17:j:65:ILE:HG13	1.67	0.42
40:v:133:TYR:HB3	40:v:138:LEU:HG	2.02	0.42
1:1:305:PRO:HG3	1:1:413:TRP:HB3	2.01	0.42
3:3:135:ARG:NH1	3:3:179:ASN:O	2.52	0.42
11:K:53:PHE:HE2	14:N:84:TRP:HE1	1.66	0.42
41:w:25:ARG:HG3	41:w:26:TRP:H	1.84	0.42
42:x:41:GLU:OE2	42:x:45:ARG:NE	2.53	0.42
1:1:42:TRP:HE1	1:1:116:HIS:HB3	1.85	0.42
4:4:67:GLU:HB3	4:4:75:LYS:HB3	2.02	0.42
11:K:55:LEU:HD13	30:l:16:TRP:HE3	1.85	0.42
8:A:55:PHE:HB2	10:J:74:MET:HE1	2.02	0.42
10:J:130:THR:HG21	35:q:123:LEU:HD12	2.02	0.42
23:d:177:ARG:NH2	54:d:401:NDP:O2N	2.46	0.42
37:s:45:MET:HB2	37:s:50:LEU:HD12	2.01	0.42
1:1:337:MET:HE1	1:1:343:ILE:HG13	2.01	0.41
5:5:74:SER:HB3	5:5:97:LEU:HB3	2.02	0.41
7:9:92:ILE:HG12	7:9:111:ILE:HG12	2.02	0.41
9:H:24:GLU:HG3	9:H:271:LEU:HD22	2.01	0.41
10:J:10:SER:O	10:J:13:PHE:HB3	2.19	0.41
13:M:75:LEU:HD23	13:M:440:HIS:CE1	2.54	0.41
23:d:100:GLU:HB2	23:d:105:ASP:HA	2.02	0.41
3:3:174:THR:HG22	3:3:183:VAL:HG22	2.02	0.41
4:4:84:HIS:NE2	6:6:130:TYR:OH	2.48	0.41
13:M:452:LYS:HE2	41:w:83:TYR:HB3	2.01	0.41
4:4:184:VAL:O	7:9:60:ARG:NH1	2.52	0.41
7:9:105:ARG:NH2	21:b:86:TYR:O	2.53	0.41
12:L:249:SER:HB2	12:L:336:LYS:HG3	2.02	0.41
12:L:373:LEU:HD21	12:L:426:ILE:HG22	2.01	0.41
13:M:379:LEU:O	13:M:383:MET:HG2	2.20	0.41
50:M:502:PC1:H251	50:M:502:PC1:H372	2.02	0.41
51:V:203:CDL:H742	51:V:204:CDL:H191	2.02	0.41
29:k:303:LYS:O	33:o:50:ARG:NH1	2.53	0.41
2:2:34:ILE:HD11	20:a:52:LEU:HD22	2.02	0.41
3:3:284:VAL:HG12	3:3:559:VAL:HG22	2.02	0.41
5:5:194:PHE:O	22:c:81:ASN:ND2	2.53	0.41
7:9:114:THR:HG21	7:9:144:HIS:CD2	2.56	0.41
49:H:401:3PE:H342	10:J:57:PHE:HE2	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:347:ILE:HD13	12:L:354:GLN:HG2	2.02	0.41
13:M:1:FME:HE2	13:M:1:FME:HB2	1.91	0.41
13:M:133:ILE:HG12	13:M:223:ALA:HB2	2.01	0.41
13:M:259:TYR:O	13:M:263:MET:HG2	2.21	0.41
18:Y:48:GLU:OE1	31:m:57:ARG:NH2	2.46	0.41
23:d:133:SER:OG	23:d:134:HIS:N	2.53	0.41
23:d:311:GLU:HG2	23:d:336:PRO:HB3	2.02	0.41
29:k:135:LEU:HD21	29:k:149:VAL:HA	2.01	0.41
33:o:43:LEU:HD22	33:o:53:VAL:HG12	2.02	0.41
4:4:94:LYS:HD2	4:4:102:TYR:HE2	1.85	0.41
12:L:316:THR:HG23	12:L:325:ALA:HB2	2.03	0.41
50:L:1002:PC1:H391	36:r:80:ILE:HG23	2.01	0.41
15:V:49:LEU:HA	15:V:52:VAL:HG22	2.02	0.41
51:V:204:CDL:H792	51:V:204:CDL:H822	1.91	0.41
4:4:109:VAL:HG11	4:4:152:MET:HG2	2.03	0.41
11:K:77:LEU:HD13	11:K:77:LEU:HA	1.91	0.41
34:p:62:PRO:O	34:p:66:ARG:HB2	2.19	0.41
3:3:350:PRO:HG2	3:3:467:LEU:HD22	2.02	0.41
49:A:202:3PE:H3H1	31:m:29:VAL:HG21	2.03	0.41
12:L:221:THR:HG21	49:L:1001:3PE:H3G1	2.03	0.41
13:M:165:ILE:HG21	14:N:268:GLN:HA	2.02	0.41
13:M:369:LEU:HD12	13:M:370:PRO:HD2	2.03	0.41
51:V:204:CDL:H351	51:V:204:CDL:H172	2.03	0.41
18:Y:59:GLY:O	18:Y:62:VAL:HB	2.21	0.41
23:d:48:PRO:HB2	23:d:73:TRP:CD1	2.56	0.41
30:l:104:ARG:NH2	35:q:80:ARG:HB3	2.36	0.41
10:J:92:THR:HG21	49:J:201:3PE:H231	2.02	0.41
13:M:71:TRP:CH2	13:M:439:LEU:HD22	2.56	0.41
14:N:20:VAL:HG11	14:N:137:ALA:HB1	2.02	0.41
51:N:403:CDL:H221	33:o:71:VAL:HG11	2.02	0.41
22:c:66:GLU:HG3	22:c:71:GLY:HA2	2.03	0.41
23:d:90:VAL:HA	23:d:128:LYS:O	2.20	0.41
24:e:23:CYS:SG	24:e:25:ARG:N	2.85	0.41
37:s:33:ARG:HH12	37:s:103:ARG:HH22	1.69	0.41
1:1:213:VAL:HG13	1:1:217:GLY:HA2	2.03	0.41
2:2:166:PRO:HA	2:2:169:ILE:HG22	2.02	0.41
3:3:431:ASP:HB3	3:3:437:HIS:HB2	2.03	0.41
3:3:540:ASP:OD1	3:3:540:ASP:N	2.54	0.41
4:4:292:ASP:OD1	4:4:292:ASP:N	2.43	0.41
6:6:36:LEU:HD13	49:6:203:3PE:H392	2.02	0.41
8:A:75:LEU:HD12	9:H:151:LEU:HD21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:45:LEU:HD23	10:J:50:SER:HA	2.03	0.41
49:L:1001:3PE:H231	49:L:1001:3PE:H262	1.86	0.41
13:M:243:MET:HB3	13:M:301:ILE:HG21	2.02	0.41
23:d:203:GLN:HB3	23:d:235:ARG:HG2	2.02	0.41
26:g:65:MET:HG3	52:g:201:ZMP:H4	2.01	0.41
28:i:9:ARG:HA	28:i:12:GLN:HG2	2.02	0.41
40:v:65:ASP:HB2	40:v:72:ASN:HA	2.02	0.41
1:1:99:GLU:OE2	1:1:107:ASP:N	2.51	0.41
4:4:387:TYR:CZ	5:5:164:LYS:HE3	2.56	0.41
9:H:70:MET:HE1	10:J:27:ILE:HG22	2.02	0.41
25:f:115:ILE:H	25:f:115:ILE:HG13	1.70	0.41
3:3:175:THR:HG21	3:3:186:TYR:HB2	2.02	0.40
4:4:35:ASP:OD2	14:N:176:ARG:NH2	2.47	0.40
4:4:324:LYS:HD3	4:4:331:SER:HB3	2.02	0.40
12:L:234:PRO:O	12:L:300:LYS:NZ	2.49	0.40
12:L:566:ILE:O	12:L:570:GLN:HG2	2.21	0.40
13:M:196:TRP:HD1	13:M:250:LEU:HB3	1.86	0.40
19:Z:159:LYS:NZ	33:o:112:VAL:O	2.51	0.40
27:h:59:ARG:HH11	27:h:59:ARG:HD2	1.76	0.40
2:2:61:LEU:HD12	2:2:90:TYR:HB3	2.03	0.40
13:M:9:MET:HE1	51:y:201:CDL:H162	2.02	0.40
13:M:191:SER:HB3	50:M:502:PC1:H31	2.03	0.40
14:N:137:ALA:O	14:N:140:SER:OG	2.32	0.40
23:d:201:VAL:HG22	23:d:237:LEU:HD23	2.03	0.40
3:3:20:VAL:HG12	3:3:32:LYS:HD3	2.03	0.40
7:9:27:TRP:HB3	7:9:30:LEU:HD12	2.02	0.40
12:L:49:ILE:HG12	19:Z:32:LEU:HD13	2.03	0.40
13:M:196:TRP:CD1	13:M:250:LEU:HB3	2.56	0.40
18:Y:21:SER:N	44:z:51:ASP:OD1	2.53	0.40
24:e:22:LEU:HD21	24:e:54:ILE:HG23	2.03	0.40
24:e:63:LYS:HD3	24:e:77:SER:HA	2.04	0.40
3:3:382:THR:HB	3:3:454:GLY:HA3	2.03	0.40
5:5:56:GLY:HA2	5:5:59:PRO:HD2	2.04	0.40
8:A:73:LEU:HD13	10:J:55:MET:HE1	2.04	0.40
51:L:1004:CDL:H631	13:M:445:LEU:HD22	2.04	0.40
51:L:1004:CDL:H181	16:W:29:ILE:HD13	2.03	0.40
13:M:91:ARG:HD3	13:M:135:ARG:HH21	1.86	0.40
14:N:128:LEU:HD13	14:N:216:PHE:HB2	2.03	0.40
16:W:128:ILE:HG21	30:l:19:ILE:HG21	2.04	0.40
41:w:114:ASP:HB3	41:w:117:LYS:HG2	2.02	0.40
1:1:97:ALA:HB3	1:1:138:ILE:HA	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:55:GLN:NE2	2:2:91:ASN:H	2.20	0.40
4:4:323:ILE:H	4:4:323:ILE:HG13	1.81	0.40
5:5:94:TYR:HB2	5:5:107:VAL:HB	2.04	0.40
6:6:63:ALA:HA	6:6:69:MET:HG2	2.02	0.40
7:9:49:ASN:O	7:9:53:GLU:N	2.54	0.40
12:L:419:THR:HA	12:L:422:TYR:CZ	2.56	0.40
22:c:60:ASP:OD1	22:c:60:ASP:N	2.53	0.40
42:x:41:GLU:OE2	42:x:44:ARG:NH2	2.43	0.40
51:y:201:CDL:H172	51:y:201:CDL:H322	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

7 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	SEP	k	36	29	8,9,10	1.62	1 (12%)	7,12,14	1.31	1 (14%)
4	2MR	4	85	4	10,12,13	2.40	3 (30%)	5,13,15	1.54	1 (20%)
27	AYA	h	1	27	6,7,8	1.34	1 (16%)	6,8,10	1.15	1 (16%)
11	FME	K	1	11	8,9,10	0.97	0	8,9,11	1.03	0
13	FME	M	1	13	8,9,10	0.96	0	8,9,11	1.11	0
15	AYA	V	1	15	6,7,8	1.23	1 (16%)	6,8,10	2.50	2 (33%)
12	FME	L	1	12	8,9,10	0.94	0	8,9,11	1.37	2 (25%)

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
29	SEP	k	36	29	-	4/6/8/10	-
4	2MR	4	85	4	-	2/10/13/15	-
27	AYA	h	1	27	-	1/5/6/8	-
11	FME	K	1	11	-	3/7/9/11	-
13	FME	M	1	13	-	3/7/9/11	-
15	AYA	V	1	15	-	2/5/6/8	-
12	FME	L	1	12	-	2/7/9/11	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	4	85	2MR	CZ-NH2	4.79	1.43	1.33
4	4	85	2MR	CZ-NE	4.68	1.44	1.34
29	k	36	SEP	P-O1P	3.55	1.61	1.50
27	h	1	AYA	CA-N	-2.81	1.43	1.46
4	4	85	2MR	CQ1-NH1	-2.39	1.41	1.46
15	V	1	AYA	CA-N	-2.19	1.44	1.46

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	V	1	AYA	CB-CA-N	4.72	115.01	109.68
15	V	1	AYA	CA-N-CT	3.21	125.64	121.50
29	k	36	SEP	OG-CB-CA	2.86	110.93	108.14
12	L	1	FME	CA-N-CN	2.64	126.89	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	h	1	AYA	CB-CA-N	2.54	112.54	109.68
12	L	1	FME	C-CA-N	2.31	113.95	109.50
4	4	85	2MR	NE-CZ-NH2	-2.08	117.57	119.48

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	K	1	FME	O1-CN-N-CA
13	M	1	FME	CB-CA-N-CN
13	M	1	FME	C-CA-CB-CG
13	M	1	FME	O-C-CA-CB
27	h	1	AYA	O-C-CA-CB
29	k	36	SEP	CB-OG-P-O2P
29	k	36	SEP	CB-OG-P-O3P
11	K	1	FME	CA-CB-CG-SD
12	L	1	FME	CA-CB-CG-SD
15	V	1	AYA	OT-CT-N-CA
15	V	1	AYA	CM-CT-N-CA
4	4	85	2MR	NE-CD-CG-CB
29	k	36	SEP	CB-OG-P-O1P
12	L	1	FME	N-CA-CB-CG
29	k	36	SEP	CA-CB-OG-P
4	4	85	2MR	CA-CB-CG-CD
11	K	1	FME	CB-CA-N-CN

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	K	1	FME	1	0
13	M	1	FME	1	0
15	V	1	AYA	3	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 44 ligands modelled in this entry, 2 are monoatomic - leaving 42 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	$\# Z > 2$
49	3PE	L	1005	-	30,30,50	0.40	0	33,35,55	0.79	1 (3%)
49	3PE	L	1001	-	50,50,50	0.30	0	53,55,55	0.38	0
45	SF4	3	802	3	0,12,12	-	-	-		
54	NDP	d	401	-	51,52,52	0.48	0	71,80,80	0.43	0
50	PC1	M	502	-	53,53,53	0.30	0	59,61,61	0.39	0
46	FMN	1	501	-	33,33,33	1.25	3 (9%)	48,50,50	1.34	8 (16%)
51	CDL	y	201	-	99,99,99	0.28	0	105,111,111	0.43	1 (0%)
49	3PE	M	501	-	43,43,50	0.32	0	46,48,55	0.43	0
47	FES	3	803	3	0,4,4	-	-	-		
49	3PE	N	402	-	30,30,50	0.39	0	33,35,55	0.39	0
51	CDL	o	201	-	89,89,99	0.30	0	95,101,111	0.43	1 (1%)
50	PC1	L	1002	-	53,53,53	0.31	0	59,61,61	0.59	1 (1%)
51	CDL	L	1004	-	99,99,99	0.26	0	105,111,111	0.33	0
51	CDL	V	204	-	84,84,99	0.28	0	90,96,111	0.25	0
55	AMP	k	501	-	25,25,25	1.41	4 (16%)	37,38,38	1.88	7 (18%)
51	CDL	N	403	-	74,74,99	0.33	0	80,86,111	0.51	1 (1%)
50	PC1	6	202	-	45,45,53	0.32	0	51,53,61	0.33	0
49	3PE	V	201	-	34,34,50	0.36	0	37,39,55	0.34	0
49	3PE	V	202	-	36,36,50	0.35	0	39,41,55	0.32	0
51	CDL	W	201	-	99,99,99	0.26	0	105,111,111	0.30	0
51	CDL	V	203	-	93,93,99	0.25	0	99,105,111	0.27	0
56	MYR	s	201	37	13,14,15	0.15	0	12,13,15	0.15	0
49	3PE	i	201	-	50,50,50	0.31	0	53,55,55	0.31	0
49	3PE	6	203	-	50,50,50	0.31	0	53,55,55	0.32	0
50	PC1	L	1003	-	53,53,53	0.31	0	59,61,61	0.40	0
49	3PE	A	202	-	50,50,50	0.30	0	53,55,55	0.38	0
50	PC1	A	201	-	36,36,53	0.36	0	42,44,61	0.61	1 (2%)
45	SF4	9	403	7	0,12,12	-	-	-		
49	3PE	H	401	-	50,50,50	0.30	0	53,55,55	0.45	1 (1%)
49	3PE	N	401	-	50,50,50	0.31	0	53,55,55	0.54	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
47	FES	2	300	2	0,4,4	-	-	-		
45	SF4	3	801	3	0,12,12	-	-	-		
49	3PE	4	501	-	39,39,50	0.34	0	42,44,55	0.40	0
49	3PE	J	201	-	39,39,50	0.33	0	42,44,55	0.43	0
52	ZMP	X	101	17	25,30,36	0.82	2 (8%)	29,37,45	1.09	3 (10%)
51	CDL	h	201	-	57,57,99	0.36	0	63,69,111	0.34	0
49	3PE	p	201	-	26,26,50	0.49	0	29,31,55	0.56	1 (3%)
52	ZMP	g	201	-	28,33,36	0.67	1 (3%)	32,40,45	1.34	4 (12%)
45	SF4	6	201	6	0,12,12	-	-	-		
45	SF4	1	500	1	0,12,12	-	-	-		
50	PC1	9	401	-	53,53,53	0.32	0	59,61,61	0.52	1 (1%)
45	SF4	9	402	7	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
49	3PE	L	1005	-	-	6/34/34/54	-
49	3PE	L	1001	-	-	13/54/54/54	-
45	SF4	3	802	3	-	-	0/6/5/5
54	NDP	d	401	-	-	11/34/77/77	0/5/5/5
50	PC1	M	502	-	-	16/57/57/57	-
46	FMN	1	501	-	-	11/18/18/18	0/3/3/3
51	CDL	y	201	-	1/1/9/9	34/110/110/110	-
49	3PE	M	501	-	-	14/47/47/54	-
47	FES	3	803	3	-	-	0/1/1/1
49	3PE	N	402	-	-	4/34/34/54	-
51	CDL	o	201	-	-	35/100/100/110	-
51	CDL	L	1004	-	1/1/9/9	32/110/110/110	-
50	PC1	L	1002	-	-	19/57/57/57	-
51	CDL	V	204	-	1/1/9/9	23/95/95/110	-
55	AMP	k	501	-	-	6/10/26/26	0/3/3/3
51	CDL	N	403	-	2/2/9/9	19/85/85/110	-
50	PC1	6	202	-	-	9/49/49/57	-
49	3PE	V	201	-	-	8/38/38/54	-
49	3PE	V	202	-	-	12/40/40/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
51	CDL	W	201	-	-	32/110/110/110	-
51	CDL	V	203	-	-	32/104/104/110	-
56	MYR	s	201	37	-	2/12/12/13	-
49	3PE	i	201	-	-	7/54/54/54	-
49	3PE	6	203	-	-	12/54/54/54	-
50	PC1	L	1003	-	-	11/57/57/57	-
49	3PE	A	202	-	-	12/54/54/54	-
50	PC1	A	201	-	-	5/40/40/57	-
45	SF4	9	403	7	-	-	0/6/5/5
49	3PE	H	401	-	-	17/54/54/54	-
49	3PE	N	401	-	-	11/54/54/54	-
47	FES	2	300	2	-	-	0/1/1/1
45	SF4	3	801	3	-	-	0/6/5/5
49	3PE	4	501	-	-	10/43/43/54	-
49	3PE	J	201	-	-	6/43/43/54	-
52	ZMP	X	101	17	-	9/35/37/43	-
51	CDL	h	201	-	-	23/68/68/110	-
49	3PE	p	201	-	-	6/27/27/54	-
52	ZMP	g	201	-	-	8/38/40/43	-
45	SF4	6	201	6	-	-	0/6/5/5
45	SF4	1	500	1	-	-	0/6/5/5
50	PC1	9	401	-	-	19/57/57/57	-
45	SF4	9	402	7	-	-	0/6/5/5

