



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 07:56 AM UTC

PDB ID : 6ZKE / pdb_00006zke
EMDB ID : EMD-11246
Title : Complex I during turnover, open2
Authors : Kampjut, D.; Sazanov, L.A.
Deposited on : 2020-06-30
Resolution : 2.60 Å(reported)
Based on initial model : 5LNK

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

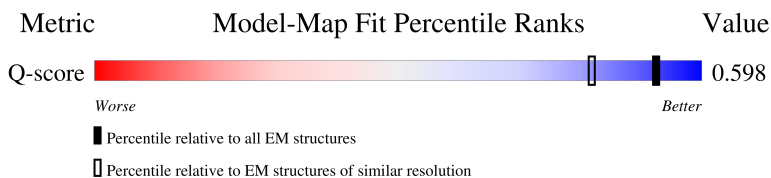
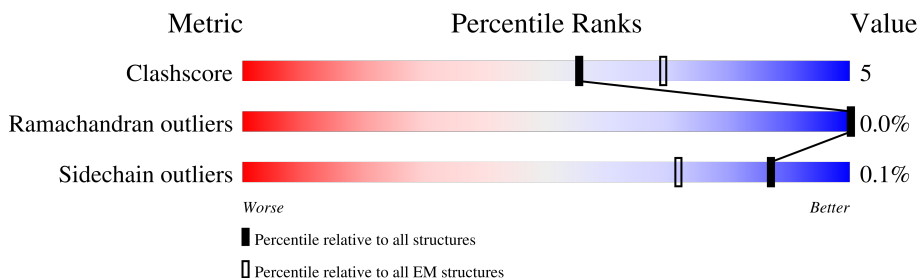
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8728 (2.10 - 3.10)

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	 78% 15% 7%
2	2	246	 72% 14% 13%
3	3	727	 80% 15% 5%
4	4	463	 73% 17% 9%

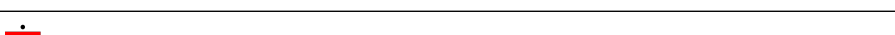
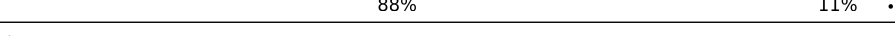
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Mol	Chain	Length	Quality of chain
5	5	266	
6	6	223	
7	9	217	
8	A	115	
9	H	318	
10	J	175	
11	K	98	
12	L	606	
13	M	459	
14	N	347	
15	V	141	
16	W	189	
17	X	157	
17	j	157	
18	Y	172	
19	Z	175	
20	a	109	
21	b	124	
22	c	170	
23	d	380	
24	e	99	
25	f	116	
26	g	140	
27	h	114	
28	i	145	

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Mol	Chain	Length	Quality of chain
29	k	355	
30	l	106	
31	m	84	
32	n	98	
33	o	122	
34	p	130	
35	q	144	
36	r	128	
37	s	137	
38	t	179	
39	u	108	
40	v	186	
41	w	154	
42	x	76	
43	y	58	
44	z	70	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
45	SF4	1	501	-	-	X	-
45	SF4	6	201	-	-	X	-
53	CDL	L	704	X	-	-	-
53	CDL	V	204	X	-	-	-
53	CDL	Y	201	X	-	-	-
53	CDL	o	502	X	-	-	-

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 67450 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 17 is a protein called Acyl carrier protein.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

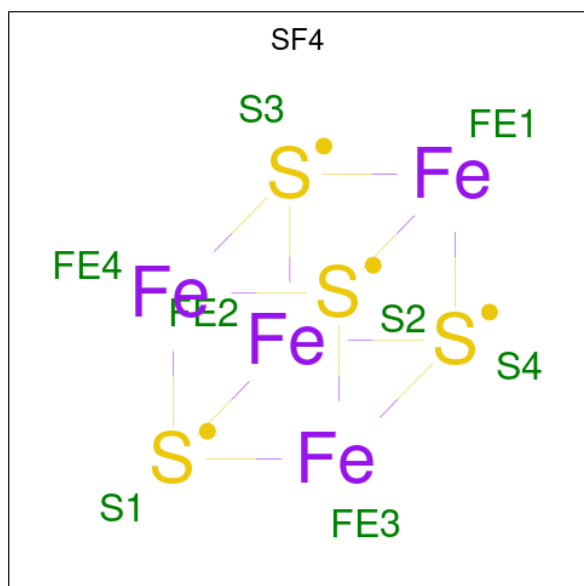
- Molecule 43 is a protein called Mitochondrial complex I, MNLL subunit.

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

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

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

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



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

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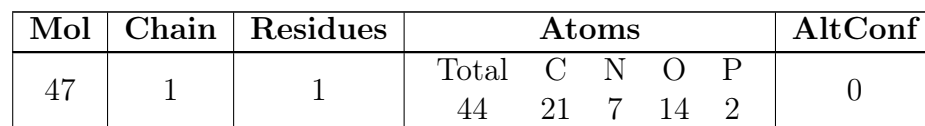
Mol	Chain	Residues	Atoms			AltConf
45	9	1	Total	Fe	S	0
			8	4	4	
45	9	1	Total	Fe	S	0
			8	4	4	

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



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

- Molecule 47 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$).



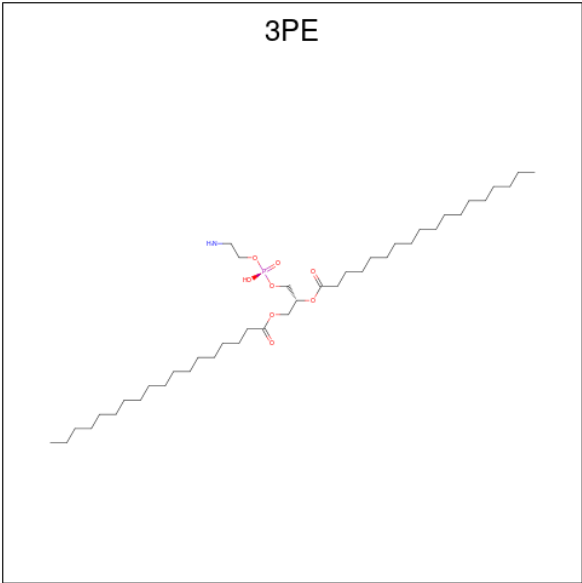
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- Diagram illustrating the structure of a ferredoxin (FES) molecule, showing a square arrangement of two iron (Fe) and two sulfur (S) atoms. The atoms are labeled S1, FE2, FE1, and S2 in green text. The bonds between the atoms are represented by lines, with some segments colored yellow and purple.

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

- 

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

- Molecule 50 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: C₄₁H₈₂NO₈P).



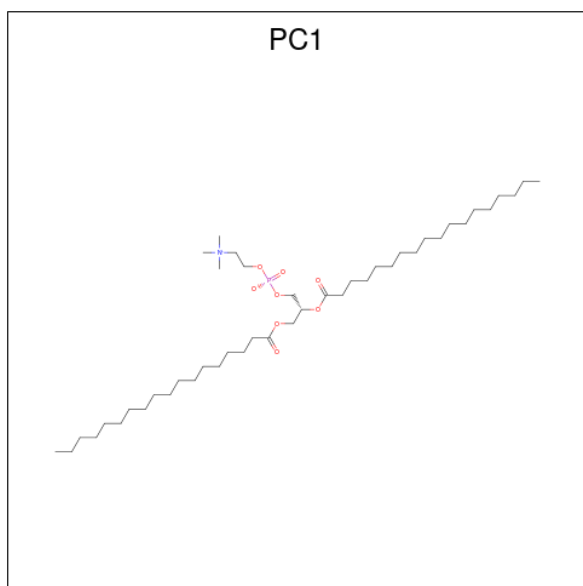
Mol	Chain	Residues	Atoms					AltConf
50	6	1	Total	C	N	O	P	0
			51	41	1	8	1	
50	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
50	H	1	Total	C	N	O	P	0
			51	41	1	8	1	
50	K	1	Total	C	N	O	P	0
			40	30	1	8	1	
50	L	1	Total	C	N	O	P	0
			40	30	1	8	1	
50	L	1	Total	C	N	O	P	0
			51	41	1	8	1	
50	L	1	Total	C	N	O	P	0
			31	21	1	8	1	
50	M	1	Total	C	N	O	P	0
			44	34	1	8	1	
50	N	1	Total	C	N	O	P	0
			51	41	1	8	1	
50	V	1	Total	C	N	O	P	0
			35	25	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
50	V	1	Total	C	N	O	P	0
			37	27	1	8	1	
50	i	1	Total	C	N	O	P	0
			51	41	1	8	1	
50	o	1	Total	C	N	O	P	0
			31	21	1	8	1	
50	p	1	Total	C	O	P		0
			27	18	8	1		

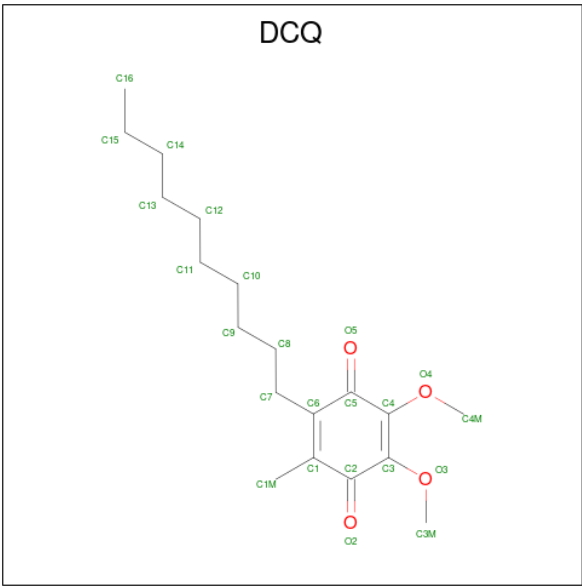
- Molecule 51 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
51	9	1	Total	C	N	O	P	0
			54	44	1	8	1	
51	A	1	Total	C	N	O	P	0
			46	36	1	8	1	
51	A	1	Total	C	N	O	P	0
			37	27	1	8	1	
51	L	1	Total	C	N	O	P	0
			54	44	1	8	1	
51	M	1	Total	C	N	O	P	0
			54	44	1	8	1	
51	w	1	Total	C	N	O	P	0
			54	44	1	8	1	

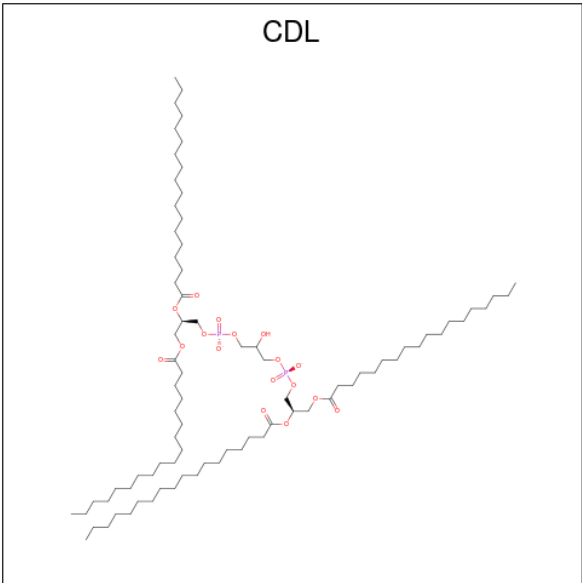
- Molecule 52 is 2-decyl-5,6-dimethoxy-3-methylcyclohexa-2,5-diene-1,4-dione (CCD ID:

DCQ) (formula: C₁₉H₃₀O₄).



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

- Molecule 53 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



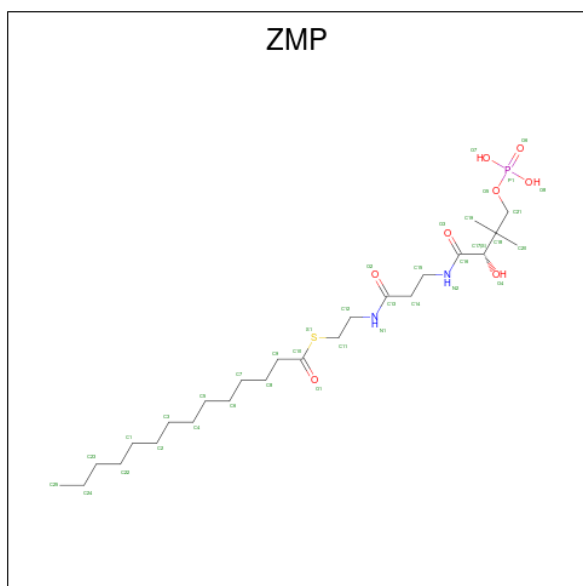
Mol	Chain	Residues	Atoms				AltConf
53	L	1	Total	C	O	P	0
			100	81	17	2	
53	M	1	Total	C	O	P	0
			90	71	17	2	

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Mol	Chain	Residues	Atoms				AltConf
53	V	1	Total	C	O	P	0
			94	75	17	2	
53	V	1	Total	C	O	P	0
			85	66	17	2	
53	W	1	Total	C	O	P	0
			100	81	17	2	
53	Y	1	Total	C	O	P	0
			100	81	17	2	
53	h	1	Total	C	O	P	0
			58	39	17	2	
53	o	1	Total	C	O	P	0
			75	56	17	2	

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

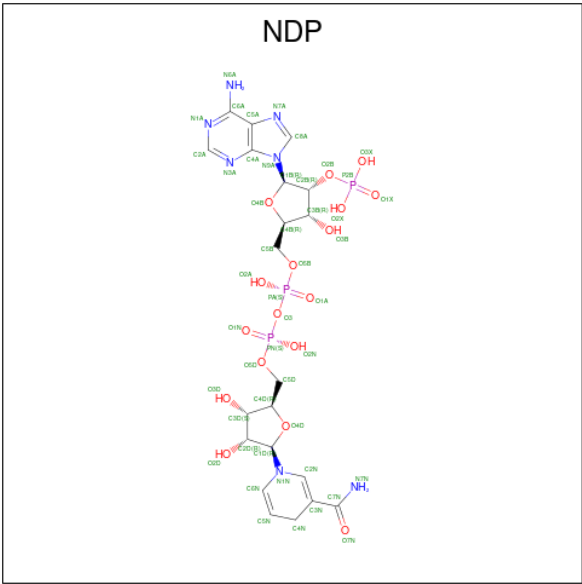


Mol	Chain	Residues	Atoms						AltConf
54	X	1	Total 31	C 20	N 2	O 7	P 1	S 1	0
54	g	1	Total 34	C 23	N 2	O 7	P 1	S 1	0

- Molecule 55 is ZINC ION (CCD ID: ZN) (formula: Zn).

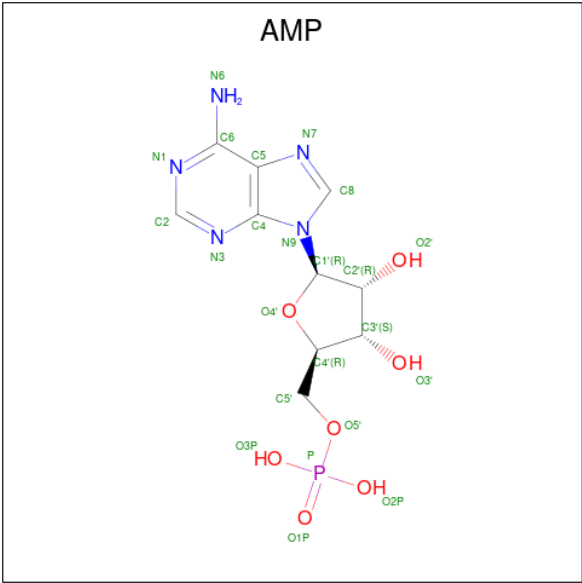
Mol	Chain	Residues	Atoms		AltConf
55	b	1	Total	Zn	0
			1	1	

- Molecule 56 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



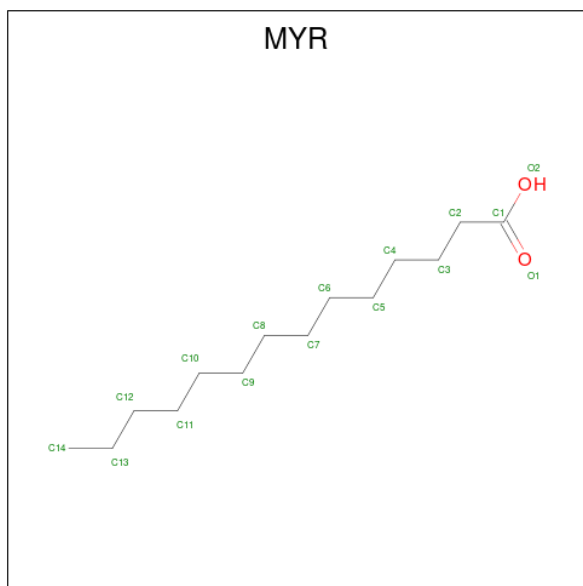
Mol	Chain	Residues	Atoms					AltConf
56	d	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 57 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: C₁₀H₁₄N₅O₇P).



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

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

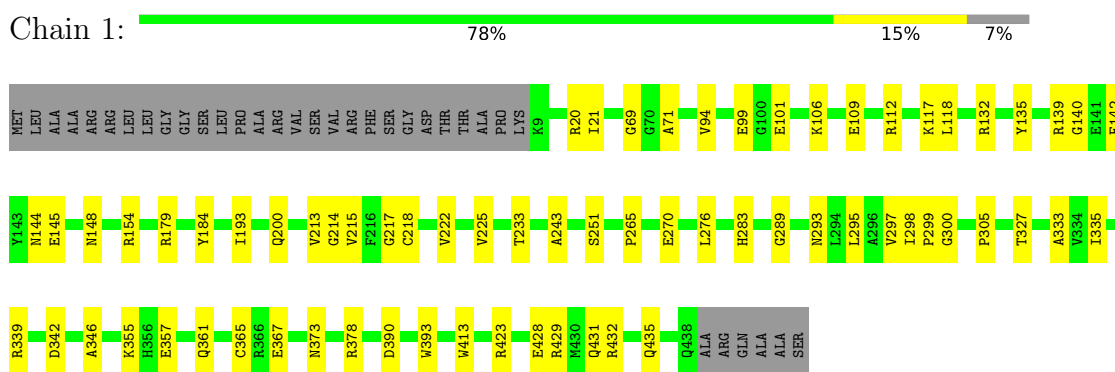


Mol	Chain	Residues	Atoms			AltConf
58	s	1	Total	C	O	0
			15	14	1	

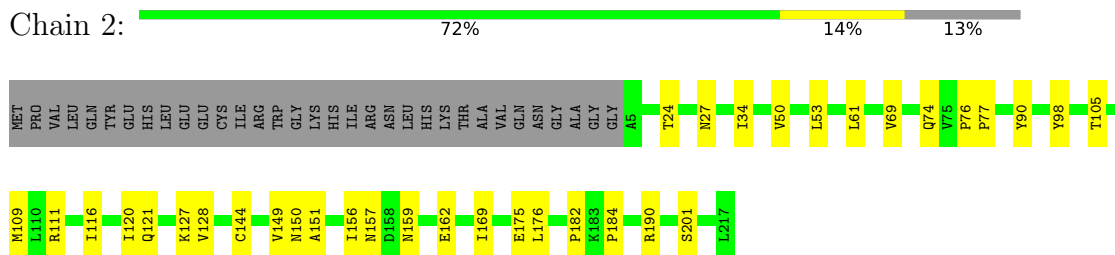
3 Residue-property plots

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.

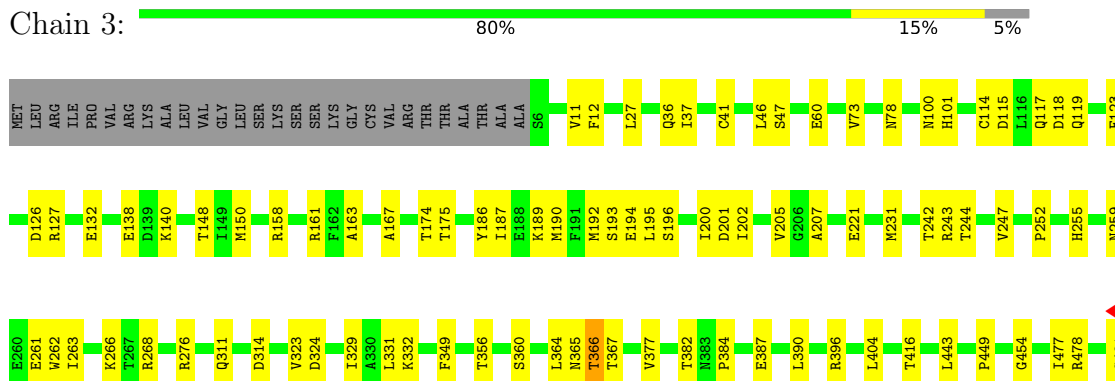
- Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



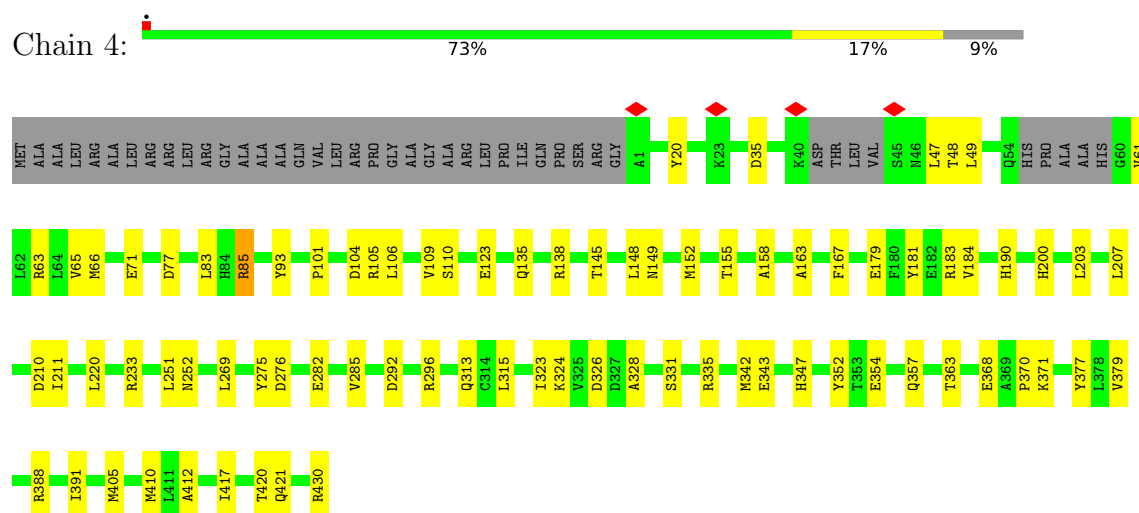
- Molecule 2: Mitochondrial complex I, 24 kDa subunit



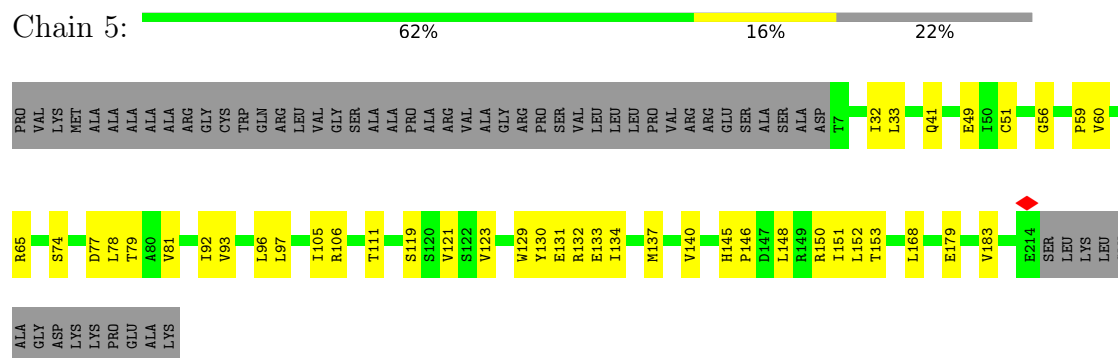
- Molecule 3: NADH:ubiquinone oxidoreductase core subunit S1



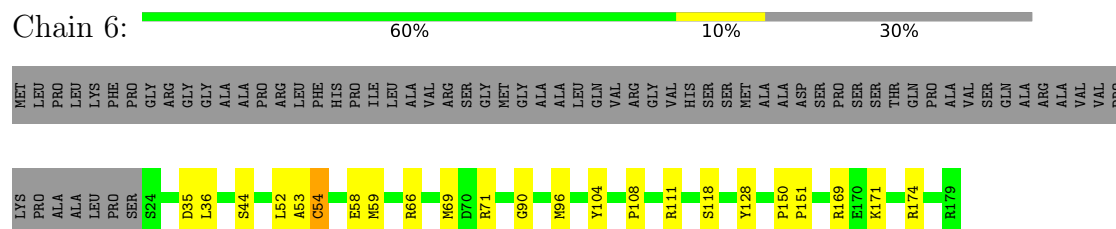
- Molecule 4: Mitochondrial complex I, 49 kDa subunit



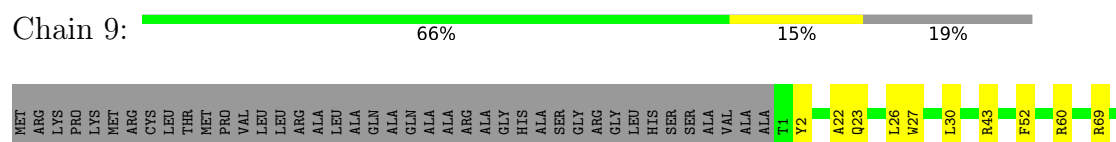
- Molecule 5: NADH:ubiquinone oxidoreductase core subunit S3



- Molecule 6: Mitochondrial complex I, PSST subunit

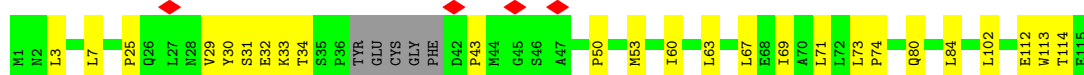
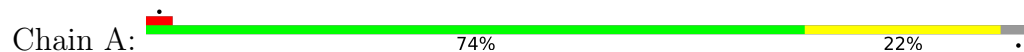


- Molecule 7: Mitochondrial complex I, TYKY subunit

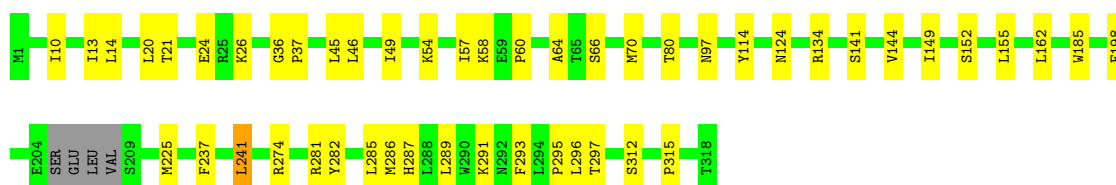
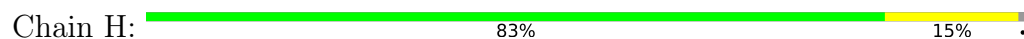




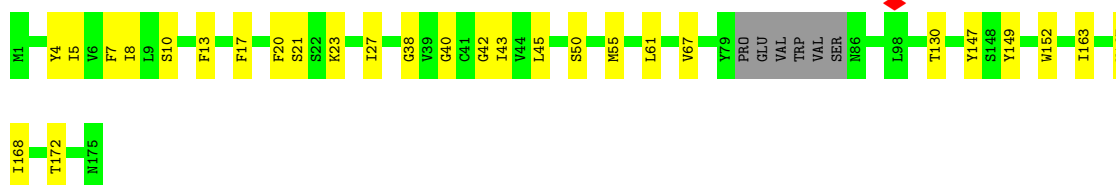
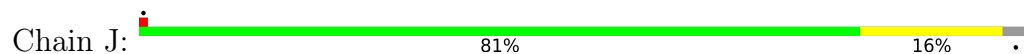
- Molecule 8: NADH-ubiquinone oxidoreductase chain 3



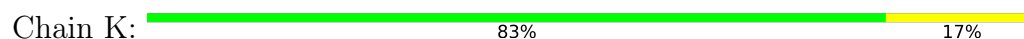
- Molecule 9: NADH-ubiquinone oxidoreductase chain 1



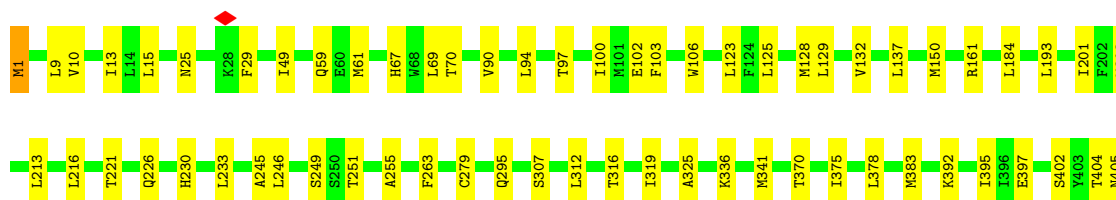
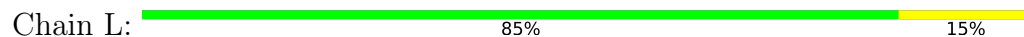
- Molecule 10: NADH-ubiquinone oxidoreductase chain 6



- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

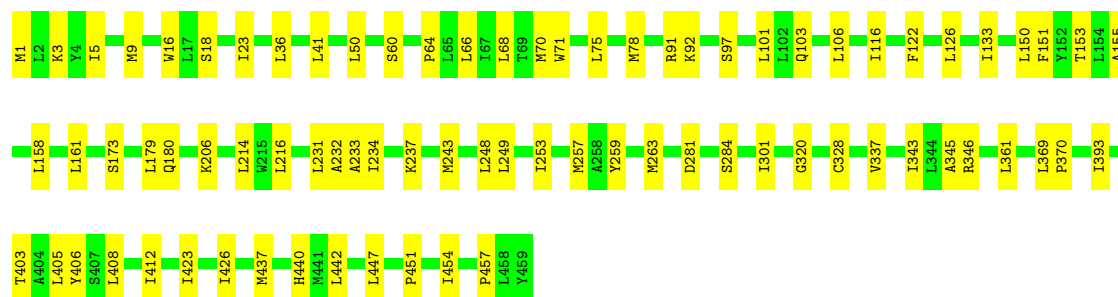
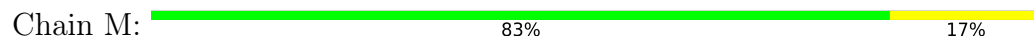


- Molecule 12: NADH-ubiquinone oxidoreductase chain 5

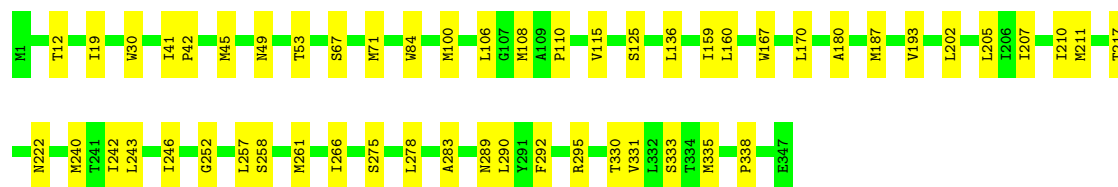
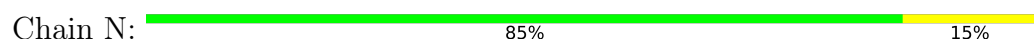




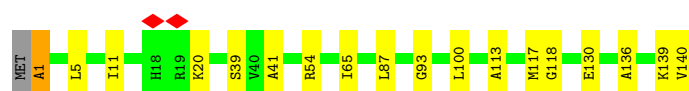
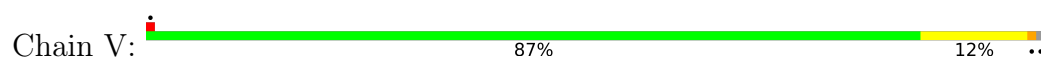
• Molecule 13: NADH-ubiquinone oxidoreductase chain 4



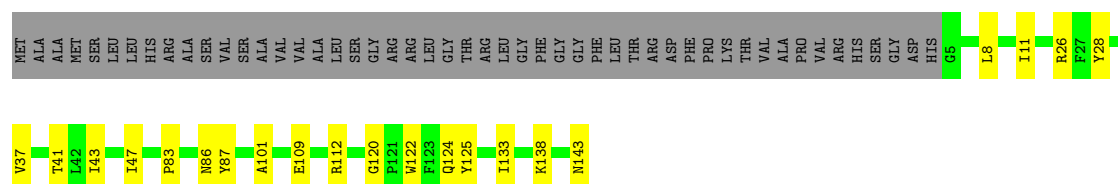
• Molecule 14: NADH-ubiquinone oxidoreductase chain 2



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



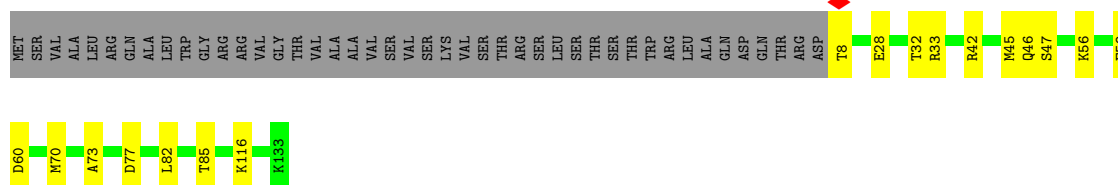
• Molecule 16: NADH:ubiquinone oxidoreductase subunit B5



• Molecule 17: Acyl carrier protein

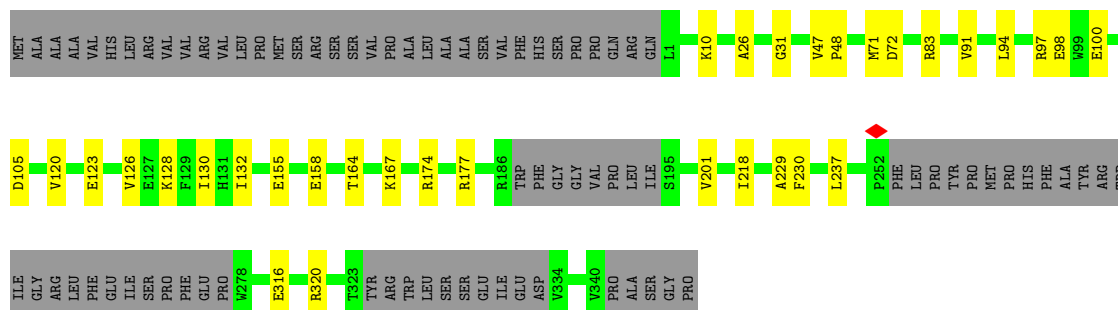


Chain c:  64% 10% 26%



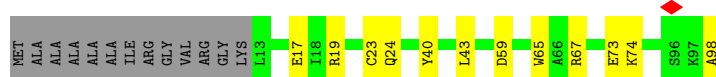
- Molecule 23: NADH:ubiquinone oxidoreductase subunit A9

Chain d:  69% 9% 22%



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

Chain e:  75% 12% 13%



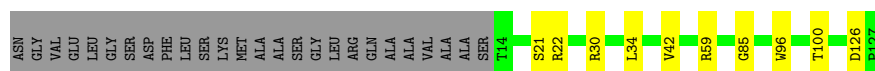
- Molecule 25: Mitochondrial complex I, B13 subunit

Chain f:  91% 7% .



