



Full wwPDB EM Validation Report ⓘ

Dec 17, 2022 – 08:46 am GMT

PDB ID : 6ZKC
EMDB ID : EMD-11244
Title : Complex I during turnover, closed
Authors : Kampjut, D.; Sazanov, L.A.
Deposited on : 2020-06-30
Resolution : 3.10 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.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

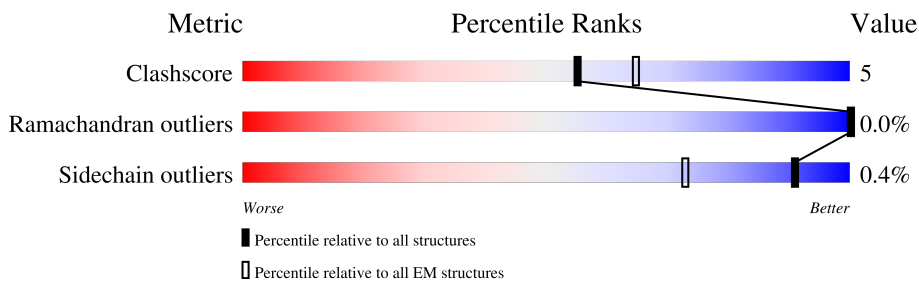
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	
2	2	246	
3	3	727	
4	4	463	
5	5	266	
6	6	223	
7	9	217	
8	A	115	

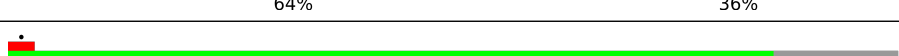
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Mol	Chain	Length	Quality of chain
9	H	318	80% 20%
10	J	175	79% 21%
11	K	98	78% 21%
12	L	606	86% 14%
13	M	459	86% 14%
14	N	347	86% 14%
15	V	141	88% 11%
16	W	189	69% 5% 26%
17	X	157	52% 45%
17	j	157	52% 48%
18	Y	172	92% 8%
19	Z	175	90% 7%
20	a	109	40% 60%
21	b	124	77% 23%
22	c	170	74% 26%
23	d	380	88% 11%
24	e	99	87% 13%
25	f	116	97%
26	g	140	81% 19%
27	h	114	83% 16%
28	i	145	100%
29	k	355	90% 10%
30	l	106	99%
31	m	84	94% 5%
32	n	98	81% 19%

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Mol	Chain	Length	Quality of chain
33	o	122	 98%
34	p	130	 98%
35	q	144	 96%
36	r	128	 77% 23%
37	s	137	 88% 11%
38	t	179	 98%
39	u	108	 60% 40%
40	v	186	 83% 17%
41	w	154	 66% 34%
42	x	76	 64% 36%
43	y	58	 86% 14%
44	z	70	 100%

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	501	-	-	X	-
53	CDL	L	1004	X	-	-	-
53	CDL	L	1005	X	-	-	-
53	CDL	M	503	X	-	-	-
53	CDL	x	101	X	-	-	-

2 Entry composition [i](#)

There are 58 unique types of molecules in this entry. The entry contains 67967 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
			Total	C	N	O	S		
1	1	430	3312	2086	593	613	20	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	4	430	3457	2207	594	631	25	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
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
			Total	C	N	O	S		
8	A	115	Total	C	N	O	S	0	0
			922	621	133	161	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	H	318	Total	C	N	O	S	0	0
			2528	1704	384	421	19		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	175	Total	C	N	O	S	0	0
			1344	904	192	235	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
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
			Total	C	N	O	S		
12	L	606	Total	C	N	O	S	0	0
			4807	3188	746	829	44		

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

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

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

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

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

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

- Molecule 17 is a protein called Acyl carrier protein.

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	d	340	2748	1775	489	478	6	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

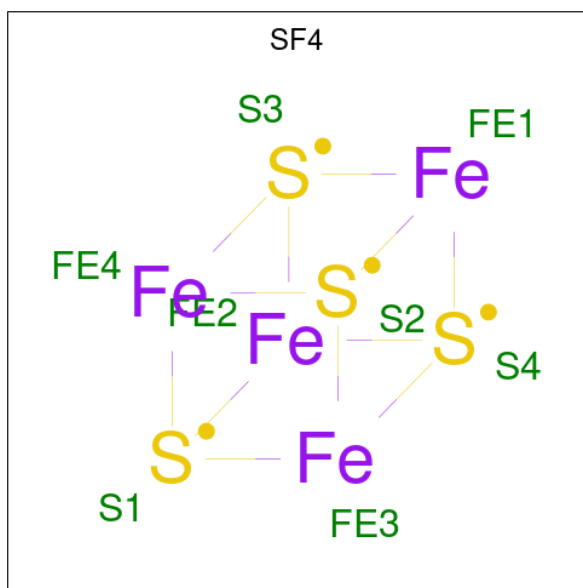
- Molecule 43 is a protein called Mitochondrial complex I, MNLL subunit.

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

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

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

- Molecule 45 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
45	1	1	8	4	4	0
45	3	1	16	8	8	0
45	3	1	16	8	8	0
45	6	1	8	4	4	0

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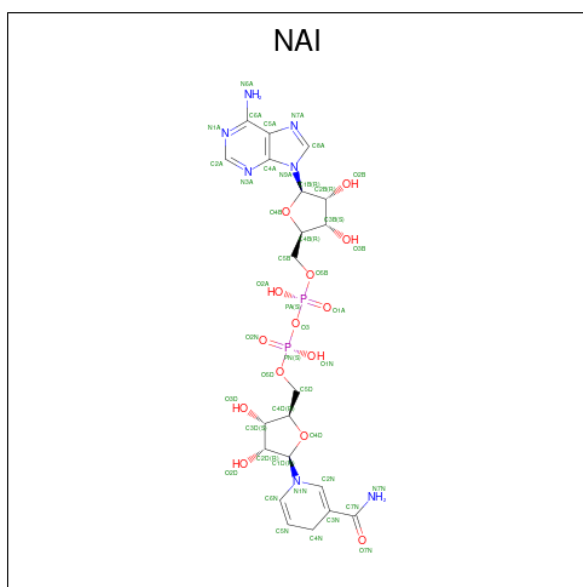
Mol	Chain	Residues	Atoms			AltConf
45	9	1	Total	Fe	S	0
			16	8	8	
45	9	1	Total	Fe	S	0
			16	8	8	

- Molecule 46 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C₁₇H₂₁N₄O₉P).



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

- Molecule 47 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: C₂₁H₂₉N₇O₁₄P₂).



Mol	Chain	Residues	Atoms				AltConf	
			Total	C	N	O		P
47	1	1	44	21	7	14	2	0

- Molecule 48 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).

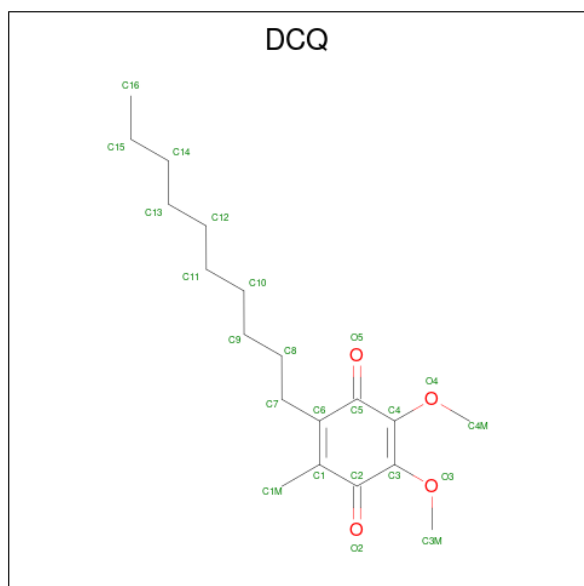


Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
48	2	1	4	2	2	0
48	3	1	4	2	2	0

- Molecule 49 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	AltConf
49	3	1	Total K 1 1	0

- Molecule 50 is 2-decyl-5,6-dimethoxy-3-methylcyclohexa-2,5-diene-1,4-dione (three-letter code: DCQ) (formula: C₁₉H₃₀O₄).



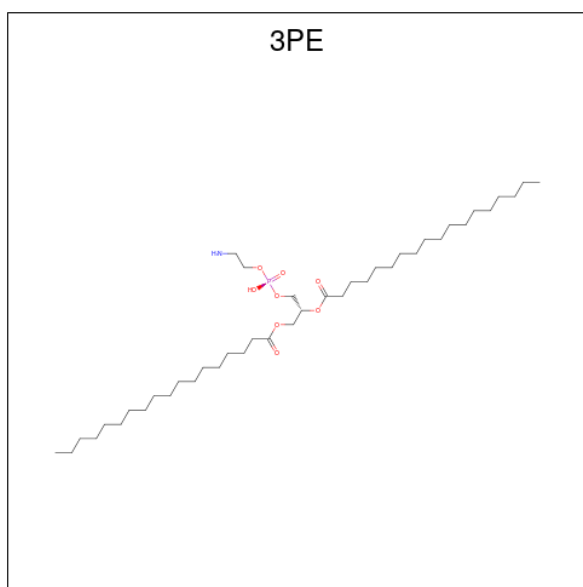
Mol	Chain	Residues	Atoms	AltConf
50	4	1	Total C O 23 19 4	0
50	H	1	Total C O 23 19 4	0

- Molecule 51 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: C₄₄H₈₈NO₈P).



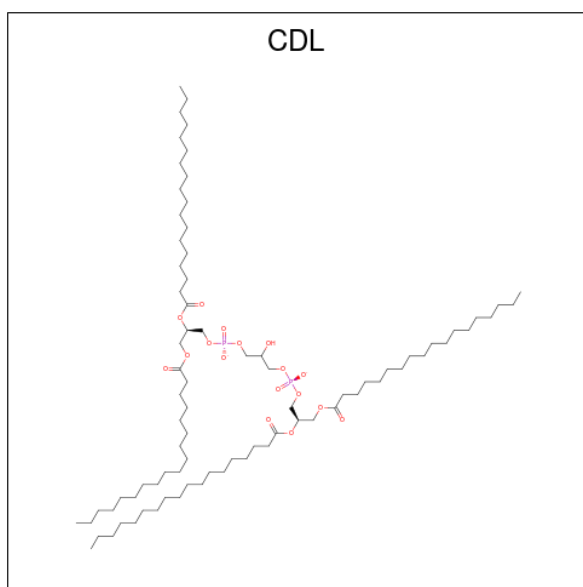
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
51	6	1	46	36	1	8	1	0
51	9	1	54	44	1	8	1	0
51	L	1	54	44	1	8	1	0
51	M	1	54	44	1	8	1	0
51	w	1	54	44	1	8	1	0

- Molecule 52 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOETHANOLAMINE (three-letter code: 3PE) (formula: C₄₁H₈₂NO₈P).



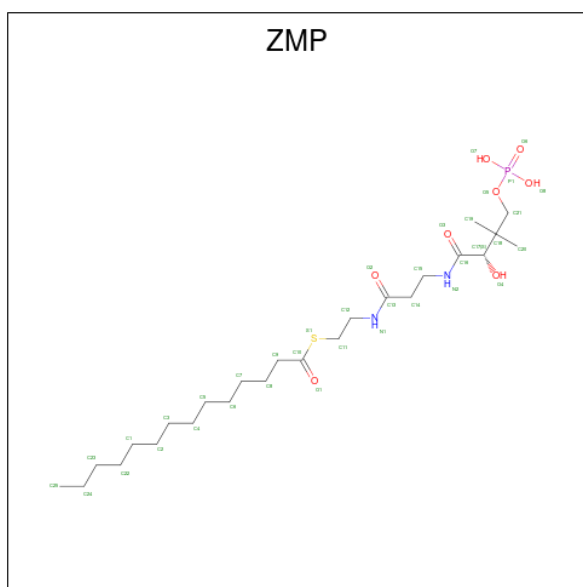
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
52	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
52	J	1	Total	C	N	O	P	0
			91	71	2	16	2	
52	J	1	Total	C	N	O	P	0
			91	71	2	16	2	
52	L	1	Total	C	N	O	P	0
			82	62	2	16	2	
52	L	1	Total	C	N	O	P	0
			82	62	2	16	2	
52	M	1	Total	C	N	O	P	0
			44	34	1	8	1	
52	N	1	Total	C	N	O	P	0
			91	71	2	16	2	
52	N	1	Total	C	N	O	P	0
			91	71	2	16	2	
52	V	1	Total	C	N	O	P	0
			37	27	1	8	1	
52	i	1	Total	C	N	O	P	0
			102	82	2	16	2	
52	i	1	Total	C	N	O	P	0
			102	82	2	16	2	
52	o	1	Total	C	N	O	P	0
			31	21	1	8	1	
52	p	1	Total	C	O	P		0
			27	18	8	1		

- Molecule 53 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
53	L	1	Total 185	C 147	O 34	P 4	0
53	L	1	Total 185	C 147	O 34	P 4	0
53	M	1	Total 100	C 81	O 17	P 2	0
53	V	1	Total 94	C 75	O 17	P 2	0
53	W	1	Total 100	C 81	O 17	P 2	0
53	h	1	Total 58	C 39	O 17	P 2	0
53	o	1	Total 90	C 71	O 17	P 2	0
53	x	1	Total 75	C 56	O 17	P 2	0

- Molecule 54 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonoxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (three-letter code: ZMP) (formula: C₂₅H₄₉N₂O₈PS).

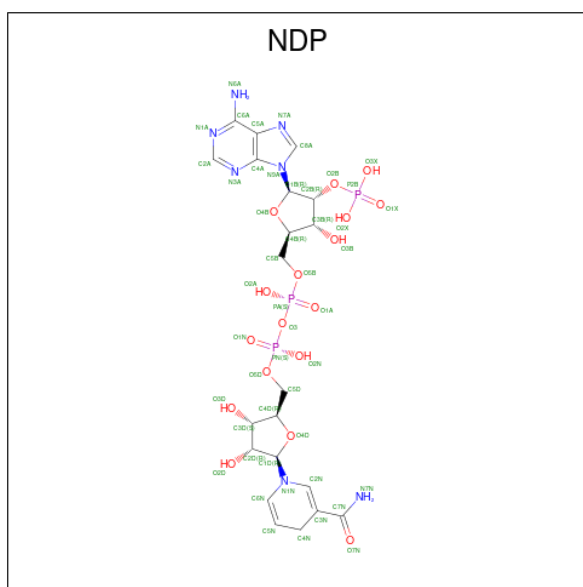


Mol	Chain	Residues	Atoms					AltConf	
			Total	C	N	O	P		S
54	X	1	31	20	2	7	1	1	0
54	g	1	34	23	2	7	1	1	0

- Molecule 55 is ZINC ION (three-letter code: ZN) (formula: Zn).

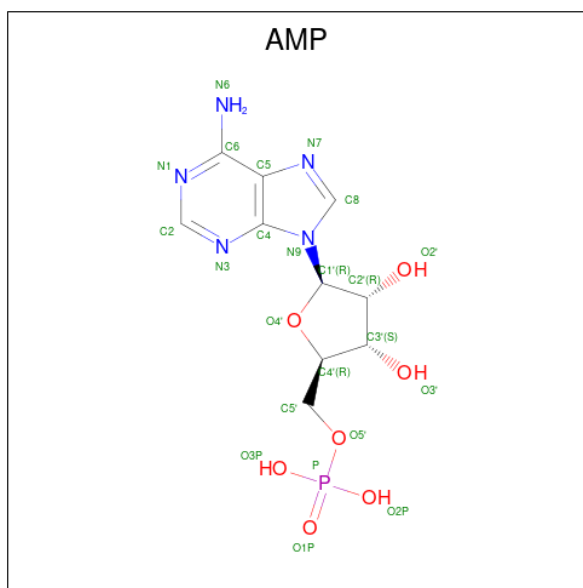
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
55	b	1	1	1	0

- Molecule 56 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



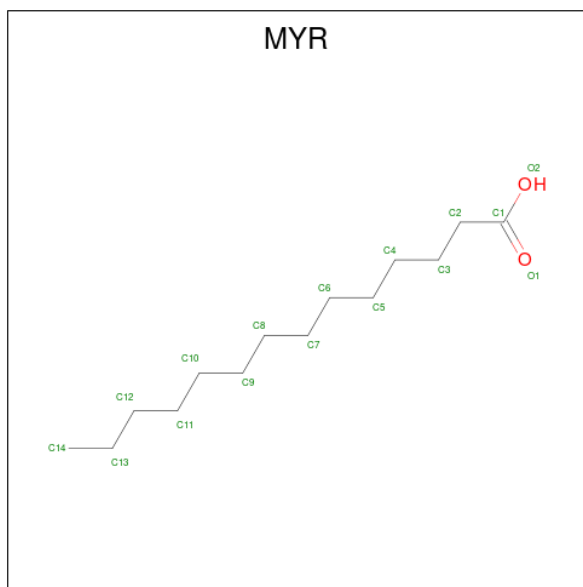
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
56	d	1	48	21	7	17	3	0

- Molecule 57 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



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

- Molecule 58 is MYRISTIC ACID (three-letter code: MYR) (formula: $C_{14}H_{28}O_2$).

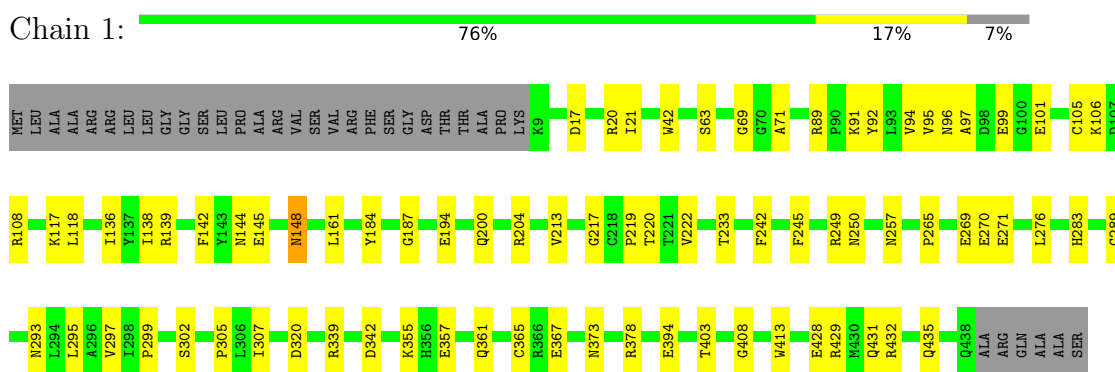


Mol	Chain	Residues	Atoms			AltConf
58	s	1	Total	C	O	0
			15	14	1	

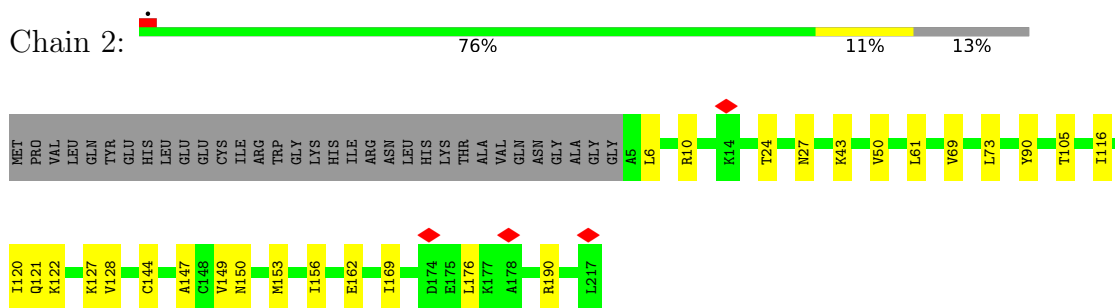
3 Residue-property plots [i](#)

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

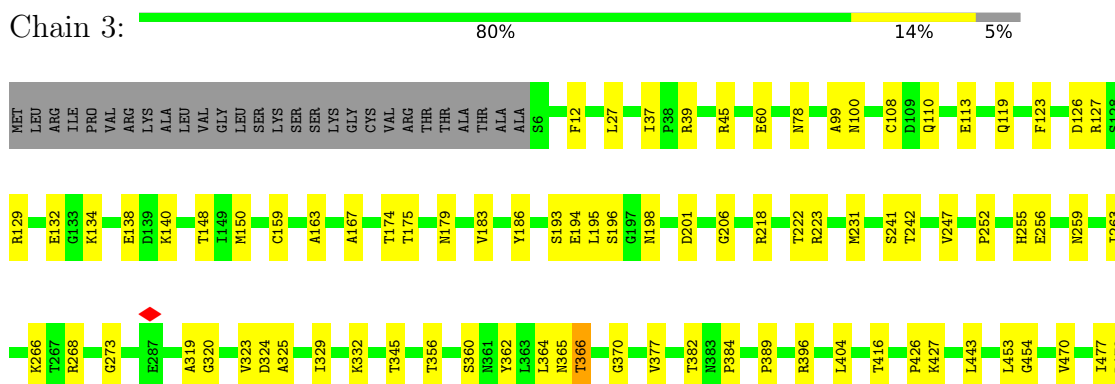
- Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



- Molecule 2: Mitochondrial complex I, 24 kDa subunit

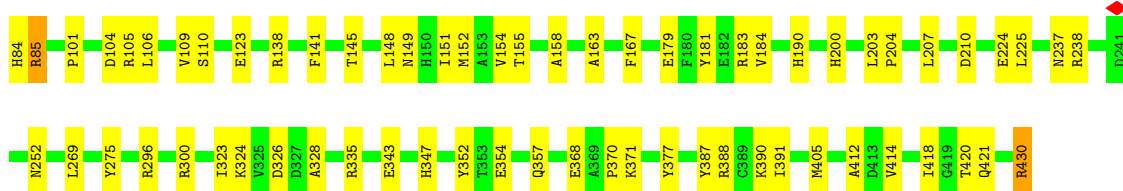
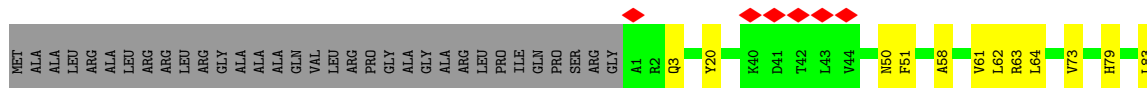
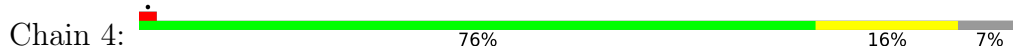


- Molecule 3: NADH:ubiquinone oxidoreductase core subunit S1

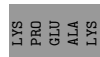
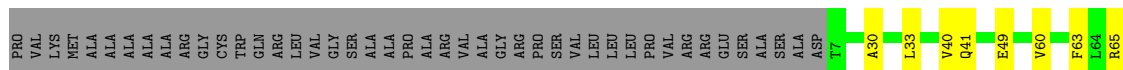




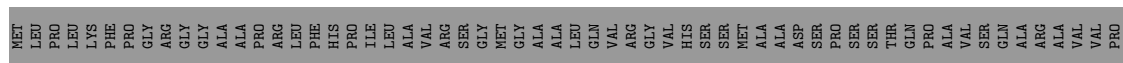
• Molecule 4: Mitochondrial complex I, 49 kDa subunit



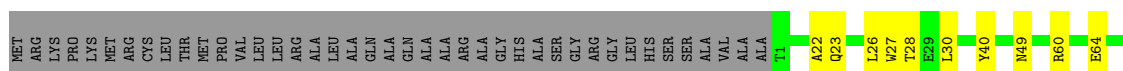
• Molecule 5: NADH:ubiquinone oxidoreductase core subunit S3




• Molecule 6: Mitochondrial complex I, PSST subunit

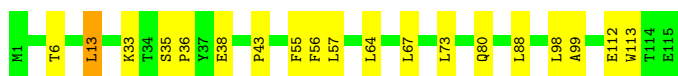


• Molecule 7: Mitochondrial complex I, TYKY subunit




- Molecule 8: NADH-ubiquinone oxidoreductase chain 3

Chain A:  83% 16%




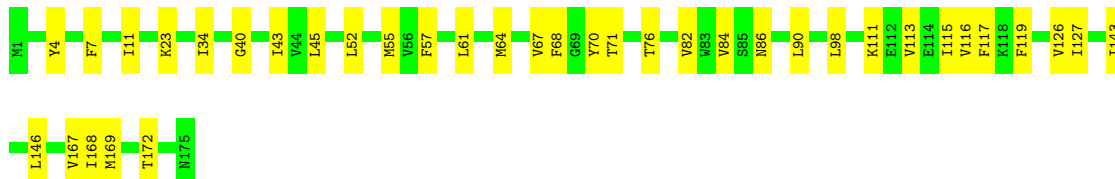
- Molecule 9: NADH-ubiquinone oxidoreductase chain 1

Chain H:  80% 20%




- Molecule 10: NADH-ubiquinone oxidoreductase chain 6

Chain J:  79% 21%




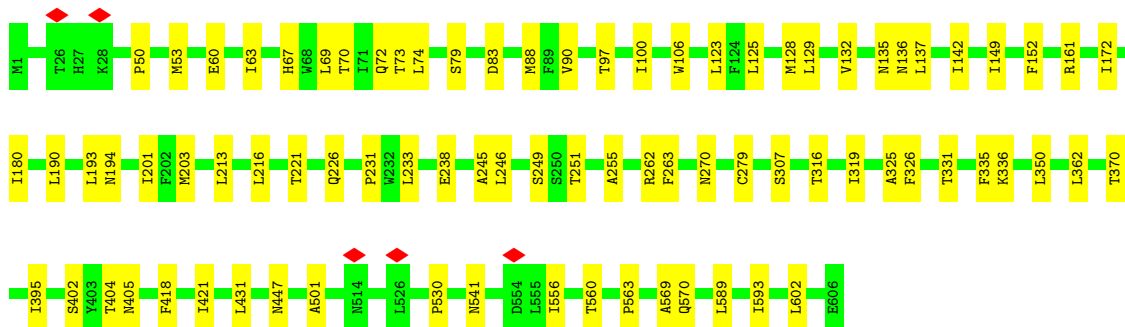
- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

Chain K:  78% 21%




- Molecule 12: NADH-ubiquinone oxidoreductase chain 5

Chain L:  86% 14%




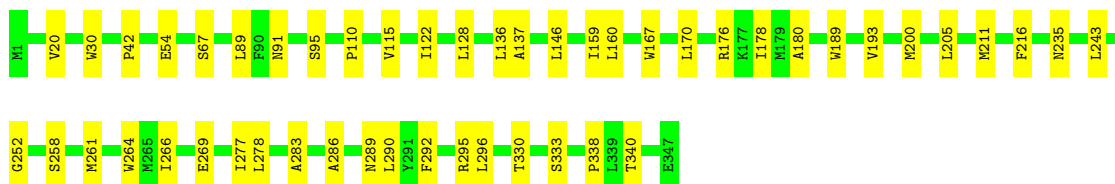
- Molecule 13: NADH-ubiquinone oxidoreductase chain 4

Chain M:  86% 14%




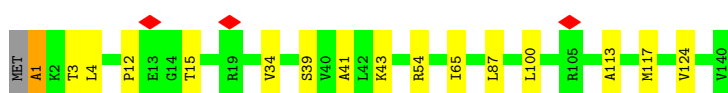
- Molecule 14: NADH-ubiquinone oxidoreductase chain 2

Chain N:  86% 14%



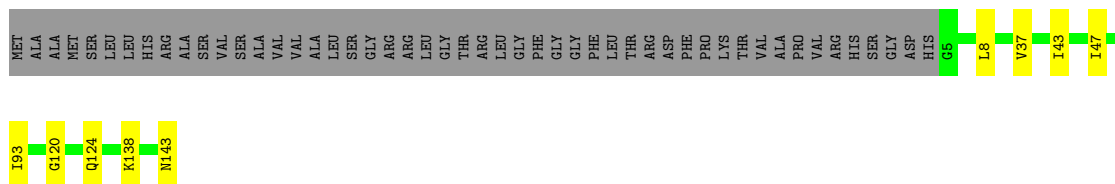
- Molecule 15: Mitochondrial complex I, B14.7 subunit

Chain V:  88% 11% ..