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	k	501	AMP	C5-C4	4.67	1.47	1.39
55	k	501	AMP	C5-C6	2.64	1.48	1.41
46	1	501	FMN	C4A-N5	2.54	1.36	1.30
55	k	501	AMP	C5-N7	-2.39	1.34	1.39
52	X	101	ZMP	C10-S1	-2.33	1.70	1.76
52	g	201	ZMP	C10-S1	-2.33	1.70	1.76
52	X	101	ZMP	C9-C10	2.32	1.53	1.50
55	k	501	AMP	C8-N7	2.20	1.35	1.31
46	1	501	FMN	C4A-C10	-2.18	1.37	1.44
46	1	501	FMN	C9A-N10	-2.07	1.37	1.41

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	k	501	AMP	C5-C4-N3	-6.07	118.36	126.72
55	k	501	AMP	N3-C4-N9	4.94	135.57	127.17
46	1	501	FMN	C4-N3-C2	-3.88	118.74	125.64
55	k	501	AMP	C2-N3-C4	3.69	120.83	111.83
52	g	201	ZMP	C15-C14-C13	-3.43	106.69	112.39
55	k	501	AMP	C4-C5-N7	-3.18	106.95	110.58
46	1	501	FMN	C4A-C10-N10	2.97	120.73	116.48
55	k	501	AMP	N3-C2-N1	-2.95	124.11	128.58
46	1	501	FMN	O4-C4-C4A	-2.92	118.83	126.53
52	g	201	ZMP	C14-C15-N2	-2.85	105.94	112.00
52	g	201	ZMP	O1-C10-C9	-2.77	120.78	123.98
51	y	201	CDL	OA8-CA6-CA4	2.69	116.14	108.40
50	L	1002	PC1	C2-O21-C21	2.63	124.10	117.80
46	1	501	FMN	C4A-C4-N3	2.62	119.92	113.25
55	k	501	AMP	C4-N9-C8	2.58	108.44	105.74
52	g	201	ZMP	C20-C18-C17	2.52	113.06	108.77
49	L	1005	3PE	C2-O21-C21	2.47	123.70	117.80
46	1	501	FMN	C4-C4A-C10	2.46	121.16	116.93
46	1	501	FMN	C4A-C10-N1	-2.38	118.75	124.59
52	X	101	ZMP	O1-C10-C9	-2.35	121.27	123.98
50	A	201	PC1	C2-O21-C21	2.33	123.38	117.80
52	X	101	ZMP	C14-C15-N2	-2.31	107.08	112.00
55	k	501	AMP	C5-N7-C8	2.30	107.07	103.45
49	H	401	3PE	O31-C3-C2	2.30	115.04	108.40
46	1	501	FMN	C4'-C3'-C2'	-2.24	109.84	113.57
49	N	401	3PE	C2-O21-C21	2.22	123.11	117.80
50	9	401	PC1	C2-O21-C21	2.21	123.08	117.80
49	p	201	3PE	O12-P-O14	2.11	119.05	110.83
46	1	501	FMN	C10-C4A-N5	-2.10	120.53	124.81
52	X	101	ZMP	C9-C10-S1	2.07	115.87	113.40
51	N	403	CDL	CB4-OB6-CB5	2.06	122.73	117.80
51	o	201	CDL	CB4-OB6-CB5	2.03	122.66	117.80

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
51	L	1004	CDL	CB4
51	N	403	CDL	CB4
51	N	403	CDL	CA4
51	V	204	CDL	CB4
51	y	201	CDL	CB4

All (494) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	1	501	FMN	N10-C1'-C2'-O2'
46	1	501	FMN	C5'-O5'-P-O2P
46	1	501	FMN	C5'-O5'-P-O3P
49	4	501	3PE	C1-O11-P-O13
49	4	501	3PE	C11-O13-P-O11
49	6	203	3PE	C1-O11-P-O12
49	6	203	3PE	C1-O11-P-O13
49	6	203	3PE	C11-O13-P-O11
49	A	202	3PE	C11-O13-P-O11
49	A	202	3PE	C11-O13-P-O12
49	A	202	3PE	C11-O13-P-O14
49	A	202	3PE	O13-C11-C12-N
49	H	401	3PE	C1-O11-P-O13
49	H	401	3PE	C11-O13-P-O11
49	H	401	3PE	C11-O13-P-O12
49	H	401	3PE	C11-O13-P-O14
49	H	401	3PE	O13-C11-C12-N
49	J	201	3PE	C1-O11-P-O13
49	L	1001	3PE	C1-O11-P-O14
49	L	1001	3PE	O13-C11-C12-N
49	L	1005	3PE	C1-O11-P-O13
49	L	1005	3PE	C2-C1-O11-P
49	M	501	3PE	C11-O13-P-O11
49	N	402	3PE	C11-O13-P-O11
49	N	402	3PE	C11-O13-P-O14
49	N	402	3PE	O13-C11-C12-N
49	V	201	3PE	C1-O11-P-O12
49	V	201	3PE	C1-O11-P-O13
49	V	201	3PE	C1-O11-P-O14
49	V	201	3PE	O13-C11-C12-N
49	V	202	3PE	C11-O13-P-O12
49	V	202	3PE	C2-C1-O11-P
49	i	201	3PE	C1-O11-P-O12
49	i	201	3PE	C1-O11-P-O13
49	i	201	3PE	C1-O11-P-O14
50	6	202	PC1	C11-O13-P-O12
50	9	401	PC1	C11-O13-P-O14
50	9	401	PC1	C11-O13-P-O11
50	A	201	PC1	C1-O11-P-O14
50	L	1002	PC1	C1-O11-P-O12
50	L	1002	PC1	C1-O11-P-O13
50	L	1002	PC1	O13-C11-C12-N

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Mol	Chain	Res	Type	Atoms
50	L	1003	PC1	C11-O13-P-O11
50	L	1003	PC1	O13-C11-C12-N
50	M	502	PC1	C11-O13-P-O12
50	M	502	PC1	C11-O13-P-O14
50	M	502	PC1	C11-O13-P-O11
51	L	1004	CDL	CA2-OA2-PA1-OA3
51	L	1004	CDL	CA3-OA5-PA1-OA2
51	L	1004	CDL	CA3-OA5-PA1-OA3
51	L	1004	CDL	CA3-OA5-PA1-OA4
51	L	1004	CDL	CB2-OB2-PB2-OB3
51	N	403	CDL	CA2-OA2-PA1-OA3
51	N	403	CDL	CA2-OA2-PA1-OA5
51	V	203	CDL	CA2-OA2-PA1-OA4
51	V	203	CDL	CA2-OA2-PA1-OA5
51	V	203	CDL	CA3-OA5-PA1-OA2
51	V	203	CDL	CA3-OA5-PA1-OA3
51	V	203	CDL	CB2-OB2-PB2-OB4
51	V	204	CDL	CA2-OA2-PA1-OA4
51	V	204	CDL	CA3-OA5-PA1-OA2
51	V	204	CDL	CA3-OA5-PA1-OA3
51	V	204	CDL	OA6-CA4-CA6-OA8
51	V	204	CDL	CB2-OB2-PB2-OB5
51	W	201	CDL	CA2-OA2-PA1-OA3
51	W	201	CDL	CA2-OA2-PA1-OA4
51	W	201	CDL	CA2-OA2-PA1-OA5
51	W	201	CDL	CA3-OA5-PA1-OA4
51	W	201	CDL	CB2-OB2-PB2-OB3
51	W	201	CDL	CB2-OB2-PB2-OB5
51	h	201	CDL	CA2-OA2-PA1-OA3
51	h	201	CDL	CA2-OA2-PA1-OA5
51	h	201	CDL	CB2-OB2-PB2-OB5
51	h	201	CDL	CB3-OB5-PB2-OB3
51	o	201	CDL	CA2-OA2-PA1-OA3
51	o	201	CDL	CA2-OA2-PA1-OA4
51	o	201	CDL	CB2-OB2-PB2-OB3
51	o	201	CDL	CB2-OB2-PB2-OB4
51	o	201	CDL	CB2-OB2-PB2-OB5
51	o	201	CDL	CB3-OB5-PB2-OB2
51	o	201	CDL	CB3-OB5-PB2-OB3
51	y	201	CDL	CA2-C1-CB2-OB2
51	y	201	CDL	CA3-OA5-PA1-OA4
51	y	201	CDL	CB2-OB2-PB2-OB3

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Mol	Chain	Res	Type	Atoms
51	y	201	CDL	CB3-OB5-PB2-OB2
52	X	101	ZMP	C16-C17-C18-C21
52	X	101	ZMP	C17-C16-N2-C15
52	g	201	ZMP	S1-C11-C12-N1
54	d	401	NDP	C2N-C3N-C7N-O7N
55	k	501	AMP	C5'-O5'-P-O1P
55	k	501	AMP	C5'-O5'-P-O2P
55	k	501	AMP	C5'-O5'-P-O3P
51	y	201	CDL	O1-C1-CB2-OB2
52	X	101	ZMP	O3-C16-N2-C15
54	d	401	NDP	O4B-C4B-C5B-O5B
55	k	501	AMP	C3'-C4'-C5'-O5'
51	L	1004	CDL	CA2-C1-CB2-OB2
50	M	502	PC1	C11-C12-N-C14
51	y	201	CDL	CB5-C51-C52-C53
51	W	201	CDL	OB6-CB4-CB6-OB8
54	d	401	NDP	C3B-C4B-C5B-O5B
55	k	501	AMP	O4'-C4'-C5'-O5'
50	M	502	PC1	C11-C12-N-C15
51	L	1004	CDL	CB7-C71-C72-C73
51	L	1004	CDL	O1-C1-CB2-OB2
51	N	403	CDL	O1-C1-CB2-OB2
51	N	403	CDL	CA7-C31-C32-C33
49	M	501	3PE	C31-C32-C33-C34
51	L	1004	CDL	CB5-C51-C52-C53
51	o	201	CDL	O1-C1-CB2-OB2
49	V	201	3PE	C31-C32-C33-C34
50	6	202	PC1	C3B-C3C-C3D-C3E
51	V	204	CDL	C71-C72-C73-C74
51	V	204	CDL	C78-C79-C80-C81
50	L	1002	PC1	C3A-C3B-C3C-C3D
51	L	1004	CDL	C21-C22-C23-C24
51	L	1004	CDL	C77-C78-C79-C80
49	A	202	3PE	C3C-C3D-C3E-C3F
51	L	1004	CDL	C56-C57-C58-C59
50	L	1002	PC1	C23-C24-C25-C26
51	L	1004	CDL	C22-C23-C24-C25
51	o	201	CDL	C81-C82-C83-C84
49	6	203	3PE	C36-C37-C38-C39
49	A	202	3PE	C2D-C2E-C2F-C2G
51	V	203	CDL	C40-C41-C42-C43
51	o	201	CDL	C78-C79-C80-C81

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Mol	Chain	Res	Type	Atoms
49	N	401	3PE	C21-C22-C23-C24
49	p	201	3PE	C21-C22-C23-C24
51	W	201	CDL	CA7-C31-C32-C33
51	W	201	CDL	CB5-C51-C52-C53
49	J	201	3PE	C34-C35-C36-C37
51	L	1004	CDL	C82-C83-C84-C85
51	V	203	CDL	C38-C39-C40-C41
51	V	204	CDL	C34-C35-C36-C37
49	i	201	3PE	C29-C2A-C2B-C2C
51	y	201	CDL	C81-C82-C83-C84
51	h	201	CDL	CB3-CB4-CB6-OB8
49	A	202	3PE	C38-C39-C3A-C3B
51	V	203	CDL	C52-C53-C54-C55
51	y	201	CDL	C52-C53-C54-C55
51	y	201	CDL	CA5-C11-C12-C13
49	H	401	3PE	C28-C29-C2A-C2B
50	L	1002	PC1	C33-C34-C35-C36
51	L	1004	CDL	C41-C42-C43-C44
51	o	201	CDL	CB5-C51-C52-C53
51	o	201	CDL	C56-C57-C58-C59
49	4	501	3PE	C25-C26-C27-C28
50	L	1002	PC1	C36-C37-C38-C39
51	V	203	CDL	C79-C80-C81-C82
49	V	201	3PE	C22-C23-C24-C25
51	V	203	CDL	C31-C32-C33-C34
51	W	201	CDL	C31-C32-C33-C34
50	L	1002	PC1	C39-C3A-C3B-C3C
50	M	502	PC1	C11-C12-N-C13
51	y	201	CDL	C15-C16-C17-C18
49	N	401	3PE	O11-C1-C2-O21
46	1	501	FMN	O3'-C3'-C4'-C5'
51	V	203	CDL	C77-C78-C79-C80
51	V	203	CDL	OB6-CB4-CB6-OB8
51	y	201	CDL	C59-C60-C61-C62
50	L	1003	PC1	C2D-C2E-C2F-C2G
56	s	201	MYR	C11-C10-C9-C8
49	L	1001	3PE	C34-C35-C36-C37
52	X	101	ZMP	C6-C7-C8-C9
51	L	1004	CDL	OB5-CB3-CB4-CB6
51	W	201	CDL	OA5-CA3-CA4-CA6
49	J	201	3PE	C24-C25-C26-C27
51	V	203	CDL	CA7-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
51	V	204	CDL	CA3-CA4-CA6-OA8
50	L	1003	PC1	C39-C3A-C3B-C3C
46	l	501	FMN	C5'-O5'-P-O1P
49	p	201	3PE	C1-O11-P-O14
50	M	502	PC1	C3A-C3B-C3C-C3D
52	X	101	ZMP	C3-C4-C5-C6
51	L	1004	CDL	C37-C38-C39-C40
51	V	204	CDL	C14-C15-C16-C17
51	V	203	CDL	C71-C72-C73-C74
49	N	401	3PE	C2C-C2D-C2E-C2F
49	N	401	3PE	C32-C33-C34-C35
51	W	201	CDL	C72-C73-C74-C75
51	L	1004	CDL	C34-C35-C36-C37
51	y	201	CDL	C63-C64-C65-C66
51	y	201	CDL	C82-C83-C84-C85
51	o	201	CDL	C84-C85-C86-C87
51	L	1004	CDL	C17-C18-C19-C20
49	H	401	3PE	O11-C1-C2-C3
50	L	1002	PC1	O11-C1-C2-C3
50	M	502	PC1	C23-C24-C25-C26
50	L	1003	PC1	C3E-C3F-C3G-C3H
51	V	203	CDL	CB3-CB4-CB6-OB8
51	V	204	CDL	CB3-CB4-CB6-OB8
51	W	201	CDL	CA3-CA4-CA6-OA8
51	h	201	CDL	CA3-CA4-CA6-OA8
51	h	201	CDL	CB7-C71-C72-C73
51	V	203	CDL	C20-C21-C22-C23
50	9	401	PC1	C22-C23-C24-C25
51	W	201	CDL	C39-C40-C41-C42
51	N	403	CDL	OA5-CA3-CA4-OA6
51	W	201	CDL	OA5-CA3-CA4-OA6
50	L	1002	PC1	C2-C1-O11-P
52	g	201	ZMP	O1-C10-S1-C11
50	L	1002	PC1	C38-C39-C3A-C3B
51	o	201	CDL	C71-C72-C73-C74
51	W	201	CDL	OA6-CA4-CA6-OA8
54	d	401	NDP	C2N-C3N-C7N-N7N
51	y	201	CDL	C57-C58-C59-C60
49	4	501	3PE	C31-C32-C33-C34
51	V	204	CDL	CA5-C11-C12-C13
52	g	201	ZMP	C22-C1-C2-C3
49	M	501	3PE	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
46	1	501	FMN	C2'-C3'-C4'-O4'
52	g	201	ZMP	C9-C10-S1-C11
51	L	1004	CDL	CA7-C31-C32-C33
51	V	203	CDL	OB5-CB3-CB4-CB6
51	y	201	CDL	C13-C14-C15-C16
49	A	202	3PE	C35-C36-C37-C38
50	9	401	PC1	C2C-C2D-C2E-C2F
51	y	201	CDL	C33-C34-C35-C36
46	1	501	FMN	O3'-C3'-C4'-O4'
49	6	203	3PE	C2D-C2E-C2F-C2G
51	W	201	CDL	C53-C54-C55-C56
51	y	201	CDL	C14-C15-C16-C17
49	H	401	3PE	O11-C1-C2-O21
49	L	1001	3PE	O11-C1-C2-O21
50	A	201	PC1	O11-C1-C2-O21
50	M	502	PC1	O11-C1-C2-O21
49	N	401	3PE	C1-C2-C3-O31
51	W	201	CDL	CB3-CB4-CB6-OB8
50	M	502	PC1	C38-C39-C3A-C3B
50	9	401	PC1	C12-C11-O13-P
50	9	401	PC1	O21-C2-C3-O31
51	V	204	CDL	OB6-CB4-CB6-OB8
51	h	201	CDL	OA6-CA4-CA6-OA8
50	L	1003	PC1	C27-C28-C29-C2A
51	V	204	CDL	C52-C53-C54-C55
51	y	201	CDL	C31-CA7-OA8-CA6
49	H	401	3PE	C2-C1-O11-P
50	9	401	PC1	O13-C11-C12-N
49	H	401	3PE	C33-C34-C35-C36
51	V	203	CDL	CA5-C11-C12-C13
49	L	1001	3PE	C35-C36-C37-C38
56	s	201	MYR	C1-C2-C3-C4
50	M	502	PC1	C39-C3A-C3B-C3C
50	9	401	PC1	C3D-C3E-C3F-C3G
52	X	101	ZMP	O3-C16-C17-O4
49	V	202	3PE	C32-C33-C34-C35
49	6	203	3PE	C25-C26-C27-C28
49	L	1001	3PE	C24-C25-C26-C27
49	L	1001	3PE	O11-C1-C2-C3
50	6	202	PC1	O11-C1-C2-C3
50	M	502	PC1	O11-C1-C2-C3
51	N	403	CDL	OA5-CA3-CA4-CA6

