



Full wwPDB EM Validation Report ⓘ

Mar 30, 2026 – 08:20 AM UTC

PDB ID : 6ZKL / pdb_00006zkl
EMDB ID : EMD-11253
Title : Complex I inhibited by rotenone, open1
Authors : Kampjut, D.; Sazanov, L.A.
Deposited on : 2020-06-30
Resolution : 3.10 Å(reported)
Based on initial model : 5LNK

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

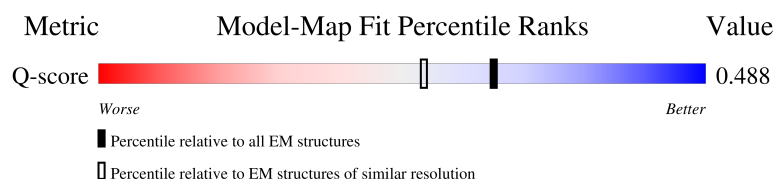
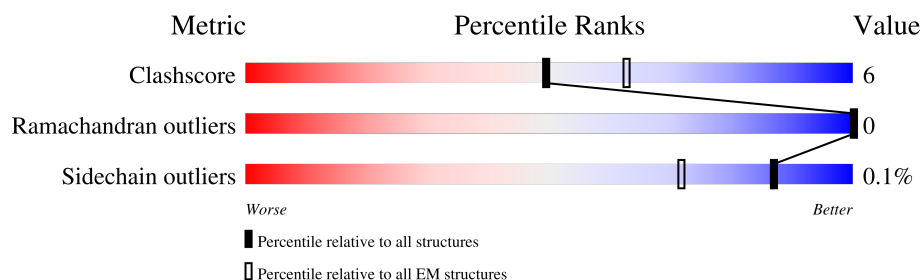
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.10 Å.

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



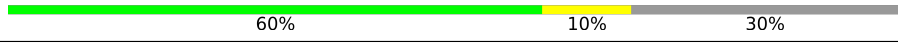
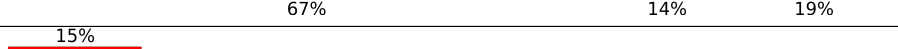
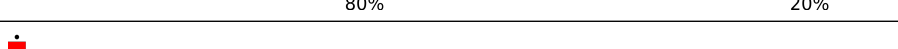
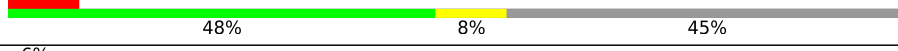
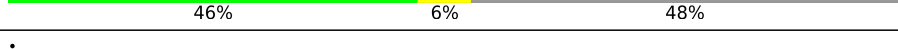
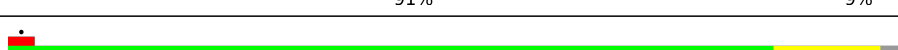
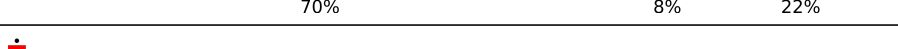
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14724 (2.60 - 3.60)

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	 75% 18% 7%
2	2	246	 71% 15% 13%
3	3	727	 79% 16% 5%
4	4	463	 5% 73% 19% 8%

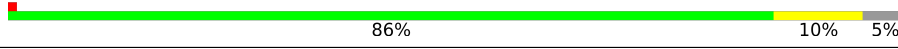
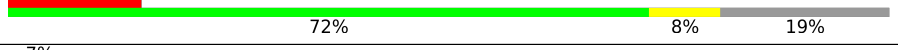
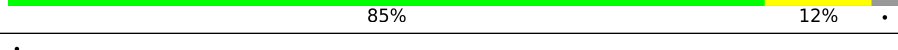
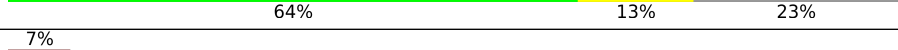
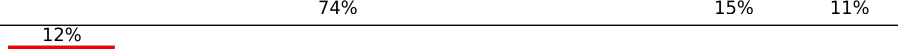
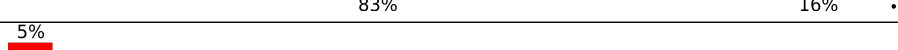
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Mol	Chain	Length	Quality of chain
5	5	266	
6	6	223	
7	9	217	
8	A	115	
9	H	318	
10	J	175	
11	K	98	
12	L	606	
13	M	459	
14	N	347	
15	V	141	
16	W	189	
17	X	157	
17	j	157	
18	Y	172	
19	Z	175	
20	a	109	
21	b	124	
22	c	170	
23	d	380	
24	e	99	
25	f	116	
26	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
53	CDL	L	704	X	-	-	-
53	CDL	V	204	X	-	-	-
53	CDL	Y	201	X	-	-	-
53	CDL	o	201	X	-	-	-

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 67492 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	426	Total	C	N	O	S	0	0
			3427	2188	590	624	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	166	Total	C	N	O	S	0	0
			1264	851	181	219	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		

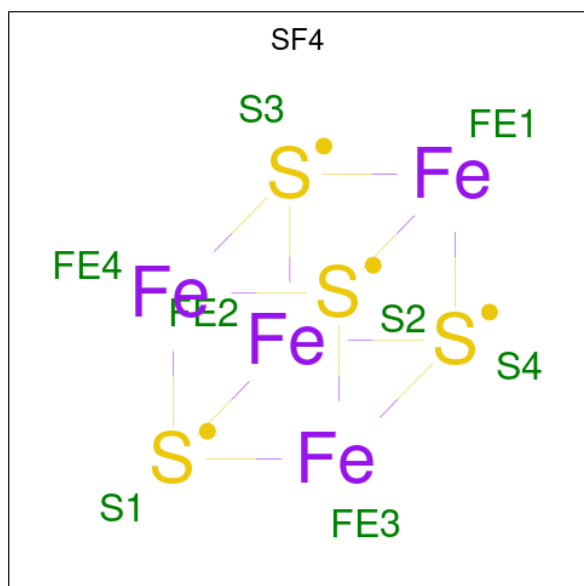
- Molecule 43 is a protein called Mitochondrial complex I, MNLL subunit.

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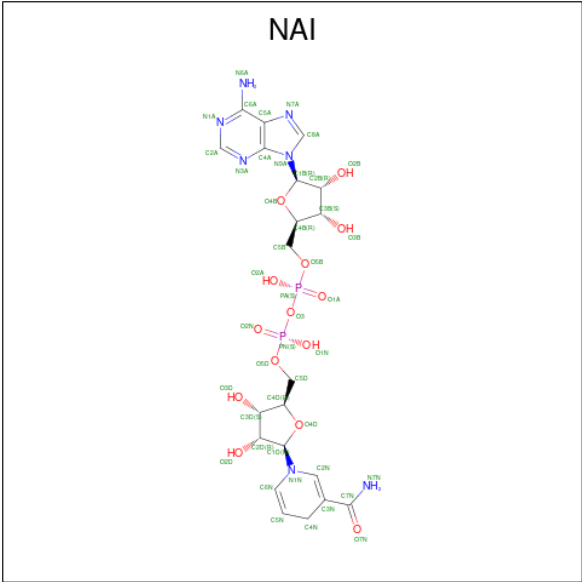
Mol	Chain	Residues	Atoms			AltConf
45	9	1	Total	Fe	S	0
			8	4	4	
45	9	1	Total	Fe	S	0
			8	4	4	

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



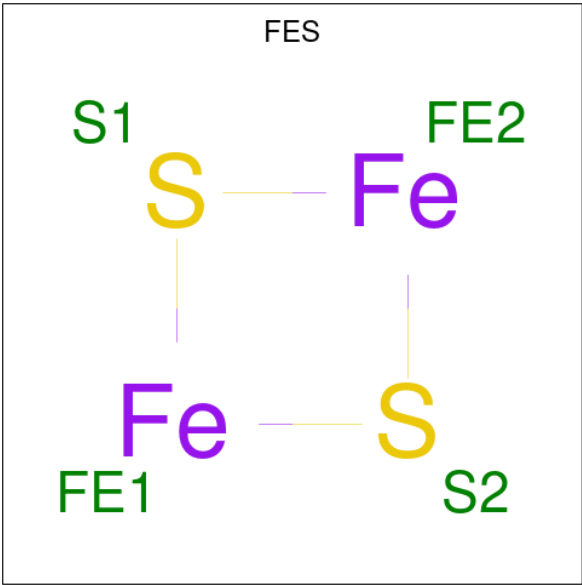
Mol	Chain	Residues	Atoms					AltConf
46	1	1	Total	C	N	O	P	0
			31	17	4	9	1	

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



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

- Molecule 48 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).

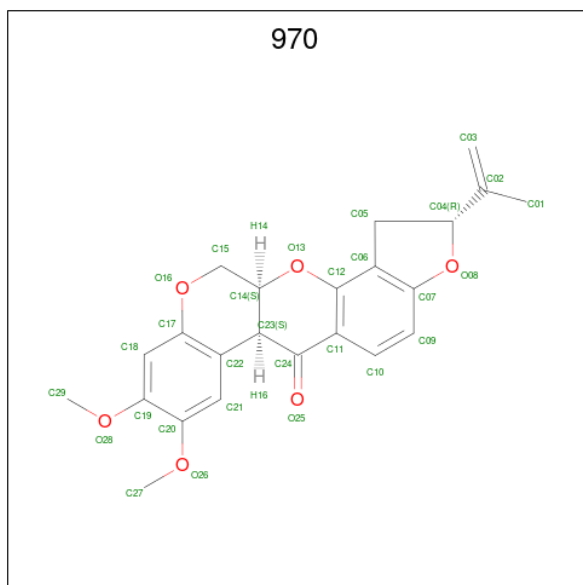


Mol	Chain	Residues	Atoms			AltConf
48	2	1	Total	Fe	S	0
			4	2	2	
48	3	1	Total	Fe	S	0
			4	2	2	

- Molecule 49 is POTASSIUM ION (CCD ID: K) (formula: K).

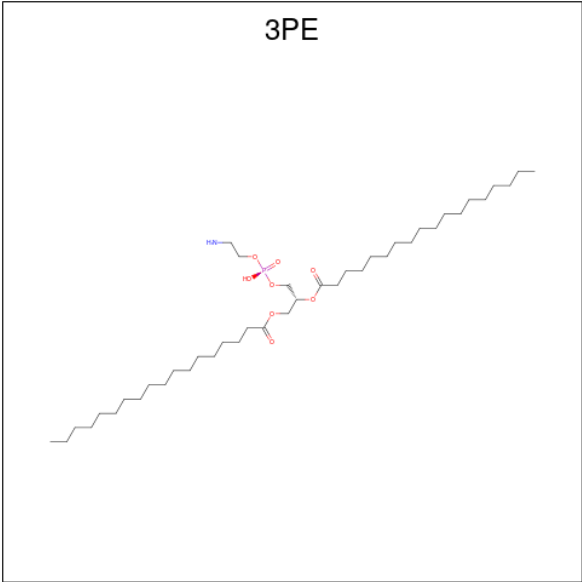
Mol	Chain	Residues	Atoms		AltConf
49	3	1	Total	K	0
			1	1	

- Molecule 50 is (2R,6aS,12aS)-8,9-dimethoxy-2-(prop-1-en-2-yl)-1,2,12,12a-tetrahydrofuro[2',3':7,8][1]benzopyrano[2,3-c][1]benzopyran-6(6aH)-one (CCD ID: 970) (formula: C₂₃H₂₂O₆) (labeled as "Ligand of Interest" by depositor).



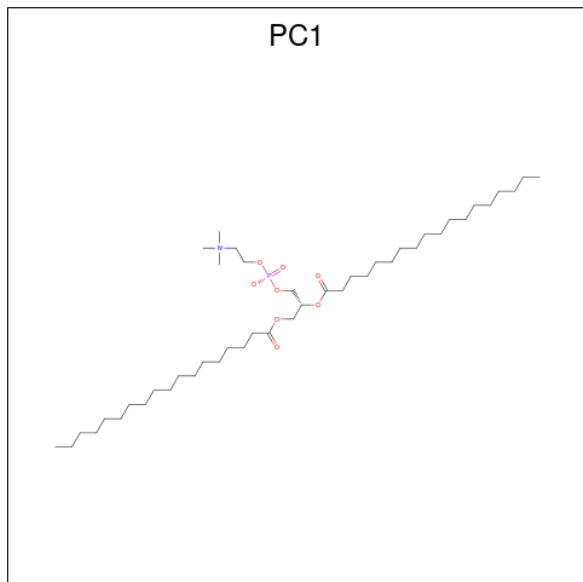
Mol	Chain	Residues	Atoms			AltConf
50	6	1	Total	C	O	0
			29	23	6	
50	H	1	Total	C	O	0
			29	23	6	

- Molecule 51 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: C₄₁H₈₂NO₈P).



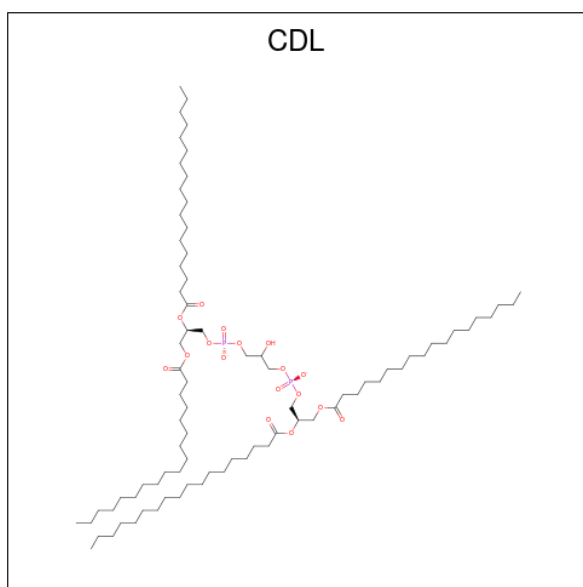
Mol	Chain	Residues	Atoms					AltConf
51	6	1	Total	C	N	O	P	0
			51	41	1	8	1	
51	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
51	J	1	Total	C	N	O	P	0
			51	41	1	8	1	
51	K	1	Total	C	N	O	P	0
			40	30	1	8	1	
51	L	1	Total	C	N	O	P	0
			40	30	1	8	1	
51	L	1	Total	C	N	O	P	0
			51	41	1	8	1	
51	L	1	Total	C	N	O	P	0
			31	21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

- Molecule 52 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



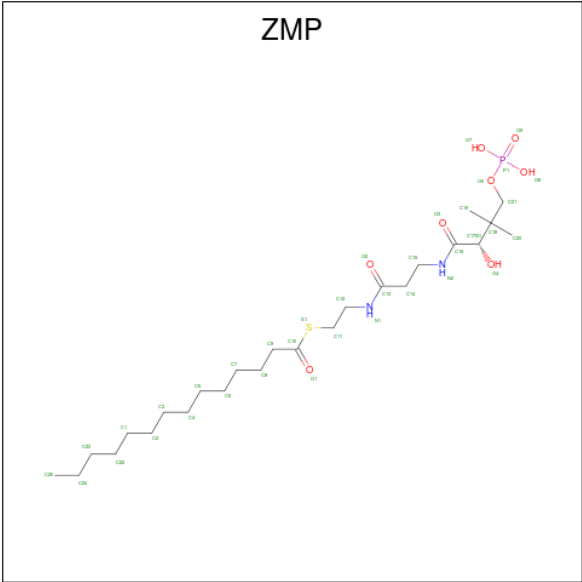
Mol	Chain	Residues	Atoms					AltConf
52	9	1	Total	C	N	O	P	0
			54	44	1	8	1	
52	A	1	Total	C	N	O	P	0
			46	36	1	8	1	
52	A	1	Total	C	N	O	P	0
			37	27	1	8	1	
52	L	1	Total	C	N	O	P	0
			54	44	1	8	1	
52	M	1	Total	C	N	O	P	0
			54	44	1	8	1	
52	w	1	Total	C	N	O	P	0
			54	44	1	8	1	

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



Mol	Chain	Residues	Atoms				AltConf
53	L	1	Total	C	O	P	0
			100	81	17	2	
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	i	1	Total	C	O	P	0
			58	39	17	2	
53	o	1	Total	C	O	P	0
			75	56	17	2	
53	o	1	Total	C	O	P	0
			90	71	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	C	N	O	P	S	0
			31	20	2	7	1	1	
54	g	1	Total	C	N	O	P	S	0
			34	23	2	7	1	1	

- 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).



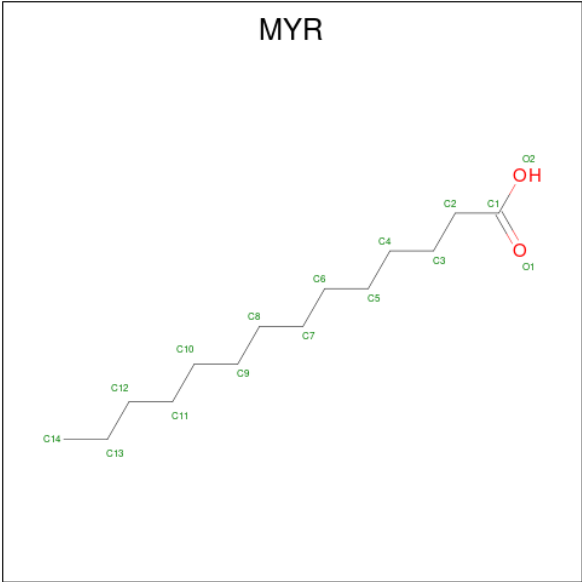
Mol	Chain	Residues	Atoms					AltConf
56	d	1	Total 48	C 21	N 7	O 17	P 3	0

- Molecule 57 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: $\text{C}_{10}\text{H}_{14}\text{N}_5\text{O}_7\text{P}$).



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

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

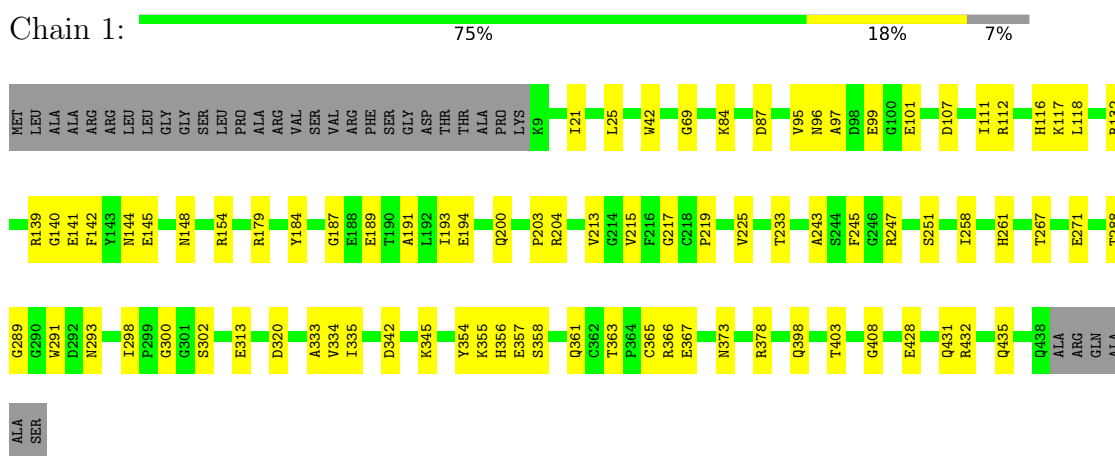


Mol	Chain	Residues	Atoms			AltConf
58	s	1	Total	C	O	0
			15	14	1	

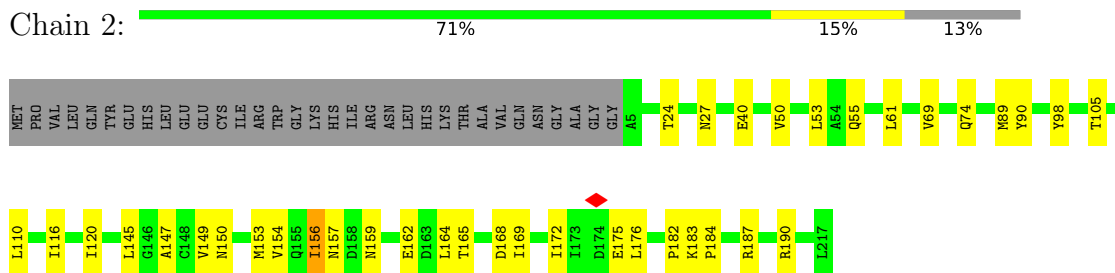
3 Residue-property plots

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.

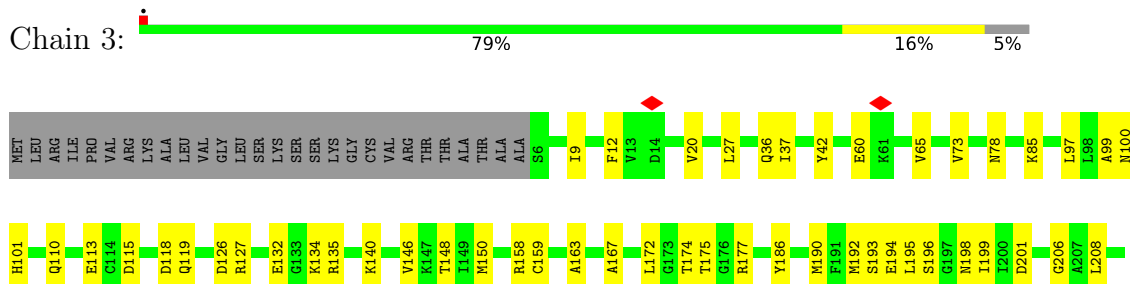
- Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

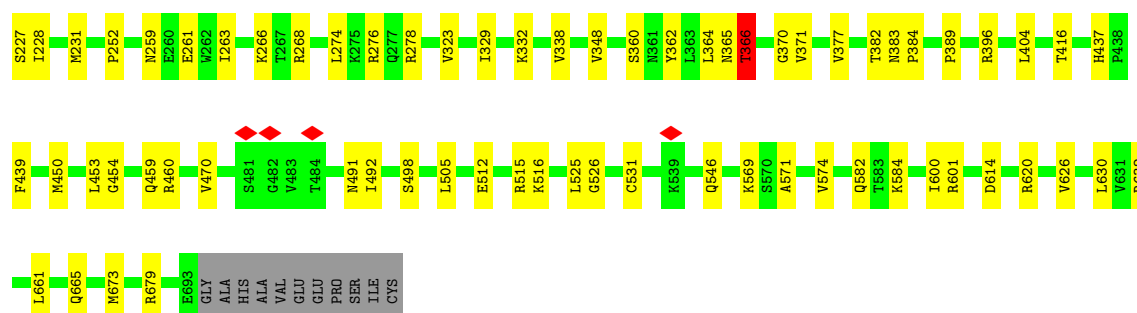


- Molecule 2: Mitochondrial complex I, 24 kDa subunit

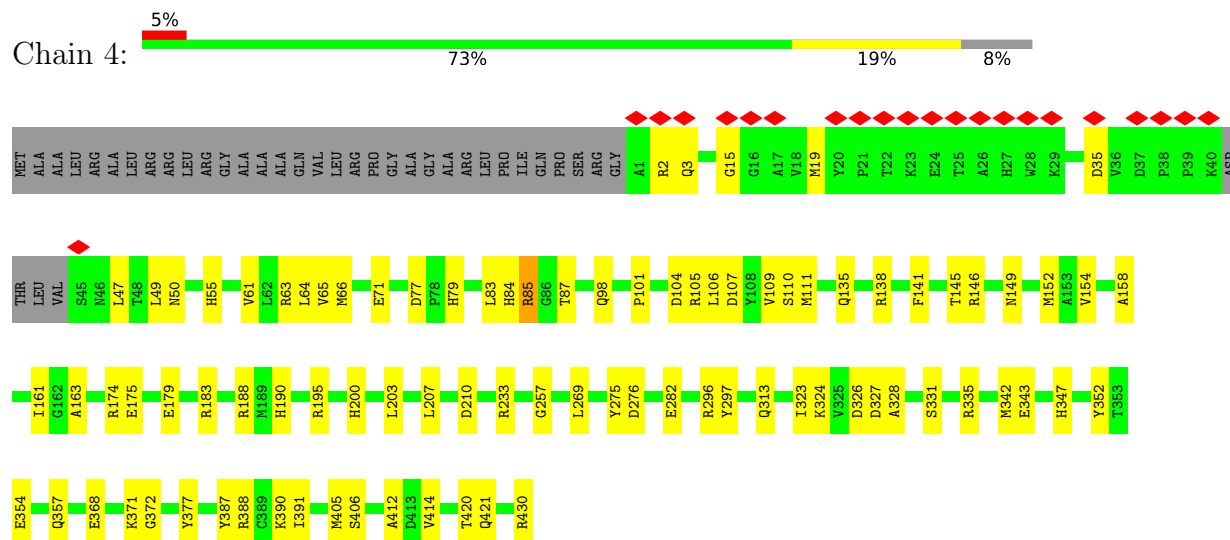


- Molecule 3: NADH:ubiquinone oxidoreductase core subunit S1

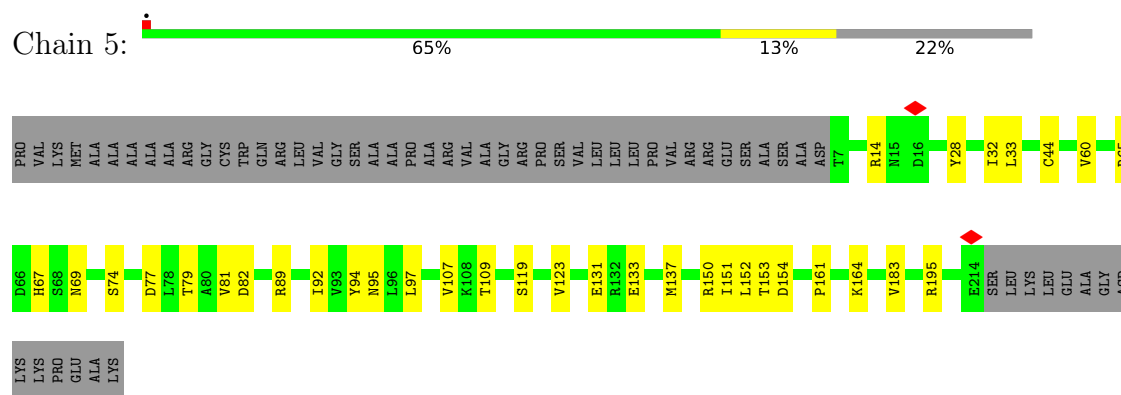




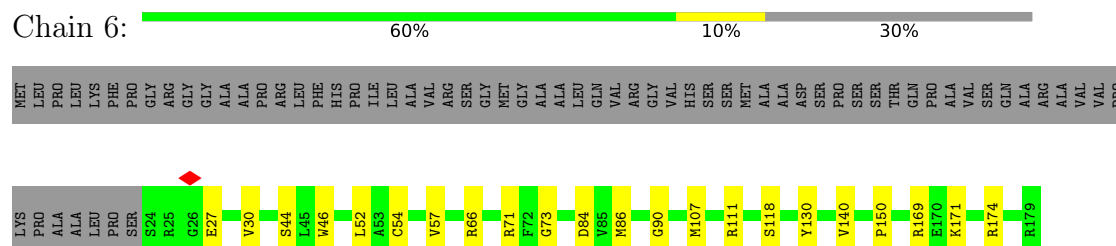
- Molecule 4: Mitochondrial complex I, 49 kDa subunit



- Molecule 5: NADH:ubiquinone oxidoreductase core subunit S3

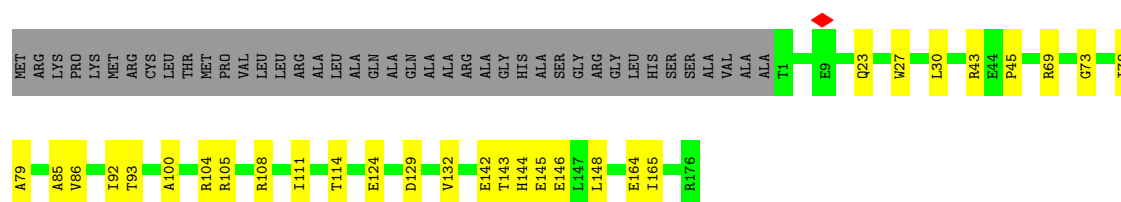


- Molecule 6: Mitochondrial complex I, PSST subunit



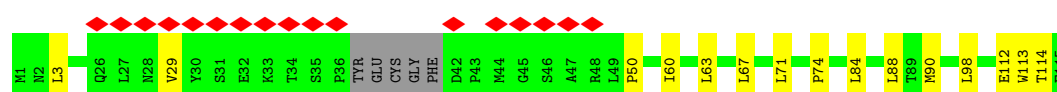
- Molecule 7: Mitochondrial complex I, TYKY subunit

Chain 9: 



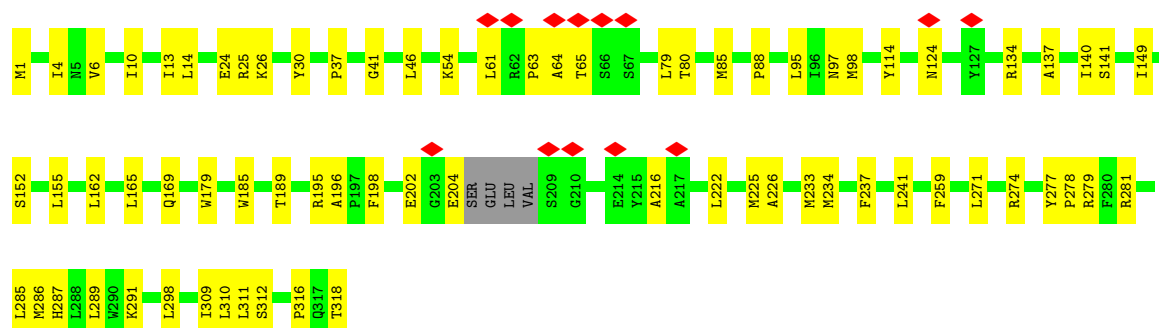
- Molecule 8: NADH-ubiquinone oxidoreductase chain 3

Chain A: 



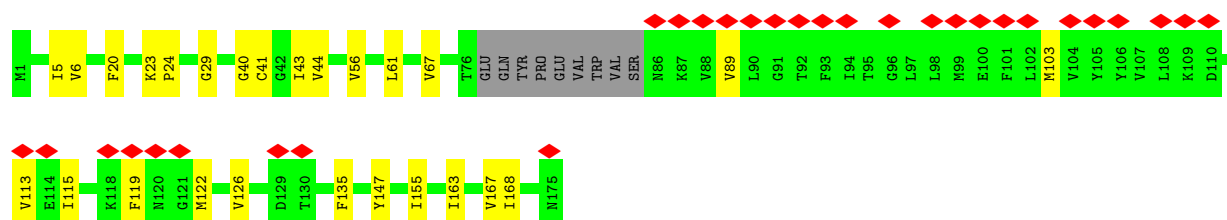
- Molecule 9: NADH-ubiquinone oxidoreductase chain 1

Chain H: 



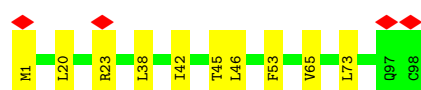
- Molecule 10: NADH-ubiquinone oxidoreductase chain 6

Chain J: 



- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

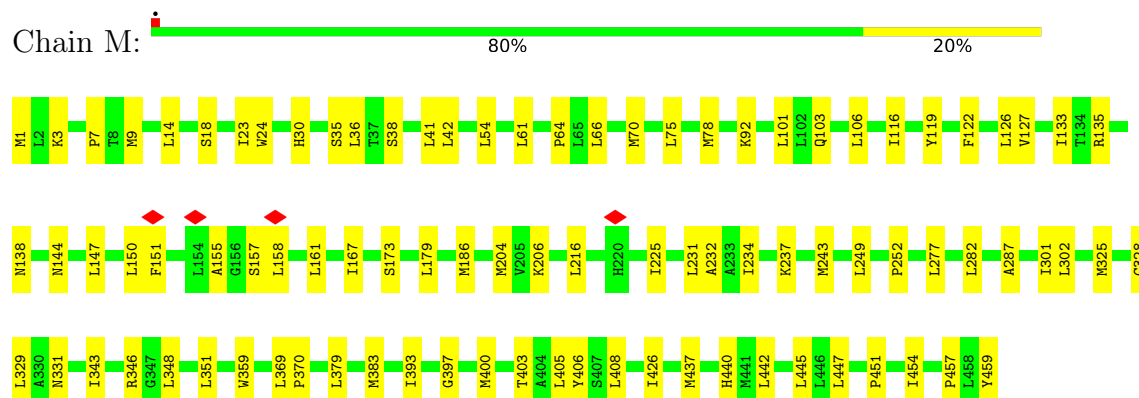
Chain K: 



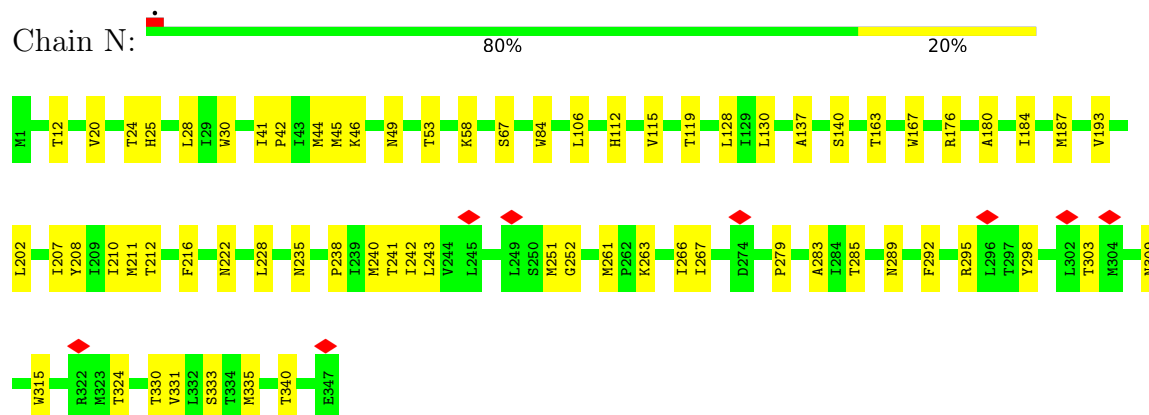
• Molecule 12: NADH-ubiquinone oxidoreductase chain 5