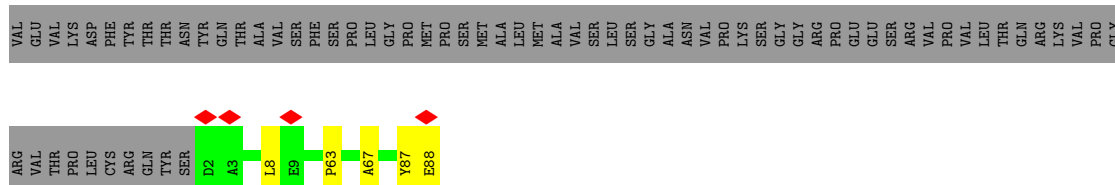
- Molecule 16: NADH:ubiquinone oxidoreductase subunit B5

Chain W:  69% 5% 26%



- Molecule 17: Acyl carrier protein

Chain X:  52% 45%




- Molecule 17: Acyl carrier protein

Chain j:  52% 48%

VAL
GLU
VAL
LYS
ASP
PHE
TYR
THR
THR
ASN
TYR
GLN
THR
ALA
VAL
SER
PHE
SER
PRO
LEU
GLY
MET
PRO
SER
MET
ALA
LEU
MET
ALA
VAL
SER
LEU
SER
GLY
ALA
ASN
VAL
PRO
LYS
SER
GLY
GLY
ARG
PRO
GLU
SER
SER
ARG
VAL
VAL
LEU
THR
GLN
LYS
VAL
PRO
GLY


ARG
VAL
THR
PRO
LEU
CYS
ARG
GLN
TYR
SER
ASP
ALA
PRO
F5
I6
E28
K38
D43
D56
E61
D85
V86
TYR
GLU

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

Chain Y:  92% 8%

MET
F1
E5
V17
K48
V19
H29
C35
M89
L44
V47
R53
M63
P119
V130
V153
W169
T170
M171

- Molecule 19: Mitochondrial complex I, PDSW subunit

Chain Z:  90% 7%

PRO
ASP
S3
W4
D5
V8
V47
I73
V81
M84
Q113
K136
D140
L155
R161
A172
A173
ALA
ALA


- Molecule 20: Mitochondrial complex I, 10 kDa subunit

Chain a:  40% 60%

MET
ALA
ALA
SER
VAL
LEU
LEU
ARG
GLN
GLY
ARG
PRO
GLY
THR
LEU
LYS
THR
VAL
LEU
LEU
GLU
ALA
GLY
PHE
ARG
GLY
LEU
ALA
ALA
VAL
VAL
LEU
LEU
SER
SER
GLY
LYS
LYS
LEU
PRO
PRO
ASN
PRO
LYS
LYS
GLN
SER
PRO
PRO
LYS
LYS
PRO
ALA
SER

ALA
ALA
PRO
THR
GLU
P32
H75

- Molecule 21: Mitochondrial complex I, 13 kDa subunit

Chain b:  77% 23%

MET
ALA
ALA
VAL
THR
PHE
LEU
ARG
LEU
LEU
GLY
ARG
GLY
GLY
ALA
VAL
THR
ARG
GLY
LEU
PRO
VAL
GLY
GLY
ALA
ARG
CYS
PHE
G1
H85
HIS

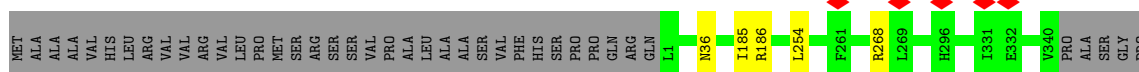
- Molecule 22: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain c:  74% 26%

MET
SER
VAL
VAL
LEU
ARG
GLN
ALA
LEU
TRP
GLY
ARG
VAL
GLY
THR
VAL
ALA
ALA
VAL
SER
SER
VAL
LYS
VAL
SER
THR
ARG
SER
LEU
LEU
SER
THR
SER
THR
TRP
ARG
LEU
ALA
GLN
ASP
GLN
THR
ASP
T8
E15
K133

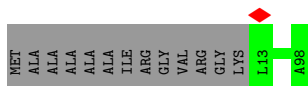
- Molecule 23: NADH:ubiquinone oxidoreductase subunit A9

Chain d: 88% 11%



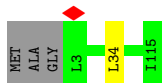
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain e: 87% 13%



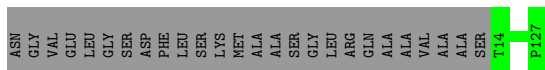
- Molecule 25: Mitochondrial complex I, B13 subunit

Chain f: 97% ..



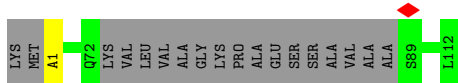
- Molecule 26: NADH:ubiquinone oxidoreductase subunit A6

Chain g: 81% 19%



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

Chain h: 83% 16%



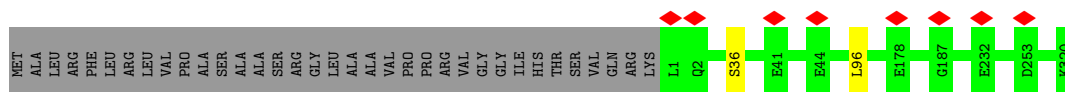
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain i: 100%

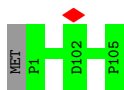


- Molecule 29: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

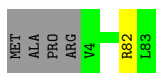
Chain k: 90% 10%



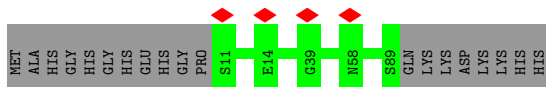
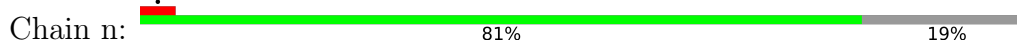
- Molecule 30: NADH:ubiquinone oxidoreductase subunit S5



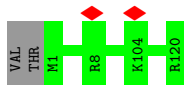
- Molecule 31: NADH:ubiquinone oxidoreductase subunit A3



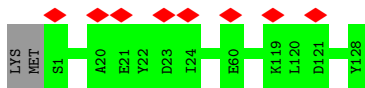
- Molecule 32: NADH:ubiquinone oxidoreductase subunit B3



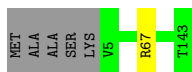
- Molecule 33: NADH dehydrogenase [ubiquinone] 1 subunit C2



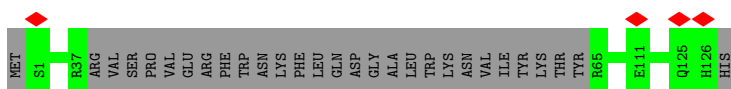
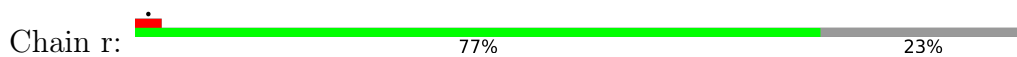
- Molecule 34: NADH:ubiquinone oxidoreductase subunit B4



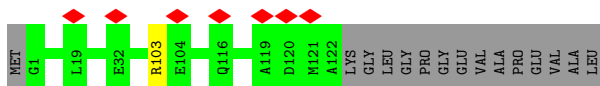
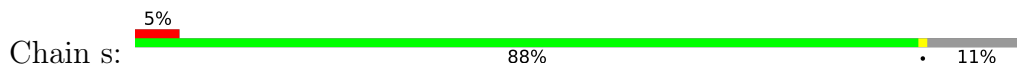
- Molecule 35: Mitochondrial complex I, B16.6 subunit



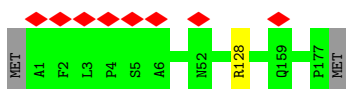
- Molecule 36: Mitochondrial complex I, B17 subunit



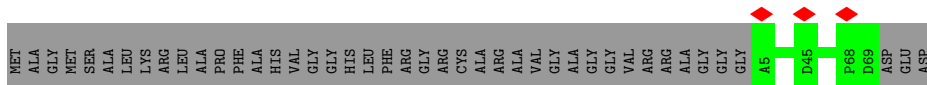
- Molecule 37: NADH:ubiquinone oxidoreductase subunit B7



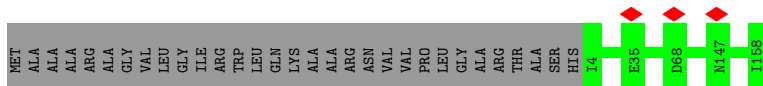
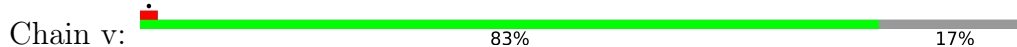
- Molecule 38: NADH:ubiquinone oxidoreductase subunit B9



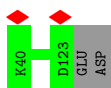
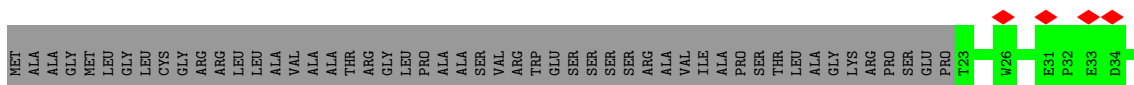
- Molecule 39: NADH:ubiquinone oxidoreductase subunit B2



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

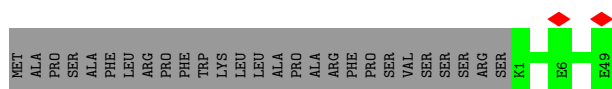


- Molecule 41: Mitochondrial complex I, ESSS subunit




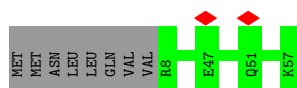
- Molecule 42: Mitochondrial complex I, KFYI subunit

Chain x:  64% 36%



- Molecule 43: Mitochondrial complex I, MNLL subunit

Chain y:  86% 14%



- Molecule 44: Mitochondrial complex I, MWFE subunit

Chain z:  100%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	15769	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	0.447	Depositor
Minimum map value	-0.150	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.029	Depositor
Recommended contour level	0.045	Depositor
Map size (Å)	170.821, 193.102, 283.287	wwPDB
Map dimensions	267, 182, 161	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.061, 1.061, 1.061	Depositor

5 Model quality i

5.1 Standard geometry i

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

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	0.37	0/3386	0.56	0/4575
2	2	0.34	0/1695	0.55	0/2306
3	3	0.37	1/5362 (0.0%)	0.55	0/7266
4	4	0.42	0/3535	0.57	0/4791
5	5	0.38	0/1776	0.55	0/2417
6	6	0.46	0/1278	0.56	1/1728 (0.1%)
7	9	0.45	0/1445	0.58	0/1956
8	A	0.37	0/947	0.63	1/1296 (0.1%)
9	H	0.40	0/2603	0.67	1/3561 (0.0%)
10	J	0.40	0/1378	0.64	2/1868 (0.1%)
11	K	0.35	0/749	0.63	1/1014 (0.1%)
12	L	0.34	0/4925	0.56	0/6700
13	M	0.35	0/3731	0.60	1/5085 (0.0%)
14	N	0.37	0/2787	0.58	1/3795 (0.0%)
15	V	0.29	0/1041	0.51	1/1412 (0.1%)
16	W	0.34	0/1188	0.50	0/1607
17	X	0.29	0/713	0.51	0/963
17	j	0.30	0/670	0.51	0/902
18	Y	0.35	0/1440	0.53	0/1942
19	Z	0.33	0/1475	0.48	0/1989
20	a	0.28	0/383	0.46	0/518
21	b	0.36	0/749	0.48	0/1009
22	c	0.35	0/1047	0.51	0/1415
23	d	0.35	0/2824	0.55	1/3830 (0.0%)
24	e	0.30	0/702	0.52	0/945
25	f	0.32	0/937	0.53	1/1271 (0.1%)
26	g	0.34	0/993	0.51	0/1336
27	h	0.34	0/779	0.53	0/1053
28	i	0.36	0/1250	0.49	0/1698
29	k	0.34	0/2646	0.51	1/3579 (0.0%)
30	l	0.35	0/896	0.51	0/1200

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	m	0.29	0/647	0.46	0/890
32	n	0.31	0/653	0.45	0/882
33	o	0.34	0/1035	0.49	0/1398
34	p	0.29	0/1085	0.48	0/1467
35	q	0.34	0/1171	0.50	0/1579
36	r	0.32	0/874	0.53	0/1188
37	s	0.30	0/1072	0.48	0/1436
38	t	0.33	0/1573	0.48	0/2130
39	u	0.29	0/590	0.46	0/810
40	v	0.31	0/1361	0.50	0/1861
41	w	0.33	0/872	0.52	0/1185
42	x	0.29	0/425	0.40	0/576
43	y	0.28	0/449	0.49	0/605
44	z	0.41	0/591	0.54	0/795
All	All	0.35	1/67728 (0.0%)	0.55	12/91829 (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
10	J	0	2
All	All	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3	159	CYS	CB-SG	-5.45	1.73	1.81

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	146	LEU	CA-CB-CG	6.03	129.17	115.30
6	6	59	MET	CA-CB-CG	5.91	123.34	113.30
23	d	254	LEU	CA-CB-CG	5.78	128.59	115.30
11	K	20	LEU	CA-CB-CG	5.62	128.22	115.30
15	V	87	LEU	CA-CB-CG	5.53	128.02	115.30
14	N	146	LEU	CA-CB-CG	5.52	128.00	115.30
29	k	96	LEU	CA-CB-CG	5.39	127.70	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	H	91	MET	C-N-CD	-5.20	109.16	120.60
25	f	34	LEU	CA-CB-CG	5.19	127.24	115.30
13	M	458	LEU	CA-CB-CG	5.16	127.16	115.30
8	A	13	LEU	CA-CB-CG	5.02	126.85	115.30
10	J	98	LEU	CA-CB-CG	5.01	126.81	115.30

There are no chirality outliers.

