



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 02:03 AM UTC

PDB ID : 6ZKM / pdb_00006zkm
EMDB ID : EMD-11254
Title : Complex I inhibited by rotenone, open2
Authors : Kampjut, D.; Sazanov, L.A.
Deposited on : 2020-06-30
Resolution : 2.80 Å(reported)
Based on initial model : 5LNK

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

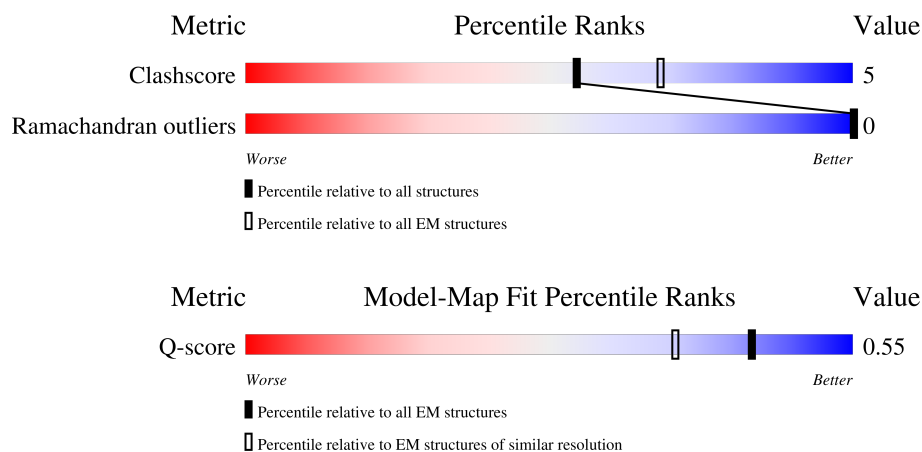
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.80 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	-
Q-score	-	25397	11806 (2.30 - 3.30)

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

Mol	Chain	Length	Quality of chain
1	1	464	
2	2	246	
3	3	727	
4	4	463	
5	5	266	

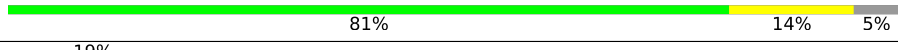
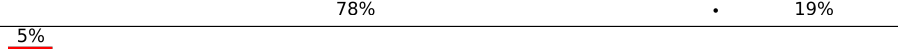
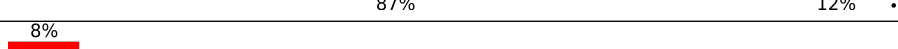
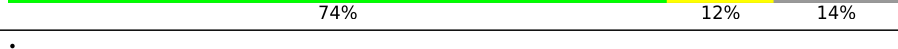
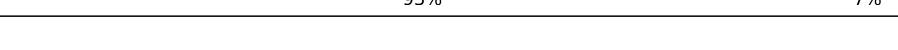
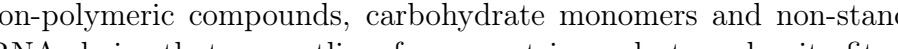
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Mol	Chain	Length	Quality of chain
6	6	223	
7	9	217	
8	A	115	
9	H	318	
10	J	175	
11	K	98	
12	L	606	
13	M	459	
14	N	347	
15	V	141	
16	W	189	
17	X	157	
17	j	157	
18	Y	172	
19	Z	175	
20	a	109	
21	b	124	
22	c	170	
23	d	380	
24	e	99	
25	f	116	
26	g	140	
27	h	114	
28	i	145	
29	k	355	

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
45	SF4	l	501	-	-	X	-
50	970	M	601	X	-	-	-
53	CDL	L	1003	X	-	-	-
53	CDL	o	502	X	-	-	-
53	CDL	y	201	X	-	-	-

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 65955 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	167	Total	C	N	O	S	0	0
			1273	856	182	222	13		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	558	Total	C	N	O	S	0	0
			4425	2935	689	759	42		

- 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	27	Total	C	N	O	S	0	0
			204	135	32	34	3		

- 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		

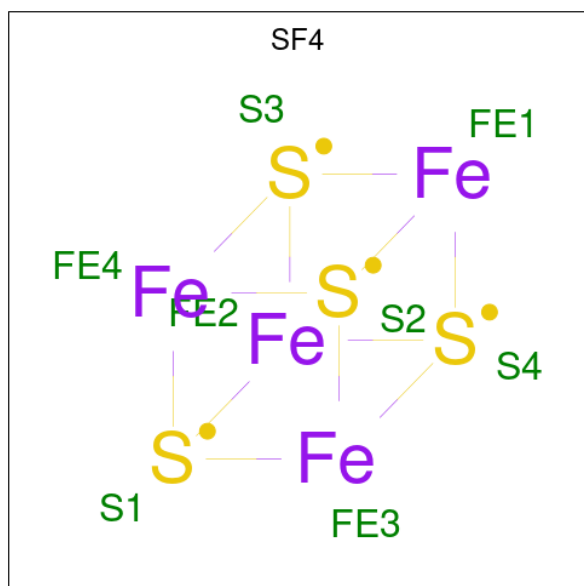
- Molecule 43 is a protein called Mitochondrial complex I, MNLL subunit.

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).



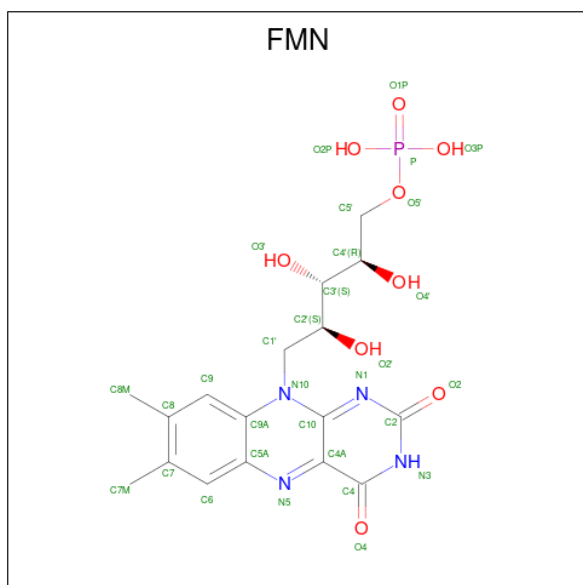
Mol	Chain	Residues	Atoms			AltConf
45	1	1	Total	Fe	S	0
			8	4	4	
45	3	1	Total	Fe	S	0
			8	4	4	
45	3	1	Total	Fe	S	0
			8	4	4	
45	6	1	Total	Fe	S	0
			8	4	4	

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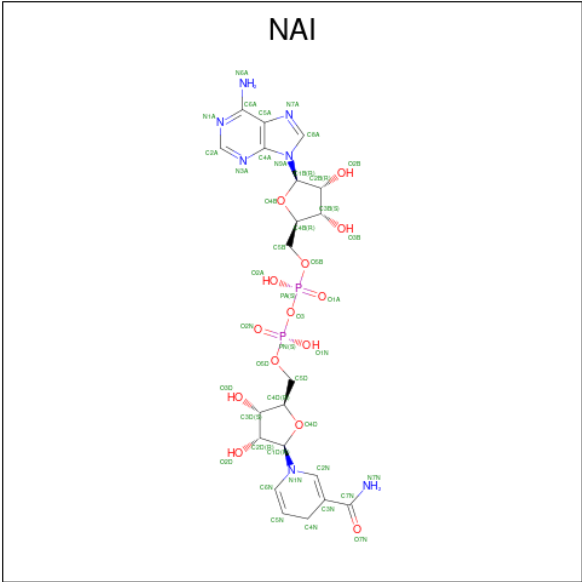
Mol	Chain	Residues	Atoms			AltConf
45	9	1	Total	Fe	S	0
			8	4	4	
45	9	1	Total	Fe	S	0
			8	4	4	

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



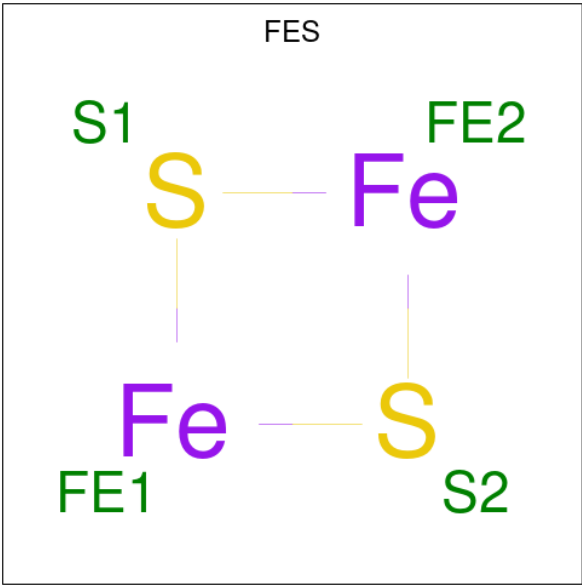
Mol	Chain	Residues	Atoms					AltConf
46	1	1	Total	C	N	O	P	0
			31	17	4	9	1	

- 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).

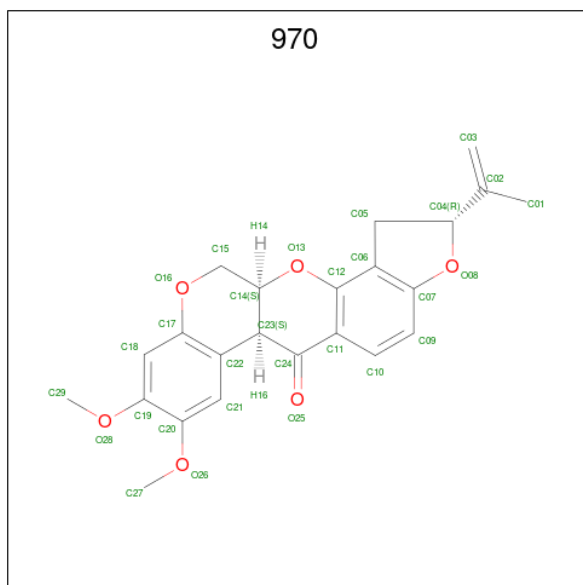


Mol	Chain	Residues	Atoms			AltConf
48	2	1	Total	Fe	S	0
			4	2	2	
48	3	1	Total	Fe	S	0
			4	2	2	

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

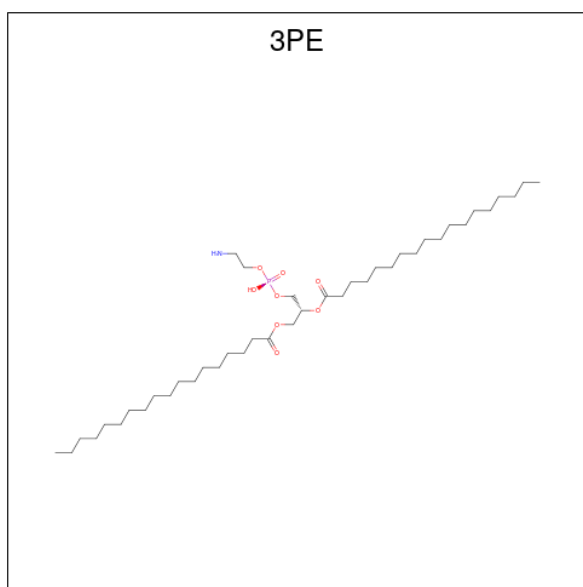
Mol	Chain	Residues	Atoms		AltConf
49	3	1	Total	K	0
			1	1	

- 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).



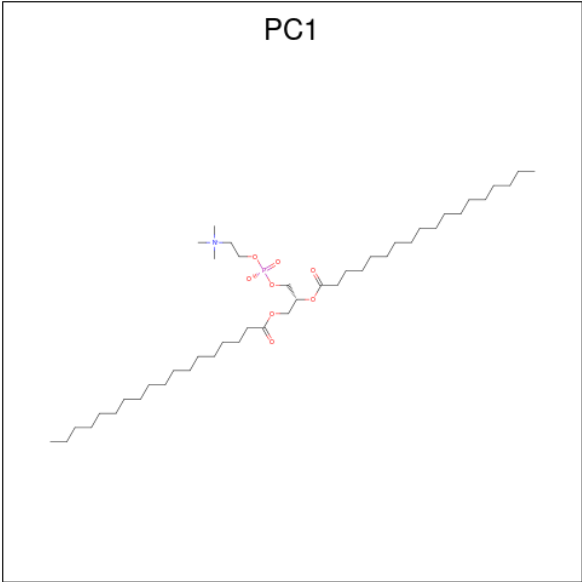
Mol	Chain	Residues	Atoms			AltConf
50	6	1	Total	C	O	0
			29	23	6	
50	H	1	Total	C	O	0
			29	23	6	
50	M	1	Total	C	O	0
			29	23	6	

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



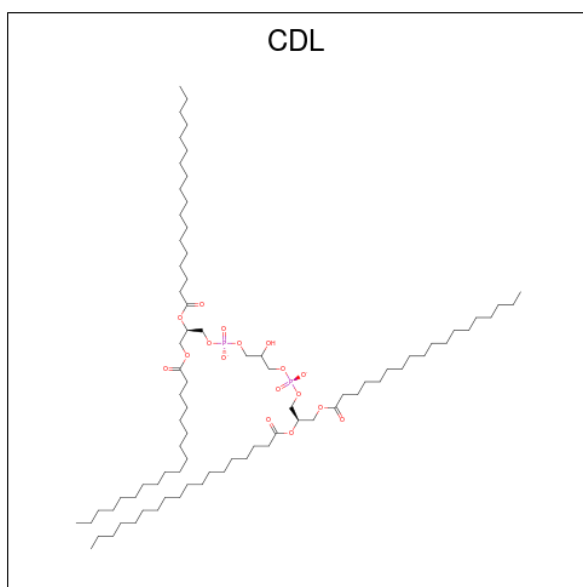
Mol	Chain	Residues	Atoms					AltConf
51	6	1	Total	C	N	O	P	0
			51	41	1	8	1	
51	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
51	H	1	Total	C	N	O	P	0
			51	41	1	8	1	
51	L	1	Total	C	N	O	P	0
			51	41	1	8	1	
51	L	1	Total	C	N	O	P	0
			31	21	1	8	1	
51	M	1	Total	C	N	O	P	0
			44	34	1	8	1	
51	N	1	Total	C	N	O	P	0
			51	41	1	8	1	
51	i	1	Total	C	N	O	P	0
			51	41	1	8	1	
51	o	1	Total	C	N	O	P	0
			31	21	1	8	1	

- Molecule 52 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: C₄₄H₈₈NO₈P).



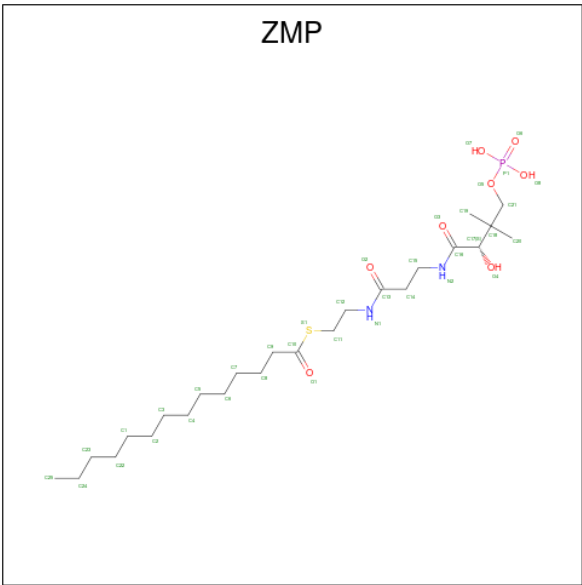
Mol	Chain	Residues	Atoms					AltConf
52	9	1	Total	C	N	O	P	0
			54	44	1	8	1	
52	A	1	Total	C	N	O	P	0
			46	36	1	8	1	
52	A	1	Total	C	N	O	P	0
			37	27	1	8	1	
52	L	1	Total	C	N	O	P	0
			54	44	1	8	1	
52	M	1	Total	C	N	O	P	0
			42	32	1	8	1	
52	w	1	Total	C	N	O	P	0
			54	44	1	8	1	

- 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	W	1	Total	C	O	P	0
			100	81	17	2	
53	h	1	Total	C	O	P	0
			58	39	17	2	
53	o	1	Total	C	O	P	0
			75	56	17	2	
53	o	1	Total	C	O	P	0
			90	71	17	2	
53	y	1	Total	C	O	P	0
			100	81	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: $C_{25}H_{49}N_2O_8PS$).

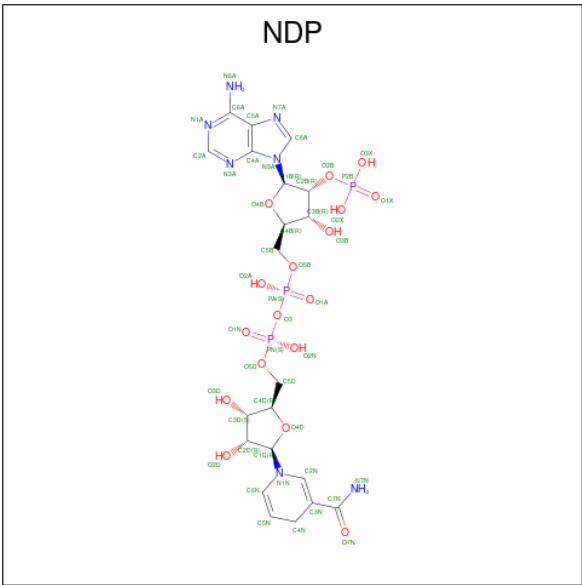


Mol	Chain	Residues	Atoms						AltConf
54	X	1	Total	C	N	O	P	S	0
			31	20	2	7	1	1	
54	g	1	Total	C	N	O	P	S	0
			34	23	2	7	1	1	

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

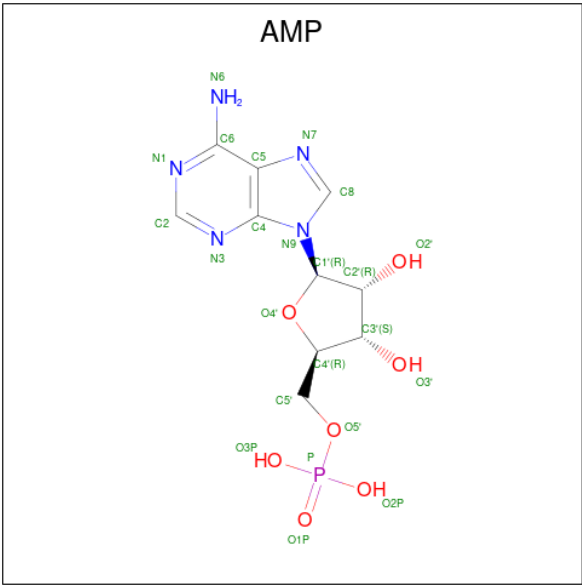
Mol	Chain	Residues	Atoms		AltConf
55	b	1	Total	Zn	0
			1	1	

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



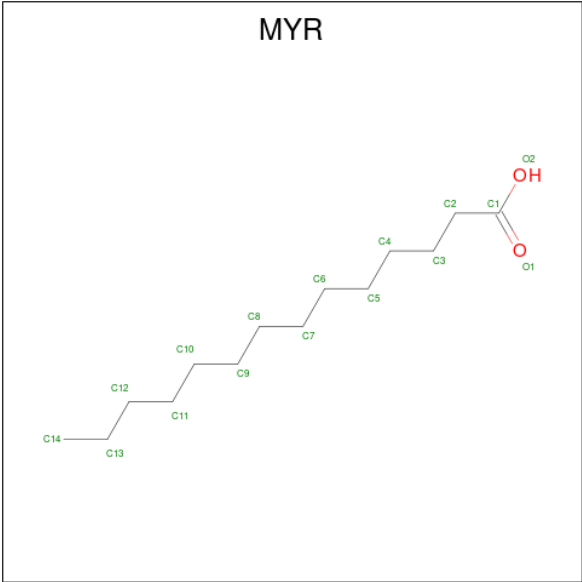
Mol	Chain	Residues	Atoms					AltConf
56	d	1	Total	C	N	O	P	0
			48	21	7	17	3	

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



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: $C_{14}H_{28}O_2$).

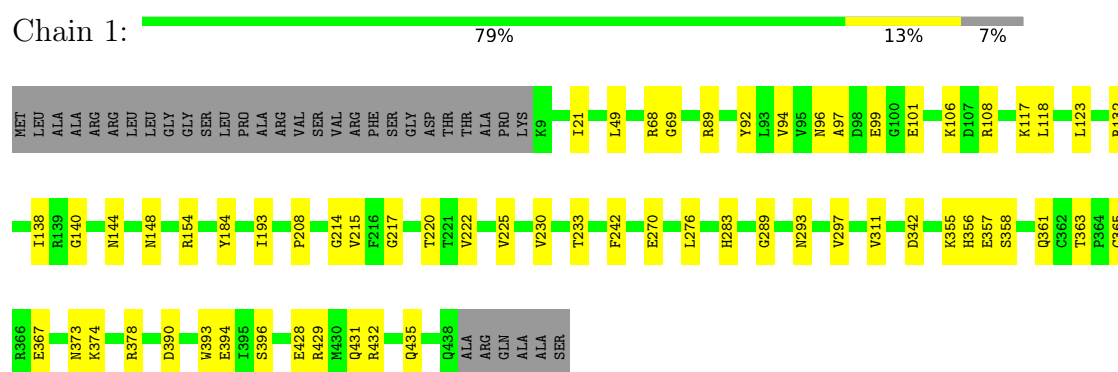


Mol	Chain	Residues	Atoms			AltConf
58	s	1	Total	C	O	0
			15	14	1	

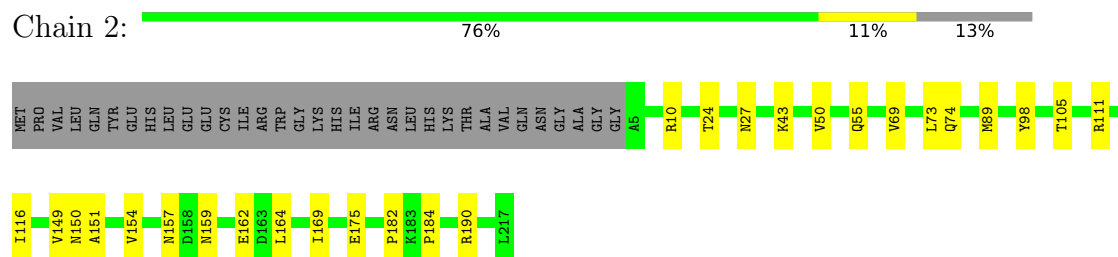
3 Residue-property plots

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.

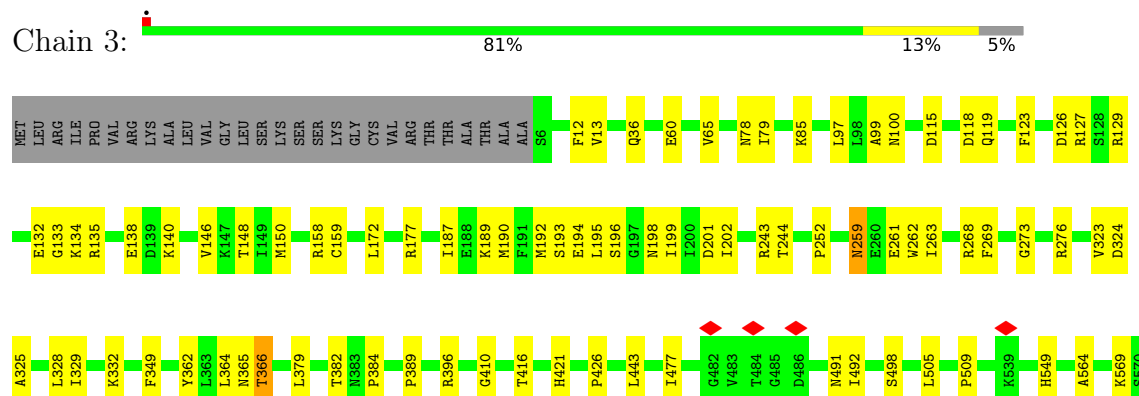
- Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

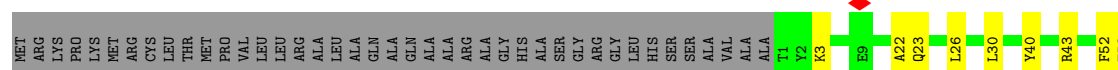


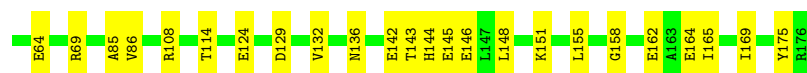
- Molecule 2: Mitochondrial complex I, 24 kDa subunit



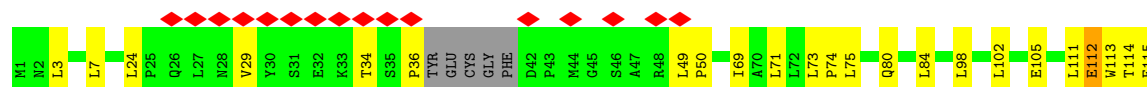
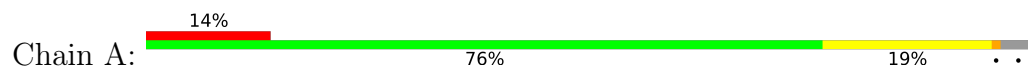
- Molecule 3: NADH:ubiquinone oxidoreductase core subunit S1



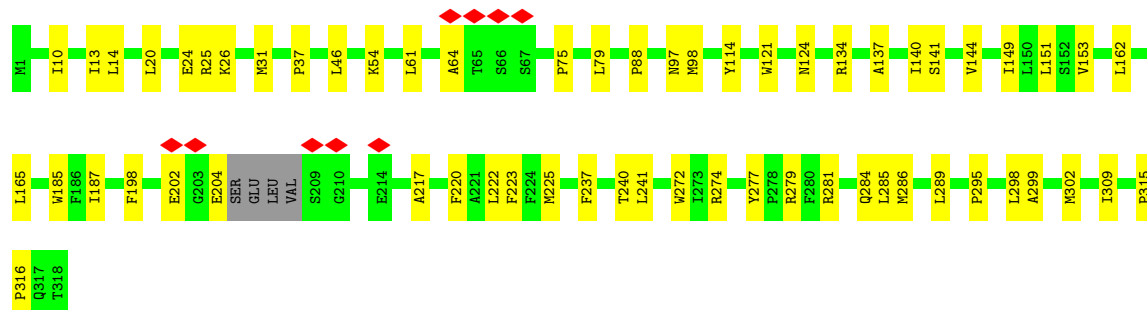
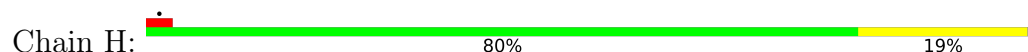




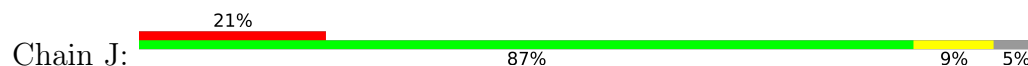
• Molecule 8: NADH-ubiquinone oxidoreductase chain 3



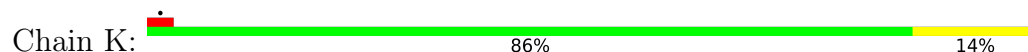
• Molecule 9: NADH-ubiquinone oxidoreductase chain 1



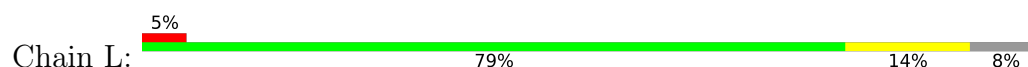
• Molecule 10: NADH-ubiquinone oxidoreductase chain 6

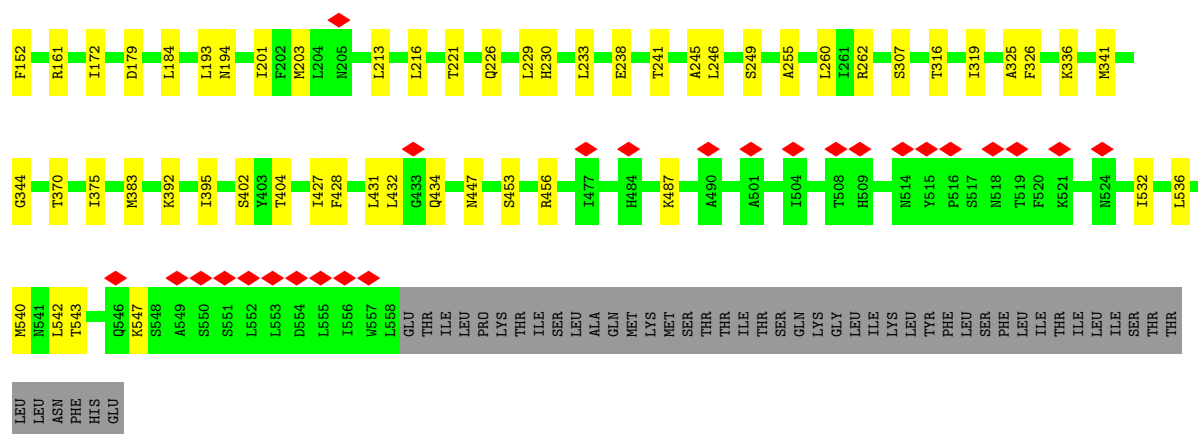


• Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

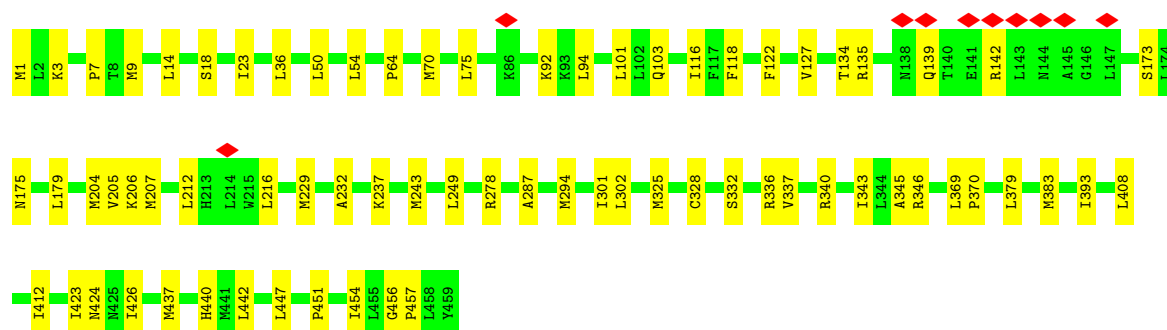
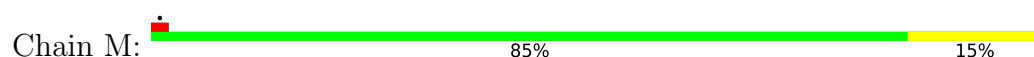