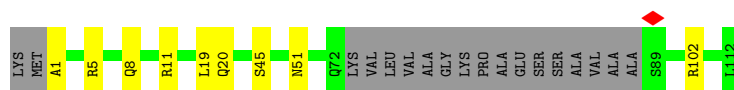
- Molecule 26: NADH:ubiquinone oxidoreductase subunit A6

Chain g:  74% 7% 19%

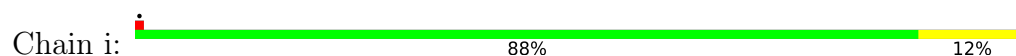


- Molecule 27: Mitochondrial complex I, B14.5a subunit

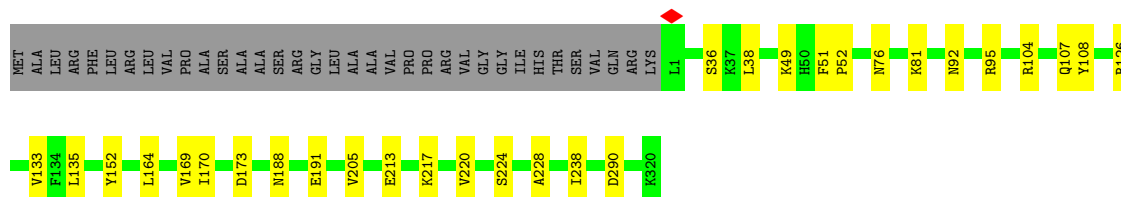
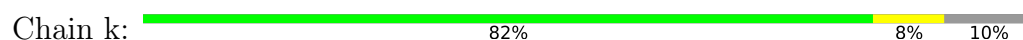
Chain h:  76% 8% 16%



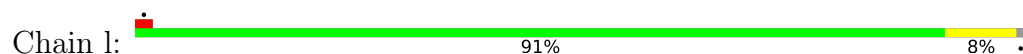
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



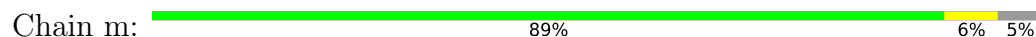
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial



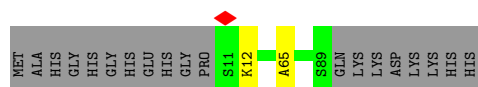
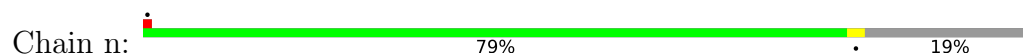
- Molecule 30: NADH:ubiquinone oxidoreductase subunit S5



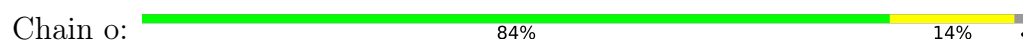
- Molecule 31: NADH:ubiquinone oxidoreductase subunit A3



- Molecule 32: NADH:ubiquinone oxidoreductase subunit B3

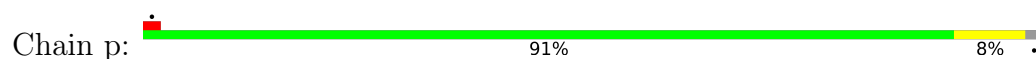


- Molecule 33: NADH dehydrogenase [ubiquinone] 1 subunit C2

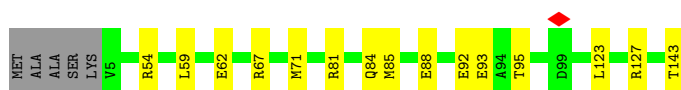
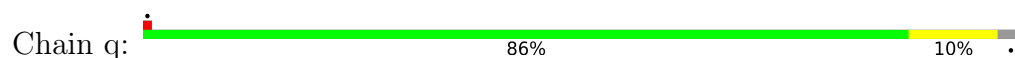




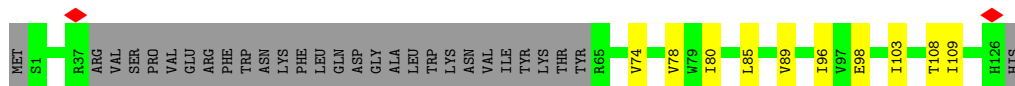
- Molecule 34: NADH:ubiquinone oxidoreductase subunit B4



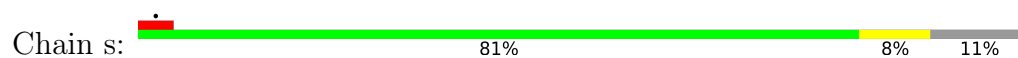
- Molecule 35: Mitochondrial complex I, B16.6 subunit



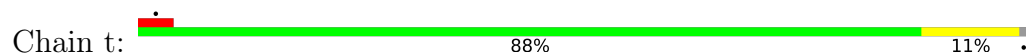
- Molecule 36: Mitochondrial complex I, B17 subunit



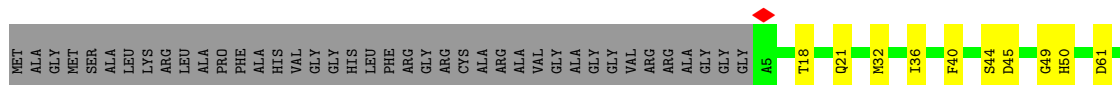
- Molecule 37: NADH:ubiquinone oxidoreductase subunit B7

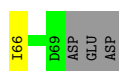


- Molecule 38: NADH:ubiquinone oxidoreductase subunit B9



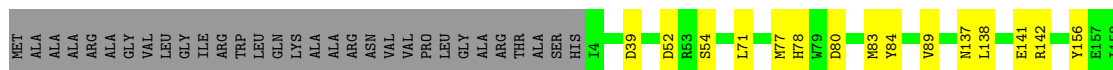
- Molecule 39: NADH:ubiquinone oxidoreductase subunit B2





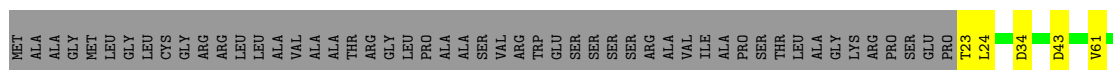
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain v: 75% 8% 17%



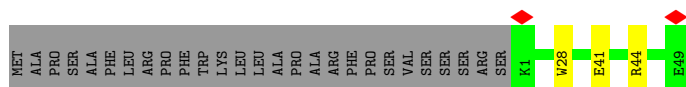
- Molecule 41: Mitochondrial complex I, ESSS subunit

Chain w: 56% 9% 34%



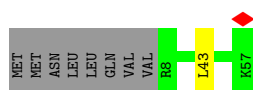
- Molecule 42: Mitochondrial complex I, KFYI subunit

Chain x: 61% 36%



- Molecule 43: Mitochondrial complex I, MNLL subunit

Chain y: 84% 14%



- Molecule 44: Mitochondrial complex I, MWFE subunit

Chain z: 93% 7%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	98436	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	0.380	Depositor
Minimum map value	-0.132	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	170.821, 196.285, 286.47	wwPDB
Map dimensions	270, 185, 161	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.061, 1.061, 1.061	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1	0.33	0/3386	0.58	0/4575
2	2	0.32	0/1695	0.57	0/2306
3	3	0.34	0/5362	0.56	2/7266 (0.0%)
4	4	0.36	0/3463	0.57	0/4687
5	5	0.34	0/1776	0.55	0/2417
6	6	0.39	0/1278	0.57	0/1728
7	9	0.40	0/1445	0.59	0/1956
8	A	0.31	0/902	0.64	2/1234 (0.2%)
9	H	0.37	0/2572	0.63	0/3517
10	J	0.32	0/1324	0.60	0/1790
11	K	0.36	0/749	0.63	0/1014
12	L	0.30	0/4924	0.58	1/6698 (0.0%)
13	M	0.35	1/3731 (0.0%)	0.59	0/5085
14	N	0.36	0/2787	0.57	0/3795
15	V	0.20	0/1041	0.44	0/1412
16	W	0.27	0/1188	0.50	0/1607
17	X	0.20	0/713	0.45	0/963
17	j	0.22	0/670	0.47	0/902
18	Y	0.27	0/1440	0.53	0/1942
19	Z	0.25	0/1475	0.46	0/1989
20	a	0.23	0/383	0.43	0/518
21	b	0.29	0/749	0.47	0/1009
22	c	0.32	0/1047	0.48	0/1415
23	d	0.28	0/2424	0.49	0/3276
24	e	0.26	0/702	0.49	0/945
25	f	0.26	0/937	0.50	0/1271
26	g	0.29	0/993	0.52	0/1336
27	h	0.30	0/779	0.54	0/1053
28	i	0.30	0/1250	0.45	0/1698
29	k	0.26	0/2646	0.45	0/3579
30	l	0.29	0/896	0.53	0/1200

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	m	0.25	0/647	0.48	0/890
32	n	0.19	0/653	0.39	0/882
33	o	0.27	0/1035	0.48	0/1398
34	p	0.23	0/1085	0.47	0/1467
35	q	0.28	0/1171	0.49	0/1579
36	r	0.25	0/874	0.48	0/1188
37	s	0.20	0/1072	0.47	0/1436
38	t	0.23	0/1573	0.52	0/2130
39	u	0.20	0/590	0.45	0/810
40	v	0.22	0/1361	0.46	0/1861
41	w	0.26	0/872	0.51	0/1185
42	x	0.21	0/425	0.38	0/576
43	y	0.33	0/449	0.52	0/605
44	z	0.34	0/591	0.56	0/795
All	All	0.31	1/67125 (0.0%)	0.54	5/90985 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	3	0	2
4	4	0	1
8	A	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	M	216	LEU	C-N	5.72	1.38	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	366	THR	CA-C-N	5.93	132.86	121.54
3	3	366	THR	C-N-CA	5.93	132.86	121.54
12	L	230	HIS	N-CA-C	5.14	121.17	109.81
8	A	112	GLU	CA-C-N	5.01	131.10	121.54
8	A	112	GLU	C-N-CA	5.01	131.10	121.54

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	3	259	ASN	Peptide
3	3	366	THR	Peptide
4	4	275	TYR	Peptide
8	A	113	TRP	Peptide

