



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 12:29 PM UTC

PDB ID : 8BPX / pdb_00008bpx
EMDB ID : EMD-16168
Title : Cryo-EM structure of the Arabidopsis thaliana I+III2 supercomplex (Complete composition)
Authors : Klusch, N.; Kuehlbrandt, W.
Deposited on : 2022-11-18
Resolution : 2.09 Å(reported)

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:

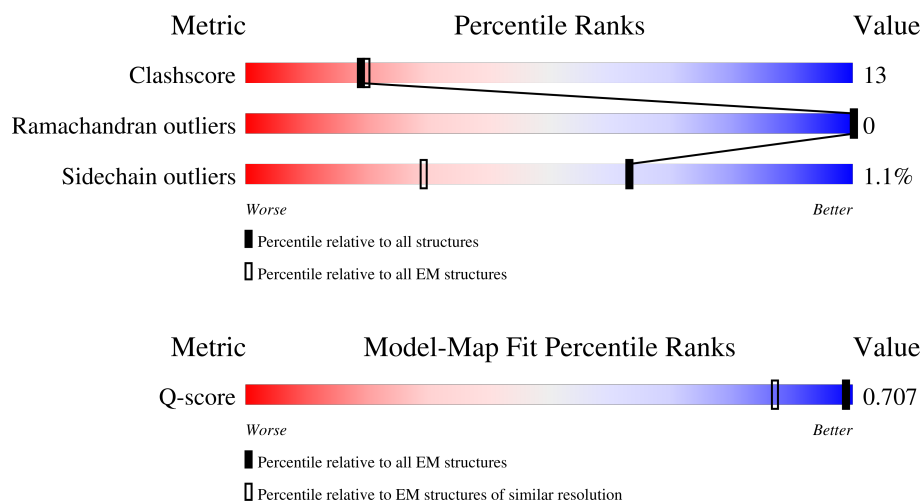
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 i

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

The reported resolution of this entry is 2.09 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2022 (1.60 - 2.59)

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	A	119	
2	B	218	
3	C	190	
4	D	394	

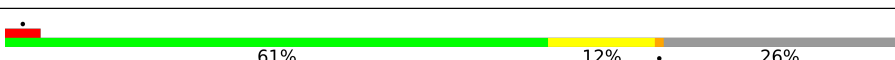
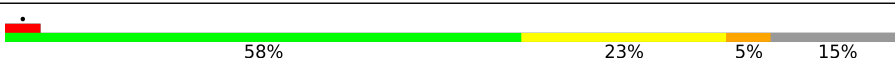
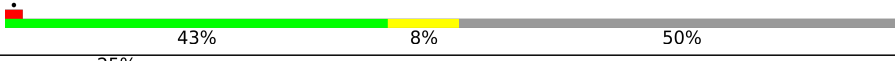
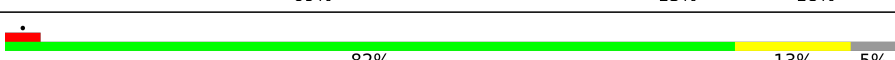
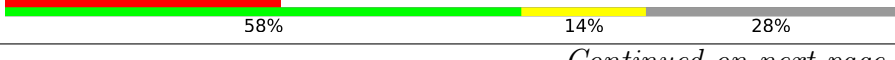
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Mol	Chain	Length	Quality of chain
5	E	255	
6	F	486	
7	G	748	
8	H	325	
9	I	222	
10	J	205	
11	K	100	
12	L	669	
13	M	495	
14	N	499	
15	O	159	
16	P	402	
17	Q	154	
18	R	110	
19	S	97	
20	T	122	
21	U	126	
22	V	169	
23	W	133	
24	X	106	
25	Y	159	
26	Z	143	
27	a	65	
28	b	65	
29	c	88	

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Mol	Chain	Length	Quality of chain
30	d	81	
31	e	83	
32	f	106	
33	g	114	
34	i	98	
35	j	69	
36	k	72	
37	l	125	
38	m	71	
39	n	117	
40	o	103	
41	p	106	
42	q	159	
43	u	63	
44	v	113	
45	x	256	
46	y	278	
47	z	275	
48	AA	503	
48	BA	503	
49	AB	531	
49	BB	531	
50	AC	393	
50	BC	393	
51	AD	272	

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Mol	Chain	Length	Quality of chain
51	BD	272	
52	AE	307	
52	BE	307	
53	AF	122	
53	BF	122	
54	AG	72	
54	BG	72	
55	AH	69	
55	BH	69	
56	AI	72	
56	BI	72	
57	AJ	57	
57	BJ	57	

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
59	SF4	I	500	-	-	X	-
73	COO	y	302	X	-	-	-

2 Entry composition

There are 76 unique types of molecules in this entry. The entry contains 104814 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-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	94	Total	C	N	O	S	0	0
			802	565	110	123	4		

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	157	Total	C	N	O	S	0	0
			1244	797	218	215	14		

- Molecule 3 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	181	Total	C	N	O	S	0	0
			1545	997	266	276	6		

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	385	Total	C	N	O	S	0	0
			3079	1957	542	556	24		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	70	LEU	SER	conflict	UNP P93306
D	227	SER	PRO	conflict	UNP P93306
D	309	LEU	SER	conflict	UNP P93306

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	192	Total	C	N	O	S	0	0
			1500	954	248	287	11		

- Molecule 6 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	434	Total	C	N	O	S	0	0
			3368	2125	600	618	25		

- Molecule 7 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	687	Total	C	N	O	S	0	0
			5243	3285	919	1000	39		

- Molecule 8 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	324	Total	C	N	O	S	0	0
			2536	1719	386	416	15		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	126	ARG	TRP	conflict	UNP P92558

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8-A, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	165	Total	C	N	O	S	0	0
			1349	849	229	261	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	174	Total	C	N	O	S	0	0
			1399	949	213	228	9		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	155	SER	PRO	conflict	UNP P60497

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	100	Total	C	N	O	S	0	0
			784	525	121	131	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	44	LEU	SER	conflict	UNP Q04614

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	665	Total	C	N	O	S	0	0
			5222	3474	808	901	39		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	91	PHE	SER	variant	UNP P29388
L	288	PHE	SER	variant	UNP P29388
L	537	LEU	PRO	variant	UNP P29388

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	494	Total	C	N	O	S	1	0
			3952	2668	610	649	25		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	146	PHE	PRO	variant	UNP P93313
M	326	LEU	PRO	variant	UNP P93313
M	383	PHE	SER	variant	UNP P93313

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	488	Total	C	N	O	S	2	0
			3839	2587	580	644	28		

- Molecule 15 is a protein called 2Fe-2S ferredoxin-like superfamily protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	123	Total	C	N	O	S	0	0
			963	603	170	186	4		

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	316	Total	C	N	O	S	0	0
			2453	1580	414	444	15		

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	105	Total	C	N	O	S	0	0
			837	536	144	156	1		

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	73	Total	C	N	O	S	0	0
			571	359	101	105	6		

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	93	Total	C	N	O	S	0	0
			727	459	129	133	6		

- Molecule 20 is a protein called Acyl carrier protein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	83	Total	C	N	O	S	0	0
			659	417	104	135	3		

- Molecule 21 is a protein called Acyl carrier protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	87	Total	C	N	O	S	0	0
			677	427	110	139	1		

- Molecule 22 is a protein called Probable NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	140	Total	C	N	O	S	0	0
			1123	712	187	219	5		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	112	Total	C	N	O	S	0	0
			904	578	161	162	3		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	98	Total	C	N	O	S	0	0
			776	486	134	144	12		

- Molecule 25 is a protein called Outer envelope pore protein 16-3, chloroplastic/mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	125	Total	C	N	O	S	0	0
			928	596	162	167	3		

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	125	Total	C	N	O	S	0	0
			997	640	175	177	5		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	a	58	Total	C	N	O	S	0	0
			469	302	84	78	5		

- Molecule 28 is a protein called At2g46540/F11C10.23.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	b	43	Total	C	N	O	S	0	0
			315	206	51	55	3		

- Molecule 29 is a protein called Transmembrane protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	c	76	Total	C	N	O	S	0	0
			617	396	115	100	6		

- Molecule 30 is a protein called Excitatory amino acid transporter.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	d	75	Total	C	N	O	S	0	0
			592	382	106	99	5		

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	e	64	Total	C	N	O	S	0	0
			546	338	102	99	7		

- Molecule 32 is a protein called At4g16450.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	f	101	Total	C	N	O	S	0	0
			765	491	126	143	5		

- Molecule 33 is a protein called ESSS subunit of NADH:ubiquinone oxidoreductase (Complex I) protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	g	79	Total	C	N	O	S	0	0
			641	412	111	115	3		

- Molecule 34 is a protein called At1g67350.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	i	83	Total	C	N	O	S	0	0
			721	458	132	126	5		

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	j	51	Total	C	N	O	S	0	0
			415	275	73	64	3		

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	k	48	Total	C	N	O	S	0	0
			382	244	72	63	3		

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	l	74	Total	C	N	O	S	0	0
			562	367	91	103	1		

- Molecule 38 is a protein called AT2G31490 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	m	70	Total	C	N	O	S	0	0
			577	370	107	98	2		

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	n	109	Total	C	N	O	S	0	0
			911	580	170	160	1		

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	o	80	Total	C	N	O	S	0	0
			657	413	115	119	10		

- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	p	90	Total	C	N	O	S	0	0
			757	479	141	133	4		

- Molecule 42 is a protein called Probable NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	q	80	Total	C	N	O	S	1	0
			669	427	120	120	2		

- Molecule 43 is a protein called Uncharacterized protein At1g67785.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	u	55	Total	C	N	O	S	0	0
			463	298	84	78	3		

- Molecule 44 is a protein called Uncharacterized protein At2g27730, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	v	29	Total	C	N	O	S	0	0
			219	142	38	39			

- Molecule 45 is a protein called Gamma carbonic anhydrase-like 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	x	210	Total	C	N	O	S	0	0
			1629	1043	280	301	5		

- Molecule 46 is a protein called Gamma carbonic anhydrase 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	y	265	Total	C	N	O	S	0	0
			2013	1258	359	388	8		

- Molecule 47 is a protein called Gamma carbonic anhydrase 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	z	233	Total	C	N	O	S	0	0
			1772	1111	325	330	6		

- Molecule 48 is a protein called Probable mitochondrial-processing peptidase subunit alpha-1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	AA	450	Total	C	N	O	S	0	0
			3431	2178	573	663	17		
48	BA	451	Total	C	N	O	S	0	0
			3436	2181	574	664	17		

- Molecule 49 is a protein called Probable mitochondrial-processing peptidase subunit beta, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	AB	487	Total	C	N	O	S	0	0
			3834	2407	672	743	12		
49	BB	487	Total	C	N	O	S	0	0
			3834	2407	672	743	12		

- Molecule 50 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	AC	387	Total	C	N	O	S	0	0
			3093	2083	487	508	15		
50	BC	387	Total	C	N	O	S	0	0
			3093	2083	487	508	15		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AC	40	SER	PRO	variant	UNP P42792
BC	40	SER	PRO	variant	UNP P42792

- Molecule 51 is a protein called Cytochrome b-c1 complex subunit Rieske-1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	AD	196	Total	C	N	O	S	0	0
			1528	978	264	281	5		
51	BD	195	Total	C	N	O	S	0	0
			1519	973	263	278	5		

- Molecule 52 is a protein called Cytochrome c1 2, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	AE	244	Total	C	N	O	S	0	0
			1917	1216	326	364	11		
52	BE	244	Total	C	N	O	S	0	0
			1917	1216	326	364	11		

- Molecule 53 is a protein called Cytochrome b-c1 complex subunit 7-2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	AF	116	Total	C	N	O	S	0	0
			976	613	186	171	6		
53	BF	116	Total	C	N	O	S	0	0
			976	613	186	171	6		

- Molecule 54 is a protein called Cytochrome b-c1 complex subunit 8-1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	AG	69	Total	C	N	O	S	0	0
			581	387	95	98	1		
54	BG	68	Total	C	N	O	S	0	0
			572	382	93	96	1		

- Molecule 55 is a protein called Cytochrome b-c1 complex subunit 6-1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	AH	64	Total	C	N	O	S	0	0
			518	334	87	91	6		
55	BH	63	Total	C	N	O	S	0	0
			511	329	86	90	6		

- Molecule 56 is a protein called Cytochrome b-c1 complex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	AI	57	Total	C	N	O	S	0	0
			476	310	85	80	1		
56	BI	57	Total	C	N	O	S	0	0
			476	310	85	80	1		

- Molecule 57 is a protein called Cytochrome b-c1 complex subunit 10, mitochondrial.

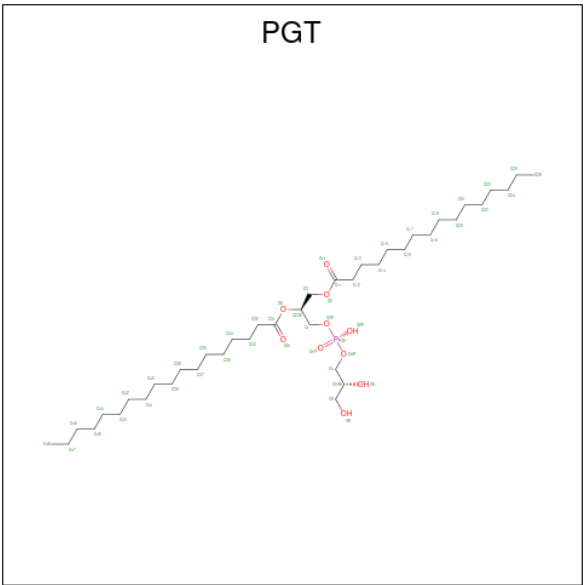
Mol	Chain	Residues	Atoms				AltConf	Trace
57	AJ	28	Total	C	N	O	0	0
			203	137	33	33		

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Mol	Chain	Residues	Atoms				AltConf	Trace
57	BJ	28	Total	C	N	O	0	0
			205	139	34	32		

- Molecule 58 is (1S)-2-{{[[(2R)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (CCD ID: PGT) (formula: C₄₀H₇₉O₁₀P) (labeled as "Ligand of Interest" by depositor).



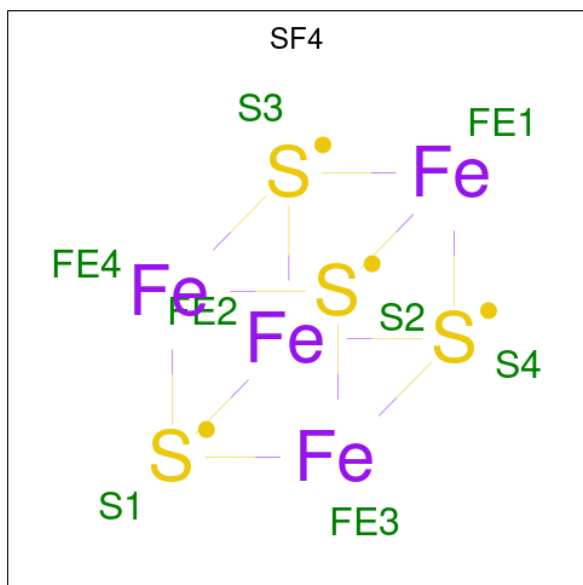
Mol	Chain	Residues	Atoms				AltConf
58	A	1	Total	C	O	P	0
			51	40	10	1	
58	L	1	Total	C	O	P	0
			36	25	10	1	
58	L	1	Total	C	O	P	0
			51	40	10	1	
58	L	1	Total	C	O	P	0
			45	34	10	1	
58	M	1	Total	C	O	P	0
			29	18	10	1	
58	y	1	Total	C	O	P	0
			41	30	10	1	
58	AC	1	Total	C	O	P	0
			41	30	10	1	
58	AC	1	Total	C	O	P	0
			51	40	10	1	
58	AF	1	Total	C	O	P	0
			51	40	10	1	

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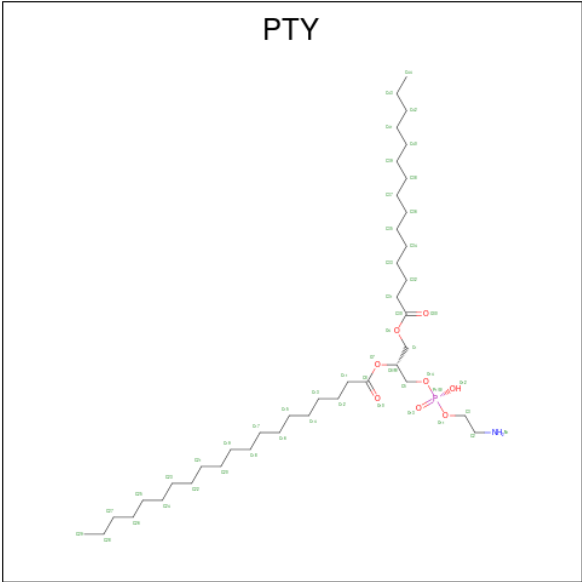
Mol	Chain	Residues	Atoms				AltConf
58	BC	1	Total	C	O	P	0
			37	26	10	1	

- Molecule 59 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



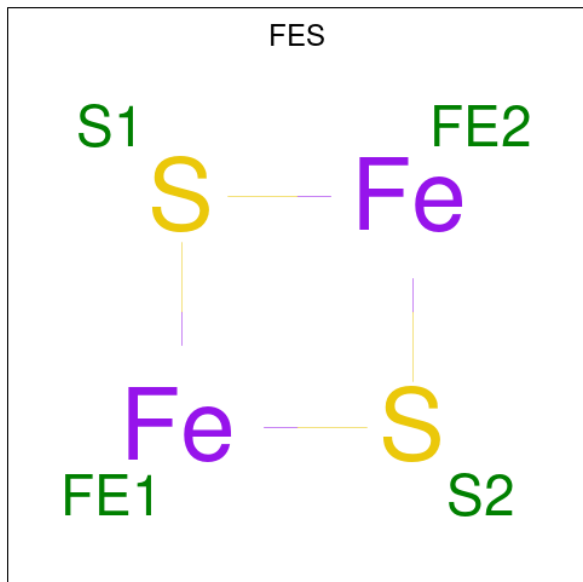
Mol	Chain	Residues	Atoms			AltConf
59	B	1	Total	Fe	S	0
			8	4	4	
59	F	1	Total	Fe	S	0
			8	4	4	
59	G	1	Total	Fe	S	0
			8	4	4	
59	G	1	Total	Fe	S	0
			8	4	4	
59	I	1	Total	Fe	S	0
			8	4	4	
59	I	1	Total	Fe	S	0
			8	4	4	

- Molecule 60 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: $\text{C}_{40}\text{H}_{80}\text{NO}_8\text{P}$) (labeled as "Ligand of Interest" by depositor).



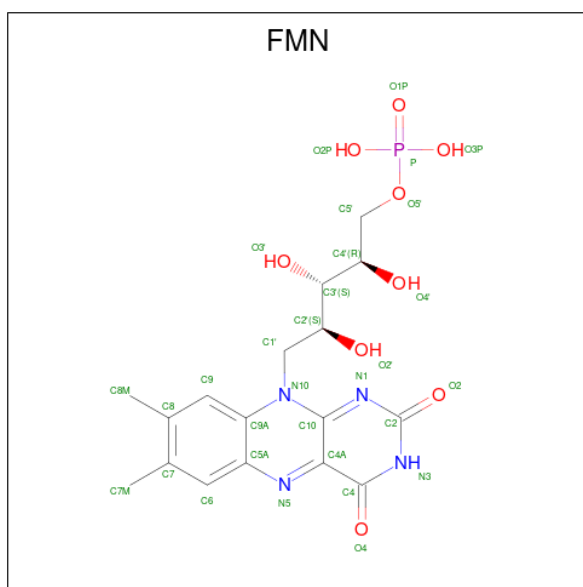
Mol	Chain	Residues	Atoms					AltConf
60	D	1	Total	C	N	O	P	0
			50	40	1	8	1	
60	L	1	Total	C	N	O	P	0
			42	32	1	8	1	
60	M	1	Total	C	N	O	P	0
			37	27	1	8	1	
60	M	1	Total	C	N	O	P	0
			50	40	1	8	1	
60	N	1	Total	C	N	O	P	0
			40	30	1	8	1	
60	N	1	Total	C	N	O	P	0
			45	35	1	8	1	
60	N	1	Total	C	N	O	P	0
			50	40	1	8	1	
60	Y	1	Total	C	N	O	P	0
			31	21	1	8	1	
60	d	1	Total	C	N	O	P	0
			39	29	1	8	1	
60	m	1	Total	C	N	O	P	0
			50	40	1	8	1	
60	z	1	Total	C	N	O	P	0
			50	40	1	8	1	
60	AB	1	Total	C	N	O	P	0
			41	31	1	8	1	
60	BB	1	Total	C	N	O	P	0
			29	19	1	8	1	
60	BF	1	Total	C	N	O	P	0
			40	30	1	8	1	

- Molecule 61 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



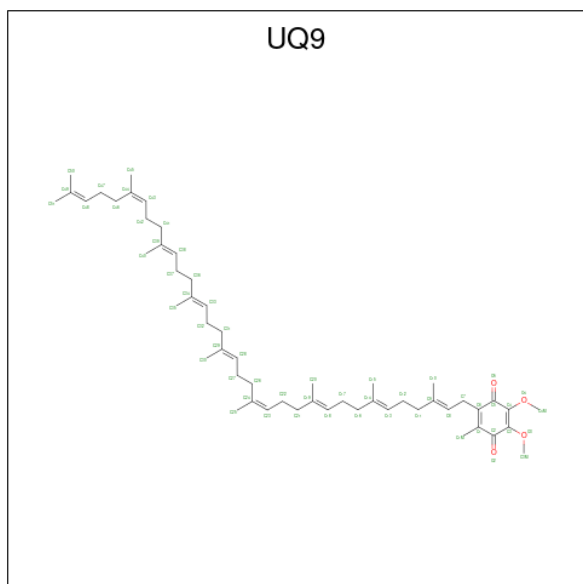
Mol	Chain	Residues	Atoms			AltConf
61	E	1	Total	Fe	S	0
			4	2	2	
61	G	1	Total	Fe	S	0
			4	2	2	
61	AD	1	Total	Fe	S	0
			4	2	2	
61	BD	1	Total	Fe	S	0
			4	2	2	

- Molecule 62 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $\text{C}_{17}\text{H}_{21}\text{N}_4\text{O}_9\text{P}$) (labeled as "Ligand of Interest" by depositor).



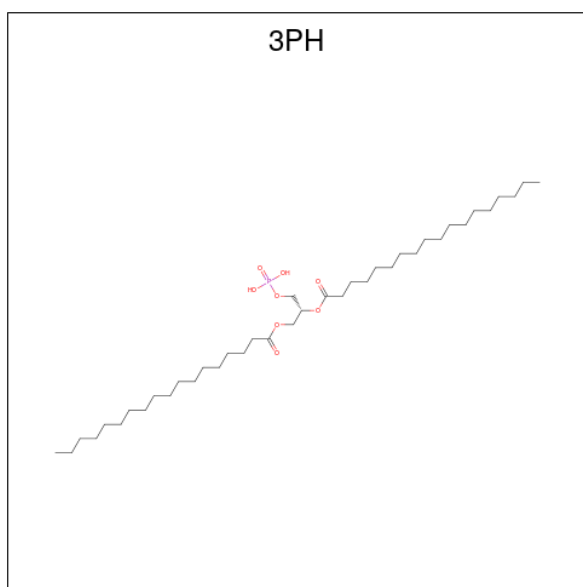
Mol	Chain	Residues	Atoms					AltConf
62	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 63 is Ubiquinone-9 (CCD ID: UQ9) (formula: $C_{54}H_{82}O_4$) (labeled as "Ligand of Interest" by depositor).



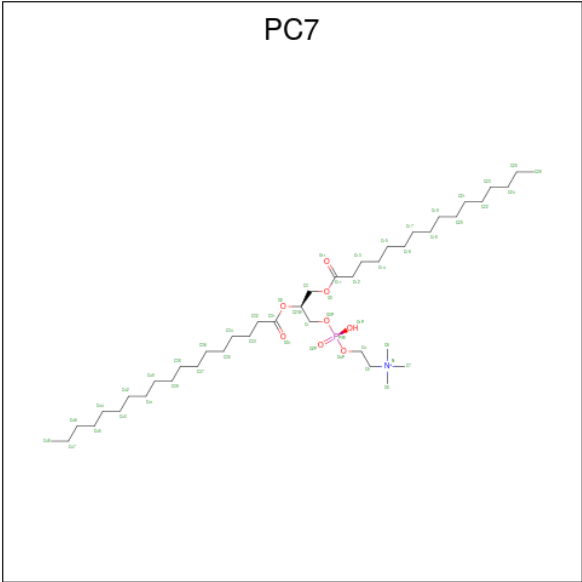
Mol	Chain	Residues	Atoms			AltConf
63	H	1	Total	C	O	0
			35	31	4	

- Molecule 64 is 2-[[[4-O-alpha-D-glucopyranosyl-alpha-D-glucopyranosyl]oxy]methyl]-4-[[[(3 beta,9beta,14beta,17beta,25R)-spirost-5-en-3-yl]oxy]butyl 4-O-alpha-D-glucopyranosyl-alpha



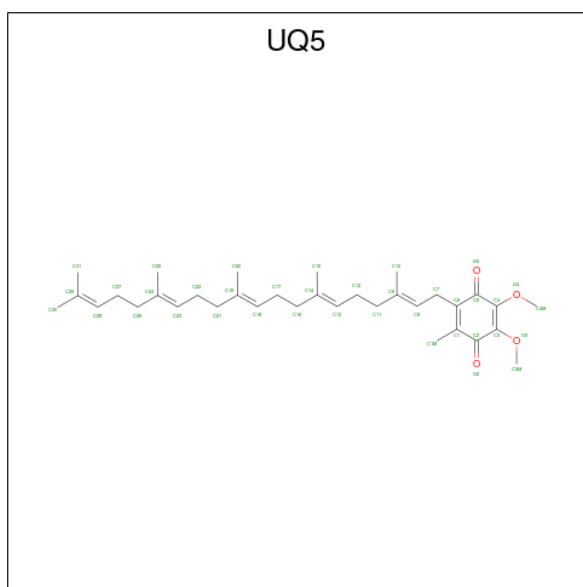
Mol	Chain	Residues	Atoms				AltConf
65	L	1	Total	C	O	P	0
			37	28	8	1	
65	M	1	Total	C	O	P	0
			41	32	8	1	
65	Y	1	Total	C	O	P	0
			33	24	8	1	
65	f	1	Total	C	O	P	0
			41	32	8	1	
65	f	1	Total	C	O	P	0
			43	34	8	1	
65	l	1	Total	C	O	P	0
			37	28	8	1	
65	AC	1	Total	C	O	P	0
			33	24	8	1	
65	AI	1	Total	C	O	P	0
			32	23	8	1	
65	BC	1	Total	C	O	P	0
			44	35	8	1	
65	BJ	1	Total	C	O	P	0
			41	32	8	1	
65	BJ	1	Total	C	O	P	0
			48	39	8	1	

- Molecule 66 is (7S)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY) METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSAN-1-AMINIUM 4-OXIDE (CCD ID: PC7) (formula: $C_{42}H_{85}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
66	L	1	Total	C	N	O	P	0
			40	30	1	8	1	
66	d	1	Total	C	N	O	P	0
			52	42	1	8	1	
66	f	1	Total	C	N	O	P	0
			48	38	1	8	1	
66	v	1	Total	C	N	O	P	0
			52	42	1	8	1	
66	AB	1	Total	C	N	O	P	0
			34	24	1	8	1	
66	AC	1	Total	C	N	O	P	0
			51	41	1	8	1	
66	AG	1	Total	C	N	O	P	0
			52	42	1	8	1	
66	BC	1	Total	C	N	O	P	0
			41	31	1	8	1	
66	BD	1	Total	C	N	O	P	0
			39	29	1	8	1	

- Molecule 67 is 2,3-DIMETHOXY-5-METHYL-6-(3,11,15,19-TETRAMETHYL-EICOSA-2,6,10,14,18-PENTAENYL)-[1,4]BENZOQUINONE (CCD ID: UQ5) (formula: C₃₄H₅₀O₄) (labeled as "Ligand of Interest" by depositor).

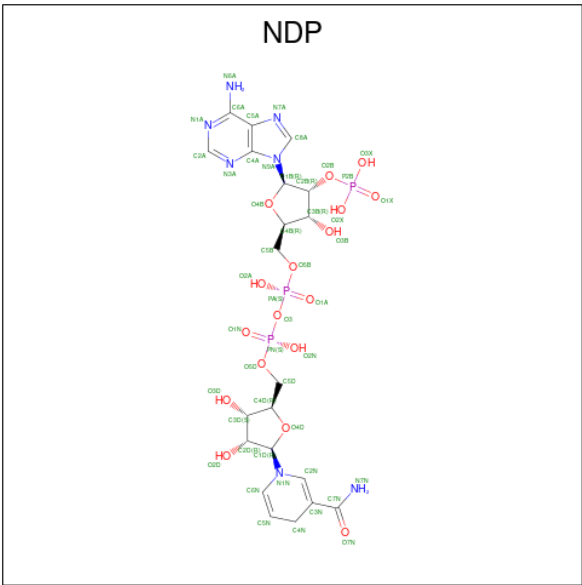


Mol	Chain	Residues	Atoms			AltConf
67	L	1	Total	C	O	0
			38	34	4	
67	AC	1	Total	C	O	0
			38	34	4	
67	AC	1	Total	C	O	0
			38	34	4	
67	BC	1	Total	C	O	0
			38	34	4	

- Molecule 68 is FE (III) ION (CCD ID: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
68	O	1	Total	Fe	0
			1	1	

- Molecule 69 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃) (labeled as "Ligand of Interest" by depositor).

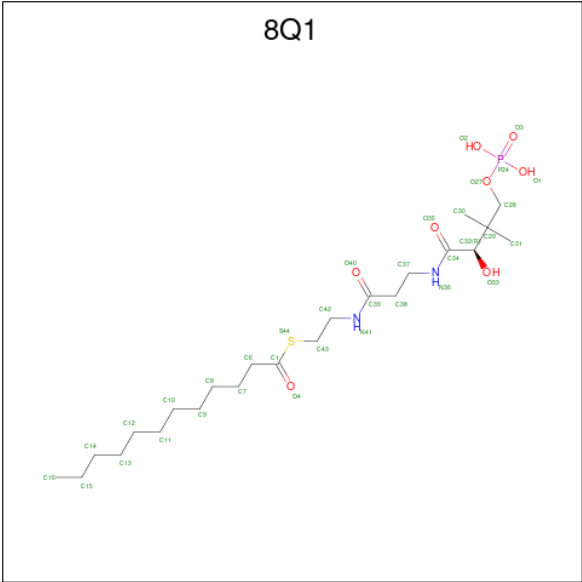


Mol	Chain	Residues	Atoms					AltConf
69	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 70 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

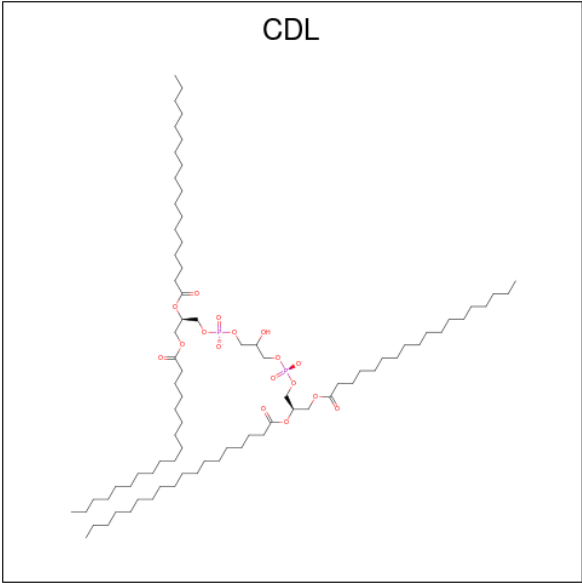
Mol	Chain	Residues	Atoms		AltConf
70	R	1	Total	Zn	0
			1	1	
70	y	1	Total	Zn	0
			1	1	
70	AB	1	Total	Zn	0
			1	1	
70	BB	1	Total	Zn	0
			1	1	

- Molecule 71 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (CCD ID: 8Q1) (formula: C₂₃H₄₅N₂O₈PS) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
71	T	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	
71	W	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	

- Molecule 72 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂) (labeled as "Ligand of Interest" by depositor).



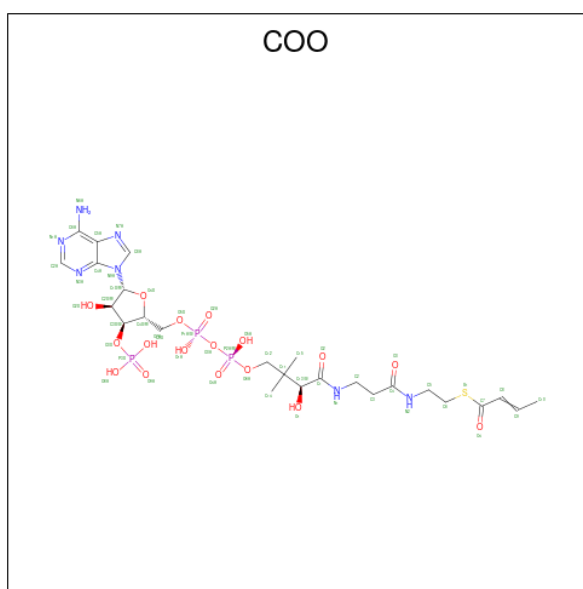
Mol	Chain	Residues	Atoms				AltConf
72	u	1	Total	C	O	P	0
			100	81	17	2	

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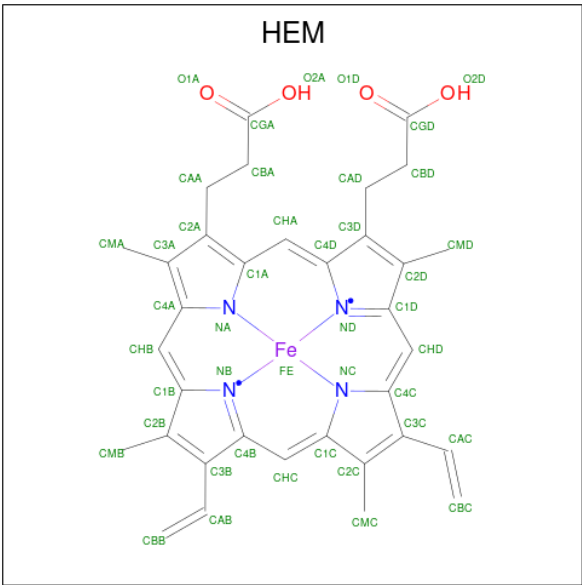
Mol	Chain	Residues	Atoms				AltConf
72	u	1	Total	C	O	P	0
			100	81	17	2	
72	AC	1	Total	C	O	P	0
			81	62	17	2	
72	AC	1	Total	C	O	P	0
			85	66	17	2	
72	AE	1	Total	C	O	P	0
			85	66	17	2	
72	BC	1	Total	C	O	P	0
			81	62	17	2	
72	BC	1	Total	C	O	P	0
			77	58	17	2	
72	BE	1	Total	C	O	P	0
			88	69	17	2	
72	BG	1	Total	C	O	P	0
			70	51	17	2	

- Molecule 73 is CROTONYL COENZYME A (CCD ID: COO) (formula: $C_{25}H_{40}N_7O_{17}P_3S$) (labeled as "Ligand of Interest" by depositor).



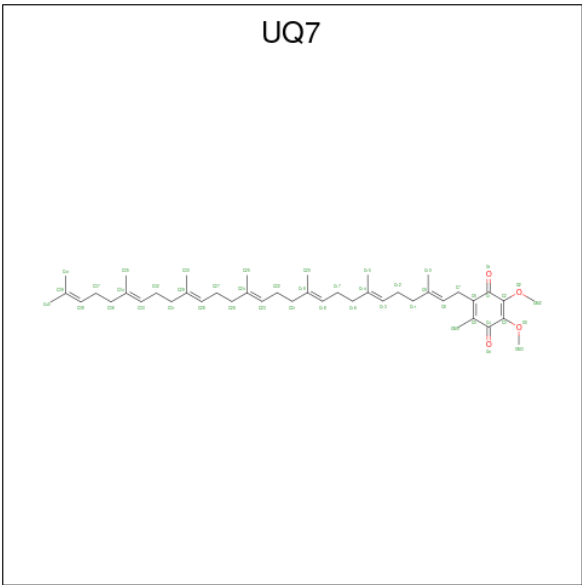
Mol	Chain	Residues	Atoms						AltConf
73	y	1	Total	C	N	O	P	S	0
			53	25	7	17	3	1	

- Molecule 74 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
74	AC	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
74	AC	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
74	AE	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
74	BC	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
74	BC	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
74	BE	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 75 is UBIQUINONE-7 (CCD ID: UQ7) (formula: C₄₄H₆₆O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
75	BC	1	Total	C	O	0
			48	44	4	

- Molecule 76 is water.

Mol	Chain	Residues	Atoms		AltConf
76	A	20	Total	O	0
			20	20	
76	B	84	Total	O	0
			84	84	
76	C	104	Total	O	0
			104	104	
76	D	226	Total	O	0
			226	226	
76	E	89	Total	O	0
			89	89	
76	F	152	Total	O	0
			152	152	
76	G	313	Total	O	0
			313	313	
76	H	129	Total	O	0
			129	129	
76	I	102	Total	O	0
			102	102	
76	J	64	Total	O	0
			64	64	
76	K	49	Total	O	0
			49	49	

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Mol	Chain	Residues	Atoms		AltConf
76	L	213	Total 213	O 213	0
76	M	158	Total 158	O 158	0
76	N	201	Total 201	O 201	0
76	O	88	Total 88	O 88	0
76	P	44	Total 44	O 44	0
76	Q	22	Total 22	O 22	0
76	R	44	Total 44	O 44	0
76	S	17	Total 17	O 17	0
76	T	13	Total 13	O 13	0
76	U	3	Total 3	O 3	0
76	V	31	Total 31	O 31	0
76	W	10	Total 10	O 10	0
76	X	19	Total 19	O 19	0
76	Y	5	Total 5	O 5	0
76	Z	53	Total 53	O 53	0
76	a	19	Total 19	O 19	0
76	b	2	Total 2	O 2	0
76	c	30	Total 30	O 30	0
76	d	21	Total 21	O 21	0
76	e	30	Total 30	O 30	0
76	f	49	Total 49	O 49	0

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Mol	Chain	Residues	Atoms		AltConf
76	g	29	Total 29	O 29	0
76	i	26	Total 26	O 26	0
76	j	3	Total 3	O 3	0
76	k	10	Total 10	O 10	0
76	l	25	Total 25	O 25	0
76	m	24	Total 24	O 24	0
76	n	52	Total 52	O 52	0
76	o	50	Total 50	O 50	0
76	p	52	Total 52	O 52	0
76	q	31	Total 31	O 31	0
76	u	10	Total 10	O 10	0
76	v	10	Total 10	O 10	0
76	x	180	Total 180	O 180	0
76	y	167	Total 167	O 167	0
76	z	121	Total 121	O 121	0
76	AA	43	Total 43	O 43	0
76	AB	259	Total 259	O 259	0
76	AC	187	Total 187	O 187	0
76	AD	60	Total 60	O 60	0
76	AE	171	Total 171	O 171	0
76	AF	109	Total 109	O 109	0

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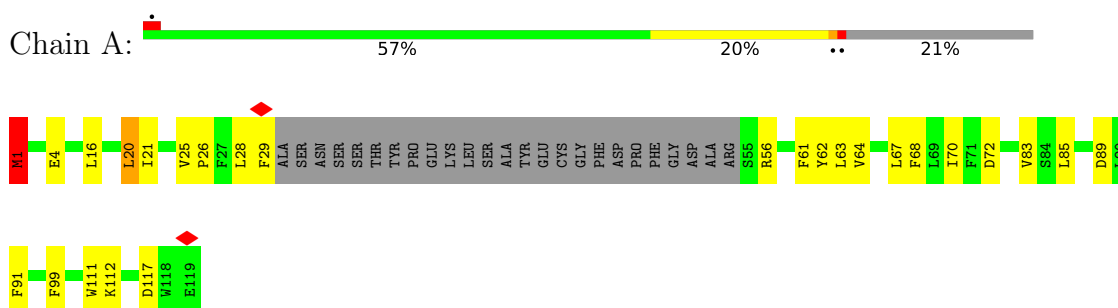
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Mol	Chain	Residues	Atoms		AltConf
76	AG	25	Total 25	O 25	0
76	AH	13	Total 13	O 13	0
76	AI	20	Total 20	O 20	0
76	BA	77	Total 77	O 77	0
76	BB	260	Total 260	O 260	0
76	BC	148	Total 148	O 148	0
76	BD	43	Total 43	O 43	0
76	BE	118	Total 118	O 118	0
76	BF	71	Total 71	O 71	0
76	BG	19	Total 19	O 19	0
76	BH	2	Total 2	O 2	0
76	BI	14	Total 14	O 14	0
76	BJ	1	Total 1	O 1	0

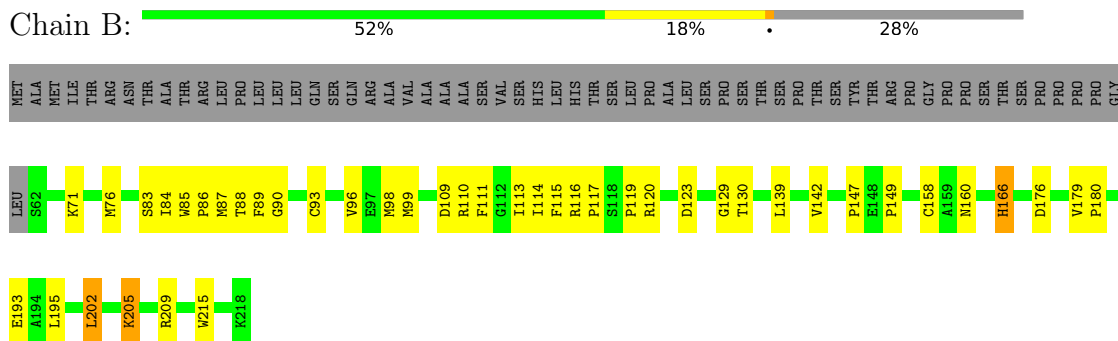
3 Residue-property plots [i](#)

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

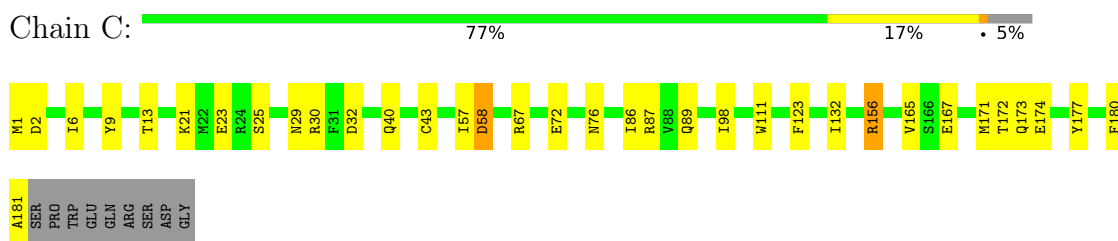
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3



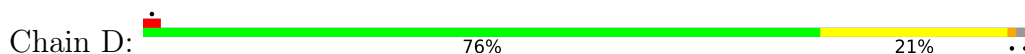
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

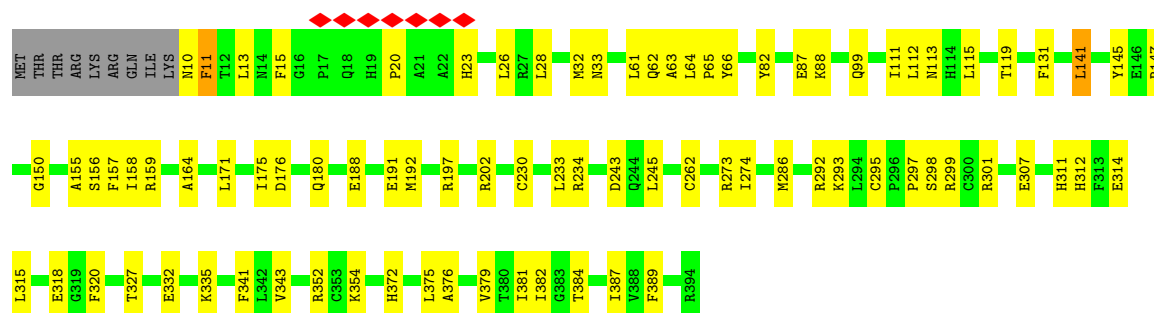


- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3

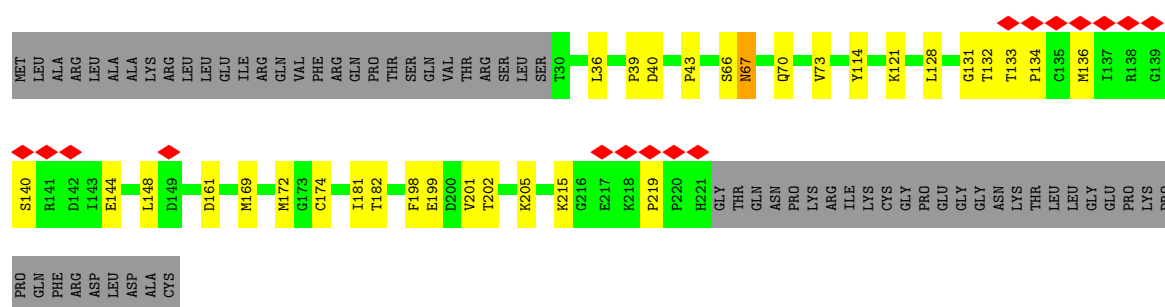


- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2

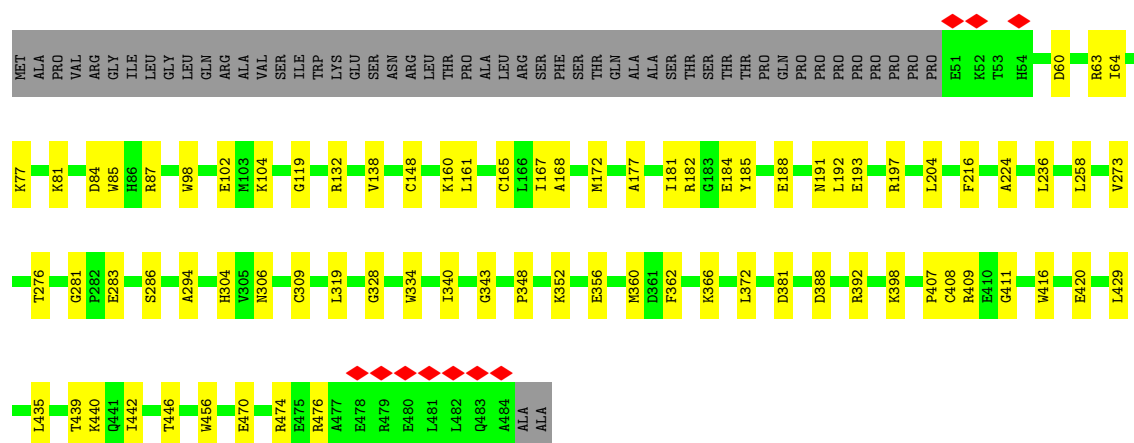




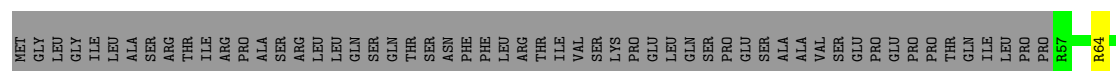
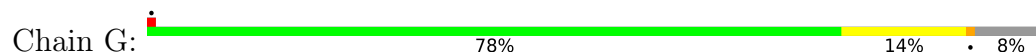
- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

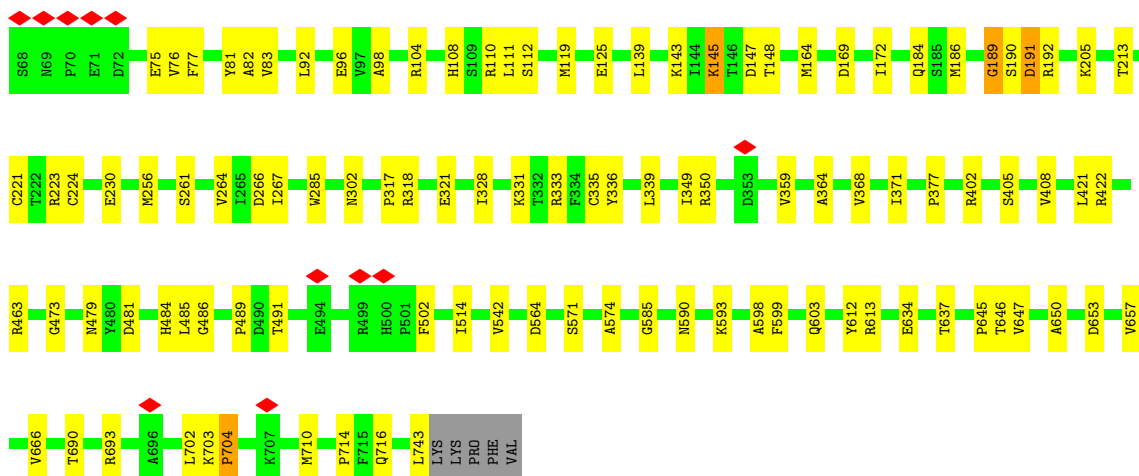


- Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



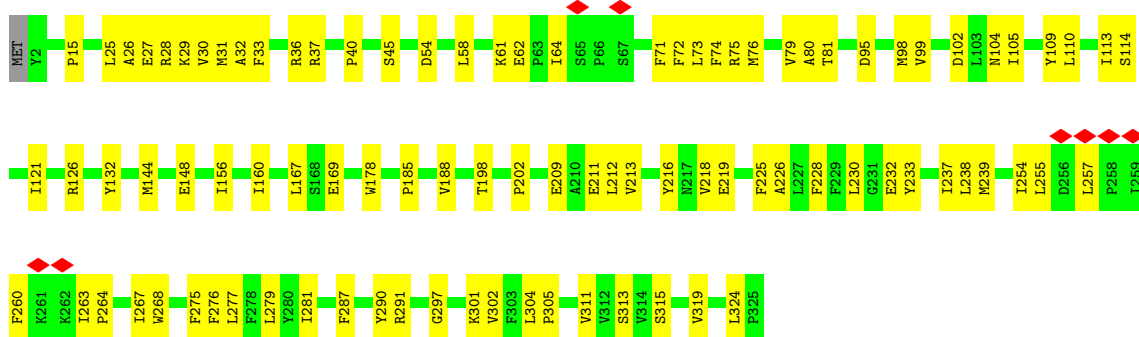
- Molecule 7: NADH dehydrogenase [ubiquinone] iron-sulfur protein 1, mitochondrial





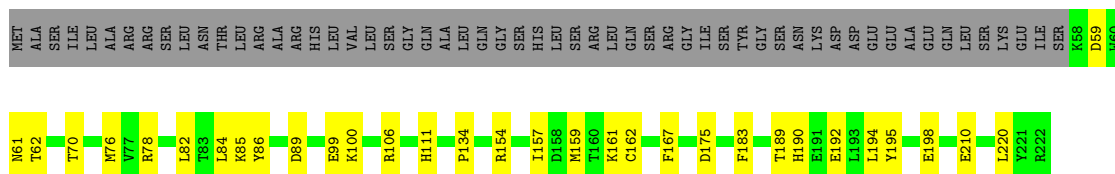
• Molecule 8: NADH-ubiquinone oxidoreductase chain 1

Chain H: 71% 29%



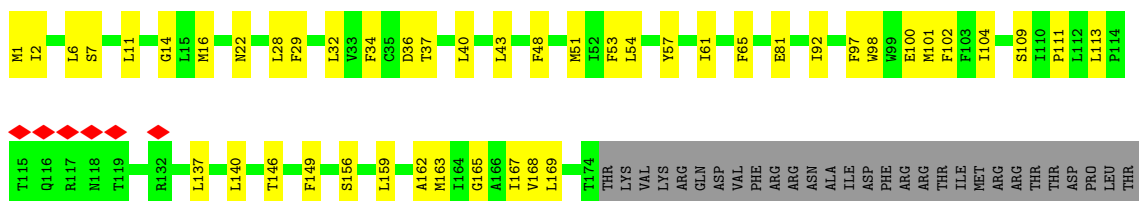
• Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8-A, mitochondrial

Chain I: 60% 14% 26%



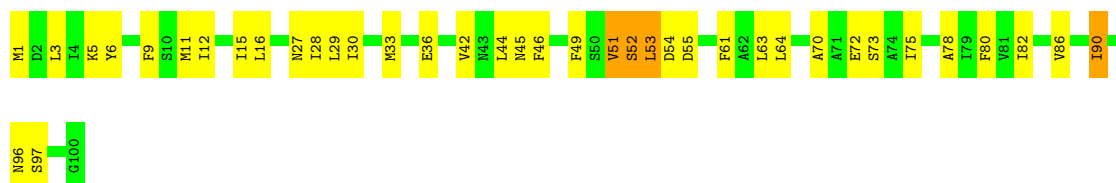
• Molecule 10: NADH-ubiquinone oxidoreductase chain 6

Chain J: 62% 22% 15%

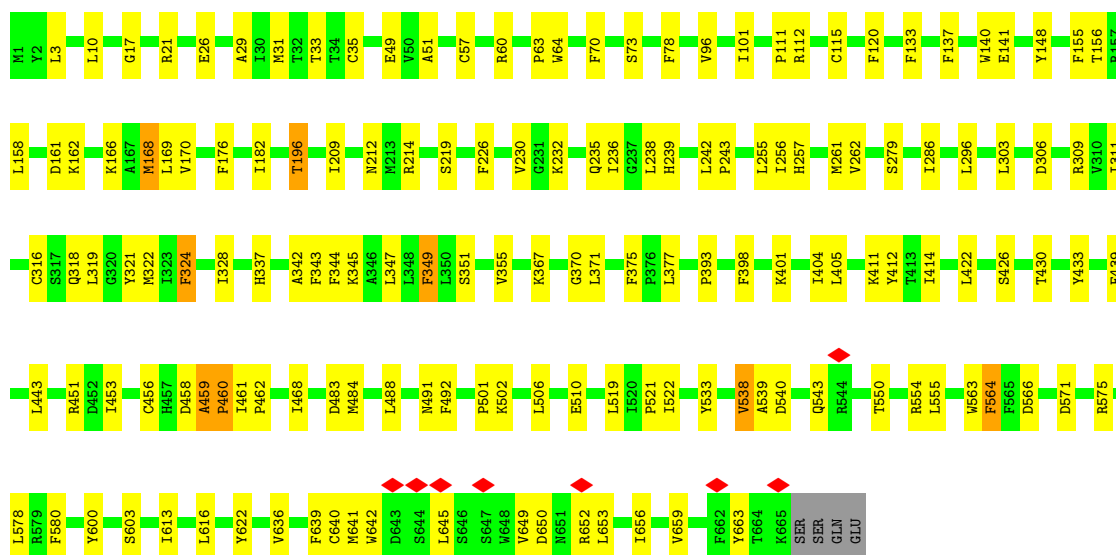


TYR

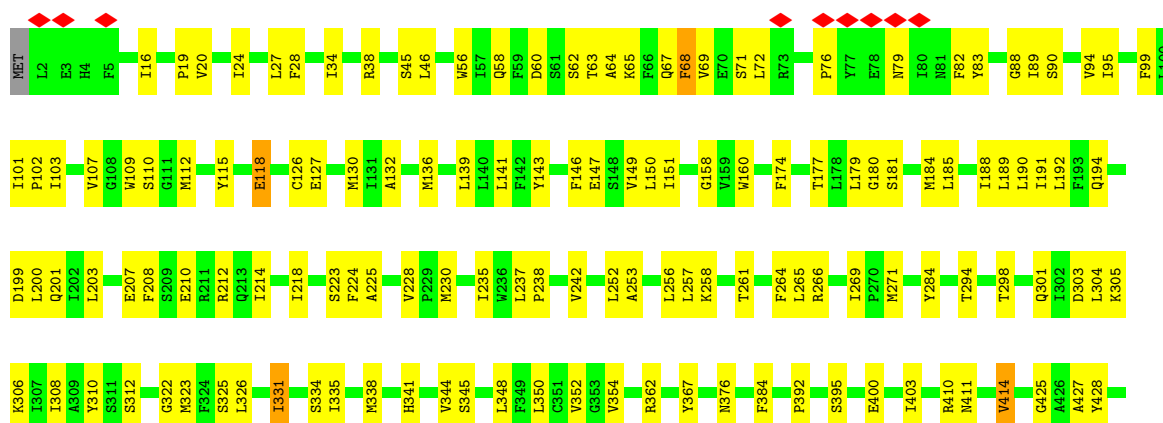
- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

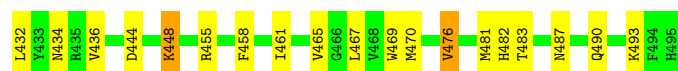
Chain K:  61% 35%

- Molecule 12: NADH-ubiquinone oxidoreductase chain 5

Chain L:  76% 22%

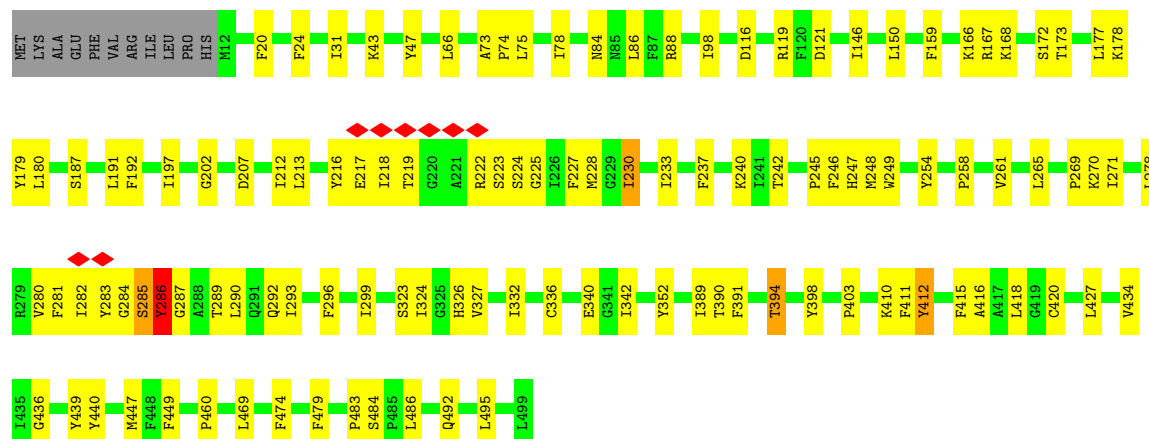
- Molecule 13: NADH-ubiquinone oxidoreductase chain 4

Chain M:  68% 31%



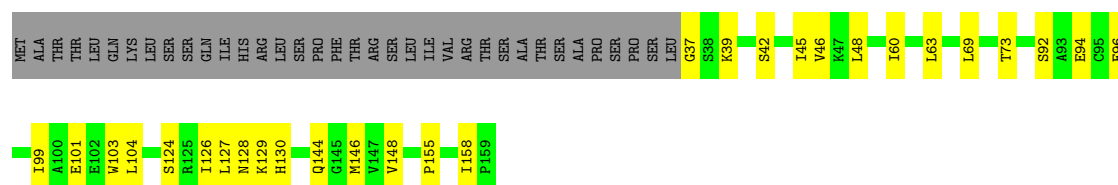
• Molecule 14: NADH-ubiquinone oxidoreductase chain 2

Chain N: 74% 22% ..



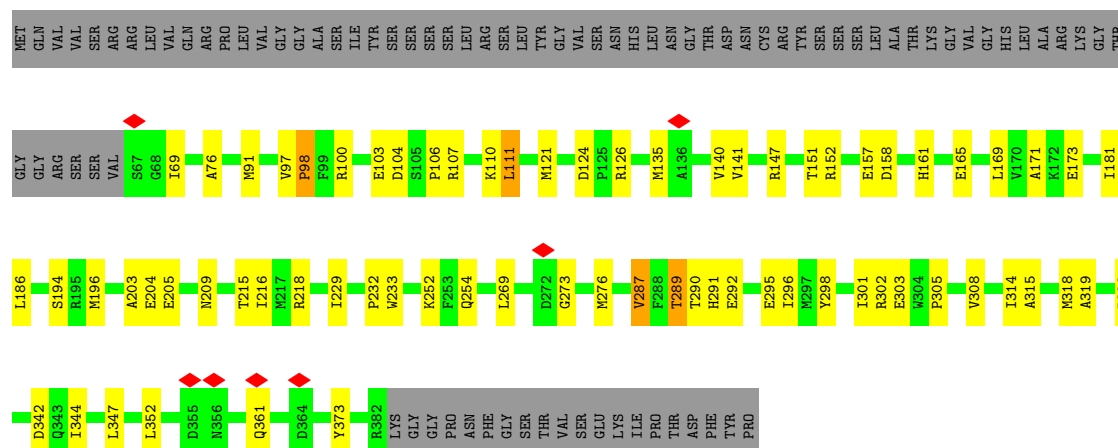
• Molecule 15: 2Fe-2S ferredoxin-like superfamily protein

Chain O: 60% 18% 23%

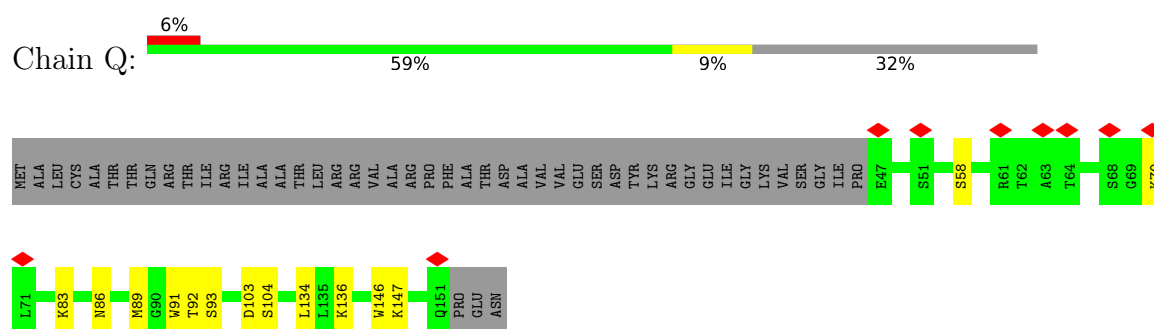


• Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

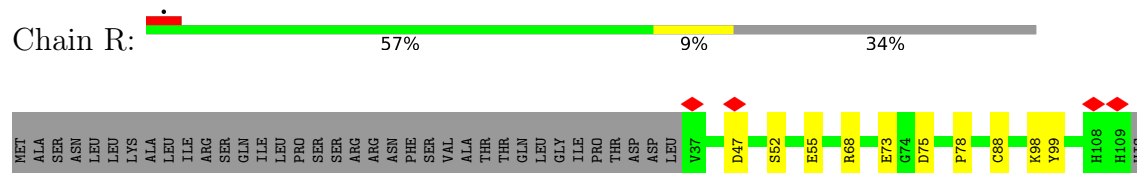
Chain P: 61% 17% 21%



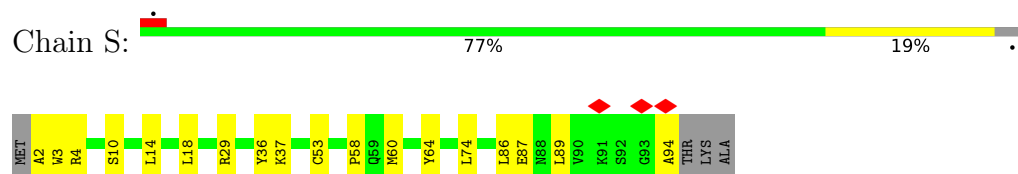
• Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



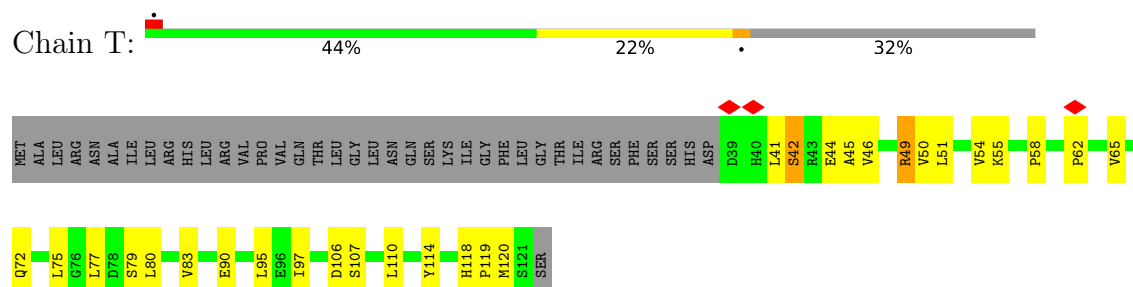
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



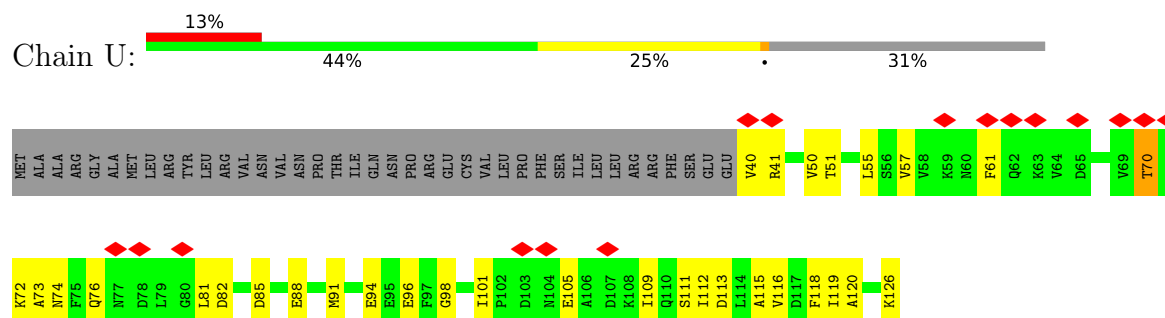
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



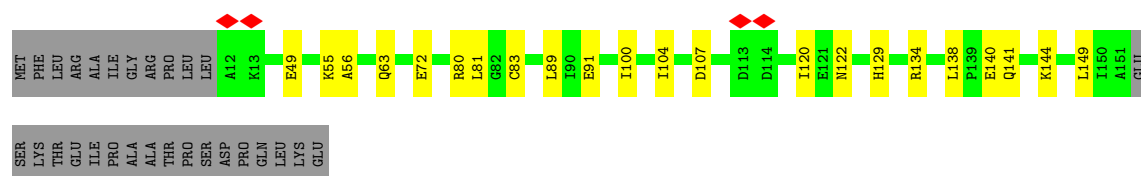
- Molecule 20: Acyl carrier protein 1, mitochondrial



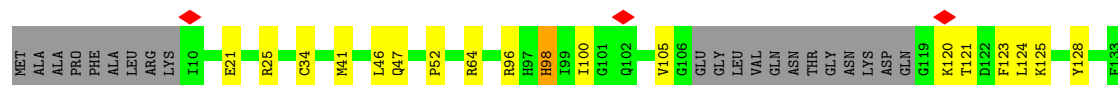
- Molecule 21: Acyl carrier protein 2, mitochondrial



- Molecule 22: Probable NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5, mitochondrial

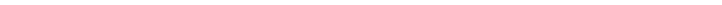


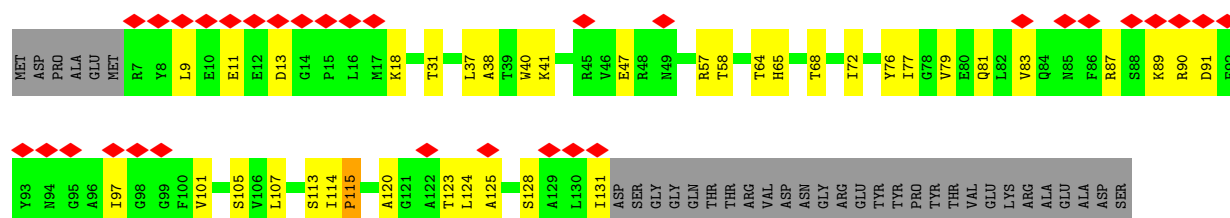
- Chain W:  71% 13% 16%

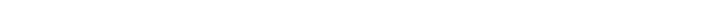


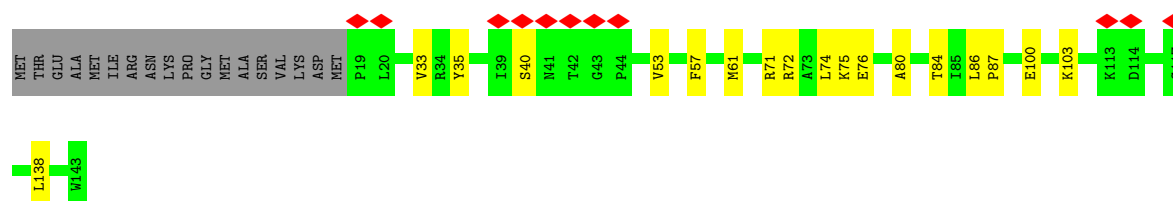
- Chain X: 

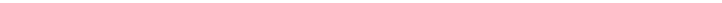


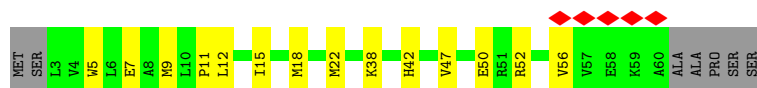
- Chain Y: 



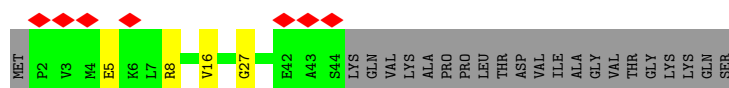
- Chain Z: 



- Chain a: 



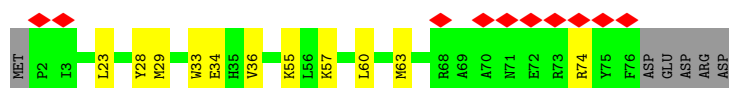
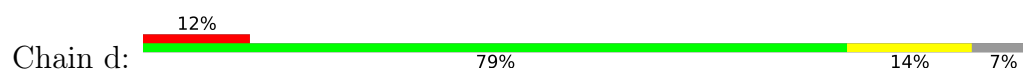
- Molecule 28: At2g46540/F11C10.23



- Molecule 29: Transmembrane protein



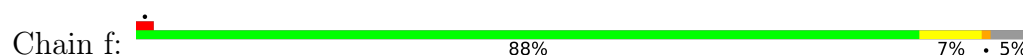
- Molecule 30: Excitatory amino acid transporter



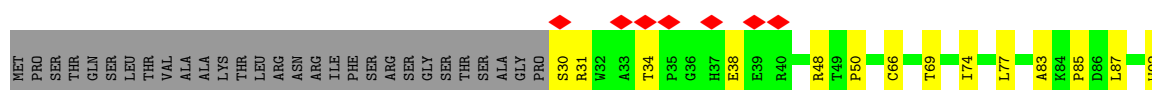
- Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5-B



- Molecule 32: At4g16450

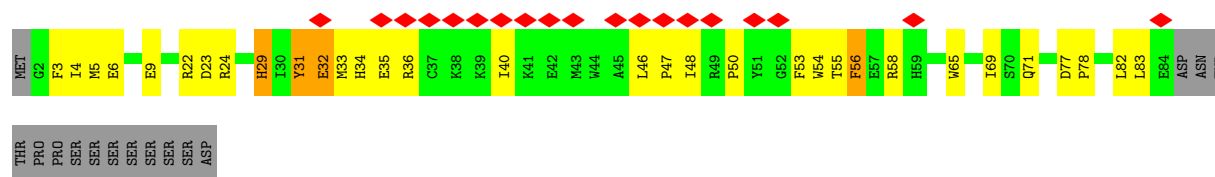


- Molecule 33: ESSS subunit of NADH:ubiquinone oxidoreductase (Complex I) protein

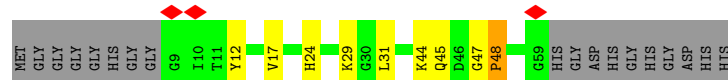




• Molecule 34: At1g67350



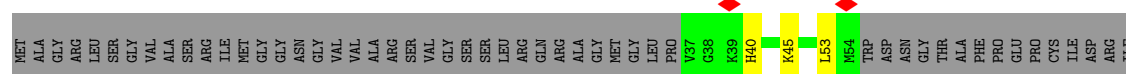
• Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2



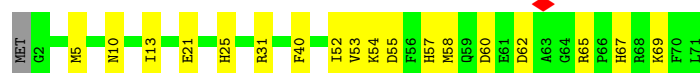
• Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3-A



• Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

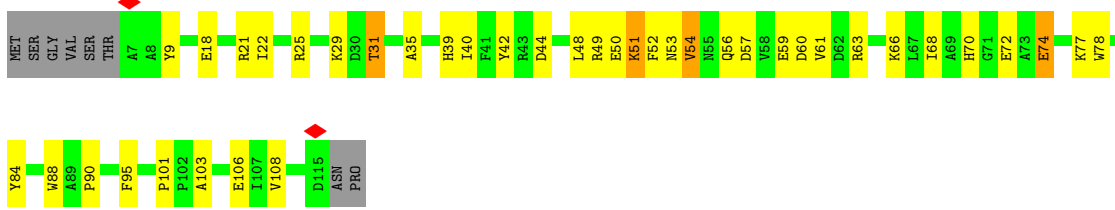


• Molecule 38: AT2G31490 protein



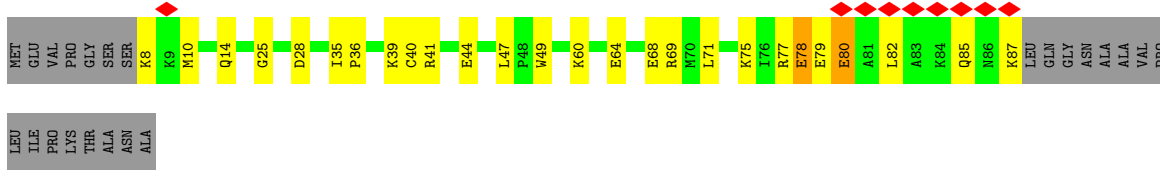
• Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

Chain n: 



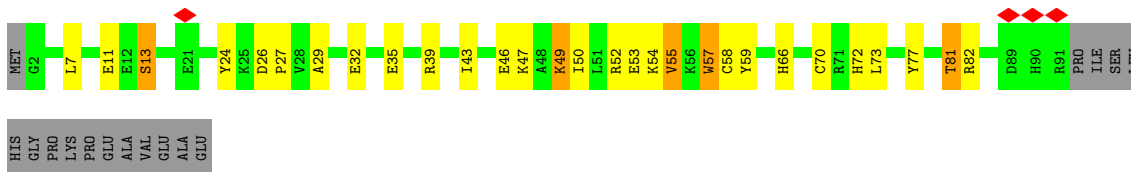
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain o: 

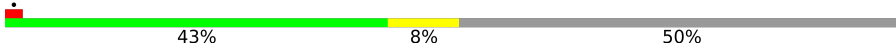


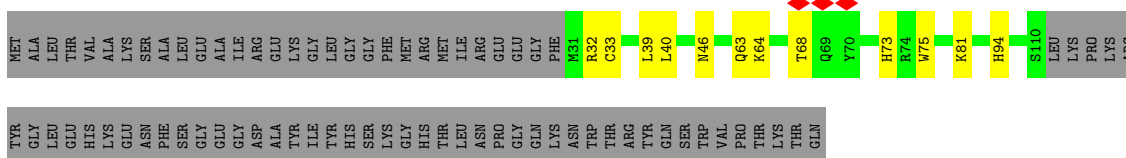
- Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10-B

Chain p: 



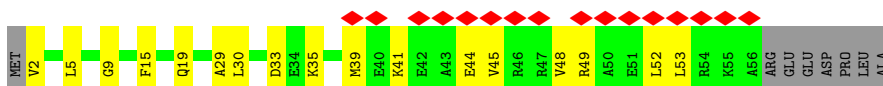
- Molecule 42: Probable NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain q: 



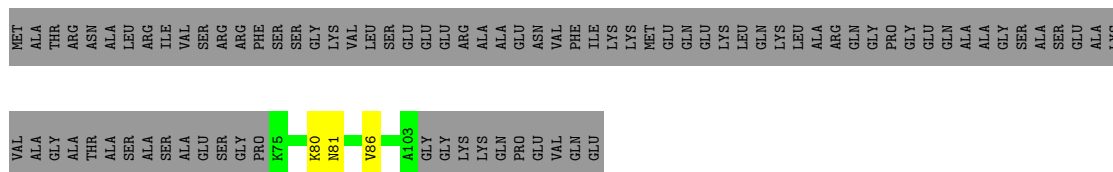
- Molecule 43: Uncharacterized protein At1g67785

Chain u: 



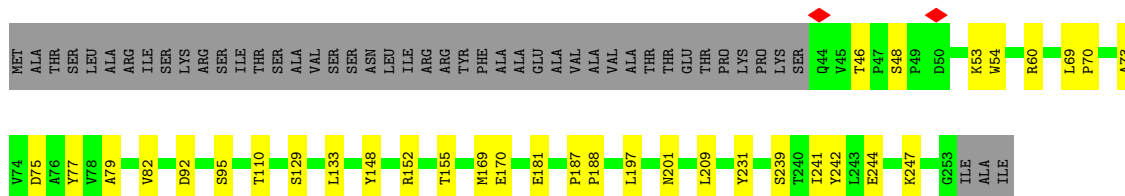
- Molecule 44: Uncharacterized protein At2g27730, mitochondrial

Chain v:  23% 74%



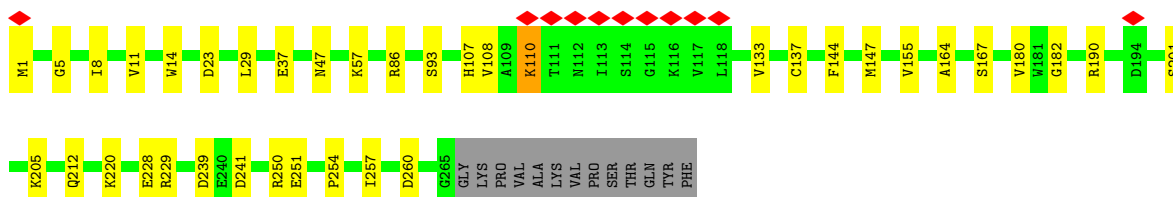
- Molecule 45: Gamma carbonic anhydrase-like 2, mitochondrial

Chain x:  69% 13% 18%



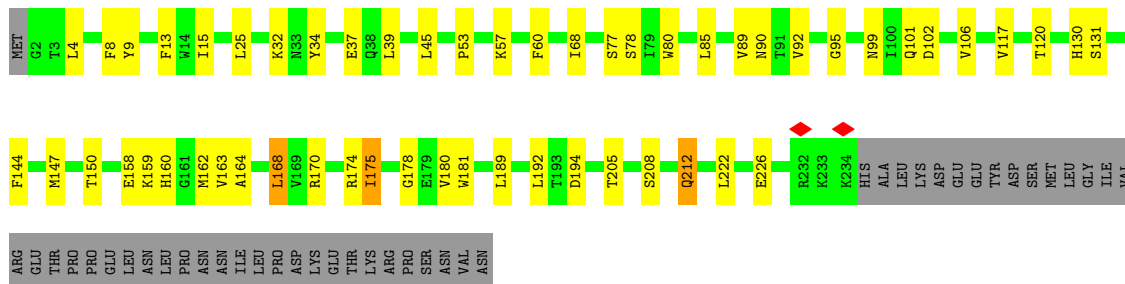
- Molecule 46: Gamma carbonic anhydrase 2, mitochondrial

Chain y:  82% 13% 5%



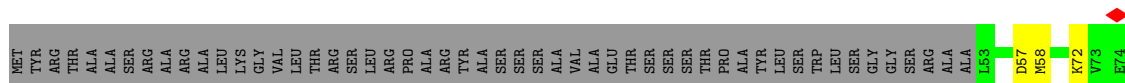
- Molecule 47: Gamma carbonic anhydrase 1, mitochondrial

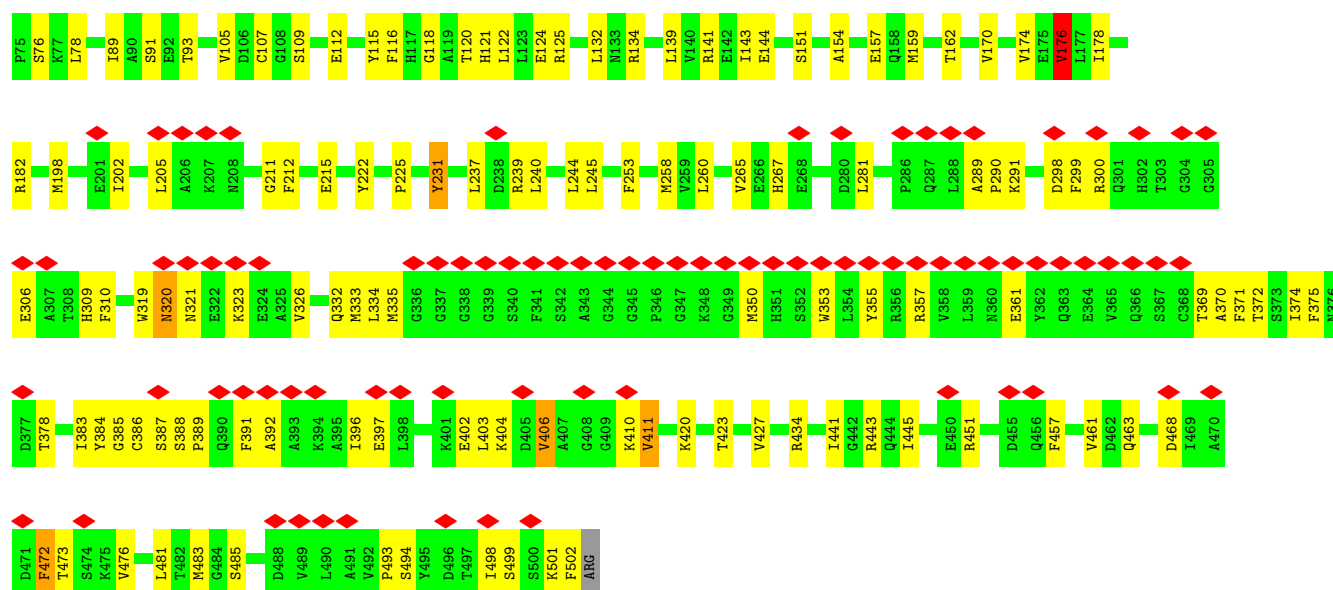
Chain z:  65% 19% 15%



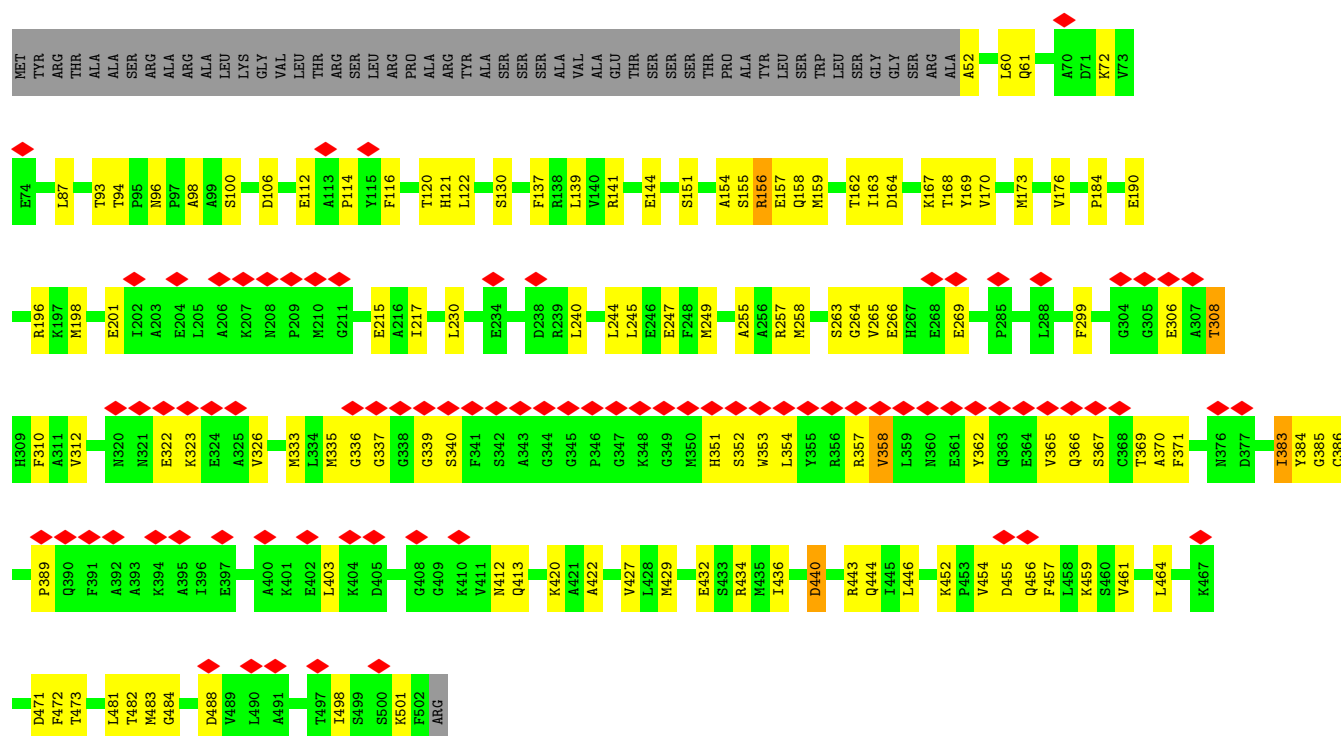
- Molecule 48: Probable mitochondrial-processing peptidase subunit alpha-1, mitochondrial

Chain AA:  17% 64% 24% 11%

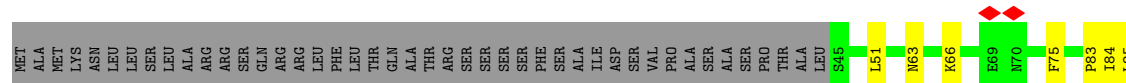
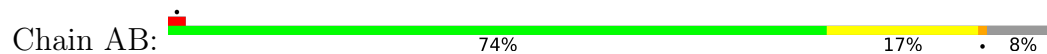


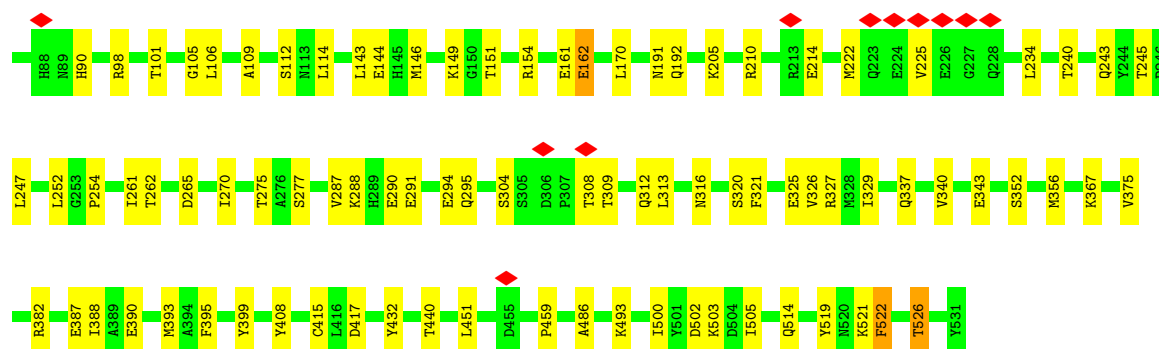


- Molecule 48: Probable mitochondrial-processing peptidase subunit alpha-1, mitochondrial



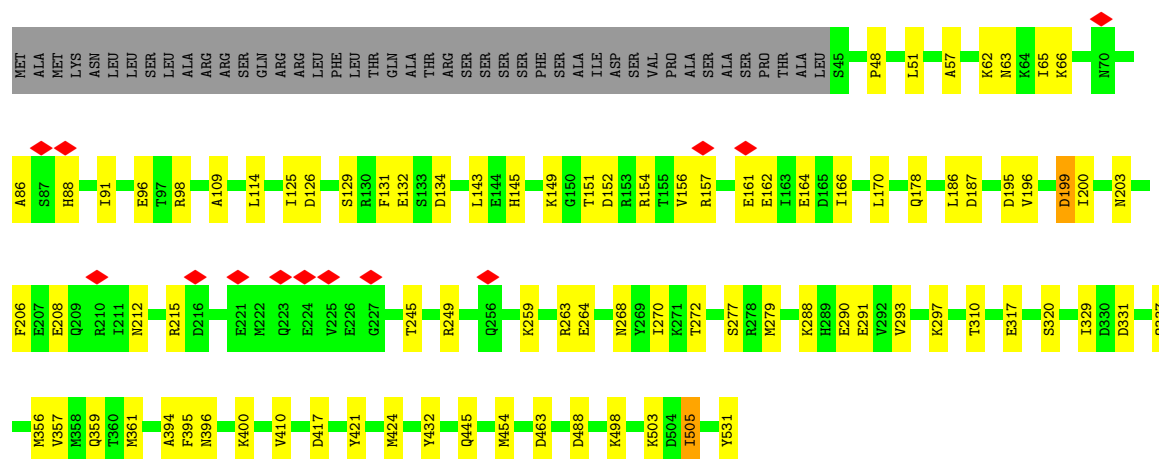
- Molecule 49: Probable mitochondrial-processing peptidase subunit beta, mitochondrial





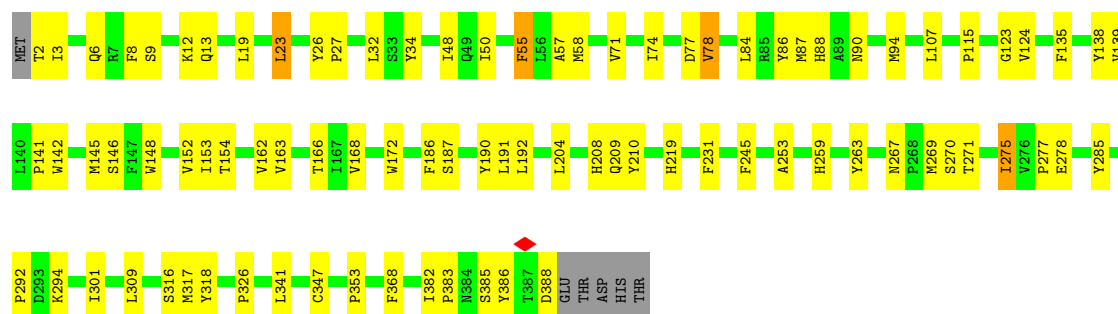
- Molecule 49: Probable mitochondrial-processing peptidase subunit beta, mitochondrial

Chain BB: 75% 16% 8%



- Molecule 50: Cytochrome b

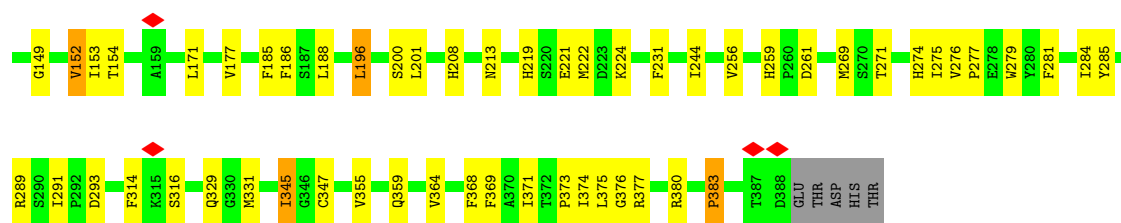
Chain AC: 76% 21% ..