• Molecule 12: NADH-ubiquinone oxidoreductase chain 5

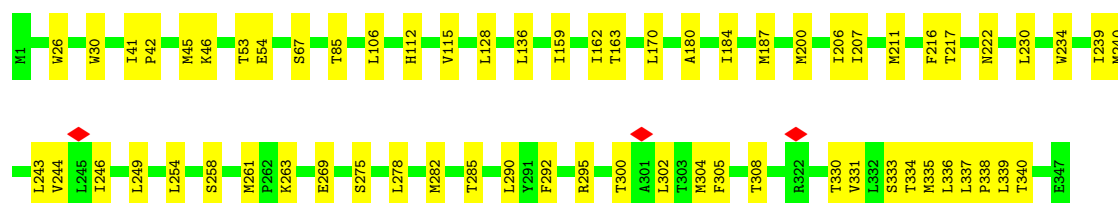
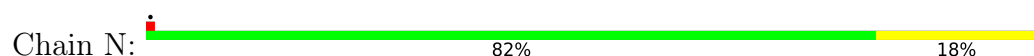




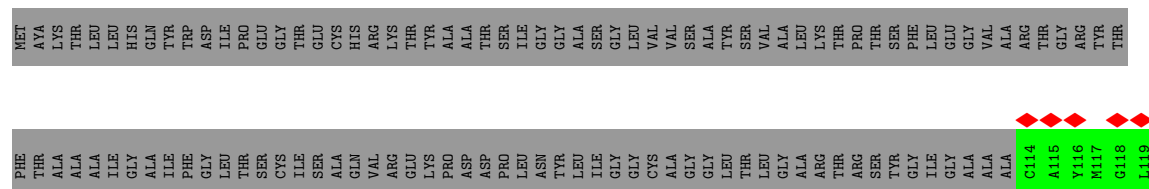
- Molecule 13: NADH-ubiquinone oxidoreductase chain 4

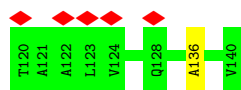


- Molecule 14: NADH-ubiquinone oxidoreductase chain 2



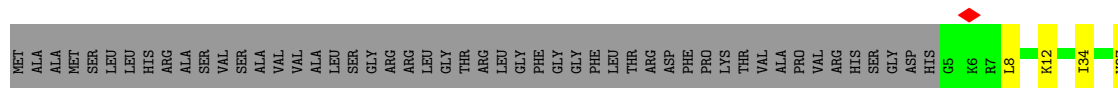
- Molecule 15: Mitochondrial complex I, B14.7 subunit





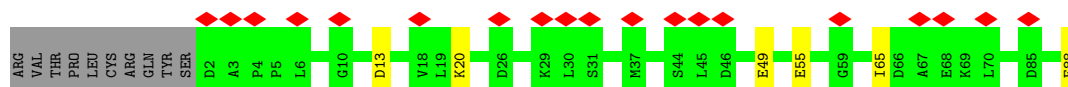
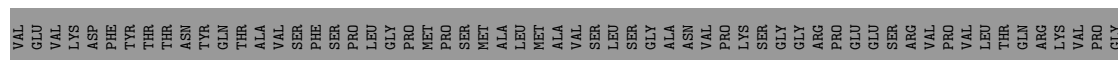
- Molecule 16: NADH:ubiquinone oxidoreductase subunit B5

Chain W: 63% 11% 26%



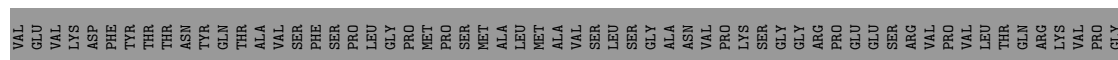
- Molecule 17: Acyl carrier protein

Chain X: 12% 52% 45%



- Molecule 17: Acyl carrier protein

Chain j: 46% 6% 48%



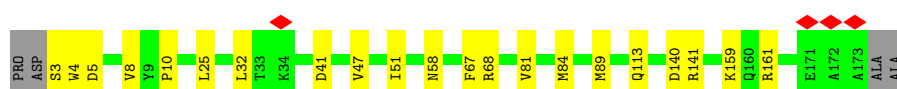
- Molecule 18: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain Y: 85% 15%

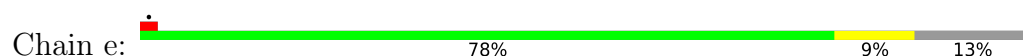


- Molecule 19: Mitochondrial complex I, PDSW subunit

Chain Z: 86% 12%



- Chain a: 

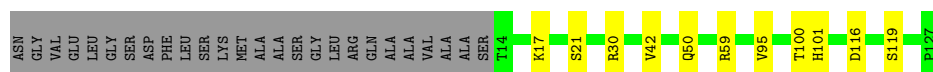


Chain f:  92% 5%



- Molecule 26: NADH:ubiquinone oxidoreductase subunit A6

Chain g:  74% 8% 19%



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

Chain h:  75% 10% 16%



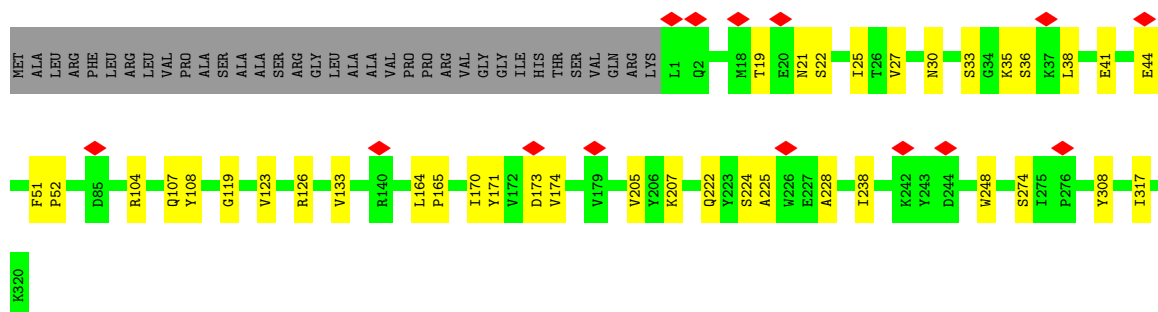
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain i:  87% 13%



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

Chain k:  79% 11% 10%



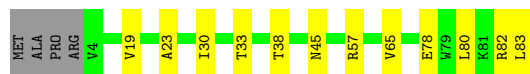
- Molecule 30: NADH:ubiquinone oxidoreductase subunit S5

Chain l:  87% 12%



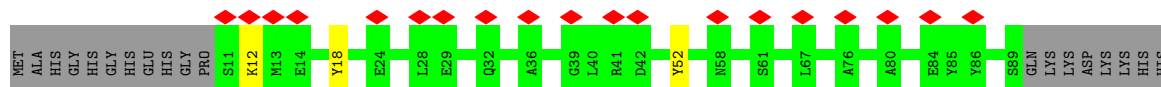
- Molecule 31: NADH:ubiquinone oxidoreductase subunit A3

Chain m:  81% 14% 5%



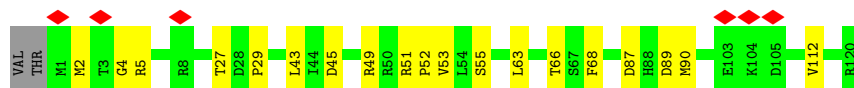
- Molecule 32: NADH:ubiquinone oxidoreductase subunit B3

Chain n:  19% 78% 19%



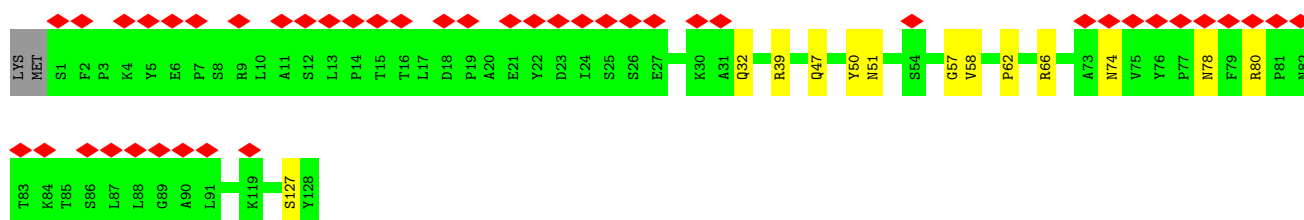
- Molecule 33: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain o:  5% 83% 16%



- Molecule 34: NADH:ubiquinone oxidoreductase subunit B4

Chain p:  34% 88% 10%



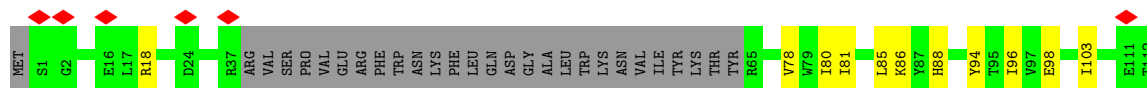
- Molecule 35: Mitochondrial complex I, B16.6 subunit

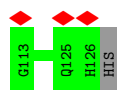
Chain q:  85% 11% 2%



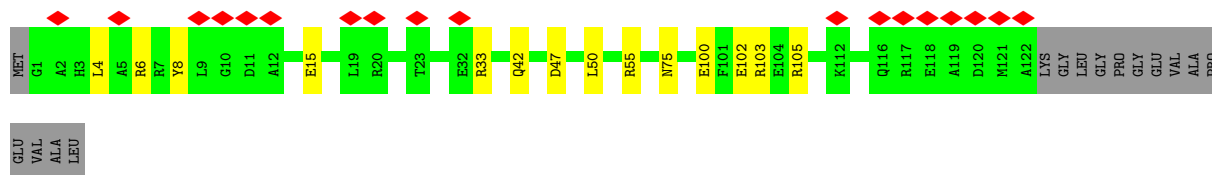
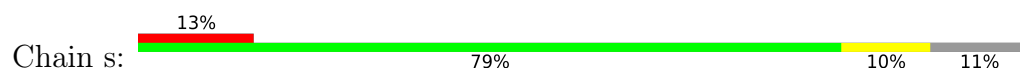
- Molecule 36: Mitochondrial complex I, B17 subunit

Chain r:  7% 69% 9% 23%

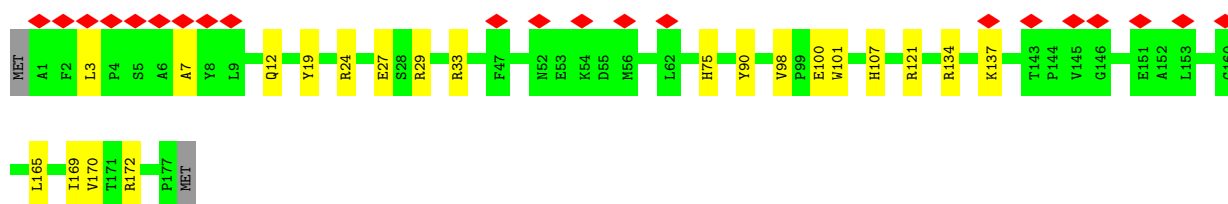
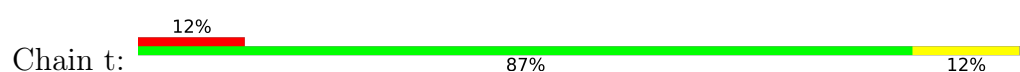




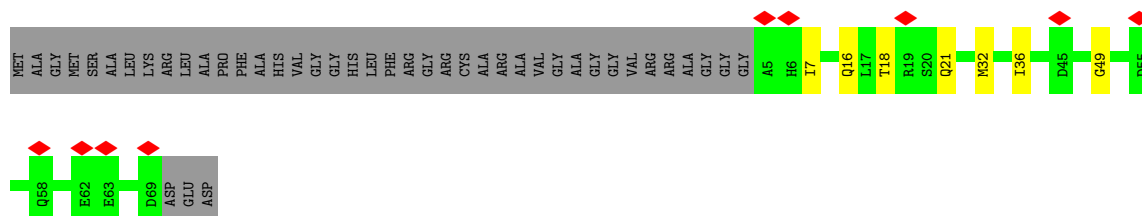
- Molecule 37: NADH:ubiquinone oxidoreductase subunit B7



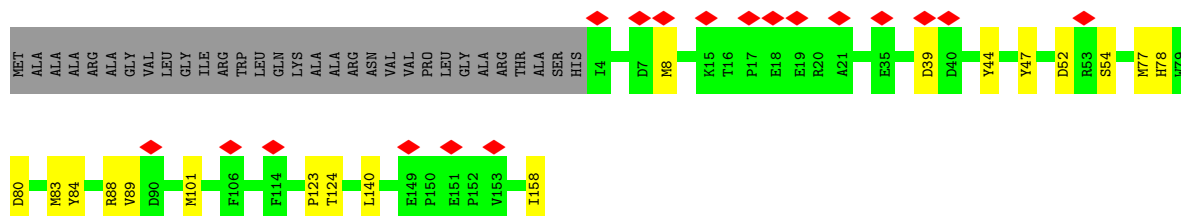
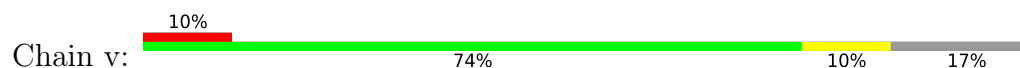
- Molecule 38: NADH:ubiquinone oxidoreductase subunit B9



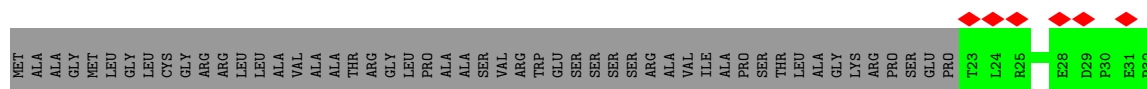
- Molecule 39: NADH:ubiquinone oxidoreductase subunit B2



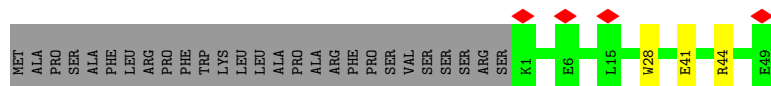
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



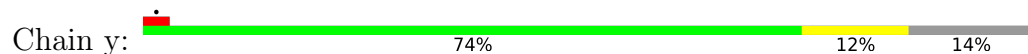
- Molecule 41: Mitochondrial complex I, ESSS subunit



- 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	61945	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	0.494	Depositor
Minimum map value	-0.206	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.033	Depositor
Recommended contour level	0.055	Depositor
Map size (Å)	172.943, 192.041, 291.775	wwPDB
Map dimensions	275, 181, 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: FME, NAI, 3PE, SF4, CDL, 970, AMP, FES, AYA, MYR, PC1, NDP, K, 2MR, ZMP, FMN, SEP, ZN

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	0.32	0/3386	0.59	1/4575 (0.0%)
2	2	0.31	0/1695	0.58	0/2306
3	3	0.33	0/5362	0.55	2/7266 (0.0%)
4	4	0.36	0/3504	0.57	0/4746
5	5	0.33	0/1776	0.56	0/2417
6	6	0.40	0/1278	0.61	0/1728
7	9	0.39	0/1445	0.59	0/1956
8	A	0.32	0/902	0.69	2/1234 (0.2%)
9	H	0.37	0/2572	0.65	0/3517
10	J	0.31	0/1302	0.58	0/1760
11	K	0.35	0/749	0.64	0/1014
12	L	0.28	0/4537	0.56	1/6176 (0.0%)
13	M	0.33	0/3731	0.60	0/5085
14	N	0.35	0/2787	0.62	0/3795
15	V	0.18	0/208	0.35	0/279
16	W	0.26	0/1188	0.50	0/1607
17	X	0.19	0/713	0.42	0/963
17	j	0.22	0/670	0.49	0/902
18	Y	0.29	0/1440	0.55	0/1942
19	Z	0.23	0/1475	0.47	0/1989
20	a	0.22	0/383	0.46	0/518
21	b	0.29	0/749	0.47	0/1009
22	c	0.31	0/1047	0.47	0/1415
23	d	0.30	0/2424	0.52	0/3276
24	e	0.25	0/702	0.48	0/945
25	f	0.26	0/937	0.51	0/1271
26	g	0.28	0/993	0.54	0/1336
27	h	0.32	0/779	0.55	0/1053
28	i	0.29	0/1250	0.47	0/1698
29	k	0.21	0/2646	0.44	0/3579
30	l	0.27	0/896	0.55	0/1200

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	m	0.25	0/647	0.52	0/890
32	n	0.18	0/653	0.40	0/882
33	o	0.25	0/1035	0.48	0/1398
34	p	0.20	0/1085	0.47	0/1467
35	q	0.28	0/1171	0.50	0/1579
36	r	0.23	0/874	0.51	0/1188
37	s	0.20	0/1072	0.49	0/1436
38	t	0.21	0/1573	0.53	0/2130
39	u	0.19	0/590	0.46	0/810
40	v	0.20	0/1361	0.48	0/1861
41	w	0.24	0/872	0.53	0/1185
42	x	0.18	0/425	0.40	0/576
43	y	0.24	0/449	0.53	0/605
44	z	0.33	0/591	0.54	0/795
All	All	0.30	0/65924	0.55	6/89359 (0.0%)