All (5) 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
10	J	115	ILE	Peptide
10	J	82	VAL	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	47	0
2	2	1655	0	1668	18	0
3	3	5275	0	5300	63	0
4	4	3457	0	3397	56	0
5	5	1726	0	1676	23	0
6	6	1247	0	1259	19	0
7	9	1414	0	1371	21	0
8	A	922	0	953	19	0
9	H	2528	0	2641	45	0
10	J	1344	0	1364	23	0
11	K	749	0	793	17	0
12	L	4807	0	4949	50	0
13	M	3647	0	3849	43	0
14	N	2723	0	2930	30	0
15	V	1028	0	1036	11	0
16	W	1155	0	1177	6	0
17	X	701	0	692	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	j	660	0	663	0	0
18	Y	1403	0	1392	6	0
19	Z	1441	0	1419	8	0
20	a	371	0	344	0	0
21	b	737	0	710	0	0
22	c	1024	0	1023	0	0
23	d	2748	0	2763	0	0
24	e	691	0	706	0	0
25	f	917	0	958	0	0
26	g	969	0	980	0	0
27	h	769	0	780	0	0
28	i	1209	0	1182	0	0
29	k	2596	0	2559	0	0
30	l	874	0	869	0	0
31	m	626	0	635	0	0
32	n	634	0	616	0	0
33	o	1004	0	995	0	0
34	p	1059	0	1062	0	0
35	q	1142	0	1137	0	0
36	r	846	0	864	0	0
37	s	1047	0	1013	0	0
38	t	1520	0	1477	0	0
39	u	563	0	509	0	0
40	v	1307	0	1207	0	0
41	w	846	0	792	0	0
42	x	412	0	411	0	0
43	y	436	0	437	0	0
44	z	576	0	570	0	0
45	1	8	0	0	2	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	0	0
47	1	44	0	27	3	0
48	2	4	0	0	1	0
48	3	4	0	0	0	0
49	3	1	0	0	0	0
50	4	23	0	30	1	0
50	H	23	0	30	2	0
51	6	46	0	69	1	0
51	9	54	0	88	1	0
51	L	54	0	88	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	M	54	0	88	3	0
51	w	54	0	88	0	0
52	A	51	0	82	3	0
52	J	91	0	136	6	0
52	L	82	0	118	1	0
52	M	44	0	65	0	0
52	N	91	0	136	1	0
52	V	37	0	48	2	0
52	i	102	0	164	0	0
52	o	31	0	36	0	0
52	p	27	0	27	0	0
53	L	185	0	276	9	0
53	M	100	0	156	9	0
53	V	94	0	141	6	0
53	W	100	0	156	3	0
53	h	58	0	60	0	0
53	o	90	0	133	0	0
53	x	75	0	97	0	0
54	X	31	0	34	1	0
54	g	34	0	40	0	0
55	b	1	0	0	0	0
56	d	48	0	26	0	0
57	k	23	0	12	0	0
58	s	15	0	27	0	0
All	All	67967	0	68894	457	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 (457) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:81:ARG:NH1	8:A:33:LYS:O	2.22	0.73
6:6:171:LYS:HG2	6:6:174:ARG:HH11	1.59	0.67
7:9:92:ILE:HG12	7:9:111:ILE:HG12	1.79	0.64
12:L:123:LEU:HD13	53:L:1005:CDL:H712	1.79	0.64
1:1:101:GLU:HB2	47:1:503:NAI:H42N	1.81	0.63
3:3:175:THR:HG21	3:3:186:TYR:HB2	1.80	0.63
4:4:405:MET:SD	4:4:421:GLN:NE2	2.72	0.62
52:J:201:3PE:H2F2	52:J:201:3PE:H371	1.81	0.62
14:N:243:LEU:HD22	14:N:330:THR:HG21	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:L:1005:CDL:H642	53:L:1005:CDL:H562	1.81	0.62
12:L:100:ILE:HG21	12:L:246:LEU:HB2	1.82	0.61
12:L:370:THR:HG23	12:L:431:LEU:HD13	1.82	0.61
5:5:129:TRP:O	5:5:132:ARG:HB3	2.00	0.61
3:3:360:SER:O	3:3:365:ASN:ND2	2.33	0.61
4:4:190:HIS:HD2	6:6:150:PRO:HD3	1.65	0.60
13:M:231:LEU:HA	13:M:235:LEU:HB2	1.81	0.60
1:1:355:LYS:HD3	1:1:373:ASN:HD22	1.65	0.60
11:K:64:LEU:O	11:K:67:ALA:HB3	2.02	0.60
3:3:252:PRO:HG3	3:3:263:ILE:HG12	1.83	0.60
12:L:221:THR:HG23	12:L:226:GLN:HB2	1.81	0.59
4:4:51:PHE:HB3	4:4:64:LEU:HB2	1.84	0.59
9:H:169:GLN:NE2	9:H:241:LEU:O	2.35	0.59
4:4:58:ALA:HB1	4:4:62:LEU:HB3	1.83	0.59
4:4:101:PRO:O	4:4:105:ARG:NH1	2.36	0.59
5:5:151:ILE:HG23	5:5:152:LEU:HG	1.84	0.59
1:1:21:ILE:O	1:1:117:LYS:NZ	2.36	0.59
3:3:194:GLU:HG3	3:3:389:PRO:HB3	1.85	0.58
6:6:81:ARG:NH2	8:A:35:SER:O	2.36	0.58
15:V:39:SER:OG	15:V:54:ARG:NH2	2.36	0.58
12:L:73:THR:HB	12:L:194:ASN:HD21	1.68	0.58
4:4:63:ARG:HB3	4:4:79:HIS:HB2	1.86	0.58
4:4:343:GLU:O	4:4:347:HIS:ND1	2.33	0.58
12:L:106:TRP:HD1	12:L:447:ASN:HD22	1.52	0.58
9:H:20:LEU:HD21	9:H:231:ILE:HD11	1.85	0.58
12:L:233:LEU:HD23	12:L:307:SER:HB3	1.85	0.58
14:N:30:TRP:NE1	14:N:67:SER:OG	2.36	0.58
18:Y:29:HIS:HB3	18:Y:119:PRO:HD2	1.84	0.58
2:2:150:ASN:HB3	2:2:162:GLU:HB3	1.84	0.58
4:4:269:LEU:HB2	4:4:368:GLU:HB2	1.86	0.58
3:3:319:ALA:HB3	3:3:345:THR:HG22	1.86	0.57
8:A:67:LEU:HD11	11:K:68:ALA:HB3	1.87	0.57
10:J:117:PHE:HE1	14:N:91:ASN:HD21	1.52	0.57
4:4:179:GLU:OE2	6:6:66:ARG:NH1	2.34	0.57
52:J:202:3PE:H11	11:K:23:ARG:HG2	1.87	0.57
18:Y:35:CYS:O	18:Y:39:ASN:ND2	2.38	0.56
12:L:231:PRO:HB3	12:L:530:PRO:HG3	1.87	0.56
53:L:1004:CDL:H141	15:V:100:LEU:HD11	1.87	0.56
14:N:159:ILE:HG21	14:N:278:LEU:HD11	1.87	0.56
4:4:20:TYR:OH	14:N:295:ARG:NH2	2.38	0.56
4:4:184:VAL:O	7:9:60:ARG:NH1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:77:ARG:HH21	50:H:501:DCQ:H4MA	1.71	0.56
3:3:362:TYR:HA	3:3:492:ILE:HD12	1.87	0.56
3:3:453:LEU:HD13	3:3:470:VAL:HG21	1.87	0.56
1:1:342:ASP:OD1	1:1:429:ARG:NH2	2.37	0.56
52:A:201:3PE:H381	9:H:295:PRO:HB3	1.87	0.56
53:L:1005:CDL:H542	53:L:1005:CDL:H722	1.87	0.56
1:1:200:GLN:NE2	3:3:174:THR:O	2.39	0.56
7:9:69:ARG:NH1	7:9:73:GLY:O	2.39	0.56
10:J:67:VAL:HG11	11:K:31:LEU:HD21	1.86	0.56
13:M:243:MET:HB3	13:M:301:ILE:HG21	1.88	0.56
5:5:150:ARG:NH1	5:5:153:THR:OG1	2.38	0.55
1:1:89:ARG:NH1	1:1:217:GLY:O	2.39	0.55
12:L:316:THR:HA	12:L:319:ILE:HG12	1.88	0.55
9:H:114:TYR:OH	10:J:61:LEU:O	2.24	0.55
10:J:52:LEU:HD22	10:J:143:ILE:HD11	1.89	0.55
3:3:201:ASP:OD2	3:3:268:ARG:NH2	2.36	0.55
6:6:107:MET:O	6:6:111:ARG:NH1	2.40	0.54
8:A:112:GLU:OE2	9:H:291:LYS:NZ	2.40	0.54
3:3:332:LYS:NZ	3:3:505:LEU:O	2.38	0.54
4:4:352:TYR:HD1	7:9:86:VAL:HG21	1.71	0.54
5:5:74:SER:HB3	5:5:97:LEU:HB3	1.90	0.54
1:1:108:ARG:NH2	2:2:162:GLU:OE2	2.40	0.54
12:L:83:ASP:OD2	12:L:262:ARG:NH1	2.40	0.54
5:5:65:ARG:NH1	5:5:123:VAL:O	2.41	0.54
1:1:378:ARG:NE	3:3:132:GLU:OE2	2.41	0.54
5:5:33:LEU:HD13	5:5:60:VAL:HG22	1.88	0.54
9:H:24:GLU:HG2	9:H:271:LEU:HD22	1.89	0.54
9:H:111:LEU:HD22	10:J:57:PHE:HZ	1.73	0.54
6:6:118:SER:N	45:6:201:SF4:S4	2.81	0.54
10:J:126:VAL:HG23	10:J:127:ILE:HG23	1.90	0.54
13:M:126:LEU:HD21	13:M:153:THR:HG21	1.90	0.54
5:5:121:VAL:HG21	5:5:146:PRO:HD3	1.90	0.54
9:H:81:LEU:HA	9:H:84:THR:HG22	1.90	0.54
12:L:69:LEU:HD13	13:M:451:PRO:HG2	1.90	0.54
2:2:105:THR:OG1	48:2:300:FES:S2	2.67	0.53
7:9:145:GLU:HA	7:9:148:LEU:HD13	1.91	0.53
8:A:73:LEU:HD12	9:H:151:LEU:HD13	1.90	0.53
12:L:90:VAL:HG22	12:L:129:LEU:HD22	1.91	0.53
9:H:141:SER:HA	9:H:290:TRP:HE1	1.74	0.53
13:M:5:ILE:HG23	13:M:104:LEU:HD11	1.89	0.53
4:4:388:ARG:HG2	5:5:81:VAL:HG22	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:87:ILE:HD12	9:H:96:ILE:HD12	1.89	0.53
10:J:84:VAL:HG12	10:J:90:LEU:HD13	1.89	0.53
1:1:428:GLU:HA	1:1:431:GLN:HG2	1.91	0.53
4:4:149:ASN:HD21	4:4:371:LYS:HG3	1.74	0.53
9:H:120:GLY:HA3	9:H:132:ALA:HB2	1.89	0.53
12:L:421:ILE:HG12	12:L:501:ALA:HB2	1.90	0.53
1:1:139:ARG:NH2	2:2:144:CYS:O	2.32	0.53
2:2:10:ARG:NH2	3:3:138:GLU:OE2	2.42	0.53
12:L:142:ILE:HG12	13:M:370:PRO:HB2	1.90	0.53
7:9:64:GLU:OE1	7:9:136:ASN:ND2	2.42	0.53
5:5:77:ASP:OD2	5:5:79:THR:OG1	2.27	0.52
2:2:147:ALA:HB3	2:2:153:MET:HG2	1.91	0.52
4:4:335:ARG:NH2	7:9:129:ASP:OD1	2.43	0.52
9:H:184:MET:SD	9:H:297:THR:OG1	2.68	0.52
10:J:23:LYS:NZ	11:K:18:GLY:O	2.40	0.52
19:Z:5:ASP:HB3	19:Z:8:VAL:HG12	1.90	0.52
1:1:270:GLU:OE1	1:1:283:HIS:NE2	2.43	0.52
13:M:64:PRO:HB3	13:M:454:ILE:HG22	1.90	0.52
1:1:365:CYS:HB3	45:1:501:SF4:S3	2.48	0.52
3:3:193:SER:H	3:3:196:SER:HB3	1.75	0.52
8:A:57:LEU:HD21	10:J:169:MET:HG2	1.92	0.52
3:3:126:ASP:HB2	4:4:328:ALA:HB3	1.92	0.52
3:3:163:ALA:HA	3:3:167:ALA:HB3	1.91	0.52
1:1:213:VAL:HG13	1:1:217:GLY:HA2	1.92	0.51
1:1:289:GLY:HA3	1:1:293:ASN:HD22	1.75	0.51
3:3:443:LEU:HD13	3:3:477:ILE:HD11	1.91	0.51
4:4:3:GLN:NE2	13:M:135:ARG:O	2.42	0.51
14:N:160:LEU:HD21	53:V:202:CDL:H191	1.93	0.51
2:2:149:VAL:O	2:2:190:ARG:NH2	2.42	0.51
3:3:255:HIS:NE2	3:3:634:ASP:OD1	2.43	0.51
4:4:224:GLU:OE2	7:9:40:TYR:OH	2.22	0.51
53:M:503:CDL:H792	14:N:338:PRO:HG3	1.91	0.51
52:A:201:3PE:H2H1	52:A:201:3PE:H292	1.93	0.51
3:3:140:LYS:HD3	3:3:150:MET:HG3	1.93	0.51
4:4:50:ASN:HB3	8:A:38:GLU:HG3	1.92	0.51
4:4:145:THR:OG1	4:4:181:TYR:OH	2.28	0.51
51:9:401:PC1:H351	9:H:187:ILE:HD12	1.92	0.51
12:L:137:LEU:HD21	12:L:263:PHE:HZ	1.76	0.51
3:3:110:GLN:NE2	3:3:113:GLU:O	2.43	0.51
13:M:6:ILE:HG23	53:M:503:CDL:H202	1.92	0.51
12:L:97:THR:HG21	12:L:125:LEU:HD22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:W:120:GLY:O	16:W:124:GLN:NE2	2.42	0.51
5:5:96:LEU:HB2	5:5:105:ILE:HG22	1.91	0.50
14:N:115:VAL:HG12	14:N:180:ALA:HB1	1.93	0.50
3:3:499:GLN:HE21	3:3:503:LEU:HD11	1.76	0.50
9:H:165:LEU:HD21	9:H:241:LEU:HA	1.93	0.50
12:L:152:PHE:HB2	12:L:172:ILE:HD11	1.93	0.50
3:3:119:GLN:HB2	3:3:123:PHE:HD2	1.76	0.50
3:3:382:THR:HG23	3:3:384:PRO:HD3	1.94	0.50
5:5:82:ASP:OD2	5:5:89:ARG:NH2	2.43	0.50
3:3:222:THR:HA	3:3:242:THR:O	2.11	0.50
4:4:141:PHE:O	4:4:145:THR:OG1	2.29	0.50
8:A:98:LEU:HD22	9:H:298:LEU:HD11	1.94	0.50
10:J:40:GLY:HA2	10:J:43:ILE:HD12	1.94	0.50
4:4:109:VAL:HG11	4:4:152:MET:HG2	1.94	0.50
15:V:65:ILE:HD11	15:V:100:LEU:HD23	1.93	0.50
19:Z:140:ASP:O	19:Z:161:ARG:NH1	2.44	0.50
4:4:300:ARG:NH2	4:4:420:THR:O	2.44	0.50
10:J:172:THR:HA	11:K:80:MET:HE3	1.94	0.50
12:L:570:GLN:OE1	14:N:167:TRP:NE1	2.42	0.50
13:M:155:ALA:HB1	51:M:502:PC1:H2H2	1.94	0.50
1:1:94:VAL:O	1:1:222:VAL:HA	2.12	0.50
12:L:67:HIS:NE2	12:L:70:THR:OG1	2.43	0.50
3:3:323:VAL:HG11	3:3:525:LEU:HD13	1.93	0.50
50:4:501:DCQ:H8	6:6:56:ALA:HB1	1.94	0.49
13:M:232:ALA:O	13:M:237:LYS:NZ	2.44	0.49
1:1:394:GLU:OE1	3:3:129:ARG:NH1	2.45	0.49
4:4:200:HIS:NE2	7:9:124:GLU:OE1	2.45	0.49
8:A:67:LEU:HD22	11:K:65:VAL:HA	1.93	0.49
12:L:350:LEU:HD11	12:L:362:LEU:HD11	1.94	0.49
6:6:52:LEU:HB2	6:6:90:GLY:HA3	1.93	0.49
13:M:180:GLN:HA	13:M:248:LEU:HD21	1.94	0.49
3:3:273:GLY:O	3:3:549:HIS:NE2	2.36	0.49
4:4:190:HIS:CD2	6:6:150:PRO:HD3	2.47	0.49
4:4:354:GLU:OE2	4:4:357:GLN:NE2	2.45	0.49
1:1:184:TYR:HB3	1:1:357:GLU:HB3	1.95	0.49
13:M:369:LEU:HD12	13:M:370:PRO:HD2	1.95	0.49
2:2:156:ILE:HD13	2:2:176:LEU:HD11	1.95	0.49
3:3:194:GLU:HG2	3:3:195:LEU:HG	1.94	0.49
1:1:144:ASN:O	1:1:148:ASN:HB2	2.13	0.49
13:M:18:SER:HB2	13:M:23:ILE:HG22	1.95	0.49
3:3:27:LEU:HA	3:3:37:ILE:HD12	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:198:ASN:OD1	3:3:268:ARG:NH2	2.38	0.49
12:L:316:THR:HG23	12:L:325:ALA:HB2	1.95	0.49
16:W:43:ILE:HG12	16:W:47:ILE:HD12	1.95	0.48
4:4:183:ARG:NH1	4:4:210:ASP:OD2	2.38	0.48
5:5:138:PHE:O	5:5:163:ARG:NE	2.44	0.48
1:1:367:GLU:OE1	3:3:100:ASN:ND2	2.43	0.48
3:3:324:ASP:N	3:3:324:ASP:OD1	2.45	0.48
5:5:60:VAL:O	5:5:63:PHE:HB3	2.13	0.48
53:L:1005:CDL:H391	53:L:1005:CDL:H171	1.94	0.48
13:M:54:LEU:HD23	16:W:93:ILE:HG23	1.95	0.48
53:M:503:CDL:H622	53:M:503:CDL:H251	1.95	0.48
3:3:99:ALA:O	3:3:134:LYS:NZ	2.46	0.48
3:3:396:ARG:NH1	3:3:416:THR:O	2.46	0.48
3:3:323:VAL:HG21	3:3:525:LEU:HB3	1.95	0.48
1:1:69:GLY:O	47:1:503:NAI:H2N	2.13	0.48
13:M:301:ILE:HA	13:M:309:TYR:HE1	1.78	0.48
15:V:1:AYA:HA	15:V:4:LEU:HD23	1.95	0.48
15:V:1:AYA:HM2	15:V:3:THR:HG22	1.96	0.48
19:Z:81:VAL:HA	19:Z:84:MET:HG2	1.94	0.48
4:4:149:ASN:HD22	4:4:370:PRO:HB2	1.79	0.48
9:H:154:LEU:HD22	9:H:157:ASN:HD22	1.79	0.48
1:1:194:GLU:OE2	1:1:204:ARG:NE	2.35	0.48
1:1:295:LEU:HB2	1:1:339:ARG:HA	1.96	0.48
3:3:140:LYS:HB2	3:3:148:THR:HG21	1.95	0.48
12:L:203:MET:HB2	19:Z:113:GLN:HG3	1.96	0.48
4:4:155:THR:HB	4:4:167:PHE:HA	1.96	0.48
12:L:63:ILE:O	12:L:79:SER:HA	2.14	0.48
4:4:64:LEU:HD11	4:4:418:ILE:HD11	1.96	0.47
5:5:192:GLN:OE1	7:9:115:LYS:NZ	2.47	0.47
9:H:205:SER:H	9:H:279:ARG:HH22	1.61	0.47
13:M:158:LEU:HD23	14:N:283:ALA:HB1	1.96	0.47
3:3:601:ARG:NH2	3:3:614:ASP:OD1	2.47	0.47
10:J:71:THR:O	10:J:76:THR:OG1	2.30	0.47
4:4:84:HIS:NE2	6:6:130:TYR:OH	2.37	0.47
18:Y:5:GLU:O	18:Y:53:ARG:NH1	2.47	0.47
3:3:45:ARG:NH2	3:3:256:GLU:OE2	2.39	0.47
9:H:251:MET:HB3	9:H:254:LEU:HD13	1.96	0.47
4:4:61:VAL:HG21	4:4:83:LEU:HB2	1.96	0.47
12:L:593:ILE:HD12	15:V:41:ALA:HB2	1.97	0.47
13:M:229:MET:O	13:M:233:ALA:HB3	2.14	0.47
1:1:305:PRO:HG3	1:1:413:TRP:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:121:GLN:HE21	2:2:128:VAL:HG23	1.80	0.47
6:6:71:ARG:HA	9:H:37:PRO:HA	1.96	0.47
11:K:21:MET:HG2	12:L:589:LEU:HD23	1.96	0.47
11:K:46:LEU:O	11:K:50:ASN:HB2	2.15	0.47
12:L:72:GLN:NE2	13:M:458:LEU:O	2.47	0.47
13:M:51:ASN:HA	13:M:57:PHE:HB2	1.97	0.47
19:Z:136:LYS:NZ	19:Z:140:ASP:OD2	2.43	0.47
2:2:121:GLN:HG2	2:2:127:LYS:HA	1.97	0.47
4:4:73:VAL:HG21	4:4:414:VAL:HG21	1.95	0.47
5:5:137:MET:HA	5:5:161:PRO:HD2	1.96	0.47
12:L:180:ILE:HD13	52:L:1001:3PE:H2H2	1.97	0.47
3:3:364:LEU:HD12	3:3:491:ASN:HB3	1.97	0.47
12:L:279:CYS:SG	12:L:405:ASN:ND2	2.88	0.47
1:1:361:GLN:N	45:1:501:SF4:S4	2.86	0.46
4:4:145:THR:HG1	4:4:181:TYR:HH	1.56	0.46
13:M:116:ILE:HD11	13:M:161:LEU:HD12	1.97	0.46
16:W:138:LYS:HB2	16:W:143:ASN:HD21	1.80	0.46
1:1:101:GLU:OE2	1:1:302:SER:N	2.48	0.46
3:3:478:ARG:NH2	3:3:485:GLY:O	2.48	0.46
13:M:352:LEU:HB3	13:M:355:MET:HB3	1.98	0.46
14:N:200:MET:HG3	14:N:269:GLU:HG3	1.97	0.46
15:V:34:VAL:HG11	53:V:202:CDL:H402	1.95	0.46
3:3:365:ASN:N	3:3:491:ASN:OD1	2.49	0.46
3:3:426:PRO:HB2	3:3:656:LEU:HD13	1.98	0.46
3:3:569:LYS:HG3	3:3:571:ALA:HB2	1.97	0.46
3:3:12:PHE:HB2	3:3:78:ASN:HA	1.97	0.46
3:3:356:THR:HG21	3:3:503:LEU:HD22	1.97	0.46
4:4:412:ALA:HB3	9:H:281:ARG:HG3	1.98	0.46
5:5:77:ASP:HB3	5:5:95:ASN:HD22	1.81	0.46
8:A:88:LEU:HD13	9:H:309:ILE:HD12	1.98	0.46
10:J:43:ILE:HG22	11:K:46:LEU:HD11	1.97	0.46
53:L:1005:CDL:H362	53:L:1005:CDL:H532	1.97	0.46
53:M:503:CDL:H741	18:Y:169:TRP:HE1	1.81	0.46
10:J:167:VAL:HG22	14:N:42:PRO:HG2	1.97	0.46
12:L:402:SER:HG	12:L:404:THR:HG1	1.58	0.46
3:3:127:ARG:NH2	4:4:326:ASP:O	2.49	0.46
1:1:96:ASN:ND2	1:1:187:GLY:O	2.40	0.46
1:1:299:PRO:HG3	1:1:307:ILE:HG12	1.98	0.46
5:5:41:GLN:NE2	5:5:49:GLU:OE1	2.43	0.46
53:M:503:CDL:H872	53:M:503:CDL:H652	1.98	0.46
1:1:265:PRO:O	2:2:190:ARG:NH1	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:M:503:CDL:HA61	53:M:503:CDL:HA21	1.98	0.46
14:N:193:VAL:HB	14:N:266:ILE:HG23	1.98	0.46
3:3:427:LYS:HD3	3:3:656:LEU:HD12	1.98	0.45
13:M:9:MET:HE2	53:M:503:CDL:H842	1.97	0.45
54:X:101:ZMP:H15	54:X:101:ZMP:H17	1.61	0.45
9:H:165:LEU:HD23	9:H:240:THR:HG22	1.98	0.45
11:K:93:LEU:HB3	14:N:54:GLU:HG3	1.97	0.45
6:6:63:ALA:HA	6:6:69:MET:HG2	1.98	0.45
11:K:56:ALA:O	11:K:59:MET:HB3	2.16	0.45
3:3:60:GLU:HG2	3:3:78:ASN:HB3	1.97	0.45
4:4:104:ASP:HB3	4:4:190:HIS:ND1	2.31	0.45
12:L:418:PHE:HD1	12:L:421:ILE:HD12	1.82	0.45
14:N:261:MET:HG3	14:N:340:THR:HG23	1.99	0.45
1:1:63:SER:HB2	1:1:242:PHE:HB3	1.98	0.45
13:M:23:ILE:HD11	13:M:92:LYS:HD2	1.99	0.45
1:1:21:ILE:HG12	1:1:233:THR:HG21	1.97	0.45
3:3:223:ARG:O	3:3:241:SER:HA	2.16	0.45
5:5:78:LEU:HB3	5:5:130:TYR:HB3	1.99	0.45
13:M:105:PHE:O	13:M:109:THR:OG1	2.23	0.45
53:V:202:CDL:H351	53:V:202:CDL:H322	1.83	0.45
1:1:71:ALA:HB2	47:1:503:NAI:H4D	1.97	0.45
8:A:55:PHE:HB3	8:A:113:TRP:CE2	2.52	0.45
12:L:50:PRO:HA	12:L:53:MET:HG2	1.98	0.45
4:4:110:SER:OG	4:4:149:ASN:ND2	2.50	0.45
9:H:86:TRP:CE2	9:H:233:MET:HB2	2.52	0.45
53:L:1005:CDL:H621	13:M:372:SER:HB3	1.99	0.45
1:1:20:ARG:HD2	1:1:269:GLU:HB3	1.99	0.45
1:1:403:THR:HG21	1:1:408:GLY:HA3	1.98	0.45
7:9:27:TRP:HB3	7:9:30:LEU:HD12	1.99	0.45
9:H:293:PHE:O	9:H:297:THR:OG1	2.27	0.45
1:1:97:ALA:HB3	1:1:138:ILE:HA	1.99	0.45
51:M:502:PC1:H2C2	51:M:502:PC1:H3B1	1.99	0.45
8:A:38:GLU:HB2	8:A:43:PRO:HG3	1.99	0.44
52:J:202:3PE:H292	11:K:14:VAL:HG22	1.98	0.44
13:M:290:SER:HA	13:M:319:HIS:HE2	1.81	0.44
13:M:343:ILE:O	13:M:346:ARG:NH1	2.48	0.44
17:X:63:PRO:O	17:X:67:ALA:N	2.50	0.44
9:H:200:LEU:HD22	9:H:282:TYR:HB3	1.98	0.44
11:K:24:SER:HA	11:K:90:VAL:HG22	2.00	0.44
1:1:17:ASP:HA	1:1:20:ARG:HG2	1.98	0.44
3:3:377:VAL:HG23	3:3:404:LEU:HD11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:64:LEU:HD11	10:J:168:ILE:HD12	1.99	0.44
53:L:1005:CDL:H741	13:M:369:LEU:HD21	1.99	0.44
14:N:89:LEU:HD12	14:N:95:SER:HA	1.98	0.44
7:9:169:ILE:O	7:9:173:TYR:HB3	2.17	0.44
9:H:152:SER:HA	9:H:155:LEU:HD12	1.98	0.44
7:9:23:GLN:HG3	7:9:28:THR:HB	1.98	0.44
7:9:172:ASP:OD2	7:9:176:ARG:NE	2.50	0.44
11:K:70:GLU:O	11:K:73:LEU:HB3	2.18	0.44
14:N:110:PRO:HD3	14:N:160:LEU:HD23	2.00	0.44
14:N:211:MET:HG2	14:N:333:SER:HB2	1.99	0.44
4:4:154:VAL:HG11	4:4:225:LEU:HD21	2.00	0.44
53:M:503:CDL:H311	53:M:503:CDL:H562	2.00	0.44
4:4:387:TYR:CZ	5:5:164:LYS:HE3	2.53	0.44
14:N:122:ILE:O	14:N:176:ARG:NH1	2.51	0.44
1:1:95:VAL:HB	1:1:136:ILE:HG12	1.99	0.43
4:4:106:LEU:HD13	4:4:391:ILE:HG21	2.00	0.43
4:4:237:ASN:O	9:H:284:GLN:NE2	2.39	0.43
9:H:6:VAL:HG22	9:H:95:LEU:HD21	1.99	0.43
1:1:91:LYS:HG2	1:1:219:PRO:HB2	1.98	0.43
3:3:382:THR:HB	3:3:454:GLY:HA3	1.99	0.43
4:4:123:GLU:OE2	4:4:138:ARG:NH2	2.51	0.43
8:A:6:THR:HG21	9:H:87:ILE:HG21	2.00	0.43
52:J:202:3PE:H222	11:K:21:MET:HB2	2.00	0.43
12:L:556:ILE:O	12:L:560:THR:N	2.51	0.43
12:L:563:PRO:HA	52:N:401:3PE:H3A1	2.00	0.43
9:H:121:TRP:HB2	10:J:68:PHE:HZ	1.83	0.43
3:3:242:THR:HG22	3:3:247:VAL:HA	2.01	0.43
3:3:231:MET:HB3	3:3:266:LYS:HD2	2.00	0.43
13:M:266:LEU:HB3	13:M:395:LEU:HD13	2.01	0.43
16:W:37:VAL:HG11	53:W:201:CDL:H862	2.01	0.43
2:2:116:ILE:HG23	2:2:169:ILE:HG21	2.01	0.43
5:5:119:SER:OG	5:5:131:GLU:OE2	2.25	0.43
7:9:114:THR:HG21	7:9:144:HIS:CD2	2.54	0.43
50:H:501:DCQ:H7A	50:H:501:DCQ:H1M	1.84	0.43
1:1:92:TYR:O	1:1:220:THR:HA	2.18	0.43
2:2:24:THR:OG1	2:2:27:ASN:OD1	2.32	0.43
6:6:176:TRP:HB2	51:6:202:PC1:H12	2.00	0.43
12:L:602:LEU:HD21	53:V:202:CDL:H422	2.01	0.43
1:1:432:ARG:HA	1:1:435:GLN:HG3	2.01	0.43
5:5:134:ILE:HG22	5:5:140:VAL:HB	2.01	0.43
8:A:80:GLN:NE2	9:H:315:PRO:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:24:GLU:HA	9:H:271:LEU:HD13	2.01	0.43
12:L:245:ALA:O	12:L:249:SER:OG	2.31	0.43
1:1:250:ASN:HD21	1:1:320:ASP:HB2	1.84	0.42
3:3:568:GLU:HB3	3:3:589:PRO:HG3	2.01	0.42
13:M:16:TRP:NE1	13:M:97:SER:OG	2.47	0.42
14:N:136:LEU:HD23	14:N:205:LEU:HD21	2.01	0.42
14:N:289:ASN:HA	14:N:292:PHE:CE1	2.54	0.42
3:3:329:ILE:HD12	3:3:329:ILE:HA	1.84	0.42
6:6:58:GLU:HG2	6:6:151:PRO:O	2.19	0.42
8:A:36:PRO:HB2	8:A:43:PRO:HG2	2.01	0.42
13:M:61:LEU:HB2	13:M:457:PRO:HG3	2.01	0.42
16:W:8:LEU:HD11	17:X:88:GLU:HG3	2.00	0.42
7:9:22:ALA:O	7:9:26:LEU:HB2	2.19	0.42
9:H:117:LEU:HD11	9:H:136:VAL:HG23	2.01	0.42
13:M:329:LEU:HB3	13:M:359:TRP:CZ2	2.54	0.42
13:M:408:LEU:O	13:M:412:ILE:N	2.50	0.42
51:M:502:PC1:H251	51:M:502:PC1:H372	2.01	0.42
4:4:430:ARG:NH2	5:5:133:GLU:OE2	2.53	0.42
6:6:62:MET:SD	6:6:69:MET:HB3	2.60	0.42
11:K:79:VAL:O	11:K:83:ASN:N	2.48	0.42
1:1:99:GLU:OE2	1:1:106:LYS:N	2.52	0.42
3:3:320:GLY:O	3:3:498:SER:OG	2.38	0.42
4:4:85:2MR:HE	4:4:85:2MR:HB3	1.69	0.42
12:L:128:MET:HG2	12:L:251:THR:HG22	2.02	0.42
13:M:379:LEU:O	13:M:383:MET:HG2	2.20	0.42
1:1:142:PHE:HB3	1:1:145:GLU:HB2	2.01	0.42
1:1:245:PHE:HB3	1:1:271:GLU:HG3	2.01	0.42
3:3:366:THR:HG22	3:3:370:GLY:HA3	2.02	0.42
4:4:203:LEU:HD22	4:4:207:LEU:HD23	2.00	0.42
7:9:95:GLU:HB2	7:9:108:ARG:HB3	2.01	0.42
8:A:99:ALA:HB1	52:A:201:3PE:H391	2.02	0.42
10:J:113:VAL:HG12	10:J:119:PHE:HB2	2.02	0.42
12:L:74:LEU:HD13	12:L:190:LEU:HD13	2.01	0.42
53:M:503:CDL:H552	53:M:503:CDL:H152	2.01	0.42
2:2:43:LYS:HE2	2:2:73:LEU:HA	2.02	0.42
2:2:120:ILE:HD11	2:2:169:ILE:HG12	2.01	0.42
9:H:89:LEU:HD11	9:H:233:MET:HG2	2.02	0.42
12:L:129:LEU:HA	12:L:132:VAL:HG22	2.01	0.42
12:L:331:THR:HG22	12:L:335:PHE:HE1	1.84	0.42
13:M:297:VAL:HG13	13:M:312:ALA:HB1	2.02	0.42
14:N:128:LEU:HD13	14:N:216:PHE:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:61:LEU:HD12	2:2:90:TYR:HB3	2.01	0.42
3:3:362:TYR:OH	3:3:504:ASP:OD1	2.32	0.42
4:4:204:PRO:HD2	4:4:207:LEU:HD22	2.01	0.42
9:H:73:LEU:HD11	52:J:201:3PE:H3H2	2.01	0.42
12:L:249:SER:HB2	12:L:336:LYS:HG3	2.01	0.42
12:L:316:THR:HB	12:L:395:ILE:HG23	2.01	0.42
14:N:258:SER:O	14:N:261:MET:HB3	2.20	0.42
53:W:201:CDL:H192	19:Z:47:VAL:HG21	2.02	0.42
1:1:95:VAL:HG11	1:1:118:LEU:HD11	2.01	0.42
4:4:149:ASN:ND2	4:4:370:PRO:HB2	2.35	0.42
10:J:4:TYR:OH	10:J:111:LYS:NZ	2.52	0.42
12:L:149:ILE:HD13	12:L:149:ILE:HA	1.91	0.42
12:L:569:ALA:HB2	53:L:1004:CDL:H541	2.01	0.42
13:M:282:LEU:HD21	13:M:359:TRP:HH2	1.84	0.42
4:4:323:ILE:HD12	4:4:324:LYS:HG3	2.02	0.41
5:5:30:ALA:HB2	5:5:40:VAL:HG21	2.02	0.41
17:X:8:LEU:H	17:X:87:TYR:HE2	1.68	0.41
19:Z:3:SER:OG	19:Z:4:TRP:N	2.52	0.41
3:3:206:GLY:N	45:3:801:SF4:S2	2.81	0.41
6:6:71:ARG:NH2	7:9:49:ASN:OD1	2.51	0.41
19:Z:73:ILE:HG23	19:Z:155:LEU:HD22	2.02	0.41
12:L:193:LEU:HD23	12:L:201:ILE:HA	2.02	0.41
3:3:324:ASP:HB3	3:3:571:ALA:HB1	2.02	0.41
7:9:132:VAL:HG11	7:9:169:ILE:HD11	2.01	0.41
51:L:1003:PC1:H372	53:W:201:CDL:H512	2.01	0.41
14:N:189:TRP:HZ2	14:N:286:ALA:HB2	1.84	0.41
15:V:43:LYS:HD3	53:V:202:CDL:HA4	2.02	0.41
1:1:105:CYS:H	1:1:257:ASN:ND2	2.18	0.41
1:1:276:LEU:HD21	1:1:297:VAL:HG11	2.03	0.41
2:2:6:LEU:HD13	2:2:10:ARG:HH12	1.85	0.41
4:4:238:ARG:NH1	9:H:279:ARG:O	2.46	0.41
9:H:58:LYS:HB3	9:H:217:ALA:HB3	2.02	0.41
10:J:34:ILE:HG13	10:J:64:MET:HG3	2.03	0.41
13:M:161:LEU:HD11	14:N:264:TRP:CD1	2.55	0.41
13:M:229:MET:O	13:M:233:ALA:CB	2.68	0.41
18:Y:17:VAL:HG12	18:Y:19:VAL:HG22	2.01	0.41
4:4:163:ALA:HB2	9:H:278:PRO:HG3	2.03	0.41
15:V:113:ALA:O	15:V:117:MET:HB2	2.20	0.41
4:4:296:ARG:HH21	4:4:420:THR:HG21	1.85	0.41
8:A:56:PHE:O	10:J:70:TYR:OH	2.37	0.41
10:J:45:LEU:HD21	52:J:201:3PE:H222	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:41:LEU:HD13	13:M:66:LEU:HD13	2.03	0.41
13:M:116:ILE:HD12	13:M:116:ILE:HA	1.97	0.41
15:V:124:VAL:HG11	53:V:202:CDL:H873	2.03	0.41
10:J:7:PHE:O	10:J:11:ILE:HG12	2.21	0.41
12:L:88:MET:HB2	12:L:326:PHE:HE2	1.85	0.41
3:3:503:LEU:HD21	3:3:509:PRO:HB3	2.01	0.41
8:A:13:LEU:HD21	9:H:10:ILE:HD11	2.01	0.41
9:H:1:MET:HG3	9:H:4:ILE:HD12	2.03	0.41
9:H:103:LEU:HD13	10:J:55:MET:HE3	2.03	0.41
12:L:136:ASN:HD21	51:L:1003:PC1:H2I1	1.86	0.41
12:L:213:LEU:HD23	12:L:216:LEU:HD12	2.02	0.41
14:N:277:ILE:HD13	52:V:201:3PE:H372	2.03	0.41
3:3:108:CYS:O	3:3:218:ARG:NH1	2.50	0.41
4:4:151:ILE:O	4:4:155:THR:OG1	2.28	0.41
7:9:158:GLY:O	7:9:162:GLU:HB2	2.21	0.41
14:N:170:LEU:O	14:N:295:ARG:NH1	2.40	0.40
14:N:178:ILE:HD13	14:N:296:LEU:HD11	2.02	0.40
3:3:325:ALA:HB1	3:3:623:LEU:HD11	2.03	0.40
4:4:145:THR:HA	4:4:148:LEU:HD12	2.03	0.40
9:H:26:LYS:HG2	9:H:36:GLY:HA3	2.03	0.40
12:L:128:MET:HE1	12:L:255:ALA:HB2	2.03	0.40
52:V:201:3PE:H322	52:V:201:3PE:H261	2.03	0.40
7:9:92:ILE:HA	7:9:110:ASP:O	2.21	0.40
12:L:60:GLU:HG2	12:L:83:ASP:HA	2.03	0.40
1:1:42:TRP:CD2	1:1:161:LEU:HD13	2.56	0.40
2:2:50:VAL:HG12	2:2:69:VAL:HG22	2.04	0.40
3:3:174:THR:HG22	3:3:183:VAL:HG22	2.03	0.40
4:4:158:ALA:HB1	4:4:163:ALA:HB3	2.04	0.40
4:4:377:TYR:HB3	4:4:390:LYS:HB3	2.03	0.40
9:H:281:ARG:HH11	9:H:281:ARG:HD3	1.78	0.40
13:M:14:LEU:O	13:M:18:SER:OG	2.37	0.40
14:N:252:GLY:HA3	14:N:290:LEU:HD13	2.02	0.40
15:V:12:PRO:HB2	15:V:15:THR:HG21	2.03	0.40
18:Y:44:LEU:HD22	18:Y:130:VAL:HB	2.03	0.40
6:6:81:ARG:NH1	9:H:61:LEU:HD21	2.36	0.40
12:L:161:ARG:NE	12:L:238:GLU:OE2	2.55	0.40
13:M:118:PHE:O	13:M:122:PHE:CB	2.69	0.40
14:N:20:VAL:HG11	14:N:137:ALA:HB1	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	428/464 (92%)	405 (95%)	23 (5%)	0	100	100
2	2	211/246 (86%)	195 (92%)	16 (8%)	0	100	100
3	3	686/727 (94%)	655 (96%)	31 (4%)	0	100	100
4	4	427/463 (92%)	403 (94%)	24 (6%)	0	100	100
5	5	206/266 (77%)	195 (95%)	11 (5%)	0	100	100
6	6	154/223 (69%)	147 (96%)	7 (4%)	0	100	100
7	9	174/217 (80%)	164 (94%)	10 (6%)	0	100	100
8	A	113/115 (98%)	106 (94%)	7 (6%)	0	100	100
9	H	316/318 (99%)	299 (95%)	17 (5%)	0	100	100
10	J	173/175 (99%)	164 (95%)	8 (5%)	1 (1%)	25	59
11	K	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
12	L	604/606 (100%)	575 (95%)	29 (5%)	0	100	100
13	M	457/459 (100%)	446 (98%)	11 (2%)	0	100	100
14	N	345/347 (99%)	335 (97%)	10 (3%)	0	100	100
15	V	138/141 (98%)	137 (99%)	1 (1%)	0	100	100
16	W	137/189 (72%)	134 (98%)	3 (2%)	0	100	100
17	X	85/157 (54%)	80 (94%)	5 (6%)	0	100	100
17	j	80/157 (51%)	75 (94%)	5 (6%)	0	100	100
18	Y	169/172 (98%)	164 (97%)	5 (3%)	0	100	100
19	Z	169/175 (97%)	167 (99%)	2 (1%)	0	100	100
20	a	42/109 (38%)	42 (100%)	0	0	100	100
21	b	93/124 (75%)	90 (97%)	3 (3%)	0	100	100
22	c	124/170 (73%)	122 (98%)	2 (2%)	0	100	100
23	d	338/380 (89%)	325 (96%)	13 (4%)	0	100	100
24	e	84/99 (85%)	81 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	f	111/116 (96%)	110 (99%)	1 (1%)	0	100	100
26	g	112/140 (80%)	108 (96%)	4 (4%)	0	100	100
27	h	92/114 (81%)	87 (95%)	5 (5%)	0	100	100
28	i	143/145 (99%)	137 (96%)	6 (4%)	0	100	100
29	k	317/355 (89%)	301 (95%)	16 (5%)	0	100	100
30	l	103/106 (97%)	97 (94%)	6 (6%)	0	100	100
31	m	78/84 (93%)	72 (92%)	6 (8%)	0	100	100
32	n	77/98 (79%)	76 (99%)	1 (1%)	0	100	100
33	o	118/122 (97%)	115 (98%)	3 (2%)	0	100	100
34	p	126/130 (97%)	123 (98%)	3 (2%)	0	100	100
35	q	137/144 (95%)	135 (98%)	2 (2%)	0	100	100
36	r	95/128 (74%)	89 (94%)	6 (6%)	0	100	100
37	s	120/137 (88%)	116 (97%)	4 (3%)	0	100	100
38	t	175/179 (98%)	170 (97%)	5 (3%)	0	100	100
39	u	63/108 (58%)	59 (94%)	4 (6%)	0	100	100
40	v	153/186 (82%)	146 (95%)	7 (5%)	0	100	100
41	w	99/154 (64%)	91 (92%)	8 (8%)	0	100	100
42	x	47/76 (62%)	46 (98%)	1 (2%)	0	100	100
43	y	48/58 (83%)	46 (96%)	2 (4%)	0	100	100
44	z	68/70 (97%)	67 (98%)	1 (2%)	0	100	100
All	All	8131/9247 (88%)	7790 (96%)	340 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	J	116	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	344/368 (94%)	342 (99%)	2 (1%)	86	94
2	2	183/210 (87%)	182 (100%)	1 (0%)	88	94
3	3	578/608 (95%)	576 (100%)	2 (0%)	92	96
4	4	370/391 (95%)	368 (100%)	2 (0%)	88	94
5	5	189/230 (82%)	189 (100%)	0	100	100
6	6	132/181 (73%)	129 (98%)	3 (2%)	50	77
7	9	151/179 (84%)	151 (100%)	0	100	100
8	A	103/103 (100%)	103 (100%)	0	100	100
9	H	278/278 (100%)	276 (99%)	2 (1%)	84	93
10	J	144/144 (100%)	143 (99%)	1 (1%)	84	93
11	K	86/86 (100%)	85 (99%)	1 (1%)	71	88
12	L	538/538 (100%)	535 (99%)	3 (1%)	86	94
13	M	411/411 (100%)	410 (100%)	1 (0%)	93	97
14	N	315/315 (100%)	314 (100%)	1 (0%)	92	96
15	V	101/102 (99%)	101 (100%)	0	100	100
16	W	122/160 (76%)	122 (100%)	0	100	100
17	X	80/141 (57%)	80 (100%)	0	100	100
17	j	76/141 (54%)	76 (100%)	0	100	100
18	Y	154/155 (99%)	152 (99%)	2 (1%)	69	87
19	Z	155/157 (99%)	155 (100%)	0	100	100
20	a	43/93 (46%)	43 (100%)	0	100	100
21	b	79/97 (81%)	79 (100%)	0	100	100
22	c	113/150 (75%)	113 (100%)	0	100	100
23	d	294/326 (90%)	290 (99%)	4 (1%)	67	86
24	e	76/82 (93%)	76 (100%)	0	100	100
25	f	101/102 (99%)	101 (100%)	0	100	100
26	g	107/124 (86%)	107 (100%)	0	100	100
27	h	84/96 (88%)	84 (100%)	0	100	100
28	i	131/131 (100%)	131 (100%)	0	100	100
29	k	283/309 (92%)	283 (100%)	0	100	100
30	l	94/95 (99%)	94 (100%)	0	100	100
31	m	69/72 (96%)	68 (99%)	1 (1%)	67	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	n	61/76 (80%)	61 (100%)	0	100	100
33	o	107/109 (98%)	107 (100%)	0	100	100
34	p	114/116 (98%)	114 (100%)	0	100	100
35	q	119/122 (98%)	118 (99%)	1 (1%)	81	92
36	r	95/122 (78%)	95 (100%)	0	100	100
37	s	110/120 (92%)	109 (99%)	1 (1%)	78	91
38	t	159/161 (99%)	158 (99%)	1 (1%)	86	94
39	u	59/84 (70%)	59 (100%)	0	100	100
40	v	140/160 (88%)	140 (100%)	0	100	100
41	w	92/130 (71%)	92 (100%)	0	100	100
42	x	44/67 (66%)	44 (100%)	0	100	100
43	y	46/54 (85%)	46 (100%)	0	100	100
44	z	59/59 (100%)	59 (100%)	0	100	100
All	All	7189/7955 (90%)	7160 (100%)	29 (0%)	91	96