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Mol	Chain	Res	Type	Atoms
51	V	204	CDL	C31-C32-C33-C34
46	1	501	FMN	N10-C1'-C2'-C3'
49	H	401	3PE	C29-C2A-C2B-C2C
50	9	401	PC1	C2-C1-O11-P
51	V	203	CDL	CA4-CA3-OA5-PA1
52	g	201	ZMP	C12-C11-S1-C10
50	6	202	PC1	O11-C1-C2-O21
51	o	201	CDL	OA5-CA3-CA4-OA6
49	M	501	3PE	C38-C39-C3A-C3B
49	A	202	3PE	C24-C25-C26-C27
50	9	401	PC1	C34-C35-C36-C37
51	h	201	CDL	OB6-CB4-CB6-OB8
51	W	201	CDL	C13-C14-C15-C16
51	y	201	CDL	C18-C19-C20-C21
51	L	1004	CDL	C60-C61-C62-C63
50	L	1003	PC1	C26-C27-C28-C29
51	W	201	CDL	C73-C74-C75-C76
49	4	501	3PE	C1-O11-P-O14
49	4	501	3PE	C11-O13-P-O14
49	6	203	3PE	C1-O11-P-O14
49	6	203	3PE	C11-O13-P-O14
49	A	202	3PE	C1-O11-P-O14
49	J	201	3PE	C1-O11-P-O14
49	L	1001	3PE	C1-O11-P-O13
49	L	1001	3PE	C11-O13-P-O14
49	L	1005	3PE	C1-O11-P-O14
49	M	501	3PE	C11-O13-P-O14
49	M	501	3PE	O13-C11-C12-N
49	N	402	3PE	C11-O13-P-O12
49	V	202	3PE	C1-O11-P-O12
49	V	202	3PE	C1-O11-P-O13
49	V	202	3PE	C1-O11-P-O14
49	i	201	3PE	C11-O13-P-O14
50	9	401	PC1	C11-O13-P-O12
50	L	1002	PC1	C1-O11-P-O14
50	L	1003	PC1	C11-O13-P-O14
50	L	1003	PC1	C1-O11-P-O14
51	N	403	CDL	CA2-OA2-PA1-OA4
51	N	403	CDL	CB3-OB5-PB2-OB2
51	N	403	CDL	CB3-OB5-PB2-OB3
51	N	403	CDL	CB3-OB5-PB2-OB4
51	V	203	CDL	CA3-OA5-PA1-OA4

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Mol	Chain	Res	Type	Atoms
51	V	203	CDL	CB3-OB5-PB2-OB2
51	V	203	CDL	CB3-OB5-PB2-OB3
51	V	203	CDL	CB3-OB5-PB2-OB4
51	V	204	CDL	CA2-OA2-PA1-OA3
51	W	201	CDL	CA3-OA5-PA1-OA2
51	W	201	CDL	CA3-OA5-PA1-OA3
51	W	201	CDL	CB2-OB2-PB2-OB4
51	h	201	CDL	CA3-OA5-PA1-OA2
51	h	201	CDL	CA3-OA5-PA1-OA3
51	h	201	CDL	CA3-OA5-PA1-OA4
51	h	201	CDL	CB2-OB2-PB2-OB3
51	h	201	CDL	CB3-OB5-PB2-OB2
51	o	201	CDL	CA2-OA2-PA1-OA5
51	o	201	CDL	CA3-OA5-PA1-OA3
51	o	201	CDL	CB3-OB5-PB2-OB4
51	y	201	CDL	CA3-OA5-PA1-OA2
51	y	201	CDL	CA3-OA5-PA1-OA3
51	y	201	CDL	CB3-OB5-PB2-OB3
52	X	101	ZMP	O4-C17-C18-C21
54	d	401	NDP	C5B-O5B-PA-O1A
54	d	401	NDP	C5B-O5B-PA-O2A
54	d	401	NDP	C5B-O5B-PA-O3
51	y	201	CDL	C32-C33-C34-C35
50	M	502	PC1	O31-C31-C32-C33
51	y	201	CDL	C80-C81-C82-C83
49	M	501	3PE	C2-C1-O11-P
50	M	502	PC1	C2-C1-O11-P
51	L	1004	CDL	C1-CA2-OA2-PA1
51	L	1004	CDL	CA4-CA3-OA5-PA1
51	V	204	CDL	C1-CA2-OA2-PA1
51	h	201	CDL	C1-CB2-OB2-PB2
51	h	201	CDL	CB4-CB3-OB5-PB2
51	o	201	CDL	CB4-CB3-OB5-PB2
51	N	403	CDL	C12-C13-C14-C15
49	p	201	3PE	C22-C23-C24-C25
49	6	203	3PE	C2E-C2F-C2G-C2H
52	g	201	ZMP	C1-C2-C3-C4
50	L	1003	PC1	C31-C32-C33-C34
51	L	1004	CDL	C58-C59-C60-C61
51	W	201	CDL	CA5-C11-C12-C13
49	N	401	3PE	O11-C1-C2-C3
51	L	1004	CDL	OB5-CB3-CB4-OB6

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Mol	Chain	Res	Type	Atoms
51	V	203	CDL	OB5-CB3-CB4-OB6
51	y	201	CDL	C1-CB2-OB2-PB2
51	o	201	CDL	OA6-CA4-CA6-OA8
49	6	203	3PE	C38-C39-C3A-C3B
50	9	401	PC1	C3A-C3B-C3C-C3D
50	A	201	PC1	O21-C21-C22-C23
55	k	501	AMP	C4'-C5'-O5'-P
50	9	401	PC1	C39-C3A-C3B-C3C
51	h	201	CDL	OA5-CA3-CA4-OA6
51	h	201	CDL	OB5-CB3-CB4-OB6
51	L	1004	CDL	C78-C79-C80-C81
50	L	1003	PC1	C3A-C3B-C3C-C3D
51	o	201	CDL	C51-C52-C53-C54
49	H	401	3PE	C32-C31-O31-C3
49	M	501	3PE	C23-C24-C25-C26
49	H	401	3PE	C36-C37-C38-C39
51	L	1004	CDL	C81-C82-C83-C84
51	V	204	CDL	C51-C52-C53-C54
51	N	403	CDL	CA2-C1-CB2-OB2
51	N	403	CDL	CB3-CB4-CB6-OB8
51	o	201	CDL	CA3-CA4-CA6-OA8
51	o	201	CDL	C72-C73-C74-C75
50	9	401	PC1	C31-C32-C33-C34
50	9	401	PC1	C3F-C3G-C3H-C3I
50	9	401	PC1	C3-C2-O21-C21
54	d	401	NDP	O4D-C1D-N1N-C6N
49	M	501	3PE	C27-C28-C29-C2A
50	L	1002	PC1	O11-C1-C2-O21
51	y	201	CDL	OB5-CB3-CB4-OB6
46	1	501	FMN	C4'-C5'-O5'-P
51	o	201	CDL	C1-CB2-OB2-PB2
51	V	203	CDL	OA5-CA3-CA4-CA6
51	y	201	CDL	OB5-CB3-CB4-CB6
51	L	1004	CDL	C19-C20-C21-C22
50	9	401	PC1	O22-C21-O21-C2
50	L	1002	PC1	C2A-C2B-C2C-C2D
51	o	201	CDL	C62-C63-C64-C65
51	y	201	CDL	C58-C59-C60-C61
50	M	502	PC1	C2F-C2G-C2H-C2I
50	6	202	PC1	O31-C31-C32-C33
49	L	1001	3PE	C3B-C3C-C3D-C3E
50	6	202	PC1	C11-C12-N-C14

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Mol	Chain	Res	Type	Atoms
46	1	501	FMN	C2'-C3'-C4'-C5'
51	o	201	CDL	C19-C20-C21-C22
49	N	401	3PE	C22-C23-C24-C25
51	V	204	CDL	C12-C13-C14-C15
49	H	401	3PE	C2F-C2G-C2H-C2I
49	J	201	3PE	C2-C1-O11-P
50	9	401	PC1	C2B-C2C-C2D-C2E
51	V	203	CDL	C19-C20-C21-C22
51	o	201	CDL	C54-C55-C56-C57
50	9	401	PC1	C22-C21-O21-C2
51	y	201	CDL	OA9-CA7-OA8-CA6
50	M	502	PC1	C25-C26-C27-C28
51	L	1004	CDL	C32-C33-C34-C35
54	d	401	NDP	C2D-C1D-N1N-C6N
49	6	203	3PE	C3D-C3E-C3F-C3G
49	4	501	3PE	C37-C38-C39-C3A
51	N	403	CDL	C52-C51-CB5-OB6
51	h	201	CDL	CA2-C1-CB2-OB2
49	H	401	3PE	C2B-C2C-C2D-C2E
49	V	202	3PE	O11-C1-C2-C3
49	4	501	3PE	O21-C2-C3-O31
50	A	201	PC1	O31-C31-C32-C33
51	V	203	CDL	C80-C81-C82-C83
49	p	201	3PE	C23-C24-C25-C26
51	V	203	CDL	C34-C35-C36-C37
51	o	201	CDL	C80-C81-C82-C83
49	V	202	3PE	O21-C21-C22-C23
49	L	1005	3PE	C1-C2-O21-C21
51	o	201	CDL	CB3-CB4-OB6-CB5
49	M	501	3PE	C39-C3A-C3B-C3C
51	h	201	CDL	C52-C53-C54-C55
50	A	201	PC1	C21-C22-C23-C24
49	6	203	3PE	C33-C34-C35-C36
52	g	201	ZMP	C3-C4-C5-C6
51	N	403	CDL	C71-C72-C73-C74
49	V	202	3PE	O11-C1-C2-O21
51	V	203	CDL	OA5-CA3-CA4-OA6
49	N	401	3PE	C38-C39-C3A-C3B
49	H	401	3PE	O32-C31-O31-C3
46	1	501	FMN	O2'-C2'-C3'-O3'
49	N	401	3PE	C36-C37-C38-C39
49	L	1001	3PE	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
52	X	101	ZMP	C16-C17-C18-C20
49	M	501	3PE	O21-C2-C3-O31
51	y	201	CDL	C72-C71-CB7-OB8
51	o	201	CDL	C72-C71-CB7-OB8
51	y	201	CDL	C71-CB7-OB8-CB6
51	W	201	CDL	C36-C37-C38-C39
54	d	401	NDP	PN-O3-PA-O2A
51	W	201	CDL	C81-C82-C83-C84
51	V	204	CDL	C32-C31-CA7-OA8
51	N	403	CDL	C14-C15-C16-C17
50	6	202	PC1	C11-C12-N-C13
50	6	202	PC1	C11-C12-N-C15
49	H	401	3PE	C3F-C3G-C3H-C3I
49	A	202	3PE	O21-C21-C22-C23
51	V	204	CDL	C23-C24-C25-C26
51	N	403	CDL	C72-C71-CB7-OB8
51	o	201	CDL	C60-C61-C62-C63
49	i	201	3PE	O21-C21-C22-C23
49	V	201	3PE	C2-C1-O11-P
49	N	401	3PE	O31-C31-C32-C33
51	V	203	CDL	OA6-CA4-CA6-OA8
49	L	1005	3PE	O21-C21-C22-C23
50	6	202	PC1	C22-C23-C24-C25
51	W	201	CDL	C79-C80-C81-C82
51	h	201	CDL	OA5-CA3-CA4-CA6
51	h	201	CDL	OB5-CB3-CB4-CB6
51	W	201	CDL	CA2-C1-CB2-OB2
49	V	202	3PE	O31-C31-C32-C33
51	V	203	CDL	C23-C24-C25-C26
49	V	202	3PE	C25-C26-C27-C28
50	L	1002	PC1	C1-C2-O21-C21
49	4	501	3PE	O31-C31-C32-C33
49	M	501	3PE	C3B-C3C-C3D-C3E
51	y	201	CDL	C56-C57-C58-C59
51	o	201	CDL	CA4-CA3-OA5-PA1
49	p	201	3PE	O21-C21-C22-C23
49	L	1001	3PE	C3A-C3B-C3C-C3D
51	o	201	CDL	C31-C32-C33-C34
51	W	201	CDL	C55-C56-C57-C58
49	A	202	3PE	O22-C21-C22-C23
49	M	501	3PE	C35-C36-C37-C38
51	y	201	CDL	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
51	V	204	CDL	C32-C31-CA7-OA9
50	L	1002	PC1	C28-C29-C2A-C2B
50	L	1002	PC1	C2D-C2E-C2F-C2G
50	L	1002	PC1	C3E-C3F-C3G-C3H
51	o	201	CDL	C53-C54-C55-C56
51	W	201	CDL	O1-C1-CB2-OB2
49	V	201	3PE	C29-C2A-C2B-C2C
49	i	201	3PE	O22-C21-C22-C23
51	N	403	CDL	C72-C71-CB7-OB9
51	o	201	CDL	C72-C71-CB7-OB9
51	y	201	CDL	C72-C71-CB7-OB9
49	L	1001	3PE	C3D-C3E-C3F-C3G
50	L	1002	PC1	C3B-C3C-C3D-C3E
49	J	201	3PE	C23-C24-C25-C26
52	X	101	ZMP	N2-C16-C17-O4
52	g	201	ZMP	N2-C16-C17-O4
49	N	401	3PE	O32-C31-C32-C33
51	L	1004	CDL	CB4-CB3-OB5-PB2
49	4	501	3PE	O32-C31-C32-C33
49	M	501	3PE	O31-C31-C32-C33
49	L	1005	3PE	O22-C21-C22-C23
49	V	202	3PE	O32-C31-C32-C33
51	W	201	CDL	C15-C16-C17-C18
51	L	1004	CDL	C39-C40-C41-C42
51	h	201	CDL	C52-C51-CB5-OB6
51	L	1004	CDL	C71-C72-C73-C74
51	N	403	CDL	C73-C74-C75-C76
51	V	203	CDL	C32-C31-CA7-OA8
54	d	401	NDP	PN-O3-PA-O1A
49	p	201	3PE	O22-C21-C22-C23
51	V	204	CDL	C52-C51-CB5-OB6
51	W	201	CDL	C22-C23-C24-C25

There are no ring outliers.

30 monomers are involved in 82 short contacts:

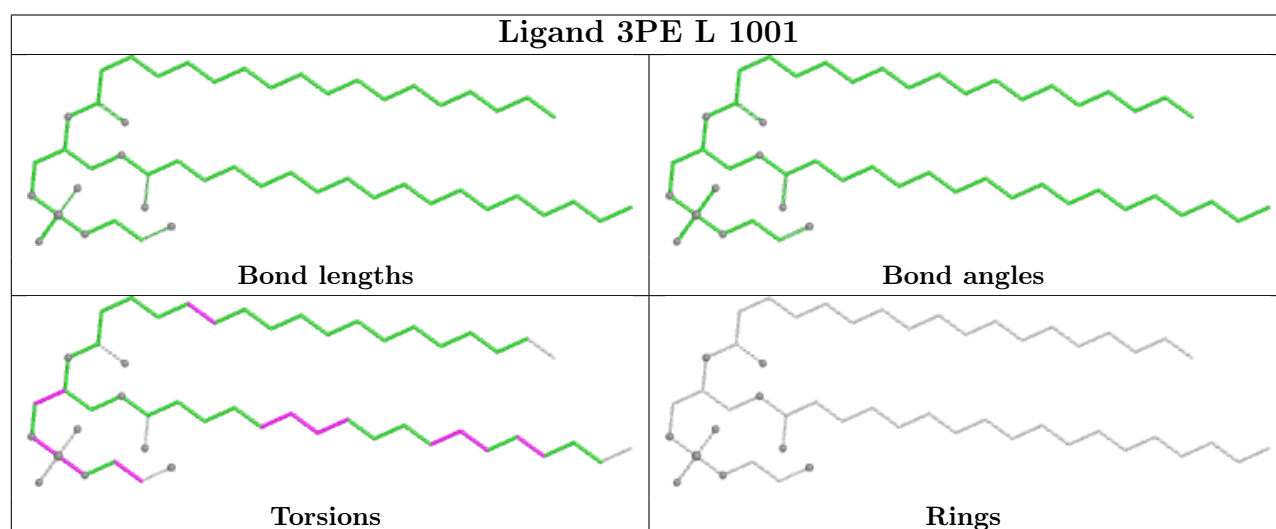
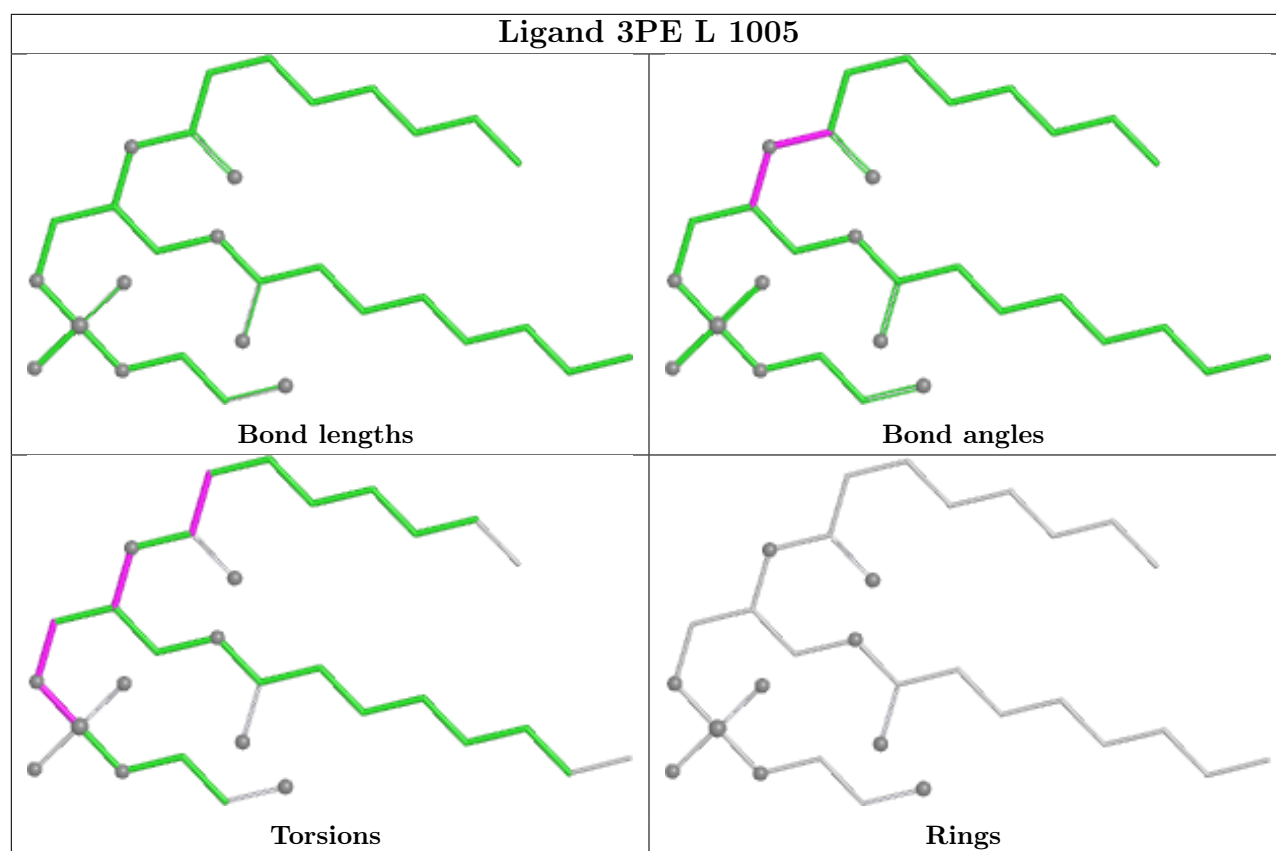
Mol	Chain	Res	Type	Clashes	Symm-Clashes
49	L	1001	3PE	2	0
54	d	401	NDP	1	0
50	M	502	PC1	4	0
46	1	501	FMN	2	0
51	y	201	CDL	5	0