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

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

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	366	THR	CA-C-N	5.80	132.62	121.54
3	3	366	THR	C-N-CA	5.80	132.62	121.54
1	1	311	VAL	N-CA-C	-5.65	107.31	112.96
12	L	230	HIS	N-CA-C	5.17	121.22	109.81
8	A	112	GLU	CA-C-N	5.02	131.12	121.54
8	A	112	GLU	C-N-CA	5.02	131.12	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
35	q	24	LEU	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	42	0
2	2	1655	0	1668	18	0
3	3	5275	0	5300	66	0
4	4	3427	0	3365	53	0
5	5	1726	0	1676	22	0
6	6	1247	0	1259	18	0
7	9	1414	0	1371	28	0
8	A	880	0	920	19	0
9	H	2498	0	2609	45	0
10	J	1273	0	1300	15	0
11	K	749	0	793	13	0
12	L	4425	0	4530	56	0
13	M	3647	0	3849	51	0
14	N	2723	0	2930	46	0
15	V	204	0	212	1	0
16	W	1155	0	1177	20	0
17	X	701	0	692	6	0
17	j	660	0	663	5	0
18	Y	1403	0	1392	18	0
19	Z	1441	0	1419	17	0
20	a	371	0	344	5	0
21	b	737	0	710	7	0
22	c	1024	0	1023	12	0
23	d	2372	0	2407	17	0
24	e	691	0	706	5	0
25	f	917	0	958	4	0
26	g	969	0	980	8	0
27	h	769	0	780	9	0
28	i	1209	0	1182	13	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	k	2596	0	2559	21	0
30	l	874	0	869	11	0
31	m	626	0	635	10	0
32	n	634	0	616	3	0
33	o	1004	0	995	15	0
34	p	1059	0	1062	12	0
35	q	1142	0	1137	15	0
36	r	846	0	864	11	0
37	s	1047	0	1015	13	0
38	t	1520	0	1477	19	0
39	u	563	0	509	5	0
40	v	1307	0	1207	15	0
41	w	846	0	792	10	0
42	x	412	0	411	2	0
43	y	436	0	437	6	0
44	z	576	0	570	4	0
45	1	8	0	0	2	0
45	3	16	0	0	0	0
45	6	8	0	0	1	0
45	9	16	0	0	0	0
46	1	31	0	19	1	0
47	1	44	0	27	2	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
50	M	29	0	0	0	0
51	6	51	0	82	3	0
51	A	51	0	82	4	0
51	H	51	0	82	3	0
51	L	82	0	118	0	0
51	M	44	0	65	0	0
51	N	51	0	82	5	0
51	i	51	0	82	2	0
51	o	31	0	36	0	0
52	9	54	0	88	3	0
52	A	83	0	117	2	0
52	L	54	0	88	10	0
52	M	42	0	58	1	0
52	w	54	0	88	7	0
53	L	100	0	156	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
53	W	100	0	156	15	0
53	h	58	0	60	1	0
53	o	165	0	230	19	0
53	y	100	0	156	11	0
54	X	31	0	34	2	0
54	g	34	0	40	0	0
55	b	1	0	0	0	0
56	d	48	0	26	2	0
57	k	23	0	12	0	0
58	s	15	0	27	0	0
All	All	65955	0	66650	673	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (673) 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)
2:2:98:TYR:HA	2:2:157:ASN:HD21	1.53	0.72
9:H:121:TRP:HE1	10:J:73:ALA:HB2	1.57	0.69
4:4:269:LEU:HB2	4:4:368:GLU:HB2	1.76	0.68
4:4:405:MET:SD	4:4:421:GLN:NE2	2.67	0.68
9:H:141:SER:HB3	9:H:289:LEU:HD22	1.78	0.66
3:3:118:ASP:OD2	22:c:46:GLN:NE2	2.28	0.66
6:6:171:LYS:HG2	6:6:174:ARG:HH11	1.62	0.65
44:z:34:ARG:NH2	44:z:61:TYR:O	2.29	0.65
12:L:241:THR:HG21	12:L:344:GLY:HA3	1.78	0.65
13:M:139:GLN:HE22	13:M:340:ARG:HH12	1.45	0.65
1:1:132:ARG:NH2	20:a:64:PRO:O	2.30	0.65
21:b:32:GLN:HE22	21:b:34:GLU:HB2	1.63	0.64
4:4:50:ASN:HD21	4:4:63:ARG:HH21	1.44	0.64
14:N:106:LEU:HD22	14:N:187:MET:HE2	1.80	0.64
31:m:83:LEU:HD13	35:q:54:ARG:HD3	1.79	0.64
4:4:63:ARG:HB3	4:4:79:HIS:HB2	1.80	0.63
18:Y:165:ARG:NH1	33:o:87:ASP:OD1	2.32	0.63
43:y:8:ARG:HG3	43:y:10:HIS:H	1.63	0.62
3:3:632:ARG:HH12	24:e:59:ASP:H	1.48	0.62
28:i:60:ARG:HH22	28:i:95:ASP:HA	1.64	0.62
36:r:85:LEU:HD22	36:r:96:ILE:HD11	1.82	0.62
34:p:66:ARG:HH21	40:v:8:MET:HB3	1.64	0.62
9:H:26:LYS:HB3	44:z:5:VAL:HG12	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:9:43:ARG:HG2	27:h:11:ARG:HD2	1.83	0.60
9:H:97:ASN:H	35:q:143:THR:HG22	1.66	0.60
53:L:1003:CDL:H532	53:L:1003:CDL:H362	1.84	0.60
2:2:150:ASN:HB3	2:2:162:GLU:HB3	1.84	0.60
4:4:233:ARG:NH2	7:9:23:GLN:O	2.35	0.60
33:o:29:PRO:HB3	53:y:201:CDL:H312	1.84	0.60
6:6:81:ARG:HD2	9:H:61:LEU:HD11	1.83	0.59
8:A:34:THR:HG21	23:d:174:ARG:HD3	1.83	0.59
53:L:1003:CDL:H642	53:L:1003:CDL:H562	1.84	0.59
16:W:124:GLN:HB2	33:o:4:GLY:HA3	1.83	0.59
25:f:49:GLN:HE22	27:h:92:LYS:HA	1.68	0.59
35:q:81:ARG:NH1	35:q:85:MET:SD	2.76	0.59
4:4:55:HIS:NE2	9:H:204:GLU:OE1	2.35	0.59
12:L:453:SER:HA	12:L:456:ARG:HH21	1.68	0.59
12:L:103:PHE:HB2	12:L:341:MET:HE3	1.84	0.59
13:M:70:MET:HG2	13:M:103:GLN:HE21	1.67	0.59
3:3:252:PRO:HG3	3:3:263:ILE:HG12	1.85	0.58
9:H:149:ILE:HG21	9:H:185:TRP:HB2	1.84	0.58
28:i:34:ARG:NH2	28:i:58:ARG:O	2.35	0.58
22:c:42:ARG:NH1	22:c:46:GLN:O	2.36	0.58
24:e:19:ARG:HB2	24:e:65:TRP:HB2	1.84	0.58
3:3:190:MET:HG2	3:3:192:MET:HG2	1.86	0.58
6:6:44:SER:O	9:H:54:LYS:NZ	2.35	0.58
14:N:45:MET:HE3	14:N:53:THR:HG22	1.85	0.58
2:2:74:GLN:O	20:a:74:ARG:NH2	2.36	0.58
13:M:343:ILE:O	13:M:346:ARG:NH1	2.36	0.58
2:2:105:THR:OG1	48:2:300:FES:S2	2.62	0.58
3:3:329:ILE:HD13	3:3:505:LEU:HD22	1.85	0.58
13:M:23:ILE:HD11	13:M:92:LYS:HD2	1.85	0.58
4:4:110:SER:OG	4:4:149:ASN:ND2	2.37	0.57
5:5:65:ARG:NH1	5:5:123:VAL:O	2.37	0.57
31:m:78:GLU:OE1	31:m:82:ARG:NH1	2.37	0.57
16:W:37:VAL:HG21	53:W:201:CDL:H811	1.86	0.57
18:Y:129:LYS:NZ	31:m:65:VAL:O	2.36	0.57
27:h:45:SER:O	27:h:51:ASN:ND2	2.37	0.57
14:N:222:ASN:HD21	14:N:240:MET:HB3	1.69	0.57
3:3:364:LEU:HD12	3:3:491:ASN:HB3	1.87	0.57
2:2:149:VAL:O	2:2:190:ARG:NH2	2.38	0.57
9:H:64:ALA:O	9:H:124:ASN:ND2	2.38	0.57
16:W:133:ILE:HD13	30:l:37:LYS:HG2	1.87	0.57
1:1:101:GLU:HB2	47:1:503:NAI:H42N	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:127:ARG:NH2	4:4:326:ASP:O	2.38	0.56
8:A:74:PRO:HG2	10:J:147:TYR:HE2	1.70	0.56
34:p:47:GLN:HA	34:p:50:TYR:HB3	1.86	0.56
9:H:24:GLU:OE2	9:H:274:ARG:NH1	2.38	0.56
36:r:103:ILE:HB	37:s:47:ASP:HB3	1.87	0.56
3:3:193:SER:H	3:3:196:SER:HB3	1.71	0.56
39:u:7:ILE:HG23	39:u:16:GLN:HB3	1.86	0.56
1:1:21:ILE:O	1:1:117:LYS:NZ	2.34	0.56
53:o:503:CDL:H652	53:o:503:CDL:H862	1.88	0.56
53:o:503:CDL:H673	53:y:201:CDL:H822	1.88	0.56
4:4:335:ARG:NH2	7:9:129:ASP:OD1	2.39	0.56
6:6:73:GLY:HA2	9:H:25:ARG:HH22	1.70	0.56
22:c:33:ARG:NH1	22:c:77:ASP:OD1	2.39	0.56
3:3:198:ASN:OD1	3:3:268:ARG:NH2	2.39	0.56
10:J:20:PHE:HB2	10:J:29:GLY:HA2	1.88	0.55
51:A:403:3PE:H381	9:H:295:PRO:HB3	1.87	0.55
12:L:543:THR:HG23	40:v:83:MET:HE1	1.87	0.55
14:N:336:LEU:HD11	53:o:502:CDL:H272	1.89	0.55
19:Z:41:ASP:OD1	36:r:86:LYS:NZ	2.39	0.55
10:J:21:SER:O	10:J:23:LYS:NZ	2.35	0.55
12:L:83:ASP:OD2	12:L:262:ARG:NH1	2.38	0.55
9:H:202:GLU:OE2	9:H:279:ARG:NH1	2.40	0.55
1:1:270:GLU:OE1	1:1:283:HIS:NE2	2.38	0.55
3:3:126:ASP:HB2	4:4:328:ALA:HB3	1.89	0.55
4:4:61:VAL:HG21	4:4:83:LEU:HB2	1.89	0.55
4:4:388:ARG:HG2	5:5:81:VAL:HG22	1.88	0.55
8:A:36:PRO:O	26:g:50:GLN:NE2	2.40	0.55
3:3:201:ASP:OD2	3:3:268:ARG:NH2	2.37	0.54
3:3:276:ARG:NH1	3:3:680:ALA:O	2.39	0.54
6:6:71:ARG:HA	9:H:37:PRO:HA	1.89	0.54
23:d:311:GLU:HG2	23:d:336:PRO:HB3	1.88	0.54
3:3:396:ARG:NH1	3:3:416:THR:O	2.40	0.54
14:N:170:LEU:HD23	14:N:292:PHE:HB3	1.87	0.54
14:N:338:PRO:HG3	53:y:201:CDL:H792	1.88	0.54
3:3:382:THR:HG23	3:3:384:PRO:HD3	1.89	0.54
1:1:365:CYS:HB3	45:1:501:SF4:S3	2.48	0.54
14:N:292:PHE:HA	14:N:295:ARG:HE	1.72	0.54
18:Y:48:GLU:OE1	31:m:57:ARG:NH2	2.39	0.54
4:4:66:MET:HE1	4:4:414:VAL:HG11	1.88	0.54
3:3:36:GLN:NE2	22:c:47:SER:O	2.34	0.54
4:4:158:ALA:HB1	4:4:163:ALA:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:9:52:PHE:HE1	28:i:77:VAL:HG21	1.73	0.54
12:L:10:VAL:HG21	36:r:78:VAL:HG22	1.90	0.54
14:N:207:ILE:HG22	14:N:211:MET:HE2	1.90	0.54
1:1:289:GLY:HA3	1:1:293:ASN:HD22	1.73	0.54
1:1:428:GLU:HA	1:1:431:GLN:HG2	1.90	0.54
4:4:109:VAL:HG11	4:4:152:MET:HG2	1.90	0.54
4:4:183:ARG:NH1	4:4:210:ASP:OD2	2.35	0.54
7:9:164:GLU:HG3	28:i:88:ARG:HG3	1.90	0.54
23:d:167:LYS:HB2	23:d:229:ALA:HA	1.90	0.54
38:t:29:ARG:HD2	38:t:75:HIS:HD2	1.73	0.54
17:j:48:VAL:HG12	17:j:52:MET:HE2	1.90	0.54
3:3:194:GLU:HG3	3:3:389:PRO:HB3	1.90	0.53
13:M:179:LEU:HD13	13:M:249:LEU:HD11	1.89	0.53
13:M:205:VAL:HG22	13:M:212:LEU:HD13	1.90	0.53
12:L:392:LYS:O	12:L:395:ILE:HB	2.09	0.53
13:M:423:ILE:HG12	34:p:58:VAL:HG22	1.90	0.53
27:h:11:ARG:NH2	27:h:20:GLN:OE1	2.42	0.53
3:3:273:GLY:O	3:3:549:HIS:NE2	2.37	0.53
19:Z:67:PHE:HD1	43:y:43:LEU:HD21	1.74	0.53
33:o:27:THR:HG21	53:y:201:CDL:H432	1.89	0.53
34:p:80:ARG:NH2	40:v:39:ASP:O	2.41	0.53
1:1:144:ASN:O	1:1:148:ASN:HB2	2.08	0.53
23:d:26:ALA:HA	23:d:31:GLY:HA3	1.89	0.53
28:i:78:ASP:HB3	28:i:81:MET:HG3	1.89	0.53
41:w:100:ARG:HB2	41:w:105:LEU:HB2	1.91	0.53
11:K:67:ALA:O	11:K:70:GLU:HB3	2.08	0.53
11:K:73:LEU:HD11	14:N:41:ILE:HG13	1.91	0.53
16:W:47:ILE:HA	19:Z:58:ASN:HD21	1.72	0.53
28:i:1:MET:HG3	28:i:3:LEU:H	1.72	0.53
3:3:148:THR:HG23	3:3:150:MET:HE3	1.89	0.53
4:4:200:HIS:NE2	7:9:124:GLU:OE1	2.42	0.53
53:W:201:CDL:H381	52:w:801:PC1:H251	1.91	0.53
9:H:10:ILE:HA	9:H:13:ILE:HD12	1.91	0.53
10:J:40:GLY:HA2	10:J:43:ILE:HD12	1.91	0.53
33:o:52:PRO:HB2	33:o:55:SER:HB2	1.89	0.53
6:6:52:LEU:HB2	6:6:90:GLY:HA3	1.91	0.52
1:1:89:ARG:NH1	1:1:217:GLY:O	2.40	0.52
12:L:69:LEU:HD13	13:M:451:PRO:HG2	1.90	0.52
14:N:243:LEU:HD22	14:N:330:THR:HG21	1.91	0.52
20:a:72:SER:OG	20:a:75:HIS:ND1	2.35	0.52
30:l:96:HIS:O	35:q:127:ARG:NH1	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:p:51:ASN:HD22	38:t:165:LEU:HD22	1.74	0.52
5:5:96:LEU:HB2	5:5:105:ILE:HG22	1.92	0.52
8:A:112:GLU:HA	8:A:115:GLU:HG3	1.92	0.52
12:L:97:THR:HG21	12:L:125:LEU:HD22	1.91	0.52
29:k:165:PRO:O	29:k:248:TRP:NE1	2.40	0.52
11:K:46:LEU:O	11:K:50:ASN:HB2	2.09	0.52
4:4:141:PHE:O	4:4:145:THR:OG1	2.28	0.52
12:L:161:ARG:NH2	38:t:90:TYR:O	2.41	0.52
52:L:1002:PC1:H32	52:w:801:PC1:H142	1.92	0.52
29:k:104:ARG:NH1	29:k:126:ARG:O	2.43	0.52
42:x:41:GLU:OE2	42:x:44:ARG:NH2	2.41	0.52
12:L:128:MET:HE1	12:L:255:ALA:HB2	1.92	0.52
13:M:456:GLY:O	41:w:84:ARG:NH2	2.43	0.52
14:N:258:SER:O	14:N:261:MET:HB3	2.09	0.52
23:d:72:ASP:O	23:d:83:ARG:NH2	2.42	0.52
14:N:115:VAL:HG12	14:N:180:ALA:HB1	1.92	0.52
14:N:159:ILE:HG21	14:N:278:LEU:HD11	1.91	0.52
1:1:367:GLU:OE1	3:3:100:ASN:ND2	2.40	0.52
3:3:261:GLU:OE1	22:c:42:ARG:NH2	2.43	0.52
4:4:5:GLN:OE1	14:N:304:MET:N	2.43	0.52
13:M:1:FME:O1	13:M:3:LYS:NZ	2.43	0.52
25:f:34:LEU:HD12	25:f:37:ILE:HD12	1.91	0.52
14:N:337:LEU:O	14:N:340:THR:OG1	2.27	0.52
18:Y:35:CYS:O	18:Y:39:ASN:ND2	2.43	0.52
23:d:128:LYS:NZ	23:d:218:ILE:O	2.39	0.52
33:o:63:LEU:HD23	53:o:502:CDL:H112	1.92	0.52
3:3:158:ARG:HB3	3:3:202:ILE:HD12	1.92	0.51
10:J:23:LYS:HD2	11:K:28:SER:HB3	1.93	0.51
12:L:370:THR:HG23	12:L:431:LEU:HD13	1.92	0.51
52:L:1002:PC1:H271	52:w:801:PC1:H281	1.91	0.51
18:Y:48:GLU:OE1	18:Y:134:ARG:NH2	2.41	0.51
19:Z:159:LYS:NZ	33:o:112:VAL:O	2.42	0.51
38:t:100:GLU:OE1	38:t:121:ARG:NH1	2.41	0.51
12:L:75:LYS:HD2	41:w:90:ARG:HH22	1.76	0.51
19:Z:140:ASP:O	19:Z:161:ARG:NH1	2.43	0.51
2:2:159:ASN:HB3	2:2:184:PRO:HB3	1.93	0.51
4:4:233:ARG:NH1	52:9:401:PC1:O12	2.43	0.51
7:9:145:GLU:HA	7:9:148:LEU:HD13	1.91	0.51
3:3:119:GLN:HB2	3:3:123:PHE:HD2	1.75	0.51
13:M:328:CYS:HB3	13:M:437:MET:HE1	1.91	0.51
33:o:45:ASP:OD2	33:o:51:ARG:NH2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:379:LEU:HD13	3:3:384:PRO:HG3	1.93	0.51
13:M:204:MET:HE1	13:M:302:LEU:HD11	1.93	0.51
14:N:239:ILE:HD13	53:o:503:CDL:H532	1.92	0.51
8:A:71:LEU:O	10:J:147:TYR:OH	2.26	0.51
14:N:211:MET:HG2	14:N:333:SER:HB2	1.93	0.51
53:W:201:CDL:H402	52:w:801:PC1:H272	1.93	0.51
8:A:3:LEU:HD23	51:H:502:3PE:H231	1.93	0.51
53:o:503:CDL:H352	53:o:503:CDL:H612	1.92	0.51
37:s:6:ARG:NH1	37:s:15:GLU:OE2	2.43	0.51
12:L:392:LYS:HA	12:L:395:ILE:HD12	1.93	0.51
29:k:19:THR:HG23	29:k:21:ASN:H	1.76	0.51
12:L:161:ARG:NE	12:L:238:GLU:OE2	2.44	0.50
3:3:674:THR:O	3:3:679:ARG:NH1	2.45	0.50
4:4:71:GLU:OE2	9:H:134:ARG:NH1	2.38	0.50
4:4:352:TYR:HD1	7:9:86:VAL:HG21	1.76	0.50
1:1:184:TYR:HB3	1:1:357:GLU:HB3	1.93	0.50
12:L:221:THR:HG23	12:L:226:GLN:HB2	1.94	0.50
4:4:282:GLU:HB3	4:4:313:GLN:HE22	1.77	0.50
12:L:233:LEU:HD23	12:L:307:SER:HB3	1.93	0.50
1:1:342:ASP:OD1	1:1:429:ARG:NH2	2.40	0.50
9:H:162:LEU:HD21	9:H:237:PHE:HE1	1.76	0.50
12:L:536:LEU:HG	12:L:540:MET:HE2	1.93	0.50
14:N:249:LEU:HB3	14:N:254:LEU:HD12	1.92	0.50
19:Z:3:SER:OG	19:Z:4:TRP:N	2.42	0.50
29:k:170:ILE:HD11	29:k:238:ILE:HD11	1.93	0.50
34:p:74:ASN:OD1	34:p:78:ASN:ND2	2.44	0.50
14:N:261:MET:HG3	14:N:340:THR:HG23	1.94	0.50
38:t:27:GLU:OE2	38:t:33:ARG:NH1	2.44	0.50
53:L:1003:CDL:H182	13:M:442:LEU:HD22	1.93	0.50
25:f:112:LYS:NZ	25:f:115:ILE:O	2.45	0.50
29:k:171:TYR:HD2	29:k:222:GLN:HG3	1.76	0.50
41:w:114:ASP:HB3	41:w:117:LYS:HG2	1.94	0.50
4:4:83:LEU:HD11	6:6:53:ALA:HB2	1.94	0.50
12:L:245:ALA:O	12:L:249:SER:OG	2.26	0.50
16:W:34:ILE:HG12	53:W:201:CDL:H831	1.93	0.50
12:L:67:HIS:HB3	52:L:1002:PC1:H111	1.93	0.49
5:5:77:ASP:OD2	5:5:79:THR:OG1	2.30	0.49
12:L:88:MET:HB2	12:L:326:PHE:HE2	1.77	0.49
17:X:65:ILE:HD13	38:t:3:LEU:HD22	1.93	0.49
24:e:40:TYR:O	24:e:43:LEU:HB3	2.11	0.49
2:2:10:ARG:NH2	3:3:138:GLU:OE2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:73:LEU:HD13	10:J:55:MET:HE1	1.94	0.49
13:M:232:ALA:O	13:M:237:LYS:NZ	2.44	0.49
28:i:44:TYR:OH	28:i:113:HIS:N	2.40	0.49
2:2:116:ILE:HG23	2:2:169:ILE:HG21	1.94	0.49
29:k:51:PHE:HB3	29:k:107:GLN:HE21	1.77	0.49
4:4:261:ARG:NH2	4:4:303:GLU:OE2	2.42	0.49
54:X:101:ZMP:O6	38:t:12:GLN:NE2	2.42	0.49
17:j:11:ILE:HG22	17:j:77:VAL:HG23	1.93	0.49
30:l:65:CYS:HA	30:l:68:ARG:HE	1.77	0.49
40:v:80:ASP:HB3	40:v:83:MET:HB3	1.93	0.49
1:1:69:GLY:O	47:1:503:NAI:H2N	2.11	0.49
4:4:179:GLU:OE2	6:6:66:ARG:NH1	2.35	0.49
13:M:122:PHE:HZ	13:M:206:LYS:HG3	1.78	0.49
26:g:116:ASP:OD1	26:g:119:SER:OG	2.23	0.49
37:s:33:ARG:HH12	37:s:103:ARG:HH22	1.61	0.49
39:u:18:THR:H	39:u:21:GLN:HE21	1.60	0.49
13:M:426:ILE:HB	38:t:101:TRP:HH2	1.77	0.49
27:h:39:LYS:H	35:q:6:LYS:HB3	1.78	0.49
1:1:432:ARG:HA	1:1:435:GLN:HG3	1.94	0.49
34:p:39:ARG:NH2	38:t:3:LEU:O	2.45	0.49
7:9:158:GLY:O	7:9:162:GLU:HB2	2.12	0.49
14:N:308:THR:HB	29:k:274:SER:HB2	1.95	0.49
13:M:18:SER:HB2	13:M:23:ILE:HG22	1.93	0.48
53:W:201:CDL:H192	19:Z:47:VAL:HG21	1.95	0.48
18:Y:44:LEU:HD22	18:Y:130:VAL:HB	1.95	0.48
40:v:54:SER:HA	40:v:84:TYR:HB3	1.94	0.48
3:3:243:ARG:HD2	3:3:244:THR:HG23	1.95	0.48
4:4:63:ARG:NH2	26:g:95:VAL:O	2.46	0.48
53:W:201:CDL:H112	19:Z:51:ILE:HD11	1.94	0.48
1:1:356:HIS:O	3:3:177:ARG:NH2	2.45	0.48
12:L:184:LEU:HD13	13:M:393:ILE:HG21	1.94	0.48
3:3:426:PRO:HG3	3:3:661:LEU:HG	1.96	0.48
13:M:337:VAL:HG11	13:M:345:ALA:HB2	1.95	0.48
14:N:162:ILE:HD13	14:N:282:MET:HG3	1.95	0.48
26:g:42:VAL:HG11	26:g:59:ARG:HG3	1.95	0.48
29:k:108:TYR:OH	29:k:164:LEU:O	2.27	0.48
14:N:335:MET:HG2	53:o:503:CDL:H661	1.95	0.48
4:4:237:ASN:O	9:H:284:GLN:NE2	2.46	0.48
6:6:118:SER:N	45:6:502:SF4:S4	2.86	0.48
7:9:145:GLU:HB2	28:i:126:PRO:HG3	1.96	0.48
16:W:12:LYS:HA	38:t:98:VAL:HG21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:k:30:ASN:O	29:k:126:ARG:NH2	2.46	0.48
38:t:107:HIS:NE2	41:w:43:ASP:OD1	2.38	0.48
37:s:102:GLU:OE2	37:s:105:ARG:NH2	2.43	0.48
53:y:201:CDL:H632	53:y:201:CDL:H571	1.95	0.48
14:N:163:THR:HA	14:N:285:THR:HG21	1.95	0.48
29:k:38:LEU:HD22	29:k:228:ALA:HB1	1.96	0.48
29:k:174:VAL:HG22	29:k:225:ALA:HB2	1.96	0.48
6:6:35:ASP:HB3	51:6:503:3PE:H331	1.95	0.48
6:6:169:ARG:NH2	7:9:142:GLU:OE2	2.47	0.48
13:M:457:PRO:O	41:w:84:ARG:NH1	2.46	0.48
27:h:3:ALA:HA	53:h:201:CDL:HA21	1.95	0.48
3:3:60:GLU:HG2	3:3:78:ASN:HB3	1.95	0.47
1:1:378:ARG:NE	3:3:132:GLU:OE2	2.38	0.47
7:9:53:GLU:OE2	28:i:34:ARG:NH2	2.39	0.47
4:4:354:GLU:OE2	4:4:357:GLN:NE2	2.48	0.47
13:M:7:PRO:HB3	43:y:16:VAL:HG13	1.95	0.47
13:M:447:LEU:HD11	52:w:801:PC1:H3F1	1.95	0.47
16:W:138:LYS:HA	30:l:27:ARG:HB3	1.96	0.47
18:Y:18:LYS:O	44:z:68:ASN:ND2	2.48	0.47
12:L:100:ILE:HG21	12:L:246:LEU:HB2	1.96	0.47
12:L:428:PHE:HA	12:L:432:LEU:HD12	1.95	0.47
9:H:217:ALA:H	9:H:220:PHE:HB3	1.80	0.47
26:g:21:SER:OG	26:g:30:ARG:NH1	2.48	0.47
4:4:406:SER:HB2	4:4:414:VAL:HG22	1.96	0.47
5:5:119:SER:OG	5:5:131:GLU:OE2	2.29	0.47
16:W:120:GLY:O	16:W:124:GLN:NE2	2.47	0.47
29:k:308:TYR:HD1	29:k:317:ILE:HG23	1.80	0.47
38:t:169:ILE:O	38:t:172:ARG:NH1	2.45	0.47
4:4:145:THR:OG1	4:4:181:TYR:OH	2.27	0.47
5:5:154:ASP:OD1	26:g:101:HIS:NE2	2.45	0.47
7:9:64:GLU:OE1	7:9:136:ASN:ND2	2.47	0.47
10:J:43:ILE:HG22	11:K:46:LEU:HD21	1.96	0.47
10:J:167:VAL:HG22	14:N:42:PRO:HG2	1.97	0.47
13:M:94:LEU:HD21	53:o:503:CDL:H551	1.96	0.47
13:M:408:LEU:O	13:M:412:ILE:N	2.45	0.47
25:f:37:ILE:O	25:f:44:ARG:NH1	2.47	0.47
29:k:133:VAL:HG12	29:k:205:VAL:HG12	1.97	0.47
30:l:96:HIS:HA	30:l:101:GLU:HG2	1.95	0.47
37:s:6:ARG:HH12	37:s:105:ARG:HD2	1.79	0.47
37:s:33:ARG:NH2	37:s:100:GLU:OE2	2.46	0.47
1:1:21:ILE:HG12	1:1:233:THR:HG21	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:390:ASP:O	1:1:393:TRP:HB3	2.15	0.47
7:9:108:ARG:NH2	28:i:128:SER:OG	2.48	0.47
52:L:1002:PC1:H262	53:W:201:CDL:H621	1.95	0.47
13:M:135:ARG:NH1	14:N:302:LEU:O	2.47	0.47
29:k:173:ASP:OD1	29:k:207:LYS:NZ	2.48	0.47
4:4:343:GLU:O	4:4:347:HIS:ND1	2.40	0.47
52:9:401:PC1:H351	9:H:187:ILE:HD12	1.97	0.47
14:N:331:VAL:HG13	14:N:335:MET:HE3	1.97	0.47
1:1:154:ARG:HA	20:a:58:LEU:HD21	1.97	0.46
3:3:574:VAL:HG21	3:3:630:LEU:HD22	1.97	0.46
4:4:323:ILE:HD12	4:4:324:LYS:HG3	1.97	0.46
8:A:49:LEU:HD12	8:A:50:PRO:HD2	1.97	0.46
8:A:102:LEU:HD23	51:A:403:3PE:H372	1.97	0.46
11:K:1:FME:H	11:K:1:FME:HG3	1.54	0.46
22:c:89:LYS:HD2	22:c:105:VAL:HG11	1.97	0.46
3:3:564:ALA:HB3	3:3:569:LYS:HD3	1.98	0.46
3:3:569:LYS:HG3	3:3:571:ALA:HB2	1.98	0.46
4:4:321:GLY:O	35:q:7:GLN:NE2	2.43	0.46
5:5:74:SER:HB3	5:5:97:LEU:HB3	1.96	0.46
13:M:243:MET:HB3	13:M:301:ILE:HG21	1.97	0.46
4:4:203:LEU:HD22	4:4:207:LEU:HD23	1.97	0.46
29:k:173:ASP:HB2	29:k:224:SER:HA	1.97	0.46
51:6:503:3PE:H221	51:i:201:3PE:H332	1.98	0.46
23:d:285:GLU:O	23:d:289:THR:OG1	2.33	0.46
35:q:22:ARG:HH21	35:q:24:LEU:HD12	1.80	0.46
1:1:363:THR:HG21	3:3:97:LEU:HG	1.97	0.46
4:4:324:LYS:HD3	4:4:331:SER:HB3	1.97	0.46
37:s:8:TYR:OH	40:v:123:PRO:O	2.31	0.46
1:1:355:LYS:HD3	1:1:373:ASN:HD22	1.80	0.46
5:5:130:TYR:O	5:5:133:GLU:HB3	2.16	0.46
7:9:22:ALA:O	7:9:26:LEU:HB2	2.15	0.46
52:L:1002:PC1:H371	53:W:201:CDL:HA4	1.97	0.46
13:M:9:MET:HB3	53:y:201:CDL:H232	1.98	0.46
14:N:112:HIS:HB2	14:N:184:ILE:HD13	1.97	0.46
19:Z:68:ARG:NH1	43:y:43:LEU:O	2.49	0.46
53:o:502:CDL:H732	53:o:502:CDL:HB4	1.98	0.46
1:1:99:GLU:OE2	1:1:106:LYS:N	2.49	0.46
13:M:14:LEU:O	13:M:18:SER:OG	2.26	0.46
13:M:36:LEU:HB2	41:w:69:VAL:HG22	1.97	0.46
14:N:136:LEU:HD11	51:N:401:3PE:H3C2	1.98	0.46
5:5:129:TRP:O	5:5:132:ARG:HB3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:84:LEU:HD11	31:m:45:ASN:HD22	1.81	0.46
51:A:403:3PE:H2A2	31:m:19:VAL:HG13	1.98	0.46
52:L:1002:PC1:H341	53:W:201:CDL:H512	1.97	0.46
18:Y:66:ALA:O	18:Y:69:PHE:HB3	2.15	0.46
19:Z:5:ASP:HB3	19:Z:8:VAL:HG12	1.97	0.46
22:c:77:ASP:HB3	22:c:80:SER:HB3	1.97	0.46
56:d:401:NDP:O7N	56:d:401:NDP:O2N	2.33	0.46
43:y:8:ARG:HE	43:y:9:ASP:H	1.64	0.46
1:1:92:TYR:O	1:1:220:THR:HA	2.15	0.46
2:2:10:ARG:HH21	21:b:77:LYS:HG2	1.80	0.46
3:3:410:GLY:O	3:3:421:HIS:NE2	2.42	0.46
23:d:100:GLU:HB2	23:d:105:ASP:HA	1.98	0.46
36:r:18:ARG:NH1	38:t:170:VAL:O	2.44	0.46
1:1:49:LEU:HD21	1:1:123:LEU:HG	1.98	0.46
2:2:55:GLN:NE2	2:2:89:MET:O	2.36	0.46
7:9:162:GLU:HB3	28:i:109:ILE:HG12	1.97	0.46
19:Z:141:ARG:HG3	41:w:112:CYS:HB2	1.96	0.46
3:3:362:TYR:HA	3:3:492:ILE:HD12	1.97	0.45
11:K:1:FME:HB3	11:K:2:SER:H	1.61	0.45
13:M:325:MET:HE3	13:M:437:MET:HB3	1.97	0.45
14:N:46:LYS:NZ	51:N:401:3PE:O12	2.43	0.45
14:N:339:LEU:HD13	53:o:502:CDL:H261	1.96	0.45
17:X:55:GLU:OE1	38:t:24:ARG:NH2	2.49	0.45
3:3:187:ILE:HG13	3:3:189:LYS:HB2	1.98	0.45
8:A:69:ILE:HD11	9:H:144:VAL:HG13	1.98	0.45
12:L:129:LEU:HA	12:L:132:VAL:HG22	1.97	0.45
13:M:64:PRO:HB3	13:M:454:ILE:HG22	1.98	0.45
52:M:603:PC1:H251	52:M:603:PC1:H372	1.98	0.45
14:N:30:TRP:NE1	14:N:67:SER:OG	2.49	0.45
14:N:206:ILE:HG23	51:N:401:3PE:H2I2	1.97	0.45
53:W:201:CDL:HB61	52:w:801:PC1:H232	1.97	0.45
37:s:33:ARG:NH1	37:s:103:ARG:HH22	2.13	0.45
12:L:547:LYS:NZ	40:v:44:TYR:OH	2.48	0.45
7:9:114:THR:HG21	7:9:144:HIS:CD2	2.50	0.45
12:L:487:LYS:HE3	39:u:49:GLY:HA2	1.98	0.45
8:A:105:GLU:HG3	8:A:111:LEU:HG	1.97	0.45
52:L:1002:PC1:H322	36:r:88:HIS:CG	2.51	0.45
14:N:128:LEU:HD13	14:N:216:PHE:HB2	1.99	0.45
51:N:401:3PE:H2H1	51:N:401:3PE:H3B2	1.98	0.45
23:d:96:GLY:HA3	56:d:401:NDP:H3D	1.98	0.45
3:3:65:VAL:HG13	3:3:85:LYS:HE2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:9:143:THR:HB	7:9:146:GLU:HG3	1.99	0.45
8:A:114:THR:HB	9:H:286:MET:HG3	1.99	0.45
18:Y:43:MET:HE3	18:Y:47:TRP:HZ3	1.81	0.45
18:Y:60:LYS:O	18:Y:64:GLN:N	2.49	0.45
23:d:22:THR:OG1	23:d:88:SER:OG	2.25	0.45
27:h:8:GLN:NE2	27:h:20:GLN:HG3	2.32	0.45
3:3:100:ASN:HB3	3:3:135:ARG:HG2	1.99	0.45
10:J:149:TYR:HD2	11:K:55:LEU:HD21	1.80	0.45
3:3:115:ASP:O	3:3:119:GLN:HG2	2.17	0.45
12:L:316:THR:HG23	12:L:325:ALA:HB2	1.98	0.45
52:L:1002:PC1:H2A1	52:L:1002:PC1:H2D2	1.73	0.45
1:1:208:PRO:HG2	22:c:119:GLY:HA3	1.99	0.45
3:3:146:VAL:HG21	3:3:199:ILE:HD11	1.98	0.45
3:3:325:ALA:HB1	3:3:623:LEU:HD11	1.99	0.45
6:6:44:SER:OG	9:H:54:LYS:NZ	2.45	0.45
12:L:40:ILE:HD11	12:L:122:LEU:HD13	1.98	0.45
14:N:200:MET:HG3	14:N:269:GLU:HG3	1.97	0.45
37:s:42:GLN:HE22	40:v:140:LEU:HD12	1.82	0.45
1:1:358:SER:OG	1:1:365:CYS:SG	2.69	0.45
12:L:106:TRP:CD1	12:L:447:ASN:HD22	2.35	0.45
12:L:193:LEU:HD23	12:L:201:ILE:HA	1.99	0.45
12:L:316:THR:HA	12:L:319:ILE:HG12	1.98	0.45
2:2:24:THR:OG1	2:2:27:ASN:OD1	2.35	0.44
2:2:50:VAL:HG12	2:2:69:VAL:HG22	1.99	0.44
4:4:71:GLU:HB3	4:4:410:MET:HG2	1.98	0.44
5:5:151:ILE:HG23	5:5:152:LEU:HG	1.99	0.44
12:L:73:THR:HB	12:L:194:ASN:HD21	1.82	0.44
52:L:1002:PC1:H3G2	36:r:80:ILE:HD13	1.99	0.44
16:W:8:LEU:HD21	17:X:88:GLU:HB2	1.98	0.44
29:k:52:PRO:O	29:k:107:GLN:NE2	2.50	0.44
41:w:34:ASP:OD1	41:w:34:ASP:N	2.50	0.44
5:5:49:GLU:HG2	5:5:106:ARG:HD2	2.00	0.44
9:H:20:LEU:HD13	44:z:12:MET:HE1	1.99	0.44
12:L:221:THR:HG22	12:L:229:LEU:HB2	2.00	0.44
37:s:50:LEU:HB2	37:s:55:ARG:HE	1.83	0.44
3:3:194:GLU:HG2	3:3:195:LEU:HG	1.98	0.44
4:4:160:ASP:O	9:H:279:ARG:NH2	2.51	0.44
9:H:46:LEU:HD21	51:i:201:3PE:H361	2.00	0.44
11:K:55:LEU:HD13	30:l:16:TRP:HE3	1.82	0.44
13:M:332:SER:O	13:M:336:ARG:NH1	2.51	0.44
18:Y:97:ARG:HD3	35:q:59:LEU:HD13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:v:88:ARG:HB3	40:v:89:VAL:H	1.64	0.44
1:1:97:ALA:HB3	1:1:138:ILE:HA	1.99	0.44
5:5:33:LEU:HD13	5:5:60:VAL:HG22	1.99	0.44
10:J:111:LYS:HA	10:J:121:GLY:HA3	2.00	0.44
4:4:135:GLN:HB3	4:4:276:ASP:HB3	1.99	0.44
23:d:26:ALA:HB3	23:d:47:VAL:HG13	1.99	0.44
33:o:5:ARG:NH2	33:o:89:ASP:OD1	2.50	0.44
12:L:542:LEU:HB2	40:v:83:MET:HE3	1.99	0.44
16:W:43:ILE:HG12	16:W:47:ILE:HD12	1.98	0.44
23:d:174:ARG:NH2	23:d:316:GLU:OE2	2.51	0.44
37:s:33:ARG:HH21	40:v:158:ILE:HB	1.82	0.44
38:t:29:ARG:HD2	38:t:75:HIS:CD2	2.53	0.44
2:2:111:ARG:HD3	2:2:151:ALA:HB3	1.98	0.44
3:3:324:ASP:OD1	3:3:324:ASP:N	2.50	0.44
53:W:201:CDL:OA3	36:r:88:HIS:NE2	2.38	0.44
18:Y:17:VAL:HG12	18:Y:19:VAL:HG22	2.00	0.44
53:o:503:CDL:CA7	53:o:503:CDL:H531	2.48	0.44
3:3:601:ARG:NH2	3:3:614:ASP:OD1	2.46	0.44
4:4:359:PRO:O	4:4:380:SER:OG	2.31	0.44
13:M:207:MET:HE3	13:M:294:MET:HB3	1.99	0.44
22:c:29:HIS:HD2	22:c:33:ARG:HH11	1.65	0.44
29:k:27:VAL:HG12	29:k:35:LYS:HD2	2.00	0.44
3:3:325:ALA:HA	3:3:328:LEU:HD12	2.00	0.44
3:3:332:LYS:NZ	3:3:505:LEU:O	2.42	0.44
53:L:1003:CDL:H802	52:w:801:PC1:H2I3	2.00	0.44
13:M:369:LEU:HD12	13:M:370:PRO:HD2	1.99	0.44
17:j:17:TYR:HA	17:j:20:LYS:HG2	2.00	0.44
30:l:85:LEU:HD22	30:l:90:LYS:HB2	1.99	0.44
40:v:47:TYR:OH	40:v:77:MET:O	2.32	0.44
8:A:24:LEU:HD11	52:A:401:PC1:H391	1.99	0.43
9:H:14:LEU:HD22	9:H:225:MET:HE2	1.98	0.43
13:M:50:LEU:HA	16:W:86:ASN:HD21	1.83	0.43
29:k:22:SER:OG	29:k:119:GLY:O	2.30	0.43
33:o:45:ASP:OD1	33:o:49:ARG:NH2	2.50	0.43
7:9:132:VAL:HG21	7:9:165:ILE:HG21	2.00	0.43
10:J:121:GLY:HA2	11:K:3:LEU:HD22	2.00	0.43
12:L:542:LEU:HB3	13:M:278:ARG:HD3	2.00	0.43
14:N:217:THR:HG23	51:N:401:3PE:H242	2.00	0.43
3:3:365:ASN:N	3:3:491:ASN:OD1	2.51	0.43
12:L:50:PRO:HA	12:L:53:MET:HG2	2.01	0.43
13:M:116:ILE:HD12	13:M:116:ILE:HA	1.91	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:216:LEU:HD23	13:M:287:ALA:HB1	2.00	0.43
17:j:37:MET:HE1	17:j:44:SER:HA	1.98	0.43
33:o:43:LEU:HD22	33:o:53:VAL:HG12	1.99	0.43
4:4:98:GLN:NE2	7:9:85:ALA:O	2.51	0.43
9:H:299:ALA:HA	9:H:302:MET:HE3	2.01	0.43
51:H:502:3PE:H2B2	51:H:502:3PE:H352	1.99	0.43
12:L:144:TRP:NE1	12:L:179:ASP:OD1	2.46	0.43
23:d:280:THR:HG23	23:d:283:LYS:H	1.83	0.43
3:3:13:VAL:HG22	3:3:79:ILE:HD12	2.00	0.43
3:3:198:ASN:ND2	3:3:262:TRP:HB3	2.33	0.43
7:9:155:LEU:HB3	21:b:36:ASN:HD22	1.84	0.43
12:L:532:ILE:HD11	40:v:101:MET:HB3	2.00	0.43
14:N:337:LEU:HD23	53:y:201:CDL:H782	2.00	0.43
20:a:57:ASP:OD1	20:a:60:LYS:NZ	2.52	0.43
3:3:269:PHE:HB3	3:3:683:THR:HG21	1.99	0.43
4:4:123:GLU:OE2	4:4:138:ARG:NH2	2.41	0.43
12:L:139:GLN:HA	12:L:142:ILE:HD12	2.00	0.43
13:M:173:SER:HB2	16:W:101:ALA:HB2	2.00	0.43
18:Y:82:THR:HA	18:Y:85:TRP:CD1	2.53	0.43
4:4:224:GLU:OE2	7:9:40:TYR:OH	2.32	0.43
5:5:41:GLN:NE2	5:5:49:GLU:OE1	2.40	0.43
12:L:383:MET:HE2	39:u:36:ILE:HD13	2.00	0.43
13:M:379:LEU:O	13:M:383:MET:HG2	2.19	0.43
18:Y:6:LEU:HD12	35:q:90:LEU:HD22	2.00	0.43
23:d:135:LEU:HA	23:d:167:LYS:HB3	1.99	0.43
30:l:74:ARG:NH2	35:q:93:GLU:OE2	2.52	0.43
35:q:92:GLU:HA	35:q:95:THR:HG22	2.00	0.43
2:2:43:LYS:HE2	2:2:73:LEU:HA	2.01	0.43
3:3:159:CYS:HB3	3:3:172:LEU:HD13	2.01	0.43
3:3:349:PHE:H	3:3:509:PRO:HB2	1.83	0.43
12:L:434:GLN:HE21	32:n:52:TYR:HA	1.82	0.43
13:M:118:PHE:O	13:M:122:PHE:HB2	2.19	0.43
14:N:234:TRP:HE1	14:N:305:PHE:HB2	1.83	0.43
3:3:329:ILE:HD11	3:3:626:VAL:HG21	2.00	0.43
7:9:132:VAL:HG11	7:9:169:ILE:HD11	2.01	0.43
16:W:133:ILE:HG23	30:l:21:SER:HB3	2.01	0.43
37:s:4:LEU:HD11	40:v:124:THR:HA	1.99	0.43
53:y:201:CDL:H122	53:y:201:CDL:H671	2.00	0.43
1:1:68:ARG:HH11	1:1:242:PHE:HZ	1.67	0.43
12:L:402:SER:OG	12:L:404:THR:OG1	2.31	0.43
14:N:230:LEU:HD11	14:N:244:VAL:HG21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:49:GLU:OE2	38:t:19:TYR:OH	2.37	0.43
3:3:140:LYS:HD3	3:3:150:MET:HG3	2.01	0.42
3:3:244:THR:HB	22:c:73:ALA:HB2	2.01	0.42
6:6:58:GLU:HG2	6:6:151:PRO:O	2.18	0.42
12:L:203:MET:HB2	19:Z:113:GLN:HG3	2.00	0.42
12:L:316:THR:HB	12:L:395:ILE:HG23	2.01	0.42
13:M:424:ASN:OD1	34:p:57:GLY:N	2.52	0.42
16:W:114:MET:HE2	16:W:121:PRO:HD2	2.00	0.42
34:p:32:GLN:HB3	38:t:7:ALA:HB1	2.00	0.42
5:5:121:VAL:HG21	5:5:146:PRO:HD3	2.00	0.42
8:A:7:LEU:HD22	51:H:502:3PE:H371	2.00	0.42
9:H:88:PRO:HB3	9:H:98:MET:HE3	2.01	0.42
9:H:165:LEU:HD21	9:H:241:LEU:HA	2.01	0.42
13:M:54:LEU:HD23	16:W:93:ILE:HG23	2.00	0.42
13:M:135:ARG:HG3	53:o:503:CDL:H742	2.01	0.42
16:W:44:ASN:HB3	53:W:201:CDL:HA31	2.00	0.42
54:X:101:ZMP:H17	54:X:101:ZMP:H15	1.65	0.42
29:k:30:ASN:N	29:k:33:SER:OG	2.50	0.42
34:p:62:PRO:O	34:p:66:ARG:HB2	2.18	0.42
1:1:374:LYS:NZ	3:3:133:GLY:O	2.52	0.42
13:M:75:LEU:HB3	13:M:229:MET:HE1	2.00	0.42
13:M:127:VAL:HG11	53:o:503:CDL:H872	2.01	0.42
9:H:316:PRO:HG3	35:q:56:ARG:HB3	2.00	0.42
12:L:59:GLN:NE2	36:r:98:GLU:OE2	2.53	0.42
12:L:73:THR:OG1	34:p:127:SER:OG	2.37	0.42
13:M:175:ASN:HD22	16:W:97:GLU:HG3	1.83	0.42
38:t:134:ARG:HA	38:t:137:LYS:HE3	2.00	0.42
41:w:77:VAL:HA	41:w:80:LEU:HG	2.01	0.42
43:y:22:PHE:O	43:y:25:TYR:HB3	2.19	0.42
1:1:94:VAL:O	1:1:222:VAL:HA	2.19	0.42
1:1:118:LEU:HD13	1:1:225:VAL:HG13	2.01	0.42
1:1:393:TRP:O	1:1:396:SER:OG	2.37	0.42
2:2:175:GLU:HG3	2:2:182:PRO:HG3	2.01	0.42
3:3:140:LYS:HB2	3:3:148:THR:HG21	2.01	0.42
13:M:101:LEU:HD21	53:o:503:CDL:H841	2.02	0.42
14:N:246:ILE:HD12	14:N:334:THR:HG21	2.02	0.42
14:N:254:LEU:HG	14:N:290:LEU:HD11	2.01	0.42
14:N:275:SER:HB3	15:V:136:ALA:HB3	2.00	0.42
16:W:122:TRP:CD1	33:o:2:MET:HG2	2.55	0.42
18:Y:29:HIS:HB3	18:Y:119:PRO:HD2	2.02	0.42
29:k:41:GLU:HA	29:k:44:GLU:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:o:503:CDL:H592	53:o:503:CDL:H791	2.01	0.42
53:o:503:CDL:H671	53:o:503:CDL:H842	2.00	0.42
3:3:443:LEU:HD13	3:3:477:ILE:HD11	2.00	0.42
4:4:197:GLY:O	4:4:325:VAL:N	2.53	0.42
6:6:46:TRP:CD1	6:6:75:VAL:HG22	2.54	0.42
33:o:66:THR:OG1	42:x:28:TRP:NE1	2.52	0.42
53:o:502:CDL:H142	53:o:502:CDL:H171	1.80	0.42
3:3:99:ALA:O	3:3:134:LYS:NZ	2.45	0.42
3:3:323:VAL:H	3:3:498:SER:HB3	1.83	0.42
5:5:72:PHE:HB3	5:5:96:LEU:HB3	2.02	0.42
5:5:175:ARG:NH2	5:5:186:GLU:OE2	2.49	0.42
6:6:46:TRP:H	6:6:84:ASP:HB2	1.84	0.42
9:H:137:ALA:HA	9:H:140:ILE:HG12	2.02	0.42
12:L:260:LEU:HD23	12:L:260:LEU:HA	1.87	0.42
14:N:26:TRP:NE1	14:N:85:THR:O	2.53	0.42
6:6:49:THR:HB	6:6:76:PHE:HB3	2.01	0.42
12:L:375:ILE:HG12	39:u:32:MET:SD	2.60	0.42
18:Y:143:SER:HB2	18:Y:146:ARG:HH12	1.85	0.42
21:b:11:VAL:HG22	21:b:17:VAL:HB	2.01	0.42
27:h:11:ARG:HG2	27:h:19:LEU:HD12	2.02	0.42
1:1:21:ILE:HG21	1:1:230:VAL:HG12	2.00	0.42
1:1:140:GLY:C	2:2:89:MET:HE1	2.45	0.42
8:A:75:LEU:HD12	9:H:151:LEU:HD21	2.01	0.42
9:H:309:ILE:HG22	31:m:38:THR:HG23	2.02	0.42
12:L:49:ILE:HG12	19:Z:32:LEU:HD13	2.02	0.42
53:o:503:CDL:H871	53:o:503:CDL:H811	2.02	0.42
3:3:324:ASP:HB3	3:3:571:ALA:HB1	2.00	0.42
8:A:98:LEU:HD22	9:H:298:LEU:HD21	2.02	0.42
9:H:75:PRO:HG3	9:H:223:PHE:CE2	2.54	0.42
12:L:213:LEU:HD23	12:L:216:LEU:HD12	2.02	0.42
13:M:122:PHE:CZ	13:M:206:LYS:HG3	2.55	0.42
14:N:300:THR:HA	14:N:305:PHE:HZ	1.84	0.42
5:5:56:GLY:HA2	5:5:59:PRO:HD2	2.02	0.41
6:6:36:LEU:HD13	51:6:503:3PE:H392	2.01	0.41
10:J:130:THR:HG21	35:q:123:LEU:HD12	2.02	0.41
12:L:427:ILE:HG23	12:L:431:LEU:HD12	2.01	0.41
14:N:263:LYS:HE2	14:N:263:LYS:HB3	1.90	0.41
22:c:69:LEU:HD13	23:d:66:GLY:HA3	2.02	0.41
24:e:13:LEU:HD22	24:e:16:ARG:HH22	1.85	0.41
7:9:151:LYS:HE2	7:9:155:LEU:HD11	2.02	0.41
53:L:1003:CDL:H851	53:W:201:CDL:H671	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:13:ASP:OD2	32:n:12:LYS:NZ	2.54	0.41
21:b:1:GLY:N	21:b:42:ASP:OD2	2.39	0.41
29:k:25:ILE:O	29:k:123:VAL:HA	2.20	0.41
4:4:412:ALA:HB3	9:H:281:ARG:HG3	2.02	0.41
5:5:183:VAL:O	26:g:100:THR:OG1	2.31	0.41
12:L:249:SER:HB2	12:L:336:LYS:HG3	2.02	0.41
17:X:20:LYS:HD2	32:n:18:TYR:CZ	2.56	0.41
1:1:193:ILE:HG23	1:1:215:VAL:HA	2.03	0.41
2:2:154:VAL:HG22	2:2:164:LEU:HD11	2.01	0.41
8:A:80:GLN:NE2	9:H:315:PRO:O	2.41	0.41
1:1:214:GLY:HA3	1:1:220:THR:HB	2.02	0.41
1:1:394:GLU:OE1	3:3:129:ARG:NH1	2.54	0.41
3:3:259:ASN:O	3:3:262:TRP:N	2.50	0.41
9:H:153:VAL:HG11	9:H:241:LEU:HD23	2.02	0.41
11:K:47:MET:HE3	11:K:47:MET:HB2	1.91	0.41
18:Y:39:ASN:HB3	35:q:72:PRO:HG2	2.02	0.41
18:Y:165:ARG:HH12	33:o:90:MET:HE1	1.85	0.41
7:9:69:ARG:NH2	21:b:38:ASN:O	2.52	0.41
28:i:9:ARG:HA	28:i:12:GLN:HG2	2.02	0.41
53:y:201:CDL:H822	53:y:201:CDL:H852	1.91	0.41
5:5:177:ASP:OD1	23:d:40:ARG:NH2	2.54	0.41
9:H:114:TYR:OH	10:J:61:LEU:O	2.31	0.41
12:L:152:PHE:HB2	12:L:172:ILE:HD11	2.02	0.41
52:L:1002:PC1:H331	53:W:201:CDL:HB21	2.03	0.41
19:Z:10:PRO:O	36:r:94:TYR:OH	2.36	0.41
21:b:68:HIS:ND1	21:b:69:PRO:O	2.52	0.41
23:d:127:GLU:O	23:d:224:ARG:NH1	2.46	0.41
24:e:81:PHE:HB3	24:e:85:GLN:HB2	2.02	0.41
1:1:96:ASN:ND2	46:1:502:FMN:O4'	2.51	0.41
4:4:302:GLU:HG2	7:9:3:LYS:HD2	2.02	0.41
9:H:31:MET:HE1	9:H:272:TRP:HB2	2.02	0.41
53:L:1003:CDL:H391	53:L:1003:CDL:H171	2.03	0.41
13:M:75:LEU:HD23	13:M:440:HIS:CE1	2.56	0.41
16:W:125:TYR:HB2	30:l:48:SER:HB3	2.03	0.41
53:W:201:CDL:H862	53:W:201:CDL:H832	1.96	0.41
3:3:588:MET:HG3	22:c:63:GLU:HA	2.02	0.41
4:4:106:LEU:HD11	4:4:391:ILE:HD13	2.01	0.41
4:4:190:HIS:CD2	6:6:150:PRO:HD3	2.55	0.41
7:9:175:TYR:CZ	27:h:38:PRO:HG3	2.56	0.41
52:9:401:PC1:H142	52:9:401:PC1:H111	1.92	0.41
9:H:198:PHE:HD1	9:H:285:LEU:HD13	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:93:LEU:HB3	14:N:54:GLU:HG3	2.03	0.41
12:L:37:LYS:HG2	12:L:98:TRP:HD1	1.86	0.41
34:p:47:GLN:HG3	38:t:165:LEU:HD13	2.02	0.41
40:v:52:ASP:OD1	40:v:78:HIS:NE2	2.40	0.41
4:4:387:TYR:CZ	5:5:164:LYS:HE3	2.55	0.41
7:9:30:LEU:O	9:H:277:TYR:OH	2.38	0.41
19:Z:25:LEU:HD12	37:s:75:ASN:HB2	2.02	0.41
31:m:80:LEU:HD12	31:m:83:LEU:HD11	2.03	0.41
1:1:276:LEU:HD21	1:1:297:VAL:HG11	2.02	0.40
4:4:149:ASN:HD21	4:4:371:LYS:HG3	1.86	0.40
9:H:79:LEU:HD11	9:H:222:LEU:HD22	2.03	0.40
9:H:165:LEU:HD23	9:H:240:THR:HG22	2.02	0.40
11:K:38:LEU:O	11:K:42:ILE:HG12	2.21	0.40
12:L:13:ILE:HG13	36:r:81:ILE:HD11	2.02	0.40
13:M:134:THR:HG22	13:M:142:ARG:HH12	1.85	0.40
17:j:49:GLU:HA	17:j:52:MET:HE3	2.02	0.40
33:o:68:PHE:HE1	53:o:502:CDL:H162	1.86	0.40
1:1:117:LYS:HE3	1:1:117:LYS:HB2	1.91	0.40
19:Z:81:VAL:HA	19:Z:84:MET:HG2	2.02	0.40
53:y:201:CDL:H321	53:y:201:CDL:HB21	2.03	0.40
5:5:72:PHE:O	5:5:124:TYR:OH	2.35	0.40
5:5:116:PRO:HG2	26:g:17:LYS:HE3	2.02	0.40
8:A:29:VAL:HB	52:A:401:PC1:H153	2.04	0.40
14:N:338:PRO:HG3	53:y:201:CDL:H762	2.03	0.40
16:W:87:TYR:HE1	19:Z:89:MET:HG3	1.87	0.40
31:m:30:ILE:O	31:m:33:THR:OG1	2.35	0.40
1:1:361:GLN:N	45:1:501:SF4:S4	2.94	0.40
3:3:12:PHE:HB2	3:3:78:ASN:HA	2.02	0.40
4:4:67:GLU:HB3	4:4:75:LYS:HB3	2.03	0.40
4:4:391:ILE:O	4:4:430:ARG:NH1	2.54	0.40
1:1:108:ARG:NH2	2:2:162:GLU:OE2	2.55	0.40
4:4:155:THR:HB	4:4:167:PHE:HA	2.03	0.40
51:A:403:3PE:H2D2	31:m:23:ALA:HA	2.03	0.40
28:i:50:GLU:HG3	28:i:89:TRP:HZ2	1.86	0.40
30:l:91:TYR:OH	35:q:92:GLU:OE1	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	428/464 (92%)	409 (96%)	19 (4%)	0	100	100
2	2	211/246 (86%)	197 (93%)	14 (7%)	0	100	100
3	3	492/727 (68%)	475 (96%)	17 (4%)	0	100	100
4	4	421/463 (91%)	405 (96%)	16 (4%)	0	100	100
5	5	206/266 (77%)	198 (96%)	8 (4%)	0	100	100
6	6	154/223 (69%)	148 (96%)	6 (4%)	0	100	100
7	9	174/217 (80%)	166 (95%)	8 (5%)	0	100	100
8	A	106/115 (92%)	96 (91%)	10 (9%)	0	100	100
9	H	310/318 (98%)	300 (97%)	10 (3%)	0	100	100
10	J	163/175 (93%)	155 (95%)	8 (5%)	0	100	100
11	K	96/98 (98%)	92 (96%)	4 (4%)	0	100	100
12	L	556/606 (92%)	532 (96%)	24 (4%)	0	100	100
13	M	457/459 (100%)	448 (98%)	9 (2%)	0	100	100
14	N	345/347 (99%)	330 (96%)	15 (4%)	0	100	100
15	V	25/141 (18%)	23 (92%)	2 (8%)	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%)	74 (92%)	6 (8%)	0	100	100
18	Y	169/172 (98%)	163 (96%)	6 (4%)	0	100	100
19	Z	169/175 (97%)	167 (99%)	2 (1%)	0	100	100
20	a	42/109 (38%)	42 (100%)	0	0	100	100
21	b	93/124 (75%)	92 (99%)	1 (1%)	0	100	100
22	c	124/170 (73%)	121 (98%)	3 (2%)	0	100	100
23	d	289/380 (76%)	283 (98%)	6 (2%)	0	100	100
24	e	84/99 (85%)	81 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	f	111/116 (96%)	110 (99%)	1 (1%)	0	100	100
26	g	112/140 (80%)	109 (97%)	3 (3%)	0	100	100
27	h	92/114 (81%)	87 (95%)	5 (5%)	0	100	100
28	i	143/145 (99%)	142 (99%)	1 (1%)	0	100	100
29	k	317/355 (89%)	305 (96%)	12 (4%)	0	100	100
30	l	103/106 (97%)	100 (97%)	3 (3%)	0	100	100
31	m	78/84 (93%)	75 (96%)	3 (4%)	0	100	100
32	n	77/98 (79%)	75 (97%)	2 (3%)	0	100	100
33	o	118/122 (97%)	116 (98%)	2 (2%)	0	100	100
34	p	126/130 (97%)	118 (94%)	8 (6%)	0	100	100
35	q	137/144 (95%)	134 (98%)	3 (2%)	0	100	100
36	r	95/128 (74%)	92 (97%)	3 (3%)	0	100	100
37	s	120/137 (88%)	116 (97%)	4 (3%)	0	100	100
38	t	175/179 (98%)	171 (98%)	4 (2%)	0	100	100
39	u	63/108 (58%)	61 (97%)	2 (3%)	0	100	100
40	v	153/186 (82%)	144 (94%)	9 (6%)	0	100	100
41	w	99/154 (64%)	95 (96%)	4 (4%)	0	100	100
42	x	47/76 (62%)	46 (98%)	1 (2%)	0	100	100
43	y	48/58 (83%)	47 (98%)	1 (2%)	0	100	100
44	z	68/70 (97%)	68 (100%)	0	0	100	100
All	All	7698/9247 (83%)	7427 (96%)	271 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	AYA	h	1	27	6,7,8	1.25	1 (16%)	6,8,10	1.03	0
13	FME	M	1	13	8,9,10	0.99	0	8,9,11	0.91	0
12	FME	L	1	12	8,9,10	0.94	0	8,9,11	1.62	2 (25%)
11	FME	K	1	11	8,9,10	0.96	0	8,9,11	0.79	0
29	SEP	k	36	29	8,9,10	1.60	1 (12%)	7,12,14	1.15	1 (14%)
4	2MR	4	85	4	10,12,13	2.32	3 (30%)	5,13,15	2.12	1 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	AYA	h	1	27	-	0/5/6/8	-
13	FME	M	1	13	-	2/7/9/11	-
12	FME	L	1	12	-	1/7/9/11	-
11	FME	K	1	11	-	6/7/9/11	-
29	SEP	k	36	29	-	3/6/8/10	-
4	2MR	4	85	4	-	1/10/13/15	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	4	85	2MR	CZ-NH2	4.74	1.43	1.33
4	4	85	2MR	CZ-NE	4.37	1.43	1.34
29	k	36	SEP	P-O1P	3.50	1.61	1.50
27	h	1	AYA	CA-N	-2.49	1.43	1.46
4	4	85	2MR	CQ1-NH1	-2.21	1.41	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	4	85	2MR	NE-CZ-NH2	-4.00	115.81	119.48
12	L	1	FME	CA-N-CN	3.36	127.98	122.82
12	L	1	FME	C-CA-N	2.81	114.92	109.50
29	k	36	SEP	OG-CB-CA	2.28	110.36	108.14