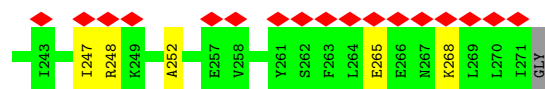
- Molecule 50: Cytochrome b

Chain BC: 76% 22% ..

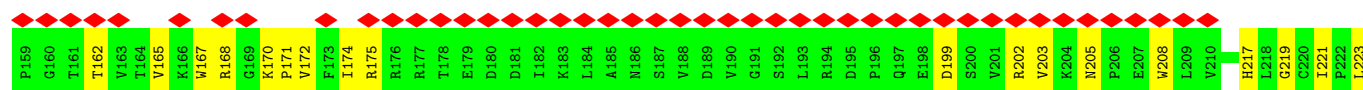
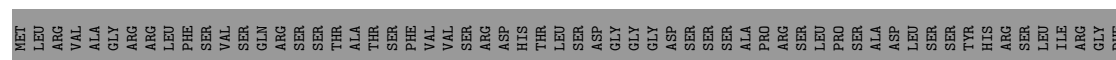




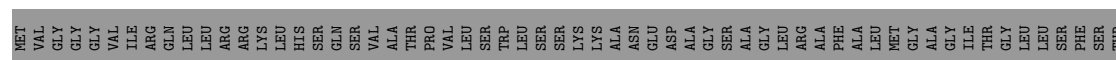
- Molecule 51: Cytochrome b-c1 complex subunit Rieske-1, mitochondrial

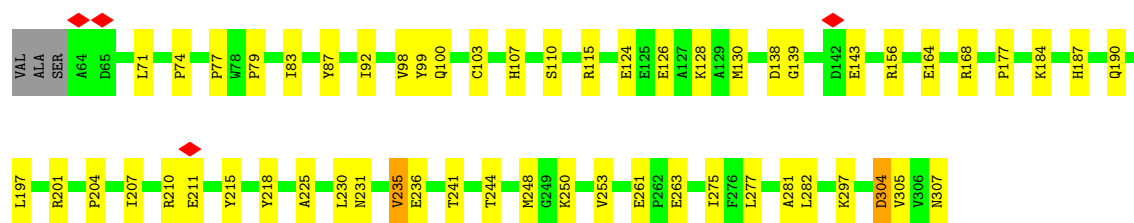


- Molecule 51: Cytochrome b-c1 complex subunit Rieske-1, mitochondrial



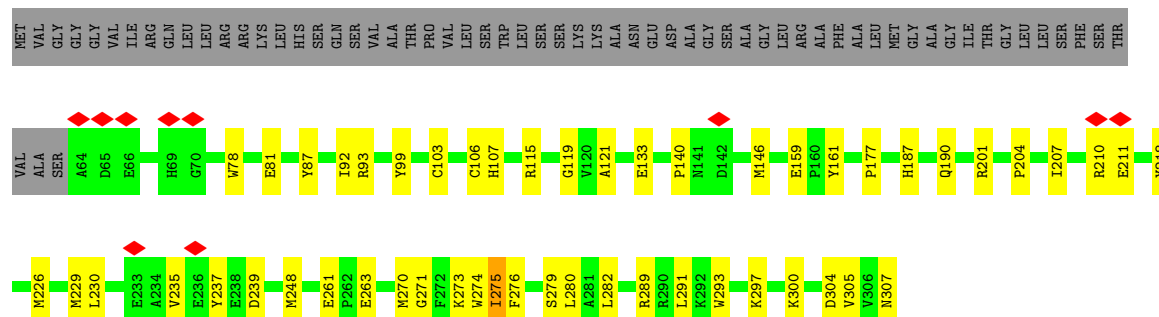
- Molecule 52: Cytochrome c1 2, heme protein, mitochondrial





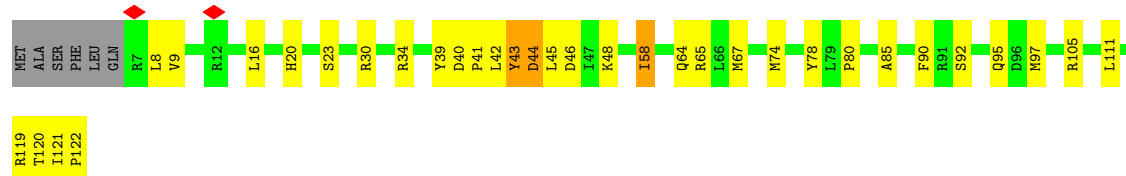
- Molecule 52: Cytochrome c1 2, heme protein, mitochondrial

Chain BE: 63% 17% 21%



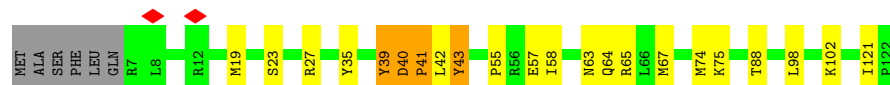
- Molecule 53: Cytochrome b-c1 complex subunit 7-2, mitochondrial

Chain AF: 67% 25% 5%



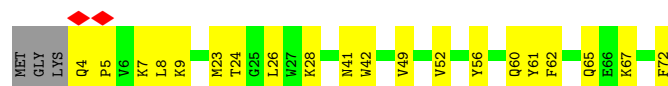
- Molecule 53: Cytochrome b-c1 complex subunit 7-2, mitochondrial

Chain BF: 77% 15% 5%



- Molecule 54: Cytochrome b-c1 complex subunit 8-1, mitochondrial

Chain AG: 68% 28% 5%



- Molecule 54: Cytochrome b-c1 complex subunit 8-1, mitochondrial

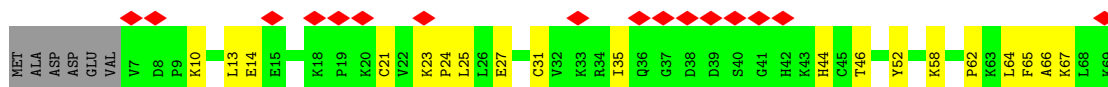
Chain BG: 76% 18% 6%



- Molecule 55: Cytochrome b-c1 complex subunit 6-1, mitochondrial



- Molecule 55: Cytochrome b-c1 complex subunit 6-1, mitochondrial



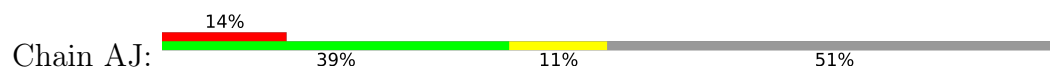
- Molecule 56: Cytochrome b-c1 complex subunit 9, mitochondrial



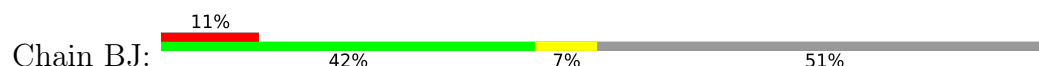
- Molecule 56: Cytochrome b-c1 complex subunit 9, mitochondrial



- Molecule 57: Cytochrome b-c1 complex subunit 10, mitochondrial



- Molecule 57: Cytochrome b-c1 complex subunit 10, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	213993	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	215000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	24.801	Depositor
Minimum map value	-12.512	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.160	Depositor
Recommended contour level	0.6	Depositor
Map size (Å)	429.75, 429.75, 429.75	wwPDB
Map dimensions	750, 750, 750	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.573, 0.573, 0.573	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UQ9, 8Q1, FE, NDP, FME, ZN, FES, HEM, Q7G, UQ7, FMN, PGT, SF4, PC7, CDL, 3PH, COO, PTY, UQ5

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	A	0.19	0/820	0.41	0/1113
2	B	0.90	6/1279 (0.5%)	0.83	0/1734
3	C	0.68	0/1590	0.75	3/2152 (0.1%)
4	D	0.75	13/3149 (0.4%)	0.73	1/4259 (0.0%)
5	E	0.79	6/1535 (0.4%)	0.78	0/2084
6	F	0.14	0/3441	0.29	0/4641
7	G	0.35	1/5338 (0.0%)	0.53	10/7231 (0.1%)
8	H	0.22	0/2609	0.41	0/3553
9	I	0.67	3/1378 (0.2%)	0.69	2/1862 (0.1%)
10	J	0.61	0/1435	0.72	0/1957
11	K	1.09	9/785 (1.1%)	1.07	5/1062 (0.5%)
12	L	0.77	13/5368 (0.2%)	0.98	15/7291 (0.2%)
13	M	0.57	2/4066 (0.0%)	0.74	5/5525 (0.1%)
14	N	0.71	9/3948 (0.2%)	0.84	7/5360 (0.1%)
15	O	0.54	1/979 (0.1%)	0.61	0/1326
16	P	0.62	2/2509 (0.1%)	0.79	3/3401 (0.1%)
17	Q	0.08	0/862	0.24	0/1166
18	R	0.43	0/585	0.59	0/793
19	S	0.51	0/739	0.61	0/996
20	T	0.77	1/671 (0.1%)	1.04	1/911 (0.1%)
21	U	0.19	0/687	0.41	0/929
22	V	0.70	2/1146 (0.2%)	0.79	0/1555
23	W	0.47	0/923	0.68	2/1249 (0.2%)
24	X	0.15	0/790	0.36	0/1060
25	Y	0.62	2/944 (0.2%)	0.70	0/1277
26	Z	0.38	0/1027	0.55	0/1392
27	a	0.22	0/481	0.38	0/646
28	b	0.16	0/320	0.39	0/434
29	c	0.48	0/637	0.60	1/860 (0.1%)
30	d	0.66	1/605 (0.2%)	0.77	0/815
31	e	0.69	0/559	0.70	0/745

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	f	0.16	0/771	0.31	0/1042
33	g	0.41	0/661	0.66	2/899 (0.2%)
34	i	0.79	3/741 (0.4%)	1.16	10/997 (1.0%)
35	j	0.60	0/433	0.90	2/592 (0.3%)
36	k	0.66	0/392	0.87	2/526 (0.4%)
37	l	0.54	0/575	0.75	1/781 (0.1%)
38	m	0.71	2/592 (0.3%)	1.03	0/793
39	n	1.00	2/938 (0.2%)	1.13	8/1273 (0.6%)
40	o	0.78	1/666 (0.2%)	1.19	5/886 (0.6%)
41	p	0.93	2/777 (0.3%)	1.23	8/1043 (0.8%)
42	q	0.25	0/690	0.38	0/936
43	u	0.13	0/472	0.22	0/632
44	v	0.13	0/222	0.29	0/300
45	x	0.67	3/1669 (0.2%)	0.62	1/2279 (0.0%)
46	y	0.52	0/2046	0.62	1/2772 (0.0%)
47	z	0.59	3/1804 (0.2%)	0.71	3/2441 (0.1%)
48	AA	0.47	1/3503 (0.0%)	0.73	7/4752 (0.1%)
48	BA	0.57	2/3508 (0.1%)	0.72	5/4759 (0.1%)
49	AB	0.46	2/3908 (0.1%)	0.61	5/5305 (0.1%)
49	BB	0.35	0/3908	0.53	2/5305 (0.0%)
50	AC	0.67	9/3208 (0.3%)	0.79	8/4395 (0.2%)
50	BC	0.67	7/3208 (0.2%)	0.83	5/4395 (0.1%)
51	AD	0.42	0/1567	0.59	0/2135
51	BD	0.49	0/1558	0.68	4/2123 (0.2%)
52	AE	0.40	0/1968	0.58	2/2672 (0.1%)
52	BE	0.45	0/1968	0.55	2/2672 (0.1%)
53	AF	0.82	5/993 (0.5%)	0.89	3/1336 (0.2%)
53	BF	0.64	3/993 (0.3%)	0.73	1/1336 (0.1%)
54	AG	0.66	1/600 (0.2%)	0.81	1/815 (0.1%)
54	BG	0.48	0/591	0.85	0/802
55	AH	0.26	0/531	0.43	0/713
55	BH	0.64	2/524 (0.4%)	0.80	1/703 (0.1%)
56	AI	0.99	4/488 (0.8%)	1.01	0/655
56	BI	0.51	0/488	0.84	2/655 (0.3%)
57	AJ	0.65	0/210	1.11	4/290 (1.4%)
57	BJ	0.23	0/212	0.39	0/291
All	All	0.58	123/98588 (0.1%)	0.72	150/133680 (0.1%)

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
1	A	0	1
14	N	0	2
All	All	0	3

All (123) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	n	51	LYS	C-O	16.00	1.42	1.24
50	AC	88	HIS	C-O	-9.50	1.13	1.24
50	AC	192	LEU	C-O	-9.23	1.15	1.24
25	Y	125	ALA	C-O	-9.15	1.13	1.24
22	V	107	ASP	C-O	-8.98	1.19	1.23
45	x	187	PRO	C-O	-8.77	1.14	1.24
50	BC	87	MET	C-O	-8.33	1.14	1.24
12	L	650	ASP	C-O	8.24	1.34	1.23
11	K	53	LEU	C-O	-8.10	1.13	1.24
54	AG	7	LYS	C-O	-8.00	1.14	1.24
53	BF	39	TYR	C-O	-7.73	1.15	1.24
15	O	42	SER	C-O	-7.71	1.14	1.24
39	n	48	LEU	C-O	7.70	1.33	1.24
22	V	129	HIS	C-O	-7.67	1.14	1.24
14	N	403	PRO	N-CD	-7.51	1.37	1.47
11	K	49	PHE	C-O	-7.44	1.15	1.24
53	BF	41	PRO	C-O	-7.34	1.14	1.24
50	AC	190	TYR	C-O	-7.27	1.15	1.24
9	I	134	PRO	C-O	-7.25	1.14	1.24
5	E	67	ASN	C-O	-7.21	1.14	1.24
12	L	484	MET	C-O	-7.15	1.15	1.24
14	N	177	LEU	C-O	-7.07	1.16	1.24
48	BA	263	SER	CA-CB	-7.02	1.43	1.53
53	BF	43	TYR	C-O	-6.96	1.16	1.24
53	AF	41	PRO	C-O	-6.94	1.15	1.24
34	i	29	HIS	C-O	-6.93	1.16	1.24
4	D	147	ARG	C-O	-6.85	1.16	1.24
2	B	147	PRO	C-O	-6.82	1.16	1.23
40	o	25	GLY	C-O	-6.81	1.16	1.24
50	AC	263	TYR	C-O	-6.59	1.15	1.24
4	D	63	ALA	C-O	-6.53	1.15	1.24
2	B	166	HIS	C-O	-6.53	1.15	1.24
56	AI	63	SER	CA-CB	-6.52	1.43	1.53
49	AB	340	VAL	C-O	-6.44	1.17	1.24
11	K	51	VAL	C-O	-6.41	1.17	1.24
4	D	65	PRO	C-O	-6.38	1.15	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	AF	58	ILE	C-O	-6.37	1.17	1.24
5	E	73	VAL	C-O	-6.33	1.16	1.24
4	D	66	TYR	C-O	-6.33	1.16	1.24
50	AC	58	MET	C-O	-6.33	1.16	1.24
56	AI	63	SER	C-O	-6.27	1.16	1.24
53	AF	43	TYR	C-O	-6.26	1.16	1.24
50	AC	57	ALA	C-O	-6.26	1.16	1.24
50	BC	188	LEU	C-O	-6.26	1.16	1.24
5	E	43	PRO	C-O	-6.25	1.16	1.24
45	x	188	PRO	C-O	-6.25	1.15	1.23
4	D	141	LEU	C-O	-6.24	1.16	1.24
2	B	180	PRO	C-O	-6.22	1.16	1.23
47	z	15	ILE	C-O	-6.18	1.17	1.24
14	N	474	PHE	C-O	-6.13	1.17	1.24
11	K	5	LYS	C-O	-6.01	1.17	1.24
14	N	394	THR	C-O	-6.00	1.17	1.24
9	I	161	LYS	C-O	-5.97	1.16	1.24
4	D	159	ARG	C-O	-5.95	1.18	1.24
14	N	178	LYS	C-O	-5.93	1.17	1.24
5	E	39	PRO	C-O	-5.85	1.16	1.24
14	N	391	PHE	C-O	-5.83	1.17	1.24
5	E	66	SER	C-O	-5.83	1.16	1.24
11	K	97	SER	C-O	-5.83	1.16	1.24
50	BC	141	PRO	C-O	-5.82	1.16	1.24
4	D	155	ALA	C-O	-5.80	1.17	1.24
38	m	40	PHE	C-O	-5.80	1.16	1.24
11	K	46	PHE	C-O	-5.79	1.17	1.24
9	I	167	PHE	C-O	-5.78	1.17	1.24
47	z	9	TYR	C-O	-5.75	1.17	1.24
4	D	158	ILE	C-O	-5.71	1.17	1.24
34	i	24	ARG	N-CA	5.71	1.53	1.46
11	K	55	ASP	C-O	-5.69	1.17	1.23
50	BC	95	PHE	C-O	-5.67	1.17	1.24
53	AF	80	PRO	C-O	-5.67	1.16	1.23
14	N	230	ILE	C-O	-5.67	1.17	1.24
2	B	202	LEU	C-O	-5.63	1.17	1.24
50	AC	187	SER	C-O	-5.63	1.17	1.24
4	D	99	GLN	C-O	-5.62	1.17	1.24
56	AI	17	TYR	C-O	-5.60	1.17	1.24
2	B	119	PRO	C-O	-5.58	1.16	1.24
12	L	622	TYR	C-O	-5.53	1.17	1.24
5	E	70	GLN	C-O	-5.51	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	M	482	HIS	C-O	-5.51	1.17	1.24
14	N	447	MET	C-O	-5.50	1.17	1.24
14	N	179	TYR	C-O	-5.49	1.17	1.24
41	p	13	SER	CA-CB	-5.49	1.45	1.53
2	B	205	LYS	C-O	-5.47	1.17	1.24
56	AI	61	ASP	C-O	-5.44	1.16	1.23
25	Y	115	PRO	N-CD	-5.44	1.40	1.47
11	K	96	ASN	C-O	-5.41	1.16	1.24
12	L	502	LYS	C-O	-5.40	1.17	1.24
50	BC	88	HIS	C-O	-5.35	1.18	1.24
30	d	23	LEU	C-O	-5.34	1.17	1.24
50	BC	185	PHE	C-O	-5.34	1.17	1.24
50	BC	196	LEU	C-O	-5.34	1.17	1.24
49	AB	321	PHE	C-O	-5.32	1.17	1.23
12	L	404	ILE	C-O	-5.30	1.18	1.24
12	L	538	VAL	C-N	-5.30	1.26	1.33
48	AA	132	LEU	C-O	-5.28	1.17	1.24
16	P	98	PRO	C-O	-5.27	1.17	1.23
50	AC	141	PRO	C-O	-5.27	1.17	1.24
12	L	155	PHE	C-O	-5.25	1.17	1.24
12	L	156	THR	C-O	-5.25	1.17	1.24
12	L	349	PHE	C-O	-5.25	1.17	1.24
53	AF	85	ALA	C-O	-5.23	1.17	1.24
4	D	87	GLU	C-O	-5.22	1.18	1.24
12	L	347	LEU	C-O	-5.21	1.18	1.24
12	L	501	PRO	C-O	-5.21	1.17	1.24
50	AC	191	LEU	C-O	-5.20	1.18	1.24
20	T	42	SER	CA-CB	-5.20	1.44	1.53
12	L	460	PRO	C-O	-5.20	1.17	1.23
55	BH	62	PRO	C-O	-5.18	1.17	1.24
7	G	147	ASP	C-O	-5.18	1.16	1.24
45	x	201	ASN	C-O	-5.17	1.18	1.24
12	L	462	PRO	C-O	-5.15	1.17	1.24
34	i	32	GLU	C-O	-5.12	1.17	1.24
47	z	131	SER	C-O	-5.12	1.16	1.23
48	BA	163	ILE	C-O	-5.12	1.18	1.24
4	D	157	PHE	C-O	-5.08	1.17	1.24
13	M	448	LYS	C-O	-5.08	1.18	1.24
55	BH	66	ALA	C-O	-5.08	1.17	1.24
38	m	53	VAL	C-O	-5.06	1.18	1.24
4	D	62	GLN	C-O	-5.05	1.17	1.24
11	K	52	SER	C-O	-5.04	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	P	287	VAL	C-O	-5.04	1.18	1.24
4	D	164	ALA	C-O	-5.02	1.18	1.24
41	p	54	LYS	N-CA	5.00	1.52	1.46

All (150) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	191	ASP	CB-CA-C	-12.13	89.52	109.53
34	i	32	GLU	CA-C-N	-11.27	101.92	122.09
34	i	32	GLU	C-N-CA	-11.27	101.92	122.09
12	L	70	PHE	CB-CA-C	10.93	125.90	110.16
40	o	79	GLU	N-CA-C	-10.50	101.52	114.75
51	BD	175	ARG	CB-CA-C	-9.54	98.92	111.42
12	L	650	ASP	CB-CA-C	-8.83	90.92	109.38
14	N	286	TYR	N-CA-C	-8.77	102.38	113.43
16	P	124	ASP	CA-CB-CG	8.46	121.06	112.60
48	AA	463	GLN	N-CA-C	-8.42	101.04	114.09
40	o	80	GLU	N-CA-C	-7.73	102.79	111.14
40	o	78	GLU	CB-CA-C	-7.54	99.37	111.06
33	g	50	PRO	N-CD-CG	-7.53	91.90	103.20
4	D	11	PHE	CA-CB-CG	7.53	121.33	113.80
12	L	344	PHE	CA-CB-CG	7.46	121.27	113.80
53	AF	40	ASP	CB-CA-C	7.42	118.44	109.31
50	BC	96	PHE	CA-C-O	-7.40	112.70	120.55
50	BC	96	PHE	CB-CA-C	7.36	123.01	110.79
57	AJ	38	VAL	N-CA-C	-7.31	99.27	109.21
53	BF	40	ASP	CA-CB-CG	7.25	119.85	112.60
14	N	286	TYR	CB-CA-C	7.13	121.62	109.65
12	L	540	ASP	CB-CA-C	7.06	121.89	109.75
37	l	116	ASN	CB-CA-C	7.02	121.70	111.73
49	AB	522	PHE	CA-CB-CG	6.85	120.65	113.80
33	g	50	PRO	CA-CB-CG	-6.73	91.71	104.50
14	N	285	SER	N-CA-C	6.73	119.05	107.28
39	n	50	GLU	O-C-N	-6.71	115.01	122.12
34	i	23	ASP	O-C-N	-6.61	114.14	122.27
35	j	29	LYS	CA-C-O	-6.60	113.83	120.90
23	W	98	HIS	N-CA-CB	-6.55	101.51	110.56
16	P	289	THR	CB-CA-C	6.47	121.15	109.83
7	G	484	HIS	CB-CA-C	6.44	120.85	110.29
47	z	205	THR	CB-CA-C	6.43	121.07	110.90
39	n	54	VAL	CA-C-N	-6.42	110.75	122.38
39	n	54	VAL	C-N-CA	-6.42	110.75	122.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	AE	304	ASP	CA-CB-CG	6.42	119.02	112.60
48	AA	323	LYS	N-CA-C	-6.39	106.11	114.04
50	BC	152	VAL	N-CA-C	6.38	116.52	110.53
7	G	473	GLY	CA-C-N	6.34	124.29	119.66
7	G	473	GLY	C-N-CA	6.34	124.29	119.66
34	i	31	TYR	N-CA-C	-6.29	104.50	111.36
13	M	68	PHE	N-CA-C	-6.28	105.20	112.86
46	y	144	PHE	CA-CB-CG	6.27	120.07	113.80
39	n	51	LYS	CA-C-N	-6.25	111.90	120.28
39	n	51	LYS	C-N-CA	-6.25	111.90	120.28
12	L	580	PHE	O-C-N	6.25	128.51	122.07
57	AJ	40	PRO	N-CA-CB	-6.23	98.64	102.81
7	G	190	SER	N-CA-CB	6.19	119.54	110.25
51	BD	114	PHE	CB-CA-C	6.15	121.14	110.68
12	L	343	PHE	CA-C-O	-6.09	114.41	120.80
34	i	24	ARG	N-CA-C	6.08	118.82	111.40
34	i	24	ARG	CB-CA-C	-6.05	100.62	110.79
48	AA	472	PHE	CA-CB-CG	6.02	119.82	113.80
11	K	6	TYR	CA-C-O	-6.01	114.18	120.55
7	G	189	GLY	CA-C-N	-6.00	111.17	122.27
7	G	189	GLY	C-N-CA	-6.00	111.17	122.27
41	p	43	ILE	CA-C-O	-5.90	114.81	120.95
41	p	55	VAL	CA-C-O	-5.87	114.95	121.17
48	AA	320	ASN	O-C-N	-5.86	115.60	122.81
40	o	79	GLU	CB-CA-C	5.85	116.71	109.16
3	C	29	ASN	N-CA-CB	5.83	118.55	109.97
36	k	4	PRO	N-CA-CB	5.83	109.42	103.00
16	P	296	ILE	N-CA-C	-5.79	104.72	110.62
52	BE	271	GLY	CA-C-O	-5.73	114.85	120.75
48	BA	164	ASP	CA-CB-CG	5.73	118.33	112.60
47	z	101	GLN	N-CA-C	5.73	117.46	110.41
12	L	539	ALA	N-CA-C	-5.72	98.94	108.32
52	BE	275	ILE	CB-CA-C	5.70	120.09	112.22
50	AC	86	TYR	CA-C-N	5.70	128.19	120.44
50	AC	86	TYR	C-N-CA	5.70	128.19	120.44
48	BA	114	PRO	CA-N-CD	-5.68	103.54	111.50
39	n	31	THR	CB-CA-C	5.68	120.21	110.79
50	AC	86	TYR	CB-CA-C	5.67	121.13	110.63
50	AC	86	TYR	CA-C-O	-5.65	113.71	120.10
53	AF	44	ASP	CA-CB-CG	5.65	118.25	112.60
13	M	301	GLN	CB-CA-C	5.64	118.83	109.53
39	n	54	VAL	O-C-N	5.60	127.30	121.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	L	564	PHE	CA-CB-CG	5.58	119.39	113.80
12	L	459	ALA	N-CA-C	5.56	117.48	109.48
20	T	49	ARG	CB-CG-CD	-5.56	98.52	111.30
55	BH	65	PHE	CB-CA-C	5.53	121.88	110.31
12	L	196	THR	CB-CA-C	5.52	119.62	110.90
41	p	57	TRP	CA-C-O	-5.51	114.58	120.42
39	n	74	GLU	CA-C-O	-5.51	115.03	120.82
56	BI	43	ASP	CA-C-O	-5.50	114.69	120.63
49	AB	519	TYR	CA-C-O	-5.47	114.76	120.55
41	p	55	VAL	O-C-N	5.46	127.26	121.91
14	N	287	GLY	N-CA-C	5.45	126.09	113.18
49	BB	199	ASP	CB-CA-C	-5.42	101.64	110.85
48	BA	156	ARG	CA-C-O	-5.41	113.98	120.10
12	L	176	PHE	CA-CB-CG	5.40	119.20	113.80
48	AA	326	VAL	N-CA-CB	-5.39	104.24	110.55
11	K	3	LEU	CA-C-O	-5.39	114.84	120.55
9	I	190	HIS	CA-CB-CG	5.37	119.17	113.80
50	AC	71	VAL	O-C-N	5.37	127.48	121.90
51	BD	115	VAL	N-CA-C	-5.36	105.31	110.72
3	C	58	ASP	N-CA-C	5.36	116.28	108.14
3	C	156	ARG	CG-CD-NE	-5.36	100.21	112.00
29	c	86	LYS	N-CA-CB	-5.36	102.25	110.44
48	BA	114	PRO	N-CD-CG	-5.35	97.38	103.80
40	o	28	ASP	CA-CB-CG	5.34	117.94	112.60
50	AC	55	PHE	CB-CA-C	5.34	119.93	110.85
11	K	45	ASN	O-C-N	-5.33	116.55	122.09
41	p	81	THR	CB-CA-C	5.31	121.09	109.99
50	AC	84	LEU	CA-C-O	-5.30	115.25	120.82
47	z	99	ASN	CA-CB-CG	5.30	117.90	112.60
45	x	188	PRO	CB-CA-C	5.28	118.34	111.64
12	L	324	PHE	CA-CB-CG	5.27	119.07	113.80
49	AB	162	GLU	CB-CA-C	-5.27	101.73	110.68
35	j	48	PRO	N-CA-C	-5.26	106.54	113.65
23	W	98	HIS	CA-CB-CG	-5.26	108.54	113.80
41	p	59	TYR	CA-C-O	-5.23	115.31	121.07
36	k	4	PRO	N-CA-C	-5.22	99.04	112.10
50	AC	87	MET	CA-C-O	-5.21	115.34	120.70
41	p	46	GLU	CB-CA-C	5.20	120.25	110.63
13	M	294	THR	CA-C-O	-5.19	115.05	120.55
7	G	704	PRO	N-CD-CG	-5.18	95.42	103.20
7	G	190	SER	O-C-N	5.17	129.63	122.08
34	i	4	ILE	O-C-N	5.16	127.27	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	AB	161	GLU	CA-C-O	-5.16	115.40	120.82
14	N	420	CYS	N-CA-C	-5.16	106.82	113.01
57	AJ	38	VAL	CA-C-O	-5.15	114.98	121.11
49	BB	152	ASP	CB-CA-C	5.15	118.89	110.96
48	AA	468	ASP	CB-CA-C	5.15	118.93	110.95
51	BD	117	SER	N-CA-C	-5.15	105.75	111.36
9	I	167	PHE	O-C-N	5.14	127.57	122.12
12	L	35	CYS	CA-C-O	-5.09	115.13	120.63
14	N	286	TYR	N-CA-CB	5.09	119.16	110.51
12	L	521	PRO	CB-CA-C	5.08	121.78	113.20
53	AF	39	TYR	CB-CA-C	5.08	118.62	110.29
34	i	23	ASP	CA-C-N	5.07	129.18	120.71
34	i	23	ASP	C-N-CA	5.07	129.18	120.71
12	L	33	THR	CB-CA-C	5.07	119.46	110.85
48	BA	440	ASP	CA-CB-CG	5.06	117.66	112.60
52	AE	235	VAL	CA-C-O	-5.04	116.52	121.67
57	AJ	39	GLN	CB-CA-C	5.04	120.50	111.12
13	M	68	PHE	CA-C-N	-5.04	113.33	120.69
13	M	68	PHE	C-N-CA	-5.04	113.33	120.69
50	BC	83	LEU	CA-C-O	-5.04	115.08	120.42
34	i	56	PHE	CA-CB-CG	5.03	118.83	113.80
11	K	45	ASN	CA-C-N	5.02	126.96	120.44
11	K	45	ASN	C-N-CA	5.02	126.96	120.44
54	AG	7	LYS	CB-CA-C	5.02	118.81	110.78
56	BI	27	TYR	CA-C-O	-5.02	115.21	120.63
49	AB	519	TYR	O-C-N	5.01	127.43	122.12
50	BC	383	PRO	N-CD-CG	-5.01	95.69	103.20
7	G	147	ASP	CB-CA-C	5.00	119.06	110.85
14	N	223	SER	N-CA-CB	5.00	117.78	109.88
41	p	50	ILE	CA-C-O	-5.00	115.87	121.17
48	AA	176	VAL	CA-C-O	-5.00	115.75	120.95

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	FME	Mainchain
14	N	411	PHE	Mainchain
14	N	412[B]	TYR	Mainchain

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	A	802	0	817	34	0
2	B	1244	0	1231	45	0
3	C	1545	0	1501	50	0
4	D	3079	0	3049	93	0
5	E	1500	0	1473	24	0
6	F	3368	0	3355	72	0
7	G	5243	0	5228	79	0
8	H	2536	0	2641	124	0
9	I	1349	0	1293	38	0
10	J	1399	0	1472	46	0
11	K	784	0	843	36	0
12	L	5222	0	5251	145	0
13	M	3952	0	4092	180	0
14	N	3839	0	3941	111	0
15	O	963	0	975	22	0
16	P	2453	0	2493	53	0
17	Q	837	0	818	26	0
18	R	571	0	559	12	0
19	S	727	0	759	21	0
20	T	659	0	644	37	0
21	U	677	0	665	27	0
22	V	1123	0	1112	19	0
23	W	904	0	901	22	0
24	X	776	0	775	13	0
25	Y	928	0	960	62	0
26	Z	997	0	979	18	0
27	a	469	0	472	11	0
28	b	315	0	338	3	0
29	c	617	0	619	18	0
30	d	592	0	610	13	0
31	e	546	0	510	11	0
32	f	765	0	766	8	0
33	g	641	0	632	24	0
34	i	721	0	695	53	0
35	j	415	0	406	7	0
36	k	382	0	380	16	0
37	l	562	0	567	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	m	577	0	564	16	0
39	n	911	0	879	46	0
40	o	657	0	669	25	0
41	p	757	0	745	39	0
42	q	669	0	630	11	0
43	u	463	0	471	73	0
44	v	219	0	227	8	0
45	x	1629	0	1636	38	0
46	y	2013	0	2024	47	0
47	z	1772	0	1771	59	0
48	AA	3431	0	3416	101	0
48	BA	3436	0	3421	89	0
49	AB	3834	0	3797	97	0
49	BB	3834	0	3797	93	0
50	AC	3093	0	3074	92	0
50	BC	3093	0	3074	115	0
51	AD	1528	0	1529	35	0
51	BD	1519	0	1523	50	0
52	AE	1917	0	1844	52	0
52	BE	1917	0	1844	51	0
53	AF	976	0	1001	40	0
53	BF	976	0	1001	41	0
54	AG	581	0	588	25	0
54	BG	572	0	582	28	0
55	AH	518	0	518	100	0
55	BH	511	0	511	11	0
56	AI	476	0	469	13	0
56	BI	476	0	469	14	0
57	AJ	203	0	197	13	0
57	BJ	205	0	203	12	0
58	A	51	0	78	7	0
58	AC	92	0	133	8	0
58	AF	51	0	78	9	0
58	BC	37	0	47	2	0
58	L	132	0	183	7	0
58	M	29	0	28	1	0
58	y	41	0	52	8	0
59	B	8	0	0	1	0
59	F	8	0	0	1	0
59	G	16	0	0	0	0
59	I	16	0	0	2	0
60	AB	41	0	58	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	BB	29	0	31	1	0
60	BF	40	0	56	16	0
60	D	50	0	79	13	0
60	L	42	0	60	2	0
60	M	87	0	126	4	0
60	N	135	0	201	9	0
60	Y	31	0	35	0	0
60	d	39	0	51	3	0
60	m	50	0	79	0	0
60	z	50	0	79	12	0
61	AD	4	0	0	0	0
61	BD	4	0	0	1	0
61	E	4	0	0	1	0
61	G	4	0	0	1	0
62	F	31	0	19	0	0
63	H	35	0	43	6	0
64	BC	78	0	0	0	0
64	H	81	0	0	3	0
64	K	81	0	0	1	0
64	M	39	0	0	0	0
64	a	39	0	0	0	0
65	AC	33	0	39	2	0
65	AI	32	0	37	3	0
65	BC	44	0	64	6	0
65	BJ	89	0	133	2	0
65	L	37	0	47	4	0
65	M	41	0	58	15	0
65	Y	33	0	39	2	0
65	f	84	0	120	5	0
65	l	37	0	47	0	0
66	AB	34	0	42	1	0
66	AC	51	0	79	3	0
66	AG	52	0	84	6	0
66	BC	41	0	56	3	0
66	BD	39	0	52	3	0
66	L	40	0	54	6	0
66	d	52	0	84	8	0
66	f	48	0	73	1	0
66	v	52	0	84	7	0
67	AC	76	0	100	10	0
67	BC	38	0	50	8	0
67	L	38	0	50	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
68	O	1	0	0	0	0
69	P	48	0	26	0	0
70	AB	1	0	0	0	0
70	BB	1	0	0	0	0
70	R	1	0	0	0	0
70	y	1	0	0	0	0
71	T	35	0	0	0	0
71	W	35	0	0	0	0
72	AC	166	0	232	15	0
72	AE	85	0	120	4	0
72	BC	158	0	210	9	0
72	BE	88	0	123	6	0
72	BG	70	0	87	6	0
72	u	200	0	312	25	0
73	y	53	0	37	5	0
74	AC	86	0	60	3	0
74	AE	43	0	30	4	0
74	BC	86	0	60	1	0
74	BE	43	0	30	6	0
75	BC	48	0	66	11	0
76	A	20	0	0	3	0
76	AA	43	0	0	2	0
76	AB	259	0	0	11	0
76	AC	187	0	0	25	0
76	AD	60	0	0	1	0
76	AE	171	0	0	13	0
76	AF	109	0	0	8	0
76	AG	25	0	0	7	0
76	AH	13	0	0	1	0
76	AI	20	0	0	2	0
76	B	84	0	0	6	0
76	BA	77	0	0	5	0
76	BB	260	0	0	17	0
76	BC	148	0	0	21	0
76	BD	43	0	0	5	0
76	BE	118	0	0	8	0
76	BF	71	0	0	5	0
76	BG	19	0	0	2	0
76	BH	2	0	0	2	0
76	BI	14	0	0	6	0
76	BJ	1	0	0	0	0
76	C	104	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
76	D	226	0	0	24	0
76	E	89	0	0	3	0
76	F	152	0	0	18	0
76	G	313	0	0	8	0
76	H	129	0	0	35	0
76	I	102	0	0	11	0
76	J	64	0	0	14	0
76	K	49	0	0	16	0
76	L	213	0	0	23	0
76	M	158	0	0	29	0
76	N	201	0	0	25	0
76	O	88	0	0	2	0
76	P	44	0	0	7	0
76	Q	22	0	0	1	0
76	R	44	0	0	4	0
76	S	17	0	0	8	0
76	T	13	0	0	2	0
76	U	3	0	0	1	0
76	V	31	0	0	4	0
76	W	10	0	0	1	0
76	X	19	0	0	1	0
76	Y	5	0	0	2	0
76	Z	53	0	0	2	0
76	a	19	0	0	2	0
76	b	2	0	0	0	0
76	c	30	0	0	3	0
76	d	21	0	0	3	0
76	e	30	0	0	2	0
76	f	49	0	0	2	0
76	g	29	0	0	7	0
76	i	26	0	0	8	0
76	j	3	0	0	1	0
76	k	10	0	0	0	0
76	l	25	0	0	0	0
76	m	24	0	0	2	0
76	n	52	0	0	17	0
76	o	50	0	0	6	0
76	p	52	0	0	11	0
76	q	31	0	0	2	0
76	u	10	0	0	0	0
76	v	10	0	0	3	0
76	x	180	0	0	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
76	y	167	0	0	11	0
76	z	121	0	0	20	0
All	All	104814	0	100597	2566	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 13.