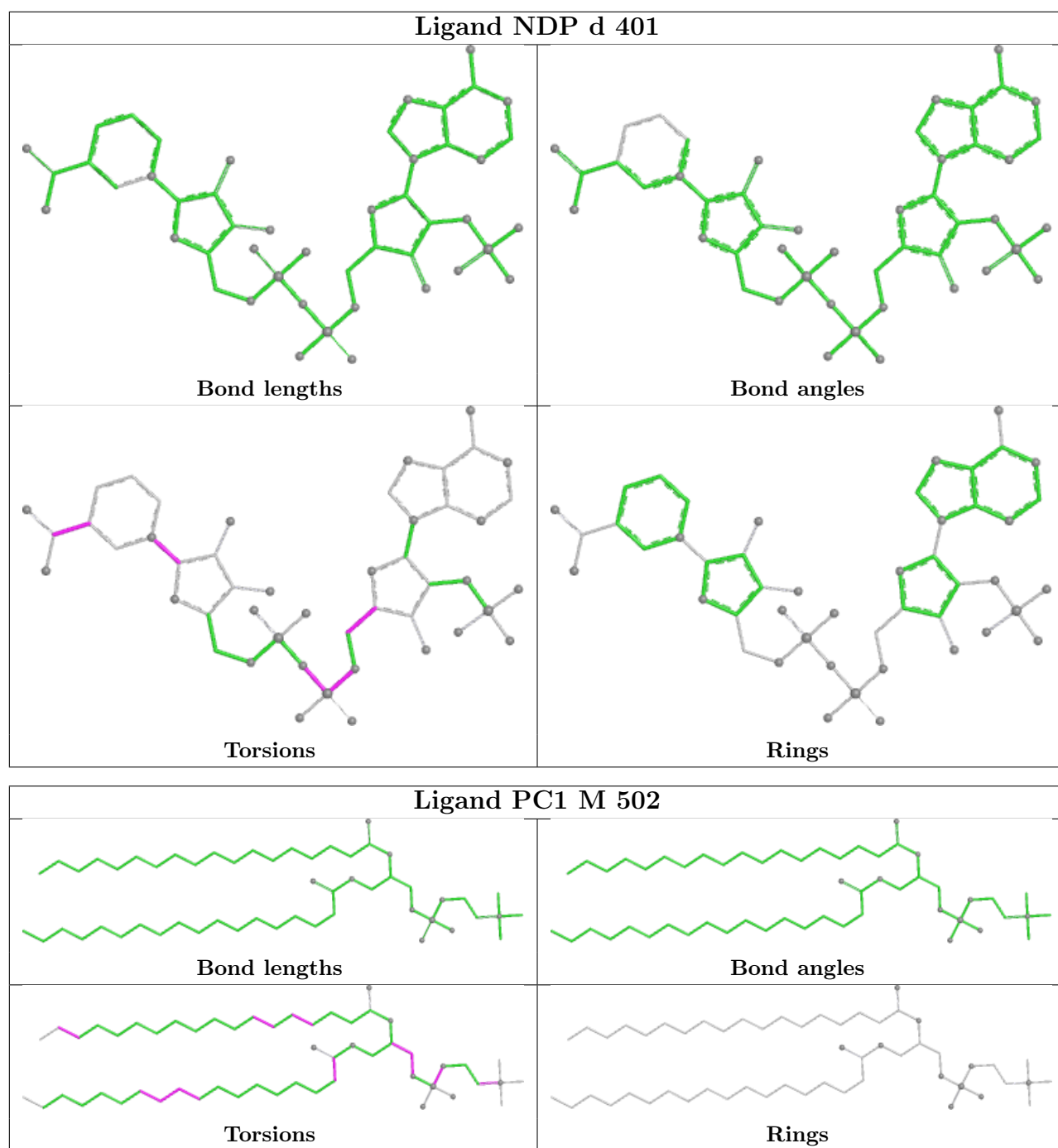
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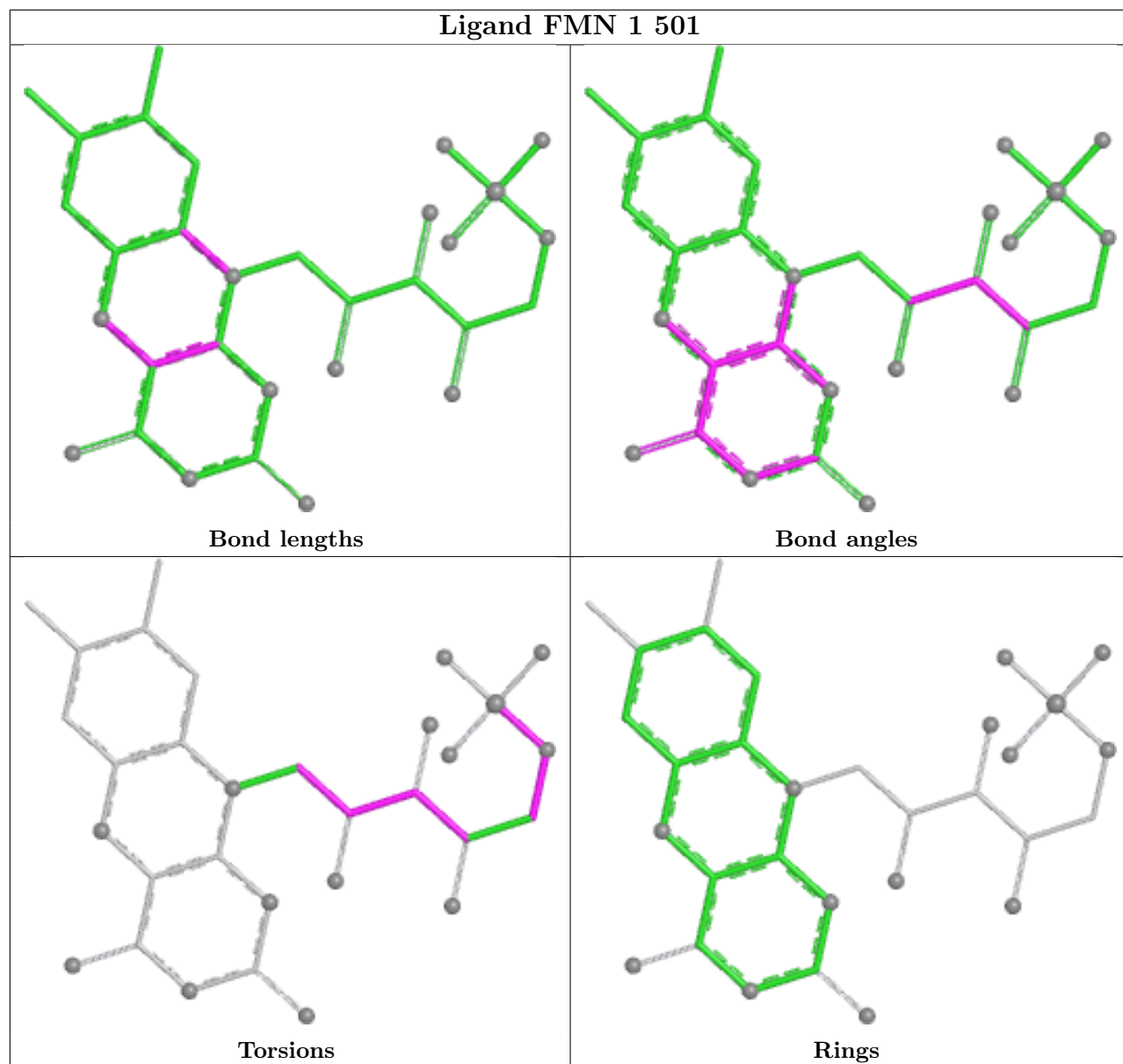
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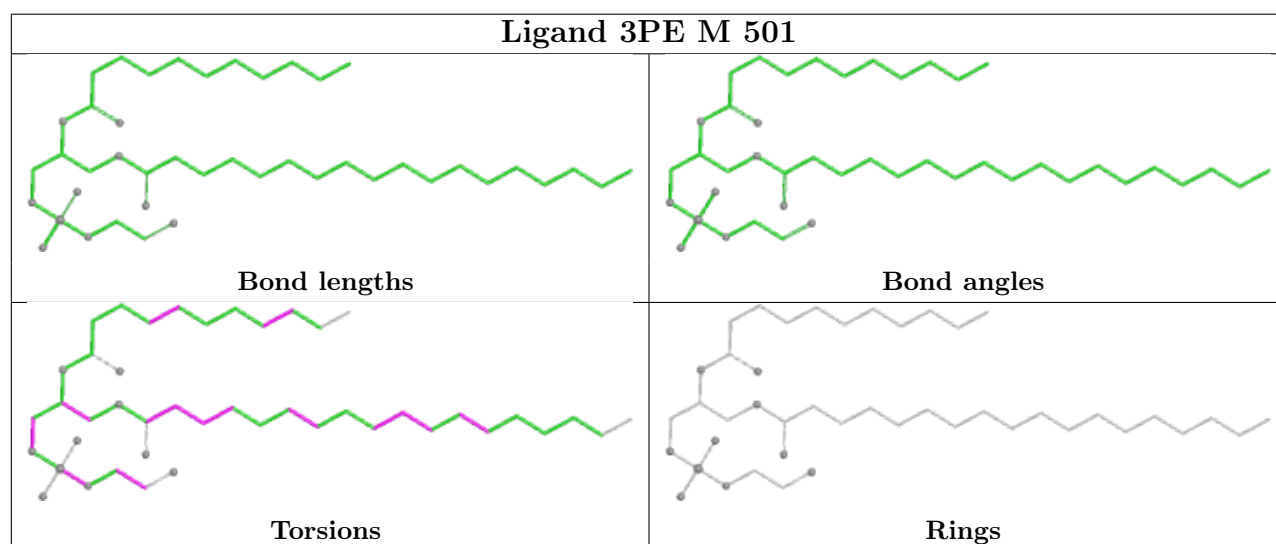
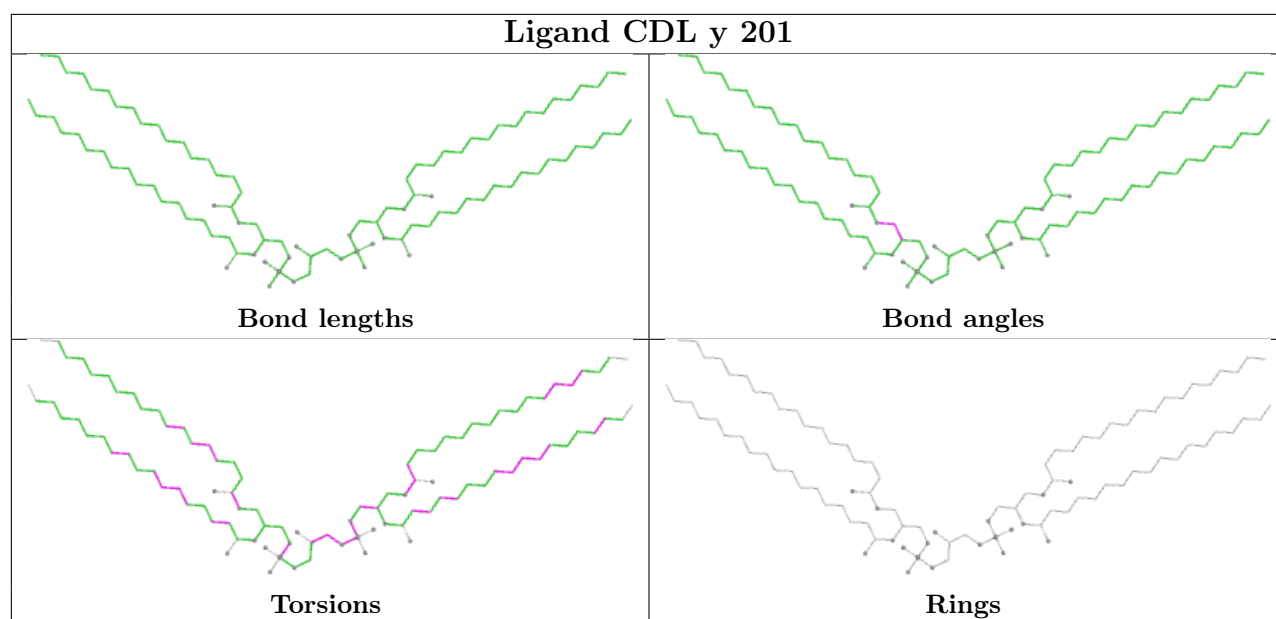
Mol	Chain	Res	Type	Clashes	Symm-Clashes
49	M	501	3PE	1	0
51	o	201	CDL	6	0
50	L	1002	PC1	4	0
51	L	1004	CDL	10	0
51	V	204	CDL	3	0
51	N	403	CDL	5	0
50	6	202	PC1	1	0
49	V	201	3PE	2	0
51	W	201	CDL	4	0
51	V	203	CDL	6	0
49	6	203	3PE	4	0
50	L	1003	PC1	3	0
49	A	202	3PE	2	0
50	A	201	PC1	2	0
49	H	401	3PE	1	0
49	N	401	3PE	2	0
47	2	300	FES	1	0
45	3	801	SF4	1	0
49	4	501	3PE	1	0
49	J	201	3PE	3	0
52	X	101	ZMP	2	0
52	g	201	ZMP	2	0
45	6	201	SF4	1	0
45	1	500	SF4	3	0
50	9	401	PC1	2	0

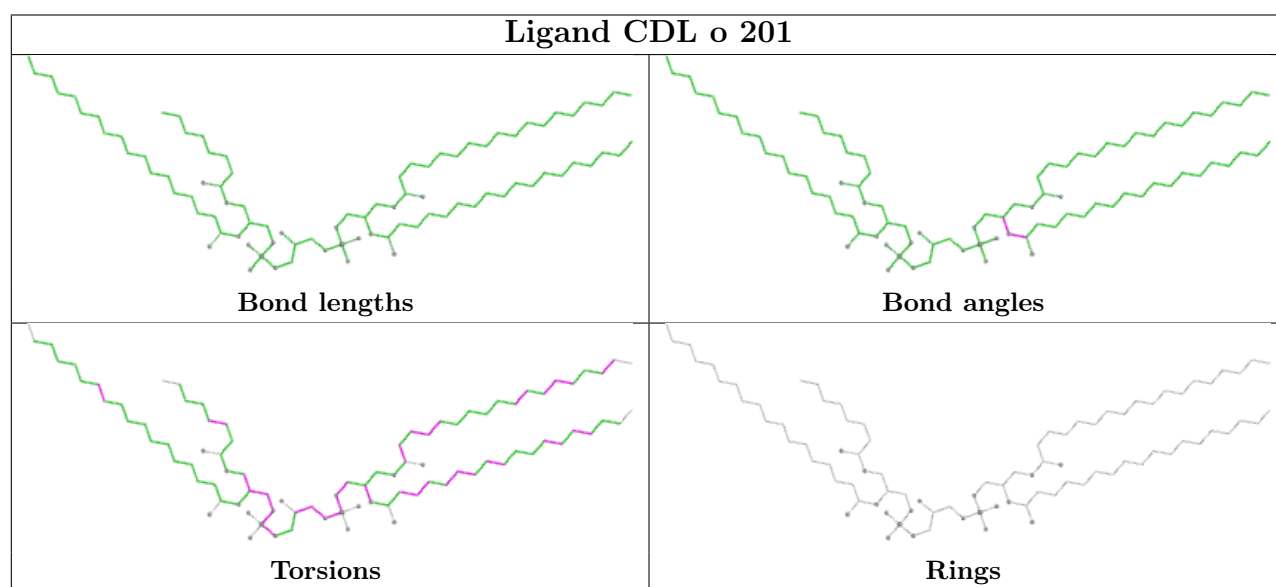
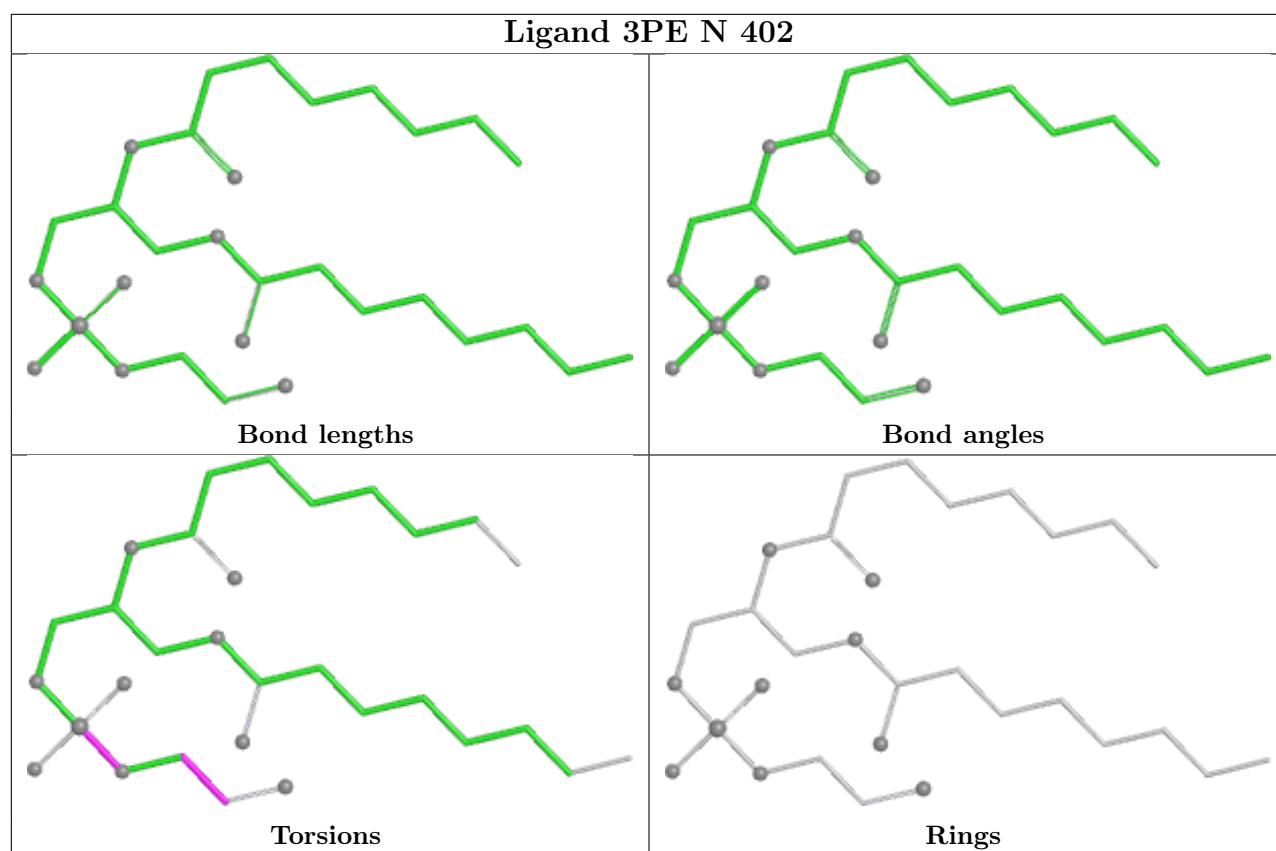
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