5.2 Too-close contacts

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	46	0
2	2	1655	0	1668	23	0
3	3	5275	0	5300	69	0
4	4	3390	0	3333	60	0
5	5	1726	0	1676	27	0
6	6	1247	0	1259	19	0
7	9	1414	0	1371	25	0
8	A	880	0	920	23	0
9	H	2498	0	2609	39	0
10	J	1294	0	1317	25	0
11	K	749	0	793	18	0
12	L	4806	0	4945	69	0
13	M	3647	0	3849	54	0
14	N	2723	0	2930	40	0
15	V	1028	0	1036	12	0
16	W	1155	0	1177	18	0
17	X	701	0	692	5	0
17	j	660	0	663	4	0
18	Y	1403	0	1392	16	0
19	Z	1441	0	1419	16	0
20	a	371	0	344	6	0
21	b	737	0	710	4	0
22	c	1024	0	1023	14	0
23	d	2372	0	2407	21	0
24	e	691	0	706	7	0
25	f	917	0	958	6	0
26	g	969	0	980	7	0
27	h	769	0	780	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	i	1209	0	1182	13	0
29	k	2596	0	2559	17	0
30	l	874	0	869	9	0
31	m	626	0	635	5	0
32	n	634	0	616	2	0
33	o	1004	0	995	13	0
34	p	1059	0	1062	8	0
35	q	1142	0	1137	12	0
36	r	846	0	864	10	0
37	s	1047	0	1015	8	0
38	t	1520	0	1477	18	0
39	u	563	0	509	7	0
40	v	1307	0	1207	11	0
41	w	846	0	792	11	0
42	x	412	0	411	2	0
43	y	436	0	437	1	0
44	z	576	0	570	5	0
45	1	8	0	0	3	0
45	3	16	0	0	0	0
45	6	8	0	0	3	0
45	9	16	0	0	0	0
46	1	31	0	19	0	0
47	1	44	0	27	4	0
48	2	4	0	0	1	0
48	3	4	0	0	0	0
49	3	1	0	0	0	0
50	6	51	0	82	3	0
50	A	51	0	82	2	0
50	H	51	0	82	6	0
50	K	40	0	54	4	0
50	L	122	0	172	1	0
50	M	44	0	65	2	0
50	N	51	0	82	2	0
50	V	72	0	92	2	0
50	i	51	0	82	2	0
50	o	31	0	36	0	0
50	p	27	0	27	1	0
51	9	54	0	88	1	0
51	A	83	0	117	0	0
51	L	54	0	88	3	0
51	M	54	0	88	4	0
51	w	54	0	88	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
52	H	23	0	30	2	0
53	L	100	0	156	7	0
53	M	90	0	133	9	0
53	V	179	0	261	4	0
53	W	100	0	156	5	0
53	Y	100	0	156	7	0
53	h	58	0	60	1	0
53	o	75	0	97	2	0
54	X	31	0	34	2	0
54	g	34	0	40	0	0
55	b	1	0	0	0	0
56	d	48	0	26	1	0
57	k	23	0	12	2	0
58	s	15	0	27	0	0
All	All	67450	0	68422	682	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 (682) 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)
3:3:632:ARG:HH12	24:e:59:ASP:H	1.42	0.68
1:1:101:GLU:HB2	47:1:503:NAI:H42N	1.77	0.66
14:N:243:LEU:HD22	14:N:330:THR:HG21	1.78	0.65
1:1:132:ARG:NH2	20:a:64:PRO:O	2.29	0.65
7:9:43:ARG:HG2	27:h:11:ARG:HD2	1.80	0.64
24:e:19:ARG:HB2	24:e:65:TRP:HB2	1.77	0.64
8:A:32:GLU:HB3	23:d:320:ARG:HH22	1.61	0.64
14:N:106:LEU:HD22	14:N:187:MET:HE2	1.79	0.64
9:H:141:SER:HB3	9:H:289:LEU:HD22	1.81	0.63
7:9:164:GLU:HG3	28:i:88:ARG:HG3	1.80	0.63
3:3:118:ASP:OD2	22:c:46:GLN:NE2	2.32	0.62
18:Y:165:ARG:NH1	33:o:87:ASP:OD1	2.32	0.62
53:L:704:CDL:H351	53:L:704:CDL:H161	1.80	0.62
35:q:81:ARG:NH1	35:q:85:MET:SD	2.73	0.62
12:L:558:LEU:HB3	13:M:214:LEU:HD21	1.82	0.62
36:r:85:LEU:HD22	36:r:96:ILE:HD11	1.82	0.62
2:2:98:TYR:HA	2:2:157:ASN:HD21	1.63	0.61
19:Z:67:PHE:HD1	43:y:43:LEU:HD21	1.65	0.61
2:2:150:ASN:HB3	2:2:162:GLU:HB3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:103:PHE:HB2	12:L:341:MET:HE3	1.82	0.61
53:L:704:CDL:H431	51:w:801:PC1:H291	1.83	0.61
5:5:151:ILE:HG23	5:5:152:LEU:HG	1.83	0.60
34:p:39:ARG:NH2	38:t:3:LEU:O	2.33	0.60
3:3:126:ASP:HB2	4:4:328:ALA:HB3	1.83	0.60
28:i:60:ARG:HH22	28:i:95:ASP:HA	1.65	0.60
6:6:44:SER:O	9:H:54:LYS:NZ	2.34	0.60
14:N:45:MET:HE3	14:N:53:THR:HG22	1.83	0.60
6:6:54:CYS:HB2	45:6:201:SF4:S2	2.41	0.60
6:6:171:LYS:HG2	6:6:174:ARG:HH11	1.66	0.60
13:M:158:LEU:HD23	14:N:283:ALA:HB1	1.84	0.60
16:W:124:GLN:HB2	33:o:4:GLY:HA3	1.84	0.60
12:L:570:GLN:OE1	14:N:167:TRP:NE1	2.34	0.59
15:V:39:SER:OG	15:V:54:ARG:NH2	2.35	0.59
4:4:109:VAL:HG11	4:4:152:MET:HG2	1.85	0.59
2:2:74:GLN:O	20:a:74:ARG:NH2	2.36	0.58
14:N:338:PRO:HG3	53:Y:201:CDL:H792	1.85	0.58
30:l:104:ARG:NH1	35:q:84:GLN:OE1	2.35	0.58
4:4:20:TYR:OH	14:N:295:ARG:NH2	2.36	0.58
37:s:6:ARG:HH12	37:s:105:ARG:HD2	1.67	0.58
41:w:114:ASP:HB3	41:w:117:LYS:HG2	1.84	0.58
4:4:269:LEU:HB2	4:4:368:GLU:HB2	1.85	0.58
4:4:391:ILE:O	4:4:430:ARG:NH1	2.37	0.58
19:Z:5:ASP:HB3	19:Z:8:VAL:HG12	1.86	0.57
12:L:233:LEU:HD23	12:L:307:SER:HB3	1.86	0.57
18:Y:66:ALA:O	18:Y:69:PHE:HB3	2.04	0.57
29:k:51:PHE:HB3	29:k:107:GLN:HE21	1.69	0.57
40:v:137:ASN:O	40:v:142:ARG:NH1	2.37	0.57
3:3:252:PRO:HG3	3:3:263:ILE:HG12	1.86	0.57
9:H:21:THR:HG21	52:H:501:DCQ:H8	1.85	0.57
18:Y:29:HIS:HB3	18:Y:119:PRO:HD2	1.87	0.57
53:M:503:CDL:H791	14:N:242:ILE:HG23	1.86	0.57
14:N:211:MET:HG2	14:N:333:SER:HB2	1.86	0.57
33:o:45:ASP:OD2	33:o:51:ARG:NH2	2.38	0.57
25:f:37:ILE:O	25:f:44:ARG:NH1	2.38	0.57
13:M:9:MET:HE1	53:Y:201:CDL:H162	1.86	0.56
2:2:121:GLN:HE21	2:2:128:VAL:HG23	1.70	0.56
9:H:64:ALA:O	9:H:124:ASN:ND2	2.39	0.56
3:3:46:LEU:O	22:c:116:LYS:NZ	2.38	0.56
3:3:396:ARG:NH1	3:3:416:THR:O	2.38	0.56
24:e:74:LYS:NZ	24:e:98:ALA:O	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:p:47:GLN:HA	34:p:50:TYR:HB3	1.87	0.56
12:L:161:ARG:NH2	38:t:90:TYR:O	2.35	0.56
9:H:26:LYS:HB3	44:z:5:VAL:HG12	1.87	0.56
12:L:90:VAL:HG22	12:L:129:LEU:HD22	1.88	0.56
12:L:249:SER:HB2	12:L:336:LYS:HG3	1.86	0.56
4:4:405:MET:SD	4:4:421:GLN:NE2	2.73	0.56
13:M:133:ILE:HD11	13:M:231:LEU:HD11	1.88	0.56
1:1:289:GLY:HA3	1:1:293:ASN:HD22	1.71	0.56
3:3:276:ARG:HA	28:i:135:GLN:HB2	1.86	0.56
4:4:200:HIS:NE2	7:9:124:GLU:OE1	2.38	0.56
28:i:34:ARG:NH2	28:i:58:ARG:O	2.36	0.56
8:A:60:ILE:HG21	10:J:168:ILE:HG21	1.88	0.56
12:L:97:THR:HG21	12:L:125:LEU:HD22	1.88	0.56
3:3:27:LEU:HA	3:3:37:ILE:HD12	1.88	0.55
2:2:105:THR:OG1	48:2:300:FES:S2	2.64	0.55
3:3:148:THR:HG23	3:3:150:MET:HE3	1.87	0.55
13:M:126:LEU:HD21	13:M:153:THR:HG21	1.89	0.55
11:K:23:ARG:HG2	50:K:101:3PE:H11	1.86	0.55
13:M:18:SER:HB2	13:M:23:ILE:HG22	1.88	0.55
4:4:335:ARG:NH2	7:9:129:ASP:OD1	2.40	0.55
25:f:69:GLU:HG3	27:h:102:ARG:HH12	1.72	0.55
1:1:20:ARG:HH12	2:2:201:SER:HB2	1.72	0.55
4:4:101:PRO:O	4:4:105:ARG:NH1	2.39	0.55
6:6:169:ARG:NH2	7:9:142:GLU:OE2	2.40	0.55
40:v:54:SER:HA	40:v:84:TYR:HB3	1.89	0.55
5:5:179:GLU:O	23:d:174:ARG:NH1	2.41	0.54
12:L:370:THR:HG23	12:L:431:LEU:HD13	1.88	0.54
50:A:403:3PE:H381	9:H:295:PRO:HB3	1.88	0.54
17:j:37:MET:HE1	17:j:44:SER:HA	1.89	0.54
9:H:46:LEU:HD21	50:i:201:3PE:H361	1.89	0.54
4:4:430:ARG:NH2	5:5:133:GLU:OE2	2.41	0.54
18:Y:35:CYS:O	18:Y:39:ASN:ND2	2.41	0.54
34:p:47:GLN:HG3	38:t:165:LEU:HD13	1.88	0.54
34:p:62:PRO:O	34:p:66:ARG:HB2	2.07	0.54
12:L:10:VAL:HG21	36:r:78:VAL:HG22	1.89	0.54
16:W:109:GLU:OE2	16:W:112:ARG:NH2	2.35	0.54
21:b:32:GLN:HE22	21:b:34:GLU:HB2	1.71	0.54
23:d:174:ARG:NH2	23:d:316:GLU:OE2	2.41	0.54
5:5:33:LEU:HD13	5:5:60:VAL:HG22	1.89	0.54
6:6:108:PRO:HB2	9:H:58:LYS:HD2	1.90	0.54
13:M:447:LEU:HD11	51:w:801:PC1:H3F1	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Y:89:ASP:OD2	44:z:34:ARG:NH1	2.41	0.54
2:2:175:GLU:HG3	2:2:182:PRO:HG3	1.89	0.53
3:3:261:GLU:OE1	22:c:42:ARG:NH2	2.41	0.53
9:H:149:ILE:HG21	9:H:185:TRP:HB2	1.90	0.53
29:k:173:ASP:HB2	29:k:224:SER:HA	1.90	0.53
2:2:149:VAL:O	2:2:190:ARG:NH2	2.38	0.53
3:3:190:MET:HG2	3:3:192:MET:HG2	1.91	0.53
9:H:24:GLU:OE2	9:H:274:ARG:NH1	2.40	0.53
11:K:67:ALA:O	11:K:70:GLU:HB3	2.07	0.53
13:M:179:LEU:HD13	13:M:249:LEU:HD11	1.89	0.53
41:w:100:ARG:HB2	41:w:105:LEU:HB2	1.90	0.53
4:4:158:ALA:HB1	4:4:163:ALA:HB3	1.91	0.53
12:L:161:ARG:HA	38:t:91:GLU:HG3	1.90	0.53
9:H:237:PHE:O	9:H:241:LEU:HB2	2.09	0.53
50:M:501:3PE:H221	15:V:87:LEU:HB2	1.91	0.53
13:M:232:ALA:O	13:M:237:LYS:NZ	2.41	0.53
24:e:40:TYR:O	24:e:43:LEU:HB3	2.08	0.53
3:3:60:GLU:HG2	3:3:78:ASN:HB3	1.91	0.53
5:5:129:TRP:O	5:5:132:ARG:HB3	2.09	0.53
22:c:42:ARG:NH1	22:c:46:GLN:O	2.42	0.53
29:k:81:LYS:HD2	29:k:92:ASN:HD22	1.73	0.53
17:j:48:VAL:HG12	17:j:52:MET:HE2	1.91	0.52
3:3:601:ARG:NH2	3:3:614:ASP:OD1	2.39	0.52
4:4:183:ARG:NH1	4:4:210:ASP:OD2	2.41	0.52
4:4:352:TYR:HD1	7:9:86:VAL:HG21	1.74	0.52
6:6:118:SER:N	45:6:201:SF4:S4	2.82	0.52
1:1:140:GLY:O	1:1:179:ARG:NH2	2.43	0.52
3:3:478:ARG:NH2	3:3:485:GLY:O	2.42	0.52
4:4:233:ARG:NH2	7:9:23:GLN:O	2.39	0.52
27:h:45:SER:O	27:h:51:ASN:ND2	2.34	0.52
9:H:10:ILE:HA	9:H:13:ILE:HD12	1.91	0.52
9:H:312:SER:HB3	35:q:54:ARG:HH21	1.75	0.52
14:N:252:GLY:HA3	14:N:290:LEU:HD13	1.90	0.52
16:W:133:ILE:HD13	30:l:37:LYS:HG2	1.92	0.52
10:J:40:GLY:HA2	10:J:43:ILE:HD12	1.91	0.52
18:Y:97:ARG:HD3	35:q:59:LEU:HD13	1.91	0.52
15:V:11:ILE:HB	15:V:20:LYS:HD3	1.91	0.52
23:d:167:LYS:HB2	23:d:229:ALA:HA	1.92	0.52
1:1:200:GLN:NE2	3:3:174:THR:O	2.42	0.52
1:1:428:GLU:HA	1:1:431:GLN:HG2	1.92	0.52
12:L:316:THR:HA	12:L:319:ILE:HG12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:35:ASP:O	14:N:49:ASN:ND2	2.43	0.52
11:K:21:MET:HE1	50:K:101:3PE:H331	1.91	0.52
3:3:193:SER:H	3:3:196:SER:HB3	1.75	0.51
12:L:25:ASN:O	16:W:26:ARG:NH2	2.40	0.51
1:1:243:ALA:HA	1:1:251:SER:HB3	1.93	0.51
13:M:1:FME:O1	13:M:3:LYS:NZ	2.43	0.51
28:i:44:TYR:OH	28:i:113:HIS:N	2.41	0.51
4:4:49:LEU:HD22	8:A:43:PRO:HB2	1.91	0.51
5:5:79:THR:HB	5:5:93:VAL:HB	1.91	0.51
13:M:36:LEU:HB2	41:w:69:VAL:HG22	1.91	0.51
13:M:337:VAL:HG11	13:M:345:ALA:HB2	1.92	0.51
53:o:502:CDL:H311	53:o:502:CDL:H511	1.93	0.51
3:3:47:SER:O	3:3:161:ARG:NH1	2.41	0.51
5:5:150:ARG:NH1	5:5:153:THR:OG1	2.41	0.51
7:9:155:LEU:HB3	21:b:36:ASN:HD22	1.75	0.51
34:p:1:SER:OG	34:p:2:PHE:N	2.44	0.51
1:1:142:PHE:HB3	1:1:145:GLU:HB2	1.92	0.51
4:4:179:GLU:OE2	6:6:66:ARG:NH1	2.40	0.51
13:M:5:ILE:HG22	13:M:9:MET:HE2	1.93	0.51
3:3:36:GLN:NE2	22:c:47:SER:O	2.43	0.51
1:1:300:GLY:HA2	1:1:333:ALA:H	1.75	0.51
1:1:367:GLU:OE1	3:3:100:ASN:ND2	2.43	0.51
3:3:201:ASP:OD2	3:3:268:ARG:NH2	2.38	0.51
54:X:101:ZMP:O6	38:t:12:GLN:NE2	2.44	0.51
18:Y:165:ARG:HH12	33:o:90:MET:HE1	1.76	0.51
3:3:377:VAL:HG23	3:3:404:LEU:HD11	1.91	0.51
8:A:63:LEU:HB2	10:J:67:VAL:HG21	1.91	0.51
11:K:21:MET:HG2	12:L:589:LEU:HD23	1.92	0.51
5:5:65:ARG:NH1	5:5:123:VAL:O	2.44	0.51
6:6:52:LEU:HB2	6:6:90:GLY:HA3	1.93	0.51
4:4:292:ASP:OD1	4:4:292:ASP:N	2.40	0.50
4:4:363:THR:O	4:4:377:TYR:HA	2.10	0.50
23:d:128:LYS:NZ	23:d:218:ILE:O	2.36	0.50
42:x:41:GLU:OE2	42:x:44:ARG:NH2	2.42	0.50
4:4:343:GLU:O	4:4:347:HIS:ND1	2.32	0.50
12:L:432:LEU:HD21	32:n:65:ALA:HB2	1.93	0.50
50:H:502:3PE:H2G1	10:J:38:GLY:HA3	1.92	0.50
13:M:328:CYS:HB3	13:M:437:MET:HE1	1.92	0.50
51:M:502:PC1:H251	51:M:502:PC1:H372	1.92	0.50
19:Z:140:ASP:O	19:Z:161:ARG:NH1	2.44	0.50
1:1:71:ALA:HB2	47:1:503:NAI:H4D	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:158:ARG:HB3	3:3:202:ILE:HD12	1.94	0.50
19:Z:26:PRO:HB2	19:Z:31:TYR:HE2	1.76	0.50
25:f:34:LEU:HD12	25:f:37:ILE:HD12	1.92	0.50
33:o:66:THR:OG1	42:x:28:TRP:NE1	2.45	0.50
3:3:244:THR:HB	22:c:73:ALA:HB2	1.94	0.50
7:9:158:GLY:O	7:9:162:GLU:HB2	2.11	0.50
8:A:67:LEU:HD22	11:K:65:VAL:HA	1.94	0.50
13:M:457:PRO:O	41:w:84:ARG:NH1	2.44	0.50
53:V:204:CDL:H362	53:V:204:CDL:H542	1.93	0.50
28:i:78:ASP:HB3	28:i:81:MET:HG3	1.93	0.50
16:W:120:GLY:O	16:W:124:GLN:NE2	2.45	0.50
1:1:378:ARG:NE	3:3:132:GLU:OE2	2.44	0.50
3:3:443:LEU:HD13	3:3:477:ILE:HD11	1.93	0.50
12:L:213:LEU:HD23	12:L:216:LEU:HD12	1.94	0.50
14:N:115:VAL:HG12	14:N:180:ALA:HB1	1.93	0.50
26:g:21:SER:OG	26:g:30:ARG:NH1	2.45	0.50
40:v:80:ASP:HB3	40:v:83:MET:HB3	1.94	0.50
3:3:329:ILE:HD13	3:3:505:LEU:HD22	1.94	0.49
5:5:77:ASP:OD2	5:5:79:THR:OG1	2.30	0.49
9:H:152:SER:HA	9:H:155:LEU:HD12	1.93	0.49
27:h:11:ARG:NH2	27:h:20:GLN:OE1	2.45	0.49
37:s:7:ARG:HH21	37:s:17:GLU:HG3	1.76	0.49
1:1:213:VAL:HG13	1:1:217:GLY:HA2	1.95	0.49
8:A:69:ILE:HD11	9:H:144:VAL:HG13	1.93	0.49
12:L:13:ILE:HD11	53:W:201:CDL:H622	1.94	0.49
12:L:123:LEU:HD13	53:L:704:CDL:H712	1.94	0.49
14:N:331:VAL:HG13	14:N:335:MET:HE3	1.94	0.49
23:d:72:ASP:O	23:d:83:ARG:NH2	2.45	0.49
1:1:154:ARG:HA	20:a:58:LEU:HD21	1.94	0.49
3:3:114:CYS:HB3	3:3:117:GLN:HB2	1.94	0.49
9:H:162:LEU:HD21	9:H:237:PHE:HE1	1.78	0.49
1:1:390:ASP:O	1:1:393:TRP:HB3	2.12	0.49
3:3:382:THR:HG23	3:3:384:PRO:HD3	1.94	0.49
12:L:100:ILE:HG21	12:L:246:LEU:HB2	1.94	0.49
12:L:536:LEU:HG	12:L:540:MET:HE2	1.94	0.49
1:1:21:ILE:O	1:1:117:LYS:NZ	2.37	0.49
1:1:21:ILE:HG12	1:1:233:THR:HG21	1.94	0.49
13:M:369:LEU:HD12	13:M:370:PRO:HD2	1.94	0.49
23:d:97:ARG:NH1	56:d:401:NDP:O1A	2.45	0.49
1:1:355:LYS:HD3	1:1:373:ASN:HD22	1.76	0.49
4:4:200:HIS:O	4:4:324:LYS:NZ	2.33	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:324:LYS:HD3	4:4:331:SER:HB3	1.94	0.49
4:4:388:ARG:HG2	5:5:81:VAL:HG22	1.94	0.49
19:Z:159:LYS:NZ	33:o:109:TYR:O	2.40	0.49
1:1:365:CYS:HB3	45:1:501:SF4:S3	2.53	0.49
3:3:349:PHE:H	3:3:509:PRO:HB2	1.78	0.49
3:3:518:PRO:HB2	3:3:538:PRO:HD3	1.94	0.49
8:A:114:THR:HB	9:H:286:MET:HG3	1.94	0.49
9:H:20:LEU:HD13	44:z:12:MET:HE1	1.94	0.49
2:2:156:ILE:HD13	2:2:176:LEU:HD11	1.95	0.49
4:4:155:THR:HB	4:4:167:PHE:HA	1.94	0.49
6:6:36:LEU:HD13	50:6:202:3PE:H392	1.94	0.49
7:9:108:ARG:NH1	22:c:70:MET:O	2.38	0.49
9:H:97:ASN:H	35:q:143:THR:HG22	1.76	0.49
11:K:63:LEU:HD13	14:N:71:MET:HE3	1.93	0.49
13:M:41:LEU:HD13	13:M:66:LEU:HD13	1.95	0.49
13:M:91:ARG:NH2	29:k:290:ASP:OD2	2.45	0.49
14:N:207:ILE:HG22	14:N:211:MET:HE2	1.95	0.49
19:Z:159:LYS:HE2	41:w:118:ILE:HG23	1.95	0.49
1:1:270:GLU:OE1	1:1:283:HIS:NE2	2.46	0.49
3:3:140:LYS:HB2	3:3:148:THR:HG21	1.94	0.49
6:6:71:ARG:HA	9:H:37:PRO:HA	1.95	0.49
10:J:43:ILE:HG22	11:K:46:LEU:HD21	1.95	0.49
12:L:15:LEU:HD11	12:L:94:LEU:HD21	1.94	0.49
12:L:221:THR:HG23	12:L:226:GLN:HB2	1.95	0.49
35:q:67:ARG:NE	35:q:71:MET:SD	2.83	0.49
38:t:100:GLU:OE1	38:t:121:ARG:NH1	2.44	0.49
6:6:35:ASP:HB3	50:6:202:3PE:H331	1.94	0.49
26:g:42:VAL:HG11	26:g:59:ARG:HG3	1.94	0.49
4:4:135:GLN:HB3	4:4:276:ASP:HB3	1.94	0.48
12:L:59:GLN:NE2	36:r:98:GLU:OE2	2.46	0.48
14:N:258:SER:O	14:N:261:MET:HB3	2.13	0.48
14:N:159:ILE:HG21	14:N:278:LEU:HD11	1.95	0.48
22:c:8:THR:OG1	26:g:22:ARG:NH1	2.46	0.48
3:3:11:VAL:HG11	3:3:73:VAL:HB	1.94	0.48
12:L:203:MET:HB2	19:Z:113:GLN:HG3	1.96	0.48
39:u:18:THR:H	39:u:21:GLN:HE21	1.62	0.48
3:3:221:GLU:OE2	3:3:243:ARG:NH1	2.46	0.48
10:J:163:ILE:HG21	14:N:12:THR:HG21	1.95	0.48
11:K:20:LEU:HB3	12:L:592:LEU:HB2	1.96	0.48
12:L:556:ILE:O	12:L:560:THR:N	2.46	0.48
53:L:704:CDL:H182	13:M:442:LEU:HD22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Y:118:ARG:NH2	35:q:62:GLU:OE2	2.46	0.48
4:4:123:GLU:OE2	4:4:138:ARG:NH2	2.44	0.48
12:L:102:GLU:OE1	12:L:456:ARG:NH1	2.46	0.48
11:K:53:PHE:HE2	14:N:84:TRP:HE1	1.62	0.48
41:w:23:THR:OG1	41:w:24:LEU:N	2.46	0.48
18:Y:100:ARG:NH1	18:Y:103:GLN:OE1	2.46	0.48
23:d:10:LYS:NZ	26:g:126:ASP:OD2	2.44	0.48
25:f:71:LEU:HD13	25:f:79:VAL:HG11	1.96	0.48
8:A:25:PRO:HB2	9:H:60:PRO:HD3	1.95	0.47
12:L:184:LEU:HD13	13:M:393:ILE:HG21	1.96	0.47
12:L:193:LEU:HD23	12:L:201:ILE:HA	1.95	0.47
19:Z:136:LYS:NZ	19:Z:140:ASP:OD2	2.44	0.47
5:5:41:GLN:NE2	5:5:49:GLU:OE1	2.41	0.47
9:H:14:LEU:HD22	9:H:225:MET:HE2	1.96	0.47
11:K:55:LEU:HD13	30:l:16:TRP:HE3	1.79	0.47
14:N:170:LEU:O	14:N:295:ARG:NH1	2.36	0.47
16:W:138:LYS:HA	30:l:27:ARG:HB3	1.96	0.47
31:m:78:GLU:OE1	31:m:82:ARG:NH1	2.47	0.47
5:5:145:HIS:HB3	5:5:148:LEU:HB2	1.97	0.47
8:A:80:GLN:NE2	9:H:315:PRO:O	2.42	0.47
23:d:155:GLU:HA	23:d:158:GLU:HG2	1.97	0.47
29:k:133:VAL:HG12	29:k:205:VAL:HG12	1.96	0.47
2:2:159:ASN:HB3	2:2:184:PRO:HB3	1.97	0.47
3:3:582:GLN:OE1	3:3:620:ARG:NH1	2.47	0.47
6:6:58:GLU:HG2	6:6:151:PRO:O	2.14	0.47
29:k:170:ILE:HD11	29:k:238:ILE:HD11	1.95	0.47
3:3:360:SER:O	3:3:365:ASN:ND2	2.36	0.47
4:4:47:LEU:HB2	8:A:50:PRO:HG3	1.96	0.47
12:L:67:HIS:NE2	12:L:70:THR:OG1	2.43	0.47
36:r:85:LEU:HA	36:r:89:VAL:HB	1.97	0.47
5:5:121:VAL:HG21	5:5:146:PRO:HD3	1.97	0.47
8:A:74:PRO:HG2	10:J:147:TYR:HE2	1.80	0.47
35:q:92:GLU:HA	35:q:95:THR:HG22	1.95	0.47
1:1:184:TYR:HB3	1:1:357:GLU:HB3	1.96	0.47
3:3:119:GLN:HB2	3:3:123:PHE:HD2	1.79	0.47
3:3:332:LYS:NZ	3:3:505:LEU:O	2.38	0.47
5:5:96:LEU:HB2	5:5:105:ILE:HG22	1.96	0.47
12:L:69:LEU:HD13	13:M:451:PRO:HG2	1.96	0.47
12:L:392:LYS:HA	12:L:395:ILE:HD12	1.96	0.47
53:L:704:CDL:H562	53:L:704:CDL:H642	1.97	0.47
13:M:70:MET:HG2	13:M:103:GLN:HE21	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:d:120:VAL:HA	23:d:123:GLU:HG2	1.96	0.47
29:k:52:PRO:O	29:k:107:GLN:NE2	2.47	0.47
29:k:169:VAL:HB	29:k:220:VAL:HG12	1.97	0.47
3:3:262:TRP:HB2	3:3:390:LEU:HD21	1.96	0.47
12:L:279:CYS:SG	12:L:405:ASN:ND2	2.88	0.47
36:r:103:ILE:HB	37:s:47:ASP:HB3	1.96	0.47
4:4:93:TYR:HD2	5:5:168:LEU:HD22	1.80	0.47
4:4:149:ASN:HD22	4:4:370:PRO:HB2	1.80	0.47
24:e:17:GLU:HG2	24:e:67:ARG:HB3	1.96	0.47
33:o:60:ARG:NH2	53:o:502:CDL:OA4	2.43	0.47
2:2:53:LEU:HD12	20:a:52:LEU:HD13	1.96	0.47
4:4:379:VAL:HB	4:4:388:ARG:HB3	1.97	0.47
7:9:22:ALA:O	7:9:26:LEU:HB2	2.15	0.47
12:L:429:PHE:O	12:L:436:ARG:NH2	2.48	0.47
26:g:34:LEU:HD21	26:g:85:GLY:HA3	1.97	0.46
31:m:83:LEU:HD13	35:q:54:ARG:HD3	1.98	0.46
50:K:101:3PE:H112	50:V:201:3PE:H121	1.97	0.46
51:M:502:PC1:H2C2	51:M:502:PC1:H3B1	1.98	0.46
15:V:65:ILE:HD11	15:V:100:LEU:HD23	1.96	0.46
53:Y:201:CDL:H152	53:Y:201:CDL:H552	1.97	0.46
34:p:80:ARG:NH2	40:v:39:ASP:O	2.48	0.46
38:t:29:ARG:HD2	38:t:75:HIS:CD2	2.49	0.46
11:K:73:LEU:HD11	14:N:41:ILE:HG13	1.96	0.46
51:L:703:PC1:H341	53:W:201:CDL:H512	1.96	0.46
38:t:107:HIS:NE2	41:w:43:ASP:OD1	2.35	0.46
4:4:149:ASN:HD21	4:4:371:LYS:HG3	1.81	0.46
7:9:132:VAL:HG11	7:9:169:ILE:HD11	1.97	0.46
12:L:543:THR:HG23	40:v:83:MET:HE1	1.97	0.46
53:M:503:CDL:H851	53:M:503:CDL:H821	1.69	0.46
53:h:201:CDL:HB22	28:i:9:ARG:HH11	1.81	0.46
9:H:70:MET:HE1	10:J:27:ILE:HG22	1.98	0.46
22:c:56:LYS:NZ	22:c:85:THR:OG1	2.44	0.46
8:A:7:LEU:HD11	50:H:502:3PE:H351	1.98	0.46
1:1:109:GLU:OE2	1:1:112:ARG:NH2	2.49	0.46
4:4:417:ILE:HA	4:4:420:THR:HG22	1.97	0.46
39:u:45:ASP:HB3	39:u:50:HIS:HA	1.97	0.46
12:L:402:SER:OG	12:L:404:THR:OG1	2.30	0.46
53:M:503:CDL:H352	53:M:503:CDL:H612	1.97	0.46
53:M:503:CDL:H661	14:N:335:MET:HG2	1.98	0.46
23:d:26:ALA:HB3	23:d:47:VAL:HG13	1.98	0.46
3:3:382:THR:HB	3:3:454:GLY:HA3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:4:TYR:O	10:J:7:PHE:HB3	2.16	0.46
12:L:129:LEU:HA	12:L:132:VAL:HG22	1.96	0.46
17:X:26:ASP:N	17:X:26:ASP:OD1	2.47	0.46
29:k:76:ASN:O	29:k:95:ARG:NE	2.43	0.46
3:3:311:GLN:H	3:3:314:ASP:HB2	1.80	0.46
6:6:104:TYR:O	6:6:111:ARG:NH1	2.49	0.46
10:J:149:TYR:HD2	11:K:55:LEU:HD21	1.80	0.46
12:L:383:MET:HE2	39:u:36:ILE:HD13	1.97	0.46
16:W:41:THR:HG23	53:W:201:CDL:HA62	1.96	0.46
2:2:111:ARG:HD3	2:2:151:ALA:HB3	1.97	0.45
3:3:449:PRO:HG3	3:3:477:ILE:HG21	1.97	0.45
3:3:525:LEU:HD21	3:3:600:ILE:HD11	1.97	0.45
4:4:145:THR:OG1	4:4:181:TYR:OH	2.31	0.45
22:c:33:ARG:NH1	22:c:77:ASP:OD1	2.43	0.45
22:c:60:ASP:N	22:c:60:ASP:OD1	2.49	0.45
3:3:356:THR:HG21	3:3:503:LEU:HD22	1.98	0.45
7:9:69:ARG:NH1	7:9:73:GLY:O	2.45	0.45
12:L:312:LEU:HD21	12:L:392:LYS:HG3	1.99	0.45
13:M:233:ALA:HA	13:M:320:GLY:HA2	1.98	0.45
53:M:503:CDL:HA61	33:o:53:VAL:HG21	1.99	0.45
8:A:53:MET:HE2	10:J:172:THR:HB	1.97	0.45
8:A:73:LEU:HD13	10:J:55:MET:HE1	1.98	0.45
12:L:1:FME:HE2	12:L:1:FME:HB2	1.73	0.45
53:L:704:CDL:H462	53:L:704:CDL:H241	1.98	0.45
18:Y:23:VAL:HG21	44:z:65:GLY:HA2	1.97	0.45
24:e:23:CYS:SG	24:e:24:GLN:N	2.89	0.45
1:1:118:LEU:HD13	1:1:225:VAL:HG13	1.98	0.45
12:L:593:ILE:HD12	15:V:41:ALA:HB2	1.98	0.45
12:L:603:ASN:ND2	15:V:1:AYA:OT	2.49	0.45
17:X:65:ILE:HD13	38:t:3:LEU:HD22	1.98	0.45
19:Z:81:VAL:HG23	19:Z:82:LEU:HD22	1.98	0.45
19:Z:119:SER:HB3	37:s:55:ARG:HH22	1.82	0.45
2:2:121:GLN:HG2	2:2:127:LYS:HA	1.99	0.45
38:t:15:VAL:HG22	38:t:63:LEU:HD13	1.99	0.45
7:9:143:THR:HB	7:9:146:GLU:HG3	1.98	0.45
51:9:401:PC1:H252	9:H:296:LEU:HD13	1.98	0.45
9:H:134:ARG:HH11	9:H:282:TYR:HB2	1.80	0.45
11:K:56:ALA:O	11:K:59:MET:HB3	2.17	0.45
30:l:74:ARG:NH2	35:q:93:GLU:OE2	2.50	0.45
40:v:52:ASP:OD1	40:v:78:HIS:NE2	2.41	0.45
1:1:432:ARG:HA	1:1:435:GLN:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:324:ASP:N	3:3:324:ASP:OD1	2.49	0.45
4:4:106:LEU:HD11	4:4:391:ILE:HD13	1.98	0.45
5:5:183:VAL:O	26:g:100:THR:OG1	2.30	0.45
7:9:52:PHE:HE1	28:i:77:VAL:HG21	1.81	0.45
53:L:704:CDL:H322	13:M:361:LEU:HD11	1.98	0.45
13:M:64:PRO:HB3	13:M:454:ILE:HG22	1.97	0.45
53:M:503:CDL:H842	53:M:503:CDL:H652	1.99	0.45
54:X:101:ZMP:H15	54:X:101:ZMP:H17	1.65	0.45
10:J:130:THR:HG21	35:q:123:LEU:HD12	1.99	0.45
12:L:392:LYS:O	12:L:395:ILE:HB	2.16	0.45
12:L:515:TYR:OH	38:t:69:GLU:OE2	2.34	0.45
39:u:61:ASP:HB3	39:u:66:ILE:HB	1.98	0.45
3:3:101:HIS:HD2	4:4:342:MET:HE2	1.82	0.45
10:J:23:LYS:HE2	11:K:23:ARG:HG3	1.98	0.45
13:M:343:ILE:O	13:M:346:ARG:NH1	2.45	0.45
53:M:503:CDL:H871	14:N:246:ILE:HG22	1.99	0.45
14:N:125:SER:HB2	50:N:401:3PE:H32	1.98	0.45
40:v:71:LEU:HD21	40:v:77:MET:HG2	1.99	0.45
1:1:295:LEU:HB2	1:1:339:ARG:HD2	1.98	0.45
12:L:106:TRP:CD1	12:L:447:ASN:HD22	2.34	0.45
12:L:137:LEU:HD21	12:L:263:PHE:HZ	1.82	0.45
50:M:501:3PE:H2A2	50:M:501:3PE:H371	1.99	0.45
14:N:222:ASN:HD21	14:N:240:MET:HB3	1.81	0.45
18:Y:136:LEU:HD23	31:m:57:ARG:HE	1.82	0.45
35:q:88:GLU:OE1	35:q:127:ARG:NH2	2.49	0.45
16:W:125:TYR:HB2	30:l:48:SER:HB3	1.98	0.44
17:X:13:ASP:OD2	32:n:12:LYS:NZ	2.50	0.44
33:o:45:ASP:OD1	33:o:49:ARG:NH2	2.50	0.44
38:t:29:ARG:HD2	38:t:75:HIS:HD2	1.83	0.44
3:3:194:GLU:HG2	3:3:195:LEU:HG	1.99	0.44
8:A:84:LEU:HD11	31:m:45:ASN:HD22	1.82	0.44
13:M:173:SER:HB2	16:W:101:ALA:HB2	1.99	0.44
18:Y:17:VAL:HG12	18:Y:19:VAL:HG22	1.99	0.44
28:i:50:GLU:HG3	28:i:89:TRP:HZ2	1.82	0.44
3:3:242:THR:HG22	3:3:247:VAL:HA	1.98	0.44
7:9:108:ARG:NH2	28:i:128:SER:OG	2.51	0.44
7:9:114:THR:HG21	7:9:144:HIS:CD2	2.53	0.44
11:K:14:VAL:HG22	50:K:101:3PE:H2B2	2.00	0.44
12:L:128:MET:HG2	12:L:251:THR:HG22	1.98	0.44
12:L:569:ALA:HB2	53:V:204:CDL:H541	1.99	0.44
21:b:49:VAL:HG22	21:b:90:GLN:HG3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:h:5:ARG:HA	27:h:8:GLN:HB3	1.99	0.44
33:o:52:PRO:HG2	33:o:56:ALA:HB2	1.98	0.44
8:A:25:PRO:HG2	9:H:60:PRO:HG3	1.99	0.44
10:J:5:ILE:HA	10:J:8:ILE:HD12	1.98	0.44
12:L:561:ILE:O	12:L:565:THR:OG1	2.36	0.44
13:M:253:ILE:HG12	13:M:257:MET:HG2	2.00	0.44
3:3:41:CYS:O	3:3:161:ARG:NH2	2.35	0.44
3:3:175:THR:HG21	3:3:186:TYR:HB2	1.99	0.44
13:M:243:MET:HB3	13:M:301:ILE:HG21	2.00	0.44
18:Y:48:GLU:OE1	18:Y:134:ARG:NH2	2.47	0.44
27:h:8:GLN:NE2	27:h:20:GLN:HG3	2.33	0.44
28:i:9:ARG:HA	28:i:12:GLN:HG2	1.99	0.44
3:3:323:VAL:HG11	3:3:525:LEU:HD13	2.00	0.44
17:X:49:GLU:OE2	38:t:19:TYR:OH	2.35	0.44
34:p:82:ASN:HA	50:p:201:3PE:H12	1.98	0.44
7:9:77:CYS:O	7:9:105:ARG:NH1	2.48	0.44
13:M:101:LEU:HD21	53:M:503:CDL:H841	1.99	0.44
38:t:137:LYS:HA	38:t:140:GLN:HG2	2.00	0.44
51:w:801:PC1:H252	51:w:801:PC1:H222	1.90	0.44
1:1:265:PRO:O	2:2:190:ARG:NH1	2.37	0.44
3:3:205:VAL:HG23	3:3:207:ALA:H	1.82	0.44
4:4:285:VAL:H	7:9:2:TYR:HA	1.82	0.44
13:M:16:TRP:NE1	13:M:97:SER:OG	2.47	0.44
14:N:110:PRO:HD3	14:N:160:LEU:HD23	2.00	0.44
23:d:130:ILE:HG12	23:d:164:THR:HB	2.00	0.44
3:3:115:ASP:O	3:3:119:GLN:HG2	2.17	0.44
4:4:110:SER:OG	4:4:149:ASN:ND2	2.51	0.44
4:4:211:ILE:HG22	4:4:315:LEU:HD11	1.99	0.44
16:W:11:ILE:HG12	38:t:103:LEU:HD11	2.00	0.44
23:d:100:GLU:HB2	23:d:105:ASP:HA	1.99	0.44
1:1:390:ASP:OD1	1:1:423:ARG:NH2	2.49	0.43
10:J:10:SER:O	10:J:13:PHE:HB3	2.18	0.43
12:L:128:MET:HE1	12:L:255:ALA:HB2	2.00	0.43
22:c:59:PHE:HE2	22:c:82:LEU:HD23	1.81	0.43
3:3:140:LYS:HD3	3:3:150:MET:HG3	1.98	0.43
8:A:67:LEU:HB3	11:K:65:VAL:HG13	2.00	0.43
8:A:102:LEU:HD23	50:A:403:3PE:H372	1.99	0.43
23:d:167:LYS:O	23:d:230:PHE:N	2.42	0.43
33:o:5:ARG:NH2	33:o:89:ASP:OD1	2.51	0.43
41:w:34:ASP:N	41:w:34:ASP:OD1	2.51	0.43
1:1:365:CYS:HB2	45:1:501:SF4:S3	2.56	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:65:VAL:HB	4:4:77:ASP:HB3	2.01	0.43
10:J:10:SER:OG	11:K:7:ASN:ND2	2.51	0.43
12:L:25:ASN:HD22	12:L:29:PHE:HE2	1.66	0.43
17:j:49:GLU:HA	17:j:52:MET:HE3	2.01	0.43
1:1:214:GLY:N	1:1:218:CYS:O	2.44	0.43
4:4:104:ASP:HB3	4:4:190:HIS:ND1	2.33	0.43
4:4:203:LEU:HD22	4:4:207:LEU:HD23	2.00	0.43
9:H:114:TYR:OH	10:J:61:LEU:O	2.28	0.43
23:d:26:ALA:HA	23:d:31:GLY:HA3	2.00	0.43
23:d:201:VAL:HG22	23:d:237:LEU:HD23	2.00	0.43
39:u:40:PHE:O	39:u:44:SER:OG	2.27	0.43
3:3:163:ALA:HA	3:3:167:ALA:HB3	1.99	0.43
13:M:423:ILE:HG12	34:p:58:VAL:HG22	2.00	0.43
4:4:61:VAL:HG11	6:6:96:MET:HE1	2.00	0.43
13:M:75:LEU:HD23	13:M:440:HIS:CE1	2.54	0.43
13:M:106:LEU:HD13	13:M:234:ILE:HG21	2.01	0.43
13:M:153:THR:HG23	13:M:206:LYS:HD3	2.00	0.43
1:1:99:GLU:OE2	1:1:106:LYS:N	2.51	0.43
1:1:298:ILE:HB	1:1:335:ILE:HB	2.01	0.43
4:4:220:LEU:HD21	27:h:19:LEU:HD23	2.01	0.43
13:M:60:SER:HB2	13:M:457:PRO:HA	2.00	0.43
13:M:180:GLN:HA	13:M:248:LEU:HD21	2.01	0.43
53:W:201:CDL:H341	53:W:201:CDL:H511	2.01	0.43
3:3:200:ILE:HG22	22:c:45:MET:HE1	2.00	0.43
12:L:538:PRO:HB2	40:v:89:VAL:HG22	2.01	0.43
16:W:138:LYS:HB2	16:W:143:ASN:HD21	1.81	0.43
3:3:187:ILE:HG13	3:3:189:LYS:HB2	2.00	0.43
4:4:83:LEU:HD11	6:6:53:ALA:HB2	2.00	0.43
4:4:190:HIS:CD2	6:6:150:PRO:HD3	2.54	0.43
12:L:565:THR:HG21	53:V:204:CDL:H751	2.00	0.43
13:M:1:FME:HE2	13:M:1:FME:HB2	1.81	0.43
3:3:622:ARG:NH2	24:e:73:GLU:OE2	2.52	0.43
4:4:184:VAL:O	7:9:60:ARG:NH1	2.51	0.43
7:9:151:LYS:HE2	7:9:155:LEU:HD11	2.01	0.43
8:A:30:TYR:OH	9:H:57:ILE:O	2.36	0.43
8:A:31:SER:HB2	8:A:33:LYS:HE3	2.01	0.43
8:A:34:THR:HG21	23:d:174:ARG:HD3	2.01	0.43
12:L:542:LEU:HB2	40:v:83:MET:HE3	2.01	0.43
53:Y:201:CDL:H641	53:Y:201:CDL:H872	2.00	0.43
1:1:193:ILE:HG23	1:1:215:VAL:HA	2.01	0.42
2:2:76:PRO:HA	2:2:77:PRO:HD3	1.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:255:HIS:NE2	3:3:634:ASP:OD1	2.47	0.42
4:4:145:THR:HA	4:4:148:LEU:HD12	2.01	0.42
12:L:316:THR:HG23	12:L:325:ALA:HB2	2.01	0.42
13:M:68:LEU:HB2	51:w:801:PC1:H3G1	2.01	0.42
14:N:100:MET:HE1	53:V:203:CDL:H272	2.01	0.42
23:d:91:VAL:HG23	23:d:126:VAL:HG11	2.00	0.42
1:1:94:VAL:O	1:1:222:VAL:HA	2.20	0.42
5:5:56:GLY:HA2	5:5:59:PRO:HD2	2.01	0.42
50:6:202:3PE:H2I3	9:H:49:ILE:HA	2.00	0.42
12:L:375:ILE:HG12	39:u:32:MET:SD	2.59	0.42
16:W:43:ILE:HG12	16:W:47:ILE:HD12	2.01	0.42
23:d:94:LEU:HD23	23:d:132:ILE:HG13	2.01	0.42
28:i:54:GLN:HB3	28:i:58:ARG:HB2	2.01	0.42
1:1:346:ALA:HA	2:2:109:MET:HE1	2.02	0.42
3:3:382:THR:OG1	3:3:387:GLU:OE1	2.34	0.42
7:9:27:TRP:HB3	7:9:30:LEU:HD12	2.01	0.42
22:c:28:GLU:O	22:c:32:THR:OG1	2.31	0.42
3:3:364:LEU:HD12	3:3:491:ASN:HB3	2.00	0.42
4:4:412:ALA:HB3	9:H:281:ARG:HG3	2.00	0.42
7:9:162:GLU:HB3	28:i:109:ILE:HG12	2.01	0.42
10:J:21:SER:O	10:J:23:LYS:NZ	2.49	0.42
12:L:245:ALA:O	12:L:249:SER:OG	2.36	0.42
13:M:116:ILE:HD11	13:M:161:LEU:HD12	2.01	0.42
16:W:28:TYR:O	41:w:67:SER:OG	2.29	0.42
19:Z:15:ARG:HB3	36:r:109:ILE:HD12	2.00	0.42
19:Z:141:ARG:HG3	41:w:112:CYS:HB2	2.01	0.42
4:4:149:ASN:ND2	4:4:370:PRO:HB2	2.35	0.42
4:4:282:GLU:HB3	4:4:313:GLN:HE22	1.85	0.42
5:5:74:SER:HB3	5:5:97:LEU:HB3	2.02	0.42
5:5:119:SER:OG	5:5:131:GLU:OE2	2.27	0.42
12:L:1:FME:HG3	12:L:61:MET:HE1	2.01	0.42
12:L:94:LEU:HD23	12:L:125:LEU:HD21	2.02	0.42
51:L:703:PC1:H3A2	36:r:80:ILE:HG12	2.02	0.42
13:M:426:ILE:HB	38:t:101:TRP:HH2	1.84	0.42
16:W:83:PRO:O	16:W:87:TYR:HB2	2.19	0.42
2:2:120:ILE:HD11	2:2:169:ILE:HG12	2.02	0.42
3:3:569:LYS:HG3	3:3:571:ALA:HB2	2.01	0.42
4:4:323:ILE:HD12	4:4:324:LYS:HG3	2.02	0.42
12:L:161:ARG:HH22	38:t:90:TYR:HB3	1.84	0.42
13:M:281:ASP:HB3	13:M:284:SER:HB2	2.01	0.42
23:d:48:PRO:HA	23:d:71:MET:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:v:138:LEU:HB3	40:v:141:GLU:HB2	2.00	0.42
9:H:26:LYS:HA	9:H:36:GLY:HA3	2.02	0.42
10:J:45:LEU:HD23	10:J:50:SER:HA	2.02	0.42
13:M:403:THR:HA	13:M:406:TYR:CE1	2.54	0.42
19:Z:18:ALA:N	36:r:108:THR:O	2.53	0.42
3:3:231:MET:HB3	3:3:266:LYS:HD2	2.01	0.42
4:4:85:2MR:HE	4:4:85:2MR:HB3	1.72	0.42
12:L:49:ILE:HG12	19:Z:32:LEU:HD13	2.01	0.42
12:L:487:LYS:HE3	39:u:49:GLY:HA2	2.01	0.42
53:M:503:CDL:H873	14:N:257:LEU:HD11	2.01	0.42
16:W:122:TRP:CD1	33:o:2:MET:HG2	2.54	0.42
4:4:354:GLU:OE2	4:4:357:GLN:NE2	2.53	0.42
5:5:78:LEU:HB3	5:5:130:TYR:HB3	2.02	0.42
10:J:152:TRP:HZ2	14:N:19:ILE:HG12	1.84	0.42
53:Y:201:CDL:H571	53:Y:201:CDL:H171	2.01	0.42
37:s:45:MET:HB2	37:s:50:LEU:HD12	2.02	0.42
37:s:102:GLU:OE2	37:s:105:ARG:NH2	2.53	0.42
2:2:34:ILE:HD11	20:a:52:LEU:HD22	2.01	0.42
14:N:136:LEU:HD23	14:N:205:LEU:HD21	2.01	0.42
29:k:49:LYS:HE3	29:k:51:PHE:HE1	1.85	0.42
3:3:138:GLU:N	21:b:74:ASN:HD22	2.18	0.41
51:L:703:PC1:H32	51:w:801:PC1:H142	2.01	0.41
19:Z:25:LEU:HD12	37:s:75:ASN:HB2	2.02	0.41
29:k:213:GLU:O	29:k:217:LYS:NZ	2.52	0.41
30:l:64:GLU:HG3	30:l:70:LYS:HD2	2.02	0.41
3:3:12:PHE:HB2	3:3:78:ASN:HA	2.01	0.41
50:H:502:3PE:H2H2	50:H:502:3PE:H3C2	2.01	0.41
12:L:9:LEU:HD12	36:r:85:LEU:HD11	2.02	0.41
14:N:217:THR:HG23	50:N:401:3PE:H242	2.02	0.41
14:N:289:ASN:HA	14:N:292:PHE:CE1	2.54	0.41
16:W:8:LEU:HD21	17:X:88:GLU:HB2	2.01	0.41
29:k:108:TYR:OH	29:k:164:LEU:O	2.27	0.41
29:k:126:ARG:NH1	57:k:501:AMP:O5'	2.53	0.41
1:1:361:GLN:N	45:1:501:SF4:S4	2.92	0.41
2:2:50:VAL:HG12	2:2:69:VAL:HG22	2.02	0.41
4:4:251:LEU:HD23	4:4:251:LEU:HA	1.92	0.41
5:5:32:ILE:HG23	25:f:43:TYR:HB2	2.01	0.41
9:H:46:LEU:HD13	9:H:49:ILE:HD13	2.02	0.41
12:L:397:GLU:HB3	12:L:482:MET:HE1	2.02	0.41
12:L:416:THR:O	12:L:419:THR:OG1	2.36	0.41
13:M:78:MET:HE2	41:w:61:VAL:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Y:44:LEU:HD22	18:Y:130:VAL:HB	2.02	0.41
18:Y:48:GLU:OE1	31:m:57:ARG:NH2	2.44	0.41
53:Y:201:CDL:H311	53:Y:201:CDL:H562	2.02	0.41
30:l:16:TRP:CD1	30:l:16:TRP:H	2.38	0.41
1:1:139:ARG:NH2	2:2:144:CYS:O	2.35	0.41
1:1:342:ASP:OD1	1:1:429:ARG:NH2	2.53	0.41
6:6:128:TYR:OH	7:9:115:LYS:NZ	2.50	0.41
9:H:80:THR:HG21	50:H:502:3PE:H3D1	2.01	0.41
12:L:295:GLN:OE1	38:t:77:GLN:NE2	2.41	0.41
13:M:50:LEU:HA	16:W:86:ASN:HD21	1.86	0.41
14:N:202:LEU:HD21	30:l:1:PRO:HD3	2.03	0.41
37:s:35:GLU:HA	40:v:156:TYR:HA	2.03	0.41
14:N:30:TRP:NE1	14:N:67:SER:OG	2.53	0.41
14:N:193:VAL:HB	14:N:266:ILE:HG23	2.02	0.41
50:i:201:3PE:H3D2	50:i:201:3PE:H3A1	1.95	0.41
29:k:38:LEU:HD22	29:k:228:ALA:HB1	2.01	0.41
3:3:495:ARG:HG3	3:3:496:ILE:HG12	2.03	0.41
8:A:3:LEU:HD23	50:H:502:3PE:H231	2.02	0.41
10:J:167:VAL:HG22	14:N:42:PRO:HG2	2.02	0.41
50:L:701:3PE:H382	13:M:151:PHE:HB3	2.01	0.41
19:Z:3:SER:OG	19:Z:4:TRP:N	2.52	0.41
1:1:184:TYR:OH	47:1:503:NAI:H5N	2.20	0.41
1:1:276:LEU:HD21	1:1:297:VAL:HG11	2.02	0.41
4:4:63:ARG:HH22	26:g:96:TRP:HA	1.86	0.41
6:6:90:GLY:HA2	45:6:201:SF4:S3	2.61	0.41
12:L:378:LEU:HB3	12:L:383:MET:HB2	2.03	0.41
13:M:23:ILE:HD11	13:M:92:LYS:HD2	2.03	0.41
1:1:94:VAL:HG22	1:1:135:TYR:HB2	2.02	0.41
2:2:61:LEU:HD12	2:2:90:TYR:HB3	2.03	0.41
3:3:243:ARG:HD2	3:3:244:THR:HG23	2.03	0.41
50:H:502:3PE:H2A2	10:J:42:GLY:HA3	2.02	0.41
13:M:126:LEU:HD13	13:M:150:LEU:HD12	2.03	0.41
23:d:98:GLU:HG3	23:d:177:ARG:HE	1.86	0.41
29:k:188:ASN:HB3	29:k:191:GLU:HB3	2.03	0.41
1:1:299:PRO:HG2	1:1:327:THR:HG21	2.03	0.41
2:2:116:ILE:HG23	2:2:169:ILE:HG21	2.03	0.41
4:4:48:THR:HA	4:4:66:MET:O	2.21	0.41
5:5:49:GLU:HG2	5:5:106:ARG:HB3	2.02	0.41
6:6:59:MET:HE2	6:6:69:MET:HE1	2.03	0.41
7:9:87:CYS:HA	7:9:88:PRO:HD3	1.96	0.41
11:K:38:LEU:O	11:K:42:ILE:HG12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:155:ALA:HB1	51:M:502:PC1:H2H2	2.03	0.41
13:M:259:TYR:O	13:M:263:MET:HG2	2.21	0.41
15:V:5:LEU:HD23	50:V:202:3PE:H231	2.03	0.41
15:V:93:GLY:HA3	15:V:118:GLY:HA2	2.02	0.41
29:k:104:ARG:HH21	57:k:501:AMP:H8	1.68	0.41
2:2:24:THR:OG1	2:2:27:ASN:OD1	2.35	0.41
3:3:331:LEU:HB2	3:3:600:ILE:HD13	2.03	0.41
8:A:71:LEU:O	10:J:147:TYR:OH	2.30	0.41
14:N:210:ILE:HG22	14:N:333:SER:HB3	2.04	0.41
16:W:37:VAL:HG21	53:W:201:CDL:H811	2.03	0.41
4:4:71:GLU:HB3	4:4:410:MET:HG2	2.03	0.40
4:4:296:ARG:HH21	4:4:420:THR:HG21	1.86	0.40
9:H:66:SER:OG	9:H:124:ASN:OD1	2.35	0.40
14:N:275:SER:HB3	15:V:136:ALA:HB3	2.03	0.40
18:Y:82:THR:HA	18:Y:85:TRP:CD1	2.56	0.40
1:1:69:GLY:O	47:1:503:NAI:H2N	2.21	0.40
3:3:127:ARG:NH2	4:4:326:ASP:O	2.54	0.40
5:5:51:CYS:HB3	25:f:111:TRP:CE2	2.56	0.40
5:5:134:ILE:HG22	5:5:140:VAL:HB	2.02	0.40
9:H:45:LEU:HD21	44:z:7:PRO:HB2	2.04	0.40
9:H:198:PHE:HD1	9:H:285:LEU:HD13	1.86	0.40
52:H:501:DCQ:H13A	52:H:501:DCQ:H10	1.88	0.40
10:J:17:PHE:HA	10:J:20:PHE:CE1	2.56	0.40
1:1:305:PRO:HG3	1:1:413:TRP:HB3	2.02	0.40
3:3:481:SER:OG	3:3:482:GLY:N	2.53	0.40
4:4:93:TYR:HE2	5:5:168:LEU:HB2	1.85	0.40
5:5:92:ILE:HD11	5:5:111:THR:HG22	2.03	0.40
12:L:123:LEU:HB2	12:L:150:MET:HE2	2.03	0.40
13:M:71:TRP:CD1	51:w:801:PC1:H3C2	2.57	0.40
29:k:135:LEU:HD22	29:k:152:TYR:CD2	2.57	0.40
33:o:13:PHE:HE2	33:o:74:TYR:HB3	1.85	0.40
1:1:144:ASN:O	1:1:148:ASN:HB2	2.21	0.40
9:H:287:HIS:HD1	9:H:291:LYS:HD2	1.86	0.40
12:L:421:ILE:HG12	12:L:501:ALA:HB2	2.03	0.40
13:M:122:PHE:CZ	13:M:206:LYS:HG3	2.57	0.40
14:N:108:MET:HB3	14:N:108:MET:HE2	1.84	0.40
15:V:113:ALA:O	15:V:117:MET:HB2	2.21	0.40
53:Y:201:CDL:H632	53:Y:201:CDL:H601	1.90	0.40
36:r:74:VAL:O	36:r:78:VAL:HG23	2.21	0.40
1:1:132:ARG:CZ	20:a:66:PRO:HD3	2.52	0.40
5:5:137:MET:HE3	5:5:152:LEU:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:293:PHE:O	9:H:297:THR:OG1	2.31	0.40
13:M:405:LEU:HD23	13:M:405:LEU:HA	1.92	0.40
13:M:408:LEU:O	13:M:412:ILE:N	2.52	0.40
51:M:502:PC1:H151	15:V:130:GLU:HB3	2.03	0.40
14:N:278:LEU:HA	14:N:278:LEU:HD12	1.93	0.40
15:V:139:LYS:HG3	15:V:140:VAL:HG13	2.02	0.40
17:j:11:ILE:HG22	17:j:77:VAL:HG23	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	428/464 (92%)	406 (95%)	22 (5%)	0	100	100
2	2	211/246 (86%)	195 (92%)	16 (8%)	0	100	100
3	3	686/727 (94%)	661 (96%)	24 (4%)	1 (0%)	48	70
4	4	414/463 (89%)	399 (96%)	15 (4%)	0	100	100
5	5	206/266 (77%)	198 (96%)	8 (4%)	0	100	100
6	6	154/223 (69%)	149 (97%)	5 (3%)	0	100	100
7	9	174/217 (80%)	166 (95%)	8 (5%)	0	100	100
8	A	106/115 (92%)	96 (91%)	10 (9%)	0	100	100
9	H	310/318 (98%)	304 (98%)	6 (2%)	0	100	100
10	J	165/175 (94%)	155 (94%)	10 (6%)	0	100	100
11	K	96/98 (98%)	94 (98%)	2 (2%)	0	100	100
12	L	604/606 (100%)	579 (96%)	25 (4%)	0	100	100
13	M	457/459 (100%)	450 (98%)	7 (2%)	0	100	100
14	N	345/347 (99%)	336 (97%)	9 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	V	138/141 (98%)	136 (99%)	2 (1%)	0	100	100
16	W	137/189 (72%)	136 (99%)	1 (1%)	0	100	100
17	X	85/157 (54%)	82 (96%)	3 (4%)	0	100	100
17	j	80/157 (51%)	77 (96%)	3 (4%)	0	100	100
18	Y	169/172 (98%)	166 (98%)	3 (2%)	0	100	100
19	Z	169/175 (97%)	166 (98%)	3 (2%)	0	100	100
20	a	42/109 (38%)	40 (95%)	2 (5%)	0	100	100
21	b	93/124 (75%)	91 (98%)	2 (2%)	0	100	100
22	c	124/170 (73%)	121 (98%)	3 (2%)	0	100	100
23	d	289/380 (76%)	283 (98%)	6 (2%)	0	100	100
24	e	84/99 (85%)	82 (98%)	2 (2%)	0	100	100
25	f	111/116 (96%)	110 (99%)	1 (1%)	0	100	100
26	g	112/140 (80%)	106 (95%)	6 (5%)	0	100	100
27	h	92/114 (81%)	86 (94%)	6 (6%)	0	100	100
28	i	143/145 (99%)	140 (98%)	3 (2%)	0	100	100
29	k	317/355 (89%)	303 (96%)	14 (4%)	0	100	100
30	l	103/106 (97%)	101 (98%)	2 (2%)	0	100	100
31	m	78/84 (93%)	74 (95%)	4 (5%)	0	100	100
32	n	77/98 (79%)	75 (97%)	2 (3%)	0	100	100
33	o	118/122 (97%)	117 (99%)	1 (1%)	0	100	100
34	p	126/130 (97%)	120 (95%)	6 (5%)	0	100	100
35	q	137/144 (95%)	135 (98%)	2 (2%)	0	100	100
36	r	95/128 (74%)	91 (96%)	4 (4%)	0	100	100
37	s	120/137 (88%)	116 (97%)	4 (3%)	0	100	100
38	t	175/179 (98%)	171 (98%)	4 (2%)	0	100	100
39	u	63/108 (58%)	61 (97%)	2 (3%)	0	100	100
40	v	153/186 (82%)	148 (97%)	5 (3%)	0	100	100
41	w	99/154 (64%)	93 (94%)	6 (6%)	0	100	100
42	x	47/76 (62%)	45 (96%)	2 (4%)	0	100	100
43	y	48/58 (83%)	47 (98%)	1 (2%)	0	100	100
44	z	68/70 (97%)	67 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	8048/9247 (87%)	7774 (97%)	273 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	3	367	THR