All (2566) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:15:PHE:CD2	8:H:212:LEU:HD13	1.18	1.68
46:y:133:VAL:HG11	47:z:147:MET:CE	1.14	1.57
25:Y:9:LEU:CD1	55:AH:20:LYS:HB2	1.10	1.55
43:u:53:LEU:CD2	55:AH:19:PRO:HG3	1.38	1.54
34:i:34:HIS:CE1	41:p:27:PRO:CG	1.93	1.51
34:i:34:HIS:HE1	41:p:27:PRO:CB	1.21	1.49
25:Y:9:LEU:HD13	55:AH:20:LYS:CB	1.03	1.47
34:i:34:HIS:CE1	41:p:27:PRO:CB	2.00	1.45
46:y:133:VAL:CG1	47:z:147:MET:HE1	1.49	1.42
49:AB:493:LYS:NZ	57:AJ:18:ILE:HD11	1.10	1.42
43:u:53:LEU:CD2	55:AH:19:PRO:CG	1.97	1.40
43:u:53:LEU:HD21	55:AH:19:PRO:CG	1.51	1.40
12:L:243:PRO:O	12:L:309:ARG:NH1	1.56	1.35
34:i:34:HIS:CE1	41:p:27:PRO:HG2	1.58	1.35
49:AB:493:LYS:NZ	57:AJ:18:ILE:CD1	1.89	1.35
34:i:34:HIS:ND1	41:p:27:PRO:HG2	1.04	1.33
4:D:15:PHE:CD2	8:H:212:LEU:CD1	2.10	1.33
25:Y:9:LEU:HD22	55:AH:20:LYS:CE	1.55	1.32
13:M:64:ALA:HB3	41:p:35:GLU:OE1	1.21	1.32
4:D:15:PHE:HD2	8:H:212:LEU:CD1	1.40	1.31
12:L:262:VAL:HB	76:L:961:HOH:O	1.30	1.30
4:D:372:HIS:HE1	76:D:619:HOH:O	1.15	1.30
13:M:194:GLN:OE1	13:M:212:ARG:CD	1.82	1.26
12:L:451:ARG:NH2	76:L:801:HOH:O	1.69	1.26
25:Y:9:LEU:CD2	55:AH:20:LYS:HE2	1.67	1.25
39:n:59:GLU:HG2	76:n:231:HOH:O	1.17	1.25
3:C:57:ILE:HA	76:D:578:HOH:O	1.31	1.24
46:y:133:VAL:CG1	47:z:147:MET:CE	2.08	1.24
43:u:49:ARG:CA	55:AH:22:VAL:HG21	1.68	1.24
4:D:15:PHE:CE2	8:H:212:LEU:HB3	1.73	1.23
43:u:53:LEU:HG	55:AH:19:PRO:CB	1.66	1.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:e:56:ARG:HD3	76:e:128:HOH:O	1.35	1.23
23:W:120:LYS:HD3	23:W:124:LEU:CD2	1.67	1.22
43:u:45:VAL:O	55:AH:22:VAL:HG11	1.32	1.22
6:F:77:LYS:HZ2	6:F:81:LYS:CE	1.51	1.22
3:C:132:ILE:HG12	76:C:266:HOH:O	1.40	1.21
34:i:34:HIS:ND1	41:p:27:PRO:CG	1.94	1.20
48:AA:441:ILE:HG12	48:AA:451:ARG:NH1	1.54	1.20
2:B:202:LEU:HA	76:B:667:HOH:O	1.38	1.20
50:BC:316:SER:HB2	76:BC:574:HOH:O	1.38	1.20
14:N:254:TYR:HA	76:N:644:HOH:O	1.38	1.19
53:BF:27:ARG:NE	60:BF:201:PTY:HC31	1.54	1.19
53:BF:27:ARG:HE	60:BF:201:PTY:C3	1.56	1.19
13:M:194:GLN:OE1	13:M:212:ARG:HD2	1.35	1.18
25:Y:9:LEU:HD22	55:AH:20:LYS:CD	1.72	1.17
9:I:159:MET:HA	76:I:692:HOH:O	1.44	1.17
49:AB:329:ILE:HG21	54:AG:8:LEU:HD11	1.21	1.17
8:H:232:GLU:HB3	76:H:501:HOH:O	1.44	1.16
49:AB:329:ILE:HG21	54:AG:8:LEU:CD1	1.74	1.16
52:AE:261:GLU:OE1	76:AE:501:HOH:O	1.63	1.15
48:AA:441:ILE:CG1	48:AA:451:ARG:NH1	2.09	1.15
14:N:116:ASP:HB3	76:f:331:HOH:O	1.47	1.14
43:u:48:VAL:HG21	55:AH:26:LEU:HD21	1.15	1.14
43:u:53:LEU:CG	55:AH:19:PRO:CB	2.26	1.13
43:u:45:VAL:HA	55:AH:26:LEU:HD12	1.28	1.12
13:M:258:LYS:NZ	13:M:341:HIS:HD2	1.48	1.12
8:H:25:LEU:HD11	76:H:549:HOH:O	1.45	1.12
49:BB:331:ASP:OD2	54:BG:8:LEU:N	1.81	1.11
50:BC:154:THR:HG22	50:BC:171:LEU:HD21	1.18	1.11
43:u:52:LEU:HD21	55:AH:18:LYS:HE2	1.25	1.11
76:Z:222:HOH:O	31:e:54:ARG:HG2	1.46	1.11
29:c:14:ASP:HB3	76:c:126:HOH:O	1.50	1.11
12:L:642:TRP:HA	12:L:645:LEU:HD12	1.33	1.11
14:N:352:TYR:HD2	76:N:634:HOH:O	1.32	1.11
60:BF:201:PTY:HC21	76:BF:305:HOH:O	1.50	1.11
49:AB:493:LYS:HZ2	57:AJ:18:ILE:CD1	1.55	1.11
6:F:77:LYS:HZ2	6:F:81:LYS:NZ	1.49	1.10
20:T:41:LEU:CD1	20:T:49:ARG:HH21	1.65	1.10
10:J:167:ILE:HA	76:J:345:HOH:O	1.51	1.10
2:B:117:PRO:CG	8:H:209:GLU:OE1	1.99	1.10
39:n:63:ARG:NE	76:n:202:HOH:O	1.83	1.09
1:A:29:PHE:CZ	2:B:76:MET:HE1	1.88	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:BB:531:TYR:CE1	57:BJ:18:ILE:HG13	1.88	1.08
43:u:49:ARG:CB	55:AH:22:VAL:HG21	1.83	1.08
1:A:56:ARG:HD3	4:D:11:PHE:HB3	1.36	1.07
39:n:60:ASP:OD1	76:n:201:HOH:O	1.69	1.07
49:BB:96:GLU:OE1	49:BB:98:ARG:HG3	1.51	1.07
13:M:82:PHE:CG	13:M:141:LEU:HD11	1.89	1.07
13:M:400:GLU:HG3	76:M:720:HOH:O	1.54	1.07
18:R:75:ASP:HB2	76:R:307:HOH:O	1.55	1.07
43:u:53:LEU:CD2	55:AH:19:PRO:CB	2.33	1.06
49:BB:134:ASP:OD1	49:BB:249:ARG:NH1	1.87	1.06
34:i:34:HIS:HE1	41:p:27:PRO:HB3	0.92	1.06
4:D:197:ARG:NH1	60:D:401:PTY:HC22	1.70	1.05
39:n:66:LYS:HD3	76:AA:637:HOH:O	1.54	1.05
12:L:261:MET:HE3	76:L:966:HOH:O	1.56	1.05
46:y:133:VAL:HG11	47:z:147:MET:HE2	1.10	1.05
49:AB:493:LYS:HZ1	57:AJ:18:ILE:CD1	1.56	1.05
53:BF:27:ARG:HG3	60:BF:201:PTY:HN11	1.21	1.05
60:z:301:PTY:HC32	76:z:495:HOH:O	1.57	1.04
34:i:3:PHE:HE2	34:i:5:MET:CB	1.69	1.04
13:M:64:ALA:CB	41:p:35:GLU:OE1	2.05	1.04
50:BC:154:THR:CG2	50:BC:171:LEU:HD21	1.86	1.04
1:A:56:ARG:HD3	4:D:11:PHE:CB	1.86	1.04
49:AB:417:ASP:OD2	50:AC:12:LYS:NZ	1.91	1.03
53:BF:27:ARG:HE	60:BF:201:PTY:HC31	0.88	1.03
23:W:120:LYS:HD3	23:W:124:LEU:HD23	1.04	1.03
34:i:3:PHE:CE2	34:i:5:MET:CB	2.42	1.03
50:AC:292:PRO:HA	76:BD:431:HOH:O	1.57	1.02
43:u:49:ARG:HA	55:AH:22:VAL:HG21	1.42	1.02
49:BB:531:TYR:CE1	57:BJ:18:ILE:CG1	2.42	1.02
43:u:53:LEU:CG	55:AH:19:PRO:HB3	1.86	1.02
50:BC:222:MET:HE1	53:BF:63:ASN:HB3	1.40	1.02
12:L:182:ILE:HA	76:L:968:HOH:O	1.59	1.02
58:y:303:PGT:H31	76:y:543:HOH:O	1.58	1.02
49:AB:275:THR:HG22	49:AB:304:SER:OG	1.58	1.02
3:C:172:THR:HG23	17:Q:86:ASN:ND2	1.74	1.01
3:C:181:ALA:C	17:Q:70:LYS:HZ2	1.68	1.01
12:L:653:LEU:HD11	25:Y:77:ILE:HD11	1.43	1.01
53:AF:23:SER:OG	58:AF:201:PGT:O1P	1.78	1.01
25:Y:9:LEU:HD22	55:AH:20:LYS:HE2	1.18	1.01
40:o:39:LYS:HE2	76:o:229:HOH:O	1.60	1.01
50:BC:154:THR:HG22	50:BC:171:LEU:CD2	1.91	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:x:60:ARG:HG3	76:z:486:HOH:O	1.60	1.00
13:M:490:GLN:HA	76:M:690:HOH:O	1.60	1.00
13:M:493:LYS:HE3	76:M:706:HOH:O	1.60	1.00
34:i:3:PHE:HE2	34:i:5:MET:HB3	1.22	1.00
43:u:53:LEU:HD21	55:AH:19:PRO:HG2	1.43	1.00
6:F:77:LYS:HZ2	6:F:81:LYS:HE3	1.22	0.99
34:i:34:HIS:CE1	41:p:27:PRO:HB3	1.84	0.99
2:B:123:ASP:OD1	8:H:61:LYS:HE3	1.61	0.99
13:M:194:GLN:OE1	13:M:212:ARG:HD3	1.60	0.99
23:W:120:LYS:CD	23:W:124:LEU:HD23	1.92	0.99
76:J:357:HOH:O	11:K:75:ILE:HD13	1.59	0.99
13:M:65:LYS:CD	76:p:243:HOH:O	2.08	0.99
8:H:232:GLU:OE2	76:H:501:HOH:O	1.79	0.99
43:u:45:VAL:HA	55:AH:26:LEU:CD1	1.92	0.99
43:u:53:LEU:HG	55:AH:19:PRO:HB3	0.99	0.99
52:AE:305:VAL:HG21	53:AF:65:ARG:HG3	1.44	0.99
52:BE:115:ARG:HD3	76:BE:608:HOH:O	1.62	0.99
3:C:172:THR:O	17:Q:93:SER:OG	1.79	0.98
4:D:145:TYR:HD1	76:D:570:HOH:O	1.47	0.98
48:AA:143:ILE:HD11	48:AA:176:VAL:HG11	1.45	0.98
52:AE:304:ASP:HB2	53:AF:64:GLN:OE1	1.62	0.98
6:F:77:LYS:NZ	6:F:81:LYS:CE	2.26	0.98
52:BE:161:TYR:O	76:BE:501:HOH:O	1.82	0.97
52:BE:307:ASN:C	53:BF:65:ARG:HD3	1.88	0.97
2:B:117:PRO:HG3	8:H:209:GLU:OE1	1.61	0.97
20:T:106:ASP:OD1	20:T:110:LEU:CD1	2.12	0.97
43:u:45:VAL:HG13	55:AH:22:VAL:HG12	1.43	0.97
58:L:704:PGT:H5	76:L:984:HOH:O	1.64	0.96
13:M:367:TYR:HB2	76:M:660:HOH:O	1.64	0.96
50:AC:385:SER:OG	76:AC:501:HOH:O	1.75	0.96
48:AA:78:LEU:HD22	48:AA:451:ARG:HD3	1.47	0.96
53:AF:121:ILE:H	50:BC:13:GLN:HE21	1.07	0.96
49:BB:417:ASP:OD2	50:BC:12:LYS:NZ	1.98	0.96
3:C:165:VAL:HB	23:W:96:ARG:CZ	1.95	0.96
12:L:232:LYS:HE2	76:L:998:HOH:O	1.65	0.96
49:AB:432:TYR:O	57:AJ:18:ILE:HD12	1.64	0.96
6:F:77:LYS:NZ	6:F:81:LYS:NZ	2.13	0.95
34:i:3:PHE:CE2	34:i:5:MET:HB2	2.01	0.95
25:Y:38:ALA:HB1	76:Y:301:HOH:O	1.63	0.95
15:O:96:GLU:OE2	76:O:301:HOH:O	1.83	0.95
20:T:41:LEU:HD21	20:T:45:ALA:CB	1.95	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:u:45:VAL:O	55:AH:22:VAL:CG1	2.15	0.95
49:BB:356:MET:HE2	76:BB:775:HOH:O	1.64	0.95
12:L:653:LEU:HD11	25:Y:77:ILE:CD1	1.97	0.95
50:BC:154:THR:CG2	50:BC:171:LEU:CD2	2.44	0.95
50:BC:222:MET:CE	53:BF:63:ASN:HB3	1.96	0.95
48:AA:441:ILE:HG12	48:AA:451:ARG:CZ	1.97	0.94
3:C:181:ALA:O	17:Q:70:LYS:NZ	2.00	0.94
13:M:261:THR:OG1	13:M:338:MET:HE3	1.68	0.94
49:AB:106:LEU:HD11	76:AB:916:HOH:O	1.68	0.94
33:g:101:LEU:HD22	76:g:225:HOH:O	1.66	0.94
49:BB:531:TYR:CD1	57:BJ:18:ILE:HG13	2.03	0.94
25:Y:9:LEU:HD13	55:AH:20:LYS:CG	1.98	0.93
50:AC:107:LEU:HB3	76:AC:613:HOH:O	1.68	0.93
6:F:309:CYS:HB2	76:F:743:HOH:O	1.67	0.93
76:M:674:HOH:O	14:N:483:PRO:HD2	1.69	0.93
43:u:53:LEU:HD21	55:AH:19:PRO:CB	1.97	0.93
60:D:401:PTY:H151	9:I:76:MET:HE2	1.51	0.93
12:L:641:MET:O	12:L:645:LEU:HD11	1.69	0.93
3:C:181:ALA:C	17:Q:70:LYS:NZ	2.27	0.93
20:T:41:LEU:CD2	20:T:45:ALA:HB3	1.98	0.93
4:D:202:ARG:NH2	8:H:211:GLU:OE2	2.02	0.92
24:X:90:ASP:OD1	26:Z:74:LEU:HD11	1.68	0.92
43:u:45:VAL:CA	55:AH:26:LEU:HD12	1.99	0.92
13:M:253:ALA:HB3	76:M:719:HOH:O	1.69	0.92
43:u:49:ARG:HG3	55:AH:19:PRO:O	1.69	0.92
13:M:79:ASN:CG	34:i:40:ILE:HG13	1.96	0.91
8:H:36:ARG:HD2	9:I:86:TYR:CE1	2.05	0.91
60:D:401:PTY:HC21	9:I:70:THR:HG23	1.50	0.91
13:M:65:LYS:HD2	76:p:243:HOH:O	1.67	0.91
13:M:258:LYS:NZ	13:M:341:HIS:CD2	2.38	0.91
43:u:49:ARG:CG	55:AH:19:PRO:O	2.19	0.91
25:Y:90:ARG:O	25:Y:91:ASP:OD1	1.88	0.91
13:M:95:ILE:HG22	65:M:501:3PH:H2H2	1.51	0.90
55:AH:6:VAL:HG12	55:AH:7:VAL:H	1.35	0.90
4:D:379:VAL:HG11	8:H:211:GLU:HG3	1.54	0.90
8:H:198:THR:HB	76:H:509:HOH:O	1.69	0.90
46:y:133:VAL:HG11	47:z:147:MET:HE1	0.91	0.90
14:N:299:ILE:HD12	60:N:501:PTY:O30	1.71	0.90
11:K:72:GLU:HG3	76:K:338:HOH:O	1.71	0.90
54:AG:28:LYS:HD2	76:AG:222:HOH:O	1.72	0.90
51:AD:99:GLU:HB2	76:AG:214:HOH:O	1.70	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:X:34:VAL:HB	76:X:202:HOH:O	1.71	0.89
25:Y:9:LEU:HD13	55:AH:20:LYS:CA	2.01	0.89
20:T:41:LEU:HD21	20:T:45:ALA:HB3	1.55	0.89
7:G:339:LEU:HG	76:G:936:HOH:O	1.72	0.89
73:y:302:COO:O7A	73:y:302:COO:H4X	1.72	0.89
13:M:79:ASN:ND2	34:i:40:ILE:HG13	1.88	0.89
16:P:194:SER:OG	16:P:342:ASP:OD1	1.89	0.89
3:C:57:ILE:HD13	76:D:578:HOH:O	1.72	0.89
14:N:167:ARG:HG3	14:N:168:LYS:HE3	1.55	0.89
48:AA:78:LEU:HD22	48:AA:451:ARG:CD	2.03	0.88
39:n:51:LYS:O	39:n:54:VAL:HG12	1.72	0.88
50:BC:274:HIS:CE1	50:BC:276:VAL:CG1	2.57	0.88
49:BB:359:GLN:OE1	49:BB:396:ASN:HB3	1.72	0.88
43:u:53:LEU:HD23	55:AH:19:PRO:HG3	0.88	0.88
12:L:543:GLN:OE1	66:L:706:PC7:H61	1.74	0.87
76:B:676:HOH:O	8:H:28:ARG:HG2	1.74	0.87
8:H:202:PRO:HB2	76:H:517:HOH:O	1.75	0.87
41:p:70:CYS:HB3	76:p:247:HOH:O	1.74	0.87
4:D:10:ASN:OD1	4:D:33:ASN:OD1	1.92	0.87
13:M:64:ALA:HB2	13:M:487:ASN:ND2	1.89	0.87
48:BA:454:VAL:CG1	76:BA:667:HOH:O	2.23	0.87
13:M:201:GLN:OE1	76:M:601:HOH:O	1.92	0.87
4:D:15:PHE:CG	8:H:212:LEU:HD13	2.06	0.87
34:i:3:PHE:HD2	34:i:6:GLU:H	1.23	0.87
52:AE:77:PRO:O	76:AE:502:HOH:O	1.92	0.87
5:E:136:MET:HB3	6:F:392:ARG:HH21	1.40	0.86
13:M:62:SER:O	76:M:602:HOH:O	1.93	0.86
55:AH:6:VAL:HG12	55:AH:7:VAL:N	1.87	0.86
4:D:115:LEU:HD12	76:D:664:HOH:O	1.74	0.86
43:u:53:LEU:HD23	55:AH:19:PRO:CG	1.80	0.86
42:q:33:CYS:HA	76:q:216:HOH:O	1.76	0.86
18:R:73:GLU:OE1	18:R:78:PRO:HG3	1.75	0.86
50:BC:222:MET:SD	53:BF:67:MET:HB2	2.16	0.86
34:i:34:HIS:CE1	41:p:27:PRO:HB2	2.10	0.86
76:AF:382:HOH:O	50:BC:6:GLN:HG2	1.73	0.86
20:T:106:ASP:OD1	20:T:110:LEU:HD12	1.73	0.86
45:x:92:ASP:OD1	76:x:301:HOH:O	1.94	0.86
19:S:4:ARG:HD3	76:S:117:HOH:O	1.75	0.85
43:u:52:LEU:CD2	55:AH:18:LYS:HB3	2.06	0.85
47:z:80:TRP:HB3	47:z:102:ASP:OD1	1.76	0.85
53:AF:121:ILE:H	50:BC:13:GLN:NE2	1.73	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:BB:359:GLN:NE2	49:BB:395:PHE:HA	1.91	0.85
47:z:90:ASN:HA	76:z:407:HOH:O	1.76	0.85
13:M:258:LYS:CE	13:M:341:HIS:HD2	1.89	0.85
10:J:61:ILE:HG12	76:K:337:HOH:O	1.77	0.84
1:A:56:ARG:CD	4:D:11:PHE:HB3	2.06	0.84
1:A:56:ARG:HD2	4:D:11:PHE:CG	2.11	0.84
1:A:56:ARG:CD	4:D:11:PHE:CG	2.60	0.84
50:BC:369:PHE:CZ	76:BC:635:HOH:O	2.29	0.84
4:D:372:HIS:CE1	76:D:619:HOH:O	2.02	0.84
21:U:120:ALA:O	76:U:201:HOH:O	1.95	0.84
49:BB:66:LYS:HG3	76:BB:745:HOH:O	1.77	0.84
49:BB:531:TYR:CE1	57:BJ:18:ILE:HG12	2.12	0.84
49:AB:493:LYS:HZ2	57:AJ:18:ILE:HD11	1.10	0.84
6:F:309:CYS:CB	76:F:743:HOH:O	2.24	0.84
47:z:181:TRP:HB2	76:z:505:HOH:O	1.77	0.84
16:P:254:GLN:HG2	16:P:287:VAL:HG22	1.60	0.83
55:AH:6:VAL:HG12	55:AH:7:VAL:HG22	1.59	0.83
49:BB:96:GLU:OE1	49:BB:98:ARG:CG	2.25	0.83
20:T:41:LEU:CD1	20:T:49:ARG:NH2	2.42	0.83
8:H:104:ASN:ND2	76:H:504:HOH:O	2.10	0.83
25:Y:11:GLU:OE2	55:AH:20:LYS:NZ	2.12	0.83
50:AC:294:LYS:HG2	51:BD:217:HIS:HD2	1.42	0.83
48:AA:441:ILE:HG13	48:AA:451:ARG:NH1	1.92	0.83
15:O:127:LEU:O	21:U:40:VAL:CG2	2.27	0.83
13:M:238:PRO:HG3	76:M:737:HOH:O	1.79	0.82
49:AB:493:LYS:HZ2	57:AJ:18:ILE:HD12	1.45	0.82
13:M:65:LYS:HD3	76:p:243:HOH:O	1.75	0.82
60:D:401:PTY:C2	9:I:70:THR:HG23	2.09	0.82
13:M:79:ASN:OD1	34:i:40:ILE:HG13	1.80	0.82
15:O:127:LEU:O	21:U:40:VAL:HG23	1.79	0.82
1:A:56:ARG:CD	4:D:11:PHE:CB	2.58	0.82
6:F:281:GLY:HA3	76:F:699:HOH:O	1.79	0.81
13:M:322:GLY:HA2	76:M:652:HOH:O	1.81	0.81
20:T:95:LEU:HD22	20:T:118:HIS:HD2	1.44	0.81
50:AC:388:ASP:HB2	53:AF:90:PHE:C	2.05	0.81
50:BC:316:SER:CA	76:BC:574:HOH:O	2.26	0.81
25:Y:9:LEU:CD2	55:AH:20:LYS:CD	2.57	0.81
43:u:48:VAL:HG21	55:AH:26:LEU:CD2	2.07	0.81
1:A:91:PHE:H	58:A:201:PGT:H5	1.44	0.81
50:BC:316:SER:HA	76:BC:574:HOH:O	1.79	0.81
8:H:36:ARG:HD2	9:I:86:TYR:CD1	2.16	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:63:GLN:HE21	22:V:141:GLN:HG2	1.44	0.81
43:u:49:ARG:HA	55:AH:22:VAL:CG2	2.11	0.81
50:BC:18:THR:HG22	76:BC:618:HOH:O	1.81	0.81
48:AA:420:LYS:HG3	48:AA:461:VAL:HG12	1.63	0.81
50:BC:154:THR:HB	50:BC:171:LEU:HD22	1.62	0.81
12:L:355:VAL:HG12	76:L:967:HOH:O	1.80	0.80
50:AC:271:THR:OG1	76:AC:502:HOH:O	1.98	0.80
51:AD:80:THR:OG1	54:AG:9:LYS:HD3	1.81	0.80
50:BC:213:ASN:HB2	76:BC:616:HOH:O	1.82	0.80
2:B:123:ASP:OD1	8:H:61:LYS:CE	2.29	0.80
25:Y:9:LEU:HD22	55:AH:20:LYS:CG	2.11	0.80
33:g:38:GLU:OE2	76:g:201:HOH:O	1.97	0.80
11:K:54:ASP:HB2	76:K:341:HOH:O	1.81	0.80
43:u:53:LEU:CG	55:AH:19:PRO:HB2	2.08	0.80
49:AB:329:ILE:CG2	54:AG:8:LEU:CD1	2.57	0.80
1:A:56:ARG:HD2	4:D:11:PHE:CD1	2.16	0.80
54:BG:32:GLU:O	54:BG:36:HIS:ND1	2.10	0.80
76:I:689:HOH:O	17:Q:89:MET:HE2	1.81	0.80
7:G:653:ASP:OD2	76:G:901:HOH:O	2.00	0.80
16:P:194:SER:CB	16:P:342:ASP:OD1	2.30	0.80
43:u:49:ARG:HB2	55:AH:22:VAL:HG21	1.63	0.80
50:BC:274:HIS:CE1	50:BC:276:VAL:HG13	2.16	0.79
45:x:53:LYS:NZ	76:x:302:HOH:O	2.16	0.79
1:A:29:PHE:CZ	2:B:76:MET:CE	2.65	0.79
1:A:29:PHE:CE2	2:B:76:MET:CE	2.66	0.79
53:BF:102:LYS:HE2	76:BF:353:HOH:O	1.83	0.79
50:BC:274:HIS:CE1	50:BC:276:VAL:HG11	2.18	0.79
2:B:114:ILE:HG21	63:H:401:UQ9:C3M	2.13	0.79
34:i:34:HIS:CE1	41:p:27:PRO:HG3	2.13	0.79
52:AE:74:PRO:HG3	55:AH:57:ASP:HB3	1.63	0.79
51:BD:91:ILE:HD11	54:BG:13:TYR:HB3	1.65	0.79
9:I:198:GLU:OE2	18:R:47:ASP:OD1	2.01	0.79
53:BF:27:ARG:CG	60:BF:201:PTY:HN11	1.95	0.78
49:AB:329:ILE:HG21	54:AG:8:LEU:HD12	1.64	0.78
12:L:243:PRO:C	12:L:309:ARG:NH1	2.40	0.78
13:M:136:MET:HE3	13:M:141:LEU:HB3	1.65	0.78
23:W:124:LEU:HD11	23:W:128:TYR:CZ	2.18	0.78
25:Y:9:LEU:HD11	55:AH:20:LYS:HB2	1.55	0.78
4:D:145:TYR:CD1	76:D:570:HOH:O	2.28	0.78
6:F:77:LYS:NZ	6:F:81:LYS:HE3	1.90	0.78
13:M:258:LYS:HZ3	13:M:341:HIS:HD2	1.31	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:AE:138:ASP:OD1	52:AE:139:GLY:N	2.17	0.78
39:n:59:GLU:CG	76:n:231:HOH:O	1.93	0.78
50:BC:77:ASP:OD1	76:BC:501:HOH:O	2.02	0.78
12:L:483:ASP:HB2	76:L:1005:HOH:O	1.84	0.77
76:v:305:HOH:O	46:y:8:ILE:HB	1.83	0.77
2:B:166:HIS:NE2	3:C:171:MET:HE1	2.00	0.77
13:M:82:PHE:CG	13:M:141:LEU:CD1	2.67	0.77
49:AB:275:THR:CG2	49:AB:304:SER:OG	2.32	0.77
5:E:132:THR:HG23	5:E:134:PRO:HD2	1.67	0.77
51:AD:265:GLU:HG2	51:AD:268:LYS:HB2	1.66	0.77
3:C:165:VAL:HB	23:W:96:ARG:NH1	1.99	0.77
14:N:299:ILE:CD1	60:N:501:PTY:O30	2.32	0.77
45:x:54:TRP:HE3	76:z:494:HOH:O	1.66	0.77
50:AC:259:HIS:CD2	76:AE:541:HOH:O	2.37	0.77
50:BC:25:ASP:OD1	76:BC:502:HOH:O	2.02	0.77
13:M:189:LEU:HB2	14:N:418:LEU:CD1	2.15	0.77
49:AB:493:LYS:CE	57:AJ:18:ILE:HD11	2.14	0.77
2:B:117:PRO:CB	8:H:209:GLU:OE1	2.33	0.77
12:L:642:TRP:CE3	12:L:645:LEU:CD1	2.68	0.77
48:AA:139:LEU:HD11	48:AA:176:VAL:HG13	1.67	0.76
50:AC:186:PHE:HE2	50:BC:186:PHE:HE2	1.31	0.76
12:L:652:ARG:O	12:L:656:ILE:HG12	1.84	0.76
49:BB:359:GLN:OE1	49:BB:396:ASN:CB	2.34	0.76
12:L:642:TRP:CA	12:L:645:LEU:HD12	2.14	0.76
16:P:319:ALA:O	76:P:601:HOH:O	2.03	0.76
52:BE:187:HIS:HB3	76:BE:609:HOH:O	1.86	0.76
25:Y:9:LEU:HB3	55:AH:20:LYS:HG3	1.68	0.76
43:u:49:ARG:CD	55:AH:19:PRO:O	2.34	0.76
50:AC:259:HIS:HD2	76:AE:541:HOH:O	1.68	0.76
10:J:2:ILE:HG22	76:J:356:HOH:O	1.85	0.76
15:O:129:LYS:HE3	15:O:130:HIS:CE1	2.20	0.76
49:BB:331:ASP:CB	54:BG:7:LYS:HE3	2.15	0.76
8:H:73:LEU:HA	8:H:76:MET:HG2	1.68	0.76
19:S:60:MET:HE2	19:S:89:LEU:HD12	1.67	0.76
8:H:62:GLU:CD	76:H:503:HOH:O	2.29	0.75
12:L:652:ARG:HD2	25:Y:131:ILE:HG21	1.66	0.75
13:M:99:PHE:CD1	65:M:501:3PH:H2E2	2.21	0.75
13:M:258:LYS:CE	13:M:341:HIS:CD2	2.69	0.75
13:M:88:GLY:O	13:M:481:MET:HG2	1.86	0.75
20:T:41:LEU:HD11	20:T:49:ARG:HH21	1.51	0.75
49:AB:329:ILE:CG2	54:AG:8:LEU:HD12	2.16	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:214:ARG:NH1	38:m:62:ASP:OD1	2.19	0.75
6:F:258:LEU:HA	76:F:713:HOH:O	1.87	0.75
49:BB:498:LYS:HA	76:BB:885:HOH:O	1.86	0.75
54:BG:9:LYS:O	76:BG:201:HOH:O	2.05	0.75
7:G:704:PRO:HA	19:S:37:LYS:HE3	1.67	0.75
39:n:63:ARG:HA	76:AA:637:HOH:O	1.86	0.75
66:v:201:PC7:H83	58:y:303:PGT:H132	1.68	0.75
46:y:212:GLN:NE2	76:y:401:HOH:O	2.20	0.75
50:BC:316:SER:CB	76:BC:574:HOH:O	2.07	0.75
3:C:72:GLU:OE1	3:C:89:GLN:NE2	2.19	0.75
18:R:73:GLU:OE2	76:R:301:HOH:O	2.03	0.75
49:BB:125:ILE:HG12	49:BB:279:MET:HG2	1.68	0.75
1:A:67:LEU:CD1	76:A:311:HOH:O	2.34	0.75
50:BC:153:ILE:HG21	75:BC:404:UQ7:H161	1.69	0.74
50:BC:145:MET:HE1	50:BC:276:VAL:H	1.51	0.74
20:T:41:LEU:HD22	20:T:46:VAL:HG23	1.69	0.74
12:L:642:TRP:HA	12:L:645:LEU:CD1	2.15	0.74
48:AA:441:ILE:HG12	48:AA:451:ARG:HH11	1.50	0.74
6:F:236:LEU:HB3	76:F:713:HOH:O	1.87	0.74
12:L:543:GLN:NE2	39:n:40:ILE:HG21	2.03	0.74
55:BH:58:LYS:HG3	76:BH:102:HOH:O	1.87	0.74
6:F:77:LYS:NZ	6:F:81:LYS:HZ1	1.82	0.74
50:BC:259:HIS:CE1	50:BC:276:VAL:HG21	2.23	0.74
13:M:99:PHE:CE1	65:M:501:3PH:H2E2	2.22	0.74
60:D:401:PTY:HC21	9:I:70:THR:CG2	2.18	0.73
19:S:4:ARG:CD	76:S:117:HOH:O	2.34	0.73
52:BE:210:ARG:NH1	52:BE:211:GLU:O	2.21	0.73
52:BE:261:GLU:OE2	76:BE:502:HOH:O	2.04	0.73
12:L:641:MET:O	12:L:645:LEU:CD1	2.36	0.73
49:AB:432:TYR:O	57:AJ:18:ILE:CD1	2.37	0.73
49:BB:145:HIS:CD2	76:BB:841:HOH:O	2.40	0.73
46:y:229:ARG:CZ	76:y:429:HOH:O	2.36	0.73
4:D:191:GLU:OE2	9:I:82:LEU:HD23	1.89	0.73
8:H:216:TYR:CD1	76:H:534:HOH:O	2.39	0.73
19:S:2:ALA:N	76:S:101:HOH:O	2.21	0.73
46:y:250:ARG:HD3	76:y:432:HOH:O	1.88	0.73
48:AA:441:ILE:CG1	48:AA:451:ARG:CZ	2.63	0.73
12:L:262:VAL:CB	76:L:961:HOH:O	2.08	0.73
21:U:70:THR:HG23	21:U:72:LYS:H	1.54	0.73
45:x:129:SER:HA	76:x:454:HOH:O	1.88	0.73
50:AC:77:ASP:OD2	76:AC:503:HOH:O	2.06	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:158:LEU:HD12	12:L:161:ASP:OD2	1.87	0.73
23:W:120:LYS:CD	23:W:124:LEU:CD2	2.58	0.73
51:BD:202:ARG:NH1	51:BD:244:SER:O	2.21	0.73
49:BB:432:TYR:HD1	57:BJ:18:ILE:HD11	1.54	0.73
45:x:170:GLU:HB3	76:x:454:HOH:O	1.88	0.72
45:x:242:TYR:HD2	47:z:34:TYR:CE1	2.07	0.72
8:H:73:LEU:HD23	8:H:76:MET:SD	2.30	0.72
10:J:43:LEU:CD1	76:J:356:HOH:O	2.36	0.72
48:AA:300:ARG:NH2	48:AA:493:PRO:O	2.22	0.72
50:BC:259:HIS:NE2	50:BC:276:VAL:HG23	2.03	0.72
23:W:120:LYS:HD3	23:W:124:LEU:HD21	1.70	0.72
43:u:52:LEU:HD23	55:AH:18:LYS:HB3	1.72	0.72
4:D:274:ILE:HG12	76:D:615:HOH:O	1.88	0.72
8:H:264:PRO:HD2	8:H:267:ILE:HD12	1.71	0.72
34:i:3:PHE:CE1	76:i:121:HOH:O	2.43	0.72
34:i:3:PHE:CE2	34:i:5:MET:HB3	2.14	0.72
12:L:182:ILE:HG12	76:L:968:HOH:O	1.89	0.71
49:AB:63:ASN:HA	49:AB:66:LYS:HE2	1.70	0.71
3:C:177:TYR:CG	17:Q:104:SER:OG	2.42	0.71
13:M:82:PHE:CD2	13:M:141:LEU:HD11	2.24	0.71
13:M:308:ILE:HD13	13:M:348:LEU:HB3	1.73	0.71
14:N:492:GLN:HG3	76:N:740:HOH:O	1.90	0.71
41:p:58:CYS:HG	41:p:70:CYS:HG	1.36	0.71
50:AC:142:TRP:HA	76:AC:568:HOH:O	1.89	0.71
52:AE:253:VAL:HG12	76:AE:636:HOH:O	1.89	0.71
13:M:304:LEU:HD23	13:M:432:LEU:HD11	1.72	0.71
48:BA:52:ALA:HB3	48:BA:60:LEU:HD11	1.72	0.71
4:D:61:LEU:HB2	76:D:709:HOH:O	1.90	0.71
4:D:311:HIS:HD2	7:G:186:MET:HE1	1.56	0.71
10:J:65:PHE:CE2	76:K:305:HOH:O	2.43	0.71
25:Y:9:LEU:CD1	55:AH:20:LYS:CA	2.65	0.71
48:AA:372:THR:HG23	48:AA:374:ILE:HD13	1.72	0.71
48:AA:289:ALA:O	48:AA:291:LYS:NZ	2.24	0.71
33:g:95:GLN:OE1	41:p:7:LEU:HD22	1.89	0.71
52:AE:190:GLN:OE1	52:AE:190:GLN:N	2.22	0.71
51:BD:265:GLU:HG2	51:BD:266:GLU:H	1.54	0.71
41:p:53:GLU:HG3	76:p:208:HOH:O	1.91	0.71
49:AB:459:PRO:HA	76:AB:940:HOH:O	1.90	0.71
49:BB:277:SER:HB3	76:BB:917:HOH:O	1.89	0.71
52:BE:280:LEU:HB3	72:BG:101:CDL:H371	1.73	0.71
12:L:209:ILE:HD12	38:m:58:MET:HE2	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:n:9:TYR:HB3	76:n:204:HOH:O	1.89	0.71
13:M:184:MET:HB2	13:M:223:SER:OG	1.89	0.70
34:i:29:HIS:O	34:i:33:MET:HG2	1.90	0.70
43:u:52:LEU:HD21	55:AH:18:LYS:HB3	1.72	0.70
50:BC:73:HIS:NE2	76:BC:505:HOH:O	2.24	0.70
13:M:174:PHE:CD1	76:M:734:HOH:O	2.43	0.70
47:z:78:SER:HB2	76:z:496:HOH:O	1.91	0.70
4:D:10:ASN:CG	4:D:33:ASN:OD1	2.33	0.70
76:K:344:HOH:O	15:O:155:PRO:HG3	1.91	0.70
4:D:311:HIS:CD2	7:G:186:MET:HE1	2.25	0.70
19:S:14:LEU:HD11	19:S:60:MET:HE3	1.74	0.70
52:BE:300:LYS:HD3	76:BE:529:HOH:O	1.90	0.70
13:M:64:ALA:HB3	41:p:35:GLU:CD	2.15	0.70
53:AF:16:LEU:HB3	58:AF:201:PGT:H162	1.74	0.70
4:D:15:PHE:CD2	8:H:212:LEU:HB3	2.26	0.70
9:I:157:ILE:HB	76:I:654:HOH:O	1.90	0.70
13:M:411:ASN:CG	38:m:55:ASP:OD2	2.34	0.70
25:Y:114:ILE:N	25:Y:115:PRO:HD2	2.07	0.70
52:BE:133:GLU:OE2	56:BI:68:ARG:NH2	2.21	0.70
50:AC:259:HIS:NE2	76:AC:508:HOH:O	2.25	0.70
13:M:189:LEU:HB2	14:N:418:LEU:HD12	1.73	0.69
19:S:3:TRP:N	76:S:101:HOH:O	2.05	0.69
43:u:49:ARG:CA	55:AH:22:VAL:CG2	2.60	0.69
1:A:29:PHE:CE2	2:B:76:MET:HE3	2.25	0.69
2:B:149:PRO:O	8:H:61:LYS:NZ	2.24	0.69
36:k:4:PRO:HG3	36:k:13:ARG:HD3	1.72	0.69
43:u:49:ARG:HD3	55:AH:19:PRO:O	1.92	0.69
46:y:93:SER:HB3	76:y:535:HOH:O	1.92	0.69
12:L:653:LEU:CD1	25:Y:77:ILE:HD11	2.21	0.69
41:p:72:HIS:CE1	76:p:202:HOH:O	2.45	0.69
46:y:260:ASP:HB3	76:y:482:HOH:O	1.91	0.69
25:Y:9:LEU:CD1	55:AH:20:LYS:CB	1.99	0.69
58:y:303:PGT:H161	60:z:301:PTY:H121	1.73	0.69
48:BA:240:LEU:HD23	48:BA:244:LEU:HD22	1.73	0.69
4:D:292:ARG:NH1	7:G:192:ARG:HA	2.08	0.69
76:n:231:HOH:O	49:AB:101:THR:HB	1.90	0.69
8:H:213:VAL:HA	76:H:505:HOH:O	1.92	0.69
14:N:460:PRO:CG	76:d:219:HOH:O	2.39	0.69
50:BC:259:HIS:NE2	50:BC:276:VAL:CG2	2.54	0.69
12:L:642:TRP:CE3	12:L:645:LEU:HD13	2.28	0.69
48:BA:366:GLN:H	48:BA:386:CYS:HB2	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:205:LYS:HB3	76:B:667:HOH:O	1.91	0.69
8:H:62:GLU:OE2	76:H:503:HOH:O	2.10	0.69
14:N:281:PHE:CG	14:N:290:LEU:HD21	2.28	0.69
44:v:80:LYS:NZ	46:y:1:MET:HG2	2.08	0.69
49:AB:415:CYS:SG	50:AC:2:THR:HG22	2.32	0.69
56:AI:17:TYR:HA	56:AI:21:MET:HG3	1.75	0.69
52:BE:78:TRP:HB2	52:BE:81:GLU:HG2	1.72	0.69
13:M:79:ASN:HD21	34:i:40:ILE:HG13	1.58	0.69
50:BC:213:ASN:CB	76:BC:616:HOH:O	2.38	0.69
5:E:121:LYS:O	76:E:601:HOH:O	2.10	0.69
14:N:460:PRO:HG2	76:d:219:HOH:O	1.93	0.69
12:L:543:GLN:HE22	39:n:35:ALA:HA	1.56	0.68
49:AB:505:ILE:HD11	49:AB:522:PHE:HB3	1.74	0.68
38:m:60:ASP:OD1	38:m:65:ARG:NH1	2.19	0.68
50:BC:285:TYR:CZ	50:BC:289:ARG:HD3	2.28	0.68
50:BC:154:THR:CB	50:BC:171:LEU:HD22	2.23	0.68
13:M:62:SER:HB3	33:g:87:LEU:O	1.93	0.68
13:M:95:ILE:CG2	65:M:501:3PH:H2H2	2.23	0.68
49:BB:215:ARG:HD3	49:BB:259:LYS:HA	1.75	0.68
52:BE:204:PRO:HG2	52:BE:207:ILE:HG13	1.73	0.68
26:Z:72:ARG:O	26:Z:76:GLU:HG2	1.94	0.68
38:m:21:GLU:OE1	76:m:201:HOH:O	2.10	0.68
2:B:88:THR:HG23	2:B:115:PHE:CD1	2.28	0.68
49:AB:505:ILE:CD1	49:AB:522:PHE:HB3	2.23	0.68
46:y:133:VAL:HG13	47:z:147:MET:HE1	1.65	0.68
49:BB:488:ASP:OD2	76:BB:701:HOH:O	2.11	0.68
8:H:230:LEU:HD11	63:H:401:UQ9:H11A	1.73	0.68
65:L:701:3PH:H221	65:L:701:3PH:H322	1.74	0.68
40:o:8:LYS:HD2	40:o:68:GLU:OE1	1.94	0.68
50:AC:347:CYS:SG	76:AC:508:HOH:O	2.52	0.68
56:BI:68:ARG:HD2	76:BI:105:HOH:O	1.94	0.68
2:B:209:ARG:NH1	16:P:104:ASP:OD2	2.27	0.68
76:v:305:HOH:O	46:y:5:GLY:HA2	1.93	0.68
50:BC:26:TYR:HD2	67:BC:403:UQ5:H3M1	1.59	0.68
12:L:29:ALA:HB1	12:L:101:ILE:HG12	1.75	0.67
13:M:258:LYS:HE2	13:M:341:HIS:CD2	2.29	0.67
34:i:50:PRO:HG2	34:i:53:PHE:HB3	1.77	0.67
49:AB:514:GLN:CD	54:AG:8:LEU:HD21	2.18	0.67
8:H:290:TYR:CD2	76:H:517:HOH:O	2.46	0.67
11:K:70:ALA:HA	76:K:337:HOH:O	1.93	0.67
36:k:13:ARG:HH11	36:k:13:ARG:HG2	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:n:63:ARG:CD	76:n:202:HOH:O	2.36	0.67
50:BC:291:ILE:H	50:BC:291:ILE:HD12	1.60	0.67
52:BE:190:GLN:N	52:BE:190:GLN:OE1	2.24	0.67
9:I:84:LEU:HA	76:I:693:HOH:O	1.94	0.67
48:AA:211:GLY:O	48:AA:215:GLU:HG3	1.94	0.67
7:G:350:ARG:NH2	7:G:612:TYR:O	2.27	0.67
12:L:31:MET:HE1	29:c:41:MET:HA	1.76	0.67
13:M:400:GLU:HA	76:M:744:HOH:O	1.93	0.67
66:v:201:PC7:H42	76:v:310:HOH:O	1.94	0.67
52:BE:159:GLU:HB3	76:BE:501:HOH:O	1.93	0.67
21:U:115:ALA:O	21:U:119:ILE:HD12	1.94	0.67
26:Z:76:GLU:OE1	76:Z:201:HOH:O	2.13	0.67
47:z:212:GLN:OE1	76:z:401:HOH:O	2.12	0.67
41:p:53:GLU:CG	76:p:208:HOH:O	2.41	0.67
47:z:130:HIS:HB2	47:z:147:MET:HE3	1.75	0.67
6:F:409:ARG:HA	76:G:1102:HOH:O	1.94	0.67
14:N:116:ASP:OD2	76:N:601:HOH:O	2.13	0.67
45:x:54:TRP:CE3	76:z:494:HOH:O	2.43	0.67
4:D:299:ARG:NH2	9:I:175:ASP:OD1	2.28	0.66
9:I:78:ARG:HH22	26:Z:40:SER:HB3	1.59	0.66
49:BB:331:ASP:HB3	54:BG:7:LYS:HE3	1.76	0.66
8:H:275:PHE:CE2	76:H:622:HOH:O	2.48	0.66
5:E:172:MET:HB3	6:F:182:ARG:NH1	2.11	0.66
39:n:106:GLU:HG2	76:n:243:HOH:O	1.95	0.66
43:u:49:ARG:CB	55:AH:22:VAL:CG2	2.69	0.66
48:BA:312:VAL:HG13	48:BA:481:LEU:HD21	1.77	0.66
12:L:26:GLU:OE1	29:c:29:ARG:NH1	2.28	0.66
39:n:106:GLU:CG	76:n:243:HOH:O	2.43	0.66
47:z:32:LYS:HB3	47:z:34:TYR:CD2	2.30	0.66
50:BC:271:THR:CG2	50:BC:275:ILE:HD11	2.25	0.66
4:D:262:CYS:SG	76:D:717:HOH:O	2.54	0.66
22:V:63:GLN:NE2	22:V:141:GLN:HG2	2.10	0.66
3:C:43:CYS:SG	76:V:230:HOH:O	2.52	0.66
47:z:212:GLN:NE2	76:z:404:HOH:O	2.23	0.66
52:AE:210:ARG:NH1	52:AE:211:GLU:O	2.29	0.66
14:N:119:ARG:NH2	76:N:607:HOH:O	2.28	0.66
14:N:168:LYS:NZ	46:y:241:ASP:OD1	2.26	0.66
43:u:53:LEU:HD11	55:AH:19:PRO:HB2	1.77	0.66
50:AC:318:TYR:CD1	53:AF:43:TYR:CE1	2.84	0.66
4:D:156:SER:HB2	76:I:666:HOH:O	1.94	0.66
8:H:114:SER:OG	8:H:148:GLU:OE1	2.12	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:312:SER:OG	76:M:603:HOH:O	2.06	0.66
48:AA:443:ARG:HG2	48:AA:443:ARG:HH11	1.60	0.66
29:c:13:GLY:HA3	39:n:101:PRO:HG2	1.77	0.66
53:AF:44:ASP:OD2	53:AF:46:ASP:HB2	1.95	0.66
40:o:8:LYS:HD2	40:o:68:GLU:CD	2.21	0.66
8:H:75:ARG:HB2	72:u:101:CDL:H522	1.78	0.65
11:K:64:LEU:HD13	14:N:150:LEU:HD11	1.78	0.65
67:L:707:UQ5:H253	60:N:501:PTY:H422	1.78	0.65
3:C:165:VAL:HG23	3:C:167:GLU:OE1	1.96	0.65
49:AB:343:GLU:HG2	76:AB:883:HOH:O	1.95	0.65
50:BC:269:MET:HE2	50:BC:269:MET:HA	1.78	0.65
48:AA:410:LYS:HG2	48:AA:410:LYS:O	1.96	0.65
2:B:160:ASN:ND2	76:B:603:HOH:O	2.29	0.65
3:C:30:ARG:HB2	76:C:232:HOH:O	1.95	0.65
20:T:41:LEU:HD21	20:T:45:ALA:HB1	1.77	0.65
20:T:41:LEU:HD22	20:T:46:VAL:CG2	2.26	0.65
48:BA:139:LEU:HD11	48:BA:176:VAL:HG13	1.77	0.65
4:D:320:PHE:HE2	76:D:709:HOH:O	1.80	0.65
27:a:18:MET:O	27:a:22:MET:HG3	1.94	0.65
73:y:302:COO:C8	76:y:404:HOH:O	2.43	0.65
49:AB:63:ASN:O	49:AB:66:LYS:HG2	1.97	0.65
61:E:500:FES:S1	76:E:685:HOH:O	2.54	0.65
21:U:50:VAL:HG12	21:U:116:VAL:HG23	1.77	0.65
48:AA:332:GLN:OE1	48:AA:372:THR:HB	1.97	0.65
6:F:398:LYS:NZ	76:F:602:HOH:O	2.29	0.65
21:U:61:PHE:HZ	21:U:88:GLU:HB3	1.62	0.65
48:BA:170:VAL:HG21	48:BA:265:VAL:HG12	1.79	0.65
13:M:107:VAL:HG21	13:M:350:LEU:HD21	1.78	0.65
14:N:283:TYR:C	76:N:627:HOH:O	2.40	0.65
52:AE:184:LYS:HG2	76:AE:520:HOH:O	1.96	0.65
50:BC:222:MET:HE1	53:BF:63:ASN:CB	2.23	0.65
43:u:53:LEU:CD1	55:AH:19:PRO:HB2	2.26	0.65
45:x:73:ALA:HB1	45:x:92:ASP:OD1	1.97	0.65
3:C:173:GLN:HB2	17:Q:91:TRP:HB3	1.79	0.65
12:L:543:GLN:OE1	66:L:706:PC7:C6	2.44	0.65
43:u:48:VAL:CG2	55:AH:26:LEU:HD21	2.10	0.65
12:L:49:GLU:HG2	29:c:69:ILE:HB	1.79	0.64
46:y:254:PRO:HA	46:y:257:ILE:HD12	1.78	0.64
50:AC:294:LYS:HG2	51:BD:217:HIS:CD2	2.30	0.64
1:A:16:LEU:O	1:A:20:LEU:HD22	1.97	0.64
12:L:543:GLN:NE2	39:n:35:ALA:HA	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:202:ARG:HH22	8:H:211:GLU:CD	2.05	0.64
14:N:436:GLY:HA2	14:N:439:TYR:CE2	2.32	0.64
49:BB:337:GLN:HG2	49:BB:410:VAL:HG22	1.79	0.64
6:F:319:LEU:HD21	6:F:340:ILE:HG21	1.79	0.64
9:I:162:CYS:HB3	76:I:692:HOH:O	1.97	0.64
20:T:41:LEU:HD13	20:T:49:ARG:NH2	2.12	0.64
25:Y:114:ILE:N	25:Y:115:PRO:CD	2.60	0.64
76:x:304:HOH:O	47:z:13:PHE:HZ	1.79	0.64
46:y:133:VAL:CG1	47:z:147:MET:HE2	1.97	0.64
49:AB:503:LYS:H	49:AB:526:THR:HG21	1.63	0.64
50:AC:163:VAL:HG12	65:BJ:101:3PH:H12	1.78	0.64
50:AC:318:TYR:HD1	53:AF:43:TYR:CD1	2.14	0.64
49:BB:151:THR:HG21	49:BB:199:ASP:CG	2.22	0.64
12:L:166:LYS:NZ	12:L:566:ASP:OD1	2.27	0.64
13:M:252:LEU:HD23	13:M:256:LEU:HD12	1.80	0.64
39:n:9:TYR:CB	76:n:204:HOH:O	2.44	0.64
48:AA:107:CYS:HB3	48:AA:159:MET:HE2	1.80	0.64
54:AG:24:THR:O	76:AG:201:HOH:O	2.15	0.64
51:BD:94:ASP:HB3	76:BF:332:HOH:O	1.97	0.64
51:BD:223:LEU:HD11	51:BD:235:PRO:HG3	1.79	0.64
12:L:659:VAL:HG11	25:Y:123:THR:HG22	1.79	0.64
13:M:425:GLY:HA2	13:M:428:TYR:CE2	2.33	0.64
49:AB:312:GLN:OE1	49:AB:312:GLN:N	2.29	0.64
49:AB:493:LYS:HZ1	57:AJ:18:ILE:CG1	2.11	0.64
7:G:264:VAL:HA	7:G:267:ILE:HG12	1.79	0.64
7:G:266:ASP:OD2	7:G:333:ARG:NH2	2.23	0.64
24:X:90:ASP:OD2	26:Z:74:LEU:HD21	1.98	0.64
43:u:49:ARG:N	55:AH:22:VAL:HG21	2.12	0.64
4:D:379:VAL:CG1	8:H:211:GLU:HG3	2.26	0.64
50:BC:275:ILE:HB	76:BC:538:HOH:O	1.97	0.64
67:L:707:UQ5:H302	60:N:501:PTY:H352	1.79	0.64
23:W:21:GLU:OE1	23:W:25:ARG:NH2	2.30	0.64
25:Y:68:THR:O	25:Y:72:ILE:HD12	1.98	0.64
6:F:77:LYS:HZ1	6:F:81:LYS:HZ1	1.45	0.64
14:N:240:LYS:HD3	76:N:612:HOH:O	1.96	0.64
50:BC:383:PRO:HG2	53:BF:39:TYR:OH	1.97	0.64
12:L:414:ILE:HD13	37:l:97:VAL:HG22	1.80	0.63
13:M:46:LEU:HD22	33:g:69:THR:HG21	1.80	0.63
21:U:81:LEU:HD22	21:U:85:ASP:HB3	1.79	0.63
23:W:47:GLN:OE1	23:W:47:GLN:N	2.21	0.63
48:BA:94:THR:HG22	48:BA:264:GLY:HA2	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:BA:454:VAL:HG12	76:BA:667:HOH:O	1.95	0.63
10:J:97:PHE:O	10:J:101:MET:HB3	1.97	0.63
13:M:190:LEU:HD11	58:M:502:PGT:H12	1.79	0.63
25:Y:9:LEU:HD23	55:AH:20:LYS:HE2	1.75	0.63
49:AB:493:LYS:HZ1	57:AJ:18:ILE:HD11	0.81	0.63
48:BA:196:ARG:HG2	48:BA:196:ARG:HH11	1.64	0.63
12:L:303:LEU:HD11	66:L:706:PC7:H341	1.80	0.63
14:N:248:MET:HG3	76:N:609:HOH:O	1.98	0.63
49:AB:486:ALA:HA	76:AB:925:HOH:O	1.99	0.63
52:BE:305:VAL:HG21	53:BF:65:ARG:HG3	1.79	0.63
50:BC:329:GLN:HE22	53:BF:27:ARG:HH22	1.46	0.63
51:BD:202:ARG:NH2	51:BD:256:LEU:O	2.32	0.63
46:y:110:LYS:HE2	46:y:110:LYS:H	1.62	0.63
60:BF:201:PTY:C2	76:BF:305:HOH:O	2.21	0.63
6:F:334:TRP:NE1	6:F:356:GLU:OE2	2.32	0.63
12:L:196:THR:HG21	41:p:52:ARG:HG3	1.81	0.63
51:AD:218:LEU:HD13	50:BC:152:VAL:HG13	1.81	0.63
13:M:258:LYS:HZ3	13:M:341:HIS:CD2	2.11	0.63
41:p:82:ARG:CZ	76:p:205:HOH:O	2.47	0.63
43:u:52:LEU:CD2	55:AH:18:LYS:CB	2.76	0.63
48:AA:332:GLN:OE1	48:AA:372:THR:CB	2.47	0.63
49:AB:312:GLN:O	49:AB:316:ASN:ND2	2.31	0.63
50:AC:271:THR:HG21	51:BD:221:ILE:O	1.99	0.63
53:AF:20:HIS:CE1	58:AF:201:PGT:H263	2.34	0.63
6:F:182:ARG:HE	6:F:184:GLU:CD	2.06	0.62
8:H:232:GLU:CB	76:H:501:HOH:O	2.21	0.62
12:L:3:LEU:HB2	29:c:55:SER:HB2	1.80	0.62
13:M:64:ALA:CB	13:M:487:ASN:ND2	2.61	0.62
29:c:14:ASP:CB	76:c:126:HOH:O	2.26	0.62
33:g:96:LYS:HB3	76:g:208:HOH:O	1.98	0.62
45:x:242:TYR:CD2	47:z:34:TYR:CE1	2.86	0.62
9:I:195:TYR:HB2	76:I:654:HOH:O	1.99	0.62
49:AB:146:MET:SD	49:AB:214:GLU:HG3	2.39	0.62
16:P:135:MET:HE1	16:P:171:ALA:HA	1.82	0.62
46:y:29:LEU:HD11	47:z:8:PHE:HD2	1.62	0.62
50:AC:253:ALA:HB2	58:AC:407:PGT:H2	1.82	0.62
72:AE:402:CDL:HB32	54:AG:26:LEU:HD21	1.80	0.62
47:z:180:VAL:HG12	47:z:189:LEU:HD12	1.80	0.62
60:D:401:PTY:H221	8:H:279:LEU:HD21	1.80	0.62
50:BC:222:MET:HE2	54:BG:8:LEU:HD23	1.80	0.62
10:J:37:THR:HG23	11:K:44:LEU:HD21	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:BB:149:LYS:HA	49:BB:156:VAL:HG12	1.80	0.62
49:BB:417:ASP:OD2	50:BC:12:LYS:CE	2.47	0.62
34:i:32:GLU:O	34:i:36:ARG:HB2	1.99	0.62
52:BE:230:LEU:HD22	52:BE:248:MET:HE3	1.80	0.62
4:D:286:MET:HE2	4:D:286:MET:HA	1.81	0.62
20:T:41:LEU:CD2	20:T:45:ALA:CB	2.65	0.62
49:AB:308:THR:HG23	49:AB:313:LEU:HD21	1.81	0.62
8:H:72:PHE:CE2	8:H:76:MET:SD	2.93	0.62
12:L:653:LEU:HD11	25:Y:77:ILE:HD12	1.81	0.62
14:N:84:ASN:HB3	76:N:733:HOH:O	2.00	0.62
40:o:8:LYS:HD2	40:o:68:GLU:OE2	1.99	0.62
58:y:303:PGT:C3	76:y:543:HOH:O	2.31	0.62
50:BC:144:GLN:NE2	76:BC:508:HOH:O	2.32	0.62
4:D:28:LEU:HD11	4:D:382:ILE:HD11	1.82	0.61
6:F:185:TYR:HB3	6:F:188:GLU:HB2	1.81	0.61
10:J:43:LEU:HD11	76:J:356:HOH:O	1.96	0.61
14:N:237:PHE:HD1	76:N:785:HOH:O	1.83	0.61
20:T:41:LEU:CD2	20:T:46:VAL:HG23	2.29	0.61
49:AB:277:SER:OG	76:AB:701:HOH:O	2.05	0.61
53:AF:16:LEU:HB3	58:AF:201:PGT:H141	1.82	0.61
48:BA:72:LYS:HB2	49:BB:114:LEU:HD12	1.82	0.61
65:BC:405:3PH:H3D1	52:BE:275:ILE:HG22	1.81	0.61
14:N:340:GLU:H	14:N:340:GLU:CD	2.07	0.61
16:P:126:ARG:NH1	16:P:158:ASP:OD2	2.33	0.61
43:u:44:GLU:HG3	55:AH:26:LEU:HD13	1.82	0.61
66:v:201:PC7:H131	66:v:201:PC7:H322	1.82	0.61
48:AA:115:TYR:HB3	48:AA:239:ARG:HH22	1.65	0.61
48:AA:472:PHE:O	48:AA:476:VAL:HG23	2.00	0.61
4:D:234:ARG:NH2	76:D:509:HOH:O	2.33	0.61
8:H:76:MET:HE1	72:u:101:CDL:H352	1.83	0.61
12:L:430:THR:HA	12:L:433:TYR:CE2	2.35	0.61
34:i:71:GLN:NE2	76:i:102:HOH:O	2.34	0.61
42:q:46:ASN:OD1	42:q:75[A]:TRP:NE1	2.31	0.61
50:BC:383:PRO:HG3	53:BF:35:TYR:HE2	1.65	0.61
3:C:172:THR:HG23	17:Q:86:ASN:HD22	1.62	0.61
14:N:43:LYS:HE2	14:N:47:TYR:OH	2.00	0.61
52:AE:225:ALA:HB3	74:AE:401:HEM:HBD2	1.83	0.61
6:F:470:GLU:OE2	6:F:474:ARG:NH2	2.33	0.61
8:H:76:MET:HE3	72:u:101:CDL:H581	1.80	0.61
13:M:132:ALA:O	13:M:136:MET:HG2	2.01	0.61
47:z:144:PHE:HB3	47:z:162:MET:HG3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:187:SER:OG	76:N:602:HOH:O	2.14	0.61
36:k:34:GLY:HA2	36:k:37:ILE:HD12	1.83	0.61
39:n:31:THR:HG23	39:n:44:ASP:HB3	1.82	0.61
1:A:29:PHE:HZ	2:B:76:MET:HE1	1.56	0.61
49:AB:63:ASN:CA	49:AB:66:LYS:HE2	2.30	0.61
51:BD:223:LEU:CD1	51:BD:235:PRO:HG3	2.30	0.61
8:H:324:LEU:O	26:Z:72:ARG:NH2	2.34	0.60
58:L:703:PGT:H251	14:N:427:LEU:HD11	1.83	0.60
52:AE:235:VAL:HG12	52:AE:248:MET:SD	2.41	0.60
49:BB:531:TYR:CD1	57:BJ:18:ILE:CG1	2.75	0.60
50:AC:139:VAL:HA	50:AC:146:SER:HB3	1.83	0.60
13:M:334:SER:HA	13:M:403:ILE:HD11	1.82	0.60
25:Y:9:LEU:HD22	55:AH:20:LYS:HG3	1.83	0.60
43:u:52:LEU:HD23	55:AH:18:LYS:CB	2.32	0.60
43:u:53:LEU:HD21	55:AH:19:PRO:HB2	1.81	0.60
43:u:53:LEU:CD2	55:AH:19:PRO:HB2	2.30	0.60
45:x:46:THR:HG23	45:x:46:THR:O	2.00	0.60
45:x:129:SER:HB2	76:x:454:HOH:O	2.01	0.60
48:AA:392:ALA:O	48:AA:396:ILE:HG12	2.02	0.60
49:AB:63:ASN:CB	49:AB:66:LYS:HE2	2.31	0.60
4:D:23:HIS:CD2	4:D:26:LEU:HD22	2.36	0.60
46:y:201:SER:O	46:y:205:LYS:HE2	2.02	0.60
48:AA:121:HIS:CE1	48:AA:198:MET:HG3	2.36	0.60
50:BC:153:ILE:HD11	75:BC:404:UQ7:C5	2.31	0.60
13:M:362:ARG:NH1	76:M:610:HOH:O	2.33	0.60
48:AA:406:VAL:HG22	48:AA:473:THR:HG21	1.84	0.60
49:AB:393:MET:HE1	49:AB:395:PHE:HB3	1.83	0.60
72:BC:408:CDL:H131	66:BC:409:PC7:H382	1.82	0.60
54:BG:27:TRP:HA	54:BG:30:LEU:HD13	1.81	0.60
8:H:126:ARG:HH22	10:J:22:ASN:HD21	1.49	0.60
13:M:56:TRP:HB2	13:M:95:ILE:HD11	1.82	0.60
13:M:191:ILE:HD13	13:M:271:MET:HE1	1.83	0.60
16:P:181:ILE:HD13	16:P:215:THR:HB	1.84	0.60
23:W:96:ARG:HD3	76:W:302:HOH:O	2.01	0.60
18:R:73:GLU:OE1	18:R:78:PRO:CG	2.49	0.60
34:i:77:ASP:OD1	34:i:78:PRO:HD2	2.01	0.60
51:BD:98:HIS:NE2	76:BD:404:HOH:O	2.32	0.60
53:BF:23:SER:HB3	60:BF:201:PTY:HC52	1.84	0.60
58:A:201:PGT:H321	65:f:202:3PH:H242	1.83	0.59
6:F:388:ASP:OD1	6:F:392:ARG:NH1	2.35	0.59
9:I:154:ARG:NH1	17:Q:89:MET:O	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:393:PRO:HA	12:L:398:PHE:CD2	2.37	0.59
19:S:53:CYS:SG	76:S:111:HOH:O	2.57	0.59
47:z:32:LYS:HD3	47:z:34:TYR:HE2	1.67	0.59
48:AA:320:ASN:O	48:AA:321:ASN:HB2	2.02	0.59
13:M:344:VAL:HG22	13:M:467:LEU:HD21	1.83	0.59
49:BB:145:HIS:CG	76:BB:841:HOH:O	2.54	0.59
49:BB:208:GLU:O	49:BB:212:ASN:ND2	2.31	0.59
51:BD:80:THR:OG1	54:BG:9:LYS:HE2	2.02	0.59
13:M:71:SER:OG	13:M:83:TYR:CE1	2.55	0.59
13:M:376:ASN:ND2	76:M:611:HOH:O	2.34	0.59
50:BC:139:VAL:HA	50:BC:146:SER:HB3	1.83	0.59
3:C:40:GLN:NE2	76:C:202:HOH:O	2.25	0.59
25:Y:101:VAL:O	25:Y:105:SER:OG	2.18	0.59
48:AA:72:LYS:HD3	49:AB:114:LEU:HB2	1.85	0.59
51:BD:115:VAL:HG11	72:BG:101:CDL:H312	1.84	0.59
76:F:686:HOH:O	7:G:164:MET:CE	2.51	0.59
7:G:92:LEU:O	7:G:96:GLU:HG2	2.02	0.59
11:K:11:MET:CE	76:K:309:HOH:O	2.50	0.59
45:x:242:TYR:HD2	47:z:34:TYR:HE1	1.48	0.59
50:AC:26:TYR:HB3	67:AC:403:UQ5:H3M1	1.83	0.59
51:AD:237:HIS:HD2	50:BC:289:ARG:HG2	1.67	0.59
65:AI:101:3PH:H241	65:AI:101:3PH:H341	1.85	0.59
48:BA:358:VAL:HG23	48:BA:365:VAL:HG21	1.84	0.59
48:BA:483:MET:CE	48:BA:498:ILE:HG21	2.32	0.59
52:BE:103:CYS:SG	74:BE:401:HEM:CAB	2.91	0.59
4:D:292:ARG:NH2	76:D:515:HOH:O	2.35	0.59
13:M:261:THR:HG1	13:M:338:MET:HE3	1.65	0.59
47:z:150:THR:HB	47:z:168:LEU:HD22	1.85	0.59
50:AC:77:ASP:HA	51:AD:142:LYS:HD2	1.84	0.59
50:AC:138:TYR:CE1	50:AC:278:GLU:OE2	2.56	0.59
72:AC:409:CDL:H132	66:AC:410:PC7:H141	1.84	0.59
48:BA:266:GLU:OE2	48:BA:269:GLU:HB2	2.03	0.59
56:BI:22:ARG:HD2	76:BI:110:HOH:O	2.03	0.59
12:L:161:ASP:OD1	12:L:162:LYS:N	2.35	0.59
12:L:316:CYS:HA	12:L:319:LEU:HD12	1.85	0.59
14:N:410:LYS:NZ	76:N:616:HOH:O	2.36	0.59
47:z:60:PHE:HD2	76:z:496:HOH:O	1.83	0.59
48:BA:151:SER:OG	48:BA:162:THR:OG1	2.21	0.59
48:BA:454:VAL:HG13	76:BA:667:HOH:O	1.97	0.59
10:J:43:LEU:HD12	76:J:356:HOH:O	1.99	0.59
14:N:460:PRO:HG3	76:d:219:HOH:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:9:LEU:HB3	55:AH:20:LYS:HA	1.84	0.59
48:AA:332:GLN:OE1	48:AA:372:THR:OG1	2.20	0.59
1:A:56:ARG:HD3	4:D:11:PHE:HB2	1.83	0.59
13:M:150:LEU:HD11	13:M:177:THR:HG21	1.85	0.59
25:Y:47:GLU:OE1	25:Y:57:ARG:NH2	2.33	0.59
45:x:181:GLU:OE2	47:z:170:ARG:NH2	2.36	0.59
1:A:25:VAL:HG23	1:A:26:PRO:HD3	1.83	0.59
1:A:117:ASP:OD2	8:H:301:LYS:NZ	2.36	0.59
14:N:197:ILE:HD11	14:N:230:ILE:HD13	1.85	0.59
12:L:554:ARG:HH12	37:l:73:VAL:HG22	1.68	0.58
16:P:314:ILE:O	16:P:318:MET:HG3	2.02	0.58
25:Y:9:LEU:CB	55:AH:20:LYS:HG3	2.32	0.58
48:BA:358:VAL:HA	48:BA:362:TYR:HB2	1.84	0.58
56:BI:19:LEU:HD22	56:BI:26:VAL:HG21	1.85	0.58
20:T:41:LEU:HD23	20:T:45:ALA:HB3	1.80	0.58
48:BA:106:ASP:HB3	48:BA:257:ARG:HB3	1.86	0.58
13:M:411:ASN:OD1	38:m:55:ASP:OD2	2.21	0.58
54:AG:4:GLN:NE2	54:AG:5:PRO:O	2.36	0.58
2:B:117:PRO:HG2	8:H:209:GLU:OE1	1.99	0.58
20:T:120:MET:HE2	39:n:88:TRP:CD1	2.39	0.58
29:c:34:ARG:HH22	33:g:34:THR:C	2.10	0.58
52:BE:99:TYR:HA	52:BE:103:CYS:SG	2.43	0.58
39:n:25:ARG:HG3	39:n:29:LYS:NZ	2.18	0.58
48:AA:78:LEU:HD22	48:AA:451:ARG:HD2	1.83	0.58
49:AB:387:GLU:OE2	50:AC:3:ILE:HD12	2.03	0.58
2:B:87:MET:HE1	2:B:142:VAL:HG11	1.85	0.58
12:L:426:SER:O	12:L:430:THR:HG22	2.04	0.58
22:V:83:CYS:HB2	22:V:89:LEU:HD21	1.85	0.58
24:X:37:LEU:HD13	34:i:82:LEU:HB3	1.86	0.58
43:u:45:VAL:CA	55:AH:26:LEU:CD1	2.70	0.58
53:AF:92:SER:HB2	76:AF:302:HOH:O	2.03	0.58
65:BC:405:3PH:H3B1	52:BE:276:PHE:HB2	1.85	0.58
52:BE:305:VAL:H	53:BF:64:GLN:HE21	1.51	0.58
8:H:31:MET:SD	76:H:578:HOH:O	2.57	0.58
13:M:189:LEU:CB	14:N:418:LEU:HD12	2.34	0.58
15:O:99:ILE:HG12	15:O:148:VAL:HG22	1.85	0.58
43:u:49:ARG:HB2	55:AH:22:VAL:CG2	2.33	0.58
52:AE:241:THR:HG23	55:AH:69:LYS:HE3	1.85	0.58
48:BA:306:GLU:HA	48:BA:389:PRO:HG3	1.85	0.58
52:BE:307:ASN:O	53:BF:65:ARG:HD3	2.04	0.58
67:L:707:UQ5:H311	14:N:296:PHE:HB3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:253:ALA:HB1	76:M:603:HOH:O	2.03	0.58
40:o:8:LYS:CE	40:o:68:GLU:CD	2.77	0.58
48:AA:121:HIS:ND1	48:AA:198:MET:HE3	2.19	0.58
3:C:171:MET:O	17:Q:93:SER:HB3	2.04	0.58
13:M:258:LYS:HZ1	13:M:341:HIS:CD2	2.17	0.58
25:Y:9:LEU:CD2	55:AH:20:LYS:HD2	2.31	0.58
33:g:99:GLU:O	33:g:103:MET:HG2	2.04	0.58
49:AB:388:ILE:HG22	50:AC:2:THR:HB	1.86	0.58
50:AC:152:VAL:HG21	67:AC:404:UQ5:O3	2.04	0.58
13:M:306:LYS:HD2	76:M:631:HOH:O	2.04	0.58
44:v:80:LYS:NZ	46:y:1:MET:CG	2.67	0.58
50:BC:376:GLY:HA3	76:BC:574:HOH:O	2.02	0.58
60:D:401:PTY:H421	26:Z:53:VAL:HG12	1.86	0.57
13:M:410:ARG:NH1	76:M:604:HOH:O	2.37	0.57
12:L:636:VAL:HG13	14:N:228:MET:HE1	1.87	0.57
50:BC:25:ASP:OD1	76:BC:503:HOH:O	2.17	0.57
4:D:23:HIS:NE2	4:D:387:ILE:HB	2.20	0.57
5:E:172:MET:HB3	6:F:182:ARG:CZ	2.34	0.57
8:H:58:LEU:HD13	8:H:226:ALA:HB2	1.86	0.57
13:M:71:SER:OG	13:M:83:TYR:CD1	2.56	0.57
47:z:4:LEU:O	47:z:8:PHE:HD1	1.86	0.57
52:AE:277:LEU:HD21	56:AI:42:VAL:HG21	1.86	0.57
55:AH:6:VAL:CG1	55:AH:7:VAL:N	2.59	0.57
3:C:172:THR:CG2	17:Q:86:ASN:ND2	2.60	0.57
39:n:25:ARG:HG3	39:n:29:LYS:HZ1	1.70	0.57
74:AE:401:HEM:HBC2	74:AE:401:HEM:HMC1	1.85	0.57
10:J:104:ILE:HG13	14:N:224:SER:OG	2.04	0.57
72:u:102:CDL:H182	72:u:102:CDL:H361	1.85	0.57
49:AB:493:LYS:NZ	57:AJ:18:ILE:HD12	2.05	0.57
52:BE:93:ARG:HB2	52:BE:121:ALA:HB1	1.86	0.57
55:BH:13:LEU:HD11	55:BH:67:LYS:HD3	1.86	0.57
12:L:370:GLY:HA2	36:k:27:GLN:HG3	1.86	0.57
34:i:46:LEU:HD23	34:i:47:PRO:HD2	1.85	0.57
49:BB:268:ASN:O	49:BB:272:THR:HG22	2.04	0.57
49:BB:331:ASP:HB2	54:BG:7:LYS:HE3	1.86	0.57
58:A:201:PGT:H41	32:f:1:FME:HB3	1.86	0.57
10:J:104:ILE:HD11	14:N:225:GLY:HA2	1.86	0.57
76:L:895:HOH:O	13:M:235:ILE:CG2	2.52	0.57
48:BA:312:VAL:HG22	48:BA:483:MET:CE	2.34	0.57
49:BB:66:LYS:CG	76:BB:745:HOH:O	2.44	0.57
67:L:707:UQ5:H272	14:N:245:PRO:HG3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:BD:265:GLU:HG2	51:BD:266:GLU:N	2.20	0.57
3:C:181:ALA:C	17:Q:70:LYS:HD2	2.30	0.57
41:p:77:TYR:CZ	41:p:81:THR:HG21	2.40	0.57
50:BC:383:PRO:HG3	53:BF:35:TYR:CE2	2.40	0.57
3:C:165:VAL:CB	23:W:96:ARG:CZ	2.77	0.57
7:G:349:ILE:HD12	7:G:359:VAL:HG21	1.86	0.57
20:T:106:ASP:OD1	20:T:110:LEU:HD11	2.04	0.57
49:AB:337:GLN:NE2	76:AB:728:HOH:O	2.37	0.57
74:AC:401:HEM:HMB2	74:AC:401:HEM:HBB2	1.86	0.57
53:BF:57:GLU:H	53:BF:57:GLU:CD	2.13	0.57
9:I:78:ARG:NH2	26:Z:40:SER:HB3	2.20	0.56
14:N:278:LEU:O	14:N:282:ILE:HB	2.05	0.56
32:f:49:TYR:HB2	32:f:62:MET:HG3	1.86	0.56
41:p:72:HIS:ND1	76:p:202:HOH:O	2.33	0.56
43:u:52:LEU:HD21	55:AH:18:LYS:CE	2.16	0.56
48:BA:168:THR:HG23	49:BB:91:ILE:HD13	1.87	0.56
8:H:238:LEU:HD23	76:H:621:HOH:O	2.05	0.56
52:BE:119:GLY:O	76:BE:504:HOH:O	2.18	0.56
3:C:181:ALA:C	17:Q:70:LYS:CE	2.78	0.56
19:S:4:ARG:CG	76:S:117:HOH:O	2.52	0.56
33:g:95:GLN:OE1	41:p:7:LEU:CD2	2.53	0.56
49:AB:415:CYS:SG	50:AC:2:THR:CG2	2.93	0.56
53:AF:30:ARG:HD2	53:AF:78:TYR:CD2	2.41	0.56
49:BB:531:TYR:HE1	57:BJ:18:ILE:HG13	1.64	0.56
50:BC:259:HIS:CE1	50:BC:276:VAL:CG2	2.88	0.56
50:BC:281:PHE:HB3	75:BC:404:UQ7:H102	1.87	0.56
53:BF:27:ARG:CD	60:BF:201:PTY:HC31	2.31	0.56
12:L:17:GLY:HA3	58:L:704:PGT:H352	1.87	0.56
12:L:640:CYS:C	12:L:641:MET:HE2	2.31	0.56
19:S:60:MET:HE1	19:S:86:LEU:HA	1.87	0.56
11:K:28:ILE:HD11	11:K:90:ILE:HD11	1.86	0.56
31:e:59:LYS:NZ	43:u:30:LEU:O	2.39	0.56
45:x:133:LEU:HB3	76:x:307:HOH:O	2.05	0.56
49:AB:240:THR:O	49:AB:243:GLN:HG3	2.06	0.56
49:BB:157:ARG:O	49:BB:161:GLU:HG3	2.05	0.56
51:BD:108:LYS:HA	76:BD:430:HOH:O	2.05	0.56
47:z:162:MET:HB2	47:z:192:LEU:HD11	1.87	0.56
48:AA:420:LYS:HE2	48:AA:461:VAL:O	2.05	0.56
50:AC:209:GLN:NE2	76:AC:518:HOH:O	2.35	0.56
51:BD:91:ILE:HD11	54:BG:13:TYR:CB	2.35	0.56
51:BD:246:ARG:HA	51:BD:255:ASN:HB3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:191:GLU:CD	9:I:82:LEU:HD23	2.31	0.56
8:H:233:TYR:CD1	76:H:501:HOH:O	2.53	0.56
12:L:212:ASN:HB3	38:m:54:LYS:NZ	2.21	0.56
13:M:143:TYR:CE1	13:M:185:LEU:HB2	2.41	0.56
19:S:18:LEU:HD13	19:S:29:ARG:HG2	1.88	0.56
39:n:9:TYR:N	76:n:204:HOH:O	2.24	0.56
40:o:47:LEU:HD13	40:o:49:TRP:CZ2	2.40	0.56
47:z:60:PHE:CD2	76:z:496:HOH:O	2.52	0.56
52:AE:99:TYR:CD1	52:AE:103:CYS:HB2	2.41	0.56
48:BA:483:MET:HE3	48:BA:498:ILE:HG21	1.87	0.56
49:BB:331:ASP:OD2	54:BG:7:LYS:HA	2.05	0.56
4:D:15:PHE:CD2	8:H:212:LEU:CG	2.87	0.56
4:D:298:SER:OG	4:D:301:ARG:HG2	2.06	0.56
13:M:64:ALA:CB	13:M:487:ASN:CG	2.79	0.56
25:Y:97:ILE:O	25:Y:101:VAL:HG12	2.06	0.56
33:g:30:SER:O	33:g:34:THR:OG1	2.24	0.56
42:q:64:LYS:HB2	42:q:73:HIS:HB3	1.87	0.56
48:AA:498:ILE:HA	48:AA:501:LYS:HD2	1.87	0.56
52:BE:99:TYR:CD1	52:BE:103:CYS:HB2	2.40	0.56
56:BI:62:ILE:HB	56:BI:65:LEU:HB2	1.88	0.56
5:E:144:GLU:O	5:E:148:LEU:HD22	2.06	0.56
9:I:99:GLU:OE2	76:I:601:HOH:O	2.17	0.56
12:L:564:PHE:CE1	37:l:73:VAL:HG21	2.41	0.56
13:M:58:GLN:HG3	13:M:68:PHE:CZ	2.41	0.56
22:V:49:GLU:O	22:V:55:LYS:NZ	2.39	0.56
34:i:65:TRP:CD2	76:i:105:HOH:O	2.59	0.56
48:AA:105:VAL:HG22	48:AA:258:MET:HG2	1.88	0.56
49:AB:63:ASN:HA	49:AB:66:LYS:HG2	1.88	0.56
49:AB:262:THR:N	49:AB:265:ASP:OD2	2.36	0.56
74:AE:401:HEM:HMB1	74:AE:401:HEM:HBB2	1.86	0.56
51:BD:167:TRP:CG	51:BD:168:ARG:H	2.23	0.56
7:G:485:LEU:HD21	7:G:502:PHE:CD2	2.41	0.56
7:G:704:PRO:HA	19:S:37:LYS:CE	2.35	0.56
8:H:74:PHE:CE2	76:H:596:HOH:O	2.53	0.56
13:M:82:PHE:CD1	13:M:141:LEU:CD1	2.89	0.56
13:M:103:ILE:O	13:M:107:VAL:HG23	2.06	0.56
50:BC:153:ILE:CG2	75:BC:404:UQ7:H161	2.35	0.56
8:H:302:VAL:HA	28:b:16:VAL:HG11	1.88	0.55
30:d:33:TRP:HB2	60:z:301:PTY:H251	1.88	0.55
45:x:242:TYR:CD2	47:z:34:TYR:HE1	2.23	0.55
4:D:15:PHE:CE2	8:H:212:LEU:CB	2.68	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:245:LEU:HB3	76:D:615:HOH:O	2.06	0.55
34:i:33:MET:HE1	34:i:36:ARG:HH21	1.70	0.55
48:AA:333:MET:HG3	48:AA:423:THR:OG1	2.06	0.55
52:AE:100:GLN:NE2	76:AE:513:HOH:O	2.32	0.55
50:BC:145:MET:CE	50:BC:276:VAL:H	2.19	0.55
52:BE:270:MET:HG2	52:BE:274:TRP:HD1	1.71	0.55
2:B:114:ILE:HG21	63:H:401:UQ9:H3MB	1.89	0.55
12:L:26:GLU:HG3	33:g:31:ARG:HE	1.72	0.55
41:p:49:LYS:HD2	41:p:52:ARG:NH2	2.21	0.55
11:K:11:MET:O	11:K:15:ILE:HG12	2.05	0.55
16:P:140:VAL:HG11	16:P:269:LEU:HD21	1.87	0.55
25:Y:79:VAL:HG11	25:Y:101:VAL:HG11	1.88	0.55
48:AA:205:LEU:HD22	48:AA:212:PHE:HD1	1.71	0.55
52:AE:126:GLU:HG2	56:AI:68:ARG:HB3	1.87	0.55
50:BC:347:CYS:SG	76:BC:642:HOH:O	2.57	0.55
51:BD:113:TYR:CZ	66:BD:302:PC7:H63	2.42	0.55
7:G:112:SER:N	76:G:931:HOH:O	2.39	0.55
19:S:10:SER:HB2	19:S:94:ALA:HB1	1.89	0.55
22:V:140:GLU:CG	22:V:144:LYS:HE3	2.37	0.55
54:AG:72:PHE:C	76:AG:204:HOH:O	2.49	0.55
50:BC:291:ILE:HD12	50:BC:291:ILE:N	2.21	0.55
2:B:88:THR:HB	2:B:98:MET:CE	2.37	0.55
4:D:292:ARG:HH11	7:G:192:ARG:HB2	1.71	0.55
10:J:159:LEU:O	10:J:163:MET:HG3	2.07	0.55
13:M:101:ILE:HG13	13:M:127:GLU:HB2	1.87	0.55
13:M:242:VAL:HG21	13:M:306:LYS:HG2	1.88	0.55
34:i:3:PHE:CZ	76:i:121:HOH:O	2.58	0.55
43:u:52:LEU:HD21	55:AH:18:LYS:CB	2.36	0.55
49:BB:156:VAL:HG23	49:BB:157:ARG:N	2.22	0.55
50:BC:271:THR:HG23	50:BC:275:ILE:HD11	1.88	0.55
8:H:297:GLY:O	8:H:301:LYS:HB2	2.06	0.55
13:M:207:GLU:C	76:M:647:HOH:O	2.49	0.55
34:i:33:MET:HE1	34:i:36:ARG:NH2	2.22	0.55
52:AE:282:LEU:HD23	72:AE:402:CDL:H561	1.89	0.55
48:BA:312:VAL:HG22	48:BA:483:MET:HE1	1.88	0.55
52:BE:307:ASN:ND2	53:BF:88:THR:OG1	2.38	0.55
10:J:109:SER:CB	76:J:307:HOH:O	2.55	0.55
19:S:37:LYS:CB	76:S:102:HOH:O	2.55	0.55
47:z:92:VAL:HG22	47:z:120:THR:HB	1.89	0.55
48:AA:159:MET:HE1	48:AA:253:PHE:HE1	1.72	0.55
50:AC:154:THR:OG1	50:AC:172:TRP:NE1	2.33	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:X:27:MET:HA	24:X:27:MET:HE3	1.88	0.55
47:z:180:VAL:HG23	47:z:192:LEU:HG	1.89	0.55
5:E:172:MET:CB	6:F:182:ARG:NH1	2.70	0.55
6:F:304:HIS:HD2	6:F:381:ASP:H	1.53	0.55
19:S:37:LYS:HB2	76:S:102:HOH:O	2.06	0.55
48:AA:170:VAL:HG11	48:AA:265:VAL:HG21	1.89	0.55
7:G:349:ILE:HD11	7:G:364:ALA:HA	1.88	0.54
52:BE:304:ASP:HB2	53:BF:64:GLN:HE22	1.72	0.54
21:U:70:THR:HG22	21:U:73:ALA:HB2	1.89	0.54
25:Y:9:LEU:CD2	55:AH:20:LYS:CE	2.37	0.54
48:AA:441:ILE:HG13	48:AA:451:ARG:HH12	1.69	0.54
67:BC:403:UQ5:H3M3	67:BC:403:UQ5:H4M2	1.87	0.54
52:BE:270:MET:HG2	52:BE:274:TRP:CD1	2.42	0.54
3:C:132:ILE:HG23	76:C:266:HOH:O	2.07	0.54
6:F:456:TRP:CE2	76:F:723:HOH:O	2.60	0.54
43:u:45:VAL:CG2	55:AH:26:LEU:HD12	2.37	0.54
51:AD:131:VAL:HG13	75:BC:404:UQ7:H361	1.89	0.54
52:AE:83:ILE:HD11	65:AI:101:3PH:H332	1.90	0.54
48:BA:299:PHE:HB3	48:BA:484:GLY:HA2	1.90	0.54
65:BC:405:3PH:H3D2	52:BE:276:PHE:HA	1.89	0.54
16:P:107:ARG:HD2	76:P:633:HOH:O	2.07	0.54
50:BC:132:VAL:HG22	75:BC:404:UQ7:H172	1.88	0.54
5:E:128:LEU:HB2	5:E:182:THR:HB	1.90	0.54
8:H:313:SER:HA	28:b:27:GLY:HA3	1.89	0.54
20:T:51:LEU:HG	20:T:65:VAL:HG12	1.90	0.54
39:n:68:ILE:O	39:n:72:GLU:HG2	2.08	0.54
50:AC:12:LYS:HA	76:AC:673:HOH:O	2.07	0.54
50:AC:385:SER:OG	53:AF:9:VAL:HG12	2.07	0.54
12:L:458:ASP:HB3	35:j:24:HIS:ND1	2.23	0.54
14:N:227:PHE:CZ	14:N:289:THR:HG21	2.43	0.54
25:Y:107:LEU:HD12	25:Y:120:ALA:HB1	1.89	0.54
43:u:2:VAL:N	72:u:102:CDL:OA4	2.40	0.54
66:v:201:PC7:H231	46:y:11:VAL:HG11	1.89	0.54
48:BA:429:MET:O	48:BA:432:GLU:HG2	2.06	0.54
51:BD:115:VAL:CG1	72:BG:101:CDL:H312	2.37	0.54
52:BE:229:MET:HE2	74:BE:401:HEM:HMC3	1.89	0.54
8:H:74:PHE:CD2	76:H:596:HOH:O	2.60	0.54
8:H:263:ILE:HD11	8:H:268:TRP:CZ2	2.42	0.54
13:M:112:MET:HA	13:M:115:TYR:HB2	1.89	0.54
51:AD:99:GLU:CA	76:AG:214:HOH:O	2.56	0.54
55:AH:57:ASP:OD1	76:AH:101:HOH:O	2.18	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:BA:459:LYS:HB3	48:BA:459:LYS:NZ	2.22	0.54
49:BB:151:THR:HG23	49:BB:203:ASN:O	2.08	0.54
13:M:305:LYS:HG3	13:M:352:VAL:HG11	1.90	0.54
20:T:107:SER:OG	20:T:110:LEU:HG	2.06	0.54
36:k:4:PRO:CG	36:k:13:ARG:HD3	2.37	0.54
50:AC:368:PHE:HB2	58:AF:201:PGT:H481	1.90	0.54
48:BA:144:GLU:OE1	49:BB:445:GLN:NE2	2.39	0.54
5:E:174:CYS:SG	76:F:747:HOH:O	2.55	0.54
6:F:181:ILE:HD11	6:F:192:LEU:HD23	1.88	0.54
12:L:642:TRP:CD2	12:L:645:LEU:CD1	2.90	0.54
13:M:65:LYS:HD3	41:p:35:GLU:OE2	2.08	0.54
76:N:740:HOH:O	30:d:60:LEU:HA	2.08	0.54
16:P:233:TRP:CH2	16:P:290:THR:HG23	2.43	0.54
48:AA:441:ILE:HA	48:AA:451:ARG:HH11	1.73	0.54
50:AC:316:SER:HB2	76:AC:633:HOH:O	2.07	0.54
50:BC:219:HIS:HE1	53:BF:42:LEU:HD11	1.73	0.54
55:BH:58:LYS:CG	76:BH:102:HOH:O	2.51	0.54
2:B:120:ARG:HG3	8:H:64:ILE:CD1	2.37	0.53
7:G:317:PRO:HG3	7:G:328:ILE:HG12	1.91	0.53
8:H:290:TYR:HD2	76:H:533:HOH:O	1.91	0.53
12:L:262:VAL:CA	76:L:961:HOH:O	2.51	0.53
13:M:79:ASN:HD21	34:i:40:ILE:HG21	1.72	0.53
16:P:205:GLU:O	16:P:209:ASN:ND2	2.40	0.53
30:d:28:TYR:CE1	66:d:102:PC7:H62	2.43	0.53
34:i:58:ARG:NH2	76:i:104:HOH:O	2.40	0.53
47:z:163:VAL:HG22	76:z:505:HOH:O	2.09	0.53
47:z:226:GLU:HB2	76:z:494:HOH:O	2.08	0.53
50:AC:162:VAL:HG23	50:AC:163:VAL:HG13	1.90	0.53
50:AC:277:PRO:HB3	67:AC:404:UQ5:C5	2.38	0.53
53:AF:105:ARG:HG2	76:AF:361:HOH:O	2.07	0.53
4:D:119:THR:HB	4:D:131:PHE:HA	1.91	0.53
6:F:348:PRO:HG3	6:F:456:TRP:HB3	1.89	0.53
15:O:128:ASN:HA	21:U:41:ARG:O	2.09	0.53
43:u:52:LEU:CD2	55:AH:18:LYS:HE2	2.17	0.53
48:AA:357:ARG:O	48:AA:361:GLU:HB2	2.08	0.53
50:BC:222:MET:CE	54:BG:8:LEU:HD23	2.38	0.53
14:N:282:ILE:HD11	14:N:342:ILE:HD11	1.89	0.53
45:x:110:THR:HG22	76:x:308:HOH:O	2.08	0.53
60:BB:602:PTY:HC31	58:BC:406:PGT:H41	1.91	0.53
51:BD:219:GLY:O	76:BD:401:HOH:O	2.19	0.53
4:D:245:LEU:HD13	4:D:274:ILE:HG23	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:315:LEU:HD12	76:D:687:HOH:O	2.08	0.53
13:M:345:SER:HB2	76:M:603:HOH:O	2.09	0.53
40:o:8:LYS:CD	40:o:68:GLU:OE1	2.56	0.53
43:u:45:VAL:CG1	55:AH:22:VAL:HG12	2.27	0.53
52:AE:305:VAL:CG2	53:AF:65:ARG:HG3	2.29	0.53
53:AF:97:MET:HE2	49:BB:65:ILE:HD11	1.90	0.53
48:BA:427:VAL:HG21	48:BA:457:PHE:CE1	2.43	0.53
72:BC:407:CDL:H211	72:BC:407:CDL:H801	1.90	0.53
52:BE:201:ARG:NH2	52:BE:218:TYR:OH	2.41	0.53
55:BH:10:LYS:HG3	55:BH:64:LEU:HD22	1.90	0.53
11:K:11:MET:HE1	14:N:192:PHE:CE2	2.42	0.53
14:N:281:PHE:CD1	14:N:290:LEU:HD21	2.43	0.53
47:z:130:HIS:HB2	47:z:147:MET:CE	2.39	0.53
50:AC:277:PRO:HB3	67:AC:404:UQ5:O5	2.07	0.53
51:BD:247:ILE:HD13	51:BD:252:ALA:HB3	1.89	0.53
53:BF:55:PRO:HD2	53:BF:58:ILE:HD12	1.89	0.53
56:BI:44:TYR:CE1	56:BI:48:LYS:HE2	2.43	0.53
25:Y:87:ARG:HE	25:Y:89:LYS:HB2	1.72	0.53
72:u:102:CDL:OA6	72:u:102:CDL:O1	2.27	0.53
50:AC:145:MET:HE1	50:AC:275:ILE:HA	1.91	0.53
52:AE:184:LYS:CG	76:AE:520:HOH:O	2.55	0.53
48:BA:169:TYR:O	48:BA:173:MET:HG3	2.09	0.53
2:B:88:THR:HG23	2:B:115:PHE:HD1	1.72	0.53
43:u:5:LEU:HB3	72:u:102:CDL:H732	1.90	0.53
44:v:80:LYS:CE	46:y:1:MET:HG2	2.38	0.53
50:AC:259:HIS:ND1	76:AC:514:HOH:O	2.32	0.53
50:BC:126:ILE:HD13	76:BC:595:HOH:O	2.09	0.53
4:D:315:LEU:CD1	76:D:687:HOH:O	2.57	0.53
6:F:148:CYS:N	76:F:620:HOH:O	2.42	0.53
6:F:306:ASN:ND2	6:F:328:GLY:O	2.34	0.53
7:G:76:VAL:HG12	7:G:139:LEU:O	2.09	0.53
13:M:99:PHE:CG	65:M:501:3PH:H2F1	2.44	0.53
13:M:110:SER:OG	13:M:455:ARG:NH2	2.42	0.53
17:Q:134:LEU:HD12	17:Q:136:LYS:HZ3	1.74	0.53
20:T:41:LEU:HD23	20:T:42:SER:O	2.09	0.53
51:BD:264:LEU:HB2	51:BD:268:LYS:HB2	1.91	0.53
7:G:336:TYR:HA	76:G:936:HOH:O	2.08	0.53
8:H:218:VAL:HG13	8:H:219:GLU:OE2	2.08	0.53
76:I:689:HOH:O	17:Q:89:MET:CE	2.49	0.53
13:M:64:ALA:HB1	13:M:487:ASN:CG	2.34	0.53
13:M:199:ASP:O	13:M:203:LEU:HG	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:269:ILE:HG13	76:M:684:HOH:O	2.07	0.53
48:AA:78:LEU:CD2	48:AA:451:ARG:HD3	2.32	0.53
49:AB:90:HIS:H	49:AB:90:HIS:CD2	2.27	0.53
48:BA:121:HIS:NE2	48:BA:201:GLU:OE2	2.39	0.53
48:BA:420:LYS:NZ	48:BA:464:LEU:O	2.40	0.53
50:BC:222:MET:HE3	53:BF:63:ASN:HB3	1.85	0.53
5:E:40:ASP:OD1	5:E:121:LYS:HD2	2.09	0.53
14:N:270:LYS:CE	76:N:667:HOH:O	2.55	0.53
25:Y:128:SER:HA	25:Y:131:ILE:HD12	1.91	0.53
48:AA:205:LEU:HD21	48:AA:215:GLU:OE1	2.09	0.53
1:A:67:LEU:HD12	76:A:311:HOH:O	2.01	0.52
1:A:99:PHE:CD1	10:J:156:SER:HB3	2.45	0.52
7:G:646:THR:OG1	7:G:650:ALA:HB3	2.09	0.52
12:L:554:ARG:NH1	37:I:73:VAL:HG22	2.24	0.52
14:N:265:LEU:HB3	76:N:772:HOH:O	2.07	0.52
19:S:58:PRO:HB2	19:S:74:LEU:HB2	1.91	0.52
29:c:13:GLY:N	29:c:16:ARG:HE	2.06	0.52
30:d:28:TYR:OH	66:d:102:PC7:H31	2.09	0.52
37:l:45:LYS:HB2	37:l:45:LYS:NZ	2.24	0.52
47:z:32:LYS:HB3	47:z:34:TYR:CE2	2.43	0.52
48:BA:336:GLY:HA3	48:BA:352:SER:HB3	1.91	0.52
50:BC:259:HIS:CD2	50:BC:276:VAL:HG23	2.44	0.52
2:B:89:PHE:CD1	2:B:139:LEU:HD23	2.44	0.52
3:C:25:SER:CB	22:V:122:ASN:HB3	2.39	0.52
4:D:230:CYS:SG	76:D:689:HOH:O	2.59	0.52
50:BC:154:THR:CG2	50:BC:171:LEU:HD22	2.30	0.52
4:D:13:LEU:HD22	8:H:132:TYR:CE1	2.43	0.52
4:D:188:GLU:O	4:D:191:GLU:HG3	2.08	0.52
10:J:51:MET:HE2	10:J:51:MET:HA	1.91	0.52
13:M:82:PHE:CD1	13:M:141:LEU:HD11	2.41	0.52
16:P:107:ARG:O	16:P:110:LYS:HG3	2.10	0.52
48:BA:121:HIS:CE1	48:BA:198:MET:HG2	2.44	0.52
48:BA:308:THR:OG1	48:BA:488:ASP:O	2.28	0.52
7:G:169:ASP:HB2	7:G:172:ILE:HG12	1.92	0.52
8:H:257:LEU:HD12	8:H:260:PHE:HE2	1.74	0.52
12:L:642:TRP:CD2	12:L:645:LEU:HD12	2.45	0.52
14:N:352:TYR:CD2	76:N:634:HOH:O	2.22	0.52
48:AA:144:GLU:OE2	49:AB:375:VAL:HA	2.09	0.52
48:AA:353:TRP:O	48:AA:357:ARG:HB2	2.10	0.52
52:AE:197:LEU:HB3	52:AE:230:LEU:HD12	1.91	0.52
49:BB:288:LYS:HB2	49:BB:291:GLU:HG3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:117:PRO:HB2	8:H:209:GLU:OE1	2.10	0.52
3:C:86:ILE:HD12	3:C:87:ARG:H	1.74	0.52
13:M:225:ALA:HA	13:M:230:MET:HG3	1.91	0.52
44:v:80:LYS:HE2	46:y:1:MET:HG2	1.92	0.52
7:G:421:LEU:HD12	7:G:703:LYS:HE3	1.92	0.52
7:G:514:ILE:HD12	7:G:542:VAL:HG11	1.91	0.52
10:J:146:THR:HB	32:f:1:FME:HE2	1.90	0.52
16:P:135:MET:HE3	16:P:141:VAL:HG21	1.90	0.52
48:AA:124:GLU:HB2	48:AA:154:ALA:HB2	1.92	0.52
50:BC:46:LEU:HD23	67:BC:403:UQ5:H202	1.90	0.52
16:P:204:GLU:HG2	16:P:216:ILE:HD12	1.92	0.52
76:T:309:HOH:O	39:n:29:LYS:HE2	2.09	0.52
50:AC:50:ILE:HA	74:AC:402:HEM:HAB	1.91	0.52
50:BC:244:ILE:HG21	72:BE:402:CDL:H382	1.92	0.52
1:A:62:TYR:OH	11:K:78:ALA:HB2	2.10	0.52
76:K:345:HOH:O	14:N:192:PHE:CD2	2.53	0.52
14:N:495:LEU:CB	30:d:63:MET:HE2	2.40	0.52
39:n:106:GLU:HG3	76:n:243:HOH:O	2.08	0.52
41:p:32:GLU:OE1	41:p:32:GLU:HA	2.10	0.52
48:AA:310:PHE:HB2	48:AA:483:MET:HE1	1.92	0.52
49:AB:225:VAL:HB	51:AD:85:LYS:HG3	1.92	0.52
53:AF:120:THR:HA	50:BC:13:GLN:HE22	1.75	0.52
10:J:28:LEU:HD22	72:u:101:CDL:H381	1.92	0.52
14:N:88:ARG:NH2	14:N:207:ASP:OD1	2.43	0.52
14:N:119:ARG:O	46:y:239:ASP:HB2	2.10	0.52
39:n:77:LYS:HE2	39:n:78:TRP:CE2	2.45	0.52
51:BD:78:PRO:HB3	52:BE:304:ASP:OD1	2.10	0.52
43:u:45:VAL:HG22	55:AH:23:LYS:HA	1.92	0.52
49:AB:254:PRO:HB3	76:AB:946:HOH:O	2.10	0.52
50:AC:275:ILE:HG21	51:BD:236:CYS:SG	2.50	0.52
58:AC:406:PGT:H41	58:AC:406:PGT:H32	1.90	0.52
51:AD:157:ILE:H	51:AD:208:TRP:HH2	1.58	0.52
57:AJ:33:GLY:O	57:AJ:37:VAL:HG23	2.10	0.52
8:H:232:GLU:CG	76:H:501:HOH:O	2.51	0.51
9:I:59:ASP:OD2	9:I:61:ASN:ND2	2.42	0.51
12:L:148:TYR:HB2	12:L:168:MET:HG2	1.92	0.51
16:P:292:GLU:HA	16:P:295:GLU:OE1	2.10	0.51
50:AC:74:ILE:HA	50:AC:78:VAL:HG13	1.92	0.51
2:B:117:PRO:HB2	8:H:209:GLU:CD	2.35	0.51
4:D:197:ARG:HH12	60:D:401:PTY:HC22	1.68	0.51
10:J:162:ALA:HA	11:K:75:ILE:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:82:ILE:HD12	14:N:173:THR:HG22	1.92	0.51
22:V:72:GLU:N	22:V:72:GLU:OE1	2.44	0.51
49:AB:144:GLU:OE1	76:AB:702:HOH:O	2.19	0.51
49:AB:222:MET:HG2	49:AB:252:LEU:HD23	1.92	0.51
53:AF:45:LEU:HD22	76:AF:323:HOH:O	2.09	0.51
50:BC:274:HIS:HE1	50:BC:276:VAL:HG11	1.74	0.51
51:BD:224:PRO:HA	51:BD:232:TRP:CD1	2.45	0.51
6:F:286:SER:HA	6:F:294:ALA:HB1	1.91	0.51
8:H:45:SER:OG	42:q:40:LEU:CD2	2.59	0.51
49:BB:126:ASP:CG	49:BB:310:THR:HG21	2.35	0.51
53:BF:27:ARG:HG3	60:BF:201:PTY:N1	2.06	0.51
3:C:180:PHE:CE1	7:G:285:TRP:CD2	2.99	0.51
4:D:314:GLU:OE1	4:D:318:GLU:HB3	2.10	0.51
60:D:401:PTY:HC22	9:I:70:THR:HG23	1.91	0.51
41:p:11:GLU:HG3	41:p:13:SER:H	1.75	0.51
52:BE:307:ASN:HB2	76:BF:309:HOH:O	2.08	0.51
4:D:292:ARG:NH1	7:G:192:ARG:HB2	2.26	0.51
12:L:653:LEU:HD23	25:Y:76:TYR:HD2	1.74	0.51
13:M:242:VAL:HG22	13:M:305:LYS:HB3	1.92	0.51
16:P:215:THR:HA	76:P:602:HOH:O	2.09	0.51
51:AD:90:LYS:NZ	76:AD:408:HOH:O	2.43	0.51
8:H:239:MET:HE3	76:H:621:HOH:O	2.09	0.51
14:N:216:TYR:O	14:N:219:THR:OG1	2.27	0.51
20:T:95:LEU:HD22	20:T:118:HIS:CD2	2.34	0.51
72:AC:408:CDL:H201	72:AC:408:CDL:H802	1.92	0.51
52:AE:263:GLU:HA	76:AE:594:HOH:O	2.11	0.51
48:BA:215:GLU:HA	48:BA:215:GLU:OE2	2.11	0.51
52:BE:282:LEU:HD23	72:BE:402:CDL:H342	1.92	0.51
9:I:82:LEU:HD12	9:I:85:LYS:HD3	1.92	0.51
15:O:103:TRP:CE2	15:O:146:MET:HA	2.44	0.51
15:O:126:ILE:HB	21:U:41:ARG:HH12	1.75	0.51
16:P:157:GLU:H	16:P:157:GLU:CD	2.19	0.51
49:AB:502:ASP:N	49:AB:526:THR:HG22	2.25	0.51
53:AF:16:LEU:CB	58:AF:201:PGT:H162	2.41	0.51
8:H:212:LEU:O	76:H:505:HOH:O	2.19	0.51
13:M:146:PHE:O	13:M:149:VAL:HG22	2.11	0.51
16:P:194:SER:CA	16:P:342:ASP:OD1	2.59	0.51
20:T:80:LEU:HG	76:T:306:HOH:O	2.09	0.51
23:W:121:THR:HG23	23:W:123:PHE:H	1.75	0.51
50:AC:12:LYS:CG	76:AC:673:HOH:O	2.58	0.51
51:AD:247:ILE:HD13	51:AD:252:ALA:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:BA:170:VAL:CG2	48:BA:265:VAL:HG12	2.40	0.51
2:B:83:SER:OG	8:H:54:ASP:OD1	2.24	0.51
7:G:83:VAL:HG11	7:G:98:ALA:HB2	1.92	0.51
12:L:375:PHE:CE2	12:L:456:CYS:HB3	2.46	0.51
20:T:118:HIS:ND1	20:T:119:PRO:HD2	2.26	0.51
38:m:57:HIS:HB3	38:m:67:HIS:NE2	2.26	0.51
39:n:70:HIS:O	39:n:74:GLU:HG2	2.11	0.51
48:BA:340:SER:OG	48:BA:365:VAL:O	2.22	0.51
4:D:112:LEU:HA	76:D:664:HOH:O	2.11	0.51
6:F:309:CYS:SG	76:F:743:HOH:O	2.59	0.51
8:H:160:ILE:HD13	8:H:315:SER:HB3	1.93	0.51
8:H:290:TYR:OH	76:H:502:HOH:O	2.05	0.51
13:M:180:GLY:O	13:M:223:SER:OG	2.23	0.51
35:j:12:TYR:HD2	36:k:21:HIS:HA	1.75	0.51
39:n:9:TYR:CZ	49:AB:105:GLY:HA2	2.45	0.51
45:x:152:ARG:NH2	73:y:302:COO:H9	2.26	0.51
52:AE:244:THR:O	52:AE:248:MET:HG3	2.11	0.51
4:D:376:ALA:HB1	8:H:211:GLU:OE2	2.11	0.50
47:z:25:LEU:HD22	60:z:301:PTY:H331	1.93	0.50
48:AA:182:ARG:HH11	48:AA:281:LEU:HG	1.76	0.50
50:AC:267:ASN:OD1	50:AC:270:SER:OG	2.29	0.50
3:C:180:PHE:HE1	7:G:285:TRP:CD2	2.29	0.50
4:D:23:HIS:HB2	4:D:26:LEU:HB2	1.93	0.50
4:D:176:ASP:O	4:D:180:GLN:HG2	2.11	0.50
11:K:11:MET:HE2	76:K:309:HOH:O	2.11	0.50
12:L:656:ILE:HG23	25:Y:124:LEU:HD22	1.93	0.50
13:M:67:GLN:C	13:M:69:VAL:N	2.68	0.50
13:M:89:ILE:HG12	13:M:335:ILE:HD11	1.94	0.50
18:R:98:LYS:HD2	76:R:313:HOH:O	2.10	0.50
47:z:194:ASP:OD1	47:z:194:ASP:N	2.44	0.50
50:AC:12:LYS:HG2	76:AC:673:HOH:O	2.11	0.50
50:AC:152:VAL:HG21	67:AC:404:UQ5:C3	2.41	0.50
58:AC:406:PGT:H351	72:AC:408:CDL:H112	1.93	0.50
52:AE:307:ASN:C	53:AF:65:ARG:HD3	2.37	0.50
54:AG:56:TYR:O	54:AG:60:GLN:HG2	2.11	0.50
49:BB:454:MET:HE1	49:BB:463:ASP:CB	2.40	0.50
50:BC:18:THR:HG23	50:BC:19:LEU:HD22	1.92	0.50
5:E:181:ILE:HG23	5:E:201:VAL:HG21	1.92	0.50
6:F:87:ARG:H	6:F:87:ARG:CZ	2.24	0.50
76:K:345:HOH:O	14:N:192:PHE:CE2	2.65	0.50
13:M:493:LYS:HD2	76:M:690:HOH:O	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:261:VAL:O	14:N:265:LEU:HG	2.11	0.50
32:f:2:ASN:HB2	76:f:345:HOH:O	2.10	0.50
39:n:59:GLU:CD	76:n:231:HOH:O	2.43	0.50
47:z:158:GLU:OE1	47:z:174:ARG:NH1	2.39	0.50
49:AB:503:LYS:H	49:AB:526:THR:CG2	2.24	0.50
48:BA:116:PHE:HZ	48:BA:247:GLU:HG2	1.76	0.50
48:BA:483:MET:HE3	48:BA:498:ILE:HD13	1.93	0.50
50:BC:97:ILE:HG13	50:BC:279:TRP:HH2	1.77	0.50
14:N:247:HIS:N	76:N:609:HOH:O	2.30	0.50
21:U:61:PHE:CZ	21:U:88:GLU:HB3	2.45	0.50
44:v:80:LYS:HZ3	46:y:1:MET:HG2	1.74	0.50
46:y:164:ALA:HB1	73:y:302:COO:N6A	2.27	0.50
47:z:175:ILE:HD12	76:z:505:HOH:O	2.11	0.50
48:AA:120:THR:HG22	48:AA:154:ALA:HB1	1.92	0.50
4:D:311:HIS:HD2	7:G:186:MET:CE	2.24	0.50
12:L:642:TRP:CG	12:L:645:LEU:HD12	2.47	0.50
13:M:118:GLU:CD	13:M:118:GLU:H	2.20	0.50
13:M:298:THR:OG1	13:M:310:TYR:HB3	2.11	0.50
19:S:64:TYR:HE1	19:S:94:ALA:HB2	1.76	0.50
26:Z:100:GLU:HA	26:Z:100:GLU:OE2	2.11	0.50
36:k:10:GLU:OE2	36:k:14:ARG:NE	2.43	0.50
12:L:170:VAL:CG1	12:L:238:LEU:HB3	2.42	0.50
27:a:12:LEU:HA	27:a:15:ILE:HD12	1.93	0.50
41:p:55:VAL:HA	76:p:247:HOH:O	2.12	0.50
48:AA:443:ARG:HG2	48:AA:443:ARG:NH1	2.26	0.50
52:AE:307:ASN:ND2	53:AF:34:ARG:NH2	2.59	0.50
1:A:1:FME:HE3	27:a:47:VAL:HG21	1.93	0.50
7:G:205:LYS:O	7:G:213:THR:OG1	2.30	0.50
12:L:309:ARG:NH2	76:L:818:HOH:O	2.44	0.50
13:M:465:VAL:HG11	65:M:501:3PH:H291	1.93	0.50
26:Z:103:LYS:HB3	26:Z:103:LYS:NZ	2.26	0.50
38:m:57:HIS:HB3	38:m:67:HIS:CE1	2.47	0.50
48:AA:369:THR:OG1	48:AA:370:ALA:N	2.45	0.50
4:D:292:ARG:NH1	7:G:192:ARG:CB	2.75	0.50
6:F:64:ILE:HG12	6:F:276:THR:HG21	1.93	0.50
12:L:488:LEU:HD22	12:L:510:GLU:OE2	2.12	0.50
14:N:218:ILE:HG23	14:N:222:ARG:HD3	1.94	0.50
22:V:91:GLU:OE2	76:V:201:HOH:O	2.18	0.50
53:AF:58:ILE:HD11	49:BB:57:ALA:HB3	1.93	0.50
48:BA:310:PHE:CZ	48:BA:385:GLY:HA3	2.46	0.50
49:BB:359:GLN:HE22	49:BB:395:PHE:HA	1.73	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:BC:32:LEU:HB2	50:BC:231:PHE:CE1	2.47	0.50
2:B:130:THR:HA	2:B:158:CYS:HB3	1.94	0.50
3:C:174:GLU:OE1	17:Q:92:THR:O	2.30	0.50
7:G:408:VAL:HG13	76:G:904:HOH:O	2.12	0.50
52:AE:99:TYR:HA	52:AE:103:CYS:SG	2.51	0.50
53:AF:8:LEU:HD21	76:AF:392:HOH:O	2.11	0.50
50:BC:285:TYR:CE1	75:BC:404:UQ7:HM32	2.46	0.50
72:BC:408:CDL:H162	66:BC:409:PC7:H392	1.93	0.50
13:M:79:ASN:OD1	34:i:40:ILE:CG1	2.56	0.49
20:T:55:LYS:HG2	20:T:62:PRO:HB3	1.94	0.49
20:T:97:ILE:HG12	20:T:114:TYR:CE1	2.46	0.49
50:AC:245:PHE:HD1	58:AC:407:PGT:H431	1.77	0.49
53:BF:27:ARG:HE	60:BF:201:PTY:C2	2.21	0.49
6:F:388:ASP:OD1	6:F:392:ARG:HD2	2.12	0.49
7:G:145:LYS:HB3	7:G:148:THR:HG23	1.94	0.49
13:M:27:LEU:HD13	66:d:102:PC7:H121	1.94	0.49
13:M:79:ASN:ND2	34:i:40:ILE:CG1	2.68	0.49
39:n:63:ARG:HD3	76:AB:743:HOH:O	2.12	0.49
9:I:111:HIS:CE1	59:I:500:SF4:S4	3.05	0.49
24:X:74:GLU:OE1	24:X:74:GLU:N	2.46	0.49
26:Z:80:ALA:O	26:Z:84:THR:HG23	2.12	0.49
48:BA:100:SER:HB2	48:BA:434:ARG:HH11	1.76	0.49
50:BC:152:VAL:HG12	50:BC:153:ILE:HD12	1.94	0.49
9:I:195:TYR:CB	76:I:654:HOH:O	2.59	0.49
12:L:112:ARG:HD3	58:L:704:PGT:O1P	2.13	0.49
13:M:436:VAL:HA	76:M:660:HOH:O	2.10	0.49
13:M:444:ASP:HB2	37:l:40:HIS:CE1	2.46	0.49
14:N:207:ASP:OD2	76:N:604:HOH:O	2.17	0.49
49:AB:514:GLN:OE1	54:AG:8:LEU:CD2	2.61	0.49
3:C:171:MET:HG2	3:C:174:GLU:HA	1.94	0.49
8:H:99:VAL:HG13	76:a:204:HOH:O	2.11	0.49
11:K:61:PHE:CZ	14:N:191:LEU:HD11	2.47	0.49
25:Y:58:THR:OG1	76:Y:301:HOH:O	1.93	0.49
43:u:44:GLU:O	55:AH:26:LEU:HD11	2.12	0.49
48:AA:151:SER:OG	48:AA:162:THR:OG1	2.30	0.49
72:AC:408:CDL:H531	72:AC:408:CDL:H752	1.93	0.49
58:A:201:PGT:H362	65:f:202:3PH:H332	1.93	0.49
8:H:61:LYS:HE2	76:H:618:HOH:O	2.13	0.49
11:K:33:MET:HA	11:K:36:GLU:OE2	2.13	0.49
12:L:115:CYS:SG	58:L:704:PGT:H371	2.52	0.49
45:x:54:TRP:CZ2	47:z:222:LEU:HD13	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:AA:107:CYS:HB3	48:AA:159:MET:CE	2.42	0.49
50:AC:388:ASP:HB2	53:AF:90:PHE:O	2.11	0.49
52:BE:140:PRO:HG3	52:BE:146:MET:HE1	1.95	0.49
54:BG:7:LYS:O	76:BG:202:HOH:O	2.19	0.49
55:BH:25:LEU:HD23	55:BH:52:TYR:CE1	2.48	0.49
60:D:401:PTY:H351	8:H:185:PRO:HB3	1.94	0.49
11:K:86:VAL:HA	76:K:302:HOH:O	2.13	0.49
12:L:564:PHE:CZ	37:l:73:VAL:HG21	2.48	0.49
12:L:603:SER:HB2	60:M:504:PTY:HC12	1.95	0.49
76:L:813:HOH:O	29:c:16:ARG:HD3	2.12	0.49
13:M:444:ASP:HB2	37:l:40:HIS:NE2	2.27	0.49
14:N:479:PHE:HA	60:d:101:PTY:H202	1.95	0.49
34:i:3:PHE:CZ	34:i:5:MET:HB2	2.48	0.49
60:z:301:PTY:H372	60:z:301:PTY:H241	1.94	0.49
50:AC:277:PRO:O	76:AC:506:HOH:O	2.20	0.49
49:BB:62:LYS:O	49:BB:66:LYS:HG3	2.13	0.49
50:BC:97:ILE:HG13	50:BC:279:TRP:CH2	2.48	0.49
53:BF:27:ARG:NE	60:BF:201:PTY:C3	2.37	0.49
4:D:197:ARG:NH1	60:D:401:PTY:C2	2.61	0.49
4:D:273:ARG:HD2	26:Z:35:TYR:CZ	2.47	0.49
10:J:109:SER:HB3	76:J:307:HOH:O	2.13	0.49
15:O:129:LYS:HE3	15:O:130:HIS:HE1	1.72	0.49
48:BA:61:GLN:OE1	48:BA:61:GLN:HA	2.12	0.49
51:BD:148:ALA:HA	51:BD:168:ARG:HD2	1.95	0.49
8:H:81:THR:HG21	8:H:228:PHE:CD1	2.47	0.49
11:K:9:PHE:O	11:K:12:ILE:HG22	2.12	0.49
12:L:64:TRP:H	12:L:73:SER:HA	1.78	0.49
48:AA:116:PHE:HE1	48:AA:244:LEU:HD22	1.77	0.49
48:AA:481:LEU:HD21	48:AA:499:SER:HA	1.94	0.49
49:AB:98:ARG:HH11	49:AB:98:ARG:HG3	1.76	0.49
48:BA:481:LEU:HD22	48:BA:482:THR:H	1.78	0.49
12:L:212:ASN:HB3	38:m:54:LYS:HZ3	1.77	0.49
12:L:543:GLN:NE2	39:n:40:ILE:CG2	2.74	0.49
14:N:324:ILE:O	14:N:327:VAL:HG22	2.13	0.49
16:P:161:HIS:HA	16:P:203:ALA:HB2	1.95	0.49
16:P:186:LEU:HA	16:P:218:ARG:HB3	1.94	0.49
27:a:9:MET:HA	27:a:9:MET:HE3	1.94	0.49
48:AA:333:MET:HE2	48:AA:333:MET:HA	1.95	0.49
49:AB:143:LEU:HD11	49:AB:270:ILE:HD11	1.95	0.49
50:AC:55:PHE:HZ	75:BC:404:UQ7:H311	1.76	0.49
50:AC:245:PHE:HZ	65:AC:405:3PH:H372	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:AC:410:PC7:H61	53:AF:78:TYR:OH	2.13	0.49
55:BH:10:LYS:O	55:BH:14:GLU:HG2	2.13	0.49
7:G:119:MET:HG2	7:G:184:GLN:HE22	1.79	0.48
13:M:208:PHE:CD2	76:M:647:HOH:O	2.66	0.48
13:M:469:TRP:CD1	65:M:501:3PH:H351	2.49	0.48
34:i:69:ILE:HG23	76:i:105:HOH:O	2.12	0.48
49:AB:367:LYS:HD3	49:AB:390:GLU:HA	1.95	0.48
51:AD:166:LYS:HG3	50:BC:269:MET:SD	2.52	0.48
4:D:312:HIS:ND1	76:D:512:HOH:O	2.34	0.48
8:H:290:TYR:N	76:H:517:HOH:O	2.46	0.48
13:M:45:SER:HB2	13:M:102:PRO:HG3	1.94	0.48
47:z:180:VAL:HG13	76:z:422:HOH:O	2.12	0.48
50:AC:386:TYR:CE1	76:AC:501:HOH:O	2.66	0.48
67:AC:403:UQ5:H151	67:AC:403:UQ5:H171	1.55	0.48
48:BA:96:ASN:HD21	48:BA:98:ALA:HB3	1.78	0.48
50:BC:371:ILE:O	50:BC:374:ILE:HG13	2.12	0.48
51:BD:237:HIS:HB2	61:BD:301:FES:S2	2.53	0.48
11:K:53:LEU:HD13	14:N:202:GLY:HA2	1.95	0.48
11:K:73:SER:HB2	76:K:337:HOH:O	2.12	0.48
12:L:226:PHE:CD1	12:L:286:ILE:HG12	2.47	0.48
16:P:173:GLU:OE2	16:P:173:GLU:HA	2.13	0.48
20:T:41:LEU:HD21	20:T:45:ALA:C	2.38	0.48
21:U:91:MET:HE2	23:W:34:CYS:HB3	1.95	0.48
24:X:19:THR:HG21	24:X:87:ASN:HB3	1.94	0.48
41:p:77:TYR:CE1	41:p:81:THR:HG21	2.48	0.48
48:AA:134:ARG:HD3	48:AA:139:LEU:HD13	1.95	0.48
48:BA:155:SER:HA	48:BA:230:LEU:HD21	1.96	0.48
13:M:284:TYR:CD2	13:M:414:VAL:HG11	2.49	0.48
14:N:486:LEU:N	76:N:622:HOH:O	2.40	0.48
40:o:77:ARG:HD3	40:o:80:GLU:OE2	2.13	0.48
46:y:251:GLU:OE1	46:y:251:GLU:HA	2.13	0.48
48:BA:312:VAL:CG2	48:BA:483:MET:HE1	2.43	0.48
48:BA:420:LYS:HE2	48:BA:464:LEU:HB2	1.95	0.48
50:BC:377:ARG:HA	50:BC:380:ARG:HD2	1.95	0.48
7:G:714:PRO:O	7:G:716:GLN:NE2	2.45	0.48
76:G:986:HOH:O	18:R:88:CYS:SG	2.60	0.48
15:O:37:GLY:C	15:O:39:LYS:H	2.22	0.48
48:AA:91:SER:OG	48:AA:267:HIS:ND1	2.29	0.48
49:AB:63:ASN:CG	49:AB:66:LYS:HE2	2.38	0.48
72:AC:409:CDL:H222	72:AC:409:CDL:H191	1.56	0.48
4:D:341:PHE:HB3	4:D:354:LYS:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:102:ASP:HB2	27:a:38:LYS:HE2	1.94	0.48
8:H:110:LEU:HD11	8:H:167:LEU:HD11	1.95	0.48
11:K:51:VAL:HA	31:e:7:ILE:HD13	1.96	0.48
14:N:323:SER:O	14:N:327:VAL:HG13	2.13	0.48
14:N:390:THR:HG21	14:N:469:LEU:HG	1.95	0.48
76:N:787:HOH:O	15:O:158:ILE:HG13	2.13	0.48
48:BA:122:LEU:HG	48:BA:245:LEU:HD11	1.95	0.48
10:J:28:LEU:HB3	72:u:101:CDL:H342	1.96	0.48
13:M:189:LEU:HD22	14:N:415:PHE:HD2	1.77	0.48
13:M:218:ILE:HD13	60:M:503:PTY:H312	1.95	0.48
14:N:412[A]:TYR:CZ	14:N:416:ALA:HB2	2.49	0.48
14:N:484:SER:OG	30:d:57:LYS:NZ	2.38	0.48
22:V:134:ARG:NH1	76:V:203:HOH:O	2.30	0.48
29:c:31:LYS:HD3	29:c:32:HIS:CE1	2.48	0.48
40:o:69:ARG:HG3	76:o:231:HOH:O	2.12	0.48
45:x:129:SER:CB	76:x:454:HOH:O	2.59	0.48
47:z:77:SER:OG	47:z:95:GLY:O	2.31	0.48
47:z:89:VAL:HG11	47:z:117:VAL:HG21	1.96	0.48
49:BB:86:ALA:HB1	49:BB:88:HIS:CE1	2.49	0.48
65:BC:405:3PH:H2C1	72:BE:402:CDL:H232	1.95	0.48
4:D:243:ASP:OD1	76:D:501:HOH:O	2.20	0.48
8:H:287:PHE:CZ	9:I:76:MET:HE3	2.48	0.48
64:H:402:Q7G:O3B	64:H:402:Q7G:O2	2.31	0.48
12:L:120:PHE:CE1	12:L:256:ILE:HG13	2.49	0.48
12:L:342:ALA:HA	76:L:954:HOH:O	2.13	0.48
13:M:79:ASN:CG	34:i:40:ILE:CG1	2.78	0.48
13:M:458:PHE:HA	13:M:461:ILE:HD12	1.94	0.48
25:Y:9:LEU:CD2	55:AH:20:LYS:CG	2.88	0.48
45:x:155:THR:HG21	76:x:311:HOH:O	2.14	0.48
48:BA:120:THR:HG23	48:BA:159:MET:SD	2.53	0.48
48:BA:383:ILE:HG13	48:BA:403:LEU:HD21	1.95	0.48
76:L:895:HOH:O	13:M:235:ILE:HG23	2.10	0.48
14:N:285:SER:O	14:N:286:TYR:HD1	1.96	0.48
16:P:273:GLY:O	16:P:276:MET:HG3	2.13	0.48
31:e:26:SER:O	34:i:55:THR:HG23	2.13	0.48
39:n:39:HIS:HA	39:n:42:TYR:CD2	2.49	0.48
40:o:36:PRO:HA	76:o:229:HOH:O	2.14	0.48
72:u:101:CDL:HA62	72:u:101:CDL:H311	1.70	0.48
48:AA:335:MET:HE2	48:AA:383:ILE:HD11	1.94	0.48
5:E:133:THR:OG1	6:F:392:ARG:HB3	2.14	0.48
7:G:169:ASP:HA	18:R:99:TYR:OH	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:422:ARG:NH1	7:G:564:ASP:OD2	2.47	0.48
64:H:402:Q7G:C5B	76:H:523:HOH:O	2.61	0.48
10:J:14:GLY:HA3	11:K:16:LEU:HD13	1.95	0.48
13:M:194:GLN:CD	13:M:212:ARG:CD	2.77	0.48
16:P:196:MET:HB3	16:P:342:ASP:OD2	2.13	0.48
38:m:69:LYS:O	76:m:202:HOH:O	2.20	0.48
40:o:8:LYS:HE3	40:o:68:GLU:CD	2.39	0.48
50:BC:314:PHE:CD2	50:BC:373:PRO:HG3	2.48	0.48
52:BE:103:CYS:SG	74:BE:401:HEM:HAB	2.54	0.48
4:D:381:ILE:O	4:D:384:THR:HG22	2.13	0.47
7:G:125:GLU:HB2	7:G:143:LYS:HB2	1.96	0.47
7:G:481:ASP:N	7:G:481:ASP:OD1	2.46	0.47
10:J:57:TYR:OH	76:J:301:HOH:O	2.18	0.47
12:L:458:ASP:HB3	35:j:24:HIS:CE1	2.49	0.47
13:M:207:GLU:HB2	41:p:24:TYR:CG	2.49	0.47
21:U:55:LEU:HD12	21:U:112:ILE:HD13	1.96	0.47
29:c:65:PRO:HG3	29:c:69:ILE:HG12	1.96	0.47
34:i:3:PHE:HD2	34:i:6:GLU:N	2.01	0.47
45:x:241:ILE:HD11	46:y:37:GLU:HB3	1.96	0.47
60:z:301:PTY:H312	60:z:301:PTY:H341	1.63	0.47
48:AA:427:VAL:HG21	48:AA:457:PHE:CE1	2.49	0.47
55:AH:27:GLU:HG3	55:AH:48:GLN:HG2	1.95	0.47
11:K:72:GLU:CG	76:K:338:HOH:O	2.44	0.47
12:L:640:CYS:SG	14:N:222:ARG:NH2	2.87	0.47
12:L:663:TYR:HB2	25:Y:107:LEU:HD13	1.96	0.47
25:Y:47:GLU:CD	25:Y:57:ARG:HH22	2.18	0.47
40:o:39:LYS:CE	76:o:229:HOH:O	2.38	0.47
46:y:180:VAL:HG12	46:y:190:ARG:O	2.14	0.47
48:BA:167:LYS:HG2	48:BA:264:GLY:O	2.14	0.47
76:F:686:HOH:O	7:G:164:MET:HE2	2.13	0.47
12:L:230:VAL:HG13	12:L:235:GLN:HB2	1.95	0.47
12:L:639:PHE:CD2	14:N:289:THR:HG23	2.49	0.47
42:q:32:ARG:HD2	42:q:32:ARG:HA	1.68	0.47
51:AD:171:PRO:HG2	51:AD:221:ILE:HD13	1.96	0.47
52:AE:115:ARG:NH1	76:AE:523:HOH:O	2.40	0.47
48:BA:158:GLN:OE1	48:BA:443:ARG:HD3	2.14	0.47
51:BD:91:ILE:CD1	54:BG:13:TYR:HB3	2.40	0.47
66:BD:302:PC7:H122	66:BD:302:PC7:H32	1.55	0.47
52:BE:226:MET:HB2	74:BE:401:HEM:C1D	2.49	0.47
4:D:11:PHE:CE1	4:D:32:MET:HB2	2.49	0.47
6:F:416:TRP:NE1	6:F:420:GLU:OE2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:d:101:PTY:H111	60:d:101:PTY:H142	1.59	0.47
41:p:26:ASP:HB3	41:p:29:ALA:HB3	1.96	0.47
50:AC:13:GLN:HE21	53:BF:121:ILE:H	1.61	0.47
56:BI:68:ARG:HG2	76:BI:105:HOH:O	2.14	0.47
2:B:110:ARG:HA	8:H:40:PRO:HA	1.95	0.47
11:K:28:ILE:HD13	11:K:80:PHE:CE2	2.50	0.47
11:K:61:PHE:CG	14:N:146:ILE:HG12	2.49	0.47
16:P:194:SER:OG	16:P:342:ASP:CG	2.55	0.47
16:P:252:LYS:HB2	16:P:352:LEU:HD11	1.96	0.47
31:e:25:MET:HE3	34:i:54:TRP:CD1	2.50	0.47
37:l:120:GLU:OE2	40:o:14:GLN:HG2	2.14	0.47
66:v:201:PC7:H212	46:y:11:VAL:HG11	1.97	0.47
48:AA:300:ARG:HH22	48:AA:494:SER:HA	1.78	0.47
48:AA:350:MET:HG2	48:AA:355:TYR:CZ	2.50	0.47
49:AB:63:ASN:OD1	49:AB:66:LYS:HE2	2.15	0.47
3:C:177:TYR:CE2	17:Q:103:ASP:O	2.66	0.47
4:D:297:PRO:HG3	76:D:515:HOH:O	2.13	0.47
4:D:307:GLU:HG2	7:G:191:ASP:O	2.15	0.47
14:N:289:THR:O	14:N:293:ILE:HG12	2.14	0.47
72:u:102:CDL:H251	72:u:102:CDL:H222	1.57	0.47
48:AA:109:SER:HA	48:AA:112:GLU:HG3	1.95	0.47
49:AB:247:LEU:HD21	49:AB:399:TYR:CD2	2.49	0.47
50:AC:208:HIS:NE2	67:AC:403:UQ5:H4M3	2.30	0.47
51:AD:188:VAL:HG11	51:AD:248:ARG:NH2	2.30	0.47
51:AD:236:CYS:SG	50:BC:275:ILE:HD12	2.54	0.47
56:AI:58:ARG:HB2	56:AI:61:ASP:OD1	2.15	0.47
56:AI:62:ILE:HA	76:AI:215:HOH:O	2.13	0.47
2:B:88:THR:HB	2:B:98:MET:HE3	1.96	0.47
7:G:224:CYS:HA	7:G:267:ILE:HD11	1.97	0.47
8:H:54:ASP:HB3	63:H:401:UQ9:H7A	1.95	0.47
8:H:109:TYR:CZ	8:H:113:ILE:HD11	2.49	0.47
12:L:483:ASP:OD2	40:o:41:ARG:HD3	2.15	0.47
24:X:51:ASP:N	24:X:51:ASP:OD1	2.47	0.47
29:c:81:LYS:HG3	41:p:57:TRP:CZ3	2.49	0.47
48:AA:306:GLU:OE1	48:AA:306:GLU:N	2.48	0.47
49:AB:85:LEU:HD13	49:AB:440:THR:HG23	1.96	0.47
49:AB:325:GLU:CD	49:AB:327:ARG:HE	2.23	0.47
49:AB:505:ILE:HD11	49:AB:522:PHE:CB	2.43	0.47
51:AD:99:GLU:HA	76:AG:214:HOH:O	2.14	0.47
48:BA:96:ASN:O	48:BA:167:LYS:HD3	2.15	0.47
48:BA:184:PRO:HG2	48:BA:249:MET:SD	2.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:BB:196:VAL:O	49:BB:200:ILE:HG23	2.15	0.47
76:BB:902:HOH:O	66:BD:302:PC7:H72	2.14	0.47
50:BC:50:ILE:HA	74:BC:402:HEM:HAB	1.96	0.47
50:BC:80:GLY:C	76:BC:557:HOH:O	2.57	0.47
50:BC:116:ARG:HD2	76:BC:616:HOH:O	2.14	0.47
50:BC:142:TRP:HH2	50:BC:177:VAL:HG12	1.78	0.47
72:BE:402:CDL:H141	72:BE:402:CDL:H111	1.62	0.47
3:C:67:ARG:O	76:C:201:HOH:O	2.20	0.47
4:D:233:LEU:HB2	4:D:332:GLU:HB2	1.97	0.47
6:F:64:ILE:HG21	6:F:273:VAL:HG12	1.97	0.47
10:J:149:PHE:N	76:J:310:HOH:O	2.47	0.47
13:M:95:ILE:HG22	65:M:501:3PH:C2H	2.34	0.47
14:N:216:TYR:O	14:N:217:GLU:C	2.57	0.47
14:N:495:LEU:HB2	30:d:63:MET:HE2	1.97	0.47
16:P:301:ILE:HG13	16:P:303:GLU:HB2	1.96	0.47
31:e:23:GLU:OE1	31:e:27:HIS:NE2	2.48	0.47
42:q:39:LEU:HB3	76:q:216:HOH:O	2.15	0.47
46:y:47:ASN:ND2	76:y:421:HOH:O	2.46	0.47
49:AB:290:GLU:O	49:AB:294:GLU:HG2	2.15	0.47
53:AF:8:LEU:CD2	76:AF:392:HOH:O	2.63	0.47
48:BA:353:TRP:HE3	48:BA:357:ARG:HG3	1.78	0.47
50:BC:126:ILE:HG23	50:BC:196:LEU:HD11	1.97	0.47
8:H:95:ASP:HB3	8:H:98:MET:HG3	1.97	0.47
10:J:53:PHE:O	10:J:57:TYR:HB2	2.15	0.47
25:Y:13:ASP:HA	25:Y:18:LYS:HE2	1.96	0.47
41:p:82:ARG:NH2	76:p:205:HOH:O	2.46	0.47
47:z:32:LYS:HB3	47:z:34:TYR:HD2	1.77	0.47
49:AB:502:ASP:H	49:AB:526:THR:HG22	1.80	0.47
50:AC:294:LYS:HE2	50:AC:294:LYS:HB3	1.72	0.47
58:AC:407:PGT:H181	58:AC:407:PGT:H212	1.75	0.47
49:BB:178:GLN:HG2	76:BB:782:HOH:O	2.15	0.47
49:BB:359:GLN:NE2	49:BB:395:PHE:CA	2.71	0.47
50:BC:291:ILE:HG22	50:BC:293:ASP:H	1.80	0.47
5:E:133:THR:CG2	76:F:739:HOH:O	2.63	0.47
6:F:132:ARG:HG2	17:Q:146:TRP:CE3	2.50	0.47
6:F:283:GLU:HG2	76:F:699:HOH:O	2.13	0.47
10:J:111:PRO:HG2	43:u:29:ALA:HB2	1.97	0.47
13:M:224:PHE:O	13:M:228:VAL:HG23	2.15	0.47
14:N:31:ILE:HG12	65:f:201:3PH:H3C2	1.97	0.47
36:k:13:ARG:HG2	36:k:13:ARG:NH1	2.25	0.47
40:o:8:LYS:CD	40:o:68:GLU:OE2	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:AA:225:PRO:HG2	48:AA:290:PRO:HB2	1.97	0.47
49:AB:149:LYS:NZ	49:AB:214:GLU:OE2	2.46	0.47
48:BA:196:ARG:HG2	48:BA:196:ARG:NH1	2.29	0.47
49:BB:154:ARG:NH2	49:BB:195:ASP:OD2	2.48	0.47
51:BD:165:VAL:HG23	51:BD:172:VAL:HB	1.97	0.47
53:BF:27:ARG:CG	60:BF:201:PTY:N1	2.69	0.47
76:L:895:HOH:O	13:M:235:ILE:HG21	2.13	0.46
13:M:395:SER:HB3	13:M:470:MET:HB3	1.95	0.46
45:x:54:TRP:HB3	76:z:494:HOH:O	2.14	0.46
48:AA:78:LEU:HD21	48:AA:445:ILE:HD11	1.97	0.46
48:AA:121:HIS:O	48:AA:125:ARG:HG2	2.15	0.46
65:AI:101:3PH:H32	65:AI:101:3PH:H321	1.48	0.46
49:BB:277:SER:CB	76:BB:917:HOH:O	2.57	0.46
50:BC:277:PRO:HB3	75:BC:404:UQ7:H71	1.96	0.46
52:BE:297:LYS:HE2	53:BF:74:MET:O	2.15	0.46
1:A:1:FME:O	76:A:301:HOH:O	2.20	0.46
4:D:15:PHE:CD2	8:H:212:LEU:CB	2.97	0.46
6:F:104:LYS:HG2	6:F:119:GLY:HA3	1.96	0.46
14:N:282:ILE:CD1	14:N:342:ILE:HD11	2.45	0.46
60:d:101:PTY:H201	60:d:101:PTY:H172	1.45	0.46
43:u:41:LYS:HE3	43:u:41:LYS:HB3	1.75	0.46
44:v:86:VAL:HA	66:v:201:PC7:H141	1.96	0.46
48:AA:58:MET:HA	48:AA:58:MET:HE3	1.97	0.46
52:AE:143:GLU:H	52:AE:143:GLU:CD	2.23	0.46
53:AF:111:LEU:HD12	48:BA:137:PHE:CE2	2.50	0.46
13:M:458:PHE:CZ	33:g:66:CYS:HB3	2.50	0.46
33:g:83:ALA:HA	34:i:9:GLU:OE2	2.16	0.46
43:u:45:VAL:CG2	55:AH:23:LYS:HA	2.44	0.46
43:u:49:ARG:HG3	55:AH:22:VAL:CG2	2.45	0.46
76:AC:523:HOH:O	53:AF:67:MET:CG	2.63	0.46
48:BA:326:VAL:HG22	48:BA:457:PHE:CE2	2.50	0.46
1:A:89:ASP:HB3	58:A:201:PGT:H61	1.97	0.46
6:F:334:TRP:O	6:F:352:LYS:NZ	2.47	0.46
6:F:362:PHE:O	6:F:366:LYS:HB2	2.16	0.46
9:I:99:GLU:OE2	42:q:75[B]:TRP:NE1	2.49	0.46
12:L:439:PHE:CD1	12:L:443:LEU:HD12	2.50	0.46
13:M:200:LEU:HD21	13:M:266:ARG:HD2	1.97	0.46
14:N:285:SER:HA	76:N:749:HOH:O	2.16	0.46
66:d:102:PC7:H171	66:d:102:PC7:H201	1.59	0.46
39:n:39:HIS:CE1	39:n:40:ILE:HG13	2.50	0.46
51:AD:159:PRO:HG3	51:AD:176:ARG:HD3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:129:GLY:HA2	59:B:500:SF4:S3	2.56	0.46
5:E:205:LYS:HE2	5:E:205:LYS:HB2	1.61	0.46
11:K:52:SER:HB2	26:Z:138:LEU:HD11	1.98	0.46
12:L:21:ARG:HD2	76:c:120:HOH:O	2.16	0.46
13:M:99:PHE:CG	65:M:501:3PH:H2E2	2.51	0.46
15:O:127:LEU:O	21:U:40:VAL:HG22	2.11	0.46
23:W:46:LEU:HD11	23:W:100:ILE:HD11	1.96	0.46
33:g:100:ARG:NE	76:g:208:HOH:O	2.49	0.46
39:n:103:ALA:HB3	76:n:205:HOH:O	2.14	0.46
49:AB:245:THR:HG21	49:AB:320:SER:H	1.80	0.46
49:AB:382:ARG:HG2	50:AC:6:GLN:NE2	2.31	0.46
72:AC:409:CDL:H441	54:AG:49:VAL:HG21	1.96	0.46
51:AD:221:ILE:HB	50:BC:271:THR:OG1	2.15	0.46
6:F:476:ARG:HB3	76:F:633:HOH:O	2.15	0.46
9:I:154:ARG:NH2	17:Q:89:MET:O	2.49	0.46
12:L:519:LEU:O	12:L:522:ILE:HG12	2.15	0.46
32:f:20:PRO:HD2	32:f:86:MET:HE3	1.97	0.46
50:AC:219:HIS:CE1	53:AF:42:LEU:HG	2.51	0.46
50:BC:26:TYR:CD2	67:BC:403:UQ5:H3M1	2.47	0.46
50:BC:213:ASN:HB3	76:BC:616:HOH:O	2.12	0.46
3:C:25:SER:HB3	22:V:122:ASN:HB3	1.96	0.46
11:K:11:MET:HE1	14:N:192:PHE:CZ	2.51	0.46
14:N:242:THR:HG22	14:N:249:TRP:CZ2	2.50	0.46
33:g:92:TRP:CZ3	41:p:39:ARG:HG2	2.51	0.46
45:x:152:ARG:NH2	73:y:302:COO:C9	2.79	0.46
45:x:231:TYR:HE2	47:z:68:ILE:HG21	1.81	0.46
48:AA:159:MET:HE1	48:AA:253:PHE:CE1	2.49	0.46
76:AC:523:HOH:O	53:AF:67:MET:HG3	2.15	0.46
49:BB:424:MET:HE2	76:BB:933:HOH:O	2.15	0.46
2:B:111:PHE:HB2	2:B:113:ILE:HD12	1.98	0.46
5:E:132:THR:HB	76:E:679:HOH:O	2.14	0.46
12:L:242:LEU:HD11	12:L:257:HIS:HB3	1.97	0.46
12:L:639:PHE:HZ	14:N:292:GLN:HB3	1.81	0.46
15:O:128:ASN:HB2	21:U:41:ARG:HH21	1.81	0.46
16:P:104:ASP:HB3	76:P:630:HOH:O	2.16	0.46
22:V:56:ALA:HB2	22:V:149:LEU:HD11	1.98	0.46
24:X:40:LYS:HD2	24:X:40:LYS:HA	1.79	0.46
40:o:8:LYS:CD	40:o:68:GLU:CD	2.88	0.46
40:o:64:GLU:OE2	76:o:201:HOH:O	2.20	0.46
48:AA:310:PHE:CZ	48:AA:385:GLY:HA3	2.51	0.46
49:AB:98:ARG:O	49:AB:109:ALA:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:AE:277:LEU:HD22	66:AG:101:PC7:H242	1.98	0.46
55:BH:31:CYS:O	55:BH:35:ILE:HG12	2.15	0.46
7:G:408:VAL:HG13	7:G:408:VAL:O	2.16	0.46
10:J:100:GLU:OE1	12:L:641:MET:HE3	2.15	0.46
13:M:184:MET:CB	13:M:223:SER:OG	2.59	0.46
20:T:41:LEU:HD21	20:T:46:VAL:N	2.31	0.46
29:c:30:PRO:HG2	29:c:33:TRP:HB3	1.98	0.46
45:x:79:ALA:HB3	45:x:82:VAL:HG23	1.98	0.46
50:AC:90:ASN:O	50:AC:94:MET:HG2	2.16	0.46
51:AD:179:GLU:HA	51:AD:182:ILE:HD12	1.97	0.46
51:BD:121:PHE:HE1	56:BI:31:ILE:HA	1.81	0.46
51:BD:157:ILE:HG13	51:BD:158:GLU:H	1.81	0.46
7:G:489:PRO:HB3	7:G:710:MET:SD	2.56	0.46
8:H:36:ARG:HH11	8:H:36:ARG:HG2	1.79	0.46
12:L:60:ARG:HH12	12:L:63:PRO:HD3	1.80	0.46
16:P:76:ALA:HB3	16:P:97:VAL:HG13	1.98	0.46
30:d:29:MET:HE3	30:d:29:MET:HB3	1.83	0.46
45:x:197:LEU:HB2	45:x:209:LEU:HD21	1.98	0.46
45:x:244:GLU:OE1	45:x:244:GLU:HA	2.15	0.46
48:AA:122:LEU:HD22	48:AA:240:LEU:HD23	1.98	0.46
56:AI:54:ASN:HA	76:AI:213:HOH:O	2.16	0.46
3:C:180:PHE:CE1	7:G:285:TRP:CG	3.05	0.45
4:D:15:PHE:HE2	4:D:375:LEU:HD11	1.81	0.45
6:F:193:GLU:HG3	6:F:197:ARG:NH1	2.31	0.45
13:M:403:ILE:HD12	76:M:744:HOH:O	2.15	0.45
16:P:69:ILE:HD12	16:P:91:MET:HE1	1.98	0.45
31:e:43:GLU:HB2	31:e:49:LYS:NZ	2.31	0.45
46:y:23:ASP:CG	76:y:420:HOH:O	2.59	0.45
49:BB:98:ARG:HG3	49:BB:98:ARG:HH11	1.81	0.45
52:BE:237:TYR:HB3	52:BE:239:ASP:OD1	2.15	0.45
53:BF:23:SER:CB	60:BF:201:PTY:HC52	2.45	0.45
56:BI:19:LEU:HB3	56:BI:26:VAL:HG11	1.96	0.45
7:G:302:ASN:HB3	7:G:318:ARG:HB3	1.98	0.45
7:G:645:PRO:HG3	17:Q:83:LYS:HG2	1.97	0.45
13:M:304:LEU:HD21	13:M:436:VAL:HG21	1.98	0.45
14:N:280:VAL:HG12	14:N:281:PHE:CD1	2.51	0.45
27:a:52:ARG:O	27:a:56:VAL:HG23	2.16	0.45
33:g:48:ARG:O	76:g:202:HOH:O	2.21	0.45
72:u:101:CDL:H442	72:u:101:CDL:H412	1.65	0.45
48:BA:412:ASN:OD1	48:BA:412:ASN:N	2.46	0.45
72:BE:402:CDL:H621	54:BG:31:PRO:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:192:MET:HG3	76:D:678:HOH:O	2.15	0.45
10:J:11:LEU:HG	11:K:12:ILE:HG12	1.98	0.45
12:L:653:LEU:CD2	25:Y:76:TYR:HD2	2.29	0.45
13:M:99:PHE:CZ	65:M:501:3PH:H2E2	2.51	0.45
13:M:448:LYS:HG2	38:m:5:MET:HG2	1.98	0.45
14:N:73:ALA:HB3	14:N:74:PRO:HD3	1.99	0.45
14:N:166:LYS:O	14:N:172:SER:HB3	2.16	0.45
34:i:3:PHE:CD2	34:i:5:MET:N	2.85	0.45
66:v:201:PC7:H482	46:y:14:TRP:HB3	1.98	0.45
46:y:107:HIS:CG	46:y:108:VAL:H	2.34	0.45
50:AC:317:MET:SD	76:AC:589:HOH:O	2.61	0.45
66:AC:410:PC7:H322	66:AC:410:PC7:H2	1.78	0.45
48:BA:413:GLN:OE1	48:BA:413:GLN:HA	2.16	0.45
50:BC:154:THR:HG21	50:BC:171:LEU:CD2	2.40	0.45
72:BC:408:CDL:H141	66:BC:409:PC7:H141	1.97	0.45
72:BC:408:CDL:H161	54:BG:48:LEU:HD21	1.97	0.45
51:BD:78:PRO:CB	52:BE:304:ASP:OD1	2.64	0.45
53:BF:98:LEU:O	53:BF:102:LYS:HD3	2.17	0.45
56:BI:68:ARG:CG	76:BI:105:HOH:O	2.63	0.45
4:D:26:LEU:HD21	4:D:382:ILE:HD13	1.98	0.45
6:F:343:GLY:HA3	6:F:372:LEU:O	2.15	0.45
12:L:488:LEU:HD12	12:L:506:LEU:HD23	1.98	0.45
19:S:64:TYR:CE1	19:S:94:ALA:HB2	2.52	0.45
25:Y:124:LEU:HD23	25:Y:124:LEU:HA	1.81	0.45
40:o:40:CYS:O	40:o:44:GLU:HG2	2.17	0.45
51:AD:121:PHE:HE2	66:AG:101:PC7:H442	1.82	0.45
48:BA:333:MET:HG2	48:BA:422:ALA:HB3	1.98	0.45
51:BD:205:ASN:HD22	51:BD:208:TRP:HD1	1.64	0.45
55:BH:21:CYS:O	55:BH:24:PRO:HD2	2.16	0.45
4:D:293:LYS:HG2	4:D:293:LYS:O	2.16	0.45
6:F:408:CYS:HB3	59:F:501:SF4:S4	2.56	0.45
6:F:456:TRP:CD2	76:F:723:HOH:O	2.55	0.45
7:G:408:VAL:CG1	76:G:904:HOH:O	2.64	0.45
67:L:707:UQ5:H101	67:L:707:UQ5:H121	1.41	0.45
18:R:52:SER:OG	18:R:55:GLU:HG3	2.16	0.45
21:U:91:MET:HE2	23:W:34:CYS:SG	2.56	0.45
31:e:21:PHE:CE1	31:e:38:ARG:HB2	2.52	0.45
39:n:56:GLN:HG3	39:n:57:ASP:OD1	2.16	0.45
60:z:301:PTY:H151	60:z:301:PTY:H122	1.75	0.45
48:AA:372:THR:CG2	48:AA:374:ILE:HD13	2.44	0.45
50:AC:48:ILE:HA	72:AC:408:CDL:H841	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:AE:143:GLU:CD	52:AE:143:GLU:N	2.75	0.45
48:BA:455:ASP:O	48:BA:459:LYS:HG3	2.17	0.45
7:G:402:ARG:CZ	7:G:666:VAL:HG13	2.47	0.45
8:H:15:PRO:HB2	27:a:22:MET:HG2	1.98	0.45
14:N:284:GLY:N	76:N:627:HOH:O	2.47	0.45
15:O:101:GLU:HA	15:O:104:LEU:HB2	1.99	0.45
16:P:135:MET:HE1	16:P:171:ALA:CA	2.45	0.45
43:u:44:GLU:C	55:AH:26:LEU:CD1	2.90	0.45
49:AB:112:SER:OG	49:AB:287:VAL:O	2.28	0.45
50:AC:123:GLY:O	74:AC:401:HEM:HMC3	2.17	0.45
52:AE:201:ARG:NH2	52:AE:218:TYR:OH	2.49	0.45
49:BB:48:PRO:HG2	49:BB:51:LEU:HB2	1.98	0.45
16:P:194:SER:HA	16:P:342:ASP:OD1	2.16	0.45
24:X:41:LYS:HD3	34:i:83:LEU:HD12	1.98	0.45
36:k:5:LEU:HD23	36:k:5:LEU:HA	1.72	0.45
72:u:101:CDL:H582	72:u:101:CDL:H551	1.73	0.45
48:AA:397:GLU:HG3	48:AA:501:LYS:HZ1	1.82	0.45
50:AC:19:LEU:O	50:AC:23:LEU:HB2	2.17	0.45
49:BB:293:VAL:HG12	49:BB:297:LYS:HE3	1.99	0.45
5:E:215:LYS:HD3	5:E:215:LYS:HA	1.67	0.45
6:F:84:ASP:OD1	6:F:160:LYS:HG2	2.16	0.45
7:G:364:ALA:O	7:G:368:VAL:HG23	2.17	0.45
8:H:254:ILE:O	8:H:255:LEU:HD23	2.16	0.45
10:J:48:PHE:CD1	10:J:137:LEU:HD13	2.51	0.45
13:M:147[A]:GLU:OE2	13:M:181:SER:HB2	2.16	0.45
20:T:41:LEU:CD2	20:T:46:VAL:N	2.80	0.45
20:T:41:LEU:HD12	20:T:49:ARG:HH21	1.68	0.45
48:AA:112:GLU:OE1	48:AA:118:GLY:N	2.39	0.45
72:AC:409:CDL:H401	72:AC:409:CDL:H431	1.47	0.45
48:BA:156:ARG:HD2	76:BA:663:HOH:O	2.17	0.45
49:BB:357:VAL:O	49:BB:361:MET:HG3	2.16	0.45
51:BD:91:ILE:HD13	51:BD:93:TYR:CZ	2.52	0.45
12:L:137:PHE:O	12:L:141:GLU:HG2	2.17	0.45
13:M:34:ILE:HD11	13:M:112:MET:HB3	1.98	0.45
14:N:24:PHE:CD1	32:f:71:MET:HE3	2.51	0.45
20:T:120:MET:HE2	39:n:88:TRP:NE1	2.32	0.45
34:i:31:TYR:O	34:i:35:GLU:HG2	2.16	0.45
43:u:5:LEU:HD22	72:u:102:CDL:H772	1.99	0.45
49:AB:290:GLU:N	49:AB:290:GLU:CD	2.75	0.45
52:AE:164:GLU:CD	52:AE:168:ARG:HE	2.24	0.45
55:BH:44:HIS:CE1	55:BH:46:THR:HB	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:BI:59:TYR:OH	76:BI:101:HOH:O	2.20	0.45
3:C:9:TYR:CZ	3:C:13:THR:HG21	2.51	0.45
66:L:706:PC7:H63	66:L:706:PC7:H41	1.66	0.45
13:M:76:PRO:HB2	30:d:57:LYS:HE2	1.99	0.45
36:k:16:ASP:OD1	36:k:19:ARG:NE	2.47	0.45
60:z:301:PTY:H111	60:z:301:PTY:HC6	1.93	0.45
48:AA:157:GLU:OE2	48:AA:375:PHE:HB3	2.17	0.45
55:AH:39:ASP:HB2	55:AH:43:LYS:HD2	1.97	0.45
48:BA:351:HIS:HB2	49:BB:164:GLU:OE2	2.17	0.45
49:BB:421:TYR:CE1	50:BC:9:SER:HB2	2.52	0.45
52:BE:106:CYS:SG	74:BE:401:HEM:CAC	3.05	0.45
72:BG:101:CDL:H431	72:BG:101:CDL:H401	1.44	0.45
20:T:72:GLN:HG2	20:T:77:LEU:O	2.17	0.44
25:Y:37:LEU:O	25:Y:41:LYS:HG3	2.17	0.44
39:n:66:LYS:HE2	48:AA:57:ASP:CG	2.43	0.44
72:AC:408:CDL:H751	51:AD:127:LEU:HB2	1.99	0.44
56:AI:60:GLU:CD	56:AI:60:GLU:H	2.26	0.44
13:M:68:PHE:O	13:M:69:VAL:C	2.59	0.44
43:u:9:GLY:HA3	72:u:102:CDL:H561	1.99	0.44
66:AG:101:PC7:H142	66:AG:101:PC7:H362	1.99	0.44
50:BC:200:SER:HB3	67:BC:403:UQ5:H161	1.98	0.44
52:BE:297:LYS:O	53:BF:75:LYS:HE2	2.16	0.44
2:B:90:GLY:HA3	4:D:20:PRO:HD3	1.99	0.44
60:D:401:PTY:H232	8:H:188:VAL:HG22	2.00	0.44
6:F:407:PRO:HG2	6:F:446:THR:HG22	1.98	0.44
13:M:194:GLN:HE21	13:M:194:GLN:HB3	1.68	0.44
13:M:265:LEU:HG	13:M:323:MET:CE	2.47	0.44
30:d:34:GLU:OE2	60:z:301:PTY:H131	2.17	0.44
45:x:244:GLU:OE1	45:x:247:LYS:HD2	2.18	0.44
52:AE:207:ILE:HD13	52:AE:207:ILE:HA	1.83	0.44
66:AG:101:PC7:H41	66:AG:101:PC7:H62	1.58	0.44
48:BA:116:PHE:CZ	48:BA:247:GLU:HG2	2.53	0.44
48:BA:120:THR:HG22	48:BA:154:ALA:HB1	2.00	0.44
5:E:161:ASP:OD1	5:E:161:ASP:N	2.48	0.44
7:G:371:ILE:HD13	7:G:599:PHE:CD1	2.53	0.44
8:H:169:GLU:OE2	26:Z:71:ARG:NH1	2.51	0.44
65:L:701:3PH:H252	65:L:701:3PH:H281	1.87	0.44
15:O:94:GLU:N	76:O:319:HOH:O	2.50	0.44
72:u:102:CDL:H551	72:u:102:CDL:H172	2.00	0.44
49:AB:83:PRO:C	49:AB:84:ILE:HD12	2.43	0.44
50:AC:294:LYS:HD3	51:BD:253:PRO:HG3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:198:PHE:CZ	5:E:219:PRO:HG2	2.53	0.44
8:H:27:GLU:HA	8:H:281:ILE:HD13	1.99	0.44
8:H:79:VAL:HG12	72:u:101:CDL:H592	1.99	0.44
9:I:111:HIS:NE2	59:I:500:SF4:S4	2.91	0.44
11:K:75:ILE:HB	76:K:324:HOH:O	2.17	0.44
12:L:461:ILE:HD13	65:L:701:3PH:O12	2.18	0.44
12:L:616:LEU:HD21	67:L:707:UQ5:H102	1.99	0.44
13:M:414:VAL:HG12	38:m:52:ILE:HG12	1.99	0.44
14:N:121:ASP:OD2	46:y:239:ASP:HB3	2.17	0.44
48:AA:410:LYS:O	48:AA:410:LYS:CG	2.63	0.44
50:AC:154:THR:O	50:AC:168:VAL:HG22	2.17	0.44
52:AE:87:TYR:HB3	52:AE:92:ILE:HD11	1.99	0.44
53:AF:105:ARG:NH1	76:AF:306:HOH:O	2.47	0.44
48:BA:471:ASP:OD1	48:BA:472:PHE:N	2.50	0.44
49:BB:454:MET:HE1	49:BB:463:ASP:CG	2.43	0.44
7:G:702:LEU:HB3	19:S:36:TYR:CD2	2.51	0.44
8:H:80:ALA:HB2	72:u:101:CDL:H591	2.00	0.44
12:L:10:LEU:HD11	58:L:704:PGT:H411	2.00	0.44
60:N:502:PTY:H211	66:f:203:PC7:H411	2.00	0.44
15:O:48:LEU:HB3	15:O:60:ILE:HG12	1.98	0.44
25:Y:18:LYS:HB3	25:Y:77:ILE:HG21	1.99	0.44
33:g:101:LEU:HB2	76:g:225:HOH:O	2.17	0.44
36:k:21:HIS:HB3	36:k:24:LEU:HB2	2.00	0.44
60:z:301:PTY:H141	60:z:301:PTY:H172	1.69	0.44
51:AD:121:PHE:HE1	56:AI:31:ILE:HA	1.82	0.44
50:BC:82:TRP:CG	52:BE:263:GLU:HG3	2.53	0.44
67:BC:403:UQ5:H272	67:BC:403:UQ5:H251	1.63	0.44
51:BD:128:ARG:HD2	57:BJ:36:TRP:CE2	2.52	0.44
52:BE:289:ARG:HE	52:BE:293:TRP:CD1	2.36	0.44
2:B:109:ASP:OD2	2:B:114:ILE:HD11	2.18	0.44
4:D:376:ALA:HB3	8:H:291:ARG:HD2	1.99	0.44
7:G:256:MET:HE2	7:G:261:SER:HB2	2.00	0.44
10:J:140:LEU:HD21	11:K:63:LEU:HD22	1.98	0.44
12:L:555:LEU:HD21	66:L:706:PC7:H361	2.00	0.44
13:M:264:PHE:HB3	13:M:323:MET:SD	2.58	0.44
60:N:501:PTY:H312	60:N:501:PTY:HC11	1.67	0.44
58:y:303:PGT:H171	58:y:303:PGT:H142	1.58	0.44
52:AE:103:CYS:SG	74:AE:401:HEM:CAB	3.06	0.44
54:AG:67:LYS:HE3	54:AG:67:LYS:HB3	1.71	0.44
50:BC:368:PHE:HB2	60:BF:201:PTY:H441	2.00	0.44
2:B:96:VAL:HA	2:B:99:MET:HE3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:2:ASP:O	3:C:6:ILE:HG13	2.18	0.44
4:D:113:ASN:OD1	4:D:335:LYS:NZ	2.51	0.44
7:G:514:ILE:HD11	7:G:542:VAL:HG21	2.00	0.44
7:G:703:LYS:HD3	7:G:703:LYS:HA	1.59	0.44
76:L:814:HOH:O	13:M:235:ILE:HG21	2.17	0.44
13:M:90:SER:O	13:M:94:VAL:HG23	2.17	0.44
13:M:107:VAL:HG21	13:M:350:LEU:CD2	2.45	0.44
14:N:159:PHE:CE2	14:N:269:PRO:HG3	2.52	0.44
15:O:92:SER:HB2	15:O:94:GLU:OE2	2.18	0.44
16:P:269:LEU:HD12	16:P:269:LEU:HA	1.88	0.44
29:c:29:ARG:H	33:g:38:GLU:CD	2.25	0.44
34:i:29:HIS:O	34:i:33:MET:N	2.50	0.44
47:z:32:LYS:HD3	47:z:34:TYR:CE2	2.50	0.44
48:AA:121:HIS:HE1	48:AA:198:MET:HG3	1.80	0.44
50:AC:163:VAL:O	50:AC:166:THR:HG22	2.18	0.44
48:BA:141:ARG:HA	48:BA:141:ARG:HD3	1.78	0.44
49:BB:424:MET:CE	76:BB:933:HOH:O	2.66	0.44
50:BC:222:MET:SD	53:BF:63:ASN:O	2.76	0.44
50:BC:375:LEU:HD23	50:BC:375:LEU:HA	1.79	0.44
1:A:68:PHE:O	1:A:72:ASP:HB2	2.18	0.44
6:F:168:ALA:HB1	6:F:172:MET:HE3	2.00	0.44
6:F:191:ASN:HB2	76:F:732:HOH:O	2.17	0.44
7:G:637:THR:HG22	7:G:690:THR:HG22	1.98	0.44
9:I:86:TYR:HA	9:I:89:ASP:OD2	2.17	0.44
12:L:322:MET:HG3	12:L:337:HIS:HD2	1.83	0.44
12:L:659:VAL:HG11	25:Y:123:THR:CG2	2.46	0.44
14:N:213:LEU:HB3	14:N:285:SER:O	2.18	0.44
31:e:13:ARG:NH1	76:e:104:HOH:O	2.40	0.44
65:f:201:3PH:O13	44:v:81:ASN:ND2	2.51	0.44
38:m:10:ASN:HB3	38:m:13:ILE:HD12	1.99	0.44
40:o:64:GLU:O	40:o:68:GLU:HG3	2.18	0.44
50:AC:13:GLN:NE2	53:BF:121:ILE:H	2.15	0.44
50:AC:115:PRO:HB2	50:AC:210:TYR:CE2	2.53	0.44
52:AE:204:PRO:HD3	52:AE:215:TYR:CZ	2.53	0.44
49:BB:98:ARG:HG3	49:BB:98:ARG:NH1	2.33	0.44
56:BI:22:ARG:CD	76:BI:110:HOH:O	2.65	0.44
6:F:429:LEU:HD22	6:F:470:GLU:HG2	2.00	0.43
7:G:634:GLU:CD	7:G:693:ARG:HH12	2.26	0.43
8:H:202:PRO:HG2	76:H:533:HOH:O	2.18	0.43
12:L:96:VAL:HG21	12:L:255:LEU:HB2	2.00	0.43
12:L:111:PRO:HB2	29:c:23:THR:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:133:PHE:HB3	12:L:182:ILE:HD13	1.99	0.43
50:AC:209:GLN:HE22	53:AF:122:PRO:CB	2.31	0.43
51:AD:176:ARG:HB2	51:AD:208:TRP:CZ3	2.53	0.43
52:AE:98:VAL:HG22	52:AE:235:VAL:HG11	2.00	0.43
48:BA:369:THR:OG1	48:BA:370:ALA:N	2.51	0.43
49:BB:264:GLU:OE2	49:BB:264:GLU:N	2.49	0.43
72:BC:407:CDL:H752	72:BC:407:CDL:H531	2.00	0.43
52:BE:107:HIS:HE1	52:BE:177:PRO:HD2	1.83	0.43
56:BI:48:LYS:HA	56:BI:48:LYS:HD3	1.79	0.43
5:E:67:ASN:O	17:Q:147:LYS:NZ	2.51	0.43
6:F:304:HIS:CD2	6:F:381:ASP:H	2.35	0.43
13:M:179:LEU:HD13	14:N:434:VAL:HG21	2.00	0.43
14:N:299:ILE:HD13	60:N:501:PTY:O30	2.18	0.43
15:O:46:VAL:HA	15:O:144:GLN:NE2	2.32	0.43
23:W:125:LYS:H	23:W:125:LYS:HG2	1.66	0.43
27:a:50:GLU:HG2	76:a:216:HOH:O	2.17	0.43
45:x:69:LEU:HD12	45:x:70:PRO:HD2	2.00	0.43
48:AA:89:ILE:HG23	48:AA:260:LEU:HD23	2.00	0.43
72:AC:408:CDL:H821	72:AC:408:CDL:H792	1.80	0.43
49:BB:259:LYS:HB3	49:BB:259:LYS:HE3	1.71	0.43
51:BD:87:PRO:O	76:BD:402:HOH:O	2.21	0.43
1:A:21:ILE:O	1:A:25:VAL:HG22	2.19	0.43
58:A:201:PGT:H62	32:f:1:FME:CN	2.48	0.43
12:L:377:LEU:HD11	12:L:468:ILE:HD11	2.00	0.43
13:M:20:VAL:O	13:M:24:ILE:HD12	2.18	0.43
13:M:207:GLU:HB2	41:p:24:TYR:CD2	2.53	0.43
13:M:384:PHE:CE1	13:M:467:LEU:HD22	2.53	0.43
14:N:240:LYS:HD2	14:N:240:LYS:HA	1.82	0.43
21:U:74:ASN:OD1	21:U:76:GLN:N	2.51	0.43
30:d:74:ARG:HH22	34:i:47:PRO:HG3	1.82	0.43
43:u:49:ARG:HG3	55:AH:22:VAL:HG23	1.99	0.43
47:z:159:LYS:HG2	47:z:160:HIS:CE1	2.53	0.43
48:AA:387:SER:OG	48:AA:388:SER:N	2.49	0.43
51:AD:171:PRO:HG3	50:BC:269:MET:HE2	2.00	0.43
52:AE:250:LYS:HE3	76:AE:652:HOH:O	2.19	0.43
54:AG:23:MET:HG3	66:AG:101:PC7:H32	2.00	0.43
49:BB:297:LYS:HB3	49:BB:297:LYS:HE2	1.83	0.43
51:BD:199:ASP:O	51:BD:203:VAL:HG22	2.17	0.43
54:BG:21:LYS:HB3	72:BG:101:CDL:HA21	2.01	0.43
1:A:4:GLU:HA	1:A:4:GLU:OE2	2.17	0.43
3:C:43:CYS:SG	76:V:222:HOH:O	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:156:ARG:NE	3:C:167:GLU:OE2	2.51	0.43
11:K:54:ASP:CB	76:K:341:HOH:O	2.53	0.43
12:L:422:LEU:HD23	12:L:422:LEU:HA	1.83	0.43
13:M:237:LEU:HD12	13:M:257:LEU:HD21	2.00	0.43
13:M:326:LEU:HA	13:M:331:ILE:HD11	1.99	0.43
14:N:284:GLY:CA	76:N:627:HOH:O	2.65	0.43
16:P:229:ILE:C	16:P:232:PRO:HD2	2.43	0.43
21:U:111:SER:OG	21:U:113:ASP:OD2	2.31	0.43
39:n:61:VAL:CG1	76:AB:701:HOH:O	2.65	0.43
72:u:102:CDL:H552	72:u:102:CDL:H521	1.65	0.43
48:AA:141:ARG:HD3	48:AA:141:ARG:HA	1.87	0.43
52:AE:187:HIS:HB3	76:AE:664:HOH:O	2.17	0.43
48:BA:440:ASP:CG	48:BA:444:GLN:HE21	2.25	0.43
50:BC:23:LEU:HD11	58:BC:406:PGT:H171	1.99	0.43
1:A:111:TRP:CE2	8:H:301:LYS:HE3	2.53	0.43
2:B:176:ASP:HB2	76:B:631:HOH:O	2.17	0.43
3:C:23:GLU:HA	22:V:120:ILE:O	2.18	0.43
6:F:360:MET:HE3	6:F:360:MET:HB3	1.86	0.43
8:H:28:ARG:NH1	63:H:401:UQ9:H1M	2.33	0.43
13:M:82:PHE:HB3	13:M:141:LEU:CD1	2.48	0.43
13:M:139:LEU:HB3	13:M:188:ILE:HG12	2.01	0.43
13:M:237:LEU:HD11	13:M:257:LEU:HD11	2.01	0.43
65:M:501:3PH:H231	65:M:501:3PH:H262	1.74	0.43
14:N:180:LEU:C	14:N:180:LEU:HD13	2.43	0.43
14:N:495:LEU:HB3	30:d:63:MET:HE2	1.99	0.43
15:O:48:LEU:HD12	15:O:48:LEU:HA	1.85	0.43
21:U:51:THR:OG1	21:U:116:VAL:HG21	2.19	0.43
47:z:57:LYS:HD3	47:z:57:LYS:HA	1.62	0.43
48:AA:178:ILE:HG22	49:AB:75:PHE:HE2	1.83	0.43
48:AA:309:HIS:CE1	48:AA:386:CYS:HG	2.32	0.43
58:AC:406:PGT:H401	58:AC:406:PGT:H371	1.70	0.43
58:AC:407:PGT:H201	52:AE:275:ILE:HG22	2.01	0.43
51:AD:171:PRO:HG2	51:AD:221:ILE:CD1	2.48	0.43
49:BB:331:ASP:HB2	54:BG:7:LYS:CE	2.48	0.43
50:BC:277:PRO:HG3	75:BC:404:UQ7:C1	2.49	0.43
50:BC:369:PHE:CE2	76:BC:635:HOH:O	2.62	0.43
52:BE:226:MET:HG3	74:BE:401:HEM:C4C	2.53	0.43
53:BF:40:ASP:HA	53:BF:41:PRO:HD2	1.91	0.43
2:B:179:VAL:C	16:P:111:LEU:HD11	2.43	0.43
8:H:32:ALA:HB1	8:H:37:ARG:HG3	2.01	0.43
8:H:36:ARG:HG2	8:H:36:ARG:NH1	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:311:VAL:HG13	76:H:597:HOH:O	2.18	0.43
64:H:402:Q7G:C3B	76:H:523:HOH:O	2.66	0.43
10:J:100:GLU:OE2	12:L:641:MET:HE3	2.18	0.43
11:K:28:ILE:HD12	11:K:29:LEU:N	2.34	0.43
12:L:261:MET:HE2	76:L:868:HOH:O	2.18	0.43
14:N:270:LYS:HD3	76:N:667:HOH:O	2.19	0.43
21:U:109:ILE:HD13	21:U:115:ALA:HA	2.00	0.43
43:u:45:VAL:HA	55:AH:26:LEU:HD11	1.88	0.43
48:AA:202:ILE:HG13	48:AA:231:TYR:HB3	2.01	0.43
48:AA:319:TRP:CD1	48:AA:374:ILE:HG22	2.53	0.43
49:AB:329:ILE:HG22	54:AG:8:LEU:HD12	1.98	0.43
50:AC:271:THR:CG2	51:BD:221:ILE:O	2.66	0.43
51:AD:80:THR:CB	54:AG:9:LYS:HD3	2.48	0.43
52:AE:231:ASN:O	52:AE:248:MET:HE1	2.18	0.43
55:AH:6:VAL:CG1	55:AH:7:VAL:HG22	2.39	0.43
50:BC:208:HIS:NE2	67:BC:403:UQ5:O3	2.52	0.43
2:B:71:LYS:HD3	2:B:71:LYS:HA	1.66	0.43
60:D:401:PTY:H231	60:D:401:PTY:H262	1.60	0.43
8:H:160:ILE:HD12	76:H:597:HOH:O	2.17	0.43
8:H:304:LEU:HB3	8:H:305:PRO:HD3	2.00	0.43
12:L:226:PHE:CE1	12:L:286:ILE:HG12	2.53	0.43
66:L:706:PC7:H332	66:L:706:PC7:H362	1.63	0.43
14:N:326[B]:HIS:CE1	14:N:352:TYR:HB2	2.54	0.43
14:N:389:ILE:HD11	66:d:102:PC7:H342	1.99	0.43
16:P:301:ILE:O	16:P:302:ARG:C	2.61	0.43
56:AI:23:ARG:HD3	56:AI:23:ARG:HA	1.75	0.43
48:BA:87:LEU:HB2	48:BA:255:ALA:HB1	2.01	0.43
48:BA:335:MET:HE1	48:BA:403:LEU:HD13	2.00	0.43
65:BC:405:3PH:H3G1	52:BE:279:SER:HB2	2.00	0.43
55:BH:23:LYS:HB2	55:BH:24:PRO:HD3	2.00	0.43
6:F:435:LEU:O	6:F:439:THR:HG23	2.19	0.43
7:G:75:GLU:OE2	7:G:82:ALA:HB1	2.19	0.43
7:G:317:PRO:HB3	7:G:328:ILE:HG23	2.01	0.43
7:G:486:GLY:HA3	7:G:491:THR:OG1	2.19	0.43
8:H:33:PHE:HZ	27:a:7:GLU:HB2	1.84	0.43
12:L:296:LEU:HD12	12:L:563:TRP:CE2	2.54	0.43
12:L:318:GLN:HE22	12:L:401:LYS:NZ	2.16	0.43
21:U:126:LYS:HB2	21:U:126:LYS:HE2	1.69	0.43
34:i:53:PHE:HA	34:i:56:PHE:CE2	2.54	0.43
38:m:31:ARG:H	72:AE:402:CDL:H472	1.83	0.43
39:n:108:VAL:HG22	76:n:235:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:y:86:ARG:O	46:y:107:HIS:HD2	2.02	0.43
47:z:208:SER:HB3	76:z:401:HOH:O	2.18	0.43
50:AC:142:TRP:CA	76:AC:568:HOH:O	2.57	0.43
72:AC:408:CDL:H142	72:AC:408:CDL:H171	1.82	0.43
65:BC:405:3PH:H322	65:BC:405:3PH:H351	1.78	0.43
56:BI:40:ARG:CZ	56:BI:40:ARG:HA	2.48	0.43
3:C:25:SER:HB2	22:V:122:ASN:HB3	2.00	0.43
6:F:60:ASP:HA	6:F:63:ARG:HG3	2.01	0.43
8:H:71:PHE:CZ	8:H:75:ARG:NH1	2.86	0.43
8:H:156:ILE:HG22	76:H:597:HOH:O	2.18	0.43
8:H:287:PHE:CE2	9:I:76:MET:HE3	2.54	0.43
10:J:16:MET:HB3	10:J:29:PHE:CD2	2.53	0.43
12:L:262:VAL:CG2	12:L:319:LEU:HD11	2.48	0.43
12:L:543:GLN:HE22	39:n:40:ILE:HG21	1.81	0.43
13:M:38:ARG:NE	76:M:612:HOH:O	2.40	0.43
60:M:503:PTY:H162	60:M:503:PTY:H131	1.84	0.43
16:P:233:TRP:HH2	16:P:290:THR:HG23	1.84	0.43
24:X:90:ASP:OD1	24:X:93:ARG:NH2	2.52	0.43
58:y:303:PGT:H371	58:y:303:PGT:H341	1.57	0.43
48:BA:357:ARG:O	48:BA:362:TYR:N	2.36	0.43
49:BB:166:ILE:HG23	76:BB:706:HOH:O	2.19	0.43
49:BB:187:ASP:OD1	49:BB:187:ASP:N	2.51	0.43
58:A:201:PGT:H391	58:A:201:PGT:H361	1.54	0.43
3:C:132:ILE:CG2	76:C:266:HOH:O	2.66	0.43
6:F:77:LYS:CG	6:F:81:LYS:HE3	2.49	0.43
6:F:138:VAL:HG21	6:F:165:CYS:SG	2.59	0.43
6:F:182:ARG:NH2	6:F:184:GLU:OE1	2.44	0.43
12:L:652:ARG:H	12:L:652:ARG:HG2	1.53	0.43
16:P:291:HIS:O	16:P:295:GLU:HG3	2.19	0.43
17:Q:58:SER:OG	76:Q:201:HOH:O	2.08	0.43
22:V:140:GLU:HG3	22:V:144:LYS:HE3	2.00	0.43
29:c:15:PHE:HB3	76:n:241:HOH:O	2.19	0.43
29:c:29:ARG:O	33:g:38:GLU:HG3	2.18	0.43
46:y:167:SER:OG	46:y:182:GLY:HA2	2.18	0.43
48:AA:493:PRO:HG2	48:AA:498:ILE:HD11	2.01	0.43
49:AB:288:LYS:HB2	49:AB:291:GLU:HG3	2.00	0.43
50:AC:32:LEU:HB2	50:AC:231:PHE:CE1	2.54	0.43
52:AE:130:MET:HG3	56:AI:68:ARG:CZ	2.49	0.43
48:BA:130:SER:OG	48:BA:190:GLU:OE2	2.34	0.43
48:BA:337:GLY:HA2	48:BA:354:LEU:HB2	2.01	0.43
49:BB:432:TYR:HD1	57:BJ:18:ILE:CD1	2.27	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:BC:408:CDL:H592	72:BE:402:CDL:H211	2.01	0.43
51:BD:142:LYS:HA	51:BD:145:LEU:HD12	2.00	0.43
51:BD:162:THR:OG1	51:BD:174:ILE:O	2.37	0.43
4:D:150:GLY:HA3	9:I:106:ARG:O	2.19	0.42
4:D:292:ARG:HH12	7:G:192:ARG:HG3	1.83	0.42
12:L:491:ASN:HB3	76:o:206:HOH:O	2.18	0.42
67:L:707:UQ5:H112	25:Y:40:TRP:CE3	2.54	0.42
13:M:151:ILE:HG21	66:d:102:PC7:H442	2.00	0.42
18:R:73:GLU:OE1	18:R:78:PRO:CB	2.67	0.42
40:o:77:ARG:HD2	40:o:80:GLU:OE1	2.19	0.42
42:q:63:GLN:HA	42:q:73:HIS:O	2.19	0.42
42:q:81:LYS:HA	42:q:81:LYS:HD3	1.81	0.42
43:u:5:LEU:HA	43:u:5:LEU:HD23	1.80	0.42
58:y:303:PGT:H191	58:y:303:PGT:H162	1.64	0.42
47:z:130:HIS:O	47:z:147:MET:HB2	2.18	0.42
48:AA:404:LYS:HE2	48:AA:502:PHE:HA	2.01	0.42
72:AC:409:CDL:H312	54:AG:41:ASN:HD22	1.84	0.42
4:D:23:HIS:CD2	4:D:389:PHE:HE2	2.37	0.42
4:D:111:ILE:HG22	76:D:664:HOH:O	2.18	0.42
5:E:136:MET:HA	5:E:140:SER:H	1.83	0.42
7:G:230:GLU:HG2	7:G:463:ARG:CZ	2.50	0.42
7:G:702:LEU:HB3	19:S:36:TYR:HD2	1.85	0.42
11:K:27:ASN:CG	11:K:30:ILE:HG12	2.44	0.42
12:L:261:MET:CE	76:L:966:HOH:O	2.35	0.42
12:L:600:TYR:OH	38:m:25:HIS:HD2	2.03	0.42
12:L:656:ILE:HG23	25:Y:124:LEU:CD2	2.48	0.42
21:U:98:GLY:O	21:U:126:LYS:NZ	2.48	0.42
23:W:41:MET:HE2	23:W:52:PRO:HG3	2.01	0.42
40:o:75:LYS:HA	40:o:78:GLU:OE1	2.19	0.42
48:AA:222:TYR:OH	48:AA:378:THR:OG1	2.22	0.42
50:AC:148:TRP:CH2	51:BD:221:ILE:HG12	2.55	0.42
67:AC:403:UQ5:H72	67:AC:403:UQ5:H1M1	1.77	0.42
51:AD:132:LEU:O	51:AD:136:VAL:HG23	2.19	0.42
56:AI:48:LYS:HD2	56:AI:48:LYS:HA	1.57	0.42
48:BA:436:ILE:HD13	48:BA:436:ILE:HA	1.92	0.42
49:BB:129:SER:HA	49:BB:132:GLU:HG3	2.01	0.42
72:BC:407:CDL:H861	51:BD:134:LEU:HD11	2.01	0.42
9:I:210:GLU:OE2	42:q:94:HIS:HB3	2.20	0.42
10:J:1:MET:SD	43:u:15:PHE:HZ	2.42	0.42
13:M:20:VAL:HG12	13:M:24:ILE:HD11	2.00	0.42
13:M:65:LYS:HE2	76:M:702:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:191:LEU:HD12	14:N:191:LEU:HA	1.87	0.42
16:P:103:GLU:HG3	76:P:640:HOH:O	2.18	0.42
16:P:298:TYR:CZ	16:P:305:PRO:HA	2.54	0.42
16:P:361:GLN:HG2	76:P:638:HOH:O	2.20	0.42
18:R:73:GLU:OE1	18:R:78:PRO:HB3	2.19	0.42
20:T:79:SER:OG	39:n:21:ARG:HD3	2.19	0.42
33:g:77:LEU:HD23	33:g:77:LEU:HA	1.89	0.42
48:AA:122:LEU:HD23	48:AA:245:LEU:HD21	2.02	0.42
48:AA:388:SER:OG	48:AA:389:PRO:HD2	2.19	0.42
49:AB:500:ILE:O	49:AB:526:THR:HG23	2.19	0.42
50:AC:388:ASP:CG	76:AC:507:HOH:O	2.62	0.42
58:AF:201:PGT:H171	76:AF:392:HOH:O	2.19	0.42
49:BB:331:ASP:OD2	54:BG:7:LYS:C	2.56	0.42
49:BB:503:LYS:HD3	49:BB:503:LYS:HA	1.85	0.42
50:BC:364:VAL:HG13	60:BF:201:PTY:H422	2.01	0.42
6:F:440:LYS:HD3	6:F:440:LYS:HA	1.82	0.42
7:G:653:ASP:O	7:G:657:VAL:HG23	2.20	0.42
8:H:81:THR:HG21	8:H:228:PHE:CE1	2.55	0.42
10:J:165:GLY:HA2	10:J:168:VAL:HG22	2.00	0.42
12:L:642:TRP:CD2	12:L:645:LEU:HD13	2.54	0.42
13:M:476:VAL:CG1	65:M:501:3PH:H31	2.50	0.42
14:N:398:TYR:HB3	14:N:440:TYR:CZ	2.55	0.42
39:n:51:LYS:O	39:n:52:PHE:C	2.61	0.42
47:z:45:LEU:HB3	47:z:53:PRO:HG2	2.01	0.42
48:AA:76:SER:HB3	48:AA:93:THR:OG1	2.19	0.42
48:AA:105:VAL:HG21	48:AA:253:PHE:CE2	2.55	0.42
72:AC:408:CDL:H582	72:AC:408:CDL:H552	1.50	0.42
1:A:112:LYS:HD2	1:A:112:LYS:HA	1.80	0.42
3:C:1:MET:HA	22:V:138:LEU:HD11	2.02	0.42
7:G:590:ASN:ND2	7:G:593:LYS:HG3	2.34	0.42
8:H:237:ILE:HA	8:H:277:LEU:HD21	2.02	0.42
8:H:276:PHE:HB3	76:H:561:HOH:O	2.19	0.42
45:x:75:ASP:OD2	76:x:301:HOH:O	2.21	0.42
46:y:137:CYS:HB2	46:y:155:VAL:O	2.20	0.42
46:y:205:LYS:HE3	46:y:205:LYS:HB2	1.94	0.42
49:AB:191:ASN:OD1	49:AB:295:GLN:HG3	2.20	0.42
50:AC:285:TYR:CZ	67:AC:404:UQ5:H3M2	2.55	0.42
49:BB:432:TYR:CD1	57:BJ:18:ILE:HD11	2.44	0.42
8:H:121:ILE:HD12	8:H:144:MET:SD	2.60	0.42
10:J:81:GLU:HA	76:J:337:HOH:O	2.20	0.42
12:L:57:CYS:HB3	12:L:78:PHE:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:28:PHE:CE1	66:d:102:PC7:H232	2.54	0.42
13:M:465:VAL:HG13	65:M:501:3PH:H382	2.02	0.42
60:M:504:PTY:H372	60:M:504:PTY:H401	1.75	0.42
21:U:94:GLU:CG	21:U:101:ILE:HG22	2.49	0.42
34:i:83:LEU:HD23	34:i:83:LEU:HA	1.85	0.42
41:p:66:HIS:HB2	41:p:70:CYS:SG	2.60	0.42
72:u:102:CDL:H791	72:u:102:CDL:H761	1.78	0.42
49:AB:337:GLN:OE1	49:AB:408:TYR:OH	2.37	0.42
58:AC:406:PGT:H441	58:AC:406:PGT:H471	1.70	0.42
48:BA:157:GLU:C	48:BA:158:GLN:HG3	2.45	0.42
57:BJ:38:VAL:O	57:BJ:40:PRO:HD3	2.19	0.42
8:H:26:ALA:HB2	27:a:11:PRO:HB2	2.00	0.42
12:L:412:TYR:HB2	76:L:1006:HOH:O	2.19	0.42
14:N:270:LYS:HE2	76:N:667:HOH:O	2.16	0.42
15:O:45:ILE:HD13	15:O:63:LEU:HD23	2.02	0.42
39:n:18:GLU:OE2	39:n:22:ILE:HD12	2.19	0.42
49:AB:205:LYS:HE2	49:AB:205:LYS:HB2	1.82	0.42
52:AE:79:PRO:HG3	76:AE:652:HOH:O	2.19	0.42
52:AE:124:GLU:HG2	52:AE:128:LYS:HE3	2.01	0.42
52:AE:204:PRO:HG3	55:AH:49:TYR:CG	2.55	0.42
53:AF:119:ARG:O	50:BC:7:ARG:NH1	2.47	0.42
48:BA:121:HIS:ND1	48:BA:198:MET:HE3	2.35	0.42
48:BA:159:MET:HE3	48:BA:159:MET:HB3	1.85	0.42
48:BA:322:GLU:C	48:BA:323:LYS:HD3	2.45	0.42
49:BB:245:THR:HG21	49:BB:320:SER:H	1.84	0.42
52:BE:307:ASN:O	53:BF:65:ARG:NH1	2.52	0.42
10:J:98:TRP:HA	10:J:102:PHE:CD1	2.55	0.42
13:M:303:ASP:HB3	13:M:306:LYS:HB2	2.01	0.42
43:u:15:PHE:O	43:u:19:GLN:HG2	2.20	0.42
43:u:45:VAL:N	55:AH:26:LEU:CD1	2.83	0.42
45:x:242:TYR:HD2	47:z:34:TYR:CD1	2.38	0.42
47:z:37:GLU:HG2	47:z:39:LEU:HG	2.01	0.42
49:AB:162:GLU:CG	49:AB:192:GLN:HE21	2.32	0.42
50:AC:34:TYR:CD2	72:AC:409:CDL:H522	2.55	0.42
50:AC:353:PRO:HG3	54:AG:62:PHE:CG	2.54	0.42
49:BB:359:GLN:NE2	49:BB:394:ALA:O	2.47	0.42
50:BC:355:VAL:O	50:BC:359:GLN:HG3	2.19	0.42
2:B:88:THR:HB	2:B:98:MET:HE1	2.01	0.42
2:B:193:GLU:HB3	9:I:183:PHE:CE2	2.55	0.42
5:E:131:GLY:HA2	5:E:169:MET:HG2	2.00	0.42
5:E:202:THR:H	5:E:205:LYS:HB3	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:221:CYS:SG	7:G:223:ARG:HG3	2.60	0.42
8:H:225:PHE:HZ	63:H:401:UQ9:H4M	1.83	0.42
10:J:113:LEU:O	76:J:302:HOH:O	2.21	0.42
12:L:367:LYS:HG3	39:n:84:TYR:CE1	2.55	0.42
12:L:550:THR:O	12:L:554:ARG:HG2	2.20	0.42
21:U:57:VAL:CG2	21:U:96:GLU:HG3	2.49	0.42
22:V:80:ARG:HE	22:V:80:ARG:HB3	1.74	0.42
25:Y:9:LEU:HB3	55:AH:20:LYS:CG	2.44	0.42
25:Y:113:SER:C	25:Y:115:PRO:HD2	2.44	0.42
26:Z:86:LEU:HB3	26:Z:87:PRO:HD3	2.02	0.42
46:y:201:SER:C	46:y:205:LYS:HE2	2.45	0.42
48:AA:300:ARG:HH22	48:AA:494:SER:CA	2.33	0.42
49:AB:309:THR:O	49:AB:313:LEU:HG	2.20	0.42
72:AE:402:CDL:H222	72:AE:402:CDL:H192	1.86	0.42
48:BA:106:ASP:HB2	48:BA:446:LEU:HD22	2.02	0.42
48:BA:112:GLU:O	48:BA:116:PHE:HB2	2.19	0.42
48:BA:371:PHE:HB3	48:BA:384:TYR:CE1	2.55	0.42
48:BA:452:LYS:HB3	48:BA:456:GLN:NE2	2.35	0.42
49:BB:48:PRO:HB2	76:BB:756:HOH:O	2.19	0.42
49:BB:331:ASP:CB	54:BG:7:LYS:CE	2.94	0.42
4:D:64:LEU:HD23	4:D:82:TYR:HD2	1.85	0.42
8:H:105:ILE:HD12	8:H:105:ILE:HA	1.94	0.42
10:J:167:ILE:HD13	76:J:345:HOH:O	2.19	0.42
13:M:210:GLU:O	13:M:214:ILE:HG12	2.20	0.42
13:M:322:GLY:HA3	13:M:403:ILE:HG12	2.02	0.42
16:P:204:GLU:OE2	16:P:216:ILE:HG21	2.19	0.42
16:P:315:ALA:HB1	16:P:344:ILE:HD13	2.01	0.42
22:V:72:GLU:CD	22:V:72:GLU:H	2.27	0.42
28:b:5:GLU:HG2	28:b:8:ARG:HD2	2.01	0.42
30:d:36:VAL:HG11	60:z:301:PTY:H282	2.02	0.42
45:x:46:THR:O	45:x:46:THR:CG2	2.66	0.42
60:z:301:PTY:HC21	76:z:424:HOH:O	2.20	0.42
48:AA:198:MET:HE2	48:AA:237:LEU:HD21	2.02	0.42
48:AA:457:PHE:O	48:AA:461:VAL:HG23	2.20	0.42
49:AB:98:ARG:HG3	49:AB:98:ARG:NH1	2.34	0.42
48:BA:339:GLY:HA3	48:BA:367:SER:HA	2.01	0.42
48:BA:461:VAL:O	48:BA:464:LEU:HD12	2.19	0.42
72:BC:408:CDL:H331	54:BG:38:VAL:HA	2.01	0.42
9:I:61:ASN:OD1	9:I:62:THR:N	2.53	0.41
11:K:61:PHE:CD1	14:N:146:ILE:HG23	2.55	0.41
12:L:321:TYR:HA	12:L:324:PHE:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:66:LEU:HD21	14:N:98:ILE:HG23	2.02	0.41
14:N:197:ILE:HD12	14:N:233:ILE:HD12	2.01	0.41
40:o:35:ILE:HB	40:o:36:PRO:HD3	2.01	0.41
72:u:101:CDL:H232	72:u:101:CDL:H202	1.68	0.41
76:x:303:HOH:O	46:y:37:GLU:HB2	2.19	0.41
48:AA:298:ASP:OD1	48:AA:299:PHE:N	2.53	0.41
48:BA:258:MET:HE1	76:BA:674:HOH:O	2.20	0.41
50:BC:221:GLU:HA	50:BC:224:LYS:HZ3	1.85	0.41
55:BH:10:LYS:HG3	55:BH:64:LEU:CD2	2.49	0.41
1:A:61:PHE:HA	1:A:64:VAL:HG12	2.02	0.41
12:L:653:LEU:HD21	25:Y:77:ILE:HG13	2.02	0.41
76:L:983:HOH:O	13:M:434:ASN:HB3	2.19	0.41
13:M:38:ARG:HG2	13:M:112:MET:HG2	2.02	0.41
21:U:82:ASP:CG	23:W:64:ARG:HH22	2.28	0.41
21:U:105:GLU:HG2	21:U:118:PHE:CE1	2.55	0.41
65:f:202:3PH:H392	65:f:202:3PH:H362	1.83	0.41
34:i:65:TRP:CE2	76:i:105:HOH:O	2.57	0.41
39:n:49:ARG:HG3	39:n:53:ASN:HD21	1.86	0.41
49:AB:51:LEU:HD12	49:AB:51:LEU:HA	1.86	0.41
49:AB:393:MET:CE	49:AB:395:PHE:HB3	2.50	0.41
1:A:83:VAL:HG21	10:J:137:LEU:HG	2.01	0.41
4:D:141:LEU:HD12	76:D:664:HOH:O	2.20	0.41
5:E:136:MET:HB3	6:F:392:ARG:NH2	2.20	0.41
6:F:138:VAL:HG11	6:F:161:LEU:HD11	2.02	0.41
8:H:178:TRP:CE3	76:H:625:HOH:O	2.71	0.41
10:J:100:GLU:CD	12:L:641:MET:HE3	2.45	0.41
11:K:42:VAL:HG11	14:N:191:LEU:HG	2.02	0.41
12:L:306:ASP:HB3	12:L:309:ARG:CG	2.50	0.41
12:L:459:ALA:HA	12:L:460:PRO:HD2	1.92	0.41
58:L:703:PGT:H362	58:L:703:PGT:H391	1.92	0.41
13:M:82:PHE:CB	13:M:141:LEU:CD1	2.98	0.41
14:N:245:PRO:HD2	14:N:246:PHE:CE2	2.54	0.41
16:P:165:GLU:O	16:P:169:LEU:HG	2.19	0.41
16:P:373:TYR:HD1	16:P:373:TYR:HA	1.71	0.41
23:W:124:LEU:HG	23:W:128:TYR:CE2	2.55	0.41
41:p:72:HIS:CD2	41:p:73:LEU:N	2.88	0.41
45:x:129:SER:CA	76:x:454:HOH:O	2.57	0.41
47:z:85:LEU:HA	47:z:106:VAL:O	2.21	0.41
50:AC:124:VAL:HG11	50:AC:309:LEU:HG	2.03	0.41
65:AC:405:3PH:H3B1	65:AC:405:3PH:H381	1.72	0.41
49:BB:98:ARG:O	49:BB:109:ALA:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:BB:331:ASP:OD2	54:BG:7:LYS:CA	2.67	0.41
52:BE:190:GLN:NE2	76:BE:526:HOH:O	2.53	0.41
7:G:377:PRO:O	7:G:405:SER:HB2	2.20	0.41
8:H:319:VAL:HG22	8:H:324:LEU:HD11	2.03	0.41
10:J:7:SER:OG	11:K:9:PHE:HD2	2.02	0.41
12:L:51:ALA:HB1	12:L:492:PHE:CE1	2.55	0.41
12:L:311:ILE:HG22	12:L:349:PHE:CE2	2.55	0.41
14:N:271:ILE:HG23	60:N:502:PTY:H431	2.02	0.41
14:N:389:ILE:CD1	66:d:102:PC7:H342	2.50	0.41
26:Z:57:PHE:O	26:Z:61:MET:HG2	2.20	0.41
33:g:83:ALA:HB2	34:i:5:MET:HE3	2.02	0.41
45:x:169:MET:HG2	46:y:147:MET:HE2	2.03	0.41
50:AC:142:TRP:C	76:AC:568:HOH:O	2.63	0.41
55:AH:23:LYS:HB3	55:AH:24:PRO:HD3	2.02	0.41
49:BB:143:LEU:HD11	49:BB:270:ILE:HD11	2.02	0.41
49:BB:170:LEU:HD23	49:BB:170:LEU:HA	1.93	0.41
49:BB:206:PHE:HB2	49:BB:263:ARG:HG3	2.01	0.41
3:C:165:VAL:CG1	23:W:96:ARG:NE	2.84	0.41
3:C:171:MET:O	17:Q:93:SER:CB	2.69	0.41
7:G:77:PHE:HA	7:G:81:TYR:O	2.21	0.41
7:G:108:HIS:HB3	7:G:111:LEU:HD12	2.01	0.41
8:H:263:ILE:HA	8:H:264:PRO:HD3	1.94	0.41
10:J:34:PHE:HE2	76:J:363:HOH:O	2.03	0.41
12:L:351:SER:O	12:L:355:VAL:HG23	2.20	0.41
13:M:158:GLY:HA3	14:N:449:PHE:CE1	2.55	0.41
14:N:75:LEU:HD12	32:f:79:GLN:HG2	2.02	0.41
22:V:81:LEU:HD23	22:V:81:LEU:HA	1.80	0.41
22:V:100:ILE:O	22:V:104:ILE:HG12	2.19	0.41
25:Y:64:THR:O	25:Y:68:THR:HG22	2.19	0.41
65:Y:201:3PH:H281	72:AC:409:CDL:H392	2.02	0.41
43:u:49:ARG:HB2	55:AH:22:VAL:CB	2.50	0.41
44:v:80:LYS:HZ1	46:y:1:MET:CG	2.33	0.41
46:y:220:LYS:NZ	46:y:228:GLU:OE1	2.49	0.41
49:BB:329:ILE:HG21	54:BG:8:LEU:HD12	2.01	0.41
1:A:70:ILE:HG13	10:J:163:MET:HG2	2.01	0.41
2:B:85:TRP:HB3	2:B:116:ARG:HG2	2.03	0.41
6:F:85:TRP:CD2	6:F:204:LEU:HD13	2.55	0.41
6:F:148:CYS:SG	76:F:747:HOH:O	2.55	0.41
7:G:571:SER:HB2	7:G:574:ALA:HB2	2.03	0.41
8:H:29:LYS:HA	8:H:29:LYS:HD2	1.82	0.41
13:M:38:ARG:HD2	13:M:109:TRP:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:68:ARG:NH2	76:R:305:HOH:O	2.53	0.41
25:Y:83:VAL:O	25:Y:87:ARG:HB3	2.20	0.41
39:n:63:ARG:HD3	76:n:202:HOH:O	2.09	0.41
47:z:13:PHE:HB3	76:z:515:HOH:O	2.21	0.41
52:AE:71:LEU:HD23	52:AE:218:TYR:CE1	2.55	0.41
49:BB:290:GLU:OE1	49:BB:291:GLU:HG2	2.20	0.41
53:BF:19:MET:HE2	53:BF:19:MET:HB3	1.95	0.41
7:G:104:ARG:HB2	61:G:801:FES:S2	2.60	0.41
7:G:110:ARG:HH22	7:G:321:GLU:CD	2.26	0.41
9:I:82:LEU:CD1	9:I:85:LYS:HD3	2.50	0.41
12:L:169:LEU:HD21	13:M:427:ALA:HA	2.02	0.41
12:L:578:LEU:HD13	37:l:53:LEU:HD22	2.02	0.41
60:L:705:PTY:H162	60:L:705:PTY:H192	1.76	0.41
14:N:332:ILE:HD13	14:N:332:ILE:HA	1.78	0.41
16:P:98:PRO:HA	16:P:121:MET:O	2.20	0.41
33:g:85:PRO:HD3	76:i:114:HOH:O	2.19	0.41
40:o:8:LYS:CE	40:o:68:GLU:OE2	2.68	0.41
43:u:35:LYS:O	43:u:39:MET:HG2	2.20	0.41
72:u:102:CDL:H422	72:u:102:CDL:H391	1.83	0.41
48:AA:170:VAL:O	48:AA:174:VAL:HG23	2.21	0.41
48:AA:388:SER:HB3	48:AA:391:PHE:HB2	2.03	0.41
52:AE:107:HIS:HE1	52:AE:177:PRO:HD2	1.86	0.41
49:BB:531:TYR:HE1	57:BJ:18:ILE:CG1	2.21	0.41
51:BD:167:TRP:CG	51:BD:168:ARG:N	2.88	0.41
3:C:181:ALA:C	17:Q:70:LYS:CD	2.93	0.41
6:F:77:LYS:HZ2	6:F:81:LYS:HZ2	1.51	0.41
13:M:160:TRP:HA	76:M:687:HOH:O	2.20	0.41
13:M:200:LEU:CD2	13:M:266:ARG:HD2	2.51	0.41
13:M:469:TRP:HB2	65:M:501:3PH:H371	2.01	0.41
20:T:58:PRO:HA	36:k:14:ARG:HH12	1.85	0.41
20:T:90:GLU:OE1	20:T:95:LEU:HB2	2.20	0.41
33:g:101:LEU:CD1	41:p:47:LYS:HD3	2.50	0.41
42:q:68:THR:HB	42:q:73:HIS:CE1	2.56	0.41
51:AD:197:GLN:HG2	51:AD:202:ARG:HD2	2.03	0.41
1:A:85:LEU:HD23	1:A:85:LEU:HA	1.93	0.41
2:B:195:LEU:HB2	76:B:681:HOH:O	2.21	0.41
4:D:88:LYS:HD3	4:D:327:THR:HG21	2.03	0.41
4:D:343:VAL:HB	4:D:352:ARG:HB3	2.03	0.41
5:E:114:TYR:HB3	6:F:224:ALA:O	2.21	0.41
6:F:177:ALA:HB2	6:F:216:PHE:CZ	2.55	0.41
7:G:585:GLY:N	7:G:603:GLN:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:598:ALA:O	7:G:613:ARG:NH2	2.44	0.41
9:I:59:ASP:HB3	9:I:62:THR:HG22	2.02	0.41
9:I:194:LEU:HB2	76:I:634:HOH:O	2.21	0.41
12:L:140:TRP:CE2	12:L:232:LYS:HG3	2.55	0.41
12:L:148:TYR:HB2	12:L:168:MET:CG	2.50	0.41
12:L:461:ILE:N	65:L:701:3PH:O14	2.45	0.41
14:N:212:ILE:HG22	14:N:213:LEU:HD23	2.02	0.41
15:O:69:LEU:O	15:O:73:THR:HG23	2.20	0.41
16:P:152:ARG:HH21	16:P:332:PRO:HG3	1.86	0.41
16:P:157:GLU:CD	16:P:157:GLU:N	2.79	0.41
25:Y:9:LEU:CB	55:AH:20:LYS:HA	2.51	0.41
25:Y:65:HIS:HA	25:Y:68:THR:HG22	2.02	0.41
65:Y:201:3PH:H262	54:AG:42:TRP:CE3	2.55	0.41
26:Z:75:LYS:HE2	26:Z:75:LYS:HB2	1.91	0.41
33:g:101:LEU:CD2	76:g:225:HOH:O	2.46	0.41
35:j:17:VAL:HB	36:k:23:MET:HE2	2.03	0.41
35:j:45:GLN:HG2	76:j:102:HOH:O	2.20	0.41
36:k:51:ILE:C	36:k:51:ILE:HD12	2.46	0.41
37:l:113:PRO:HG3	40:o:10:MET:SD	2.60	0.41
39:n:90:PRO:HA	39:n:95:PHE:CD2	2.56	0.41
40:o:60:LYS:HG2	40:o:64:GLU:OE2	2.21	0.41
45:x:48:SER:HB3	46:y:57:LYS:HG2	2.03	0.41
45:x:239:SER:OG	45:x:241:ILE:HG12	2.21	0.41
49:AB:514:GLN:OE1	54:AG:8:LEU:HD21	2.19	0.41
50:AC:8:PHE:O	50:AC:9:SER:C	2.64	0.41
50:AC:204:LEU:HA	76:AC:648:HOH:O	2.21	0.41
50:AC:316:SER:HB2	76:AC:573:HOH:O	2.20	0.41
50:AC:326:PRO:HD2	53:AF:20:HIS:CE1	2.56	0.41
50:AC:341:LEU:HD21	54:AG:52:VAL:HA	2.03	0.41
67:AC:404:UQ5:H151	67:AC:404:UQ5:H171	1.82	0.41
51:AD:122:VAL:HG11	52:AE:281:ALA:HB2	2.02	0.41
52:AE:297:LYS:HE2	53:AF:74:MET:O	2.21	0.41
49:BB:151:THR:HG23	49:BB:203:ASN:HB2	2.02	0.41
49:BB:505:ILE:HG21	76:BB:933:HOH:O	2.20	0.41
3:C:21:LYS:HB2	3:C:32:ASP:HB2	2.02	0.41
3:C:98:ILE:O	3:C:123:PHE:HA	2.21	0.41
7:G:479:ASN:OD1	7:G:479:ASN:N	2.50	0.41
9:I:189:THR:OG1	9:I:192:GLU:HG3	2.21	0.41
12:L:219:SER:HA	12:L:279:SER:OG	2.21	0.41
13:M:476:VAL:HG11	65:M:501:3PH:H31	2.03	0.41
14:N:166:LYS:HG3	14:N:258:PRO:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:X:66:ASP:OD2	24:X:66:ASP:C	2.63	0.41
24:X:90:ASP:CG	26:Z:74:LEU:HD11	2.41	0.41
47:z:164:ALA:N	76:z:422:HOH:O	2.54	0.41
48:AA:402:GLU:O	48:AA:406:VAL:HG13	2.21	0.41
49:AB:63:ASN:O	49:AB:66:LYS:CG	2.67	0.41
49:AB:149:LYS:HD3	49:AB:149:LYS:HA	1.60	0.41
49:AB:352:SER:O	49:AB:356:MET:HG3	2.21	0.41
50:AC:135:PHE:CZ	50:AC:153:ILE:HB	2.56	0.41
50:AC:383:PRO:HB2	53:AF:95:GLN:HG3	2.02	0.41
51:AD:99:GLU:CB	76:AG:214:HOH:O	2.44	0.41
51:AD:121:PHE:CE1	56:AI:31:ILE:HA	2.56	0.41
66:AG:101:PC7:H441	66:AG:101:PC7:H412	1.91	0.41
49:BB:264:GLU:N	49:BB:264:GLU:CD	2.79	0.41
51:BD:223:LEU:HA	51:BD:224:PRO:HD3	1.96	0.41
2:B:215:TRP:CZ2	16:P:332:PRO:HG2	2.56	0.40
4:D:13:LEU:HD22	8:H:132:TYR:HE1	1.86	0.40
4:D:171:LEU:O	4:D:175:ILE:HG13	2.21	0.40
8:H:71:PHE:N	76:H:529:HOH:O	2.54	0.40
8:H:76:MET:HB2	72:u:101:CDL:H582	2.03	0.40
10:J:169:LEU:HD13	76:K:336:HOH:O	2.21	0.40
12:L:533:TYR:HE2	36:k:28:MET:HE2	1.86	0.40
60:L:705:PTY:H401	60:L:705:PTY:H371	1.67	0.40
13:M:60:ASP:OD2	34:i:22:ARG:NH2	2.55	0.40
13:M:192:LEU:HD23	14:N:415:PHE:HE2	1.86	0.40
13:M:325:SER:HA	76:M:604:HOH:O	2.21	0.40
20:T:50:VAL:O	20:T:54:VAL:HG23	2.20	0.40
48:AA:115:TYR:HA	48:AA:239:ARG:HH12	1.85	0.40
49:AB:146:MET:HE1	49:AB:210:ARG:HB3	2.02	0.40
49:AB:151:THR:O	49:AB:205:LYS:NZ	2.43	0.40
76:AB:890:HOH:O	50:AC:8:PHE:HB3	2.20	0.40
51:AD:199:ASP:O	51:AD:203:VAL:HG12	2.21	0.40
52:AE:110:SER:O	52:AE:156:ARG:HD2	2.21	0.40
53:AF:121:ILE:HD12	50:BC:13:GLN:HG3	2.04	0.40
48:BA:217:ILE:HD12	48:BA:217:ILE:C	2.47	0.40
49:BB:63:ASN:HB3	76:BB:930:HOH:O	2.21	0.40
50:BC:77:ASP:HA	51:BD:142:LYS:HE3	2.02	0.40
54:BG:21:LYS:NZ	72:BG:101:CDL:OB4	2.53	0.40
65:BJ:101:3PH:H2A2	65:BJ:102:3PH:H371	2.03	0.40
1:A:63:LEU:HD23	1:A:63:LEU:HA	1.94	0.40
6:F:411:GLY:HA3	6:F:442:ILE:HD11	2.03	0.40
6:F:416:TRP:O	6:F:420:GLU:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:64:ARG:NH1	17:Q:134:LEU:HD23	2.36	0.40
7:G:743:LEU:HD23	7:G:743:LEU:HA	1.96	0.40
8:H:216:TYR:CG	76:H:534:HOH:O	2.70	0.40
12:L:101:ILE:HA	76:L:1003:HOH:O	2.21	0.40
12:L:141:GLU:HG3	13:M:392:PRO:HG2	2.01	0.40
12:L:328:ILE:HB	12:L:411:LYS:HD3	2.01	0.40
12:L:653:LEU:HD23	25:Y:76:TYR:CD2	2.55	0.40
16:P:100:ARG:HD2	76:P:639:HOH:O	2.19	0.40
20:T:79:SER:O	20:T:83:VAL:HG23	2.21	0.40
35:j:12:TYR:HB3	36:k:21:HIS:CD2	2.56	0.40
43:u:44:GLU:CG	55:AH:26:LEU:HD13	2.51	0.40
72:u:102:CDL:H762	72:u:102:CDL:H562	2.03	0.40
48:AA:334:LEU:HD21	48:AA:411:VAL:HG21	2.03	0.40
49:AB:290:GLU:CD	49:AB:290:GLU:H	2.29	0.40
50:AC:269:MET:HE3	51:BD:171:PRO:HG3	2.03	0.40
54:AG:61:TYR:O	54:AG:65:GLN:HG2	2.21	0.40
56:AI:58:ARG:HB2	56:AI:58:ARG:HE	1.56	0.40
50:BC:201:LEU:HD23	67:BC:403:UQ5:H152	2.04	0.40
3:C:58:ASP:HB2	3:C:111:TRP:NE1	2.36	0.40
7:G:331:LYS:O	7:G:335:CYS:HB3	2.22	0.40
8:H:33:PHE:CE2	27:a:5:TRP:HA	2.56	0.40
10:J:6:LEU:HB3	10:J:36:ASP:OD1	2.20	0.40
10:J:54:LEU:HD13	64:K:201:Q7G:C79	2.52	0.40
12:L:371:LEU:HG	12:L:375:PHE:CE1	2.56	0.40
12:L:571:ASP:HA	12:L:575:ARG:NH2	2.36	0.40
35:j:47:GLY:N	35:j:48:PRO:CD	2.84	0.40
45:x:77:TYR:O	45:x:95:SER:HA	2.22	0.40
46:y:229:ARG:NH2	76:y:429:HOH:O	2.49	0.40
47:z:178:GLY:C	47:z:192:LEU:HD12	2.46	0.40
49:AB:63:ASN:OD1	49:AB:66:LYS:CE	2.69	0.40
49:AB:451:LEU:HD23	49:AB:451:LEU:HA	1.81	0.40
50:AC:26:TYR:HA	50:AC:27:PRO:HD3	1.97	0.40
51:AD:150:LEU:HD23	51:AD:150:LEU:HA	1.90	0.40
53:AF:20:HIS:HE1	58:AF:201:PGT:H263	1.83	0.40
58:AF:201:PGT:H242	58:AF:201:PGT:H211	1.82	0.40
55:AH:18:LYS:N	55:AH:19:PRO:HD2	2.35	0.40
48:BA:498:ILE:HA	48:BA:501:LYS:HE2	2.03	0.40
49:BB:131:PHE:HZ	49:BB:400:LYS:HE3	1.87	0.40
50:BC:149:GLY:HA2	75:BC:404:UQ7:O2	2.21	0.40
52:BE:87:TYR:HB3	52:BE:92:ILE:HD11	2.04	0.40
54:BG:8:LEU:HD22	54:BG:9:LYS:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:76:ASN:ND2	3:C:87:ARG:HG3	2.36	0.40
4:D:295:CYS:O	4:D:311:HIS:CE1	2.75	0.40
6:F:98:TRP:O	6:F:102:GLU:HG2	2.21	0.40
12:L:236:ILE:O	12:L:239:HIS:ND1	2.54	0.40
13:M:63:THR:C	13:M:483:THR:HG21	2.47	0.40
13:M:126:CYS:C	13:M:130:MET:HE2	2.46	0.40
47:z:106:VAL:HG13	47:z:120:THR:HG21	2.04	0.40
48:AA:371:PHE:HB3	48:AA:384:TYR:CE2	2.56	0.40
50:AC:317:MET:HG2	76:AC:573:HOH:O	2.20	0.40
50:BC:145:MET:HG2	50:BC:261:ASP:HB2	2.02	0.40
50:BC:316:SER:OG	53:BF:43:TYR:OH	2.19	0.40
2:B:84:ILE:O	2:B:86:PRO:HD3	2.21	0.40
7:G:189:GLY:C	7:G:191:ASP:H	2.29	0.40
8:H:30:VAL:HB	8:H:281:ILE:HG21	2.03	0.40
12:L:405:LEU:HD23	12:L:405:LEU:HA	1.91	0.40
13:M:16:ILE:O	13:M:19:PRO:HD2	2.21	0.40
13:M:38:ARG:HD2	13:M:109:TRP:CE2	2.57	0.40
60:N:503:PTY:N1	58:y:303:PGT:H321	2.37	0.40
16:P:103:GLU:O	16:P:106:PRO:HD2	2.21	0.40
16:P:302:ARG:NH1	16:P:302:ARG:HG3	2.36	0.40
19:S:3:TRP:CZ2	19:S:87:GLU:HB2	2.57	0.40
23:W:98:HIS:O	23:W:105:VAL:N	2.49	0.40
25:Y:77:ILE:O	25:Y:81:GLN:HG2	2.21	0.40
31:e:49:LYS:HB2	31:e:49:LYS:HE2	1.74	0.40
72:u:102:CDL:H171	72:u:102:CDL:H342	2.04	0.40
66:AB:603:PC7:H81	51:AD:113:TYR:CZ	2.57	0.40
50:AC:152:VAL:HG23	50:AC:153:ILE:HD12	2.02	0.40
50:AC:382:ILE:HA	76:AC:501:HOH:O	2.20	0.40
52:AE:74:PRO:CG	55:AH:57:ASP:HB3	2.44	0.40
49:BB:329:ILE:O	54:BG:9:LYS:HA	2.22	0.40
50:BC:345:ILE:HD13	50:BC:345:ILE:HA	1.83	0.40
51:BD:108:LYS:HA	51:BD:108:LYS:HD3	1.90	0.40
51:BD:172:VAL:HG11	51:BD:271:ILE:HD13	2.03	0.40
52:BE:291:LEU:HA	54:BG:22:ILE:HD12	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	90/119 (76%)	89 (99%)	1 (1%)	0	100	100
2	B	155/218 (71%)	149 (96%)	6 (4%)	0	100	100
3	C	179/190 (94%)	176 (98%)	3 (2%)	0	100	100
4	D	383/394 (97%)	366 (96%)	17 (4%)	0	100	100
5	E	190/255 (74%)	178 (94%)	12 (6%)	0	100	100
6	F	432/486 (89%)	421 (98%)	11 (2%)	0	100	100
7	G	676/748 (90%)	660 (98%)	16 (2%)	0	100	100
8	H	322/325 (99%)	314 (98%)	8 (2%)	0	100	100
9	I	163/222 (73%)	161 (99%)	2 (1%)	0	100	100
10	J	172/205 (84%)	168 (98%)	4 (2%)	0	100	100
11	K	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
12	L	663/669 (99%)	637 (96%)	26 (4%)	0	100	100
13	M	493/495 (100%)	487 (99%)	6 (1%)	0	100	100
14	N	488/499 (98%)	474 (97%)	14 (3%)	0	100	100
15	O	121/159 (76%)	117 (97%)	4 (3%)	0	100	100
16	P	314/402 (78%)	301 (96%)	13 (4%)	0	100	100
17	Q	103/154 (67%)	100 (97%)	3 (3%)	0	100	100
18	R	71/110 (64%)	70 (99%)	1 (1%)	0	100	100
19	S	91/97 (94%)	89 (98%)	2 (2%)	0	100	100
20	T	81/122 (66%)	78 (96%)	3 (4%)	0	100	100
21	U	85/126 (68%)	77 (91%)	8 (9%)	0	100	100
22	V	138/169 (82%)	135 (98%)	3 (2%)	0	100	100
23	W	108/133 (81%)	99 (92%)	9 (8%)	0	100	100
24	X	96/106 (91%)	95 (99%)	1 (1%)	0	100	100
25	Y	123/159 (77%)	117 (95%)	6 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	Z	123/143 (86%)	122 (99%)	1 (1%)	0	100	100
27	a	56/65 (86%)	55 (98%)	1 (2%)	0	100	100
28	b	41/65 (63%)	39 (95%)	2 (5%)	0	100	100
29	c	74/88 (84%)	73 (99%)	1 (1%)	0	100	100
30	d	73/81 (90%)	71 (97%)	2 (3%)	0	100	100
31	e	62/83 (75%)	61 (98%)	1 (2%)	0	100	100
32	f	99/106 (93%)	98 (99%)	1 (1%)	0	100	100
33	g	77/114 (68%)	77 (100%)	0	0	100	100
34	i	81/98 (83%)	79 (98%)	2 (2%)	0	100	100
35	j	49/69 (71%)	47 (96%)	2 (4%)	0	100	100
36	k	46/72 (64%)	45 (98%)	1 (2%)	0	100	100
37	l	70/125 (56%)	69 (99%)	1 (1%)	0	100	100
38	m	68/71 (96%)	67 (98%)	1 (2%)	0	100	100
39	n	107/117 (92%)	106 (99%)	1 (1%)	0	100	100
40	o	78/103 (76%)	75 (96%)	3 (4%)	0	100	100
41	p	88/106 (83%)	86 (98%)	2 (2%)	0	100	100
42	q	79/159 (50%)	75 (95%)	4 (5%)	0	100	100
43	u	53/63 (84%)	53 (100%)	0	0	100	100
44	v	27/113 (24%)	27 (100%)	0	0	100	100
45	x	208/256 (81%)	206 (99%)	2 (1%)	0	100	100
46	y	263/278 (95%)	261 (99%)	2 (1%)	0	100	100
47	z	231/275 (84%)	228 (99%)	3 (1%)	0	100	100
48	AA	448/503 (89%)	431 (96%)	17 (4%)	0	100	100
48	BA	449/503 (89%)	431 (96%)	18 (4%)	0	100	100
49	AB	485/531 (91%)	475 (98%)	10 (2%)	0	100	100
49	BB	485/531 (91%)	476 (98%)	9 (2%)	0	100	100
50	AC	385/393 (98%)	375 (97%)	10 (3%)	0	100	100
50	BC	385/393 (98%)	374 (97%)	11 (3%)	0	100	100
51	AD	194/272 (71%)	182 (94%)	12 (6%)	0	100	100
51	BD	193/272 (71%)	181 (94%)	12 (6%)	0	100	100
52	AE	242/307 (79%)	238 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	BE	242/307 (79%)	238 (98%)	4 (2%)	0	100	100
53	AF	114/122 (93%)	114 (100%)	0	0	100	100
53	BF	114/122 (93%)	114 (100%)	0	0	100	100
54	AG	67/72 (93%)	67 (100%)	0	0	100	100
54	BG	66/72 (92%)	65 (98%)	1 (2%)	0	100	100
55	AH	62/69 (90%)	61 (98%)	1 (2%)	0	100	100
55	BH	61/69 (88%)	59 (97%)	2 (3%)	0	100	100
56	AI	55/72 (76%)	53 (96%)	2 (4%)	0	100	100
56	BI	55/72 (76%)	53 (96%)	2 (4%)	0	100	100
57	AJ	26/57 (46%)	25 (96%)	1 (4%)	0	100	100
57	BJ	26/57 (46%)	23 (88%)	3 (12%)	0	100	100
All	All	12042/14108 (85%)	11709 (97%)	333 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	85/105 (81%)	83 (98%)	2 (2%)	43	49
2	B	132/184 (72%)	131 (99%)	1 (1%)	73	81
3	C	171/179 (96%)	171 (100%)	0	100	100
4	D	331/340 (97%)	331 (100%)	0	100	100
5	E	166/220 (76%)	164 (99%)	2 (1%)	63	72
6	F	353/396 (89%)	352 (100%)	1 (0%)	86	91
7	G	570/625 (91%)	568 (100%)	2 (0%)	84	89
8	H	271/272 (100%)	271 (100%)	0	100	100
9	I	147/195 (75%)	145 (99%)	2 (1%)	59	67
10	J	156/186 (84%)	153 (98%)	3 (2%)	50	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	K	85/85 (100%)	84 (99%)	1 (1%)	63	72
12	L	564/568 (99%)	558 (99%)	6 (1%)	65	74
13	M	434/434 (100%)	428 (99%)	6 (1%)	59	67
14	N	408/416 (98%)	402 (98%)	6 (2%)	57	65
15	O	108/141 (77%)	107 (99%)	1 (1%)	70	78
16	P	263/334 (79%)	257 (98%)	6 (2%)	44	51
17	Q	89/128 (70%)	89 (100%)	0	100	100
18	R	64/97 (66%)	64 (100%)	0	100	100
19	S	82/85 (96%)	82 (100%)	0	100	100
20	T	78/112 (70%)	76 (97%)	2 (3%)	40	46
21	U	78/113 (69%)	77 (99%)	1 (1%)	61	69
22	V	123/148 (83%)	123 (100%)	0	100	100
23	W	98/114 (86%)	98 (100%)	0	100	100
24	X	88/94 (94%)	88 (100%)	0	100	100
25	Y	92/120 (77%)	91 (99%)	1 (1%)	65	74
26	Z	100/115 (87%)	99 (99%)	1 (1%)	68	76
27	a	48/53 (91%)	47 (98%)	1 (2%)	47	54
28	b	35/53 (66%)	35 (100%)	0	100	100
29	c	66/71 (93%)	66 (100%)	0	100	100
30	d	60/66 (91%)	59 (98%)	1 (2%)	53	62
31	e	59/73 (81%)	59 (100%)	0	100	100
32	f	80/83 (96%)	80 (100%)	0	100	100
33	g	68/96 (71%)	66 (97%)	2 (3%)	37	42
34	i	75/90 (83%)	74 (99%)	1 (1%)	61	69
35	j	42/51 (82%)	40 (95%)	2 (5%)	23	23
36	k	39/60 (65%)	39 (100%)	0	100	100
37	l	60/97 (62%)	58 (97%)	2 (3%)	33	37
38	m	58/59 (98%)	58 (100%)	0	100	100
39	n	92/99 (93%)	92 (100%)	0	100	100
40	o	70/87 (80%)	66 (94%)	4 (6%)	18	17
41	p	80/93 (86%)	79 (99%)	1 (1%)	61	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	q	69/133 (52%)	69 (100%)	0	100	100
43	u	47/54 (87%)	46 (98%)	1 (2%)	47	54
44	v	22/84 (26%)	22 (100%)	0	100	100
45	x	179/216 (83%)	178 (99%)	1 (1%)	78	86
46	y	221/232 (95%)	220 (100%)	1 (0%)	81	88
47	z	188/228 (82%)	185 (98%)	3 (2%)	55	64
48	AA	369/408 (90%)	362 (98%)	7 (2%)	50	58
48	BA	369/408 (90%)	364 (99%)	5 (1%)	59	67
49	AB	415/452 (92%)	408 (98%)	7 (2%)	53	62
49	BB	415/452 (92%)	411 (99%)	4 (1%)	68	76
50	AC	330/336 (98%)	326 (99%)	4 (1%)	63	72
50	BC	330/336 (98%)	323 (98%)	7 (2%)	47	54
51	AD	170/232 (73%)	166 (98%)	4 (2%)	43	49
51	BD	169/232 (73%)	168 (99%)	1 (1%)	78	86
52	AE	200/247 (81%)	199 (100%)	1 (0%)	81	88
52	BE	200/247 (81%)	198 (99%)	2 (1%)	68	76
53	AF	105/110 (96%)	104 (99%)	1 (1%)	68	76
53	BF	105/110 (96%)	105 (100%)	0	100	100
54	AG	63/65 (97%)	63 (100%)	0	100	100
54	BG	62/65 (95%)	62 (100%)	0	100	100
55	AH	58/62 (94%)	58 (100%)	0	100	100
55	BH	57/62 (92%)	56 (98%)	1 (2%)	51	60
56	AI	48/59 (81%)	47 (98%)	1 (2%)	47	54
56	BI	48/59 (81%)	48 (100%)	0	100	100
57	AJ	16/41 (39%)	16 (100%)	0	100	100
57	BJ	16/41 (39%)	16 (100%)	0	100	100
All	All	10339/11908 (87%)	10230 (99%)	109 (1%)	63	74

