



## Full wwPDB EM Validation Report ⓘ

Nov 11, 2025 – 08:00 PM JST

PDB ID : 8ZO8 / pdb\_00008zo8  
EMDB ID : EMD-60284  
Title : Respirasome open state 3 in presence of metformin (SC-MetO3)  
Authors : Teng, F.; He, Z.X.; Hu, Y.Q.; Xu, C.Y.; Guo, R.Y.; Zhou, L.  
Deposited on : 2024-05-28  
Resolution : 3.24 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev129  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
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) : 2.46

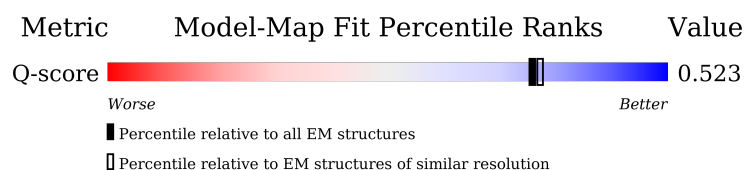
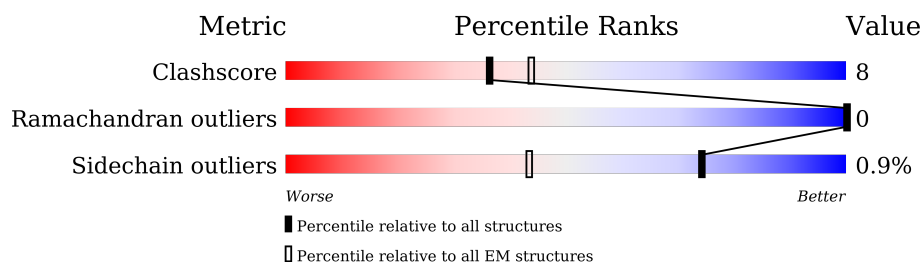
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.24 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	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	14594 ( 2.74 - 3.74 )

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  $\geq 3$ , 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	4L	98	 82% 18%
2	5A	102	 71% 29%
3	5B	95	 71% 29%
4	6A	75	 75% 25%







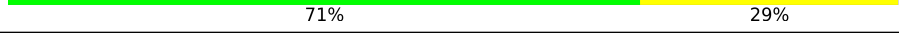
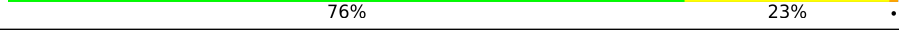
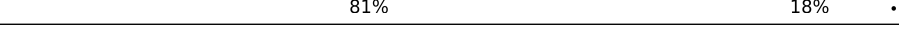
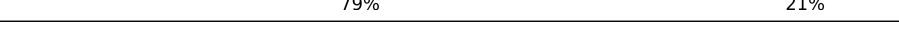
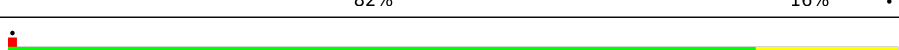

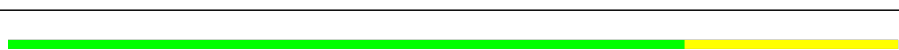

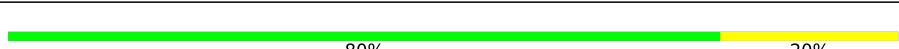





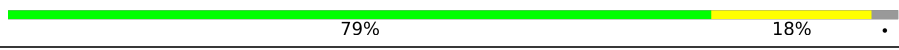
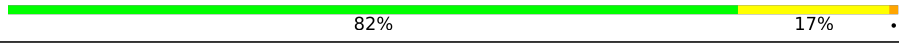



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Mol	Chain	Length	Quality of chain
5	6B	82	
6	6C	70	
7	7A	57	
8	7B	50	
9	7C	47	
10	8B	43	
11	A1	70	
12	A2	85	
13	A3	83	
14	A5	112	
15	A6	114	
16	A7	112	
17	A8	171	
18	A9	341	
19	AB	156	
19	AC	156	
20	AK	320	
21	AL	140	
22	AM	143	
23	AN	142	
24	B1	56	
25	B2	67	
26	B3	79	
27	B4	128	
28	B5	138	






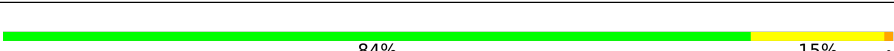
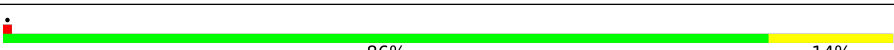

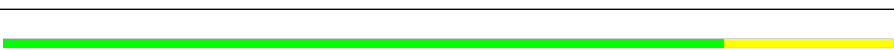

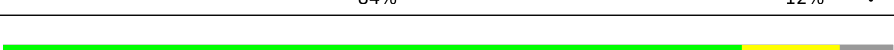
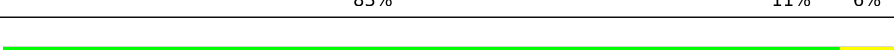
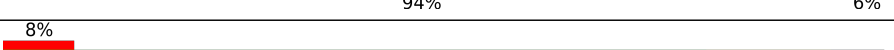
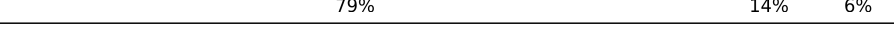
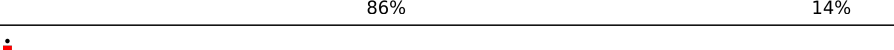
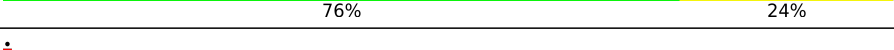





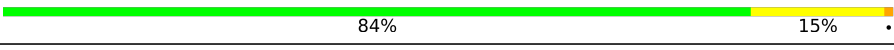
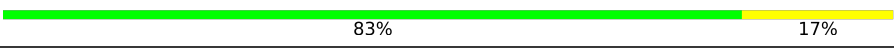


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Mol	Chain	Length	Quality of chain
29	B6	126	
30	B7	125	
31	B8	156	
32	B9	178	
33	BK	176	
34	BL	102	
35	C1	514	
36	C2	228	
37	C3	260	
38	C4	138	
39	CA	49	
40	CB	121	
41	N1	318	
42	N2	347	
43	N3	115	
44	N4	459	
45	N5	603	
46	N6	173	
47	QA	419	
47	Qa	419	
48	QB	446	
48	Qb	446	
49	QC	379	
49	Qc	379	
50	QD	241	

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Mol	Chain	Length	Quality of chain
50	Qd	241	
51	QE	196	
51	Qe	196	
52	QF	67	
52	Qf	67	
53	QG	101	
53	Qg	101	
54	QH	79	
54	Qh	79	
55	QI	64	
55	Qi	64	
56	QJ	49	
57	QK	78	
58	Qj	51	
59	S1	689	
60	S2	430	
61	S3	207	
62	S4	124	
63	S5	100	
64	S6	96	
65	S7	156	
66	S8	176	
67	V1	431	
68	V2	217	
69	V3	42	

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
85	FES	QE	304	-	-	X	-
86	SF4	S8	302	-	-	X	-

## 2 Entry composition

There are 87 unique types of molecules in this entry. The entry contains 116743 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 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	4L	98	Total	C	N	O	S	0	0
			748	493	113	128	14		