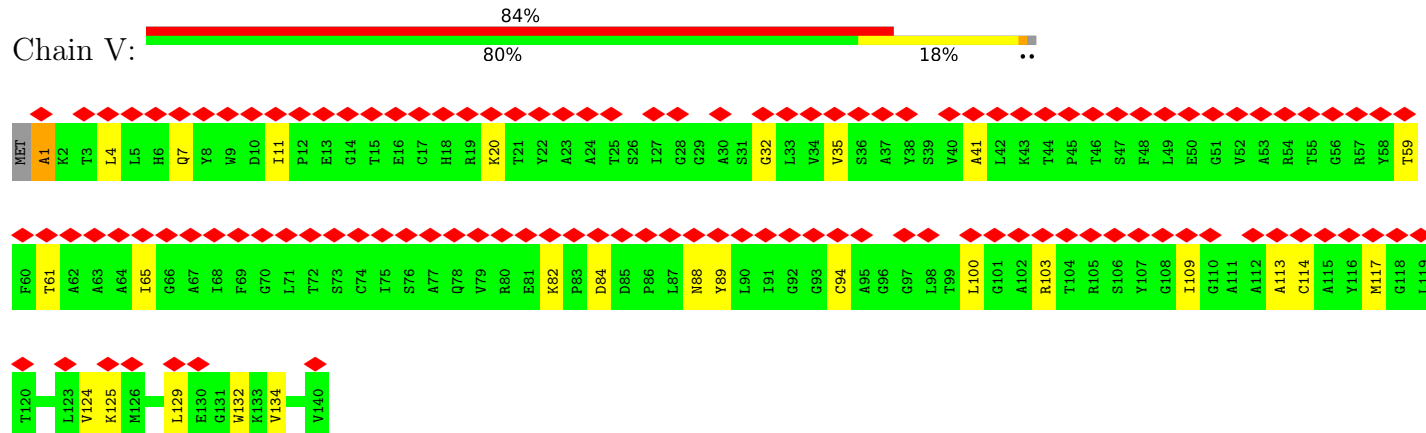
• Molecule 13: NADH-ubiquinone oxidoreductase chain 4



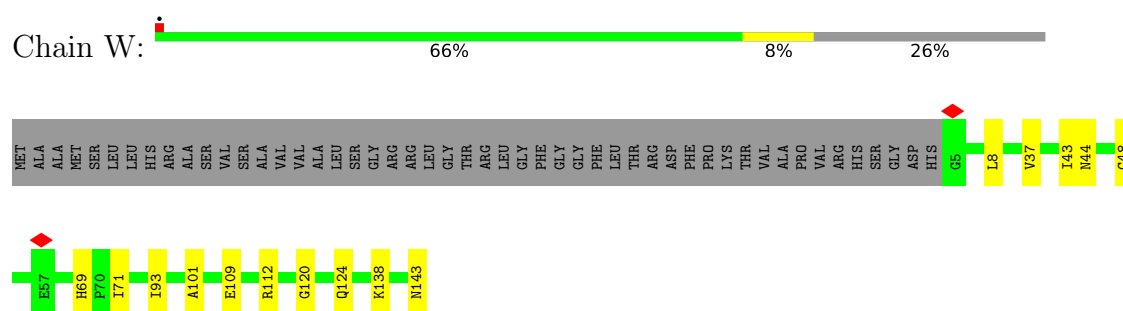
• Molecule 14: NADH-ubiquinone oxidoreductase chain 2



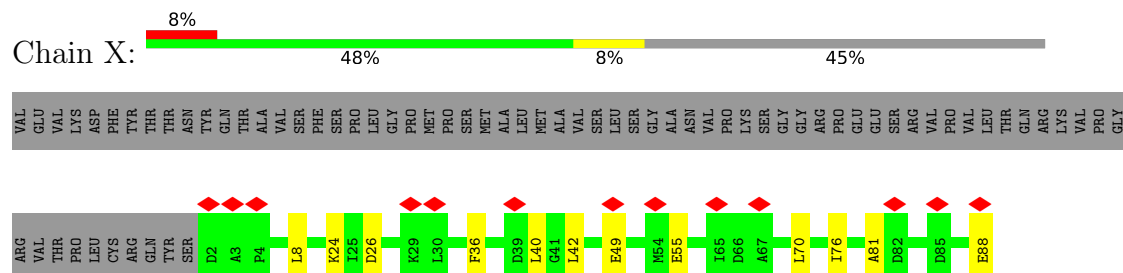
- Molecule 15: Mitochondrial complex I, B14.7 subunit



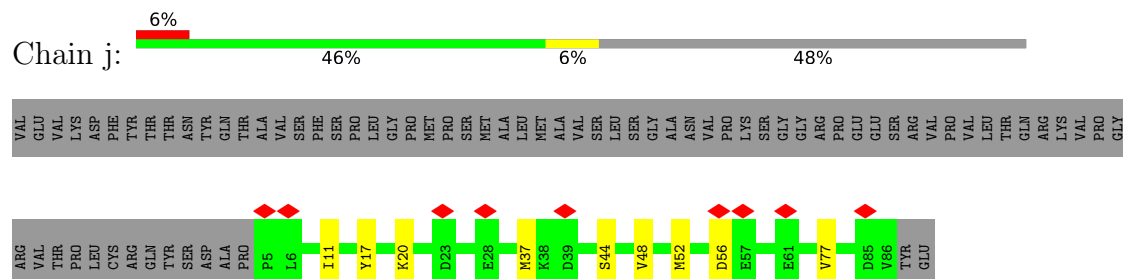
- Molecule 16: NADH:ubiquinone oxidoreductase subunit B5



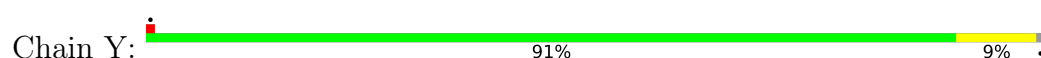
- Molecule 17: Acyl carrier protein

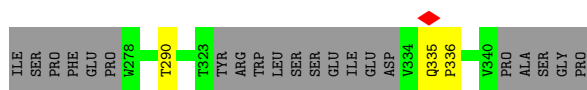


- Molecule 17: Acyl carrier protein



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





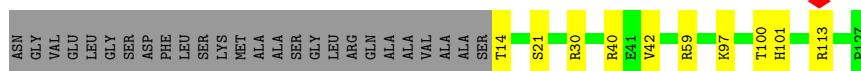
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



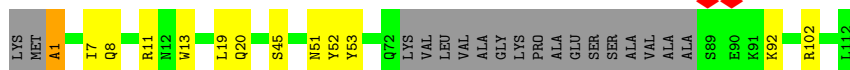
- Molecule 25: Mitochondrial complex I, B13 subunit



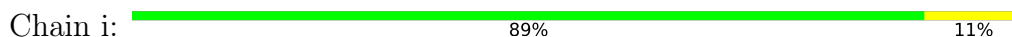
- Molecule 26: NADH:ubiquinone oxidoreductase subunit A6



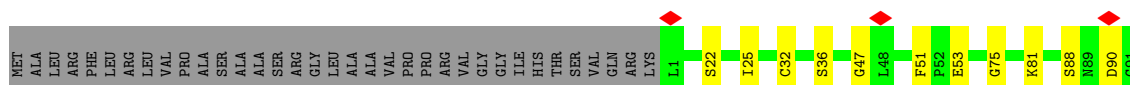
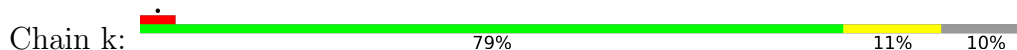
- Molecule 27: Mitochondrial complex I, B14.5a subunit

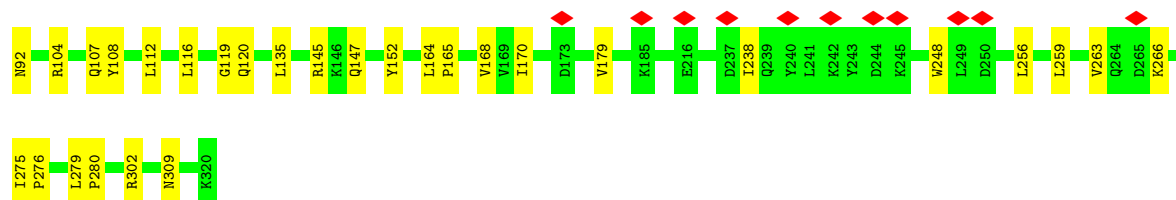


- Molecule 28: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

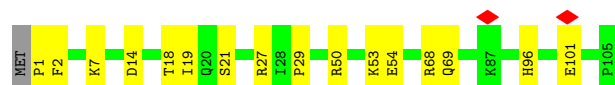
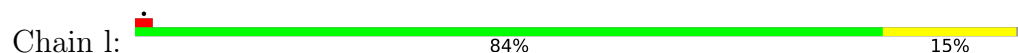


- Molecule 29: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

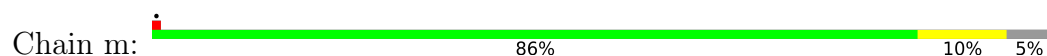




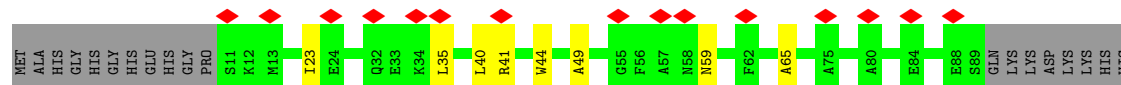
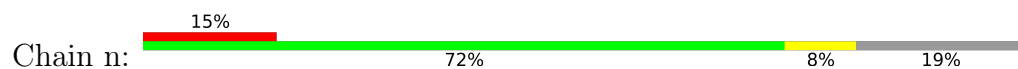
- Molecule 30: NADH:ubiquinone oxidoreductase subunit S5



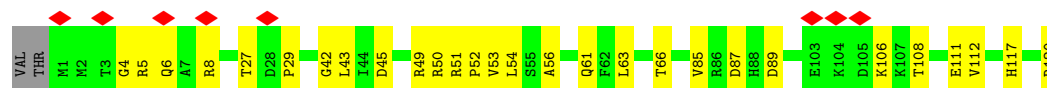
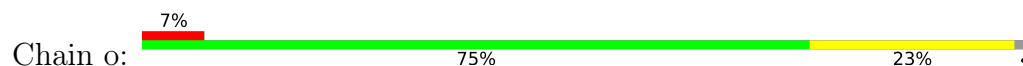
- Molecule 31: NADH:ubiquinone oxidoreductase subunit A3



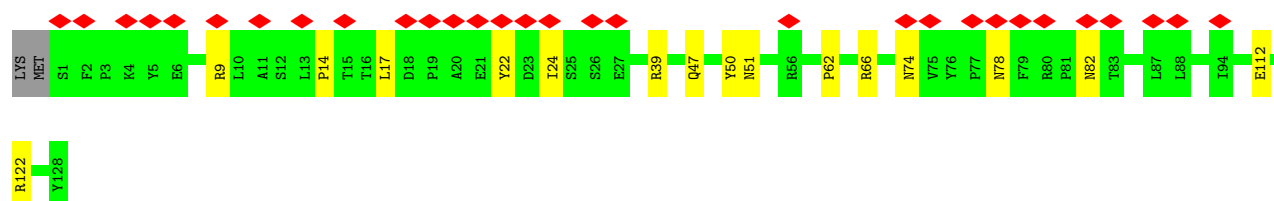
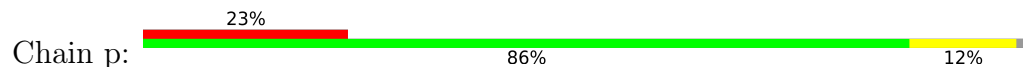
- Molecule 32: NADH:ubiquinone oxidoreductase subunit B3



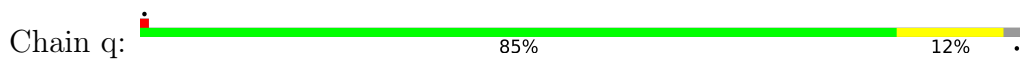
- Molecule 33: NADH dehydrogenase [ubiquinone] 1 subunit C2



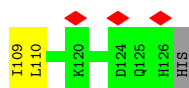
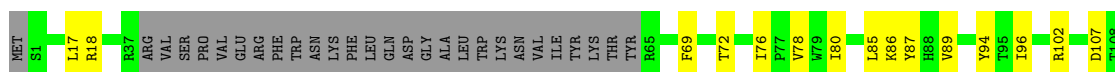
- Molecule 34: NADH:ubiquinone oxidoreductase subunit B4



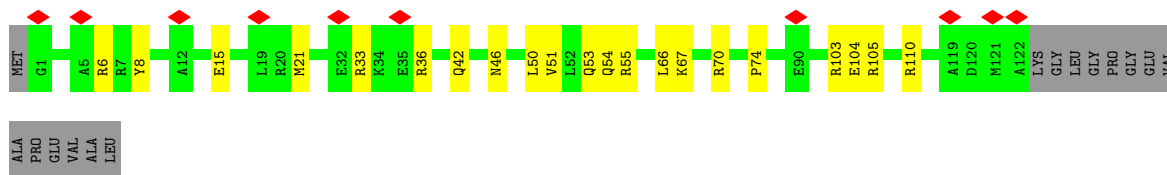
- Molecule 35: Mitochondrial complex I, B16.6 subunit



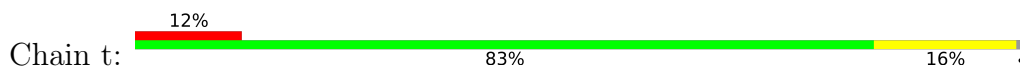
- Molecule 36: Mitochondrial complex I, B17 subunit



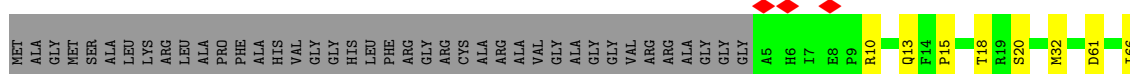
- Molecule 37: NADH:ubiquinone oxidoreductase subunit B7



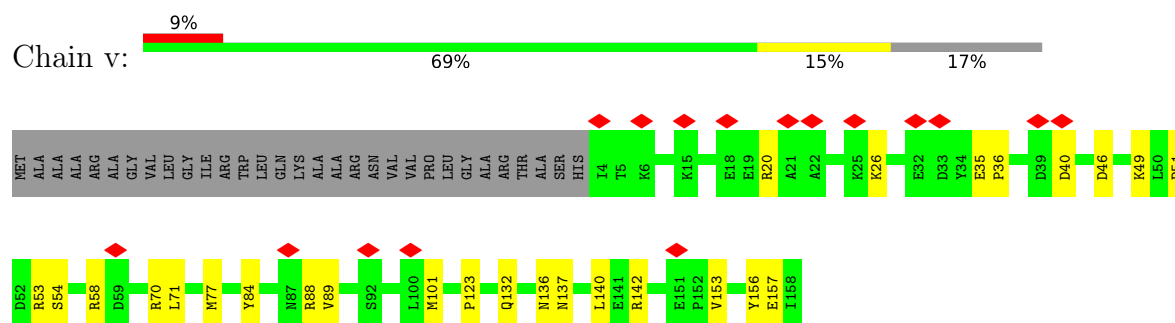
- Molecule 38: NADH:ubiquinone oxidoreductase subunit B9



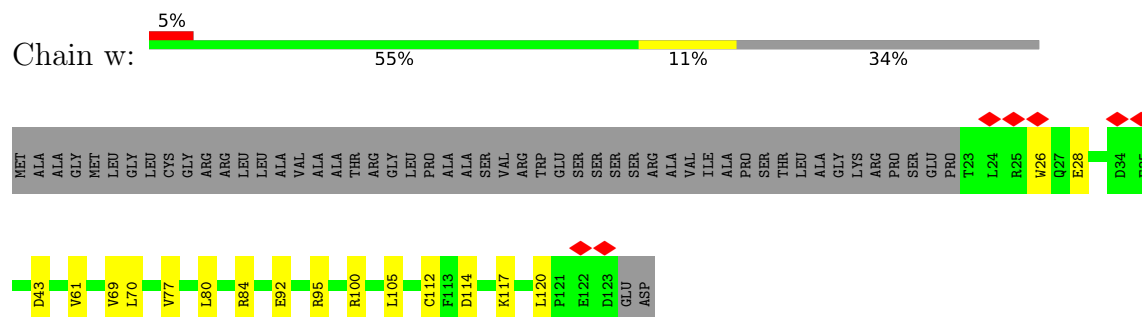
- Molecule 39: NADH:ubiquinone oxidoreductase subunit B2



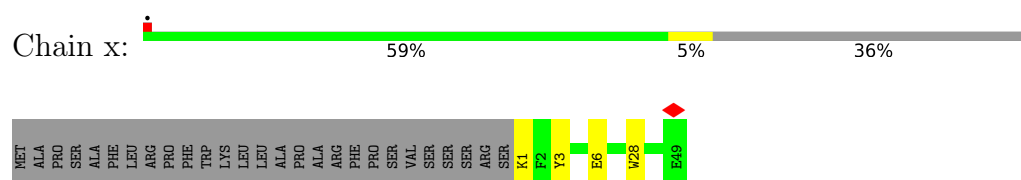
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



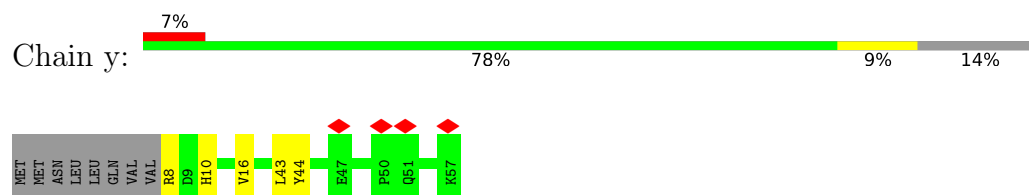
- Molecule 41: Mitochondrial complex I, ESSS subunit



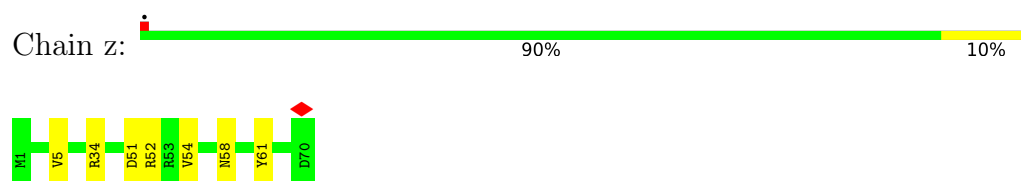
- Molecule 42: Mitochondrial complex I, KFYI subunit



- Molecule 43: Mitochondrial complex I, MNLL subunit



- Molecule 44: Mitochondrial complex I, MWFE subunit



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	21296	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	0.467	Depositor
Minimum map value	-0.150	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.032	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	172.943, 190.98, 289.65298	wwPDB
Map dimensions	273, 180, 163	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: NDP, ZMP, SF4, MYR, ZN, AMP, 2MR, FMN, 970, K, FME, CDL, FES, PC1, SEP, 3PE, AYA, NAI

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1	0.27	0/3386	0.56	0/4575
2	2	0.26	0/1695	0.59	2/2306 (0.1%)
3	3	0.25	0/5362	0.54	3/7266 (0.0%)
4	4	0.28	0/3504	0.53	0/4746
5	5	0.25	0/1776	0.54	0/2417
6	6	0.29	0/1278	0.56	0/1728
7	9	0.28	0/1445	0.56	0/1956
8	A	0.26	0/902	0.63	2/1234 (0.2%)
9	H	0.30	0/2572	0.60	0/3517
10	J	0.26	0/1293	0.57	0/1748
11	K	0.29	0/749	0.58	0/1014
12	L	0.27	0/4924	0.58	0/6698
13	M	0.27	0/3731	0.57	0/5085
14	N	0.29	0/2787	0.57	0/3795
15	V	0.21	0/1041	0.45	0/1412
16	W	0.22	0/1188	0.50	0/1607
17	X	0.19	0/713	0.45	0/963
17	j	0.21	0/670	0.50	0/902
18	Y	0.22	0/1440	0.53	0/1942
19	Z	0.20	0/1475	0.48	0/1989
20	a	0.17	0/383	0.43	0/518
21	b	0.20	0/749	0.45	0/1009
22	c	0.23	0/1047	0.44	0/1415
23	d	0.22	0/2424	0.48	0/3276
24	e	0.20	0/702	0.47	0/945
25	f	0.21	0/937	0.51	0/1271
26	g	0.24	0/993	0.52	0/1336
27	h	0.23	0/779	0.53	0/1053
28	i	0.21	0/1250	0.43	0/1698
29	k	0.19	0/2646	0.44	0/3579
30	l	0.24	0/896	0.56	0/1200

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	m	0.22	0/647	0.48	0/890
32	n	0.19	0/653	0.41	0/882
33	o	0.21	0/1035	0.45	0/1398
34	p	0.18	0/1085	0.48	0/1467
35	q	0.22	0/1171	0.49	0/1579
36	r	0.21	0/874	0.54	0/1188
37	s	0.19	0/1072	0.48	0/1436
38	t	0.19	0/1573	0.54	0/2130
39	u	0.19	0/590	0.46	0/810
40	v	0.19	0/1361	0.48	0/1861
41	w	0.23	0/872	0.51	0/1185
42	x	0.16	0/425	0.38	0/576
43	y	0.21	0/449	0.54	0/605
44	z	0.24	0/591	0.49	0/795
All	All	0.24	0/67135	0.53	7/91002 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	3	0	2
4	4	0	1
8	A	0	2
All	All	0	5

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	338	VAL	N-CA-C	-6.95	106.23	112.90
3	3	366	THR	CA-C-N	5.77	132.56	121.54
3	3	366	THR	C-N-CA	5.77	132.56	121.54
2	2	156	ILE	CA-C-N	5.65	132.34	121.54
2	2	156	ILE	C-N-CA	5.65	132.34	121.54
8	A	112	GLU	CA-C-N	5.01	131.11	121.54
8	A	112	GLU	C-N-CA	5.01	131.11	121.54

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	3	259	ASN	Peptide
3	3	366	THR	Peptide
4	4	275	TYR	Peptide
8	A	113	TRP	Peptide
8	A	29	VAL	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	54	0
2	2	1655	0	1668	23	0
3	3	5275	0	5300	73	0
4	4	3427	0	3365	64	0
5	5	1726	0	1676	24	0
6	6	1247	0	1259	15	0
7	9	1414	0	1370	24	0
8	A	880	0	920	13	0
9	H	2498	0	2609	51	0
10	J	1264	0	1294	22	0
11	K	749	0	793	12	0
12	L	4806	0	4945	82	0
13	M	3647	0	3849	66	0
14	N	2723	0	2930	45	0
15	V	1028	0	1036	16	0
16	W	1155	0	1177	12	0
17	X	701	0	692	9	0
17	j	660	0	663	5	0
18	Y	1403	0	1392	11	0
19	Z	1441	0	1419	17	0
20	a	371	0	344	6	0
21	b	737	0	710	6	0
22	c	1024	0	1023	12	0
23	d	2372	0	2407	18	0
24	e	691	0	706	12	0
25	f	917	0	958	7	0
26	g	969	0	980	8	0
27	h	769	0	780	12	0
28	i	1209	0	1182	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	k	2596	0	2559	22	0
30	l	874	0	869	14	0
31	m	626	0	635	6	0
32	n	634	0	616	6	0
33	o	1004	0	995	22	0
34	p	1059	0	1062	13	0
35	q	1142	0	1137	15	0
36	r	846	0	864	16	0
37	s	1047	0	1015	19	0
38	t	1520	0	1477	23	0
39	u	563	0	509	7	0
40	v	1307	0	1207	18	0
41	w	846	0	792	16	0
42	x	412	0	411	4	0
43	y	436	0	437	5	0
44	z	576	0	570	5	0
45	1	8	0	0	1	0
45	3	16	0	0	1	0
45	6	8	0	0	1	0
45	9	16	0	0	0	0
46	1	31	0	19	2	0
47	1	44	0	27	5	0
48	2	4	0	0	1	0
48	3	4	0	0	0	0
49	3	1	0	0	0	0
50	6	29	0	0	0	0
50	H	29	0	0	0	0
51	6	51	0	82	1	0
51	A	51	0	82	0	0
51	J	51	0	82	3	0
51	K	40	0	54	1	0
51	L	122	0	172	3	0
51	M	44	0	65	2	0
51	N	51	0	82	2	0
51	V	72	0	92	2	0
51	i	51	0	82	1	0
51	l	31	0	36	0	0
51	p	27	0	27	0	0
52	9	54	0	88	2	0
52	A	83	0	117	1	0
52	L	54	0	88	4	0
52	M	54	0	88	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
52	w	54	0	88	4	0
53	L	100	0	156	7	0
53	V	179	0	261	10	0
53	W	100	0	156	8	0
53	Y	100	0	156	7	0
53	i	58	0	60	1	0
53	o	165	0	230	11	0
54	X	31	0	34	1	0
54	g	34	0	40	0	0
55	b	1	0	0	0	0
56	d	48	0	26	1	0
57	k	23	0	12	0	0
58	s	15	0	27	0	0
All	All	67492	0	68400	776	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 6.