There are no chirality outliers.

All (13) 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
29	k	36	SEP	CB-OG-P-O1P
29	k	36	SEP	CB-OG-P-O2P
29	k	36	SEP	CB-OG-P-O3P
12	L	1	FME	CA-CB-CG-SD
11	K	1	FME	N-CA-CB-CG
11	K	1	FME	CB-CA-N-CN
13	M	1	FME	CB-CA-N-CN
11	K	1	FME	CA-CB-CG-SD
11	K	1	FME	C-CA-CB-CG
4	4	85	2MR	NE-CD-CG-CB

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	M	1	FME	1	0
11	K	1	FME	2	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 41 ligands modelled in this entry, 2 are monoatomic - leaving 39 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
54	ZMP	g	201	-	28,33,36	0.64	1 (3%)	32,40,45	1.20	4 (12%)
52	PC1	M	603	-	41,41,53	0.35	0	47,49,61	0.49	0
53	CDL	y	201	-	99,99,99	0.29	0	105,111,111	0.30	0
45	SF4	6	502	6	0,12,12	-	-	-	-	-
54	ZMP	X	101	17	25,30,36	0.80	1 (4%)	29,37,45	0.98	2 (6%)
45	SF4	3	802	3	0,12,12	-	-	-	-	-
52	PC1	L	1002	-	53,53,53	0.31	0	59,61,61	0.64	2 (3%)
48	FES	2	300	2	0,4,4	-	-	-	-	-
51	3PE	o	501	-	30,30,50	0.38	0	33,35,55	0.43	0
51	3PE	H	502	-	50,50,50	0.31	0	53,55,55	0.53	1 (1%)
56	NDP	d	401	-	51,52,52	0.46	0	71,80,80	0.37	0
46	FMN	1	502	-	33,33,33	1.08	2 (6%)	48,50,50	1.36	8 (16%)
47	NAI	1	503	-	47,48,48	0.39	0	64,73,73	1.84	4 (6%)
48	FES	3	803	3	0,4,4	-	-	-	-	-
51	3PE	L	1001	-	50,50,50	0.30	0	53,55,55	0.35	0
52	PC1	A	402	-	36,36,53	0.36	0	42,44,61	0.63	2 (4%)
52	PC1	A	401	-	45,45,53	0.32	0	51,53,61	0.34	0
52	PC1	9	401	-	53,53,53	0.31	0	59,61,61	0.51	1 (1%)
51	3PE	6	503	-	50,50,50	0.31	0	53,55,55	0.31	0
50	970	6	501	-	33,33,33	0.46	0	48,50,50	0.62	0
45	SF4	1	501	1	0,12,12	-	-	-	-	-
58	MYR	s	201	37	13,14,15	0.19	0	12,13,15	0.14	0
51	3PE	M	602	-	43,43,50	0.32	0	46,48,55	0.48	0
53	CDL	o	503	-	89,89,99	0.30	0	95,101,111	0.39	1 (1%)
52	PC1	w	801	-	53,53,53	0.29	0	59,61,61	0.38	0
45	SF4	3	801	3	0,12,12	-	-	-	-	-
53	CDL	W	201	-	99,99,99	0.28	0	105,111,111	0.30	0
45	SF4	9	402	7	0,12,12	-	-	-	-	-
50	970	H	501	-	33,33,33	0.37	0	48,50,50	0.72	2 (4%)
53	CDL	L	1003	-	99,99,99	0.26	0	105,111,111	0.30	0
51	3PE	L	1004	-	30,30,50	0.41	0	33,35,55	0.78	1 (3%)
50	970	M	601	-	33,33,33	0.40	0	48,50,50	1.13	4 (8%)
53	CDL	o	502	-	74,74,99	0.28	0	80,86,111	0.47	1 (1%)
53	CDL	h	201	-	57,57,99	0.37	0	63,69,111	0.30	0
51	3PE	A	403	-	50,50,50	0.30	0	53,55,55	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	SF4	9	403	7	0,12,12	-	-	-		
57	AMP	k	501	-	25,25,25	1.43	4 (16%)	37,38,38	1.96	7 (18%)
51	3PE	i	201	-	50,50,50	0.29	0	53,55,55	0.30	0
51	3PE	N	401	-	50,50,50	0.32	0	53,55,55	0.53	2 (3%)

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
54	ZMP	g	201	-	-	15/38/40/43	-
53	CDL	y	201	-	1/1/9/9	32/110/110/110	-
52	PC1	M	603	-	-	15/45/45/57	-
54	ZMP	X	101	17	-	15/35/37/43	-
45	SF4	6	502	6	-	-	0/6/5/5
45	SF4	3	802	3	-	-	0/6/5/5
52	PC1	L	1002	-	-	18/57/57/57	-
51	3PE	o	501	-	-	1/34/34/54	-
48	FES	2	300	2	-	-	0/1/1/1
51	3PE	H	502	-	-	13/54/54/54	-
56	NDP	d	401	-	-	5/34/77/77	0/5/5/5
46	FMN	1	502	-	-	10/18/18/18	0/3/3/3
47	NAI	1	503	-	-	6/29/72/72	0/5/5/5
48	FES	3	803	3	-	-	0/1/1/1
51	3PE	L	1001	-	-	9/54/54/54	-
52	PC1	A	402	-	-	9/40/40/57	-
52	PC1	A	401	-	-	15/49/49/57	-
52	PC1	9	401	-	-	12/57/57/57	-
51	3PE	6	503	-	-	10/54/54/54	-
50	970	6	501	-	-	4/8/41/41	0/5/5/5
45	SF4	1	501	1	-	-	0/6/5/5
58	MYR	s	201	37	-	2/12/12/13	-
51	3PE	M	602	-	-	20/47/47/54	-
53	CDL	o	503	-	-	30/100/100/110	-
52	PC1	w	801	-	-	8/57/57/57	-
53	CDL	W	201	-	-	24/110/110/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	SF4	3	801	3	-	-	0/6/5/5
45	SF4	9	402	7	-	-	0/6/5/5
50	970	H	501	-	-	3/8/41/41	0/5/5/5
53	CDL	L	1003	-	1/1/9/9	27/110/110/110	-
53	CDL	o	502	-	2/2/9/9	20/85/85/110	-
50	970	M	601	-	1/1/5/5	4/8/41/41	0/5/5/5
51	3PE	L	1004	-	-	15/34/34/54	-
53	CDL	h	201	-	-	18/68/68/110	-
51	3PE	A	403	-	-	16/54/54/54	-
45	SF4	9	403	7	-	-	0/6/5/5
57	AMP	k	501	-	-	6/10/26/26	0/3/3/3
51	3PE	i	201	-	-	7/54/54/54	-
51	3PE	N	401	-	-	12/54/54/54	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	k	501	AMP	C5-C4	4.82	1.47	1.39
46	1	502	FMN	C4A-N5	2.91	1.37	1.30
57	k	501	AMP	C5-C6	2.63	1.48	1.41
57	k	501	AMP	C5-N7	-2.52	1.34	1.39
57	k	501	AMP	C8-N7	2.16	1.35	1.31
54	X	101	ZMP	C9-C10	2.15	1.53	1.50
46	1	502	FMN	C10-N1	2.05	1.37	1.33
54	g	201	ZMP	C9-C10	2.03	1.52	1.50