- Molecule 2 is a protein called Cytochrome c oxidase subunit 5A, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	5A	102	Total	C	N	O	S	0	0
			825	528	139	156	2		

- Molecule 3 is a protein called Cytochrome c oxidase subunit 5B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	5B	95	Total	C	N	O	S	0	0
			724	449	128	141	6		

- Molecule 4 is a protein called Cytochrome c oxidase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	6A	75	Total	C	N	O	S	0	0
			620	401	118	100	1		

- Molecule 5 is a protein called Cytochrome c oxidase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	6B	82	Total	C	N	O	S	0	0
			684	431	125	123	5		

- Molecule 6 is a protein called Cytochrome c oxidase subunit 6C.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6C	70	Total	C	N	O	S	0	0
			574	375	101	95	3		

- Molecule 7 is a protein called Cytochrome c oxidase subunit 7A1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	7A	57	Total	C	N	O	S	0	0
			447	287	76	81	3		

- Molecule 8 is a protein called Cytochrome c oxidase subunit 7B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7B	50	Total	C	N	O	S	0	0
			392	254	66	71	1		

- Molecule 9 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	7C	47	Total	C	N	O	S	0	0
			387	257	65	63	2		

- Molecule 10 is a protein called Cytochrome c oxidase subunit 8.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	8B	43	Total	C	N	O	0	0
			338	222	57	59		

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	A1	70	Total	C	N	O	S	0	0
			562	361	101	94	6		

- Molecule 12 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	A2	85	Total	C	N	O	S	0	0
			686	431	128	125	2		

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	A3	83	Total	C	N	O	S	0	0
			643	417	110	115	1		



- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	A5	112	Total	C	N	O	S	0	0
			910	588	154	165	3		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	A6	114	Total	C	N	O	S	0	0
			967	617	178	167	5		

- Molecule 16 is a protein called Complex I-B14.5a.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	A7	97	Total	C	N	O	S	0	0
			780	491	147	139	3		

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	A8	171	Total	C	N	O	S	0	0
			1398	887	250	251	10		

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	A9	337	Total	C	N	O	S	0	0
			2703	1750	472	472	9		

- Molecule 19 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AB	77	Total	C	N	O	S	0	0
			624	402	93	124	5		
19	AC	87	Total	C	N	O	S	0	0
			702	452	103	142	5		

- Molecule 20 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AK	320	Total	C	N	O	S	0	0
			2590	1649	440	491	10		

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AL	140	Total	C	N	O	S	0	0
			1021	651	174	190	6		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	AM	143	Total	C	N	O	S	0	0
			1195	764	216	211	4		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	AN	142	Total	C	N	O	S	0	0
			1173	755	203	206	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
24	B1	56	Total	C	N	O	S	0	0
			479	311	88	79	1		

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	B2	67	Total	C	N	O	S	0	0
			584	385	95	103	1		

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	B3	79	Total	C	N	O	S	0	0
			632	413	106	112	1		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	B4	128	Total	C	N	O	S	0	0
			1062	691	182	189			

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	B5	138	Total	C	N	O	S	0	0
			1151	754	195	199	3		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	B6	101	Total	C	N	O	S	0	0
			861	562	153	145	1		

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	B7	125	Total	C	N	O	S	0	0
			1068	663	204	190	11		

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	B8	156	Total	C	N	O	S	0	0
			1315	853	213	241	8		

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	B9	178	Total	C	N	O	S	0	0
			1534	982	279	265	8		

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	BK	174	Total	C	N	O	S	0	0
			1456	913	264	271	8		

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	BL	99	Total	C	N	O	S	0	0
			828	531	137	156	4		

- Molecule 35 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	C1	514	Total	C	N	O	S	0	0
			4024	2692	625	675	32		

- Molecule 36 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	C2	228	Total	C	N	O	S	0	0
			1833	1193	282	340	18		

- Molecule 37 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	C3	260	Total	C	N	O	S	0	0
			2103	1403	337	353	10		

- Molecule 38 is a protein called Cytochrome c oxidase subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	C4	138	Total	C	N	O	S	0	0
			1153	751	188	210	4		

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	CA	49	Total	C	N	O	0	0
			417	276	71	70		

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	CB	121	Total	C	N	O	S	0	0
			1000	650	173	171	6		

- Molecule 41 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	N1	311	Total	C	N	O	S	0	0
			2457	1644	377	415	21		

- Molecule 42 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	N2	347	Total	C	N	O	S	0	0
			2710	1782	420	462	46		

- Molecule 43 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	N3	98	Total	C	N	O	S	0	0
			786	535	114	132	5		

- Molecule 44 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	N4	459	Total	C	N	O	S	0	0
			3631	2412	572	609	38		

- Molecule 45 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	N5	603	Total	C	N	O	S	0	0
			4785	3173	741	820	51		

- Molecule 46 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	N6	163	Total	C	N	O	S	0	0
			1236	831	177	217	11		

- Molecule 47 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	QA	419	Total	C	N	O	S	0	0
			3147	1971	557	611	8		
47	Qa	419	Total	C	N	O	S	0	0
			3147	1971	557	611	8		

- Molecule 48 is a protein called Cytochrome b-c1 complex subunit 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	QB	446	Total	C	N	O	S	0	0
			3459	2161	605	674	19		
48	Qb	433	Total	C	N	O	S	0	0
			3367	2103	592	653	19		

- Molecule 49 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	QC	379	Total	C	N	O	S	0	0
			3025	2031	471	502	21		
49	Qc	379	Total	C	N	O	S	0	0
			3025	2031	471	502	21		

- Molecule 50 is a protein called Cytochrome c domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	QD	241	Total	C	N	O	S	0	0
			1921	1225	330	350	16		
50	Qd	239	Total	C	N	O	S	0	0
			1904	1215	327	346	16		

- Molecule 51 is a protein called Rieske domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	QE	196	Total	C	N	O	S	0	0
			1517	955	265	290	7		
51	Qe	196	Total	C	N	O	S	0	0
			1517	955	265	290	7		

- Molecule 52 is a protein called Cytochrome b-c1 complex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	QF	67	Total	C	N	O	S	0	0
			552	336	100	111	5		
52	Qf	64	Total	C	N	O	S	0	0
			528	320	97	106	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
53	QG	101	Total	C	N	O	S	0	0
			893	572	157	162	2		
53	Qg	101	Total	C	N	O	S	0	0
			893	572	157	162	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
54	QH	78	Total	C	N	O	S	0	0
			662	432	121	107	2		
54	Qh	79	Total	C	N	O	S	0	0
			666	434	122	108	2		

- Molecule 55 is a protein called Ubiquinol-cytochrome c reductase complex.

Mol	Chain	Residues	Atoms				AltConf	Trace
55	QI	62	Total	C	N	O	0	0
			507	331	90	86		
55	Qi	60	Total	C	N	O	0	0
			493	322	87	84		

- Molecule 56 is a protein called Cytochrome b-c1 complex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	QJ	49	Total	C	N	O	S	0	0
			405	269	71	63	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
57	QK	73	Total	C	N	O	S	0	0
			520	328	98	92	2		

- Molecule 58 is a protein called Cytochrome b-c1 complex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	Qj	51	Total	C	N	O	S	0	0
			421	281	74	65	1		

- Molecule 59 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	S1	689	Total	C	N	O	S	0	0
			5290	3317	922	1012	39		

- Molecule 60 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	S2	421	Total	C	N	O	S	0	0
			3391	2169	580	618	24		

- Molecule 61 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	S3	207	Total	C	N	O	S	0	0
			1729	1119	297	311	2		

- Molecule 62 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	S4	124	Total	C	N	O	S	0	0
			1007	637	179	188	3		

- Molecule 63 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	S5	100	Total	C	N	O	S	0	0
			825	525	153	141	6		

- Molecule 64 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.