5.3.2 Protein sidechains ⓘ

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%)	344 (100%)	0	100	100
2	2	183/210 (87%)	183 (100%)	0	100	100
3	3	578/608 (95%)	578 (100%)	0	100	100
4	4	363/391 (93%)	362 (100%)	1 (0%)	86	94
5	5	189/230 (82%)	189 (100%)	0	100	100
6	6	132/181 (73%)	131 (99%)	1 (1%)	73	88
7	9	151/179 (84%)	150 (99%)	1 (1%)	76	89
8	A	99/103 (96%)	98 (99%)	1 (1%)	68	86
9	H	274/278 (99%)	273 (100%)	1 (0%)	84	93
10	J	138/144 (96%)	138 (100%)	0	100	100
11	K	86/86 (100%)	86 (100%)	0	100	100
12	L	538/538 (100%)	538 (100%)	0	100	100
13	M	411/411 (100%)	411 (100%)	0	100	100
14	N	315/315 (100%)	315 (100%)	0	100	100
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	Y	154/155 (99%)	154 (100%)	0	100	100
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	255/326 (78%)	255 (100%)	0	100	100
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%)	69 (100%)	0	100	100
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%)	119 (100%)	0	100	100
36	r	95/122 (78%)	95 (100%)	0	100	100
37	s	110/120 (92%)	110 (100%)	0	100	100
38	t	159/161 (99%)	159 (100%)	0	100	100
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	7129/7955 (90%)	7124 (100%)	5 (0%)	87	96

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	4	252	ASN

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Mol	Chain	Res	Type
6	6	54	CYS
7	9	78	ILE
8	A	29	VAL
9	H	241	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	148	ASN
1	1	150	GLN
1	1	293	ASN
1	1	361	GLN
1	1	373	ASN
1	1	402	HIS
1	1	421	HIS
2	2	101	GLN
2	2	121	GLN
2	2	155	GLN
3	3	237	ASN
3	3	277	GLN
3	3	581	GLN
4	4	149	ASN
4	4	252	ASN
5	5	19	HIS
5	5	160	HIS
9	H	235	ASN
9	H	247	HIS
12	L	175	ASN
12	L	192	ASN
12	L	269	ASN
12	L	354	GLN
12	L	405	ASN
12	L	442	ASN
12	L	603	ASN
13	M	144	ASN
13	M	169	ASN
13	M	374	ASN
14	N	232	HIS
14	N	235	ASN
15	V	18	HIS
16	W	143	ASN
18	Y	29	HIS

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Mol	Chain	Res	Type
18	Y	76	HIS
18	Y	142	HIS
19	Z	77	HIS
19	Z	123	ASN
19	Z	143	HIS
20	a	40	ASN
21	b	16	GLN
21	b	36	ASN
23	d	103	ASN
23	d	148	ASN
25	f	49	GLN
26	g	125	HIS
27	h	24	GLN
28	i	69	ASN
28	i	72	ASN
29	k	107	GLN
29	k	141	GLN
29	k	200	GLN
29	k	251	GLN
29	k	288	GLN
30	l	97	HIS
30	l	100	GLN
31	m	51	ASN
33	o	61	GLN
37	s	46	ASN
38	t	32	HIS
38	t	50	HIS
39	u	21	GLN
40	v	55	GLN
40	v	87	ASN
41	w	57	ASN
42	x	34	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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
27	AYA	h	1	27	6,7,8	1.24	1 (16%)	6,8,10	1.09	0
4	2MR	4	85	4	10,12,13	2.34	3 (30%)	5,13,15	1.17	0
29	SEP	k	36	29	8,9,10	1.61	1 (12%)	7,12,14	1.19	1 (14%)
12	FME	L	1	12	8,9,10	0.94	0	8,9,11	1.13	1 (12%)
13	FME	M	1	13	8,9,10	0.94	0	8,9,11	1.03	0
11	FME	K	1	11	8,9,10	0.99	0	8,9,11	0.92	0
15	AYA	V	1	15	6,7,8	1.23	1 (16%)	6,8,10	1.91	2 (33%)

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
27	AYA	h	1	27	-	0/5/6/8	-
4	2MR	4	85	4	-	4/10/13/15	-
29	SEP	k	36	29	-	4/6/8/10	-
12	FME	L	1	12	-	3/7/9/11	-
13	FME	M	1	13	-	2/7/9/11	-
11	FME	K	1	11	-	4/7/9/11	-
15	AYA	V	1	15	-	2/5/6/8	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	4	85	2MR	CZ-NH2	4.79	1.43	1.33
4	4	85	2MR	CZ-NE	4.45	1.43	1.34
29	k	36	SEP	P-O1P	3.53	1.61	1.50
27	h	1	AYA	CA-N	-2.38	1.44	1.46
15	V	1	AYA	CA-N	-2.21	1.44	1.46
4	4	85	2MR	CQ1-NH1	-2.13	1.42	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	V	1	AYA	CB-CA-N	3.23	113.32	109.68
15	V	1	AYA	CA-N-CT	2.91	125.25	121.50
29	k	36	SEP	OG-CB-CA	2.44	110.52	108.14
12	L	1	FME	C-CA-N	2.16	113.67	109.50

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	K	1	FME	O1-CN-N-CA
13	M	1	FME	C-CA-CB-CG
29	k	36	SEP	CB-OG-P-O1P
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
12	L	1	FME	CA-CB-CG-SD
12	L	1	FME	CB-CG-SD-CE
12	L	1	FME	N-CA-CB-CG
4	4	85	2MR	CA-CB-CG-CD
4	4	85	2MR	NE-CD-CG-CB
11	K	1	FME	CA-CB-CG-SD
11	K	1	FME	CB-CG-SD-CE
13	M	1	FME	CB-CA-N-CN
11	K	1	FME	CB-CA-N-CN
29	k	36	SEP	CA-CB-OG-P
4	4	85	2MR	N-CA-CB-CG

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	4	85	2MR	1	0
12	L	1	FME	2	0
13	M	1	FME	2	0
15	V	1	AYA	1	0

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 46 ligands modelled in this entry, 2 are monoatomic - leaving 44 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
46	FMN	1	502	-	33,33,33	1.12	3 (9%)	48,50,50	1.36	8 (16%)
51	PC1	A	402	-	36,36,53	0.37	0	42,44,61	0.60	2 (4%)
50	3PE	K	101	-	39,39,50	0.34	0	42,44,55	0.40	0
48	FES	3	803	3	0,4,4	-	-	-	-	-
53	CDL	V	203	-	93,93,99	0.26	0	99,105,111	0.25	0
53	CDL	Y	201	-	99,99,99	0.26	0	105,111,111	0.36	1 (0%)
45	SF4	1	501	1	0,12,12	-	-	-	-	-
52	DCQ	H	501	-	23,23,23	0.21	0	27,29,29	0.50	0
47	NAI	1	503	-	47,48,48	0.38	0	64,73,73	1.80	4 (6%)
56	NDP	d	401	-	51,52,52	0.42	0	71,80,80	0.43	0
50	3PE	o	501	-	30,30,50	0.38	0	33,35,55	0.33	0
50	3PE	V	201	-	34,34,50	0.36	0	37,39,55	0.31	0
50	3PE	L	702	-	50,50,50	0.30	0	53,55,55	0.39	0
50	3PE	p	201	-	26,26,50	0.49	0	29,31,55	0.52	1 (3%)
53	CDL	W	201	-	99,99,99	0.28	0	105,111,111	0.29	0
53	CDL	h	201	-	57,57,99	0.37	0	63,69,111	0.34	0
45	SF4	9	403	7	0,12,12	-	-	-	-	-
50	3PE	V	202	-	36,36,50	0.35	0	39,41,55	0.33	0
53	CDL	o	502	-	74,74,99	0.31	0	80,86,111	0.47	1 (1%)
58	MYR	s	201	37	13,14,15	0.18	0	12,13,15	0.14	0
51	PC1	9	401	-	53,53,53	0.30	0	59,61,61	0.50	0
54	ZMP	g	201	-	28,33,36	0.62	1 (3%)	32,40,45	1.30	4 (12%)
50	3PE	N	401	-	50,50,50	0.31	0	53,55,55	0.55	1 (1%)
45	SF4	3	802	3	0,12,12	-	-	-	-	-
48	FES	2	300	2	0,4,4	-	-	-	-	-
50	3PE	A	403	-	50,50,50	0.31	0	53,55,55	0.41	0
50	3PE	H	502	-	50,50,50	0.30	0	53,55,55	0.44	1 (1%)
50	3PE	i	201	-	50,50,50	0.30	0	53,55,55	0.32	0
51	PC1	w	801	-	53,53,53	0.29	0	59,61,61	0.39	0
57	AMP	k	501	-	25,25,25	1.43	4 (16%)	37,38,38	2.05	8 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
50	3PE	L	701	-	39,39,50	0.33	0	42,44,55	0.34	0
51	PC1	A	401	-	45,45,53	0.31	0	51,53,61	0.34	0
45	SF4	6	201	6	0,12,12	-	-	-		
50	3PE	6	202	-	50,50,50	0.30	0	53,55,55	0.32	0
53	CDL	V	204	-	84,84,99	0.27	0	90,96,111	0.27	0
50	3PE	L	705	-	30,30,50	0.40	0	33,35,55	0.80	2 (6%)
53	CDL	L	704	-	99,99,99	0.25	0	105,111,111	0.32	0
51	PC1	M	502	-	53,53,53	0.31	0	59,61,61	0.40	0
45	SF4	3	801	3	0,12,12	-	-	-		
51	PC1	L	703	-	53,53,53	0.31	0	59,61,61	0.62	2 (3%)
53	CDL	M	503	-	89,89,99	0.30	0	95,101,111	0.42	0
50	3PE	M	501	-	43,43,50	0.32	0	46,48,55	0.49	0
45	SF4	9	402	7	0,12,12	-	-	-		
54	ZMP	X	101	17	25,30,36	0.82	1 (4%)	29,37,45	1.16	3 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	FMN	1	502	-	-	5/18/18/18	0/3/3/3
51	PC1	A	402	-	-	6/40/40/57	-
50	3PE	K	101	-	-	7/43/43/54	-
48	FES	3	803	3	-	-	0/1/1/1
53	CDL	V	203	-	-	33/104/104/110	-
53	CDL	Y	201	-	1/1/9/9	23/110/110/110	-
45	SF4	1	501	1	-	-	0/6/5/5
52	DCQ	H	501	-	-	1/14/38/38	0/1/1/1
47	NAI	1	503	-	-	10/29/72/72	0/5/5/5
56	NDP	d	401	-	-	7/34/77/77	0/5/5/5
50	3PE	o	501	-	-	2/34/34/54	-
50	3PE	V	201	-	-	1/38/38/54	-
50	3PE	L	702	-	-	11/54/54/54	-
50	3PE	p	201	-	-	4/27/27/54	-
53	CDL	W	201	-	-	31/110/110/110	-
53	CDL	h	201	-	-	21/68/68/110	-
53	CDL	o	502	-	2/2/9/9	19/85/85/110	-
50	3PE	V	202	-	-	12/40/40/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	SF4	9	403	7	-	-	0/6/5/5
58	MYR	s	201	37	-	2/12/12/13	-
51	PC1	9	401	-	-	16/57/57/57	-
54	ZMP	g	201	-	-	6/38/40/43	-
50	3PE	N	401	-	-	14/54/54/54	-
45	SF4	3	802	3	-	-	0/6/5/5
48	FES	2	300	2	-	-	0/1/1/1
50	3PE	A	403	-	-	12/54/54/54	-
50	3PE	H	502	-	-	20/54/54/54	-
50	3PE	i	201	-	-	7/54/54/54	-
51	PC1	w	801	-	-	10/57/57/57	-
57	AMP	k	501	-	-	7/10/26/26	0/3/3/3
50	3PE	L	701	-	-	8/43/43/54	-
51	PC1	A	401	-	-	14/49/49/57	-
53	CDL	V	204	-	1/1/9/9	34/95/95/110	-
50	3PE	6	202	-	-	15/54/54/54	-
45	SF4	6	201	6	-	-	0/6/5/5
53	CDL	L	704	-	1/1/9/9	32/110/110/110	-
50	3PE	L	705	-	-	8/34/34/54	-
51	PC1	M	502	-	-	20/57/57/57	-
45	SF4	3	801	3	-	-	0/6/5/5
51	PC1	L	703	-	-	21/57/57/57	-
53	CDL	M	503	-	-	31/100/100/110	-
50	3PE	M	501	-	-	12/47/47/54	-
45	SF4	9	402	7	-	-	0/6/5/5
54	ZMP	X	101	17	-	8/35/37/43	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	k	501	AMP	C5-C4	4.88	1.47	1.39
46	1	502	FMN	C4A-N5	2.79	1.36	1.30
57	k	501	AMP	C5-C6	2.57	1.48	1.41
57	k	501	AMP	C5-N7	-2.53	1.34	1.39
54	X	101	ZMP	C9-C10	2.52	1.53	1.50
54	g	201	ZMP	C9-C10	2.43	1.53	1.50
46	1	502	FMN	C10-N1	2.21	1.37	1.33
46	1	502	FMN	C4A-C10	-2.08	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	k	501	AMP	C8-N7	2.04	1.35	1.31

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	1	503	NAI	O5B-PA-O1A	-9.99	69.35	108.94
47	1	503	NAI	O2A-PA-O1A	-7.99	75.29	112.44
57	k	501	AMP	C5-C4-N3	-6.86	117.28	126.72
57	k	501	AMP	N3-C4-N9	5.75	136.94	127.17
47	1	503	NAI	O3-PA-O1A	-5.68	93.63	110.70
57	k	501	AMP	C2-N3-C4	4.14	121.95	111.83
46	1	502	FMN	C4-N3-C2	-3.75	118.98	125.64
57	k	501	AMP	N3-C2-N1	-3.36	123.50	128.58
54	g	201	ZMP	O1-C10-C9	-3.25	120.23	123.98
54	X	101	ZMP	C15-C14-C13	-3.23	107.01	112.39
57	k	501	AMP	C4-C5-N7	-2.93	107.24	110.58
54	g	201	ZMP	C14-C15-N2	-2.86	105.91	112.00
46	1	502	FMN	O4-C4-C4A	-2.81	119.12	126.53
46	1	502	FMN	C4A-C10-N10	2.79	120.47	116.48
54	g	201	ZMP	C15-C14-C13	-2.74	107.82	112.39
46	1	502	FMN	C4A-C4-N3	2.72	120.19	113.25
51	L	703	PC1	C2-O21-C21	2.54	123.87	117.80
50	N	401	3PE	O21-C2-C1	2.53	117.42	108.34
54	g	201	ZMP	C9-C10-S1	2.52	116.40	113.40
46	1	502	FMN	C4A-C10-N1	-2.49	118.48	124.59
50	L	705	3PE	C2-O21-C21	2.45	123.66	117.80
54	X	101	ZMP	O1-C10-C9	-2.44	121.17	123.98
51	A	402	PC1	C2-O21-C21	2.33	123.37	117.80
46	1	502	FMN	C4-C4A-C10	2.29	120.86	116.93
57	k	501	AMP	C1'-N9-C8	-2.26	122.08	127.09
50	H	502	3PE	O31-C3-C2	2.26	114.90	108.40
47	1	503	NAI	O2A-PA-O5B	2.25	117.76	107.57
57	k	501	AMP	C5-N7-C8	2.24	106.97	103.45
51	L	703	PC1	O21-C2-C1	2.22	116.30	108.34
46	1	502	FMN	C10-C4A-N5	-2.19	120.33	124.81
53	o	502	CDL	CB4-OB6-CB5	2.13	122.90	117.80
50	p	201	3PE	O12-P-O14	2.12	119.08	110.83
50	L	705	3PE	O21-C2-C3	2.11	115.90	108.34
57	k	501	AMP	C4-N9-C8	2.08	107.93	105.74
51	A	402	PC1	O21-C2-C3	2.07	115.78	108.34
54	X	101	ZMP	C9-C10-S1	2.04	115.84	113.40
53	Y	201	CDL	OA8-CA6-CA4	2.04	114.28	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	1	502	FMN	C6-C5A-C9A	2.02	121.82	119.05

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
53	L	704	CDL	CB4
53	V	204	CDL	CB4
53	Y	201	CDL	CB4
53	o	502	CDL	CB4
53	o	502	CDL	CA4