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	1	503	NAI	O5B-PA-O1A	-9.66	70.67	108.94
47	1	503	NAI	O2A-PA-O1A	-8.58	72.55	112.44
57	k	501	AMP	C5-C4-N3	-6.50	117.77	126.72
47	1	503	NAI	O3-PA-O1A	-5.71	93.53	110.70
57	k	501	AMP	N3-C4-N9	5.40	136.34	127.17
50	M	601	970	C22-C23-C14	-4.20	103.63	109.64
57	k	501	AMP	C2-N3-C4	3.88	121.31	111.83
46	1	502	FMN	C4-N3-C2	-3.58	119.28	125.64
50	M	601	970	C12-O13-C14	-3.42	110.51	116.07
57	k	501	AMP	N3-C2-N1	-3.12	123.86	128.58
46	1	502	FMN	C4A-C10-N10	3.11	120.94	116.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	g	201	ZMP	O1-C10-C9	-3.10	120.40	123.98
57	k	501	AMP	C4-C5-N7	-3.03	107.12	110.58
51	H	502	3PE	O31-C3-C2	2.88	116.71	108.40
52	L	1002	PC1	C2-O21-C21	2.67	124.19	117.80
46	l	502	FMN	C4A-C4-N3	2.60	119.86	113.25
54	g	201	ZMP	C14-C15-N2	-2.60	106.48	112.00
54	g	201	ZMP	C15-C14-C13	-2.58	108.10	112.39
47	l	503	NAI	O2A-PA-O5B	2.52	118.98	107.57
46	l	502	FMN	C10-C4A-N5	-2.50	119.70	124.81
51	L	1004	3PE	C2-O21-C21	2.47	123.71	117.80
46	l	502	FMN	O4-C4-C4A	-2.44	120.09	126.53
46	l	502	FMN	C4A-C10-N1	-2.41	118.67	124.59
54	X	101	ZMP	O1-C10-C9	-2.38	121.23	123.98
50	M	601	970	O13-C14-C15	2.31	109.61	106.61
52	L	1002	PC1	O21-C2-C1	2.29	116.55	108.34
54	g	201	ZMP	C9-C10-S1	2.27	116.10	113.40
52	A	402	PC1	C2-O21-C21	2.26	123.21	117.80
57	k	501	AMP	C5-N7-C8	2.26	107.00	103.45
57	k	501	AMP	C4-N9-C8	2.25	108.11	105.74
52	A	402	PC1	O21-C2-C3	2.24	116.39	108.34
46	l	502	FMN	C4-C4A-C10	2.19	120.68	116.93
51	N	401	3PE	O21-C2-C1	2.18	116.15	108.34
46	l	502	FMN	C1'-C2'-C3'	2.12	115.40	109.66
53	o	503	CDL	CB4-OB6-CB5	2.11	122.85	117.80
50	H	501	970	O08-C07-C06	2.06	114.22	112.99
52	9	401	PC1	O21-C2-C1	2.05	115.70	108.34
50	H	501	970	C12-O13-C14	2.05	119.40	116.07
51	N	401	3PE	C2-O21-C21	2.05	122.70	117.80
53	o	502	CDL	CB4-OB6-CB5	2.03	122.67	117.80
50	M	601	970	C15-O16-C17	2.03	119.35	115.29
54	X	101	ZMP	C15-C14-C13	-2.01	109.05	112.39

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
50	M	601	970	C14
53	L	1003	CDL	CB4
53	o	502	CDL	CB4
53	o	502	CDL	CA4
53	y	201	CDL	CB4

All (401) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	1	502	FMN	N10-C1'-C2'-O2'
46	1	502	FMN	N10-C1'-C2'-C3'
46	1	502	FMN	C5'-O5'-P-O2P
46	1	502	FMN	C5'-O5'-P-O3P
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	C01-C02-C04-O08
50	M	601	970	C03-C02-C04-C05
50	M	601	970	C03-C02-C04-O08
51	6	503	3PE	C1-O11-P-O12
51	6	503	3PE	O13-C11-C12-N
51	A	403	3PE	C1-O11-P-O12
51	A	403	3PE	C1-O11-P-O13
51	A	403	3PE	C11-O13-P-O11
51	A	403	3PE	C11-O13-P-O12
51	A	403	3PE	O13-C11-C12-N
51	H	502	3PE	C11-O13-P-O11
51	H	502	3PE	C11-O13-P-O12
51	H	502	3PE	O13-C11-C12-N
51	L	1001	3PE	C1-O11-P-O13
51	L	1001	3PE	C1-O11-P-O14
51	L	1001	3PE	C11-O13-P-O11
51	L	1001	3PE	O13-C11-C12-N
51	L	1004	3PE	C1-O11-P-O12
51	L	1004	3PE	C1-O11-P-O13
51	L	1004	3PE	C1-O11-P-O14
51	L	1004	3PE	C11-O13-P-O11
51	L	1004	3PE	C11-O13-P-O12
51	L	1004	3PE	O13-C11-C12-N
51	M	602	3PE	C1-O11-P-O12
51	M	602	3PE	C1-O11-P-O13
51	M	602	3PE	C1-O11-P-O14
51	M	602	3PE	C11-O13-P-O11
51	N	401	3PE	C11-O13-P-O14
51	N	401	3PE	O13-C11-C12-N
51	i	201	3PE	C1-O11-P-O12
51	i	201	3PE	C1-O11-P-O13
52	9	401	PC1	C1-O11-P-O12
52	9	401	PC1	C1-O11-P-O13
52	A	401	PC1	C11-O13-P-O12
52	A	401	PC1	C11-O13-P-O14

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Mol	Chain	Res	Type	Atoms
52	A	401	PC1	C11-O13-P-O11
52	A	401	PC1	C1-O11-P-O14
52	A	402	PC1	C11-O13-P-O12
52	A	402	PC1	C11-O13-P-O11
52	A	402	PC1	C1-O11-P-O14
52	A	402	PC1	C1-O11-P-O13
52	L	1002	PC1	C1-O11-P-O12
52	L	1002	PC1	C1-O11-P-O14
52	L	1002	PC1	C1-O11-P-O13
52	M	603	PC1	C11-O13-P-O14
52	M	603	PC1	C1-O11-P-O12
52	w	801	PC1	C11-O13-P-O11
53	L	1003	CDL	CA2-OA2-PA1-OA3
53	L	1003	CDL	CA3-OA5-PA1-OA2
53	L	1003	CDL	CA3-OA5-PA1-OA3
53	L	1003	CDL	CA3-OA5-PA1-OA4
53	L	1003	CDL	CB2-OB2-PB2-OB3
53	W	201	CDL	CB3-OB5-PB2-OB2
53	W	201	CDL	CB3-OB5-PB2-OB3
53	W	201	CDL	CB3-OB5-PB2-OB4
53	h	201	CDL	CA2-OA2-PA1-OA3
53	h	201	CDL	CA2-OA2-PA1-OA4
53	h	201	CDL	CA2-OA2-PA1-OA5
53	h	201	CDL	CB2-OB2-PB2-OB4
53	h	201	CDL	CB2-OB2-PB2-OB5
53	o	502	CDL	CA2-OA2-PA1-OA3
53	o	502	CDL	CA2-OA2-PA1-OA4
53	o	502	CDL	CA2-OA2-PA1-OA5
53	o	502	CDL	CA3-OA5-PA1-OA2
53	o	502	CDL	CA3-OA5-PA1-OA3
53	o	502	CDL	CA3-OA5-PA1-OA4
53	o	503	CDL	CA2-OA2-PA1-OA4
53	o	503	CDL	CA3-OA5-PA1-OA2
53	o	503	CDL	CA3-OA5-PA1-OA3
53	o	503	CDL	CB2-OB2-PB2-OB3
53	o	503	CDL	CB2-OB2-PB2-OB4
53	o	503	CDL	CB2-OB2-PB2-OB5
53	y	201	CDL	CA2-C1-CB2-OB2
53	y	201	CDL	CB3-OB5-PB2-OB2
53	y	201	CDL	CB3-OB5-PB2-OB4
54	X	101	ZMP	C17-C18-C21-O5
54	X	101	ZMP	C16-C17-C18-C21

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Mol	Chain	Res	Type	Atoms
54	X	101	ZMP	O3-C16-C17-O4
54	X	101	ZMP	C17-C16-N2-C15
54	g	201	ZMP	S1-C11-C12-N1
54	g	201	ZMP	C12-C11-S1-C10
57	k	501	AMP	C5'-O5'-P-O1P
57	k	501	AMP	C5'-O5'-P-O2P
57	k	501	AMP	C5'-O5'-P-O3P
53	h	201	CDL	O1-C1-CB2-OB2
53	y	201	CDL	O1-C1-CB2-OB2
54	X	101	ZMP	O3-C16-N2-C15
57	k	501	AMP	C3'-C4'-C5'-O5'
53	W	201	CDL	CA2-C1-CB2-OB2
53	W	201	CDL	O1-C1-CB2-OB2
53	W	201	CDL	OB5-CB3-CB4-OB6
52	M	603	PC1	C11-C12-N-C14
53	L	1003	CDL	CB7-C71-C72-C73
53	o	502	CDL	O1-C1-CB2-OB2
53	h	201	CDL	CA2-C1-CB2-OB2
52	M	603	PC1	C11-C12-N-C15
52	A	402	PC1	C22-C23-C24-C25
53	o	503	CDL	CB5-C51-C52-C53
51	A	403	3PE	C2C-C2D-C2E-C2F
53	L	1003	CDL	C56-C57-C58-C59
51	6	503	3PE	C3C-C3D-C3E-C3F
53	L	1003	CDL	C82-C83-C84-C85
51	A	403	3PE	C2E-C2F-C2G-C2H
51	N	401	3PE	C32-C33-C34-C35
51	i	201	3PE	C29-C2A-C2B-C2C
53	o	503	CDL	C78-C79-C80-C81
53	W	201	CDL	C72-C73-C74-C75
53	y	201	CDL	C12-C13-C14-C15
53	W	201	CDL	C78-C79-C80-C81
53	W	201	CDL	C35-C36-C37-C38
52	9	401	PC1	C3C-C3D-C3E-C3F
53	L	1003	CDL	C21-C22-C23-C24
52	A	401	PC1	C3B-C3C-C3D-C3E
52	9	401	PC1	C3B-C3C-C3D-C3E
52	9	401	PC1	C2B-C2C-C2D-C2E
53	L	1003	CDL	C77-C78-C79-C80
53	y	201	CDL	C13-C14-C15-C16
54	X	101	ZMP	C3-C4-C5-C6
53	L	1003	CDL	C41-C42-C43-C44

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Mol	Chain	Res	Type	Atoms
52	M	603	PC1	C11-C12-N-C13
53	L	1003	CDL	C17-C18-C19-C20
51	N	401	3PE	C21-C22-C23-C24
53	W	201	CDL	CB5-C51-C52-C53
52	9	401	PC1	C22-C21-O21-C2
53	W	201	CDL	C31-C32-C33-C34
51	H	502	3PE	C28-C29-C2A-C2B
52	L	1002	PC1	C3A-C3B-C3C-C3D
53	o	503	CDL	C19-C20-C21-C22
53	W	201	CDL	C82-C83-C84-C85
53	y	201	CDL	C59-C60-C61-C62
53	y	201	CDL	C81-C82-C83-C84
54	g	201	ZMP	C3-C4-C5-C6
57	k	501	AMP	O4'-C4'-C5'-O5'
53	L	1003	CDL	CB5-C51-C52-C53
52	9	401	PC1	C27-C28-C29-C2A
54	X	101	ZMP	C5-C6-C7-C8
53	L	1003	CDL	C22-C23-C24-C25
51	H	502	3PE	O11-C1-C2-C3
53	L	1003	CDL	OB5-CB3-CB4-CB6
53	W	201	CDL	OA5-CA3-CA4-CA6
53	o	503	CDL	C56-C57-C58-C59
54	g	201	ZMP	C1-C2-C3-C4
52	9	401	PC1	O22-C21-O21-C2
51	N	401	3PE	C1-C2-C3-O31
53	h	201	CDL	CA3-CA4-CA6-OA8
53	y	201	CDL	CA3-CA4-CA6-OA8
53	o	503	CDL	C76-C77-C78-C79
46	1	502	FMN	C5'-O5'-P-O1P
53	o	503	CDL	C81-C82-C83-C84
52	L	1002	PC1	C38-C39-C3A-C3B
53	y	201	CDL	C15-C16-C17-C18
53	o	503	CDL	C84-C85-C86-C87
54	g	201	ZMP	O4-C17-C18-C20
52	M	603	PC1	C23-C24-C25-C26
51	L	1004	3PE	C2-C1-O11-P
52	9	401	PC1	C2-C1-O11-P
53	L	1003	CDL	C1-CA2-OA2-PA1
53	h	201	CDL	CB7-C71-C72-C73
52	L	1002	PC1	O11-C1-C2-C3
51	6	503	3PE	C33-C34-C35-C36
51	N	401	3PE	C2C-C2D-C2E-C2F

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Mol	Chain	Res	Type	Atoms
52	9	401	PC1	C22-C23-C24-C25
51	M	602	3PE	C23-C24-C25-C26
51	N	401	3PE	C31-C32-C33-C34
53	h	201	CDL	C52-C53-C54-C55
54	g	201	ZMP	N2-C16-C17-O4
53	L	1003	CDL	C32-C33-C34-C35
52	w	801	PC1	C26-C27-C28-C29
53	o	503	CDL	C64-C65-C66-C67
53	L	1003	CDL	OB5-CB3-CB4-OB6
53	W	201	CDL	OA5-CA3-CA4-OA6
53	o	502	CDL	OB5-CB3-CB4-OB6
51	H	502	3PE	C2-C1-O11-P
53	o	503	CDL	CB4-CB3-OB5-PB2
53	W	201	CDL	OB6-CB4-CB6-OB8
53	y	201	CDL	OA6-CA4-CA6-OA8
53	y	201	CDL	CB7-C71-C72-C73
53	L	1003	CDL	C37-C38-C39-C40
54	g	201	ZMP	C22-C1-C2-C3
53	y	201	CDL	C57-C58-C59-C60
53	y	201	CDL	C37-C38-C39-C40
51	6	503	3PE	C36-C37-C38-C39
52	M	603	PC1	O11-C1-C2-C3
53	W	201	CDL	OB5-CB3-CB4-CB6
53	h	201	CDL	C1-CB2-OB2-PB2
52	L	1002	PC1	C3F-C3G-C3H-C3I
53	o	503	CDL	C71-C72-C73-C74
52	w	801	PC1	C39-C3A-C3B-C3C
53	y	201	CDL	C11-C12-C13-C14
51	L	1004	3PE	O11-C1-C2-O21
52	A	402	PC1	O11-C1-C2-O21
52	L	1002	PC1	O11-C1-C2-O21
52	M	603	PC1	O11-C1-C2-O21
46	1	502	FMN	C2'-C3'-C4'-O4'
51	A	403	3PE	C12-C11-O13-P
51	H	502	3PE	C12-C11-O13-P
54	X	101	ZMP	C16-C17-C18-C19
54	X	101	ZMP	C16-C17-C18-C20
54	g	201	ZMP	C16-C17-C18-C20
51	N	401	3PE	C3C-C3D-C3E-C3F
51	N	401	3PE	O21-C2-C3-O31
53	L	1003	CDL	OA6-CA4-CA6-OA8
53	h	201	CDL	OA6-CA4-CA6-OA8

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Mol	Chain	Res	Type	Atoms
53	o	503	CDL	OA6-CA4-CA6-OA8
52	L	1002	PC1	C21-C22-C23-C24
52	L	1002	PC1	C23-C24-C25-C26
51	A	403	3PE	C35-C36-C37-C38
51	M	602	3PE	C36-C37-C38-C39
52	w	801	PC1	O13-C11-C12-N
51	M	602	3PE	C3D-C3E-C3F-C3G
58	s	201	MYR	C1-C2-C3-C4
52	A	401	PC1	C11-C12-N-C14
51	H	502	3PE	C32-C31-O31-C3
52	L	1002	PC1	C3E-C3F-C3G-C3H
53	o	502	CDL	OB5-CB3-CB4-CB6
53	o	503	CDL	OB5-CB3-CB4-CB6
53	y	201	CDL	OB5-CB3-CB4-CB6
50	M	601	970	C01-C02-C04-C05
54	X	101	ZMP	C19-C18-C21-O5
54	X	101	ZMP	C20-C18-C21-O5
54	g	201	ZMP	C16-C17-C18-C21
52	L	1002	PC1	C2-C1-O11-P
53	W	201	CDL	C1-CA2-OA2-PA1
50	M	601	970	C01-C02-C04-O08
51	H	502	3PE	O11-C1-C2-O21
53	y	201	CDL	OB5-CB3-CB4-OB6
52	A	401	PC1	C11-C12-N-C13
52	w	801	PC1	C3E-C3F-C3G-C3H
53	L	1003	CDL	CA3-CA4-CA6-OA8
53	h	201	CDL	CB3-CB4-CB6-OB8
53	o	503	CDL	CA3-CA4-CA6-OA8
53	o	503	CDL	C31-C32-C33-C34
53	L	1003	CDL	C58-C59-C60-C61
58	s	201	MYR	C11-C10-C9-C8
51	A	403	3PE	C38-C39-C3A-C3B
53	o	502	CDL	CA7-C31-C32-C33
47	1	503	NAI	C5B-O5B-PA-O1A
51	6	503	3PE	C1-O11-P-O14
51	A	403	3PE	C11-O13-P-O14
51	L	1001	3PE	C11-O13-P-O14
51	L	1004	3PE	C11-O13-P-O14
51	M	602	3PE	C11-O13-P-O14
51	i	201	3PE	C1-O11-P-O14
51	i	201	3PE	C11-O13-P-O14
52	A	401	PC1	C1-O11-P-O12

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Mol	Chain	Res	Type	Atoms
52	A	401	PC1	C1-O11-P-O13
52	A	402	PC1	C1-O11-P-O12
52	M	603	PC1	C11-O13-P-O11
52	M	603	PC1	C1-O11-P-O14
52	M	603	PC1	C1-O11-P-O13
52	w	801	PC1	C11-O13-P-O14
52	w	801	PC1	C1-O11-P-O14
53	h	201	CDL	CB2-OB2-PB2-OB3
53	h	201	CDL	CB3-OB5-PB2-OB2
53	o	503	CDL	CA2-OA2-PA1-OA3
53	o	503	CDL	CA2-OA2-PA1-OA5
53	o	503	CDL	CB3-OB5-PB2-OB3
53	y	201	CDL	CB3-OB5-PB2-OB3
54	X	101	ZMP	O4-C17-C18-C21
54	g	201	ZMP	O4-C17-C18-C21
53	o	502	CDL	C12-C13-C14-C15
46	1	502	FMN	C4'-C5'-O5'-P
51	M	602	3PE	C2-C1-O11-P
52	M	603	PC1	C2-C1-O11-P
53	L	1003	CDL	CA4-CA3-OA5-PA1
53	h	201	CDL	CB4-CB3-OB5-PB2
53	o	502	CDL	CA4-CA3-OA5-PA1
53	y	201	CDL	C1-CB2-OB2-PB2
53	y	201	CDL	C56-C57-C58-C59
53	y	201	CDL	OA5-CA3-CA4-CA6
51	M	602	3PE	O11-C1-C2-O21
53	y	201	CDL	C32-C33-C34-C35
52	A	402	PC1	O21-C21-C22-C23
54	g	201	ZMP	O4-C17-C18-C19
56	d	401	NDP	PN-O3-PA-O1A
51	H	502	3PE	C33-C34-C35-C36
46	1	502	FMN	O3'-C3'-C4'-C5'
53	o	502	CDL	C71-C72-C73-C74
51	H	502	3PE	O32-C31-O31-C3
51	A	403	3PE	C24-C25-C26-C27
52	A	401	PC1	C11-C12-N-C15
51	N	401	3PE	C2B-C2C-C2D-C2E
53	y	201	CDL	C58-C59-C60-C61
53	L	1003	CDL	C60-C61-C62-C63
47	1	503	NAI	O4D-C1D-N1N-C2N
56	d	401	NDP	O4D-C1D-N1N-C6N
52	L	1002	PC1	C2A-C2B-C2C-C2D

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Mol	Chain	Res	Type	Atoms
53	o	502	CDL	C14-C15-C16-C17
51	A	403	3PE	C2-C1-O11-P
52	L	1002	PC1	C29-C2A-C2B-C2C
53	o	502	CDL	CA2-C1-CB2-OB2
54	X	101	ZMP	N2-C16-C17-O4
51	M	602	3PE	C32-C33-C34-C35
52	9	401	PC1	C3-C2-O21-C21
52	L	1002	PC1	C1-C2-O21-C21
53	y	201	CDL	CA5-C11-C12-C13
51	6	503	3PE	C25-C26-C27-C28
52	A	401	PC1	C26-C27-C28-C29
53	o	502	CDL	OA6-CA4-CA6-OA8
51	L	1001	3PE	C24-C25-C26-C27
47	1	503	NAI	C2N-C3N-C7N-N7N
51	H	502	3PE	C2F-C2G-C2H-C2I
51	M	602	3PE	C34-C35-C36-C37
56	d	401	NDP	C2B-O2B-P2B-O1X
56	d	401	NDP	PN-O3-PA-O2A
47	1	503	NAI	PN-O3-PA-O5B
54	X	101	ZMP	C7-C8-C9-C10
53	L	1003	CDL	C39-C40-C41-C42
51	A	403	3PE	C22-C23-C24-C25
51	M	602	3PE	C26-C27-C28-C29
52	M	603	PC1	O21-C21-C22-C23
53	o	502	CDL	C52-C51-CB5-OB6
53	o	502	CDL	CA3-CA4-CA6-OA8
51	L	1001	3PE	C35-C36-C37-C38
51	M	602	3PE	C37-C38-C39-C3A
46	1	502	FMN	C2'-C3'-C4'-C5'
53	o	503	CDL	C34-C35-C36-C37
53	L	1003	CDL	C79-C80-C81-C82
51	L	1004	3PE	O11-C1-C2-C3
51	M	602	3PE	O11-C1-C2-C3
51	L	1004	3PE	C33-C34-C35-C36
51	A	403	3PE	O21-C2-C3-O31
53	L	1003	CDL	C1-CB2-OB2-PB2
57	k	501	AMP	C4'-C5'-O5'-P
51	6	503	3PE	C23-C24-C25-C26
46	1	502	FMN	O3'-C3'-C4'-O4'
53	W	201	CDL	CA5-C11-C12-C13
51	6	503	3PE	O21-C21-C22-C23
51	N	401	3PE	C3-C2-O21-C21

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Mol	Chain	Res	Type	Atoms
53	o	503	CDL	CB3-CB4-OB6-CB5
53	y	201	CDL	C36-C37-C38-C39
51	o	501	3PE	C25-C26-C27-C28
51	M	602	3PE	C33-C34-C35-C36
51	M	602	3PE	C27-C28-C29-C2A
53	W	201	CDL	CB3-CB4-CB6-OB8
54	g	201	ZMP	C16-C17-C18-C19
51	6	503	3PE	C37-C38-C39-C3A
51	L	1004	3PE	O21-C21-C22-C23
51	i	201	3PE	O21-C21-C22-C23
47	1	503	NAI	C2D-C1D-N1N-C2N
52	A	402	PC1	O13-C11-C12-N
52	L	1002	PC1	O13-C11-C12-N
54	g	201	ZMP	C6-C7-C8-C9
52	L	1002	PC1	C31-C32-C33-C34
51	M	602	3PE	O21-C21-C22-C23
53	y	201	CDL	C12-C11-CA5-OA6
53	o	503	CDL	CA5-C11-C12-C13
54	g	201	ZMP	O3-C16-C17-C18
53	W	201	CDL	C19-C20-C21-C22
56	d	401	NDP	C2B-O2B-P2B-O2X
53	o	503	CDL	CA4-CA3-OA5-PA1
52	L	1002	PC1	C33-C34-C35-C36
51	L	1004	3PE	C23-C24-C25-C26
53	y	201	CDL	C63-C64-C65-C66
53	o	503	CDL	C72-C71-CB7-OB8
53	y	201	CDL	C72-C73-C74-C75
52	M	603	PC1	O31-C31-C32-C33
50	H	501	970	C01-C02-C04-C05
51	H	502	3PE	C29-C2A-C2B-C2C
51	L	1004	3PE	C1-C2-O21-C21
53	o	502	CDL	CB6-CB4-OB6-CB5
54	g	201	ZMP	N2-C16-C17-C18
51	i	201	3PE	O22-C21-C22-C23
54	X	101	ZMP	C6-C7-C8-C9
50	H	501	970	C03-C02-C04-O08
52	A	401	PC1	O31-C31-C32-C33
53	o	502	CDL	C72-C71-CB7-OB8
53	y	201	CDL	C52-C51-CB5-OB6
51	L	1004	3PE	O22-C21-C22-C23
52	A	401	PC1	C35-C36-C37-C38
53	y	201	CDL	C12-C11-CA5-OA7

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Mol	Chain	Res	Type	Atoms
51	L	1001	3PE	C3B-C3C-C3D-C3E
52	M	603	PC1	C28-C29-C2A-C2B
52	A	401	PC1	C22-C23-C24-C25
53	o	503	CDL	C72-C73-C74-C75
51	M	602	3PE	O22-C21-C22-C23
53	y	201	CDL	C60-C61-C62-C63
52	w	801	PC1	C34-C35-C36-C37
53	h	201	CDL	C52-C51-CB5-OB6
53	W	201	CDL	C14-C15-C16-C17
52	A	401	PC1	C24-C25-C26-C27
52	9	401	PC1	C2D-C2E-C2F-C2G
51	A	403	3PE	O11-C1-C2-C3
53	o	503	CDL	C72-C71-CB7-OB9
51	N	401	3PE	O31-C31-C32-C33
47	1	503	NAI	PN-O3-PA-O2A
53	h	201	CDL	C52-C51-CB5-OB7
53	y	201	CDL	C52-C51-CB5-OB7
53	W	201	CDL	C53-C54-C55-C56
53	W	201	CDL	C83-C84-C85-C86
51	L	1001	3PE	C23-C24-C25-C26
53	W	201	CDL	CA7-C31-C32-C33
51	M	602	3PE	C35-C36-C37-C38

There are no ring outliers.