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	LEU
1	A	28	LEU

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Mol	Chain	Res	Type
2	B	93	CYS
5	E	36	LEU
5	E	199	GLU
6	F	167	ILE
7	G	145	LYS
7	G	647	VAL
9	I	100	LYS
9	I	220	LEU
10	J	32	LEU
10	J	40	LEU
10	J	92	ILE
11	K	90	ILE
12	L	168	MET
12	L	345	LYS
12	L	453	ILE
12	L	538	VAL
12	L	613	ILE
12	L	649	VAL
13	M	72	LEU
13	M	118	GLU
13	M	331	ILE
13	M	354	VAL
13	M	414	VAL
13	M	476	VAL
14	N	20	PHE
14	N	78	ILE
14	N	86	LEU
14	N	286	TYR
14	N	336	CYS
14	N	394	THR
15	O	124	SER
16	P	111	LEU
16	P	147	ARG
16	P	151	THR
16	P	289	THR
16	P	308	VAL
16	P	347	LEU
20	T	44	GLU
20	T	75	LEU
21	U	70	THR
25	Y	31	THR
26	Z	33	VAL

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Mol	Chain	Res	Type
27	a	42	HIS
30	d	55	LYS
33	g	74	ILE
33	g	106	LEU
34	i	48	ILE
35	j	31	LEU
35	j	44	LYS
37	l	73	VAL
37	l	116	ASN
40	o	71	LEU
40	o	82	LEU
40	o	85	GLN
40	o	87	LYS
41	p	49	LYS
43	u	33	ASP
45	x	148	TYR
46	y	110	LYS
47	z	168	LEU
47	z	175	ILE
47	z	212	GLN
48	AA	176	VAL
48	AA	231	TYR
48	AA	403	LEU
48	AA	406	VAL
48	AA	411	VAL
48	AA	434	ARG
48	AA	485	SER
49	AB	154	ARG
49	AB	170	LEU
49	AB	234	LEU
49	AB	261	ILE
49	AB	326	VAL
49	AB	521	LYS
49	AB	526	THR
50	AC	23	LEU
50	AC	78	VAL
50	AC	275	ILE
50	AC	301	ILE
51	AD	77	VAL
51	AD	108	LYS
51	AD	172	VAL
51	AD	194	ARG

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Mol	Chain	Res	Type
52	AE	236	GLU
53	AF	48	LYS
56	AI	21	MET
48	BA	93	THR
48	BA	308	THR
48	BA	358	VAL
48	BA	383	ILE
48	BA	473	THR
49	BB	162	GLU
49	BB	186	LEU
49	BB	317	GLU
49	BB	505	ILE
50	BC	44	ILE
50	BC	98	VAL
50	BC	122	LEU
50	BC	256	VAL
50	BC	284	ILE
50	BC	331	MET
50	BC	345	ILE
51	BD	170	LYS
52	BE	235	VAL
52	BE	273	LYS
55	BH	27	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (93) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	201	GLN
2	B	203	GLN
3	C	76	ASN
4	D	23	HIS
4	D	281	GLN
4	D	311	HIS
4	D	372	HIS
5	E	196	ASN
6	F	72	HIS
6	F	187	ASN
7	G	284	ASN
7	G	455	ASN
7	G	548	ASN
8	H	50	GLN
8	H	70	ASN

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Mol	Chain	Res	Type
8	H	104	ASN
10	J	73	HIS
10	J	136	ASN
12	L	305	ASN
12	L	318	GLN
12	L	330	ASN
12	L	417	ASN
12	L	457	HIS
12	L	547	GLN
12	L	560	ASN
13	M	31	ASN
13	M	79	ASN
13	M	341	HIS
13	M	491	HIS
14	N	85	ASN
15	O	66	GLN
16	P	94	GLN
16	P	327	ASN
17	Q	65	GLN
18	R	109	HIS
20	T	118	HIS
22	V	45	GLN
23	W	54	GLN
23	W	66	ASN
25	Y	85	ASN
26	Z	66	GLN
26	Z	126	ASN
27	a	30	HIS
27	a	34	HIS
29	c	27	ASN
29	c	63	HIS
30	d	47	ASN
34	i	60	ASN
37	l	99	ASN
38	m	25	HIS
39	n	39	HIS
43	u	31	HIS
43	u	32	GLN
46	y	38	HIS
46	y	42	HIS
46	y	47	ASN
47	z	107	HIS

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Mol	Chain	Res	Type
48	AA	133	ASN
49	AB	70	ASN
49	AB	113	ASN
49	AB	169	HIS
49	AB	192	GLN
49	AB	316	ASN
49	AB	453	HIS
50	AC	6	GLN
50	AC	13	GLN
50	AC	20	ASN
50	AC	209	GLN
50	AC	348	GLN
50	AC	384	ASN
52	AE	80	HIS
53	AF	20	HIS
54	AG	36	HIS
54	AG	41	ASN
54	AG	70	HIS
48	BA	149	ASN
48	BA	320	ASN
49	BB	63	ASN
49	BB	467	GLN
49	BB	497	ASN
50	BC	5	ASN
50	BC	13	GLN
50	BC	144	GLN
50	BC	219	HIS
50	BC	259	HIS
50	BC	274	HIS
50	BC	329	GLN
51	BD	96	HIS
52	BE	163	ASN
52	BE	307	ASN
53	BF	64	GLN
53	BF	76	HIS
55	BH	54	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 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	$\# Z > 2$
32	FME	f	1	32	8,9,10	1.77	1 (12%)	8,9,11	1.51	1 (12%)
1	FME	A	1	1	8,9,10	1.77	1 (12%)	8,9,11	1.58	1 (12%)
11	FME	K	1	11	8,9,10	0.82	0	8,9,11	1.99	3 (37%)

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
32	FME	f	1	32	-	5/7/9/11	-
1	FME	A	1	1	-	0/7/9/11	-
11	FME	K	1	11	-	5/7/9/11	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	f	1	FME	O-C	4.32	1.36	1.20
1	A	1	FME	O-C	4.29	1.36	1.20

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	FME	O-C-CA	-3.76	115.10	124.77
11	K	1	FME	C-CA-N	3.47	116.19	109.50
32	f	1	FME	O-C-CA	-3.45	115.89	124.77
11	K	1	FME	O-C-CA	-3.02	116.99	124.77
11	K	1	FME	CG-CB-CA	-2.15	106.29	112.87

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	K	1	FME	O1-CN-N-CA
11	K	1	FME	N-CA-CB-CG
32	f	1	FME	O1-CN-N-CA
32	f	1	FME	C-CA-CB-CG
32	f	1	FME	O-C-CA-CB
32	f	1	FME	CA-CB-CG-SD
11	K	1	FME	CA-CB-CG-SD
11	K	1	FME	C-CA-CB-CG
32	f	1	FME	CB-CG-SD-CE
11	K	1	FME	CB-CG-SD-CE