All (490) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	1	502	FMN	N10-C1'-C2'-O2'
46	1	502	FMN	C5'-O5'-P-O1P
47	1	503	NAI	C5D-O5D-PN-O3
50	6	202	3PE	C1-O11-P-O12
50	6	202	3PE	C1-O11-P-O13
50	6	202	3PE	C1-O11-P-O14
50	6	202	3PE	C11-O13-P-O11
50	6	202	3PE	C11-O13-P-O12
50	6	202	3PE	C11-O13-P-O14
50	6	202	3PE	O13-C11-C12-N
50	A	403	3PE	C11-O13-P-O12
50	A	403	3PE	O13-C11-C12-N
50	H	502	3PE	C1-O11-P-O12
50	H	502	3PE	C11-O13-P-O11
50	H	502	3PE	C11-O13-P-O12
50	H	502	3PE	C11-O13-P-O14
50	H	502	3PE	O13-C11-C12-N
50	K	101	3PE	C1-O11-P-O12
50	K	101	3PE	C1-O11-P-O13
50	K	101	3PE	C1-O11-P-O14
50	K	101	3PE	O13-C11-C12-N
50	L	701	3PE	C11-O13-P-O11
50	L	701	3PE	C11-O13-P-O12
50	L	701	3PE	O13-C11-C12-N
50	L	702	3PE	C1-O11-P-O13
50	L	702	3PE	C1-O11-P-O14
50	L	705	3PE	C1-O11-P-O12
50	L	705	3PE	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
50	M	501	3PE	C11-O13-P-O11
50	N	401	3PE	C11-O13-P-O11
50	N	401	3PE	C11-O13-P-O14
50	V	202	3PE	C1-O11-P-O12
50	V	202	3PE	C1-O11-P-O13
50	V	202	3PE	C11-O13-P-O11
50	V	202	3PE	C11-O13-P-O12
50	V	202	3PE	C11-O13-P-O14
50	V	202	3PE	O13-C11-C12-N
50	i	201	3PE	C1-O11-P-O12
50	p	201	3PE	C1-O11-P-O12
50	p	201	3PE	C1-O11-P-O13
51	9	401	PC1	C11-O13-P-O12
51	9	401	PC1	C11-O13-P-O11
51	9	401	PC1	C1-O11-P-O12
51	9	401	PC1	C1-O11-P-O13
51	A	401	PC1	C11-O13-P-O12
51	A	401	PC1	C11-O13-P-O11
51	A	401	PC1	C1-O11-P-O14
51	A	402	PC1	C1-O11-P-O14
51	L	703	PC1	C1-O11-P-O12
51	M	502	PC1	C11-O13-P-O11
51	M	502	PC1	C1-O11-P-O12
51	w	801	PC1	C11-O13-P-O14
53	L	704	CDL	CA3-OA5-PA1-OA2
53	L	704	CDL	CA3-OA5-PA1-OA3
53	L	704	CDL	CA3-OA5-PA1-OA4
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	M	503	CDL	CB2-OB2-PB2-OB5
53	M	503	CDL	CB3-OB5-PB2-OB3
53	V	203	CDL	CA2-OA2-PA1-OA5
53	V	203	CDL	CB2-OB2-PB2-OB3
53	V	203	CDL	CB2-OB2-PB2-OB4
53	V	203	CDL	CB2-OB2-PB2-OB5
53	V	203	CDL	CB3-OB5-PB2-OB3
53	V	203	CDL	CB3-OB5-PB2-OB4
53	V	204	CDL	O1-C1-CB2-OB2
53	V	204	CDL	CA2-OA2-PA1-OA3
53	V	204	CDL	CA2-OA2-PA1-OA4
53	V	204	CDL	CA2-OA2-PA1-OA5

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Mol	Chain	Res	Type	Atoms
53	V	204	CDL	CB2-OB2-PB2-OB3
53	V	204	CDL	CB2-OB2-PB2-OB5
53	V	204	CDL	CB3-OB5-PB2-OB2
53	V	204	CDL	CB3-OB5-PB2-OB3
53	W	201	CDL	CA3-OA5-PA1-OA4
53	W	201	CDL	CB2-OB2-PB2-OB3
53	Y	201	CDL	O1-C1-CB2-OB2
53	Y	201	CDL	CA2-C1-CB2-OB2
53	Y	201	CDL	CB3-OB5-PB2-OB2
53	Y	201	CDL	CB3-OB5-PB2-OB3
53	h	201	CDL	CA2-C1-CB2-OB2
53	h	201	CDL	CA2-OA2-PA1-OA4
53	h	201	CDL	CA2-OA2-PA1-OA5
53	h	201	CDL	CA3-OA5-PA1-OA2
53	h	201	CDL	CA3-OA5-PA1-OA3
53	h	201	CDL	CB2-OB2-PB2-OB3
53	h	201	CDL	CB2-OB2-PB2-OB4
53	h	201	CDL	CB2-OB2-PB2-OB5
53	h	201	CDL	CB3-OB5-PB2-OB2
53	h	201	CDL	CB3-OB5-PB2-OB3
53	o	502	CDL	CA2-OA2-PA1-OA3
53	o	502	CDL	CA2-OA2-PA1-OA4
53	o	502	CDL	CA2-OA2-PA1-OA5
53	o	502	CDL	CA3-OA5-PA1-OA4
54	X	101	ZMP	C17-C18-C21-O5
54	X	101	ZMP	C16-C17-C18-C21
54	X	101	ZMP	C17-C16-N2-C15
54	g	201	ZMP	S1-C11-C12-N1
54	g	201	ZMP	C12-C11-S1-C10
57	k	501	AMP	C5'-O5'-P-O1P
57	k	501	AMP	C5'-O5'-P-O2P
57	k	501	AMP	C5'-O5'-P-O3P
53	h	201	CDL	O1-C1-CB2-OB2
53	o	502	CDL	O1-C1-CB2-OB2
54	X	101	ZMP	O3-C16-N2-C15
51	L	703	PC1	C2-C1-O11-P
53	V	204	CDL	CA2-C1-CB2-OB2
53	W	201	CDL	CB2-C1-CA2-OA2
51	A	401	PC1	C11-C12-N-C14
53	W	201	CDL	O1-C1-CA2-OA2
53	V	204	CDL	OA6-CA4-CA6-OA8
57	k	501	AMP	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
51	A	401	PC1	C11-C12-N-C15
53	L	704	CDL	CB5-C51-C52-C53
53	o	502	CDL	CA5-C11-C12-C13
50	N	401	3PE	C21-C22-C23-C24
53	o	502	CDL	CA2-C1-CB2-OB2
50	V	201	3PE	C31-C32-C33-C34
53	L	704	CDL	O1-C1-CB2-OB2
53	M	503	CDL	C1-CA2-OA2-PA1
50	H	502	3PE	C33-C34-C35-C36
53	L	704	CDL	C77-C78-C79-C80
53	L	704	CDL	C56-C57-C58-C59
51	9	401	PC1	C3C-C3D-C3E-C3F
51	A	401	PC1	C3B-C3C-C3D-C3E
50	6	202	3PE	C36-C37-C38-C39
53	L	704	CDL	C21-C22-C23-C24
53	W	201	CDL	C72-C73-C74-C75
53	L	704	CDL	CB7-C71-C72-C73
53	V	204	CDL	C71-C72-C73-C74
50	K	101	3PE	C34-C35-C36-C37
53	L	704	CDL	C41-C42-C43-C44
53	M	503	CDL	C78-C79-C80-C81
53	V	203	CDL	C40-C41-C42-C43
53	Y	201	CDL	C80-C81-C82-C83
51	L	703	PC1	C38-C39-C3A-C3B
53	W	201	CDL	C35-C36-C37-C38
53	L	704	CDL	CA2-C1-CB2-OB2
53	V	203	CDL	C79-C80-C81-C82
53	W	201	CDL	CA5-C11-C12-C13
53	W	201	CDL	CB5-C51-C52-C53
53	Y	201	CDL	CB5-C51-C52-C53
53	V	203	CDL	C38-C39-C40-C41
53	W	201	CDL	C31-C32-C33-C34
51	A	401	PC1	C11-C12-N-C13
53	L	704	CDL	C82-C83-C84-C85
53	Y	201	CDL	C81-C82-C83-C84
53	Y	201	CDL	C63-C64-C65-C66
50	6	202	3PE	C3C-C3D-C3E-C3F
53	Y	201	CDL	C52-C53-C54-C55
50	K	101	3PE	C24-C25-C26-C27
53	V	203	CDL	CA7-C31-C32-C33
53	V	204	CDL	C34-C35-C36-C37
50	L	702	3PE	C3B-C3C-C3D-C3E

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Mol	Chain	Res	Type	Atoms
51	L	703	PC1	C23-C24-C25-C26
53	M	503	CDL	CB5-C51-C52-C53
53	V	204	CDL	C14-C15-C16-C17
56	d	401	NDP	O4B-C4B-C5B-O5B
53	V	203	CDL	C31-C32-C33-C34
51	M	502	PC1	C11-C12-N-C14
51	L	703	PC1	C33-C34-C35-C36
50	A	403	3PE	C2E-C2F-C2G-C2H
51	9	401	PC1	C22-C21-O21-C2
50	A	403	3PE	C2C-C2D-C2E-C2F
50	L	701	3PE	C31-C32-C33-C34
51	A	401	PC1	C23-C24-C25-C26
53	V	203	CDL	C20-C21-C22-C23
53	V	204	CDL	C1-CA2-OA2-PA1
53	V	204	CDL	C15-C16-C17-C18
53	V	203	CDL	O1-C1-CB2-OB2
53	L	704	CDL	C34-C35-C36-C37
51	M	502	PC1	C11-C12-N-C15
54	X	101	ZMP	O3-C16-C17-O4
50	M	501	3PE	C31-C32-C33-C34
53	Y	201	CDL	C79-C80-C81-C82
50	H	502	3PE	O11-C1-C2-C3
51	M	502	PC1	O11-C1-C2-C3
53	L	704	CDL	OB5-CB3-CB4-CB6
51	9	401	PC1	C3B-C3C-C3D-C3E
52	H	501	DCQ	C11-C12-C13-C14
51	w	801	PC1	C27-C28-C29-C2A
57	k	501	AMP	O4'-C4'-C5'-O5'
53	W	201	CDL	CA7-C31-C32-C33
53	M	503	CDL	C82-C83-C84-C85
51	9	401	PC1	C2C-C2D-C2E-C2F
53	Y	201	CDL	C32-C33-C34-C35
53	M	503	CDL	C56-C57-C58-C59
53	V	204	CDL	CA3-CA4-CA6-OA8
51	M	502	PC1	C11-C12-N-C13
51	M	502	PC1	C3A-C3B-C3C-C3D
53	Y	201	CDL	C57-C58-C59-C60
50	A	403	3PE	C38-C39-C3A-C3B
51	w	801	PC1	C21-C22-C23-C24
53	o	502	CDL	CB7-C71-C72-C73
53	V	203	CDL	CA2-C1-CB2-OB2
50	N	401	3PE	O11-C1-C2-O21

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Mol	Chain	Res	Type	Atoms
51	M	502	PC1	C25-C26-C27-C28
51	L	703	PC1	C37-C38-C39-C3A
53	W	201	CDL	O1-C1-CB2-OB2
54	g	201	ZMP	C1-C2-C3-C4
51	w	801	PC1	C3E-C3F-C3G-C3H
47	1	503	NAI	C2D-C1D-N1N-C2N
51	9	401	PC1	C22-C23-C24-C25
53	M	503	CDL	C51-C52-C53-C54
56	d	401	NDP	PN-O3-PA-O1A
53	Y	201	CDL	C15-C16-C17-C18
51	L	703	PC1	C2A-C2B-C2C-C2D
54	g	201	ZMP	C5-C6-C7-C8
50	H	502	3PE	C2-C1-O11-P
50	V	202	3PE	C2-C1-O11-P
53	h	201	CDL	C1-CB2-OB2-PB2
53	h	201	CDL	CB4-CB3-OB5-PB2
50	N	401	3PE	C32-C33-C34-C35
50	6	202	3PE	C23-C24-C25-C26
50	i	201	3PE	C27-C28-C29-C2A
53	M	503	CDL	C76-C77-C78-C79
53	W	201	CDL	OA5-CA3-CA4-CA6
53	M	503	CDL	C71-C72-C73-C74
50	p	201	3PE	C21-C22-C23-C24
51	L	703	PC1	C3F-C3G-C3H-C3I
53	W	201	CDL	C53-C54-C55-C56
53	L	704	CDL	C22-C23-C24-C25
50	N	401	3PE	C1-C2-C3-O31
53	V	204	CDL	CB3-CB4-CB6-OB8
53	W	201	CDL	CA3-CA4-CA6-OA8
54	X	101	ZMP	N2-C16-C17-O4
53	L	704	CDL	C31-C32-C33-C34
51	9	401	PC1	O22-C21-O21-C2
50	L	702	3PE	O11-C1-C2-O21
53	V	203	CDL	OB5-CB3-CB4-OB6
53	W	201	CDL	OA5-CA3-CA4-OA6
50	L	705	3PE	C2-C1-O11-P
53	M	503	CDL	OA6-CA4-CA6-OA8
53	W	201	CDL	OA6-CA4-CA6-OA8
53	W	201	CDL	OB6-CB4-CB6-OB8
53	Y	201	CDL	OA6-CA4-CA6-OA8
50	A	403	3PE	C3A-C3B-C3C-C3D
50	i	201	3PE	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
51	w	801	PC1	C39-C3A-C3B-C3C
47	1	503	NAI	PN-O3-PA-O5B
50	H	502	3PE	C36-C37-C38-C39
53	Y	201	CDL	C37-C38-C39-C40
50	6	202	3PE	C3D-C3E-C3F-C3G
53	Y	201	CDL	CA5-C11-C12-C13
51	L	703	PC1	C36-C37-C38-C39
53	M	503	CDL	C84-C85-C86-C87
50	M	501	3PE	C3B-C3C-C3D-C3E
50	L	702	3PE	O11-C1-C2-C3
53	V	203	CDL	OA5-CA3-CA4-CA6
53	V	203	CDL	OB5-CB3-CB4-CB6
53	V	204	CDL	OA5-CA3-CA4-CA6
53	V	203	CDL	C77-C78-C79-C80
51	M	502	PC1	C31-C32-C33-C34
53	L	704	CDL	C17-C18-C19-C20
47	1	503	NAI	C2D-C1D-N1N-C6N
50	L	702	3PE	C35-C36-C37-C38
53	Y	201	CDL	C59-C60-C61-C62
51	w	801	PC1	C3A-C3B-C3C-C3D
51	A	402	PC1	O11-C1-C2-O21
51	M	502	PC1	O11-C1-C2-O21
53	V	203	CDL	OA5-CA3-CA4-OA6
53	V	204	CDL	OA5-CA3-CA4-OA6
53	Y	201	CDL	CA3-CA4-CA6-OA8
53	h	201	CDL	CB3-CB4-CB6-OB8
53	W	201	CDL	C79-C80-C81-C82
50	H	502	3PE	C12-C11-O13-P
50	L	701	3PE	C12-C11-O13-P
50	M	501	3PE	O21-C2-C3-O31
50	N	401	3PE	O21-C2-C3-O31
53	V	204	CDL	OB6-CB4-CB6-OB8
50	N	401	3PE	C38-C39-C3A-C3B
53	Y	201	CDL	C14-C15-C16-C17
47	1	503	NAI	PA-O3-PN-O2N
51	9	401	PC1	O13-C11-C12-N
51	w	801	PC1	O13-C11-C12-N
53	W	201	CDL	CA2-C1-CB2-OB2
50	p	201	3PE	C22-C23-C24-C25
50	N	401	3PE	C2C-C2D-C2E-C2F
53	o	502	CDL	C71-C72-C73-C74
58	s	201	MYR	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
53	L	704	CDL	C80-C81-C82-C83
51	9	401	PC1	C34-C35-C36-C37
51	L	703	PC1	O11-C1-C2-C3
53	V	203	CDL	C43-C44-C45-C46
46	1	502	FMN	N10-C1'-C2'-C3'
54	X	101	ZMP	C19-C18-C21-O5
54	X	101	ZMP	C20-C18-C21-O5
50	K	101	3PE	C2-C1-O11-P
51	M	502	PC1	C2-C1-O11-P
53	M	503	CDL	CB4-CB3-OB5-PB2
50	H	502	3PE	C2F-C2G-C2H-C2I
50	H	502	3PE	O11-C1-C2-O21
51	L	703	PC1	O11-C1-C2-O21
53	L	704	CDL	OB5-CB3-CB4-OB6
53	L	704	CDL	C37-C38-C39-C40
53	V	203	CDL	OA6-CA4-CA6-OA8
50	M	501	3PE	C1-C2-C3-O31
53	M	503	CDL	CA3-CA4-CA6-OA8
53	h	201	CDL	CA3-CA4-CA6-OA8
50	6	202	3PE	C2D-C2E-C2F-C2G
47	1	503	NAI	C5B-O5B-PA-O2A
47	1	503	NAI	C5D-O5D-PN-O1N
50	A	403	3PE	C11-O13-P-O11
50	A	403	3PE	C11-O13-P-O14
50	H	502	3PE	C1-O11-P-O13
50	H	502	3PE	C1-O11-P-O14
50	L	702	3PE	C1-O11-P-O12
50	L	702	3PE	C11-O13-P-O12
50	L	705	3PE	C1-O11-P-O14
50	M	501	3PE	C11-O13-P-O14
50	V	202	3PE	C1-O11-P-O14
50	i	201	3PE	C1-O11-P-O13
50	i	201	3PE	C1-O11-P-O14
51	A	401	PC1	C11-O13-P-O14
51	A	401	PC1	C1-O11-P-O12
51	A	401	PC1	C1-O11-P-O13
51	A	402	PC1	C1-O11-P-O13
51	L	703	PC1	C1-O11-P-O14
51	L	703	PC1	C1-O11-P-O13
51	M	502	PC1	C11-O13-P-O14
51	M	502	PC1	C1-O11-P-O14
51	M	502	PC1	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
53	L	704	CDL	CA2-OA2-PA1-OA3
53	L	704	CDL	CA2-OA2-PA1-OA4
53	L	704	CDL	CA2-OA2-PA1-OA5
53	M	503	CDL	CA2-OA2-PA1-OA3
53	M	503	CDL	CA2-OA2-PA1-OA4
53	M	503	CDL	CA2-OA2-PA1-OA5
53	M	503	CDL	CA3-OA5-PA1-OA3
53	M	503	CDL	CB2-OB2-PB2-OB4
53	V	203	CDL	CB3-OB5-PB2-OB2
53	V	204	CDL	CA3-OA5-PA1-OA3
53	V	204	CDL	CB2-OB2-PB2-OB4
53	V	204	CDL	CB3-OB5-PB2-OB4
53	W	201	CDL	CA3-OA5-PA1-OA2
53	W	201	CDL	CA3-OA5-PA1-OA3
53	W	201	CDL	CB2-OB2-PB2-OB4
53	W	201	CDL	CB2-OB2-PB2-OB5
53	Y	201	CDL	CA2-OA2-PA1-OA5
53	h	201	CDL	CA3-OA5-PA1-OA4
53	h	201	CDL	CB3-OB5-PB2-OB4
53	o	502	CDL	CA3-OA5-PA1-OA2
53	o	502	CDL	CA3-OA5-PA1-OA3
56	d	401	NDP	C5B-O5B-PA-O1A
53	L	704	CDL	CA4-CA3-OA5-PA1
53	V	204	CDL	C1-CB2-OB2-PB2
53	W	201	CDL	C1-CA2-OA2-PA1
57	k	501	AMP	C4'-C5'-O5'-P
51	A	401	PC1	C3E-C3F-C3G-C3H
51	9	401	PC1	C3-C2-O21-C21
50	6	202	3PE	C33-C34-C35-C36
51	L	703	PC1	C29-C2A-C2B-C2C
53	L	704	CDL	C55-C56-C57-C58
47	1	503	NAI	O4D-C1D-N1N-C2N
53	o	502	CDL	CA7-C31-C32-C33
53	V	203	CDL	OB6-CB4-CB6-OB8
53	h	201	CDL	OA6-CA4-CA6-OA8
51	M	502	PC1	O31-C31-C32-C33
53	W	201	CDL	CB3-CB4-CB6-OB8
47	1	503	NAI	O4D-C1D-N1N-C6N
51	M	502	PC1	C2B-C2C-C2D-C2E
51	w	801	PC1	C26-C27-C28-C29
50	M	501	3PE	C35-C36-C37-C38
53	V	204	CDL	C52-C53-C54-C55

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Mol	Chain	Res	Type	Atoms
53	V	204	CDL	C78-C79-C80-C81
53	V	204	CDL	CB2-C1-CA2-OA2
50	H	502	3PE	C32-C31-O31-C3
46	1	502	FMN	C4'-C5'-O5'-P
53	V	203	CDL	C41-C42-C43-C44
53	Y	201	CDL	C13-C14-C15-C16
51	L	703	PC1	C3E-C3F-C3G-C3H
56	d	401	NDP	O4D-C1D-N1N-C6N
53	o	502	CDL	C13-C14-C15-C16
53	W	201	CDL	C81-C82-C83-C84
53	V	203	CDL	CB3-CB4-CB6-OB8
53	M	503	CDL	C81-C82-C83-C84
54	g	201	ZMP	C2-C1-C22-C23
50	L	705	3PE	C1-C2-O21-C21
50	M	501	3PE	C23-C24-C25-C26
53	M	503	CDL	C64-C65-C66-C67
53	M	503	CDL	CA5-C11-C12-C13
53	V	204	CDL	C77-C78-C79-C80
51	9	401	PC1	C2D-C2E-C2F-C2G
54	g	201	ZMP	O1-C10-S1-C11
47	1	503	NAI	C2N-C3N-C7N-N7N
50	H	502	3PE	C26-C27-C28-C29
50	A	403	3PE	C22-C23-C24-C25
53	o	502	CDL	C15-C16-C17-C18
51	A	402	PC1	O21-C21-C22-C23
51	9	401	PC1	C3F-C3G-C3H-C3I
51	w	801	PC1	C2C-C2D-C2E-C2F
50	L	701	3PE	C27-C28-C29-C2A
51	M	502	PC1	C3B-C3C-C3D-C3E
51	L	703	PC1	C2C-C2D-C2E-C2F
50	M	501	3PE	C2-C1-O11-P
53	V	203	CDL	CA4-CA3-OA5-PA1
53	Y	201	CDL	C1-CB2-OB2-PB2
53	L	704	CDL	C78-C79-C80-C81
53	W	201	CDL	C58-C59-C60-C61
50	H	502	3PE	O32-C31-O31-C3
51	A	401	PC1	O31-C31-C32-C33
53	L	704	CDL	CA7-C31-C32-C33
50	o	501	3PE	C22-C23-C24-C25
51	L	703	PC1	O31-C31-C32-C33
51	M	502	PC1	O21-C21-C22-C23
50	H	502	3PE	C29-C2A-C2B-C2C

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Mol	Chain	Res	Type	Atoms
50	N	401	3PE	O11-C1-C2-C3
53	M	503	CDL	OB5-CB3-CB4-CB6
50	M	501	3PE	C34-C35-C36-C37
53	h	201	CDL	OB6-CB4-CB6-OB8
53	V	203	CDL	C78-C79-C80-C81
53	V	203	CDL	C71-C72-C73-C74
46	1	502	FMN	C5'-O5'-P-O2P
50	H	502	3PE	C3F-C3G-C3H-C3I
51	L	703	PC1	C1-C2-O21-C21
53	L	704	CDL	C58-C59-C60-C61
51	A	401	PC1	C3F-C3G-C3H-C3I
53	o	502	CDL	CA4-CA3-OA5-PA1
50	6	202	3PE	O11-C1-C2-O21
53	M	503	CDL	C53-C54-C55-C56
53	M	503	CDL	C83-C84-C85-C86
50	L	701	3PE	O21-C21-C22-C23
53	V	203	CDL	C32-C31-CA7-OA8
57	k	501	AMP	O4'-C1'-N9-C8
50	6	202	3PE	C32-C33-C34-C35
50	V	202	3PE	O31-C31-C32-C33
50	V	202	3PE	O11-C1-C2-C3
53	L	704	CDL	C72-C73-C74-C75
58	s	201	MYR	C11-C10-C9-C8
50	A	403	3PE	C2D-C2E-C2F-C2G
50	i	201	3PE	O21-C21-C22-C23
50	M	501	3PE	C3E-C3F-C3G-C3H
51	L	703	PC1	O13-C11-C12-N
50	L	705	3PE	O21-C21-C22-C23
53	V	203	CDL	C11-C12-C13-C14
53	M	503	CDL	C72-C73-C74-C75
50	N	401	3PE	O31-C31-C32-C33
51	L	703	PC1	C2D-C2E-C2F-C2G
50	A	403	3PE	C35-C36-C37-C38
50	M	501	3PE	C33-C34-C35-C36
53	h	201	CDL	C52-C51-CB5-OB6
50	N	401	3PE	C22-C23-C24-C25
53	L	704	CDL	C39-C40-C41-C42
53	W	201	CDL	C83-C84-C85-C86
53	L	704	CDL	C72-C71-CB7-OB8
53	V	204	CDL	C32-C31-CA7-OA8
50	L	702	3PE	C34-C35-C36-C37
51	A	402	PC1	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
51	A	402	PC1	C22-C23-C24-C25
53	V	204	CDL	C51-C52-C53-C54
50	H	502	3PE	C3C-C3D-C3E-C3F
51	L	703	PC1	C3A-C3B-C3C-C3D
51	w	801	PC1	C2D-C2E-C2F-C2G
50	N	401	3PE	C3-C2-O21-C21
53	M	503	CDL	CB3-CB4-OB6-CB5
53	o	502	CDL	CB3-CB4-OB6-CB5
56	d	401	NDP	C3B-C4B-C5B-O5B
53	W	201	CDL	C15-C16-C17-C18
53	V	203	CDL	C37-C38-C39-C40
53	M	503	CDL	C31-C32-C33-C34
50	i	201	3PE	O22-C21-C22-C23
51	M	502	PC1	C39-C3A-C3B-C3C
50	o	501	3PE	C25-C26-C27-C28
56	d	401	NDP	C2B-O2B-P2B-O1X
53	V	204	CDL	C52-C51-CB5-OB6
50	L	705	3PE	O11-C1-C2-O21
53	o	502	CDL	OB5-CB3-CB4-OB6
53	o	502	CDL	C72-C71-CB7-OB8
50	L	705	3PE	O22-C21-C22-C23
51	9	401	PC1	O31-C31-C32-C33
53	o	502	CDL	C73-C74-C75-C76
50	V	202	3PE	O32-C31-C32-C33
53	V	203	CDL	C32-C31-CA7-OA9
53	V	204	CDL	C32-C31-CA7-OA9
51	M	502	PC1	C2F-C2G-C2H-C2I
53	V	204	CDL	CA5-C11-C12-C13
50	L	701	3PE	O22-C21-C22-C23
50	N	401	3PE	O32-C31-C32-C33
53	V	204	CDL	C12-C11-CA5-OA6
53	V	203	CDL	C80-C81-C82-C83
53	W	201	CDL	C12-C11-CA5-OA6
53	L	704	CDL	C72-C71-CB7-OB9
53	Y	201	CDL	CB7-C71-C72-C73
50	A	403	3PE	O21-C21-C22-C23
50	L	702	3PE	O31-C31-C32-C33
56	d	401	NDP	PN-O3-PA-O2A
50	V	202	3PE	O21-C21-C22-C23
53	h	201	CDL	C52-C51-CB5-OB7
50	L	702	3PE	C23-C24-C25-C26
53	W	201	CDL	C19-C20-C21-C22

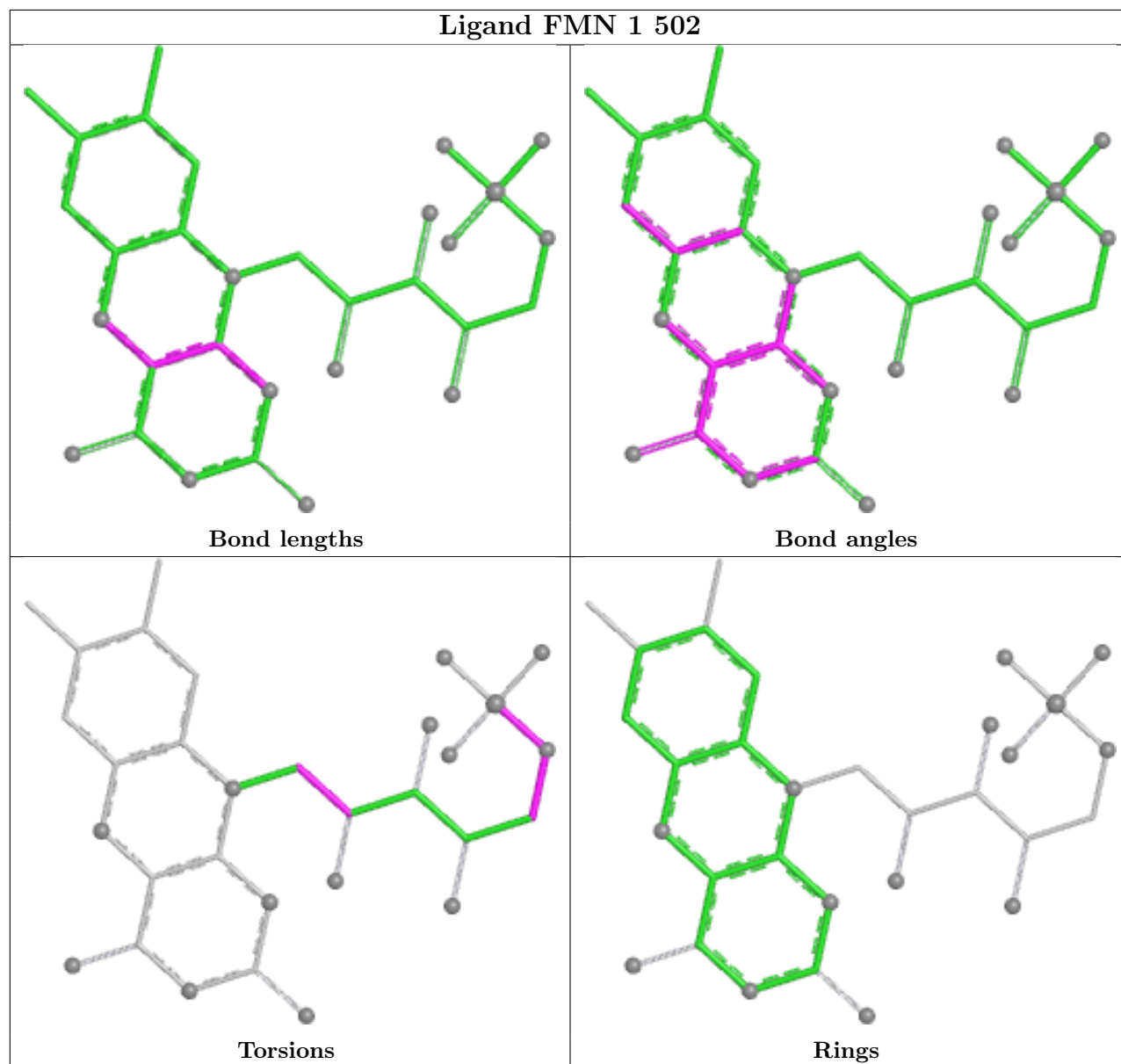
There are no ring outliers.