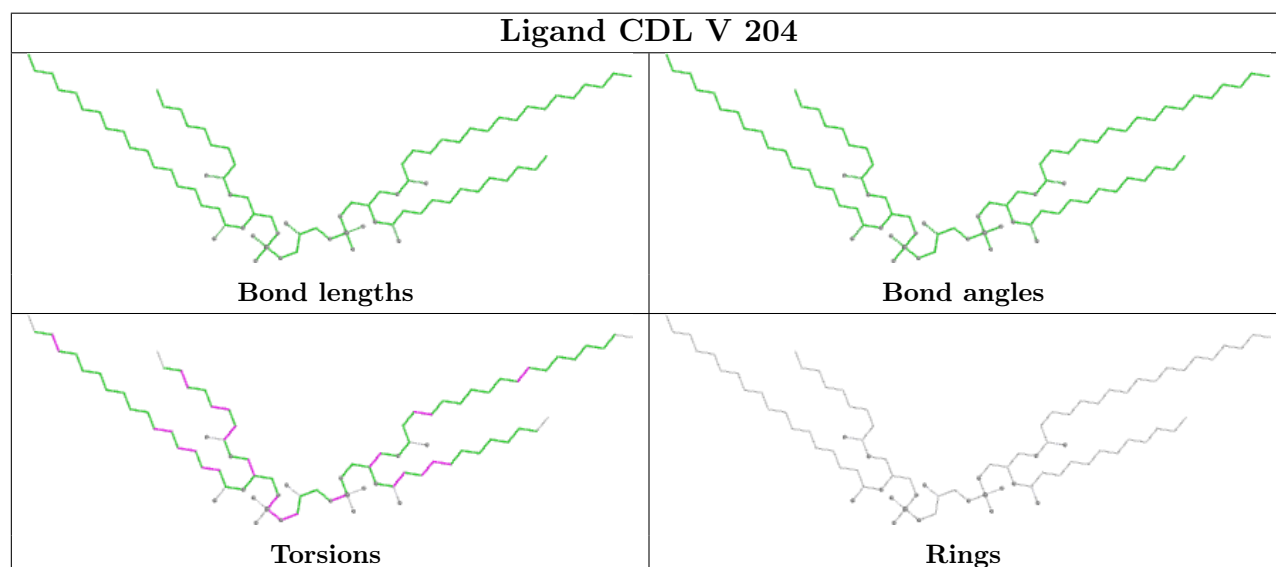
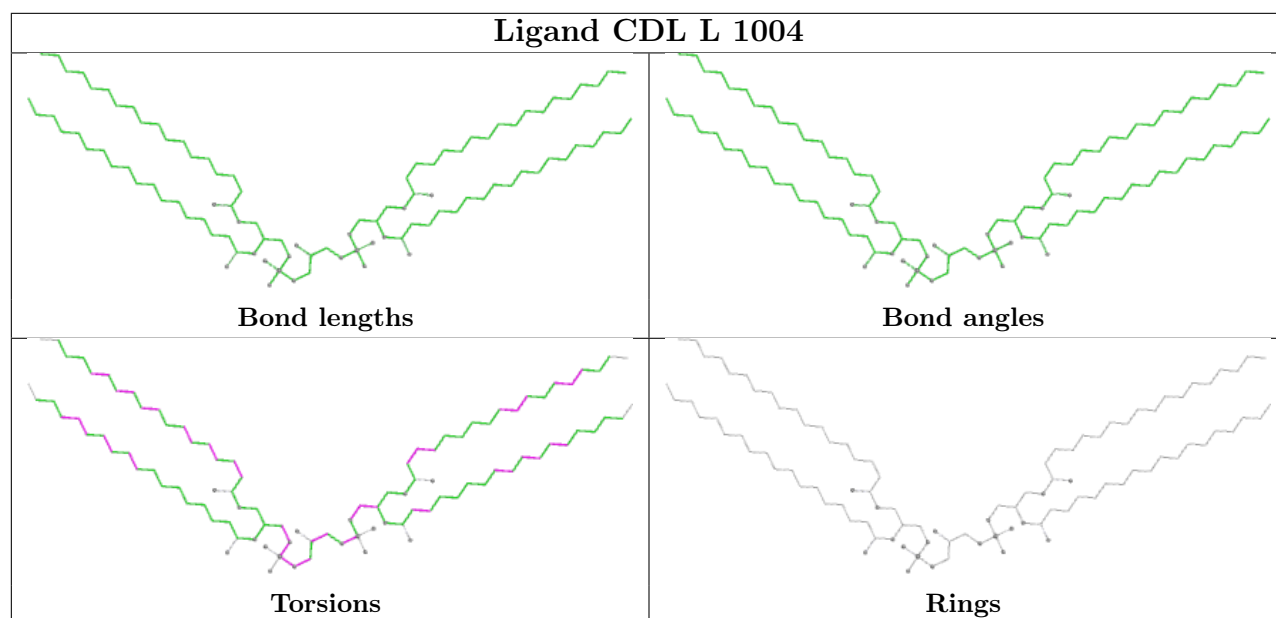
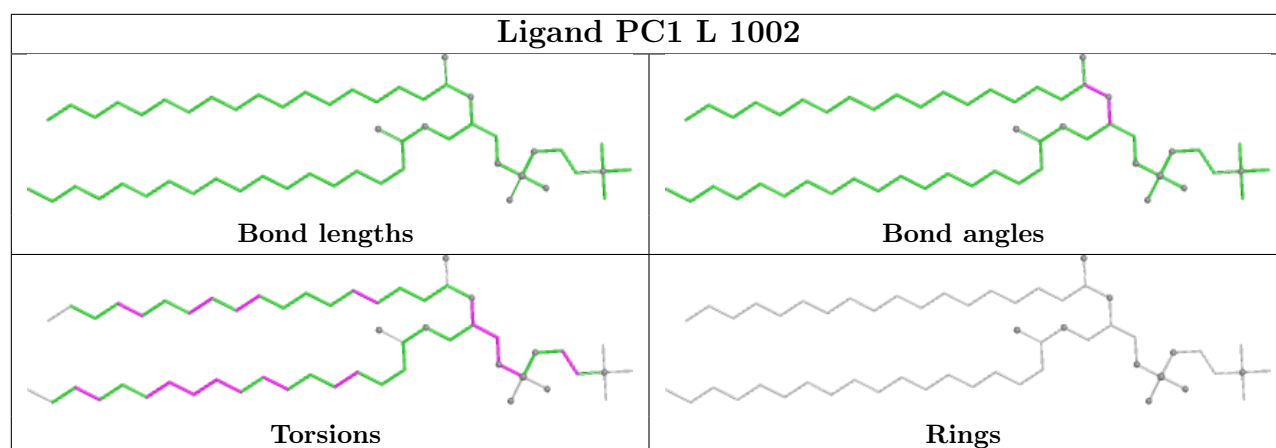


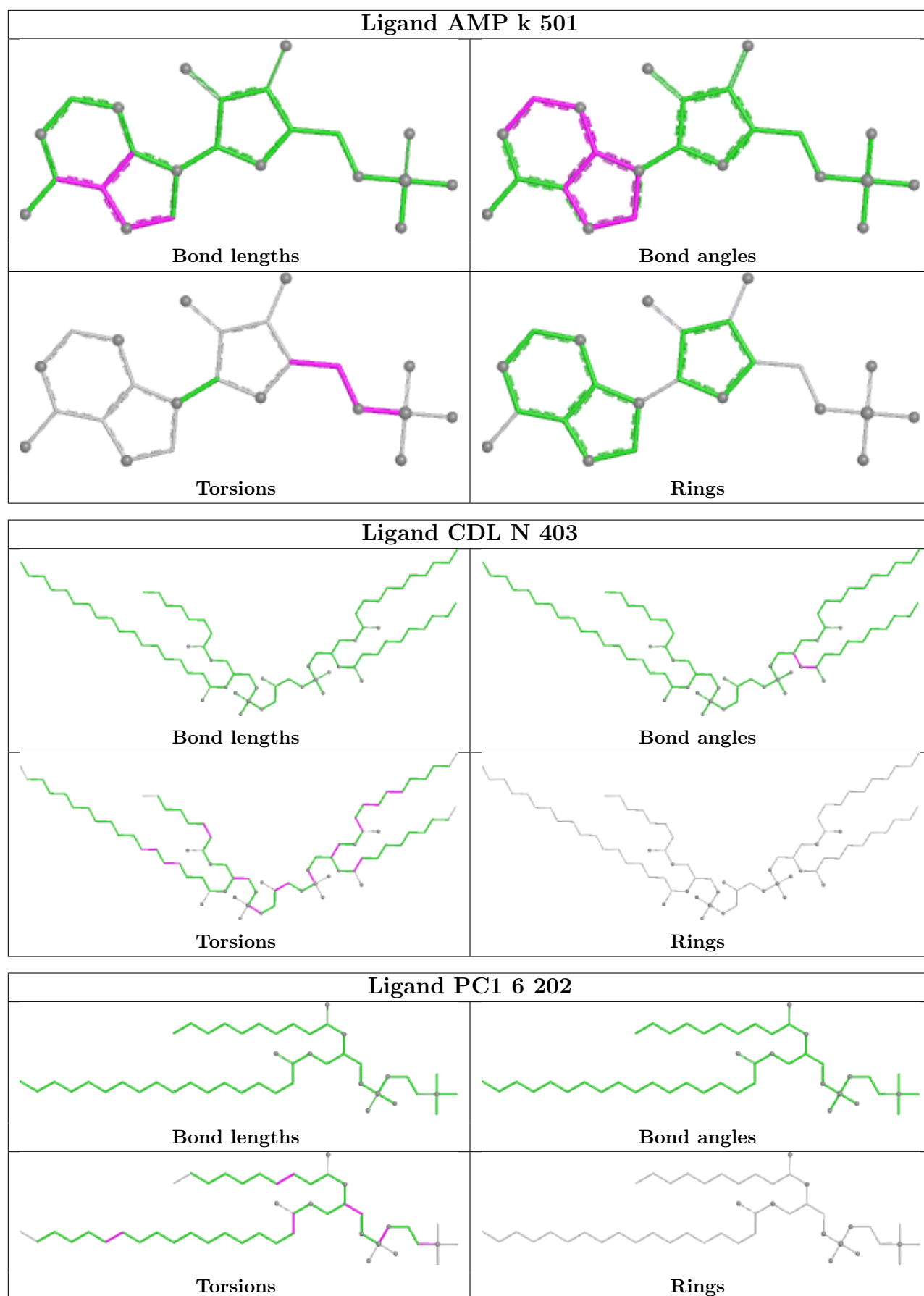


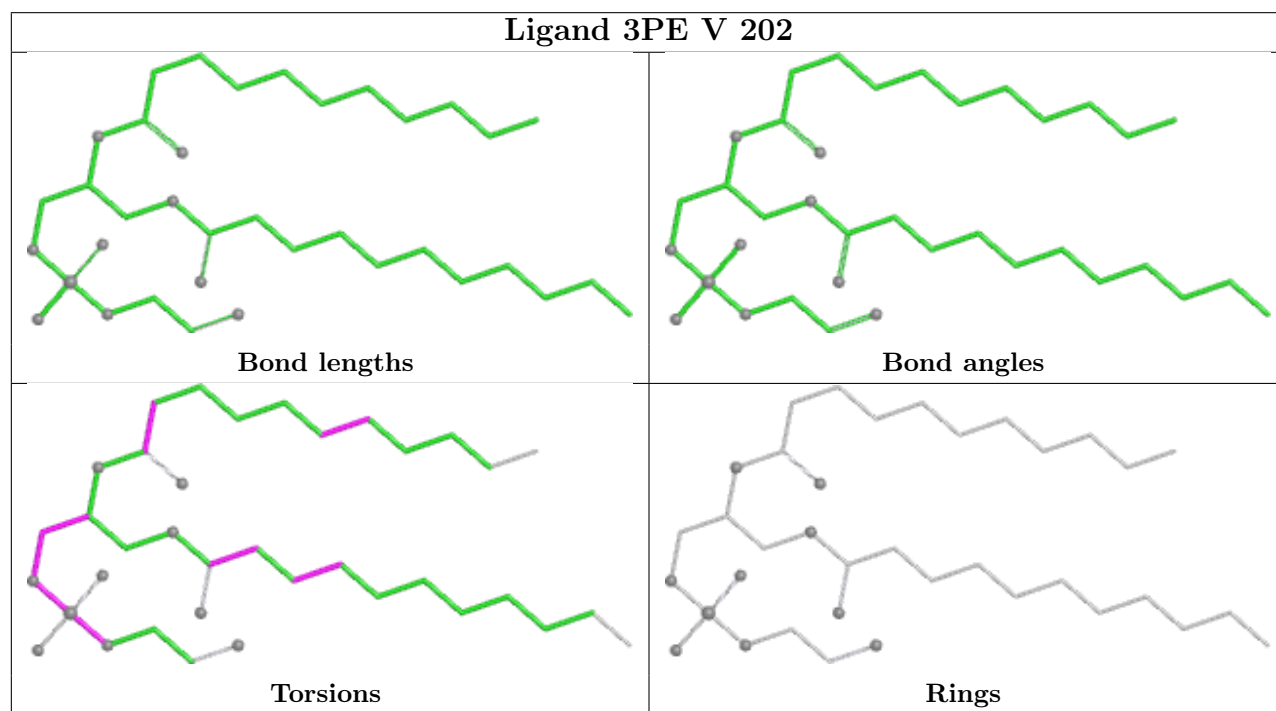
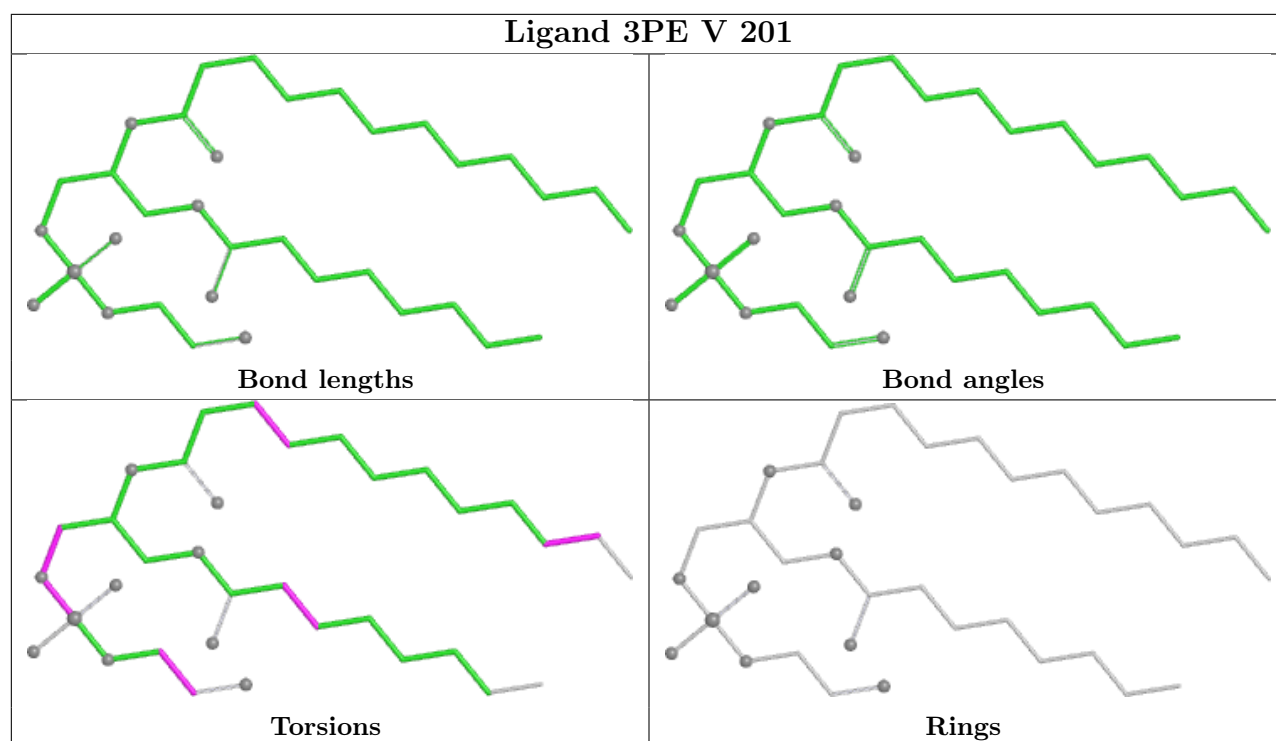