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	f	1	FME	3	0
1	A	1	FME	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 91 ligands modelled in this entry, 5 are monoatomic - leaving 86 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	$\# Z > 2$
67	UQ5	AC	404	-	38,38,38	0.46	0	48,49,49	0.84	2 (4%)
60	PTY	D	401	-	49,49,49	0.89	4 (8%)	52,54,54	1.03	2 (3%)
72	CDL	u	101	-	99,99,99	0.89	7 (7%)	105,111,111	1.08	5 (4%)
72	CDL	BC	408	-	76,76,99	0.31	0	82,88,111	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
74	HEM	BC	402	50	50,50,50	2.10	13 (26%)	67,82,82	1.67	16 (23%)
59	SF4	B	500	2	0,12,12	-	-	-		
66	PC7	BD	302	-	38,38,51	0.34	0	44,46,59	0.47	0
73	COO	y	302	-	51,55,55	4.32	18 (35%)	73,81,81	3.99	20 (27%)
72	CDL	BE	402	-	87,87,99	0.94	8 (9%)	93,99,111	1.12	4 (4%)
60	PTY	N	502	-	44,44,49	0.30	0	47,49,54	0.42	0
60	PTY	N	503	-	49,49,49	0.28	0	52,54,54	0.36	0
72	CDL	AE	402	-	84,84,99	0.29	0	90,96,111	0.36	0
61	FES	BD	301	51	0,4,4	-	-	-		
72	CDL	BC	407	-	80,80,99	0.31	0	86,92,111	0.39	0
64	Q7G	K	201	-	90,90,90	0.80	3 (3%)	134,138,138	1.40	19 (14%)
71	8Q1	T	200	-	32,34,34	0.38	0	39,43,43	1.15	3 (7%)
63	UQ9	H	401	-	35,35,58	2.53	12 (34%)	43,45,73	2.23	13 (30%)
60	PTY	d	101	-	38,38,49	0.32	0	41,43,54	0.41	0
60	PTY	Y	202	-	30,30,49	0.35	0	33,35,54	0.37	0
60	PTY	N	501	-	39,39,49	0.30	0	42,44,54	0.35	0
74	HEM	BC	401	50	50,50,50	2.02	18 (36%)	67,82,82	1.71	20 (29%)
75	UQ7	BC	404	-	48,48,48	0.67	2 (4%)	60,61,61	0.76	2 (3%)
66	PC7	BC	409	-	40,40,51	0.34	0	46,48,59	0.52	0
58	PGT	AC	407	-	50,50,50	1.11	4 (8%)	53,56,56	1.05	2 (3%)
65	3PH	AI	101	-	31,31,47	0.77	1 (3%)	34,36,52	0.77	2 (5%)
58	PGT	AC	406	-	40,40,50	0.32	0	43,46,56	0.34	0
72	CDL	AC	409	-	84,84,99	0.32	0	90,96,111	0.36	0
58	PGT	L	704	-	44,44,50	1.16	4 (9%)	47,50,56	1.07	2 (4%)
60	PTY	BF	201	-	39,39,49	0.98	4 (10%)	42,44,54	1.07	2 (4%)
61	FES	AD	301	51	0,4,4	-	-	-		
64	Q7G	H	402	-	90,90,90	0.71	3 (3%)	134,138,138	1.23	14 (10%)
60	PTY	m	101	-	49,49,49	0.27	0	52,54,54	0.36	0
59	SF4	I	501	9	0,12,12	-	-	-		
66	PC7	AC	410	-	50,50,51	0.36	0	56,58,59	0.47	0
58	PGT	AF	201	-	50,50,50	1.09	4 (8%)	53,56,56	1.07	2 (3%)
65	3PH	L	701	-	36,36,47	0.57	1 (2%)	39,41,52	0.73	2 (5%)
58	PGT	L	703	-	50,50,50	0.30	0	53,56,56	0.32	0
64	Q7G	M	505	-	44,44,90	0.88	1 (2%)	64,68,138	1.85	17 (26%)
66	PC7	L	706	-	39,39,51	1.10	3 (7%)	45,47,59	1.12	3 (6%)
66	PC7	d	102	-	51,51,51	0.43	0	57,59,59	0.53	0
72	CDL	BG	101	-	69,69,99	1.05	8 (11%)	75,81,111	1.18	5 (6%)
59	SF4	G	802	7	0,12,12	-	-	-		
66	PC7	AB	603	-	33,33,51	0.38	0	39,41,59	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
59	SF4	I	500	9	0,12,12	-	-	-		
65	3PH	Y	201	-	32,32,47	0.35	0	35,37,52	0.34	0
65	3PH	BC	405	-	43,43,47	0.66	1 (2%)	46,48,52	0.62	1 (2%)
58	PGT	A	201	-	50,50,50	1.10	4 (8%)	53,56,56	1.09	3 (5%)
66	PC7	f	203	-	47,47,51	0.28	0	53,55,59	0.32	0
72	CDL	u	102	-	99,99,99	0.89	8 (8%)	105,111,111	1.08	4 (3%)
61	FES	G	801	7	0,4,4	-	-	-		
66	PC7	v	201	-	51,51,51	0.99	4 (7%)	57,59,59	1.14	3 (5%)
60	PTY	AB	602	-	40,40,49	0.30	0	43,45,54	0.33	0
74	HEM	BE	401	52	50,50,50	2.05	16 (32%)	67,82,82	2.04	20 (29%)
66	PC7	AG	101	-	51,51,51	0.98	4 (7%)	57,59,59	1.02	2 (3%)
59	SF4	G	803	7	0,12,12	-	-	-		
58	PGT	BC	406	-	36,36,50	0.34	0	39,42,56	0.46	0
69	NDP	P	500	-	51,52,52	0.58	0	71,80,80	0.70	0
58	PGT	L	702	-	35,35,50	0.31	0	38,41,56	0.41	0
72	CDL	AC	408	-	80,80,99	0.31	0	86,92,111	0.36	0
59	SF4	F	501	6	0,12,12	-	-	-		
67	UQ5	L	707	-	38,38,38	0.76	1 (2%)	48,49,49	0.88	4 (8%)
71	8Q1	W	200	-	32,34,34	0.33	0	39,43,43	0.46	0
64	Q7G	BC	410	-	44,44,90	0.77	1 (2%)	64,68,138	1.51	10 (15%)
67	UQ5	BC	403	-	38,38,38	0.49	0	48,49,49	0.62	1 (2%)
60	PTY	M	504	-	49,49,49	0.31	0	52,54,54	0.41	0
65	3PH	f	201	-	40,40,47	0.67	1 (2%)	43,45,52	0.74	2 (4%)
60	PTY	M	503	-	36,36,49	0.32	0	39,41,54	0.47	0
60	PTY	BB	602	-	28,28,49	0.36	0	31,33,54	0.53	0
61	FES	E	500	5	0,4,4	-	-	-		
67	UQ5	AC	403	-	38,38,38	0.78	2 (5%)	48,49,49	0.61	1 (2%)
58	PGT	M	502	-	28,28,50	0.34	0	31,34,56	0.39	0
65	3PH	M	501	-	40,40,47	0.71	1 (2%)	43,45,52	0.67	2 (4%)
74	HEM	AC	402	50	50,50,50	2.00	13 (26%)	67,82,82	1.62	11 (16%)
62	FMN	F	500	-	33,33,33	0.63	0	48,50,50	0.66	1 (2%)
64	Q7G	a	101	-	44,44,90	0.68	0	64,68,138	1.40	10 (15%)
74	HEM	AC	401	50	50,50,50	1.48	8 (16%)	67,82,82	1.17	4 (5%)
60	PTY	L	705	-	41,41,49	0.98	4 (9%)	44,46,54	1.08	2 (4%)
65	3PH	BJ	101	-	40,40,47	0.68	1 (2%)	43,45,52	0.65	1 (2%)
58	PGT	y	303	-	40,40,50	1.19	5 (12%)	43,46,56	1.12	2 (4%)
65	3PH	l	201	-	36,36,47	0.72	1 (2%)	39,41,52	0.71	1 (2%)
64	Q7G	BC	411	-	44,44,90	0.79	2 (4%)	64,68,138	1.44	13 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
65	3PH	AC	405	-	32,32,47	0.34	0	35,37,52	0.41	0
65	3PH	BJ	102	-	47,47,47	0.64	1 (2%)	50,52,52	0.59	1 (2%)
74	HEM	AE	401	52	50,50,50	1.45	7 (14%)	67,82,82	1.17	8 (11%)
65	3PH	f	202	-	42,42,47	0.68	1 (2%)	45,47,52	0.64	2 (4%)
60	PTY	z	301	-	49,49,49	0.87	3 (6%)	52,54,54	1.17	3 (5%)

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
67	UQ5	AC	404	-	-	13/33/57/57	0/1/1/1
60	PTY	D	401	-	-	17/53/53/53	-
72	CDL	u	101	-	-	48/110/110/110	-
72	CDL	BC	408	-	-	36/87/87/110	-
74	HEM	BC	402	50	-	4/14/54/54	-
59	SF4	B	500	2	-	-	0/6/5/5
73	COO	y	302	-	1/1/12/16	12/54/70/70	0/3/3/3
66	PC7	BD	302	-	-	17/42/42/55	-
72	CDL	BE	402	-	-	33/98/98/110	-
60	PTY	N	502	-	-	29/48/48/53	-
60	PTY	N	503	-	-	16/53/53/53	-
72	CDL	AE	402	-	-	41/95/95/110	-
61	FES	BD	301	51	-	-	0/1/1/1
72	CDL	BC	407	-	-	45/91/91/110	-
64	Q7G	K	201	-	-	6/32/200/200	0/10/10/10
71	8Q1	T	200	-	-	23/41/41/41	-
63	UQ9	H	401	-	-	9/30/54/81	0/1/1/1
60	PTY	d	101	-	-	25/42/42/53	-
60	PTY	Y	202	-	-	4/34/34/53	-
60	PTY	N	501	-	-	11/43/43/53	-
74	HEM	BC	401	50	-	2/14/54/54	-
75	UQ7	BC	404	-	-	19/45/69/69	0/1/1/1
66	PC7	BC	409	-	-	25/44/44/55	-
58	PGT	AC	407	-	-	22/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
65	3PH	AI	101	-	-	15/33/33/49	-
58	PGT	AC	406	-	-	21/45/45/55	-
72	CDL	AC	409	-	-	50/95/95/110	-
58	PGT	L	704	-	-	27/49/49/55	-
60	PTY	BF	201	-	-	18/43/43/53	-
61	FES	AD	301	51	-	-	0/1/1/1
64	Q7G	H	402	-	-	12/32/200/200	0/10/10/10
60	PTY	m	101	-	-	16/53/53/53	-
66	PC7	AC	410	-	-	20/54/54/55	-
59	SF4	I	501	9	-	-	0/6/5/5
58	PGT	AF	201	-	-	37/55/55/55	-
65	3PH	L	701	-	-	14/38/38/49	-
58	PGT	L	703	-	-	11/55/55/55	-
64	Q7G	M	505	-	-	6/12/100/200	0/6/6/10
66	PC7	L	706	-	-	17/43/43/55	-
66	PC7	d	102	-	-	26/55/55/55	-
72	CDL	BG	101	-	-	37/80/80/110	-
59	SF4	G	802	7	-	-	0/6/5/5
66	PC7	AB	603	-	-	18/37/37/55	-
65	3PH	Y	201	-	-	17/34/34/49	-
65	3PH	BC	405	-	-	20/45/45/49	-
59	SF4	I	500	9	-	-	0/6/5/5
58	PGT	A	201	-	-	25/55/55/55	-
66	PC7	f	203	-	-	25/51/51/55	-
72	CDL	u	102	-	-	43/110/110/110	-
61	FES	G	801	7	-	-	0/1/1/1
66	PC7	v	201	-	-	24/55/55/55	-
60	PTY	AB	602	-	-	24/44/44/53	-
74	HEM	BE	401	52	-	4/14/54/54	-
66	PC7	AG	101	-	-	21/55/55/55	-
59	SF4	G	803	7	-	-	0/6/5/5
58	PGT	BC	406	-	-	25/41/41/55	-
69	NDP	P	500	-	-	6/34/77/77	0/5/5/5
58	PGT	L	702	-	-	18/40/40/55	-
72	CDL	AC	408	-	-	49/91/91/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	SF4	F	501	6	-	-	0/6/5/5
67	UQ5	L	707	-	-	16/33/57/57	0/1/1/1
71	8Q1	W	200	-	-	11/41/41/41	-
64	Q7G	BC	410	-	-	6/12/100/200	0/6/6/10
67	UQ5	BC	403	-	-	9/33/57/57	0/1/1/1
60	PTY	M	504	-	-	33/53/53/53	-
65	3PH	f	201	-	-	15/42/42/49	-
60	PTY	M	503	-	-	22/40/40/53	-
60	PTY	BB	602	-	-	15/32/32/53	-
61	FES	E	500	5	-	-	0/1/1/1
67	UQ5	AC	403	-	-	15/33/57/57	0/1/1/1
58	PGT	M	502	-	-	18/33/33/55	-
65	3PH	M	501	-	-	19/42/42/49	-
74	HEM	AC	402	50	-	6/14/54/54	-
62	FMN	F	500	-	-	2/18/18/18	0/3/3/3
64	Q7G	a	101	-	-	3/12/100/200	0/6/6/10
74	HEM	AC	401	50	-	2/14/54/54	-
60	PTY	L	705	-	-	19/45/45/53	-
65	3PH	BJ	101	-	-	14/42/42/49	-
58	PGT	y	303	-	-	25/45/45/55	-
65	3PH	l	201	-	-	11/38/38/49	-
64	Q7G	BC	411	-	-	4/12/100/200	0/6/6/10
65	3PH	AC	405	-	-	22/34/34/49	-
65	3PH	BJ	102	-	-	13/49/49/49	-
74	HEM	AE	401	52	-	2/14/54/54	-
65	3PH	f	202	-	-	18/44/44/49	-
60	PTY	z	301	-	-	24/53/53/53	-

All (207) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
73	y	302	COO	C2A-N1A	-15.93	1.05	1.33
73	y	302	COO	C5A-C4A	13.17	1.62	1.39
63	H	401	UQ9	C6-C1	9.98	1.53	1.35
73	y	302	COO	C2A-N3A	-8.97	1.18	1.33
73	y	302	COO	C6A-N1A	-8.11	1.13	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
73	y	302	COO	C5A-N7A	-7.71	1.25	1.39
74	BC	402	HEM	FE-NB	7.17	2.17	1.94
73	y	302	COO	C1-N1	6.96	1.49	1.33
73	y	302	COO	P1A-O3A	6.91	1.67	1.59
73	y	302	COO	C4-N2	6.51	1.48	1.33
74	BC	402	HEM	C1B-NB	-6.31	1.29	1.40
73	y	302	COO	P2A-O3A	6.12	1.66	1.59
74	AC	402	HEM	FE-NB	6.11	2.13	1.94
74	AC	402	HEM	FE-NC	5.80	2.14	1.95
74	BE	401	HEM	C1B-NB	-5.57	1.30	1.40
74	BC	401	HEM	FE-NC	5.29	2.12	1.95
74	BE	401	HEM	FE-NB	5.20	2.10	1.94
74	BC	401	HEM	FE-NB	5.05	2.10	1.94
63	H	401	UQ9	C4-C3	4.95	1.54	1.36
73	y	302	COO	C4A-N3A	4.94	1.43	1.34
74	BC	402	HEM	FE-NC	4.85	2.11	1.95
74	BC	401	HEM	C1B-NB	-4.80	1.31	1.40
73	y	302	COO	C6A-N6A	4.43	1.45	1.34
74	BE	401	HEM	FE-NC	4.30	2.09	1.95
74	AC	401	HEM	FE-ND	4.02	2.07	1.94
74	AC	402	HEM	C1B-NB	-4.02	1.33	1.40
74	BC	401	HEM	C4D-ND	-3.95	1.33	1.40
74	AC	401	HEM	FE-NB	3.93	2.07	1.94
74	BC	402	HEM	C4D-ND	-3.91	1.33	1.40
63	H	401	UQ9	C7-C8	3.87	1.56	1.50
74	BE	401	HEM	C4B-NB	-3.87	1.31	1.38
74	AC	402	HEM	C4D-ND	-3.83	1.33	1.40
74	AE	401	HEM	FE-NA	3.83	2.07	1.95
74	BC	402	HEM	C4B-NB	-3.80	1.31	1.38
74	BE	401	HEM	C4D-ND	-3.61	1.34	1.40
74	AC	402	HEM	C4B-NB	-3.61	1.31	1.38
74	AE	401	HEM	FE-NC	3.54	2.06	1.95
74	BE	401	HEM	C1C-C2C	-3.50	1.38	1.45
73	y	302	COO	P3X-O3X	3.50	1.65	1.59
74	BC	401	HEM	O2A-CGA	-3.43	1.19	1.30
65	M	501	3PH	P-O11	3.35	1.70	1.60
74	BC	402	HEM	C1D-ND	-3.33	1.32	1.38
65	f	202	3PH	P-O11	3.32	1.70	1.60
65	BJ	102	3PH	P-O11	3.32	1.70	1.60
65	AI	101	3PH	P-O11	3.30	1.70	1.60
65	BC	405	3PH	P-O11	3.29	1.70	1.60
65	BJ	101	3PH	P-O11	3.28	1.70	1.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
65	l	201	3PH	P-O11	3.27	1.70	1.60
65	f	201	3PH	P-O11	3.26	1.70	1.60
58	A	201	PGT	O3-C11	3.17	1.42	1.33
58	AF	201	PGT	O3-C11	3.16	1.42	1.33
73	y	302	COO	O4X-C1X	3.13	1.49	1.42
58	AC	407	PGT	O3-C11	3.10	1.42	1.33
58	L	704	PGT	O3-C11	3.10	1.42	1.33
74	AE	401	HEM	CAC-C3C	3.09	1.55	1.47
74	AC	401	HEM	CAC-C3C	3.07	1.55	1.47
58	AC	407	PGT	O2-C31	3.07	1.43	1.34
74	BC	401	HEM	C1C-C2C	-3.07	1.39	1.45
74	AC	402	HEM	C1C-NC	-3.06	1.33	1.39
74	BE	401	HEM	O2A-CGA	-3.06	1.20	1.30
74	AC	401	HEM	CAB-C3B	3.06	1.55	1.47
74	AC	402	HEM	O2D-CGD	-3.02	1.20	1.30
74	BE	401	HEM	C1D-ND	-3.00	1.33	1.38
74	BE	401	HEM	C3C-C4C	-2.99	1.40	1.46
72	u	101	CDL	OA6-CA4	-2.97	1.39	1.46
64	K	201	Q7G	O1B-C1B	2.96	1.45	1.40
74	AE	401	HEM	CAB-C3B	2.93	1.55	1.47
74	BC	402	HEM	O2A-CGA	-2.92	1.21	1.30
74	BC	401	HEM	C3C-C4C	-2.92	1.40	1.46
58	AF	201	PGT	O2-C31	2.90	1.42	1.34
72	BG	101	CDL	OA6-CA4	-2.88	1.39	1.46
72	u	102	CDL	OA6-CA4	-2.88	1.39	1.46
58	A	201	PGT	O2-C31	2.87	1.42	1.34
58	y	303	PGT	O2-C31	2.87	1.42	1.34
74	AE	401	HEM	FE-ND	2.85	2.03	1.94
74	AC	402	HEM	C1D-ND	-2.84	1.33	1.38
74	BC	401	HEM	C1D-ND	-2.84	1.33	1.38
67	L	707	UQ5	C4-C5	-2.83	1.40	1.48
74	AC	401	HEM	FE-NC	2.81	2.04	1.95
66	L	706	PC7	O2-C2	-2.81	1.40	1.46
60	z	301	PTY	O7-C6	-2.80	1.40	1.46
58	y	303	PGT	O3-C11	2.79	1.41	1.33
74	BC	401	HEM	C1C-NC	-2.78	1.34	1.39
74	BE	401	HEM	C1A-C2A	-2.77	1.39	1.44
66	AG	101	PC7	O2-C2	-2.76	1.40	1.46
73	y	302	COO	C12-C11	2.76	1.57	1.52
72	BG	101	CDL	OB6-CB4	-2.75	1.40	1.46
74	AC	401	HEM	FE-NA	2.75	2.04	1.95
60	L	705	PTY	O7-C6	-2.72	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	L	704	PGT	O2-C31	2.72	1.42	1.34
67	AC	403	UQ5	C3-C2	-2.72	1.41	1.48
64	BC	410	Q7G	C11-C08	-2.72	1.51	1.56
74	AC	402	HEM	O2A-CGA	-2.72	1.21	1.30
64	H	402	Q7G	C11-C08	-2.72	1.51	1.56
72	BE	402	CDL	OB6-CB4	-2.71	1.40	1.46
74	BC	401	HEM	C1A-C2A	-2.71	1.39	1.44
60	D	401	PTY	O7-C6	-2.68	1.40	1.46
74	AE	401	HEM	FE-NB	2.68	2.03	1.94
60	BF	201	PTY	O7-C6	-2.67	1.40	1.46
64	M	505	Q7G	C11-C08	-2.65	1.51	1.56
74	BE	401	HEM	C4A-NA	-2.65	1.34	1.39
72	u	102	CDL	OB6-CB4	-2.65	1.40	1.46
74	BE	401	HEM	FE-ND	-2.60	1.86	1.94
60	z	301	PTY	O4-C1	-2.60	1.39	1.45
63	H	401	UQ9	C11-C9	2.59	1.56	1.51
74	BE	401	HEM	O2D-CGD	-2.57	1.22	1.30
74	BC	401	HEM	O2D-CGD	-2.55	1.22	1.30
74	BC	402	HEM	C1A-C2A	-2.54	1.39	1.44
74	AC	402	HEM	C1C-C2C	-2.53	1.40	1.45
72	u	101	CDL	OA8-CA7	2.53	1.40	1.33
66	v	201	PC7	O2-C2	-2.52	1.40	1.46
74	BC	401	HEM	C4B-NB	-2.52	1.33	1.38
64	BC	411	Q7G	C11-C08	-2.52	1.52	1.56
72	u	101	CDL	OB6-CB5	2.51	1.41	1.34
72	u	101	CDL	OB8-CB7	2.50	1.40	1.33
63	H	401	UQ9	C16-C14	2.48	1.56	1.51
73	y	302	COO	C3-C4	2.47	1.56	1.51
60	L	705	PTY	O4-C30	2.47	1.40	1.33
72	u	102	CDL	OB8-CB7	2.47	1.40	1.33
72	BG	101	CDL	OB8-CB7	2.47	1.40	1.33
74	BC	401	HEM	C4C-NC	-2.47	1.35	1.39
72	BG	101	CDL	OA8-CA7	2.46	1.40	1.33
66	v	201	PC7	O3-C11	2.45	1.40	1.33
72	BE	402	CDL	OA8-CA7	2.44	1.40	1.33
74	BC	402	HEM	O2D-CGD	-2.43	1.22	1.30
75	BC	404	UQ7	C3-C4	-2.42	1.41	1.48
72	BE	402	CDL	OB8-CB7	2.42	1.40	1.33
60	D	401	PTY	O4-C30	2.41	1.40	1.33
66	L	706	PC7	O3-C11	2.41	1.40	1.33
66	v	201	PC7	O3-C3	-2.41	1.39	1.45
74	BC	401	HEM	C3D-C2D	-2.40	1.31	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
63	H	401	UQ9	C21-C19	2.40	1.56	1.51
72	u	102	CDL	OA8-CA7	2.40	1.40	1.33
74	BE	401	HEM	C4C-NC	-2.39	1.35	1.39
66	AG	101	PC7	O3-C11	2.39	1.40	1.33
74	AC	402	HEM	C4A-NA	-2.38	1.35	1.39
73	y	302	COO	P1A-O5X	2.37	1.68	1.59
63	H	401	UQ9	O4-C4M	-2.37	1.40	1.45
74	BC	401	HEM	C4A-NA	-2.36	1.35	1.39
63	H	401	UQ9	C26-C24	2.35	1.56	1.51
60	BF	201	PTY	O4-C30	2.35	1.40	1.33
67	AC	403	UQ5	C4-C5	-2.35	1.42	1.48
58	AC	407	PGT	P-O3P	2.33	1.68	1.59
74	AC	402	HEM	C4C-NC	-2.33	1.35	1.39
72	u	101	CDL	OA8-CA6	-2.33	1.40	1.45
73	y	302	COO	O3-C4	-2.33	1.18	1.23
60	L	705	PTY	O4-C1	-2.32	1.40	1.45
72	BE	402	CDL	OA6-CA5	2.31	1.40	1.34
58	L	704	PGT	O2-C2	-2.30	1.41	1.46
72	BE	402	CDL	OA6-CA4	-2.30	1.41	1.46
74	BC	402	HEM	C3C-C4C	-2.29	1.42	1.46
58	L	704	PGT	P-O3P	2.28	1.68	1.59
58	A	201	PGT	O2-C2	-2.27	1.41	1.46
64	K	201	Q7G	O1C-C1C	2.26	1.44	1.40
58	y	303	PGT	P-O3P	2.26	1.68	1.59
58	AF	201	PGT	P-O3P	2.24	1.68	1.59
58	A	201	PGT	P-O3P	2.24	1.68	1.59
66	AG	101	PC7	O3-C3	-2.22	1.40	1.45
72	BE	402	CDL	OA8-CA6	-2.21	1.40	1.45
74	BE	401	HEM	C1C-NC	-2.21	1.35	1.39
72	u	101	CDL	OB6-CB4	-2.20	1.41	1.46
74	AC	401	HEM	CMB-C2B	2.20	1.55	1.50
72	BG	101	CDL	OA8-CA6	-2.19	1.40	1.45
60	D	401	PTY	O4-C1	-2.19	1.40	1.45
72	BE	402	CDL	OB8-CB6	-2.19	1.40	1.45
74	BC	402	HEM	C4A-NA	-2.19	1.35	1.39
72	u	102	CDL	OB6-CB5	2.18	1.40	1.34
60	BF	201	PTY	O7-C8	2.18	1.40	1.34
60	L	705	PTY	O7-C8	2.17	1.40	1.34
74	AC	402	HEM	FE-NA	2.16	2.02	1.95
60	BF	201	PTY	O4-C1	-2.16	1.40	1.45
66	L	706	PC7	O3-C3	-2.16	1.40	1.45
72	BG	101	CDL	OB8-CB6	-2.15	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
74	BC	401	HEM	C1B-C2B	-2.15	1.40	1.44
60	D	401	PTY	O7-C8	2.15	1.40	1.34
74	BC	401	HEM	C4A-C3A	-2.15	1.38	1.43
63	H	401	UQ9	C17-C18	2.14	1.56	1.50
58	y	303	PGT	O3-C3	-2.13	1.40	1.45
75	BC	404	UQ7	C2-C1	-2.13	1.42	1.48
72	BG	101	CDL	OA6-CA5	2.13	1.40	1.34
72	BE	402	CDL	OB6-CB5	2.13	1.40	1.34
58	y	303	PGT	O2-C2	-2.13	1.41	1.46
64	H	402	Q7G	O1B-C1B	2.12	1.43	1.40
64	H	402	Q7G	O1C-C1C	2.12	1.43	1.40
72	BG	101	CDL	OB6-CB5	2.12	1.40	1.34
74	BC	401	HEM	C1A-NA	-2.10	1.35	1.39
74	BE	401	HEM	C1B-C2B	-2.10	1.40	1.44
73	y	302	COO	O2-C1	-2.10	1.19	1.23
66	AG	101	PC7	O2-C31	2.10	1.40	1.34
63	H	401	UQ9	C6-C5	2.10	1.52	1.46
72	u	102	CDL	OA8-CA6	-2.09	1.40	1.45
74	BC	402	HEM	C1C-C2C	-2.09	1.41	1.45
66	v	201	PC7	O2-C31	2.09	1.40	1.34
72	u	101	CDL	OB8-CB6	-2.09	1.40	1.45
72	u	102	CDL	OB8-CB6	-2.08	1.40	1.45
64	K	201	Q7G	C11-C08	-2.08	1.52	1.56
58	AF	201	PGT	O2-C2	-2.06	1.41	1.46
60	z	301	PTY	O4-C30	2.05	1.39	1.33
63	H	401	UQ9	O5-C5	-2.05	1.18	1.23
72	u	102	CDL	OA6-CA5	2.04	1.40	1.34
74	AC	401	HEM	CMA-C3A	2.04	1.55	1.50
74	BC	402	HEM	C3B-C4B	2.04	1.48	1.44
64	BC	411	Q7G	C11-C13	-2.03	1.49	1.52
74	AE	401	HEM	CMC-C2C	2.03	1.54	1.50
65	L	701	3PH	P-O14	-2.02	1.47	1.54
58	AC	407	PGT	O2-C2	-2.02	1.41	1.46
63	H	401	UQ9	O3-C3	2.00	1.41	1.36

All (269) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
73	y	302	COO	C5A-C4A-N3A	-14.32	107.00	126.72
73	y	302	COO	C6A-C5A-N7A	13.89	158.86	132.09
73	y	302	COO	C4A-C5A-N7A	-13.78	94.83	110.58
73	y	302	COO	C4A-N9A-C8A	-10.70	94.50	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
73	y	302	COO	C6-S1-C7	8.17	109.48	99.85
74	BE	401	HEM	CHC-C4B-NB	8.03	133.06	124.42
73	y	302	COO	C6A-C5A-C4A	-7.97	106.30	117.18
63	H	401	UQ9	C7-C8-C9	-7.74	113.50	126.83
73	y	302	COO	N3A-C4A-N9A	7.63	140.15	127.17
73	y	302	COO	C5A-C4A-N9A	6.40	112.79	105.81
73	y	302	COO	C5A-N7A-C8A	6.39	113.49	103.45
73	y	302	COO	C2A-N3A-C4A	5.43	125.09	111.83
64	M	505	Q7G	C05-C06-C02	-5.36	97.49	103.85
74	AC	402	HEM	C1B-NB-C4B	5.23	111.40	105.21
74	BC	402	HEM	C1B-NB-C4B	5.22	111.38	105.21
63	H	401	UQ9	C7-C6-C1	-5.20	115.97	124.89
74	BE	401	HEM	CHD-C1D-ND	5.17	129.98	124.42
74	BE	401	HEM	C1B-NB-C4B	4.83	110.92	105.21
73	y	302	COO	C2A-N1A-C6A	4.79	126.60	118.73
63	H	401	UQ9	C7-C6-C5	4.76	124.05	118.52
74	BC	402	HEM	CHC-C4B-NB	4.70	129.48	124.42
74	AC	402	HEM	C3B-C4B-NB	-4.69	106.10	109.47
74	AC	402	HEM	CHC-C4B-NB	4.68	129.46	124.42
74	BE	401	HEM	O2A-CGA-O1A	-4.62	111.45	123.33
64	K	201	Q7G	C76-C73-C74	-4.58	107.36	115.66
64	K	201	Q7G	C15-C07-C06	-4.49	104.58	110.93
66	v	201	PC7	O2-C31-C32	4.34	120.86	111.48
72	BE	402	CDL	OA6-CA5-C11	4.29	120.76	111.48
71	T	200	8Q1	C37-C38-C39	-4.22	105.37	112.39
74	BC	401	HEM	CHC-C4B-NB	4.21	128.96	124.42
73	y	302	COO	C2X-C1X-N9A	-4.19	102.90	113.30
64	M	505	Q7G	C76-C73-C74	-4.08	108.26	115.66
58	A	201	PGT	O2-C31-C32	4.07	120.28	111.48
64	K	201	Q7G	O80-C73-C76	-4.06	107.22	110.76
64	BC	410	Q7G	C02-C06-C07	-4.05	108.66	114.41
72	u	102	CDL	OB6-CB5-C51	4.04	120.22	111.48
64	M	505	Q7G	C09-C08-C11	-4.00	108.16	113.08
64	M	505	Q7G	C16-C13-C11	3.96	121.50	116.42
60	z	301	PTY	O7-C8-C11	3.96	120.05	111.48
72	BG	101	CDL	OA6-CA5-C11	3.94	120.00	111.48
58	L	704	PGT	O2-C31-C32	3.92	119.96	111.48
58	AC	407	PGT	O2-C31-C32	3.92	119.96	111.48
58	y	303	PGT	O2-C31-C32	3.91	119.95	111.48
72	BE	402	CDL	OB6-CB5-C51	3.89	119.89	111.48
72	BG	101	CDL	OB6-CB5-C51	3.87	119.86	111.48
74	BC	401	HEM	C1B-NB-C4B	3.86	109.78	105.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	AF	201	PGT	O2-C31-C32	3.86	119.83	111.48
60	L	705	PTY	O7-C8-C11	3.85	119.80	111.48
60	BF	201	PTY	O7-C8-C11	3.81	119.72	111.48
66	AG	101	PC7	O2-C31-C32	3.80	119.69	111.48
72	u	101	CDL	OA6-CA5-C11	3.73	119.54	111.48
67	AC	404	UQ5	C7-C6-C5	-3.71	114.21	118.52
74	BC	402	HEM	CHA-C4D-ND	3.70	128.94	124.37
73	y	302	COO	C5A-C6A-N1A	3.70	126.90	117.51
74	BE	401	HEM	C3B-C4B-NB	-3.68	106.82	109.47
64	M	505	Q7G	C09-C10-C02	-3.68	106.53	112.74
64	K	201	Q7G	C16-C13-C14	-3.63	115.65	120.57
60	D	401	PTY	O7-C8-C11	3.58	119.23	111.48
72	u	102	CDL	OA6-CA5-C11	3.55	119.16	111.48
64	BC	410	Q7G	C02-C03-C74	-3.55	110.00	120.50
73	y	302	COO	C3X-C2X-C1X	3.53	107.65	99.89
66	L	706	PC7	O2-C31-C32	3.53	119.11	111.48
74	BC	401	HEM	O2A-CGA-O1A	-3.50	114.34	123.33
64	a	101	Q7G	C76-C73-C74	-3.50	109.33	115.66
64	BC	410	Q7G	C12-C11-C08	-3.48	107.75	111.66
74	BC	401	HEM	CHD-C1D-ND	3.43	128.12	124.42
64	M	505	Q7G	C02-C03-C74	-3.43	110.35	120.50
63	H	401	UQ9	C1M-C1-C6	-3.39	118.87	124.45
74	BC	401	HEM	CMD-C2D-C1D	3.37	130.29	125.03
64	M	505	Q7G	O80-C79-C78	-3.36	107.85	112.17
64	a	101	Q7G	C02-C06-C07	-3.35	109.65	114.41
64	BC	410	Q7G	C76-C73-C74	-3.32	109.64	115.66
64	BC	410	Q7G	C07-C15-C14	-3.31	108.17	112.76
64	BC	411	Q7G	C19-C11-C08	3.28	113.07	108.74
72	u	101	CDL	OB6-CB5-C51	3.26	118.54	111.48
64	H	402	Q7G	C3B-C4B-C5B	-3.22	103.79	110.93
63	H	401	UQ9	C22-C23-C24	-3.22	120.26	127.62
72	u	101	CDL	OA8-CA7-C31	3.21	121.64	111.83
64	BC	411	Q7G	C02-C06-C07	-3.21	109.86	114.41
74	AC	402	HEM	O2D-CGD-O1D	-3.20	115.10	123.33
63	H	401	UQ9	C17-C18-C19	-3.20	120.30	127.62
74	BE	401	HEM	CHD-C1D-C2D	-3.19	120.00	125.03
73	y	302	COO	C5A-C6A-N6A	-3.18	115.41	123.29
74	BE	401	HEM	O2A-CGA-CBA	3.16	124.00	114.00
63	H	401	UQ9	C8-C7-C6	3.14	119.81	112.08
64	H	402	Q7G	C09-C10-C02	-3.13	107.45	112.74
74	BC	401	HEM	C2A-C1A-NA	-3.11	106.70	110.15
74	BC	402	HEM	O2D-CGD-O1D	-3.11	115.32	123.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
63	H	401	UQ9	C12-C13-C14	-3.10	120.53	127.62
64	H	402	Q7G	C02-C03-C74	-3.09	111.35	120.50
64	H	402	Q7G	C76-C73-C74	-3.09	110.07	115.66
64	BC	411	Q7G	C12-C11-C08	-3.05	108.23	111.66
66	L	706	PC7	O3-C11-C12	3.04	121.10	111.83
74	BC	402	HEM	CHD-C1D-ND	3.03	127.68	124.42
74	BC	402	HEM	C4D-ND-C1D	3.02	108.79	105.21
64	a	101	Q7G	C02-C03-C74	-3.02	111.56	120.50
64	K	201	Q7G	C81-C78-C79	-3.01	106.39	111.03
58	AF	201	PGT	O3-C11-C12	2.97	120.90	111.83
73	y	302	COO	O4X-C1X-N9A	2.97	113.78	108.09
74	BE	401	HEM	CHA-C4D-ND	2.96	128.03	124.37
64	BC	411	Q7G	C02-C03-C74	-2.95	111.78	120.50
64	M	505	Q7G	C19-C11-C13	2.93	113.79	108.74
64	K	201	Q7G	C02-C03-C74	-2.93	111.84	120.50
66	v	201	PC7	O3-C11-C12	2.92	120.74	111.83
74	BC	401	HEM	CHA-C4D-ND	2.92	127.97	124.37
64	M	505	Q7G	C02-C06-C07	-2.91	110.28	114.41
74	AC	402	HEM	CHA-C4D-ND	2.90	127.95	124.37
64	H	402	Q7G	C09-C08-C11	-2.89	109.52	113.08
64	K	201	Q7G	O1B-C1B-C2B	2.88	112.65	108.27
74	BC	401	HEM	C3B-C4B-NB	-2.85	107.42	109.47
67	L	707	UQ5	C1-C6-C5	-2.82	116.88	119.62
64	M	505	Q7G	C12-C11-C08	-2.82	108.50	111.66
63	H	401	UQ9	C20-C19-C21	2.81	120.10	115.23
74	AC	401	HEM	C4D-ND-C1D	2.80	108.52	105.21
74	BE	401	HEM	O2D-CGD-O1D	-2.79	116.16	123.33
72	u	102	CDL	OB8-CB7-C71	2.79	120.33	111.83
64	BC	410	Q7G	C11-C08-C07	-2.78	108.66	112.71
64	H	402	Q7G	C05-C06-C02	-2.76	100.58	103.85
64	H	402	Q7G	C12-C11-C08	-2.76	108.57	111.66
64	BC	411	Q7G	C76-C73-C74	-2.76	110.67	115.66
64	M	505	Q7G	C75-C74-C03	-2.75	109.00	114.50
64	a	101	Q7G	O80-C79-C78	-2.74	108.65	112.17
60	D	401	PTY	O4-C30-C31	2.74	120.18	111.83
74	AC	401	HEM	C1B-NB-C4B	2.74	108.45	105.21
72	u	101	CDL	OB8-CB7-C71	2.72	120.14	111.83
74	AC	402	HEM	CHD-C1D-ND	2.71	127.34	124.42
74	BC	402	HEM	O2D-CGD-CBD	2.71	122.56	114.00
64	K	201	Q7G	O80-C73-C74	2.68	115.24	107.26
74	BC	401	HEM	O2D-CGD-CBD	2.68	122.45	114.00
58	y	303	PGT	O3-C11-C12	2.67	119.99	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	L	707	UQ5	C7-C6-C5	2.67	121.62	118.52
72	BE	402	CDL	OA8-CA7-C31	2.66	119.94	111.83
64	a	101	Q7G	C12-C11-C08	-2.65	108.68	111.66
64	a	101	Q7G	C75-C74-C73	-2.65	110.67	114.94
64	BC	411	Q7G	C09-C10-C02	-2.64	108.29	112.74
72	BG	101	CDL	OB8-CB7-C71	2.63	119.86	111.83
60	BF	201	PTY	O4-C30-C31	2.63	119.85	111.83
64	H	402	Q7G	C75-C74-C73	-2.63	110.70	114.94
58	AC	407	PGT	O3-C11-C12	2.63	119.85	111.83
72	u	102	CDL	OA8-CA7-C31	2.62	119.83	111.83
67	L	707	UQ5	C3-C4-C5	-2.61	115.90	120.69
74	BC	401	HEM	CHB-C1B-NB	2.61	127.59	124.37
72	BG	101	CDL	OA8-CA7-C31	2.60	119.77	111.83
66	AG	101	PC7	O3-C11-C12	2.60	119.77	111.83
74	BE	401	HEM	C1A-CHA-C4D	-2.60	120.14	126.25
73	y	302	COO	C10-C9-C8	-2.60	120.06	125.28
64	a	101	Q7G	C08-C11-C13	2.57	113.42	109.65
63	H	401	UQ9	C25-C24-C26	2.57	119.69	115.23
74	BC	402	HEM	C4B-C3B-C2B	-2.57	104.92	107.28
74	BC	401	HEM	CBD-CAD-C3D	-2.57	105.44	112.53
74	BC	402	HEM	O2A-CGA-O1A	-2.56	116.74	123.33
74	AE	401	HEM	CAA-CBA-CGA	-2.56	106.87	113.67
64	BC	411	Q7G	C11-C08-C07	-2.55	108.99	112.71
72	BE	402	CDL	OB8-CB7-C71	2.55	119.60	111.83
66	v	201	PC7	C2-O2-C31	-2.55	111.70	117.80
58	A	201	PGT	O3-C11-C12	2.53	119.56	111.83
58	L	704	PGT	O3-C11-C12	2.53	119.56	111.83
64	M	505	Q7G	C15-C07-C08	-2.52	106.81	109.72
64	K	201	Q7G	C76-C77-C78	-2.52	106.65	111.67
64	K	201	Q7G	O72-C73-C76	2.52	113.64	108.54
74	BE	401	HEM	CHA-C1A-NA	2.50	128.40	123.86
64	BC	410	Q7G	C09-C08-C11	-2.50	110.00	113.08
74	AC	401	HEM	C2A-C1A-NA	-2.50	107.38	110.15
74	BE	401	HEM	CHC-C4B-C3B	-2.49	120.10	125.07
64	K	201	Q7G	C05-C06-C02	-2.49	100.90	103.85
64	H	402	Q7G	CF1-O11-C4C	-2.49	112.08	117.98
63	H	401	UQ9	C15-C14-C16	2.47	119.52	115.23
64	M	505	Q7G	C01-C02-C06	-2.47	107.21	111.68
74	BC	401	HEM	CHD-C1D-C2D	-2.46	121.14	125.03
74	BC	402	HEM	CBD-CAD-C3D	-2.46	105.72	112.53
73	y	302	COO	C1X-N9A-C8A	-2.46	121.63	127.09
65	f	202	3PH	O13-P-O11	-2.45	100.28	106.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
74	AC	402	HEM	C4C-NC-C1C	2.45	109.81	105.82
64	M	505	Q7G	C10-C02-C03	-2.43	111.89	115.36
64	K	201	Q7G	C77-C76-C73	-2.43	108.12	111.93
60	z	301	PTY	O4-C30-C31	2.43	119.24	111.83
74	AC	402	HEM	CBD-CAD-C3D	-2.43	105.82	112.53
73	y	302	COO	N9A-C8A-N7A	-2.42	110.50	113.94
64	BC	411	Q7G	C17-C16-C13	-2.42	107.88	111.45
74	BC	401	HEM	O2A-CGA-CBA	2.41	121.62	114.00
64	M	505	Q7G	C16-C13-C14	-2.41	117.30	120.57
74	AE	401	HEM	C1B-NB-C4B	2.39	108.04	105.21
65	f	201	3PH	C3-C2-C1	2.39	117.36	111.78
74	BC	401	HEM	O2D-CGD-O1D	-2.38	117.20	123.33
60	L	705	PTY	O4-C30-C31	2.38	119.08	111.83
74	BC	402	HEM	C3B-C4B-NB	-2.36	107.77	109.47
64	BC	411	Q7G	C15-C07-C06	-2.36	107.59	110.93
72	BG	101	CDL	CA4-OA6-CA5	-2.36	112.14	117.80
66	L	706	PC7	C2-O2-C31	-2.35	112.17	117.80
74	AE	401	HEM	C3B-C2B-C1B	2.34	108.17	106.41
65	l	201	3PH	O13-P-O11	-2.34	100.56	106.67
64	BC	411	Q7G	C75-C74-C03	-2.34	109.83	114.50
65	BC	405	3PH	O13-P-O11	-2.33	100.58	106.67
64	BC	411	Q7G	C16-C13-C14	-2.33	117.41	120.57
64	BC	410	Q7G	C75-C74-C03	-2.33	109.84	114.50
64	K	201	Q7G	C61-C51-C41	-2.32	107.33	113.02
64	K	201	Q7G	C1C-O5C-C5C	2.32	118.25	113.72
65	M	501	3PH	O13-P-O11	-2.32	100.63	106.67
75	BC	404	UQ7	C7-C6-C5	-2.31	120.92	124.89
64	K	201	Q7G	C03-C02-C06	-2.30	97.17	100.18
74	AE	401	HEM	C3D-C4D-ND	-2.30	107.65	110.17
75	BC	404	UQ7	C17-C16-C14	2.30	120.79	113.19
74	AE	401	HEM	C4D-ND-C1D	2.29	107.92	105.21
65	L	701	3PH	O21-C21-C22	-2.28	106.54	111.48
67	AC	403	UQ5	C7-C6-C1	-2.28	120.98	124.89
74	BC	401	HEM	CHD-C4C-NC	2.28	126.94	124.45
64	a	101	Q7G	C07-C15-C14	-2.26	109.63	112.76
64	M	505	Q7G	C10-C02-C06	2.25	110.62	107.25
74	BE	401	HEM	CHB-C1B-NB	2.24	127.14	124.37
63	H	401	UQ9	C6-C1-C2	2.24	120.94	119.17
74	BE	401	HEM	C1C-CHC-C4B	-2.23	121.28	126.02
74	BE	401	HEM	CHD-C4C-NC	2.23	126.88	124.45
64	BC	410	Q7G	C09-C10-C02	-2.22	108.99	112.74
74	BC	401	HEM	CHA-C1A-NA	2.22	127.89	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
65	L	701	3PH	C3-C2-C1	2.22	116.96	111.78
64	a	101	Q7G	C75-C74-C03	-2.22	110.07	114.50
65	f	201	3PH	O13-P-O11	-2.21	100.92	106.67
74	AC	401	HEM	C3D-C4D-ND	-2.20	107.76	110.17
65	BJ	101	3PH	O13-P-O11	-2.20	100.94	106.67
74	AC	402	HEM	CHB-C1B-NB	2.19	127.08	124.37
65	AI	101	3PH	O13-P-O11	-2.19	100.97	106.67
74	BC	401	HEM	C4A-NA-C1A	2.18	109.38	105.82
64	BC	411	Q7G	C16-C13-C11	2.16	119.19	116.42
62	F	500	FMN	C4-N3-C2	-2.16	121.81	125.64
73	y	302	COO	C2X-C3X-C4X	2.16	107.01	103.24
74	BC	402	HEM	O2A-CGA-CBA	2.15	120.80	114.00
74	BC	401	HEM	C4B-C3B-C2B	-2.15	105.30	107.28
64	K	201	Q7G	C08-C07-C06	-2.15	106.28	109.09
60	z	301	PTY	C6-O7-C8	-2.15	112.66	117.80
74	BC	401	HEM	C4C-NC-C1C	2.15	109.32	105.82
64	K	201	Q7G	C19-C11-C08	2.14	111.57	108.74
65	BJ	102	3PH	O13-P-O11	-2.14	101.09	106.67
74	AE	401	HEM	C2A-C1A-NA	-2.12	107.80	110.15
74	AC	402	HEM	C2A-C1A-NA	-2.12	107.80	110.15
74	BE	401	HEM	CBD-CAD-C3D	-2.11	106.69	112.53
74	BC	402	HEM	CAA-C2A-C1A	2.11	129.06	124.94
64	M	505	Q7G	O80-C73-C76	-2.11	108.92	110.76
63	H	401	UQ9	C10-C9-C8	-2.10	118.23	123.63
74	BE	401	HEM	C4D-ND-C1D	2.10	107.69	105.21
74	AE	401	HEM	CBD-CAD-C3D	-2.09	106.75	112.53
67	AC	404	UQ5	C12-C13-C14	2.09	132.40	127.62
74	BC	401	HEM	CAD-C3D-C4D	2.09	128.33	124.70
74	BE	401	HEM	CBA-CAA-C2A	2.09	118.30	112.53
67	L	707	UQ5	C7-C6-C1	-2.08	121.33	124.89
67	BC	403	UQ5	C6-C1-C2	2.08	120.81	119.17
65	f	202	3PH	O14-P-O13	2.07	115.57	107.80
74	BE	401	HEM	CAA-CBA-CGA	-2.07	108.17	113.67
74	AE	401	HEM	CHC-C4B-NB	2.07	126.65	124.42
64	BC	411	Q7G	C77-C76-C73	-2.07	108.70	111.93
64	H	402	Q7G	C08-C07-C06	-2.06	106.39	109.09
58	A	201	PGT	C2-O2-C31	-2.06	112.86	117.80
74	BE	401	HEM	C2A-C1A-NA	-2.06	107.86	110.15
65	AI	101	3PH	C3-C2-C1	2.06	116.58	111.78
64	K	201	Q7G	C11-C13-C14	2.06	125.93	122.93
74	BC	402	HEM	CHA-C4D-C3D	-2.06	121.44	125.23
64	H	402	Q7G	C02-C06-C07	-2.06	111.50	114.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
72	u	101	CDL	OA8-CA7-OA9	-2.05	118.51	123.63
64	BC	410	Q7G	C15-C14-C13	-2.05	121.57	125.02
71	T	200	8Q1	C42-N41-C39	2.04	126.62	122.82
64	H	402	Q7G	O5B-C1B-C2B	2.03	114.55	110.37
64	H	402	Q7G	C1-O1-C4B	-2.03	113.16	117.98
74	BC	402	HEM	C4C-NC-C1C	2.03	109.13	105.82
74	AC	402	HEM	C4A-NA-C1A	2.03	109.13	105.82
71	T	200	8Q1	C37-N36-C34	2.02	126.18	122.55
64	H	402	Q7G	O5B-C5B-C4B	-2.02	105.55	109.72
74	BC	402	HEM	CMC-C2C-C1C	2.02	128.28	124.73
64	K	201	Q7G	C12-C11-C08	-2.01	109.41	111.66
64	a	101	Q7G	C17-C16-C13	-2.01	108.49	111.45
65	M	501	3PH	O31-C3-C2	2.01	114.18	108.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
73	y	302	COO	C13

All (1447) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	A	201	PGT	C32-C31-O2-C2
58	A	201	PGT	O4P-C4-C5-O5
58	L	702	PGT	C32-C31-O2-C2
58	L	702	PGT	O31-C31-O2-C2
58	L	704	PGT	C32-C31-O2-C2
58	L	704	PGT	O2-C2-C3-O3
58	L	704	PGT	C1-O3P-P-O1P
58	M	502	PGT	C1-O3P-P-O1P
58	M	502	PGT	C4-O4P-P-O3P
58	M	502	PGT	C4-O4P-P-O1P
58	M	502	PGT	C4-O4P-P-O2P
58	M	502	PGT	C4-C5-C6-O6
58	y	303	PGT	O2-C2-C3-O3
58	y	303	PGT	C4-O4P-P-O3P
58	AC	406	PGT	C1-O3P-P-O1P
58	AC	406	PGT	C4-O4P-P-O1P
58	AC	406	PGT	C4-O4P-P-O2P
58	AC	406	PGT	C4-C5-C6-O6
58	AC	407	PGT	C32-C31-O2-C2
58	AC	407	PGT	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
58	AF	201	PGT	C1-O3P-P-O2P
58	AF	201	PGT	C1-O3P-P-O4P
58	AF	201	PGT	C4-O4P-P-O2P
58	BC	406	PGT	C32-C31-O2-C2
58	BC	406	PGT	O31-C31-O2-C2
58	BC	406	PGT	C1-O3P-P-O1P
58	BC	406	PGT	C1-O3P-P-O2P
58	BC	406	PGT	C1-O3P-P-O4P
58	BC	406	PGT	C4-O4P-P-O3P
58	BC	406	PGT	C4-O4P-P-O2P
58	BC	406	PGT	O4P-C4-C5-C6
58	BC	406	PGT	C4-C5-C6-O6
60	D	401	PTY	C3-O11-P1-O12
60	D	401	PTY	C3-O11-P1-O14
60	L	705	PTY	N1-C2-C3-O11
60	L	705	PTY	C2-C3-O11-P1
60	M	503	PTY	C11-C8-O7-C6
60	M	503	PTY	C3-O11-P1-O14
60	M	504	PTY	N1-C2-C3-O11
60	M	504	PTY	O10-C8-O7-C6
60	M	504	PTY	C11-C8-O7-C6
60	M	504	PTY	C3-O11-P1-O14
60	N	501	PTY	C3-O11-P1-O13
60	N	501	PTY	C5-O14-P1-O11
60	N	501	PTY	C5-O14-P1-O12
60	N	502	PTY	C2-C3-O11-P1
60	N	502	PTY	C3-O11-P1-O12
60	N	502	PTY	C3-O11-P1-O14
60	N	503	PTY	N1-C2-C3-O11
60	Y	202	PTY	O10-C8-O7-C6
60	Y	202	PTY	C11-C8-O7-C6
60	d	101	PTY	C3-O11-P1-O12
60	d	101	PTY	C3-O11-P1-O14
60	m	101	PTY	C5-O14-P1-O11
60	m	101	PTY	C5-O14-P1-O12
60	z	301	PTY	O10-C8-O7-C6
60	z	301	PTY	C11-C8-O7-C6
60	AB	602	PTY	N1-C2-C3-O11
60	AB	602	PTY	C3-O11-P1-O14
60	BB	602	PTY	N1-C2-C3-O11
60	BB	602	PTY	O10-C8-O7-C6
60	BB	602	PTY	C11-C8-O7-C6

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Mol	Chain	Res	Type	Atoms
60	BF	201	PTY	N1-C2-C3-O11
60	BF	201	PTY	C3-O11-P1-O12
60	BF	201	PTY	C3-O11-P1-O14
63	H	401	UQ9	C1-C6-C7-C8
63	H	401	UQ9	C5-C6-C7-C8
64	H	402	Q7G	CG1-C22-C23-C48
64	H	402	Q7G	C48-C23-C24-O1B
64	K	201	Q7G	C2B-C1B-O1B-C24
64	K	201	Q7G	O5B-C1B-O1B-C24
64	M	505	Q7G	C22-CG1-O20-C17
64	a	101	Q7G	C18-C17-O20-CG1
65	L	701	3PH	C22-C21-O21-C2
65	Y	201	3PH	C1-O11-P-O13
65	Y	201	3PH	C1-O11-P-O14
65	f	201	3PH	C1-O11-P-O13
65	f	201	3PH	C1-O11-P-O12
65	f	202	3PH	C22-C21-O21-C2
65	l	201	3PH	O22-C21-O21-C2
65	l	201	3PH	C22-C21-O21-C2
65	AC	405	3PH	C1-O11-P-O13
65	AC	405	3PH	C1-O11-P-O14
65	AC	405	3PH	O22-C21-O21-C2
65	AC	405	3PH	C22-C21-O21-C2
65	AI	101	3PH	C1-O11-P-O13
65	AI	101	3PH	C1-O11-P-O14
65	AI	101	3PH	C32-C31-O31-C3
65	BJ	101	3PH	C1-O11-P-O13
66	L	706	PC7	C32-C31-O2-C2
66	L	706	PC7	O31-C31-O2-C2
66	L	706	PC7	C4-O4P-P-O3P
66	L	706	PC7	C4-O4P-P-O2P
66	L	706	PC7	O4P-C4-C5-N
66	f	203	PC7	C32-C31-O2-C2
66	f	203	PC7	O31-C31-O2-C2
66	f	203	PC7	C4-O4P-P-O3P
66	f	203	PC7	C4-O4P-P-O1P
66	AB	603	PC7	C32-C31-O2-C2
66	AB	603	PC7	O31-C31-O2-C2
66	AB	603	PC7	C1-O3P-P-O2P
66	AB	603	PC7	C1-O3P-P-O4P
66	AC	410	PC7	C32-C31-O2-C2
66	AC	410	PC7	O31-C31-O2-C2

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Mol	Chain	Res	Type	Atoms
66	AG	101	PC7	C32-C31-O2-C2
66	BC	409	PC7	C32-C31-O2-C2
66	BC	409	PC7	O2-C2-C3-O3
66	BC	409	PC7	C1-O3P-P-O1P
66	BC	409	PC7	C4-O4P-P-O3P
66	BC	409	PC7	C4-O4P-P-O2P
66	BD	302	PC7	C32-C31-O2-C2
67	L	707	UQ5	C7-C8-C9-C10
67	L	707	UQ5	C7-C8-C9-C11
67	L	707	UQ5	C27-C28-C29-C31
67	AC	403	UQ5	C7-C8-C9-C10
67	AC	403	UQ5	C7-C8-C9-C11
67	AC	403	UQ5	C12-C13-C14-C15
67	AC	403	UQ5	C17-C18-C19-C20
71	T	200	8Q1	C28-C29-C32-C34
71	T	200	8Q1	C30-C29-C32-C34
71	T	200	8Q1	C30-C29-C32-O33
71	T	200	8Q1	C31-C29-C32-C34
71	T	200	8Q1	C32-C34-N36-C37
71	T	200	8Q1	O35-C34-N36-C37
71	T	200	8Q1	C38-C39-N41-C42
71	T	200	8Q1	O40-C39-N41-C42
71	T	200	8Q1	N41-C42-C43-S44
71	T	200	8Q1	C42-C43-S44-C1
71	T	200	8Q1	C28-O27-P24-O2
71	T	200	8Q1	C28-O27-P24-O1
71	W	200	8Q1	O27-C28-C29-C30
71	W	200	8Q1	O27-C28-C29-C31
71	W	200	8Q1	O27-C28-C29-C32
71	W	200	8Q1	C29-C28-O27-P24
71	W	200	8Q1	C28-C29-C32-C34
71	W	200	8Q1	C28-C29-C32-O33
71	W	200	8Q1	C30-C29-C32-O33
71	W	200	8Q1	C31-C29-C32-C34
71	W	200	8Q1	C31-C29-C32-O33
71	W	200	8Q1	C28-O27-P24-O1
72	u	101	CDL	O1-C1-CB2-OB2
72	u	101	CDL	OA9-CA7-OA8-CA6
72	u	101	CDL	C31-CA7-OA8-CA6
72	u	102	CDL	CB3-OB5-PB2-OB2
72	u	102	CDL	CB3-OB5-PB2-OB4
72	u	102	CDL	OB7-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
72	u	102	CDL	C51-CB5-OB6-CB4
72	AC	408	CDL	CA2-OA2-PA1-OA4
72	AC	408	CDL	CA2-OA2-PA1-OA5
72	AC	408	CDL	C11-CA5-OA6-CA4
72	AC	408	CDL	CB2-OB2-PB2-OB4
72	AC	408	CDL	CB2-OB2-PB2-OB5
72	AC	408	CDL	OB5-CB3-CB4-OB6
72	AC	408	CDL	C51-CB5-OB6-CB4
72	AC	409	CDL	CA2-C1-CB2-OB2
72	AC	409	CDL	CB2-OB2-PB2-OB3
72	AC	409	CDL	CB2-OB2-PB2-OB5
72	AC	409	CDL	CB3-OB5-PB2-OB2
72	AE	402	CDL	C11-CA5-OA6-CA4
72	AE	402	CDL	CB3-OB5-PB2-OB2
72	AE	402	CDL	CB3-OB5-PB2-OB4
72	BC	407	CDL	CA2-OA2-PA1-OA3
72	BC	407	CDL	OA7-CA5-OA6-CA4
72	BC	407	CDL	C11-CA5-OA6-CA4
72	BC	407	CDL	CB2-OB2-PB2-OB3
72	BC	407	CDL	CB2-OB2-PB2-OB4
72	BC	407	CDL	CB2-OB2-PB2-OB5
72	BC	408	CDL	CB2-OB2-PB2-OB4
72	BC	408	CDL	CB2-OB2-PB2-OB5
72	BC	408	CDL	CB3-OB5-PB2-OB2
72	BC	408	CDL	CB3-OB5-PB2-OB3
72	BC	408	CDL	CB3-OB5-PB2-OB4
72	BE	402	CDL	CA6-CA4-OA6-CA5
72	BE	402	CDL	C11-CA5-OA6-CA4
72	BE	402	CDL	CB3-OB5-PB2-OB2
72	BE	402	CDL	CB3-OB5-PB2-OB3
72	BE	402	CDL	CB3-OB5-PB2-OB4
72	BG	101	CDL	CA3-OA5-PA1-OA3
72	BG	101	CDL	CA3-OA5-PA1-OA4
72	BG	101	CDL	C11-CA5-OA6-CA4
72	BG	101	CDL	CB2-OB2-PB2-OB5
72	BG	101	CDL	CB4-CB3-OB5-PB2
73	y	302	COO	C5X-O5X-P1A-O3A
73	y	302	COO	C5X-O5X-P1A-O2A
73	y	302	COO	C5X-O5X-P1A-O1A
73	y	302	COO	C5-C6-S1-C7
73	y	302	COO	S1-C7-C8-C9
74	BC	402	HEM	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
75	BC	404	UQ7	C17-C18-C19-C20
75	BC	404	UQ7	C17-C18-C19-C21
58	M	502	PGT	O11-C11-O3-C3
60	N	501	PTY	O30-C30-O4-C1
60	BB	602	PTY	O30-C30-O4-C1
65	AI	101	3PH	O32-C31-O31-C3
66	BD	302	PC7	O11-C11-O3-C3
72	AC	409	CDL	OB9-CB7-OB8-CB6
67	L	707	UQ5	C27-C28-C29-C30
58	M	502	PGT	C12-C11-O3-C3
60	N	501	PTY	C31-C30-O4-C1
60	BB	602	PTY	C31-C30-O4-C1
66	BD	302	PC7	C12-C11-O3-C3
72	AC	409	CDL	C71-CB7-OB8-CB6
58	AF	201	PGT	O11-C11-O3-C3
60	M	503	PTY	O30-C30-O4-C1
65	BC	405	3PH	O32-C31-O31-C3
65	BJ	101	3PH	O32-C31-O31-C3
72	AE	402	CDL	OB9-CB7-OB8-CB6
72	BG	101	CDL	OB9-CB7-OB8-CB6
58	A	201	PGT	O31-C31-O2-C2
58	L	704	PGT	O31-C31-O2-C2
58	AC	407	PGT	O31-C31-O2-C2
60	M	503	PTY	O10-C8-O7-C6
60	N	502	PTY	O10-C8-O7-C6
65	L	701	3PH	O22-C21-O21-C2
66	AG	101	PC7	O31-C31-O2-C2
66	BC	409	PC7	O31-C31-O2-C2
72	AC	408	CDL	OA7-CA5-OA6-CA4
72	AC	408	CDL	OB7-CB5-OB6-CB4
72	AE	402	CDL	OA7-CA5-OA6-CA4
72	BG	101	CDL	OA7-CA5-OA6-CA4
65	BJ	101	3PH	C32-C31-O31-C3
72	BG	101	CDL	C71-CB7-OB8-CB6
60	N	502	PTY	C11-C8-O7-C6
72	AE	402	CDL	OA9-CA7-OA8-CA6
63	H	401	UQ9	C12-C11-C9-C10
75	BC	404	UQ7	C20-C19-C21-C22
63	H	401	UQ9	C12-C11-C9-C8
75	BC	404	UQ7	C18-C19-C21-C22
58	AF	201	PGT	C12-C11-O3-C3
60	M	503	PTY	C31-C30-O4-C1

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Mol	Chain	Res	Type	Atoms
60	M	504	PTY	C31-C30-O4-C1
65	BC	405	3PH	C32-C31-O31-C3
66	d	102	PC7	C12-C11-O3-C3
72	AE	402	CDL	C71-CB7-OB8-CB6
67	L	707	UQ5	C17-C18-C19-C20
67	L	707	UQ5	C17-C18-C19-C21
67	AC	403	UQ5	C17-C18-C19-C21
66	d	102	PC7	O11-C11-O3-C3
65	f	202	3PH	O22-C21-O21-C2
66	BD	302	PC7	O31-C31-O2-C2
72	BE	402	CDL	OA7-CA5-OA6-CA4
58	BC	406	PGT	O4P-C4-C5-O5
72	BE	402	CDL	O1-C1-CA2-OA2
72	BG	101	CDL	O1-C1-CA2-OA2
58	L	702	PGT	C12-C11-O3-C3
60	d	101	PTY	C31-C30-O4-C1
72	AE	402	CDL	C31-CA7-OA8-CA6
72	AC	409	CDL	C51-CB5-OB6-CB4
67	L	707	UQ5	C12-C11-C9-C10
75	BC	404	UQ7	C25-C24-C26-C27
67	L	707	UQ5	C12-C11-C9-C8
67	AC	403	UQ5	C13-C14-C16-C17
75	BC	404	UQ7	C23-C24-C26-C27
60	M	504	PTY	O30-C30-O4-C1
67	L	707	UQ5	C9-C11-C12-C13
67	L	707	UQ5	C14-C16-C17-C18
67	L	707	UQ5	C19-C21-C22-C23
67	AC	404	UQ5	C14-C16-C17-C18
67	AC	404	UQ5	C19-C21-C22-C23
67	AC	404	UQ5	C24-C26-C27-C28
67	BC	403	UQ5	C9-C11-C12-C13
67	BC	403	UQ5	C19-C21-C22-C23
66	v	201	PC7	C2-C1-O3P-P
58	L	702	PGT	O11-C11-O3-C3
60	d	101	PTY	O30-C30-O4-C1
73	y	302	COO	C4X-C3X-O3X-P3X
58	L	702	PGT	O4P-C4-C5-C6
58	y	303	PGT	O4P-C4-C5-C6
72	BG	101	CDL	CB2-C1-CA2-OA2
58	y	303	PGT	C12-C11-O3-C3
65	L	701	3PH	C32-C31-O31-C3
72	u	101	CDL	C71-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
66	v	201	PC7	C4-C5-N-C6
66	AC	410	PC7	C4-C5-N-C8
66	AC	410	PC7	C4-C5-N-C6
60	d	101	PTY	C17-C18-C19-C20
66	f	203	PC7	C41-C42-C43-C44
72	AC	409	CDL	C19-C20-C21-C22
60	N	502	PTY	C12-C13-C14-C15
72	AC	408	CDL	C55-C56-C57-C58
72	AC	409	CDL	C40-C41-C42-C43
67	AC	403	UQ5	C15-C14-C16-C17
67	BC	403	UQ5	C25-C24-C26-C27
75	BC	404	UQ7	C15-C14-C16-C17
67	BC	403	UQ5	C23-C24-C26-C27
75	BC	404	UQ7	C13-C14-C16-C17
60	AB	602	PTY	C15-C16-C17-C18
60	M	504	PTY	C8-C11-C12-C13
58	L	702	PGT	O4P-C4-C5-O5
72	BC	407	CDL	C56-C57-C58-C59
65	L	701	3PH	O32-C31-O31-C3
72	AC	409	CDL	OB7-CB5-OB6-CB4
58	BC	406	PGT	O2-C2-C3-O3
60	AB	602	PTY	C31-C30-O4-C1
72	BC	407	CDL	C71-CB7-OB8-CB6
65	AC	405	3PH	C31-C32-C33-C34
72	u	101	CDL	CB5-C51-C52-C53
65	L	701	3PH	C22-C23-C24-C25
58	A	201	PGT	O5-C5-C6-O6
58	AC	407	PGT	O5-C5-C6-O6
58	BC	406	PGT	O5-C5-C6-O6
67	AC	403	UQ5	C12-C13-C14-C16
72	BC	408	CDL	C71-CB7-OB8-CB6
58	y	303	PGT	C14-C15-C16-C17
65	BC	405	3PH	C21-C22-C23-C24
67	AC	403	UQ5	C9-C11-C12-C13
75	BC	404	UQ7	C29-C31-C32-C33
60	D	401	PTY	C35-C36-C37-C38
60	m	101	PTY	C30-C31-C32-C33
65	BJ	102	3PH	C31-C32-C33-C34
72	AC	409	CDL	CB5-C51-C52-C53
60	AB	602	PTY	O30-C30-O4-C1
58	L	703	PGT	C32-C31-O2-C2
58	L	702	PGT	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
58	L	704	PGT	C31-C32-C33-C34
60	z	301	PTY	C8-C11-C12-C13
65	L	701	3PH	C21-C22-C23-C24
65	BJ	101	3PH	C21-C22-C23-C24
72	AC	408	CDL	CA5-C11-C12-C13
72	AE	402	CDL	CA5-C11-C12-C13
72	BC	408	CDL	CA7-C31-C32-C33
58	AC	406	PGT	C44-C45-C46-C47
72	BG	101	CDL	C40-C41-C42-C43
60	z	301	PTY	C31-C32-C33-C34
60	z	301	PTY	C38-C39-C40-C41
66	d	102	PC7	C17-C18-C19-C20
58	L	704	PGT	O4P-C4-C5-O5
58	M	502	PGT	O4P-C4-C5-O5
58	y	303	PGT	O4P-C4-C5-O5
72	AC	408	CDL	C31-CA7-OA8-CA6
72	BG	101	CDL	C31-CA7-OA8-CA6
58	y	303	PGT	O11-C11-O3-C3
72	u	101	CDL	OB9-CB7-OB8-CB6
72	BC	407	CDL	OB9-CB7-OB8-CB6
58	L	702	PGT	C11-C12-C13-C14
60	AB	602	PTY	C8-C11-C12-C13
65	Y	201	3PH	C21-C22-C23-C24
72	u	101	CDL	CA5-C11-C12-C13
60	d	101	PTY	C11-C8-O7-C6
72	u	101	CDL	C32-C33-C34-C35
72	BC	408	CDL	OB9-CB7-OB8-CB6
58	y	303	PGT	C12-C13-C14-C15
69	P	500	NDP	C2D-C1D-N1N-C6N
58	A	201	PGT	C17-C18-C19-C20
60	N	501	PTY	C8-C11-C12-C13
72	AC	409	CDL	CA7-C31-C32-C33
58	L	703	PGT	O31-C31-O2-C2
60	d	101	PTY	O10-C8-O7-C6
58	A	201	PGT	O4P-C4-C5-C6
58	L	704	PGT	O4P-C4-C5-C6
58	M	502	PGT	O4P-C4-C5-C6
58	AF	201	PGT	O4P-C4-C5-C6
72	u	101	CDL	CA2-C1-CB2-OB2
72	BE	402	CDL	CB2-C1-CA2-OA2
64	H	402	Q7G	C22-C23-C24-O1B
66	v	201	PC7	C4-C5-N-C8

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Mol	Chain	Res	Type	Atoms
66	BC	409	PC7	C4-C5-N-C7
66	BC	409	PC7	C4-C5-N-C8
66	BC	409	PC7	C4-C5-N-C6
72	AE	402	CDL	CB5-C51-C52-C53
72	AE	402	CDL	C14-C15-C16-C17
72	BC	407	CDL	C31-CA7-OA8-CA6
60	d	101	PTY	C8-C11-C12-C13
65	M	501	3PH	C31-C32-C33-C34
67	BC	403	UQ5	C12-C11-C9-C10
66	v	201	PC7	C32-C31-O2-C2
72	BC	408	CDL	C11-CA5-OA6-CA4
64	K	201	Q7G	C22-CG1-O20-C17
72	BC	408	CDL	OA7-CA5-OA6-CA4
67	BC	403	UQ5	C14-C16-C17-C18
67	BC	403	UQ5	C24-C26-C27-C28
58	AC	407	PGT	O4P-C4-C5-O5
58	AF	201	PGT	O4P-C4-C5-O5
72	AC	408	CDL	O1-C1-CB2-OB2
72	AC	409	CDL	O1-C1-CB2-OB2
58	A	201	PGT	C36-C37-C38-C39
72	BG	101	CDL	OA9-CA7-OA8-CA6
58	A	201	PGT	C4-C5-C6-O6
58	L	704	PGT	C4-C5-C6-O6
58	AF	201	PGT	C4-C5-C6-O6
64	BC	410	Q7G	C16-C17-O20-CG1
64	BC	410	Q7G	C18-C17-O20-CG1
60	L	705	PTY	C16-C17-C18-C19
58	AF	201	PGT	C2-C3-O3-C11
60	AB	602	PTY	C11-C8-O7-C6
65	M	501	3PH	C22-C21-O21-C2
72	AC	408	CDL	C71-CB7-OB8-CB6
66	v	201	PC7	C4-C5-N-C7
66	AC	410	PC7	C4-C5-N-C7
58	AC	406	PGT	C11-C12-C13-C14
65	M	501	3PH	C21-C22-C23-C24
72	BC	408	CDL	CB5-C51-C52-C53
58	AC	407	PGT	C15-C16-C17-C18
58	BC	406	PGT	C15-C16-C17-C18
60	BF	201	PTY	C34-C35-C36-C37
65	Y	201	3PH	C33-C34-C35-C36
72	BC	408	CDL	C35-C36-C37-C38
58	L	704	PGT	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
60	L	705	PTY	C35-C36-C37-C38
65	M	501	3PH	C36-C37-C38-C39
65	f	202	3PH	C2C-C2D-C2E-C2F
66	d	102	PC7	C32-C33-C34-C35
66	AC	410	PC7	C36-C37-C38-C39
66	BC	409	PC7	C33-C34-C35-C36
72	AC	409	CDL	C73-C74-C75-C76
72	AE	402	CDL	C22-C23-C24-C25
72	BC	408	CDL	C13-C14-C15-C16
72	BE	402	CDL	C15-C16-C17-C18
66	L	706	PC7	C31-C32-C33-C34
58	AF	201	PGT	C42-C43-C44-C45
60	N	503	PTY	C11-C12-C13-C14
66	BC	409	PC7	C32-C33-C34-C35
72	AE	402	CDL	C35-C36-C37-C38
72	AC	408	CDL	OA9-CA7-OA8-CA6
58	y	303	PGT	C33-C34-C35-C36
58	AC	407	PGT	C40-C41-C42-C43
60	M	504	PTY	C32-C33-C34-C35
60	z	301	PTY	C33-C34-C35-C36
65	AI	101	3PH	C33-C34-C35-C36
66	d	102	PC7	C39-C40-C41-C42
66	f	203	PC7	C39-C40-C41-C42
66	AC	410	PC7	C15-C16-C17-C18
72	u	101	CDL	C76-C77-C78-C79
72	u	102	CDL	C37-C38-C39-C40
72	BC	408	CDL	C52-C53-C54-C55
58	AC	406	PGT	O5-C5-C6-O6
58	AF	201	PGT	O5-C5-C6-O6
60	L	705	PTY	C33-C34-C35-C36
60	d	101	PTY	C14-C15-C16-C17
66	f	203	PC7	C33-C34-C35-C36
66	AG	101	PC7	C21-C22-C23-C24
72	AC	409	CDL	C16-C17-C18-C19
72	BC	407	CDL	C78-C79-C80-C81
72	BE	402	CDL	C12-C13-C14-C15
66	L	706	PC7	C11-C12-C13-C14
58	A	201	PGT	C15-C16-C17-C18
58	BC	406	PGT	C13-C14-C15-C16
65	AC	405	3PH	C34-C35-C36-C37
66	AC	410	PC7	C17-C18-C19-C20
72	AC	408	CDL	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
72	BC	407	CDL	C16-C17-C18-C19
60	d	101	PTY	C13-C14-C15-C16
60	d	101	PTY	C18-C19-C20-C21
60	AB	602	PTY	C36-C37-C38-C39
60	M	503	PTY	C31-C32-C33-C34
60	N	503	PTY	C13-C14-C15-C16
65	AI	101	3PH	C22-C23-C24-C25
72	AC	409	CDL	O1-C1-CA2-OA2
58	BC	406	PGT	C11-C12-C13-C14
60	AB	602	PTY	C30-C31-C32-C33
72	BG	101	CDL	CB7-C71-C72-C73
58	A	201	PGT	C20-C21-C22-C23
58	AC	407	PGT	C18-C19-C20-C21
60	N	503	PTY	C21-C22-C23-C24
60	d	101	PTY	C11-C12-C13-C14
65	AI	101	3PH	C38-C39-C3A-C3B
66	d	102	PC7	C37-C38-C39-C40
66	AG	101	PC7	C39-C40-C41-C42
72	u	101	CDL	C36-C37-C38-C39
72	AC	408	CDL	C83-C84-C85-C86
72	AE	402	CDL	C37-C38-C39-C40
72	BC	407	CDL	C80-C81-C82-C83
58	y	303	PGT	C13-C14-C15-C16
58	AF	201	PGT	C37-C38-C39-C40
60	M	504	PTY	C18-C19-C20-C21
60	d	101	PTY	C16-C17-C18-C19
65	BJ	101	3PH	C22-C23-C24-C25
60	N	502	PTY	C20-C21-C22-C23
60	m	101	PTY	C13-C14-C15-C16
72	AC	408	CDL	CA7-C31-C32-C33
65	AI	101	3PH	C36-C37-C38-C39
66	v	201	PC7	O31-C31-O2-C2
58	L	704	PGT	C33-C34-C35-C36
60	N	502	PTY	C37-C38-C39-C40
65	Y	201	3PH	C28-C29-C2A-C2B
66	v	201	PC7	C38-C39-C40-C41
72	BC	407	CDL	C59-C60-C61-C62
58	AC	407	PGT	O4P-C4-C5-C6
72	BC	408	CDL	CA2-C1-CB2-OB2
65	M	501	3PH	C32-C31-O31-C3
66	v	201	PC7	C12-C13-C14-C15
72	AC	409	CDL	C54-C55-C56-C57

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Mol	Chain	Res	Type	Atoms
72	BC	408	CDL	C11-C12-C13-C14
73	y	302	COO	O4-C7-C8-C9
60	BB	602	PTY	C30-C31-C32-C33
72	BE	402	CDL	CB7-C71-C72-C73
58	A	201	PGT	C13-C14-C15-C16
58	L	704	PGT	C17-C18-C19-C20
58	AF	201	PGT	C16-C17-C18-C19
65	f	202	3PH	C28-C29-C2A-C2B
66	d	102	PC7	C43-C44-C45-C46
66	AB	603	PC7	C13-C14-C15-C16
72	AC	408	CDL	C57-C58-C59-C60
72	BE	402	CDL	C19-C20-C21-C22
72	BC	407	CDL	OA9-CA7-OA8-CA6
60	D	401	PTY	C17-C18-C19-C20
72	BC	407	CDL	C13-C14-C15-C16
66	L	706	PC7	C39-C40-C41-C42
66	v	201	PC7	C18-C19-C20-C21
71	T	200	8Q1	C11-C10-C9-C8
72	AC	409	CDL	C71-C72-C73-C74
58	L	704	PGT	C18-C19-C20-C21
58	AF	201	PGT	C40-C41-C42-C43
65	AC	405	3PH	C33-C34-C35-C36
66	BD	302	PC7	C17-C18-C19-C20
65	AC	405	3PH	C21-C22-C23-C24
72	u	101	CDL	CB7-C71-C72-C73
72	AE	402	CDL	CB7-C71-C72-C73
72	AC	408	CDL	OB9-CB7-OB8-CB6
58	AC	406	PGT	C37-C38-C39-C40
58	AC	407	PGT	C13-C14-C15-C16
60	L	705	PTY	C40-C41-C42-C43
60	N	502	PTY	C38-C39-C40-C41
72	AC	409	CDL	C39-C40-C41-C42
72	u	102	CDL	C11-CA5-OA6-CA4
72	BC	408	CDL	C51-CB5-OB6-CB4
58	L	703	PGT	C14-C15-C16-C17
60	M	504	PTY	C15-C16-C17-C18
66	f	203	PC7	C43-C44-C45-C46
58	A	201	PGT	C22-C23-C24-C25
72	u	102	CDL	CA5-C11-C12-C13
72	AE	402	CDL	CA7-C31-C32-C33
60	M	503	PTY	C15-C16-C17-C18
66	v	201	PC7	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
58	L	704	PGT	C20-C21-C22-C23
60	D	401	PTY	C33-C34-C35-C36
60	AB	602	PTY	O10-C8-O7-C6
65	M	501	3PH	O22-C21-O21-C2
69	P	500	NDP	C2D-C1D-N1N-C2N
60	D	401	PTY	C14-C15-C16-C17
60	N	503	PTY	C32-C33-C34-C35
65	AC	405	3PH	C36-C37-C38-C39
72	AE	402	CDL	C16-C17-C18-C19
75	BC	404	UQ7	C12-C13-C14-C16
67	BC	403	UQ5	C12-C11-C9-C8
72	u	101	CDL	C51-C52-C53-C54
72	AC	409	CDL	C36-C37-C38-C39
58	A	201	PGT	C34-C35-C36-C37
58	y	303	PGT	C38-C39-C40-C41
58	AC	407	PGT	C19-C20-C21-C22
60	d	101	PTY	C19-C20-C21-C22
65	M	501	3PH	C25-C26-C27-C28
72	AC	409	CDL	C38-C39-C40-C41
72	AE	402	CDL	C31-C32-C33-C34
58	L	702	PGT	C13-C14-C15-C16
58	BC	406	PGT	C17-C18-C19-C20
60	N	503	PTY	C24-C25-C26-C27
65	M	501	3PH	C2C-C2D-C2E-C2F
72	AC	408	CDL	C75-C76-C77-C78
60	M	504	PTY	C35-C36-C37-C38
72	BC	408	CDL	C56-C57-C58-C59
58	AC	406	PGT	C42-C43-C44-C45
58	AC	407	PGT	C33-C34-C35-C36
60	z	301	PTY	C32-C33-C34-C35
65	Y	201	3PH	C27-C28-C29-C2A
60	N	502	PTY	C8-C11-C12-C13
75	BC	404	UQ7	C37-C38-C39-C40
58	y	303	PGT	C15-C16-C17-C18
72	AC	409	CDL	C18-C19-C20-C21
72	BC	408	CDL	O1-C1-CB2-OB2
58	y	303	PGT	C34-C35-C36-C37
66	d	102	PC7	C36-C37-C38-C39
58	AC	406	PGT	C32-C31-O2-C2
65	AI	101	3PH	C22-C21-O21-C2
72	BC	407	CDL	C51-CB5-OB6-CB4
72	BC	407	CDL	OB7-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
60	N	502	PTY	C14-C15-C16-C17
60	BF	201	PTY	C40-C41-C42-C43
65	f	202	3PH	C38-C39-C3A-C3B
66	L	706	PC7	C32-C33-C34-C35
71	T	200	8Q1	C12-C13-C14-C15
64	H	402	Q7G	O5-C1-O1-C4B
58	L	702	PGT	C34-C35-C36-C37
60	N	503	PTY	C8-C11-C12-C13
65	l	201	3PH	C32-C33-C34-C35
66	d	102	PC7	C15-C16-C17-C18
60	N	502	PTY	C19-C20-C21-C22
66	AC	410	PC7	C32-C33-C34-C35
66	AB	603	PC7	C11-C12-C13-C14
60	D	401	PTY	C12-C13-C14-C15
60	D	401	PTY	C37-C38-C39-C40
60	N	502	PTY	C40-C41-C42-C43
66	d	102	PC7	C18-C19-C20-C21
72	u	101	CDL	C61-C62-C63-C64
72	BC	407	CDL	C77-C78-C79-C80
58	AC	406	PGT	C39-C40-C41-C42
60	M	504	PTY	C33-C34-C35-C36
60	d	101	PTY	C15-C16-C17-C18
65	BC	405	3PH	C31-C32-C33-C34
72	BC	408	CDL	CB7-C71-C72-C73
66	v	201	PC7	C33-C34-C35-C36
66	BC	409	PC7	C35-C36-C37-C38
72	AC	408	CDL	C17-C18-C19-C20
58	AC	406	PGT	O31-C31-O2-C2
72	BC	407	CDL	OB5-CB3-CB4-OB6
58	L	703	PGT	C15-C16-C17-C18
58	M	502	PGT	C32-C31-O2-C2
74	BC	402	HEM	C4C-C3C-CAC-CBC
60	AB	602	PTY	C13-C14-C15-C16
66	f	203	PC7	C16-C17-C18-C19
60	M	504	PTY	C37-C38-C39-C40
72	AC	409	CDL	C58-C59-C60-C61
60	L	705	PTY	C32-C33-C34-C35
66	BD	302	PC7	C32-C33-C34-C35
60	N	503	PTY	C20-C21-C22-C23
65	L	701	3PH	C26-C27-C28-C29
65	BC	405	3PH	C33-C34-C35-C36
72	AC	408	CDL	C80-C81-C82-C83

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Mol	Chain	Res	Type	Atoms
58	L	704	PGT	C36-C37-C38-C39
58	AF	201	PGT	C36-C37-C38-C39
60	d	101	PTY	C20-C21-C22-C23
65	AC	405	3PH	C32-C33-C34-C35
72	AC	409	CDL	C35-C36-C37-C38
65	AC	405	3PH	C37-C38-C39-C3A
66	AC	410	PC7	C34-C35-C36-C37
66	AC	410	PC7	C18-C19-C20-C21
72	AC	409	CDL	C41-C42-C43-C44
65	BC	405	3PH	C34-C35-C36-C37
66	AG	101	PC7	C20-C21-C22-C23
72	AE	402	CDL	C21-C22-C23-C24
60	M	504	PTY	C34-C35-C36-C37
65	AC	405	3PH	C38-C39-C3A-C3B
65	AI	101	3PH	O22-C21-O21-C2
72	BC	408	CDL	OB7-CB5-OB6-CB4
58	L	704	PGT	C34-C35-C36-C37
60	N	502	PTY	C15-C16-C17-C18
65	Y	201	3PH	C23-C24-C25-C26
65	Y	201	3PH	C24-C25-C26-C27
66	BD	302	PC7	C15-C16-C17-C18
72	BE	402	CDL	C79-C80-C81-C82
60	BF	201	PTY	C13-C14-C15-C16
72	AE	402	CDL	C32-C33-C34-C35
60	N	503	PTY	C30-C31-C32-C33
65	M	501	3PH	O32-C31-O31-C3
60	N	503	PTY	C33-C34-C35-C36
58	AC	406	PGT	C33-C34-C35-C36
60	AB	602	PTY	C38-C39-C40-C41
72	u	102	CDL	C16-C17-C18-C19
58	AC	407	PGT	C43-C44-C45-C46
58	BC	406	PGT	C20-C21-C22-C23
72	AC	408	CDL	C12-C13-C14-C15
72	AE	402	CDL	C71-C72-C73-C74
64	H	402	Q7G	C2-C1-O1-C4B
65	L	701	3PH	C2D-C2E-C2F-C2G
65	BJ	102	3PH	C32-C33-C34-C35
58	L	702	PGT	O3P-C1-C2-C3
60	z	301	PTY	O14-C5-C6-C1
65	Y	201	3PH	O11-C1-C2-C3
65	f	202	3PH	O11-C1-C2-C3
65	l	201	3PH	O11-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
66	L	706	PC7	O3P-C1-C2-C3
72	u	102	CDL	OB5-CB3-CB4-CB6
65	f	201	3PH	C23-C24-C25-C26
72	u	102	CDL	C53-C54-C55-C56
72	AC	408	CDL	C76-C77-C78-C79
72	BC	408	CDL	C41-C42-C43-C44
65	M	501	3PH	C27-C28-C29-C2A
72	u	102	CDL	C51-C52-C53-C54
73	y	302	COO	O4X-C4X-C5X-O5X
66	AB	603	PC7	C35-C36-C37-C38
60	z	301	PTY	C34-C35-C36-C37
72	u	102	CDL	C77-C78-C79-C80
58	y	303	PGT	C36-C37-C38-C39
65	Y	201	3PH	C29-C2A-C2B-C2C
58	BC	406	PGT	C31-C32-C33-C34
63	H	401	UQ9	C24-C26-C27-C28
66	v	201	PC7	C32-C33-C34-C35
72	AC	409	CDL	C57-C58-C59-C60
71	T	200	8Q1	C11-C12-C13-C14
64	BC	410	Q7G	C22-CG1-O20-C17
72	u	102	CDL	OA7-CA5-OA6-CA4
72	AC	408	CDL	C14-C15-C16-C17
58	L	704	PGT	C1-C2-C3-O3
60	L	705	PTY	O4-C1-C6-C5
60	N	502	PTY	O4-C1-C6-C5
65	AC	405	3PH	C1-C2-C3-O31
66	d	102	PC7	C1-C2-C3-O3
66	f	203	PC7	C1-C2-C3-O3
66	BC	409	PC7	C1-C2-C3-O3
72	AC	408	CDL	CA3-CA4-CA6-OA8
72	AE	402	CDL	CB3-CB4-CB6-OB8
72	BC	407	CDL	CA3-CA4-CA6-OA8
72	BE	402	CDL	CA3-CA4-CA6-OA8
72	BG	101	CDL	CB3-CB4-CB6-OB8
75	BC	404	UQ7	C9-C11-C12-C13
58	AF	201	PGT	C38-C39-C40-C41
66	L	706	PC7	C33-C34-C35-C36
64	H	402	Q7G	O5C-C5C-C6C-O6C
60	L	705	PTY	C31-C32-C33-C34
72	u	102	CDL	C58-C59-C60-C61
66	AG	101	PC7	C14-C15-C16-C17
72	u	101	CDL	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
72	AC	408	CDL	C54-C55-C56-C57
72	AC	409	CDL	CA5-C11-C12-C13
65	f	202	3PH	C23-C24-C25-C26
72	AC	409	CDL	C20-C21-C22-C23
60	D	401	PTY	C15-C16-C17-C18
72	u	102	CDL	CB5-C51-C52-C53
58	A	201	PGT	C12-C13-C14-C15
67	AC	404	UQ5	C18-C19-C21-C22
72	AC	408	CDL	C1-CB2-OB2-PB2
67	AC	403	UQ5	C27-C28-C29-C30
65	Y	201	3PH	C1-O11-P-O12
65	AC	405	3PH	C1-O11-P-O12
65	AI	101	3PH	C1-O11-P-O12
60	AB	602	PTY	C31-C32-C33-C34
72	AC	409	CDL	C53-C54-C55-C56
65	f	201	3PH	C3F-C3G-C3H-C3I
65	AC	405	3PH	C39-C3A-C3B-C3C
64	H	402	Q7G	C3C-C4C-O11-CF1
72	AC	409	CDL	C23-C24-C25-C26
72	AE	402	CDL	C40-C41-C42-C43
65	BJ	102	3PH	C32-C31-O31-C3
60	M	503	PTY	C1-C6-O7-C8
71	T	200	8Q1	C7-C8-C9-C10
72	BG	101	CDL	C38-C39-C40-C41
66	f	203	PC7	C15-C16-C17-C18
72	AE	402	CDL	C11-C12-C13-C14
72	BC	407	CDL	C73-C74-C75-C76
66	d	102	PC7	C33-C34-C35-C36
60	d	101	PTY	C30-C31-C32-C33
65	f	202	3PH	C35-C36-C37-C38
60	z	301	PTY	C36-C37-C38-C39
72	u	102	CDL	C12-C13-C14-C15
58	AF	201	PGT	O3P-C1-C2-O2
65	f	201	3PH	C37-C38-C39-C3A
66	AG	101	PC7	C32-C33-C34-C35
60	Y	202	PTY	C31-C30-O4-C1
65	f	202	3PH	C32-C31-O31-C3
60	N	502	PTY	C17-C18-C19-C20
60	z	301	PTY	C20-C21-C22-C23
72	AC	409	CDL	C52-C53-C54-C55
66	AC	410	PC7	C44-C45-C46-C47
58	AC	407	PGT	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
66	v	201	PC7	C16-C17-C18-C19
75	BC	404	UQ7	C11-C12-C13-C14
58	y	303	PGT	C35-C36-C37-C38
60	M	504	PTY	C14-C15-C16-C17
60	N	503	PTY	C22-C23-C24-C25
65	M	501	3PH	C22-C23-C24-C25
72	BC	408	CDL	C37-C38-C39-C40
58	AC	406	PGT	C13-C14-C15-C16
71	T	200	8Q1	C13-C14-C15-C16
58	L	702	PGT	O2-C2-C3-O3
60	BB	602	PTY	O4-C1-C6-O7
66	BC	409	PC7	C41-C42-C43-C44
72	u	101	CDL	C44-C45-C46-C47
58	AC	406	PGT	C45-C46-C47-C48
75	BC	404	UQ7	C37-C38-C39-C41
60	m	101	PTY	C37-C38-C39-C40
65	AC	405	3PH	C25-C26-C27-C28
66	AG	101	PC7	C15-C16-C17-C18
72	u	101	CDL	C11-C12-C13-C14
72	BC	407	CDL	C75-C76-C77-C78
64	BC	411	Q7G	C23-C48-O1C-C1C
60	AB	602	PTY	C32-C33-C34-C35
71	T	200	8Q1	C6-C7-C8-C9
60	N	502	PTY	C21-C22-C23-C24
66	f	203	PC7	C45-C46-C47-C48
64	BC	410	Q7G	C23-C22-CG1-O20
64	BC	411	Q7G	C23-C22-CG1-O20
58	M	502	PGT	C13-C14-C15-C16
71	T	200	8Q1	C31-C29-C32-O33
60	M	503	PTY	C36-C37-C38-C39
58	AC	407	PGT	C42-C43-C44-C45
65	BJ	102	3PH	C23-C24-C25-C26
72	u	101	CDL	C33-C34-C35-C36
72	AC	409	CDL	C22-C23-C24-C25
69	P	500	NDP	PN-O3-PA-O1A
58	BC	406	PGT	C12-C11-O3-C3
66	BC	409	PC7	C36-C37-C38-C39
72	u	101	CDL	C11-CA5-OA6-CA4
60	N	503	PTY	C41-C42-C43-C44
58	AC	407	PGT	C31-C32-C33-C34
58	A	201	PGT	C37-C38-C39-C40
72	u	102	CDL	C79-C80-C81-C82