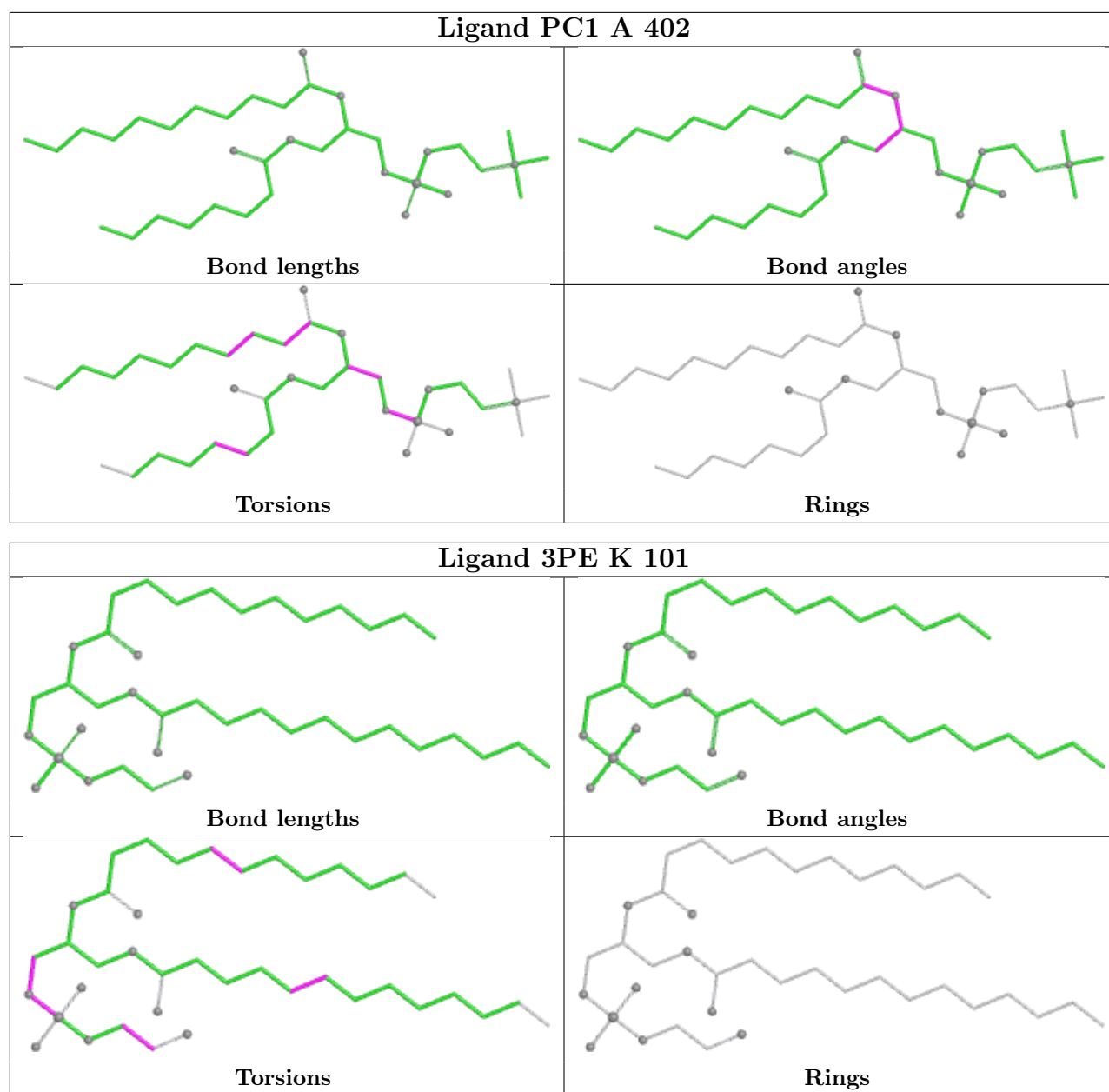
31 monomers are involved in 88 short contacts:

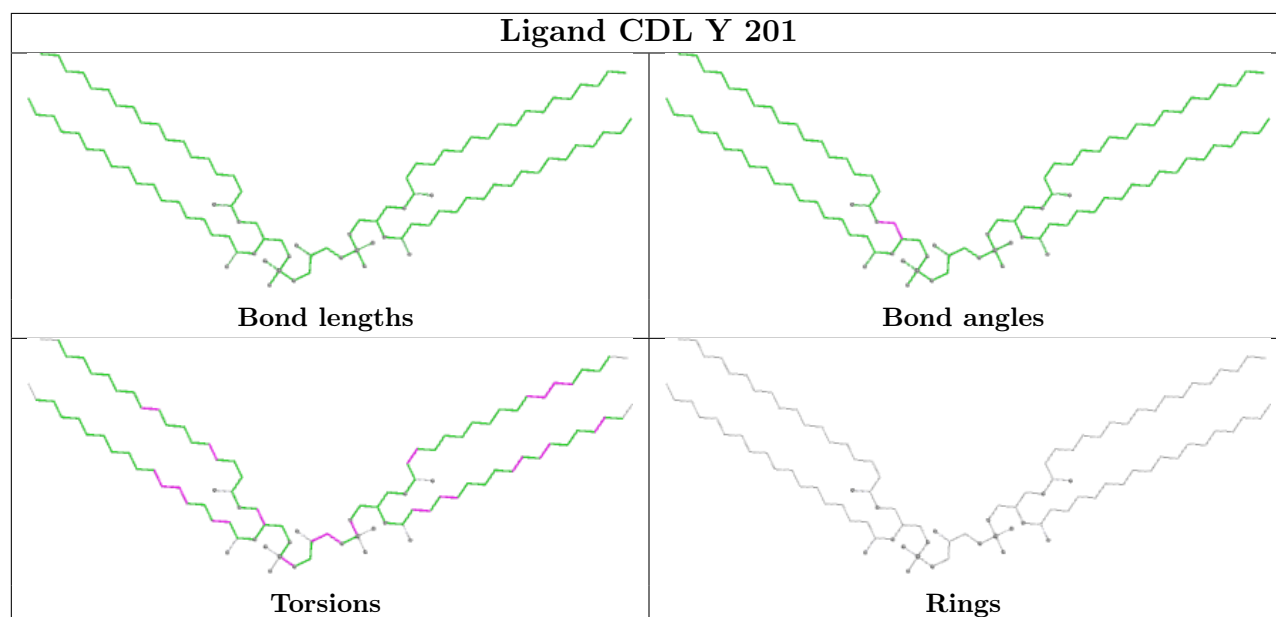
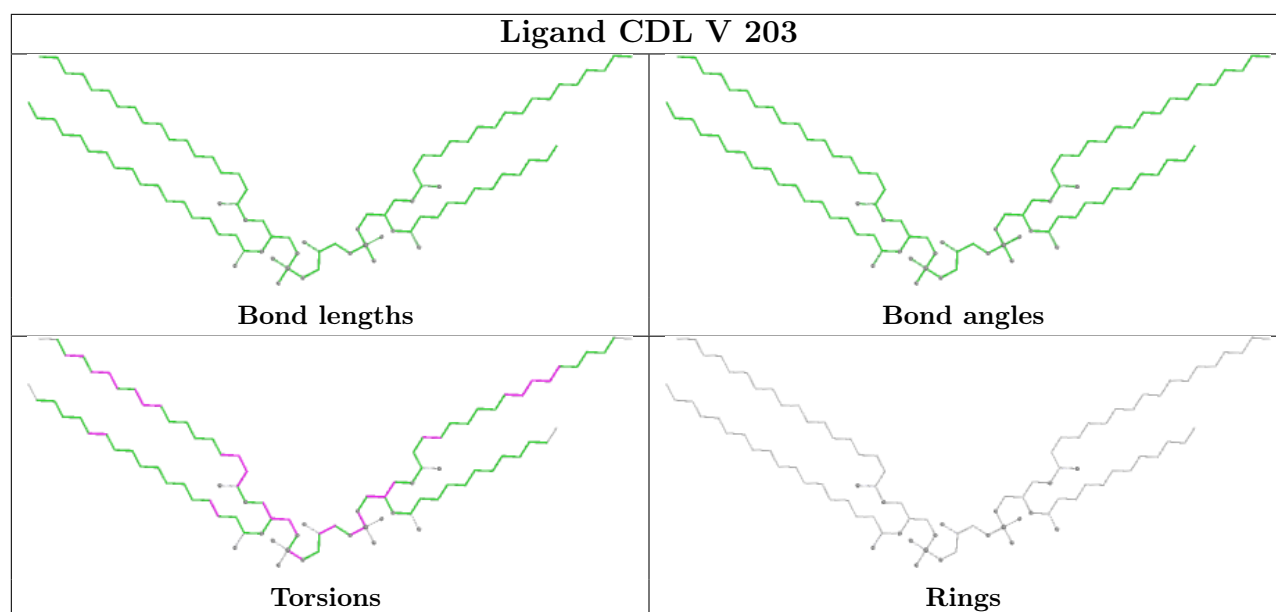
Mol	Chain	Res	Type	Clashes	Symm-Clashes
50	K	101	3PE	4	0
53	V	203	CDL	1	0
53	Y	201	CDL	7	0
45	1	501	SF4	3	0
52	H	501	DCQ	2	0
47	1	503	NAI	4	0
56	d	401	NDP	1	0
50	V	201	3PE	1	0
50	p	201	3PE	1	0
53	W	201	CDL	5	0
53	h	201	CDL	1	0
50	V	202	3PE	1	0
53	o	502	CDL	2	0
51	9	401	PC1	1	0
50	N	401	3PE	2	0
48	2	300	FES	1	0
50	A	403	3PE	2	0
50	H	502	3PE	6	0
50	i	201	3PE	2	0
51	w	801	PC1	6	0
57	k	501	AMP	2	0
50	L	701	3PE	1	0
45	6	201	SF4	3	0
50	6	202	3PE	3	0
53	V	204	CDL	3	0
53	L	704	CDL	7	0
51	M	502	PC1	4	0
51	L	703	PC1	3	0
53	M	503	CDL	9	0
50	M	501	3PE	2	0
54	X	101	ZMP	2	0

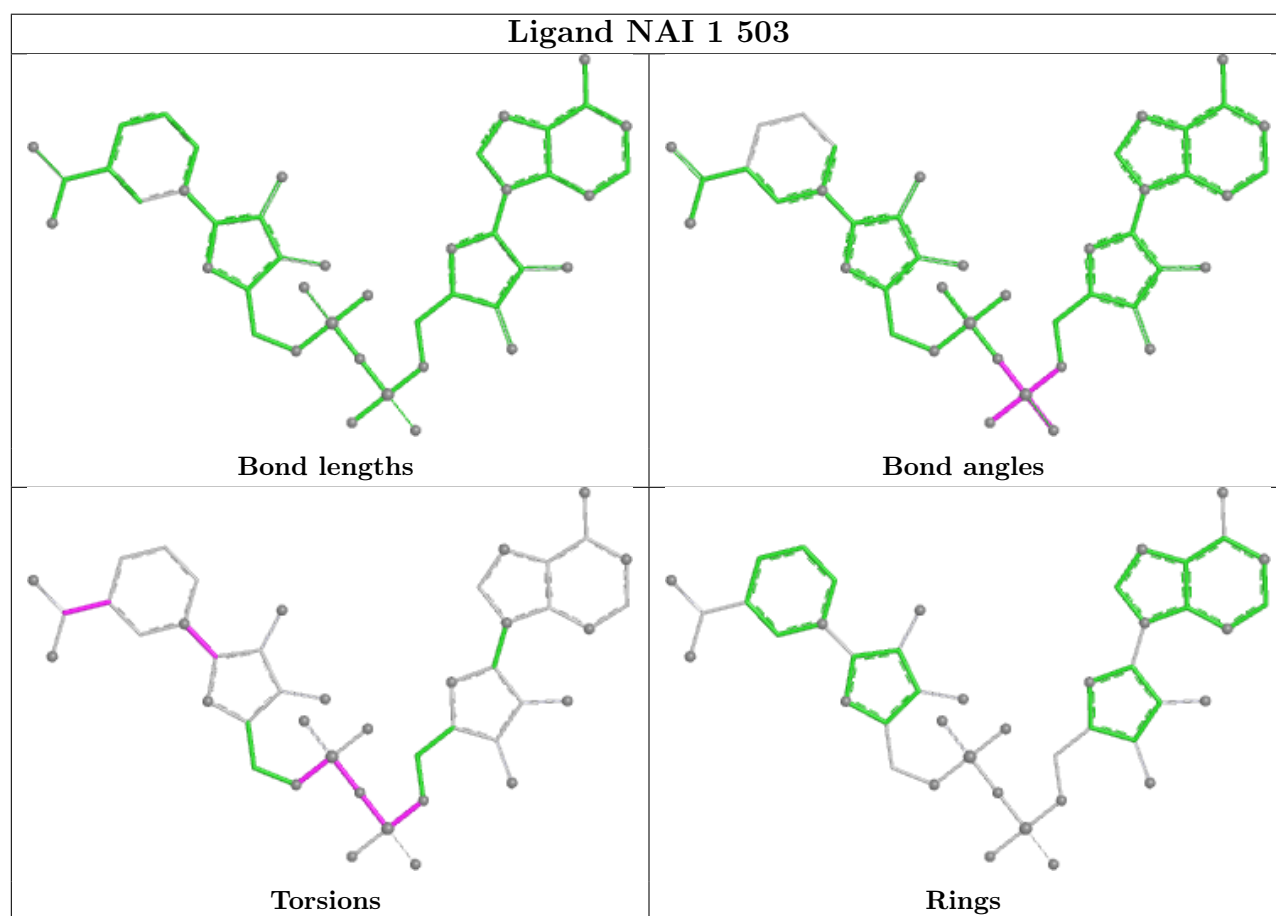
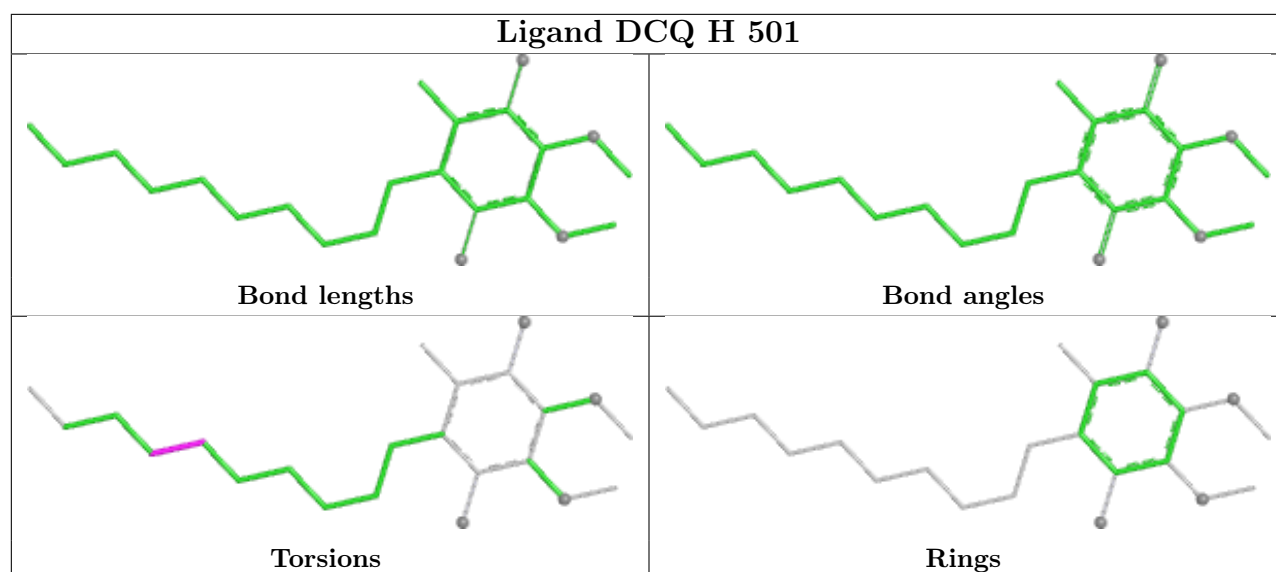
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

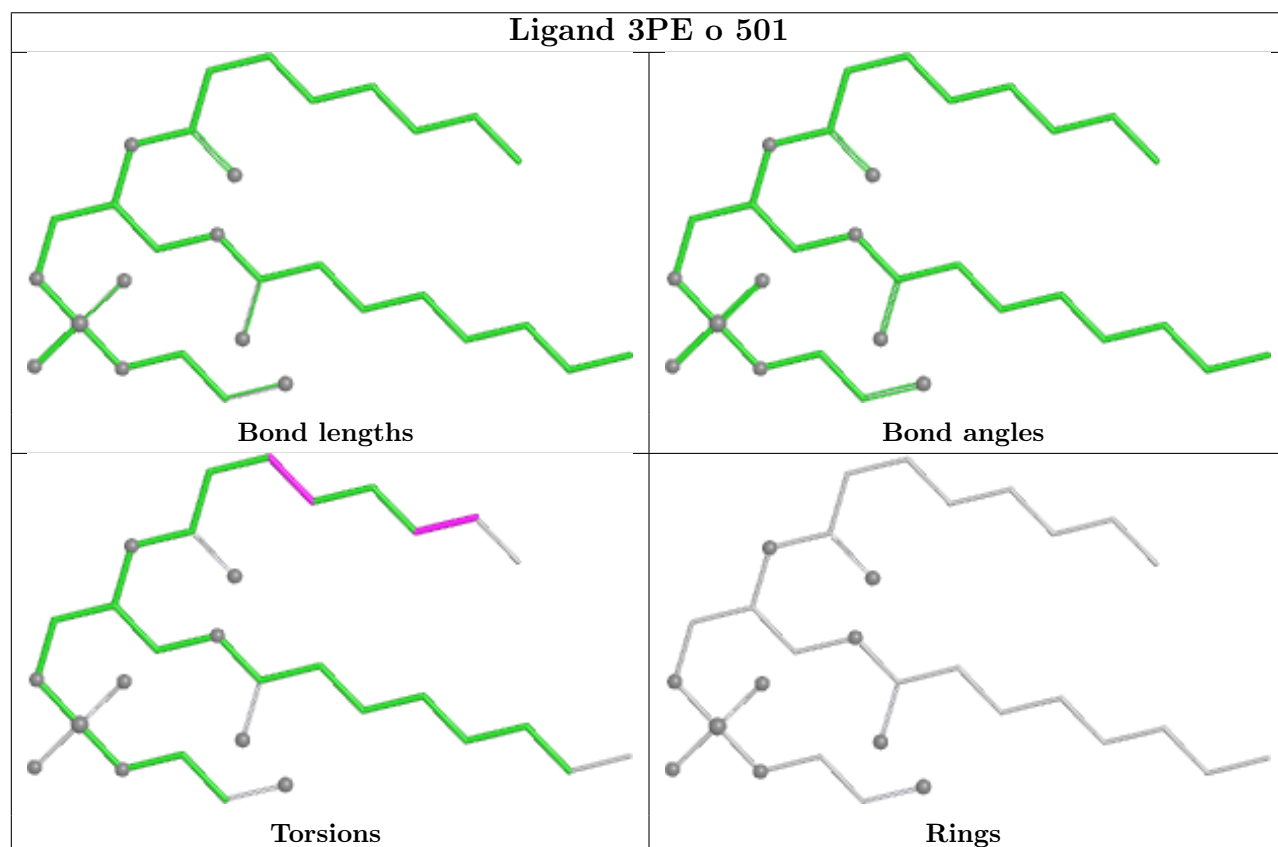
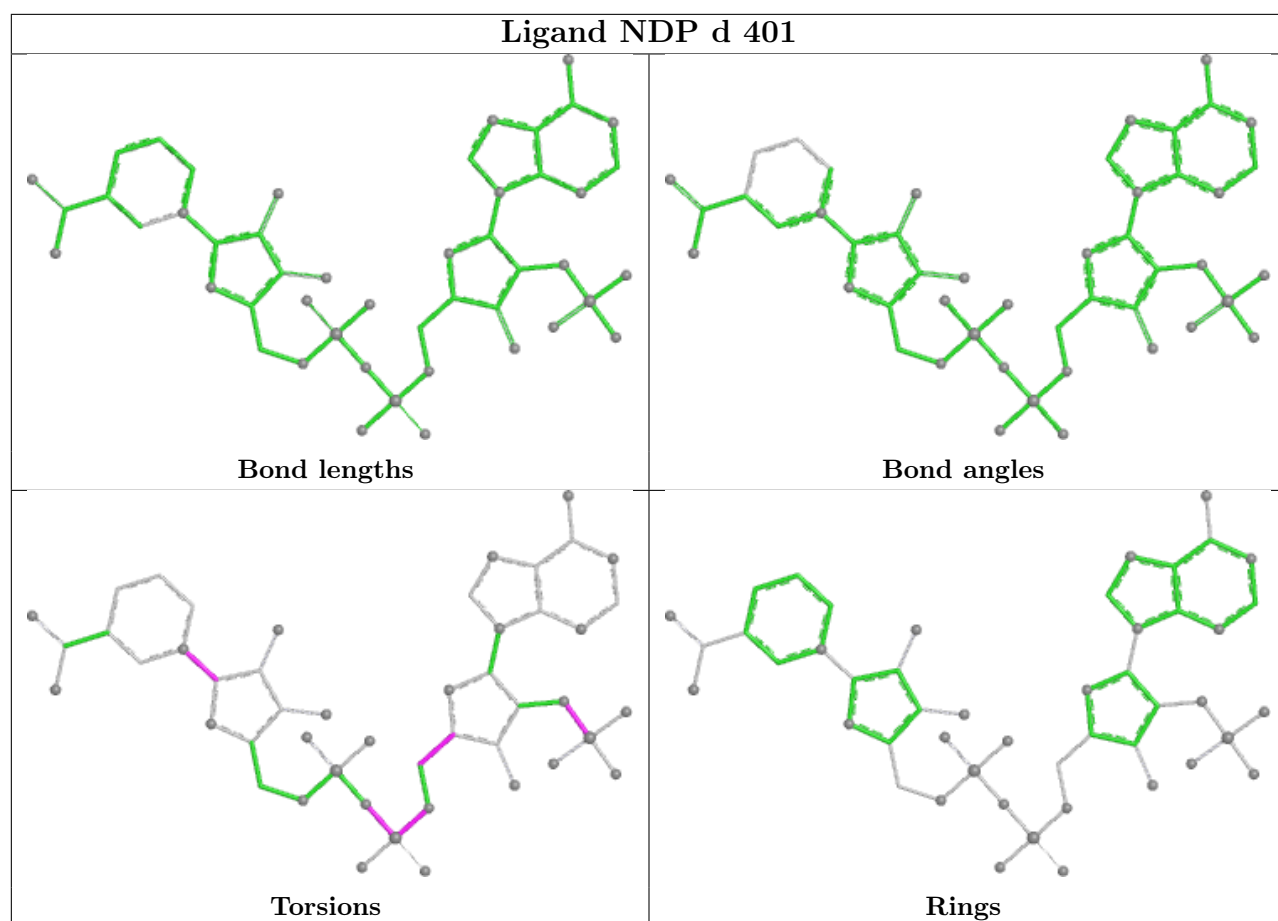
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