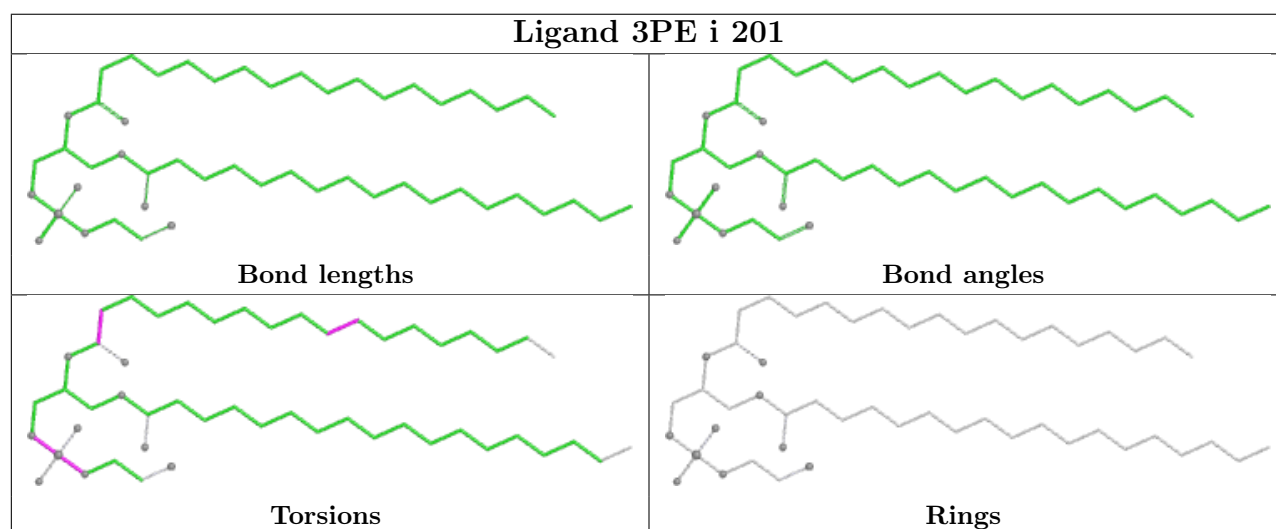
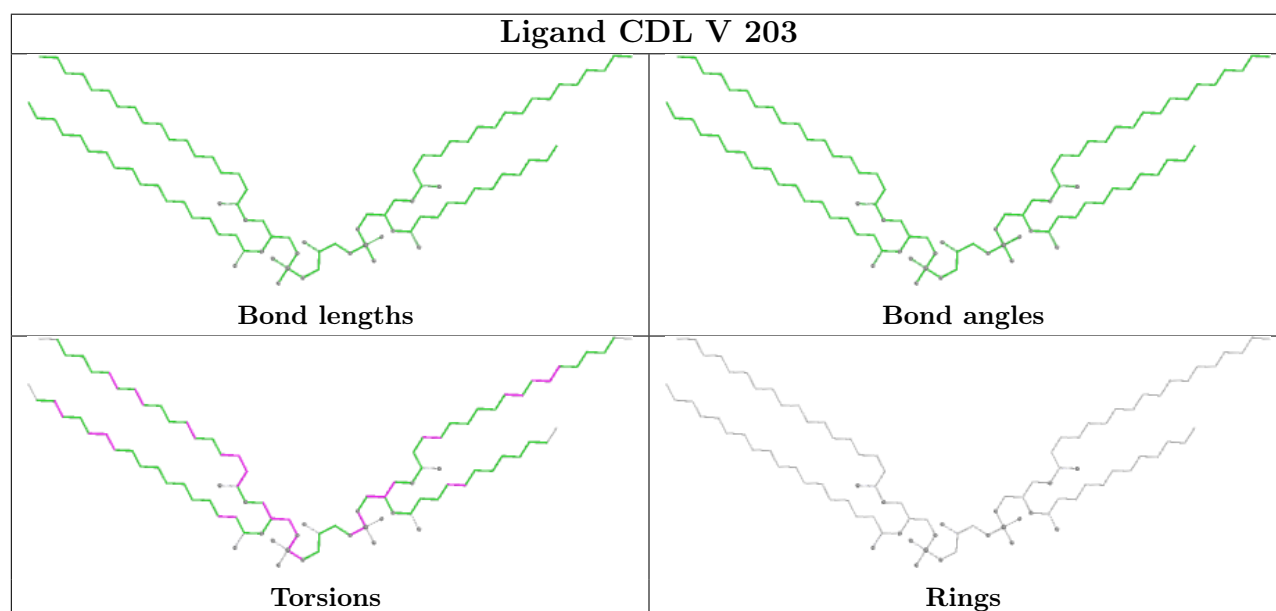
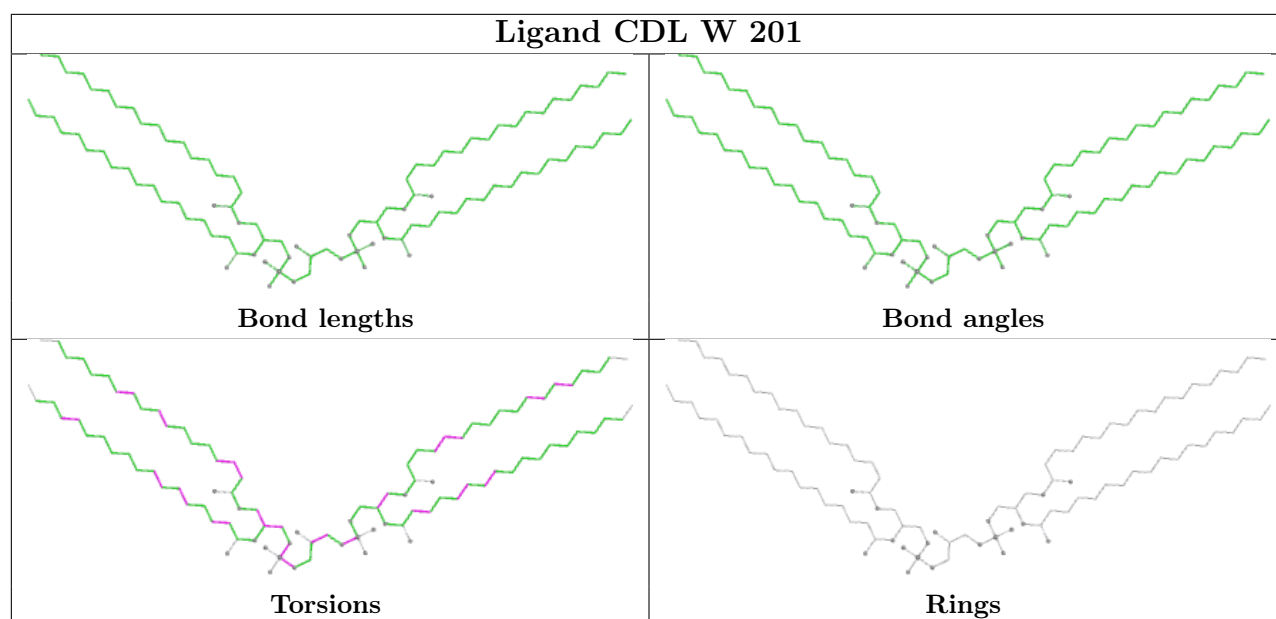


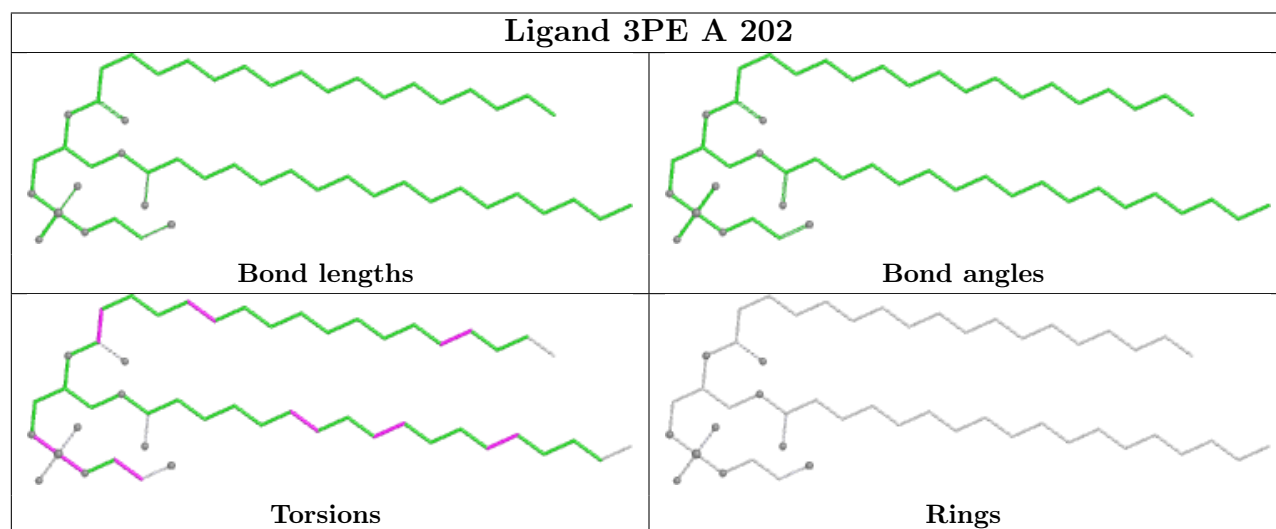
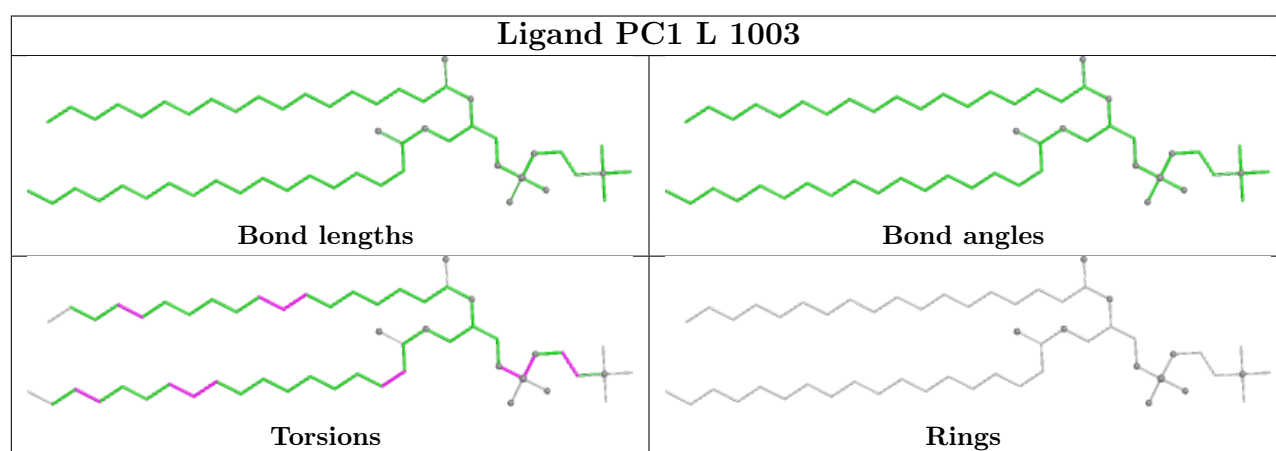
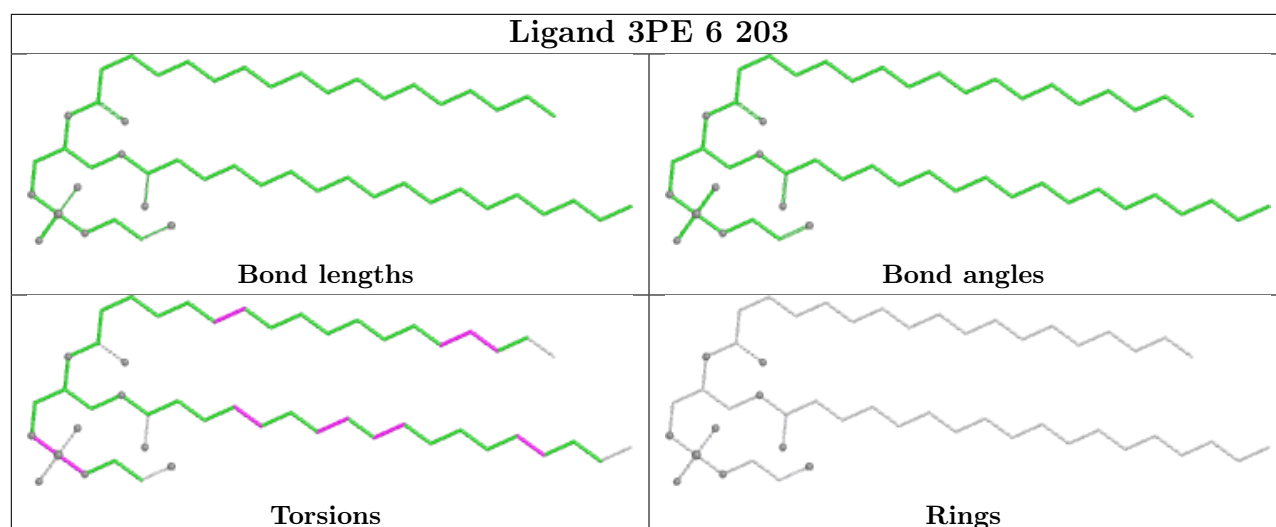