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Mol	Chain	Res	Type	Atoms
67	AC	404	UQ5	C20-C19-C21-C22
66	BD	302	PC7	C21-C22-C23-C24
58	AF	201	PGT	C21-C22-C23-C24
65	M	501	3PH	C23-C24-C25-C26
60	d	101	PTY	C22-C23-C24-C25
60	AB	602	PTY	C33-C34-C35-C36
58	M	502	PGT	O5-C5-C6-O6
58	y	303	PGT	O5-C5-C6-O6
65	BJ	102	3PH	C35-C36-C37-C38
72	BC	407	CDL	C18-C19-C20-C21
58	AC	406	PGT	C5-C4-O4P-P
65	Y	201	3PH	C2-C1-O11-P
72	u	102	CDL	C44-C45-C46-C47
60	d	101	PTY	C23-C24-C25-C26
72	AE	402	CDL	C74-C75-C76-C77
72	AC	408	CDL	C15-C16-C17-C18
64	H	402	Q7G	C2C-C1C-O1C-C48
65	BJ	101	3PH	C35-C36-C37-C38
66	v	201	PC7	C21-C22-C23-C24
66	v	201	PC7	C45-C46-C47-C48
72	BC	407	CDL	C19-C20-C21-C22
60	d	101	PTY	O14-C5-C6-C1
65	L	701	3PH	O11-C1-C2-C3
66	d	102	PC7	O3P-C1-C2-C3
72	BC	407	CDL	OB5-CB3-CB4-CB6
65	M	501	3PH	C2D-C2E-C2F-C2G
72	u	102	CDL	C34-C35-C36-C37
60	BB	602	PTY	C11-C12-C13-C14
64	H	402	Q7G	C5C-C4C-O11-CF1
72	AC	409	CDL	C11-C12-C13-C14
65	l	201	3PH	C21-C22-C23-C24
60	AB	602	PTY	C39-C40-C41-C42
60	L	705	PTY	C41-C42-C43-C44
60	d	101	PTY	C31-C32-C33-C34
67	AC	404	UQ5	C12-C11-C9-C10
65	l	201	3PH	C26-C27-C28-C29
58	L	704	PGT	C21-C22-C23-C24
72	BE	402	CDL	C11-C12-C13-C14
66	v	201	PC7	C40-C41-C42-C43
72	BC	407	CDL	C53-C54-C55-C56
58	AF	201	PGT	C32-C31-O2-C2
65	f	202	3PH	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
58	M	502	PGT	O31-C31-O2-C2
72	BC	407	CDL	C64-C65-C66-C67
58	y	303	PGT	C1-C2-C3-O3
58	BC	406	PGT	C1-C2-C3-O3
60	M	503	PTY	O4-C1-C6-C5
60	M	504	PTY	O4-C1-C6-C5
60	m	101	PTY	O4-C1-C6-C5
60	z	301	PTY	O4-C1-C6-C5
60	BB	602	PTY	O4-C1-C6-C5
65	l	201	3PH	C1-C2-C3-O31
66	BD	302	PC7	C1-C2-C3-O3
72	u	101	CDL	CA3-CA4-CA6-OA8
72	u	102	CDL	CA3-CA4-CA6-OA8
65	BC	405	3PH	C2B-C2C-C2D-C2E
60	BF	201	PTY	C11-C12-C13-C14
72	AC	408	CDL	C56-C57-C58-C59
60	M	504	PTY	C40-C41-C42-C43
72	AC	408	CDL	C82-C83-C84-C85
65	AC	405	3PH	C24-C25-C26-C27
65	M	501	3PH	C2A-C2B-C2C-C2D
67	AC	404	UQ5	C12-C11-C9-C8
60	Y	202	PTY	O30-C30-O4-C1
65	f	202	3PH	C36-C37-C38-C39
60	M	504	PTY	C21-C22-C23-C24
72	BC	407	CDL	C15-C16-C17-C18
72	BC	407	CDL	C79-C80-C81-C82
58	L	703	PGT	O3P-C1-C2-O2
65	l	201	3PH	O11-C1-C2-O21
66	d	102	PC7	O3P-C1-C2-O2
66	v	201	PC7	C41-C42-C43-C44
58	L	702	PGT	C35-C36-C37-C38
72	u	102	CDL	C72-C71-CB7-OB8
58	BC	406	PGT	C2-C1-O3P-P
60	BB	602	PTY	C8-C11-C12-C13
60	D	401	PTY	C39-C40-C41-C42
60	M	503	PTY	C32-C33-C34-C35
64	M	505	Q7G	C48-C23-C24-O1B
64	M	505	Q7G	C24-C23-C48-O1C
64	BC	410	Q7G	C24-C23-C48-O1C
65	BJ	102	3PH	O32-C31-O31-C3
58	A	201	PGT	C32-C33-C34-C35
58	y	303	PGT	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
60	M	503	PTY	C16-C17-C18-C19
60	AB	602	PTY	C16-C17-C18-C19
72	AE	402	CDL	C56-C57-C58-C59
60	L	705	PTY	O4-C1-C6-O7
60	M	503	PTY	O4-C1-C6-O7
60	N	502	PTY	O4-C1-C6-O7
65	l	201	3PH	O21-C2-C3-O31
66	BD	302	PC7	O2-C2-C3-O3
72	AC	408	CDL	OB6-CB4-CB6-OB8
72	AC	409	CDL	OA6-CA4-CA6-OA8
72	BG	101	CDL	OB6-CB4-CB6-OB8
72	AE	402	CDL	C24-C25-C26-C27
66	d	102	PC7	C38-C39-C40-C41
58	AC	407	PGT	C34-C35-C36-C37
72	u	101	CDL	C31-C32-C33-C34
60	M	504	PTY	C11-C12-C13-C14
66	BD	302	PC7	C12-C13-C14-C15
72	BE	402	CDL	C52-C53-C54-C55
58	AF	201	PGT	C41-C42-C43-C44
65	BJ	101	3PH	C36-C37-C38-C39
66	BD	302	PC7	C14-C15-C16-C17
72	AC	408	CDL	C52-C53-C54-C55
60	M	504	PTY	C30-C31-C32-C33
72	u	102	CDL	C36-C37-C38-C39
58	L	702	PGT	C16-C17-C18-C19
60	N	501	PTY	C13-C14-C15-C16
66	AB	603	PC7	C4-C5-N-C7
60	M	504	PTY	C23-C24-C25-C26
58	AF	201	PGT	C34-C35-C36-C37
64	H	402	Q7G	CG1-C22-C23-C24
60	N	503	PTY	C18-C19-C20-C21
72	BC	408	CDL	C74-C75-C76-C77
65	l	201	3PH	C32-C31-O31-C3
73	y	302	COO	C2X-C3X-O3X-P3X
72	AC	409	CDL	C11-CA5-OA6-CA4
58	AC	406	PGT	O4P-C4-C5-C6
58	L	704	PGT	C22-C23-C24-C25
60	L	705	PTY	C15-C16-C17-C18
66	AG	101	PC7	C17-C18-C19-C20
72	BE	402	CDL	C18-C19-C20-C21
58	M	502	PGT	O3P-C1-C2-C3
72	AC	408	CDL	OB5-CB3-CB4-CB6

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Mol	Chain	Res	Type	Atoms
72	BG	101	CDL	OA5-CA3-CA4-CA6
60	M	503	PTY	C35-C36-C37-C38
72	u	101	CDL	C12-C13-C14-C15
66	AC	410	PC7	C35-C36-C37-C38
66	AG	101	PC7	C16-C17-C18-C19
75	BC	404	UQ7	C12-C13-C14-C15
58	AC	406	PGT	C38-C39-C40-C41
66	L	706	PC7	C13-C14-C15-C16
72	AC	408	CDL	C84-C85-C86-C87
73	y	302	COO	C3X-C4X-C5X-O5X
60	z	301	PTY	C21-C22-C23-C24
72	u	102	CDL	C20-C21-C22-C23
65	f	202	3PH	O32-C31-O31-C3
67	L	707	UQ5	C1-C6-C7-C8
60	M	503	PTY	C34-C35-C36-C37
60	N	502	PTY	C13-C14-C15-C16
72	u	101	CDL	OA7-CA5-OA6-CA4
74	BE	401	HEM	C2B-C3B-CAB-CBB
58	L	704	PGT	C37-C38-C39-C40
60	M	503	PTY	C14-C15-C16-C17
64	M	505	Q7G	C22-C23-C24-O1B
65	AC	405	3PH	C3-C2-O21-C21
72	u	101	CDL	CB6-CB4-OB6-CB5
72	AC	409	CDL	CB3-CB4-OB6-CB5
60	D	401	PTY	C23-C24-C25-C26
72	AC	408	CDL	C58-C59-C60-C61
58	A	201	PGT	C33-C34-C35-C36
72	BC	407	CDL	C83-C84-C85-C86
72	BG	101	CDL	C41-C42-C43-C44
72	AC	409	CDL	C74-C75-C76-C77
58	BC	406	PGT	O11-C11-O3-C3
72	AC	408	CDL	C79-C80-C81-C82
65	f	201	3PH	C3A-C3B-C3C-C3D
72	BG	101	CDL	C43-C44-C45-C46
58	AF	201	PGT	O31-C31-O2-C2
60	d	101	PTY	O14-C5-C6-O7
65	L	701	3PH	O11-C1-C2-O21
65	BJ	102	3PH	O11-C1-C2-O21
66	f	203	PC7	O3P-C1-C2-O2
58	AF	201	PGT	C17-C18-C19-C20
58	L	702	PGT	C1-C2-C3-O3
58	AF	201	PGT	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
72	AC	409	CDL	CA3-CA4-CA6-OA8
72	u	101	CDL	CA7-C31-C32-C33
66	d	102	PC7	C12-C13-C14-C15
72	u	101	CDL	C14-C15-C16-C17
72	BG	101	CDL	C51-C52-C53-C54
60	m	101	PTY	C2-C3-O11-P1
60	BF	201	PTY	C2-C3-O11-P1
71	W	200	8Q1	C30-C29-C32-C34
72	AC	409	CDL	C24-C25-C26-C27
58	AF	201	PGT	O2-C2-C3-O3
60	M	504	PTY	O4-C1-C6-O7
60	m	101	PTY	O4-C1-C6-O7
60	z	301	PTY	O4-C1-C6-O7
60	AB	602	PTY	O4-C1-C6-O7
66	f	203	PC7	O2-C2-C3-O3
66	v	201	PC7	O2-C2-C3-O3
66	AB	603	PC7	O2-C2-C3-O3
72	u	101	CDL	OA6-CA4-CA6-OA8
72	u	101	CDL	OB6-CB4-CB6-OB8
72	u	102	CDL	OA6-CA4-CA6-OA8
72	AE	402	CDL	OB6-CB4-CB6-OB8
72	BE	402	CDL	OB6-CB4-CB6-OB8
60	L	705	PTY	C14-C15-C16-C17
72	BC	408	CDL	C55-C56-C57-C58
65	f	202	3PH	C2D-C2E-C2F-C2G
72	BC	408	CDL	C31-C32-C33-C34
64	M	505	Q7G	C23-C48-O1C-C1C
69	P	500	NDP	O4D-C1D-N1N-C6N
72	BC	408	CDL	C57-C58-C59-C60
60	z	301	PTY	C40-C41-C42-C43
72	BG	101	CDL	CB4-CB6-OB8-CB7
60	L	705	PTY	C11-C12-C13-C14
65	l	201	3PH	O32-C31-O31-C3
72	u	102	CDL	C75-C76-C77-C78
72	AE	402	CDL	C23-C24-C25-C26
66	BD	302	PC7	C33-C34-C35-C36
72	AE	402	CDL	C20-C21-C22-C23
58	A	201	PGT	C12-C11-O3-C3
58	L	704	PGT	C14-C15-C16-C17
72	BC	408	CDL	C38-C39-C40-C41
58	L	702	PGT	C36-C37-C38-C39
66	v	201	PC7	C12-C11-O3-C3

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Mol	Chain	Res	Type	Atoms
67	AC	404	UQ5	C25-C24-C26-C27
65	BC	405	3PH	C39-C3A-C3B-C3C
66	BD	302	PC7	C34-C35-C36-C37
72	AC	409	CDL	C42-C43-C44-C45
58	L	703	PGT	O3P-C1-C2-C3
58	AF	201	PGT	O3P-C1-C2-C3
60	M	504	PTY	O14-C5-C6-C1
60	BB	602	PTY	O14-C5-C6-C1
65	M	501	3PH	O11-C1-C2-C3
65	BJ	102	3PH	O11-C1-C2-C3
66	f	203	PC7	O3P-C1-C2-C3
72	AC	409	CDL	OA7-CA5-OA6-CA4
72	BG	101	CDL	C13-C14-C15-C16
62	F	500	FMN	N10-C1'-C2'-O2'
62	F	500	FMN	N10-C1'-C2'-C3'
72	BC	407	CDL	C12-C13-C14-C15
60	D	401	PTY	C40-C41-C42-C43
72	BG	101	CDL	C31-C32-C33-C34
58	L	704	PGT	C5-C4-O4P-P
58	M	502	PGT	C2-C1-O3P-P
72	AC	408	CDL	CB4-CB3-OB5-PB2
65	BJ	101	3PH	C33-C34-C35-C36
58	L	702	PGT	O3P-C1-C2-O2
60	M	504	PTY	O14-C5-C6-O7
60	z	301	PTY	O14-C5-C6-O7
60	BB	602	PTY	O14-C5-C6-O7
65	M	501	3PH	O11-C1-C2-O21
65	Y	201	3PH	O11-C1-C2-O21
65	f	202	3PH	O11-C1-C2-O21
66	L	706	PC7	O3P-C1-C2-O2
72	u	102	CDL	OB5-CB3-CB4-OB6
72	BG	101	CDL	OA5-CA3-CA4-OA6
66	AB	603	PC7	C4-C5-N-C6
60	z	301	PTY	C25-C26-C27-C28
64	BC	411	Q7G	C22-CG1-O20-C17
66	d	102	PC7	C13-C14-C15-C16
66	BC	409	PC7	C34-C35-C36-C37
66	BC	409	PC7	C40-C41-C42-C43
69	P	500	NDP	O4D-C1D-N1N-C2N
65	BC	405	3PH	O21-C2-C3-O31
72	AC	408	CDL	OA6-CA4-CA6-OA8
72	BC	407	CDL	OA6-CA4-CA6-OA8

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Mol	Chain	Res	Type	Atoms
72	BC	407	CDL	OB6-CB4-CB6-OB8
72	BE	402	CDL	OA6-CA4-CA6-OA8
60	M	504	PTY	C19-C20-C21-C22
65	L	701	3PH	C32-C33-C34-C35
66	AC	410	PC7	C33-C34-C35-C36
66	BC	409	PC7	C31-C32-C33-C34
60	AB	602	PTY	O4-C1-C6-C5
66	AB	603	PC7	C1-C2-C3-O3
65	BC	405	3PH	C36-C37-C38-C39
72	u	102	CDL	C22-C23-C24-C25
66	v	201	PC7	O11-C11-O3-C3
72	u	101	CDL	OB7-CB5-OB6-CB4
63	H	401	UQ9	C5-C4-O4-C4M
67	AC	403	UQ5	C2-C3-O3-C3M
67	AC	404	UQ5	C2-C3-O3-C3M
72	BC	408	CDL	C16-C17-C18-C19
66	AC	410	PC7	C41-C42-C43-C44
58	A	201	PGT	C41-C42-C43-C44
58	A	201	PGT	C1-O3P-P-O1P
58	L	703	PGT	C1-O3P-P-O1P
58	L	704	PGT	C4-O4P-P-O1P
58	y	303	PGT	C4-O4P-P-O1P
58	AC	406	PGT	C4-O4P-P-O3P
58	AF	201	PGT	C1-O3P-P-O1P
58	AF	201	PGT	C4-O4P-P-O3P
58	AF	201	PGT	C4-O4P-P-O1P
60	D	401	PTY	C3-O11-P1-O13
60	L	705	PTY	C3-O11-P1-O12
60	M	503	PTY	C3-O11-P1-O13
60	M	504	PTY	C3-O11-P1-O13
60	N	502	PTY	N1-C2-C3-O11
60	N	502	PTY	C5-O14-P1-O11
60	N	502	PTY	C5-O14-P1-O12
60	N	502	PTY	C5-O14-P1-O13
60	d	101	PTY	C3-O11-P1-O13
60	m	101	PTY	N1-C2-C3-O11
60	m	101	PTY	C3-O11-P1-O13
60	m	101	PTY	C5-O14-P1-O13
60	z	301	PTY	C3-O11-P1-O12
60	z	301	PTY	C3-O11-P1-O13
60	z	301	PTY	C3-O11-P1-O14
60	z	301	PTY	C5-O14-P1-O13

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Mol	Chain	Res	Type	Atoms
60	AB	602	PTY	C3-O11-P1-O13
60	BF	201	PTY	C3-O11-P1-O13
66	L	706	PC7	C4-O4P-P-O1P
66	d	102	PC7	C4-C5-N-C8
66	f	203	PC7	C1-O3P-P-O1P
66	f	203	PC7	C1-O3P-P-O2P
66	f	203	PC7	C1-O3P-P-O4P
66	f	203	PC7	C4-O4P-P-O2P
66	AB	603	PC7	C1-O3P-P-O1P
66	AG	101	PC7	C4-O4P-P-O2P
66	BC	409	PC7	C1-O3P-P-O2P
66	BC	409	PC7	C1-O3P-P-O4P
66	BC	409	PC7	C4-O4P-P-O1P
71	T	200	8Q1	C28-C29-C32-O33
72	u	101	CDL	CB2-OB2-PB2-OB3
72	u	101	CDL	CB2-OB2-PB2-OB5
72	u	101	CDL	CB3-OB5-PB2-OB2
72	u	101	CDL	CB3-OB5-PB2-OB3
72	u	101	CDL	CB3-OB5-PB2-OB4
72	u	102	CDL	CB3-OB5-PB2-OB3
72	AC	408	CDL	CA3-OA5-PA1-OA2
72	AC	408	CDL	CB2-OB2-PB2-OB3
72	AC	409	CDL	CB2-OB2-PB2-OB4
72	AE	402	CDL	CB3-OB5-PB2-OB3
72	BG	101	CDL	CA3-OA5-PA1-OA2
72	BG	101	CDL	CB2-OB2-PB2-OB3
66	AG	101	PC7	C13-C14-C15-C16
67	AC	403	UQ5	C27-C28-C29-C31
66	f	203	PC7	C37-C38-C39-C40
67	AC	404	UQ5	C15-C14-C16-C17
65	M	501	3PH	C32-C33-C34-C35
65	f	202	3PH	C39-C3A-C3B-C3C
58	y	303	PGT	C11-C12-C13-C14
66	AB	603	PC7	C31-C32-C33-C34
58	L	704	PGT	C2-C1-O3P-P
58	AF	201	PGT	C5-C4-O4P-P
60	N	502	PTY	C6-C5-O14-P1
65	AC	405	3PH	C2-C1-O11-P
65	AI	101	3PH	C2-C1-O11-P
72	u	102	CDL	CB4-CB3-OB5-PB2
72	BE	402	CDL	CB4-CB3-OB5-PB2
66	BC	409	PC7	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
65	f	201	3PH	C22-C23-C24-C25
72	u	101	CDL	C37-C38-C39-C40
66	f	203	PC7	C44-C45-C46-C47
65	BJ	101	3PH	C1-O11-P-O12
60	N	503	PTY	C35-C36-C37-C38
58	A	201	PGT	C19-C20-C21-C22
58	L	704	PGT	O5-C5-C6-O6
58	AC	407	PGT	C35-C36-C37-C38
58	AF	201	PGT	C31-C32-C33-C34
72	u	102	CDL	CB7-C71-C72-C73
66	d	102	PC7	C19-C20-C21-C22
58	A	201	PGT	O11-C11-O3-C3
58	BC	406	PGT	C1-C2-O2-C31
58	BC	406	PGT	C3-C2-O2-C31
72	BC	407	CDL	CA6-CA4-OA6-CA5
72	AC	409	CDL	C33-C34-C35-C36
67	AC	403	UQ5	C14-C16-C17-C18
60	m	101	PTY	C31-C32-C33-C34
66	d	102	PC7	C4-C5-N-C7
58	M	502	PGT	C33-C34-C35-C36
58	A	201	PGT	C21-C22-C23-C24
72	BC	407	CDL	C58-C59-C60-C61
72	BG	101	CDL	CA2-C1-CB2-OB2
58	M	502	PGT	O3P-C1-C2-O2
72	BC	407	CDL	OA5-CA3-CA4-OA6
64	H	402	Q7G	O5C-C1C-O1C-C48
72	u	101	CDL	C41-C42-C43-C44
60	BF	201	PTY	C41-C42-C43-C44
58	A	201	PGT	C42-C43-C44-C45
72	AE	402	CDL	C53-C54-C55-C56
75	BC	404	UQ7	C4-C3-O3-CM3
58	AF	201	PGT	C19-C20-C21-C22
65	AC	405	3PH	O21-C2-C3-O31
66	d	102	PC7	O2-C2-C3-O3
60	m	101	PTY	C24-C25-C26-C27
66	BC	409	PC7	C14-C15-C16-C17
65	BJ	101	3PH	C22-C21-O21-C2
72	u	101	CDL	C51-CB5-OB6-CB4
64	BC	410	Q7G	C22-C23-C48-O1C
71	T	200	8Q1	N36-C37-C38-C39
72	AC	408	CDL	C59-C60-C61-C62
72	BE	402	CDL	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
64	BC	411	Q7G	C23-C24-O1B-C1B
65	BJ	101	3PH	O22-C21-O21-C2
72	AC	408	CDL	C32-C31-CA7-OA8
66	f	203	PC7	C18-C19-C20-C21
72	u	102	CDL	C59-C60-C61-C62
72	AC	408	CDL	CB3-CB4-CB6-OB8
69	P	500	NDP	PN-O3-PA-O2A
72	AC	408	CDL	C64-C65-C66-C67
58	A	201	PGT	C39-C40-C41-C42
72	u	102	CDL	C78-C79-C80-C81
66	L	706	PC7	C37-C38-C39-C40
58	AC	406	PGT	C35-C36-C37-C38
72	AE	402	CDL	C19-C20-C21-C22
60	D	401	PTY	C22-C23-C24-C25
74	AC	402	HEM	C2A-CAA-CBA-CGA
60	M	504	PTY	C41-C42-C43-C44
72	u	101	CDL	OA5-CA3-CA4-OA6
60	AB	602	PTY	C17-C18-C19-C20
74	BE	401	HEM	C4B-C3B-CAB-CBB
72	u	102	CDL	C56-C57-C58-C59
72	u	102	CDL	C72-C73-C74-C75
66	AB	603	PC7	C4-C5-N-C8
72	u	102	CDL	C42-C43-C44-C45
60	N	501	PTY	O10-C8-O7-C6
72	BC	408	CDL	C40-C41-C42-C43
72	u	102	CDL	C73-C74-C75-C76
60	M	504	PTY	C25-C26-C27-C28
66	AB	603	PC7	C33-C34-C35-C36
65	BJ	102	3PH	C29-C2A-C2B-C2C
64	K	201	Q7G	C3C-C4C-O11-CF1
60	AB	602	PTY	C34-C35-C36-C37
60	BB	602	PTY	C32-C33-C34-C35
74	BC	402	HEM	CAD-CBD-CGD-O2D
66	BC	409	PC7	C16-C17-C18-C19
66	AC	410	PC7	C22-C23-C24-C25
58	AF	201	PGT	C11-C12-C13-C14
58	AF	201	PGT	C15-C16-C17-C18
66	d	102	PC7	C4-C5-N-C6
74	BC	402	HEM	CAD-CBD-CGD-O1D
72	BC	407	CDL	C63-C64-C65-C66
72	BE	402	CDL	C78-C79-C80-C81
74	AC	402	HEM	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
64	K	201	Q7G	C5C-C4C-O11-CF1
58	L	703	PGT	C16-C17-C18-C19
65	f	201	3PH	C1-C2-O21-C21
66	d	102	PC7	C14-C15-C16-C17
72	AE	402	CDL	C54-C55-C56-C57
60	L	705	PTY	C37-C38-C39-C40
65	f	202	3PH	C2B-C2C-C2D-C2E
72	AC	409	CDL	C59-C60-C61-C62
74	BE	401	HEM	CAA-CBA-CGA-O2A
60	N	501	PTY	C11-C8-O7-C6
74	AE	401	HEM	CAA-CBA-CGA-O1A
74	BC	401	HEM	CAA-CBA-CGA-O1A
60	D	401	PTY	C6-C5-O14-P1
72	u	102	CDL	C21-C22-C23-C24
72	AE	402	CDL	C44-C45-C46-C47
63	H	401	UQ9	C15-C14-C16-C17
65	BC	405	3PH	C32-C33-C34-C35
75	BC	404	UQ7	C26-C27-C28-C29
65	Y	201	3PH	C32-C33-C34-C35
74	BE	401	HEM	CAA-CBA-CGA-O1A
72	AC	408	CDL	C63-C64-C65-C66
74	AC	402	HEM	CAD-CBD-CGD-O1D
60	d	101	PTY	C24-C25-C26-C27
65	BJ	102	3PH	C26-C27-C28-C29
58	L	703	PGT	C32-C33-C34-C35
66	AG	101	PC7	C12-C11-O3-C3
72	BC	407	CDL	C74-C75-C76-C77
72	AC	408	CDL	C74-C75-C76-C77
67	L	707	UQ5	C15-C14-C16-C17
67	L	707	UQ5	C20-C19-C21-C22
73	y	302	COO	C3X-O3X-P3X-O9A
72	AC	408	CDL	C78-C79-C80-C81
58	L	702	PGT	C37-C38-C39-C40
65	BJ	102	3PH	C39-C3A-C3B-C3C
60	z	301	PTY	C26-C27-C28-C29
60	M	503	PTY	C13-C14-C15-C16
66	v	201	PC7	C17-C18-C19-C20
74	BC	401	HEM	CAA-CBA-CGA-O2A
60	BF	201	PTY	O10-C8-O7-C6
65	BC	405	3PH	O22-C21-O21-C2
65	BJ	102	3PH	O22-C21-O21-C2
72	u	101	CDL	C81-C82-C83-C84

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Mol	Chain	Res	Type	Atoms
65	f	202	3PH	C24-C25-C26-C27
67	AC	403	UQ5	C22-C23-C24-C25
67	L	707	UQ5	C25-C24-C26-C27
65	f	201	3PH	C2-C1-O11-P
63	H	401	UQ9	C13-C14-C16-C17
67	AC	404	UQ5	C23-C24-C26-C27
60	N	502	PTY	C31-C30-O4-C1
72	AC	409	CDL	C44-C45-C46-C47
74	AC	401	HEM	CAA-CBA-CGA-O2A
74	AE	401	HEM	CAA-CBA-CGA-O2A
65	f	201	3PH	C24-C25-C26-C27
65	BC	405	3PH	C37-C38-C39-C3A
66	v	201	PC7	C1-C2-C3-O3
64	a	101	Q7G	CG1-C22-C23-C24
60	N	502	PTY	O30-C30-O4-C1
72	BE	402	CDL	C37-C38-C39-C40
58	y	303	PGT	O3P-C1-C2-O2
65	BC	405	3PH	O11-C1-C2-O21
72	AE	402	CDL	OB5-CB3-CB4-OB6
72	BG	101	CDL	OB5-CB3-CB4-OB6
65	BJ	102	3PH	C22-C21-O21-C2
72	BE	402	CDL	C34-C35-C36-C37
58	y	303	PGT	C37-C38-C39-C40
58	AC	407	PGT	C36-C37-C38-C39
72	u	101	CDL	C62-C63-C64-C65
72	u	102	CDL	C72-C71-CB7-OB9
60	BF	201	PTY	C39-C40-C41-C42
58	AC	407	PGT	C41-C42-C43-C44
66	BC	409	PC7	O3P-C1-C2-C3
72	BG	101	CDL	OB5-CB3-CB4-CB6
72	AC	409	CDL	OB6-CB4-CB6-OB8
65	BC	405	3PH	C22-C23-C24-C25
72	u	101	CDL	C21-C22-C23-C24
60	AB	602	PTY	C11-C12-C13-C14
72	BE	402	CDL	C77-C78-C79-C80
65	BC	405	3PH	C3F-C3G-C3H-C3I
72	AE	402	CDL	C72-C73-C74-C75
60	BF	201	PTY	C12-C13-C14-C15
60	M	504	PTY	C26-C27-C28-C29
72	u	102	CDL	C24-C25-C26-C27
72	BG	101	CDL	O1-C1-CB2-OB2
66	AG	101	PC7	O11-C11-O3-C3

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Mol	Chain	Res	Type	Atoms
65	L	701	3PH	C1-O11-P-O14
65	f	201	3PH	C1-O11-P-O14
65	BJ	101	3PH	C1-O11-P-O14
71	T	200	8Q1	C28-O27-P24-O3
66	v	201	PC7	O3-C11-C12-C13
66	BD	302	PC7	C16-C17-C18-C19
72	AE	402	CDL	C59-C60-C61-C62
72	BG	101	CDL	C11-C12-C13-C14
60	M	503	PTY	C11-C12-C13-C14
74	AC	402	HEM	C2B-C3B-CAB-CBB
60	BF	201	PTY	C16-C17-C18-C19
58	M	502	PGT	C32-C33-C34-C35
72	BC	407	CDL	CA7-C31-C32-C33
66	AB	603	PC7	C36-C37-C38-C39
74	AC	401	HEM	CAA-CBA-CGA-O1A
60	d	101	PTY	C6-C5-O14-P1
72	BC	408	CDL	CB4-CB3-OB5-PB2
72	BC	407	CDL	CA2-C1-CB2-OB2
60	D	401	PTY	C21-C22-C23-C24
72	u	101	CDL	CB3-CB4-CB6-OB8
72	u	102	CDL	CB3-CB4-CB6-OB8
72	BC	407	CDL	CB3-CB4-CB6-OB8
74	AC	402	HEM	C4B-C3B-CAB-CBB
72	BE	402	CDL	C76-C77-C78-C79
72	BG	101	CDL	C36-C37-C38-C39
58	L	704	PGT	C35-C36-C37-C38
66	L	706	PC7	O3-C11-C12-C13
67	AC	404	UQ5	C13-C14-C16-C17
72	BC	408	CDL	C12-C13-C14-C15
65	f	201	3PH	O31-C31-C32-C33
72	BC	408	CDL	C72-C73-C74-C75
60	N	502	PTY	C32-C33-C34-C35
65	BC	405	3PH	C22-C21-O21-C2
66	d	102	PC7	C23-C24-C25-C26
58	y	303	PGT	O3P-C1-C2-C3
65	BC	405	3PH	O11-C1-C2-C3
72	u	101	CDL	OA5-CA3-CA4-CA6
72	AC	409	CDL	OA5-CA3-CA4-CA6
67	AC	404	UQ5	C4-C3-O3-C3M
60	M	504	PTY	C12-C11-C8-O7
64	K	201	Q7G	C23-C22-CG1-O20
60	L	705	PTY	O10-C8-O7-C6

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Mol	Chain	Res	Type	Atoms
60	N	502	PTY	C36-C37-C38-C39
66	f	203	PC7	C17-C18-C19-C20
66	BD	302	PC7	C18-C19-C20-C21
66	AC	410	PC7	C12-C13-C14-C15
72	u	101	CDL	C40-C41-C42-C43
72	u	102	CDL	C43-C44-C45-C46
66	AG	101	PC7	O4P-C4-C5-N
72	BC	408	CDL	C12-C11-CA5-OA6
66	AC	410	PC7	C23-C24-C25-C26
65	f	201	3PH	O22-C21-O21-C2
60	BF	201	PTY	C11-C8-O7-C6
72	BG	101	CDL	C32-C31-CA7-OA8
65	Y	201	3PH	C2A-C2B-C2C-C2D
60	M	503	PTY	C18-C19-C20-C21
58	y	303	PGT	O3-C11-C12-C13
65	Y	201	3PH	O31-C31-C32-C33
60	m	101	PTY	C16-C17-C18-C19
58	L	703	PGT	C13-C14-C15-C16
72	BE	402	CDL	C32-C31-CA7-OA8
60	BB	602	PTY	C31-C32-C33-C34
65	f	202	3PH	C31-C32-C33-C34
72	BC	407	CDL	CB5-C51-C52-C53
66	AC	410	PC7	C16-C17-C18-C19
72	BC	407	CDL	C51-C52-C53-C54
72	BG	101	CDL	C72-C71-CB7-OB8
66	d	102	PC7	C45-C46-C47-C48
65	AI	101	3PH	O31-C31-C32-C33
65	L	701	3PH	C23-C24-C25-C26
65	AI	101	3PH	C1-C2-C3-O31
65	BC	405	3PH	C1-C2-C3-O31
72	AC	409	CDL	CB3-CB4-CB6-OB8
72	BE	402	CDL	CB3-CB4-CB6-OB8
75	BC	404	UQ7	C14-C16-C17-C18
64	H	402	Q7G	C23-C22-CG1-O20
64	M	505	Q7G	C23-C22-CG1-O20
60	N	503	PTY	C17-C18-C19-C20
60	L	705	PTY	C11-C8-O7-C6
60	BF	201	PTY	O4-C30-C31-C32
66	AG	101	PC7	O2-C31-C32-C33
72	AC	409	CDL	C52-C51-CB5-OB6
60	L	705	PTY	C17-C18-C19-C20
65	BJ	101	3PH	C37-C38-C39-C3A

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Mol	Chain	Res	Type	Atoms
72	AE	402	CDL	C73-C74-C75-C76
60	AB	602	PTY	C35-C36-C37-C38
66	f	203	PC7	C14-C15-C16-C17
60	M	503	PTY	O4-C30-C31-C32
60	N	501	PTY	O4-C30-C31-C32
66	AG	101	PC7	O3-C11-C12-C13
72	u	101	CDL	C17-C18-C19-C20
72	u	102	CDL	C52-C53-C54-C55
60	BF	201	PTY	C33-C34-C35-C36
58	AC	407	PGT	C39-C40-C41-C42
63	H	401	UQ9	C3-C4-O4-C4M
75	BC	404	UQ7	C2-C3-O3-CM3
66	AB	603	PC7	O3-C11-C12-C13
58	AF	201	PGT	C44-C45-C46-C47
71	T	200	8Q1	C37-C38-C39-N41
65	M	501	3PH	C2E-C2F-C2G-C2H
66	AG	101	PC7	C22-C23-C24-C25
60	N	502	PTY	C18-C19-C20-C21
65	M	501	3PH	C28-C29-C2A-C2B
60	z	301	PTY	C15-C16-C17-C18
65	AC	405	3PH	C3A-C3B-C3C-C3D
58	y	303	PGT	O11-C11-C12-C13
72	u	101	CDL	C54-C55-C56-C57
72	BC	408	CDL	C12-C11-CA5-OA7
72	BG	101	CDL	C72-C71-CB7-OB9
66	AG	101	PC7	C43-C44-C45-C46
72	AC	409	CDL	OA5-CA3-CA4-OA6
60	m	101	PTY	C21-C22-C23-C24
65	BJ	101	3PH	C39-C3A-C3B-C3C
72	BE	402	CDL	C72-C71-CB7-OB8
67	BC	403	UQ5	C16-C17-C18-C19
60	M	504	PTY	C39-C40-C41-C42
72	BE	402	CDL	C13-C14-C15-C16
72	u	101	CDL	C43-C44-C45-C46
58	AC	407	PGT	C20-C21-C22-C23
72	BG	101	CDL	C32-C31-CA7-OA9
66	AC	410	PC7	C19-C20-C21-C22
72	BC	408	CDL	C34-C35-C36-C37
60	D	401	PTY	C41-C42-C43-C44
65	Y	201	3PH	O32-C31-C32-C33
66	AG	101	PC7	O31-C31-C32-C33
65	f	201	3PH	O32-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
66	AG	101	PC7	O11-C11-C12-C13
60	M	504	PTY	C12-C11-C8-O10
66	L	706	PC7	O11-C11-C12-C13
60	N	503	PTY	O4-C30-C31-C32
65	BC	405	3PH	O21-C21-C22-C23
66	BD	302	PC7	C11-C12-C13-C14
72	u	101	CDL	C35-C36-C37-C38
73	y	302	COO	N1-C1-C13-O1
60	M	504	PTY	O4-C30-C31-C32
67	L	707	UQ5	C13-C14-C16-C17
74	AC	402	HEM	C2C-C3C-CAC-CBC
72	AE	402	CDL	C36-C37-C38-C39
60	M	503	PTY	O30-C30-C31-C32
60	BF	201	PTY	O30-C30-C31-C32
66	AB	603	PC7	O11-C11-C12-C13
65	L	701	3PH	C2E-C2F-C2G-C2H
65	f	201	3PH	C22-C21-O21-C2
58	AC	406	PGT	C40-C41-C42-C43
72	AE	402	CDL	C12-C11-CA5-OA6
64	a	101	Q7G	C23-C48-O1C-C1C
58	L	703	PGT	C11-C12-C13-C14
60	m	101	PTY	C19-C20-C21-C22
65	AI	101	3PH	O32-C31-C32-C33
72	BE	402	CDL	C32-C31-CA7-OA9
58	BC	406	PGT	O2-C31-C32-C33
66	d	102	PC7	C21-C22-C23-C24
72	BE	402	CDL	C59-C60-C61-C62
58	AF	201	PGT	C45-C46-C47-C48
58	L	704	PGT	C11-C12-C13-C14
58	L	704	PGT	O2-C31-C32-C33
60	z	301	PTY	O4-C30-C31-C32
60	BB	602	PTY	C12-C11-C8-O7
65	AC	405	3PH	O31-C31-C32-C33
72	u	102	CDL	C32-C31-CA7-OA8
60	N	501	PTY	O30-C30-C31-C32
66	f	203	PC7	C31-C32-C33-C34
72	BE	402	CDL	CB5-C51-C52-C53
72	BC	407	CDL	C32-C31-CA7-OA8
67	AC	403	UQ5	C22-C23-C24-C26
66	v	201	PC7	C11-C12-C13-C14
58	AF	201	PGT	C12-C13-C14-C15

There are no ring outliers.

68 monomers are involved in 299 short contacts:

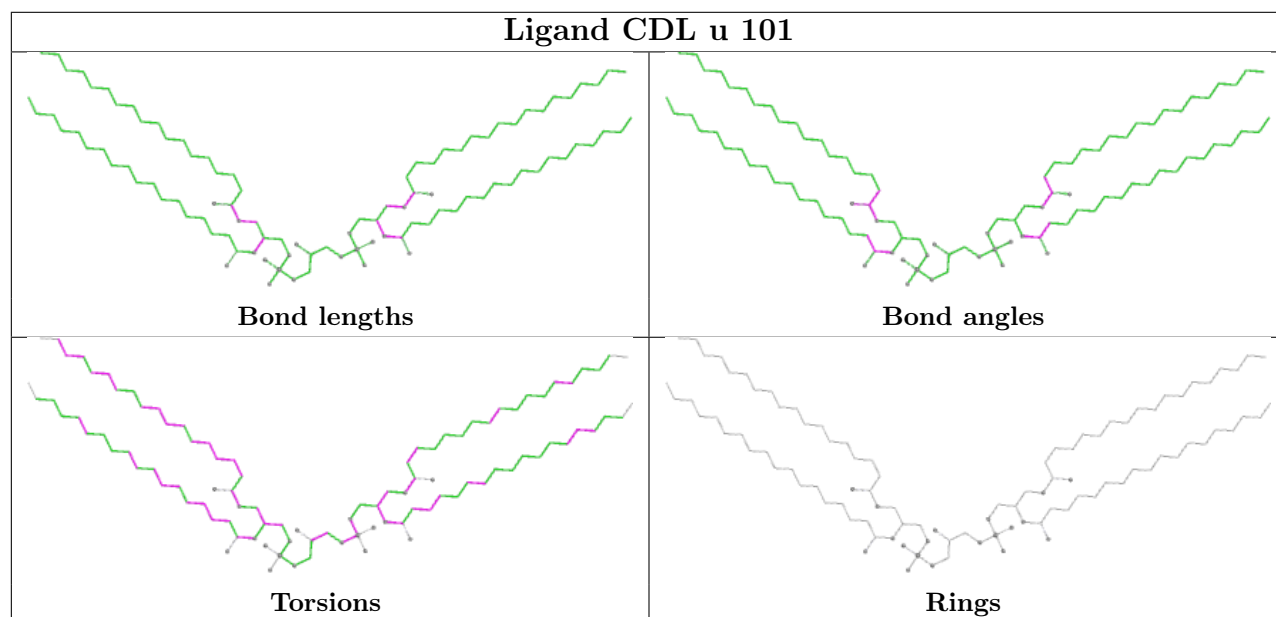
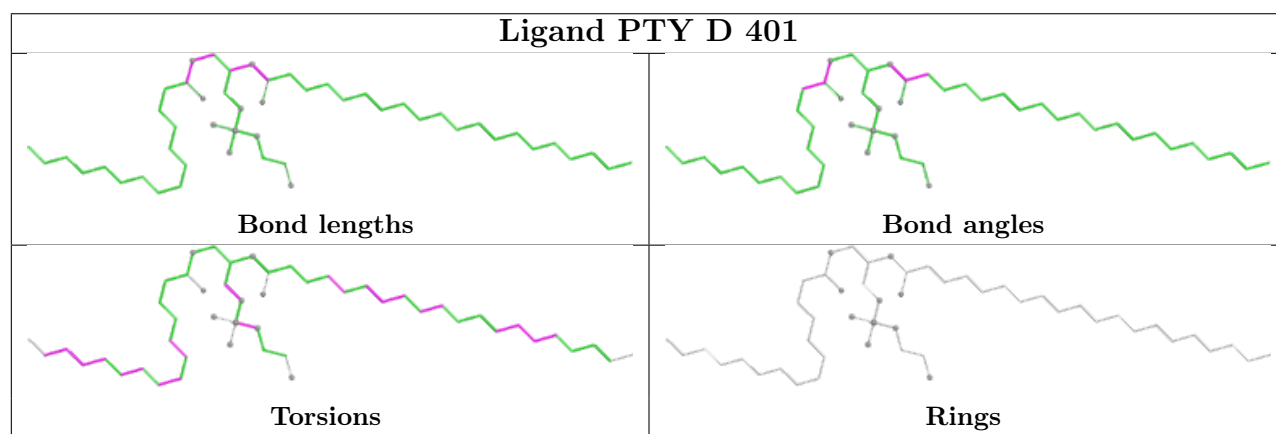
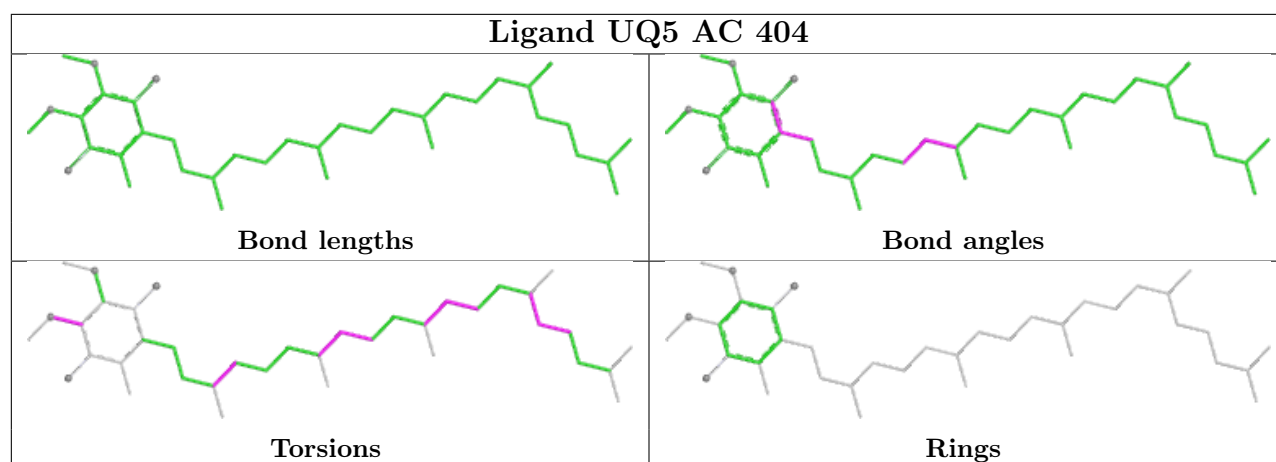
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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60	D	401	PTY	13	0
72	u	101	CDL	12	0
72	BC	408	CDL	6	0
74	BC	402	HEM	1	0
59	B	500	SF4	1	0
66	BD	302	PC7	3	0
73	y	302	COO	5	0
72	BE	402	CDL	6	0
60	N	502	PTY	2	0
60	N	503	PTY	1	0
72	AE	402	CDL	4	0
61	BD	301	FES	1	0
72	BC	407	CDL	3	0
64	K	201	Q7G	1	0
63	H	401	UQ9	6	0
60	d	101	PTY	3	0
60	N	501	PTY	6	0
75	BC	404	UQ7	11	0
66	BC	409	PC7	3	0
58	AC	407	PGT	4	0
65	AI	101	3PH	3	0
58	AC	406	PGT	4	0
72	AC	409	CDL	7	0
58	L	704	PGT	5	0
60	BF	201	PTY	16	0
64	H	402	Q7G	3	0
66	AC	410	PC7	3	0
58	AF	201	PGT	9	0
65	L	701	3PH	4	0
58	L	703	PGT	2	0
66	L	706	PC7	6	0
66	d	102	PC7	8	0
72	BG	101	CDL	6	0
66	AB	603	PC7	1	0
59	I	500	SF4	2	0
65	Y	201	3PH	2	0
65	BC	405	3PH	6	0
58	A	201	PGT	7	0
66	f	203	PC7	1	0
72	u	102	CDL	13	0
61	G	801	FES	1	0

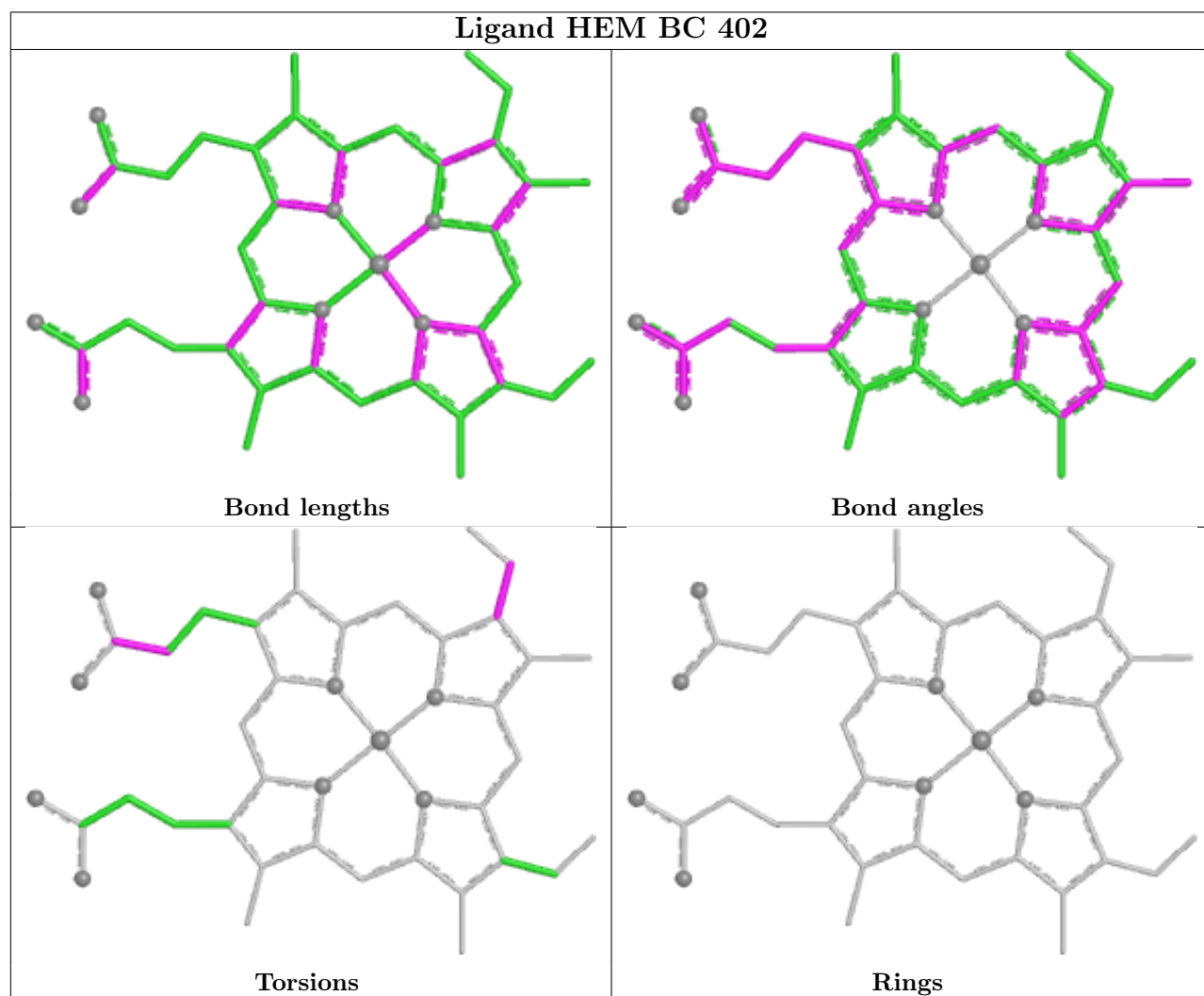
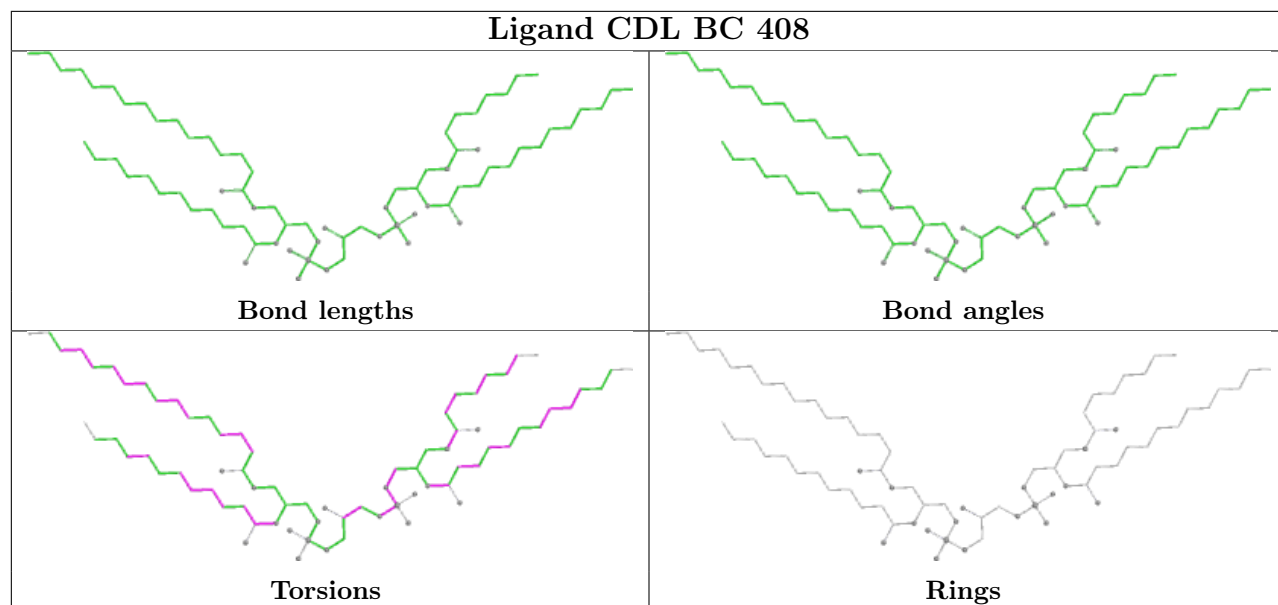
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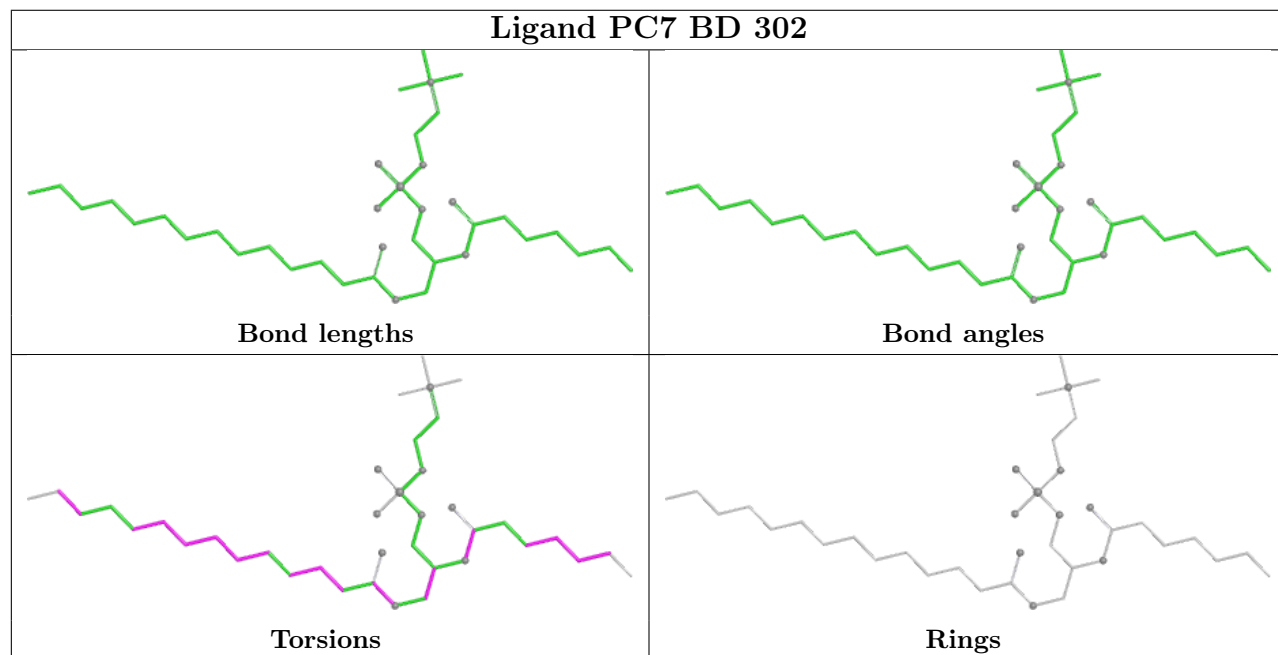
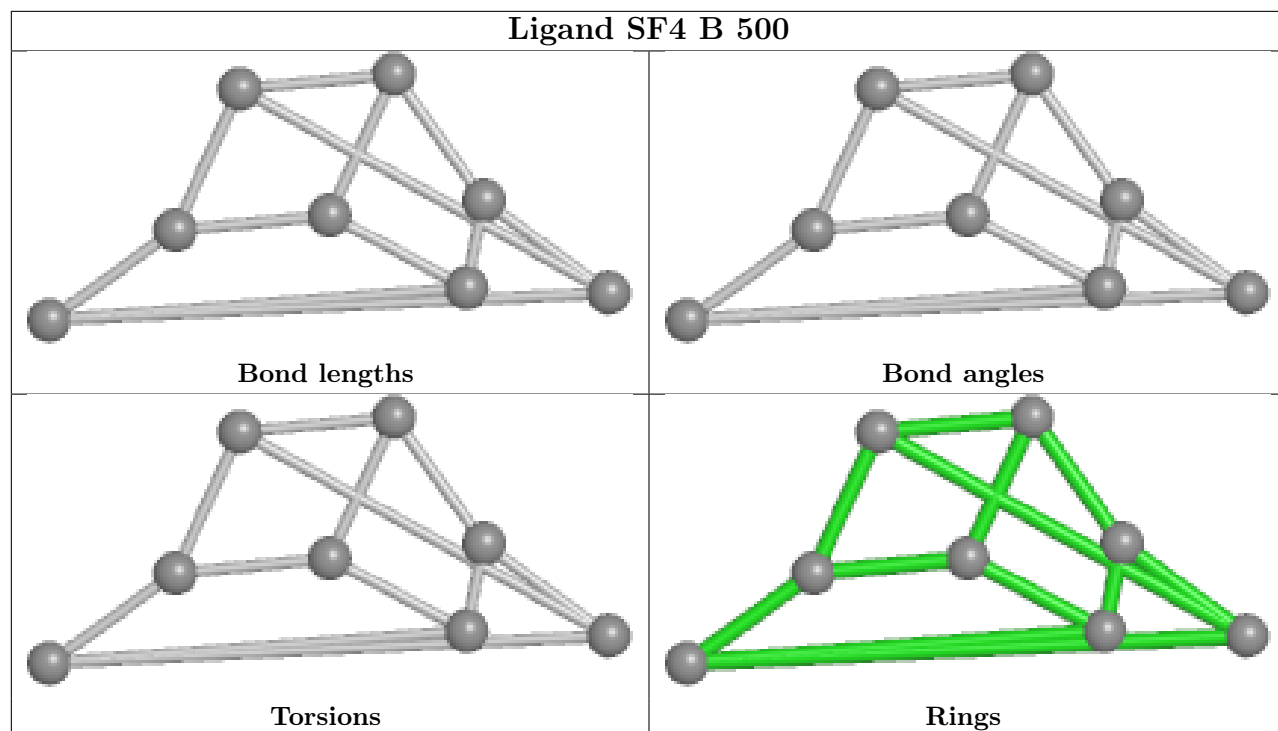
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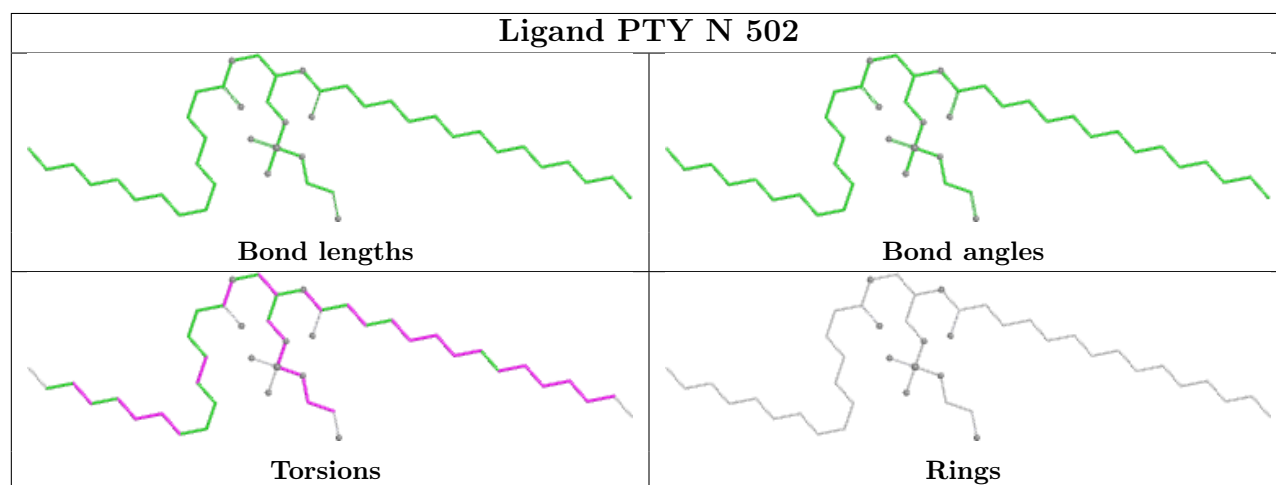
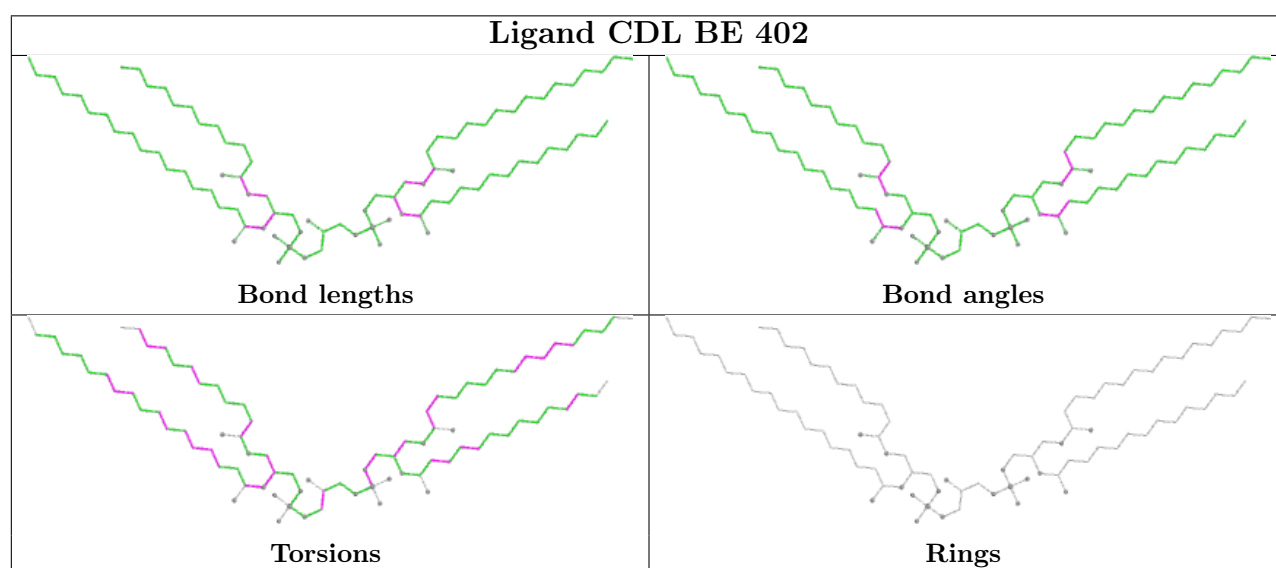
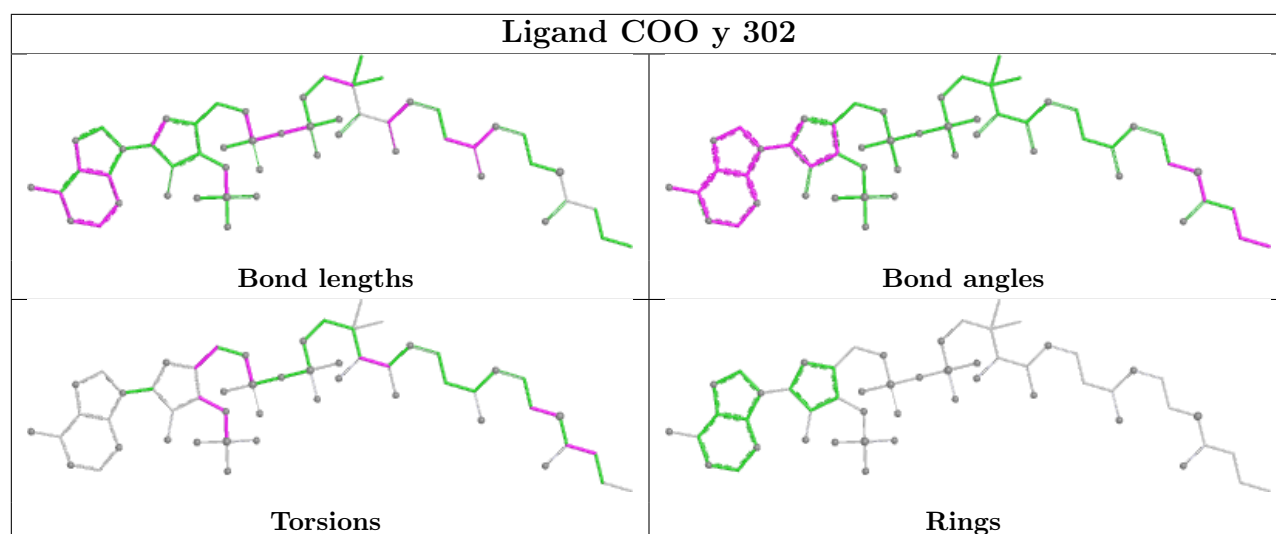
Mol	Chain	Res	Type	Clashes	Symm-Clashes
66	v	201	PC7	7	0
74	BE	401	HEM	6	0
66	AG	101	PC7	6	0
58	BC	406	PGT	2	0
72	AC	408	CDL	8	0
59	F	501	SF4	1	0
67	L	707	UQ5	7	0
67	BC	403	UQ5	8	0
60	M	504	PTY	2	0
65	f	201	3PH	2	0
60	M	503	PTY	2	0
60	BB	602	PTY	1	0
61	E	500	FES	1	0
67	AC	403	UQ5	4	0
58	M	502	PGT	1	0
65	M	501	3PH	15	0
74	AC	402	HEM	1	0
74	AC	401	HEM	2	0
60	L	705	PTY	2	0
65	BJ	101	3PH	2	0
58	y	303	PGT	8	0
65	AC	405	3PH	2	0
65	BJ	102	3PH	1	0
74	AE	401	HEM	4	0
65	f	202	3PH	3	0
60	z	301	PTY	12	0

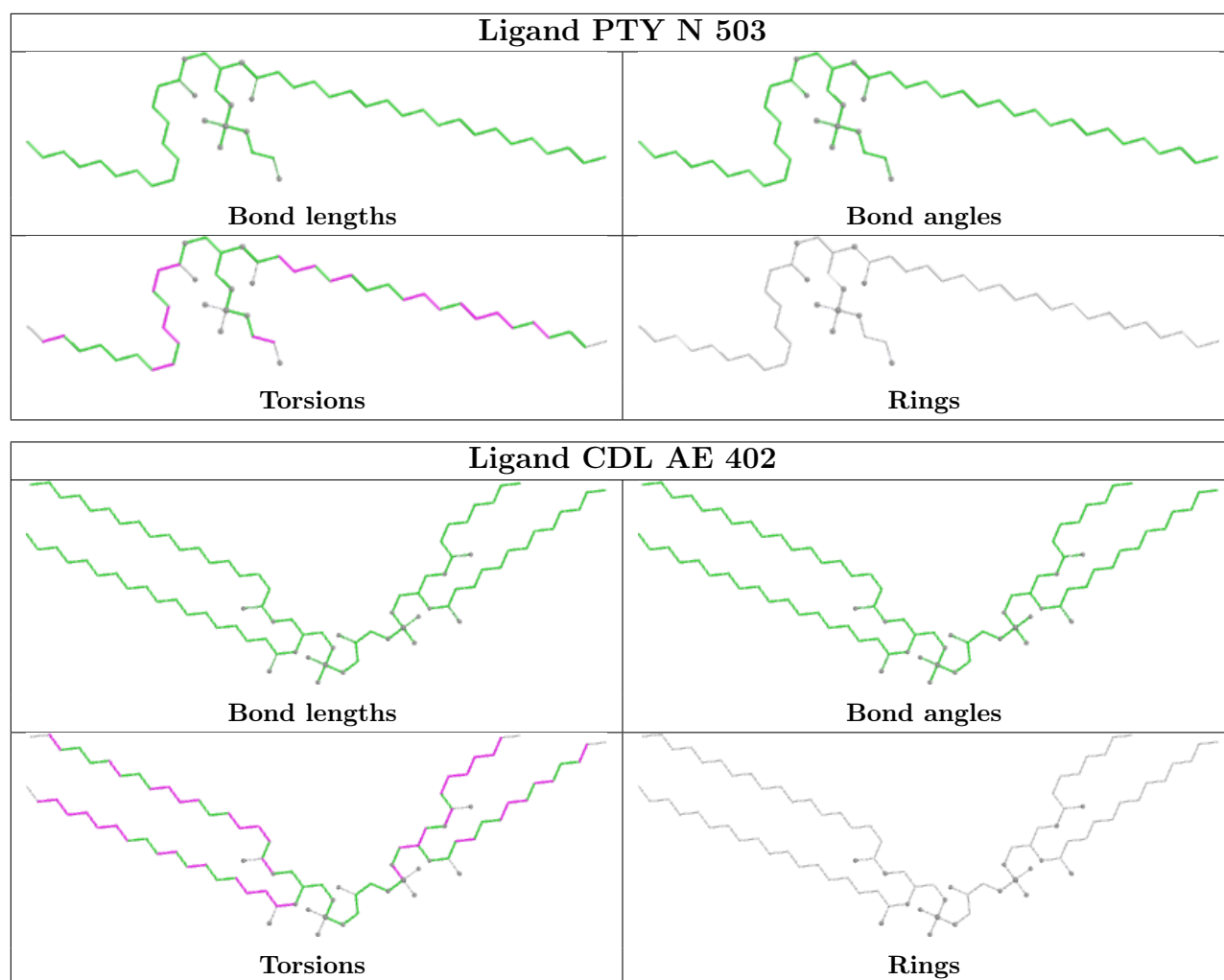
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

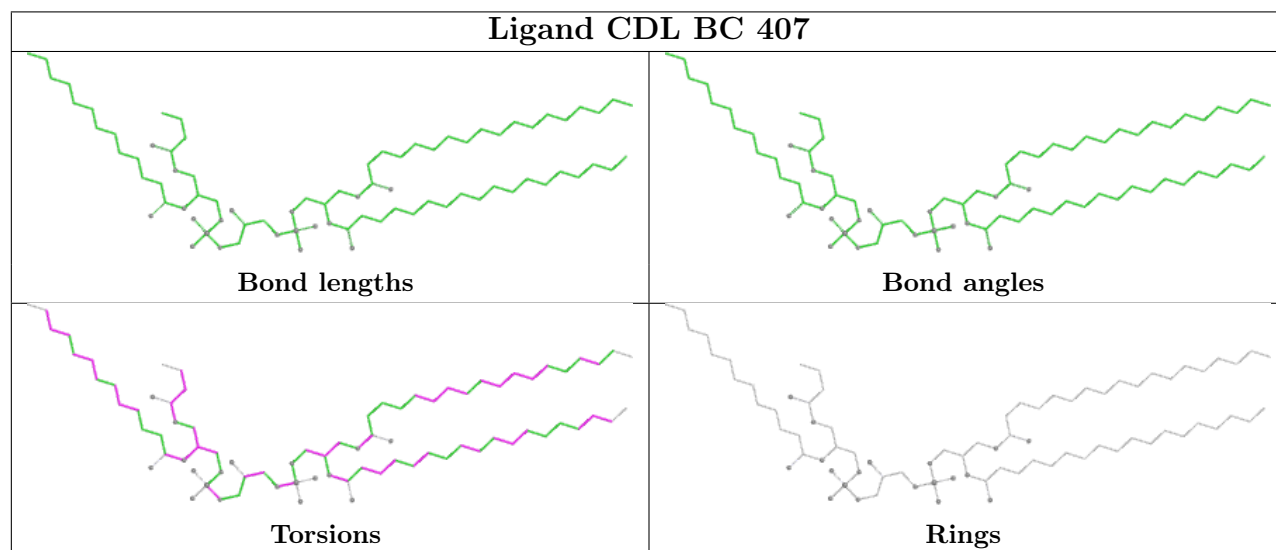
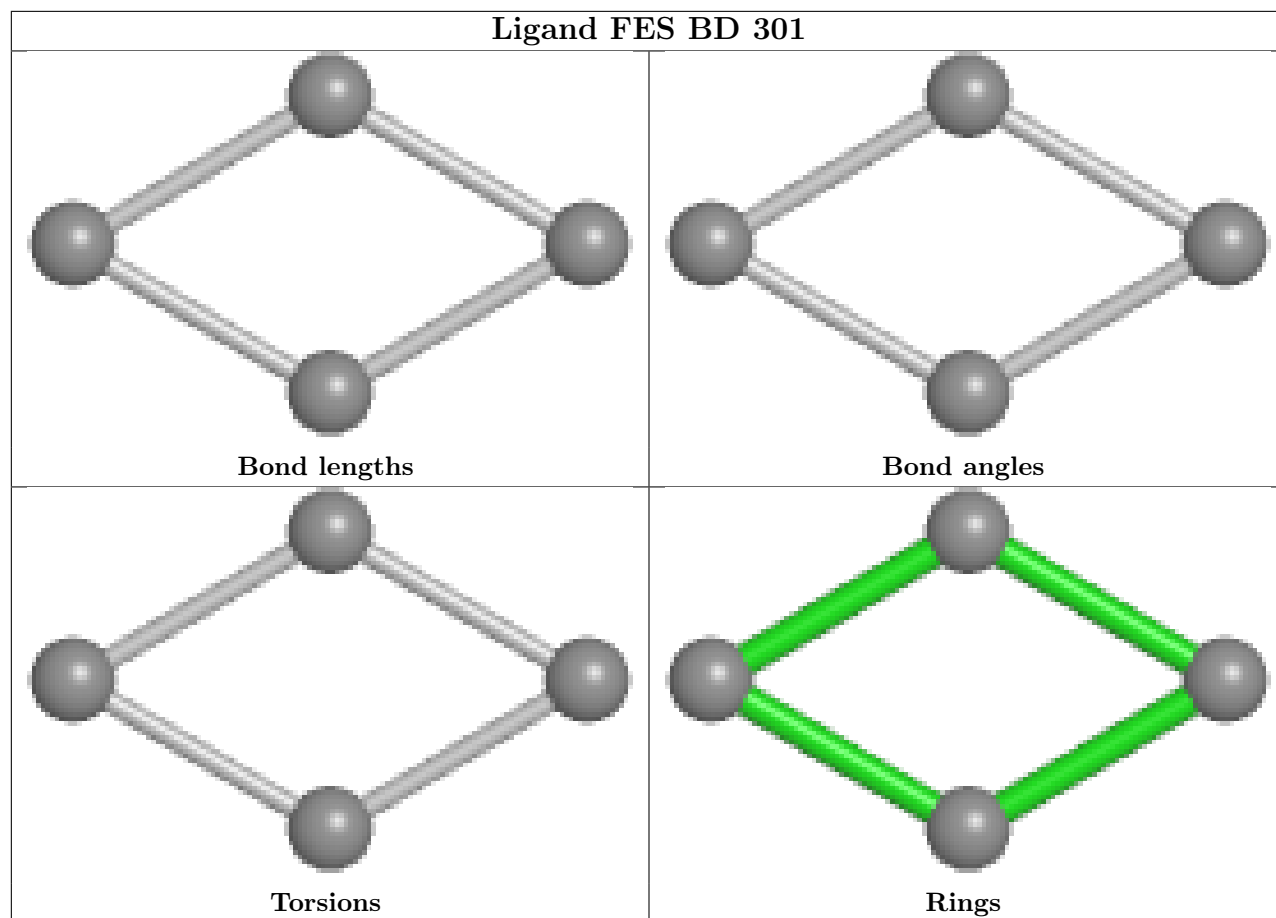


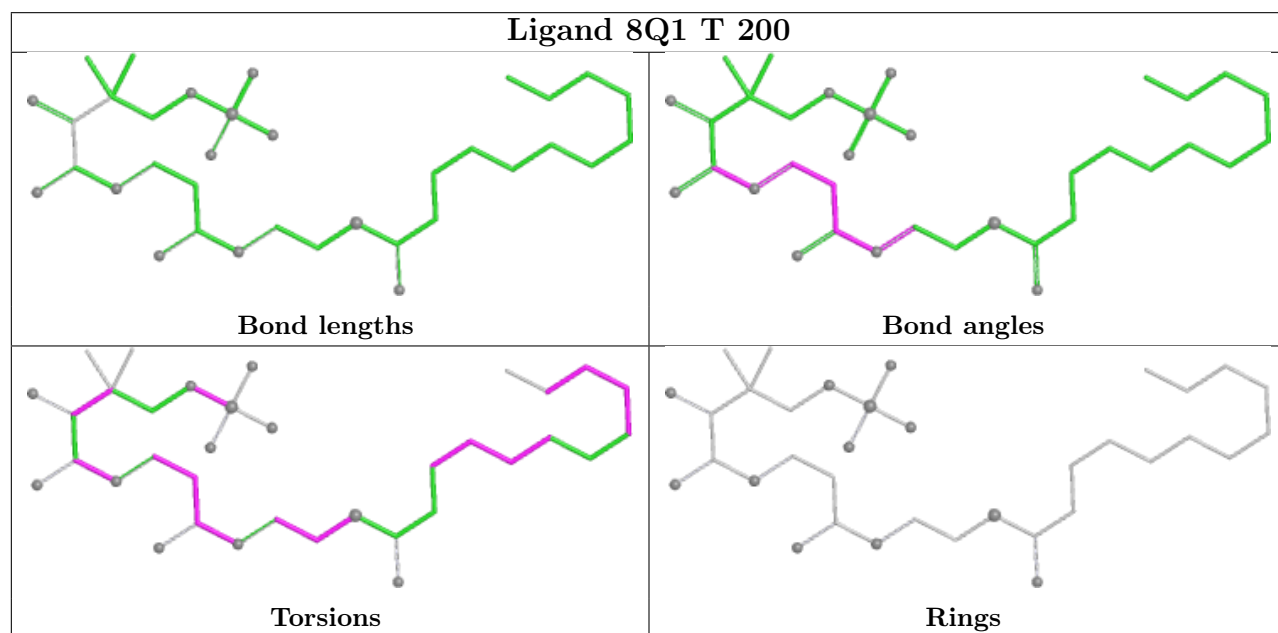
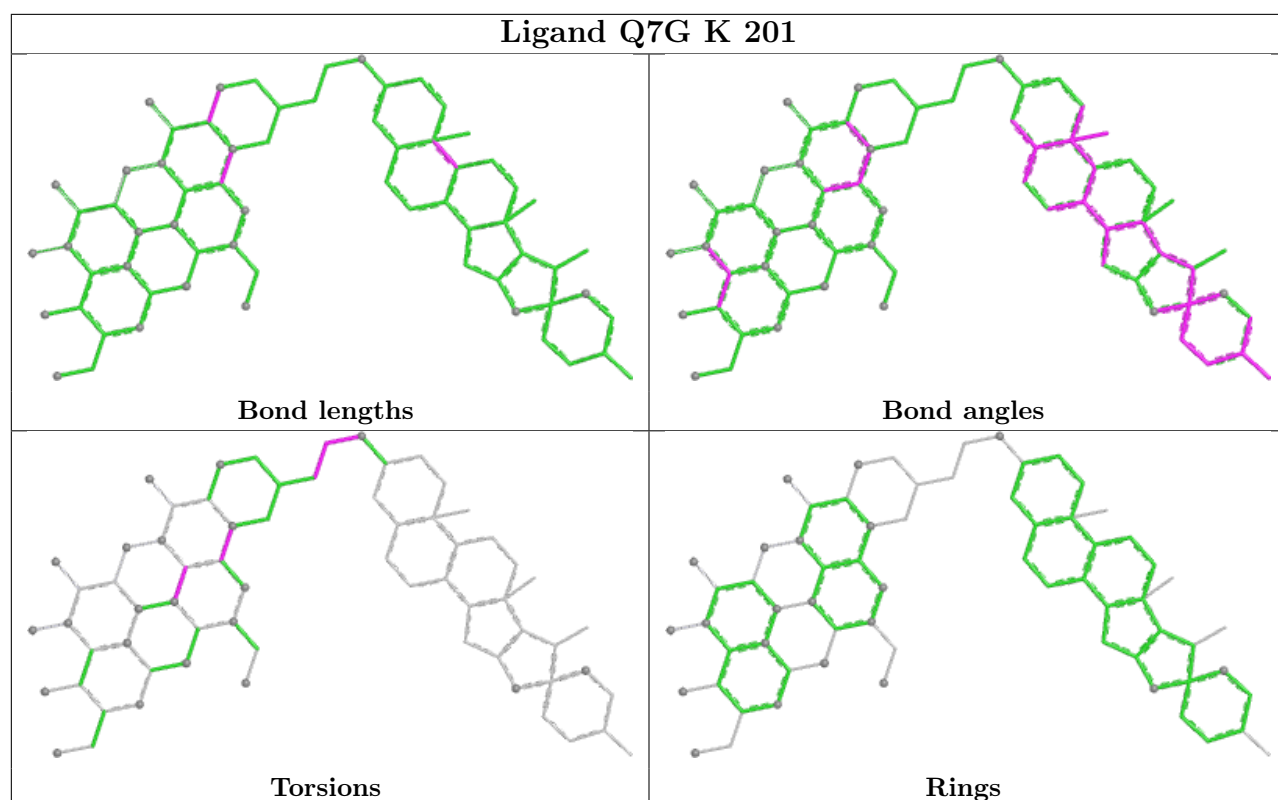


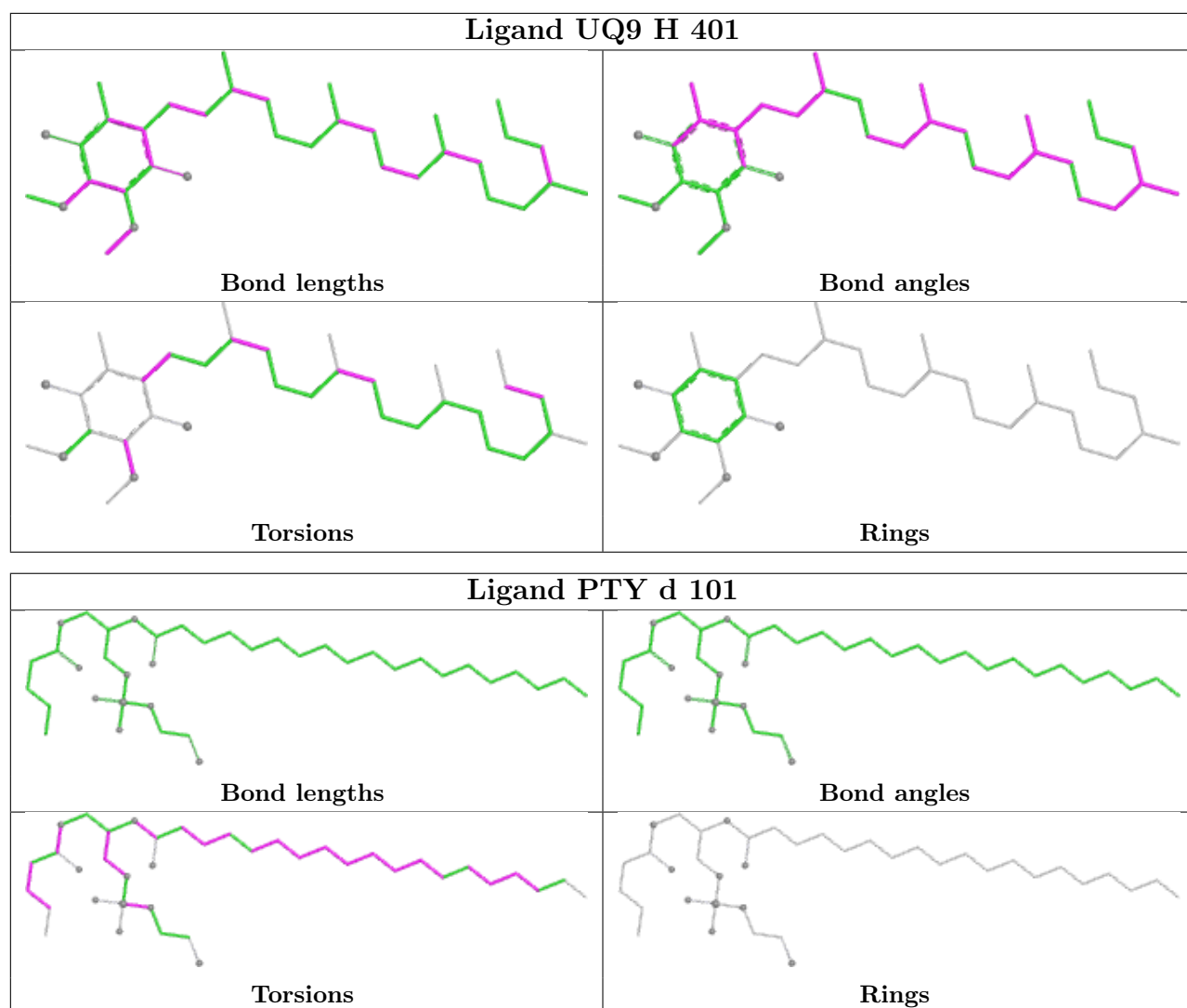


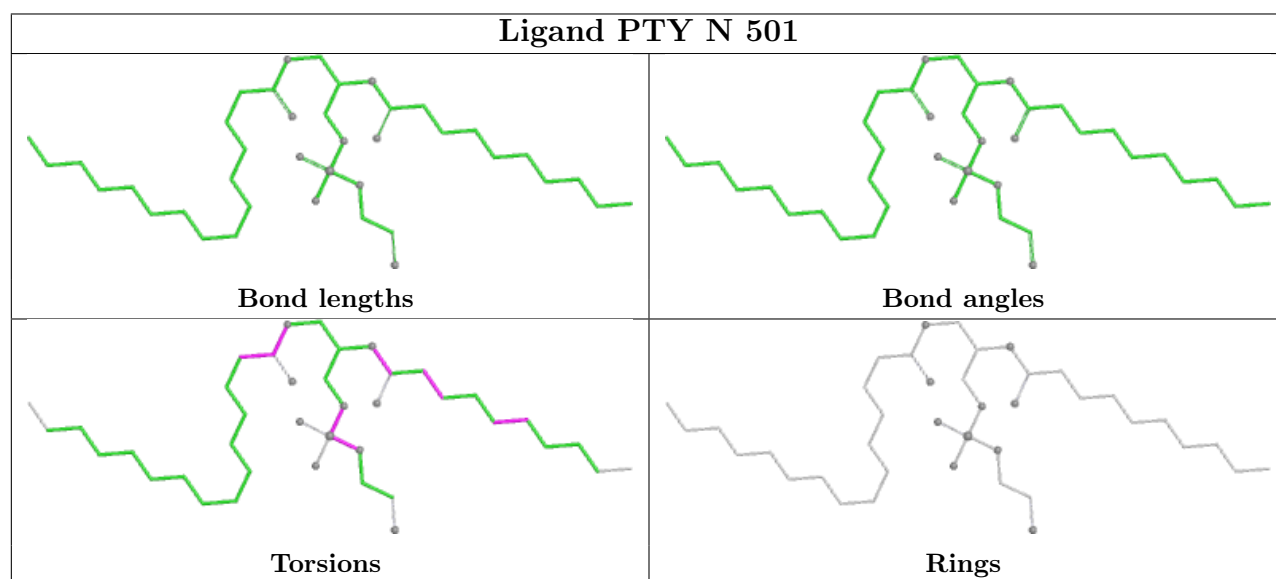
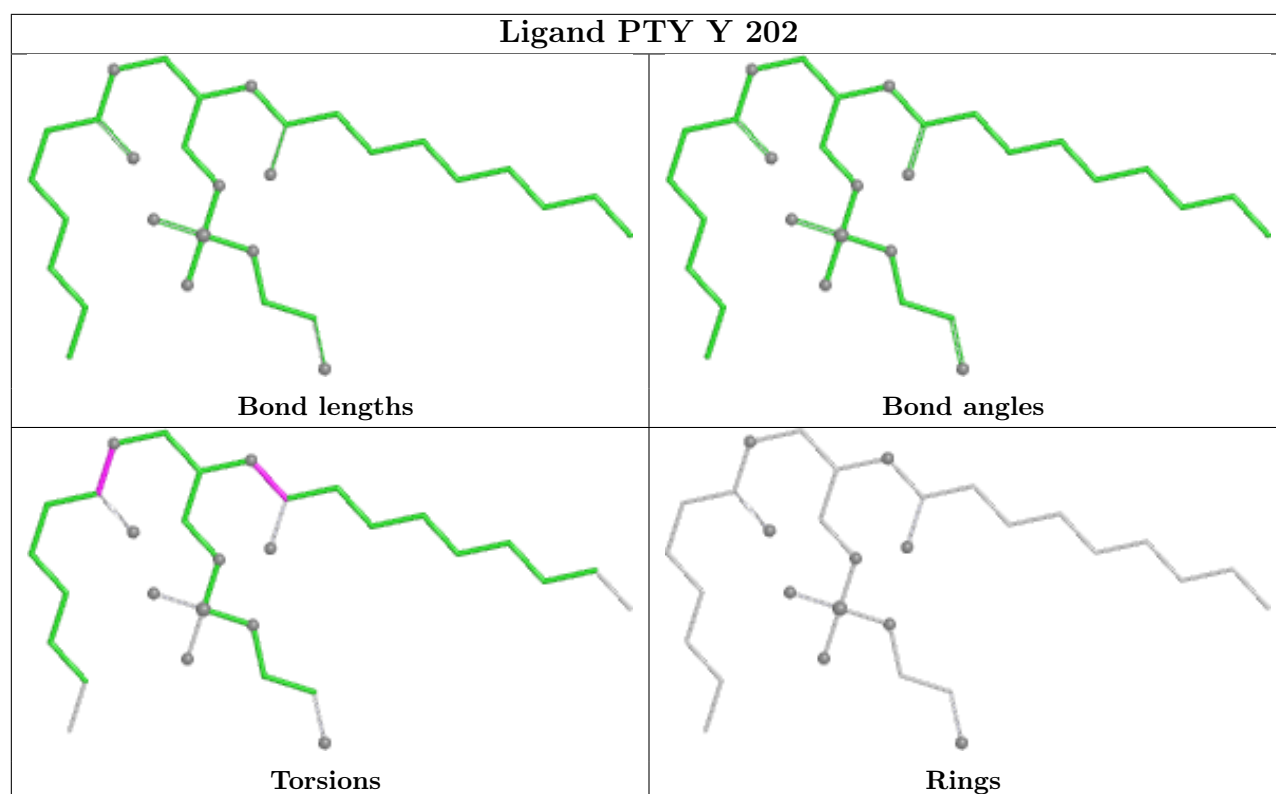