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	148	ASN
1	1	249	ARG
2	2	122	LYS
3	3	39	ARG
3	3	179	ASN
4	4	252	ASN
4	4	430	ARG
6	6	54	CYS
6	6	59	MET
6	6	111	ARG
9	H	193	THR
9	H	274	ARG
10	J	86	ASN
11	K	50	ASN
12	L	135	ASN
12	L	270	ASN
12	L	541	ASN
13	M	138	ASN
14	N	235	ASN

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Mol	Chain	Res	Type
18	Y	47	TRP
18	Y	63	ASN
23	d	36	ASN
23	d	185	ILE
23	d	186	ARG
23	d	268	ARG
31	m	82	ARG
35	q	67	ARG
37	s	103	ARG
38	t	128	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	148	ASN
1	1	150	GLN
1	1	250	ASN
1	1	373	ASN
2	2	121	GLN
3	3	401	HIS
3	3	499	GLN
4	4	149	ASN
4	4	252	ASN
5	5	95	ASN
9	H	230	ASN
9	H	235	ASN
10	J	46	ASN
11	K	83	ASN
12	L	135	ASN
12	L	199	GLN
12	L	210	ASN
12	L	270	ASN
12	L	446	ASN
19	Z	123	ASN
19	Z	143	HIS
20	a	40	ASN
21	b	36	ASN
23	d	87	HIS
23	d	288	HIS
25	f	36	HIS
25	f	49	GLN
26	g	125	HIS

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Mol	Chain	Res	Type
30	l	6	GLN
33	o	61	GLN
34	p	78	ASN
38	t	138	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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
11	FME	K	1	11	8,9,10	0.99	0	7,9,11	0.93	0
12	FME	L	1	12	8,9,10	0.92	0	7,9,11	1.05	0
27	AYA	h	1	27	6,7,8	1.26	1 (16%)	5,8,10	1.24	1 (20%)
4	2MR	4	85	4	10,12,13	2.34	3 (30%)	5,13,15	1.20	1 (20%)
15	AYA	V	1	15	6,7,8	1.17	1 (16%)	5,8,10	1.74	2 (40%)
13	FME	M	1	13	8,9,10	0.95	0	7,9,11	0.75	0
29	SEP	k	36	29	8,9,10	1.55	1 (12%)	8,12,14	1.51	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
11	FME	K	1	11	-	2/7/9/11	-
12	FME	L	1	12	-	1/7/9/11	-
27	AYA	h	1	27	-	0/4/6/8	-
4	2MR	4	85	4	-	3/10/13/15	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	AYA	V	1	15	-	2/4/6/8	-
13	FME	M	1	13	-	4/7/9/11	-
29	SEP	k	36	29	-	4/5/8/10	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	4	85	2MR	CZ-NE	4.84	1.44	1.34
4	4	85	2MR	CZ-NH2	4.57	1.43	1.33
29	k	36	SEP	P-O1P	3.38	1.61	1.50
27	h	1	AYA	CA-N	-2.50	1.43	1.46
4	4	85	2MR	CQ1-NH1	-2.20	1.42	1.46
15	V	1	AYA	CA-N	-2.04	1.44	1.46

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	k	36	SEP	P-OG-CB	-3.11	109.74	118.30
27	h	1	AYA	CB-CA-N	2.49	112.38	109.61
15	V	1	AYA	CB-CA-N	2.40	112.28	109.61
4	4	85	2MR	CQ2-NH2-CZ	-2.33	118.71	123.86
29	k	36	SEP	OG-CB-CA	2.27	110.36	108.14
15	V	1	AYA	CA-N-CT	2.23	124.76	121.52

There are no chirality outliers.

All (16) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
29	k	36	SEP	CA-CB-OG-P
13	M	1	FME	N-CA-CB-CG
11	K	1	FME	CB-CA-N-CN
13	M	1	FME	CB-CA-N-CN

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	4	85	2MR	1	0
15	V	1	AYA	2	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 45 ligands modelled in this entry, 2 are monoatomic - leaving 43 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	$\# Z > 2$
52	3PE	p	201	-	26,26,50	0.48	0	30,31,55	0.59	1 (3%)
52	3PE	L	1001	-	50,50,50	0.30	0	53,55,55	0.39	0
46	FMN	1	502	-	33,33,33	1.11	2 (6%)	48,50,50	1.24	7 (14%)
53	CDL	M	503	-	99,99,99	0.26	0	105,111,111	0.31	0
45	SF4	3	802	3	0,12,12	-	-	-	-	-
51	PC1	9	401	-	53,53,53	0.31	0	59,61,61	0.50	1 (1%)
48	FES	3	803	3	0,4,4	-	-	-	-	-
52	3PE	J	202	-	39,39,50	0.36	0	42,44,55	0.37	0
52	3PE	N	401	-	39,39,50	0.33	0	42,44,55	0.34	0
58	MYR	s	201	37	14,14,15	0.18	0	13,13,15	0.23	0
47	NAI	1	503	-	42,48,48	0.58	0	47,73,73	1.94	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
52	3PE	i	501	-	50,50,50	0.30	0	53,55,55	0.29	0
54	ZMP	g	201	-	27,33,36	0.62	1 (3%)	32,40,45	1.20	4 (12%)
51	PC1	w	801	-	53,53,53	0.29	0	59,61,61	0.37	0
53	CDL	W	201	-	99,99,99	0.27	0	105,111,111	0.30	0
57	AMP	k	501	-	22,25,25	0.89	1 (4%)	25,38,38	1.24	2 (8%)
56	NDP	d	401	-	45,52,52	0.55	0	53,80,80	0.57	1 (1%)
51	PC1	M	502	-	53,53,53	0.31	0	59,61,61	0.37	0
52	3PE	i	502	-	50,50,50	0.30	0	53,55,55	0.29	0
53	CDL	L	1004	-	84,84,99	0.29	0	90,96,111	0.27	0
45	SF4	1	501	1	0,12,12	-	-	-	-	-
52	3PE	A	201	-	50,50,50	0.31	0	53,55,55	0.34	0
48	FES	2	300	2	0,4,4	-	-	-	-	-
52	3PE	L	1002	-	30,30,50	0.42	0	33,35,55	0.77	1 (3%)
53	CDL	o	502	-	89,89,99	0.29	0	95,101,111	0.41	0
52	3PE	o	501	-	30,30,50	0.38	0	33,35,55	0.42	0
51	PC1	L	1003	-	53,53,53	0.32	0	59,61,61	0.60	2 (3%)
53	CDL	x	101	-	74,74,99	0.31	0	80,86,111	0.44	1 (1%)
45	SF4	9	403	7	0,12,12	-	-	-	-	-
52	3PE	N	402	-	50,50,50	0.33	0	53,55,55	0.55	1 (1%)
45	SF4	6	201	6	0,12,12	-	-	-	-	-
50	DCQ	H	501	-	23,23,23	0.21	0	26,29,29	0.54	0
53	CDL	V	202	-	93,93,99	0.26	0	99,105,111	0.27	0
54	ZMP	X	101	17	24,30,36	0.82	1 (4%)	29,37,45	1.03	2 (6%)
53	CDL	h	201	-	57,57,99	0.34	0	63,69,111	0.28	0
50	DCQ	4	501	-	23,23,23	0.19	0	26,29,29	0.51	0
52	3PE	J	201	-	50,50,50	0.31	0	53,55,55	0.31	0
45	SF4	9	402	7	0,12,12	-	-	-	-	-
53	CDL	L	1005	-	99,99,99	0.26	0	105,111,111	0.31	0
52	3PE	M	501	-	43,43,50	0.34	0	46,48,55	0.49	1 (2%)
51	PC1	6	202	-	45,45,53	0.32	0	51,53,61	0.32	0
52	3PE	V	201	-	36,36,50	0.35	0	39,41,55	0.32	0
45	SF4	3	801	3	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
53	CDL	M	503	-	1/1/9/9	31/110/110/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
52	3PE	L	1001	-	-	14/54/54/54	-
46	FMN	1	502	-	-	7/18/18/18	0/3/3/3
52	3PE	p	201	-	-	3/27/27/54	-
45	SF4	3	801	3	-	-	0/6/5/5
45	SF4	3	802	3	-	-	0/6/5/5
51	PC1	9	401	-	-	15/57/57/57	-
52	3PE	N	401	-	-	11/43/43/54	-
52	3PE	J	202	-	-	13/43/43/54	-
58	MYR	s	201	37	-	2/11/12/13	-
48	FES	3	803	3	-	-	0/1/1/1
47	NAI	1	503	-	-	8/25/72/72	0/5/5/5
52	3PE	i	501	-	-	9/54/54/54	-
54	ZMP	g	201	-	-	11/38/40/43	-
51	PC1	w	801	-	-	13/57/57/57	-
53	CDL	W	201	-	-	24/110/110/110	-
57	AMP	k	501	-	-	5/6/26/26	0/3/3/3
56	NDP	d	401	-	-	4/30/77/77	0/5/5/5
51	PC1	M	502	-	-	18/57/57/57	-
52	3PE	i	502	-	-	11/54/54/54	-
53	CDL	L	1004	-	1/1/9/9	31/95/95/110	-
45	SF4	1	501	1	-	-	0/6/5/5
52	3PE	A	201	-	-	13/54/54/54	-
52	3PE	L	1002	-	-	9/34/34/54	-
48	FES	2	300	2	-	-	0/1/1/1
53	CDL	o	502	-	-	31/100/100/110	-
52	3PE	o	501	-	-	7/34/34/54	-
51	PC1	L	1003	-	-	19/57/57/57	-
53	CDL	x	101	-	2/2/9/9	20/85/85/110	-
45	SF4	9	403	7	-	-	0/6/5/5
52	3PE	N	402	-	-	18/54/54/54	-
45	SF4	6	201	6	-	-	0/6/5/5
50	DCQ	H	501	-	-	5/14/38/38	0/1/1/1
54	ZMP	X	101	17	-	12/35/37/43	-
53	CDL	h	201	-	-	15/68/68/110	-
50	DCQ	4	501	-	-	5/14/38/38	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
52	3PE	J	201	-	-	11/54/54/54	-
45	SF4	9	402	7	-	-	0/6/5/5
53	CDL	L	1005	-	1/1/9/9	35/110/110/110	-
52	3PE	M	501	-	-	11/47/47/54	-
51	PC1	6	202	-	-	7/49/49/57	-
52	3PE	V	201	-	-	13/40/40/54	-
53	CDL	V	202	-	-	20/104/104/110	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	1	502	FMN	C4A-N5	3.42	1.37	1.30
54	X	101	ZMP	C9-C10	2.60	1.53	1.50
46	1	502	FMN	C10-N1	2.46	1.38	1.33
57	k	501	AMP	C5-C4	2.42	1.47	1.40
54	g	201	ZMP	C9-C10	2.27	1.53	1.50

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	1	503	NAI	O5B-PA-O1A	-9.70	71.15	109.07
47	1	503	NAI	O2A-PA-O1A	-7.96	72.91	112.24
46	1	502	FMN	C4-N3-C2	-3.26	119.61	125.64
57	k	501	AMP	N3-C2-N1	-3.22	123.64	128.68
54	g	201	ZMP	O1-C10-C9	-3.03	120.42	123.99
57	k	501	AMP	C4-C5-N7	-2.83	106.45	109.40
54	g	201	ZMP	C14-C15-N2	-2.76	106.33	111.90
46	1	502	FMN	C4A-C4-N3	2.73	120.13	113.19
46	1	502	FMN	O4-C4-C4A	-2.67	119.51	126.60
54	g	201	ZMP	C15-C14-C13	-2.52	108.16	112.36
54	X	101	ZMP	O1-C10-C9	-2.52	121.01	123.99
46	1	502	FMN	C4A-C10-N1	-2.48	118.97	124.73
46	1	502	FMN	C4A-C10-N10	2.45	120.06	116.48
51	L	1003	PC1	C2-O21-C21	2.43	123.78	117.79
47	1	503	NAI	O2A-PA-O5B	2.38	118.80	107.75
52	L	1002	3PE	C2-O21-C21	2.37	123.63	117.79
56	d	401	NDP	C5A-C6A-N6A	2.31	123.86	120.35
52	N	402	3PE	C2-O21-C21	2.27	123.39	117.79
47	1	503	NAI	C5A-C6A-N6A	2.17	123.66	120.35
46	1	502	FMN	C10-C4A-N5	-2.15	120.30	124.86
51	L	1003	PC1	O21-C2-C1	2.14	116.16	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	1	502	FMN	C4-C4A-C10	2.13	120.36	116.79
54	X	101	ZMP	C9-C10-S1	2.11	115.92	113.46
54	g	201	ZMP	C9-C10-S1	2.07	115.87	113.46
53	x	101	CDL	CB4-OB6-CB5	2.05	122.84	117.79
52	p	201	3PE	O12-P-O14	2.04	118.66	110.68
51	9	401	PC1	C2-O21-C21	2.02	122.77	117.79
52	M	501	3PE	O21-C2-C3	-2.01	101.13	108.40

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
53	L	1004	CDL	CB4
53	L	1005	CDL	CB4
53	M	503	CDL	CB4
53	x	101	CDL	CA4
53	x	101	CDL	CB4

All (481) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
47	1	503	NAI	C5B-O5B-PA-O1A
51	6	202	PC1	C1-O11-P-O12
51	9	401	PC1	C11-O13-P-O14
51	9	401	PC1	C1-O11-P-O14
51	L	1003	PC1	C11-O13-P-O14
51	L	1003	PC1	C1-O11-P-O12
51	M	502	PC1	C11-O13-P-O14
52	A	201	3PE	C11-O13-P-O11
52	A	201	3PE	C11-O13-P-O12
52	A	201	3PE	C11-O13-P-O14
52	J	201	3PE	C1-O11-P-O13
52	J	201	3PE	C1-O11-P-O14
52	J	201	3PE	C11-O13-P-O12
52	J	201	3PE	C11-O13-P-O14
52	J	202	3PE	C1-O11-P-O14
52	J	202	3PE	O13-C11-C12-N
52	L	1001	3PE	C11-O13-P-O11
52	L	1001	3PE	C11-O13-P-O14
52	L	1001	3PE	O13-C11-C12-N
52	L	1002	3PE	C1-O11-P-O12
52	L	1002	3PE	C1-O11-P-O13
52	L	1002	3PE	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
52	L	1002	3PE	O13-C11-C12-N
52	M	501	3PE	C11-O13-P-O12
52	M	501	3PE	C11-O13-P-O14
52	M	501	3PE	O13-C11-C12-N
52	N	401	3PE	C1-O11-P-O12
52	N	401	3PE	O13-C11-C12-N
52	N	402	3PE	C1-O11-P-O12
52	N	402	3PE	C1-O11-P-O14
52	N	402	3PE	C11-O13-P-O14
52	N	402	3PE	O13-C11-C12-N
52	V	201	3PE	O13-C11-C12-N
52	i	501	3PE	C11-O13-P-O11
52	i	502	3PE	C1-O11-P-O12
52	i	502	3PE	C1-O11-P-O14
52	i	502	3PE	O13-C11-C12-N
52	o	501	3PE	C11-O13-P-O12
52	o	501	3PE	C11-O13-P-O14
52	o	501	3PE	O13-C11-C12-N
53	L	1004	CDL	O1-C1-CA2-OA2
53	L	1004	CDL	CA2-OA2-PA1-OA3
53	L	1004	CDL	CA2-OA2-PA1-OA4
53	L	1004	CDL	CA2-OA2-PA1-OA5
53	L	1004	CDL	CA3-OA5-PA1-OA2
53	L	1004	CDL	CA3-OA5-PA1-OA3
53	L	1004	CDL	CA3-OA5-PA1-OA4
53	L	1004	CDL	CB2-OB2-PB2-OB4
53	L	1005	CDL	CA3-OA5-PA1-OA3
53	L	1005	CDL	CA3-OA5-PA1-OA4
53	L	1005	CDL	CB3-OB5-PB2-OB3
53	M	503	CDL	O1-C1-CB2-OB2
53	M	503	CDL	CA2-C1-CB2-OB2
53	M	503	CDL	CB2-OB2-PB2-OB3
53	V	202	CDL	CB2-OB2-PB2-OB3
53	W	201	CDL	CA2-OA2-PA1-OA4
53	W	201	CDL	CA2-OA2-PA1-OA5
53	W	201	CDL	CA3-OA5-PA1-OA3
53	W	201	CDL	CA3-OA5-PA1-OA4
53	h	201	CDL	CA2-OA2-PA1-OA3
53	h	201	CDL	CA2-OA2-PA1-OA4
53	h	201	CDL	CA3-OA5-PA1-OA3
53	h	201	CDL	CB3-OB5-PB2-OB3
53	o	502	CDL	CA2-C1-CB2-OB2

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Mol	Chain	Res	Type	Atoms
53	o	502	CDL	CA2-OA2-PA1-OA4
53	o	502	CDL	CB2-OB2-PB2-OB3
53	o	502	CDL	CB2-OB2-PB2-OB4
53	o	502	CDL	CB2-OB2-PB2-OB5
53	o	502	CDL	CB3-OB5-PB2-OB3
53	x	101	CDL	CA2-OA2-PA1-OA4
53	x	101	CDL	CA3-OA5-PA1-OA3
53	x	101	CDL	CA4-CA3-OA5-PA1
53	x	101	CDL	CB2-OB2-PB2-OB4
54	X	101	ZMP	O4-C17-C18-C21
54	X	101	ZMP	C16-C17-C18-C21
54	X	101	ZMP	O4-C17-C18-C19
54	X	101	ZMP	C16-C17-C18-C19
54	X	101	ZMP	C16-C17-C18-C20
54	X	101	ZMP	C17-C16-N2-C15
54	g	201	ZMP	S1-C11-C12-N1
57	k	501	AMP	C5'-O5'-P-O1P
57	k	501	AMP	C5'-O5'-P-O2P
57	k	501	AMP	C5'-O5'-P-O3P
50	4	501	DCQ	C6-C7-C8-C9
53	h	201	CDL	O1-C1-CB2-OB2
53	o	502	CDL	O1-C1-CB2-OB2
54	X	101	ZMP	O3-C16-N2-C15
52	V	201	3PE	C2-C1-O11-P
53	L	1005	CDL	C1-CA2-OA2-PA1
53	L	1004	CDL	CB2-C1-CA2-OA2
53	h	201	CDL	CA2-C1-CB2-OB2
52	J	201	3PE	O21-C2-C3-O31
51	L	1003	PC1	C2-C1-O11-P
51	6	202	PC1	C11-C12-N-C14
51	M	502	PC1	C11-C12-N-C14
53	M	503	CDL	CB5-C51-C52-C53
51	6	202	PC1	C1-O11-P-O13
51	9	401	PC1	C1-O11-P-O13
52	J	201	3PE	C11-O13-P-O11
52	J	202	3PE	C1-O11-P-O13
52	M	501	3PE	C11-O13-P-O11
52	N	402	3PE	C1-O11-P-O13
52	V	201	3PE	C1-O11-P-O13
52	V	201	3PE	C11-O13-P-O11
52	i	502	3PE	C1-O11-P-O13
52	o	501	3PE	C11-O13-P-O11