All (776) 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)
4:4:50:ASN:HD21	4:4:63:ARG:HH21	1.35	0.71
24:e:19:ARG:HB2	24:e:65:TRP:HB2	1.73	0.69
7:9:43:ARG:HG2	27:h:11:ARG:HD2	1.73	0.69
37:s:33:ARG:HH12	37:s:103:ARG:HH22	1.41	0.67
9:H:237:PHE:O	9:H:241:LEU:HB2	1.94	0.66
4:4:405:MET:SD	4:4:421:GLN:NE2	2.68	0.65
35:q:81:ARG:NH1	35:q:85:MET:SD	2.69	0.65
3:3:118:ASP:OD2	22:c:46:GLN:NE2	2.29	0.65
4:4:377:TYR:HB3	4:4:390:LYS:HB3	1.78	0.64
13:M:158:LEU:HD23	14:N:283:ALA:HB1	1.79	0.64
12:L:241:THR:HG21	12:L:344:GLY:HA3	1.79	0.64
1:1:132:ARG:NH2	20:a:64:PRO:O	2.30	0.63
16:W:69:HIS:HD1	16:W:71:ILE:H	1.46	0.63
7:9:92:ILE:HG12	7:9:111:ILE:HG12	1.81	0.62
4:4:55:HIS:NE2	9:H:204:GLU:OE1	2.33	0.62
17:j:48:VAL:HG12	17:j:52:MET:HE2	1.81	0.62
18:Y:165:ARG:NH1	33:o:87:ASP:OD1	2.32	0.62
7:9:145:GLU:HA	7:9:148:LEU:HD13	1.82	0.61
9:H:141:SER:HB3	9:H:289:LEU:HD22	1.81	0.61
11:K:73:LEU:HD11	14:N:41:ILE:HG13	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:V:11:ILE:HB	15:V:20:LYS:HD3	1.82	0.61
18:Y:89:ASP:OD2	44:z:34:ARG:NH1	2.33	0.61
44:z:52:ARG:NH1	44:z:58:ASN:OD1	2.33	0.61
1:1:101:GLU:HB2	47:1:503:NAI:H42N	1.82	0.61
4:4:233:ARG:NH2	7:9:23:GLN:O	2.32	0.61
15:V:4:LEU:HD13	15:V:7:GLN:HE21	1.66	0.61
38:t:153:LEU:HD11	38:t:165:LEU:HD12	1.83	0.61
13:M:133:ILE:HD11	13:M:231:LEU:HD11	1.82	0.60
28:i:34:ARG:NH2	28:i:58:ARG:O	2.34	0.60
13:M:7:PRO:HB3	43:y:16:VAL:HG13	1.83	0.60
10:J:40:GLY:HA2	10:J:43:ILE:HD12	1.83	0.60
4:4:2:ARG:O	13:M:138:ASN:ND2	2.35	0.60
14:N:45:MET:HE3	14:N:53:THR:HG22	1.84	0.60
53:Y:201:CDL:H632	53:Y:201:CDL:H571	1.84	0.60
12:L:103:PHE:HB2	12:L:341:MET:HE3	1.83	0.59
12:L:145:GLU:OE2	12:L:176:ARG:NH1	2.34	0.59
24:e:13:LEU:HD22	24:e:16:ARG:HH22	1.66	0.59
3:3:127:ARG:NH2	4:4:326:ASP:O	2.35	0.59
6:6:44:SER:O	9:H:54:LYS:NZ	2.35	0.59
3:3:252:PRO:HG3	3:3:263:ILE:HG12	1.84	0.59
2:2:149:VAL:O	2:2:190:ARG:NH2	2.35	0.59
11:K:23:ARG:HG2	51:K:101:3PE:H11	1.85	0.59
3:3:126:ASP:HB2	4:4:328:ALA:HB3	1.84	0.59
12:L:106:TRP:HD1	12:L:447:ASN:HD22	1.50	0.59
53:L:704:CDL:H631	13:M:445:LEU:HD22	1.84	0.59
3:3:632:ARG:NH1	24:e:57:CYS:SG	2.76	0.59
3:3:332:LYS:NZ	3:3:505:LEU:O	2.36	0.59
2:2:159:ASN:HB3	2:2:184:PRO:HB3	1.85	0.58
13:M:54:LEU:HD23	16:W:93:ILE:HG23	1.86	0.58
37:s:6:ARG:HH12	37:s:105:ARG:HD2	1.68	0.58
3:3:193:SER:H	3:3:196:SER:HB3	1.68	0.58
52:L:703:PC1:H372	53:W:201:CDL:H512	1.85	0.58
22:c:42:ARG:NH1	22:c:46:GLN:O	2.36	0.58
23:d:167:LYS:HB2	23:d:229:ALA:HA	1.86	0.58
36:r:85:LEU:HD22	36:r:96:ILE:HD11	1.86	0.58
5:5:151:ILE:HG23	5:5:152:LEU:HG	1.86	0.58
12:L:184:LEU:HD13	13:M:393:ILE:HG21	1.85	0.58
40:v:20:ARG:HH12	40:v:36:PRO:HD3	1.68	0.58
24:e:23:CYS:SG	24:e:24:GLN:N	2.76	0.58
1:1:21:ILE:O	1:1:117:LYS:NZ	2.36	0.58
38:t:100:GLU:O	38:t:121:ARG:NH1	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:p:39:ARG:NH2	38:t:3:LEU:O	2.37	0.58
4:4:183:ARG:NH1	4:4:210:ASP:OD2	2.37	0.57
1:1:428:GLU:HA	1:1:431:GLN:HG2	1.87	0.57
1:1:403:THR:HG21	1:1:408:GLY:HA3	1.86	0.57
14:N:207:ILE:HG22	14:N:211:MET:HE2	1.86	0.57
21:b:32:GLN:HE22	21:b:34:GLU:HB2	1.70	0.57
51:6:503:3PE:H2G2	52:A:401:PC1:H3H2	1.87	0.57
25:f:34:LEU:HD12	25:f:37:ILE:HD12	1.86	0.57
2:2:150:ASN:HB3	2:2:162:GLU:HB3	1.86	0.57
25:f:37:ILE:O	25:f:44:ARG:NH1	2.38	0.57
28:i:78:ASP:HB3	28:i:81:MET:HG3	1.87	0.57
12:L:161:ARG:NH2	38:t:90:TYR:O	2.37	0.56
4:4:388:ARG:HG2	5:5:81:VAL:HG22	1.86	0.56
6:6:118:SER:N	45:6:502:SF4:S4	2.78	0.56
2:2:74:GLN:O	20:a:74:ARG:NH2	2.38	0.56
5:5:65:ARG:NH1	5:5:123:VAL:O	2.39	0.56
9:H:26:LYS:HB3	44:z:5:VAL:HG12	1.86	0.56
53:L:704:CDL:H391	53:L:704:CDL:H171	1.88	0.56
53:Y:201:CDL:H122	53:Y:201:CDL:H671	1.87	0.56
34:p:82:ASN:ND2	40:v:40:ASP:O	2.38	0.56
23:d:72:ASP:O	23:d:83:ARG:NH2	2.38	0.56
24:e:17:GLU:OE2	24:e:19:ARG:NH1	2.38	0.56
37:s:36:ARG:NH1	40:v:132:GLN:OE1	2.38	0.56
3:3:140:LYS:HB2	3:3:148:THR:HG21	1.88	0.56
4:4:269:LEU:HB2	4:4:368:GLU:HB2	1.87	0.56
3:3:276:ARG:HA	28:i:135:GLN:HB2	1.87	0.56
6:6:171:LYS:HG2	6:6:174:ARG:HH11	1.70	0.56
1:1:184:TYR:HB3	1:1:357:GLU:HB3	1.88	0.56
9:H:149:ILE:HG21	9:H:185:TRP:HB2	1.88	0.56
29:k:51:PHE:HB3	29:k:107:GLN:HE21	1.70	0.56
34:p:47:GLN:HA	34:p:50:TYR:HB3	1.86	0.56
13:M:155:ALA:HB1	52:M:502:PC1:H2H2	1.87	0.56
18:Y:63:ASN:OD1	35:q:80:ARG:NH2	2.39	0.56
27:h:11:ARG:NH2	27:h:20:GLN:OE1	2.39	0.56
7:9:69:ARG:NH1	7:9:73:GLY:O	2.39	0.56
12:L:9:LEU:HD11	12:L:63:ILE:HG21	1.88	0.56
1:1:200:GLN:NE2	3:3:174:THR:O	2.39	0.56
9:H:46:LEU:HD21	51:i:201:3PE:H361	1.87	0.56
12:L:370:THR:HG23	12:L:431:LEU:HD13	1.88	0.56
2:2:53:LEU:HD12	20:a:52:LEU:HD13	1.88	0.55
12:L:69:LEU:HD23	12:L:76:LEU:HD12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:309:ASN:ND2	29:k:75:GLY:O	2.35	0.55
27:h:45:SER:O	27:h:51:ASN:ND2	2.37	0.55
1:1:243:ALA:HA	1:1:251:SER:HB3	1.88	0.55
3:3:274:LEU:O	3:3:278:ARG:NH1	2.38	0.55
4:4:354:GLU:OE2	4:4:357:GLN:NE2	2.39	0.55
9:H:14:LEU:HD22	9:H:225:MET:HE2	1.88	0.55
1:1:142:PHE:HB3	1:1:145:GLU:HB2	1.88	0.55
9:H:312:SER:HB3	35:q:54:ARG:HH21	1.70	0.55
12:L:453:SER:HA	12:L:456:ARG:HH21	1.70	0.55
23:d:138:ASP:HB3	23:d:141:SER:HB2	1.87	0.55
3:3:382:THR:HB	3:3:454:GLY:HA3	1.87	0.55
9:H:165:LEU:HD21	9:H:241:LEU:HA	1.87	0.55
16:W:124:GLN:HB2	33:o:4:GLY:HA3	1.88	0.55
13:M:343:ILE:O	13:M:346:ARG:NH1	2.40	0.55
13:M:41:LEU:HD13	13:M:66:LEU:HD13	1.88	0.55
53:Y:201:CDL:H432	33:o:27:THR:HG21	1.89	0.55
37:s:50:LEU:HB2	37:s:55:ARG:HE	1.72	0.55
4:4:61:VAL:HG21	4:4:83:LEU:HB2	1.89	0.55
9:H:10:ILE:HA	9:H:13:ILE:HD12	1.89	0.55
12:L:268:GLU:OE1	37:s:53:GLN:NE2	2.40	0.55
18:Y:35:CYS:O	18:Y:39:ASN:ND2	2.40	0.55
3:3:198:ASN:OD1	3:3:268:ARG:NH2	2.35	0.55
12:L:432:LEU:HD21	32:n:65:ALA:HB2	1.89	0.55
41:w:26:TRP:NE1	41:w:28:GLU:OE1	2.31	0.55
3:3:190:MET:HG2	3:3:192:MET:HG2	1.88	0.54
4:4:3:GLN:NE2	13:M:135:ARG:O	2.41	0.54
29:k:108:TYR:OH	29:k:164:LEU:O	2.24	0.54
6:6:169:ARG:NH2	7:9:142:GLU:OE2	2.40	0.54
19:Z:15:ARG:HB3	36:r:109:ILE:HD12	1.88	0.54
34:p:47:GLN:HG3	38:t:165:LEU:HD13	1.88	0.54
3:3:65:VAL:HG13	3:3:85:LYS:HE2	1.90	0.54
3:3:601:ARG:NH2	3:3:614:ASP:OD1	2.39	0.54
29:k:25:ILE:HG12	29:k:168:VAL:HB	1.90	0.54
14:N:243:LEU:HD22	14:N:330:THR:HG21	1.90	0.54
36:r:72:THR:HA	36:r:76:ILE:HD12	1.89	0.54
40:v:137:ASN:O	40:v:142:ARG:NH1	2.40	0.54
5:5:28:TYR:OH	5:5:67:HIS:NE2	2.38	0.54
13:M:447:LEU:HD11	52:w:801:PC1:H3F1	1.88	0.54
3:3:201:ASP:OD2	3:3:268:ARG:NH2	2.36	0.54
12:L:446:ASN:ND2	39:u:18:THR:OG1	2.41	0.54
24:e:41:VAL:HG12	24:e:45:LYS:HE2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:35:ASP:O	14:N:49:ASN:ND2	2.41	0.54
12:L:510:TYR:O	38:t:35:LYS:NZ	2.39	0.54
13:M:70:MET:HG2	13:M:103:GLN:HE21	1.71	0.54
15:V:1:AYA:HA	15:V:4:LEU:HD23	1.90	0.54
25:f:69:GLU:HG3	27:h:102:ARG:HH12	1.73	0.54
29:k:145:ARG:NH1	29:k:147:GLN:OE1	2.40	0.54
34:p:62:PRO:O	34:p:66:ARG:HB2	2.08	0.54
4:4:138:ARG:NH2	4:4:195:ARG:O	2.41	0.53
19:Z:140:ASP:O	19:Z:161:ARG:NH1	2.40	0.53
22:c:28:GLU:O	22:c:32:THR:OG1	2.26	0.53
3:3:329:ILE:HD13	3:3:505:LEU:HD22	1.88	0.53
3:3:673:MET:HB3	3:3:679:ARG:HG2	1.90	0.53
12:L:97:THR:HG21	12:L:125:LEU:HD22	1.91	0.53
25:f:49:GLN:HE22	27:h:92:LYS:HA	1.73	0.53
9:H:24:GLU:OE2	9:H:274:ARG:NH1	2.41	0.53
12:L:106:TRP:CD1	12:L:447:ASN:HD22	2.26	0.53
17:X:36:PHE:O	17:X:42:LEU:N	2.40	0.53
33:o:66:THR:OG1	42:x:28:TRP:NE1	2.41	0.53
4:4:110:SER:OG	4:4:149:ASN:ND2	2.42	0.53
5:5:33:LEU:HD13	5:5:60:VAL:HG22	1.90	0.53
5:5:82:ASP:OD2	5:5:89:ARG:NH2	2.39	0.53
53:V:203:CDL:H511	53:V:204:CDL:H151	1.90	0.53
3:3:12:PHE:HB2	3:3:78:ASN:HA	1.91	0.53
12:L:137:LEU:H	12:L:196:TRP:HB3	1.74	0.53
5:5:74:SER:HB3	5:5:97:LEU:HB3	1.91	0.53
39:u:18:THR:HG22	39:u:20:SER:H	1.73	0.53
1:1:298:ILE:HB	1:1:335:ILE:HB	1.89	0.53
1:1:356:HIS:O	3:3:177:ARG:NH2	2.42	0.53
5:5:32:ILE:HG23	25:f:43:TYR:HB2	1.90	0.53
13:M:64:PRO:HB3	13:M:454:ILE:HG22	1.90	0.53
53:W:201:CDL:H341	53:W:201:CDL:H511	1.91	0.53
1:1:96:ASN:ND2	46:1:502:FMN:O4'	2.42	0.53
2:2:105:THR:OG1	48:2:300:FES:S2	2.67	0.53
17:j:17:TYR:HA	17:j:20:LYS:HG2	1.91	0.53
13:M:42:LEU:HD13	41:w:80:LEU:HD11	1.91	0.53
37:s:51:VAL:HG12	37:s:53:GLN:H	1.74	0.53
3:3:515:ARG:NH2	3:3:531:CYS:O	2.43	0.52
41:w:114:ASP:HB3	41:w:117:LYS:HG2	1.90	0.52
3:3:261:GLU:OE1	22:c:42:ARG:NH2	2.42	0.52
4:4:391:ILE:O	4:4:430:ARG:NH1	2.43	0.52
12:L:561:ILE:HB	53:V:204:CDL:H801	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:W:44:ASN:ND2	53:W:201:CDL:OB4	2.41	0.52
23:d:26:ALA:HA	23:d:31:GLY:HA3	1.90	0.52
41:w:92:GLU:OE2	41:w:95:ARG:NH2	2.40	0.52
1:1:144:ASN:O	1:1:148:ASN:HB2	2.09	0.52
1:1:358:SER:OG	1:1:365:CYS:SG	2.66	0.52
3:3:194:GLU:HG3	3:3:389:PRO:HB3	1.90	0.52
5:5:77:ASP:OD2	5:5:79:THR:OG1	2.27	0.52
13:M:167:ILE:HD13	13:M:249:LEU:HD13	1.91	0.52
17:X:24:LYS:HG2	32:n:41:ARG:HH22	1.75	0.52
1:1:291:TRP:NE1	1:1:313:GLU:OE1	2.42	0.52
4:4:84:HIS:NE2	6:6:130:TYR:OH	2.39	0.52
13:M:459:TYR:H	41:w:84:ARG:HH22	1.58	0.52
1:1:84:LYS:HZ1	1:1:219:PRO:HB3	1.74	0.52
1:1:289:GLY:HA3	1:1:293:ASN:HD22	1.75	0.52
12:L:231:PRO:HB3	12:L:530:PRO:HG3	1.91	0.52
1:1:288:THR:O	1:1:293:ASN:ND2	2.43	0.52
4:4:343:GLU:O	4:4:347:HIS:ND1	2.39	0.52
9:H:64:ALA:O	9:H:124:ASN:ND2	2.41	0.52
13:M:277:LEU:O	40:v:88:ARG:NH2	2.36	0.52
40:v:51:PRO:O	40:v:53:ARG:NH1	2.43	0.52
4:4:412:ALA:HB3	9:H:281:ARG:HG3	1.92	0.52
14:N:140:SER:HA	30:l:1:PRO:HD2	1.92	0.52
25:f:5:LYS:NZ	25:f:68:GLU:OE2	2.39	0.52
38:t:30:CYS:HB3	38:t:35:LYS:HD3	1.91	0.52
40:v:136:ASN:HA	40:v:153:VAL:HB	1.91	0.52
4:4:101:PRO:O	4:4:105:ARG:NH1	2.42	0.51
7:9:108:ARG:NH1	22:c:70:MET:O	2.38	0.51
12:L:69:LEU:HD13	13:M:451:PRO:HG2	1.91	0.51
3:3:569:LYS:HG3	3:3:571:ALA:HB2	1.92	0.51
14:N:30:TRP:NE1	14:N:67:SER:OG	2.42	0.51
1:1:140:GLY:O	1:1:179:ARG:NH2	2.43	0.51
14:N:242:ILE:HG21	53:o:202:CDL:H562	1.92	0.51
41:w:100:ARG:HB2	41:w:105:LEU:HB2	1.93	0.51
12:L:316:THR:HA	12:L:319:ILE:HG12	1.91	0.51
51:L:701:3PE:O32	13:M:144:ASN:ND2	2.43	0.51
36:r:18:ARG:NH1	38:t:170:VAL:O	2.38	0.51
38:t:137:LYS:HA	38:t:140:GLN:HG2	1.92	0.51
1:1:355:LYS:HD3	1:1:373:ASN:HD22	1.76	0.51
4:4:149:ASN:HD21	4:4:371:LYS:HG3	1.76	0.51
12:L:520:PHE:O	12:L:524:ASN:HB2	2.11	0.51
12:L:539:TYR:OH	34:p:9:ARG:NH2	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:o:201:CDL:H191	53:o:201:CDL:H762	1.93	0.51
4:4:430:ARG:NH2	5:5:133:GLU:OE2	2.44	0.51
8:A:74:PRO:HG2	10:J:147:TYR:HE2	1.76	0.51
52:M:502:PC1:H251	52:M:502:PC1:H372	1.92	0.51
24:e:64:LEU:HB3	24:e:76:VAL:HB	1.92	0.51
12:L:13:ILE:HD11	53:W:201:CDL:H622	1.93	0.51
12:L:421:ILE:HG12	12:L:501:ALA:HB2	1.92	0.51
13:M:24:TRP:HE1	13:M:92:LYS:HD3	1.75	0.51
13:M:328:CYS:HB3	13:M:437:MET:HE1	1.92	0.51
30:l:68:ARG:NH2	35:q:119:MET:SD	2.84	0.51
37:s:33:ARG:NE	40:v:157:GLU:O	2.44	0.51
3:3:632:ARG:HH12	24:e:59:ASP:H	1.57	0.51
53:o:202:CDL:H352	53:o:202:CDL:H612	1.92	0.51
39:u:10:ARG:HD2	39:u:15:PRO:HA	1.92	0.51
3:3:163:ALA:HA	3:3:167:ALA:HB3	1.94	0.51
3:3:206:GLY:N	45:3:801:SF4:S2	2.83	0.51
4:4:323:ILE:HD12	4:4:324:LYS:HG3	1.93	0.51
5:5:119:SER:OG	5:5:131:GLU:OE2	2.25	0.51
19:Z:3:SER:OG	19:Z:4:TRP:N	2.44	0.51
5:5:94:TYR:HB2	5:5:107:VAL:HB	1.92	0.50
12:L:245:ALA:O	12:L:249:SER:OG	2.28	0.50
12:L:570:GLN:OE1	14:N:167:TRP:NE1	2.44	0.50
3:3:512:GLU:O	3:3:516:LYS:HB2	2.11	0.50
18:Y:43:MET:HE3	18:Y:47:TRP:HZ3	1.75	0.50
29:k:263:VAL:O	29:k:266:LYS:NZ	2.43	0.50
29:k:53:GLU:HG3	29:k:104:ARG:HH12	1.76	0.50
3:3:364:LEU:HD12	3:3:491:ASN:HB3	1.93	0.50
4:4:282:GLU:HB3	4:4:313:GLN:HE22	1.77	0.50
26:g:42:VAL:HG11	26:g:59:ARG:HG3	1.92	0.50
33:o:6:GLN:HE22	33:o:85:VAL:HG11	1.77	0.50
37:s:6:ARG:NH1	37:s:15:GLU:OE2	2.45	0.50
3:3:27:LEU:HA	3:3:37:ILE:HD12	1.94	0.50
6:6:107:MET:O	6:6:111:ARG:NH1	2.44	0.50
1:1:95:VAL:HG11	1:1:118:LEU:HD11	1.93	0.50
3:3:175:THR:HG21	3:3:186:TYR:HB2	1.94	0.50
12:L:139:GLN:HA	12:L:142:ILE:HD12	1.93	0.50
15:V:84:ASP:HB2	15:V:129:LEU:HD21	1.93	0.50
29:k:112:LEU:HD13	29:k:259:LEU:HD21	1.94	0.50
9:H:85:MET:HG3	9:H:233:MET:HE2	1.93	0.50
14:N:335:MET:HG2	53:o:202:CDL:H661	1.94	0.50
16:W:120:GLY:O	16:W:124:GLN:NE2	2.39	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:v:26:LYS:NZ	40:v:46:ASP:OD2	2.44	0.50
40:v:71:LEU:HD21	40:v:77:MET:HG2	1.93	0.50
1:1:154:ARG:HA	20:a:58:LEU:HD21	1.93	0.49
12:L:433:GLY:O	32:n:59:ASN:ND2	2.39	0.49
12:L:536:LEU:HG	12:L:540:MET:HE2	1.94	0.49
19:Z:41:ASP:OD1	36:r:86:LYS:NZ	2.37	0.49
1:1:118:LEU:HD13	1:1:225:VAL:HG13	1.93	0.49
4:4:335:ARG:NH2	7:9:129:ASP:OD1	2.46	0.49
9:H:79:LEU:HD11	9:H:222:LEU:HD22	1.94	0.49
16:W:138:LYS:HA	30:l:27:ARG:HB3	1.94	0.49
17:X:55:GLU:OE1	38:t:24:ARG:NH2	2.45	0.49
53:Y:201:CDL:H312	33:o:29:PRO:HB3	1.93	0.49
36:r:102:ARG:O	37:s:70:ARG:NH1	2.45	0.49
1:1:189:GLU:OE2	47:1:503:NAI:O2B	2.30	0.49
2:2:183:LYS:O	2:2:187:ARG:NH1	2.45	0.49
6:6:86:MET:HE1	6:6:140:VAL:HG11	1.95	0.49
10:J:103:MET:HE3	10:J:115:ILE:HG13	1.95	0.49
12:L:144:TRP:NE1	12:L:179:ASP:OD1	2.43	0.49
19:Z:68:ARG:NH1	43:y:43:LEU:O	2.45	0.49
3:3:360:SER:O	3:3:365:ASN:ND2	2.30	0.49
3:3:582:GLN:OE1	3:3:620:ARG:NH1	2.46	0.49
8:A:90:MET:HE1	10:J:155:ILE:HG13	1.95	0.49
14:N:44:MET:HE2	14:N:130:LEU:HD12	1.95	0.49
14:N:211:MET:HG2	14:N:333:SER:HB2	1.93	0.49
21:b:19:ASP:HB2	21:b:22:ASP:HB2	1.94	0.49
4:4:233:ARG:NH1	52:9:401:PC1:O12	2.46	0.49
5:5:137:MET:HA	5:5:161:PRO:HD2	1.95	0.49
4:4:406:SER:HB2	4:4:414:VAL:HG22	1.94	0.49
10:J:163:ILE:HG21	14:N:12:THR:HG21	1.94	0.49
14:N:106:LEU:HD22	14:N:187:MET:HE2	1.94	0.49
29:k:170:ILE:HD11	29:k:238:ILE:HD11	1.95	0.49
38:t:107:HIS:NE2	41:w:43:ASP:OD1	2.38	0.49
3:3:36:GLN:NE2	22:c:47:SER:O	2.37	0.49
13:M:243:MET:HB3	13:M:301:ILE:HG21	1.94	0.49
52:M:502:PC1:H272	51:V:202:3PE:H392	1.95	0.49
1:1:247:ARG:HH22	1:1:320:ASP:HB2	1.78	0.49
4:4:200:HIS:NE2	7:9:124:GLU:OE1	2.45	0.49
8:A:84:LEU:HD11	31:m:45:ASN:HD22	1.77	0.49
37:s:21:MET:HE2	37:s:104:GLU:HG3	1.94	0.49
3:3:574:VAL:HG21	3:3:630:LEU:HD22	1.95	0.48
2:2:175:GLU:HG3	2:2:182:PRO:HG3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:196:ALA:HB3	9:H:274:ARG:HB2	1.94	0.48
11:K:1:FME:HCN	30:l:69:GLN:HG2	1.94	0.48
8:A:67:LEU:HD22	11:K:65:VAL:HA	1.95	0.48
14:N:222:ASN:HD21	14:N:240:MET:HB3	1.79	0.48
15:V:61:THR:HG23	15:V:103:ARG:HG3	1.95	0.48
3:3:382:THR:HG23	3:3:384:PRO:HD3	1.96	0.48
12:L:40:ILE:HD11	12:L:122:LEU:HD13	1.95	0.48
12:L:416:THR:O	12:L:419:THR:OG1	2.31	0.48
53:L:704:CDL:H473	53:W:201:CDL:H741	1.95	0.48
1:1:194:GLU:OE2	1:1:204:ARG:NE	2.35	0.48
29:k:309:ASN:HD22	42:x:3:TYR:HH	1.55	0.48
34:p:14:PRO:HD2	34:p:17:LEU:HD12	1.96	0.48
3:3:453:LEU:HB2	3:3:470:VAL:HG11	1.96	0.48
5:5:154:ASP:OD1	26:g:101:HIS:NE2	2.44	0.48
12:L:593:ILE:HD12	15:V:41:ALA:HB2	1.96	0.48
13:M:204:MET:HE1	13:M:302:LEU:HD11	1.96	0.48
14:N:46:LYS:NZ	51:N:401:3PE:O12	2.41	0.48
23:d:91:VAL:HG23	23:d:126:VAL:HG11	1.95	0.48
33:o:45:ASP:OD1	33:o:49:ARG:NH2	2.47	0.48
2:2:172:ILE:HG23	2:2:182:PRO:HG2	1.96	0.48
5:5:77:ASP:HB3	5:5:95:ASN:HB2	1.95	0.48
7:9:108:ARG:NH2	28:i:128:SER:OG	2.45	0.48
12:L:172:ILE:HG21	13:M:408:LEU:HD12	1.96	0.48
12:L:474:PRO:HD2	37:s:66:LEU:HD21	1.96	0.48
13:M:282:LEU:HD21	13:M:359:TRP:HH2	1.79	0.48
13:M:426:ILE:HB	38:t:101:TRP:HH2	1.78	0.48
27:h:11:ARG:HG2	27:h:19:LEU:HD12	1.96	0.48
4:4:141:PHE:O	4:4:145:THR:OG1	2.32	0.48
6:6:46:TRP:H	6:6:84:ASP:HB2	1.77	0.48
23:d:200:THR:HB	23:d:238:LEU:HB2	1.96	0.48
30:l:7:LYS:NZ	33:o:8:ARG:O	2.42	0.48
34:p:51:ASN:OD1	38:t:168:HIS:ND1	2.40	0.48
1:1:193:ILE:HG23	1:1:215:VAL:HA	1.96	0.48
28:i:44:TYR:OH	28:i:113:HIS:N	2.47	0.48
29:k:32:CYS:HB2	29:k:179:VAL:HG13	1.95	0.48
1:1:139:ARG:NE	1:1:141:GLU:OE1	2.40	0.47
12:L:80:PHE:HB3	12:L:82:MET:HE3	1.96	0.47
15:V:94:CYS:HA	15:V:114:CYS:HA	1.96	0.47
19:Z:159:LYS:NZ	33:o:112:VAL:O	2.46	0.47
37:s:8:TYR:OH	40:v:123:PRO:O	2.26	0.47
40:v:35:GLU:HG3	40:v:49:LYS:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:v:58:ARG:HB2	40:v:70:ARG:HD3	1.96	0.47
3:3:159:CYS:HB3	3:3:172:LEU:HD13	1.96	0.47
4:4:106:LEU:HD13	4:4:391:ILE:HG21	1.95	0.47
13:M:325:MET:HE3	13:M:437:MET:HB3	1.95	0.47
35:q:92:GLU:HA	35:q:95:THR:HG22	1.95	0.47
38:t:169:ILE:O	38:t:172:ARG:NH1	2.45	0.47
3:3:199:ILE:HD12	3:3:208:LEU:HD13	1.95	0.47
10:J:5:ILE:HG21	35:q:141:TRP:HZ2	1.79	0.47
11:K:20:LEU:HB3	12:L:592:LEU:HB2	1.96	0.47
14:N:115:VAL:HG12	14:N:180:ALA:HB1	1.96	0.47
12:L:538:PRO:HB2	40:v:89:VAL:HG22	1.97	0.47
13:M:232:ALA:O	13:M:237:LYS:NZ	2.48	0.47
3:3:371:VAL:HG22	3:3:450:MET:HE1	1.95	0.47
13:M:119:TYR:HE1	13:M:157:SER:HB2	1.79	0.47
23:d:52:GLU:HG3	23:d:54:TYR:H	1.79	0.47
1:1:42:TRP:HE1	1:1:116:HIS:HB3	1.80	0.47
3:3:231:MET:HB3	3:3:266:LYS:HD2	1.95	0.47
4:4:49:LEU:O	4:4:66:MET:N	2.46	0.47
15:V:35:VAL:HG22	53:V:203:CDL:H342	1.95	0.47
23:d:27:THR:HG1	56:d:401:NDP:HO3A	1.56	0.47
4:4:179:GLU:OE2	6:6:66:ARG:NH1	2.33	0.47
7:9:69:ARG:HH12	21:b:40:ALA:HB2	1.80	0.47
9:H:1:MET:HA	9:H:4:ILE:HD12	1.96	0.47
11:K:20:LEU:HD13	12:L:588:PHE:HD1	1.79	0.47
12:L:180:ILE:HD13	51:L:702:3PE:H2H2	1.96	0.47
13:M:101:LEU:HD21	53:o:202:CDL:H841	1.97	0.47
13:M:116:ILE:HD11	13:M:161:LEU:HD12	1.95	0.47
13:M:348:LEU:HD23	13:M:351:LEU:HD12	1.95	0.47
14:N:261:MET:HG3	14:N:340:THR:HG23	1.97	0.47
53:V:203:CDL:H202	53:V:203:CDL:H372	1.97	0.47
19:Z:136:LYS:NZ	19:Z:140:ASP:OD2	2.44	0.47
22:c:57:MET:HB3	22:c:84:LEU:HB2	1.97	0.47
34:p:22:TYR:HE1	38:t:63:LEU:HD23	1.80	0.47
4:4:174:ARG:HH12	6:6:57:VAL:HG13	1.80	0.47
12:L:161:ARG:HA	38:t:91:GLU:HG3	1.96	0.47
13:M:18:SER:HB2	13:M:23:ILE:HG22	1.96	0.47
15:V:109:ILE:HG23	53:V:204:CDL:H331	1.96	0.47
4:4:154:VAL:HG13	4:4:297:TYR:HE1	1.80	0.47
4:4:296:ARG:HH21	4:4:420:THR:HG21	1.80	0.47
18:Y:48:GLU:OE1	31:m:57:ARG:NH2	2.41	0.47
5:5:150:ARG:NH1	5:5:153:THR:OG1	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:L:704:CDL:H202	41:w:70:LEU:HD23	1.95	0.47
14:N:25:HIS:HB3	14:N:28:LEU:HD23	1.97	0.47
19:Z:10:PRO:O	36:r:94:TYR:OH	2.31	0.47
22:c:33:ARG:NH1	22:c:77:ASP:OD1	2.48	0.47
2:2:40:GLU:HB2	20:a:67:SER:HA	1.96	0.46
9:H:169:GLN:NE2	9:H:241:LEU:O	2.45	0.46
12:L:232:TRP:O	12:L:236:ALA:CB	2.62	0.46
1:1:213:VAL:HG13	1:1:217:GLY:HA2	1.98	0.46
5:5:14:ARG:NH2	5:5:44:CYS:O	2.48	0.46
7:9:79:ALA:HB3	7:9:104:ARG:HG2	1.97	0.46
12:L:232:TRP:O	12:L:236:ALA:HB2	2.15	0.46
36:r:85:LEU:HA	36:r:89:VAL:HB	1.97	0.46
13:M:186:MET:H	13:M:252:PRO:HD2	1.80	0.46
1:1:367:GLU:OE1	3:3:100:ASN:ND2	2.38	0.46
7:9:164:GLU:OE2	28:i:87:HIS:ND1	2.44	0.46
11:K:53:PHE:HE2	14:N:84:TRP:HE1	1.62	0.46
19:Z:144:ASP:OD2	34:p:122:ARG:NH1	2.48	0.46
21:b:49:VAL:HG22	21:b:90:GLN:HG3	1.97	0.46
1:1:361:GLN:N	45:1:501:SF4:S4	2.86	0.46
2:2:55:GLN:NE2	2:2:89:MET:O	2.48	0.46
3:3:377:VAL:HG23	3:3:404:LEU:HD11	1.96	0.46
14:N:119:THR:HG22	14:N:176:ARG:HB3	1.97	0.46
53:V:203:CDL:H581	53:V:204:CDL:H221	1.98	0.46
17:X:8:LEU:HD21	17:X:81:ALA:HB2	1.97	0.46
1:1:69:GLY:O	47:1:503:NAI:H2N	2.16	0.46
2:2:50:VAL:HG12	2:2:69:VAL:HG22	1.97	0.46
12:L:128:MET:HG2	12:L:251:THR:HG22	1.97	0.46
18:Y:82:THR:HA	18:Y:85:TRP:CD1	2.50	0.46
36:r:17:LEU:HD11	38:t:162:LEU:HD22	1.98	0.46
1:1:141:GLU:HG2	2:2:145:LEU:HD22	1.98	0.46
3:3:42:TYR:O	3:3:158:ARG:NH2	2.47	0.46
3:3:383:ASN:ND2	3:3:665:GLN:O	2.41	0.46
4:4:257:GLY:HA3	4:4:372:GLY:HA2	1.97	0.46
6:6:73:GLY:HA2	9:H:25:ARG:HH22	1.81	0.46
12:L:12:LEU:HB3	53:W:201:CDL:H651	1.97	0.46
19:Z:77:HIS:HB3	33:o:106:LYS:HE2	1.97	0.46
3:3:329:ILE:HD11	3:3:626:VAL:HG21	1.97	0.46
14:N:289:ASN:HA	14:N:292:PHE:CE1	2.50	0.46
23:d:26:ALA:HB3	23:d:47:VAL:HG13	1.98	0.46
30:l:50:ARG:O	30:l:54:GLU:HB2	2.16	0.46
33:o:45:ASP:OD2	33:o:51:ARG:NH2	2.39	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:u:10:ARG:HB3	39:u:13:GLN:HE21	1.81	0.46
8:A:71:LEU:O	10:J:147:TYR:OH	2.29	0.46
14:N:324:THR:H	51:N:401:3PE:H241	1.81	0.46
23:d:128:LYS:NZ	23:d:218:ILE:O	2.37	0.46
33:o:5:ARG:NH2	33:o:89:ASP:OD1	2.48	0.46
4:4:64:LEU:HB3	4:4:66:MET:HE2	1.97	0.45
12:L:69:LEU:O	12:L:76:LEU:N	2.48	0.45
13:M:369:LEU:HD12	13:M:370:PRO:HD2	1.97	0.45
14:N:210:ILE:HG22	14:N:333:SER:HB3	1.98	0.45
10:J:24:PRO:HA	10:J:89:VAL:HG21	1.98	0.45
13:M:225:ILE:HD13	13:M:331:ASN:HB2	1.99	0.45
14:N:24:THR:HG22	30:l:2:PHE:HZ	1.82	0.45
17:j:37:MET:HE1	17:j:44:SER:HA	1.98	0.45
1:1:112:ARG:HB2	1:1:145:GLU:HG3	1.97	0.45
12:L:552:LEU:HA	12:L:556:ILE:HD12	1.98	0.45
1:1:342:ASP:HB3	1:1:345:LYS:HE3	1.98	0.45
5:5:92:ILE:N	5:5:109:THR:O	2.49	0.45
8:A:98:LEU:HD22	9:H:298:LEU:HD11	1.99	0.45
10:J:20:PHE:HB2	10:J:29:GLY:HA2	1.99	0.45
15:V:32:GLY:HA3	15:V:59:THR:HA	1.98	0.45
32:n:23:ILE:HG22	32:n:49:ALA:HB2	1.98	0.45
2:2:98:TYR:HA	2:2:157:ASN:HD21	1.80	0.45
4:4:158:ALA:HB1	4:4:163:ALA:HB3	1.98	0.45
6:6:52:LEU:HB2	6:6:90:GLY:HA3	1.97	0.45
9:H:152:SER:HA	9:H:155:LEU:HD12	1.99	0.45
10:J:167:VAL:HG22	14:N:42:PRO:HG2	1.98	0.45
19:Z:81:VAL:HA	19:Z:84:MET:HG2	1.97	0.45
38:t:139:LEU:O	38:t:143:THR:OG1	2.30	0.45
40:v:54:SER:HA	40:v:84:TYR:HB3	1.98	0.45
3:3:148:THR:HG23	3:3:150:MET:HE3	1.99	0.45
9:H:79:LEU:HD23	9:H:226:ALA:HB2	1.98	0.45
12:L:249:SER:HB2	12:L:336:LYS:HG3	1.99	0.45
13:M:126:LEU:HD13	13:M:150:LEU:HD12	1.99	0.45
29:k:309:ASN:ND2	42:x:3:TYR:OH	2.38	0.45
37:s:42:GLN:O	37:s:46:ASN:HB2	2.17	0.45
41:w:77:VAL:HA	41:w:80:LEU:HG	1.99	0.45
1:1:87:ASP:N	1:1:87:ASP:OD1	2.49	0.45
1:1:99:GLU:OE2	1:1:107:ASP:N	2.48	0.45
3:3:348:VAL:N	3:3:459:GLN:OE1	2.50	0.45
36:r:107:ASP:OD1	37:s:67:LYS:NZ	2.49	0.45
42:x:1:LYS:NZ	42:x:6:GLU:OE1	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:203:LEU:HD22	4:4:207:LEU:HD23	1.99	0.45
4:4:111:MET:SD	4:4:111:MET:N	2.90	0.45
9:H:6:VAL:HG22	9:H:95:LEU:HD21	1.98	0.45
12:L:68:TRP:CE2	52:L:703:PC1:H2E2	2.52	0.45
15:V:82:LYS:O	15:V:88:ASN:ND2	2.50	0.45
35:q:81:ARG:NH2	35:q:124:TYR:OH	2.49	0.45
38:t:100:GLU:OE1	38:t:121:ARG:NH1	2.49	0.45
23:d:115:GLN:NE2	23:d:119:GLN:OE1	2.44	0.44
27:h:7:ILE:HD11	53:i:202:CDL:H111	1.99	0.44
29:k:22:SER:OG	29:k:119:GLY:O	2.26	0.44
1:1:378:ARG:NE	3:3:132:GLU:OE2	2.37	0.44
4:4:352:TYR:HD1	7:9:86:VAL:HG21	1.81	0.44
7:9:27:TRP:HB3	7:9:30:LEU:HD12	1.99	0.44
52:9:401:PC1:H2A1	31:m:24:ILE:HD11	1.99	0.44
12:L:152:PHE:HB2	12:L:172:ILE:HD11	1.99	0.44
12:L:233:LEU:HD23	12:L:307:SER:HB3	2.00	0.44
14:N:208:TYR:O	14:N:212:THR:OG1	2.33	0.44
24:e:17:GLU:HG2	24:e:67:ARG:HB3	1.97	0.44
29:k:47:GLY:O	29:k:120:GLN:NE2	2.50	0.44
31:m:68:HIS:N	31:m:71:ASP:OD2	2.50	0.44
18:Y:97:ARG:HD3	35:q:59:LEU:HD13	1.99	0.44
12:L:304:PHE:HZ	12:L:526:LEU:HD22	1.81	0.44
12:L:539:TYR:HH	34:p:9:ARG:HH21	1.65	0.44
12:L:566:ILE:HG12	53:V:204:CDL:H582	1.98	0.44
15:V:89:TYR:CD2	15:V:125:LYS:HB2	2.53	0.44
18:Y:17:VAL:HG12	18:Y:19:VAL:HG22	2.00	0.44
31:m:44:ILE:HG12	31:m:80:LEU:HD13	1.98	0.44
3:3:323:VAL:H	3:3:498:SER:HB3	1.83	0.44
7:9:143:THR:HB	7:9:146:GLU:HG3	1.99	0.44
12:L:9:LEU:HD12	36:r:85:LEU:HD11	2.00	0.44
12:L:375:ILE:HG12	39:u:32:MET:SD	2.57	0.44
13:M:397:GLY:HA2	13:M:400:MET:HE3	2.00	0.44
16:W:8:LEU:HD11	17:X:88:GLU:HG3	1.98	0.44
53:W:201:CDL:H381	52:w:801:PC1:H251	2.00	0.44
1:1:97:ALA:HB1	1:1:111:ILE:HD11	1.99	0.44
3:3:362:TYR:HA	3:3:492:ILE:HD12	1.99	0.44
4:4:146:ARG:NH2	4:4:368:GLU:O	2.45	0.44
10:J:41:CYS:HB2	10:J:56:VAL:HG11	2.00	0.44
12:L:524:ASN:O	38:t:77:GLN:NE2	2.51	0.44
53:L:704:CDL:H241	53:L:704:CDL:H442	1.98	0.44
13:M:122:PHE:HZ	13:M:206:LYS:HG3	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:V:65:ILE:HD11	15:V:100:LEU:HD23	1.98	0.44
18:Y:118:ARG:NH2	35:q:62:GLU:OE2	2.50	0.44
23:d:200:THR:HG23	23:d:290:THR:HA	1.98	0.44
8:A:60:ILE:HG21	10:J:168:ILE:HG21	1.99	0.44
9:H:310:LEU:HD12	9:H:311:LEU:HG	1.99	0.44
12:L:316:THR:HG23	12:L:325:ALA:HB2	1.99	0.44
14:N:235:ASN:O	14:N:315:TRP:NE1	2.47	0.44
20:a:72:SER:OG	20:a:75:HIS:ND1	2.39	0.44
12:L:62:ILE:HG12	12:L:81:LYS:HA	2.00	0.44
52:L:703:PC1:H3A1	36:r:80:ILE:HG23	2.00	0.44
53:V:203:CDL:OB4	53:V:204:CDL:OA7	2.36	0.44
23:d:164:THR:OG1	23:d:223:ALA:O	2.30	0.44
4:4:87:THR:HG21	4:4:106:LEU:HD21	1.99	0.44
9:H:318:THR:HG21	10:J:135:PHE:HB3	1.98	0.44
14:N:20:VAL:HG11	14:N:137:ALA:HB1	1.99	0.44
1:1:69:GLY:O	47:1:503:NAI:N7N	2.45	0.43
3:3:460:ARG:HH21	3:3:661:LEU:HD23	1.83	0.43
4:4:71:GLU:OE2	9:H:134:ARG:NH1	2.50	0.43
5:5:183:VAL:O	26:g:100:THR:OG1	2.27	0.43
9:H:88:PRO:HB3	9:H:98:MET:HE3	2.00	0.43
13:M:9:MET:HB3	53:Y:201:CDL:H232	2.00	0.43
13:M:179:LEU:HD13	13:M:249:LEU:HD21	1.99	0.43
28:i:9:ARG:HA	28:i:12:GLN:HG2	1.99	0.43
12:L:532:ILE:HD11	40:v:101:MET:HB3	2.01	0.43
13:M:329:LEU:HB3	13:M:359:TRP:CZ2	2.53	0.43
14:N:267:ILE:HG12	14:N:279:PRO:HB2	2.00	0.43
29:k:165:PRO:O	29:k:248:TRP:NE1	2.34	0.43
38:t:153:LEU:HD12	38:t:164:PRO:HG2	2.01	0.43
44:z:34:ARG:NH2	44:z:61:TYR:O	2.36	0.43
13:M:459:TYR:H	41:w:84:ARG:NH2	2.17	0.43
53:Y:201:CDL:H592	53:Y:201:CDL:H192	2.01	0.43
53:o:202:CDL:H842	53:o:202:CDL:H652	2.00	0.43
34:p:74:ASN:OD1	34:p:78:ASN:ND2	2.52	0.43
1:1:300:GLY:HA2	1:1:333:ALA:H	1.84	0.43
3:3:584:LYS:HE3	22:c:36:ARG:HD2	2.01	0.43
12:L:69:LEU:HB3	12:L:76:LEU:HB2	2.01	0.43
12:L:292:ALA:HB2	12:L:304:PHE:HB3	2.00	0.43
13:M:78:MET:HE2	41:w:61:VAL:HG22	2.00	0.43
19:Z:163:LEU:HG	41:w:120:LEU:HD12	1.99	0.43
3:3:366:THR:HG22	3:3:370:GLY:HA3	2.00	0.43
8:A:88:LEU:HD13	9:H:309:ILE:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:23:LYS:O	11:K:23:ARG:NH1	2.51	0.43
14:N:252:GLY:O	14:N:263:LYS:NZ	2.52	0.43
19:Z:16:THR:HG23	36:r:110:LEU:HB2	2.01	0.43
19:Z:141:ARG:HG3	41:w:112:CYS:HB2	1.99	0.43
4:4:98:GLN:NE2	7:9:85:ALA:O	2.51	0.43
12:L:50:PRO:HA	12:L:53:MET:HG2	2.01	0.43
12:L:290:MET:O	12:L:523:SER:OG	2.28	0.43
53:L:704:CDL:H362	53:L:704:CDL:H532	2.00	0.43
30:l:14:ASP:O	30:l:18:THR:OG1	2.36	0.43
52:w:801:PC1:H2B1	52:w:801:PC1:H282	1.86	0.43
1:1:191:ALA:HB2	1:1:203:PRO:HG3	2.00	0.43
8:A:114:THR:HB	9:H:286:MET:HG3	2.01	0.43
12:L:173:LEU:HD12	13:M:405:LEU:HD21	2.01	0.43
17:X:26:ASP:OD1	17:X:26:ASP:N	2.51	0.43
19:Z:5:ASP:HB3	19:Z:8:VAL:HG12	1.99	0.43
27:h:1:AYA:HA	27:h:20:GLN:HE22	1.83	0.43
38:t:29:ARG:HD2	38:t:75:HIS:HD2	1.84	0.43
1:1:21:ILE:HG12	1:1:233:THR:HG21	2.00	0.43
2:2:24:THR:OG1	2:2:27:ASN:OD1	2.31	0.43
6:6:27:GLU:HA	6:6:30:VAL:HG22	2.01	0.43
9:H:316:PRO:HG3	35:q:56:ARG:HB3	2.00	0.43
12:L:7:LEU:HD22	12:L:46:THR:HG23	2.01	0.43
17:X:49:GLU:HB3	32:n:44:TRP:HE1	1.83	0.43
1:1:261:HIS:NE2	2:2:110:LEU:O	2.45	0.43
3:3:115:ASP:O	3:3:119:GLN:HG2	2.19	0.43
3:3:146:VAL:HG21	3:3:199:ILE:HD11	2.01	0.43
3:3:396:ARG:NH1	3:3:416:THR:O	2.52	0.43
9:H:162:LEU:HD21	9:H:237:PHE:HE1	1.84	0.43
13:M:30:HIS:HB3	43:y:16:VAL:HG21	2.01	0.43
17:X:36:PHE:HA	17:X:40:LEU:HB2	2.00	0.43
28:i:26:VAL:O	28:i:30:ALA:HB3	2.19	0.43
29:k:88:SER:OG	29:k:90:ASP:OD1	2.31	0.43
2:2:116:ILE:HG23	2:2:169:ILE:HG21	2.00	0.43
54:X:101:ZMP:H15	54:X:101:ZMP:H17	1.71	0.43
30:l:96:HIS:HA	30:l:101:GLU:HG2	2.00	0.43
33:o:108:THR:OG1	33:o:111:GLU:OE1	2.30	0.43
4:4:109:VAL:HG11	4:4:152:MET:HG2	2.00	0.42
10:J:6:VAL:HG13	10:J:43:ILE:HG23	2.01	0.42
12:L:243:VAL:O	12:L:247:LEU:HB2	2.19	0.42
16:W:37:VAL:HG11	53:W:201:CDL:H832	2.01	0.42
24:e:30:GLN:OE1	24:e:33:ARG:NH1	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:t:142:GLU:OE2	38:t:157:ARG:NH2	2.52	0.42
1:1:258:ILE:HA	1:1:334:VAL:HB	2.01	0.42
2:2:147:ALA:HB3	2:2:153:MET:HG2	2.01	0.42
3:3:60:GLU:HG2	3:3:78:ASN:HB3	2.01	0.42
3:3:526:GLY:N	3:3:546:GLN:O	2.48	0.42
10:J:23:LYS:HE2	11:K:23:ARG:HG3	2.01	0.42
12:L:584:ILE:HG12	14:N:58:LYS:HE2	2.01	0.42
53:L:704:CDL:H182	13:M:442:LEU:HD22	2.00	0.42
13:M:147:LEU:HD22	13:M:151:PHE:HE2	1.84	0.42
7:9:132:VAL:HG21	7:9:165:ILE:HG21	2.00	0.42
8:A:3:LEU:HD23	51:J:201:3PE:H231	2.02	0.42
9:H:114:TYR:OH	10:J:61:LEU:O	2.28	0.42
14:N:298:TYR:O	14:N:303:THR:OG1	2.30	0.42
23:d:10:LYS:O	26:g:113:ARG:NH1	2.52	0.42
13:M:252:PRO:HG3	33:o:117:HIS:CD2	2.54	0.42
16:W:143:ASN:HD22	30:l:29:PRO:HB3	1.84	0.42
43:y:8:ARG:HG3	43:y:10:HIS:H	1.85	0.42
5:5:195:ARG:HH12	7:9:93:THR:HA	1.85	0.42
9:H:63:PRO:HG2	9:H:65:THR:HG23	2.00	0.42
9:H:198:PHE:HD1	9:H:285:LEU:HD13	1.83	0.42
10:J:43:ILE:HG22	11:K:46:LEU:HD21	2.00	0.42
12:L:331:THR:HG22	12:L:335:PHE:HE1	1.85	0.42
13:M:36:LEU:HD23	41:w:69:VAL:HA	2.01	0.42
13:M:127:VAL:HG11	53:o:202:CDL:H872	2.02	0.42
13:M:403:THR:HA	13:M:406:TYR:CE1	2.55	0.42
53:Y:201:CDL:H322	53:Y:201:CDL:H172	2.02	0.42
22:c:13:VAL:O	26:g:14:THR:OG1	2.37	0.42
3:3:100:ASN:HB3	3:3:135:ARG:HG2	2.02	0.42
3:3:101:HIS:HD2	4:4:342:MET:HE2	1.84	0.42
4:4:107:ASP:OD1	4:4:371:LYS:NZ	2.53	0.42
7:9:30:LEU:O	9:H:277:TYR:OH	2.37	0.42
12:L:39:THR:HA	36:r:69:PHE:HZ	1.84	0.42
18:Y:6:LEU:HD12	35:q:90:LEU:HD22	2.00	0.42
24:e:57:CYS:SG	24:e:58:SER:N	2.91	0.42
1:1:398:GLN:HE21	27:h:52:TYR:HE1	1.68	0.42
4:4:19:MET:HG2	14:N:295:ARG:CZ	2.50	0.42
4:4:161:ILE:HG22	9:H:278:PRO:HB2	2.02	0.42
14:N:202:LEU:HD21	30:l:1:PRO:HD3	2.02	0.42
29:k:116:LEU:HD21	29:k:256:LEU:HD22	2.02	0.42
30:l:96:HIS:O	35:q:127:ARG:NH1	2.52	0.42
39:u:61:ASP:HB3	39:u:66:ILE:HB	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:120:ILE:HD11	2:2:169:ILE:HG12	2.01	0.42
5:5:67:HIS:CD2	5:5:69:ASN:H	2.38	0.42
13:M:36:LEU:HB2	41:w:69:VAL:HG22	2.02	0.42
14:N:211:MET:HB3	14:N:251:MET:HG2	2.02	0.42
29:k:279:LEU:HA	29:k:280:PRO:HD3	1.94	0.42
53:o:202:CDL:CA7	53:o:202:CDL:H531	2.49	0.42
1:1:363:THR:HG21	3:3:97:LEU:HG	2.01	0.42
3:3:227:SER:OG	3:3:228:ILE:N	2.52	0.42
3:3:453:LEU:HD13	3:3:470:VAL:HG21	2.01	0.42
9:H:202:GLU:OE2	9:H:279:ARG:NH1	2.53	0.42
12:L:418:PHE:HD1	12:L:421:ILE:HD12	1.84	0.42
13:M:1:FME:O1	13:M:3:LYS:NZ	2.47	0.42
26:g:21:SER:OG	26:g:30:ARG:NH1	2.53	0.42
27:h:8:GLN:NE2	27:h:20:GLN:HG3	2.35	0.42
1:1:245:PHE:HB3	1:1:271:GLU:HG3	2.01	0.42
46:1:502:FMN:O2'	47:1:503:NAI:O2N	2.33	0.42
9:H:80:THR:HG21	51:J:201:3PE:H3D1	2.01	0.42
14:N:112:HIS:HB2	14:N:184:ILE:HD13	2.02	0.42
14:N:238:PRO:O	14:N:241:THR:OG1	2.29	0.42
28:i:50:GLU:HG3	28:i:89:TRP:HZ2	1.84	0.42
29:k:302:ARG:O	33:o:50:ARG:NH1	2.53	0.42
37:s:42:GLN:HE22	40:v:140:LEU:HD12	1.85	0.42
1:1:302:SER:OG	1:1:354:TYR:OH	2.29	0.41
3:3:9:ILE:HD11	3:3:73:VAL:HG23	2.02	0.41
3:3:525:LEU:HD21	3:3:600:ILE:HD11	2.01	0.41
10:J:44:VAL:HG13	11:K:45:THR:HG21	2.01	0.41
10:J:122:MET:HE2	10:J:126:VAL:HG11	2.01	0.41
13:M:173:SER:HB2	16:W:101:ALA:HB2	2.02	0.41
32:n:35:LEU:HB3	32:n:40:LEU:HB2	2.02	0.41
52:w:801:PC1:H153	52:w:801:PC1:H111	1.88	0.41
3:3:194:GLU:HG2	3:3:195:LEU:HG	2.02	0.41
5:5:137:MET:HE3	5:5:152:LEU:HB2	2.02	0.41
7:9:100:ALA:HB3	21:b:41:ILE:HD11	2.03	0.41
13:M:106:LEU:HD13	13:M:234:ILE:HG21	2.01	0.41
14:N:128:LEU:HD13	14:N:216:PHE:HB2	2.02	0.41
24:e:18:ILE:HD12	24:e:52:ILE:HG12	2.02	0.41
3:3:20:VAL:HG21	3:3:73:VAL:HG21	2.01	0.41
3:3:110:GLN:NE2	3:3:113:GLU:O	2.54	0.41
12:L:350:LEU:HD11	12:L:362:LEU:HD11	2.03	0.41
12:L:396:ILE:HG21	12:L:490:ALA:HB2	2.01	0.41
13:M:379:LEU:O	13:M:383:MET:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:j:11:ILE:HG22	17:j:77:VAL:HG23	2.02	0.41
4:4:47:LEU:HB2	8:A:50:PRO:HG3	2.02	0.41
8:A:63:LEU:HB2	10:J:67:VAL:HG21	2.02	0.41
9:H:233:MET:HE3	9:H:233:MET:HB3	1.99	0.41
14:N:331:VAL:HG13	14:N:335:MET:HE3	2.02	0.41
27:h:13:TRP:NE1	35:q:27:ARG:HH12	2.18	0.41
33:o:52:PRO:HG2	33:o:56:ALA:HB2	2.02	0.41
3:3:329:ILE:HD12	3:3:329:ILE:HA	1.86	0.41
4:4:175:GLU:OE2	4:4:188:ARG:NH1	2.53	0.41
12:L:10:VAL:HG21	36:r:78:VAL:HG22	2.02	0.41
12:L:176:ARG:NH2	13:M:400:MET:HB3	2.35	0.41
13:M:75:LEU:HD23	13:M:440:HIS:CE1	2.56	0.41
22:c:42:ARG:HD3	22:c:49:VAL:HG12	2.02	0.41
29:k:81:LYS:HD2	29:k:92:ASN:HD22	1.86	0.41
43:y:43:LEU:HD22	43:y:44:TYR:CZ	2.55	0.41
2:2:156:ILE:HD13	2:2:176:LEU:HD11	2.02	0.41
8:A:3:LEU:HD22	51:J:201:3PE:H32	2.02	0.41
12:L:94:LEU:HD23	12:L:125:LEU:HD21	2.02	0.41
52:L:703:PC1:H142	52:L:703:PC1:H111	1.84	0.41
51:M:501:3PE:H3I1	53:V:204:CDL:H812	2.03	0.41
26:g:97:LYS:HB3	26:g:101:HIS:HB2	2.02	0.41
30:l:19:ILE:HD12	30:l:21:SER:HB2	2.03	0.41
44:z:51:ASP:HA	44:z:54:VAL:HG22	2.03	0.41
4:4:63:ARG:HB3	4:4:79:HIS:HB2	2.02	0.41
4:4:65:VAL:HB	4:4:77:ASP:HB3	2.03	0.41
9:H:41:GLY:HA3	9:H:46:LEU:H	1.85	0.41
9:H:97:ASN:H	35:q:143:THR:HG22	1.86	0.41
9:H:189:THR:HG22	9:H:234:MET:HE3	2.02	0.41
12:L:60:GLU:HG2	12:L:83:ASP:HA	2.01	0.41
12:L:316:THR:HB	12:L:395:ILE:HG23	2.01	0.41
33:o:42:GLY:HA3	33:o:61:GLN:HG2	2.01	0.41
33:o:63:LEU:HD23	53:o:201:CDL:H112	2.02	0.41
1:1:25:LEU:HD21	1:1:267:THR:HG22	2.02	0.41
1:1:96:ASN:ND2	1:1:187:GLY:O	2.38	0.41
1:1:432:ARG:HA	1:1:435:GLN:HG3	2.02	0.41
4:4:85:2MR:HE	4:4:85:2MR:HB3	1.77	0.41
4:4:327:ASP:OD1	27:h:53:TYR:OH	2.38	0.41
9:H:179:TRP:HE1	35:q:42:LEU:HG	1.86	0.41
12:L:419:THR:HA	12:L:422:TYR:CE1	2.56	0.41
51:M:501:3PE:H3B1	53:V:204:CDL:H852	2.03	0.41
26:g:40:ARG:NH1	17:j:56:ASP:OD1	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:o:54:LEU:HD21	53:o:202:CDL:H142	2.02	0.41
1:1:361:GLN:O	1:1:366:ARG:NH1	2.54	0.41
2:2:154:VAL:HG22	2:2:164:LEU:HD11	2.02	0.41
3:3:99:ALA:O	3:3:134:LYS:NZ	2.53	0.41
4:4:15:GLY:HA3	14:N:228:LEU:HD22	2.02	0.41
4:4:104:ASP:HB3	4:4:190:HIS:ND1	2.35	0.41
4:4:324:LYS:HD3	4:4:331:SER:HB3	2.03	0.41
6:6:71:ARG:HA	9:H:37:PRO:HA	2.03	0.41
9:H:287:HIS:HD1	9:H:291:LYS:HD2	1.85	0.41
10:J:113:VAL:HG12	10:J:119:PHE:HB2	2.03	0.41
13:M:14:LEU:O	13:M:18:SER:OG	2.30	0.41
13:M:457:PRO:O	41:w:84:ARG:NH1	2.53	0.41
14:N:163:THR:HA	14:N:285:THR:HG21	2.02	0.41
17:X:70:LEU:HB3	17:X:76:ILE:HG12	2.02	0.41
22:c:69:LEU:HD11	28:i:126:PRO:HG2	2.03	0.41
23:d:90:VAL:HG21	23:d:218:ILE:HG12	2.01	0.41
23:d:155:GLU:HA	23:d:158:GLU:HG2	2.02	0.41
30:l:53:LYS:HG3	30:l:54:GLU:HG3	2.03	0.41
31:m:77:LEU:HD13	31:m:80:LEU:HD23	2.02	0.41
33:o:43:LEU:HD22	33:o:53:VAL:HG12	2.03	0.41
37:s:110:ARG:NH1	39:u:69:ASP:OD2	2.54	0.41
11:K:38:LEU:O	11:K:42:ILE:HG12	2.21	0.41
12:L:90:VAL:HG22	12:L:129:LEU:HD22	2.02	0.41
13:M:122:PHE:CZ	13:M:206:LYS:HG3	2.55	0.41
13:M:216:LEU:HD23	13:M:287:ALA:HB1	2.03	0.41
4:4:135:GLN:HB3	4:4:276:ASP:HB3	2.02	0.40
5:5:77:ASP:HB3	5:5:95:ASN:HD22	1.86	0.40
7:9:114:THR:HG21	7:9:144:HIS:CD2	2.55	0.40
9:H:24:GLU:CD	9:H:195:ARG:HH22	2.29	0.40
13:M:61:LEU:HB2	13:M:457:PRO:HD3	2.04	0.40
15:V:113:ALA:O	15:V:117:MET:HB2	2.20	0.40
16:W:43:ILE:O	16:W:48:GLY:N	2.47	0.40
16:W:109:GLU:OE2	16:W:112:ARG:NH2	2.39	0.40
19:Z:48:ARG:HG2	36:r:87:TYR:CE1	2.56	0.40
33:o:54:LEU:HD11	53:o:202:CDL:H132	2.02	0.40
4:4:387:TYR:CZ	5:5:164:LYS:HE3	2.56	0.40
15:V:124:VAL:HA	51:V:202:3PE:H351	2.02	0.40
23:d:335:GLN:HA	23:d:336:PRO:HD3	1.91	0.40
29:k:135:LEU:HD22	29:k:152:TYR:CD2	2.57	0.40
4:4:190:HIS:CD2	6:6:150:PRO:HD3	2.56	0.40
12:L:477:ILE:HD11	37:s:54:GLN:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:M:502:PC1:H222	15:V:132:TRP:CD2	2.56	0.40
14:N:193:VAL:HB	14:N:266:ILE:HG23	2.04	0.40
29:k:275:ILE:HA	29:k:276:PRO:HD3	1.91	0.40
37:s:33:ARG:HG2	40:v:156:TYR:HB3	2.03	0.40
2:2:61:LEU:HD12	2:2:90:TYR:HB3	2.03	0.40
7:9:45:PRO:HG3	9:H:30:TYR:HE1	1.86	0.40
7:9:105:ARG:NH2	21:b:86:TYR:O	2.54	0.40
51:L:702:3PE:H392	51:L:702:3PE:H362	1.90	0.40
19:Z:27:ASN:HB3	37:s:74:PRO:HD3	2.04	0.40
25:f:34:LEU:HD11	25:f:44:ARG:HA	2.02	0.40
2:2:165:THR:H	2:2:168:ASP:HB2	1.87	0.40
3:3:437:HIS:CD2	3:3:439:PHE:H	2.40	0.40
9:H:24:GLU:HA	9:H:271:LEU:HD13	2.02	0.40
9:H:61:LEU:HB2	9:H:216:ALA:HB3	2.03	0.40
9:H:137:ALA:HA	9:H:140:ILE:HG12	2.04	0.40
13:M:35:SER:O	13:M:38:SER:OG	2.32	0.40
23:d:166:ILE:HG22	23:d:168:PRO:HD3	2.03	0.40
33:o:120:ARG:NH2	34:p:112:GLU:OE2	2.55	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%)	407 (95%)	21 (5%)	0	100	100
2	2	211/246 (86%)	194 (92%)	17 (8%)	0	100	100
3	3	686/727 (94%)	657 (96%)	29 (4%)	0	100	100
4	4	421/463 (91%)	409 (97%)	12 (3%)	0	100	100
5	5	206/266 (77%)	199 (97%)	7 (3%)	0	100	100
6	6	154/223 (69%)	146 (95%)	8 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	9	174/217 (80%)	167 (96%)	7 (4%)	0	100	100
8	A	106/115 (92%)	96 (91%)	10 (9%)	0	100	100
9	H	310/318 (98%)	297 (96%)	13 (4%)	0	100	100
10	J	162/175 (93%)	154 (95%)	8 (5%)	0	100	100
11	K	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
12	L	604/606 (100%)	573 (95%)	31 (5%)	0	100	100
13	M	457/459 (100%)	444 (97%)	13 (3%)	0	100	100
14	N	345/347 (99%)	335 (97%)	10 (3%)	0	100	100
15	V	138/141 (98%)	135 (98%)	3 (2%)	0	100	100
16	W	137/189 (72%)	136 (99%)	1 (1%)	0	100	100
17	X	85/157 (54%)	83 (98%)	2 (2%)	0	100	100
17	j	80/157 (51%)	78 (98%)	2 (2%)	0	100	100
18	Y	169/172 (98%)	166 (98%)	3 (2%)	0	100	100
19	Z	169/175 (97%)	164 (97%)	5 (3%)	0	100	100
20	a	42/109 (38%)	42 (100%)	0	0	100	100
21	b	93/124 (75%)	91 (98%)	2 (2%)	0	100	100
22	c	124/170 (73%)	120 (97%)	4 (3%)	0	100	100
23	d	289/380 (76%)	281 (97%)	8 (3%)	0	100	100
24	e	84/99 (85%)	82 (98%)	2 (2%)	0	100	100
25	f	111/116 (96%)	108 (97%)	3 (3%)	0	100	100
26	g	112/140 (80%)	107 (96%)	5 (4%)	0	100	100
27	h	92/114 (81%)	86 (94%)	6 (6%)	0	100	100
28	i	143/145 (99%)	142 (99%)	1 (1%)	0	100	100
29	k	317/355 (89%)	302 (95%)	15 (5%)	0	100	100
30	l	103/106 (97%)	100 (97%)	3 (3%)	0	100	100
31	m	78/84 (93%)	73 (94%)	5 (6%)	0	100	100
32	n	77/98 (79%)	75 (97%)	2 (3%)	0	100	100
33	o	118/122 (97%)	118 (100%)	0	0	100	100
34	p	126/130 (97%)	121 (96%)	5 (4%)	0	100	100
35	q	137/144 (95%)	135 (98%)	2 (2%)	0	100	100
36	r	95/128 (74%)	89 (94%)	6 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	s	120/137 (88%)	114 (95%)	6 (5%)	0	100	100
38	t	175/179 (98%)	168 (96%)	7 (4%)	0	100	100
39	u	63/108 (58%)	58 (92%)	5 (8%)	0	100	100
40	v	153/186 (82%)	144 (94%)	9 (6%)	0	100	100
41	w	99/154 (64%)	93 (94%)	6 (6%)	0	100	100
42	x	47/76 (62%)	46 (98%)	1 (2%)	0	100	100
43	y	48/58 (83%)	46 (96%)	2 (4%)	0	100	100
44	z	68/70 (97%)	66 (97%)	2 (3%)	0	100	100
All	All	8052/9247 (87%)	7740 (96%)	312 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	366/391 (94%)	366 (100%)	0	100	100
5	5	189/230 (82%)	189 (100%)	0	100	100
6	6	132/181 (73%)	131 (99%)	1 (1%)	73	81
7	9	151/179 (84%)	150 (99%)	1 (1%)	76	82
8	A	99/103 (96%)	99 (100%)	0	100	100
9	H	274/278 (99%)	273 (100%)	1 (0%)	84	86
10	J	135/144 (94%)	135 (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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	N	315/315 (100%)	315 (100%)	0	100	100
15	V	101/102 (99%)	100 (99%)	1 (1%)	68	79
16	W	122/160 (76%)	122 (100%)	0	100	100
17	X	80/141 (57%)	80 (100%)	0	100	100
17	j	76/141 (54%)	76 (100%)	0	100	100
18	Y	154/155 (99%)	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%)	113 (99%)	1 (1%)	70	80
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	z	59/59 (100%)	59 (100%)	0	100	100
All	All	7129/7955 (90%)	7124 (100%)	5 (0%)	87	90