Mol	Chain	Residues	Atoms					AltConf	Trace
64	S6	96	Total	C	N	O	S	0	0
			741	452	140	146	3		

- Molecule 65 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	S7	156	Total	C	N	O	S	0	0
			1248	794	227	213	14		

- Molecule 66 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	S8	176	Total	C	N	O	S	0	0
			1412	887	243	269	13		

- Molecule 67 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	V1	431	Total	C	N	O	S	0	0
			3316	2092	592	612	20		

- Molecule 68 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	V2	217	Total	C	N	O	S	0	0
			1671	1065	281	315	10		

- Molecule 69 is a protein called NADH:ubiquinone oxidoreductase subunit V3.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	V3	42	Total	C	N	O	S	0	0
			355	219	67	68	1		

- Molecule 70 is ZINC ION (CCD ID: ZN) (formula: Zn).

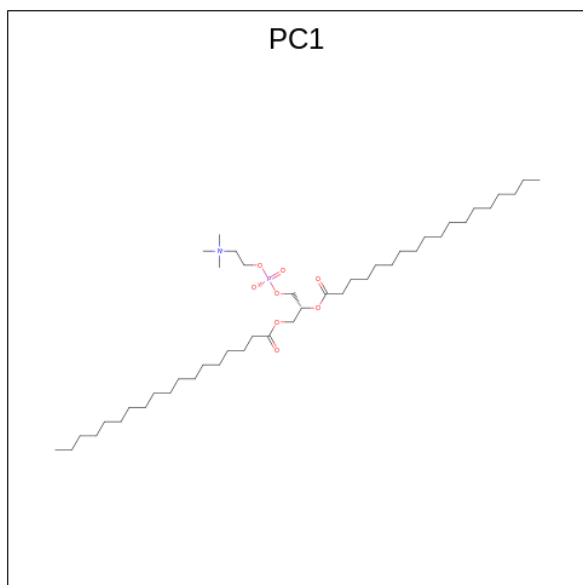
Mol	Chain	Residues	Atoms		AltConf
70	5B	1	Total	Zn	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
70	S6	1	Total	Zn	0
			1	1	

- Molecule 71 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula:  $C_{44}H_{88}NO_8P$ ).



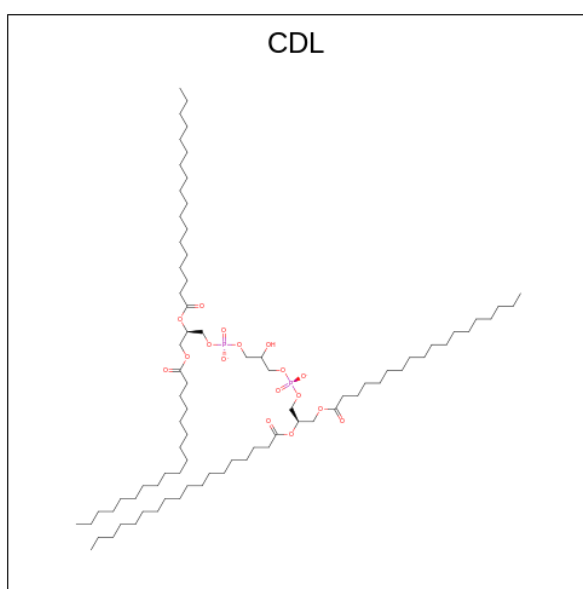
Mol	Chain	Residues	Atoms					AltConf
71	6A	1	Total	C	N	O	P	0
			45	35	1	8	1	
71	7B	1	Total	C	N	O	P	0
			54	44	1	8	1	
71	AL	1	Total	C	N	O	P	0
			54	44	1	8	1	
71	C1	1	Total	C	N	O	P	0
			54	44	1	8	1	
71	C1	1	Total	C	N	O	P	0
			46	36	1	8	1	
71	C3	1	Total	C	N	O	P	0
			49	39	1	8	1	
71	C3	1	Total	C	N	O	P	0
			43	33	1	8	1	
71	N5	1	Total	C	N	O	P	0
			54	44	1	8	1	
71	N6	1	Total	C	N	O	P	0
			54	44	1	8	1	
71	QC	1	Total	C	N	O	P	0
			54	44	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
71	QC	1	Total	C	N	O	P	0
			54	44	1	8	1	
71	QH	1	Total	C	N	O	P	0
			54	44	1	8	1	
71	Qb	1	Total	C	N	O	P	0
			29	19	1	8	1	
71	Qj	1	Total	C	N	O	P	0
			54	44	1	8	1	

- Molecule 72 is CARDIOLIPIN (CCD ID: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ).



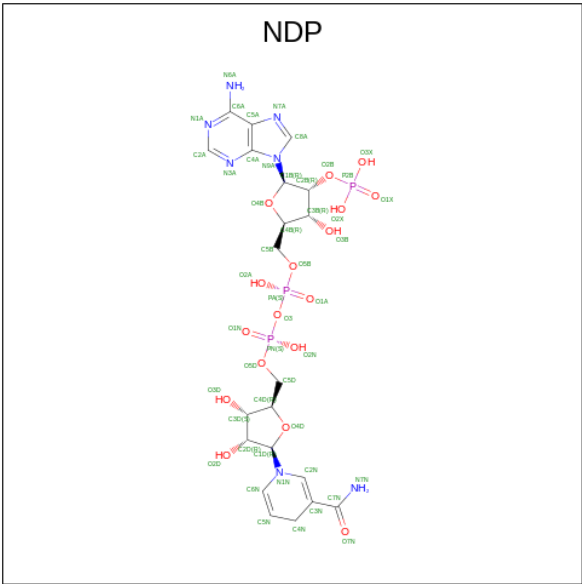
Mol	Chain	Residues	Atoms				AltConf
72	6A	1	Total	C	O	P	0
			69	50	17	2	
72	A8	1	Total	C	O	P	0
			83	64	17	2	
72	AL	1	Total	C	O	P	0
			84	65	17	2	
72	AL	1	Total	C	O	P	0
			93	74	17	2	
72	AL	1	Total	C	O	P	0
			80	61	17	2	
72	AM	1	Total	C	O	P	0
			51	32	17	2	
72	B5	1	Total	C	O	P	0
			100	81	17	2	