23 monomers are involved in 90 short contacts:

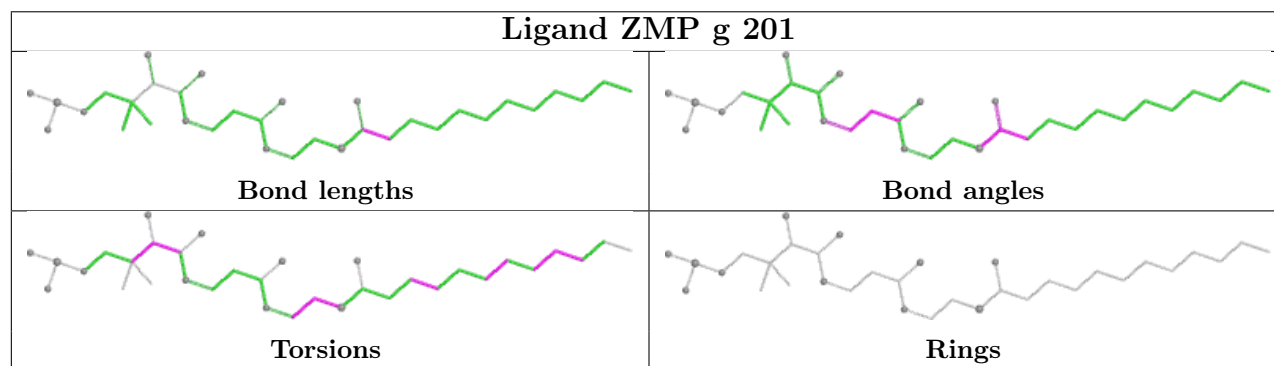
Mol	Chain	Res	Type	Clashes	Symm-Clashes
52	M	603	PC1	1	0
53	y	201	CDL	11	0
45	6	502	SF4	1	0
54	X	101	ZMP	2	0
52	L	1002	PC1	10	0
48	2	300	FES	1	0
51	H	502	3PE	3	0
56	d	401	NDP	2	0
46	1	502	FMN	1	0
47	1	503	NAI	2	0
52	A	401	PC1	2	0
52	9	401	PC1	3	0
51	6	503	3PE	3	0
45	1	501	SF4	2	0
53	o	503	CDL	13	0

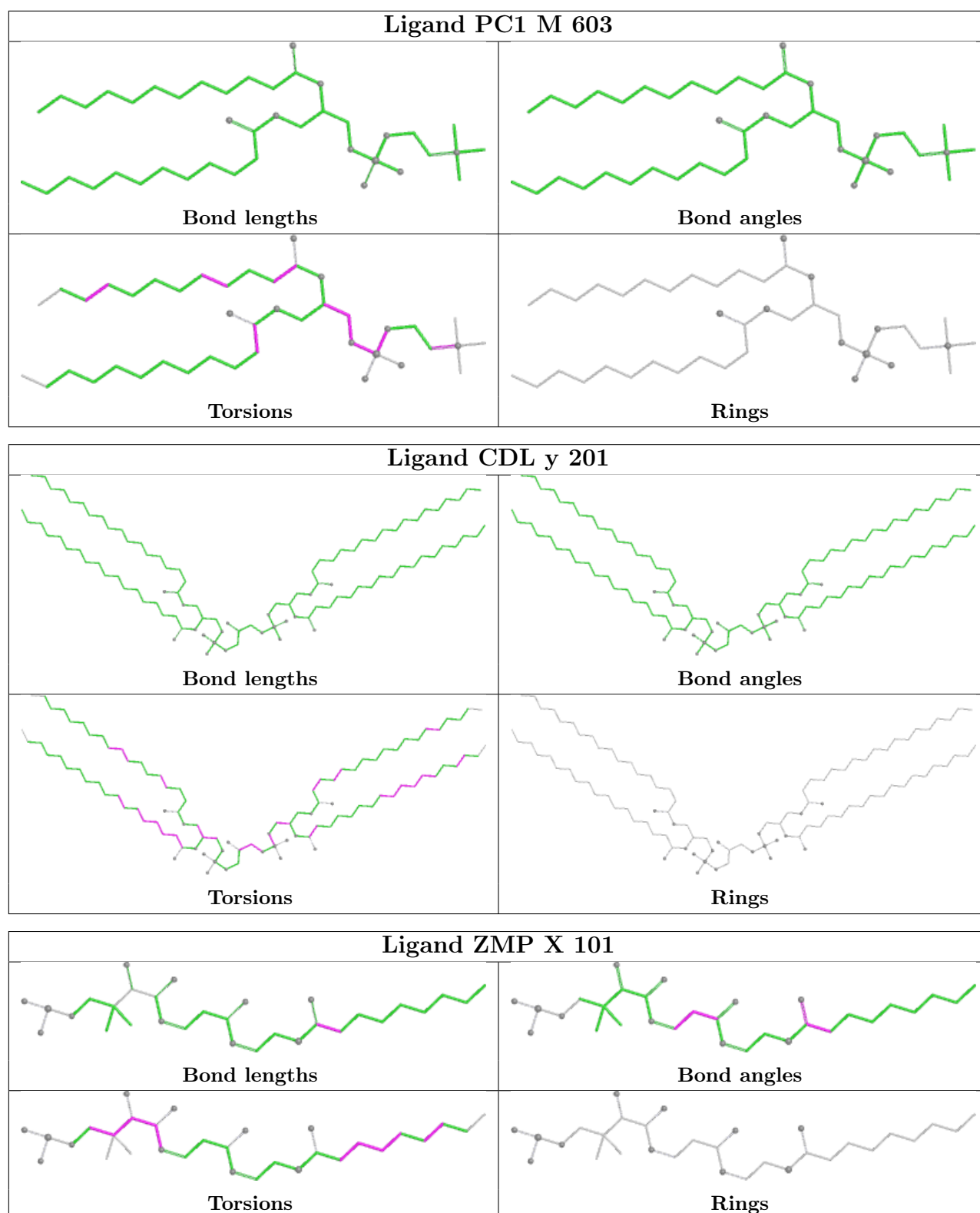
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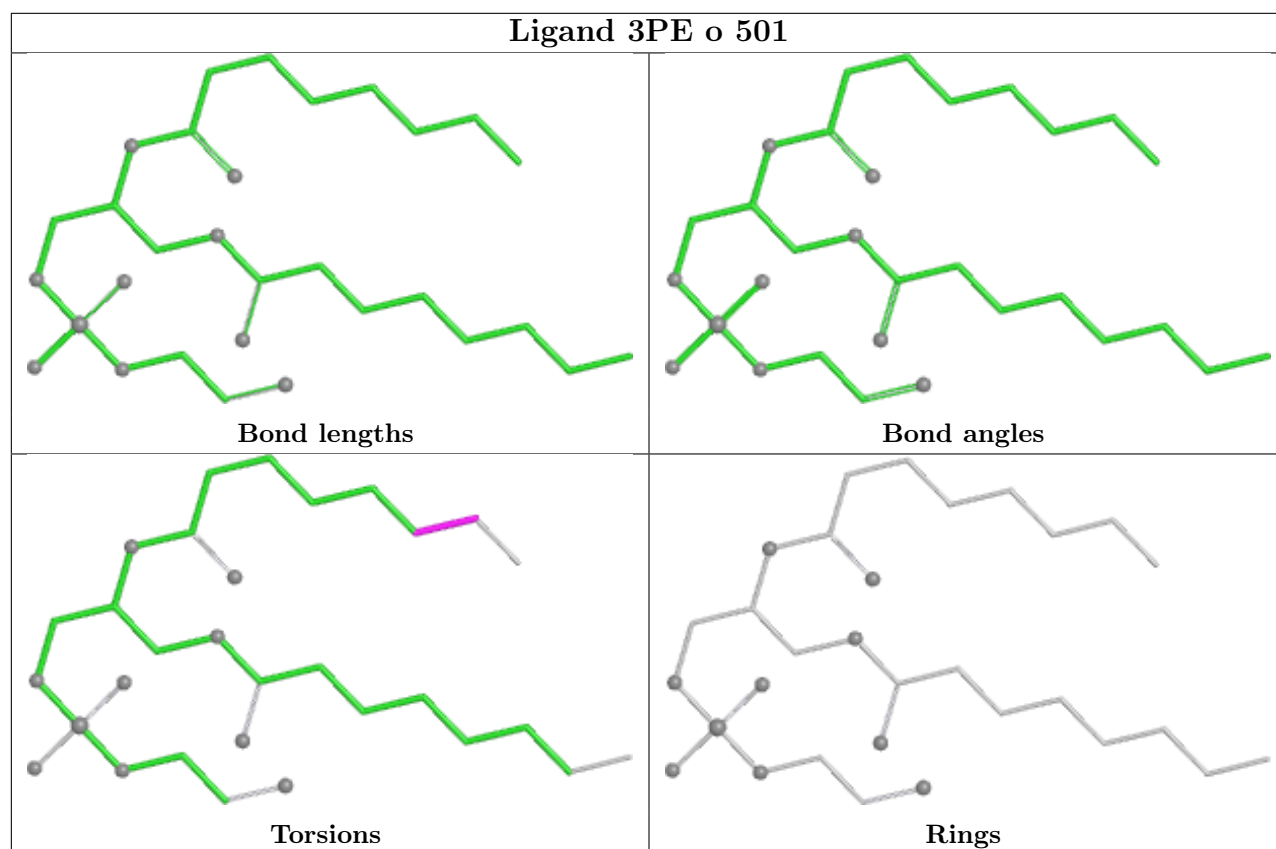
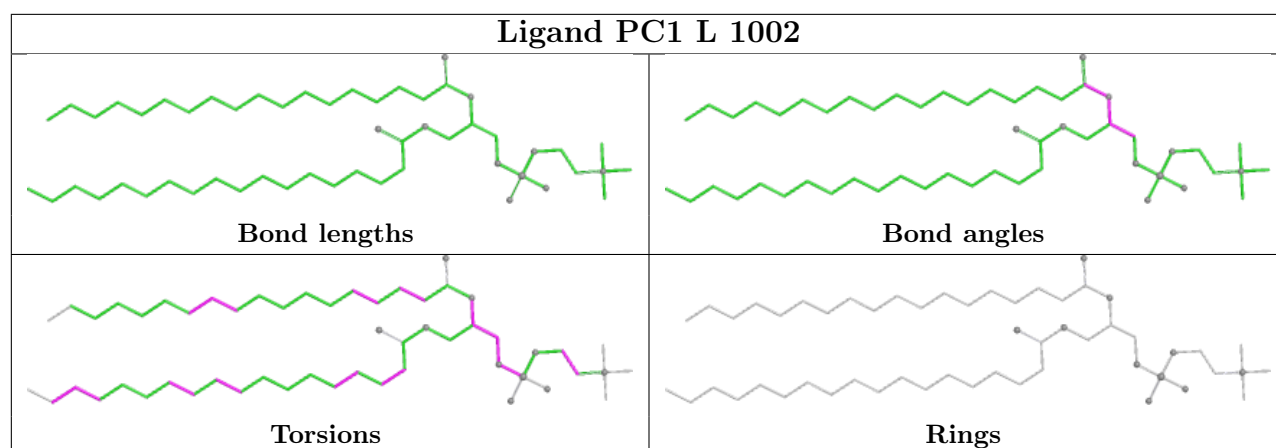
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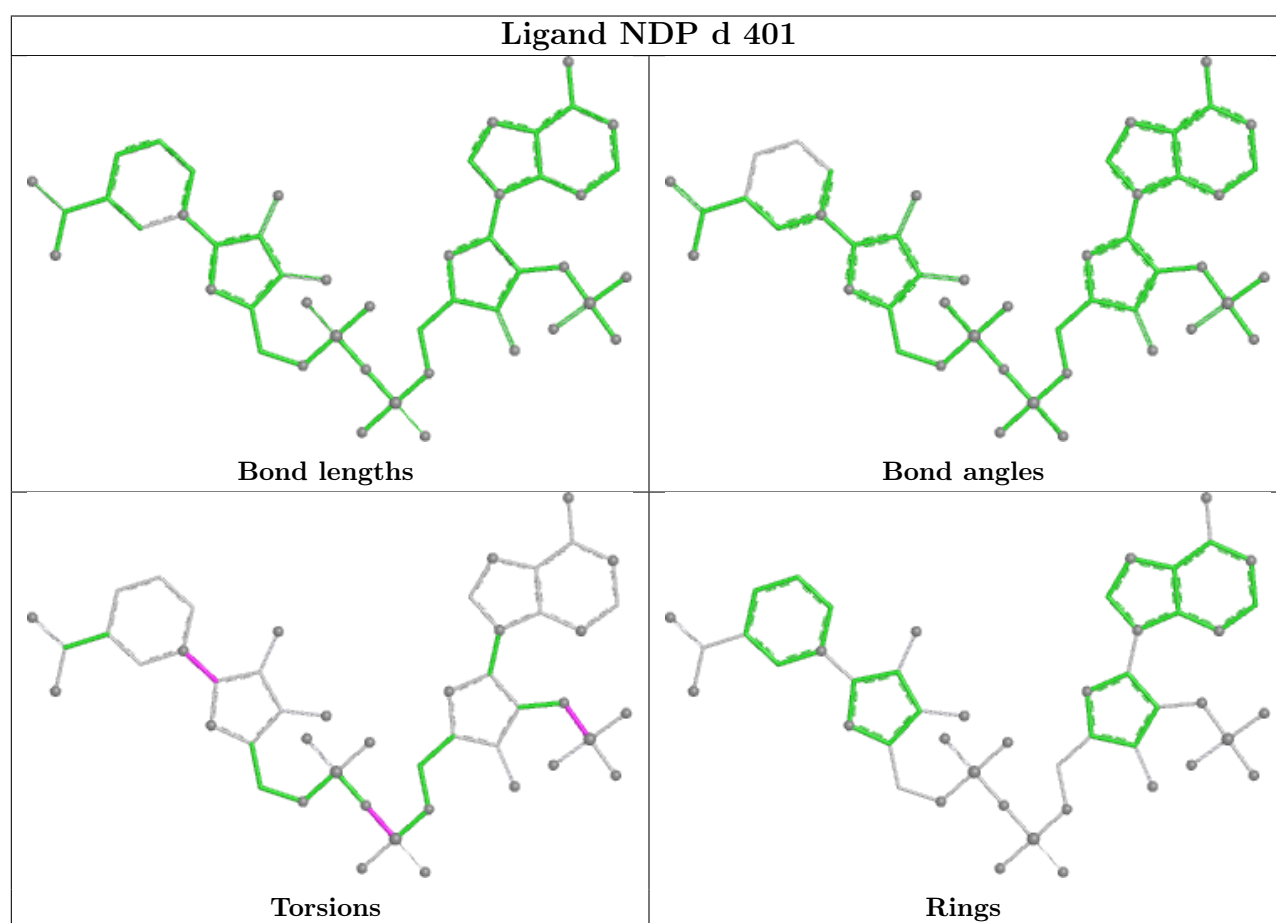
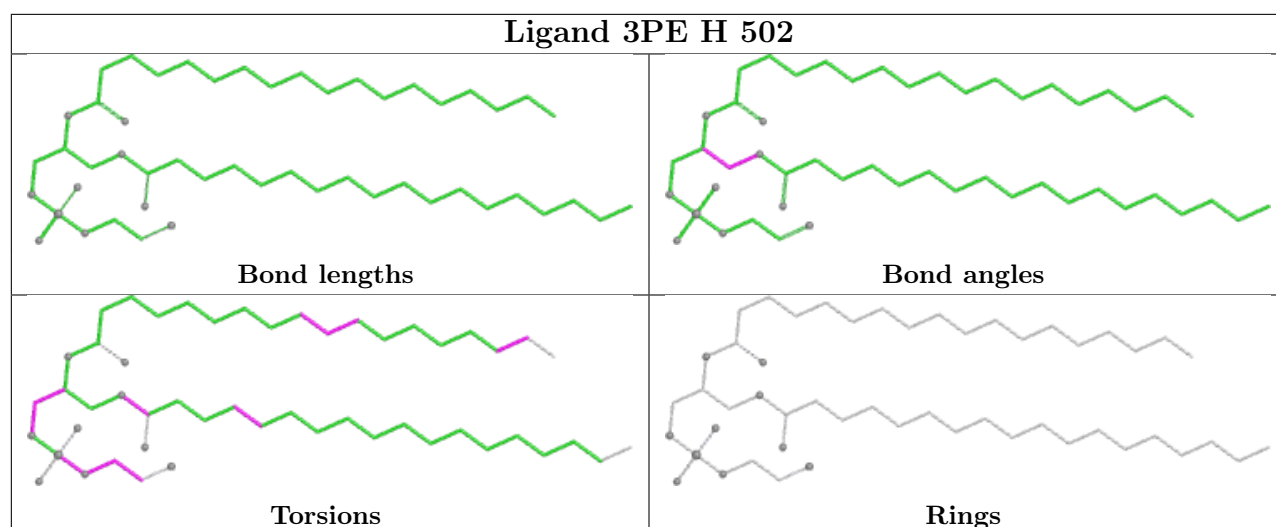
Mol	Chain	Res	Type	Clashes	Symm-Clashes
52	w	801	PC1	7	0
53	W	201	CDL	15	0
53	L	1003	CDL	6	0
53	o	502	CDL	6	0
53	h	201	CDL	1	0
51	A	403	3PE	4	0
51	i	201	3PE	2	0
51	N	401	3PE	5	0

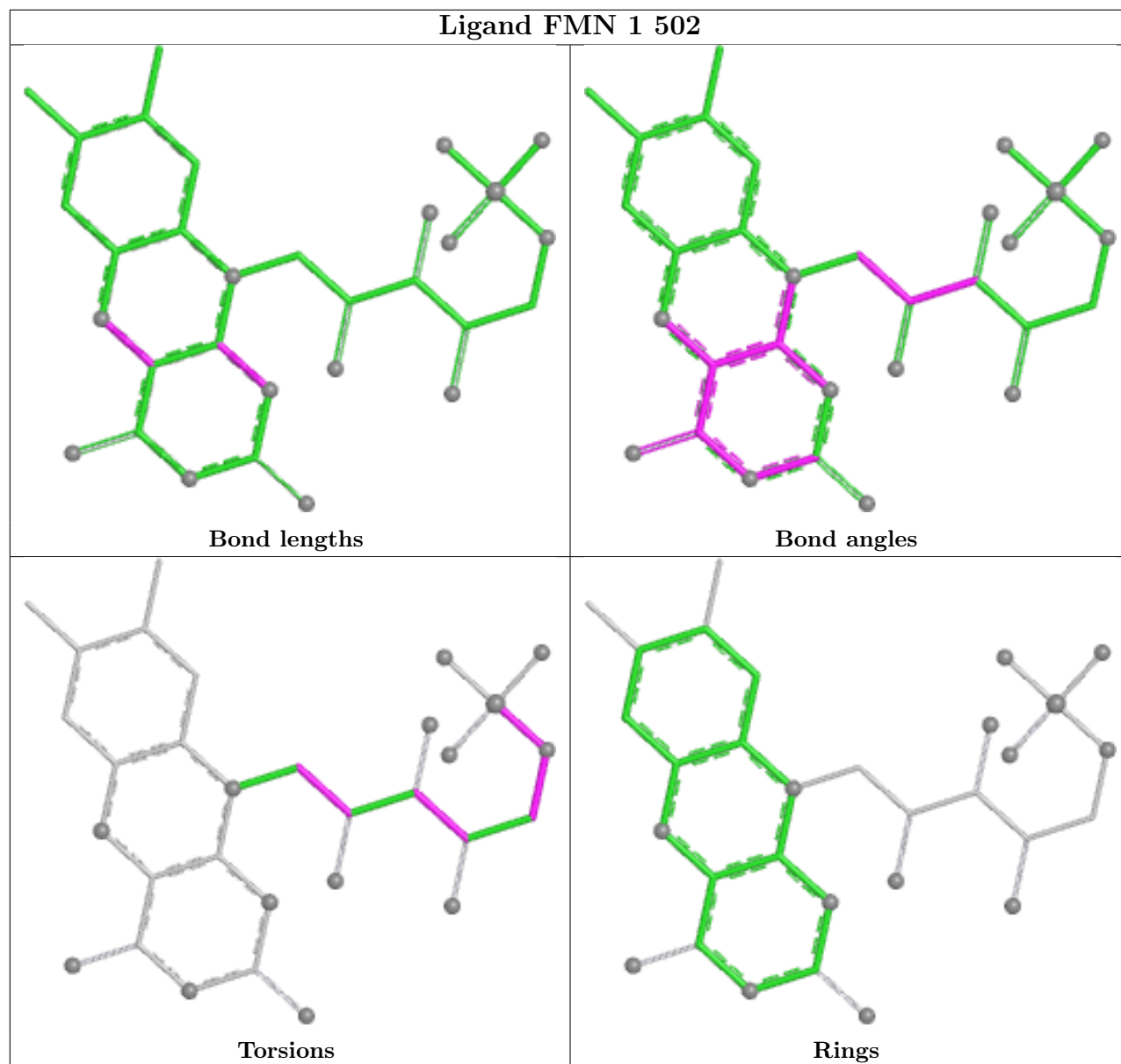
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

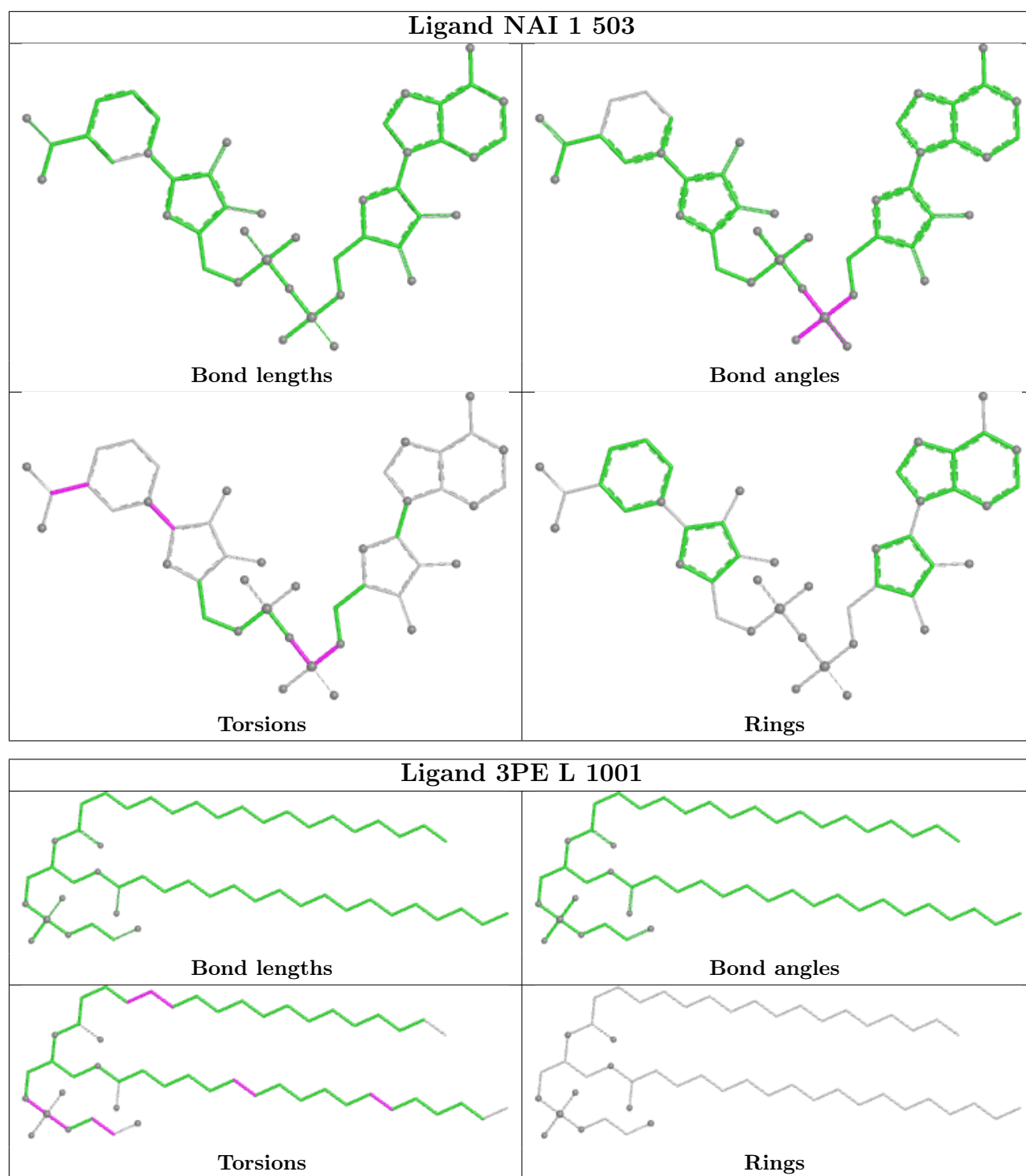


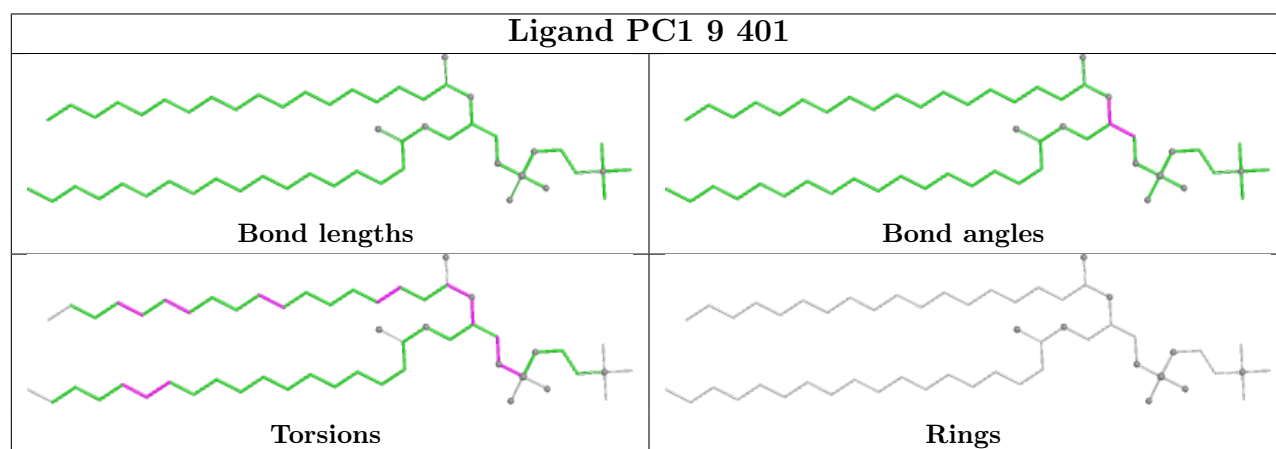
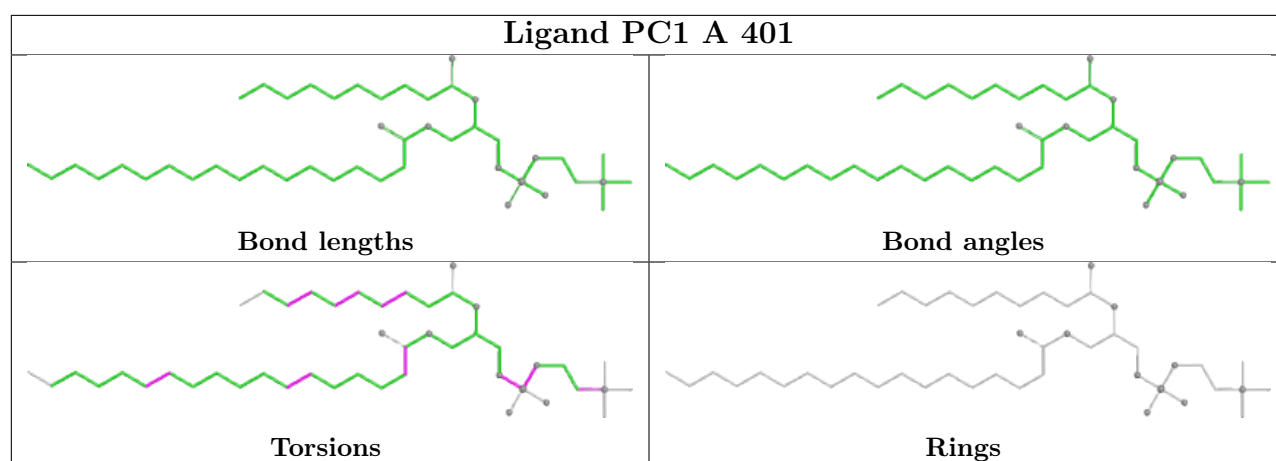
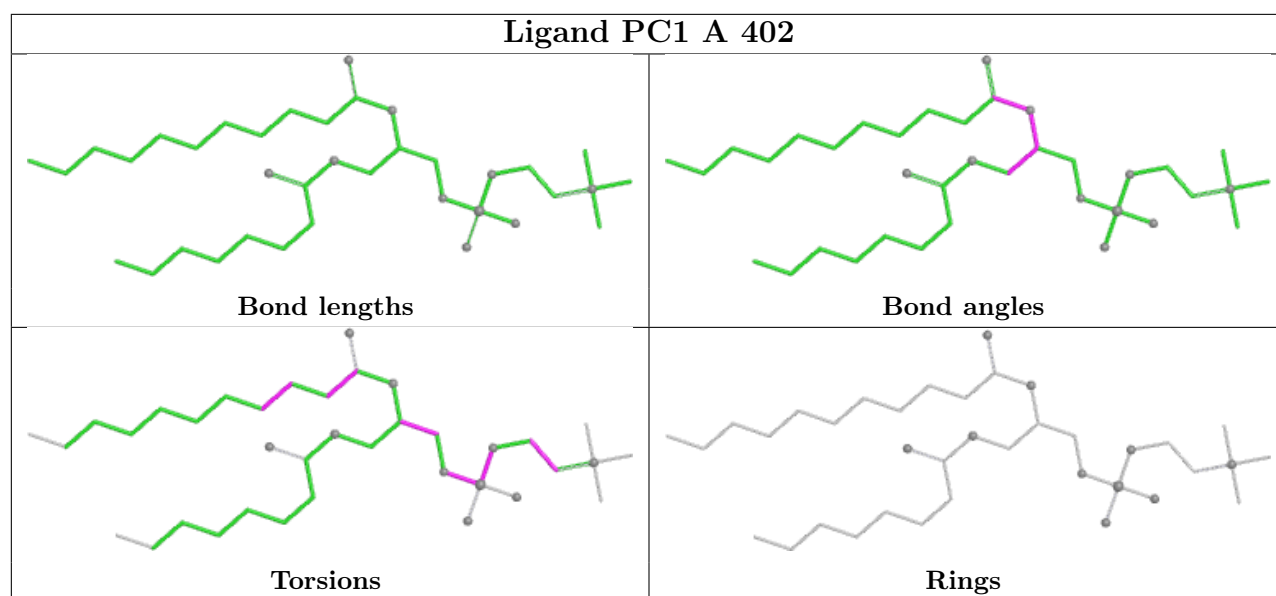