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Mol	Chain	Res	Type	Atoms
53	L	1004	CDL	CB2-OB2-PB2-OB5
53	L	1005	CDL	CA2-OA2-PA1-OA5
53	L	1005	CDL	CA3-OA5-PA1-OA2
53	L	1005	CDL	CB3-OB5-PB2-OB2
53	W	201	CDL	CA3-OA5-PA1-OA2
53	h	201	CDL	CA2-OA2-PA1-OA5
53	h	201	CDL	CB3-OB5-PB2-OB2
53	o	502	CDL	CA2-OA2-PA1-OA5
53	x	101	CDL	CA2-OA2-PA1-OA5
53	x	101	CDL	CA3-OA5-PA1-OA2
53	x	101	CDL	CB2-OB2-PB2-OB5
53	x	101	CDL	CB3-OB5-PB2-OB2
53	M	503	CDL	CA7-C31-C32-C33
51	M	502	PC1	C11-C12-N-C15
53	W	201	CDL	C35-C36-C37-C38
51	9	401	PC1	C3B-C3C-C3D-C3E
52	i	502	3PE	C29-C2A-C2B-C2C
53	W	201	CDL	C82-C83-C84-C85
53	o	502	CDL	C78-C79-C80-C81
50	H	501	DCQ	C11-C10-C9-C8
53	L	1005	CDL	C21-C22-C23-C24
53	L	1005	CDL	C77-C78-C79-C80
53	M	503	CDL	C81-C82-C83-C84
53	L	1004	CDL	C1-CA2-OA2-PA1
52	i	501	3PE	C3C-C3D-C3E-C3F
53	M	503	CDL	C12-C13-C14-C15
53	M	503	CDL	C63-C64-C65-C66
53	L	1005	CDL	C22-C23-C24-C25
53	L	1005	CDL	C82-C83-C84-C85
53	W	201	CDL	CB5-C51-C52-C53
51	L	1003	PC1	C38-C39-C3A-C3B
52	N	402	3PE	C37-C38-C39-C3A
53	L	1004	CDL	C13-C14-C15-C16
53	L	1004	CDL	C78-C79-C80-C81
53	V	202	CDL	C79-C80-C81-C82
53	o	502	CDL	C81-C82-C83-C84
51	9	401	PC1	C3C-C3D-C3E-C3F
53	o	502	CDL	CB5-C51-C52-C53
51	9	401	PC1	C2C-C2D-C2E-C2F
51	6	202	PC1	C11-C12-N-C15
53	M	503	CDL	C52-C53-C54-C55
52	J	202	3PE	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
53	L	1005	CDL	C56-C57-C58-C59
53	o	502	CDL	C52-C53-C54-C55
52	J	202	3PE	C26-C27-C28-C29
52	L	1001	3PE	C34-C35-C36-C37
51	M	502	PC1	C3A-C3B-C3C-C3D
52	A	201	3PE	C38-C39-C3A-C3B
52	J	201	3PE	C21-C22-C23-C24
51	6	202	PC1	C3B-C3C-C3D-C3E
52	J	202	3PE	C32-C33-C34-C35
51	6	202	PC1	C11-C12-N-C13
52	N	402	3PE	C2B-C2C-C2D-C2E
51	L	1003	PC1	C31-C32-C33-C34
52	L	1002	3PE	C21-C22-C23-C24
52	A	201	3PE	C2E-C2F-C2G-C2H
53	V	202	CDL	C39-C40-C41-C42
52	A	201	3PE	C2C-C2D-C2E-C2F
52	J	202	3PE	C34-C35-C36-C37
52	A	201	3PE	C35-C36-C37-C38
52	N	402	3PE	O21-C2-C3-O31
51	M	502	PC1	C11-C12-N-C13
53	M	503	CDL	C11-C12-C13-C14
46	1	502	FMN	C2'-C3'-C4'-O4'
51	L	1003	PC1	C11-O13-P-O11
51	L	1003	PC1	C1-O11-P-O13
53	L	1004	CDL	CB3-OB5-PB2-OB2
53	M	503	CDL	CB2-OB2-PB2-OB5
53	V	202	CDL	CB2-OB2-PB2-OB5
51	L	1003	PC1	O11-C1-C2-C3
51	M	502	PC1	O11-C1-C2-C3
53	W	201	CDL	OA5-CA3-CA4-CA6
51	w	801	PC1	C3E-C3F-C3G-C3H
52	J	201	3PE	C1-C2-C3-O31
52	J	202	3PE	C1-C2-C3-O31
53	M	503	CDL	CA3-CA4-CA6-OA8
52	N	402	3PE	C29-C2A-C2B-C2C
51	L	1003	PC1	C23-C24-C25-C26
53	M	503	CDL	C35-C36-C37-C38
53	L	1005	CDL	C41-C42-C43-C44
53	o	502	CDL	C62-C63-C64-C65
54	X	101	ZMP	C2-C3-C4-C5
53	V	202	CDL	OB5-CB3-CB4-OB6
54	g	201	ZMP	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
52	V	201	3PE	C33-C34-C35-C36
53	h	201	CDL	C57-C58-C59-C60
53	L	1005	CDL	OA6-CA4-CA6-OA8
54	X	101	ZMP	O4-C17-C18-C20
54	g	201	ZMP	O4-C17-C18-C20
53	L	1004	CDL	C72-C73-C74-C75
53	V	202	CDL	C34-C35-C36-C37
53	M	503	CDL	C14-C15-C16-C17
53	M	503	CDL	C36-C37-C38-C39
53	o	502	CDL	OB5-CB3-CB4-CB6
52	L	1002	3PE	C2-C1-O11-P
58	s	201	MYR	C11-C10-C9-C8
53	L	1005	CDL	CA3-CA4-CA6-OA8
53	L	1004	CDL	CB7-C71-C72-C73
53	M	503	CDL	C59-C60-C61-C62
52	N	401	3PE	C1-O11-P-O13
53	o	502	CDL	CB3-OB5-PB2-OB2
51	L	1003	PC1	O11-C1-C2-O21
52	L	1001	3PE	O11-C1-C2-O21
53	V	202	CDL	OA5-CA3-CA4-OA6
53	W	201	CDL	OB5-CB3-CB4-OB6
53	V	202	CDL	C71-C72-C73-C74
53	L	1004	CDL	CA5-C11-C12-C13
53	W	201	CDL	C31-C32-C33-C34
53	L	1005	CDL	C17-C18-C19-C20
52	o	501	3PE	C2-C1-O11-P
53	L	1005	CDL	CA4-CA3-OA5-PA1
53	h	201	CDL	C1-CB2-OB2-PB2
53	o	502	CDL	C1-CA2-OA2-PA1
52	p	201	3PE	C22-C23-C24-C25
53	o	502	CDL	C12-C13-C14-C15
54	X	101	ZMP	O1-C10-S1-C11
54	g	201	ZMP	O1-C10-S1-C11
51	M	502	PC1	C25-C26-C27-C28
47	1	503	NAI	PN-O3-PA-O5B
53	V	202	CDL	OA5-CA3-CA4-CA6
53	V	202	CDL	OB5-CB3-CB4-CB6
52	i	501	3PE	C36-C37-C38-C39
52	M	501	3PE	C32-C31-O31-C3
54	g	201	ZMP	C9-C10-S1-C11
50	4	501	DCQ	C2-C3-O3-C3M
50	H	501	DCQ	C5-C4-O4-C4M

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Mol	Chain	Res	Type	Atoms
51	M	502	PC1	C2-C1-O11-P
52	N	402	3PE	C1-C2-C3-O31
51	w	801	PC1	O11-C1-C2-O21
53	L	1004	CDL	OA5-CA3-CA4-OA6
53	W	201	CDL	OA5-CA3-CA4-OA6
52	M	501	3PE	C34-C35-C36-C37
53	V	202	CDL	C77-C78-C79-C80
54	g	201	ZMP	C22-C1-C2-C3
53	W	201	CDL	C16-C17-C18-C19
53	M	503	CDL	OA6-CA4-CA6-OA8
53	M	503	CDL	C57-C58-C59-C60
47	1	503	NAI	C5D-O5D-PN-O3
53	L	1004	CDL	C73-C74-C75-C76
51	9	401	PC1	C11-O13-P-O11
52	N	402	3PE	C11-O13-P-O11
53	W	201	CDL	CB3-OB5-PB2-OB2
53	M	503	CDL	C58-C59-C60-C61
51	9	401	PC1	C34-C35-C36-C37
53	L	1005	CDL	C1-CB2-OB2-PB2
53	V	202	CDL	CA4-CA3-OA5-PA1
53	h	201	CDL	CB4-CB3-OB5-PB2
51	9	401	PC1	C1-O11-P-O12
51	L	1003	PC1	C11-O13-P-O12
51	L	1003	PC1	C1-O11-P-O14
52	N	401	3PE	C1-O11-P-O14
52	V	201	3PE	C1-O11-P-O12
52	V	201	3PE	C1-O11-P-O14
52	V	201	3PE	C11-O13-P-O14
52	i	501	3PE	C11-O13-P-O12
53	L	1004	CDL	CB2-OB2-PB2-OB3
53	L	1004	CDL	CB3-OB5-PB2-OB3
53	L	1004	CDL	CB3-OB5-PB2-OB4
53	L	1005	CDL	CA2-OA2-PA1-OA3
53	L	1005	CDL	CA2-OA2-PA1-OA4
53	L	1005	CDL	CB3-OB5-PB2-OB4
53	M	503	CDL	CB2-OB2-PB2-OB4
53	V	202	CDL	CB2-OB2-PB2-OB4
53	W	201	CDL	CA2-OA2-PA1-OA3
53	h	201	CDL	CB3-OB5-PB2-OB4
53	o	502	CDL	CA2-OA2-PA1-OA3
53	x	101	CDL	CA2-OA2-PA1-OA3
53	x	101	CDL	CA3-OA5-PA1-OA4

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Mol	Chain	Res	Type	Atoms
53	L	1005	CDL	CB7-C71-C72-C73
53	L	1004	CDL	OA5-CA3-CA4-CA6
52	N	402	3PE	C23-C24-C25-C26
53	L	1005	CDL	C37-C38-C39-C40
53	o	502	CDL	C76-C77-C78-C79
52	J	202	3PE	C21-C22-C23-C24
53	L	1005	CDL	C38-C39-C40-C41
46	1	502	FMN	N10-C1'-C2'-O2'
51	M	502	PC1	O11-C1-C2-O21
46	1	502	FMN	O3'-C3'-C4'-C5'
51	w	801	PC1	C31-C32-C33-C34
53	W	201	CDL	CA5-C11-C12-C13
47	1	503	NAI	C2D-C1D-N1N-C2N
51	9	401	PC1	O13-C11-C12-N
51	L	1003	PC1	O13-C11-C12-N
52	J	202	3PE	C25-C26-C27-C28
54	g	201	ZMP	O4-C17-C18-C21
52	J	202	3PE	O21-C2-C3-O31
53	L	1005	CDL	C58-C59-C60-C61
52	J	201	3PE	C27-C28-C29-C2A
52	M	501	3PE	C31-C32-C33-C34
53	L	1005	CDL	C42-C43-C44-C45
54	X	101	ZMP	O3-C16-C17-O4
46	1	502	FMN	O3'-C3'-C4'-O4'
47	1	503	NAI	O4D-C1D-N1N-C2N
52	o	501	3PE	C25-C26-C27-C28
51	9	401	PC1	C3-C2-O21-C21
52	L	1001	3PE	O11-C1-C2-C3
51	L	1003	PC1	C39-C3A-C3B-C3C
53	o	502	CDL	CA5-C11-C12-C13
51	w	801	PC1	C27-C28-C29-C2A
53	L	1004	CDL	CA4-CA3-OA5-PA1
53	x	101	CDL	OB5-CB3-CB4-OB6
52	A	201	3PE	C2D-C2E-C2F-C2G
53	x	101	CDL	C52-C51-CB5-OB6
53	L	1004	CDL	C12-C13-C14-C15
51	M	502	PC1	C11-O13-P-O11
51	w	801	PC1	C11-O13-P-O11
52	A	201	3PE	C1-O11-P-O13
52	N	401	3PE	C11-O13-P-O11
52	i	502	3PE	C11-O13-P-O11
53	L	1005	CDL	CB2-OB2-PB2-OB5

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Mol	Chain	Res	Type	Atoms
53	M	503	CDL	CB3-OB5-PB2-OB2
53	V	202	CDL	CA2-OA2-PA1-OA5
53	o	502	CDL	CA3-OA5-PA1-OA2
51	9	401	PC1	C22-C21-O21-C2
56	d	401	NDP	O4D-C1D-N1N-C6N
51	M	502	PC1	C39-C3A-C3B-C3C
52	o	501	3PE	C22-C23-C24-C25
53	V	202	CDL	C19-C20-C21-C22
53	o	502	CDL	C1-CB2-OB2-PB2
53	o	502	CDL	CB4-CB3-OB5-PB2
53	W	201	CDL	CB7-C71-C72-C73
52	M	501	3PE	O32-C31-O31-C3
51	w	801	PC1	C2B-C2C-C2D-C2E
52	i	501	3PE	C23-C24-C25-C26
51	w	801	PC1	O11-C1-C2-C3
52	J	202	3PE	C29-C2A-C2B-C2C
53	o	502	CDL	C19-C20-C21-C22
52	N	402	3PE	C24-C25-C26-C27
57	k	501	AMP	C4'-C5'-O5'-P
51	9	401	PC1	O22-C21-O21-C2
56	d	401	NDP	C2D-C1D-N1N-C6N
53	o	502	CDL	C72-C73-C74-C75
51	9	401	PC1	C22-C23-C24-C25
53	o	502	CDL	CB3-CB4-CB6-OB8
53	x	101	CDL	C16-C17-C18-C19
53	W	201	CDL	O1-C1-CB2-OB2
46	1	502	FMN	C2'-C3'-C4'-C5'
52	N	402	3PE	C27-C28-C29-C2A
51	M	502	PC1	C2F-C2G-C2H-C2I
54	g	201	ZMP	C1-C2-C3-C4
51	L	1003	PC1	C1-C2-O21-C21
52	L	1002	3PE	C1-C2-O21-C21
53	L	1005	CDL	C33-C34-C35-C36
52	p	201	3PE	C26-C27-C28-C29
50	4	501	DCQ	C4-C3-O3-C3M
50	H	501	DCQ	C3-C4-O4-C4M
51	L	1003	PC1	C36-C37-C38-C39
53	M	503	CDL	OB5-CB3-CB4-CB6
52	J	201	3PE	C2A-C2B-C2C-C2D
53	L	1005	CDL	C76-C77-C78-C79
51	M	502	PC1	C2B-C2C-C2D-C2E
51	w	801	PC1	C39-C3A-C3B-C3C

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Mol	Chain	Res	Type	Atoms
50	H	501	DCQ	C2-C3-O3-C3M
54	g	201	ZMP	C12-C11-S1-C10
51	M	502	PC1	C31-C32-C33-C34
52	M	501	3PE	C37-C38-C39-C3A
52	i	502	3PE	C32-C33-C34-C35
53	W	201	CDL	CA2-C1-CB2-OB2
47	l	503	NAI	C2D-C1D-N1N-C6N
52	i	501	3PE	C33-C34-C35-C36
52	A	201	3PE	C3C-C3D-C3E-C3F
52	L	1001	3PE	C3A-C3B-C3C-C3D
53	V	202	CDL	C40-C41-C42-C43
52	V	201	3PE	O21-C21-C22-C23
52	L	1001	3PE	C1-C2-C3-O31
52	N	401	3PE	C32-C33-C34-C35
52	N	402	3PE	C28-C29-C2A-C2B
53	L	1004	CDL	C72-C71-CB7-OB8
52	p	201	3PE	C21-C22-C23-C24
51	M	502	PC1	C3B-C3C-C3D-C3E
53	M	503	CDL	OB5-CB3-CB4-OB6
53	h	201	CDL	CB7-C71-C72-C73
52	V	201	3PE	C32-C33-C34-C35
53	L	1005	CDL	C55-C56-C57-C58
53	W	201	CDL	OB5-CB3-CB4-CB6
51	L	1003	PC1	O31-C31-C32-C33
52	J	202	3PE	C2-C1-O11-P
53	M	503	CDL	C12-C11-CA5-OA6
51	w	801	PC1	C28-C29-C2A-C2B
54	X	101	ZMP	C19-C18-C21-O5
53	W	201	CDL	C75-C76-C77-C78
53	V	202	CDL	C44-C45-C46-C47
53	x	101	CDL	CB6-CB4-OB6-CB5
51	L	1003	PC1	C24-C25-C26-C27
52	L	1002	3PE	C25-C26-C27-C28
51	6	202	PC1	O31-C31-C32-C33
52	i	502	3PE	C36-C37-C38-C39
53	M	503	CDL	C72-C71-CB7-OB8
53	o	502	CDL	C72-C71-CB7-OB8
50	4	501	DCQ	C5-C4-O4-C4M
53	L	1004	CDL	C54-C55-C56-C57
52	A	201	3PE	O21-C21-C22-C23
52	N	402	3PE	O21-C21-C22-C23
52	V	201	3PE	O31-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
53	M	503	CDL	C52-C51-CB5-OB6
53	x	101	CDL	C72-C71-CB7-OB8
51	w	801	PC1	C11-C12-N-C14
56	d	401	NDP	O4B-C4B-C5B-O5B
53	L	1005	CDL	C11-C12-C13-C14
53	h	201	CDL	C52-C51-CB5-OB6
54	g	201	ZMP	C16-C17-C18-C20
52	L	1001	3PE	O21-C21-C22-C23
52	N	401	3PE	O21-C21-C22-C23
47	l	503	NAI	O4D-C1D-N1N-C6N
52	V	201	3PE	O11-C1-C2-C3
51	L	1003	PC1	C3C-C3D-C3E-C3F
53	L	1005	CDL	C34-C35-C36-C37
53	L	1004	CDL	OA6-CA4-CA6-OA8
53	V	202	CDL	OB6-CB4-CB6-OB8
54	g	201	ZMP	O4-C17-C18-C19
56	d	401	NDP	C5B-O5B-PA-O3
51	9	401	PC1	C31-C32-C33-C34
52	N	401	3PE	C31-C32-C33-C34
52	L	1001	3PE	O31-C31-C32-C33
53	o	502	CDL	C32-C31-CA7-OA8
58	s	201	MYR	C7-C8-C9-C10
53	L	1005	CDL	C32-C31-CA7-OA8
51	M	502	PC1	C28-C29-C2A-C2B
50	4	501	DCQ	C3-C4-O4-C4M
50	H	501	DCQ	C4-C3-O3-C3M
57	k	501	AMP	O4'-C4'-C5'-O5'
52	A	201	3PE	C24-C25-C26-C27
53	L	1005	CDL	CB5-C51-C52-C53
53	M	503	CDL	C12-C11-CA5-OA7
53	o	502	CDL	C72-C71-CB7-OB9
52	M	501	3PE	O21-C21-C22-C23
52	A	201	3PE	O22-C21-C22-C23
52	V	201	3PE	O32-C31-C32-C33
53	x	101	CDL	C72-C71-CB7-OB9
53	V	202	CDL	C31-C32-C33-C34
53	M	503	CDL	CB2-C1-CA2-OA2
52	N	402	3PE	O22-C21-C22-C23
53	M	503	CDL	C72-C71-CB7-OB9
51	w	801	PC1	C24-C25-C26-C27
53	M	503	CDL	C52-C51-CB5-OB7
53	L	1004	CDL	C33-C34-C35-C36

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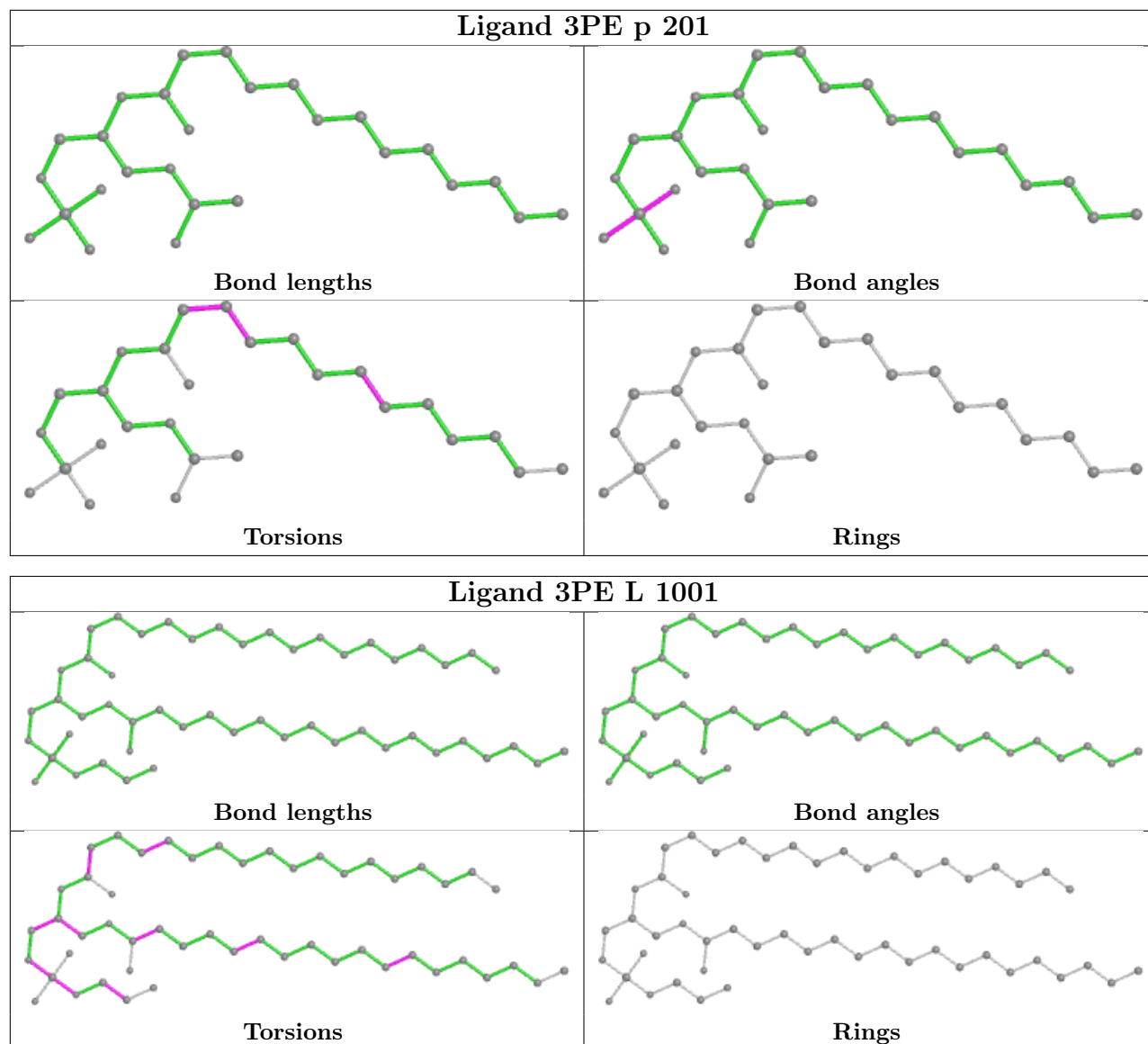
Mol	Chain	Res	Type	Atoms
53	h	201	CDL	C52-C51-CB5-OB7
52	i	501	3PE	C3D-C3E-C3F-C3G
46	1	502	FMN	C4'-C5'-O5'-P
53	x	101	CDL	CB4-CB3-OB5-PB2
52	L	1001	3PE	C23-C24-C25-C26
47	1	503	NAI	C2N-C3N-C7N-N7N
52	L	1001	3PE	C1-O11-P-O14
52	i	501	3PE	C1-O11-P-O12
52	i	501	3PE	C1-O11-P-O14
52	i	502	3PE	C11-O13-P-O14
53	M	503	CDL	CB3-OB5-PB2-OB3
53	W	201	CDL	CB3-OB5-PB2-OB4
53	x	101	CDL	CB3-OB5-PB2-OB3
53	x	101	CDL	CB3-OB5-PB2-OB4
52	L	1001	3PE	O32-C31-C32-C33
52	L	1001	3PE	O22-C21-C22-C23
53	L	1005	CDL	C32-C31-CA7-OA9
51	M	502	PC1	C3F-C3G-C3H-C3I
52	N	401	3PE	O22-C21-C22-C23
52	J	201	3PE	C12-C11-O13-P
52	N	402	3PE	C1-C2-O21-C21
53	o	502	CDL	CB3-CB4-OB6-CB5
53	V	202	CDL	CA7-C31-C32-C33
51	w	801	PC1	C2E-C2F-C2G-C2H
53	x	101	CDL	C75-C76-C77-C78
52	N	401	3PE	C27-C28-C29-C2A
52	L	1002	3PE	O21-C21-C22-C23
52	N	401	3PE	O31-C31-C32-C33
52	i	502	3PE	O21-C21-C22-C23
53	W	201	CDL	C14-C15-C16-C17
53	L	1004	CDL	CB4-CB3-OB5-PB2
46	1	502	FMN	N10-C1'-C2'-C3'
51	w	801	PC1	C26-C27-C28-C29
52	i	502	3PE	O22-C21-C22-C23
53	L	1004	CDL	C32-C31-CA7-OA8
52	M	501	3PE	O22-C21-C22-C23
53	o	502	CDL	C32-C31-CA7-OA9
53	W	201	CDL	C81-C82-C83-C84
51	M	502	PC1	C35-C36-C37-C38

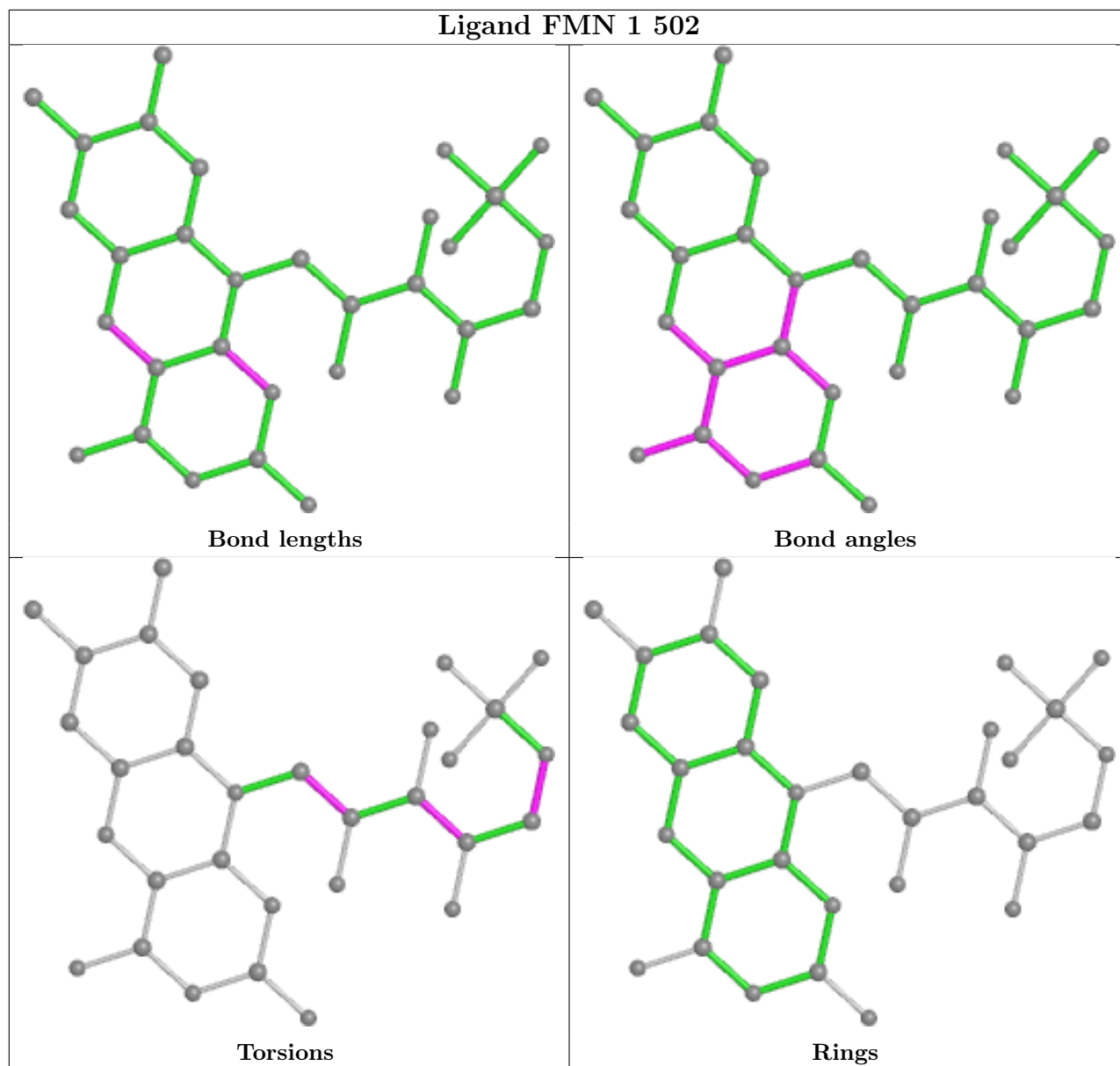
There are no ring outliers.