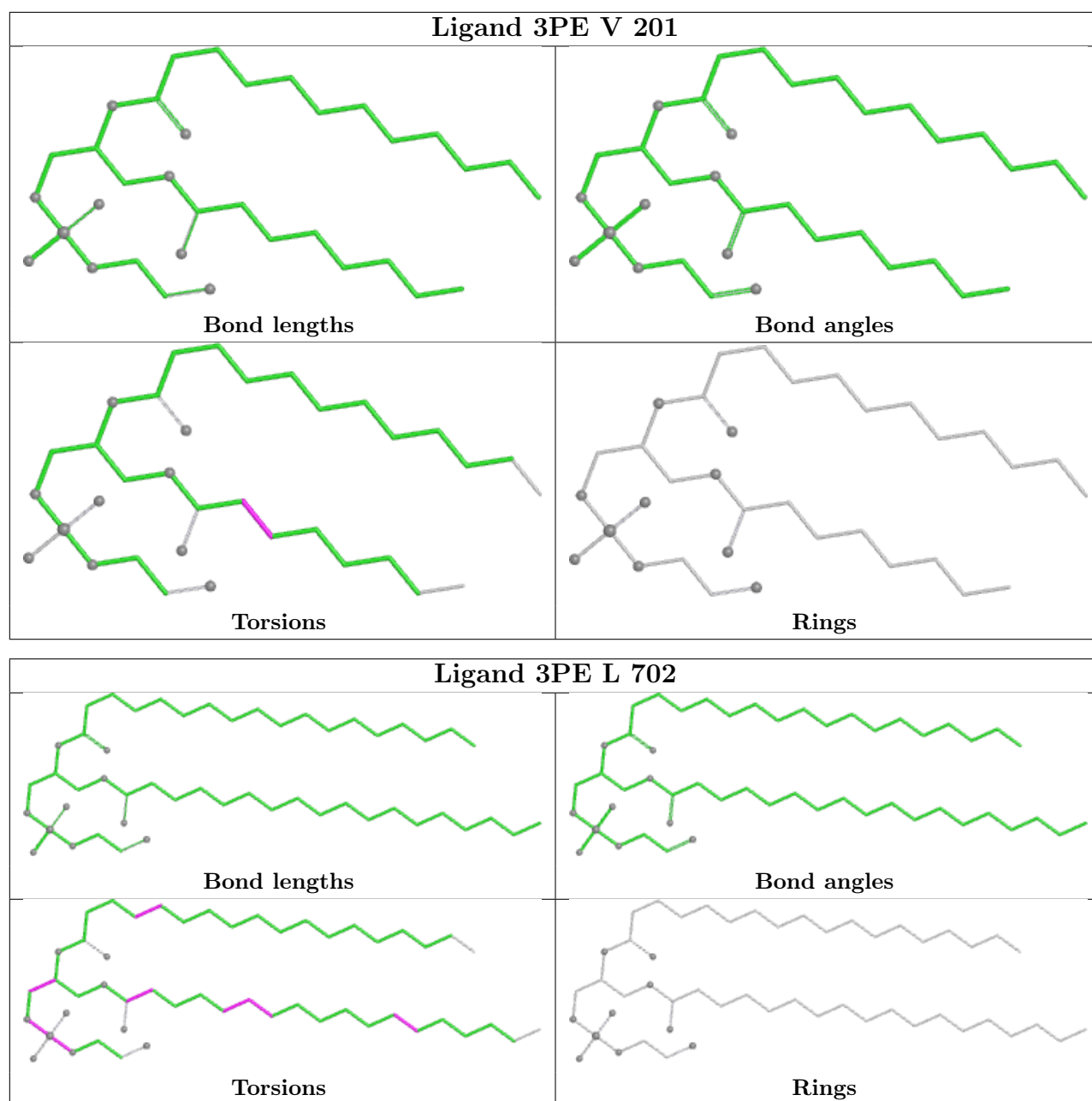


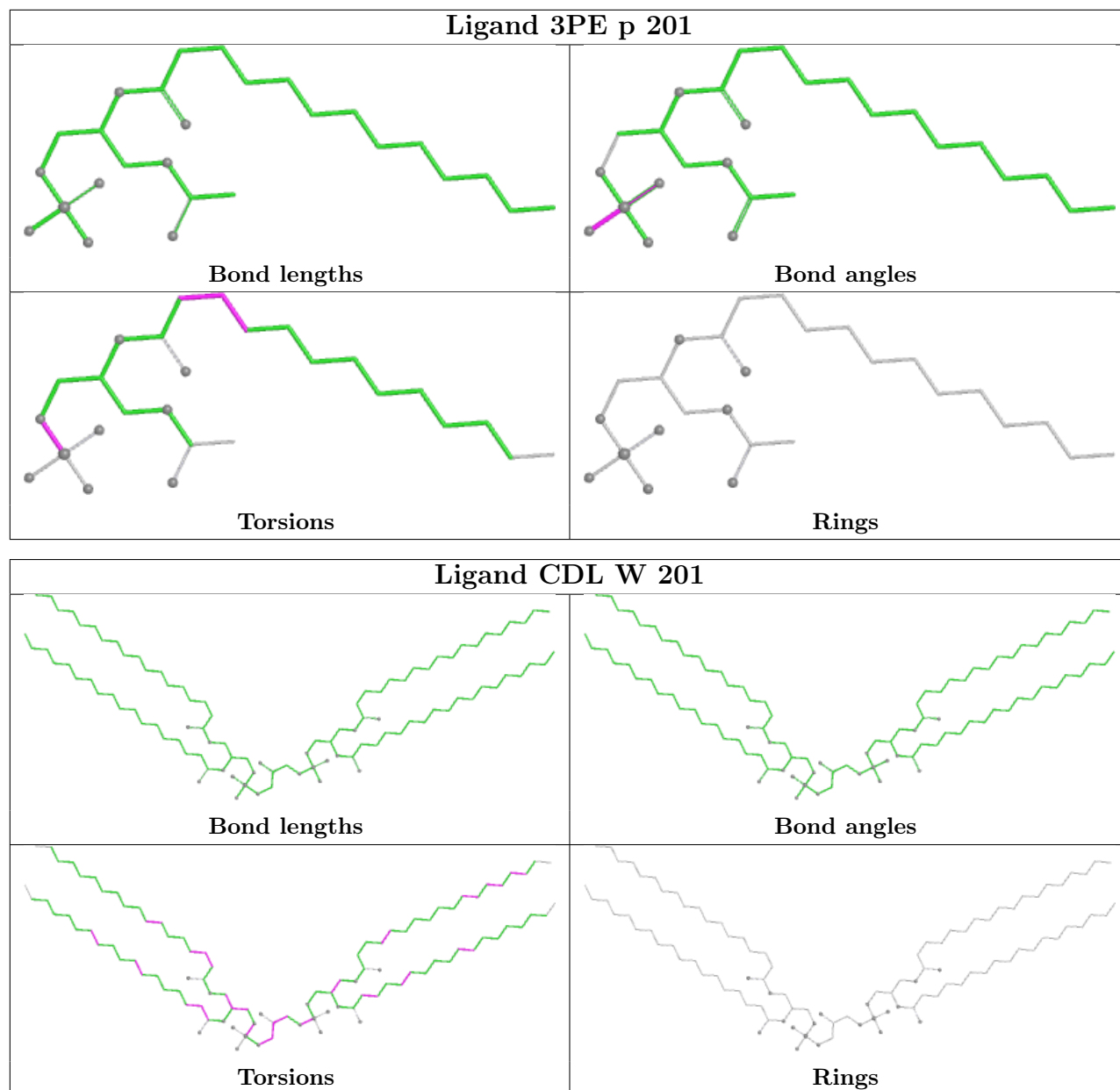


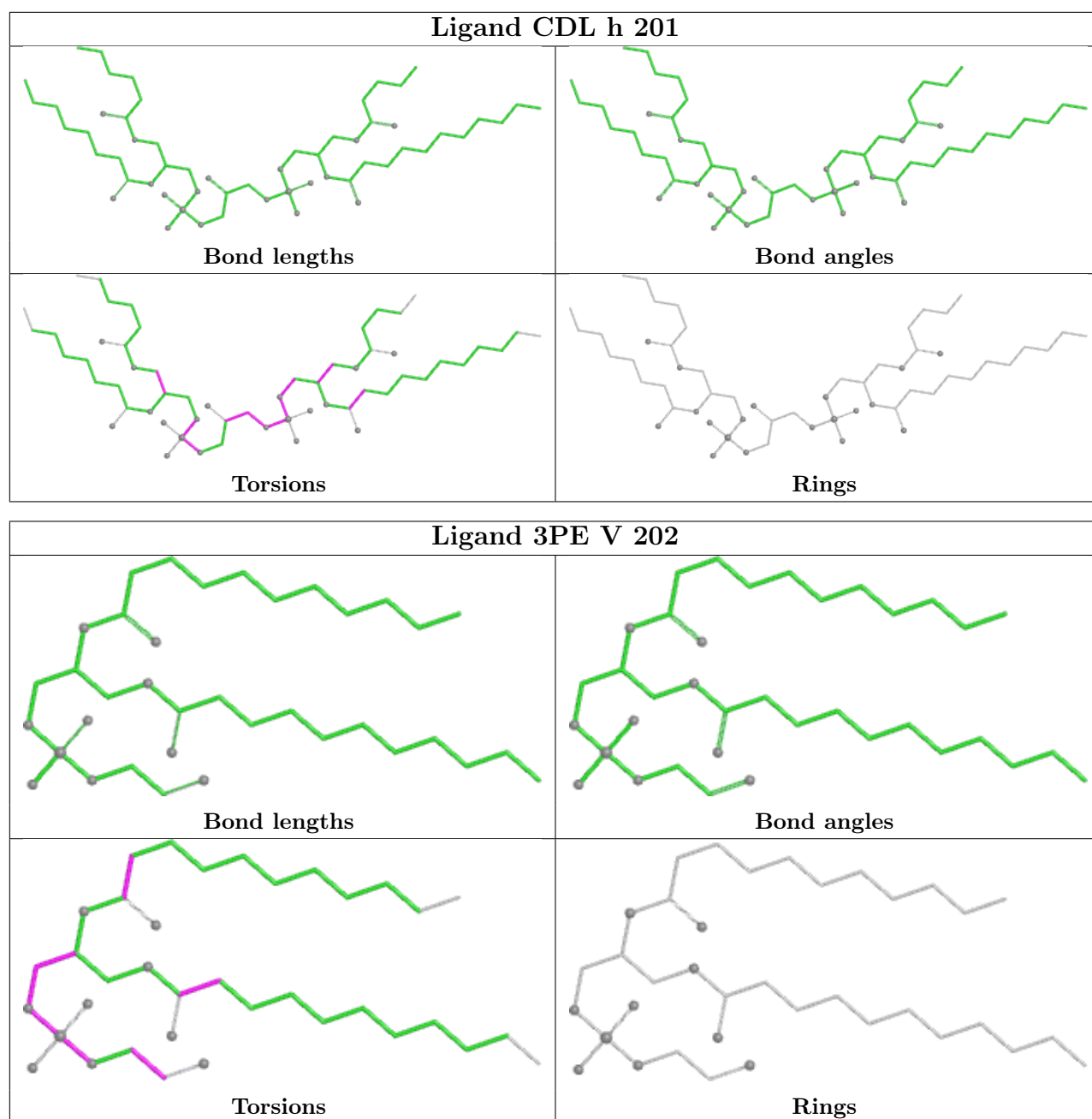


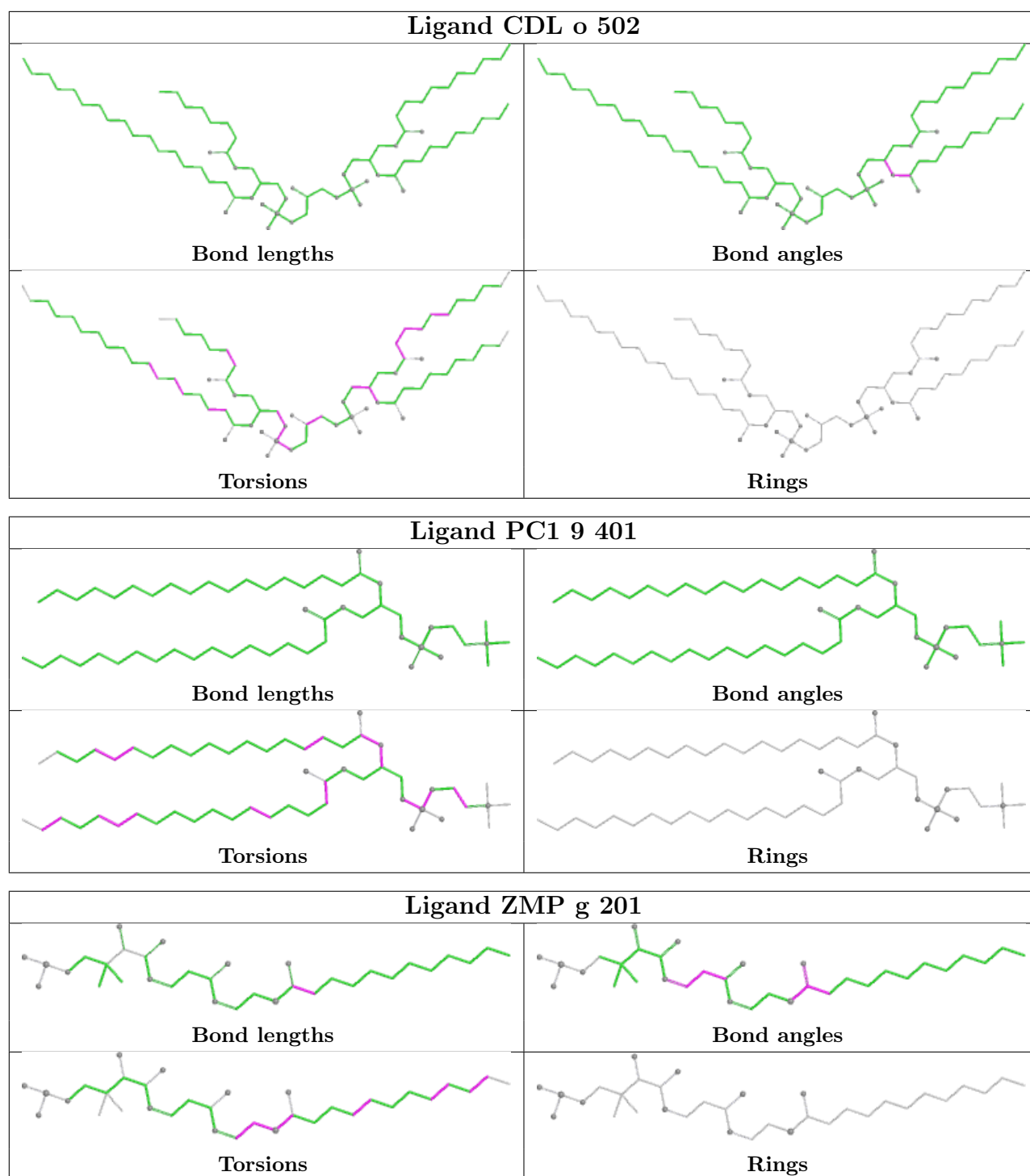


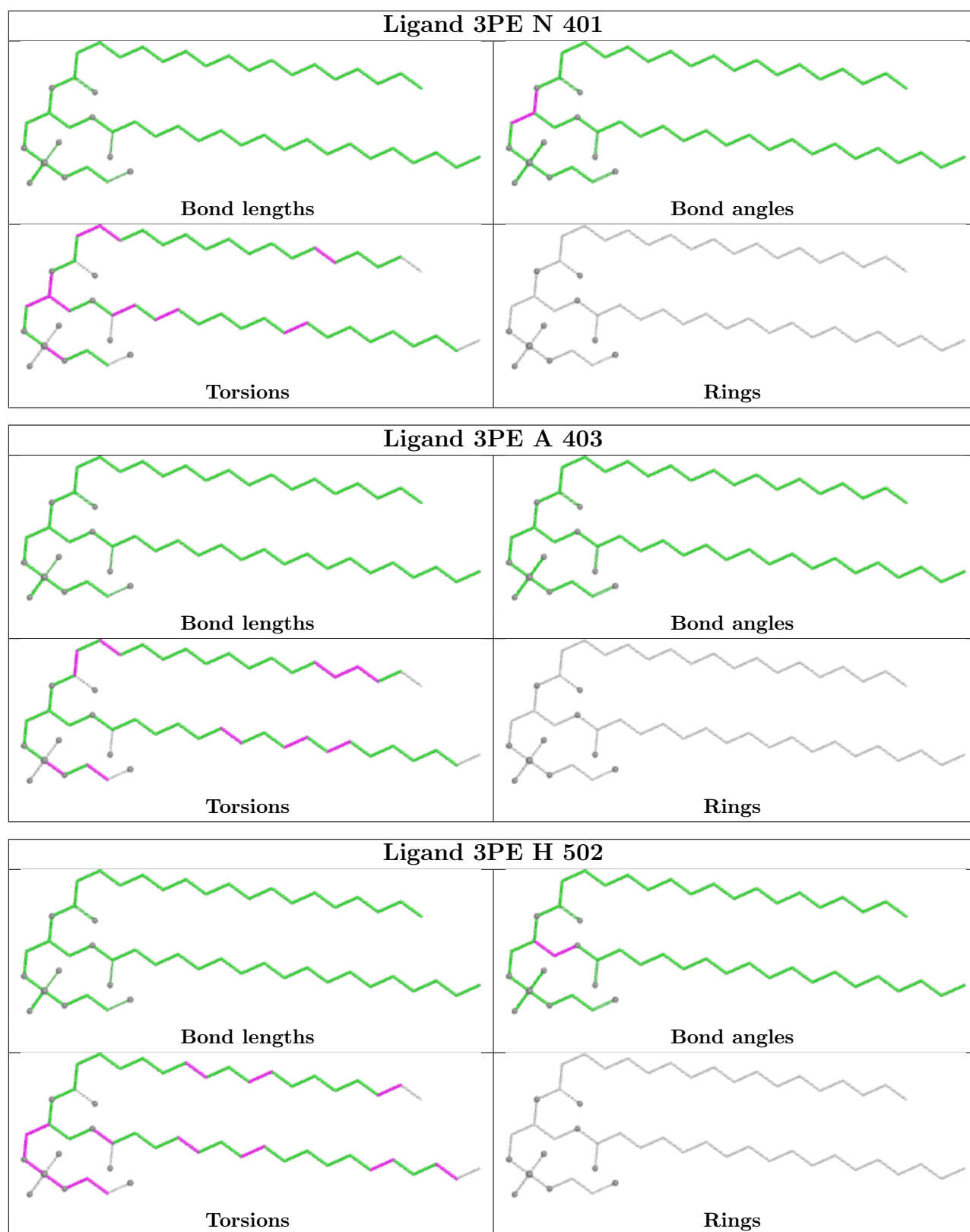


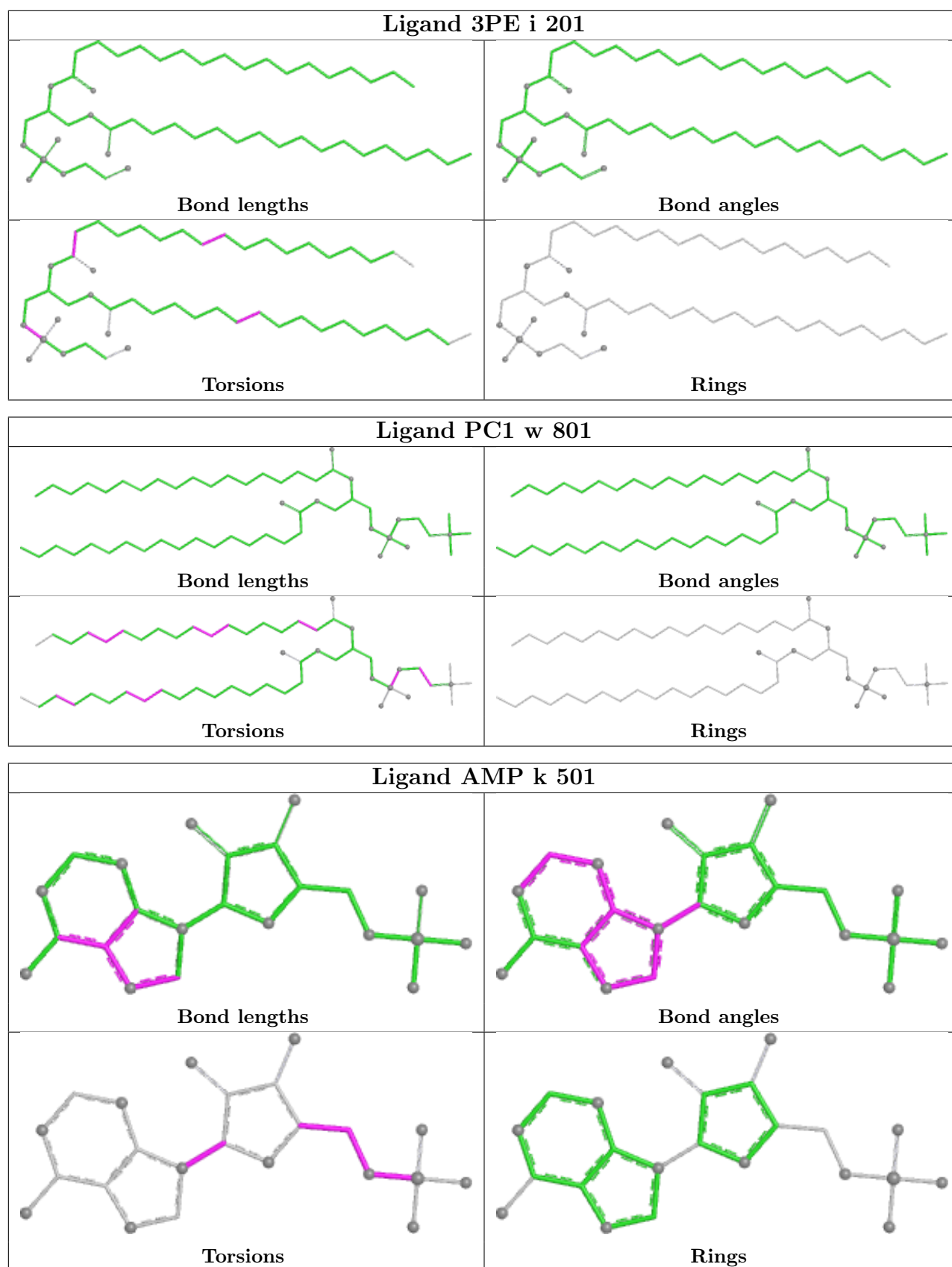


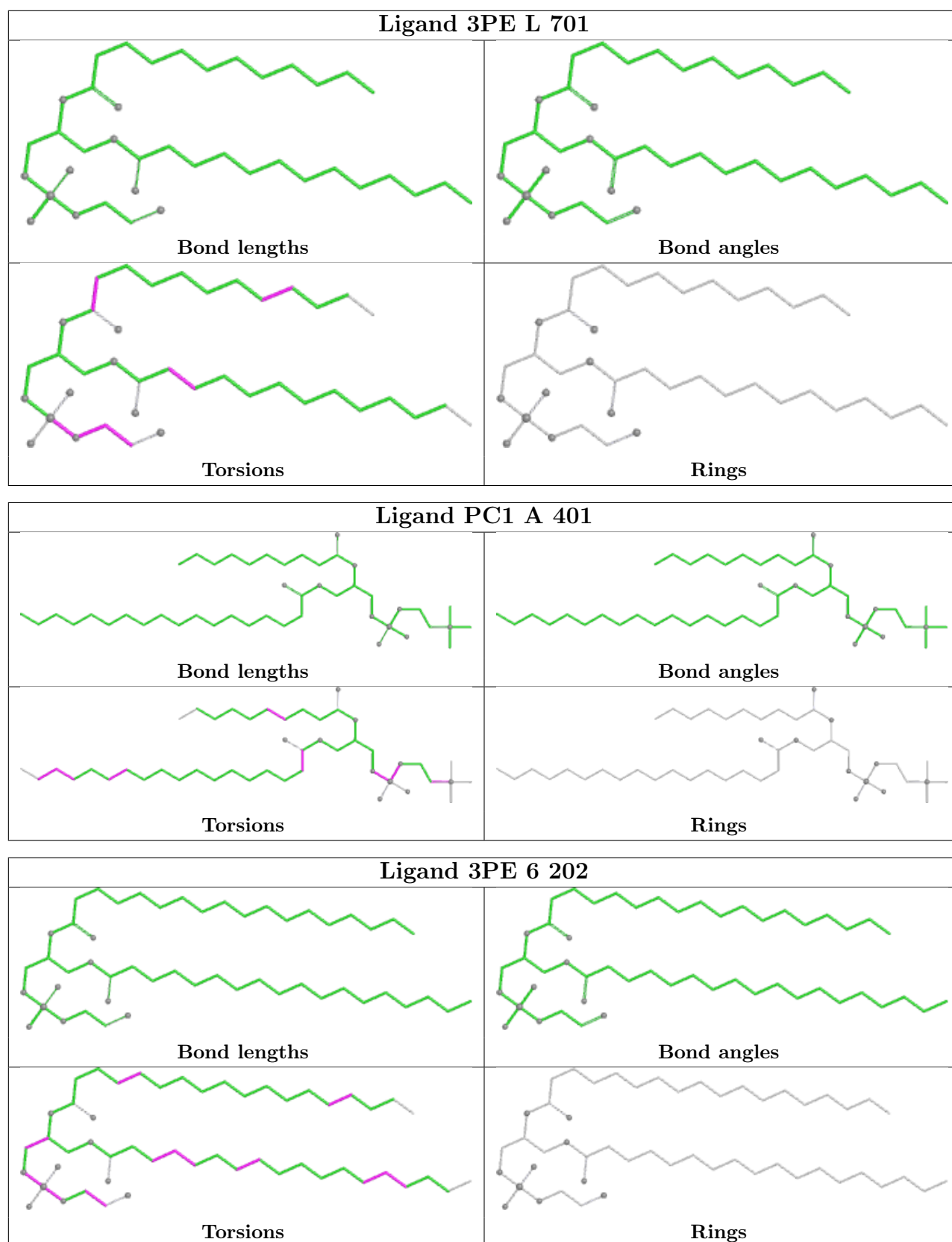


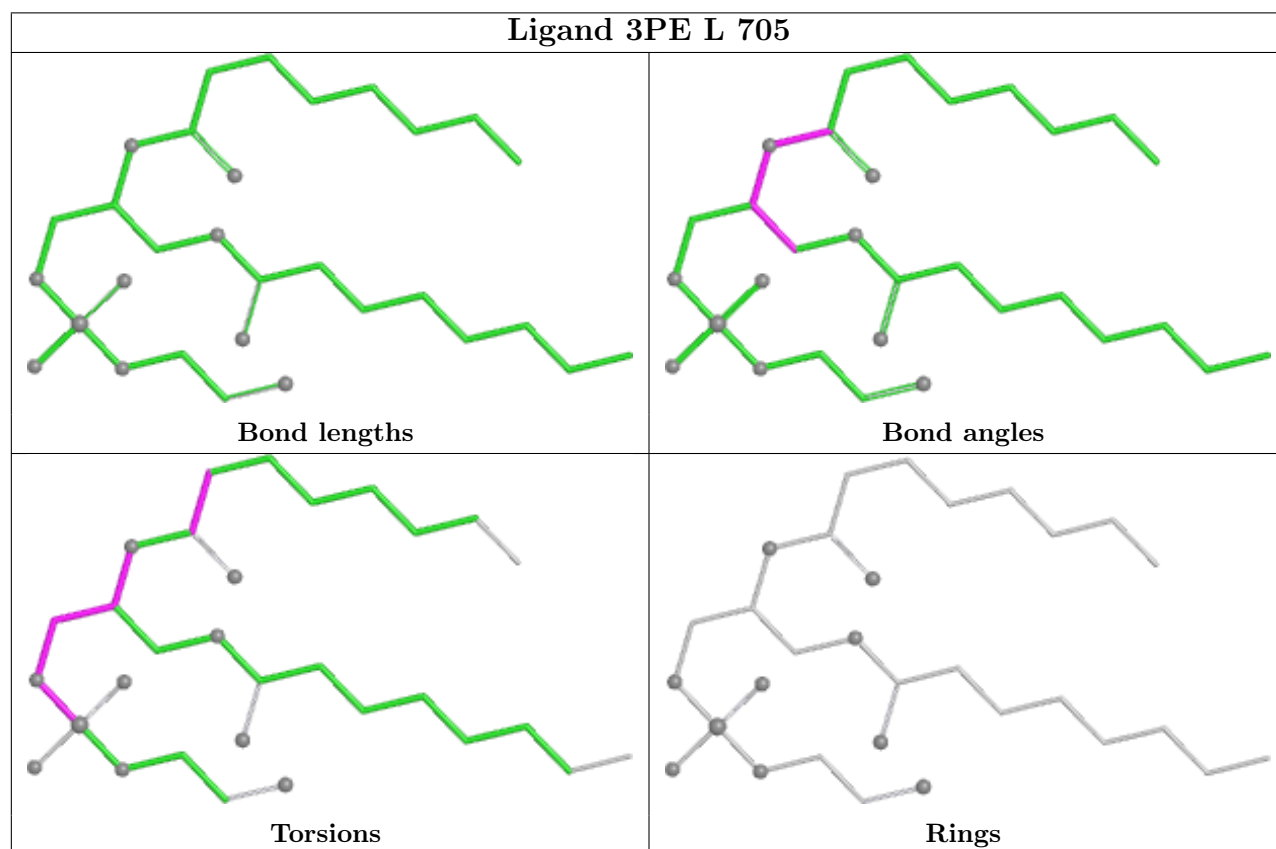
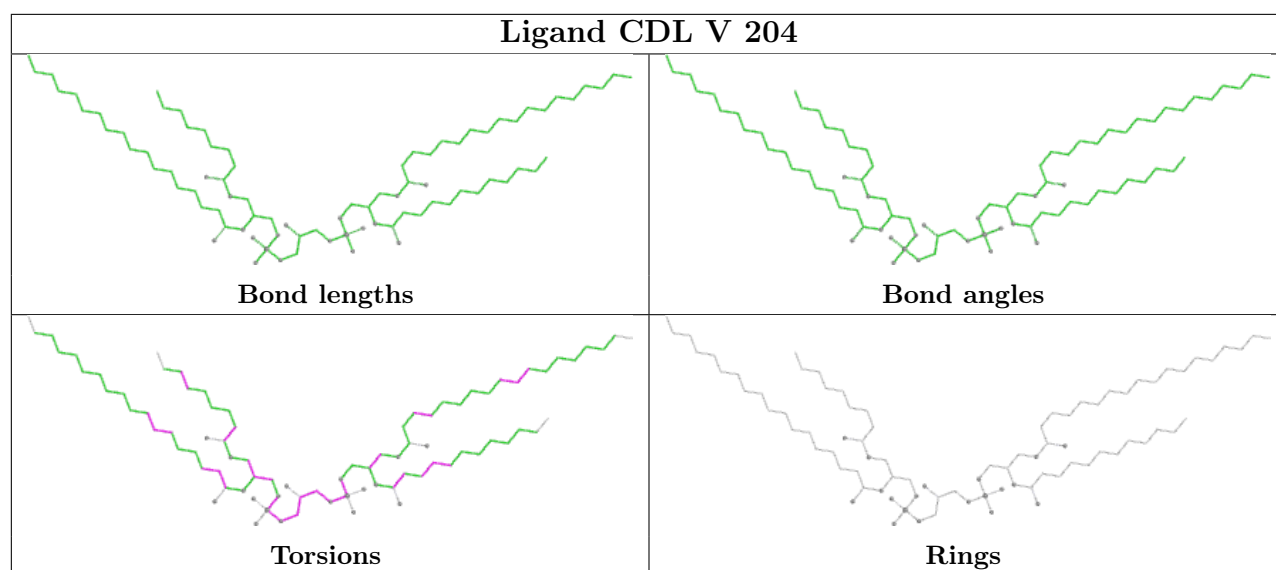


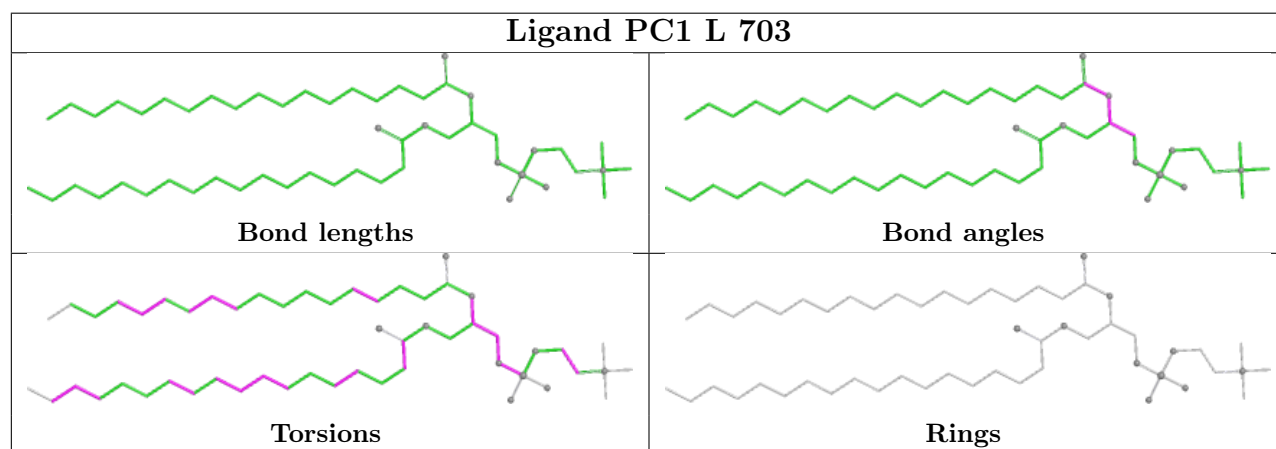
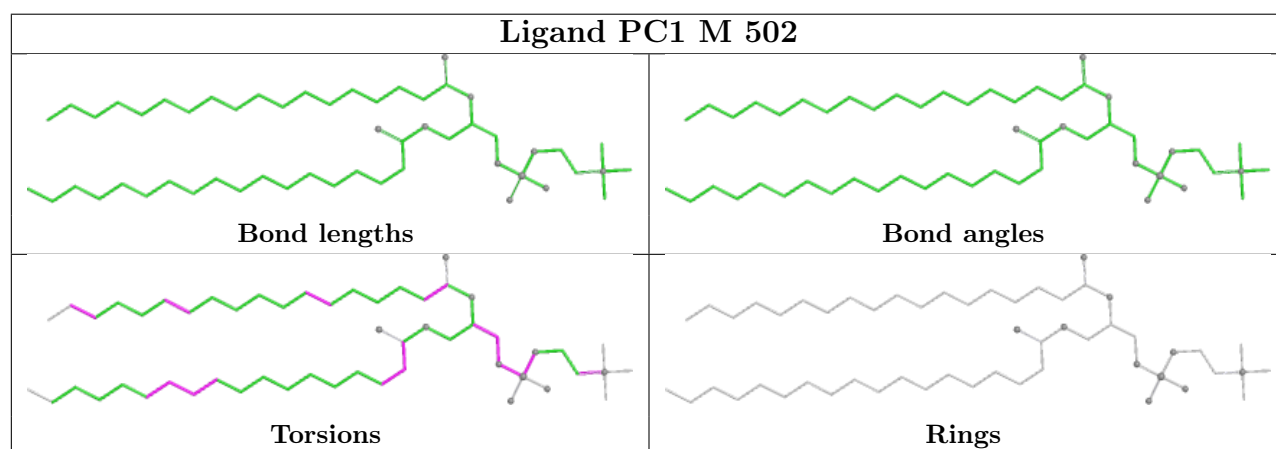
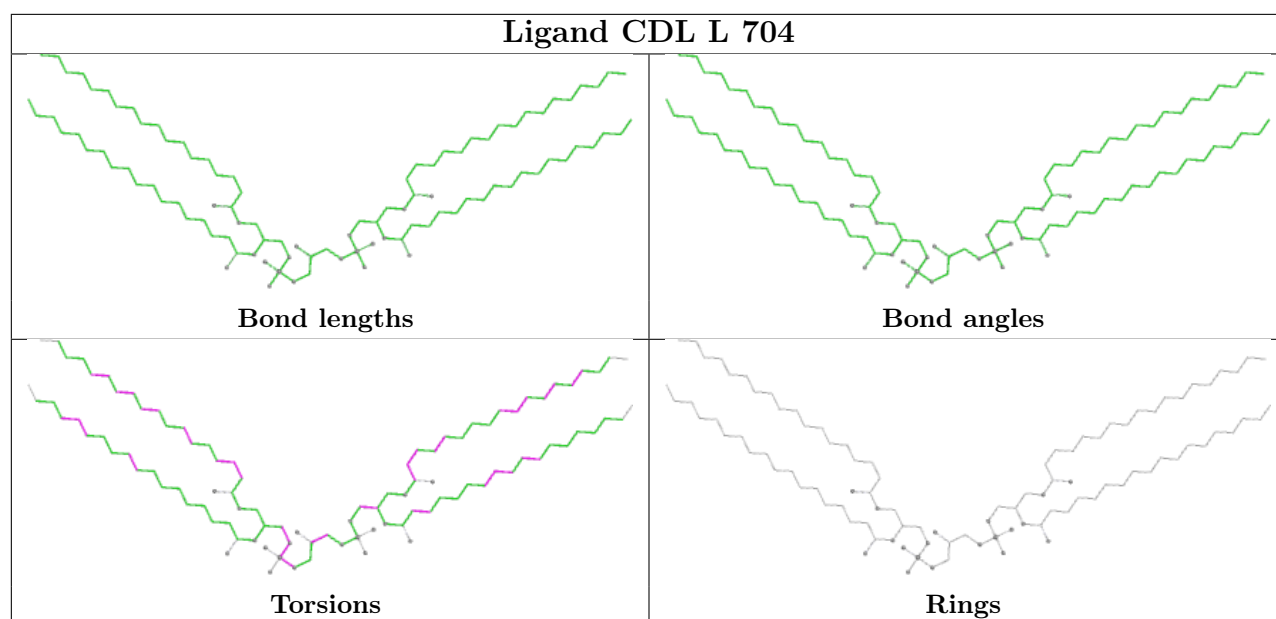


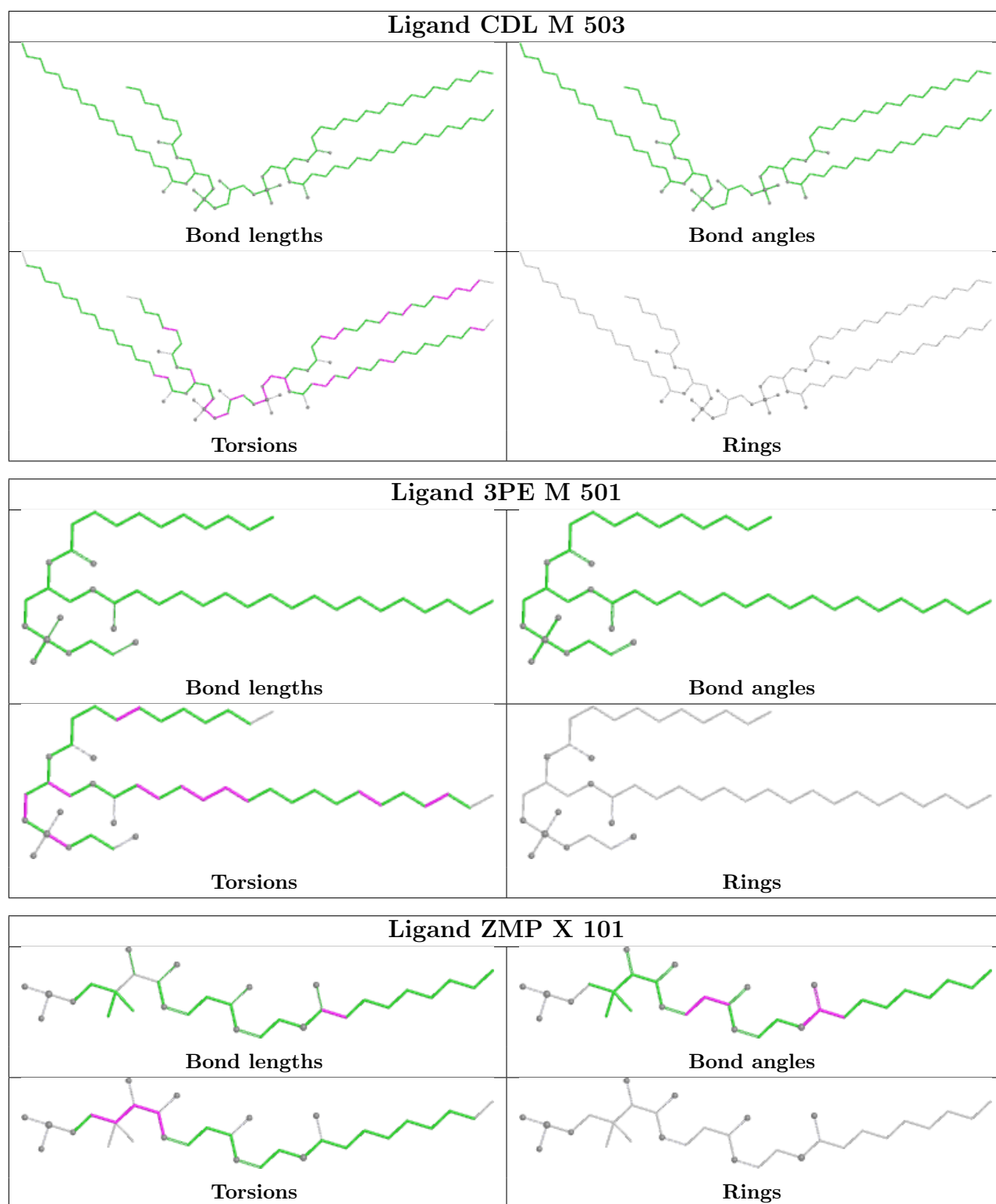












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

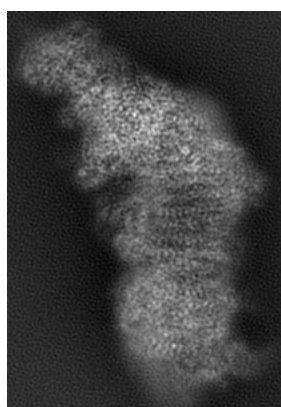
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11246. These allow visual inspection of the internal detail of the map and identification of artifacts.