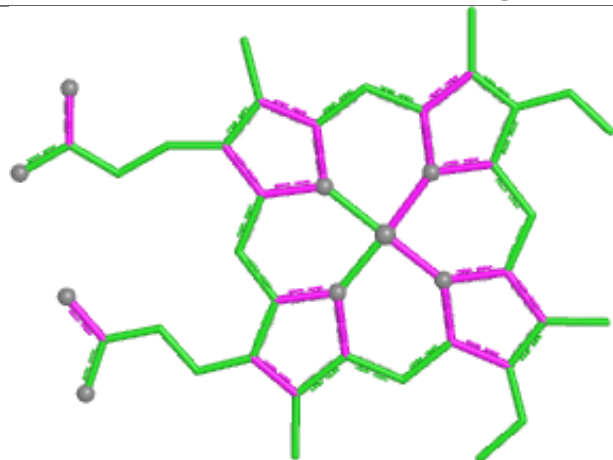




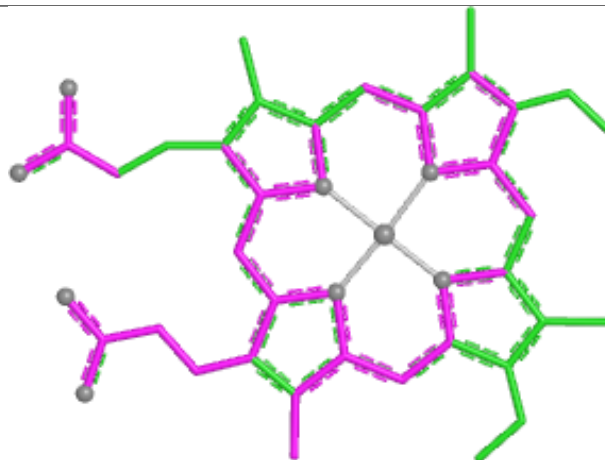




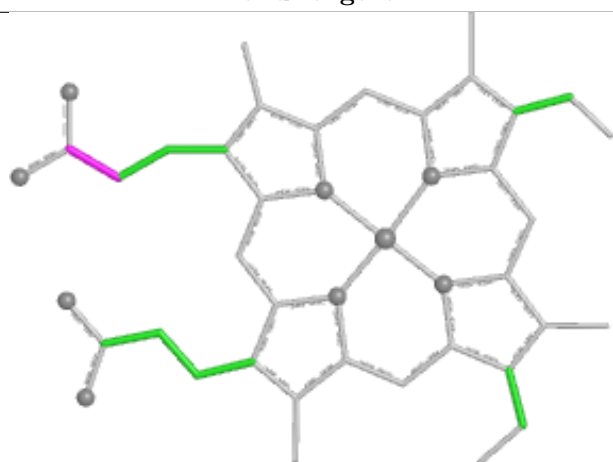
Ligand HEM BC 401



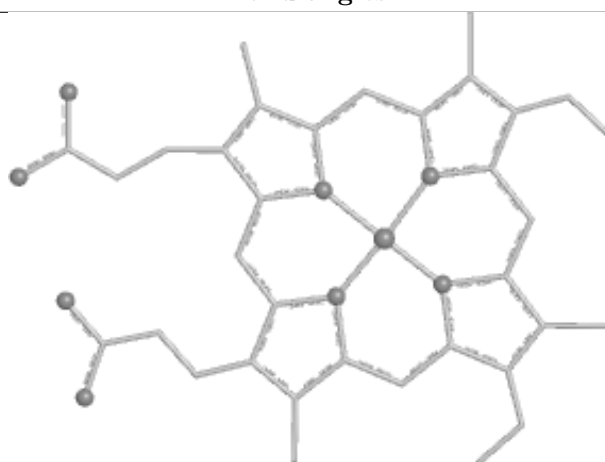
Bond lengths



Bond angles

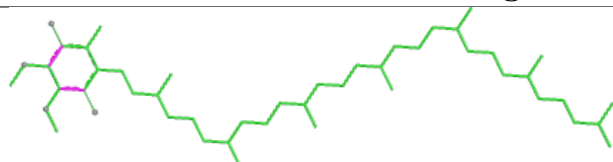


Torsions

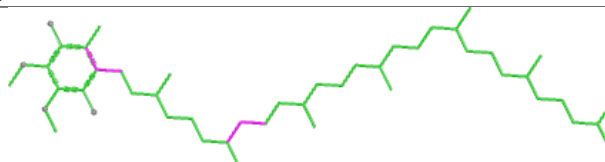


Rings

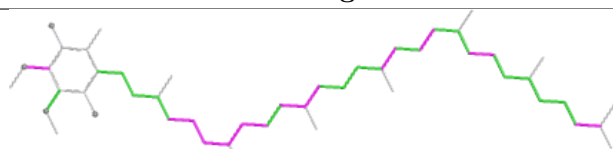
Ligand UQ7 BC 404



Bond lengths



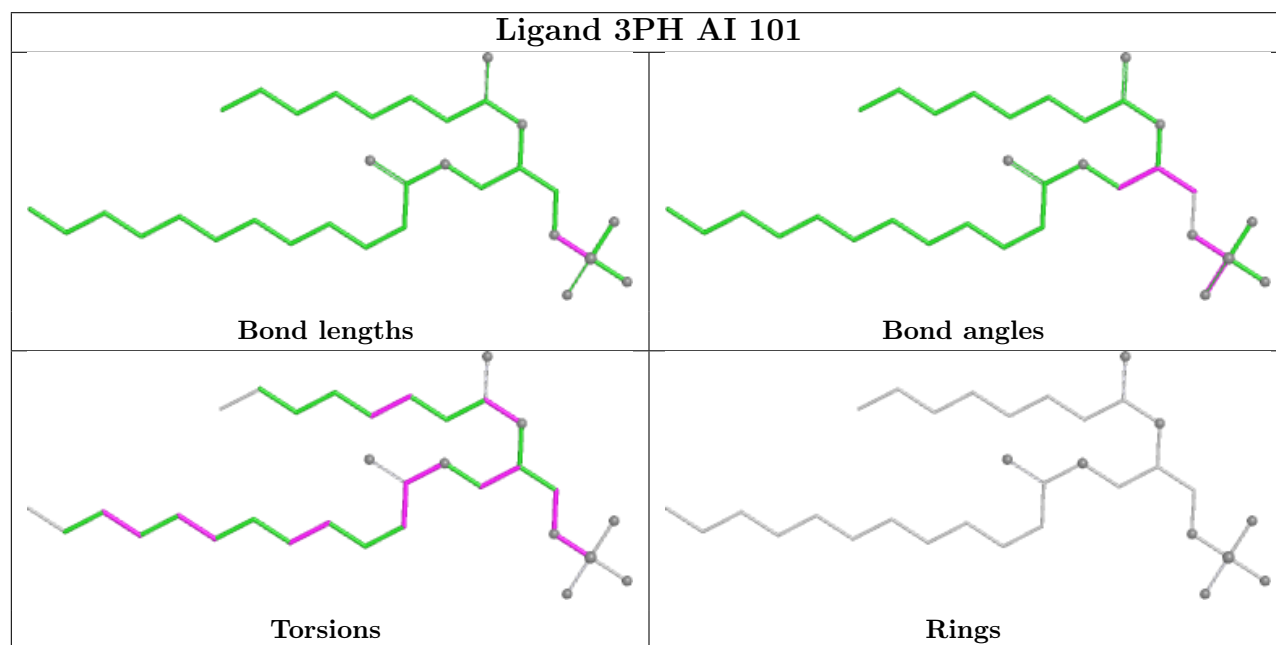
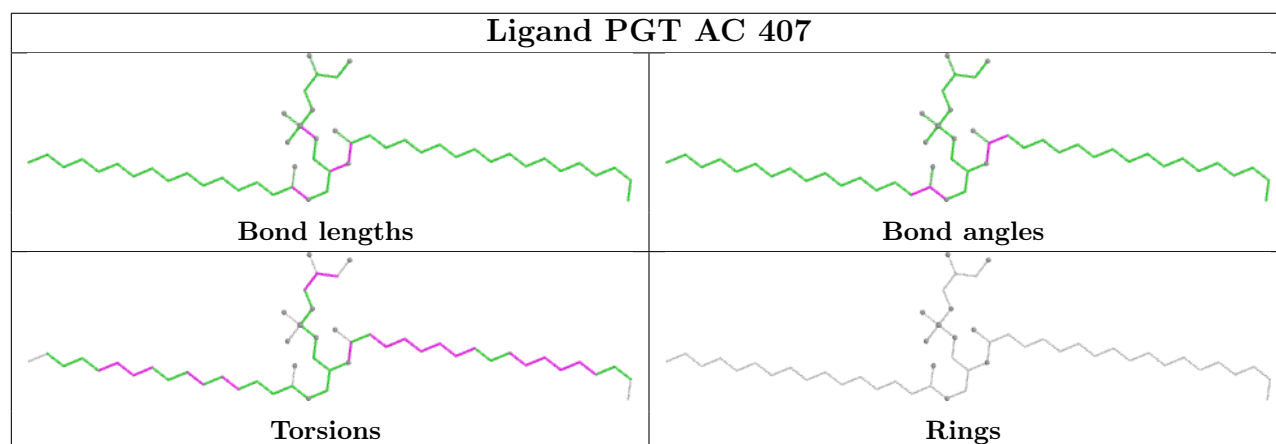
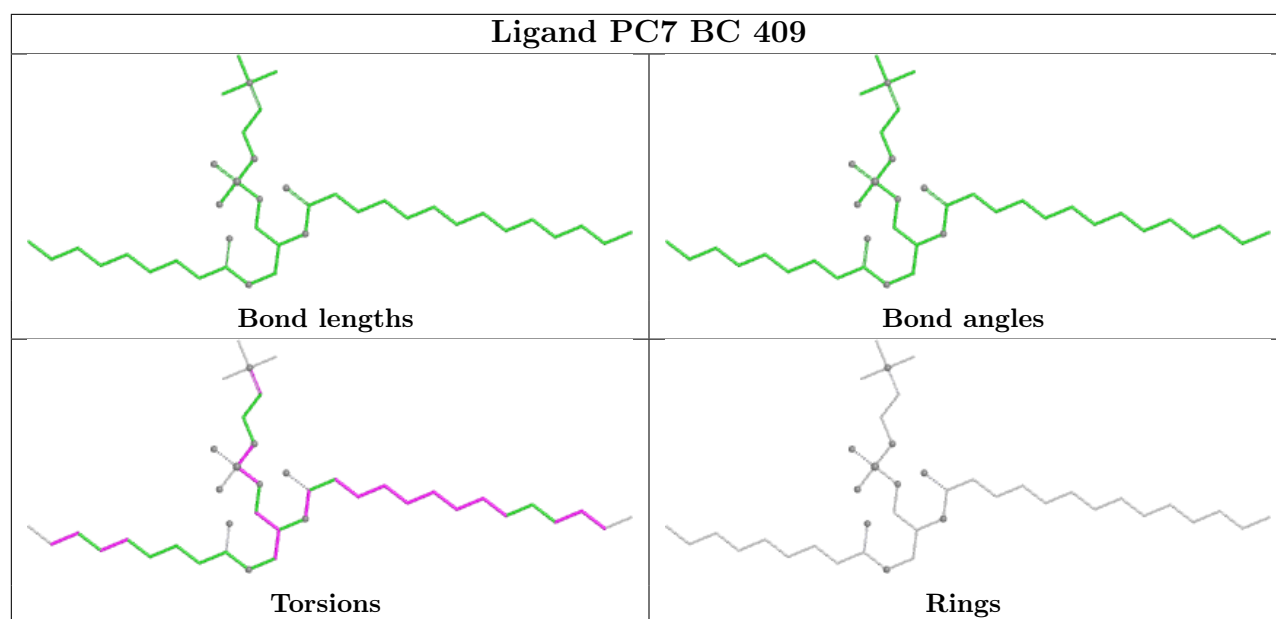
Bond angles

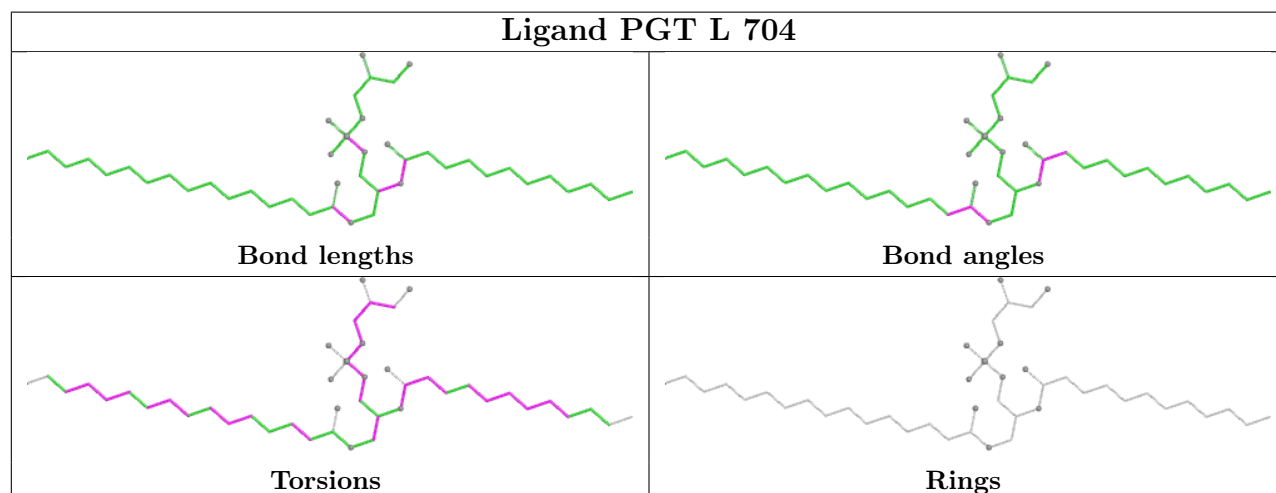
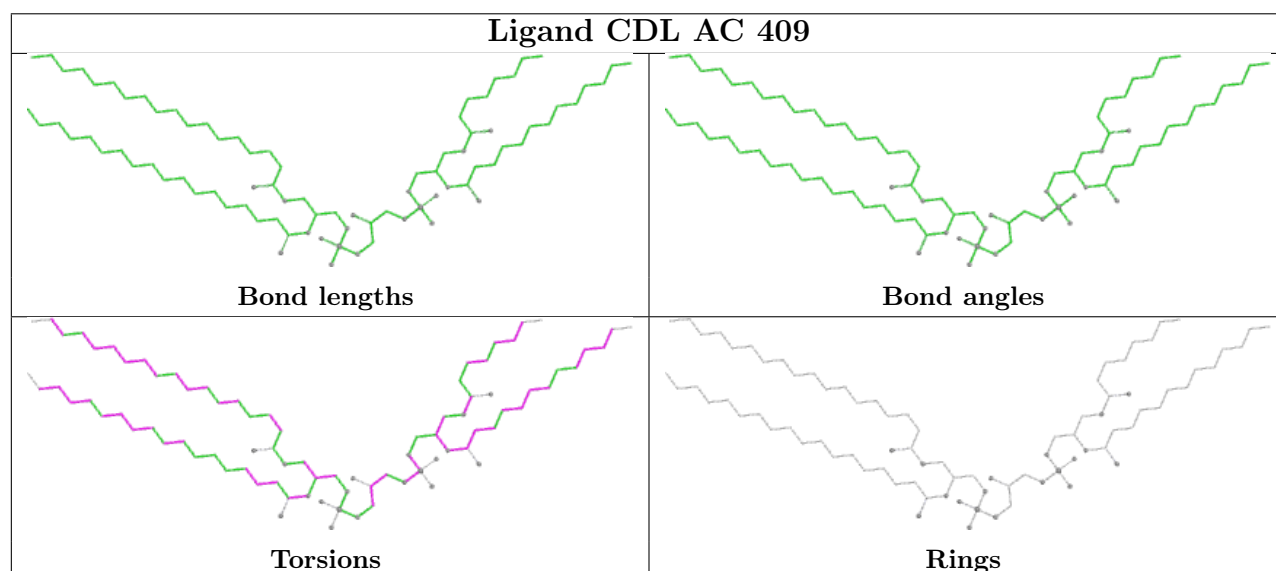
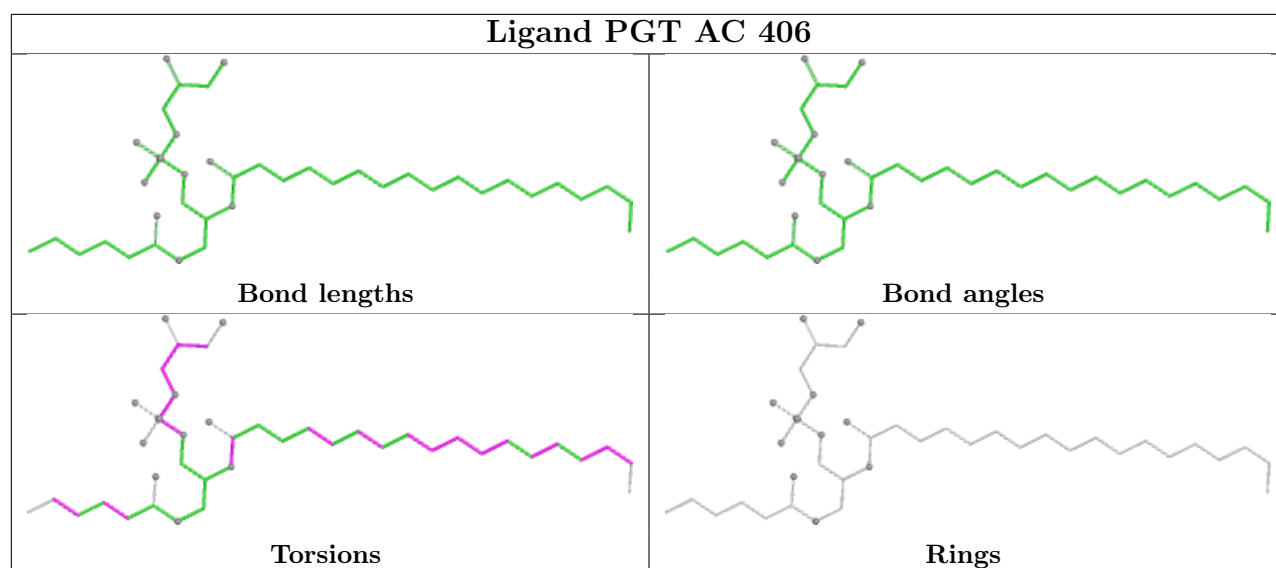


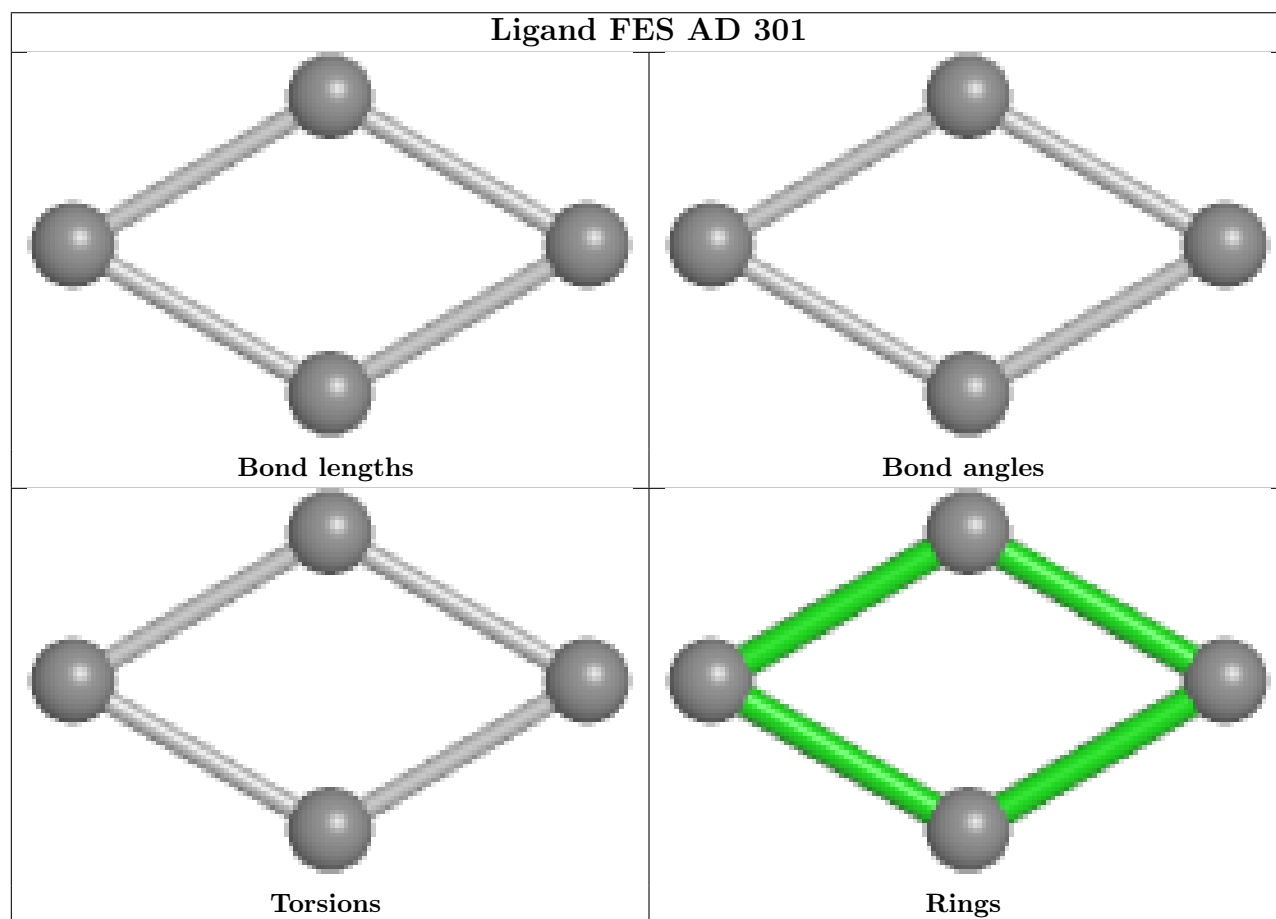
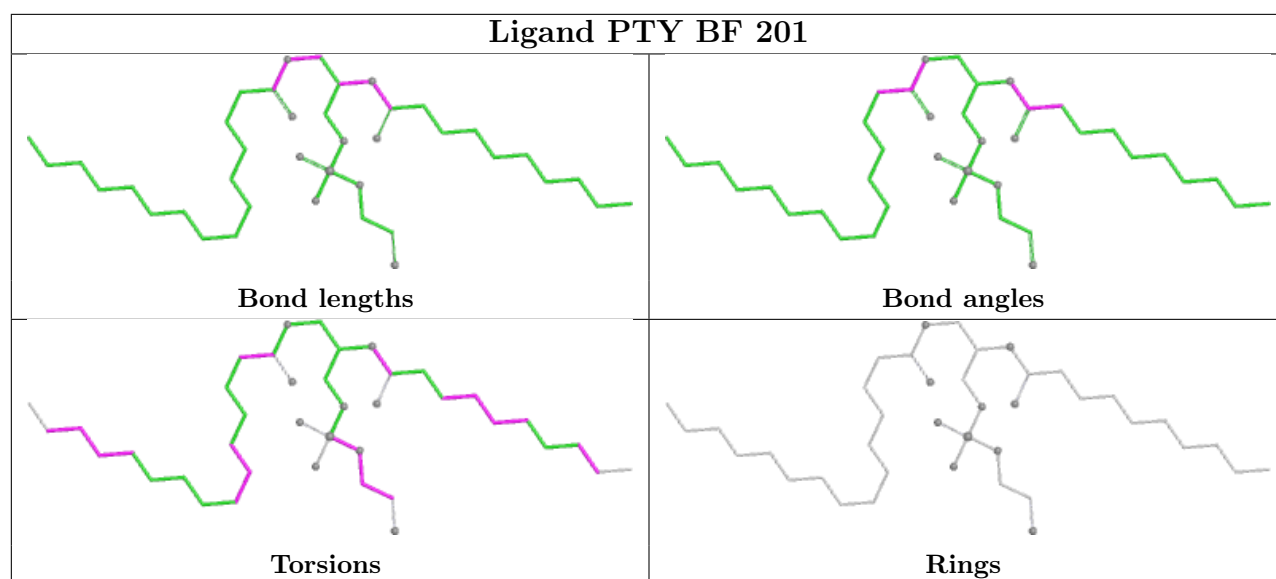
Torsions

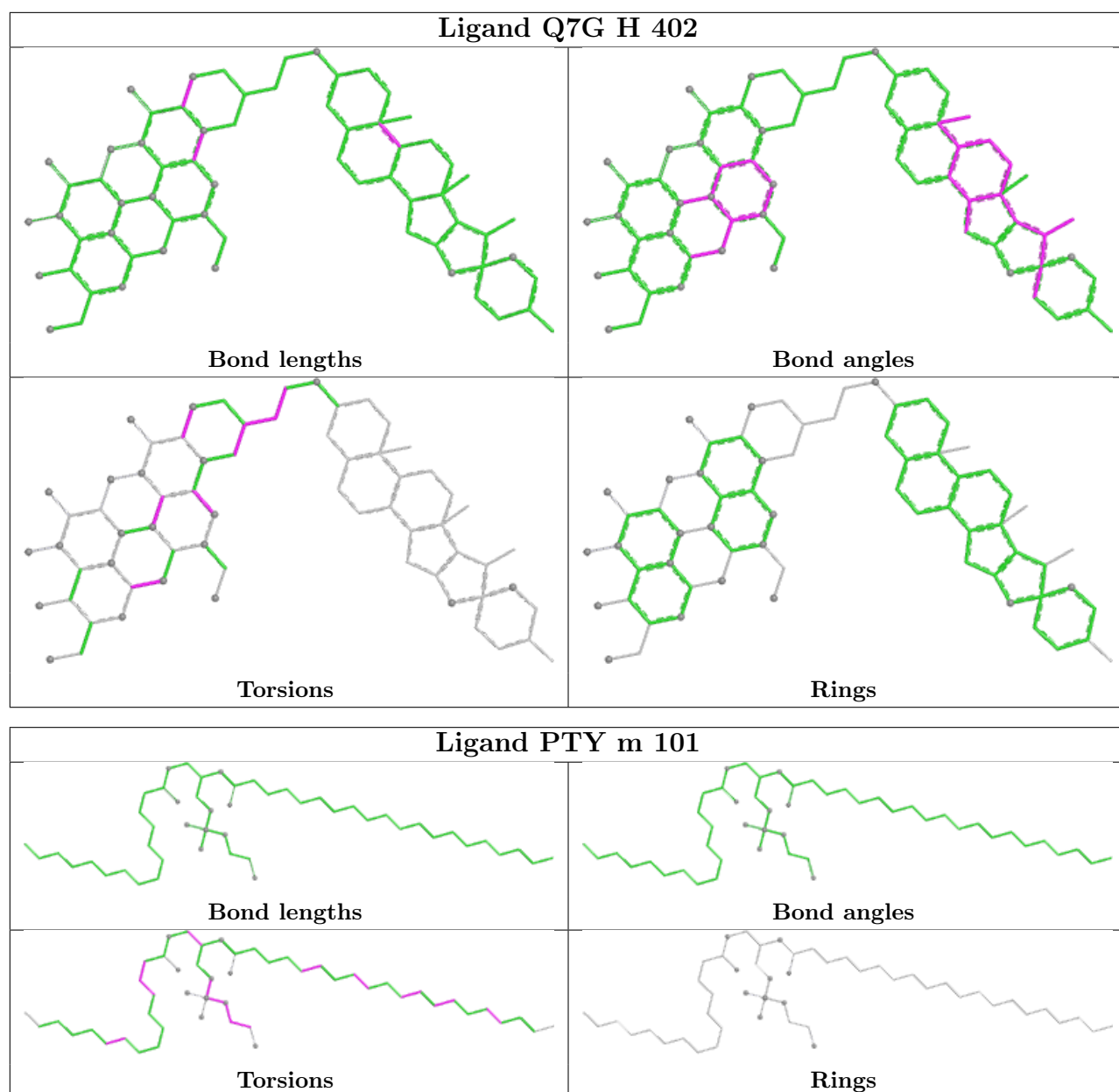


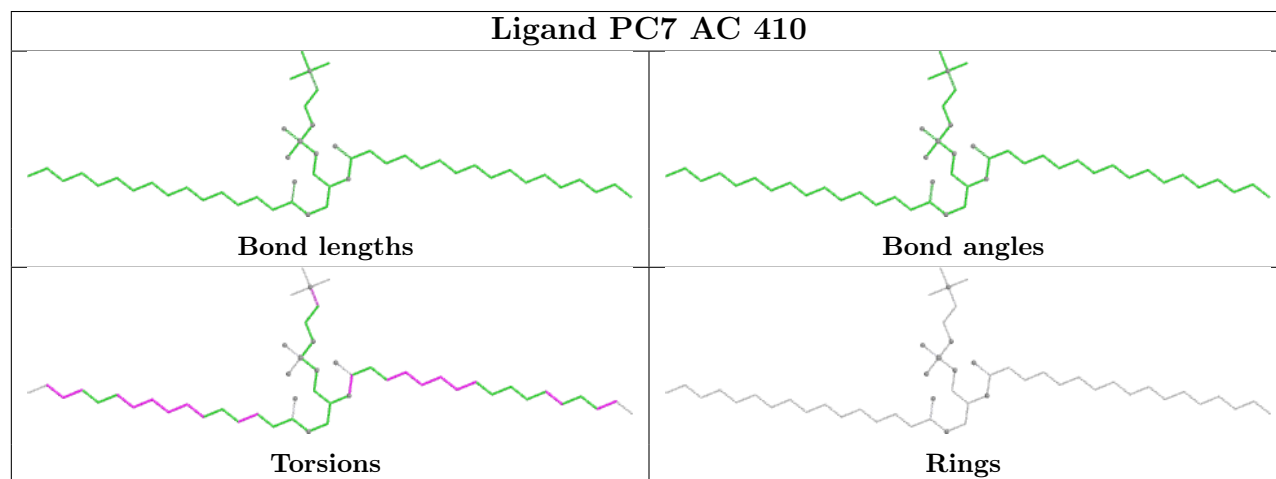
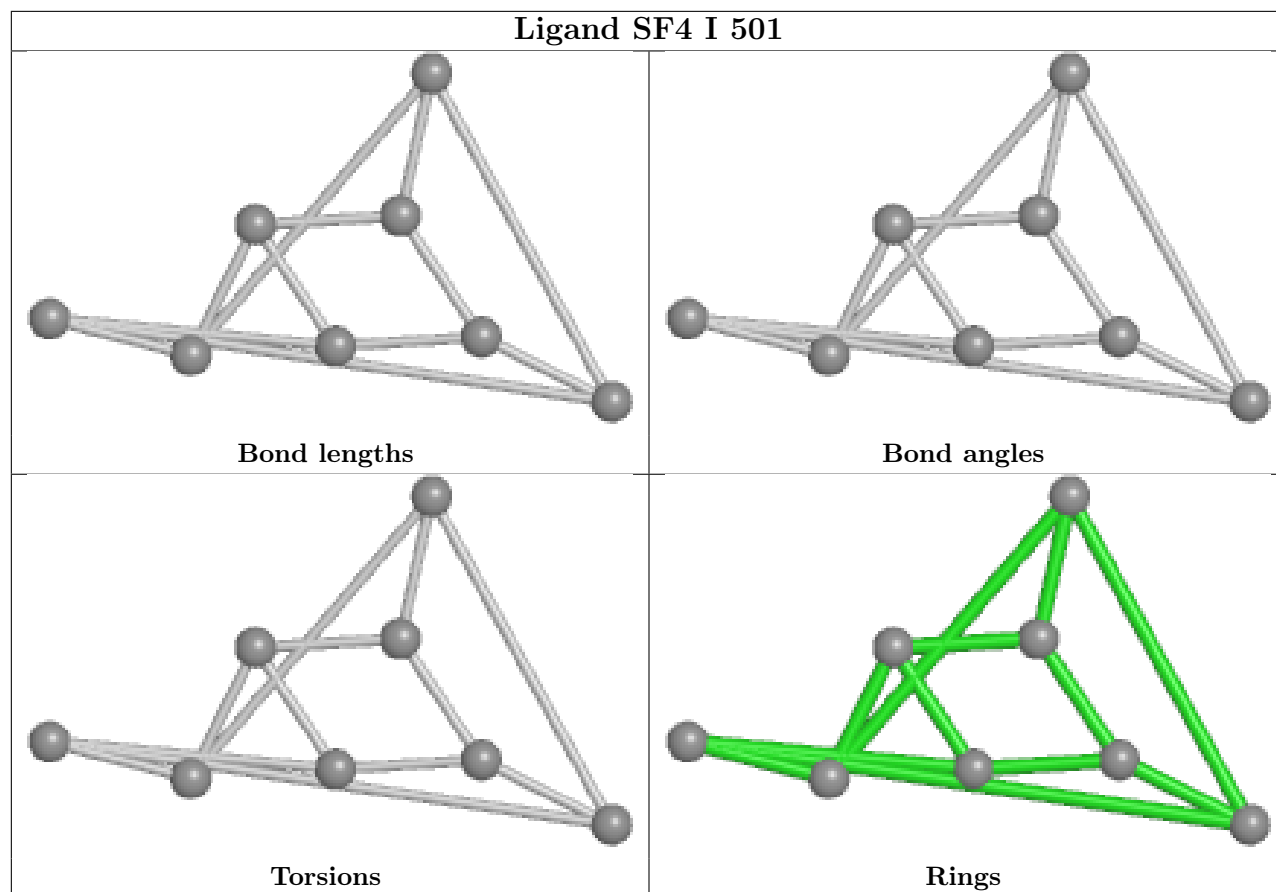
Rings

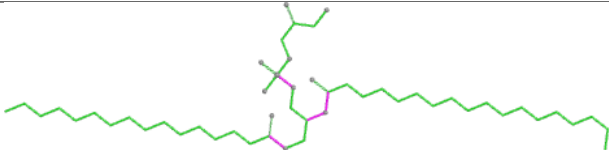
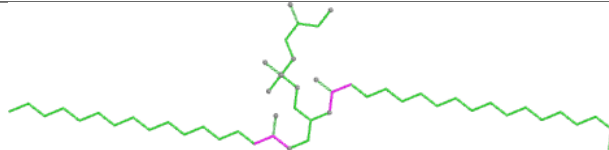
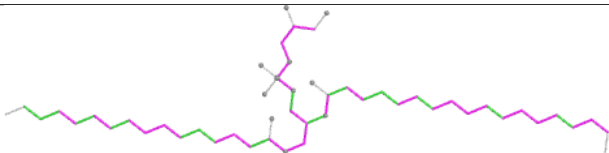
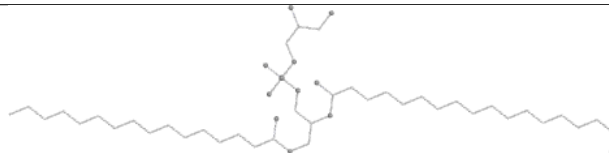


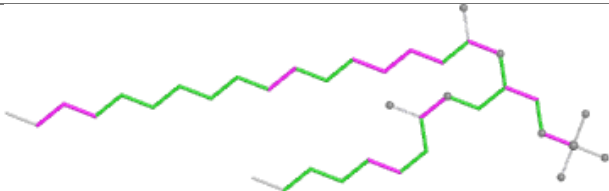


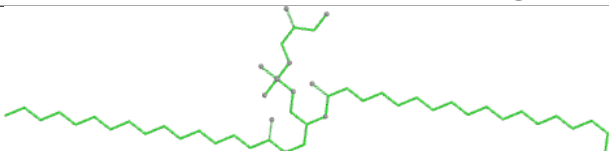
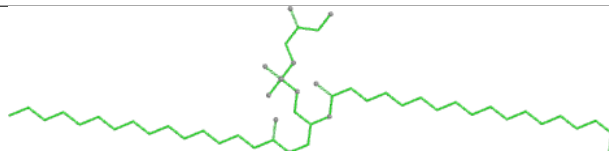
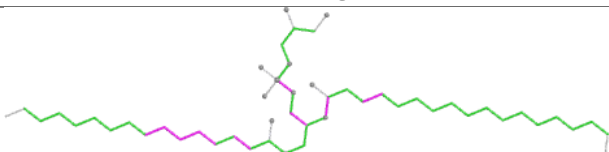
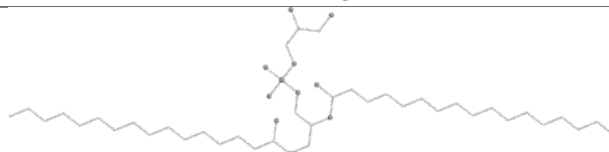


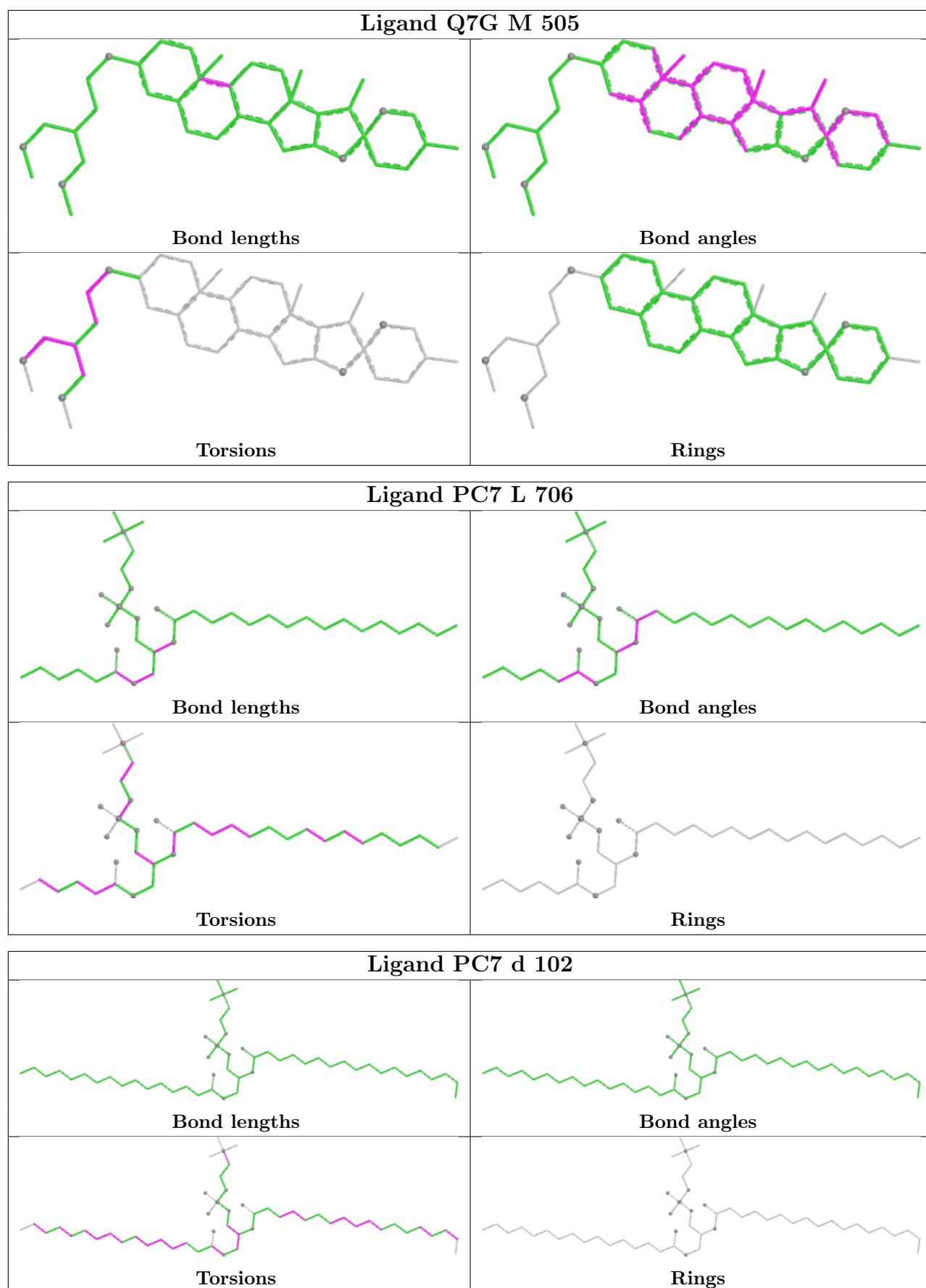


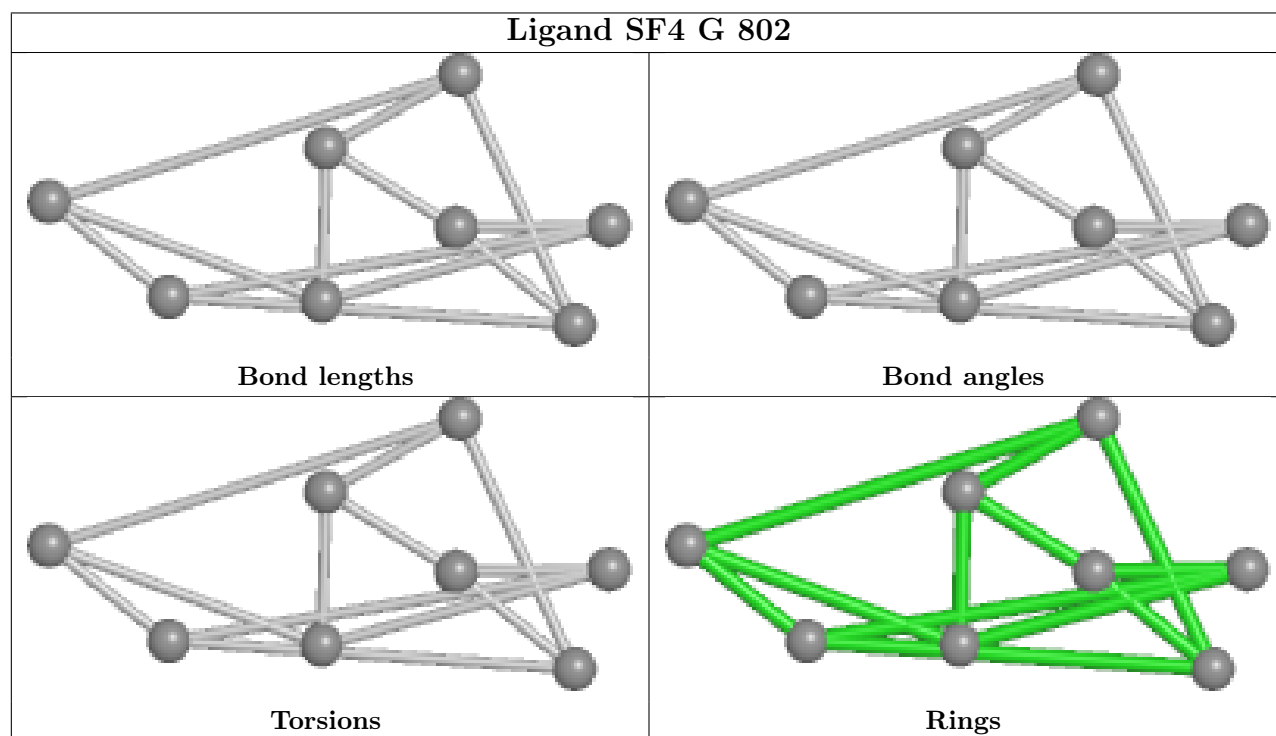
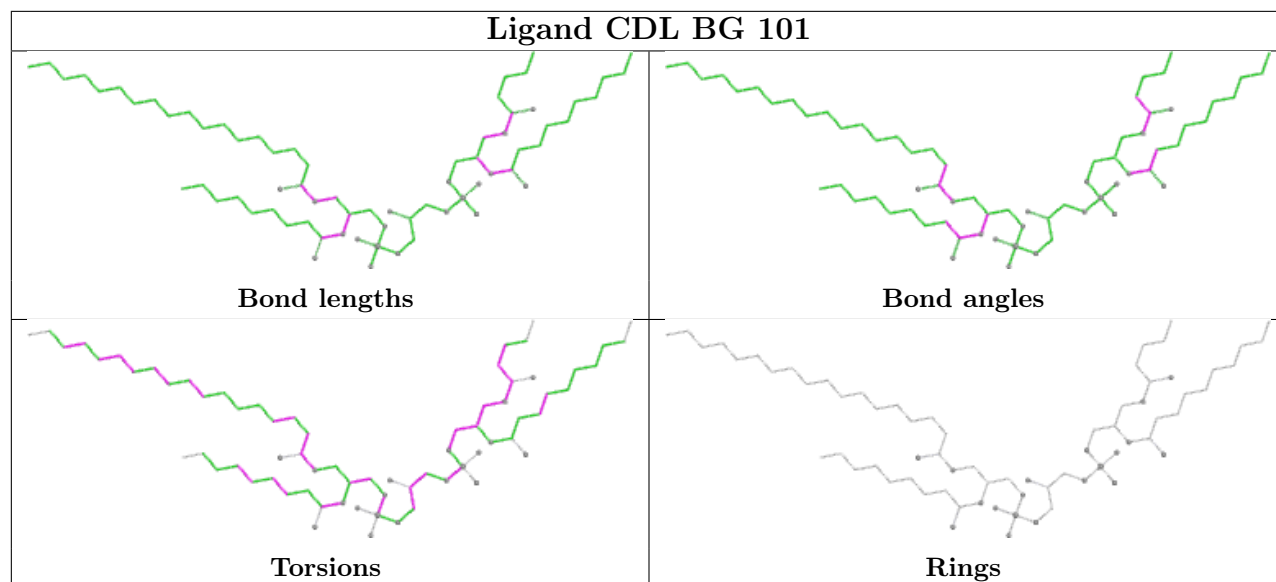


Ligand PGT AF 201	
	
Bond lengths	Bond angles
	
Torsions	Rings

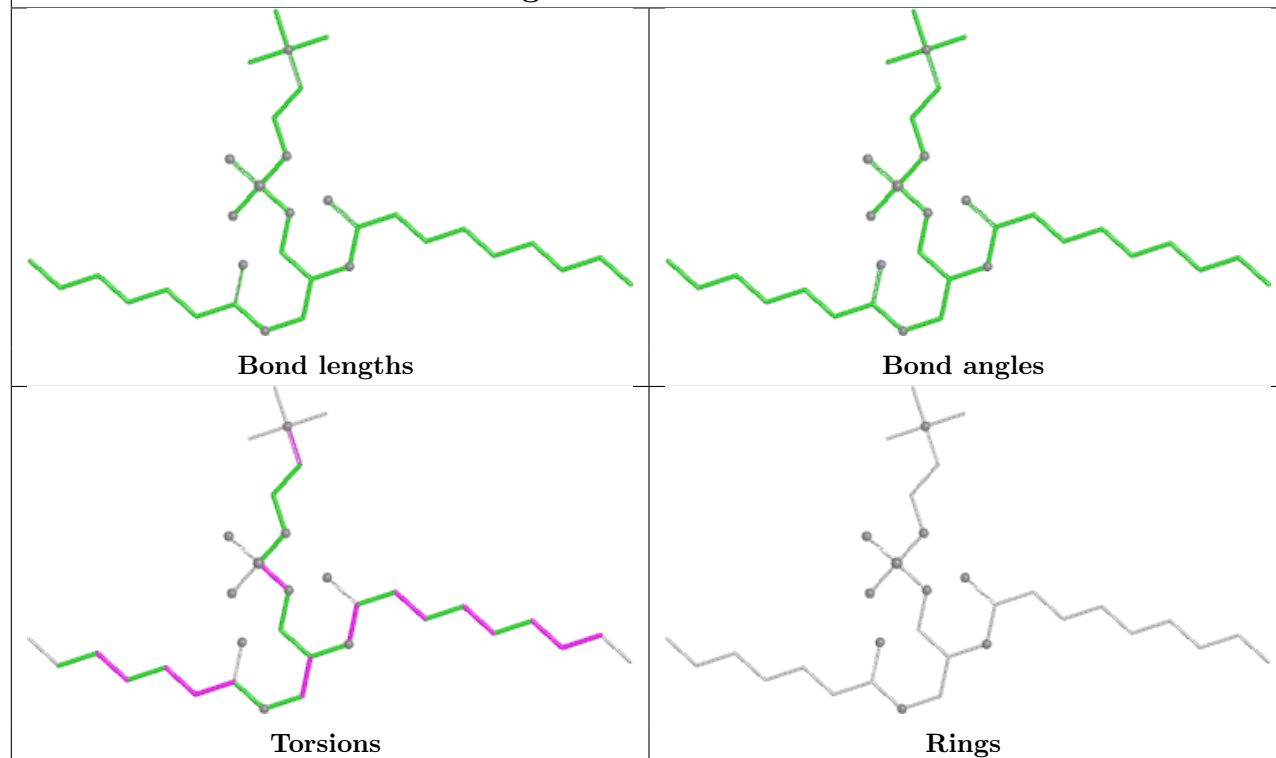
Ligand 3PH L 701	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PGT L 703	
	
Bond lengths	Bond angles
	
Torsions	Rings

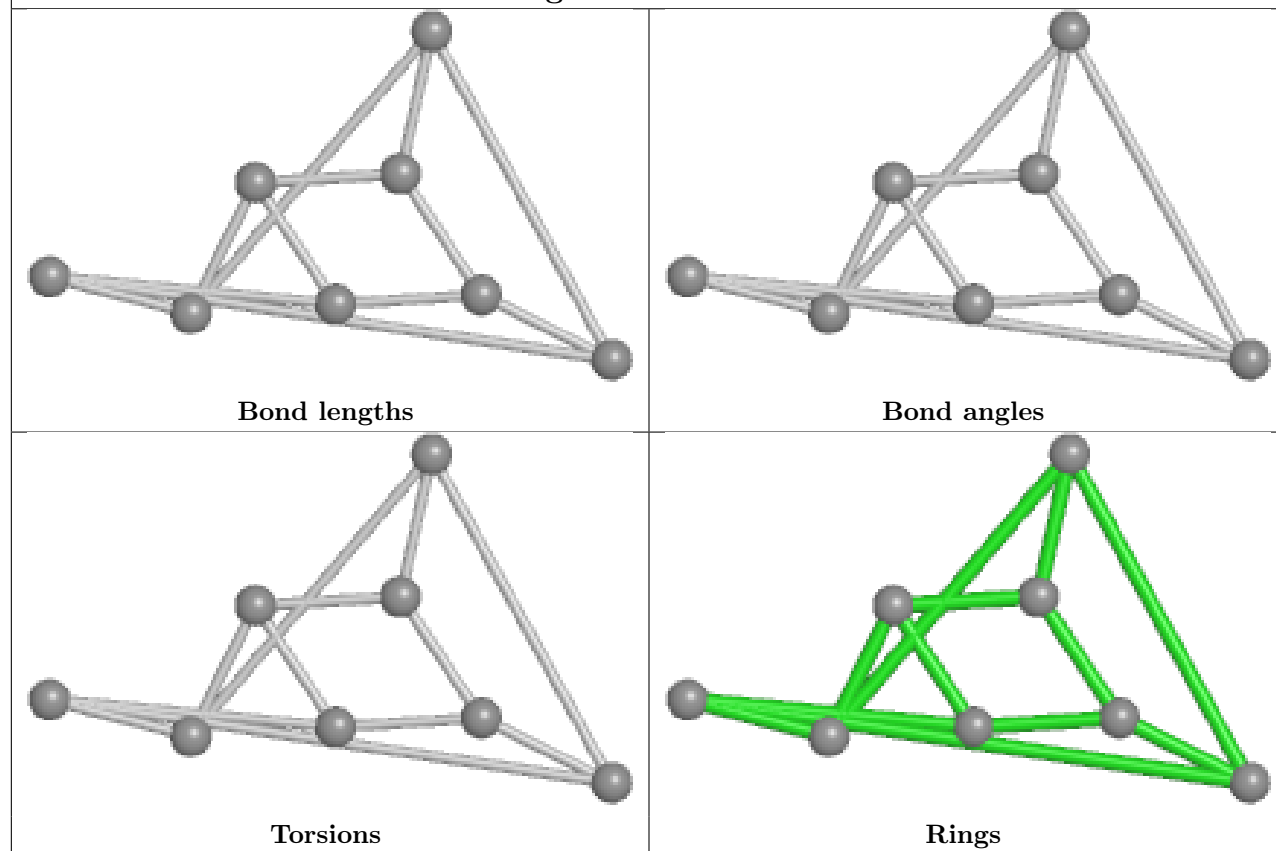


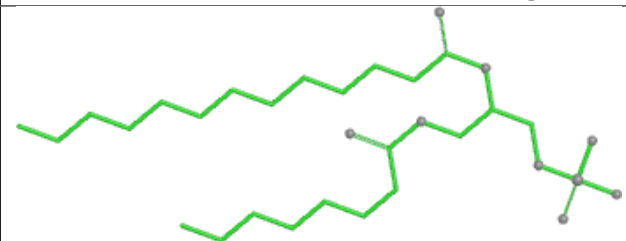
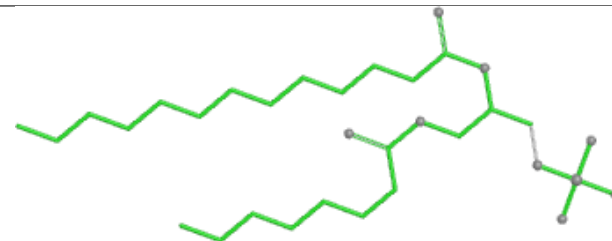
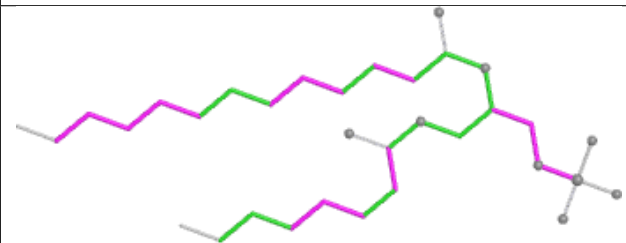


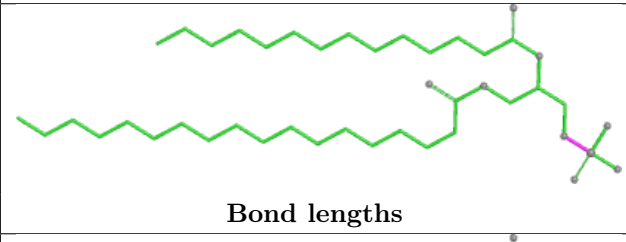
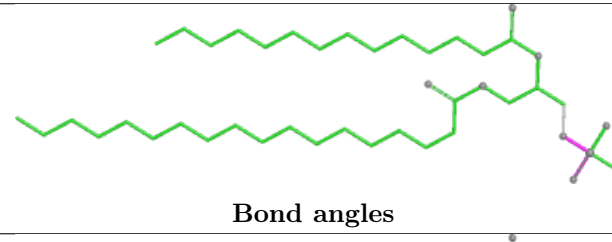
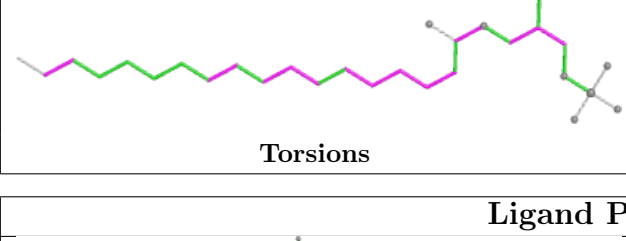
Ligand PC7 AB 603

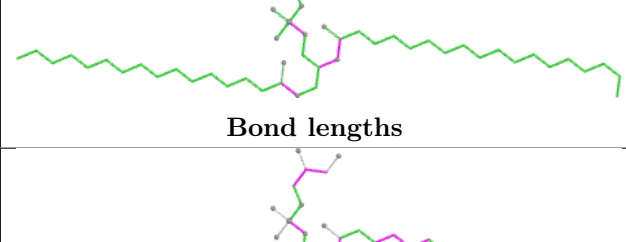
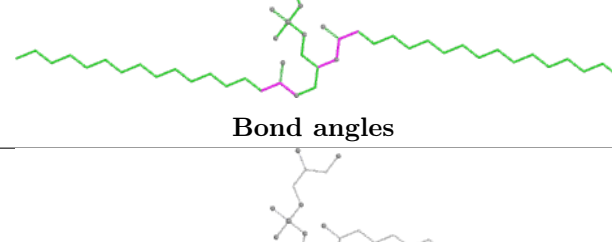
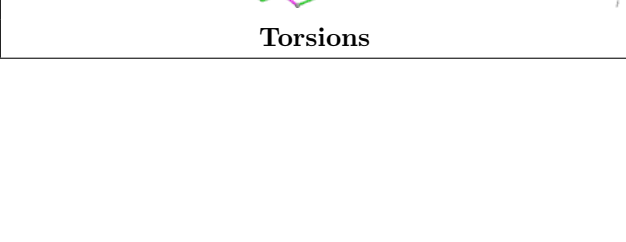
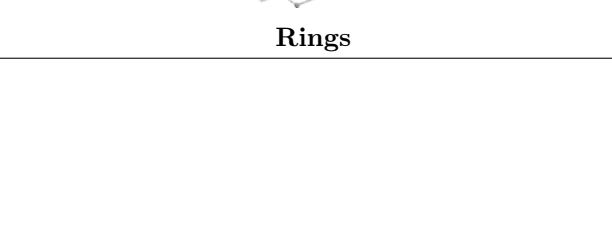


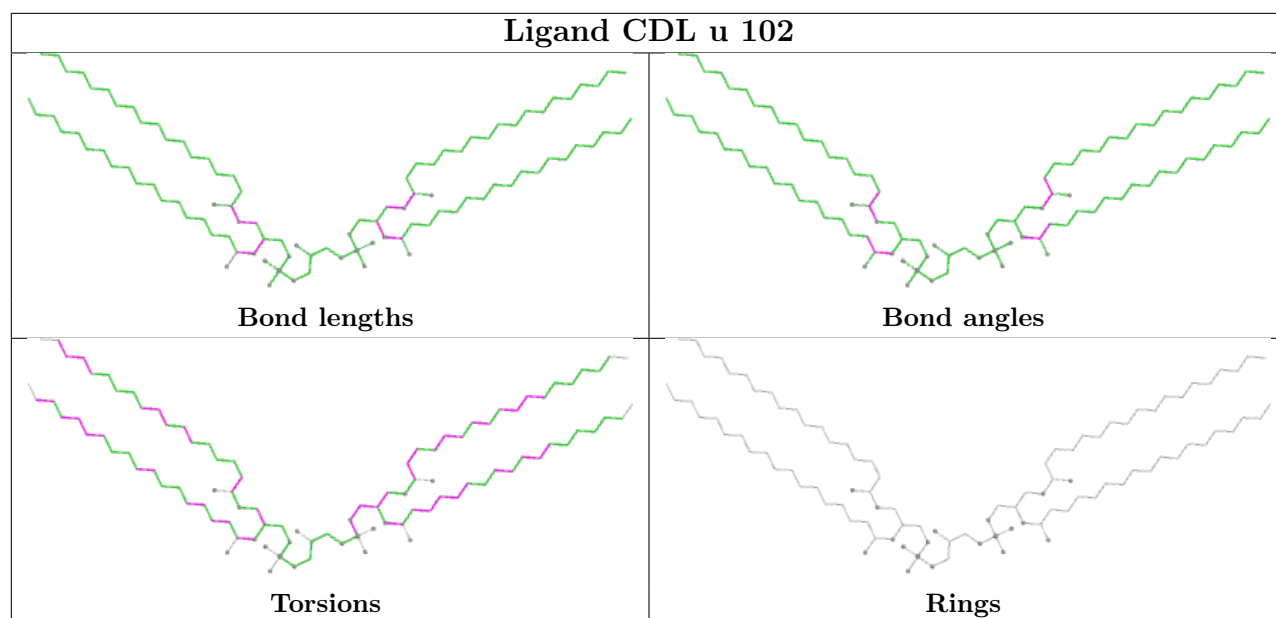
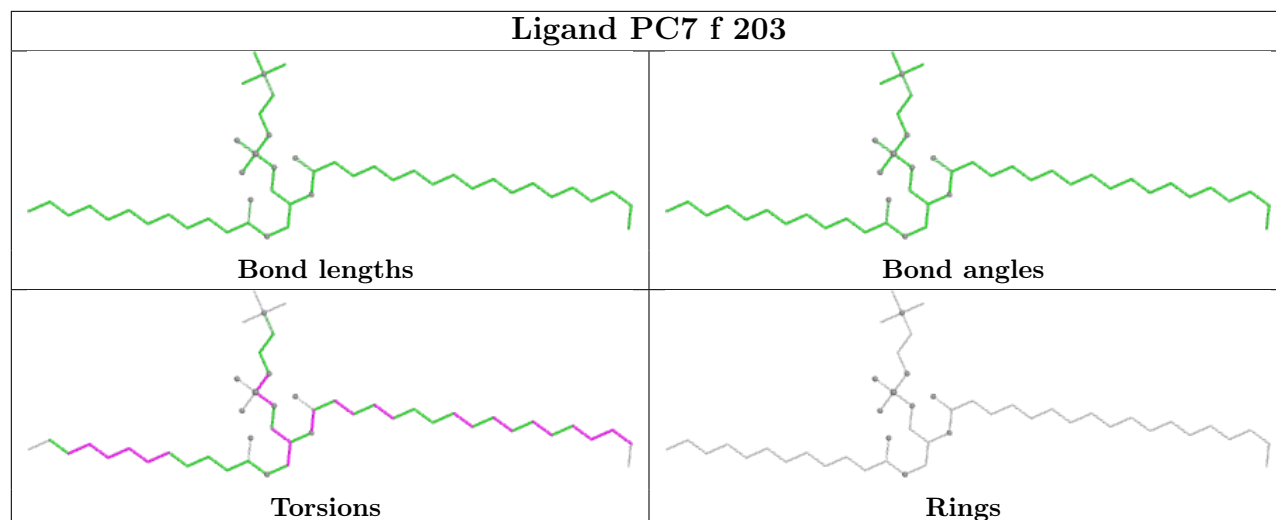
Ligand SF4 I 500

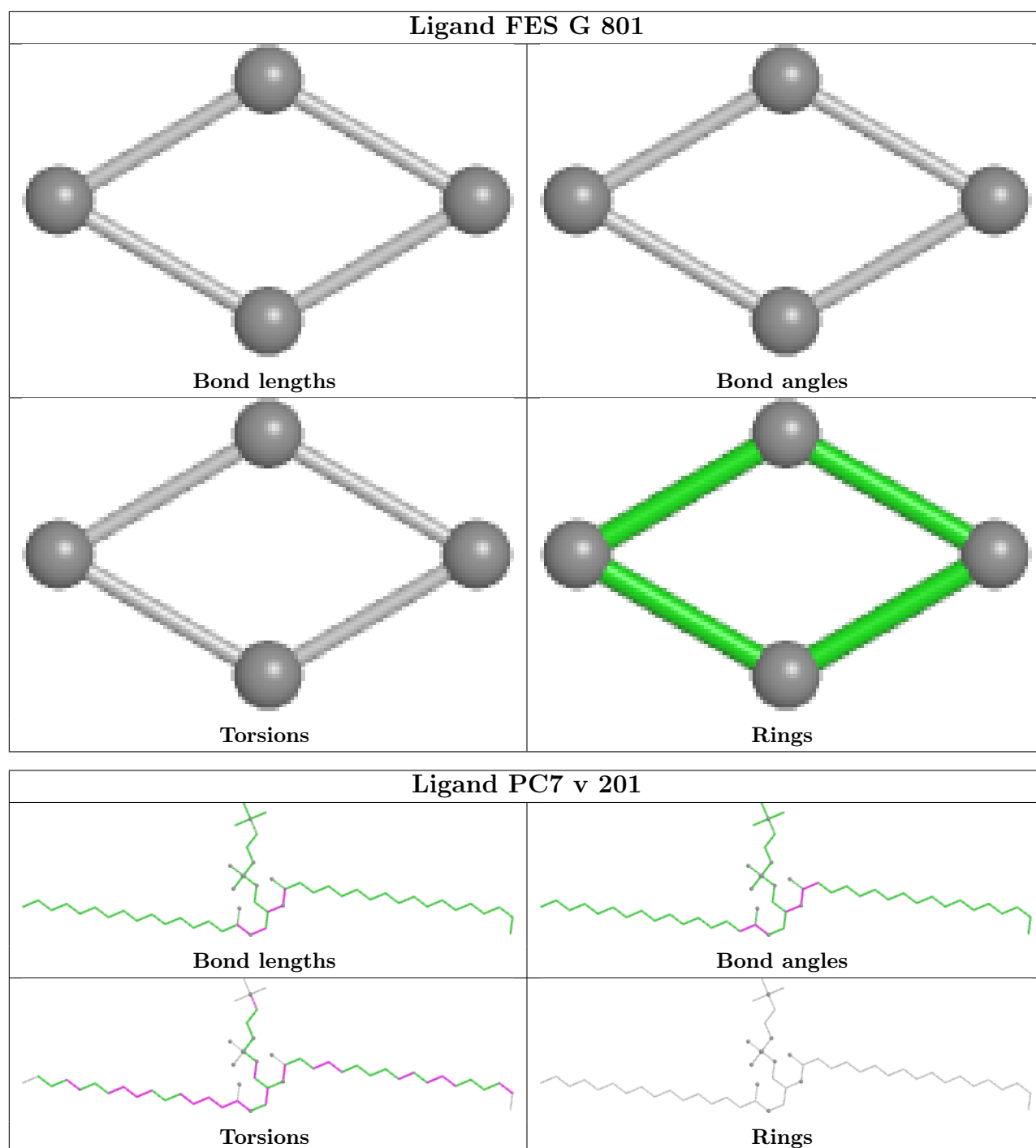


Ligand 3PH Y 201	
	
Bond lengths	Bond angles
	
Torsions	Rings

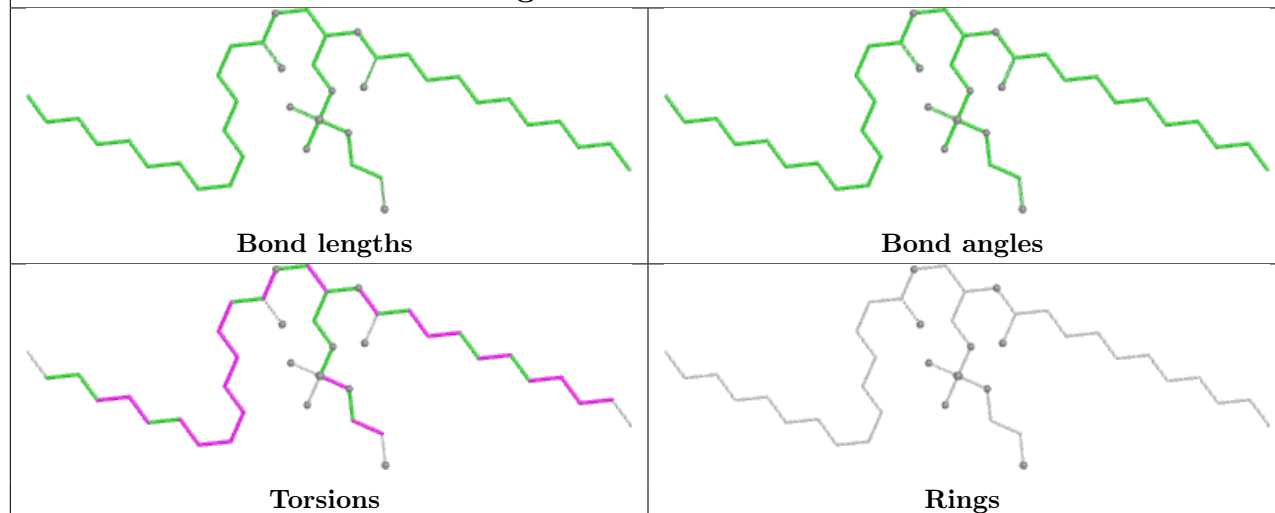
Ligand 3PH BC 405	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PGT A 201	
	
Bond lengths	Bond angles
	
Torsions	Rings

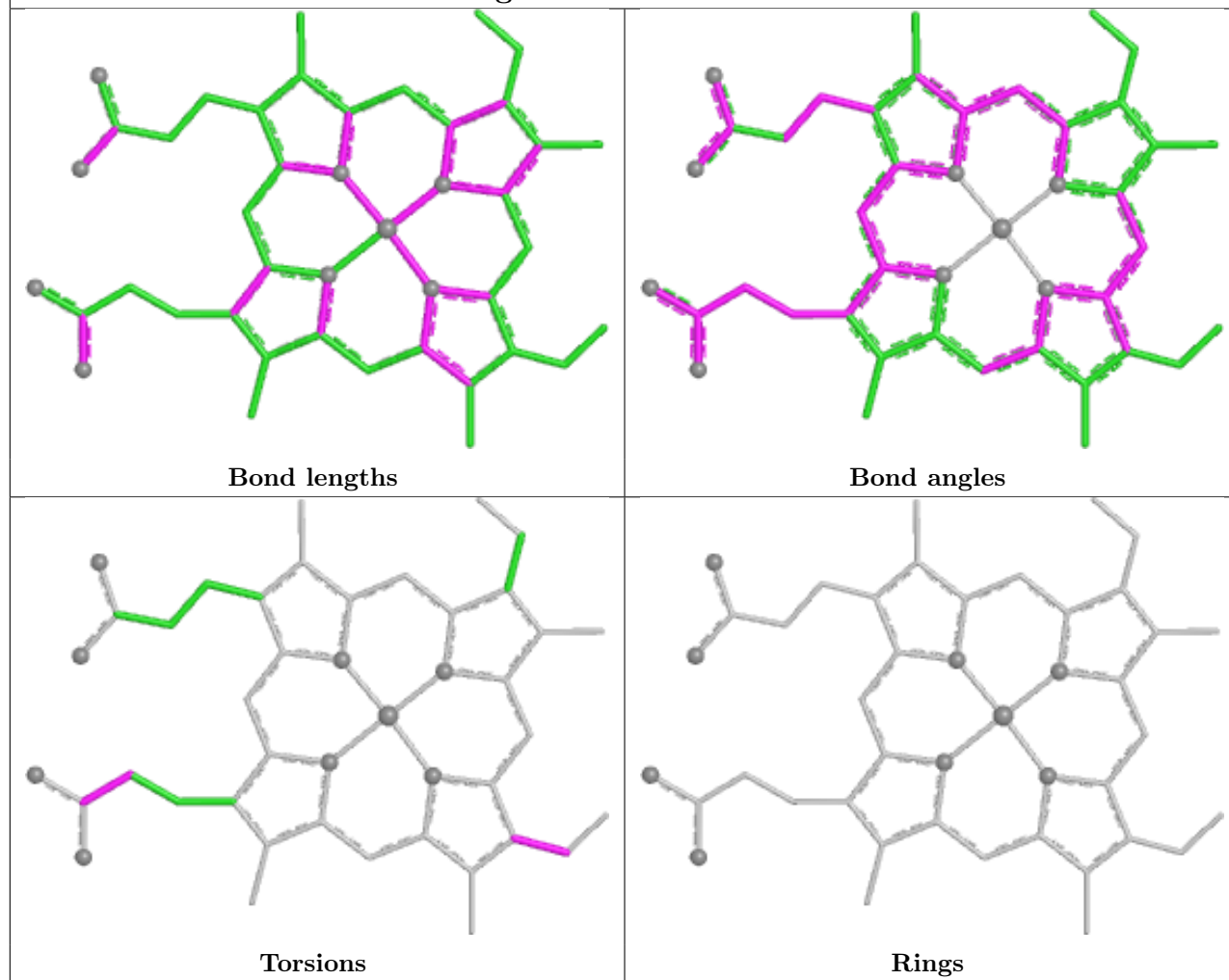


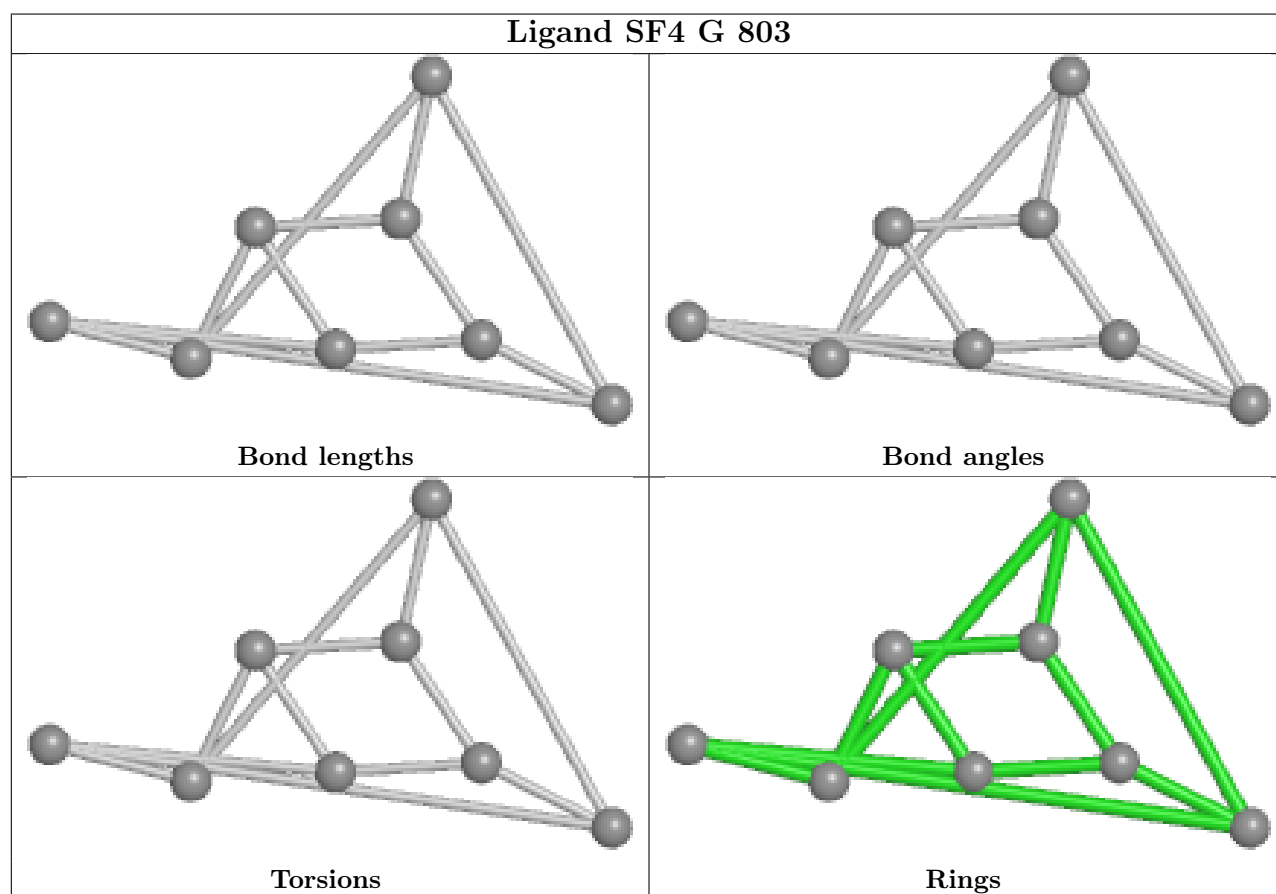
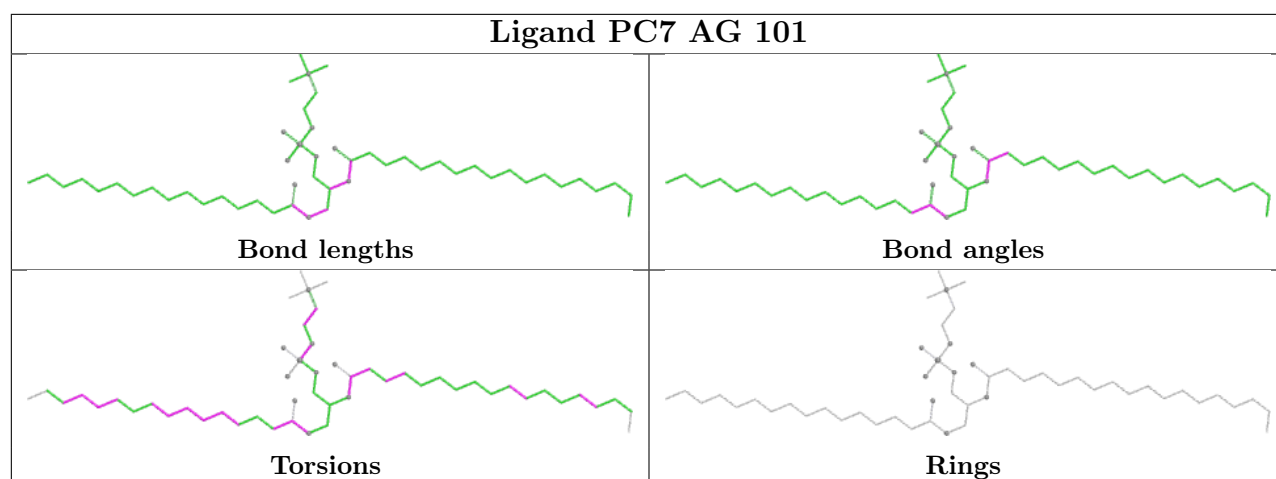


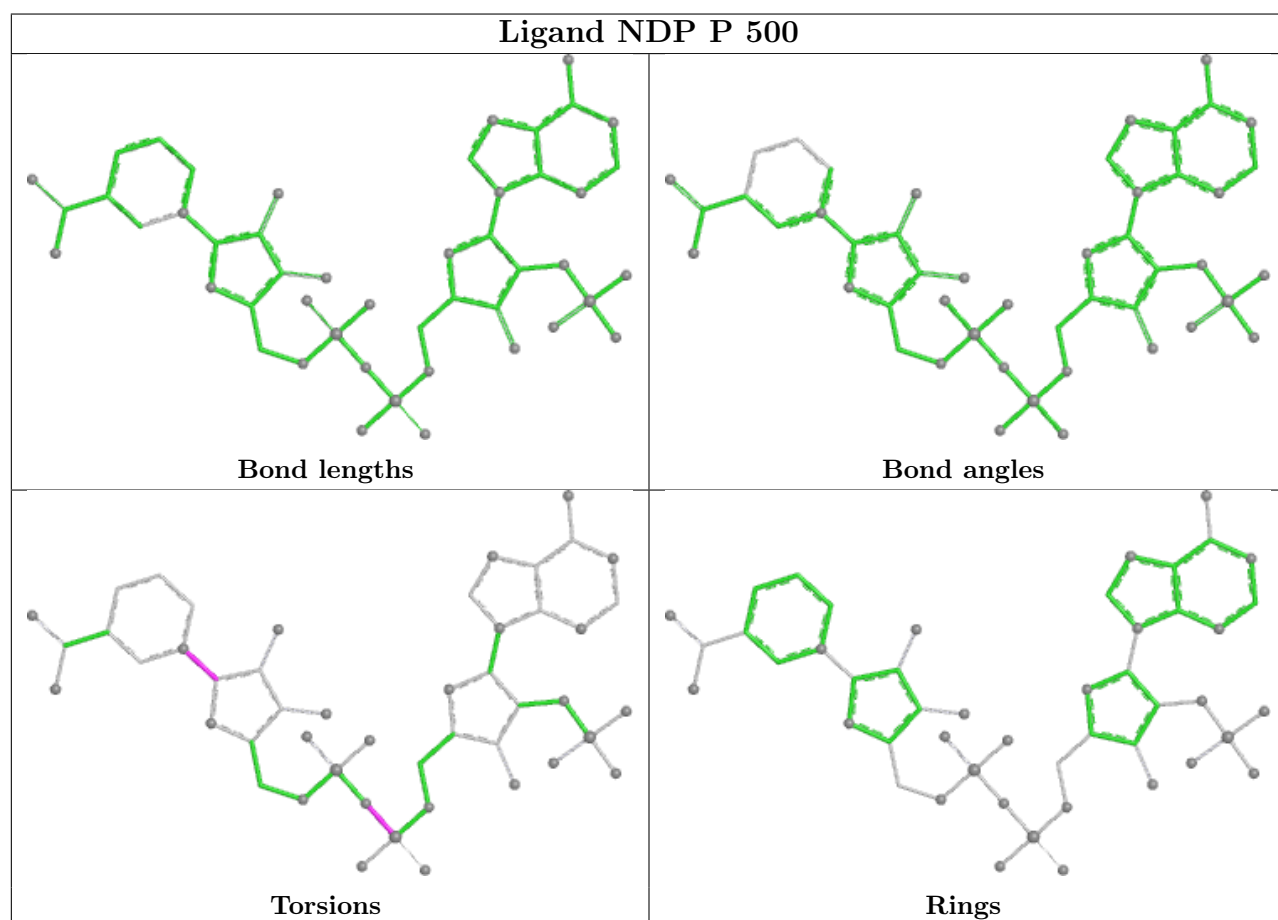
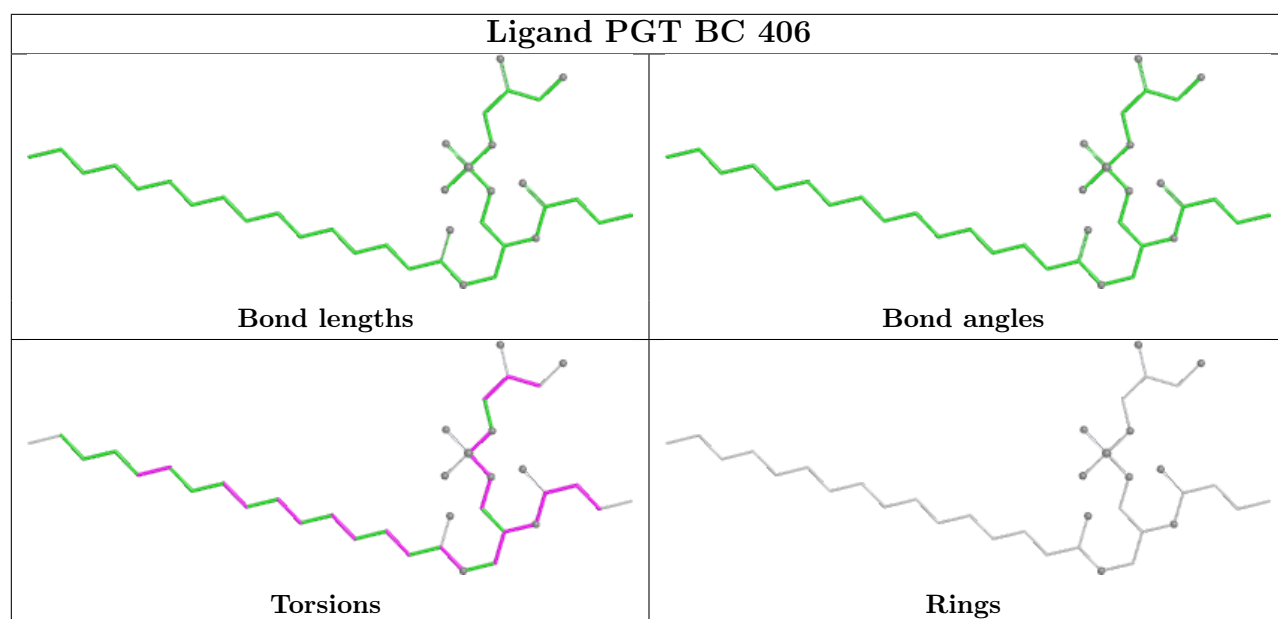
Ligand PTY AB 602

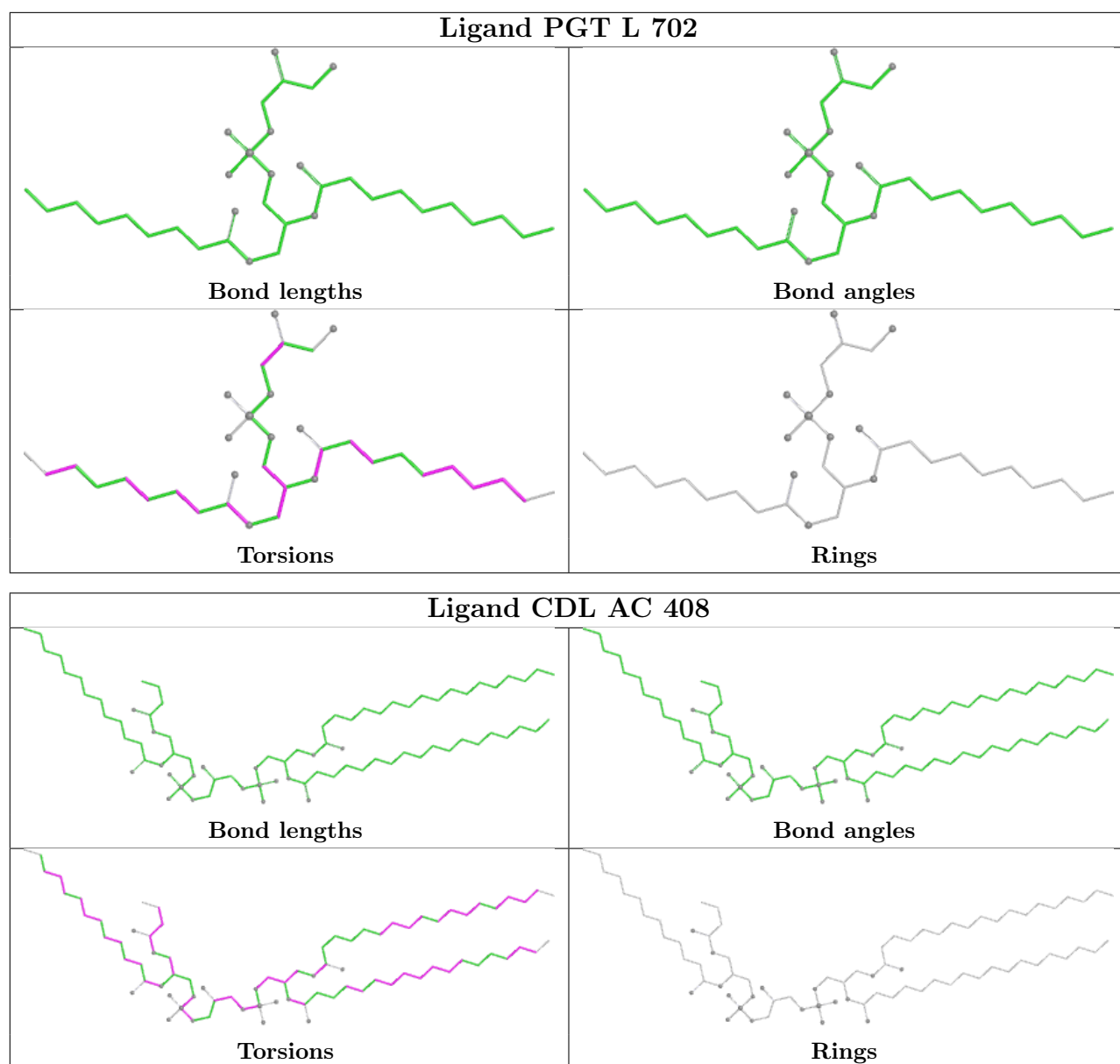


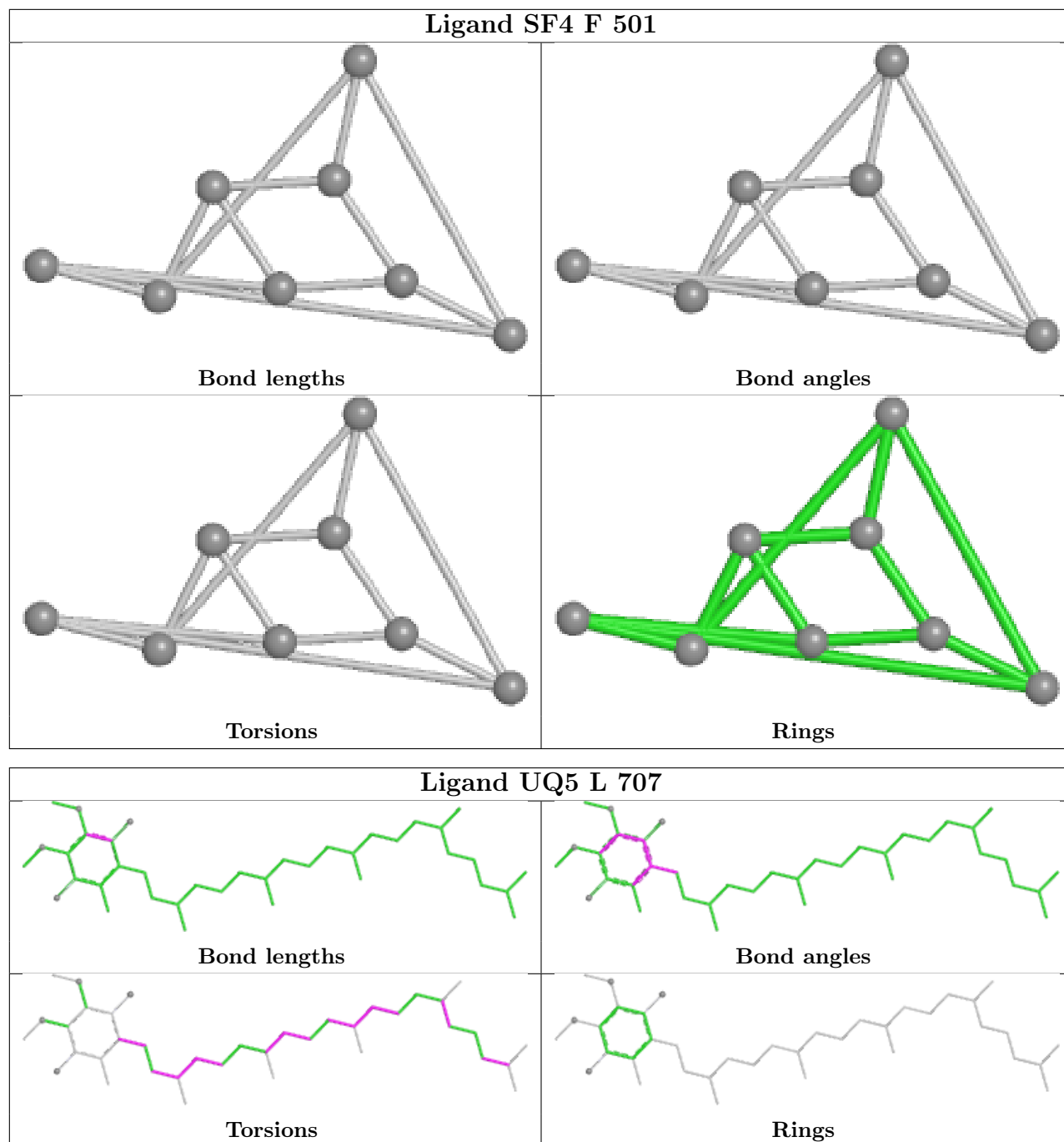
Ligand HEM BE 401

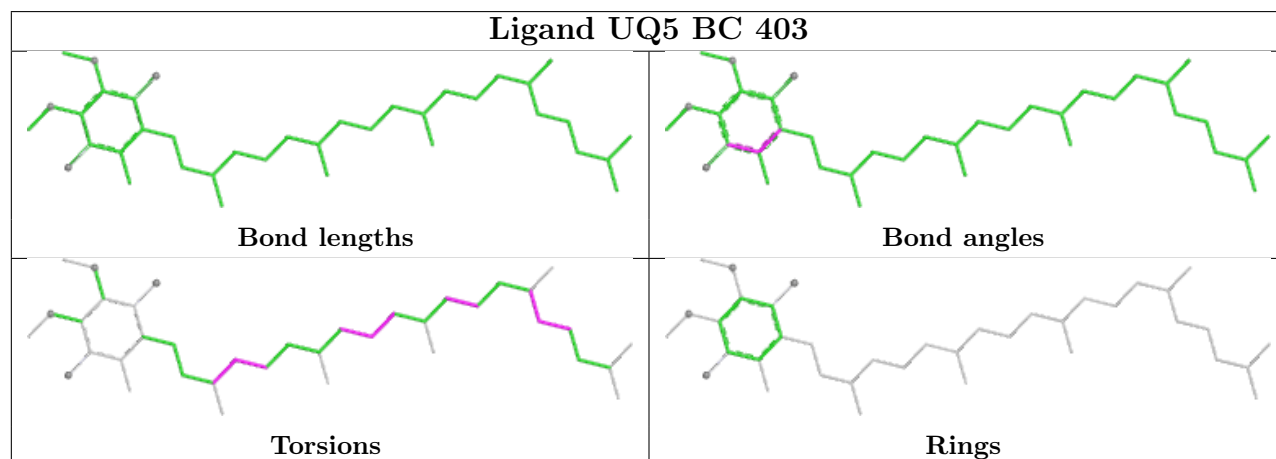
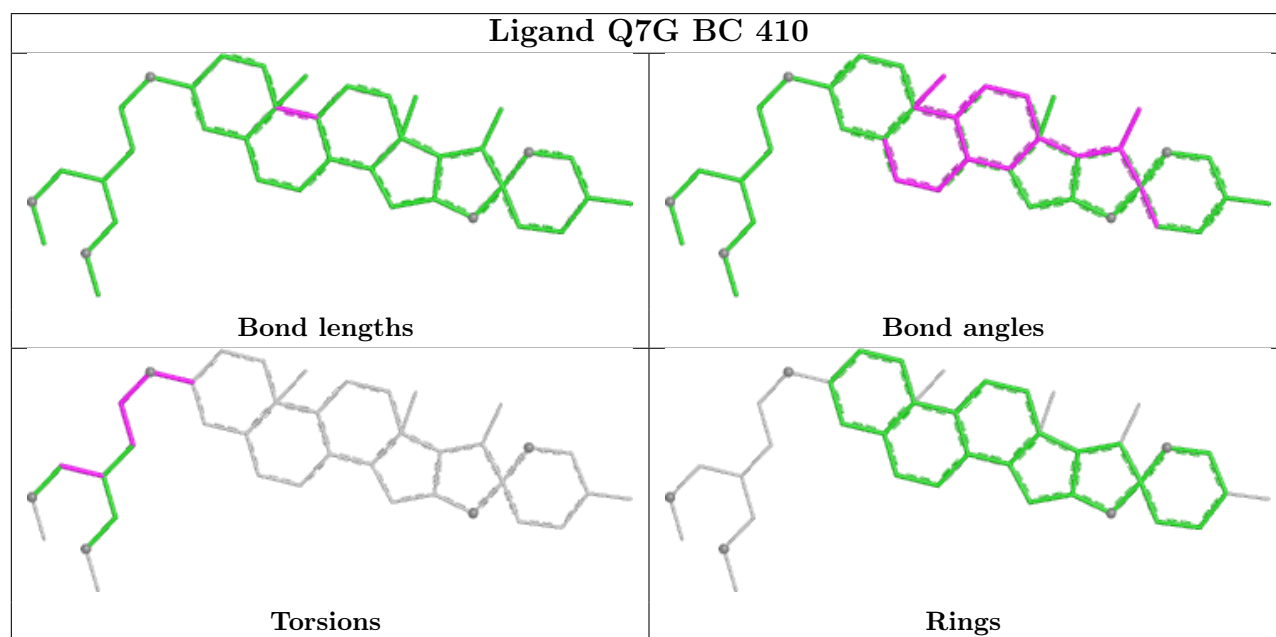
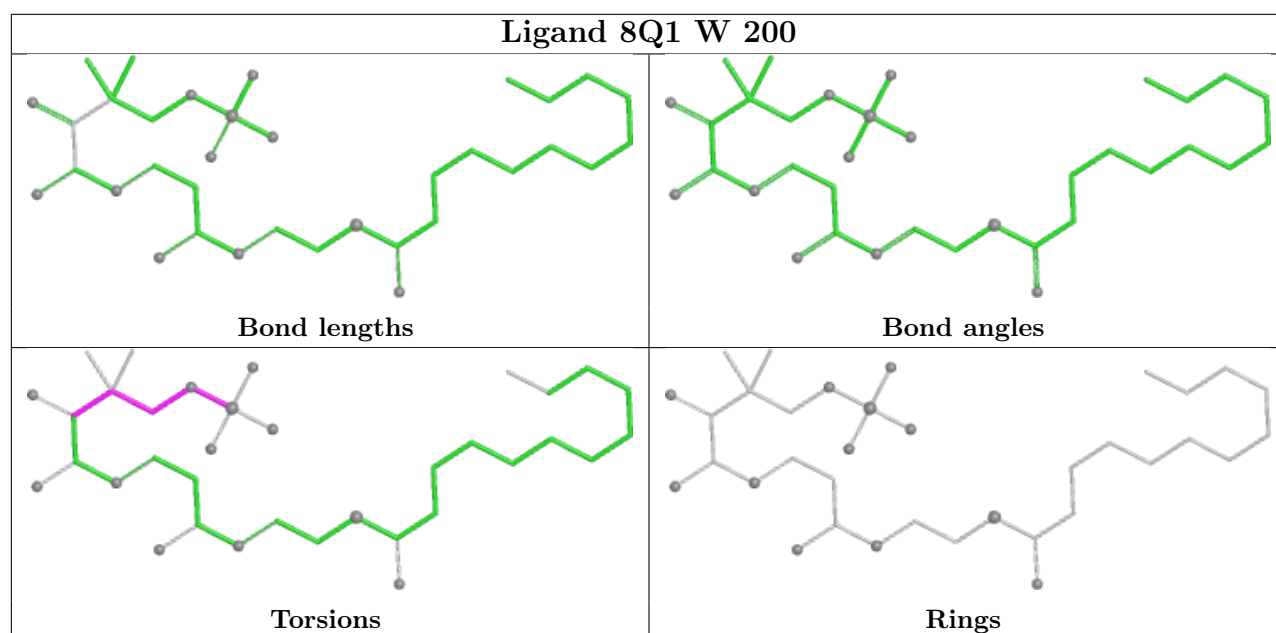