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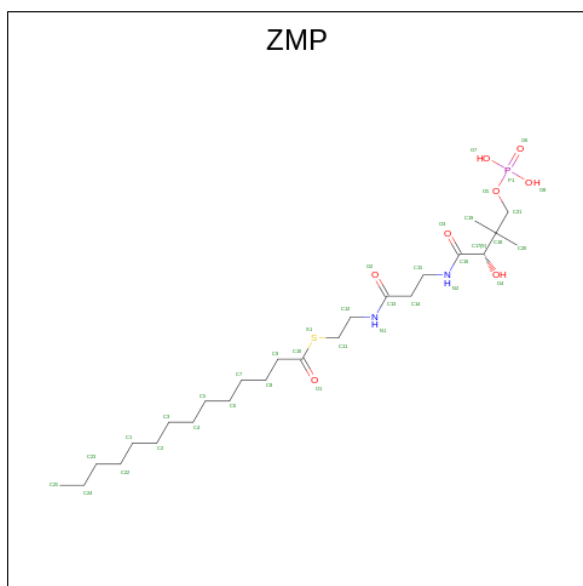
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
72	CB	1	Total 100	81	17	2	0
72	N2	1	Total 68	49	17	2	0
72	N5	1	Total 89	70	17	2	0
72	N5	1	Total 100	81	17	2	0
72	QB	1	Total 64	45	17	2	0
72	QC	1	Total 94	75	17	2	0
72	QC	1	Total 55	36	17	2	0
72	QH	1	Total 61	42	17	2	0
72	Qb	1	Total 64	45	17	2	0
72	Qd	1	Total 64	45	17	2	0
72	Qh	1	Total 64	45	17	2	0

- Molecule 73 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C<sub>21</sub>H<sub>30</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



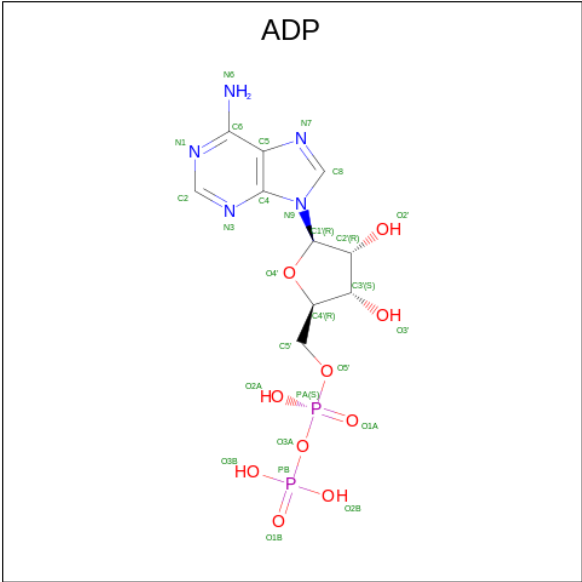
Mol	Chain	Residues	Atoms					AltConf
73	A9	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 74 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (CCD ID: ZMP) (formula: C<sub>25</sub>H<sub>49</sub>N<sub>2</sub>O<sub>8</sub>PS).



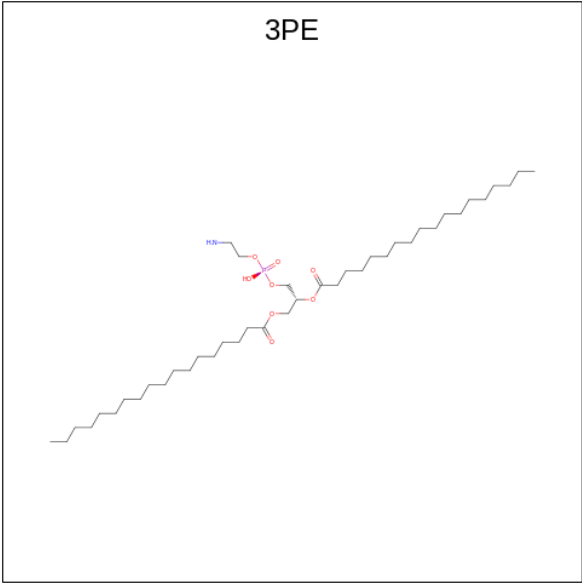
Mol	Chain	Residues	Atoms						AltConf
74	AB	1	Total 36	C 25	N 2	O 7	P 1	S 1	0
74	AC	1	Total 36	C 25	N 2	O 7	P 1	S 1	0

- Molecule 75 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					AltConf
75	AK	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 76 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula:  $C_{41}H_{82}NO_8P$ ).



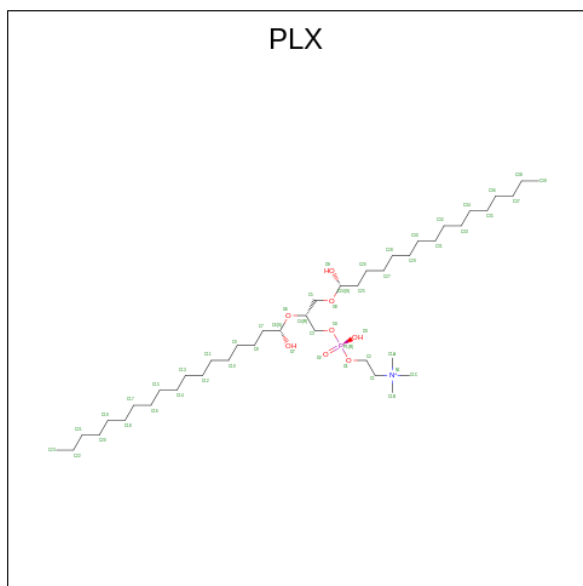
Mol	Chain	Residues	Atoms					AltConf
76	AL	1	Total	C	N	O	P	0
			51	41	1	8	1	
76	C1	1	Total	C	N	O	P	0
			51	41	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
76	C1	1	Total	C	N	O	P	0
			44	34	1	8	1	
76	CA	1	Total	C	N	O	P	0
			51	41	1	8	1	
76	CB	1	Total	C	N	O	P	0
			46	36	1	8	1	
76	N4	1	Total	C	N	O	P	0
			51	41	1	8	1	
76	QE	1	Total	C	N	O	P	0
			44	34	1	8	1	
76	S7	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 77 is (9R,11S)-9-({[(1S)-1-HYDROXYHEXADECYL]OXY}METHYL)-2,2-DIMETHYL-5,7,10-TRIOXA-2LAMBDA 5 -AZA-6LAMBDA 5 -PHOSPHAOCTACOSANE-6,6,11-TRIOL (CCD ID: PLX) (formula: C<sub>42</sub>H<sub>89</sub>NO<sub>8</sub>P).



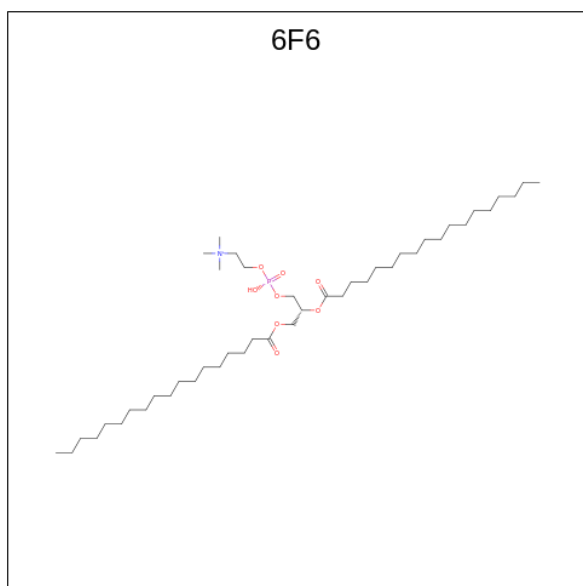
Mol	Chain	Residues	Atoms					AltConf
77	AL	1	Total	C	N	O	P	0
			47	37	1	8	1	
77	AM	1	Total	C	N	O	P	0
			52	42	1	8	1	
77	AM	1	Total	C	N	O	P	0
			52	42	1	8	1	
77	B5	1	Total	C	N	O	P	0
			52	42	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
77	C2	1	Total	C	N	O	P	0
			43	33	1	8	1	
77	CB	1	Total	C	N	O	P	0
			52	42	1	8	1	
77	N4	1	Total	C	N	O	P	0
			52	42	1	8	1	
77	QE	1	Total	C	N	O	P	0
			46	36	1	8	1	
77	QI	1	Total	C	N	O	P	0
			52	42	1	8	1	