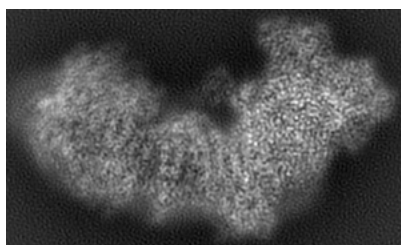
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

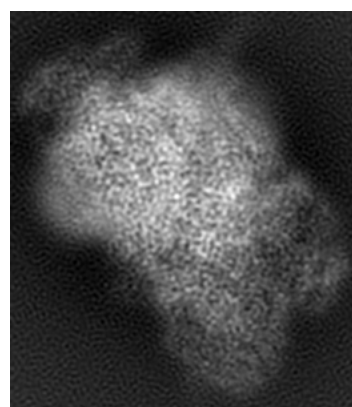
6.1.1 Primary map



X



Y

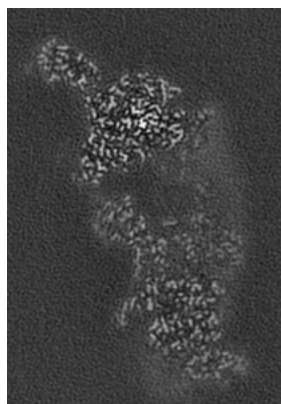


Z

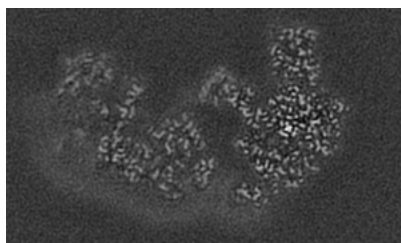
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

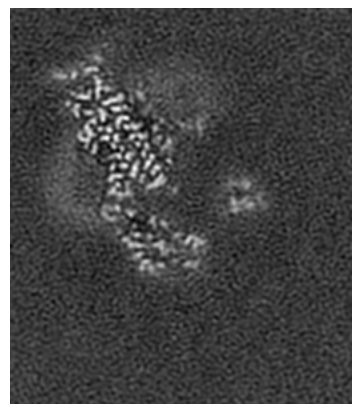
6.2.1 Primary map



X Index: 80



Y Index: 92

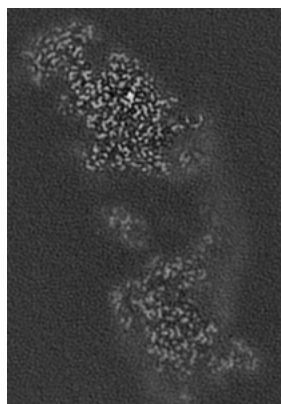


Z Index: 135

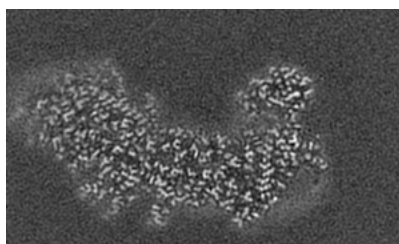
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

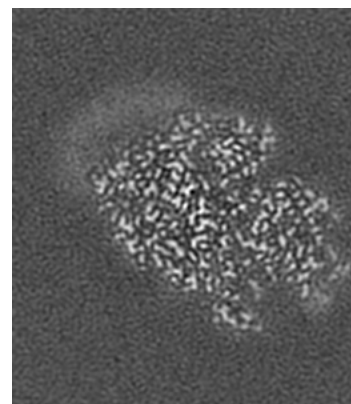
6.3.1 Primary map



X Index: 90



Y Index: 120

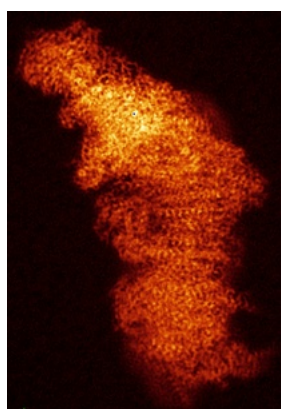


Z Index: 196

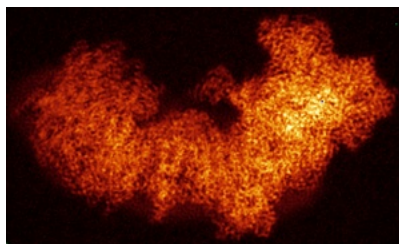
The images above show the largest variance slices of the map in three orthogonal directions.

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

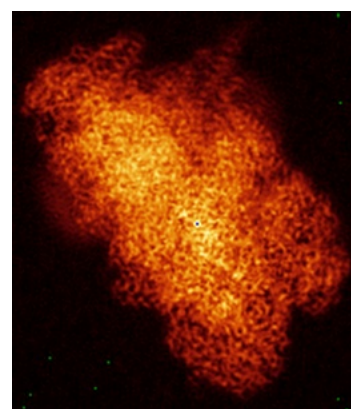
6.4.1 Primary map



X



Y

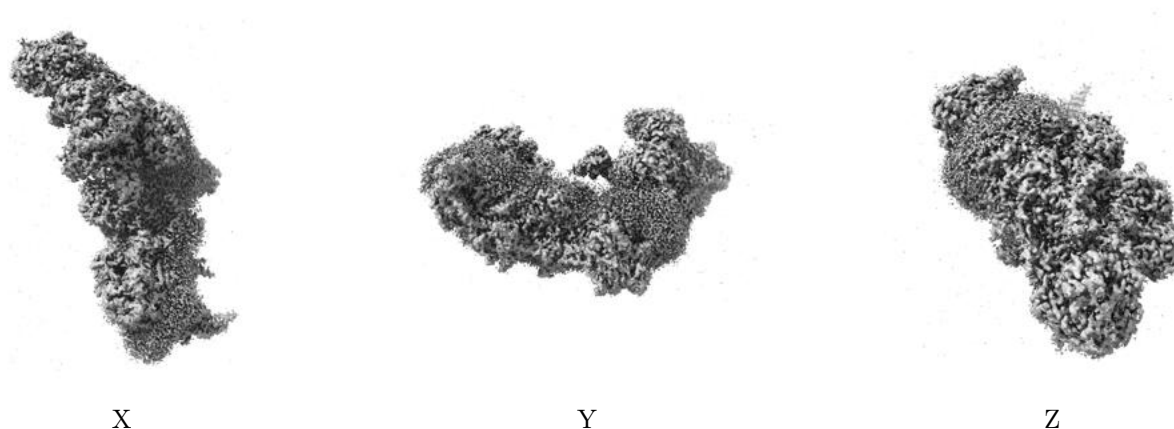


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

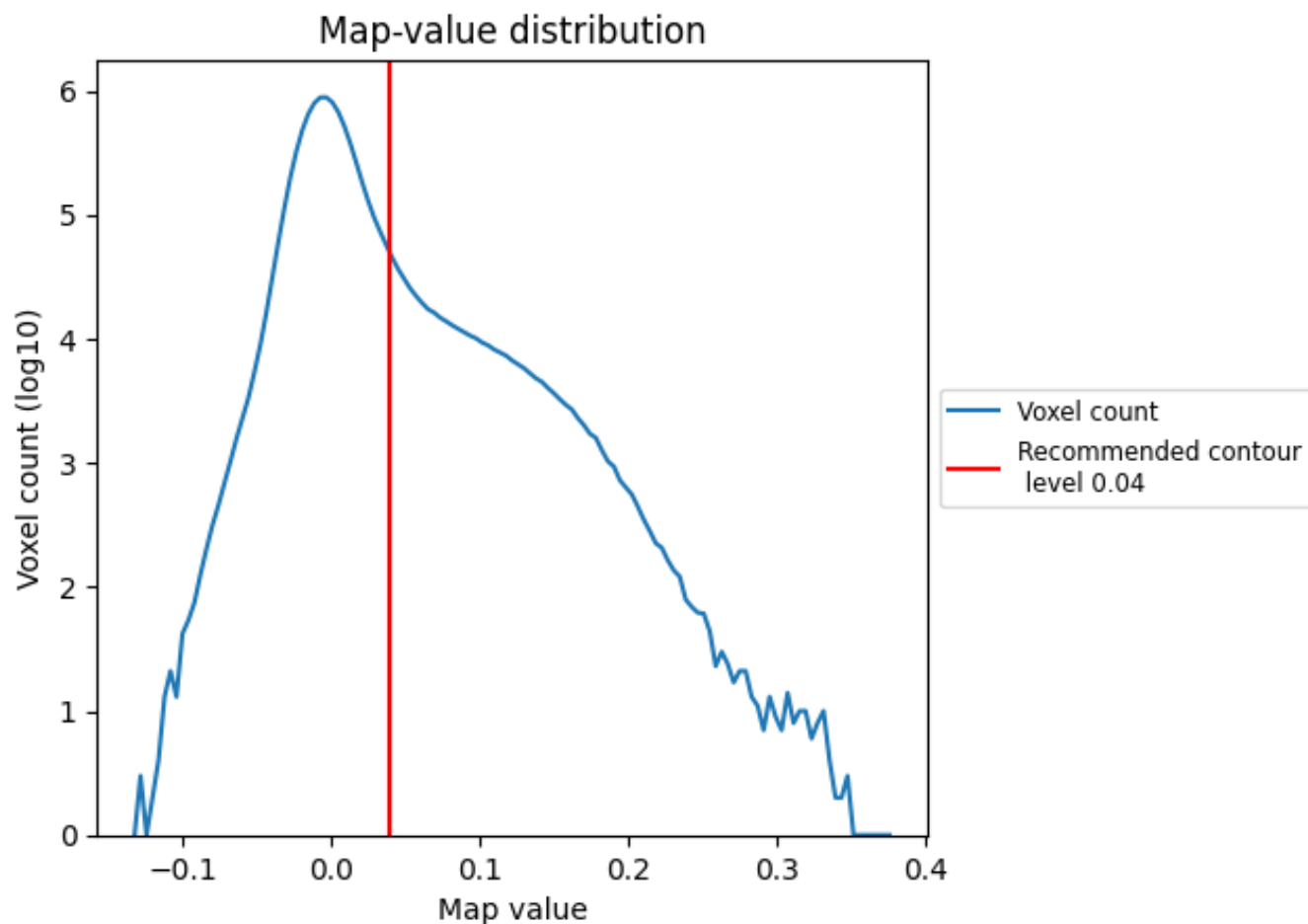
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

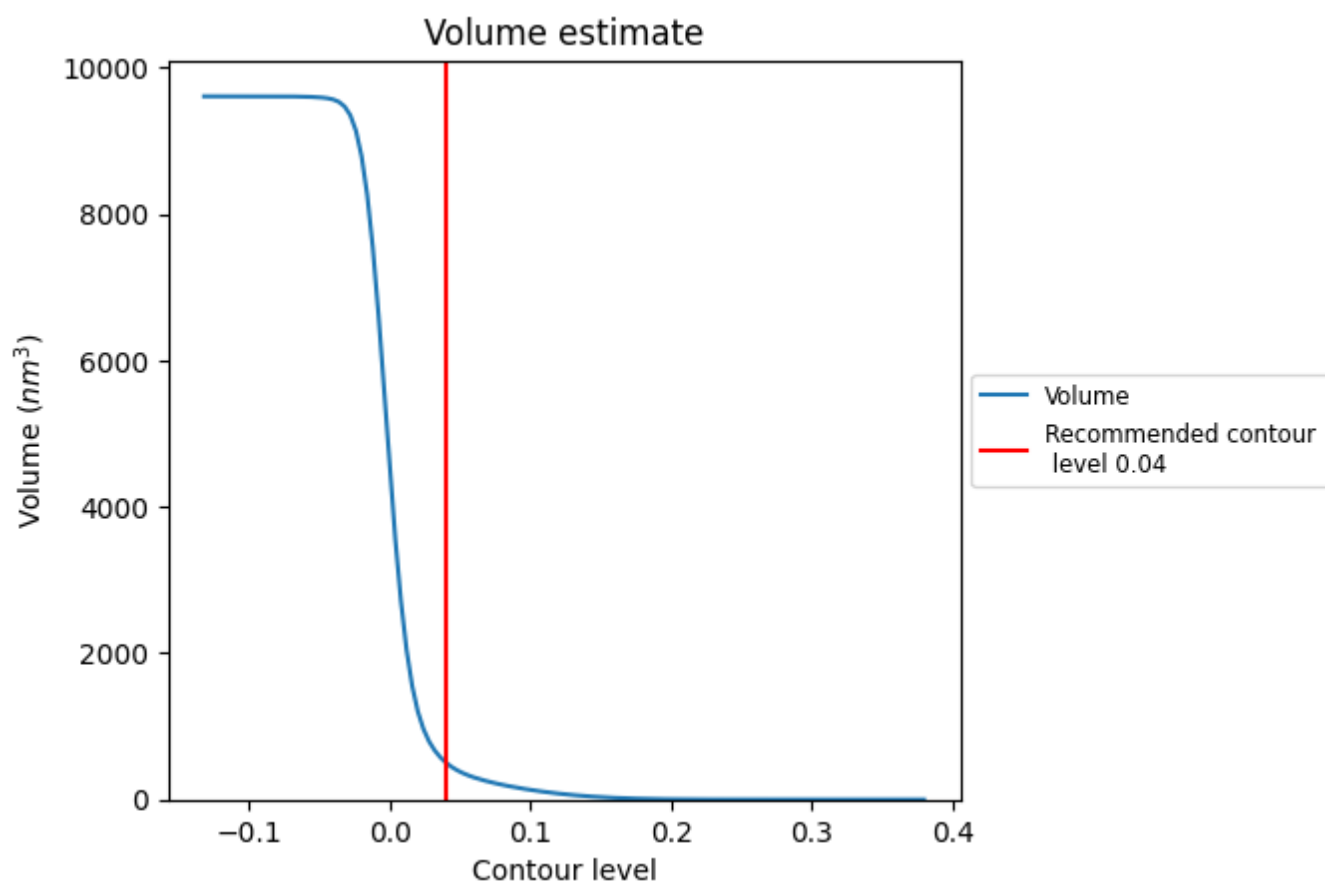
This section contains the results of statistical analysis of the map.

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 504 nm³; this corresponds to an approximate mass of 455 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.

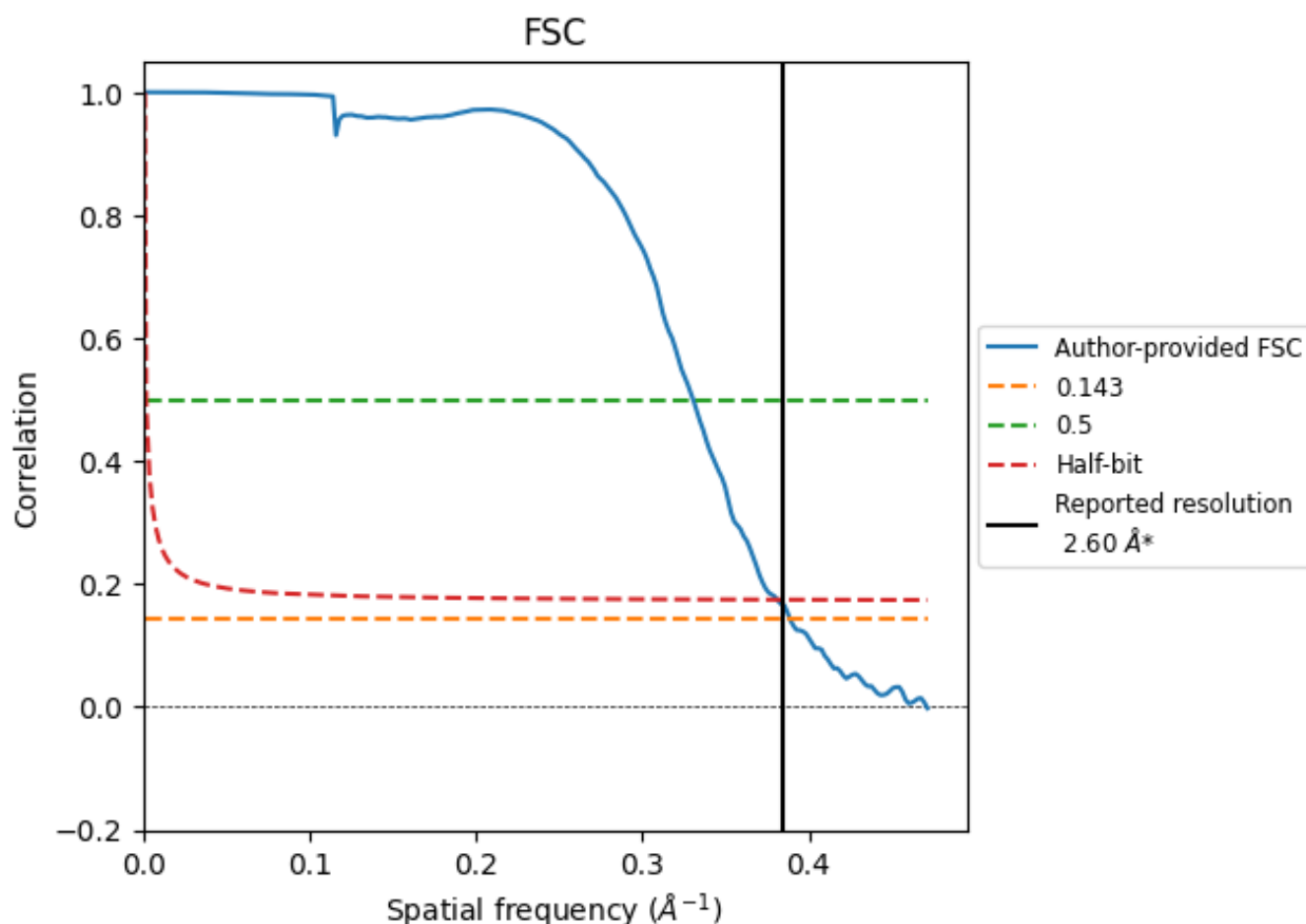
7.3 Rotationally averaged power spectrum [i](#)

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 0.385 Å⁻¹

8.2 Resolution estimates [i](#)

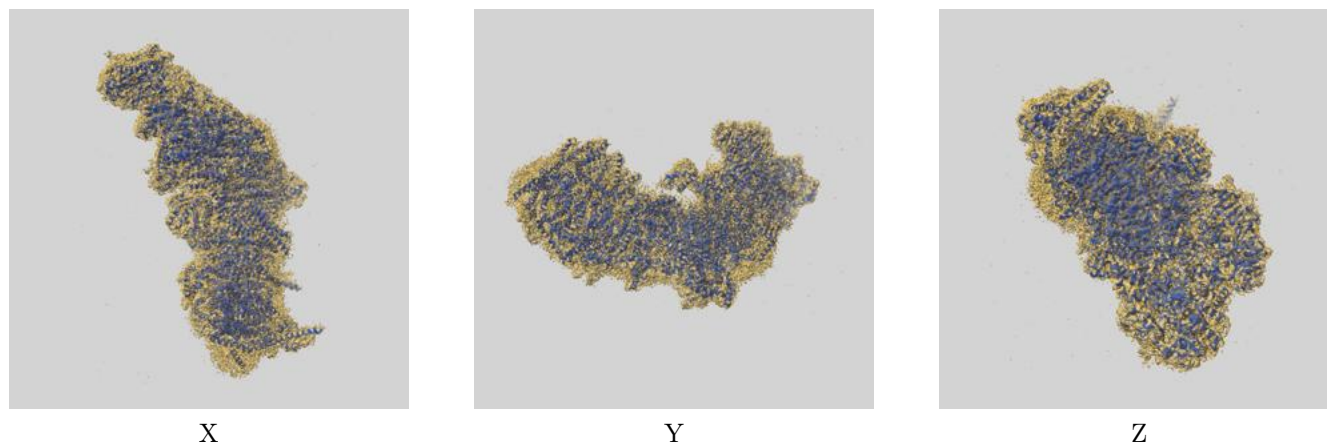
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	2.57	3.03	2.62
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

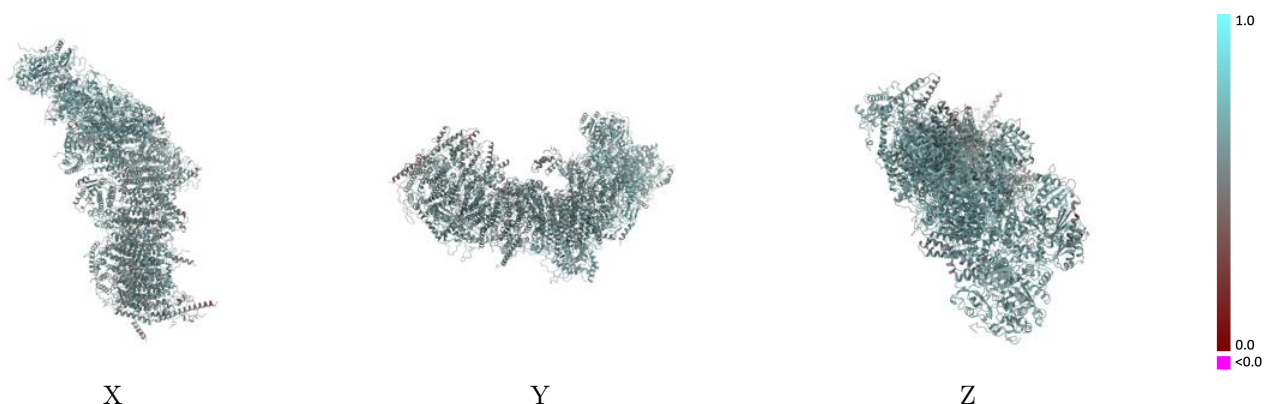
This section contains information regarding the fit between EMDB map EMD-11246 and PDB model 6ZKE. Per-residue inclusion information can be found in section [3](#) on page [20](#).

9.1 Map-model overlay [i](#)



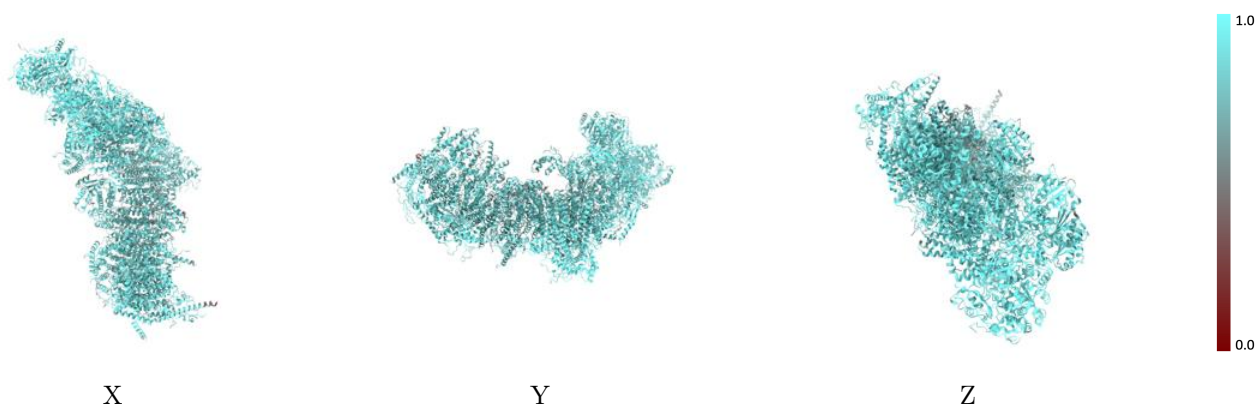
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



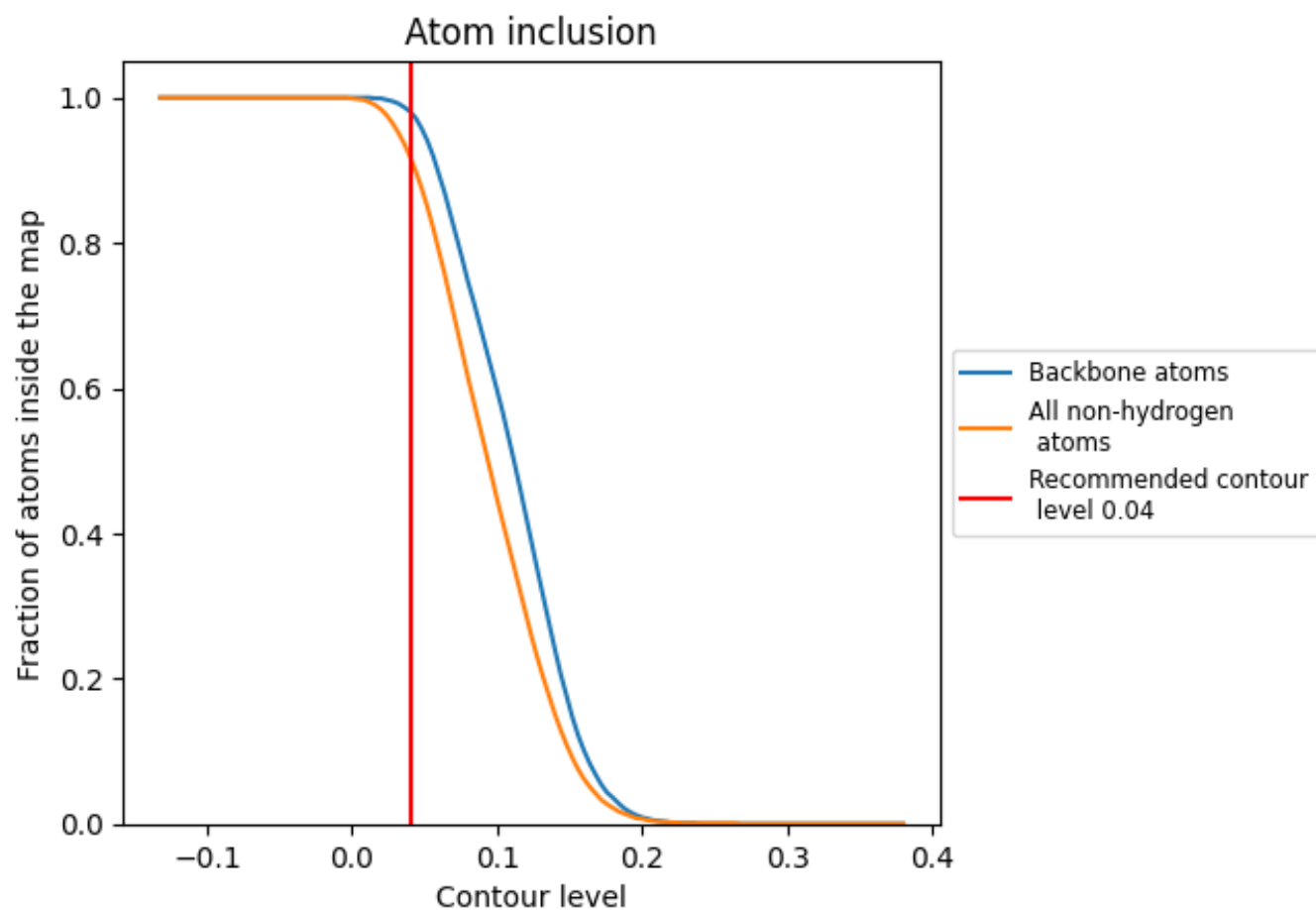
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.04).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 92% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9190	 0.5980
1	 0.9600	 0.6140
2	 0.9380	 0.6020
3	 0.9510	 0.6240
4	 0.9540	 0.6400
5	 0.9610	 0.6500
6	 0.9570	 0.6360
9	 0.9690	 0.6500
A	 0.8500	 0.5700
H	 0.9440	 0.6250
J	 0.9030	 0.5840
K	 0.9260	 0.6190
L	 0.9100	 0.5880
M	 0.9450	 0.6230
N	 0.9550	 0.6310
V	 0.7450	 0.5270
W	 0.9120	 0.6030
X	 0.8350	 0.5200
Y	 0.9120	 0.5950
Z	 0.9010	 0.5770
a	 0.9310	 0.6010
b	 0.9460	 0.6320
c	 0.9370	 0.6350
d	 0.9230	 0.5930
e	 0.9060	 0.5660
f	 0.9180	 0.6050
g	 0.9250	 0.6120
h	 0.9240	 0.6150
i	 0.9430	 0.6270
j	 0.8050	 0.5010
k	 0.9000	 0.5820
l	 0.9060	 0.5810
m	 0.9320	 0.5910
n	 0.8400	 0.4920
o	 0.9140	 0.5970



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Chain	Atom inclusion	Q-score
p	 0.8600	 0.5540
q	 0.9450	 0.6080
r	 0.8710	 0.5420
s	 0.8540	 0.4930
t	 0.8710	 0.5370
u	 0.8760	 0.5190
v	 0.8850	 0.5600
w	 0.8700	 0.5680
x	 0.8540	 0.5550
y	 0.8610	 0.5570
z	 0.9570	 0.6140