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

Mol	Chain	Res	Type
6	6	54	CYS
7	9	78	ILE
9	H	259	PHE
15	V	134	VAL
34	p	24	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (72) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	150	GLN
1	1	293	ASN
1	1	373	ASN
1	1	398	GLN
1	1	437	HIS
2	2	55	GLN
2	2	157	ASN
4	4	135	GLN
4	4	149	ASN
4	4	252	ASN
5	5	19	HIS
5	5	144	ASN
5	5	160	HIS
5	5	211	GLN
6	6	38	ASN
7	9	156	ASN
9	H	247	HIS
11	K	7	ASN
12	L	269	ASN
12	L	348	HIS
12	L	354	GLN
12	L	434	GLN
12	L	446	ASN
12	L	509	HIS
12	L	546	GLN
13	M	81	GLN

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Mol	Chain	Res	Type
13	M	103	GLN
13	M	138	ASN
13	M	184	GLN
13	M	338	HIS
13	M	374	ASN
13	M	390	ASN
14	N	48	HIS
15	V	7	GLN
16	W	44	ASN
18	Y	29	HIS
18	Y	72	GLN
18	Y	142	HIS
19	Z	114	GLN
19	Z	143	HIS
20	a	40	ASN
21	b	32	GLN
23	d	44	GLN
23	d	87	HIS
23	d	148	ASN
23	d	250	HIS
25	f	20	HIS
25	f	49	GLN
26	g	25	ASN
28	i	31	ASN
29	k	114	HIS
29	k	141	GLN
29	k	190	HIS
29	k	287	HIS
29	k	288	GLN
30	l	76	ASN
30	l	97	HIS
30	l	100	GLN
32	n	20	GLN
33	o	12	GLN
33	o	61	GLN
34	p	78	ASN
37	s	42	GLN
38	t	13	GLN
39	u	13	GLN
40	v	55	GLN
40	v	137	ASN
41	w	119	GLN

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Mol	Chain	Res	Type
42	x	9	HIS
42	x	34	GLN
43	y	10	HIS
43	y	13	HIS

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
13	FME	M	1	13	8,9,10	0.98	0	8,9,11	1.03	0
11	FME	K	1	11	8,9,10	0.97	0	8,9,11	0.85	0
4	2MR	4	85	4	10,12,13	2.49	3 (30%)	5,13,15	1.19	1 (20%)
15	AYA	V	1	15	6,7,8	1.16	0	6,8,10	2.06	2 (33%)
29	SEP	k	36	29	8,9,10	1.61	1 (12%)	7,12,14	1.54	1 (14%)
27	AYA	h	1	27	6,7,8	1.26	1 (16%)	6,8,10	1.04	1 (16%)
12	FME	L	1	12	8,9,10	0.94	0	8,9,11	1.68	2 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	FME	M	1	13	-	2/7/9/11	-
11	FME	K	1	11	-	3/7/9/11	-
4	2MR	4	85	4	-	3/10/13/15	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	AYA	V	1	15	-	3/5/6/8	-
29	SEP	k	36	29	-	4/6/8/10	-
27	AYA	h	1	27	-	1/5/6/8	-
12	FME	L	1	12	-	1/7/9/11	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	4	85	2MR	CZ-NH2	5.15	1.44	1.33
4	4	85	2MR	CZ-NE	5.10	1.45	1.34
29	k	36	SEP	P-O1P	3.51	1.61	1.50
27	h	1	AYA	CA-N	-2.34	1.44	1.46
4	4	85	2MR	CQ1-NH1	-2.17	1.42	1.46

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	L	1	FME	CA-N-CN	3.63	128.40	122.82
29	k	36	SEP	OG-CB-CA	3.56	111.61	108.14
15	V	1	AYA	CA-N-CT	3.35	125.83	121.50
15	V	1	AYA	CB-CA-N	3.23	113.33	109.68
12	L	1	FME	C-CA-N	2.82	114.94	109.50
4	4	85	2MR	CD-NE-CZ	2.25	127.59	123.36
27	h	1	AYA	CB-CA-N	2.24	112.20	109.68

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	K	1	FME	O1-CN-N-CA
11	K	1	FME	O-C-CA-CB
13	M	1	FME	C-CA-CB-CG
15	V	1	AYA	O-C-CA-CB
27	h	1	AYA	O-C-CA-CB
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
12	L	1	FME	CA-CB-CG-SD
15	V	1	AYA	OT-CT-N-CA
15	V	1	AYA	CM-CT-N-CA

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

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	M	1	FME	1	0
11	K	1	FME	1	0
4	4	85	2MR	1	0
15	V	1	AYA	1	0
27	h	1	AYA	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 47 ligands modelled in this entry, 2 are monoatomic - leaving 45 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	$\# Z > 2$
45	SF4	3	801	3	0,12,12	-	-	-		
45	SF4	1	501	1	0,12,12	-	-	-		
51	3PE	K	101	-	39,39,50	0.34	0	42,44,55	0.32	0
51	3PE	V	202	-	36,36,50	0.35	0	39,41,55	0.33	0
53	CDL	W	201	-	99,99,99	0.27	0	105,111,111	0.26	0
53	CDL	i	202	-	57,57,99	0.35	0	63,69,111	0.28	0
57	AMP	k	501	-	25,25,25	1.45	4 (16%)	37,38,38	2.07	7 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
54	ZMP	X	101	17	25,30,36	0.81	1 (4%)	29,37,45	0.92	1 (3%)
48	FES	3	803	3	0,4,4	-	-	-		
51	3PE	L	702	-	50,50,50	0.30	0	53,55,55	0.35	0
52	PC1	9	401	-	53,53,53	0.30	0	59,61,61	0.51	1 (1%)
46	FMN	1	502	-	33,33,33	1.07	2 (6%)	48,50,50	1.32	8 (16%)
45	SF4	9	403	7	0,12,12	-	-	-		
51	3PE	V	201	-	34,34,50	0.35	0	37,39,55	0.30	0
51	3PE	J	201	-	50,50,50	0.30	0	53,55,55	0.45	1 (1%)
45	SF4	6	502	6	0,12,12	-	-	-		
45	SF4	9	402	7	0,12,12	-	-	-		
51	3PE	L	705	-	30,30,50	0.42	0	33,35,55	0.84	3 (9%)
51	3PE	N	401	-	50,50,50	0.32	0	53,55,55	0.55	2 (3%)
51	3PE	l	501	-	30,30,50	0.38	0	33,35,55	0.39	0
52	PC1	M	502	-	53,53,53	0.29	0	59,61,61	0.33	0
54	ZMP	g	201	-	28,33,36	0.68	1 (3%)	32,40,45	1.12	3 (9%)
50	970	H	501	-	33,33,33	0.32	0	48,50,50	0.71	1 (2%)
52	PC1	L	703	-	53,53,53	0.30	0	59,61,61	0.63	2 (3%)
51	3PE	L	701	-	39,39,50	0.34	0	42,44,55	0.34	0
53	CDL	V	204	-	84,84,99	0.29	0	90,96,111	0.26	0
53	CDL	o	202	-	89,89,99	0.27	0	95,101,111	0.41	1 (1%)
52	PC1	w	801	-	53,53,53	0.29	0	59,61,61	0.39	0
50	970	6	501	-	33,33,33	0.28	0	48,50,50	0.51	0
53	CDL	V	203	-	93,93,99	0.25	0	99,105,111	0.26	0
45	SF4	3	802	3	0,12,12	-	-	-		
51	3PE	M	501	-	43,43,50	0.33	0	46,48,55	0.47	0
51	3PE	i	201	-	50,50,50	0.30	0	53,55,55	0.29	0
53	CDL	L	704	-	99,99,99	0.26	0	105,111,111	0.26	0
48	FES	2	300	2	0,4,4	-	-	-		
47	NAI	1	503	-	47,48,48	0.40	0	64,73,73	1.81	4 (6%)
52	PC1	A	401	-	45,45,53	0.31	0	51,53,61	0.35	0
52	PC1	A	402	-	36,36,53	0.36	0	42,44,61	0.63	1 (2%)
53	CDL	o	201	-	74,74,99	0.29	0	80,86,111	0.49	1 (1%)
51	3PE	A	403	-	50,50,50	0.32	0	53,55,55	0.45	1 (1%)
53	CDL	Y	201	-	99,99,99	0.27	0	105,111,111	0.36	1 (0%)
51	3PE	6	503	-	50,50,50	0.30	0	53,55,55	0.32	0
51	3PE	p	201	-	26,26,50	0.49	0	29,31,55	0.54	1 (3%)
56	NDP	d	401	-	51,52,52	0.35	0	71,80,80	0.37	0
58	MYR	s	201	37	13,14,15	0.19	0	12,13,15	0.14	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	SF4	3	801	3	-	-	0/6/5/5
45	SF4	1	501	1	-	-	0/6/5/5
51	3PE	K	101	-	-	6/43/43/54	-
51	3PE	V	202	-	-	12/40/40/54	-
53	CDL	W	201	-	-	27/110/110/110	-
53	CDL	i	202	-	-	16/68/68/110	-
57	AMP	k	501	-	-	8/10/26/26	0/3/3/3
54	ZMP	X	101	17	-	16/35/37/43	-
48	FES	3	803	3	-	-	0/1/1/1
51	3PE	L	702	-	-	9/54/54/54	-
52	PC1	9	401	-	-	19/57/57/57	-
46	FMN	1	502	-	-	6/18/18/18	0/3/3/3
45	SF4	9	403	7	-	-	0/6/5/5
51	3PE	V	201	-	-	6/38/38/54	-
51	3PE	J	201	-	-	17/54/54/54	-
45	SF4	6	502	6	-	-	0/6/5/5
45	SF4	9	402	7	-	-	0/6/5/5
51	3PE	L	705	-	-	15/34/34/54	-
51	3PE	N	401	-	-	14/54/54/54	-
51	3PE	l	501	-	-	4/34/34/54	-
52	PC1	M	502	-	-	18/57/57/57	-
54	ZMP	g	201	-	-	6/38/40/43	-
50	970	H	501	-	-	4/8/41/41	0/5/5/5
52	PC1	L	703	-	-	17/57/57/57	-
51	3PE	L	701	-	-	15/43/43/54	-
53	CDL	V	204	-	1/1/9/9	35/95/95/110	-
53	CDL	o	202	-	-	22/100/100/110	-
52	PC1	w	801	-	-	17/57/57/57	-
50	970	6	501	-	-	4/8/41/41	0/5/5/5
53	CDL	V	203	-	-	31/104/104/110	-
45	SF4	3	802	3	-	-	0/6/5/5
51	3PE	M	501	-	-	10/47/47/54	-
53	CDL	L	704	-	1/1/9/9	33/110/110/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
51	3PE	i	201	-	-	14/54/54/54	-
48	FES	2	300	2	-	-	0/1/1/1
47	NAI	1	503	-	-	10/29/72/72	0/5/5/5
52	PC1	A	401	-	-	10/49/49/57	-
52	PC1	A	402	-	-	12/40/40/57	-
53	CDL	o	201	-	2/2/9/9	17/85/85/110	-
51	3PE	A	403	-	-	18/54/54/54	-
53	CDL	Y	201	-	1/1/9/9	28/110/110/110	-
51	3PE	6	503	-	-	11/54/54/54	-
51	3PE	p	201	-	-	6/27/27/54	-
56	NDP	d	401	-	-	5/34/77/77	0/5/5/5
58	MYR	s	201	37	-	2/12/12/13	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	k	501	AMP	C5-C4	5.05	1.48	1.39
46	1	502	FMN	C4A-N5	2.99	1.37	1.30
54	X	101	ZMP	C9-C10	2.92	1.53	1.50
57	k	501	AMP	C5-C6	2.75	1.48	1.41
57	k	501	AMP	C5-N7	-2.50	1.34	1.39
54	g	201	ZMP	C9-C10	2.47	1.53	1.50
46	1	502	FMN	C10-N1	2.20	1.37	1.33
57	k	501	AMP	C8-N7	2.13	1.35	1.31