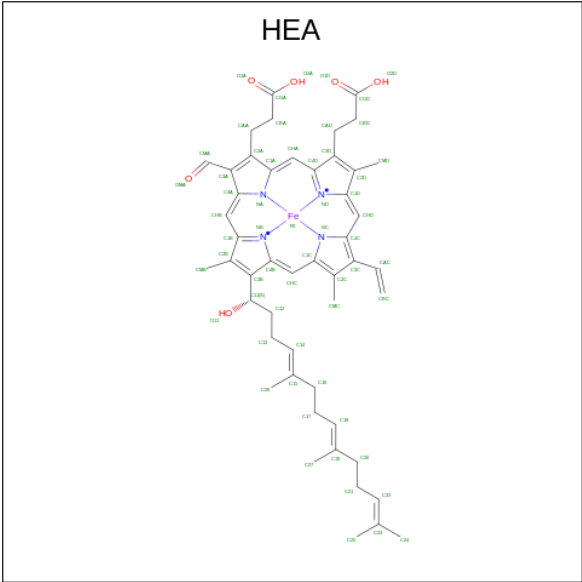
- Molecule 78 is (4S,7R)-4-hydroxy-N,N,N-trimethyl-7-(octadecanoyloxy)-4,10-dioxo-3,5,9-tri-oxa-4lambda 5 -phosphaheptacosan-1-aminium (CCD ID: 6F6) (formula: C<sub>44</sub>H<sub>89</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms					AltConf
78	B5	1	Total	C	N	O	P	0
			54	44	1	8	1	
78	QJ	1	Total	C	N	O	P	0
			54	44	1	8	1	
78	Qc	1	Total	C	N	O	P	0
			54	44	1	8	1	

- Molecule 79 is HEME-A (CCD ID: HEA) (formula: C<sub>49</sub>H<sub>56</sub>FeN<sub>4</sub>O<sub>6</sub>).





Mol	Chain	Residues	Atoms					AltConf
79	C1	1	Total 60	C 49	Fe 1	N 4	O 6	0
79	C1	1	Total 60	C 49	Fe 1	N 4	O 6	0

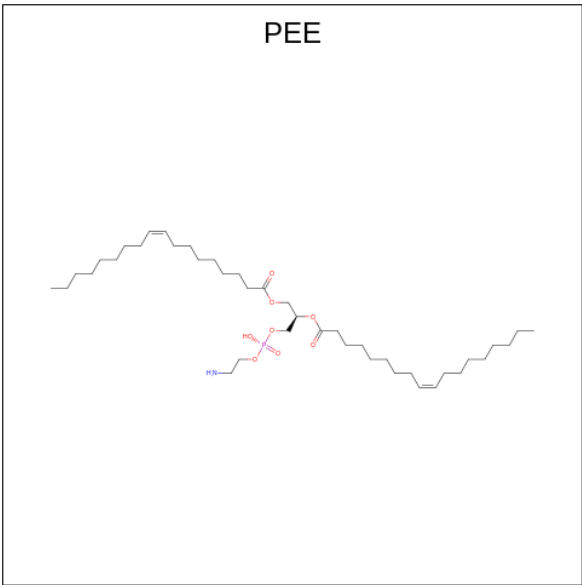
- Molecule 80 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		AltConf
80	C1	1	Total	Cu	0
			1	1	
80	C2	2	Total	Cu	0
			2	2	

- Molecule 81 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
81	C1	1	Total	Mg	0
			1	1	
81	S1	1	Total	Mg	0
			1	1	

- Molecule 82 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: C<sub>41</sub>H<sub>78</sub>NO<sub>8</sub>P).



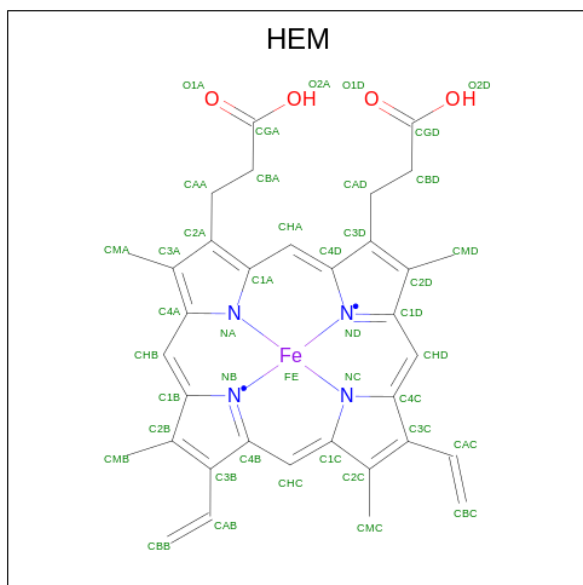
Mol	Chain	Residues	Atoms					AltConf
82	C1	1	Total	C	N	O	P	0
			51	41	1	8	1	
82	N1	1	Total	C	N	O	P	0
			38	28	1	8	1	
82	N3	1	Total	C	N	O	P	0
			51	41	1	8	1	
82	N5	1	Total	C	N	O	P	0
			46	36	1	8	1	
82	QB	1	Total	C	N	O	P	0
			27	17	1	8	1	
82	QB	1	Total	C	N	O	P	0
			51	41	1	8	1	
82	QC	1	Total	C	N	O	P	0
			51	41	1	8	1	
82	QC	1	Total	C	N	O	P	0
			38	28	1	8	1	
82	QE	1	Total	C	N	O	P	0
			47	37	1	8	1	
82	Qc	1	Total	C	N	O	P	0
			42	32	1	8	1	
82	Qd	1	Total	C	N	O	P	0
			51	41	1	8	1	
82	Qh	1	Total	C	N	O	P	0
			41	31	1	8	1	
82	Qh	1	Total	C	N	O	P	0
			51	41	1	8	1	
82	S2	1	Total	C	N	O	P	0
			48	38	1	8	1	

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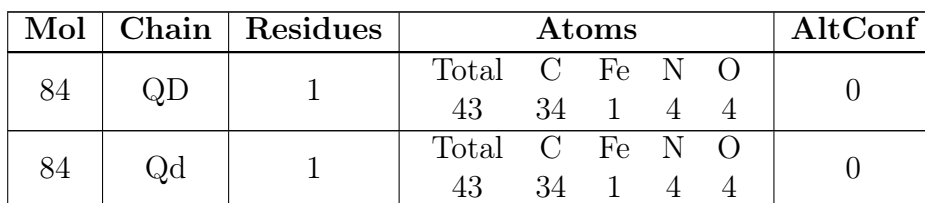
Mol	Chain	Residues	Atoms					AltConf
82	S8	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 83 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



Mol	Chain	Residues	Atoms					AltConf
83	QC	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
83	QC	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
83	Qc	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
83	Qc	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 84 is HEME C (CCD ID: HEC) (formula:  $C_{34}H_{34}FeN_4O_4$ ).