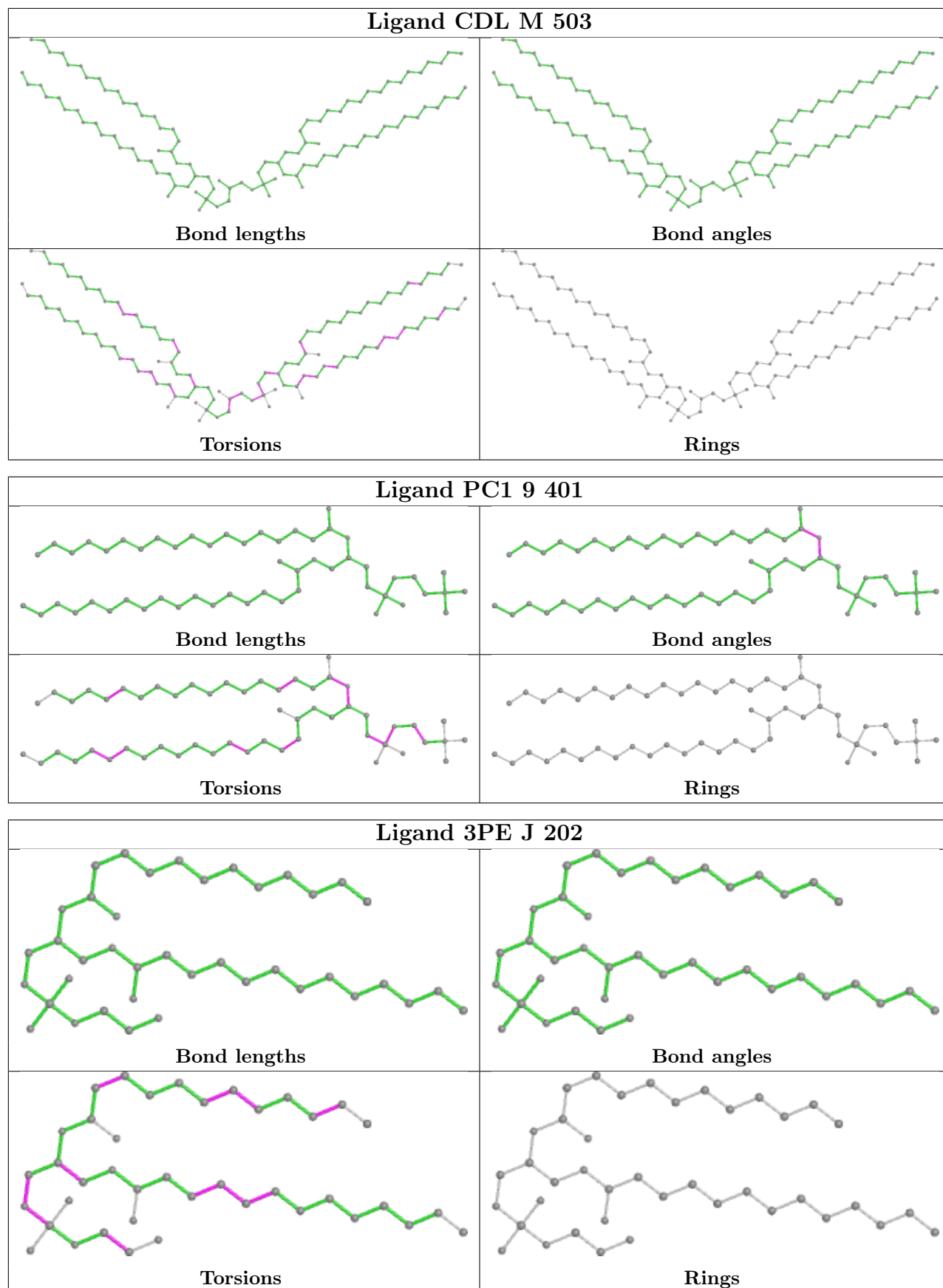
23 monomers are involved in 58 short contacts:

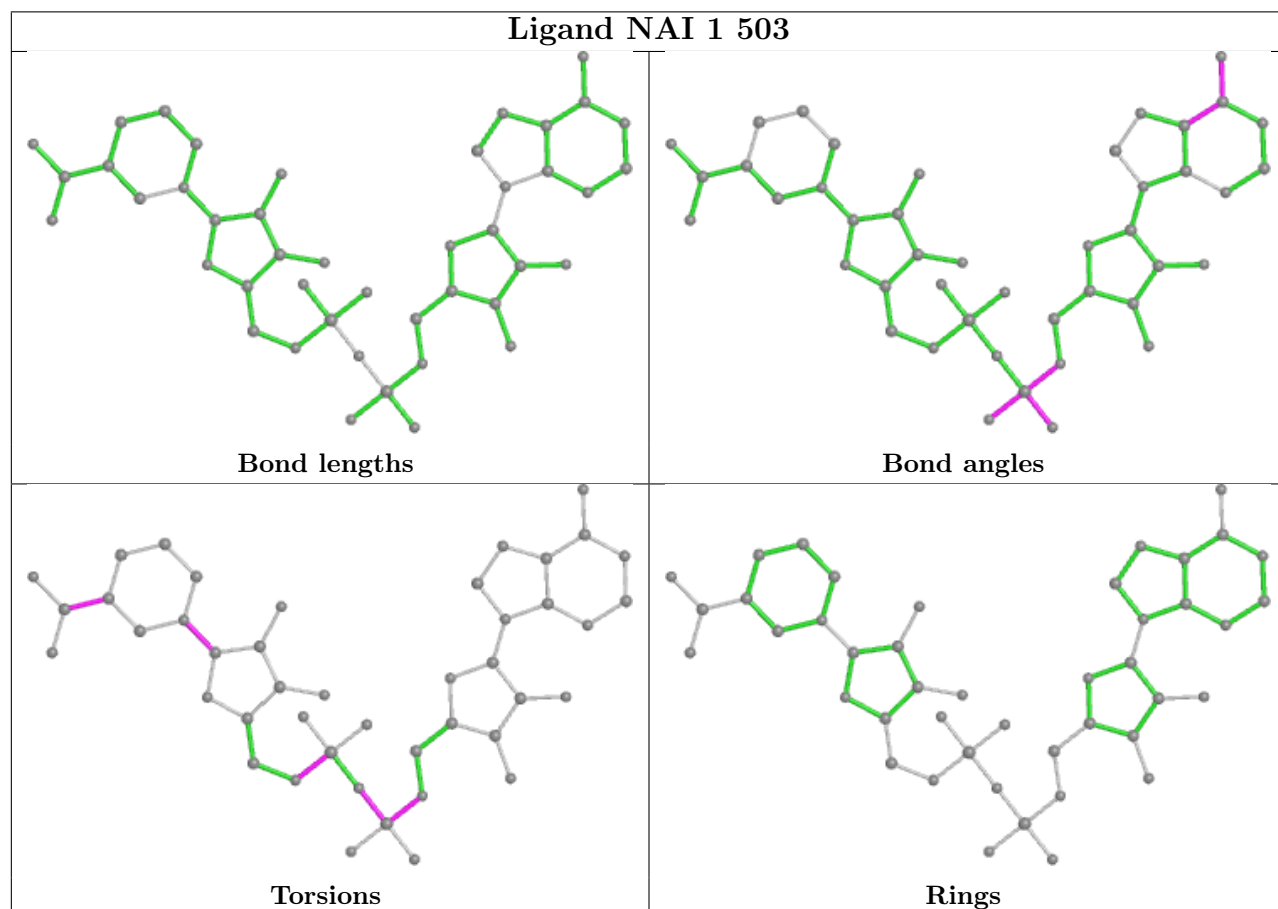
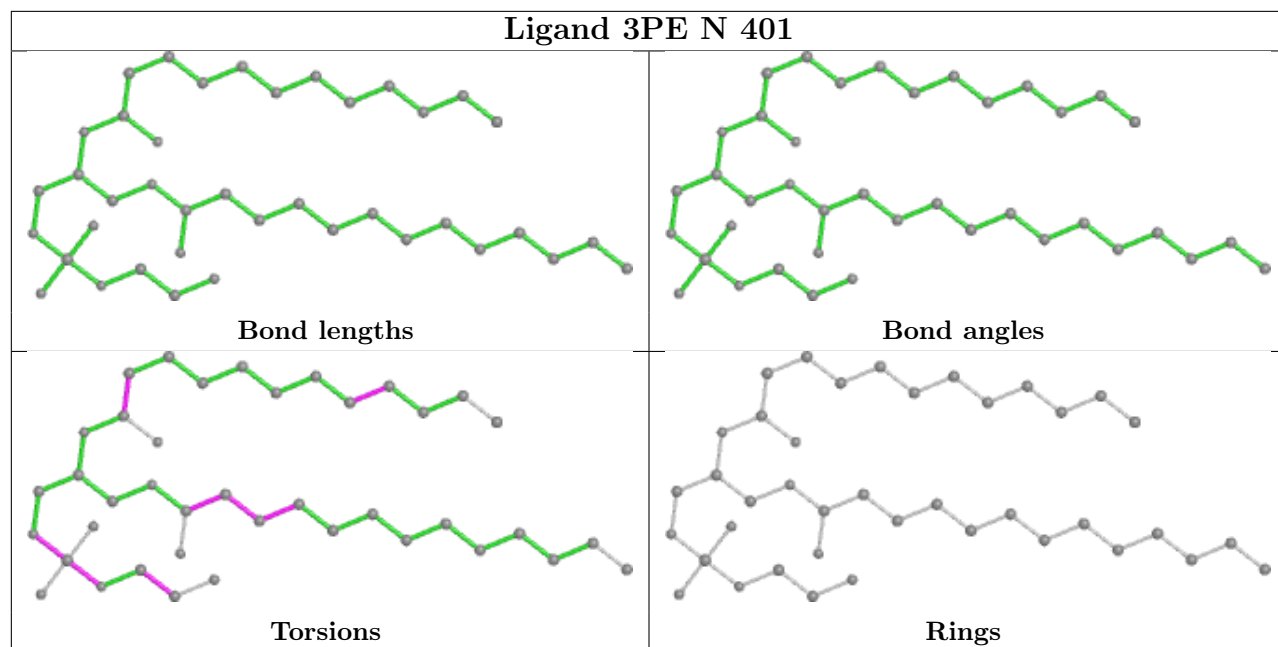
Mol	Chain	Res	Type	Clashes	Symm-Clashes
52	L	1001	3PE	1	0
53	M	503	CDL	9	0
51	9	401	PC1	1	0
52	J	202	3PE	3	0
52	N	401	3PE	1	0
47	1	503	NAI	3	0
53	W	201	CDL	3	0
51	M	502	PC1	3	0
53	L	1004	CDL	2	0
45	1	501	SF4	2	0
52	A	201	3PE	3	0
48	2	300	FES	1	0
51	L	1003	PC1	2	0
45	6	201	SF4	1	0
50	H	501	DCQ	2	0
53	V	202	CDL	6	0
54	X	101	ZMP	1	0
50	4	501	DCQ	1	0
52	J	201	3PE	3	0
53	L	1005	CDL	7	0
51	6	202	PC1	1	0
52	V	201	3PE	2	0
45	3	801	SF4	1	0

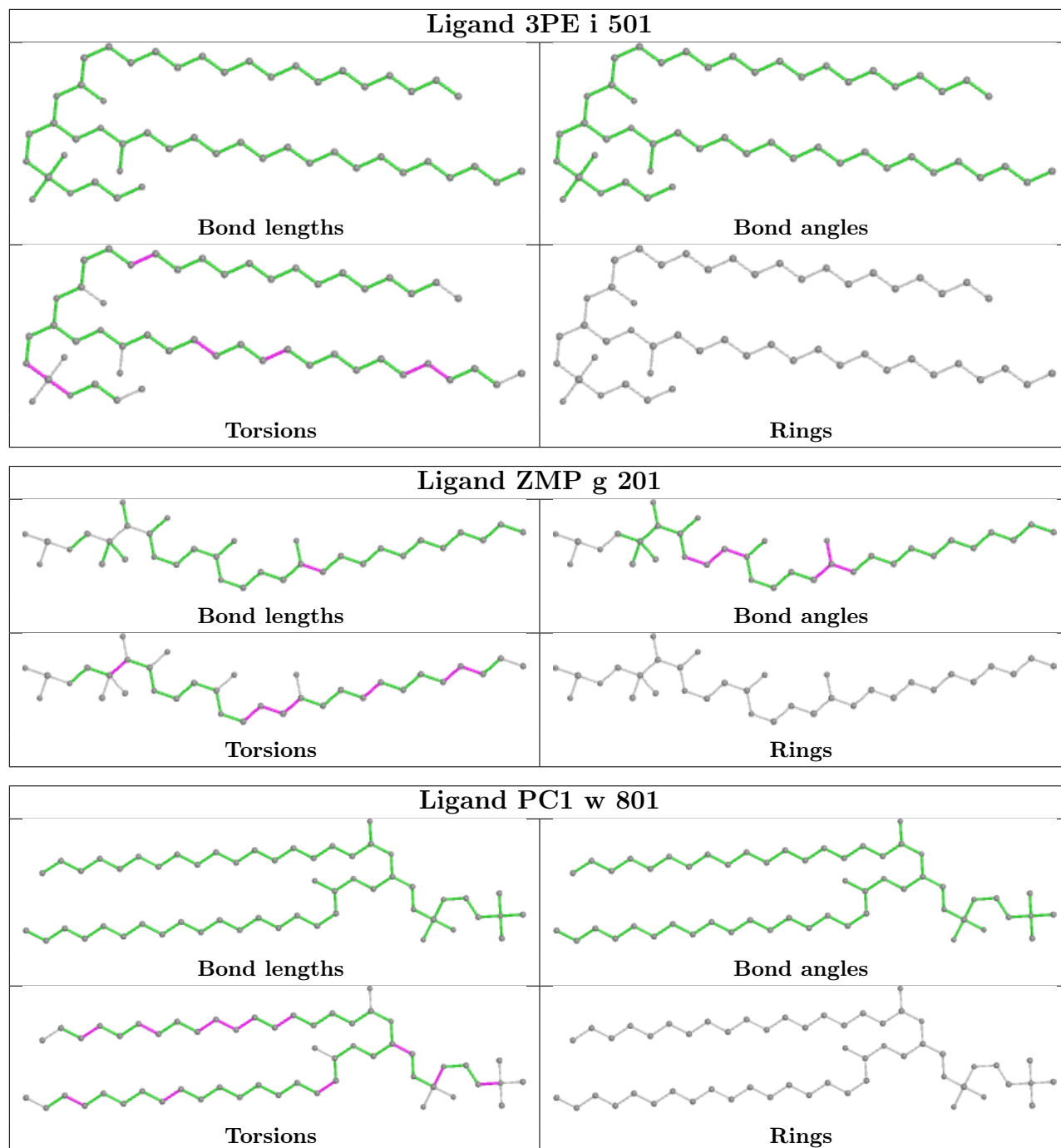
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

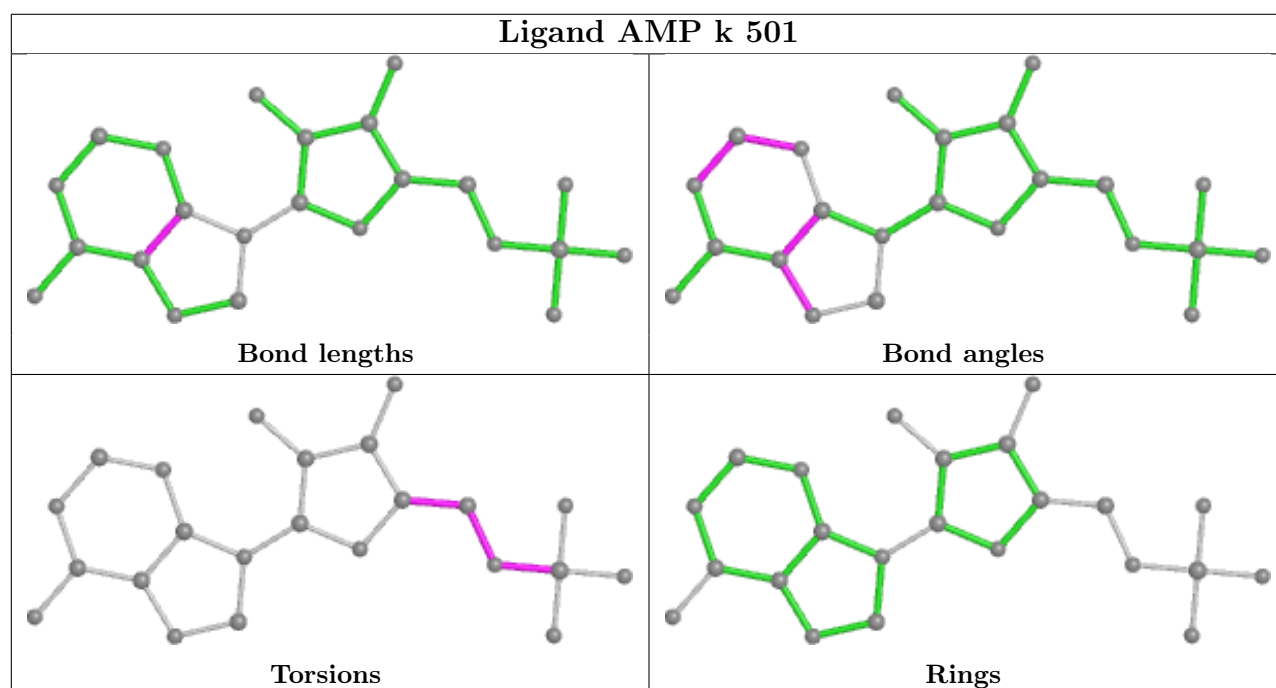
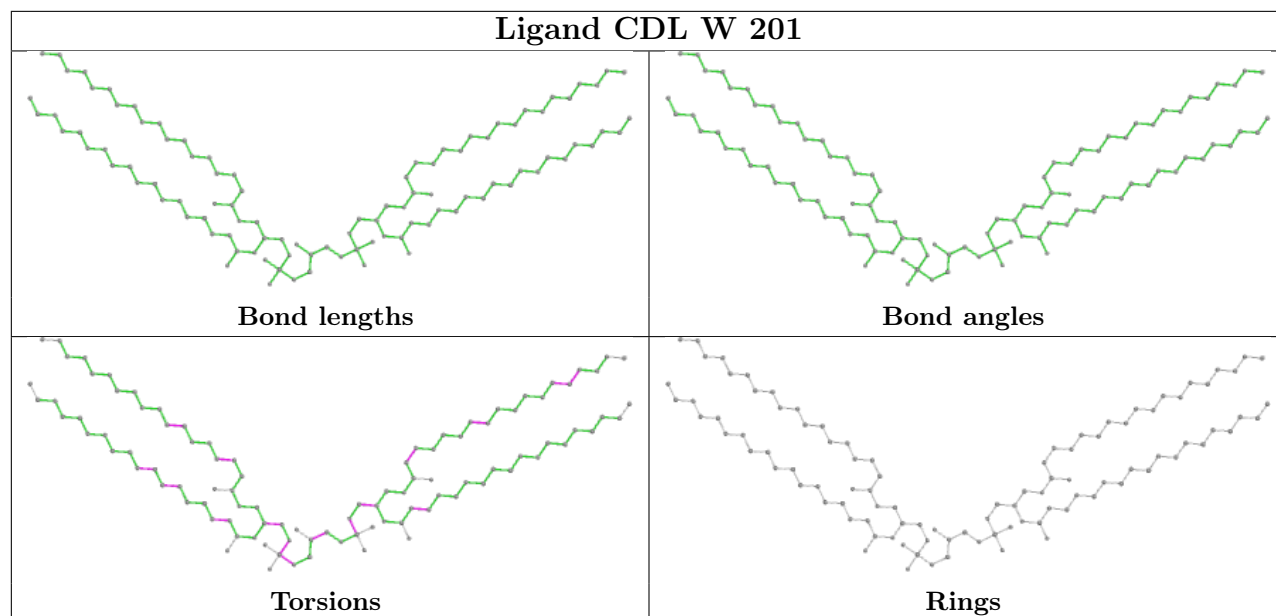