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	1	503	NAI	O5B-PA-O1A	-9.64	70.75	108.94
47	1	503	NAI	O2A-PA-O1A	-8.17	74.46	112.44
57	k	501	AMP	C5-C4-N3	-7.02	117.05	126.72
47	1	503	NAI	O3-PA-O1A	-5.90	92.94	110.70
57	k	501	AMP	N3-C4-N9	5.67	136.81	127.17
57	k	501	AMP	C2-N3-C4	4.14	121.95	111.83
46	1	502	FMN	C4-N3-C2	-3.59	119.27	125.64
57	k	501	AMP	C4-C5-N7	-3.20	106.92	110.58
57	k	501	AMP	N3-C2-N1	-3.09	123.90	128.58
46	1	502	FMN	C4A-C10-N10	2.93	120.68	116.48
54	g	201	ZMP	O1-C10-C9	-2.77	120.79	123.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	1	502	FMN	O4-C4-C4A	-2.65	119.53	126.53
46	1	502	FMN	C4A-C4-N3	2.62	119.93	113.25
57	k	501	AMP	C1'-N9-C8	-2.56	121.41	127.09
54	X	101	ZMP	O1-C10-C9	-2.55	121.04	123.98
52	L	703	PC1	O21-C2-C1	2.50	117.33	108.34
52	L	703	PC1	C2-O21-C21	2.48	123.72	117.80
54	g	201	ZMP	C15-C14-C13	-2.48	108.27	112.39
51	J	201	3PE	O31-C3-C2	2.42	115.36	108.40
46	1	502	FMN	C4A-C10-N1	-2.42	118.67	124.59
47	1	503	NAI	O2A-PA-O5B	2.40	118.46	107.57
51	L	705	3PE	C2-O21-C21	2.38	123.49	117.80
57	k	501	AMP	C5-N7-C8	2.37	107.18	103.45
54	g	201	ZMP	C14-C15-N2	-2.36	106.98	112.00
51	L	705	3PE	O31-C3-C2	2.35	115.17	108.40
52	A	402	PC1	C2-O21-C21	2.35	123.41	117.80
46	1	502	FMN	C4'-C3'-C2'	-2.34	109.67	113.57
46	1	502	FMN	C4-C4A-C10	2.25	120.80	116.93
50	H	501	970	C12-O13-C14	2.24	119.71	116.07
51	N	401	3PE	O21-C2-C1	2.23	116.35	108.34
46	1	502	FMN	C10-C4A-N5	-2.23	120.25	124.81
53	Y	201	CDL	OA8-CA6-CA4	2.21	114.77	108.40
52	9	401	PC1	O21-C2-C1	2.18	116.16	108.34
51	A	403	3PE	O31-C3-C2	2.15	114.59	108.40
51	L	705	3PE	O21-C2-C1	2.12	115.96	108.34
53	o	201	CDL	CB4-OB6-CB5	2.10	122.82	117.80
51	N	401	3PE	C2-O21-C21	2.10	122.81	117.80
51	p	201	3PE	O12-P-O14	2.09	119.00	110.83
53	o	202	CDL	CB4-OB6-CB5	2.02	122.64	117.80

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	201	CDL	CA4
53	o	201	CDL	CB4

All (520) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	1	502	FMN	C5'-O5'-P-O2P

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Mol	Chain	Res	Type	Atoms
46	1	502	FMN	C5'-O5'-P-O3P
47	1	503	NAI	C5B-O5B-PA-O2A
47	1	503	NAI	C5D-O5D-PN-O3
47	1	503	NAI	C5D-O5D-PN-O1N
47	1	503	NAI	C5D-O5D-PN-O2N
50	6	501	970	C01-C02-C04-C05
50	6	501	970	C01-C02-C04-O08
50	6	501	970	C03-C02-C04-C05
50	6	501	970	C03-C02-C04-O08
50	H	501	970	C03-C02-C04-C05
50	H	501	970	C03-C02-C04-O08
51	6	503	3PE	C11-O13-P-O12
51	A	403	3PE	C1-O11-P-O13
51	A	403	3PE	C1-O11-P-O14
51	A	403	3PE	C11-O13-P-O11
51	A	403	3PE	C11-O13-P-O12
51	A	403	3PE	C11-O13-P-O14
51	J	201	3PE	C1-O11-P-O12
51	J	201	3PE	C11-O13-P-O11
51	J	201	3PE	C11-O13-P-O12
51	J	201	3PE	C11-O13-P-O14
51	J	201	3PE	O13-C11-C12-N
51	K	101	3PE	C1-O11-P-O13
51	K	101	3PE	C1-O11-P-O14
51	K	101	3PE	O13-C11-C12-N
51	L	701	3PE	C1-O11-P-O12
51	L	701	3PE	C1-O11-P-O13
51	L	701	3PE	C1-O11-P-O14
51	L	701	3PE	C11-O13-P-O11
51	L	701	3PE	C11-O13-P-O12
51	L	701	3PE	O21-C2-C3-O31
51	L	702	3PE	C11-O13-P-O12
51	L	702	3PE	O13-C11-C12-N
51	L	705	3PE	C1-O11-P-O12
51	L	705	3PE	C1-O11-P-O13
51	L	705	3PE	C1-O11-P-O14
51	L	705	3PE	C11-O13-P-O11
51	L	705	3PE	C11-O13-P-O12
51	L	705	3PE	C11-O13-P-O14
51	N	401	3PE	C11-O13-P-O11
51	N	401	3PE	O13-C11-C12-N
51	V	201	3PE	C1-O11-P-O12

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Mol	Chain	Res	Type	Atoms
51	V	201	3PE	C1-O11-P-O13
51	V	201	3PE	C11-O13-P-O11
51	V	202	3PE	C11-O13-P-O12
51	V	202	3PE	O13-C11-C12-N
51	i	201	3PE	C1-O11-P-O13
51	i	201	3PE	C1-O11-P-O14
51	i	201	3PE	C11-O13-P-O11
51	i	201	3PE	C11-O13-P-O12
51	i	201	3PE	C11-O13-P-O14
51	l	501	3PE	C11-O13-P-O14
51	l	501	3PE	O13-C11-C12-N
51	p	201	3PE	C1-O11-P-O12
51	p	201	3PE	C1-O11-P-O13
51	p	201	3PE	C1-O11-P-O14
52	9	401	PC1	C11-O13-P-O14
52	9	401	PC1	C11-O13-P-O11
52	9	401	PC1	O13-C11-C12-N
52	A	401	PC1	C11-O13-P-O11
52	A	401	PC1	O13-C11-C12-N
52	A	402	PC1	C11-O13-P-O12
52	A	402	PC1	C11-O13-P-O11
52	A	402	PC1	C1-O11-P-O12
52	A	402	PC1	C1-O11-P-O14
52	A	402	PC1	C1-O11-P-O13
52	A	402	PC1	O13-C11-C12-N
52	L	703	PC1	C11-O13-P-O14
52	L	703	PC1	C1-O11-P-O12
52	M	502	PC1	C11-O13-P-O14
52	w	801	PC1	C11-O13-P-O12
52	w	801	PC1	C11-O13-P-O14
52	w	801	PC1	C11-O13-P-O11
52	w	801	PC1	C1-O11-P-O12
52	w	801	PC1	C1-O11-P-O14
52	w	801	PC1	C1-O11-P-O13
52	w	801	PC1	O13-C11-C12-N
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	L	704	CDL	CB2-OB2-PB2-OB5
53	L	704	CDL	CB3-OB5-PB2-OB2
53	L	704	CDL	CB3-OB5-PB2-OB3
53	V	203	CDL	CA2-OA2-PA1-OA4

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Mol	Chain	Res	Type	Atoms
53	V	203	CDL	CA3-OA5-PA1-OA2
53	V	203	CDL	CA3-OA5-PA1-OA3
53	V	203	CDL	CB2-OB2-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-OA4
53	V	204	CDL	CA3-OA5-PA1-OA2
53	V	204	CDL	CA3-OA5-PA1-OA4
53	V	204	CDL	CB3-OB5-PB2-OB2
53	V	204	CDL	CB3-OB5-PB2-OB3
53	W	201	CDL	CA3-OA5-PA1-OA2
53	W	201	CDL	CA3-OA5-PA1-OA3
53	W	201	CDL	CB2-OB2-PB2-OB3
53	W	201	CDL	CB2-OB2-PB2-OB5
53	W	201	CDL	CB3-OB5-PB2-OB2
53	W	201	CDL	CB3-OB5-PB2-OB3
53	W	201	CDL	OB5-CB3-CB4-OB6
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	i	202	CDL	CA2-OA2-PA1-OA3
53	i	202	CDL	CA2-OA2-PA1-OA5
53	o	201	CDL	CA2-OA2-PA1-OA3
53	o	201	CDL	CA2-OA2-PA1-OA4
53	o	201	CDL	CA2-OA2-PA1-OA5
53	o	201	CDL	CB2-OB2-PB2-OB3
53	o	201	CDL	CB2-OB2-PB2-OB5
53	o	202	CDL	CB2-OB2-PB2-OB4
53	o	202	CDL	CB2-OB2-PB2-OB5
53	o	202	CDL	CB3-OB5-PB2-OB2
53	o	202	CDL	CB3-OB5-PB2-OB3
53	o	202	CDL	CB3-OB5-PB2-OB4
54	X	101	ZMP	O4-C17-C18-C21
54	X	101	ZMP	C16-C17-C18-C21
54	X	101	ZMP	O3-C16-C17-O4
54	X	101	ZMP	C17-C16-N2-C15
54	X	101	ZMP	S1-C11-C12-N1
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

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Mol	Chain	Res	Type	Atoms
53	Y	201	CDL	O1-C1-CB2-OB2
53	o	202	CDL	O1-C1-CB2-OB2
54	X	101	ZMP	O3-C16-N2-C15
57	k	501	AMP	C3'-C4'-C5'-O5'
51	V	202	3PE	C2-C1-O11-P
52	w	801	PC1	C11-C12-N-C15
51	A	403	3PE	O21-C2-C3-O31
53	L	704	CDL	CB5-C51-C52-C53
53	V	203	CDL	CA7-C31-C32-C33
52	M	502	PC1	C11-C12-N-C14
53	o	202	CDL	CB5-C51-C52-C53
53	Y	201	CDL	CA7-C31-C32-C33
53	W	201	CDL	CA5-C11-C12-C13
53	V	204	CDL	CA2-C1-CB2-OB2
52	M	502	PC1	C11-C12-N-C15
51	i	201	3PE	C36-C37-C38-C39
52	w	801	PC1	C11-C12-N-C14
52	L	703	PC1	C37-C38-C39-C3A
52	M	502	PC1	C3A-C3B-C3C-C3D
53	V	204	CDL	C71-C72-C73-C74
51	l	501	3PE	C22-C23-C24-C25
54	g	201	ZMP	C3-C4-C5-C6
52	9	401	PC1	C2C-C2D-C2E-C2F
53	W	201	CDL	C72-C73-C74-C75
53	L	704	CDL	C21-C22-C23-C24
53	V	203	CDL	C31-C32-C33-C34
52	L	703	PC1	C21-C22-C23-C24
57	k	501	AMP	O4'-C4'-C5'-O5'
52	L	703	PC1	C2C-C2D-C2E-C2F
53	V	203	CDL	C82-C83-C84-C85
51	6	503	3PE	C3C-C3D-C3E-C3F
52	9	401	PC1	C22-C23-C24-C25
53	V	203	CDL	C79-C80-C81-C82
52	9	401	PC1	C3A-C3B-C3C-C3D
53	V	203	CDL	C38-C39-C40-C41
53	V	204	CDL	CB3-CB4-CB6-OB8
53	Y	201	CDL	C59-C60-C61-C62
53	L	704	CDL	CB7-C71-C72-C73
53	W	201	CDL	CB5-C51-C52-C53
51	6	503	3PE	C36-C37-C38-C39
53	L	704	CDL	C41-C42-C43-C44
53	V	203	CDL	C40-C41-C42-C43

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Mol	Chain	Res	Type	Atoms
51	A	403	3PE	C2C-C2D-C2E-C2F
53	V	203	CDL	C20-C21-C22-C23
52	w	801	PC1	C11-C12-N-C13
53	L	704	CDL	C31-C32-C33-C34
53	L	704	CDL	C82-C83-C84-C85
53	W	201	CDL	C31-C32-C33-C34
52	9	401	PC1	C22-C21-O21-C2
51	N	401	3PE	C21-C22-C23-C24
51	i	201	3PE	C29-C2A-C2B-C2C
52	9	401	PC1	C3C-C3D-C3E-C3F
53	Y	201	CDL	C81-C82-C83-C84
53	Y	201	CDL	C15-C16-C17-C18
52	A	401	PC1	C3B-C3C-C3D-C3E
53	Y	201	CDL	C54-C55-C56-C57
51	N	401	3PE	C2B-C2C-C2D-C2E
53	L	704	CDL	C54-C55-C56-C57
52	L	703	PC1	C38-C39-C3A-C3B
53	o	202	CDL	C71-C72-C73-C74
51	A	403	3PE	C2E-C2F-C2G-C2H
53	o	202	CDL	C77-C78-C79-C80
52	M	502	PC1	C11-C12-N-C13
51	N	401	3PE	C2D-C2E-C2F-C2G
53	W	201	CDL	CA7-C31-C32-C33
52	L	703	PC1	C36-C37-C38-C39
53	o	202	CDL	OA6-CA4-CA6-OA8
52	L	703	PC1	C2-C1-O11-P
51	L	705	3PE	C21-C22-C23-C24
52	L	703	PC1	C33-C34-C35-C36
51	V	202	3PE	C33-C34-C35-C36
52	L	703	PC1	C29-C2A-C2B-C2C
53	Y	201	CDL	C12-C13-C14-C15
52	L	703	PC1	O11-C1-C2-C3
53	L	704	CDL	OB5-CB3-CB4-CB6
53	W	201	CDL	OB5-CB3-CB4-CB6
51	M	501	3PE	C33-C34-C35-C36
51	A	403	3PE	C1-C2-C3-O31
53	i	202	CDL	CA3-CA4-CA6-OA8
51	6	503	3PE	C39-C3A-C3B-C3C
51	J	201	3PE	C28-C29-C2A-C2B
51	p	201	3PE	C22-C23-C24-C25
53	V	204	CDL	C15-C16-C17-C18
52	w	801	PC1	C3E-C3F-C3G-C3H

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Mol	Chain	Res	Type	Atoms
53	o	202	CDL	C56-C57-C58-C59
52	9	401	PC1	O22-C21-O21-C2
46	1	502	FMN	C5'-O5'-P-O1P
56	d	401	NDP	O4B-C4B-C5B-O5B
54	g	201	ZMP	C5-C6-C7-C8
53	o	202	CDL	C84-C85-C86-C87
53	i	202	CDL	C57-C58-C59-C60
51	N	401	3PE	C3F-C3G-C3H-C3I
52	M	502	PC1	C31-C32-C33-C34
53	Y	201	CDL	C19-C20-C21-C22
52	9	401	PC1	C3B-C3C-C3D-C3E
53	Y	201	CDL	C41-C42-C43-C44
53	Y	201	CDL	C58-C59-C60-C61
53	L	704	CDL	C17-C18-C19-C20
51	L	705	3PE	C2-C1-O11-P
52	M	502	PC1	O11-C1-C2-C3
52	w	801	PC1	O11-C1-C2-C3
53	V	203	CDL	OB5-CB3-CB4-CB6
52	M	502	PC1	O31-C31-C32-C33
53	V	204	CDL	C52-C53-C54-C55
54	X	101	ZMP	C3-C4-C5-C6
51	L	701	3PE	C34-C35-C36-C37
51	K	101	3PE	C34-C35-C36-C37
52	9	401	PC1	C29-C2A-C2B-C2C
53	W	201	CDL	CA3-CA4-CA6-OA8
53	o	202	CDL	CA3-CA4-CA6-OA8
51	J	201	3PE	C36-C37-C38-C39
51	K	101	3PE	C23-C24-C25-C26
53	W	201	CDL	C35-C36-C37-C38
53	L	704	CDL	C77-C78-C79-C80
52	L	703	PC1	O11-C1-C2-O21
52	M	502	PC1	O11-C1-C2-O21
53	L	704	CDL	OB5-CB3-CB4-OB6
53	V	203	CDL	OB5-CB3-CB4-OB6
53	V	204	CDL	C31-C32-C33-C34
51	J	201	3PE	C2-C1-O11-P
53	V	203	CDL	C11-C12-C13-C14
51	M	501	3PE	C3B-C3C-C3D-C3E
52	A	402	PC1	O21-C21-C22-C23
53	V	204	CDL	OA6-CA4-CA6-OA8
53	Y	201	CDL	C11-C12-C13-C14
47	1	503	NAI	PA-O3-PN-O5D

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Mol	Chain	Res	Type	Atoms
54	X	101	ZMP	C7-C8-C9-C10
53	V	203	CDL	C35-C36-C37-C38
53	Y	201	CDL	CB5-C51-C52-C53
53	o	202	CDL	CA2-C1-CB2-OB2
53	V	203	CDL	C51-C52-C53-C54
51	J	201	3PE	O11-C1-C2-C3
53	V	204	CDL	OA5-CA3-CA4-CA6
51	A	403	3PE	C23-C24-C25-C26
53	L	704	CDL	C81-C82-C83-C84
53	V	204	CDL	C14-C15-C16-C17
53	V	204	CDL	C23-C24-C25-C26
51	L	702	3PE	C35-C36-C37-C38
51	L	701	3PE	C23-C24-C25-C26
51	J	201	3PE	O11-C1-C2-O21
53	V	204	CDL	OA5-CA3-CA4-OA6
51	N	401	3PE	C1-C2-C3-O31
53	i	202	CDL	CB3-CB4-CB6-OB8
51	J	201	3PE	C12-C11-O13-P
51	L	701	3PE	C12-C11-O13-P
54	X	101	ZMP	C16-C17-C18-C20
53	Y	201	CDL	CB7-C71-C72-C73
51	N	401	3PE	O21-C2-C3-O31
53	W	201	CDL	OA6-CA4-CA6-OA8
53	i	202	CDL	OA6-CA4-CA6-OA8
51	M	501	3PE	C25-C26-C27-C28
51	N	401	3PE	C32-C33-C34-C35
52	M	502	PC1	C3B-C3C-C3D-C3E
53	Y	201	CDL	C36-C37-C38-C39
51	M	501	3PE	C2-C1-O11-P
53	L	704	CDL	C56-C57-C58-C59
51	6	503	3PE	C23-C24-C25-C26
58	s	201	MYR	C1-C2-C3-C4
53	V	204	CDL	C21-C22-C23-C24
53	Y	201	CDL	OB5-CB3-CB4-CB6
51	J	201	3PE	C34-C35-C36-C37
52	w	801	PC1	C27-C28-C29-C2A
46	1	502	FMN	N10-C1'-C2'-O2'
46	1	502	FMN	N10-C1'-C2'-C3'
50	H	501	970	C01-C02-C04-C05
52	9	401	PC1	C2-C1-O11-P
52	M	502	PC1	C2-C1-O11-P
53	V	204	CDL	C1-CB2-OB2-PB2

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Mol	Chain	Res	Type	Atoms
53	o	202	CDL	CA4-CA3-OA5-PA1
50	H	501	970	C01-C02-C04-O08
54	X	101	ZMP	C12-C11-S1-C10
51	A	403	3PE	O11-C1-C2-O21
52	A	402	PC1	O11-C1-C2-O21
52	w	801	PC1	O11-C1-C2-O21
53	Y	201	CDL	OB5-CB3-CB4-OB6
53	o	201	CDL	OA5-CA3-CA4-OA6
52	A	402	PC1	C21-C22-C23-C24
53	o	202	CDL	C64-C65-C66-C67
53	o	202	CDL	C20-C21-C22-C23
53	V	204	CDL	OB6-CB4-CB6-OB8
51	L	701	3PE	C1-C2-C3-O31
52	M	502	PC1	C2B-C2C-C2D-C2E
53	V	204	CDL	C13-C14-C15-C16
53	V	204	CDL	C77-C78-C79-C80
53	W	201	CDL	C14-C15-C16-C17
51	6	503	3PE	O13-C11-C12-N
51	A	403	3PE	C1-O11-P-O12
51	J	201	3PE	C1-O11-P-O13
51	J	201	3PE	C1-O11-P-O14
51	L	702	3PE	C11-O13-P-O11
51	L	702	3PE	C11-O13-P-O14
51	M	501	3PE	C1-O11-P-O14
51	N	401	3PE	C11-O13-P-O14
51	V	201	3PE	C1-O11-P-O14
51	V	201	3PE	C11-O13-P-O14
51	V	201	3PE	O13-C11-C12-N
51	V	202	3PE	C1-O11-P-O12
51	V	202	3PE	C1-O11-P-O13
51	V	202	3PE	C1-O11-P-O14
51	V	202	3PE	C11-O13-P-O11
51	V	202	3PE	C11-O13-P-O14
52	9	401	PC1	C11-O13-P-O12
52	A	401	PC1	C11-O13-P-O14
52	A	401	PC1	C1-O11-P-O14
52	L	703	PC1	C1-O11-P-O14
53	L	704	CDL	CA2-OA2-PA1-OA3
53	L	704	CDL	CB2-OB2-PB2-OB3
53	L	704	CDL	CB3-OB5-PB2-OB4
53	V	203	CDL	CA2-OA2-PA1-OA3
53	V	203	CDL	CA2-OA2-PA1-OA5

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Mol	Chain	Res	Type	Atoms
53	V	203	CDL	CA3-OA5-PA1-OA4
53	V	203	CDL	CB2-OB2-PB2-OB5
53	V	203	CDL	CB3-OB5-PB2-OB2
53	V	204	CDL	CA2-OA2-PA1-OA3
53	V	204	CDL	CA2-OA2-PA1-OA5
53	V	204	CDL	CB2-OB2-PB2-OB3
53	V	204	CDL	CB3-OB5-PB2-OB4
53	W	201	CDL	CB2-OB2-PB2-OB4
53	W	201	CDL	CB3-OB5-PB2-OB4
53	Y	201	CDL	CB2-OB2-PB2-OB3
53	i	202	CDL	CA2-OA2-PA1-OA4
53	o	201	CDL	CB3-OB5-PB2-OB3
56	d	401	NDP	C5B-O5B-PA-O1A
46	l	502	FMN	C4'-C5'-O5'-P
51	A	403	3PE	C2-C1-O11-P
53	L	704	CDL	CA4-CA3-OA5-PA1
53	V	203	CDL	CA4-CA3-OA5-PA1
53	i	202	CDL	C1-CB2-OB2-PB2
54	g	201	ZMP	C1-C2-C3-C4
51	i	201	3PE	C37-C38-C39-C3A
53	o	201	CDL	CA7-C31-C32-C33
53	o	201	CDL	OA5-CA3-CA4-CA6
53	V	204	CDL	C51-C52-C53-C54
52	A	401	PC1	O11-C1-C2-O21
53	L	704	CDL	C18-C19-C20-C21
53	o	202	CDL	C1-CA2-OA2-PA1
52	A	401	PC1	O31-C31-C32-C33
51	L	701	3PE	C25-C26-C27-C28
52	L	703	PC1	C2A-C2B-C2C-C2D
51	6	503	3PE	C26-C27-C28-C29
51	l	501	3PE	C21-C22-C23-C24
53	L	704	CDL	C58-C59-C60-C61
56	d	401	NDP	PN-O3-PA-O2A
51	6	503	3PE	C25-C26-C27-C28
53	o	202	CDL	C63-C64-C65-C66
53	Y	201	CDL	C32-C33-C34-C35
51	A	403	3PE	O11-C1-C2-C3
51	M	501	3PE	C34-C35-C36-C37
53	W	201	CDL	C15-C16-C17-C18
53	V	204	CDL	C19-C20-C21-C22
52	A	401	PC1	C25-C26-C27-C28
53	L	704	CDL	C80-C81-C82-C83

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Mol	Chain	Res	Type	Atoms
54	g	201	ZMP	C4-C5-C6-C7
47	l	503	NAI	O4D-C1D-N1N-C2N
56	d	401	NDP	O4D-C1D-N1N-C6N
51	L	702	3PE	C26-C27-C28-C29
51	L	702	3PE	C2-C1-O11-P
53	Y	201	CDL	C1-CB2-OB2-PB2
53	o	202	CDL	CB4-CB3-OB5-PB2
53	Y	201	CDL	C56-C57-C58-C59
52	M	502	PC1	O32-C31-C32-C33
52	9	401	PC1	C25-C26-C27-C28
51	L	705	3PE	C1-C2-O21-C21
52	9	401	PC1	C3-C2-O21-C21
52	L	703	PC1	C1-C2-O21-C21
53	o	201	CDL	CB6-CB4-OB6-CB5
53	L	704	CDL	OA5-CA3-CA4-OA6
54	X	101	ZMP	O2-C13-C14-C15
53	W	201	CDL	O1-C1-CA2-OA2
52	w	801	PC1	C31-C32-C33-C34
53	W	201	CDL	C22-C23-C24-C25
53	Y	201	CDL	C14-C15-C16-C17
53	i	202	CDL	OB6-CB4-CB6-OB8
47	l	503	NAI	C2N-C3N-C7N-N7N
51	A	403	3PE	C2A-C2B-C2C-C2D
53	o	201	CDL	C72-C73-C74-C75
53	L	704	CDL	C84-C85-C86-C87
53	o	201	CDL	O1-C1-CA2-OA2
51	K	101	3PE	C2-C1-O11-P
53	i	202	CDL	CB4-CB3-OB5-PB2
52	w	801	PC1	C37-C38-C39-C3A
51	M	501	3PE	C1-C2-C3-O31
53	V	204	CDL	CA3-CA4-CA6-OA8
53	i	202	CDL	C32-C33-C34-C35
53	V	203	CDL	OA5-CA3-CA4-OA6
51	6	503	3PE	C33-C34-C35-C36
51	L	705	3PE	C25-C26-C27-C28
51	i	201	3PE	C3A-C3B-C3C-C3D
51	i	201	3PE	C35-C36-C37-C38
53	V	203	CDL	OA5-CA3-CA4-CA6
53	W	201	CDL	OB6-CB4-CB6-OB8
52	A	402	PC1	O22-C21-C22-C23
51	p	201	3PE	C23-C24-C25-C26
51	L	701	3PE	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
52	M	502	PC1	C2F-C2G-C2H-C2I
52	9	401	PC1	C23-C24-C25-C26
47	1	503	NAI	C2D-C1D-N1N-C2N
51	L	705	3PE	C1-C2-C3-O31
52	w	801	PC1	C28-C29-C2A-C2B
52	A	402	PC1	C24-C25-C26-C27
53	o	201	CDL	C14-C15-C16-C17
52	9	401	PC1	C12-C11-O13-P
54	X	101	ZMP	C16-C17-C18-C19
52	M	502	PC1	C2C-C2D-C2E-C2F
57	k	501	AMP	C2'-C1'-N9-C4
57	k	501	AMP	O4'-C1'-N9-C8
51	M	501	3PE	O21-C2-C3-O31
53	L	704	CDL	OA6-CA4-CA6-OA8
51	L	701	3PE	O21-C21-C22-C23
53	Y	201	CDL	C12-C11-CA5-OA6
51	i	201	3PE	O11-C1-C2-C3
52	A	401	PC1	O11-C1-C2-C3
52	A	402	PC1	O11-C1-C2-C3
53	L	704	CDL	C37-C38-C39-C40
53	W	201	CDL	C16-C17-C18-C19
51	V	202	3PE	C26-C27-C28-C29
54	X	101	ZMP	O4-C17-C18-C19
53	W	201	CDL	C52-C53-C54-C55
51	6	503	3PE	C2D-C2E-C2F-C2G
56	d	401	NDP	PN-O3-PA-O1A
51	A	403	3PE	O21-C21-C22-C23
52	L	703	PC1	O31-C31-C32-C33
51	6	503	3PE	C3D-C3E-C3F-C3G
52	M	502	PC1	C23-C24-C25-C26
53	V	204	CDL	C22-C23-C24-C25
54	X	101	ZMP	N1-C13-C14-C15
53	L	704	CDL	C20-C21-C22-C23
53	V	204	CDL	C52-C51-CB5-OB6
53	Y	201	CDL	C31-C32-C33-C34
51	L	705	3PE	O21-C21-C22-C23
51	J	201	3PE	C26-C27-C28-C29
51	i	201	3PE	O21-C21-C22-C23
53	V	204	CDL	C35-C36-C37-C38
53	o	201	CDL	C72-C71-CB7-OB8
51	J	201	3PE	O31-C31-C32-C33
51	L	705	3PE	O31-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
53	i	202	CDL	C12-C11-CA5-OA6
53	i	202	CDL	C52-C51-CB5-OB6
53	W	201	CDL	C12-C11-CA5-OA6
51	A	403	3PE	C3C-C3D-C3E-C3F
51	V	202	3PE	O31-C31-C32-C33
53	L	704	CDL	C32-C31-CA7-OA8
52	M	502	PC1	C25-C26-C27-C28
51	N	401	3PE	C3-C2-O21-C21
53	o	202	CDL	CB6-CB4-OB6-CB5
51	L	701	3PE	O31-C31-C32-C33
53	V	203	CDL	C32-C31-CA7-OA8
51	L	702	3PE	C3B-C3C-C3D-C3E
53	Y	201	CDL	C57-C58-C59-C60
51	N	401	3PE	O31-C31-C32-C33
54	X	101	ZMP	C13-C14-C15-N2
53	o	201	CDL	CA4-CA3-OA5-PA1
57	k	501	AMP	C4'-C5'-O5'-P
51	N	401	3PE	C35-C36-C37-C38
51	i	201	3PE	O11-C1-C2-O21
52	A	401	PC1	C23-C24-C25-C26
53	W	201	CDL	C19-C20-C21-C22
51	i	201	3PE	O22-C21-C22-C23
53	V	204	CDL	C52-C51-CB5-OB7
53	i	202	CDL	C12-C11-CA5-OA7
53	V	203	CDL	CA5-C11-C12-C13
53	L	704	CDL	C32-C31-CA7-OA9
53	V	203	CDL	C32-C31-CA7-OA9
51	L	701	3PE	O22-C21-C22-C23
53	Y	201	CDL	C12-C11-CA5-OA7
51	A	403	3PE	O22-C21-C22-C23
51	L	705	3PE	O32-C31-C32-C33
53	o	201	CDL	C72-C71-CB7-OB9
51	L	702	3PE	C23-C24-C25-C26
53	V	203	CDL	C41-C42-C43-C44
53	o	201	CDL	C73-C74-C75-C76
52	L	703	PC1	C3E-C3F-C3G-C3H
53	o	202	CDL	C74-C75-C76-C77
54	X	101	ZMP	N2-C16-C17-O4
58	s	201	MYR	C11-C10-C9-C8
51	L	705	3PE	O22-C21-C22-C23
51	V	202	3PE	O32-C31-C32-C33
51	M	501	3PE	C27-C28-C29-C2A

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Mol	Chain	Res	Type	Atoms
52	9	401	PC1	O31-C31-C32-C33
53	V	204	CDL	C32-C31-CA7-OA8
53	V	204	CDL	C32-C31-CA7-OA9
51	p	201	3PE	O21-C21-C22-C23
52	M	502	PC1	O21-C21-C22-C23
53	V	203	CDL	C44-C45-C46-C47
52	9	401	PC1	C3D-C3E-C3F-C3G
47	1	503	NAI	PN-O3-PA-O2A
47	1	503	NAI	PA-O3-PN-O1N
51	N	401	3PE	O32-C31-C32-C33
53	i	202	CDL	C52-C51-CB5-OB7
53	i	202	CDL	CB7-C71-C72-C73
51	M	501	3PE	C23-C24-C25-C26
53	V	203	CDL	C72-C71-CB7-OB8
51	J	201	3PE	O32-C31-C32-C33

There are no ring outliers.