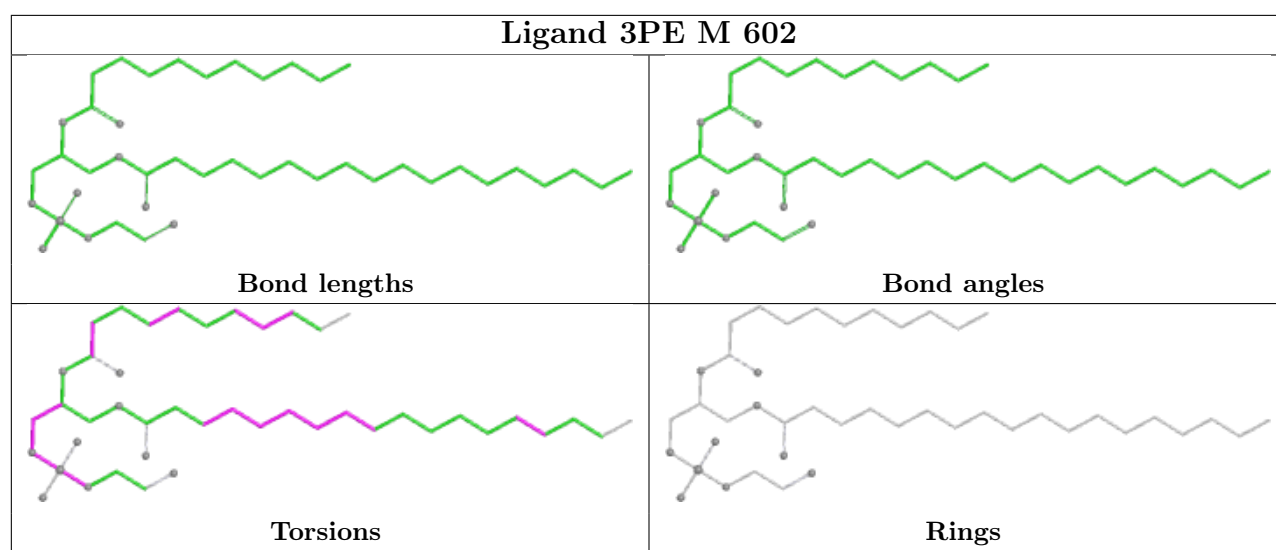
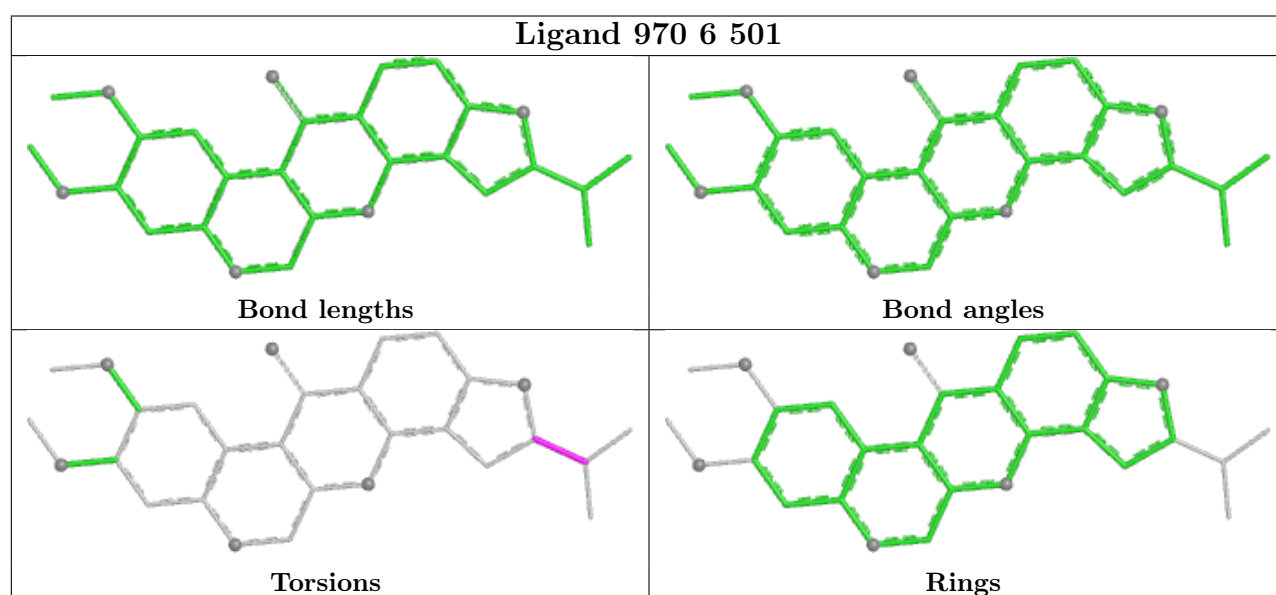
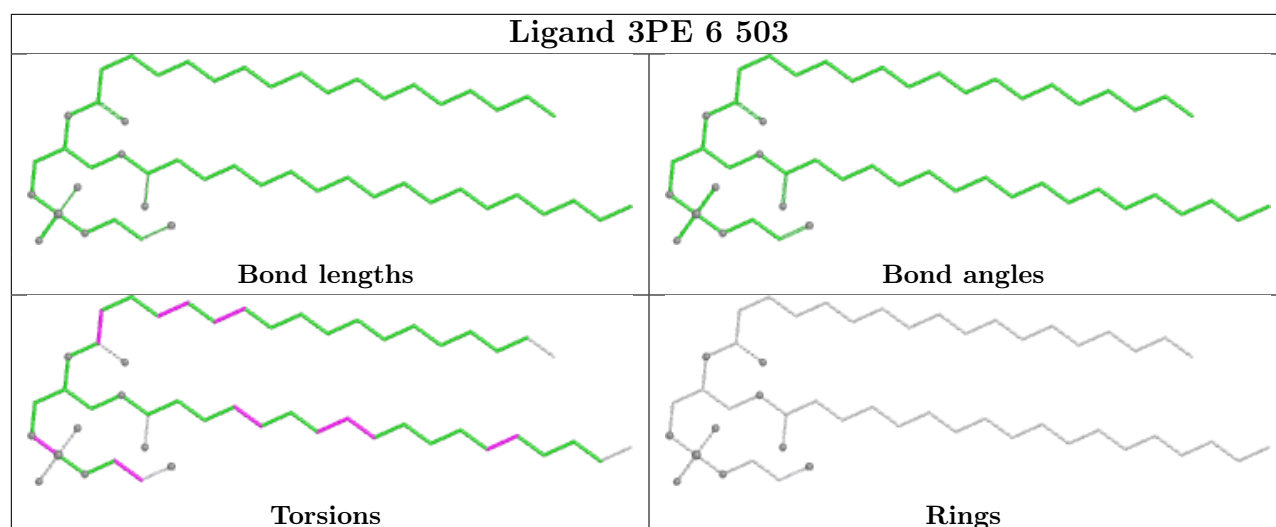


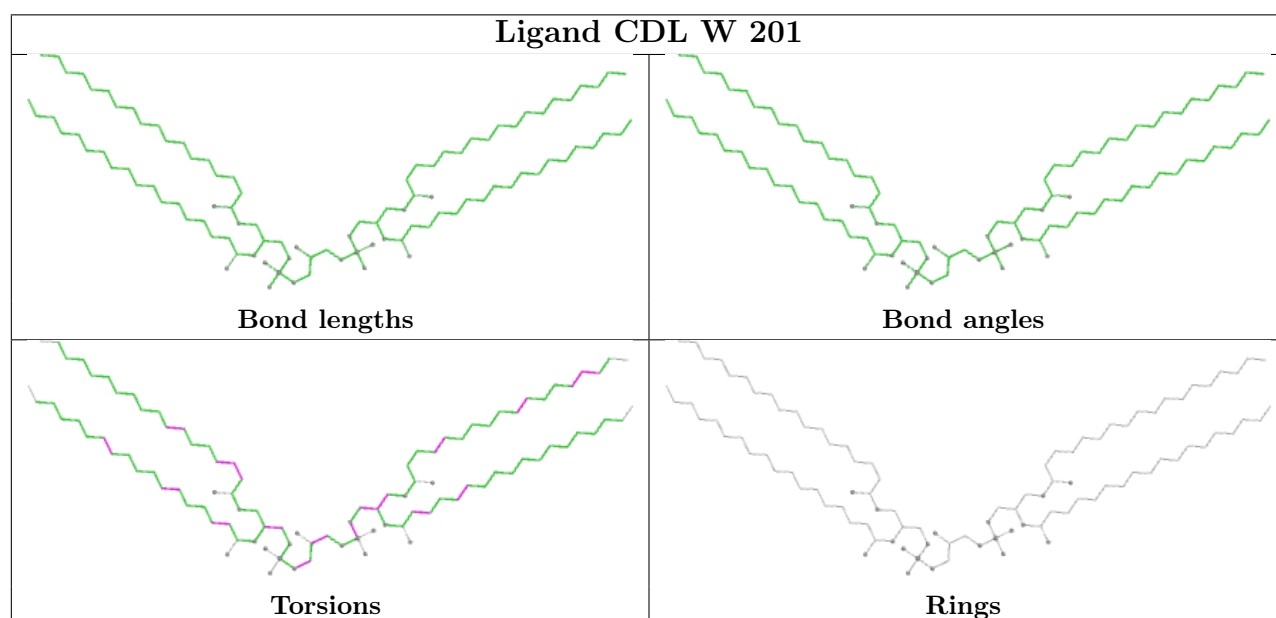
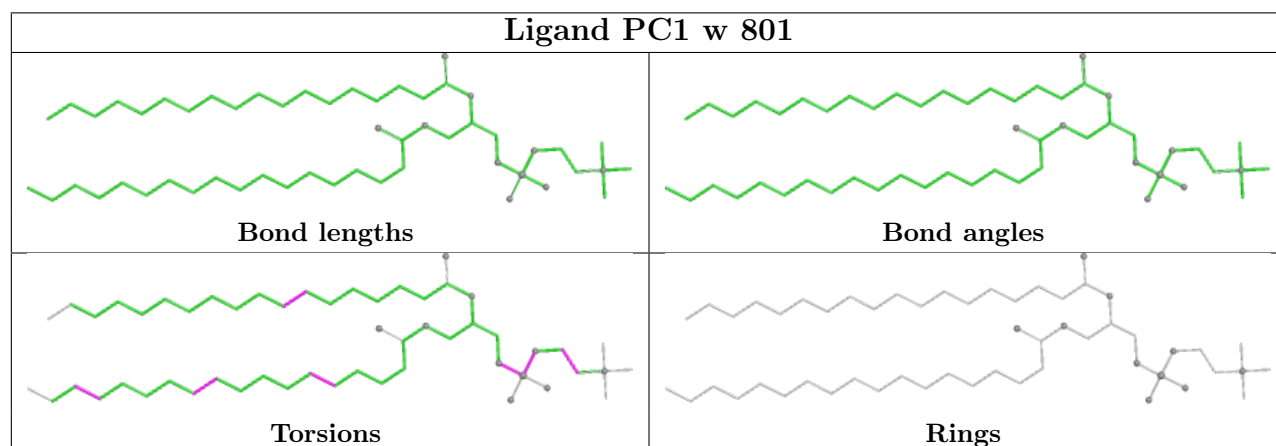
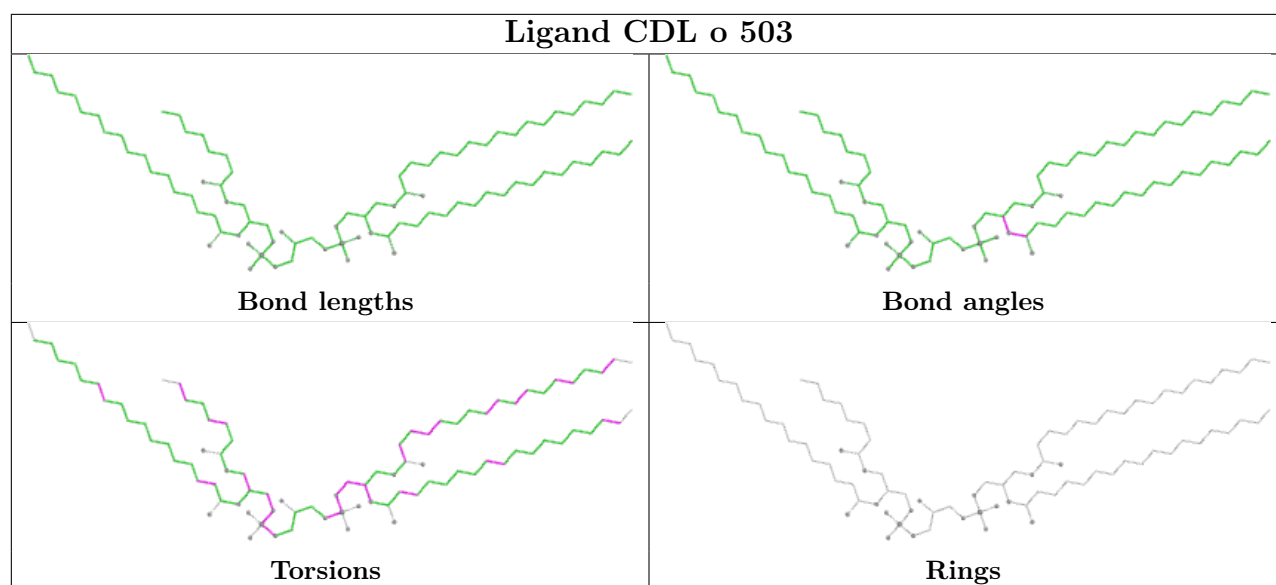


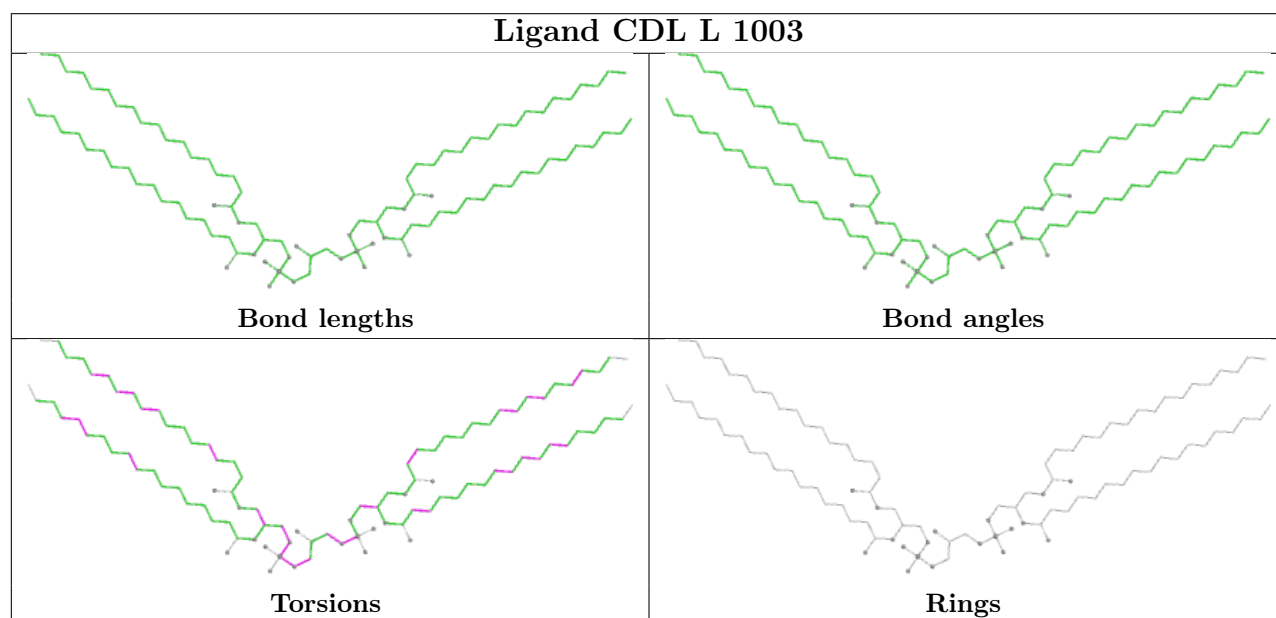
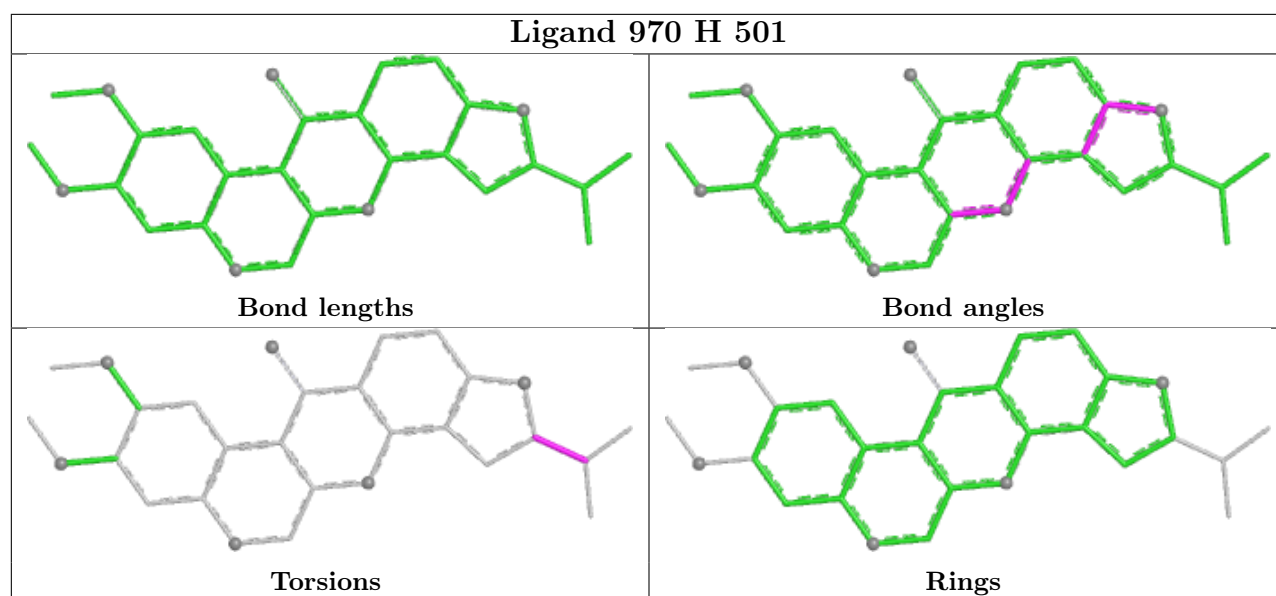


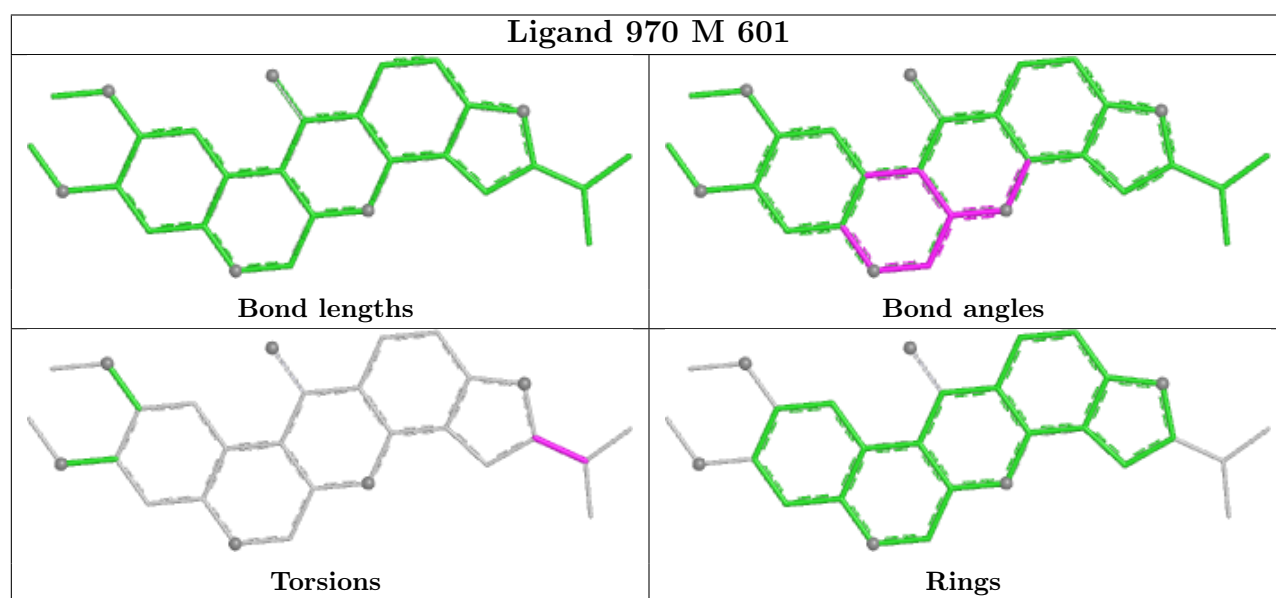
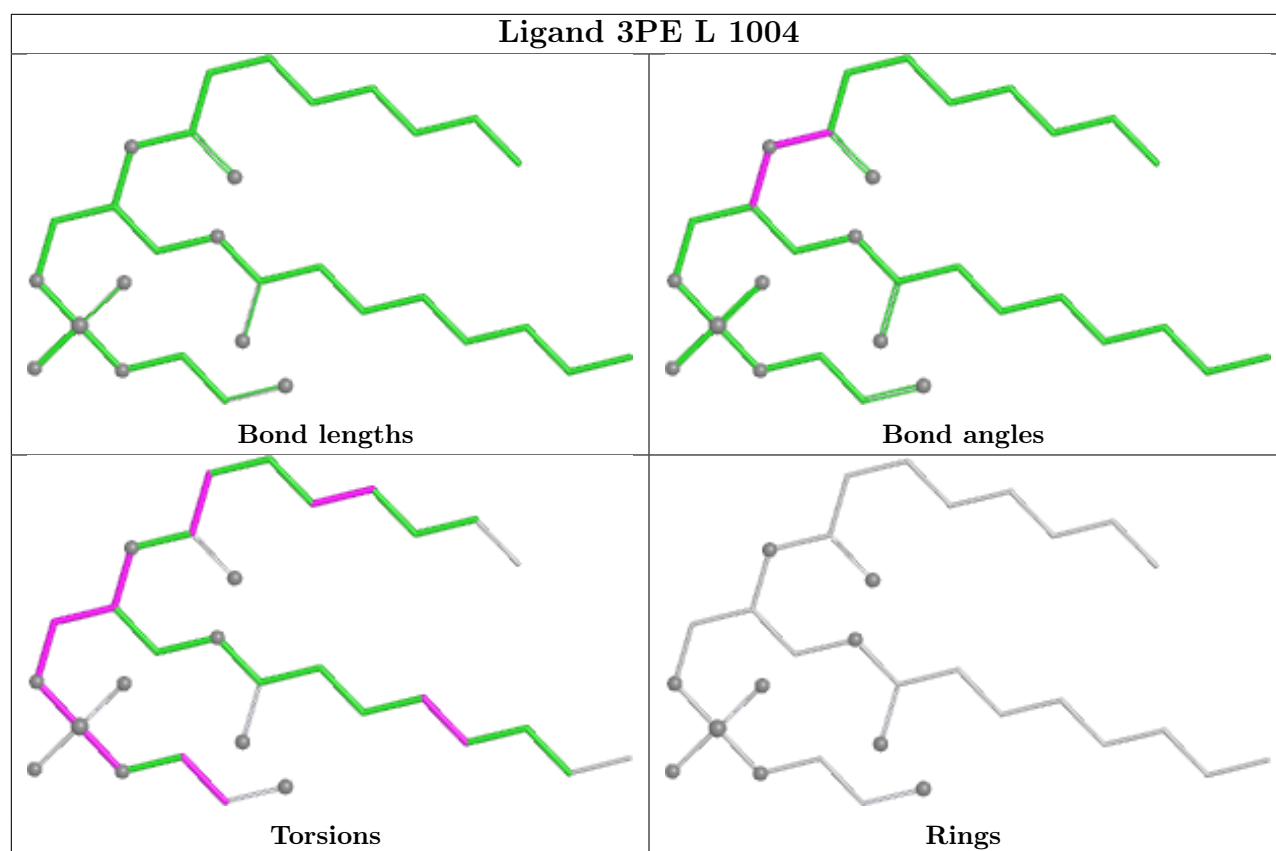


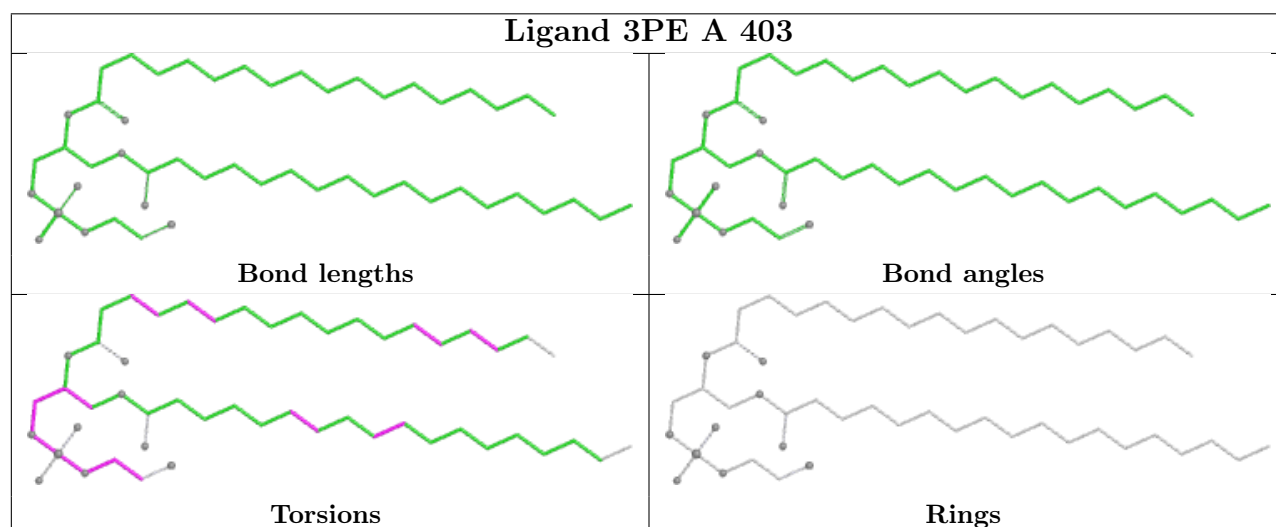
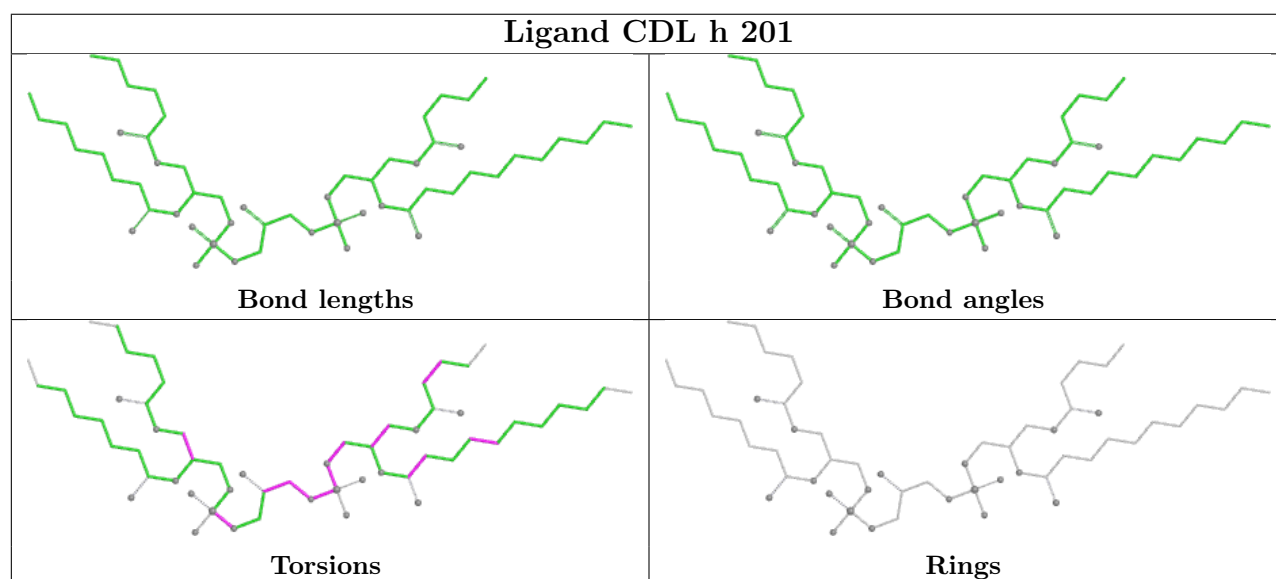
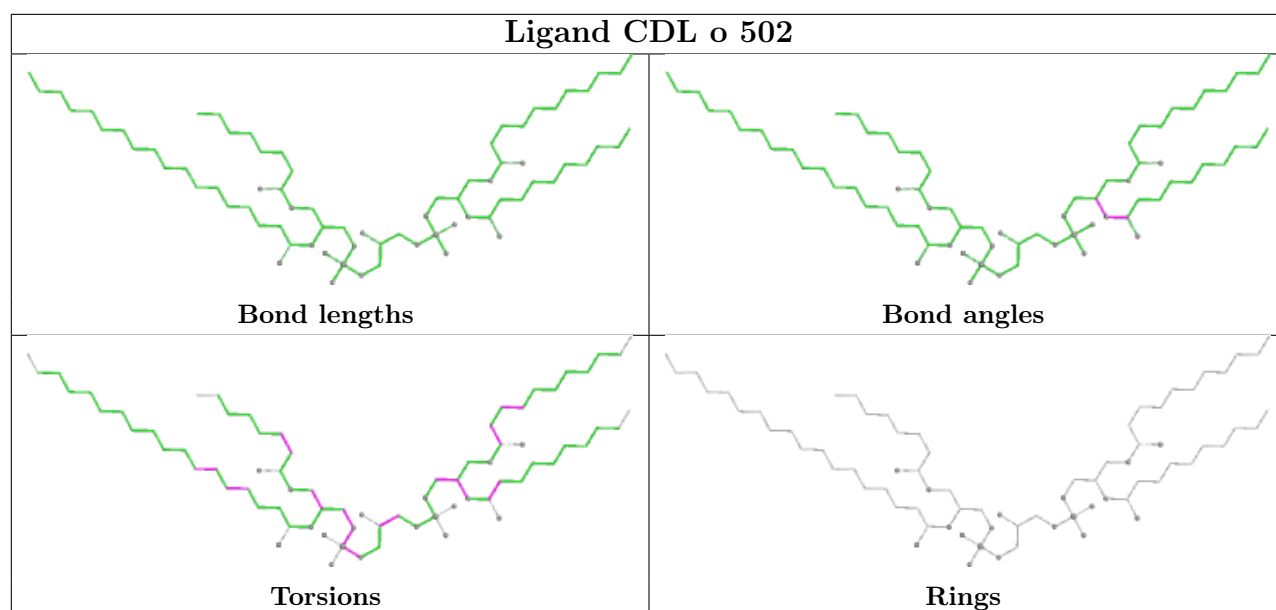


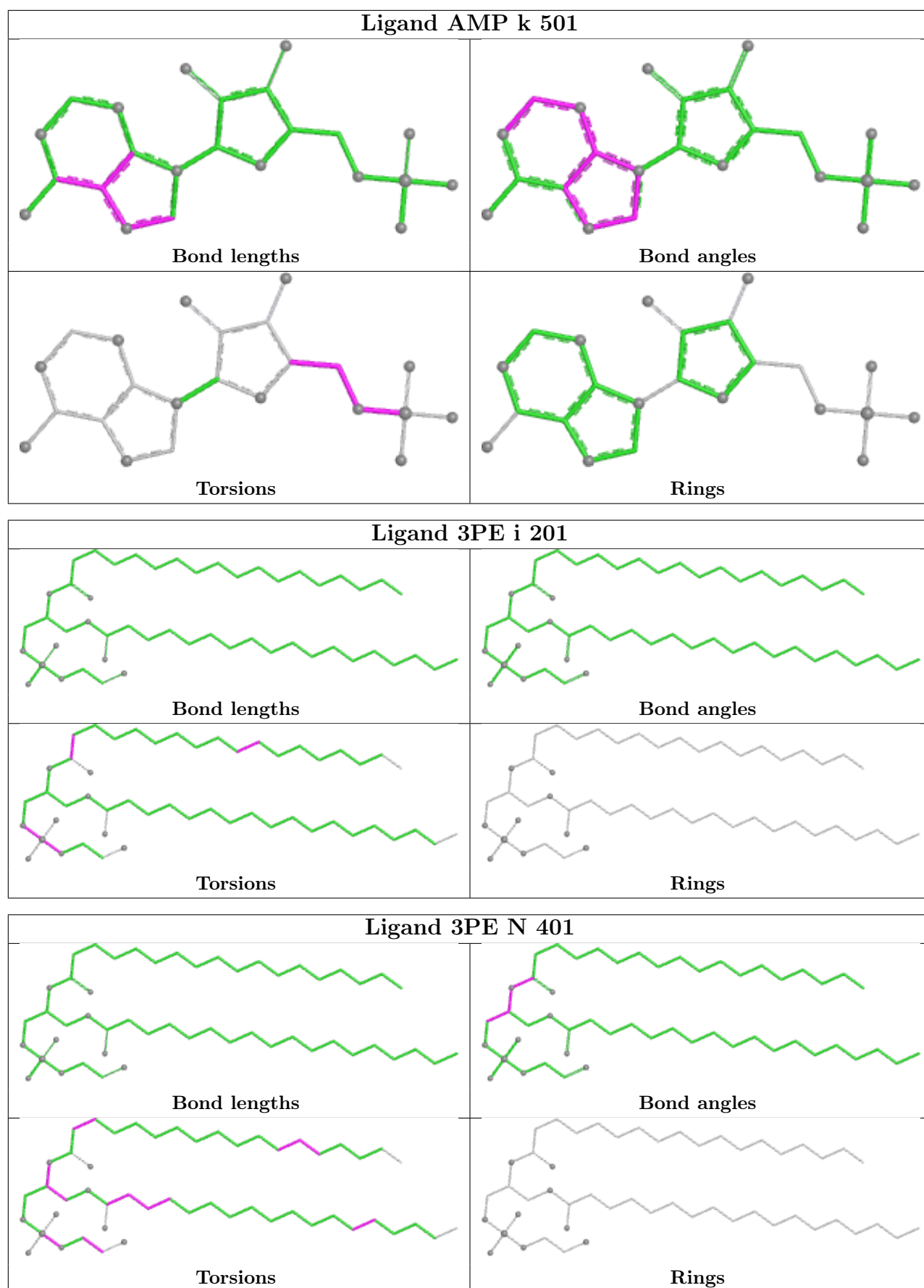












5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

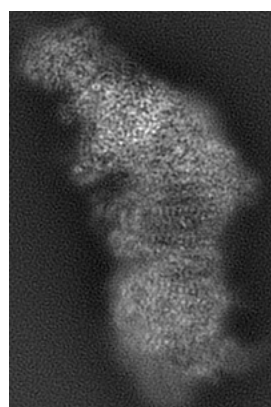
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11254. These allow visual inspection of the internal detail of the map and identification of artifacts.