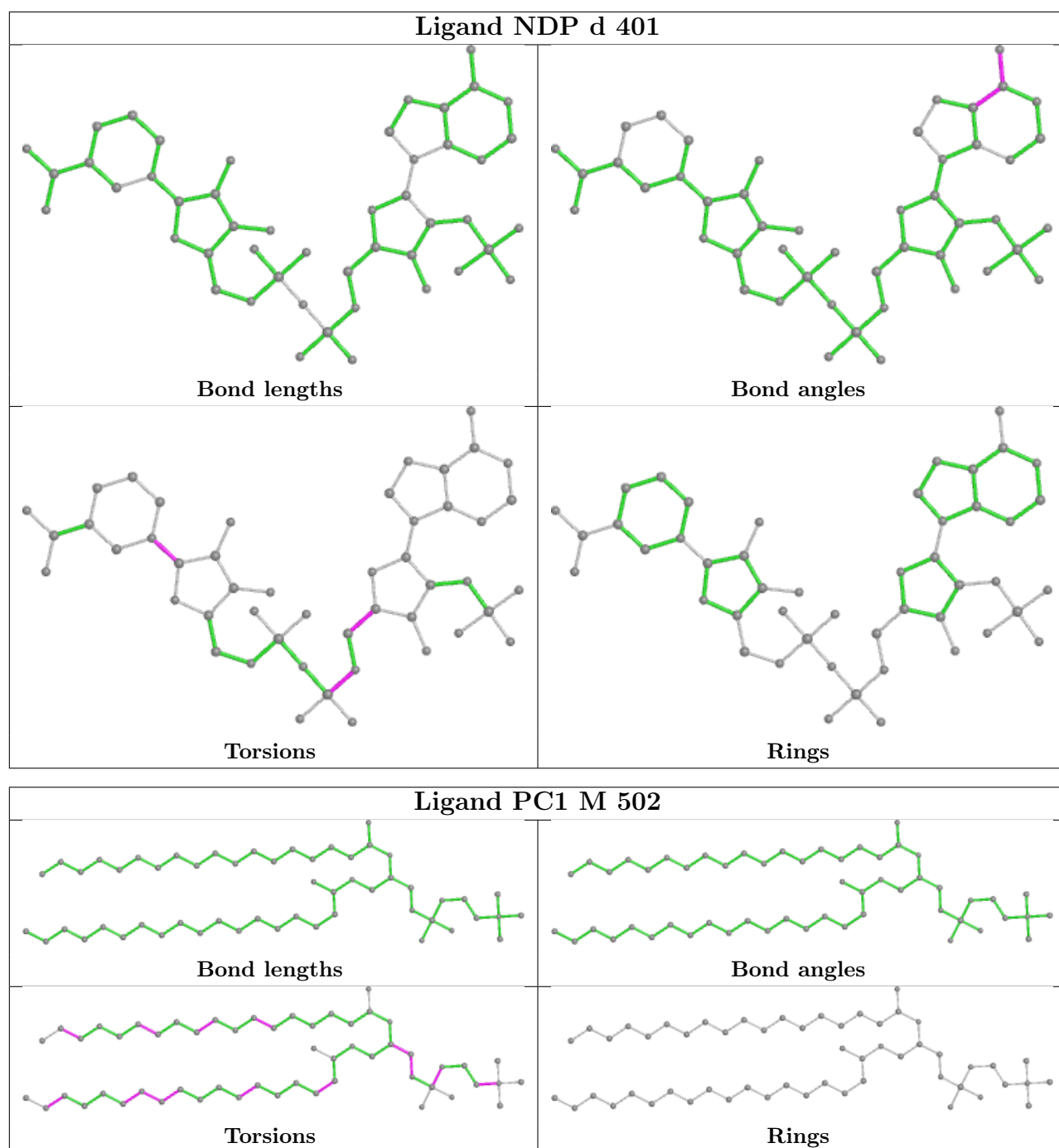


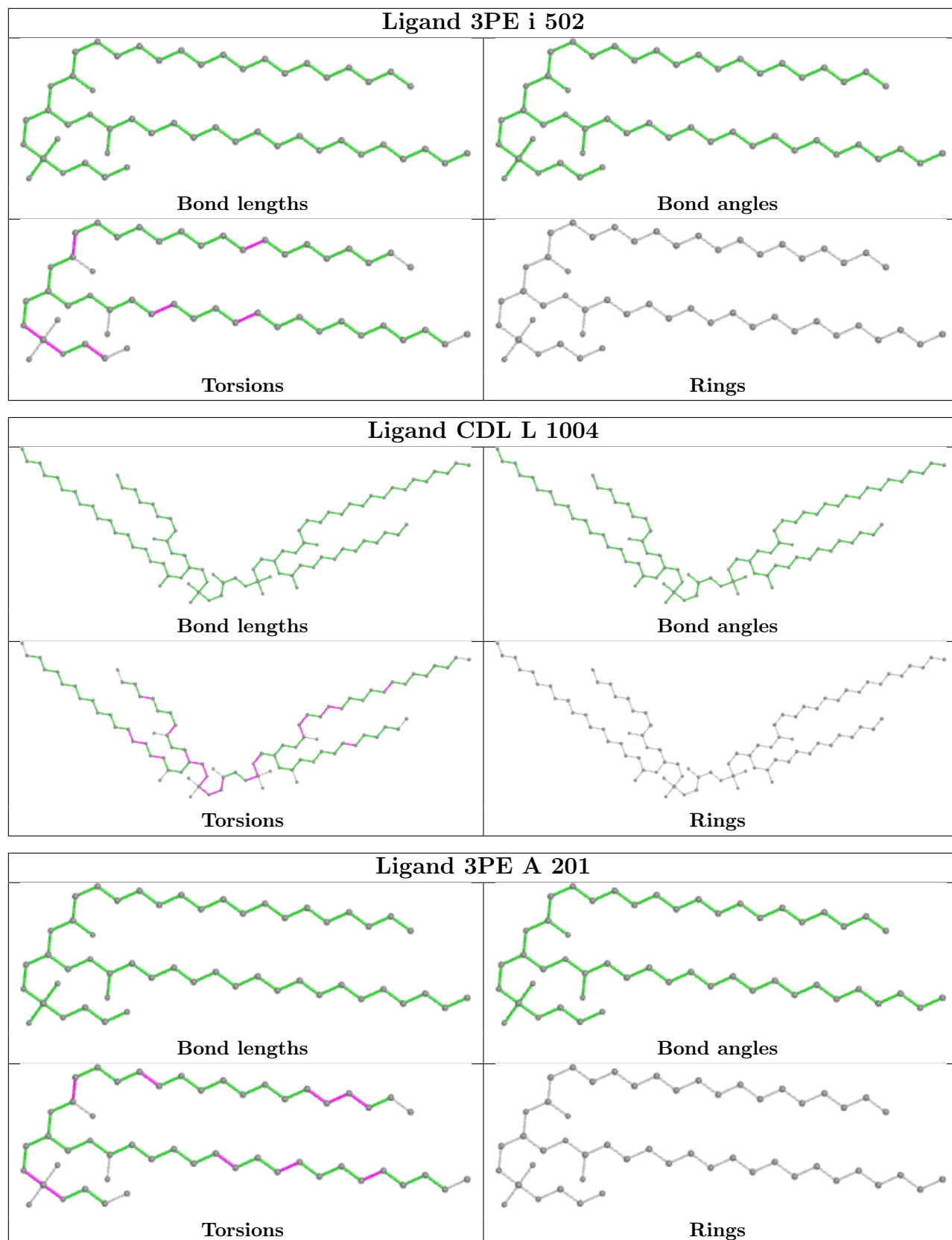


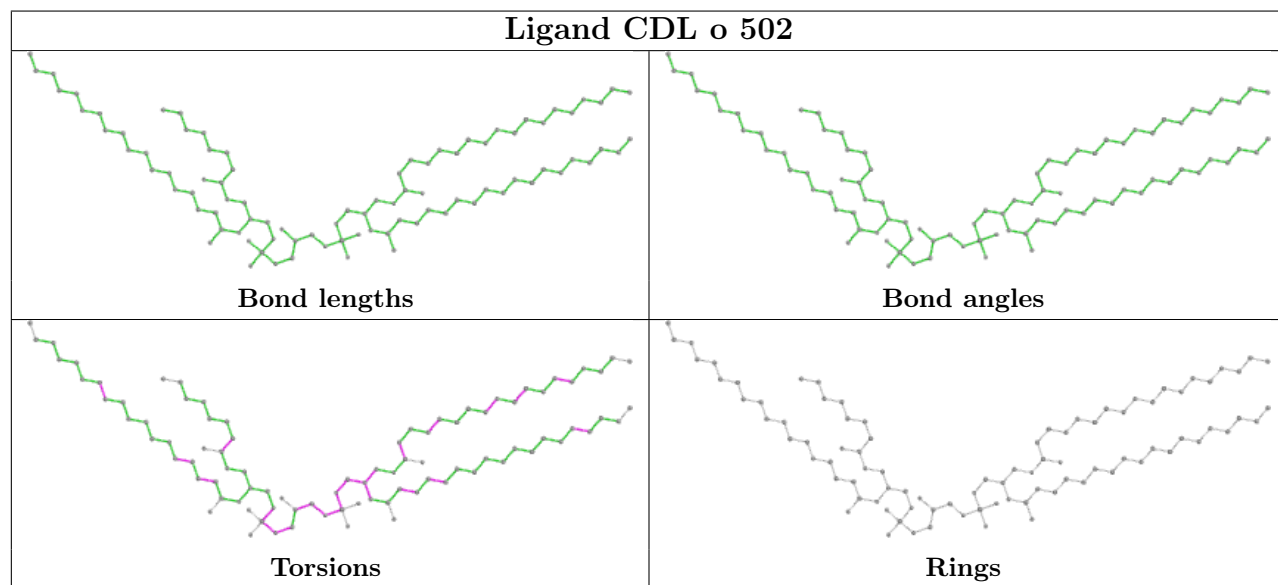
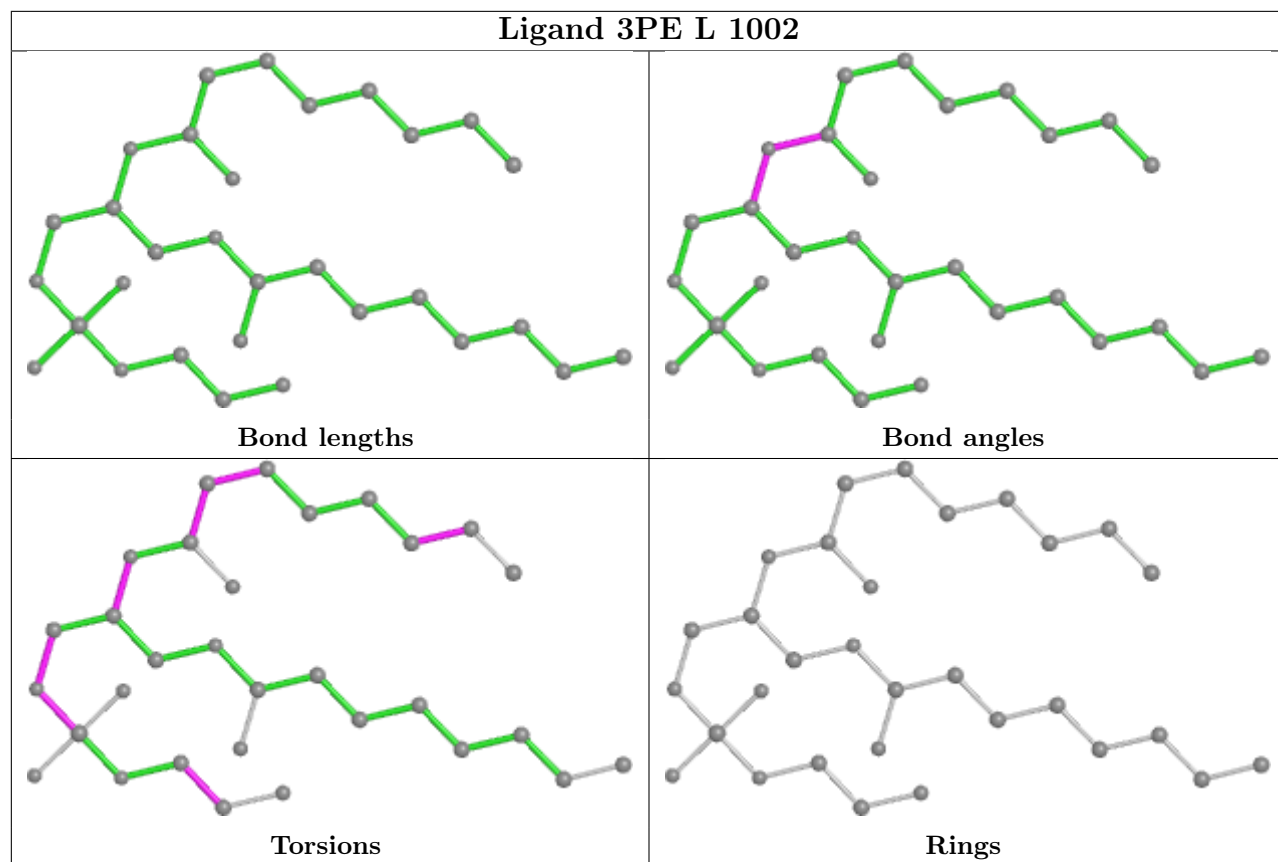


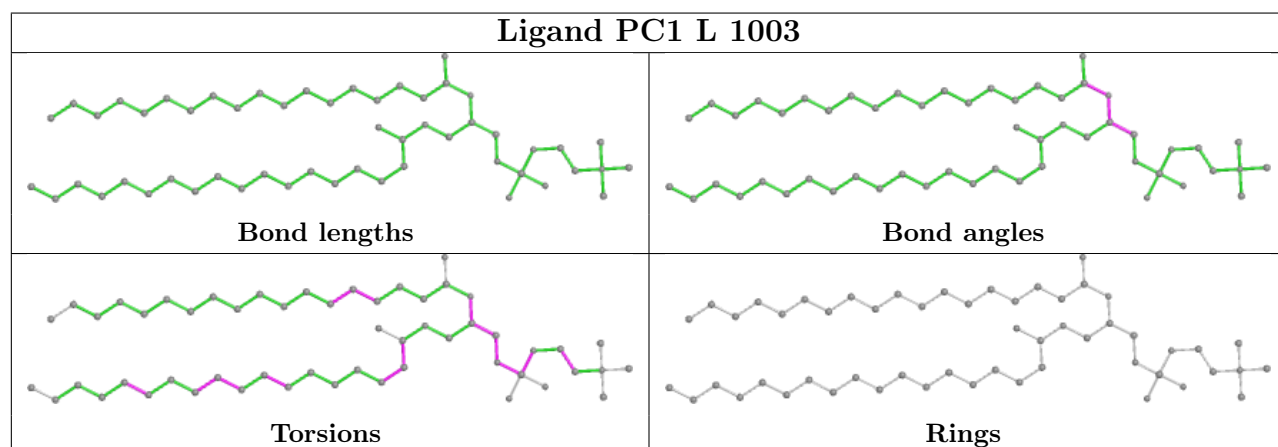
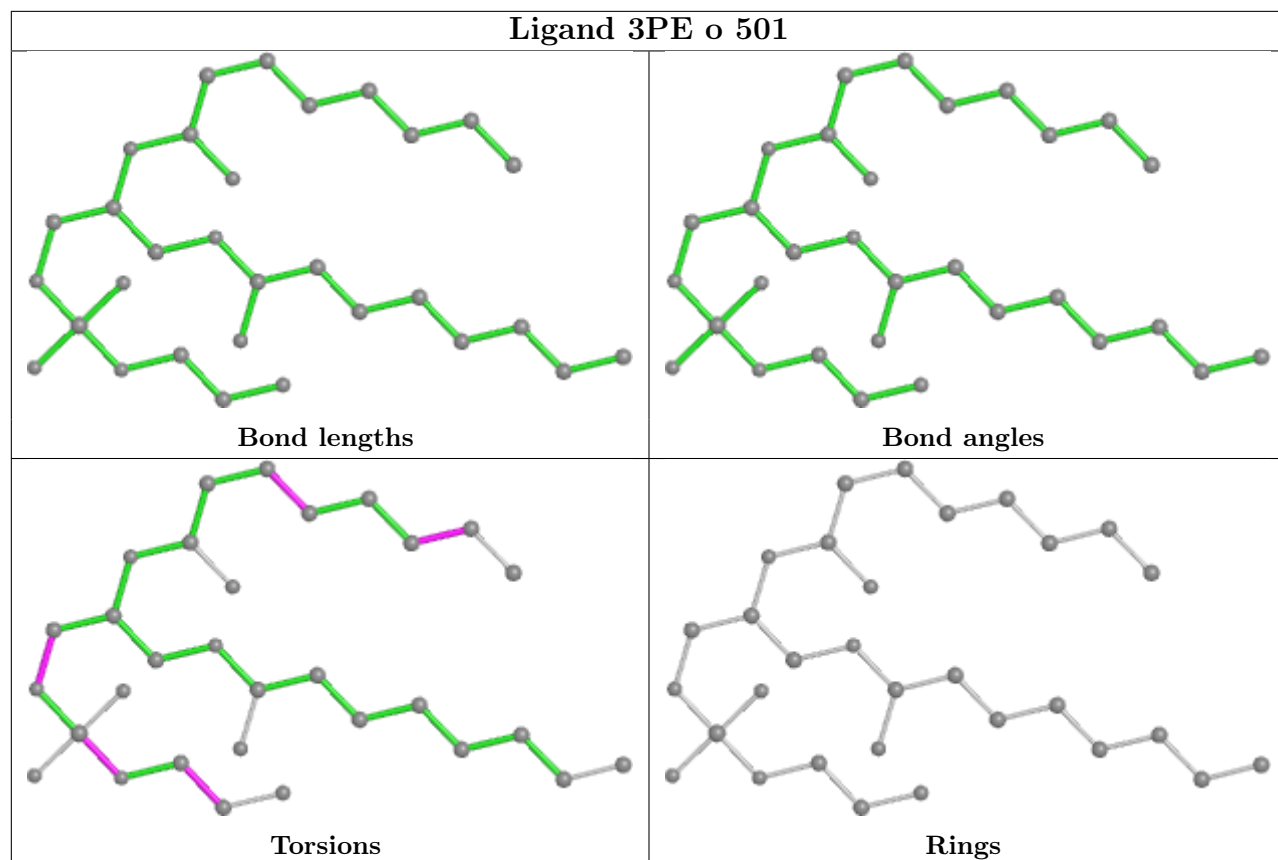


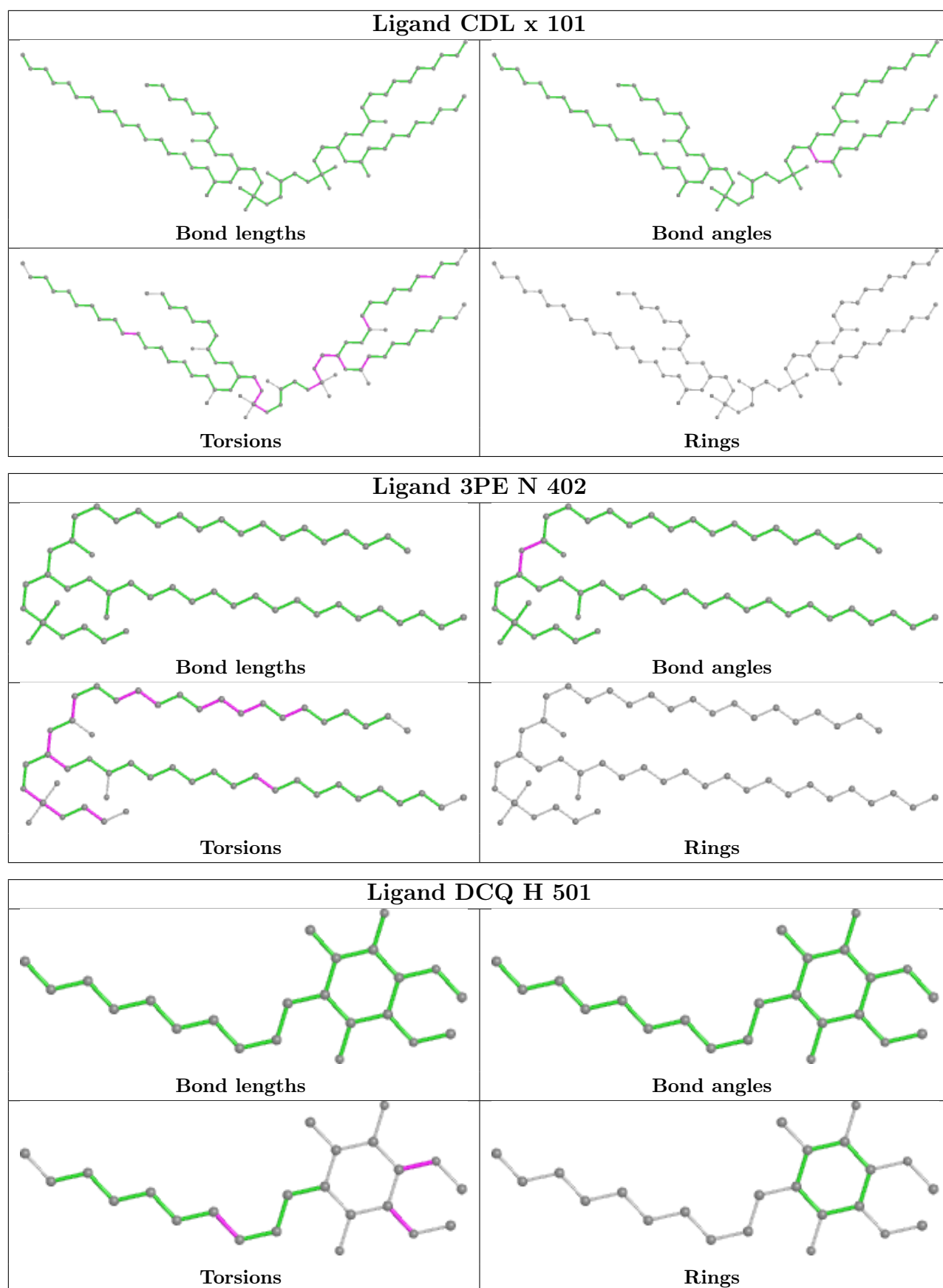


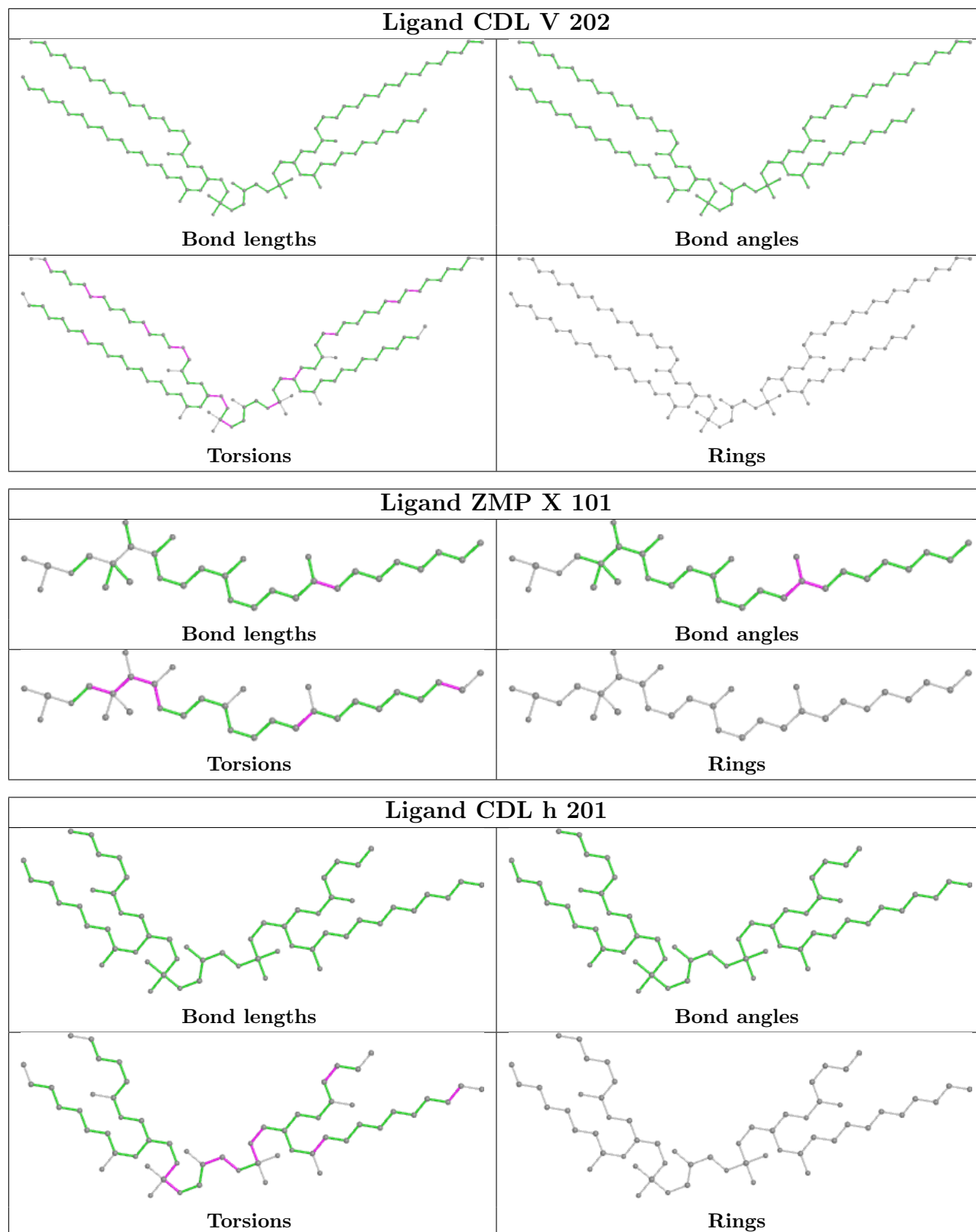


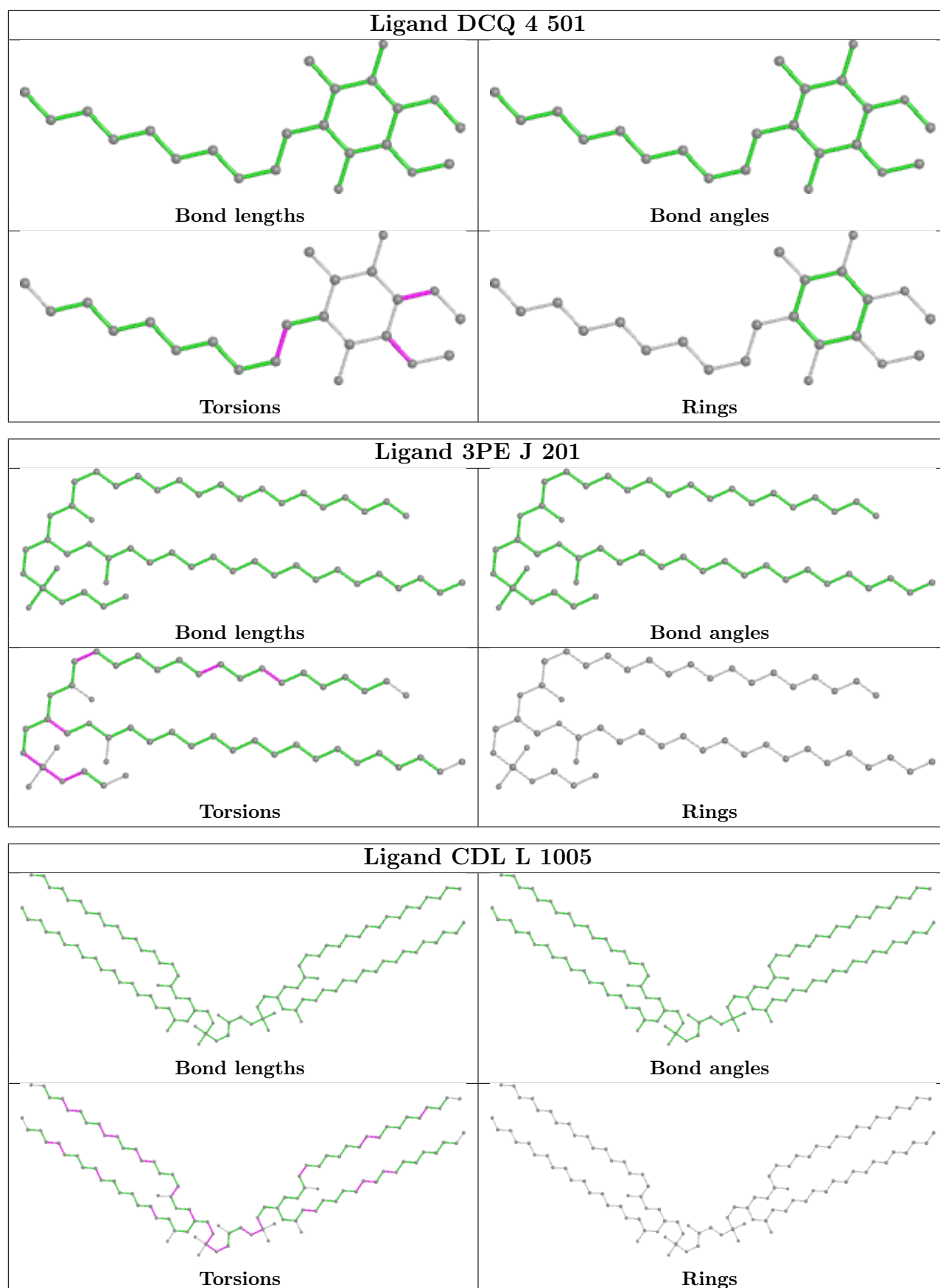


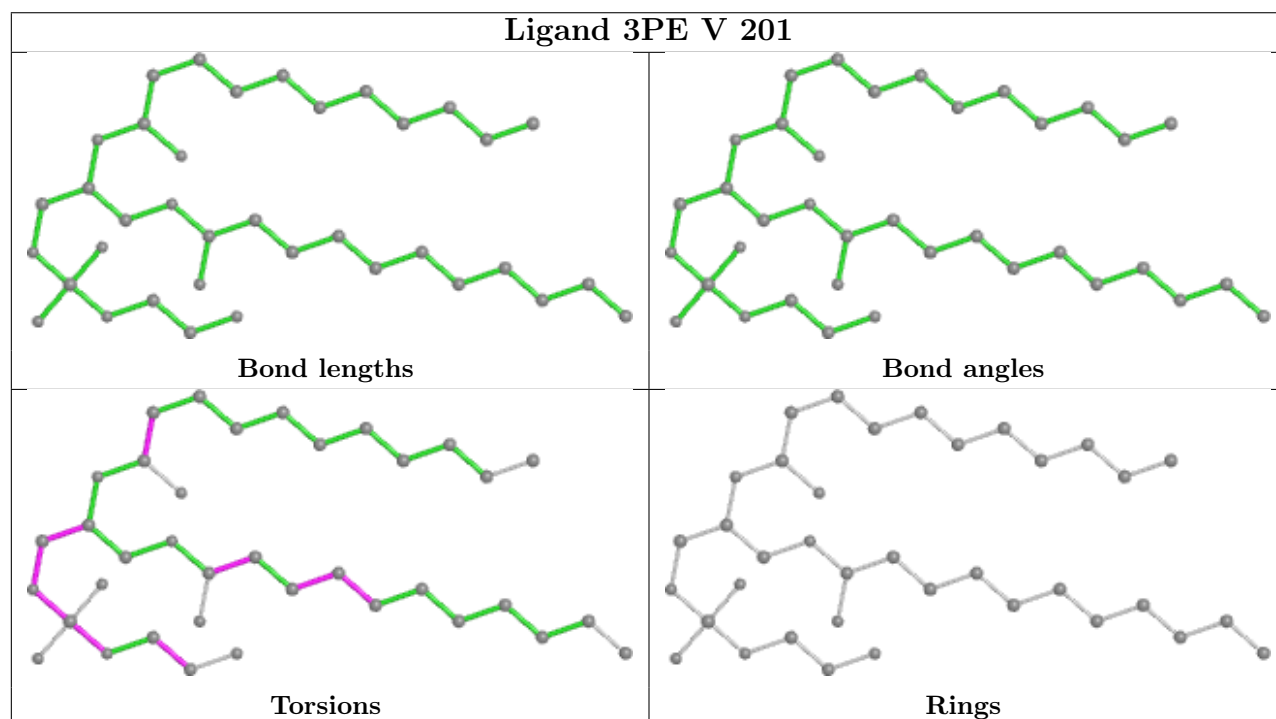
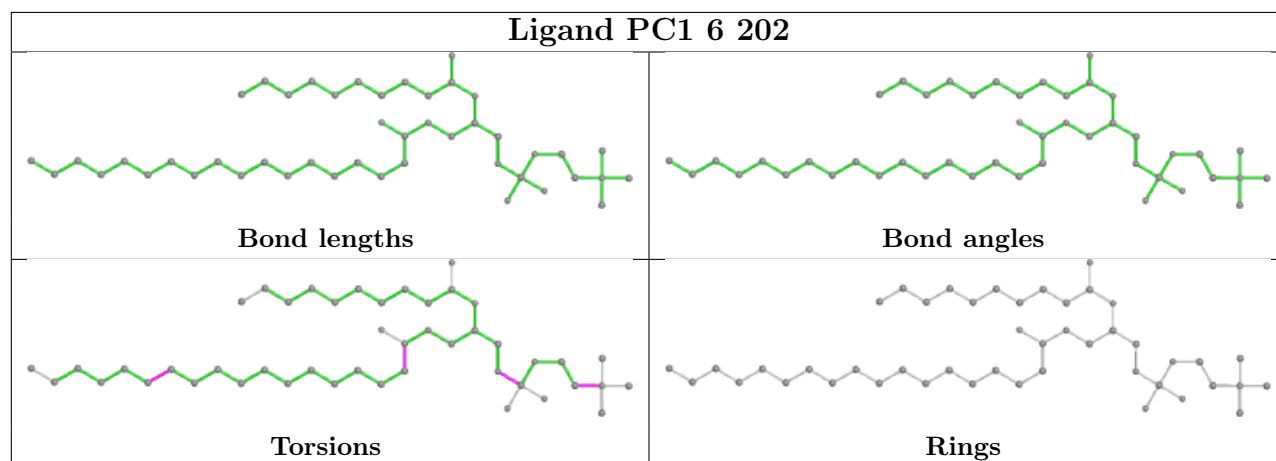
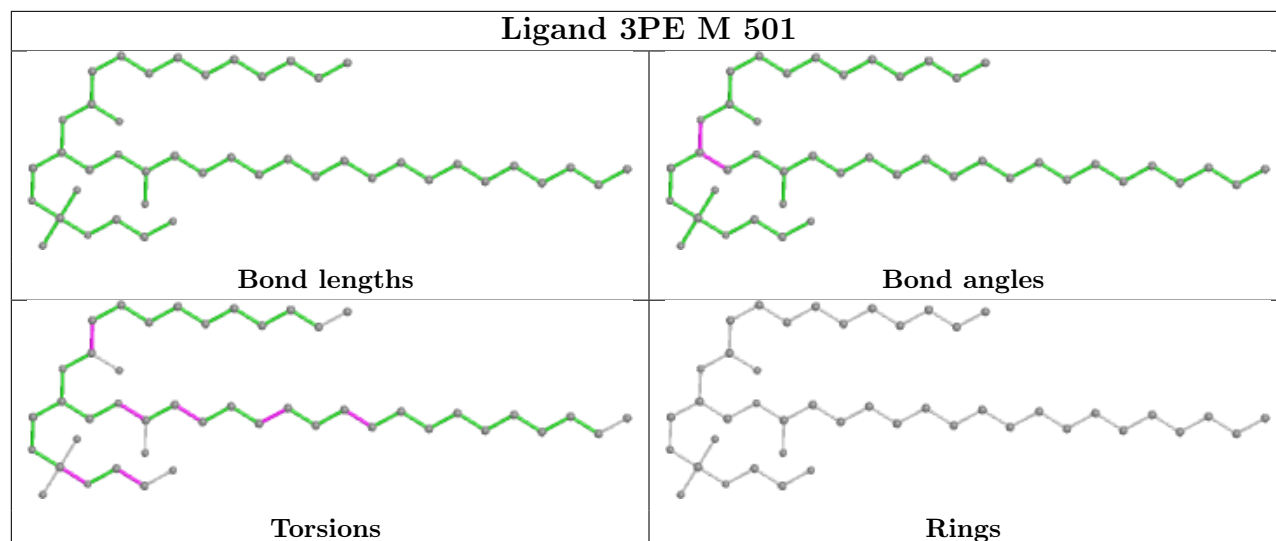












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

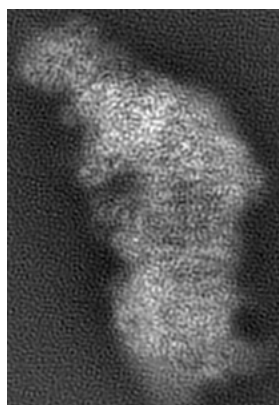
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11244. These allow visual inspection of the internal detail of the map and identification of artifacts.