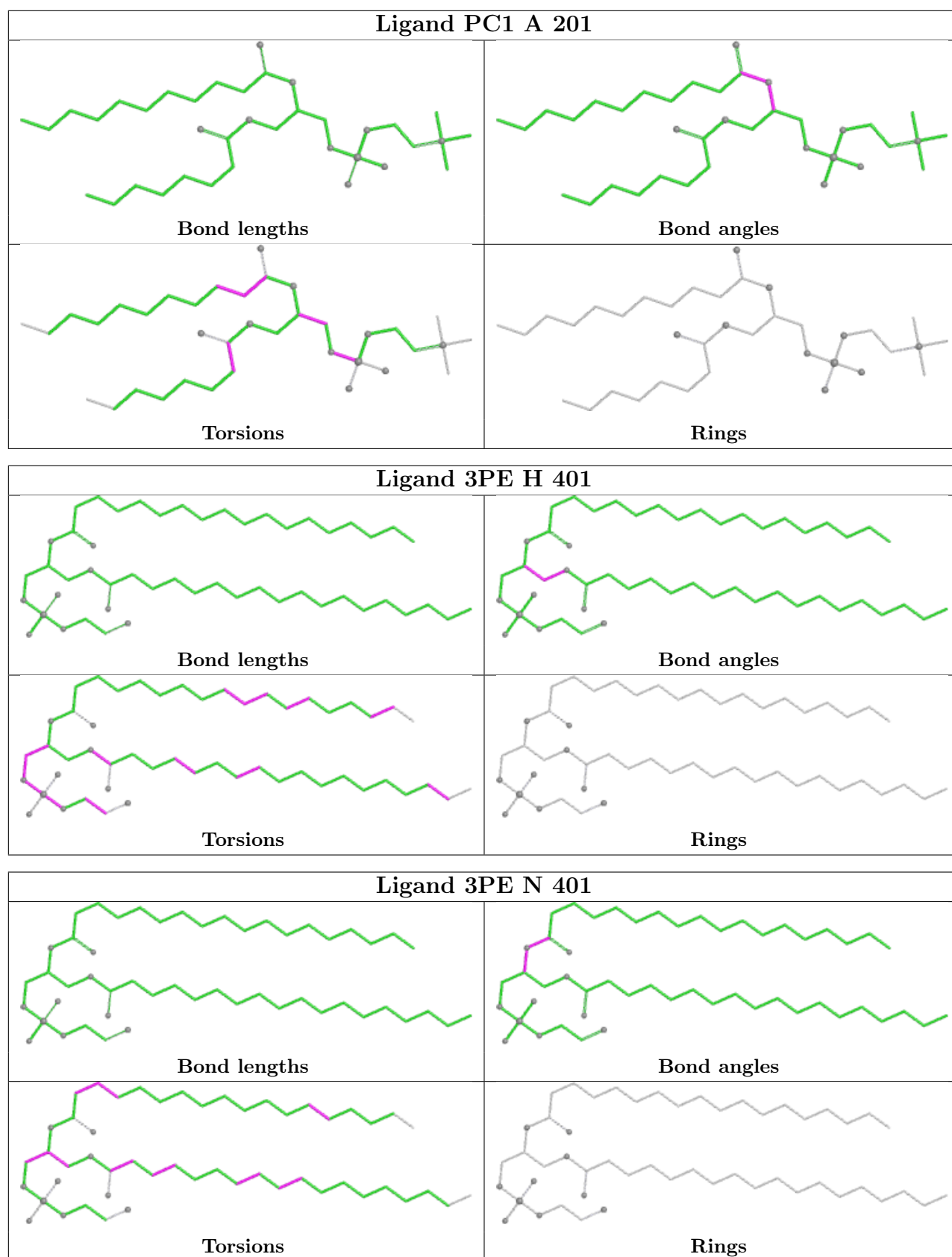


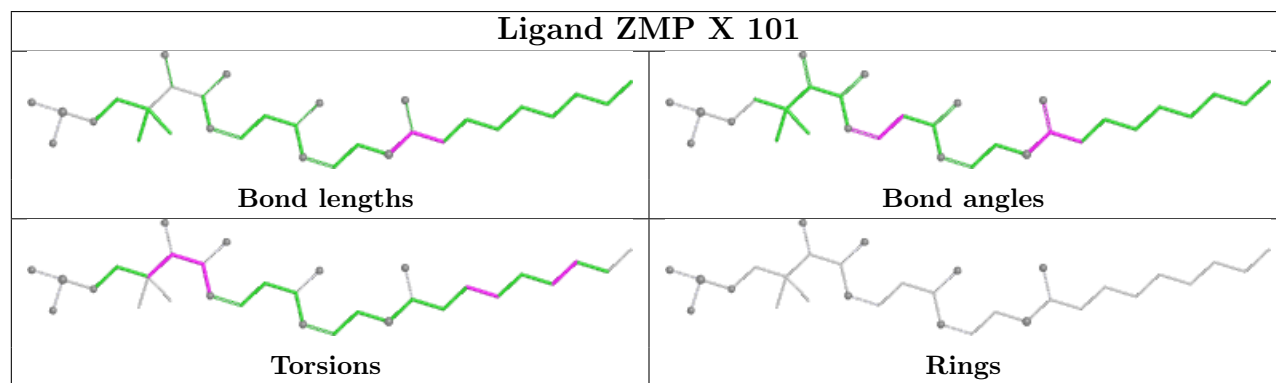
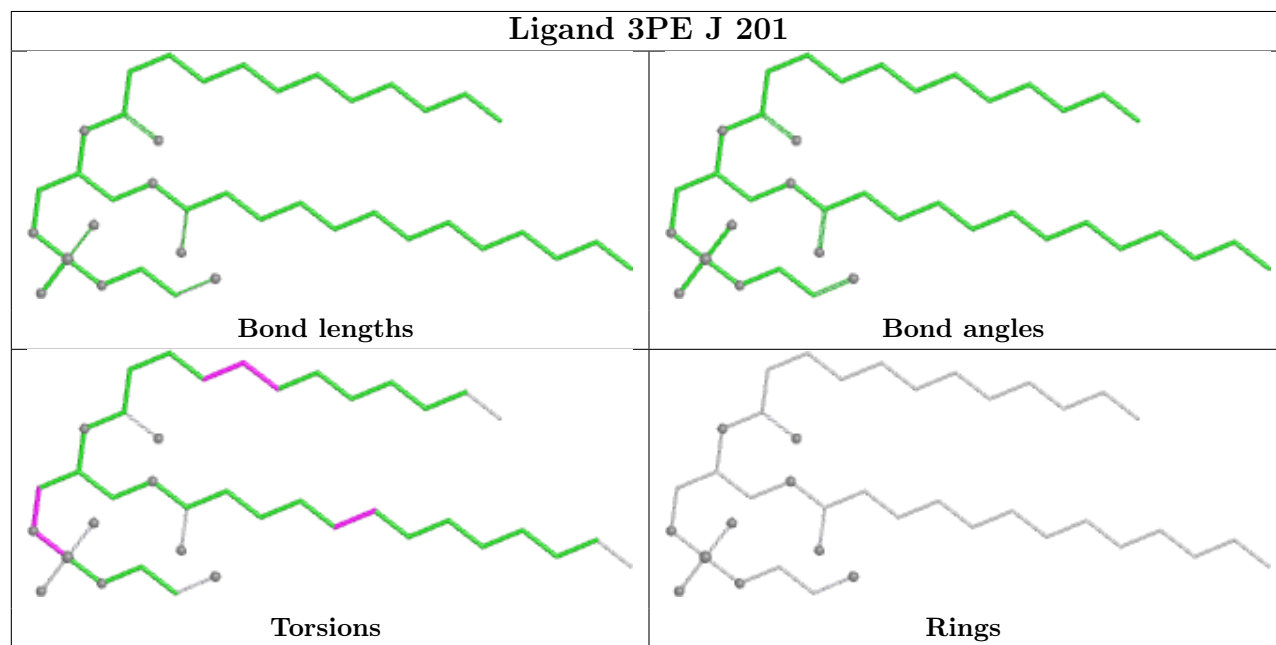
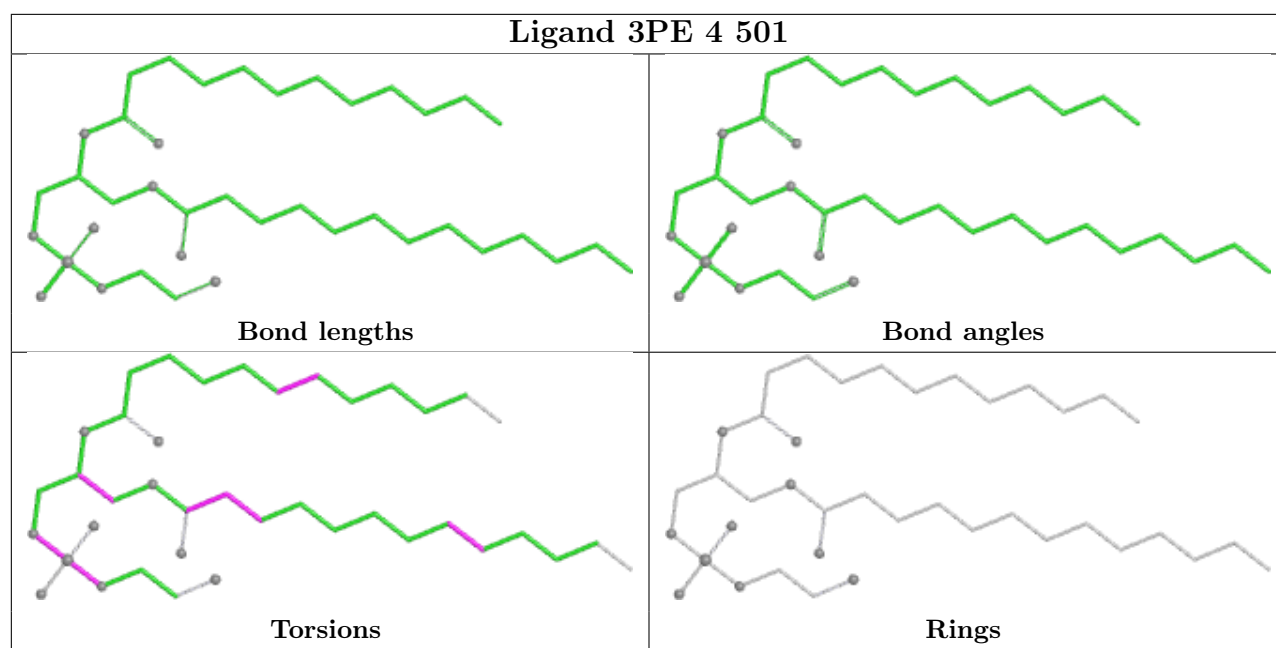


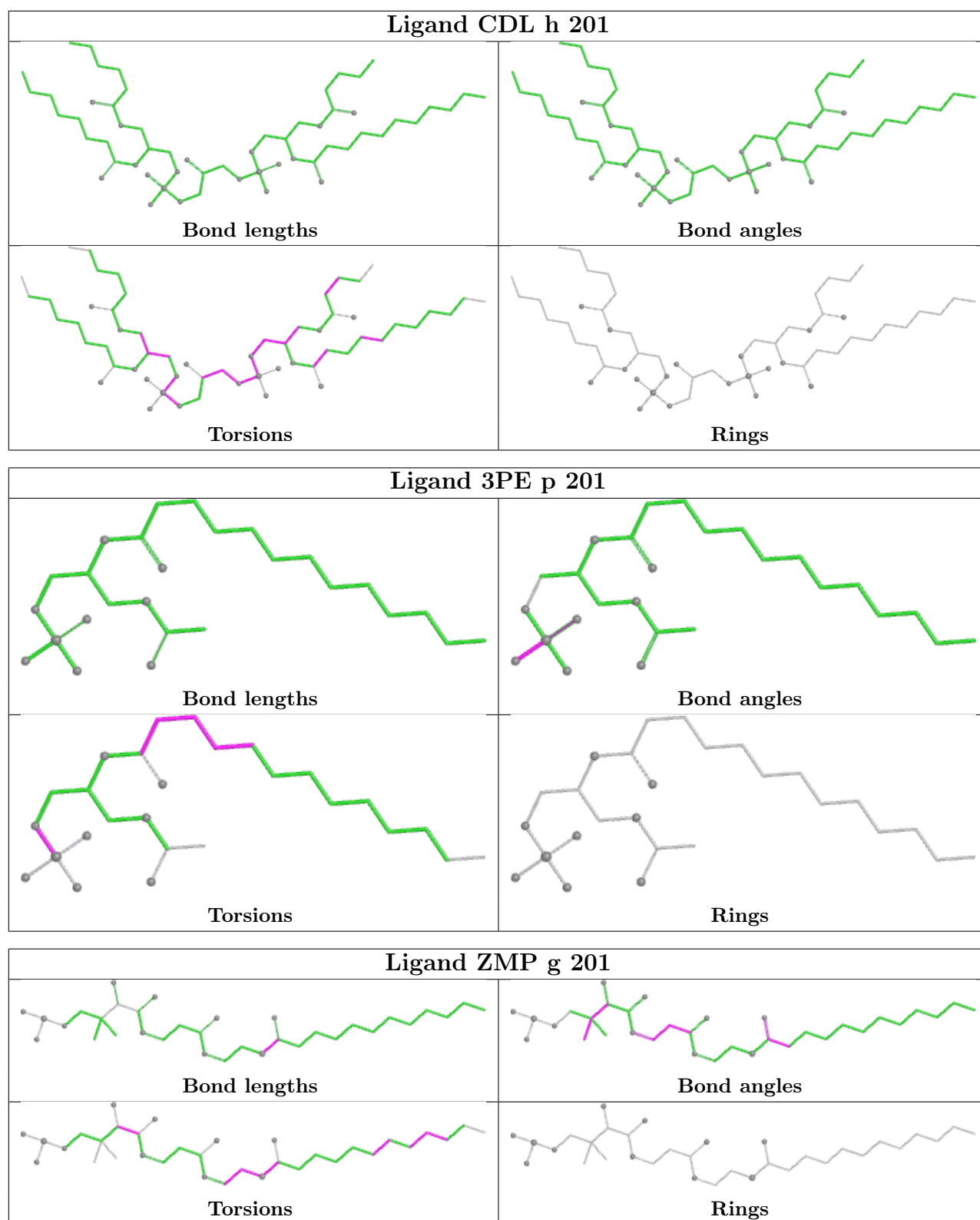


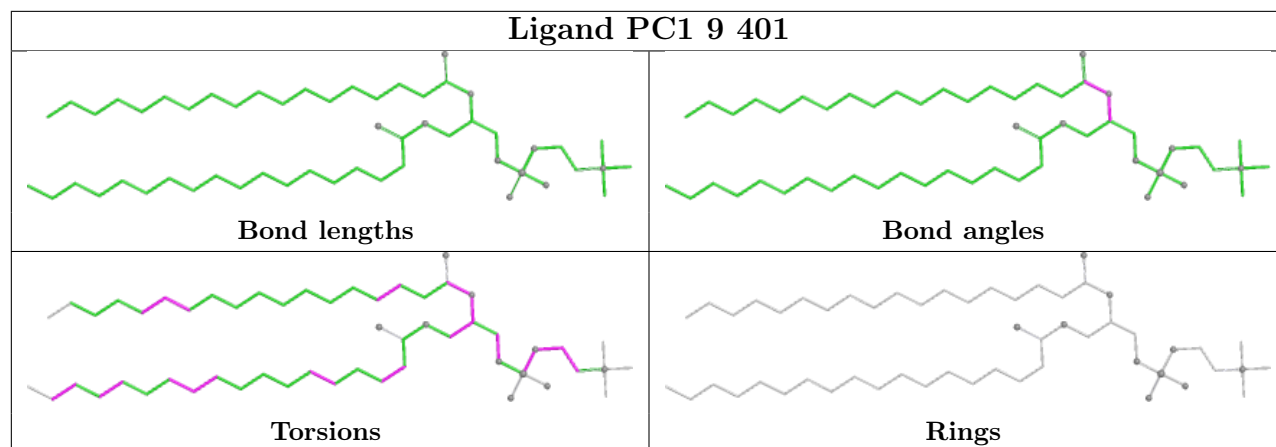












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

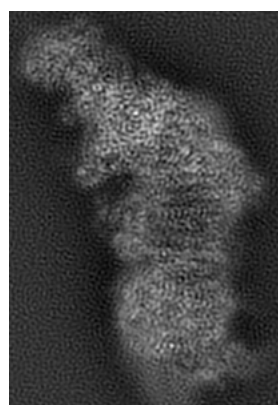
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11257. These allow visual inspection of the internal detail of the map and identification of artifacts.

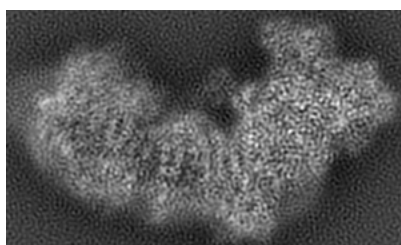
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

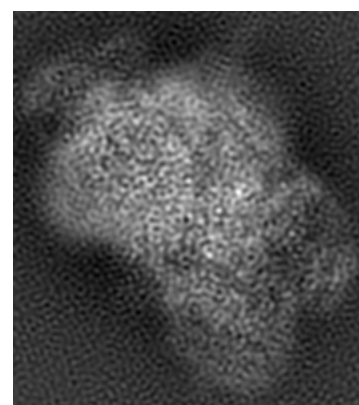
6.1.1 Primary map



X



Y

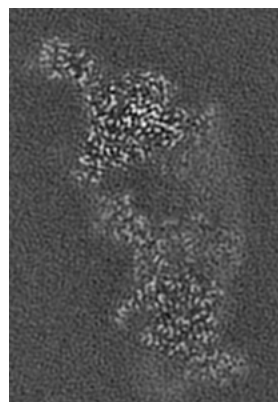


Z

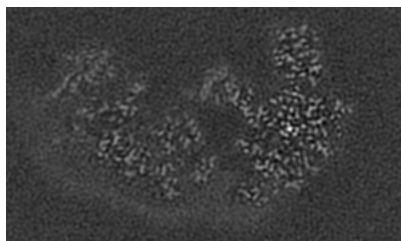
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

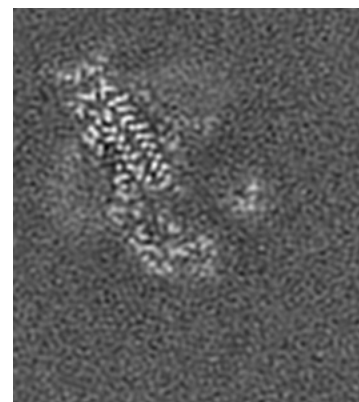
6.2.1 Primary map



X Index: 103



Y Index: 116

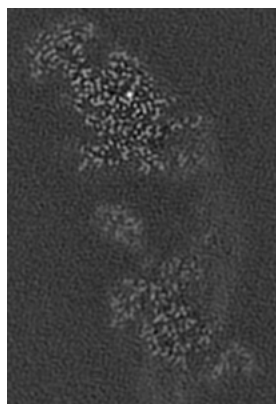


Z Index: 172

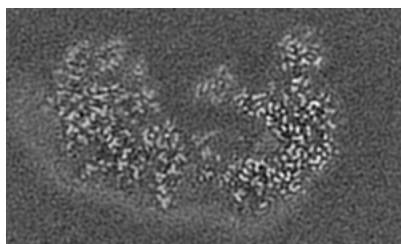
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

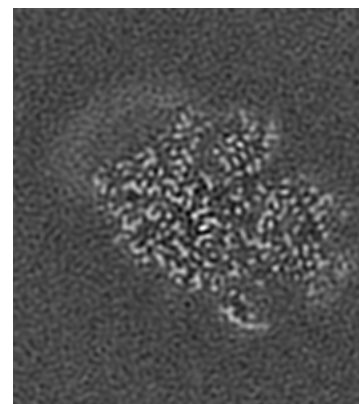
6.3.1 Primary map



X Index: 115



Y Index: 127

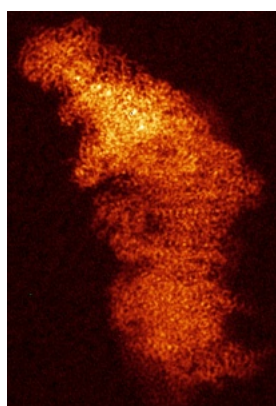


Z Index: 252

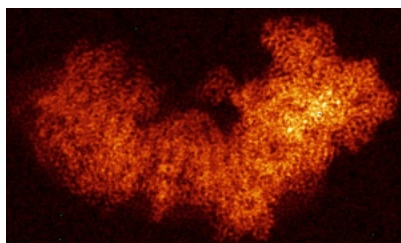
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

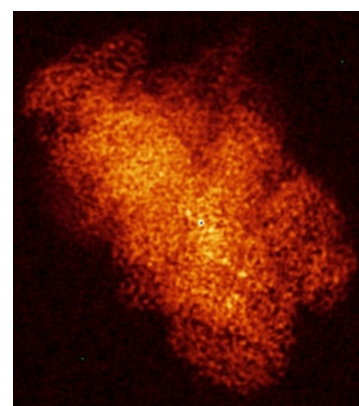
6.4.1 Primary map



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

This section was not generated.