30 monomers are involved in 79 short contacts:

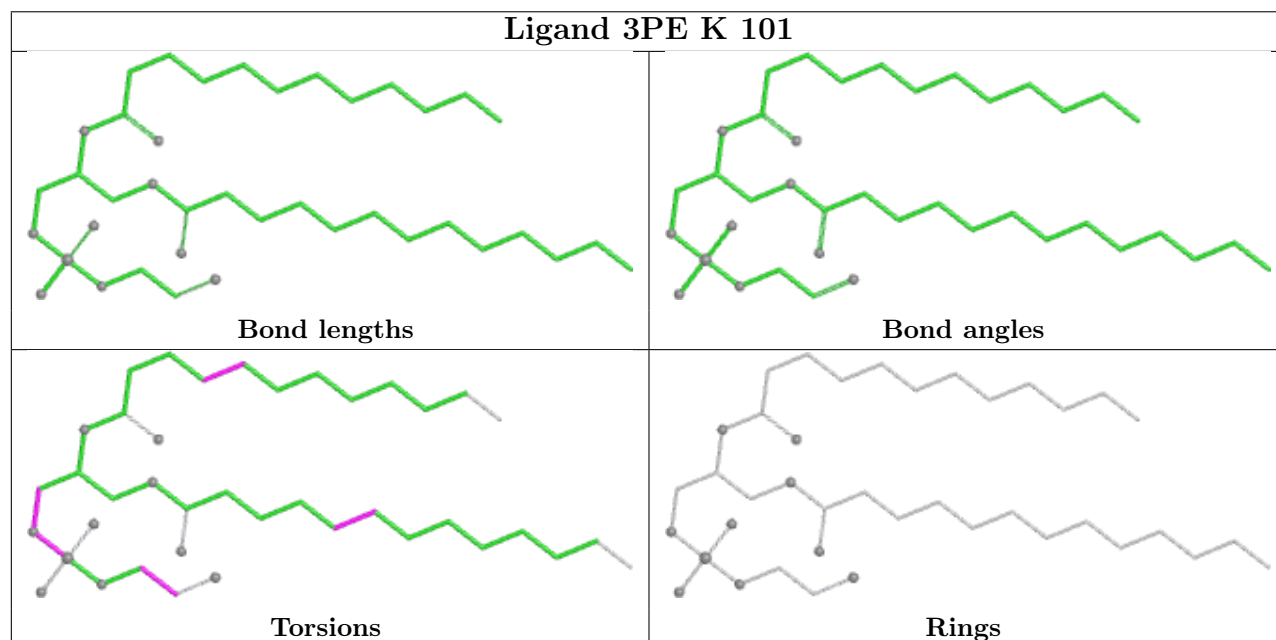
Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	3	801	SF4	1	0
45	1	501	SF4	1	0
51	K	101	3PE	1	0
51	V	202	3PE	2	0
53	W	201	CDL	8	0
53	i	202	CDL	1	0
54	X	101	ZMP	1	0
51	L	702	3PE	2	0
52	9	401	PC1	2	0
46	1	502	FMN	2	0
51	J	201	3PE	3	0
45	6	502	SF4	1	0
51	N	401	3PE	2	0
52	M	502	PC1	4	0
52	L	703	PC1	4	0
51	L	701	3PE	1	0
53	V	204	CDL	8	0
53	o	202	CDL	9	0
52	w	801	PC1	4	0
53	V	203	CDL	5	0
51	M	501	3PE	2	0
51	i	201	3PE	1	0

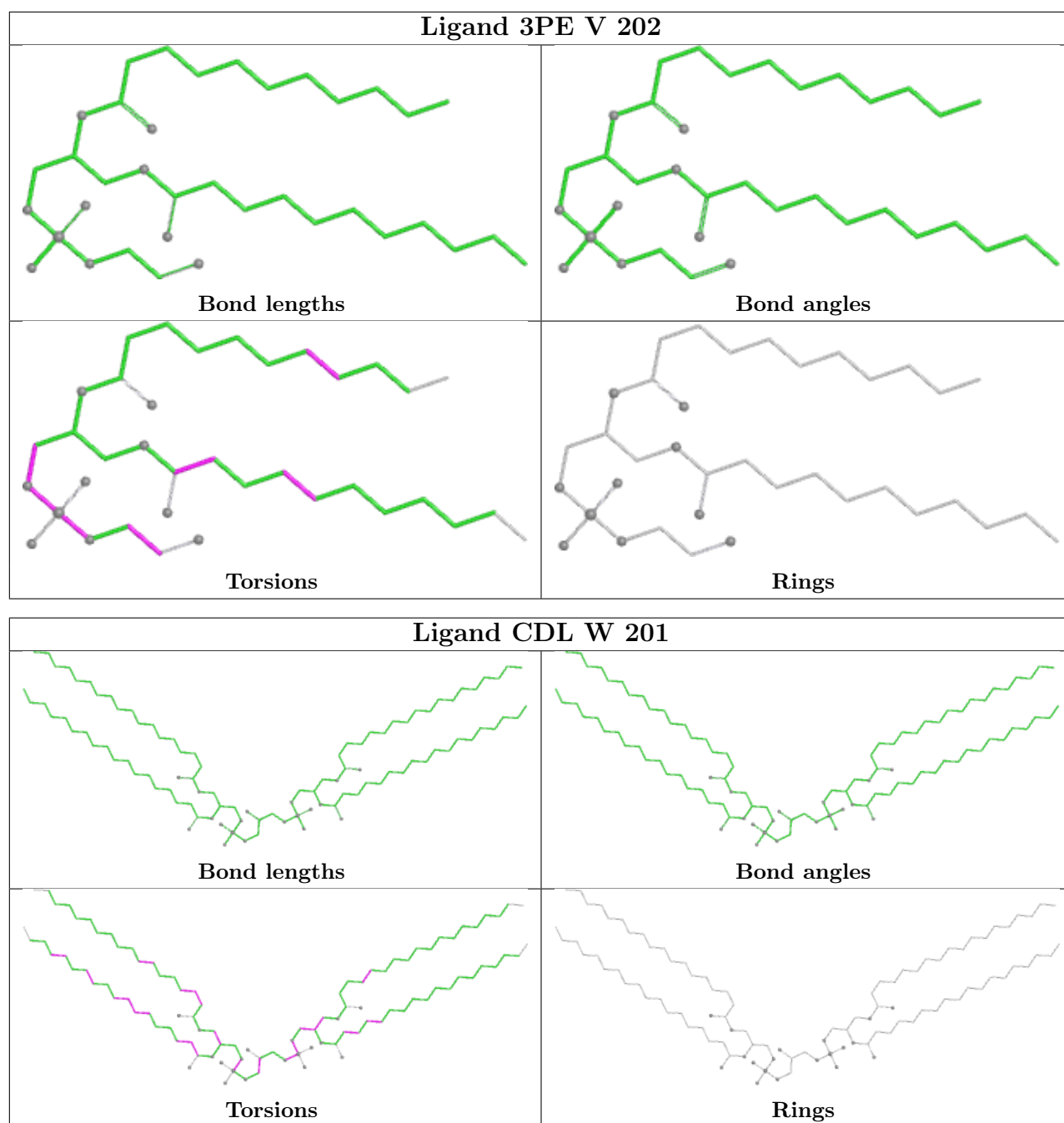
Continued on next page...

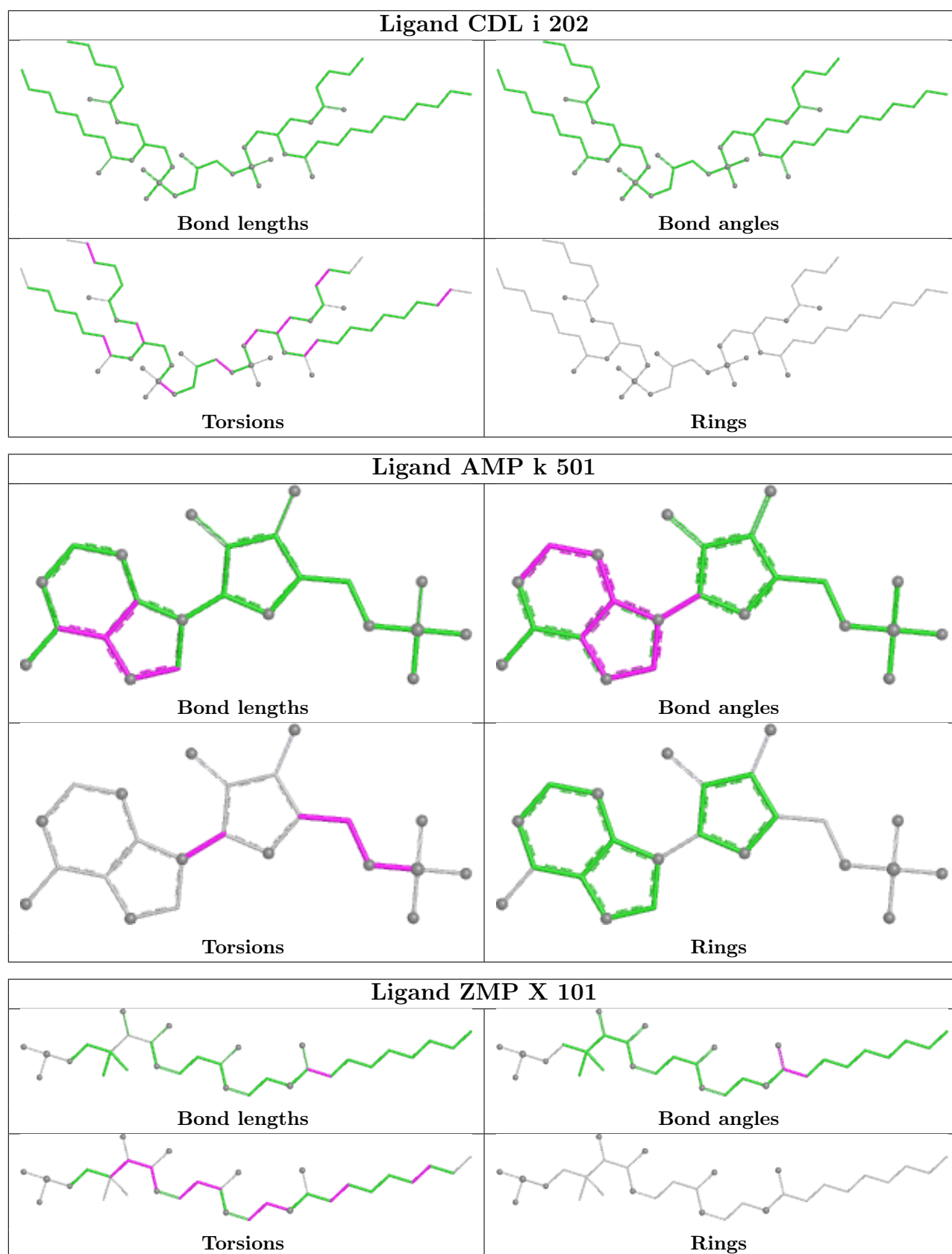
Continued from previous page...

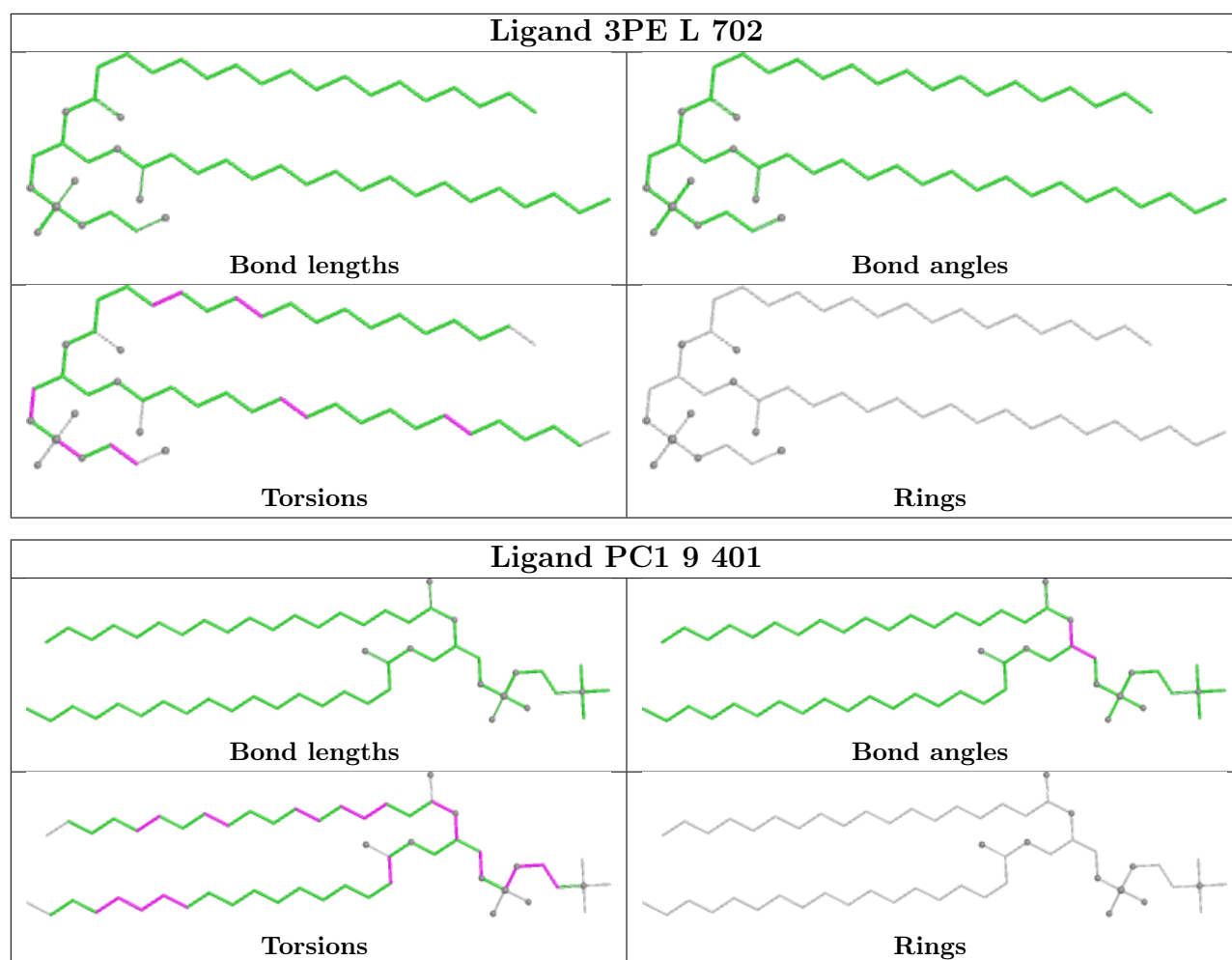
Mol	Chain	Res	Type	Clashes	Symm-Clashes
53	L	704	CDL	7	0
48	2	300	FES	1	0
47	1	503	NAI	5	0
52	A	401	PC1	1	0
53	o	201	CDL	2	0
53	Y	201	CDL	7	0
51	6	503	3PE	1	0
56	d	401	NDP	1	0

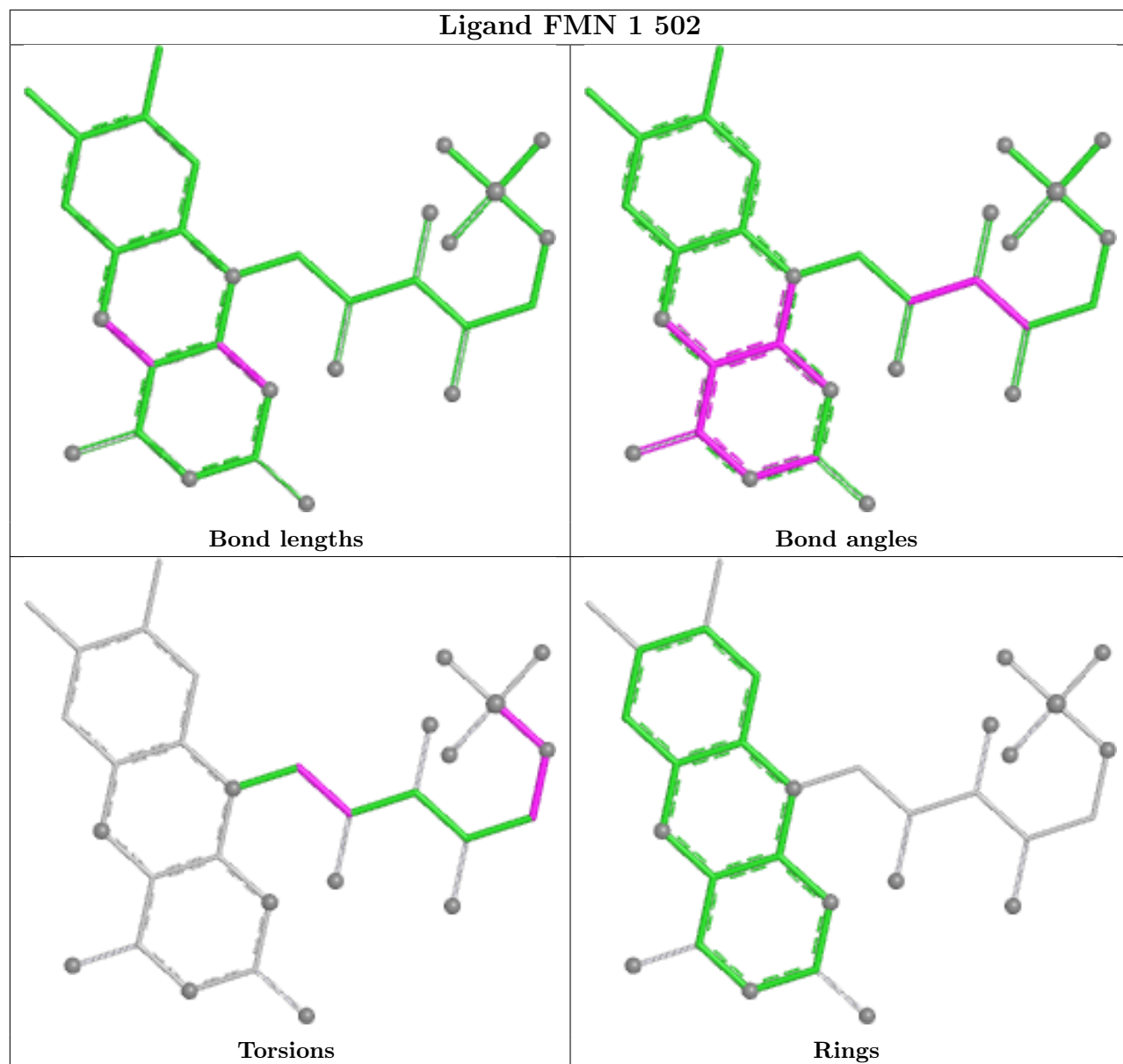
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

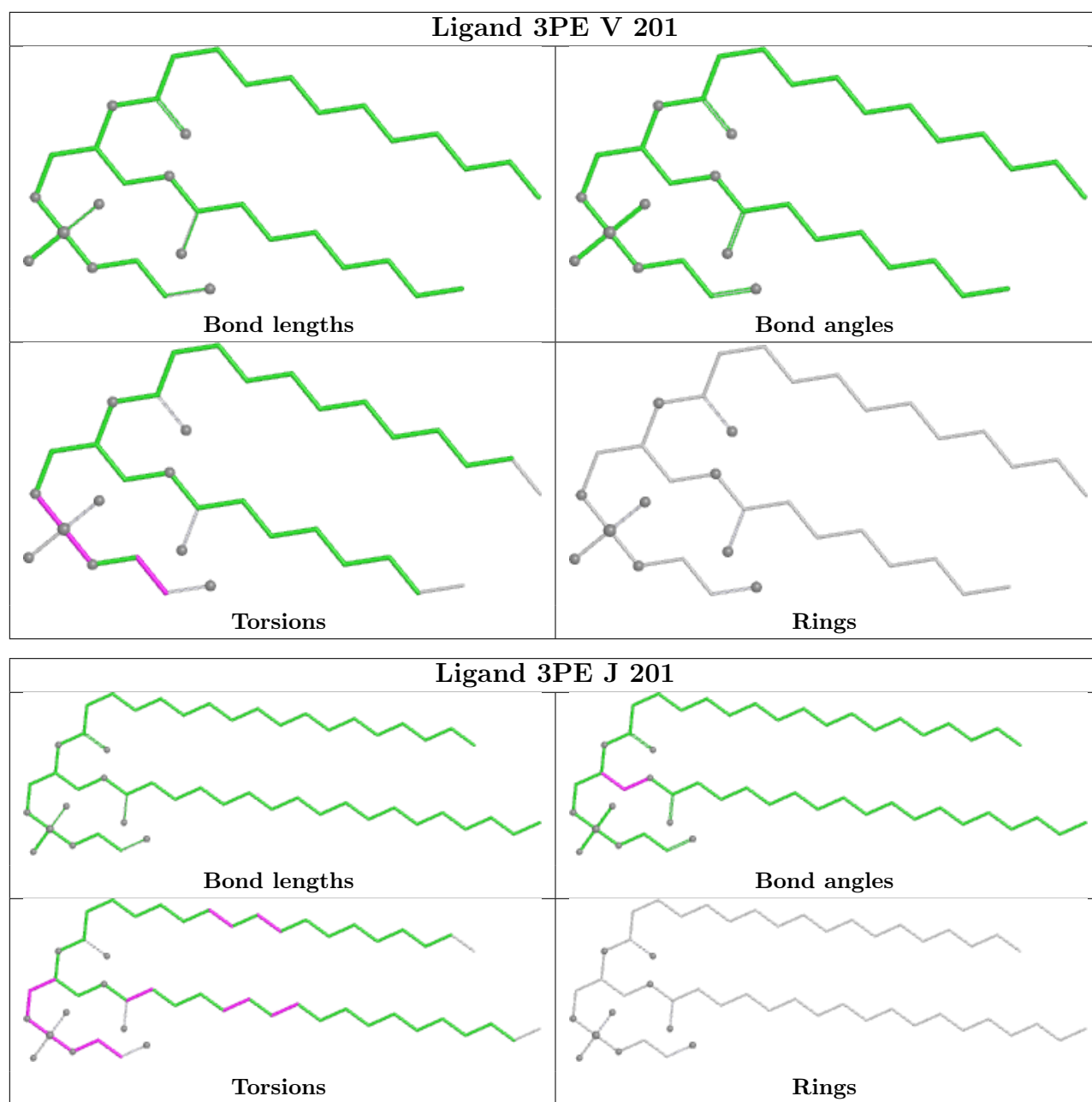


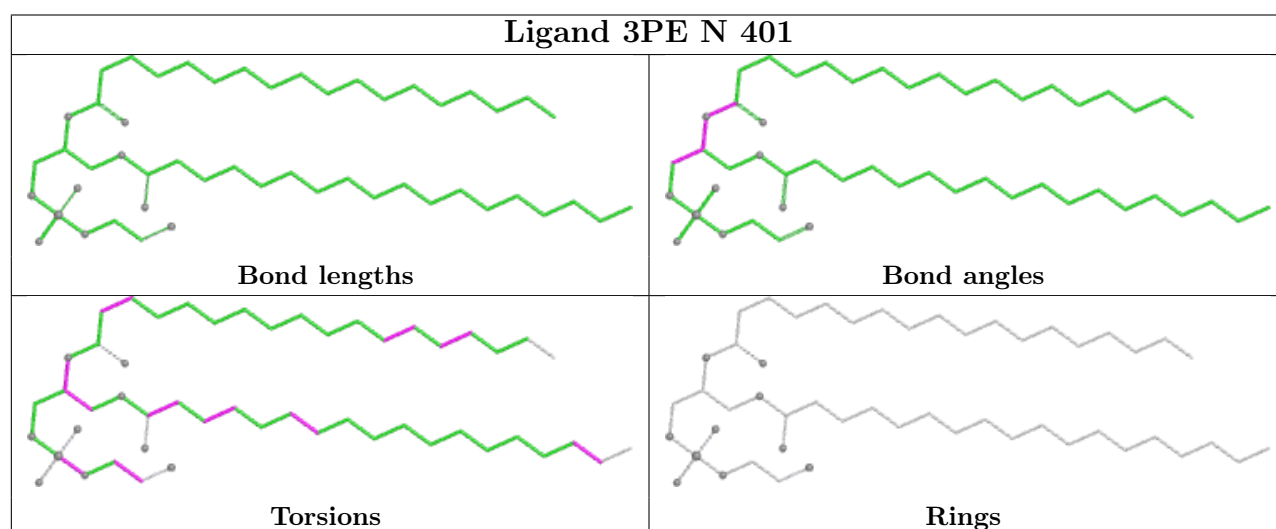
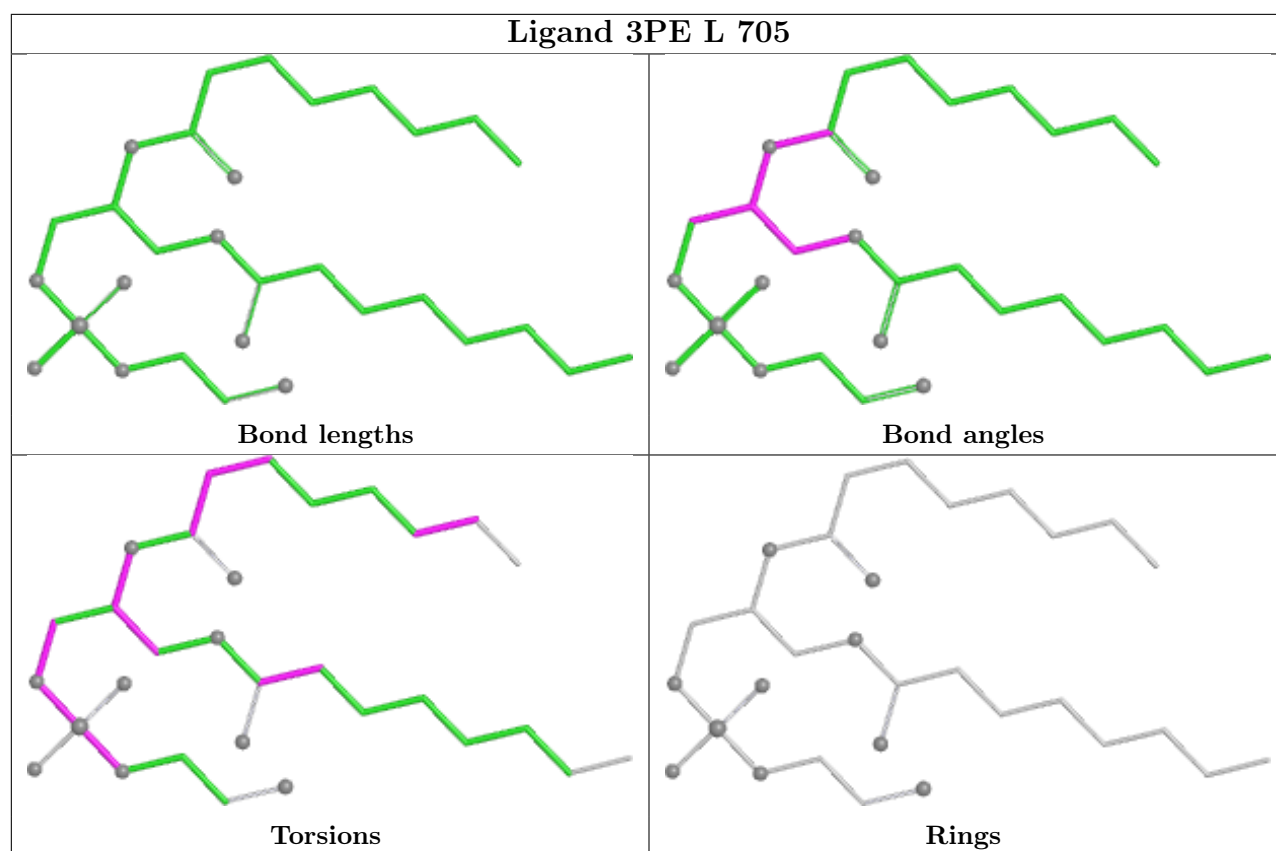


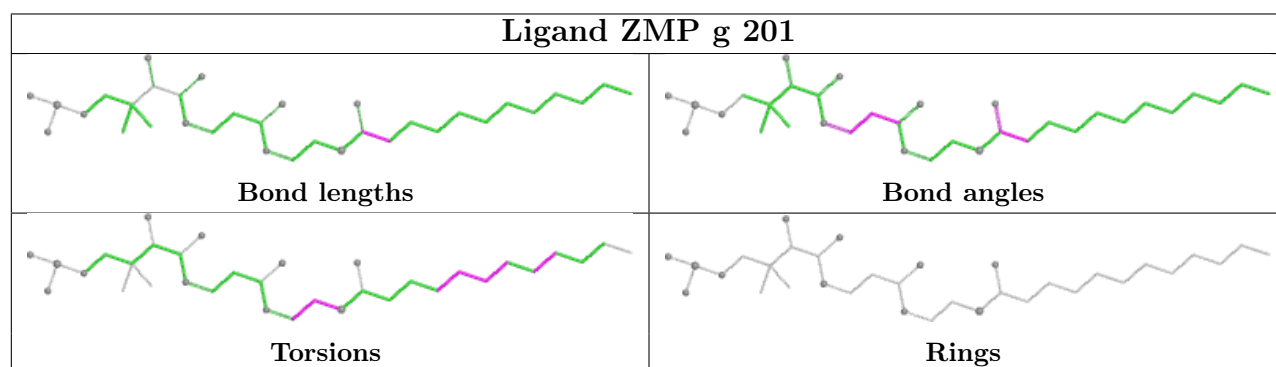
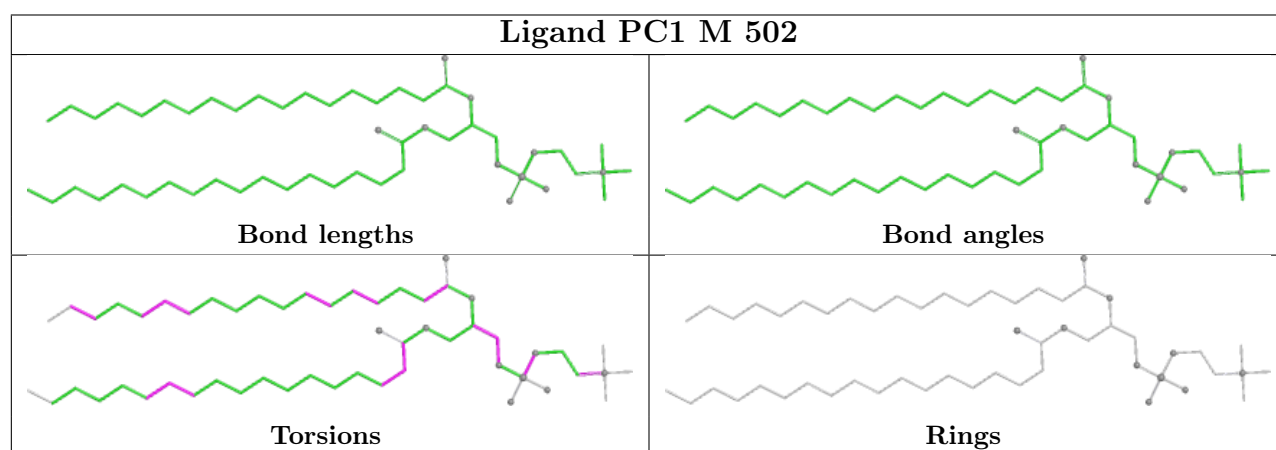
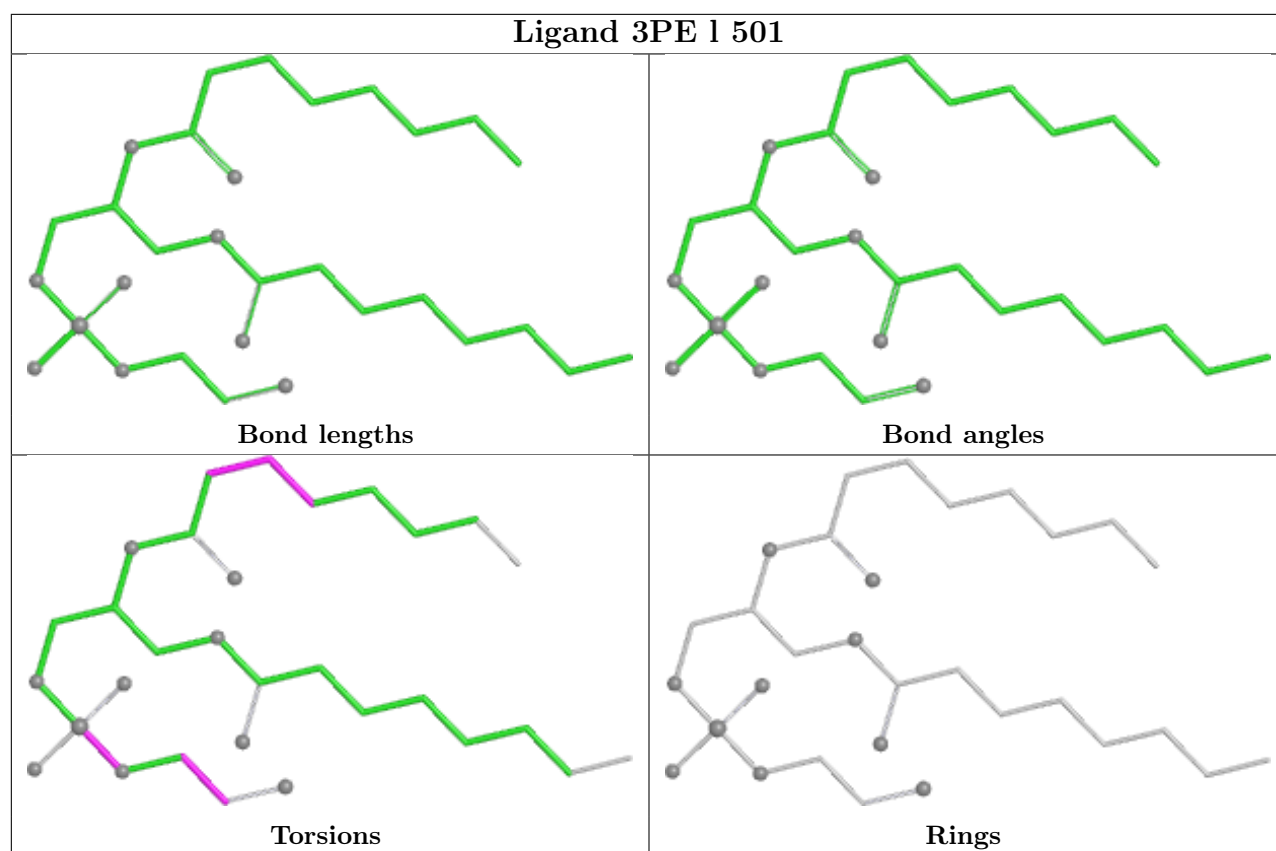