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

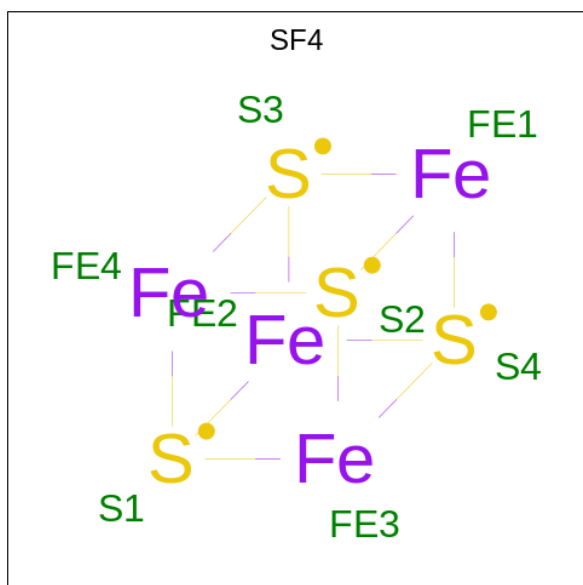
Mol	Chain	Residues	Atoms			AltConf
85	QE	1	Total 4	Fe 2	S 2	0
85	Qe	1	Total 4	Fe 2	S 2	0

WORLDWIDE  
**PDB**  
PROTEIN DATA BANK

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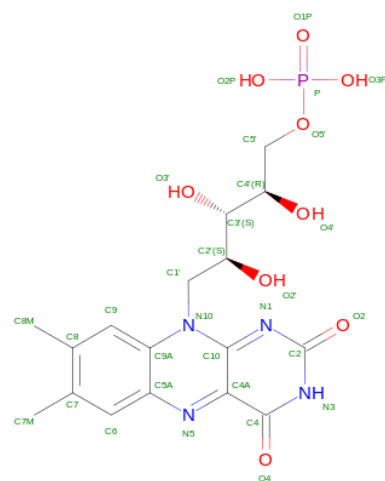
Mol	Chain	Residues	Atoms			AltConf
85	S1	1	Total	Fe	S	0
			4	2	2	
85	V2	1	Total	Fe	S	0
			4	2	2	

- Molecule 86 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ).



Mol	Chain	Residues	Atoms			AltConf
86	S1	1	Total	Fe	S	0
			8	4	4	
86	S1	1	Total	Fe	S	0
			8	4	4	
86	S7	1	Total	Fe	S	0
			8	4	4	
86	S8	1	Total	Fe	S	0
			8	4	4	
86	S8	1	Total	Fe	S	0
			8	4	4	
86	V1	1	Total	Fe	S	0
			8	4	4	

- Molecule 87 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula:  $\text{C}_{17}\text{H}_{21}\text{N}_4\text{O}_9\text{P}$ ).




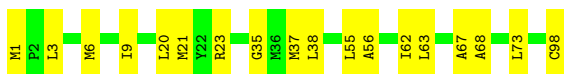
Mol	Chain	Residues	Atoms					AltConf
87	V1	1	Total 31	C 17	N 4	O 9	P 1	0

### 3 Residue-property plots

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

- Molecule 1: NADH-ubiquinone oxidoreductase chain 4L

Chain 4L:  82% 18%



- Molecule 2: Cytochrome c oxidase subunit 5A, mitochondrial

Chain 5A:  71% 29%




- Molecule 3: Cytochrome c oxidase subunit 5B, mitochondrial

Chain 5B:  71% 29%



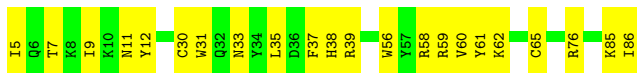
- Molecule 4: Cytochrome c oxidase subunit

Chain 6A:  75% 25%




- Molecule 5: Cytochrome c oxidase subunit

Chain 6B:  73% 27%



- Molecule 6: Cytochrome c oxidase subunit 6C

Chain 6C:  79% 21%




- Molecule 7: Cytochrome c oxidase subunit 7A1, mitochondrial

Chain 7A:  74% 25%



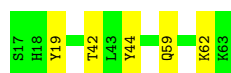
- Molecule 8: Cytochrome c oxidase subunit 7B, mitochondrial

Chain 7B:  86% 14%



- Molecule 9: Cytochrome c oxidase subunit 7C, mitochondrial

Chain 7C:  89% 11%



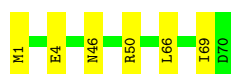
- Molecule 10: Cytochrome c oxidase subunit 8

Chain 8B:  72% 28%



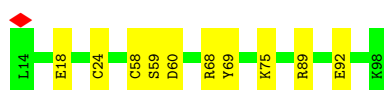
- Molecule 11: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain A1:  91% 9%



- Molecule 12: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain A2:  88% 12%



- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

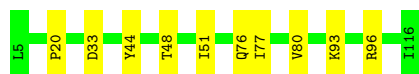


Chain A3:  96% .




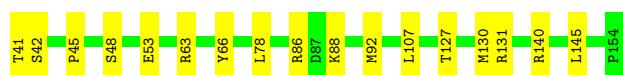
- Molecule 14: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

Chain A5:  91% 9%




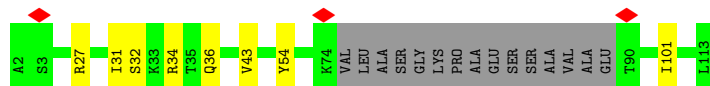
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain A6:  85% 15%




- Molecule 16: Complex I-B14.5a

Chain A7:  79% 7% 13%




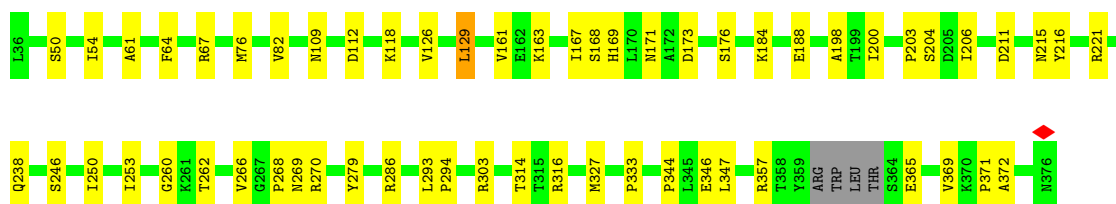
- Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain A8:  85% 15%



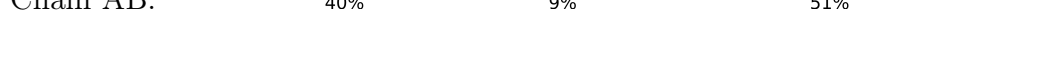
- Molecule 18: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain A9:  82% 17% .