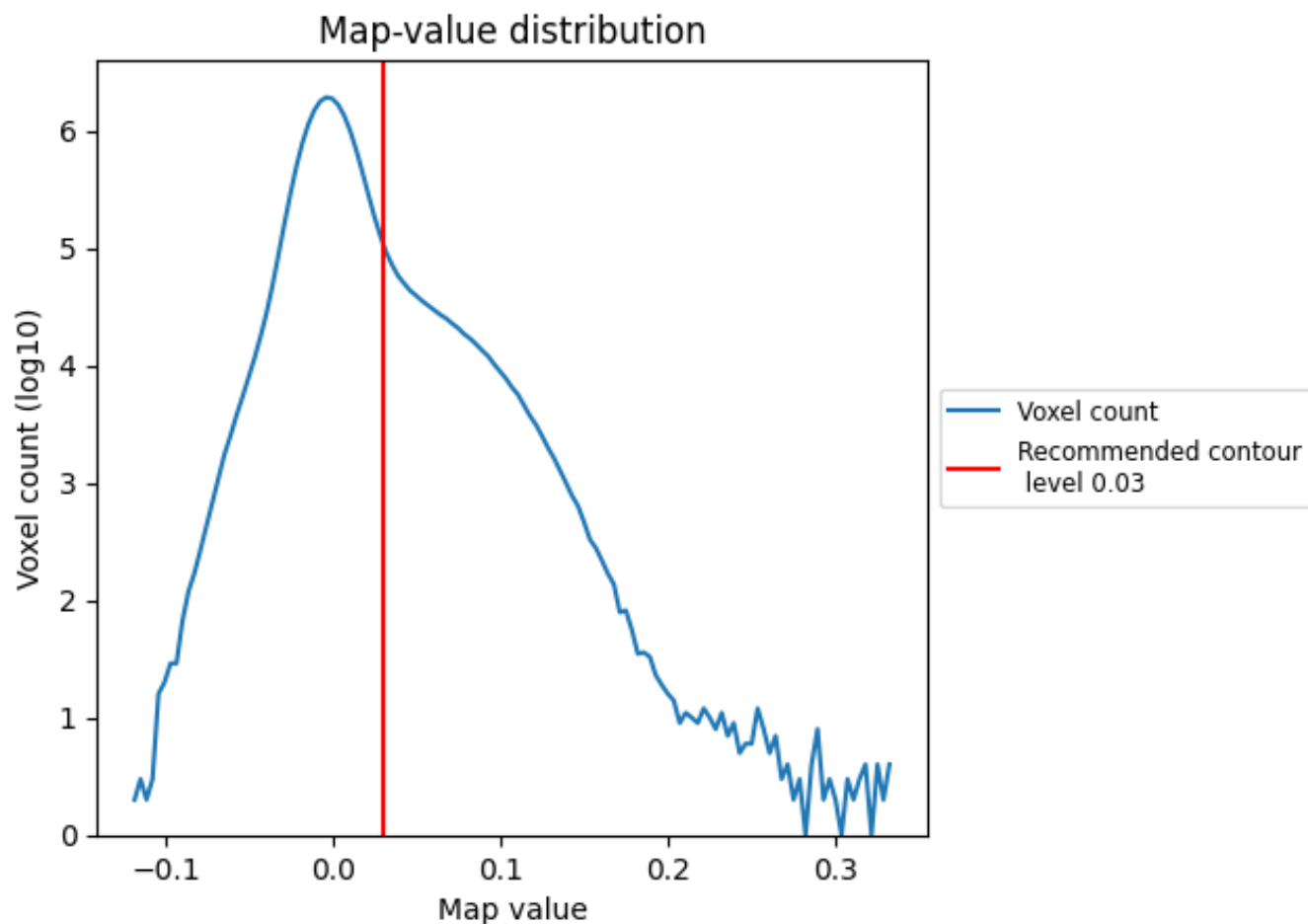
6.6 Mask visualisation

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

7 Map analysis [i](#)

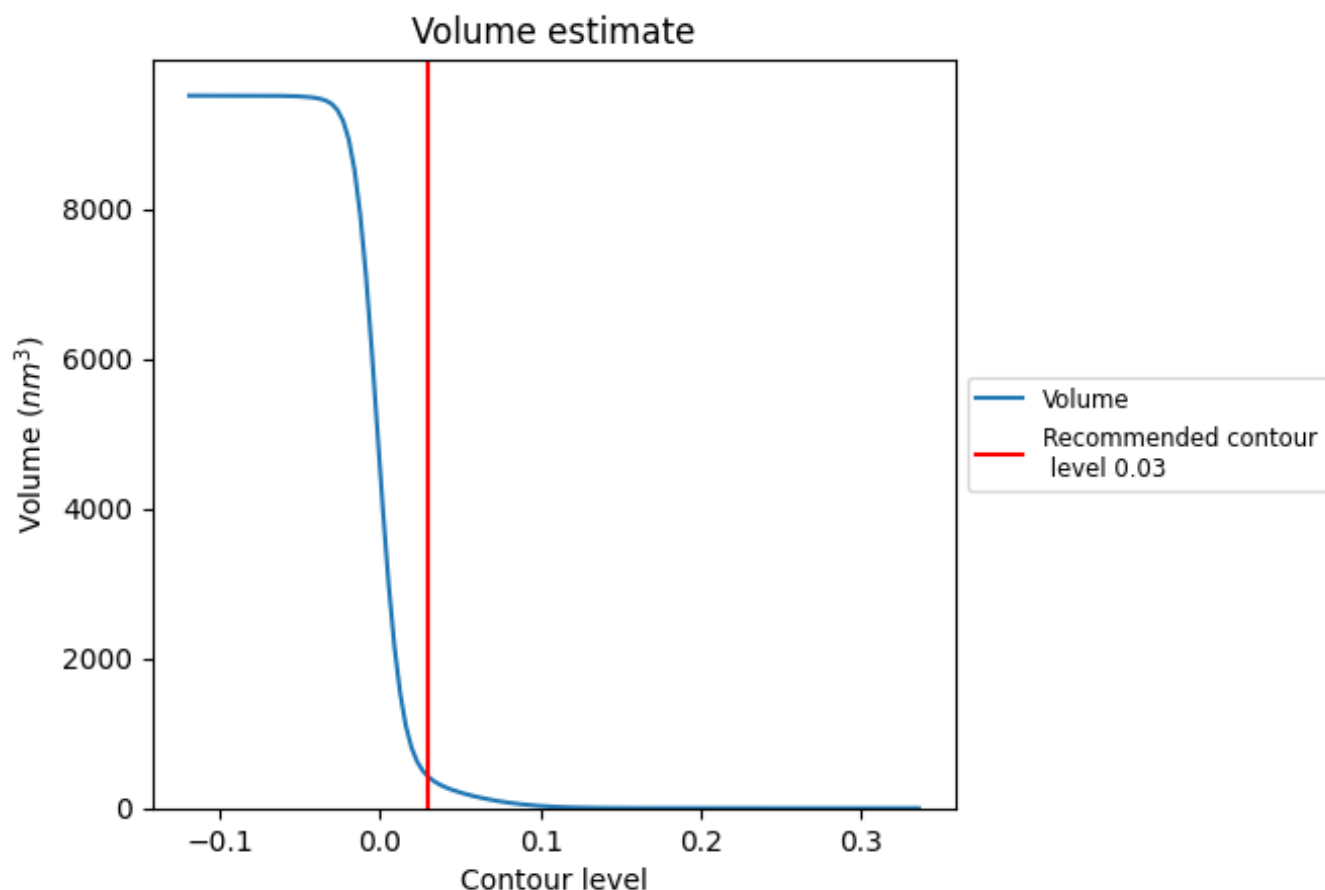
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate [i](#)



The volume at the recommended contour level is 422 nm^3 ; this corresponds to an approximate mass of 381 kDa.

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

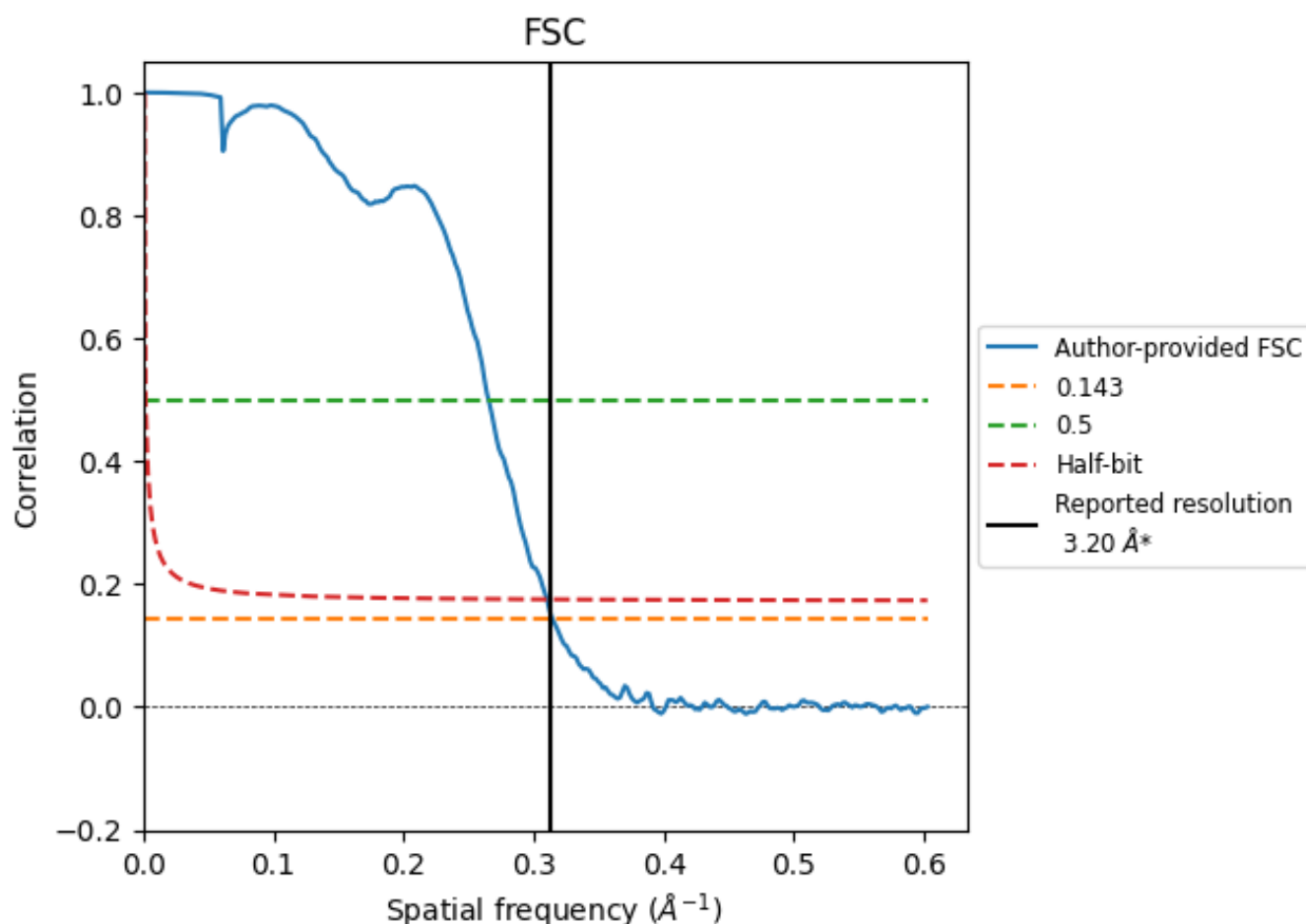
7.3 Rotationally averaged power spectrum [i](#)

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

8 Fourier-Shell correlation [i](#)

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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

8.2 Resolution estimates [i](#)

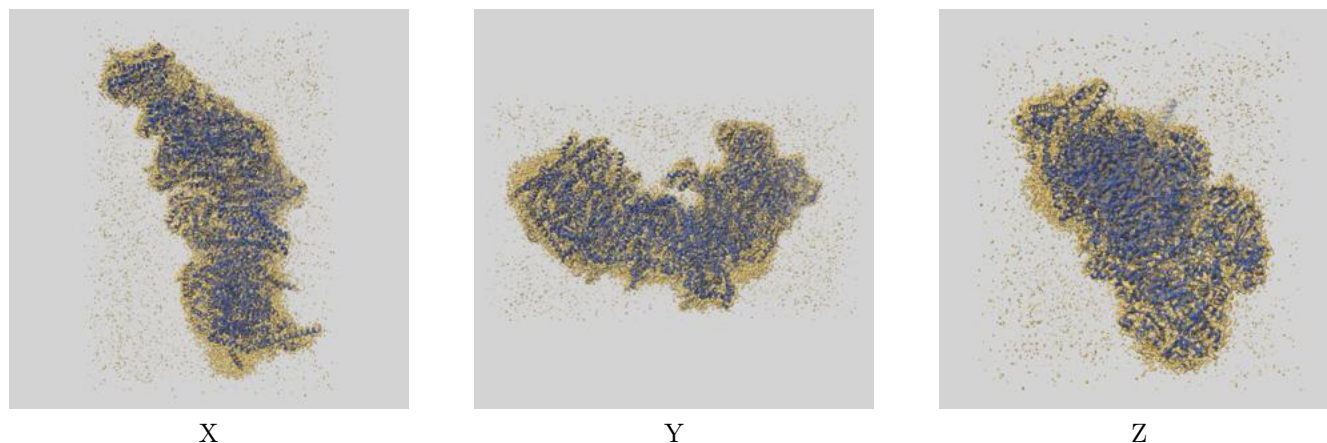
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.18	3.77	3.22
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

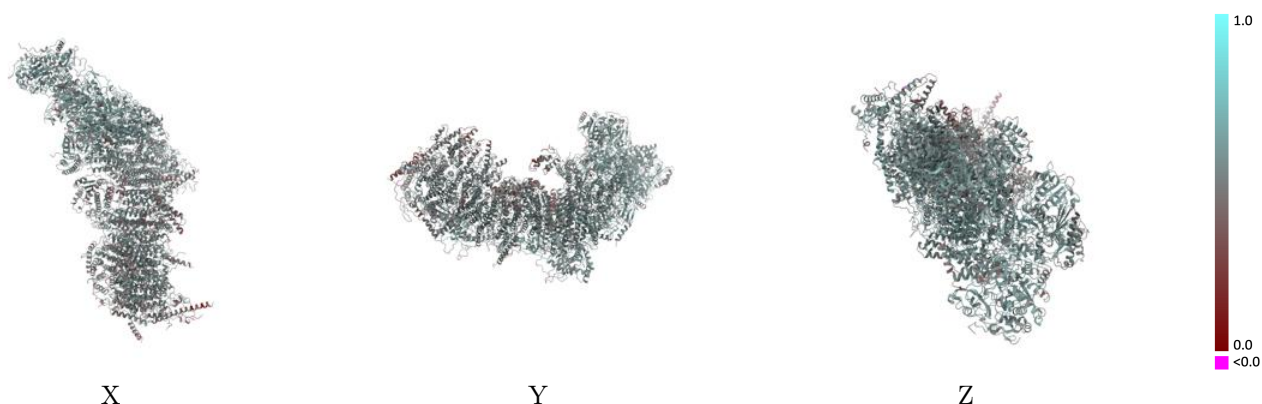
This section contains information regarding the fit between EMDB map EMD-11257 and PDB model 6ZKP. Per-residue inclusion information can be found in section 3 on page 20.

9.1 Map-model overlay [i](#)



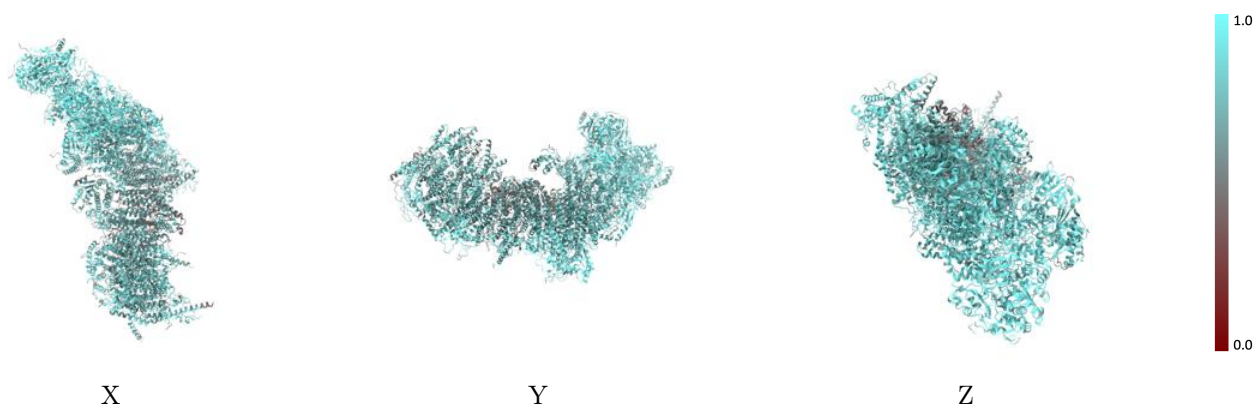
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



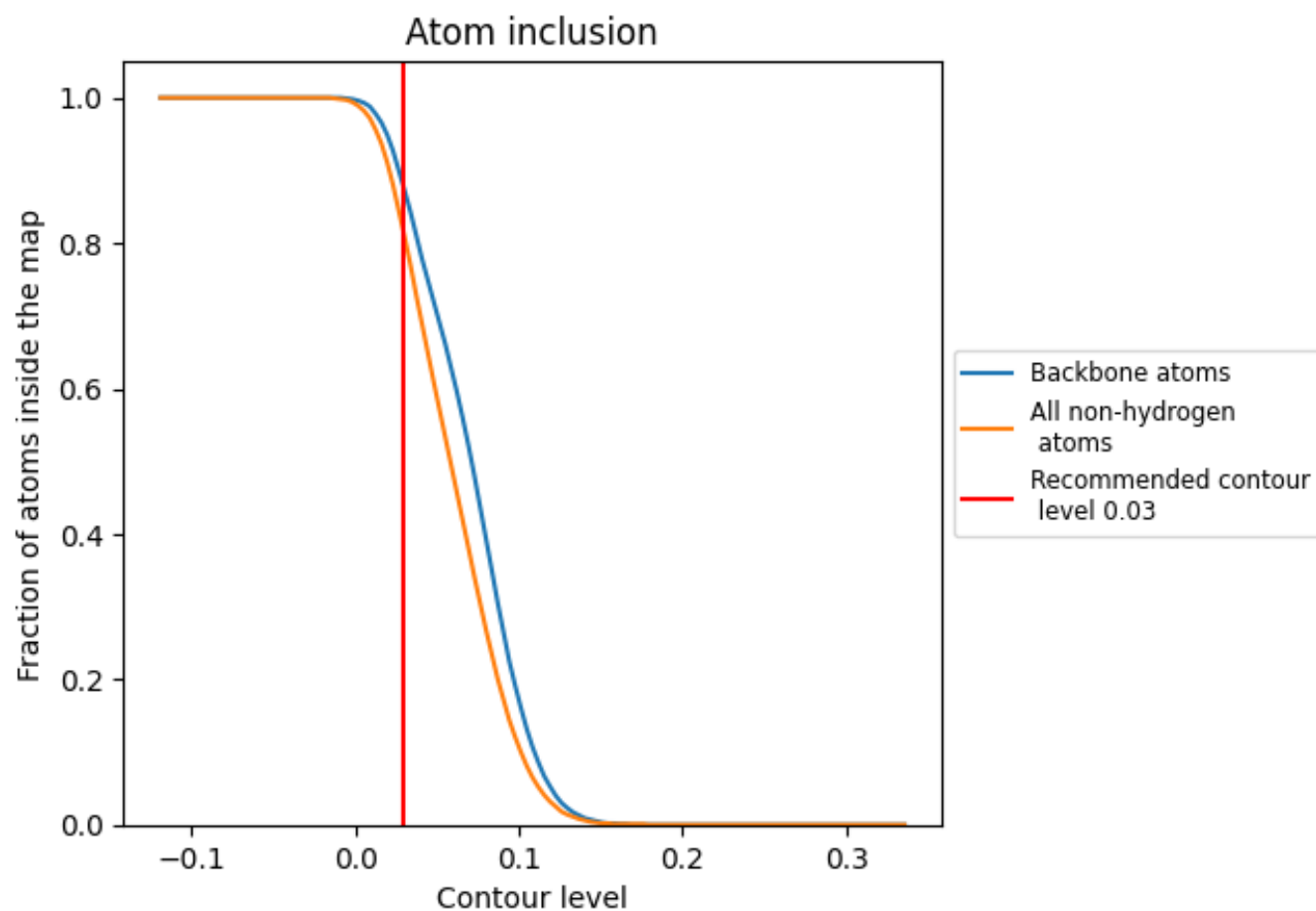
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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 (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 81% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8120	 0.5330
1	 0.8830	 0.5520
2	 0.8760	 0.5440
3	 0.8720	 0.5620
4	 0.8460	 0.5700
5	 0.8950	 0.5830
6	 0.8670	 0.5640
9	 0.8990	 0.5810
A	 0.6960	 0.5070
H	 0.8240	 0.5600
J	 0.7070	 0.5080
K	 0.7890	 0.5450
L	 0.7600	 0.5220
M	 0.8170	 0.5570
N	 0.8020	 0.5570
V	 0.5300	 0.4350
W	 0.7960	 0.5380
X	 0.7160	 0.4670
Y	 0.8550	 0.5340
Z	 0.7920	 0.5060
a	 0.8810	 0.5350
b	 0.8910	 0.5690
c	 0.8590	 0.5630
d	 0.8410	 0.5310
e	 0.8480	 0.5190
f	 0.8260	 0.5370
g	 0.8300	 0.5480
h	 0.8630	 0.5670
i	 0.8650	 0.5630
j	 0.6930	 0.4170
k	 0.7850	 0.5080
l	 0.8050	 0.5210
m	 0.8290	 0.5270
n	 0.7330	 0.4440
o	 0.7780	 0.5260



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Chain	Atom inclusion	Q-score
p	 0.7200	 0.4800
q	 0.8590	 0.5500
r	 0.7600	 0.4760
s	 0.7500	 0.4450
t	 0.7720	 0.4750
u	 0.7880	 0.4660
v	 0.7730	 0.5020
w	 0.7770	 0.5070
x	 0.7890	 0.5100
y	 0.7250	 0.5000
z	 0.8610	 0.5480