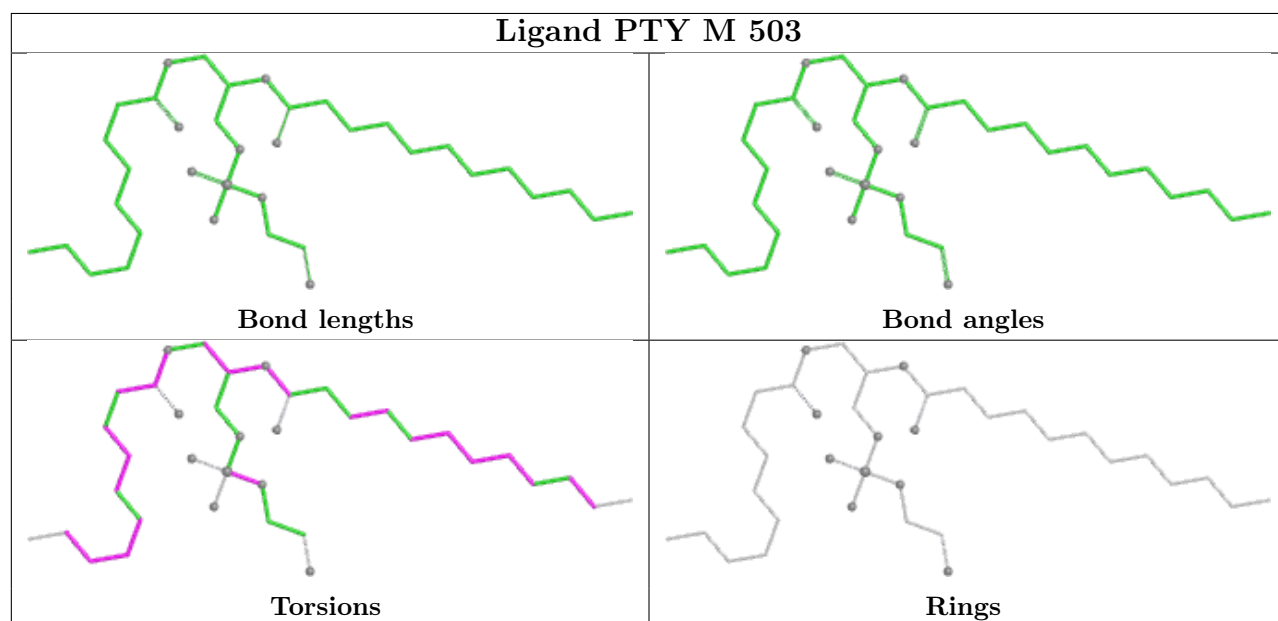
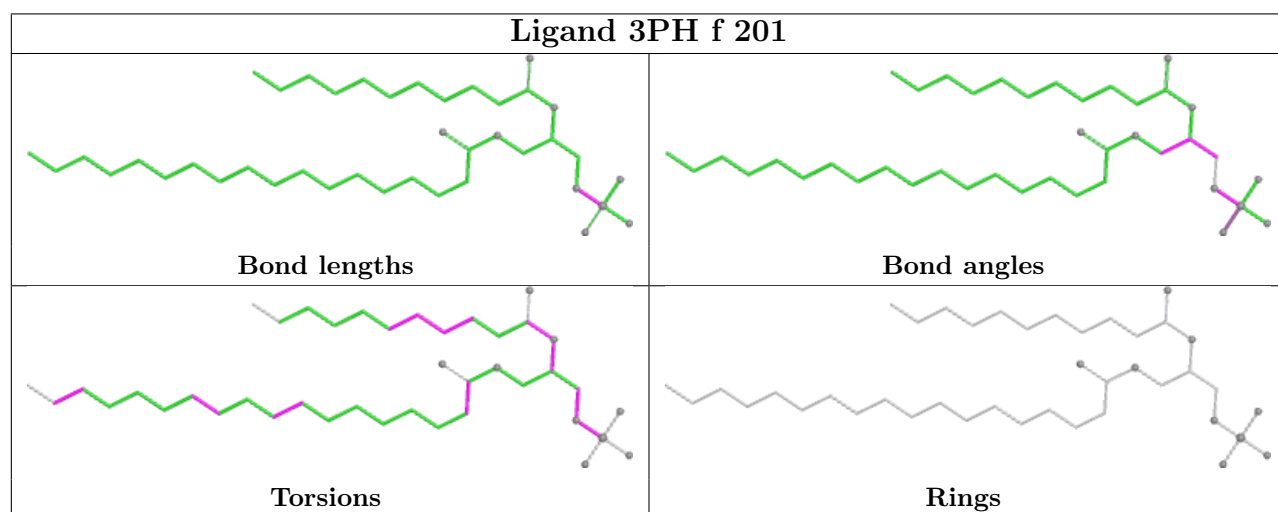
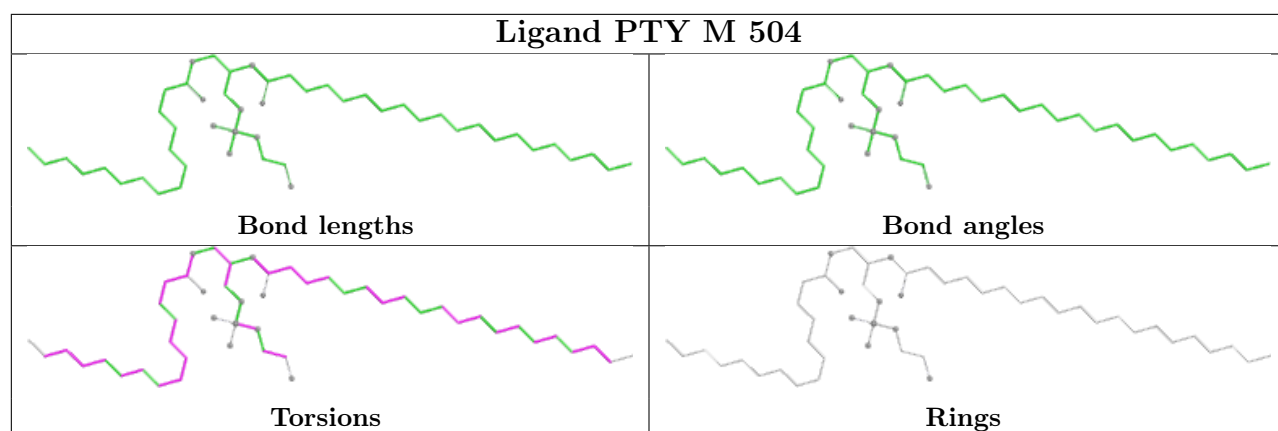


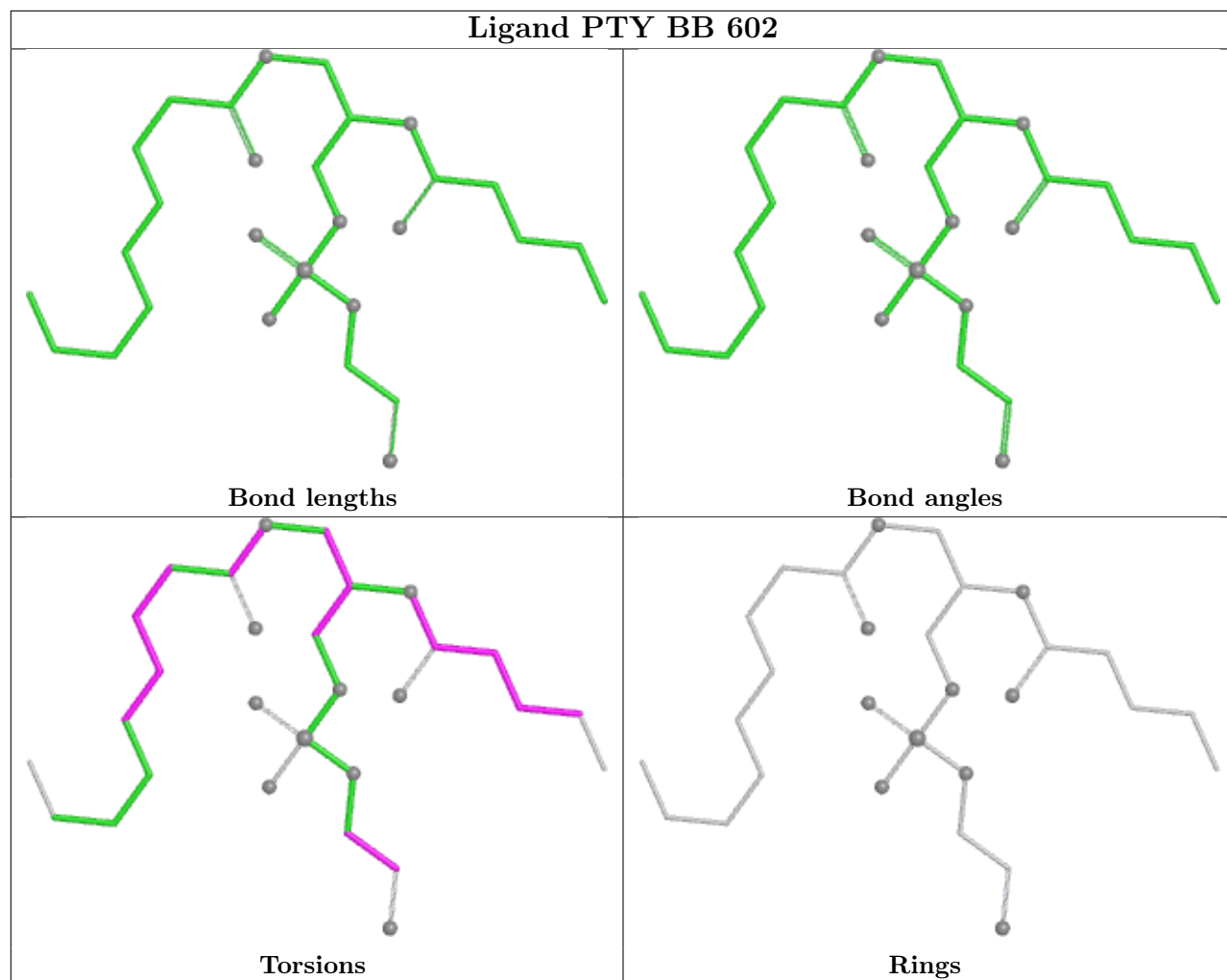


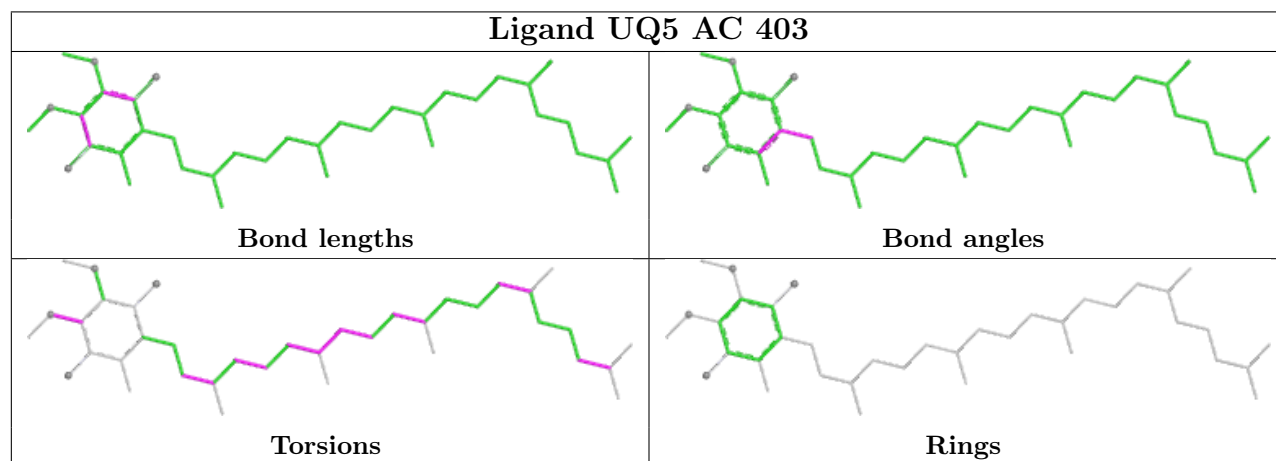
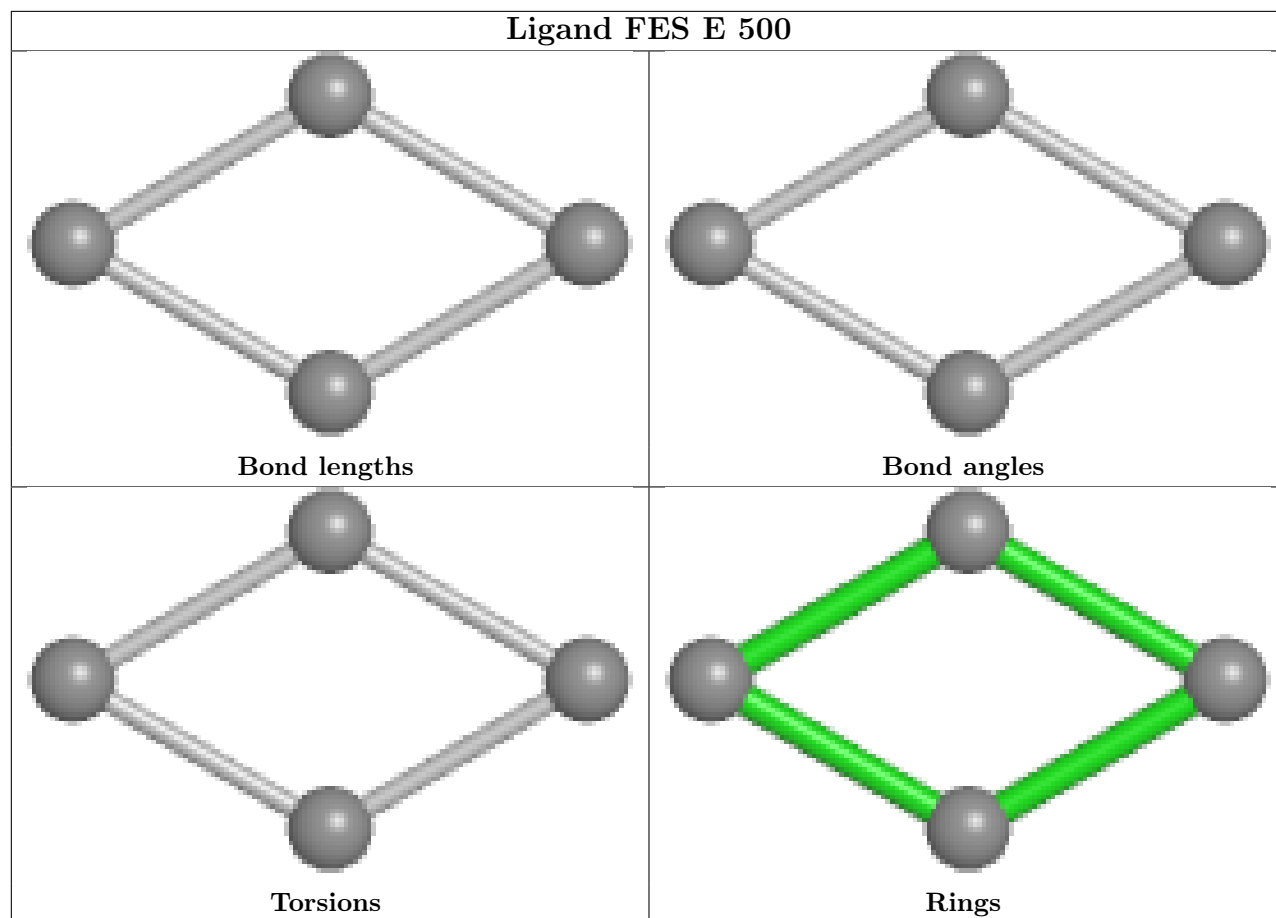


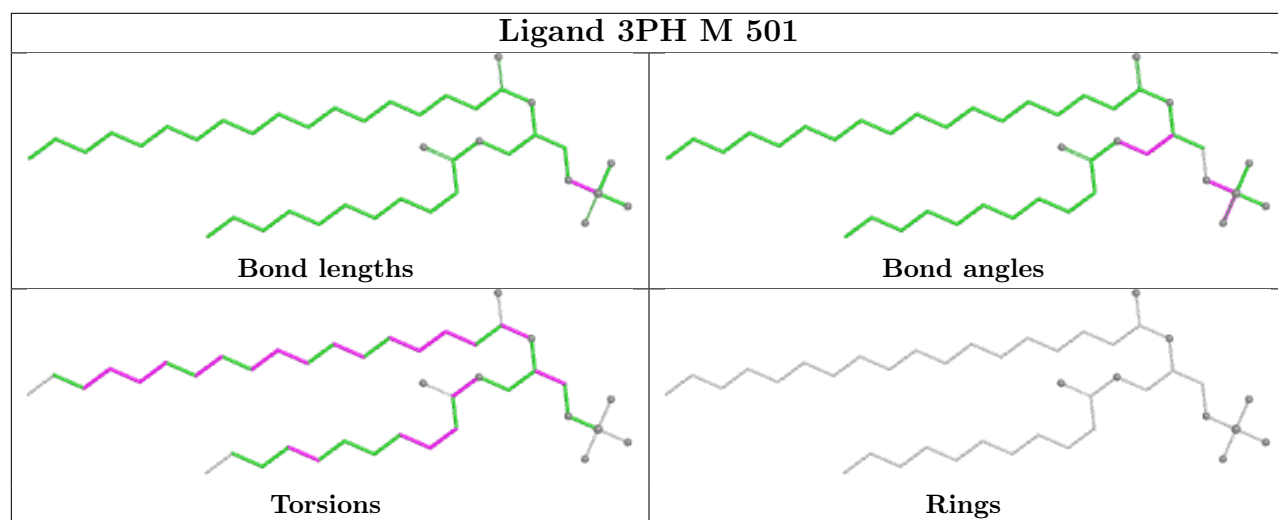
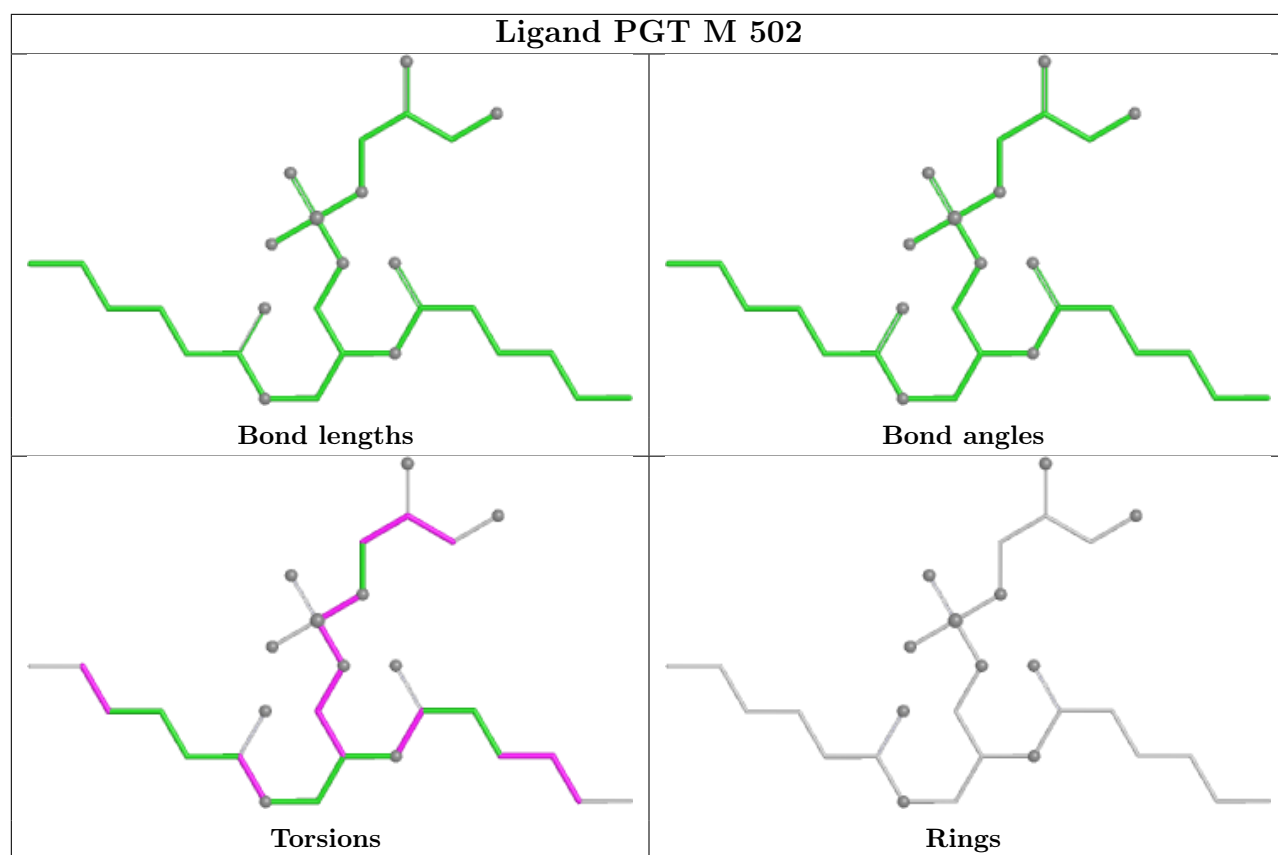




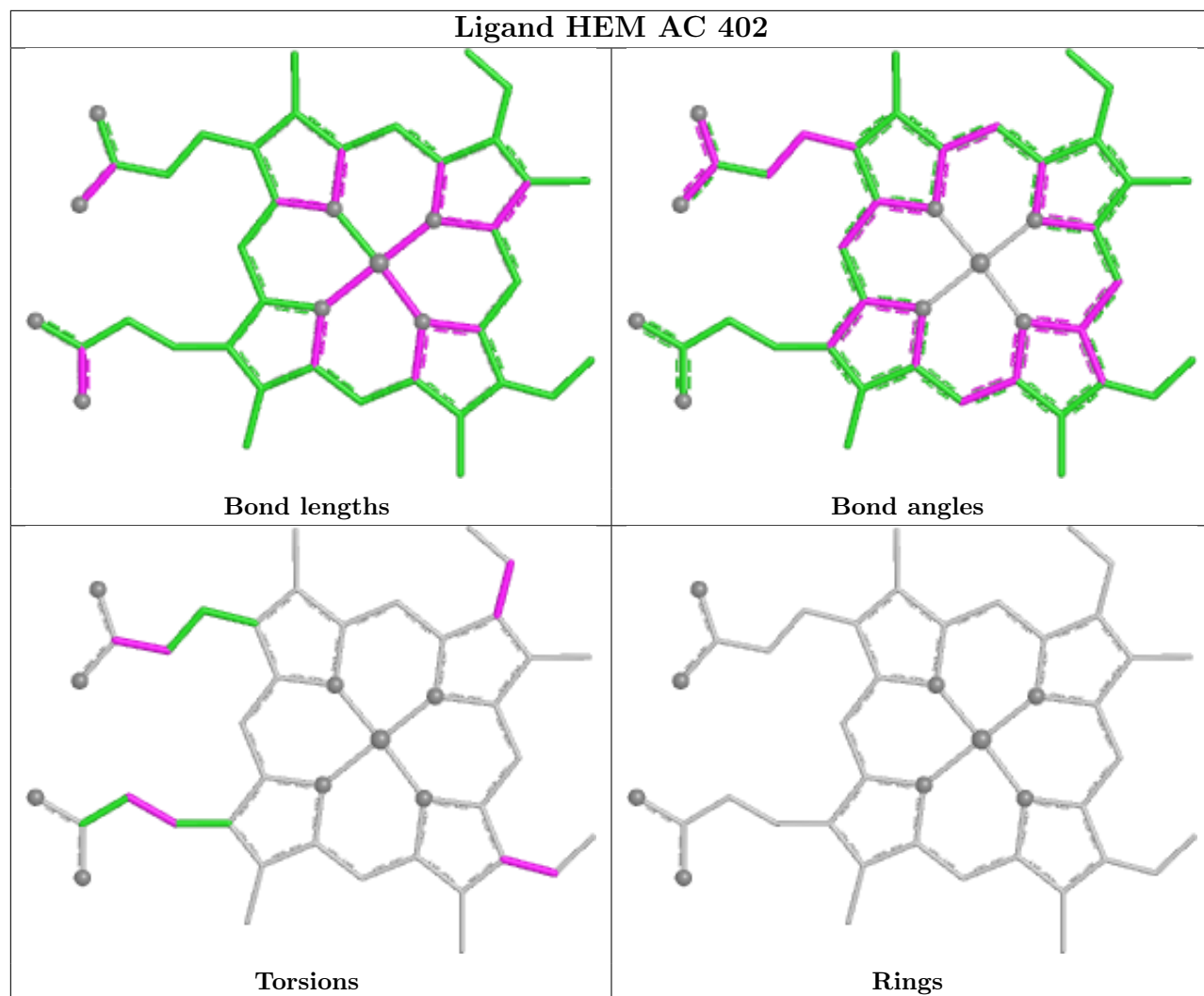


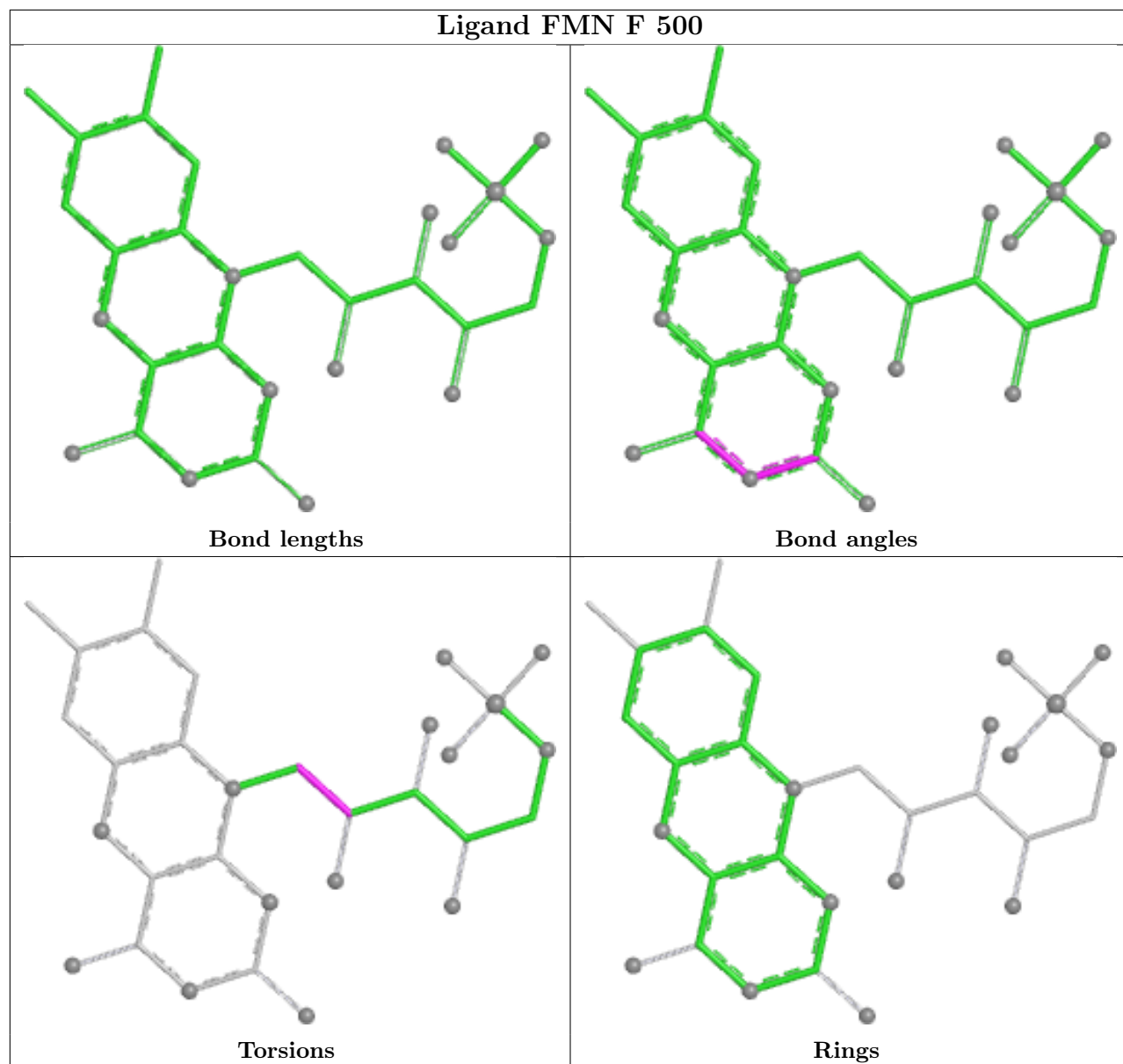


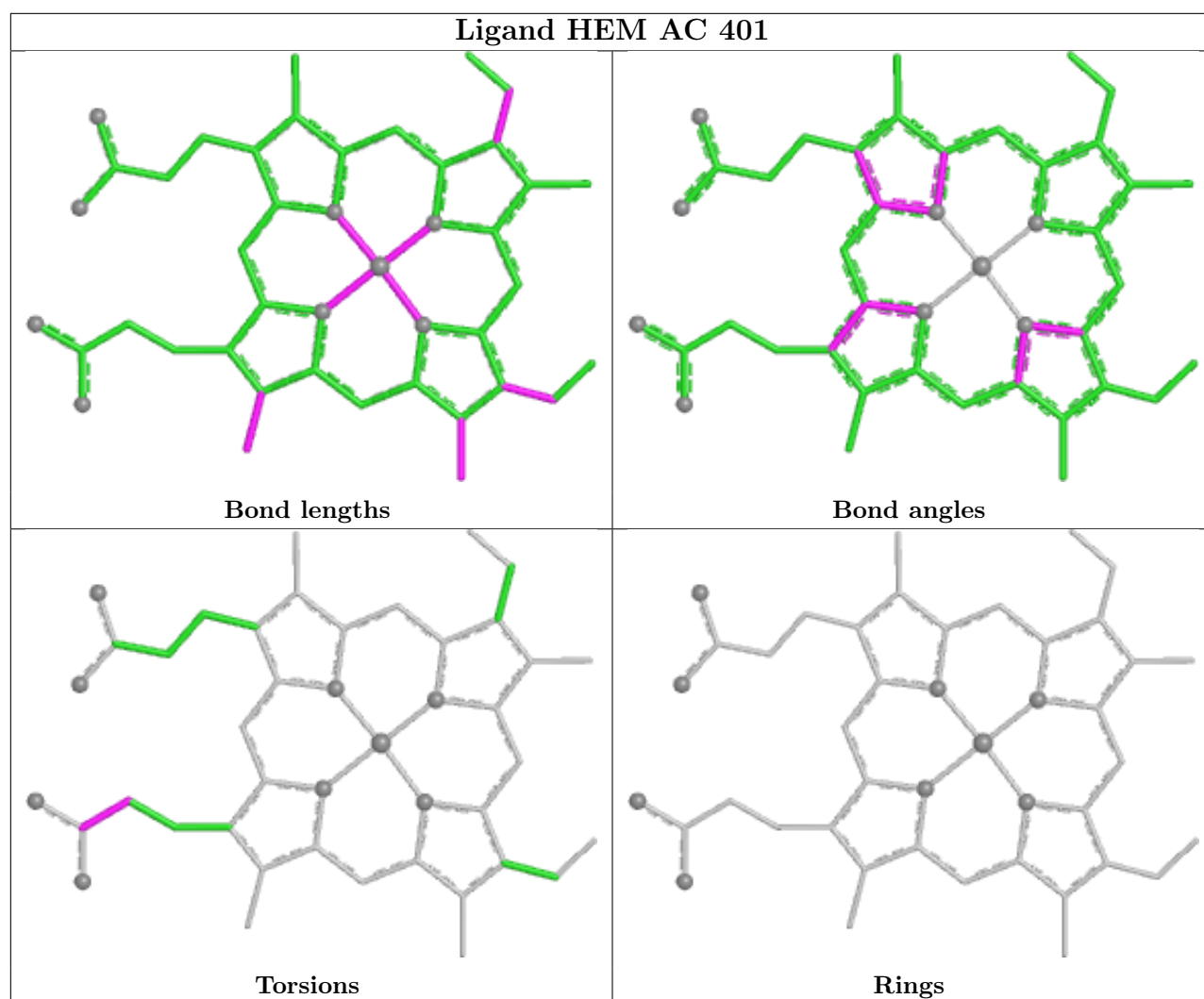
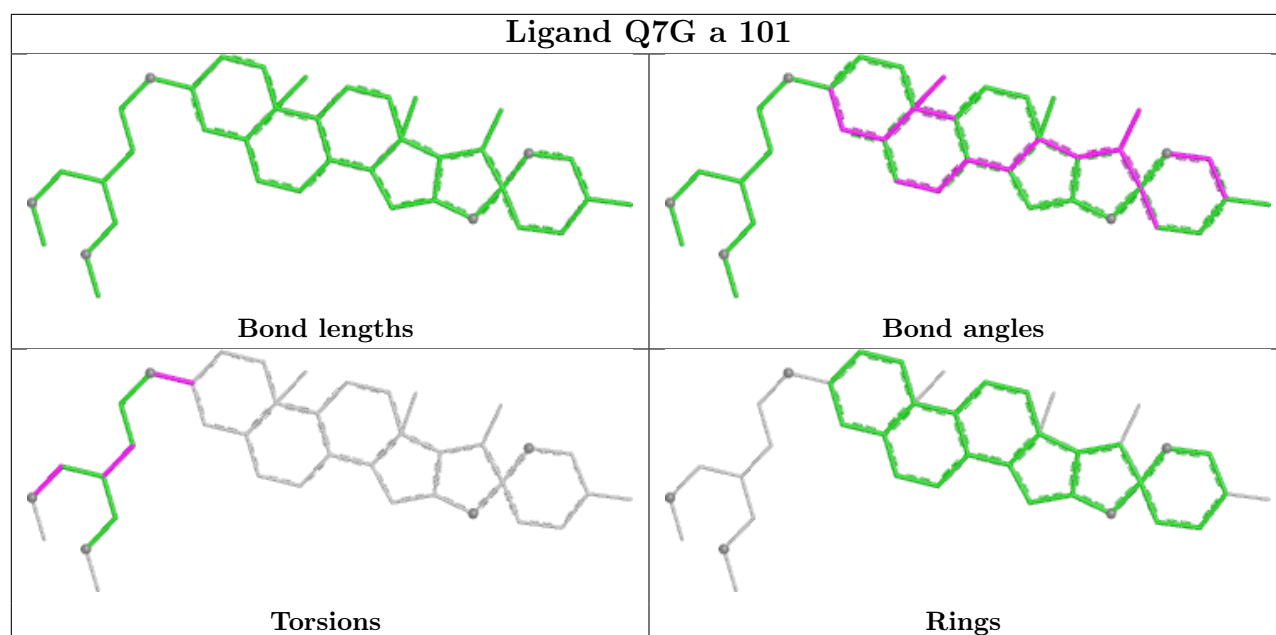


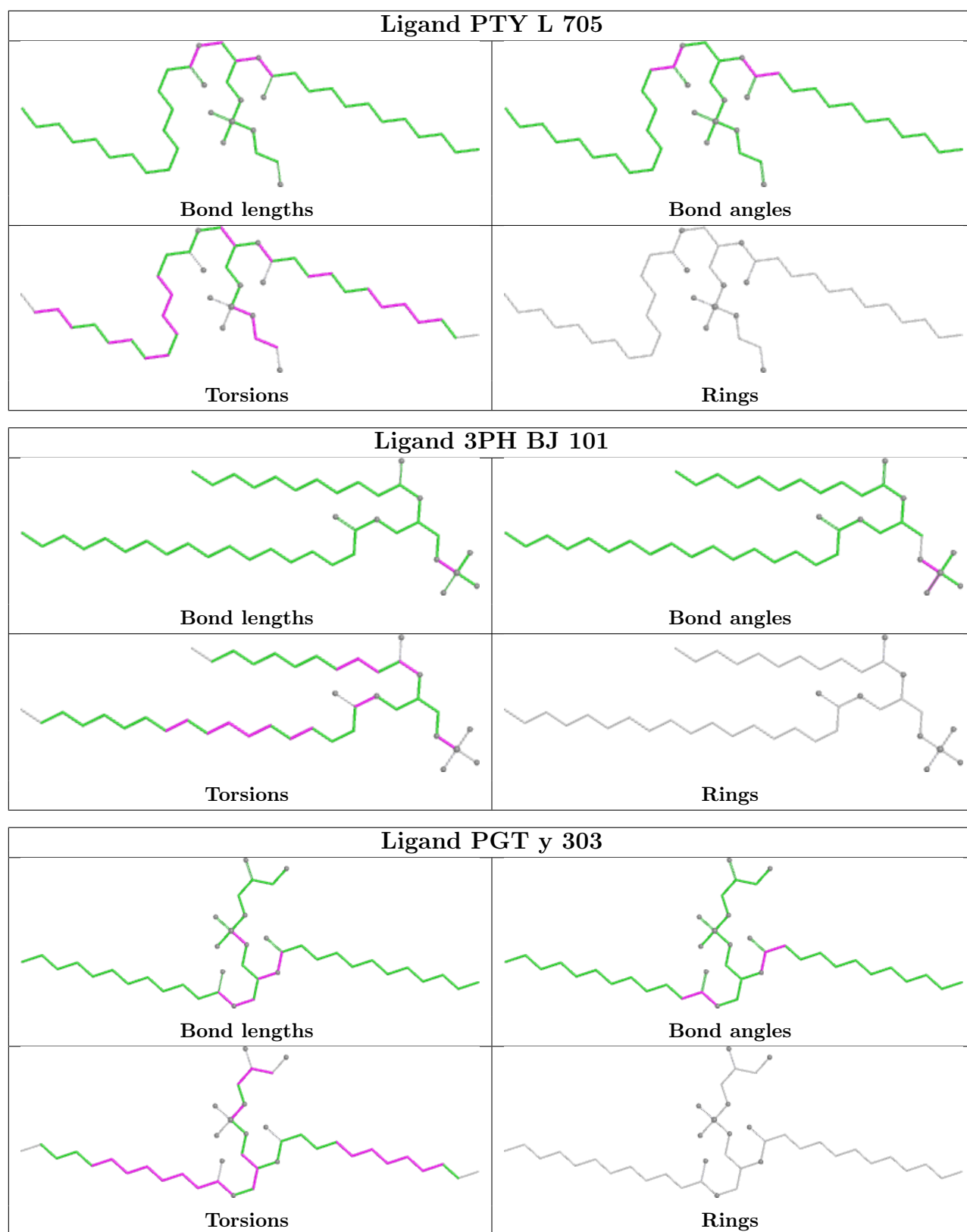


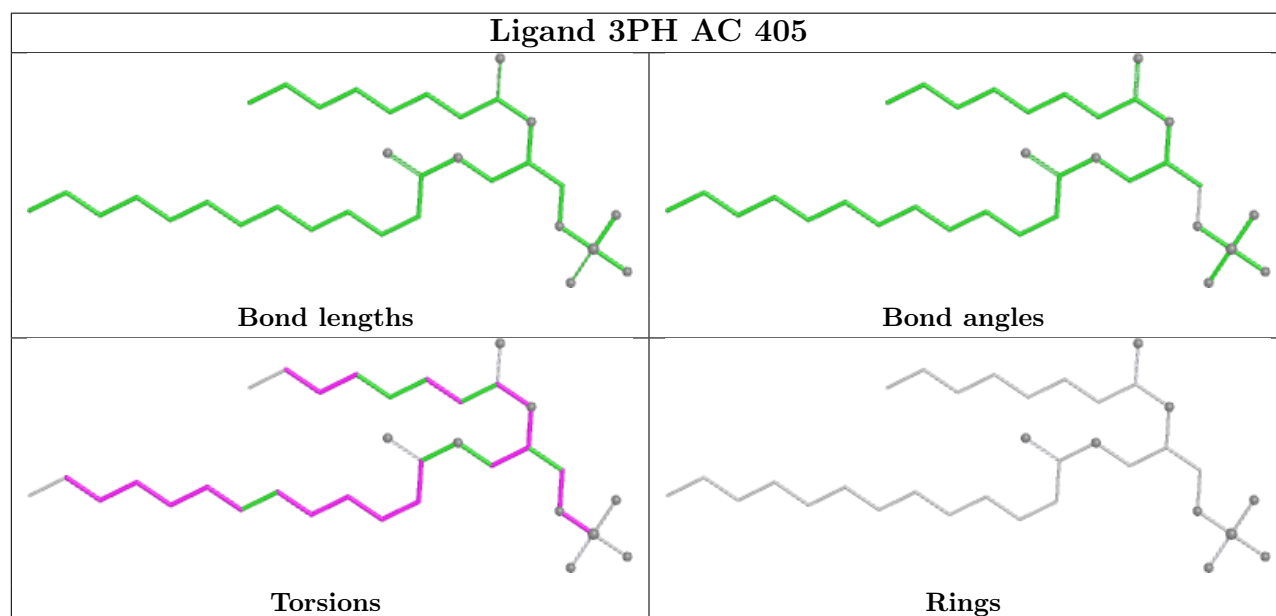
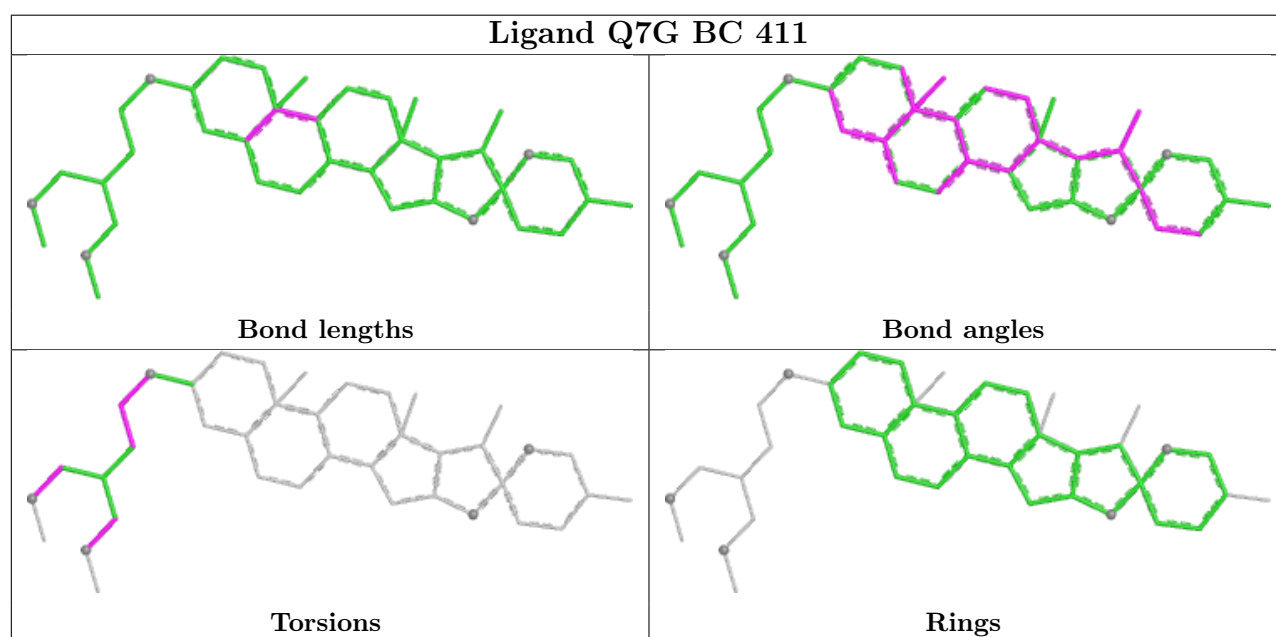
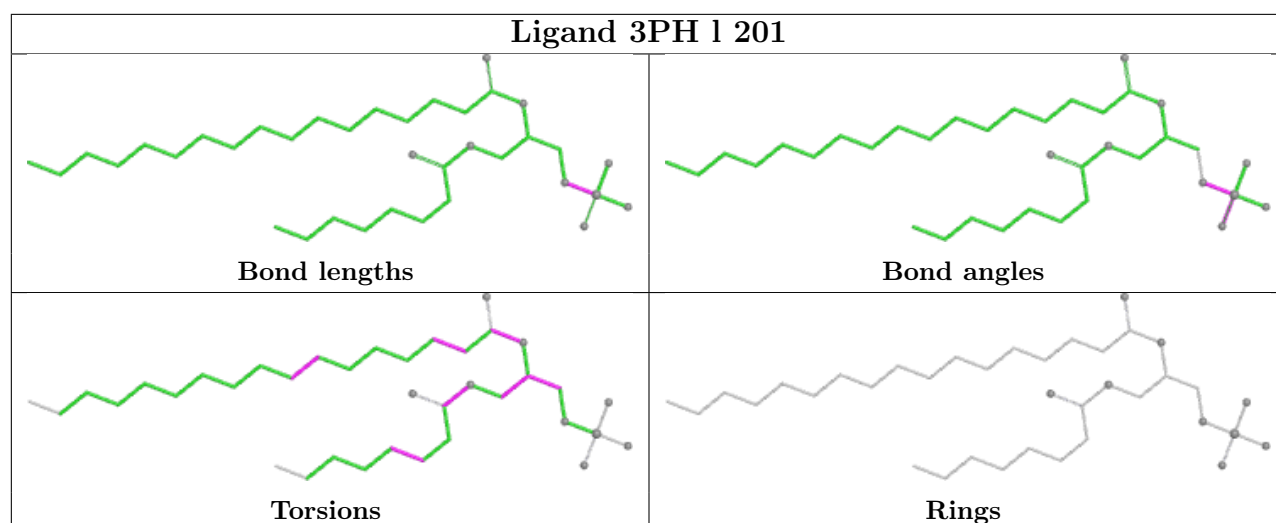
Ligand HEM AC 402

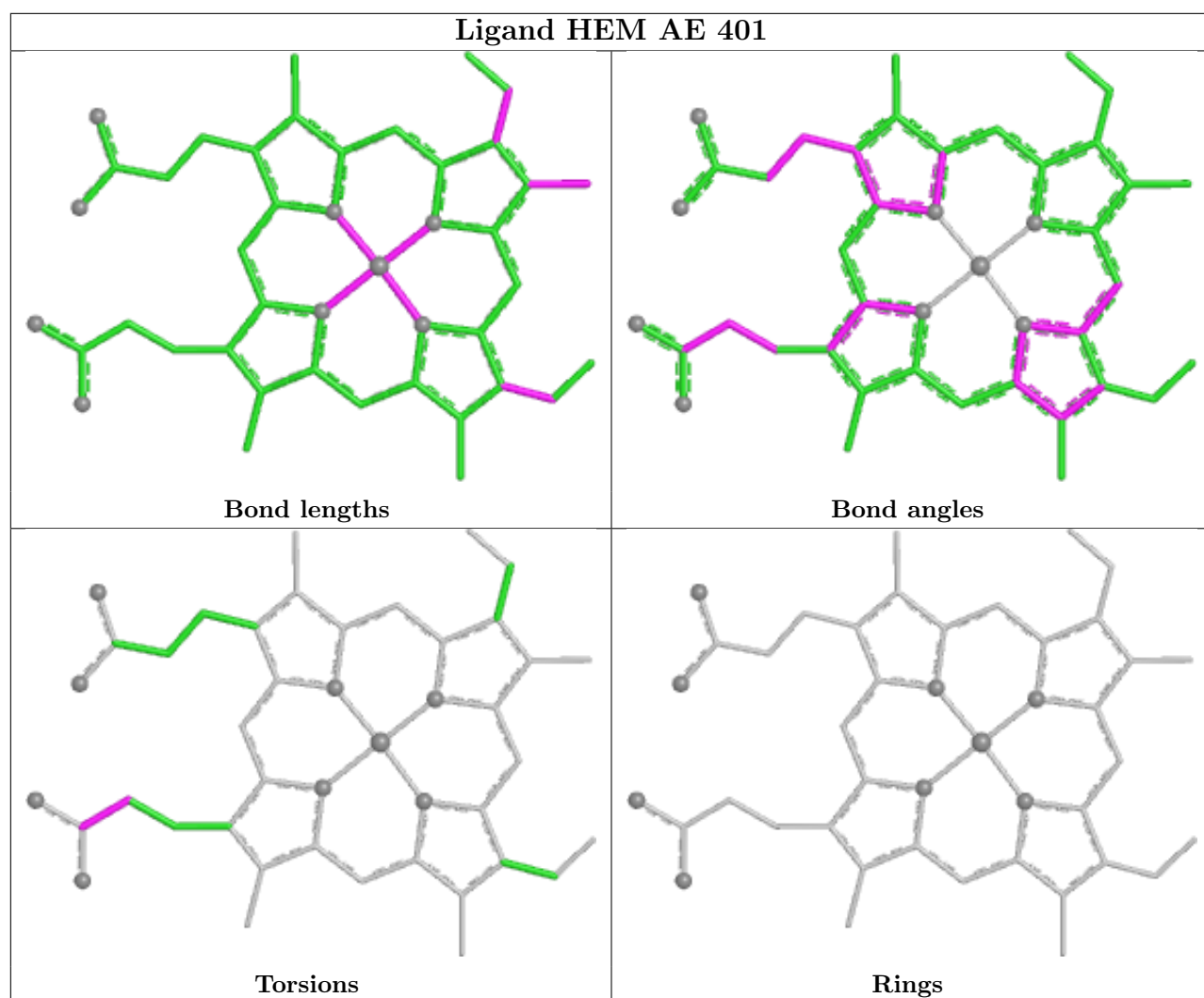
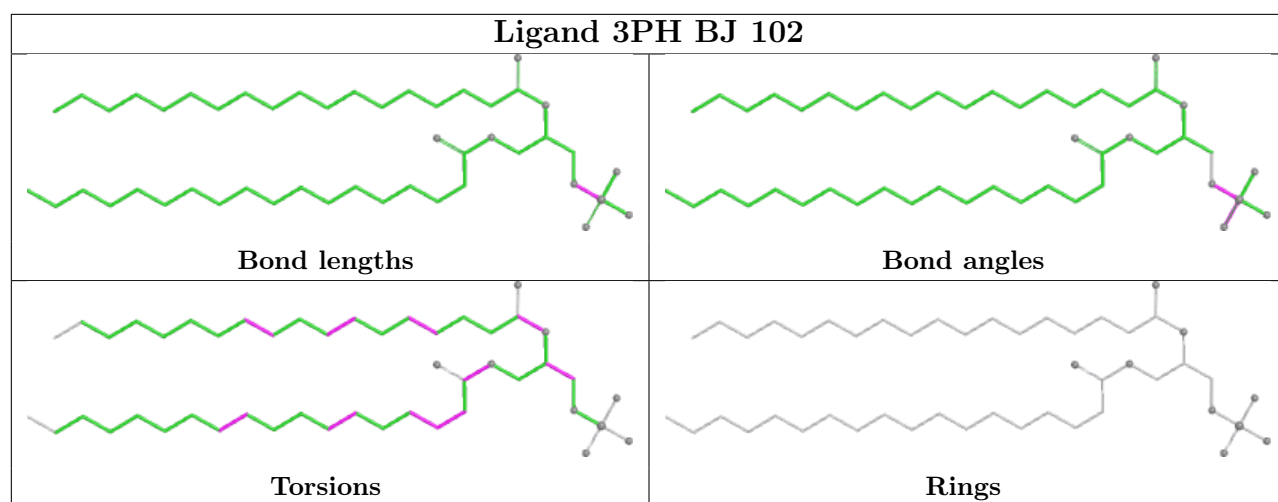


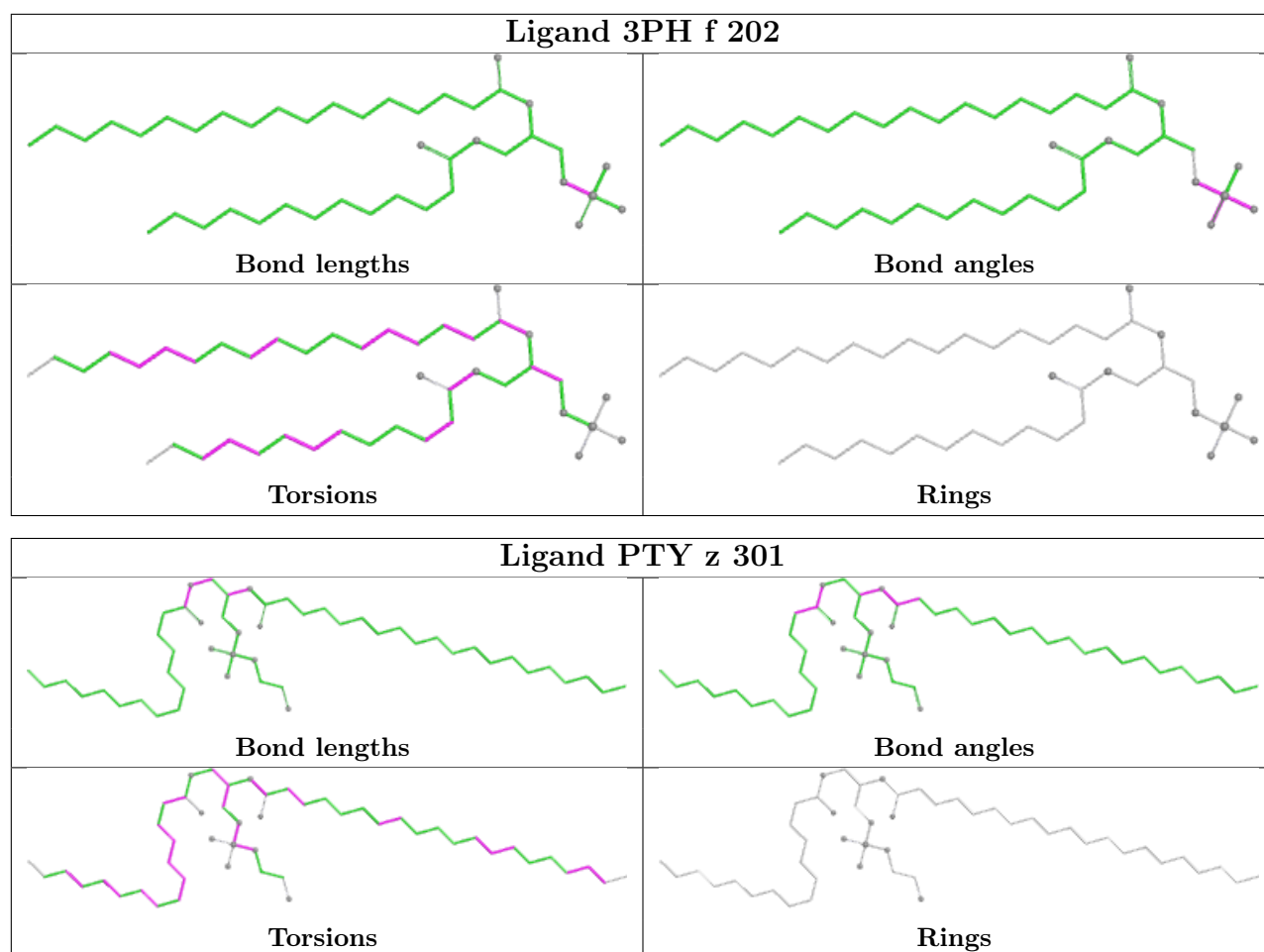












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

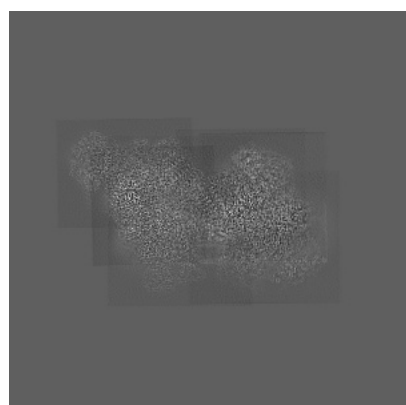
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16168. 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](#)

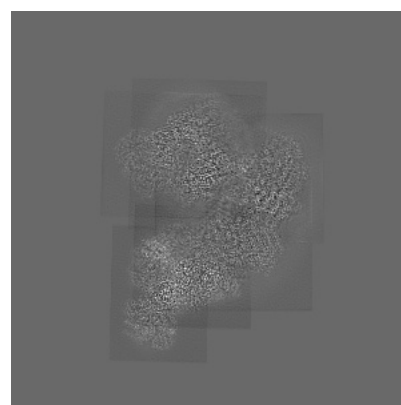
6.1.1 Primary map



X



Y

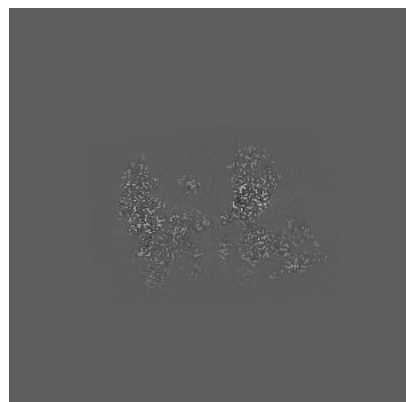


Z

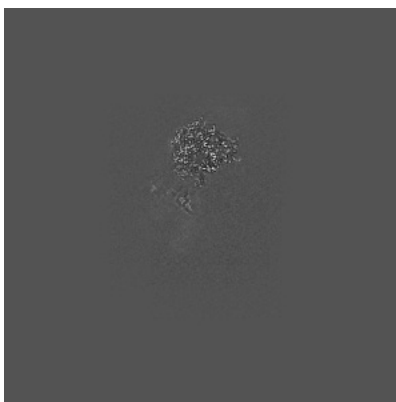
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

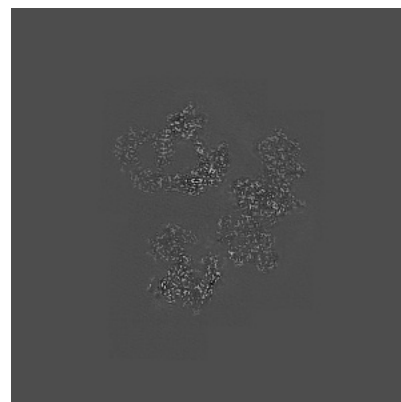
6.2.1 Primary map



X Index: 375



Y Index: 375



Z Index: 375

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

6.3 Largest variance slices [i](#)

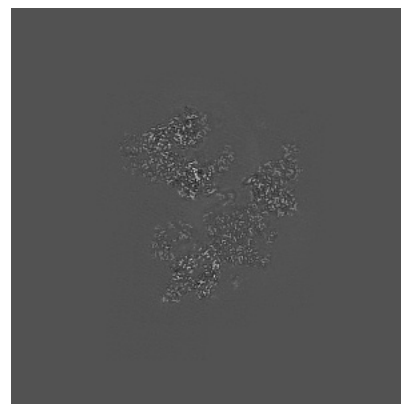
6.3.1 Primary map



X Index: 289



Y Index: 236

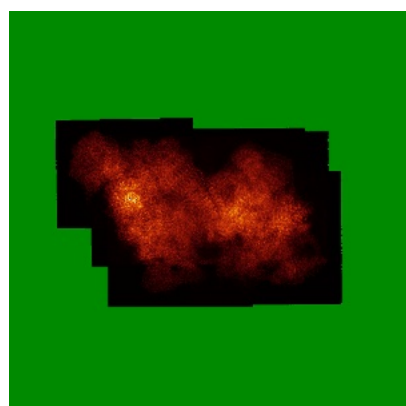


Z Index: 355

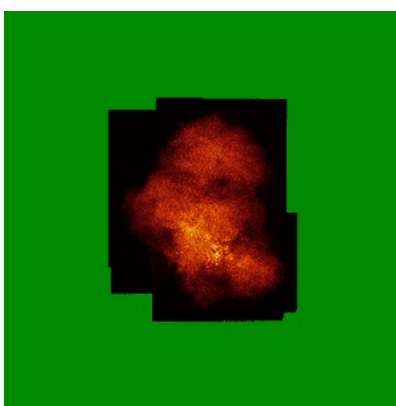
The images above show the largest variance slices of the map in three orthogonal directions.

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

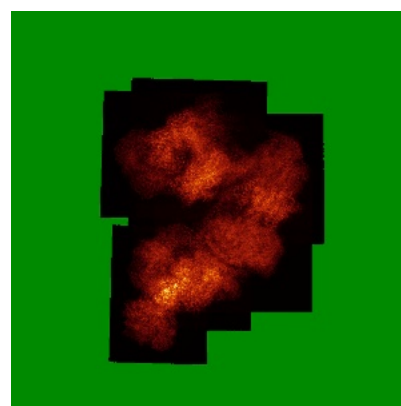
6.4.1 Primary map



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.

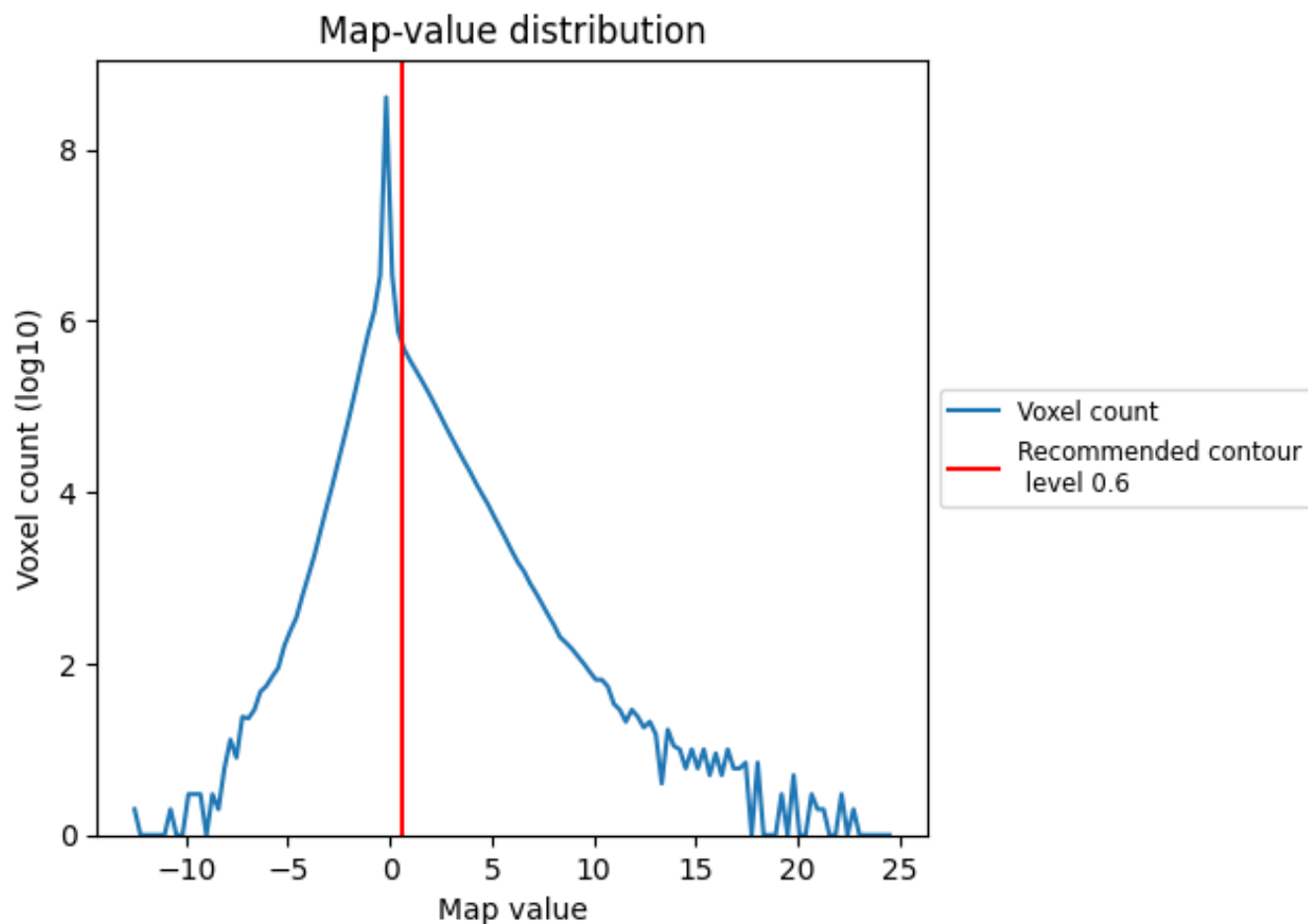
6.6 Mask visualisation

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

7 Map analysis [i](#)

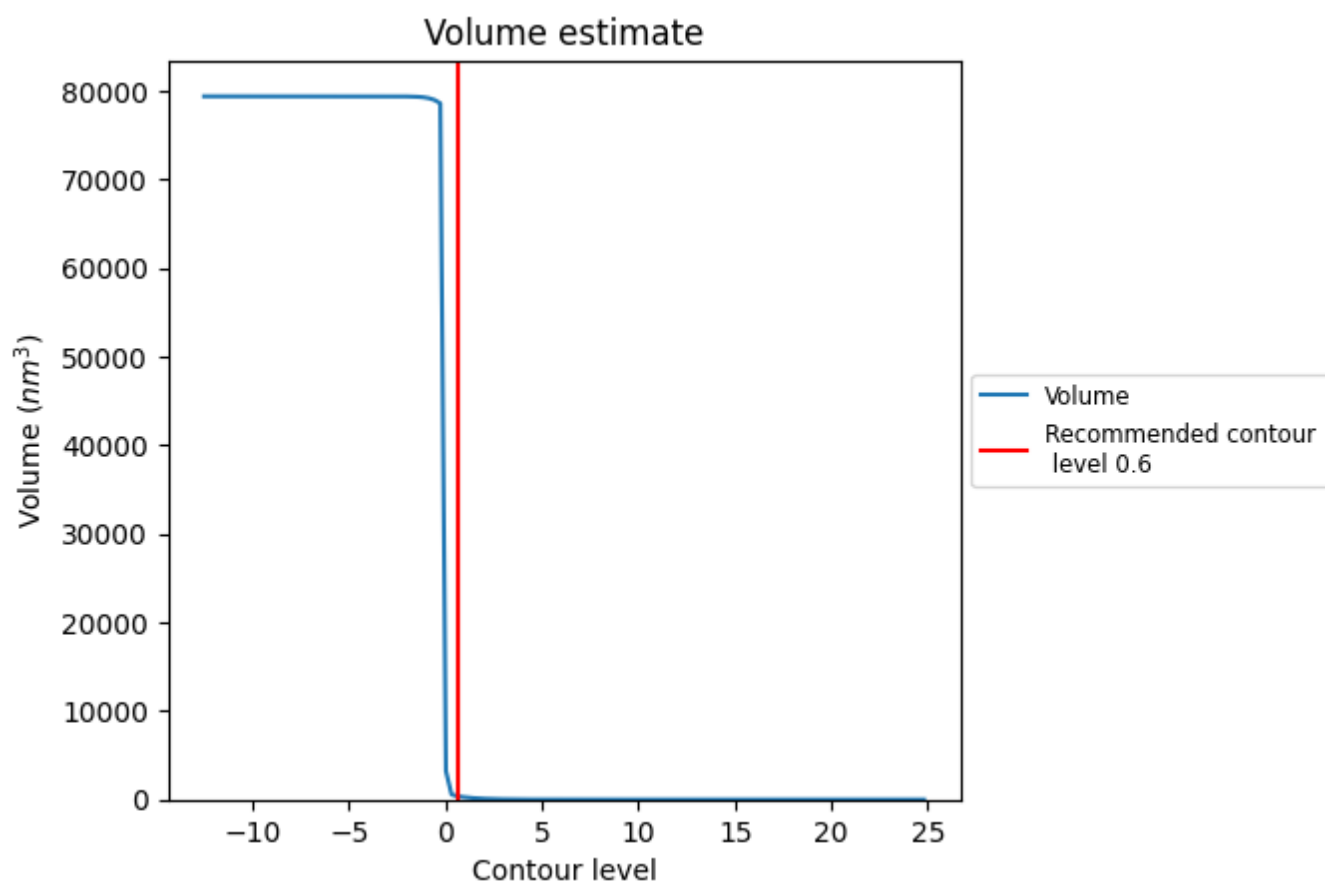
This section contains the results of statistical analysis of the map.

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.

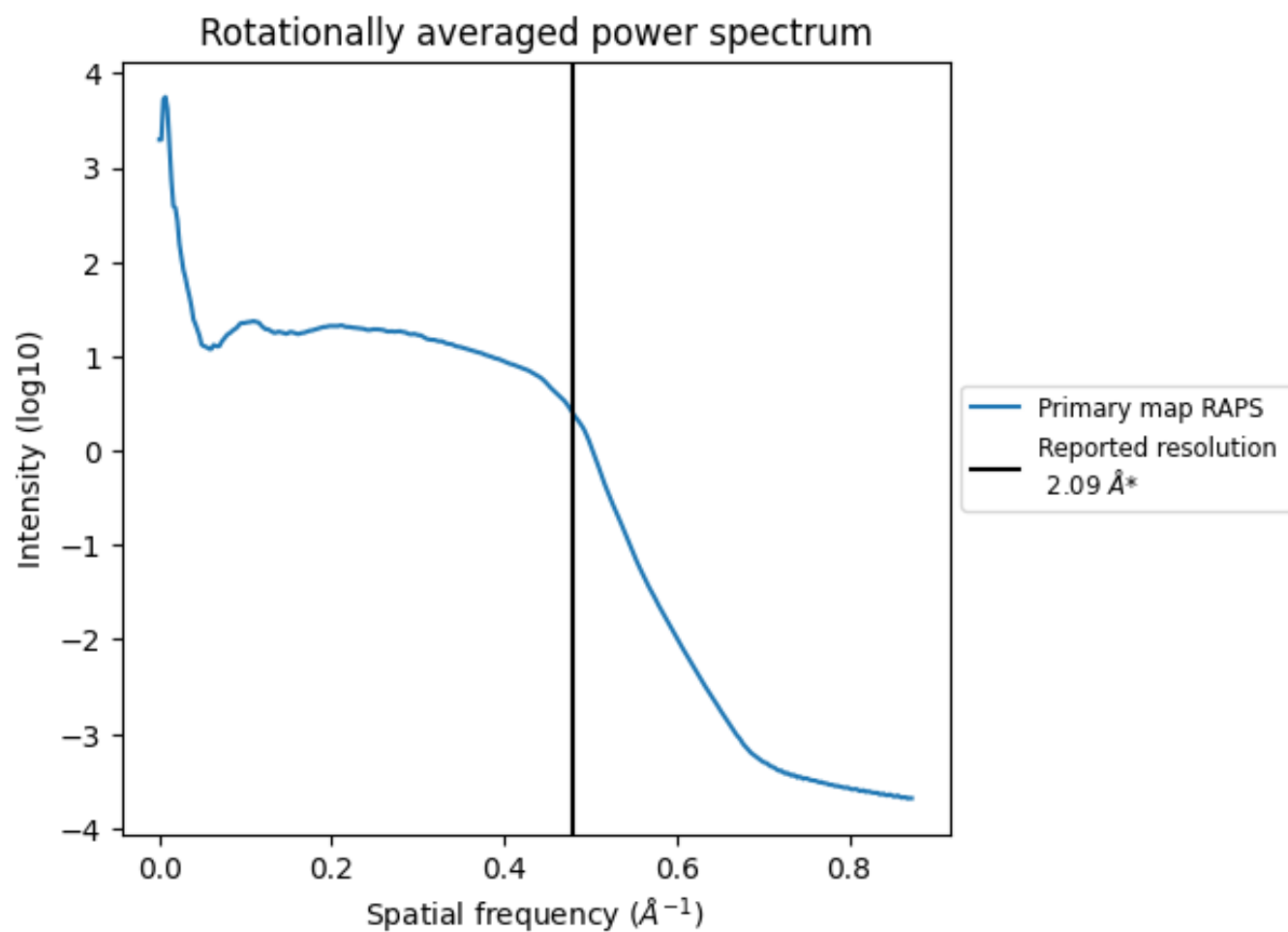
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 390 nm^3 ; this corresponds to an approximate mass of 352 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 ⓘ

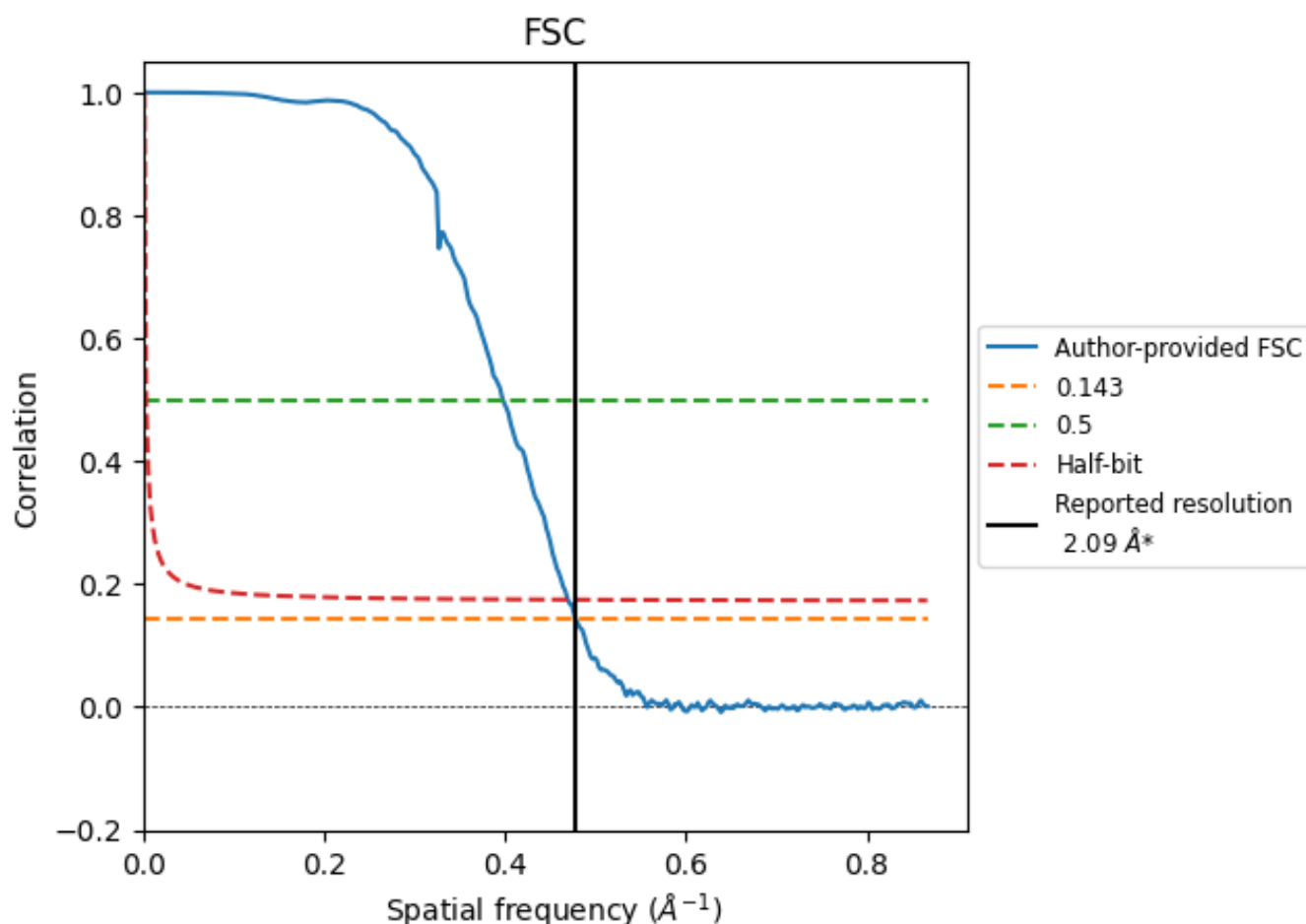


*Reported resolution corresponds to spatial frequency of 0.478 Å⁻¹

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 0.478 Å⁻¹

8.2 Resolution estimates [i](#)

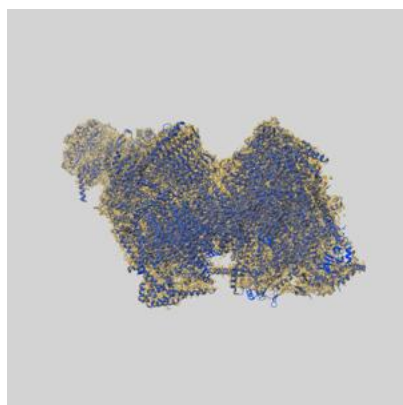
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.09	-	-
Author-provided FSC curve	2.09	2.51	2.13
Unmasked-calculated*	-	-	-

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

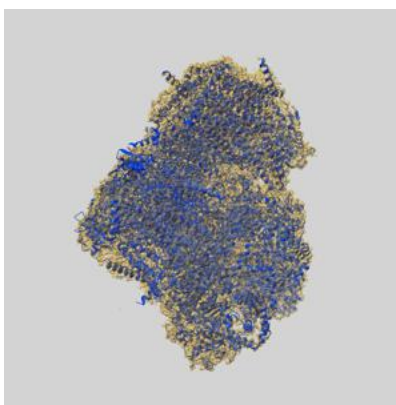
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-16168 and PDB model 8BPX. Per-residue inclusion information can be found in section 3 on page 33.

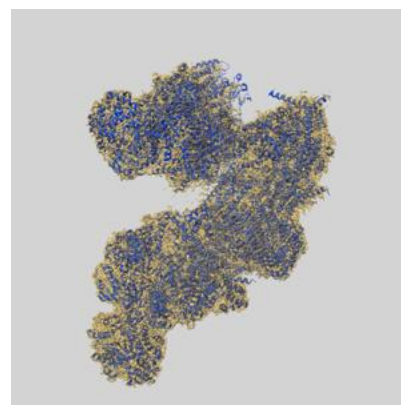
9.1 Map-model overlay [i](#)



X



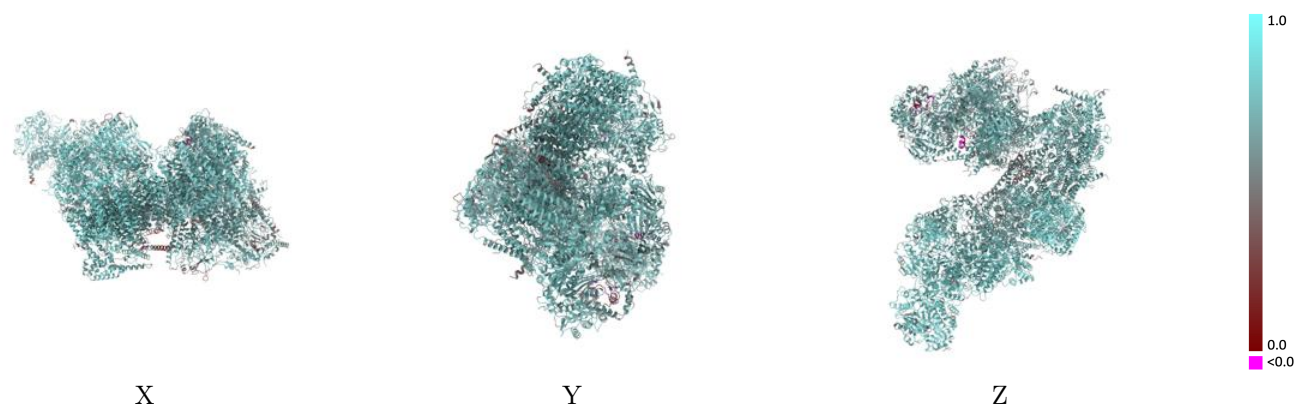
Y



Z

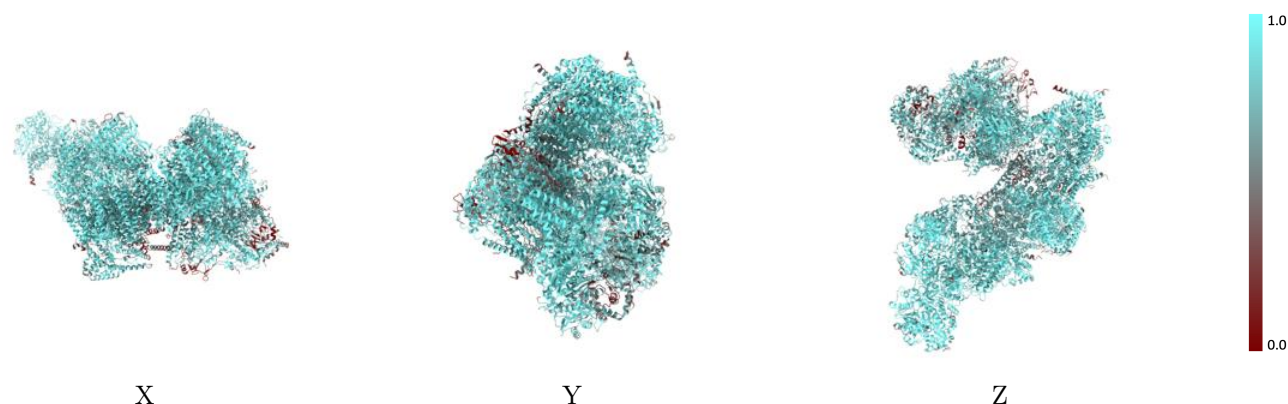
The images above show the 3D surface view of the map at the recommended contour level 0.6 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



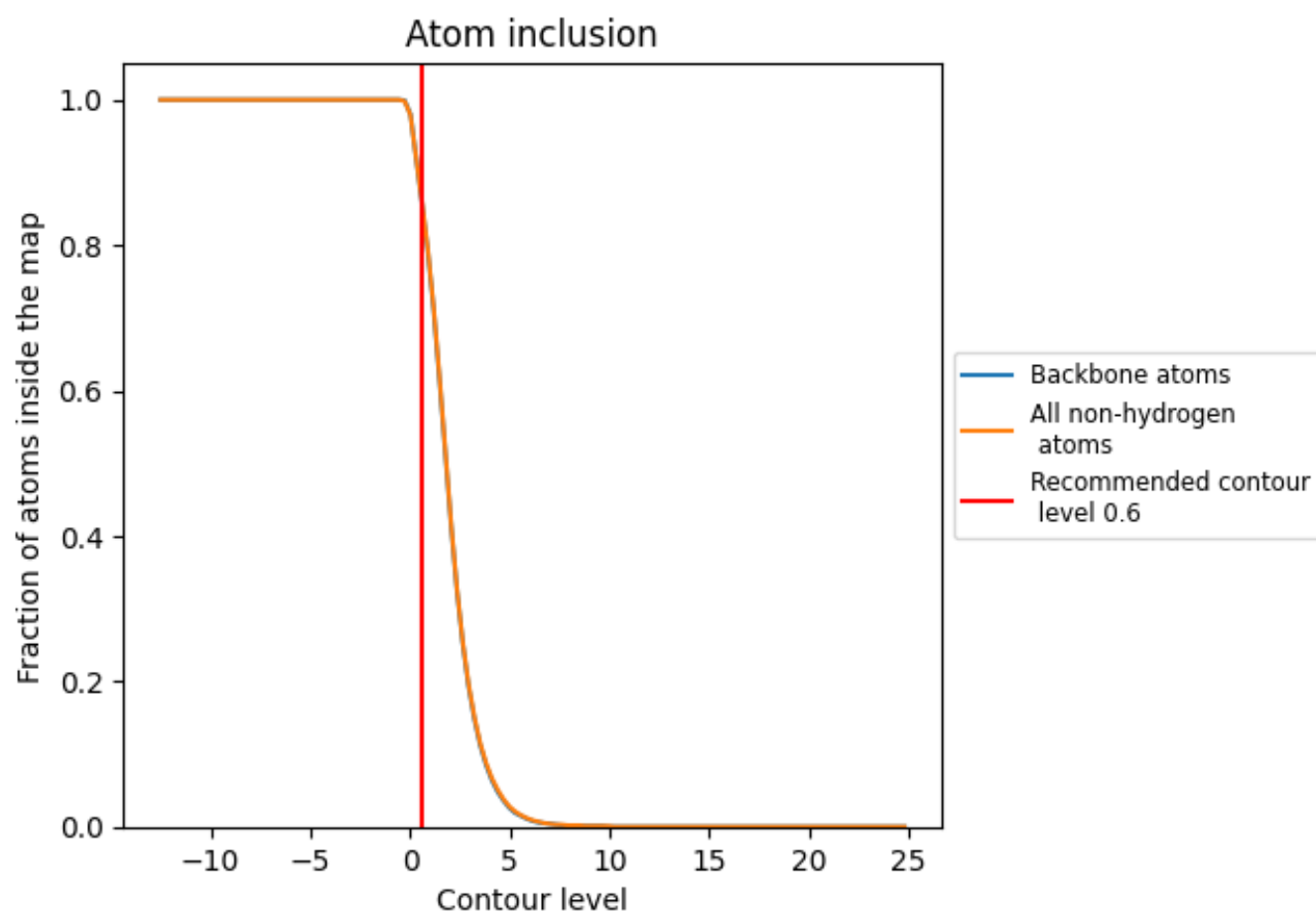
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.6).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 86% 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 (0.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8590	 0.7070
A	 0.9390	 0.7560
AA	 0.6670	 0.5930
AB	 0.8810	 0.7020
AC	 0.9060	 0.7190
AD	 0.5260	 0.5880
AE	 0.9120	 0.7220
AF	 0.9330	 0.7300
AG	 0.8570	 0.6890
AH	 0.7710	 0.6450
AI	 0.8330	 0.6880
AJ	 0.5700	 0.5930
B	 0.9790	 0.8060
BA	 0.6820	 0.6050
BB	 0.8730	 0.7010
BC	 0.8880	 0.7010
BD	 0.5720	 0.5910
BE	 0.8800	 0.6940
BF	 0.9170	 0.6960
BG	 0.7870	 0.6430
BH	 0.6090	 0.5780
BI	 0.7820	 0.6380
BJ	 0.5730	 0.5980
C	 0.9580	 0.7940
D	 0.9530	 0.7910
E	 0.8470	 0.6810
F	 0.9330	 0.7460
G	 0.9220	 0.7420
H	 0.9250	 0.7710
I	 0.9650	 0.7850
J	 0.9060	 0.7450
K	 0.9170	 0.7600
L	 0.9240	 0.7200
M	 0.9270	 0.7270
N	 0.9420	 0.7730



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Chain	Atom inclusion	Q-score
O	 0.9360	 0.7570
P	 0.8670	 0.6930
Q	 0.8190	 0.6700
R	 0.8840	 0.7270
S	 0.9100	 0.7020
T	 0.8290	 0.6560
U	 0.6240	 0.5640
V	 0.8690	 0.7290
W	 0.8390	 0.6900
X	 0.8100	 0.7000
Y	 0.5890	 0.5500
Z	 0.8420	 0.7090
a	 0.8430	 0.7150
b	 0.7520	 0.6610
c	 0.9220	 0.7100
d	 0.7720	 0.6850
e	 0.8670	 0.7180
f	 0.8850	 0.7520
g	 0.7840	 0.6390
i	 0.6430	 0.5780
j	 0.8420	 0.6610
k	 0.8080	 0.6400
l	 0.8100	 0.6520
m	 0.8630	 0.6840
n	 0.9130	 0.6840
o	 0.8270	 0.6810
p	 0.8610	 0.6780
q	 0.9190	 0.7380
u	 0.5850	 0.5480
v	 0.8830	 0.7440
x	 0.9600	 0.7990
y	 0.9120	 0.7580
z	 0.9050	 0.7460