- Molecule 19: Acyl carrier protein

Chain AB:  40% 9% 51%



MET ALA ALA ARG VAL LEU CYS CYS VAL VAL ARG LEU PRO ALA ALA PHE ALA PRO LEU PRO ILE PRO THR VAL VAL ALA ALA ARG ARG PRO LEU SER THR THR PHE PRO THR THR GLY ALA GLN ALA ARG SER ARG ALA ALA LEU GLN PRO ALA LEU VAL LEU LEU LEU GLN ALA ALA PRO GLY GLY

VAL THR GLN LEU CYS ARG ARG TYR SER CYS VAL ASP ALA ARG PRO PRO LEU THR L76 E77 A78 D81 I93 F104 L108 S112 Q115 V116 I119 M120 E129 A135 L138 I144 K151 K152 ASP VAL TYR GLU


• Molecule 19: Acyl carrier protein

Chain AC:  44% 11% 44%

MET ALA ALA ARG VAL LEU CYS CYS VAL ASP ALA ARG PRO PRO LEU THR L76 E77 A78 D81 I93 F104 L108 S112 Q115 V116 I119 M120 E129 A135 L138 I144 K151 K152 ASP VAL TYR GLU

VAL THR GLN LEU CYS ARG ARG TYR SER CYS VAL ASP ALA ARG PRO PRO LEU THR L76 E77 A78 D81 I93 F104 L108 S112 Q115 V116 I119 M120 E129 A135 L138 I144 K151 K152 ASP VAL TYR GLU

• Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain AK:  79% 20%

L38 G41 I62 T63 V64 D65 G66 N67 I68 K72 G73 G92 I93 H94 Y95 D97 P105 G112 Y131 Q134 S135 K279 W136 Y138 R141 L142 Y145 A148 L152 V159 V160 I165 L172 R182 K183 Q184 C185 H188 Y189 L201

H204 V205 V206 D210 V211 I216 K222 Q237 N241 K244 K245 L248 C255 E256 V257 L258 D267 L278 K279 C280 D281 K282 G283 P286 R297 K298 L299 V300 L316 P317 E318 I319 D327 Q331 K340 Y341 S342 Y345 K357

• Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain AL:  88% 12%


A2 K3 T4 K8 E14 E17 R20 K21 A22 T26 L43 R81 N89 R106 C115 M118 G119 L120 T121 P139 K140 V141

• Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain AM:  88% 12%

E2 Q5 R8 Q12 G16 F28 R34 D42 M46 F55 F56 G57 R58 D76 E85 W86 H87 R88 M93 R106 I109 Y144

• Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain AN:  82% 18%

A3 S4 K5 V6 K7 Y16 I19 L43 S49 M50 M51 E56 R57 R58 R59 E63 A70 P73 D80 R88 E92 E93 E94 A95 M96 V101 V106 P119 M120 E123 L124 T144

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

Chain B1:  91% 9%




- Molecule 25: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

Chain B2:  90% 10%




- Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain B3:  85% 15%




- Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

Chain B4:  88% 12%



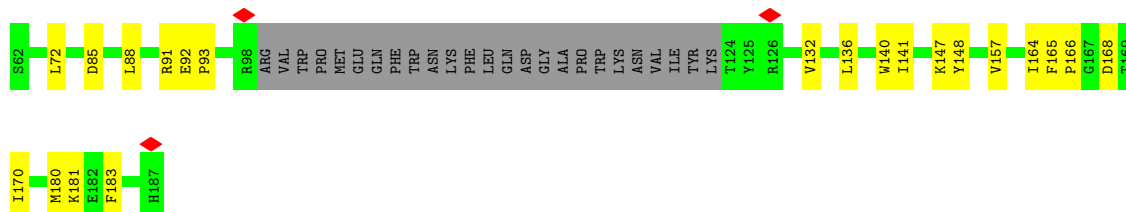
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain B5:  86% 14%




- Molecule 29: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain B6:  63% 17% 20%




- Molecule 30: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain B7:  84% 16%




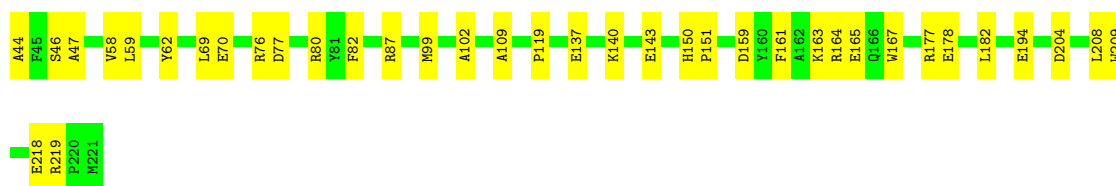
- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain B8:  89% 11%



- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

Chain B9:  79% 21%




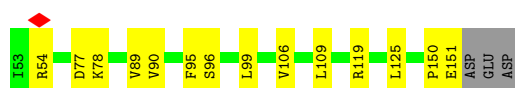
- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

Chain BK:  89% 10%



- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain BL:  83% 14%



- Molecule 35: Cytochrome c oxidase subunit 1

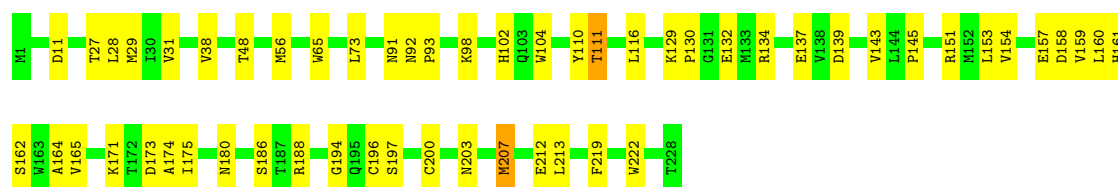
Chain C1:  71% 29%





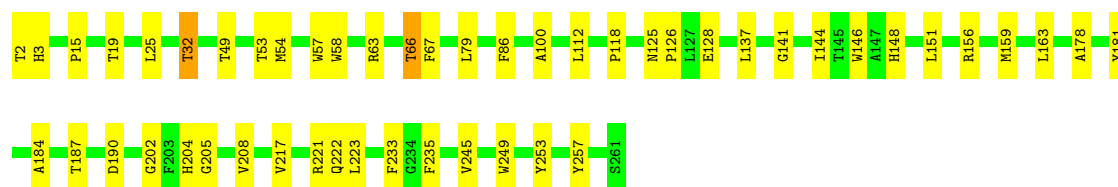
• Molecule 36: Cytochrome c oxidase subunit 2

Chain C2: 76% 23% .



• Molecule 37: Cytochrome c oxidase subunit 3

Chain C3: 81% 18% .



• Molecule 38: Cytochrome c oxidase subunit 4

Chain C4: 79% 21% .



• Molecule 39: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

Chain CA: 82% 16% .



• Molecule 40: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain CB: 84% 16% .



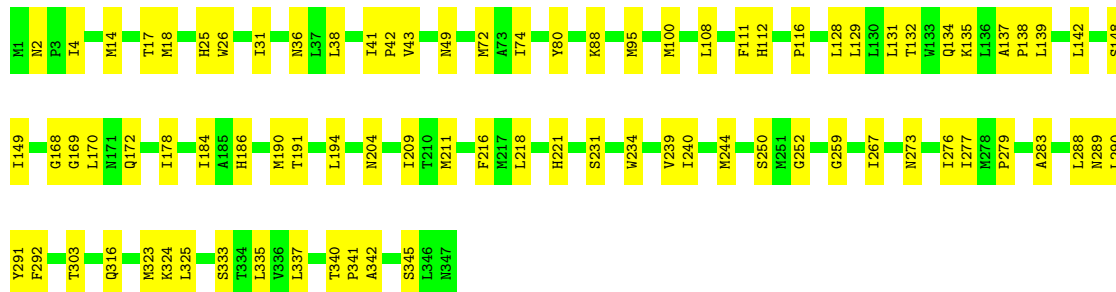
• Molecule 41: NADH-ubiquinone oxidoreductase chain 1