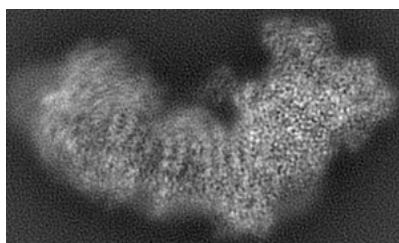
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

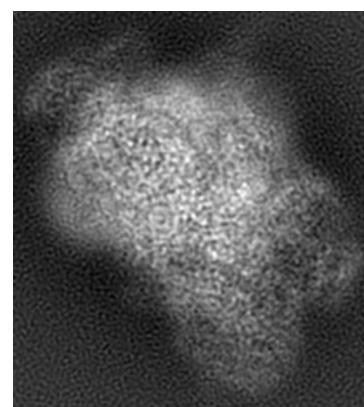
6.1.1 Primary map



X



Y

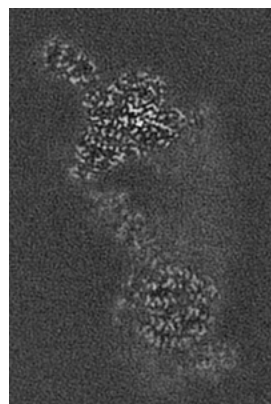


Z

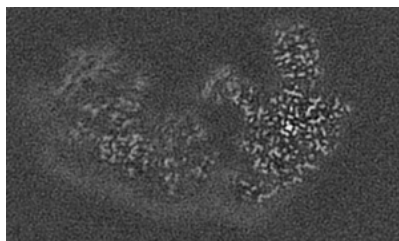
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

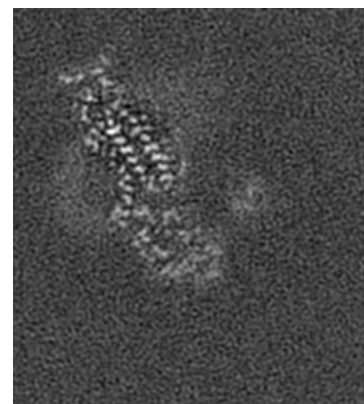
6.2.1 Primary map



X Index: 81



Y Index: 90

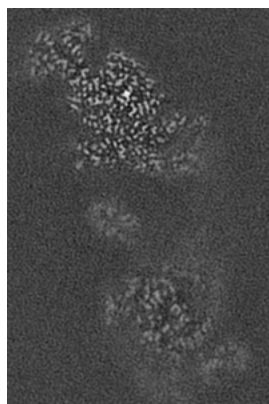


Z Index: 137

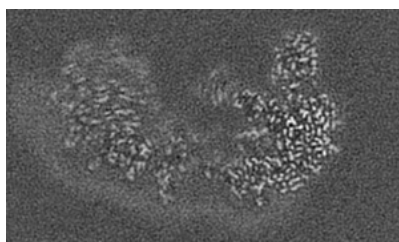
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

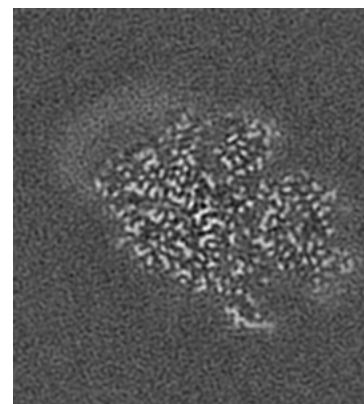
6.3.1 Primary map



X Index: 91



Y Index: 96

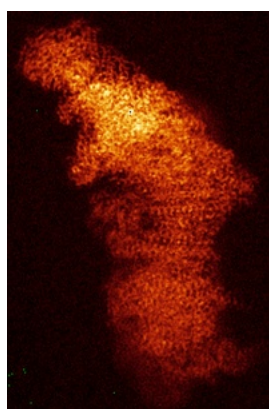


Z Index: 201

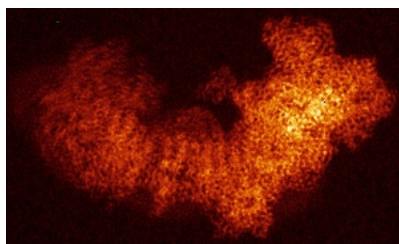
The images above show the largest variance slices of the map in three orthogonal directions.

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

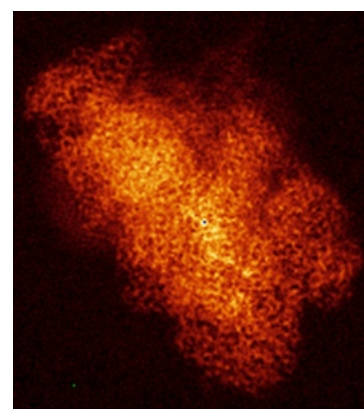
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views

This section was not generated.

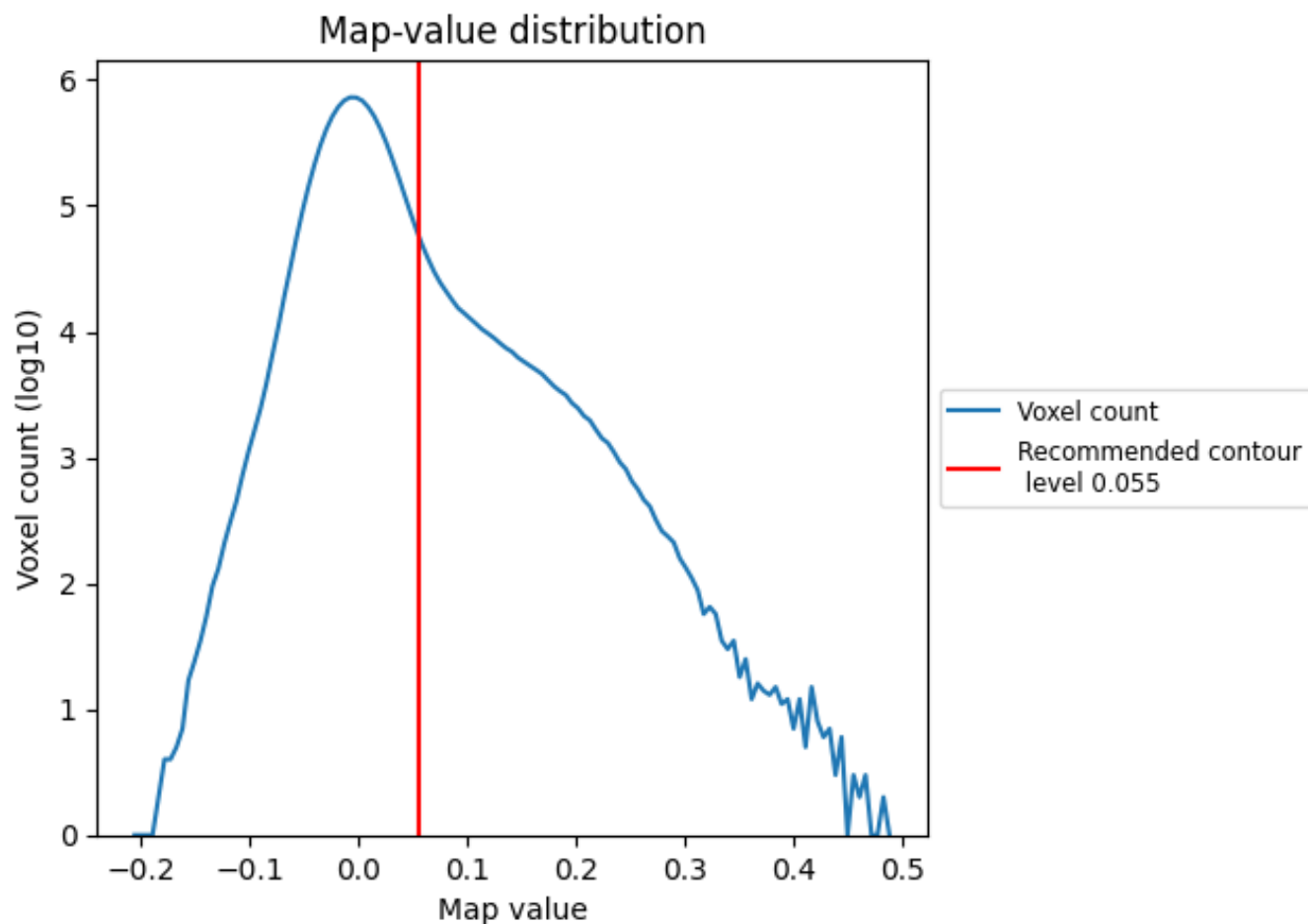
6.6 Mask visualisation

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

7 Map analysis [i](#)

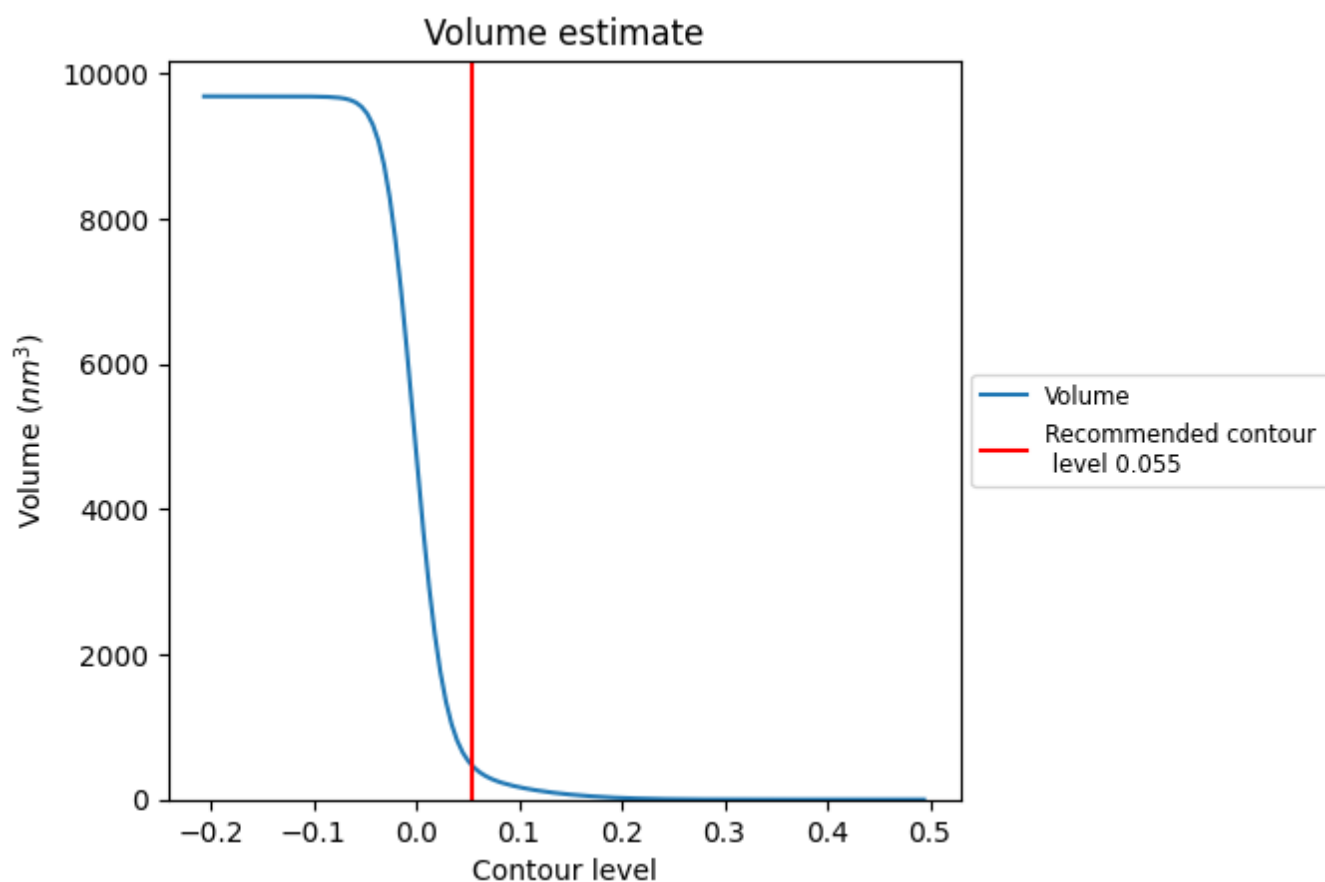
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

7.2 Volume estimate [i](#)



The volume at the recommended contour level is 462 nm³; this corresponds to an approximate mass of 418 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.

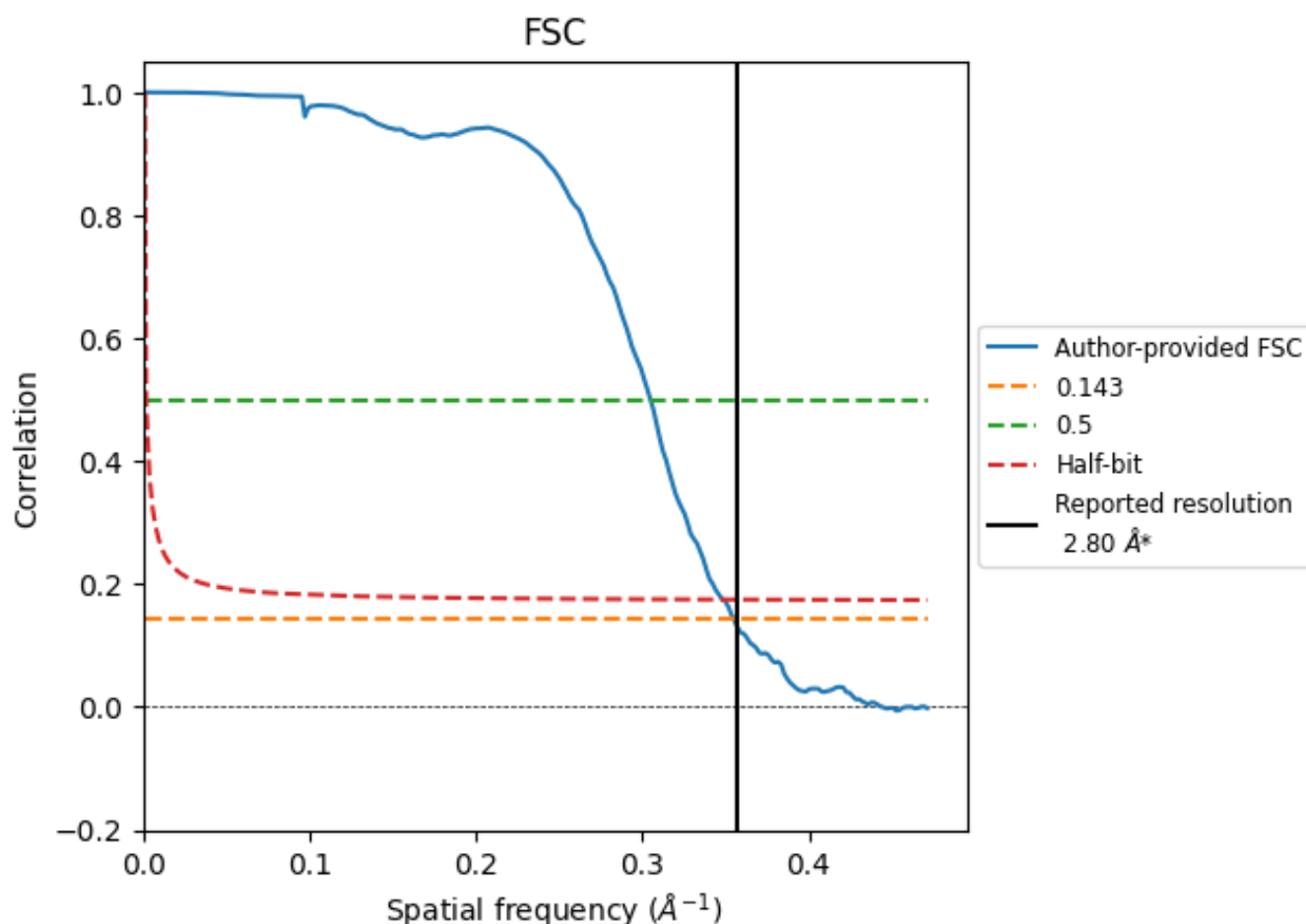
7.3 Rotationally averaged power spectrum [i](#)

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 0.357 Å⁻¹

8.2 Resolution estimates [i](#)

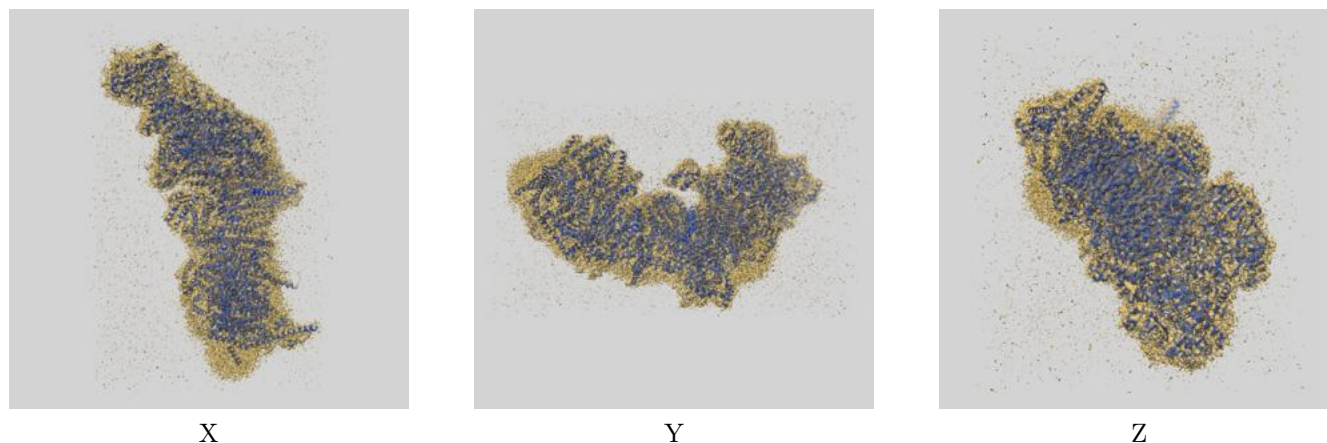
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.82	3.28	2.87
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

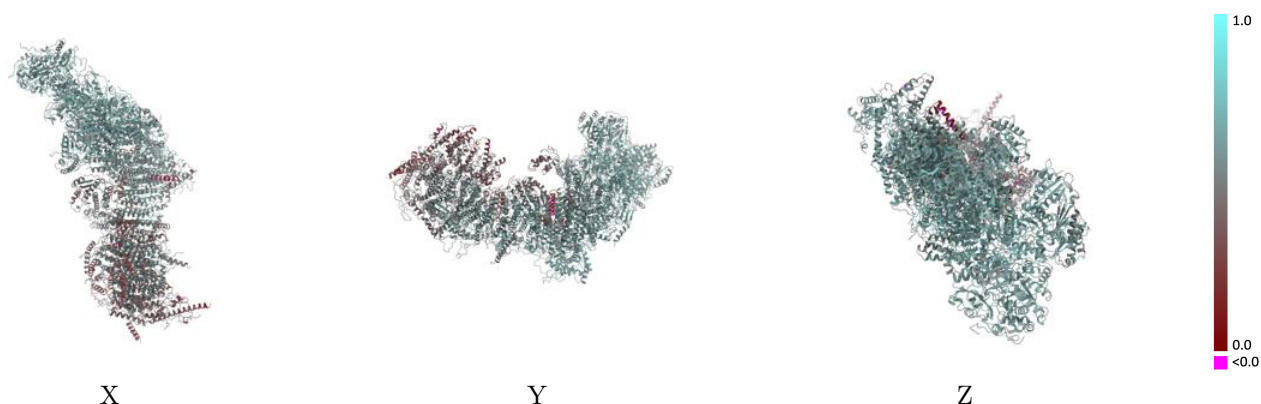
This section contains information regarding the fit between EMDB map EMD-11254 and PDB model 6ZKM. Per-residue inclusion information can be found in section [3](#) on page [21](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.055 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](#)

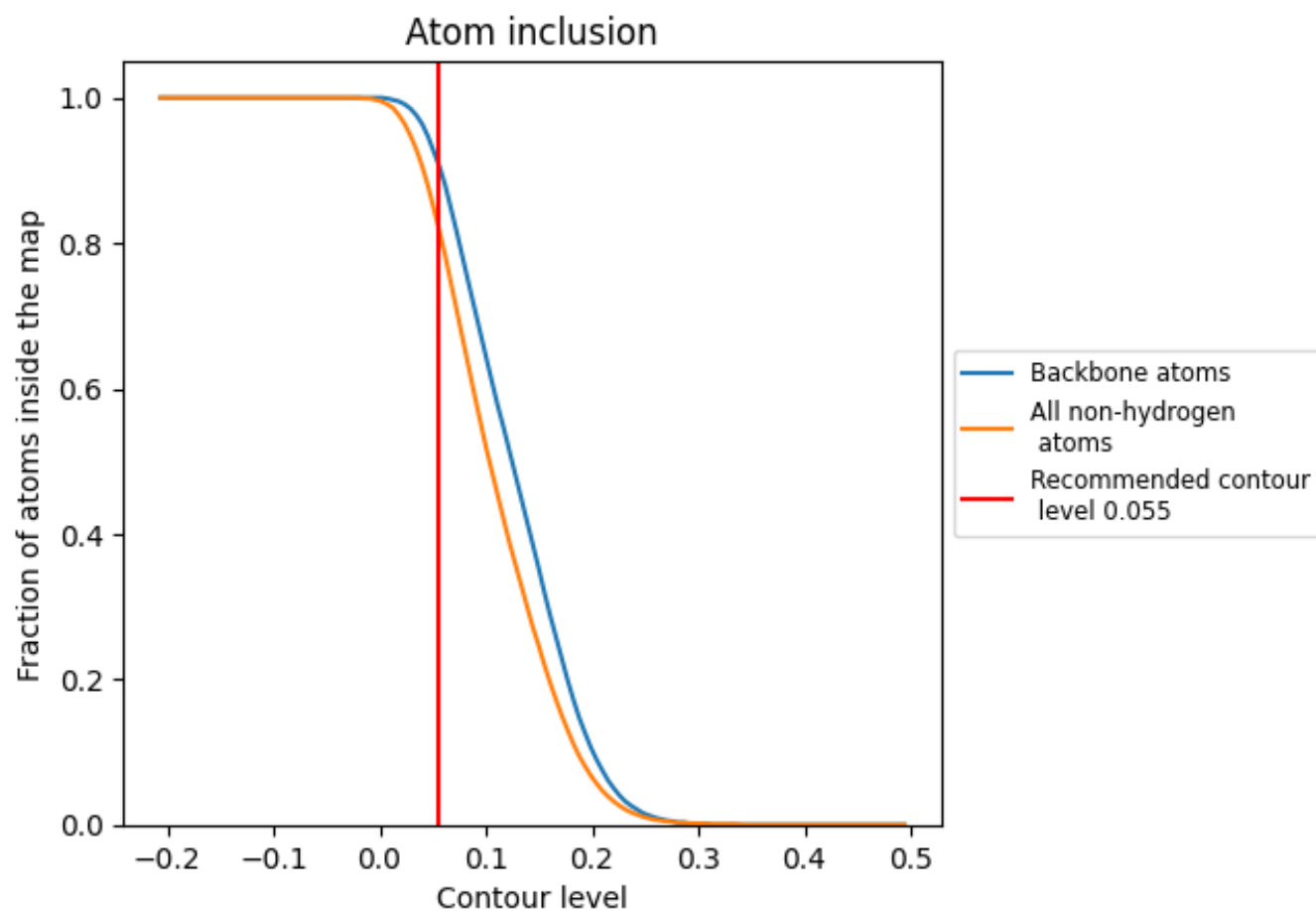


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion ⓘ



At the recommended contour level, 91% of all backbone atoms, 82% 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 (0.055) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8240	 0.5500
1	 0.9350	 0.6050
2	 0.8850	 0.5850
3	 0.9180	 0.6110
4	 0.8800	 0.6130
5	 0.9400	 0.6390
6	 0.9370	 0.6310
9	 0.9470	 0.6460
A	 0.7080	 0.5280
H	 0.8930	 0.6040
J	 0.6780	 0.4790
K	 0.8320	 0.5720
L	 0.7070	 0.4860
M	 0.8430	 0.5680
N	 0.8670	 0.5840
V	 0.5300	 0.4050
W	 0.8230	 0.5520
X	 0.5960	 0.3510
Y	 0.8880	 0.5860
Z	 0.7800	 0.5010
a	 0.9170	 0.5760
b	 0.9280	 0.6230
c	 0.9080	 0.6220
d	 0.8800	 0.5780
e	 0.8620	 0.5520
f	 0.8680	 0.5800
g	 0.8590	 0.5850
h	 0.8930	 0.5990
i	 0.8960	 0.6170
j	 0.6700	 0.4160
k	 0.7350	 0.4880
l	 0.8310	 0.5460
m	 0.9020	 0.5840
n	 0.5780	 0.3450
o	 0.7750	 0.5430



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Chain	Atom inclusion	Q-score
p	 0.5870	 0.4080
q	 0.8900	 0.5880
r	 0.7160	 0.4360
s	 0.6380	 0.3700
t	 0.6720	 0.4040
u	 0.6640	 0.3860
v	 0.6720	 0.4220
w	 0.7440	 0.5170
x	 0.7150	 0.4760
y	 0.7150	 0.4810
z	 0.9170	 0.6050