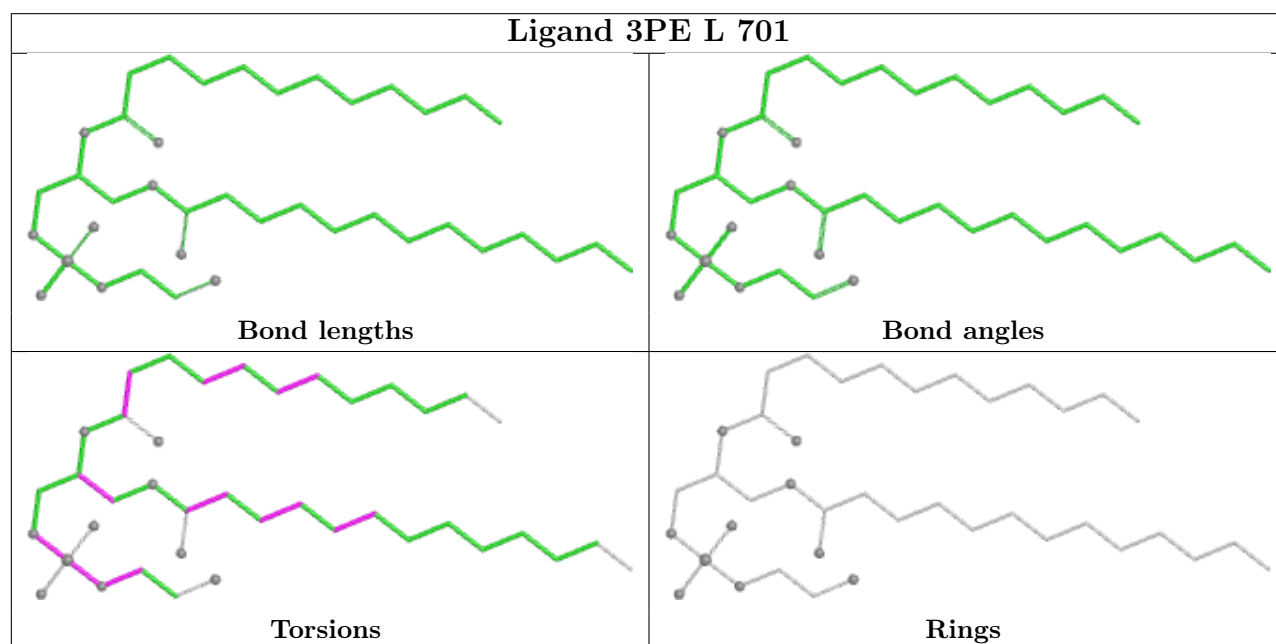
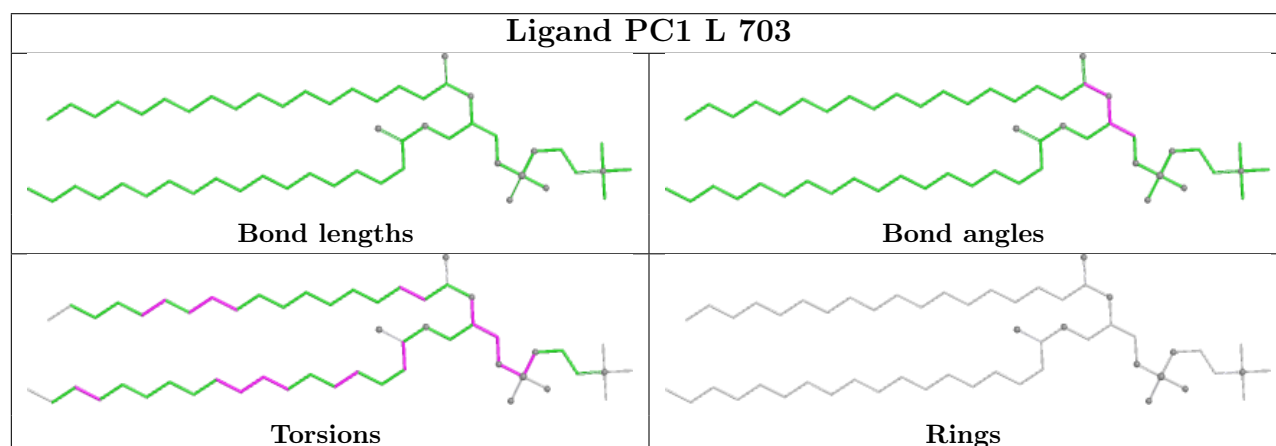
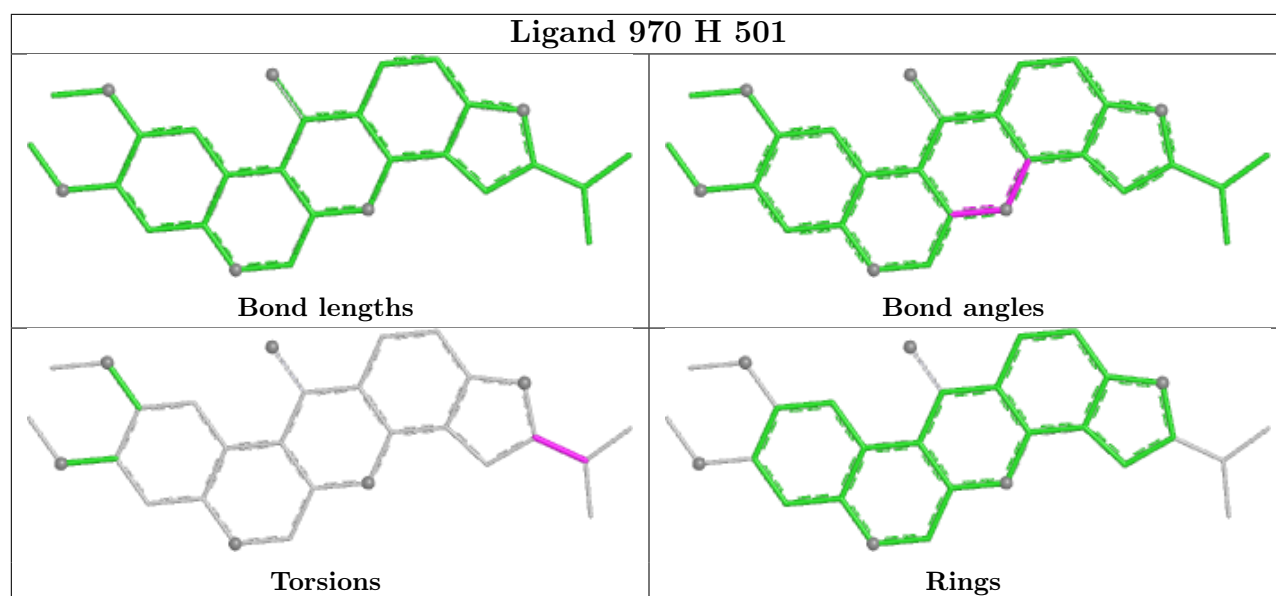


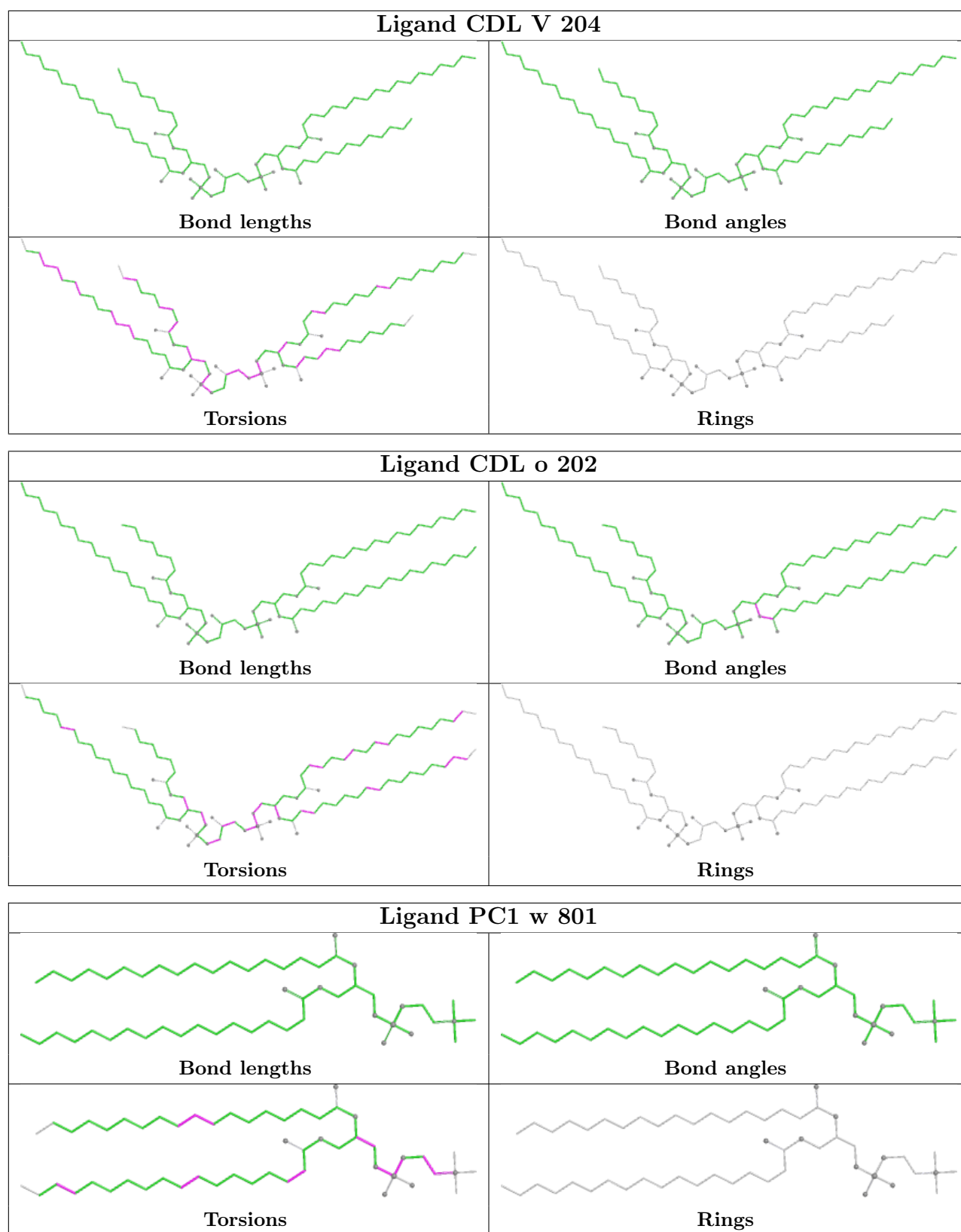


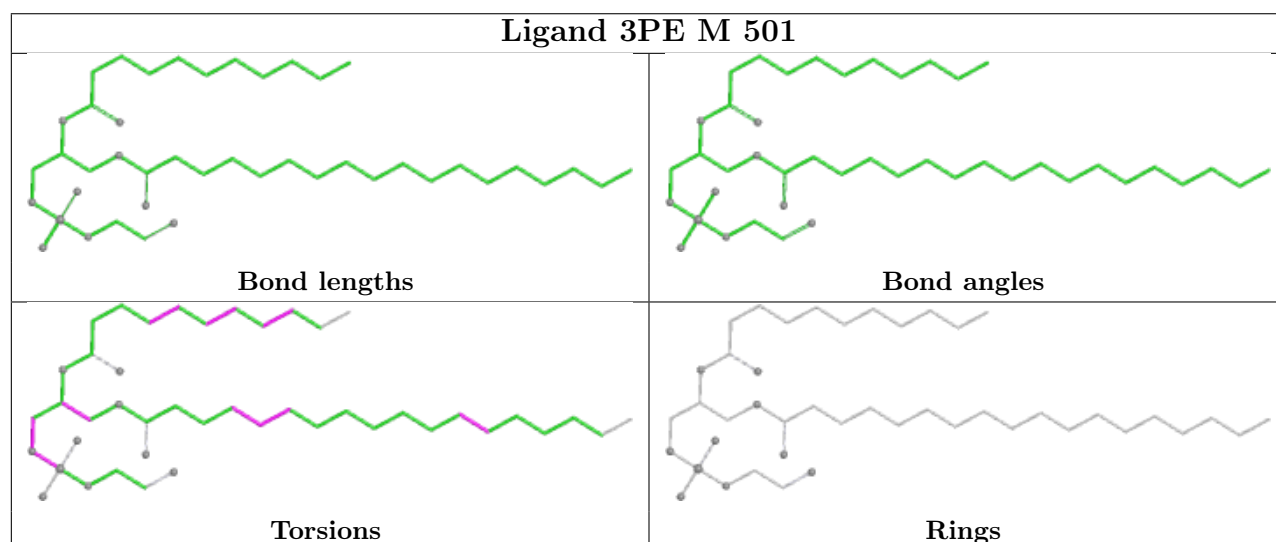
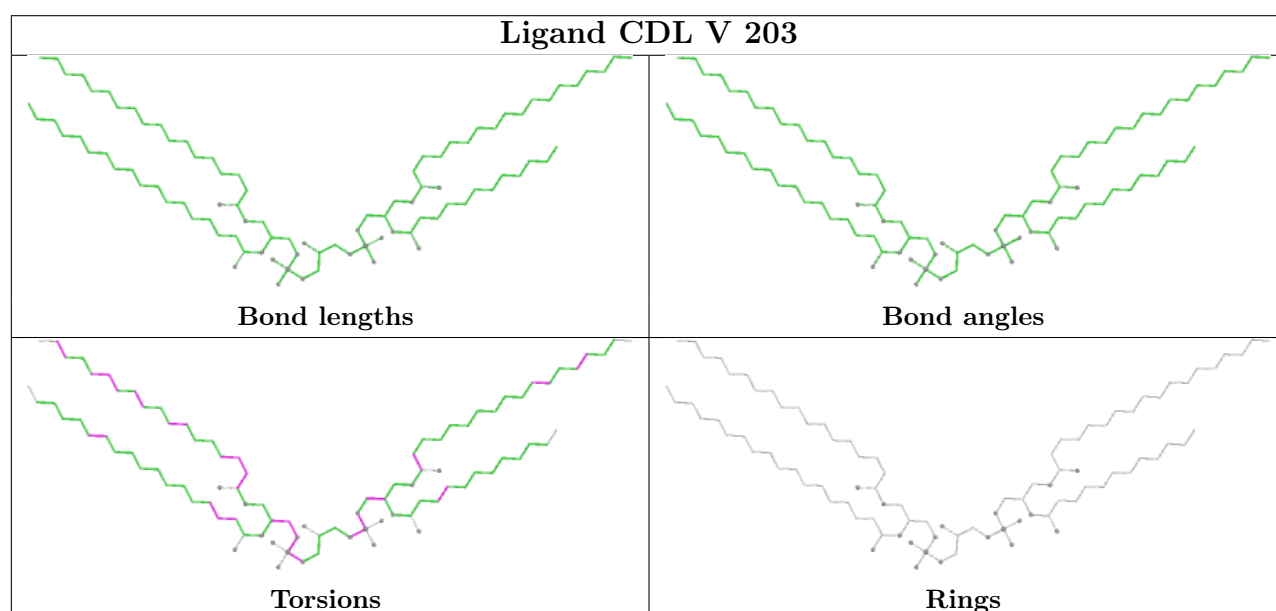
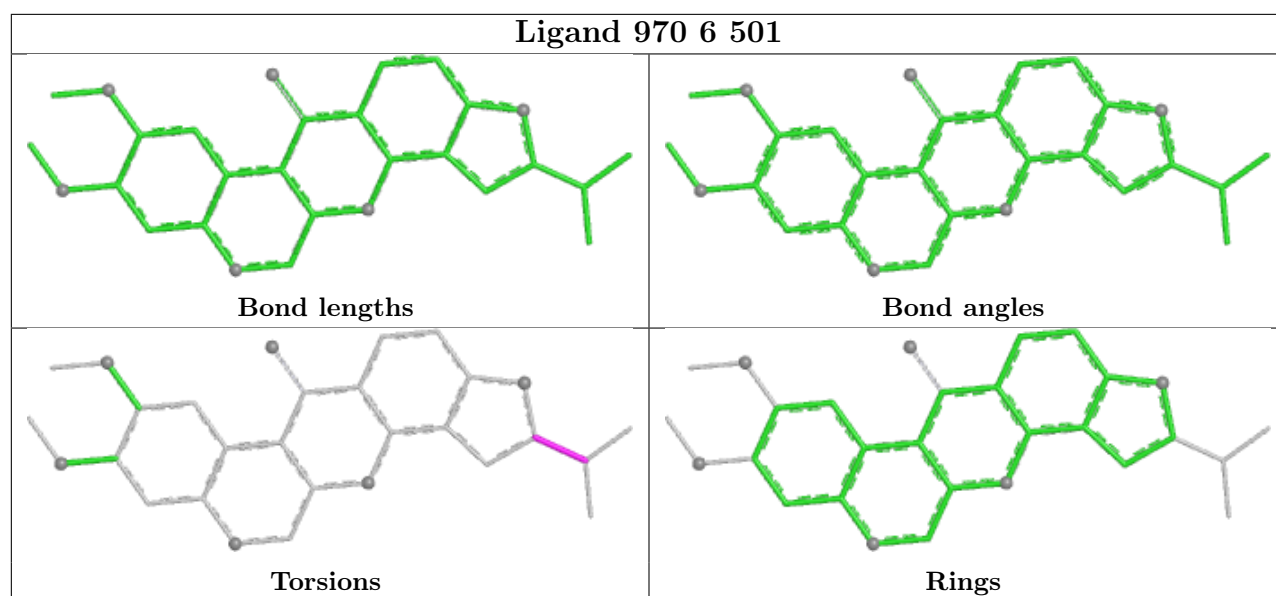


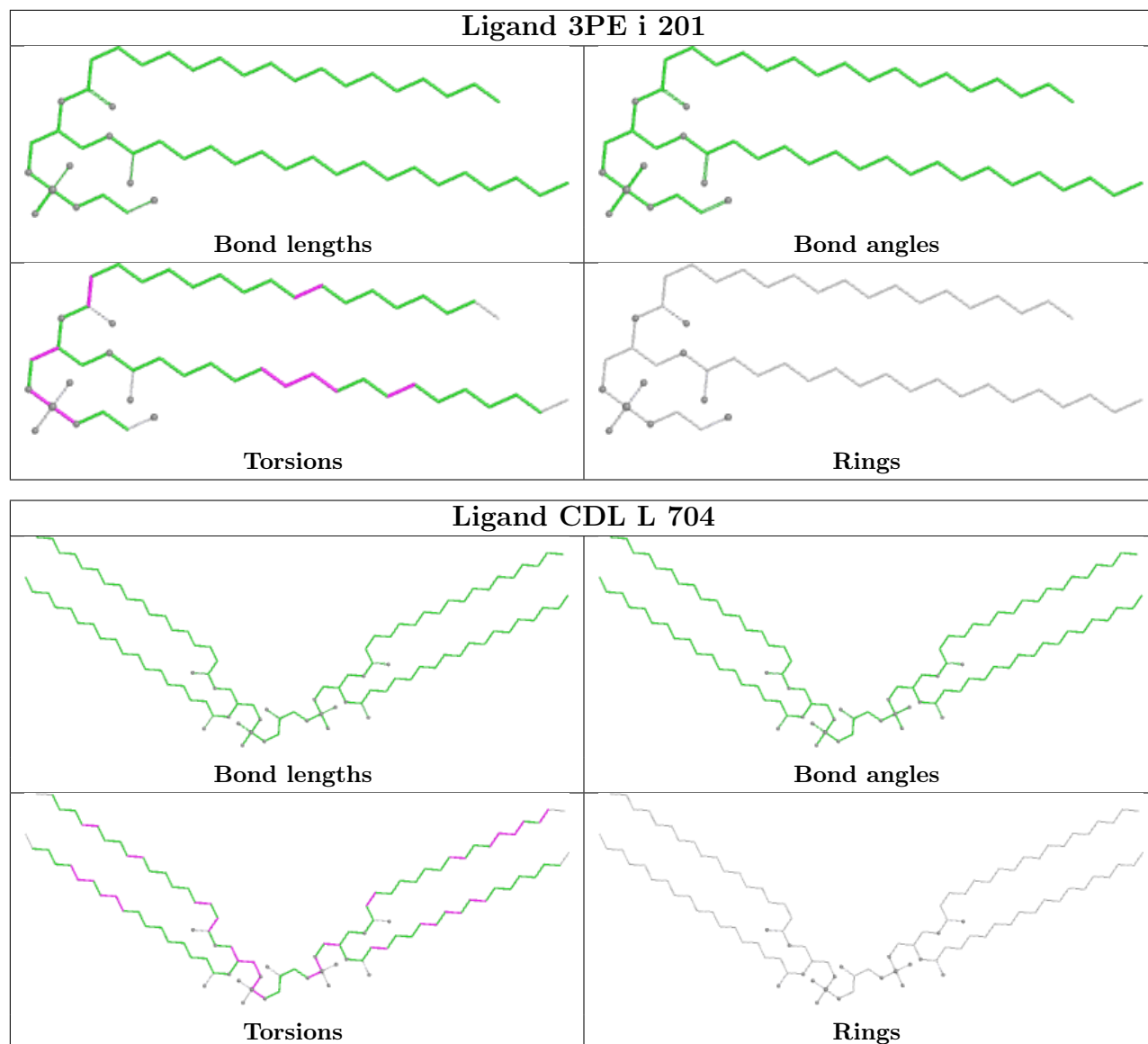


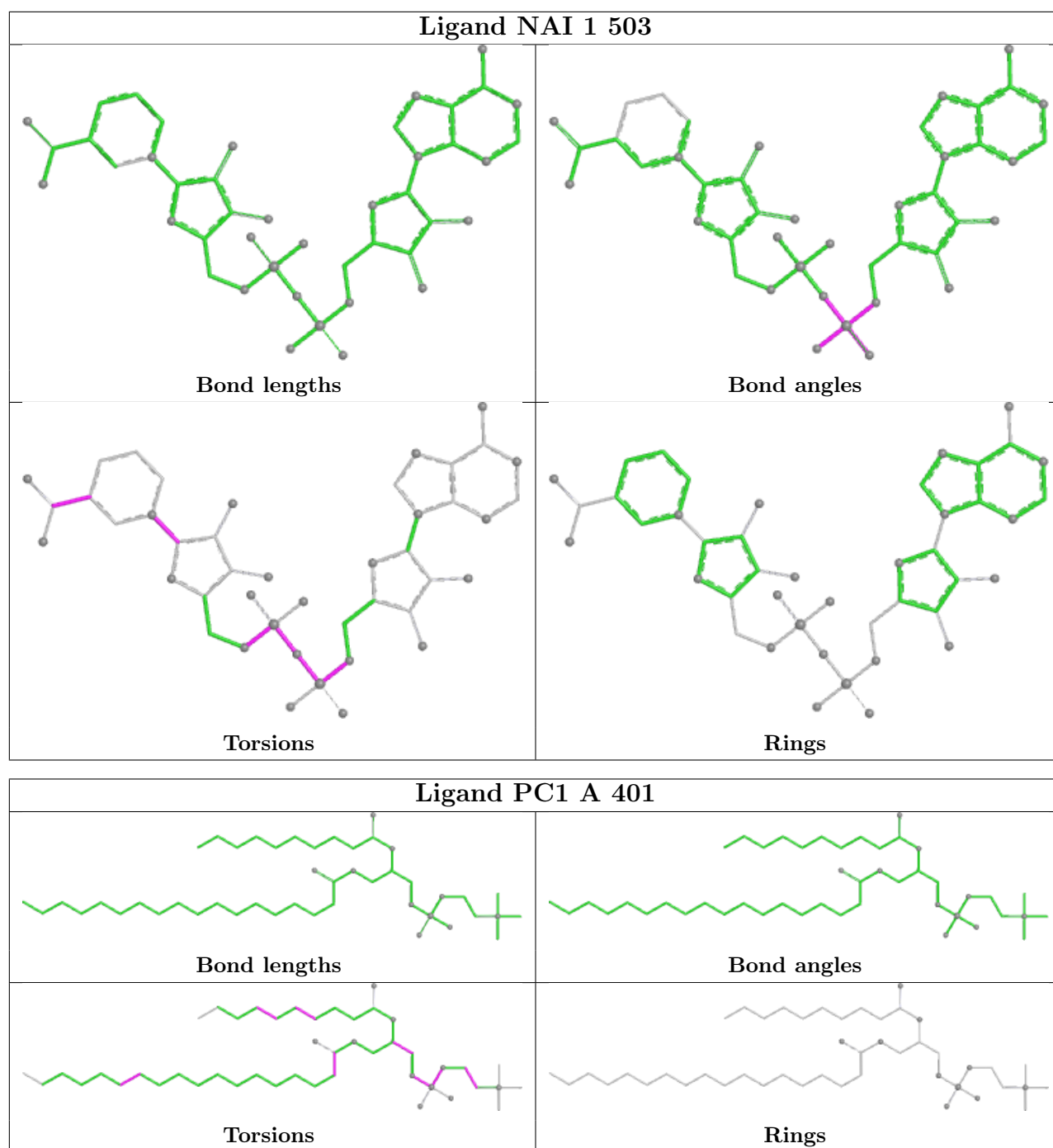


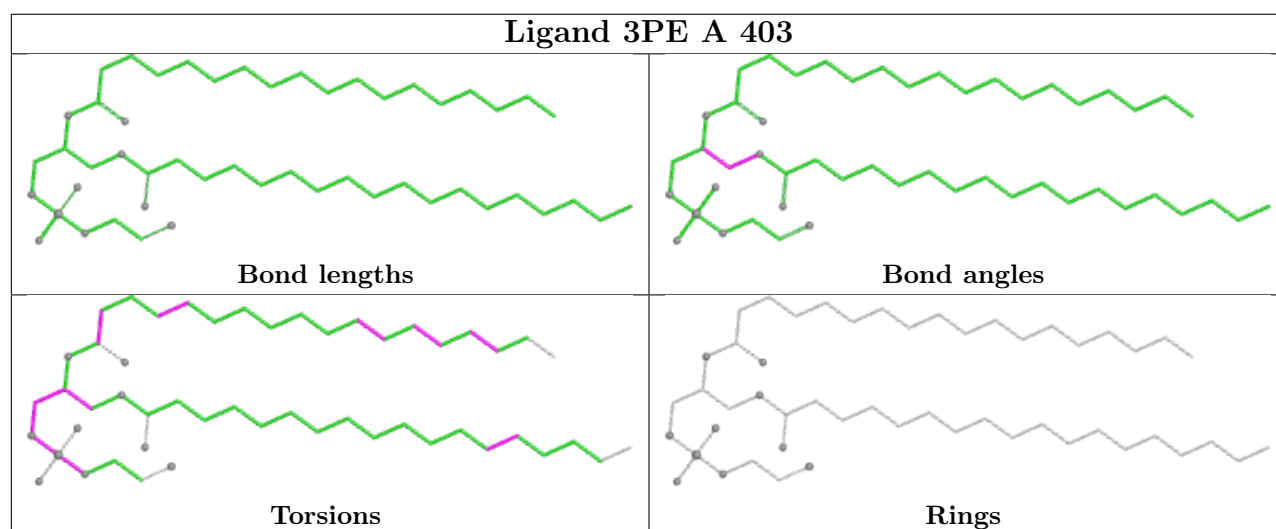
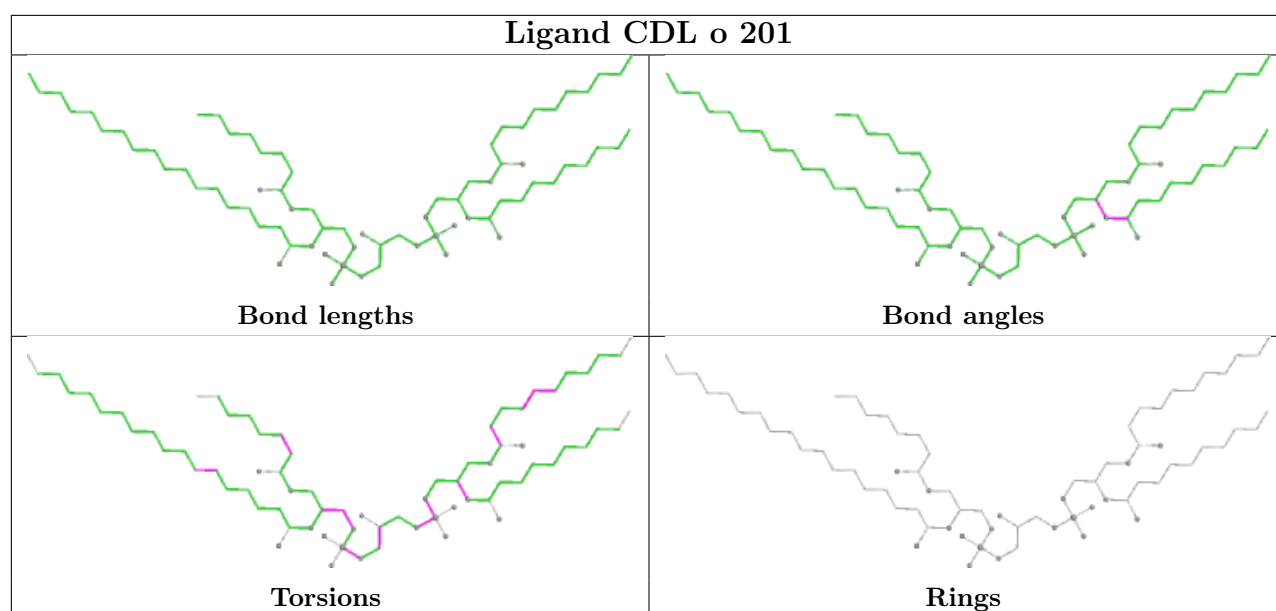
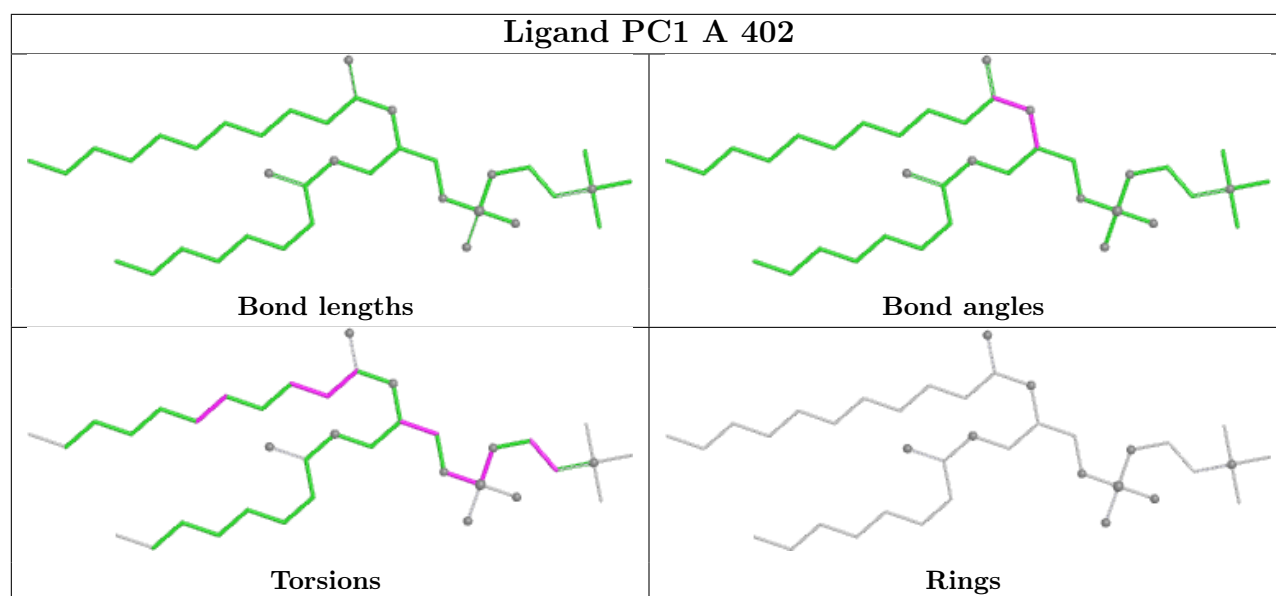


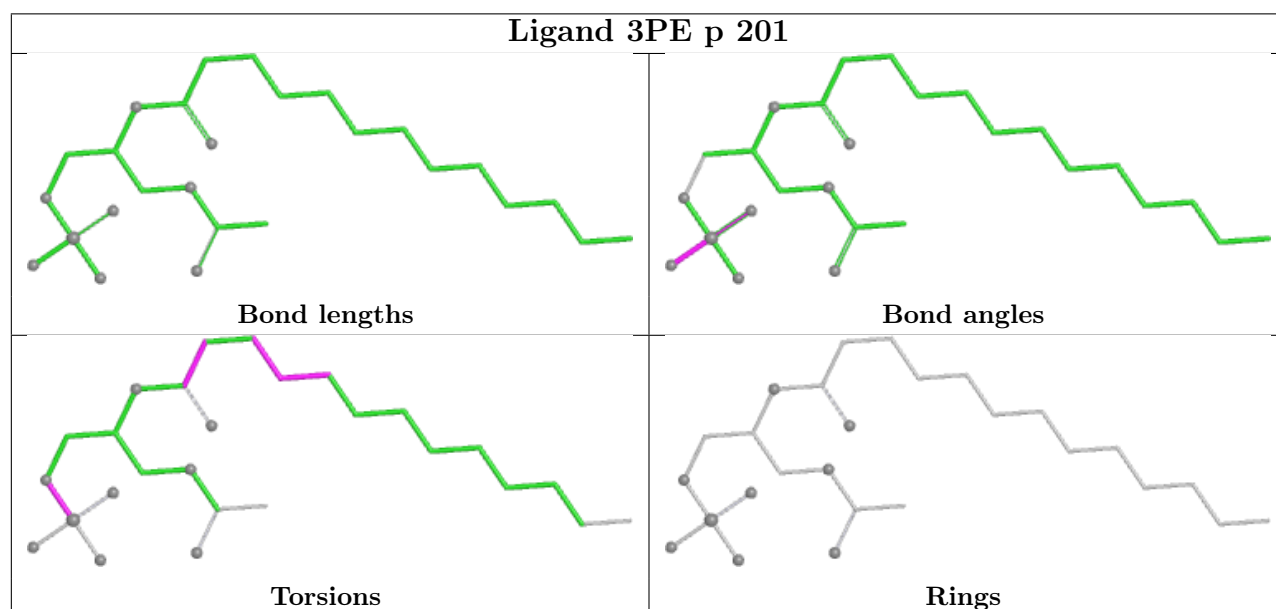
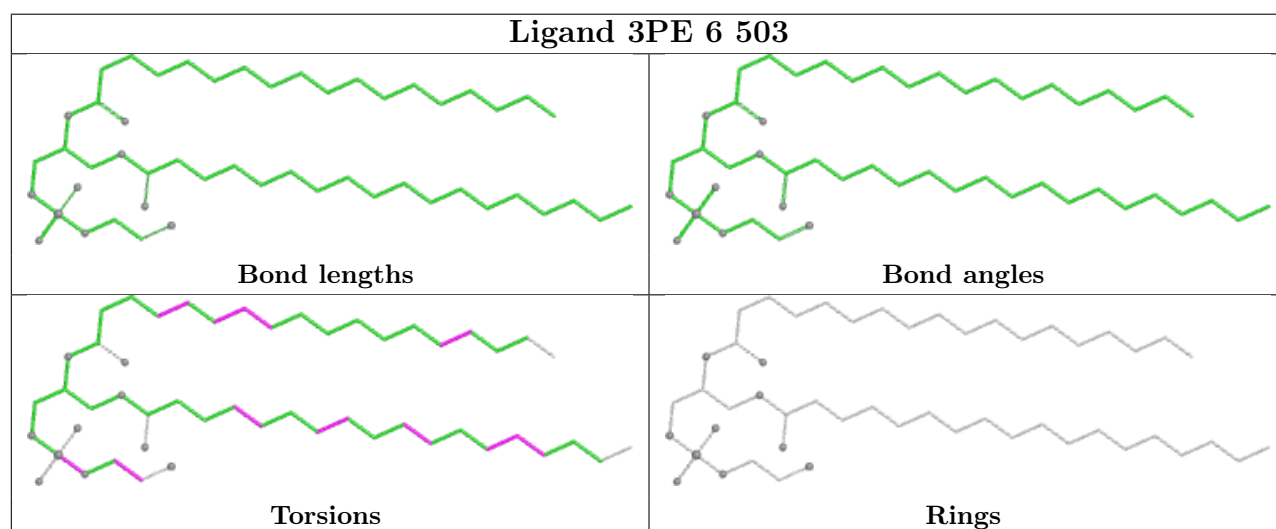
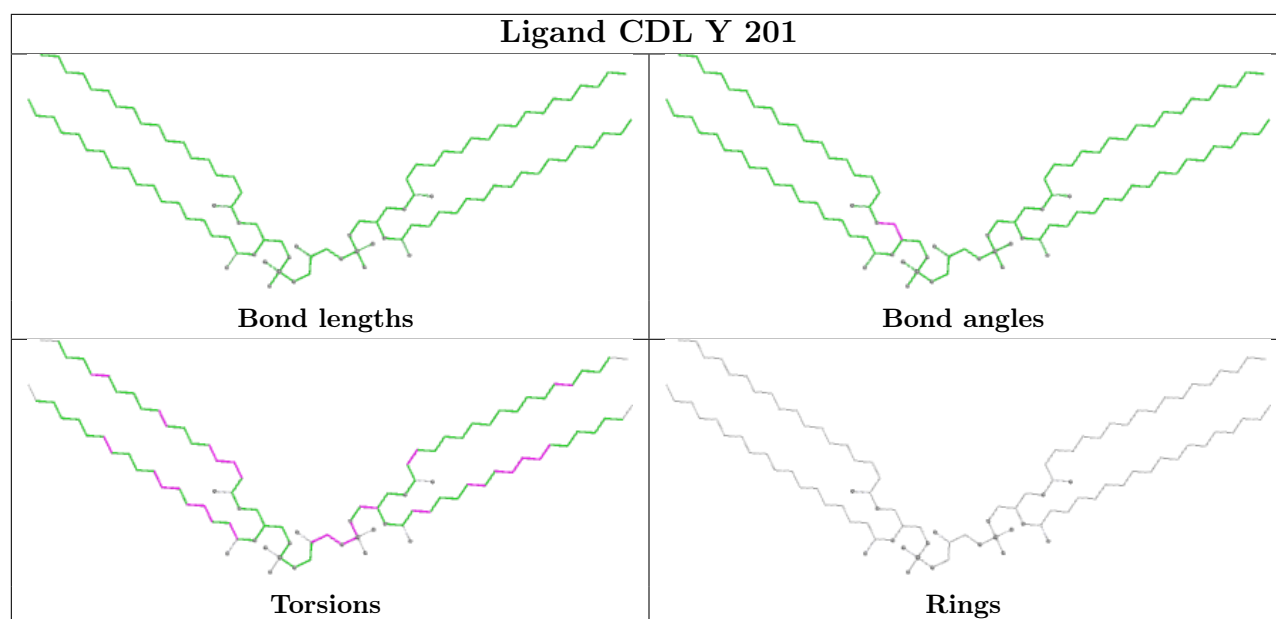