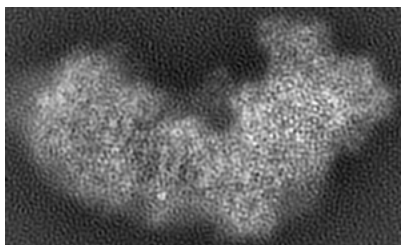
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

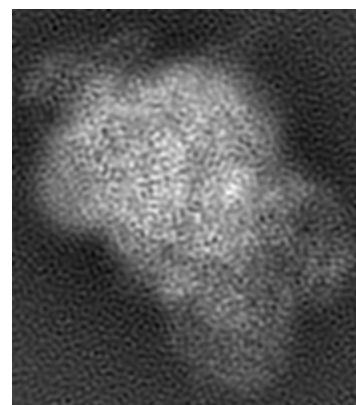
6.1.1 Primary map



X



Y

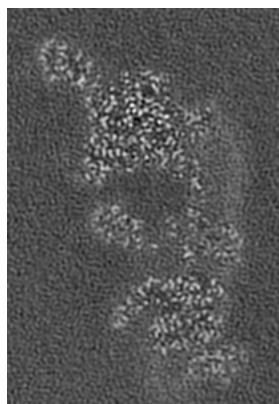


Z

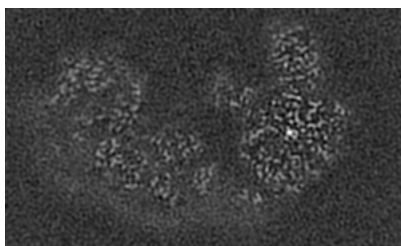
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

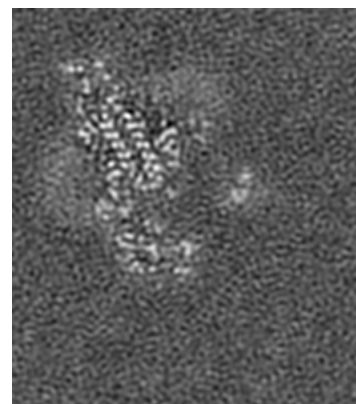
6.2.1 Primary map



X Index: 80



Y Index: 91

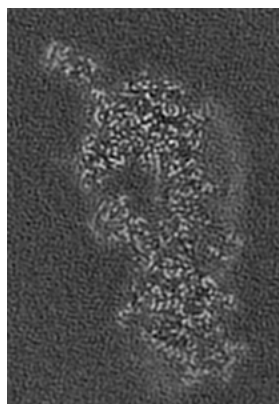


Z Index: 133

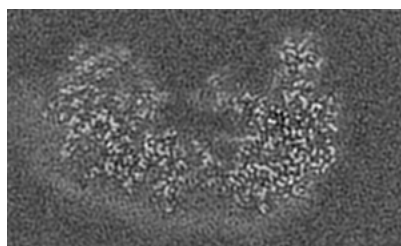
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

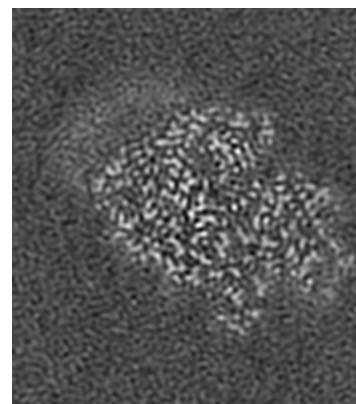
6.3.1 Primary map



X Index: 74



Y Index: 100



Z Index: 195

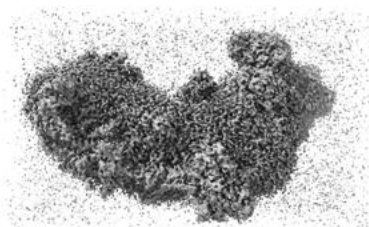
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

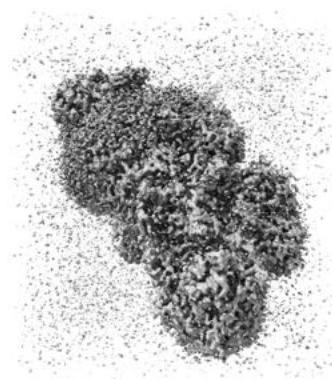
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.045. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

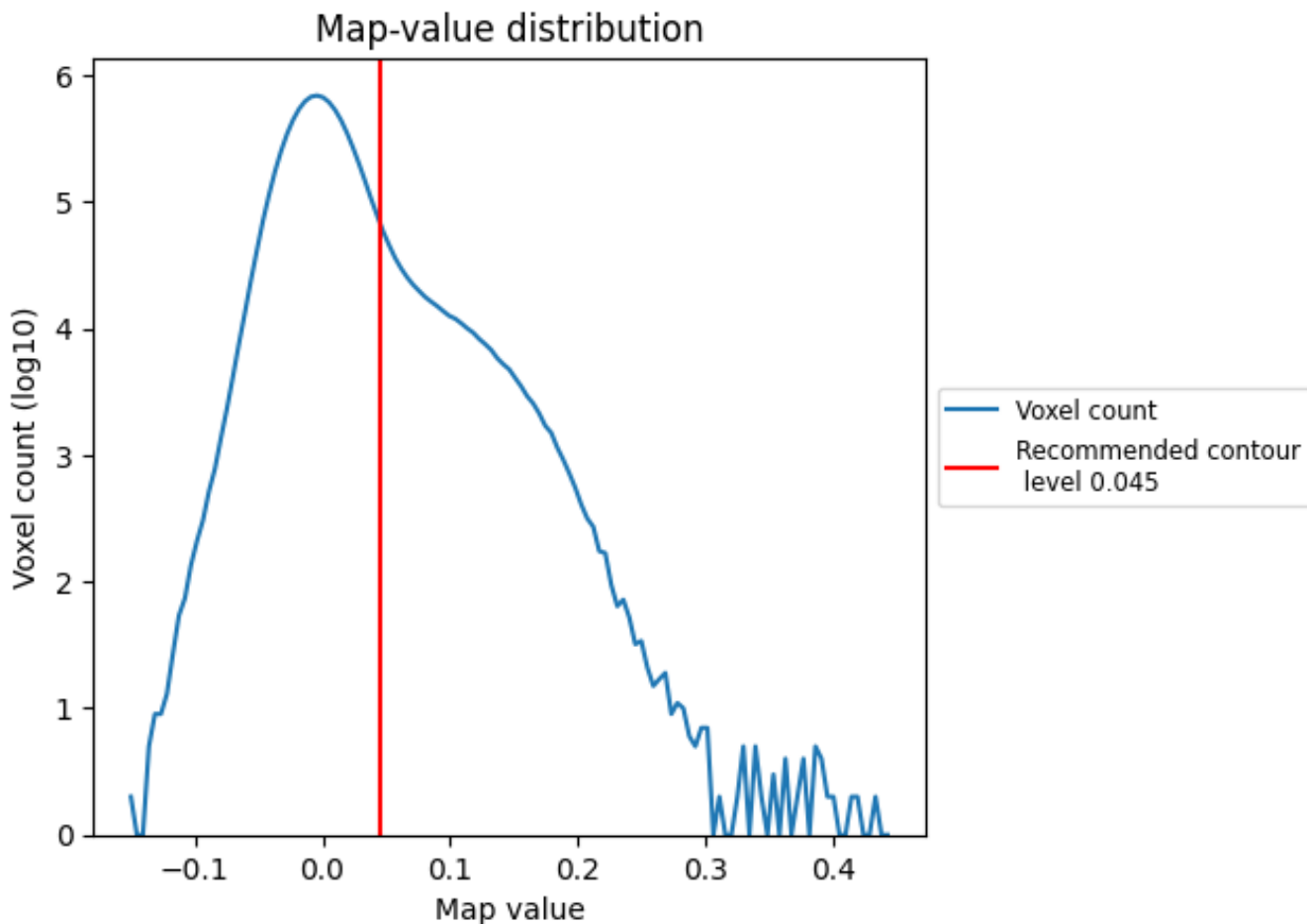
6.5 Mask visualisation

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

7 Map analysis [i](#)

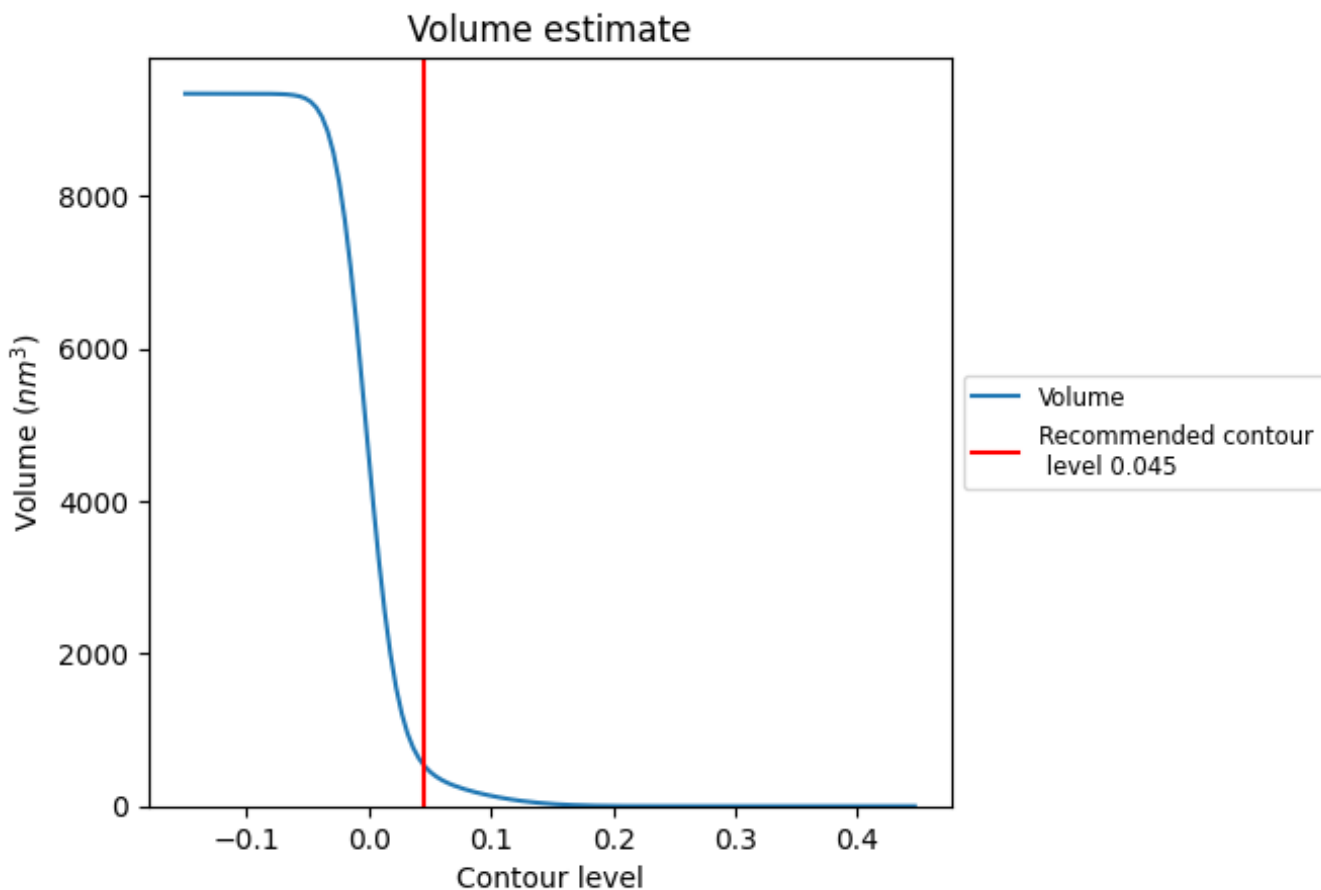
This section contains the results of statistical analysis of the map.

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 543 nm^3 ; this corresponds to an approximate mass of 491 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.

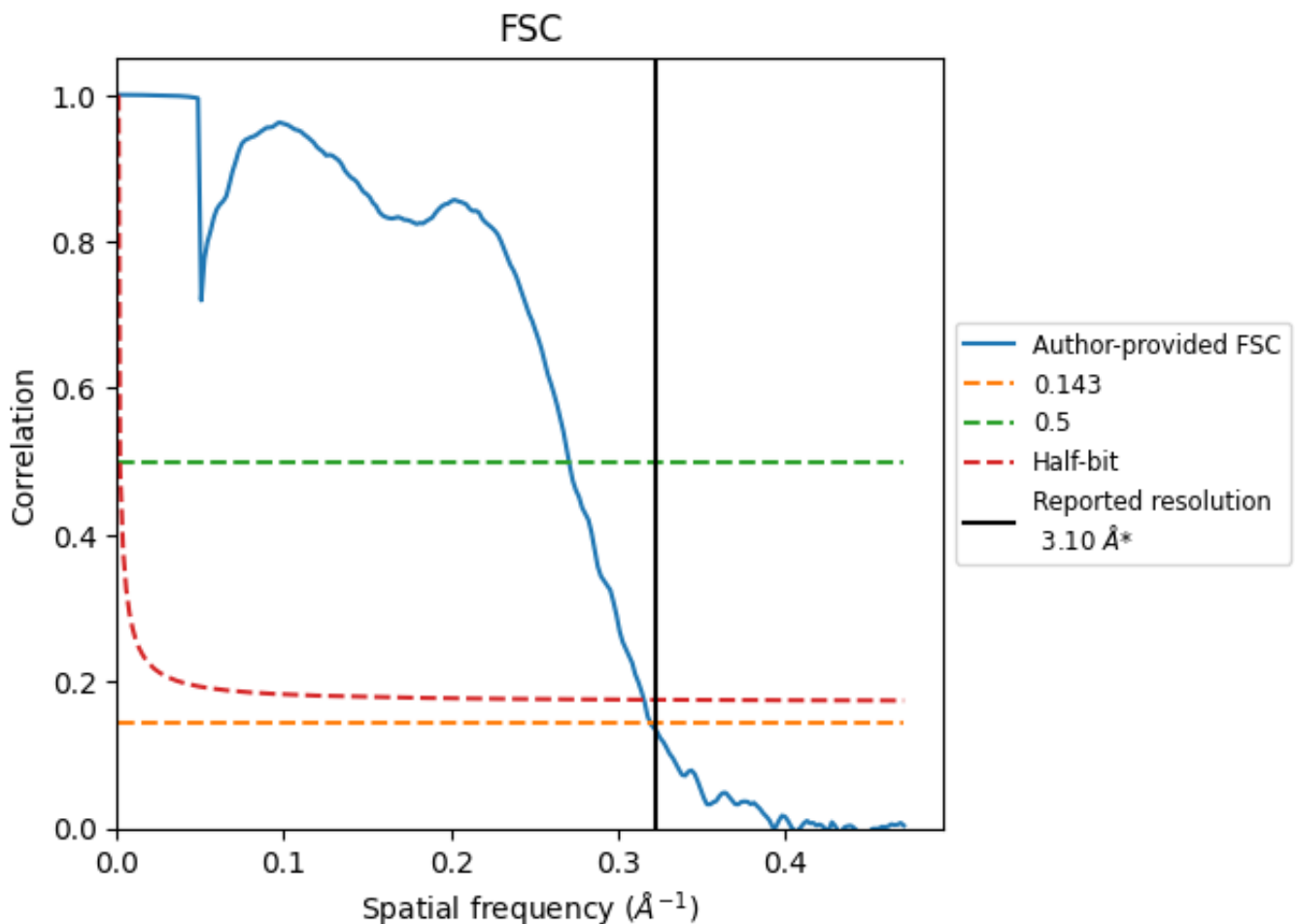
7.3 Rotationally averaged power spectrum [i](#)

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 0.323 Å⁻¹

8.2 Resolution estimates [i](#)

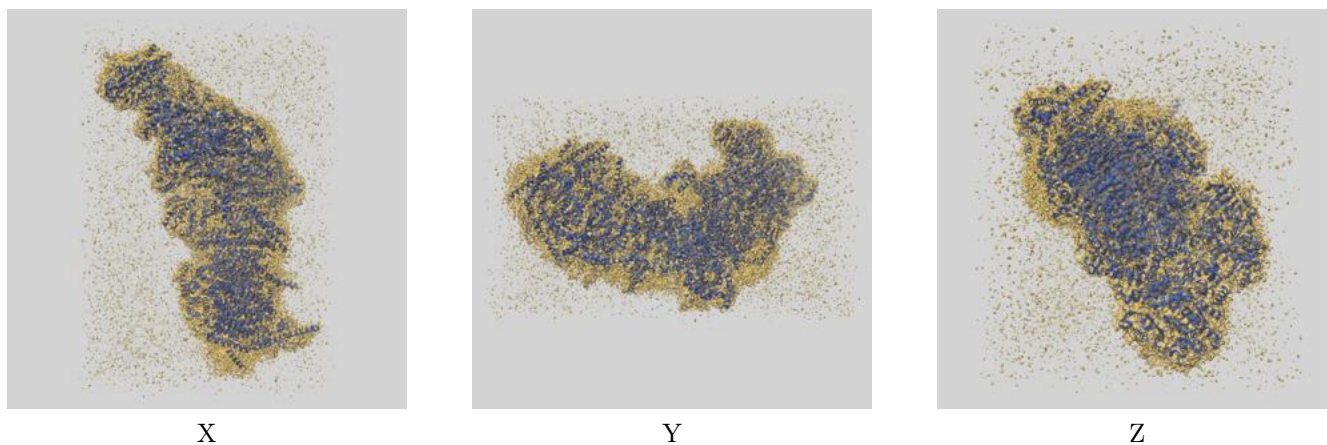
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.13	3.69	3.17
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

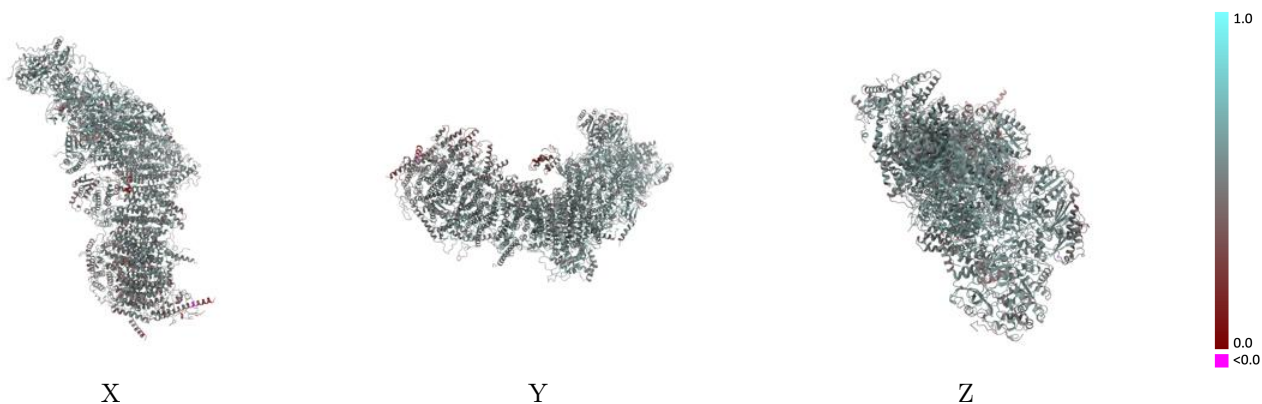
This section contains information regarding the fit between EMDB map EMD-11244 and PDB model 6ZKC. Per-residue inclusion information can be found in section 3 on page 21.

9.1 Map-model overlay [i](#)



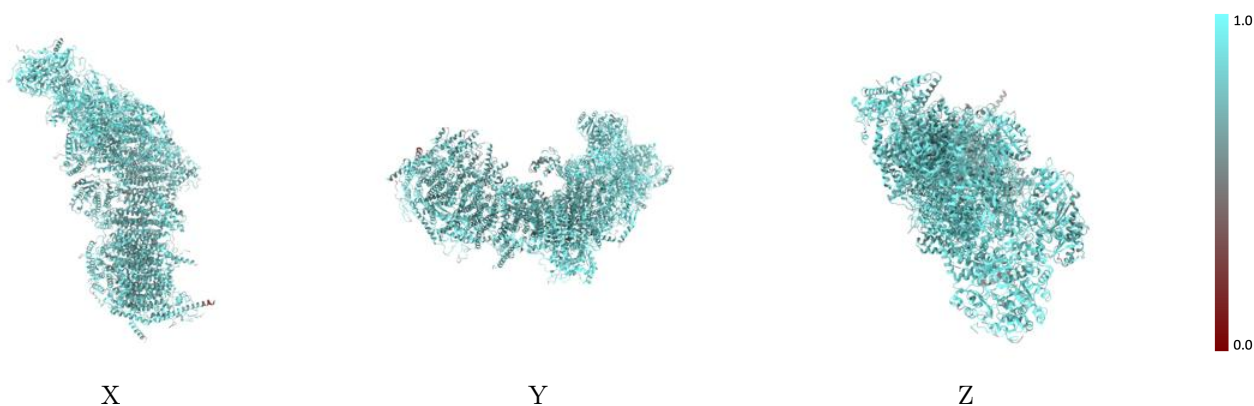
The images above show the 3D surface view of the map at the recommended contour level 0.045 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



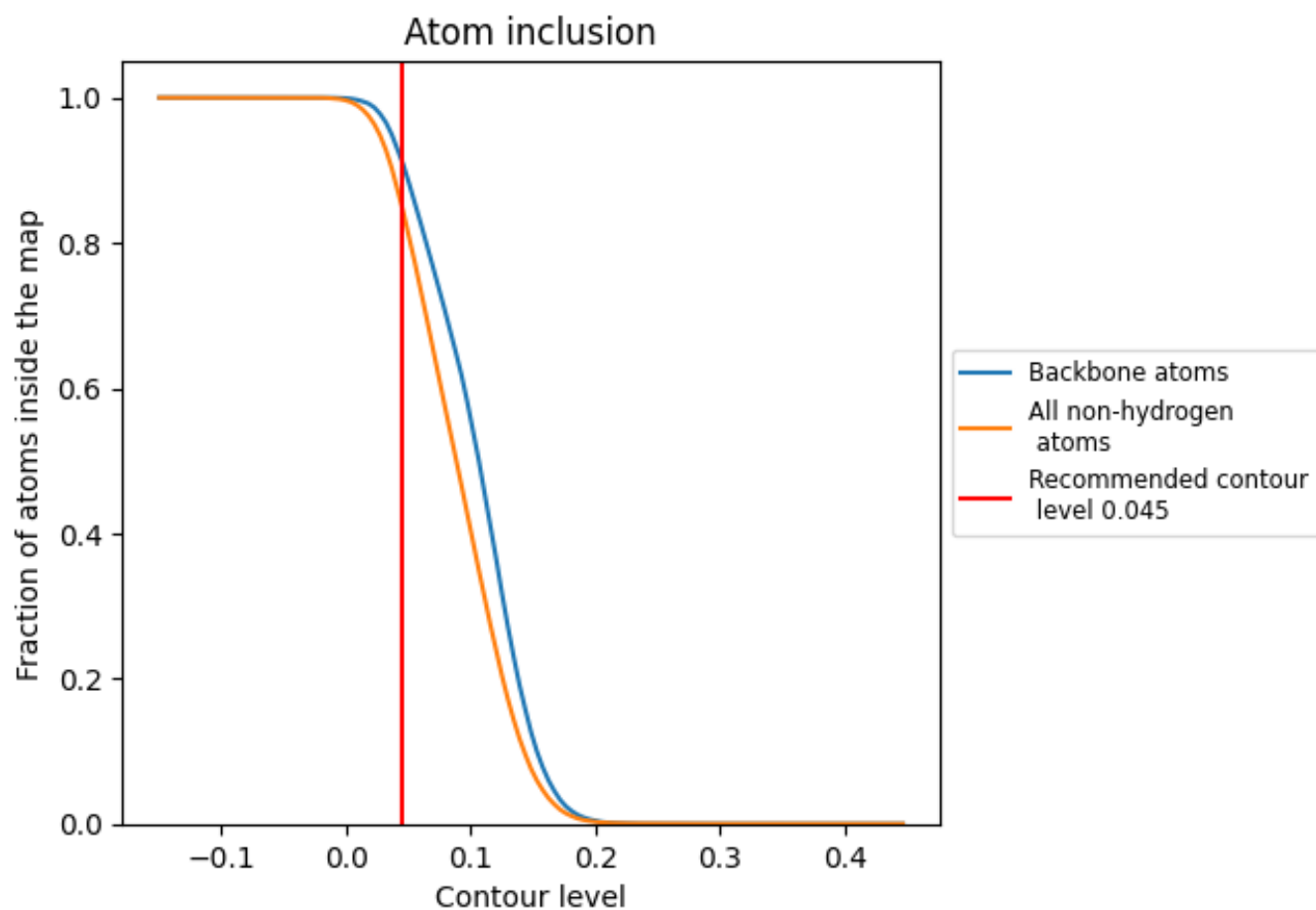
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.045).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 85% 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 (0.045) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8484	 0.5230
1	 0.8918	 0.5250
2	 0.8733	 0.5210
3	 0.8811	 0.5400
4	 0.8788	 0.5590
5	 0.9136	 0.5680
6	 0.9163	 0.5670
9	 0.9112	 0.5680
A	 0.8150	 0.5420
H	 0.8815	 0.5550
J	 0.8384	 0.5390
K	 0.8304	 0.5400
L	 0.8031	 0.5100
M	 0.8658	 0.5520
N	 0.8629	 0.5540
V	 0.7777	 0.4860
W	 0.8409	 0.5360
X	 0.7576	 0.4540
Y	 0.8691	 0.5190
Z	 0.8304	 0.5030
a	 0.8729	 0.5060
b	 0.8928	 0.5500
c	 0.8651	 0.5510
d	 0.8687	 0.5360
e	 0.8393	 0.4930
f	 0.8496	 0.5220
g	 0.8480	 0.5360
h	 0.8552	 0.5320
i	 0.8625	 0.5450
j	 0.6931	 0.3810
k	 0.8245	 0.5020
l	 0.8335	 0.5170
m	 0.8583	 0.5190
n	 0.7524	 0.4260
o	 0.8297	 0.5230



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Chain	Atom inclusion	Q-score
p	 0.7777	 0.4740
q	 0.8811	 0.5320
r	 0.8088	 0.4690
s	 0.7879	 0.4260
t	 0.7962	 0.4610
u	 0.8248	 0.4570
v	 0.7978	 0.4700
w	 0.7991	 0.5020
x	 0.7908	 0.4950
y	 0.7778	 0.4810
z	 0.8716	 0.5270