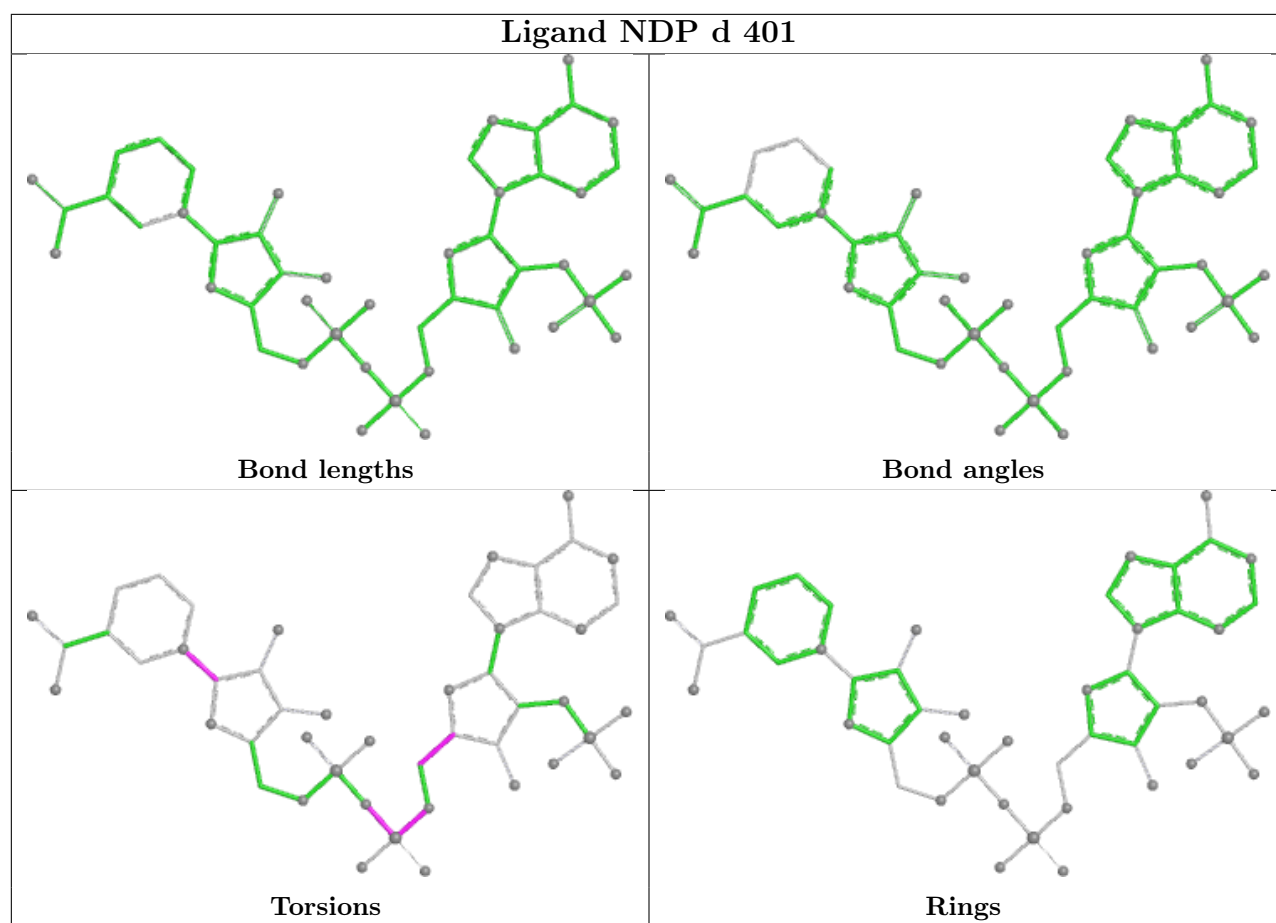












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

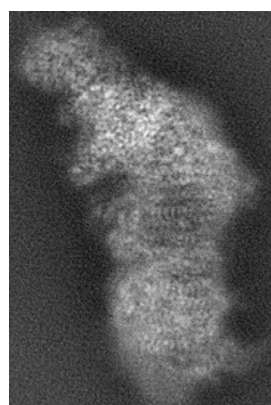
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11253. These allow visual inspection of the internal detail of the map and identification of artifacts.

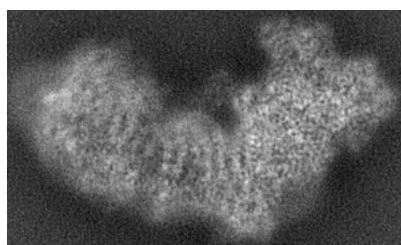
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

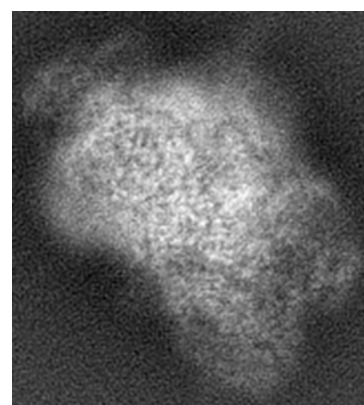
6.1.1 Primary map



X



Y

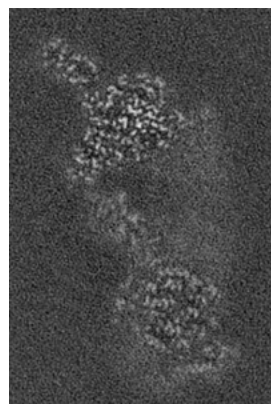


Z

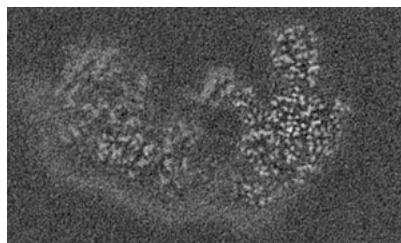
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

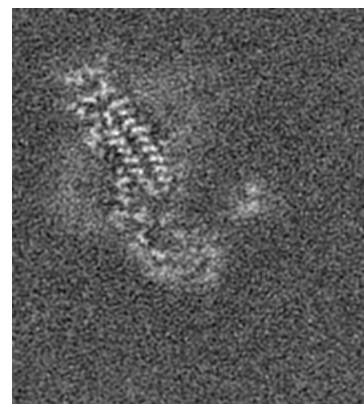
6.2.1 Primary map



X Index: 81



Y Index: 90

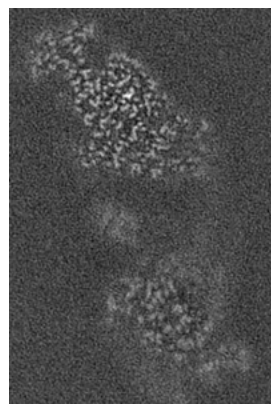


Z Index: 136

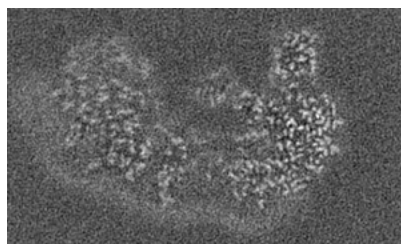
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

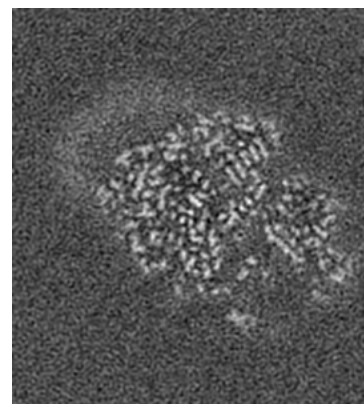
6.3.1 Primary map



X Index: 92



Y Index: 95

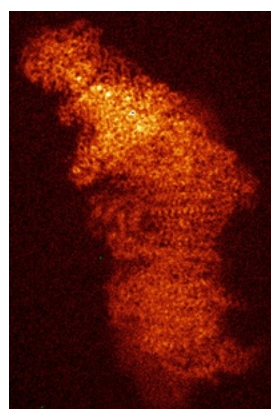


Z Index: 195

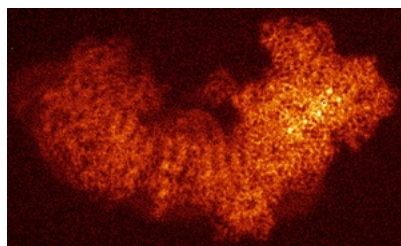
The images above show the largest variance slices of the map in three orthogonal directions.

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

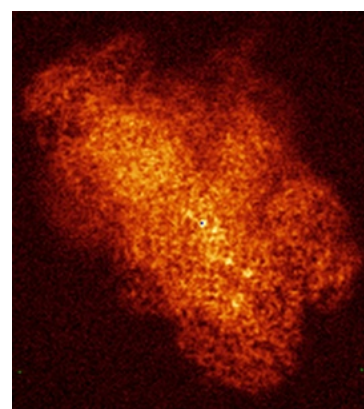
6.4.1 Primary map



X



Y



Z

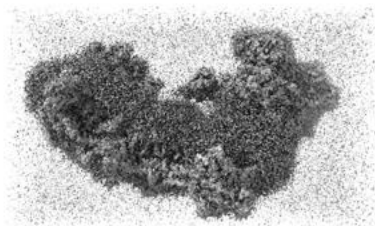
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

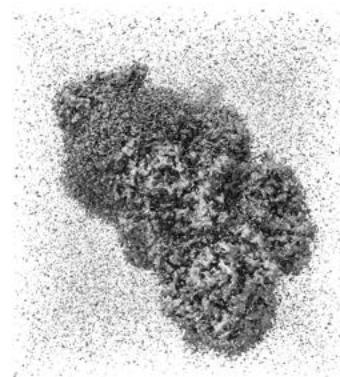
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

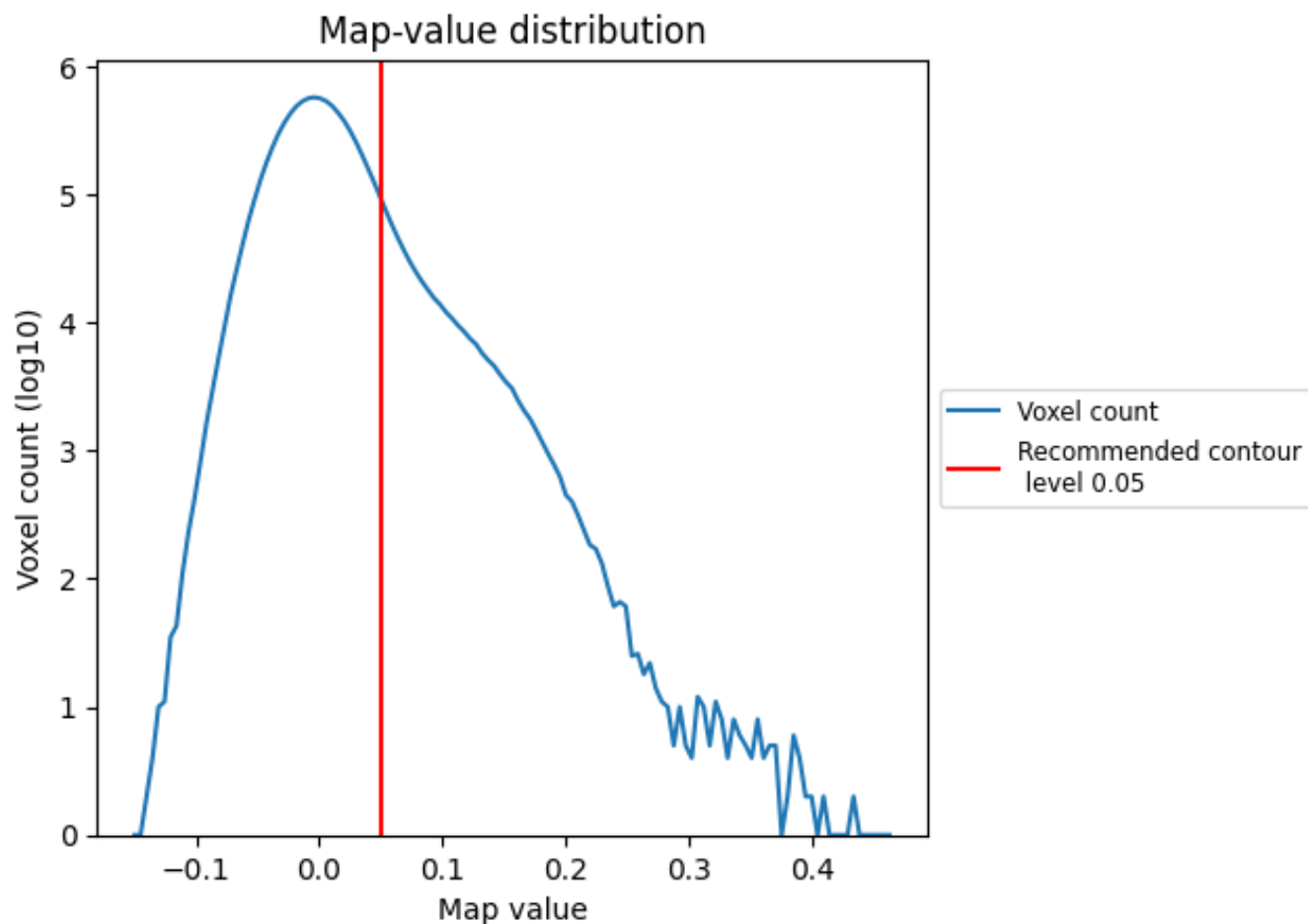
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

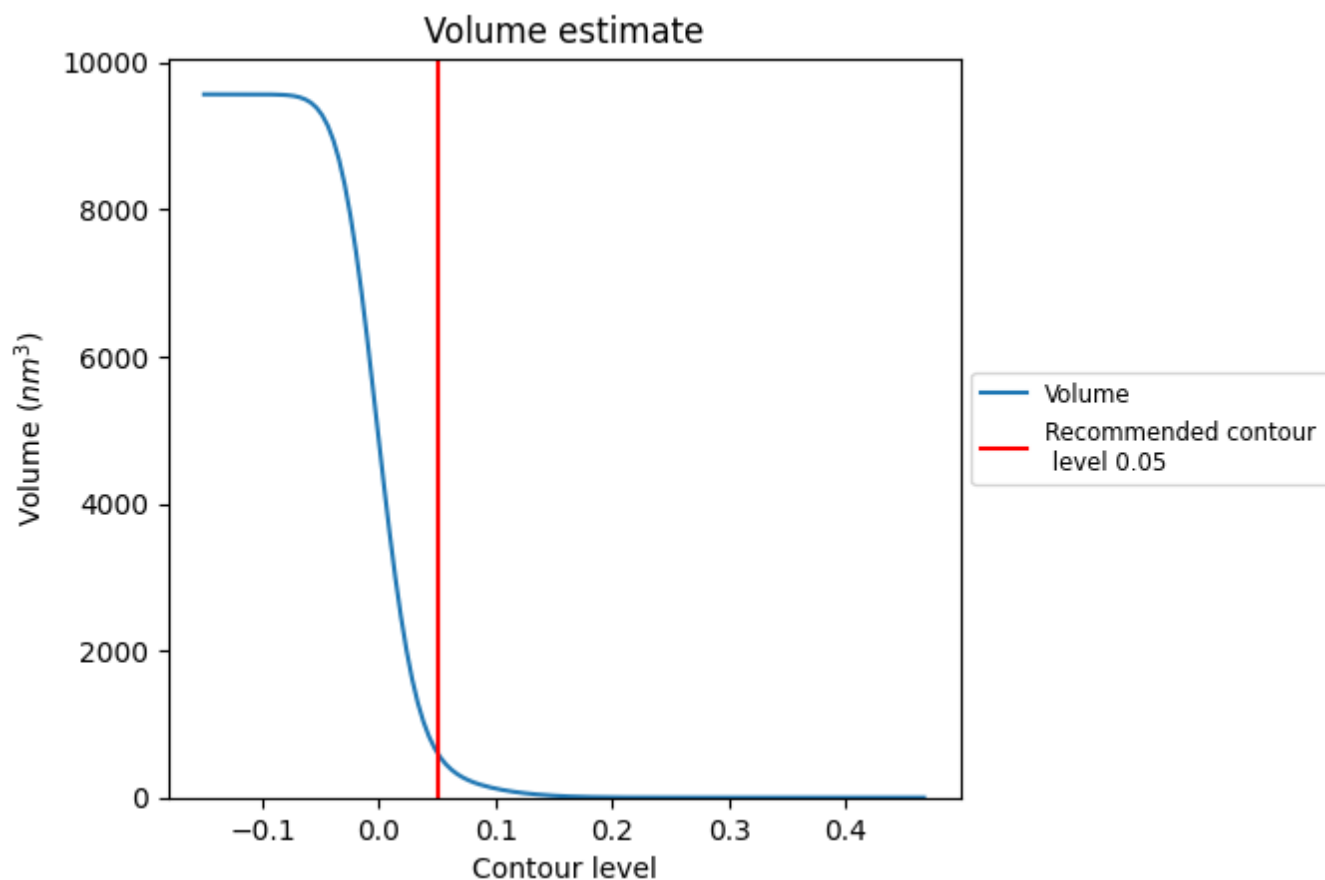
This section contains the results of statistical analysis of the map.

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 614 nm³; this corresponds to an approximate mass of 555 kDa.

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

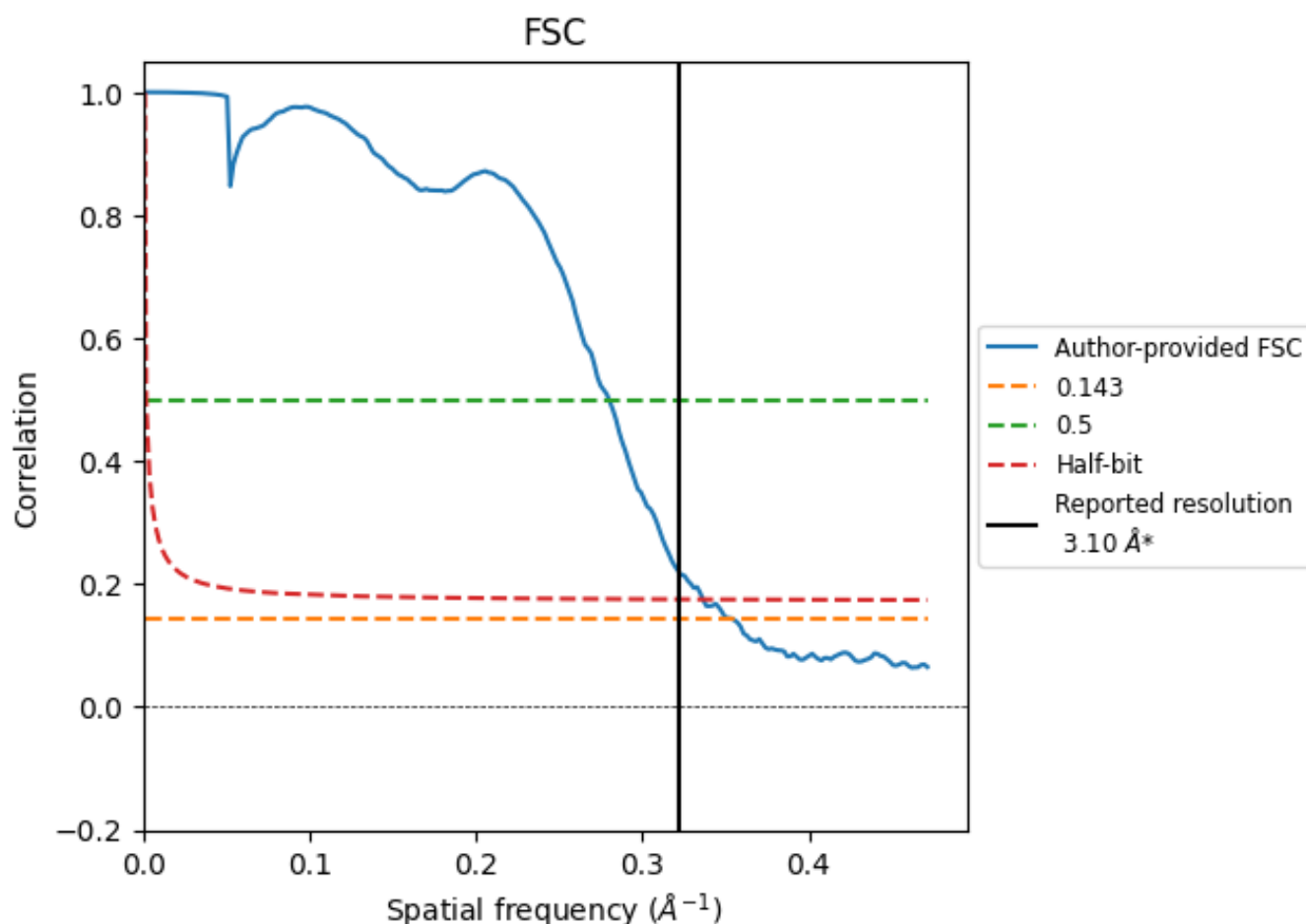
7.3 Rotationally averaged power spectrum [i](#)

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

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

8.2 Resolution estimates [i](#)

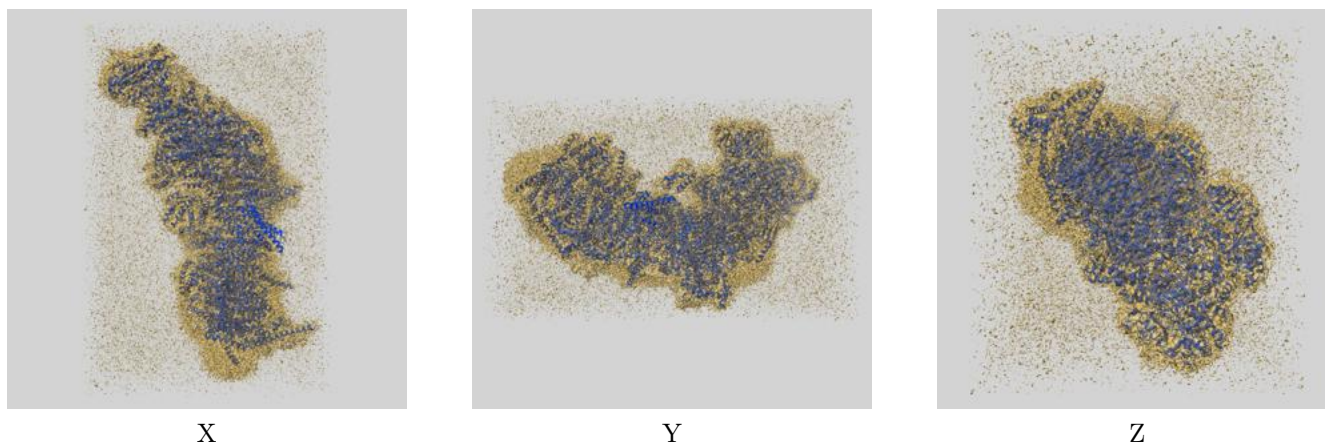
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	2.82	3.57	2.97
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

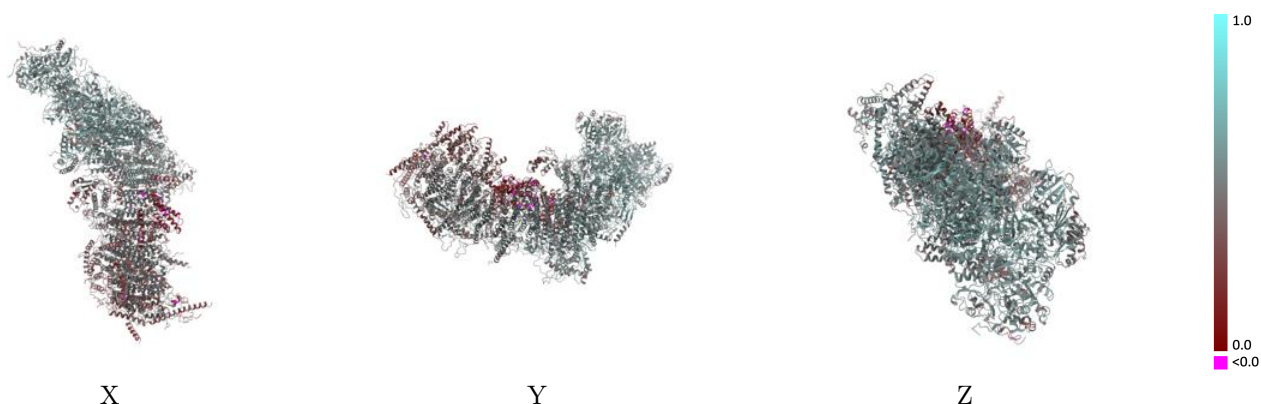
This section contains information regarding the fit between EMDB map EMD-11253 and PDB model 6ZKL. Per-residue inclusion information can be found in [section 3](#) on [page 21](#).

9.1 Map-model overlay [i](#)



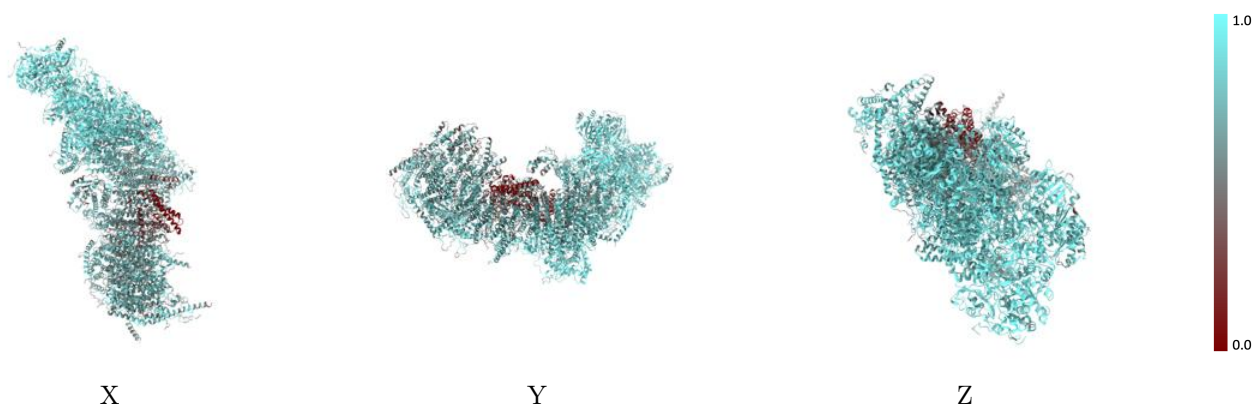
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



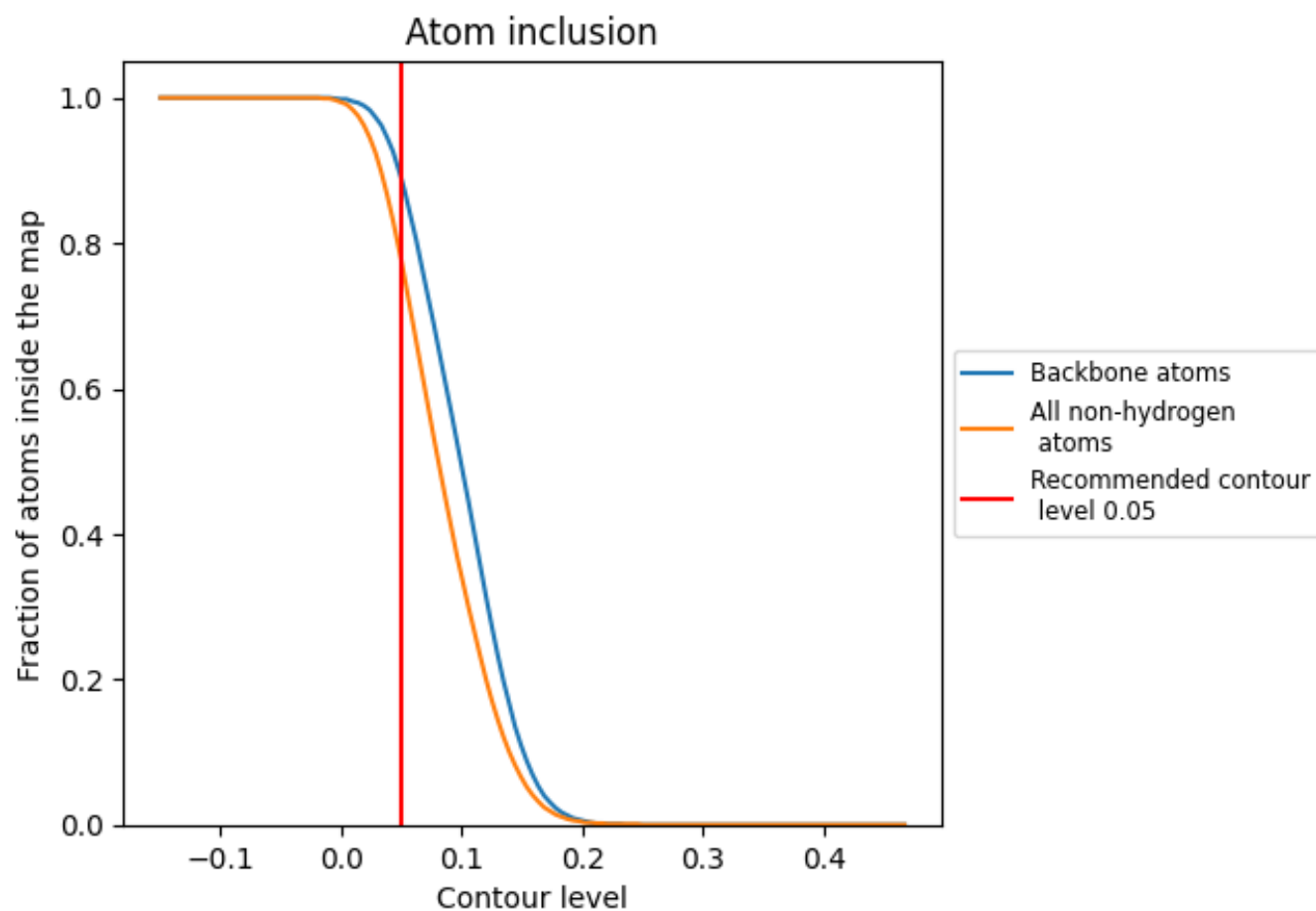
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.05).

9.4 Atom inclusion ⓘ



At the recommended contour level, 89% of all backbone atoms, 78% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7750	 0.4880
1	 0.8900	 0.5390
2	 0.8560	 0.5240
3	 0.8780	 0.5570
4	 0.8430	 0.5620
5	 0.8990	 0.5880
6	 0.8970	 0.5780
9	 0.9080	 0.5870
A	 0.6490	 0.4650
H	 0.8170	 0.5430
J	 0.6460	 0.4430
K	 0.7330	 0.5090
L	 0.6690	 0.4240
M	 0.7710	 0.5050
N	 0.7880	 0.5230
V	 0.1710	 0.2130
W	 0.7730	 0.4880
X	 0.6010	 0.3480
Y	 0.8150	 0.5000
Z	 0.7570	 0.4360
a	 0.8650	 0.5030
b	 0.8890	 0.5750
c	 0.8650	 0.5750
d	 0.8480	 0.5270
e	 0.8420	 0.4910
f	 0.8290	 0.5250
g	 0.8060	 0.5350
h	 0.8560	 0.5600
i	 0.8670	 0.5570
j	 0.6660	 0.3920
k	 0.7130	 0.4250
l	 0.7950	 0.4910
m	 0.8370	 0.5110
n	 0.6070	 0.3080
o	 0.7110	 0.4620



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Chain	Atom inclusion	Q-score
p	 0.5950	 0.3620
q	 0.8460	 0.5200
r	 0.7190	 0.3900
s	 0.6910	 0.3490
t	 0.6710	 0.3550
u	 0.7120	 0.3640
v	 0.6700	 0.3860
w	 0.7230	 0.4650
x	 0.7300	 0.4000
y	 0.7190	 0.4380
z	 0.8700	 0.5400