Chain N1: 77% 21%



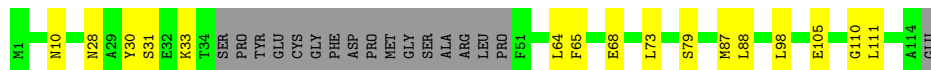
• Molecule 42: NADH-ubiquinone oxidoreductase chain 2

Chain N2: 76% 24%



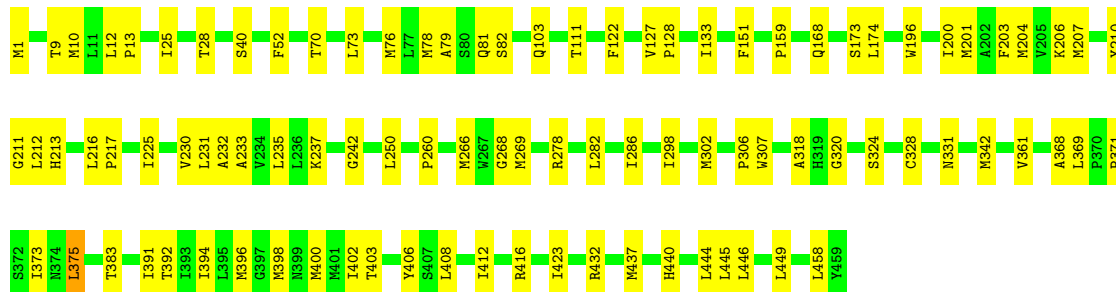
• Molecule 43: NADH-ubiquinone oxidoreductase chain 3

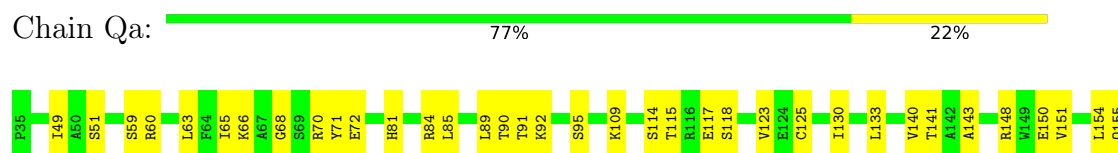
Chain N3: 71% 14% 15%

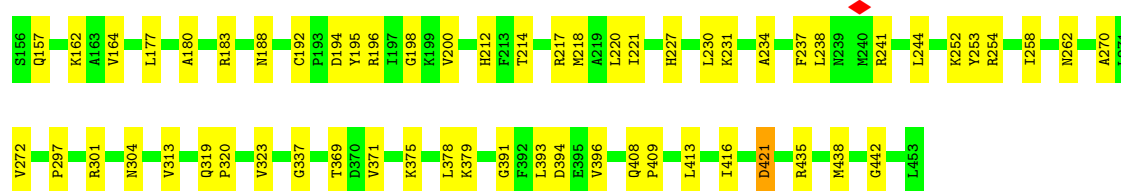


• Molecule 44: NADH-ubiquinone oxidoreductase chain 4

Chain N4: 80% 20%

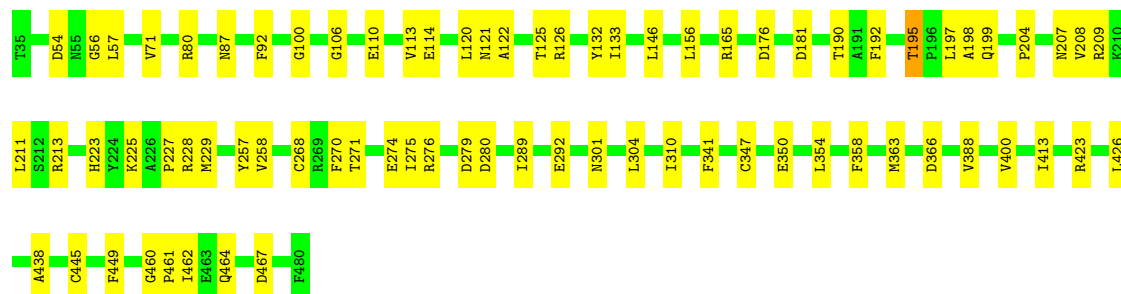






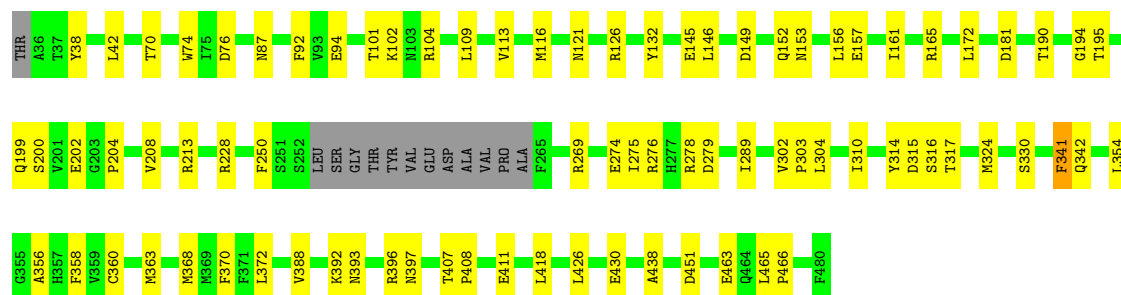
- Molecule 48: Cytochrome b-c1 complex subunit 1, mitochondrial

Chain QB: 83% 17%



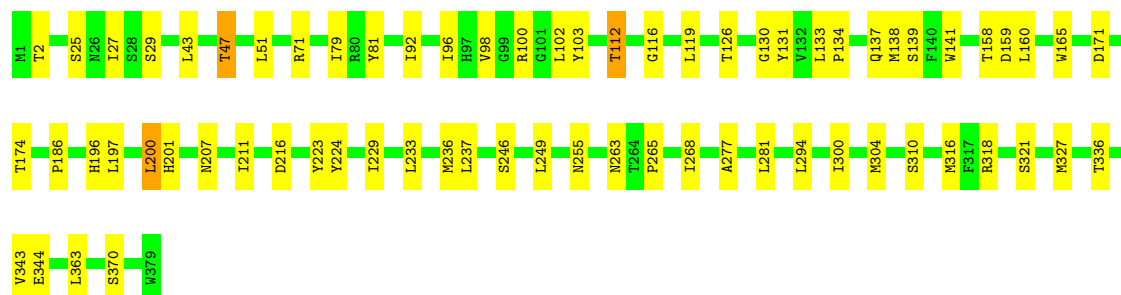
- Molecule 48: Cytochrome b-c1 complex subunit 1, mitochondrial

Chain Qb: 79% 18%



- Molecule 49: Cytochrome b

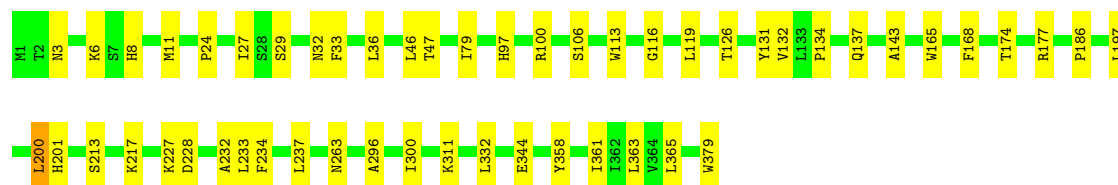
Chain QC: 82% 17%



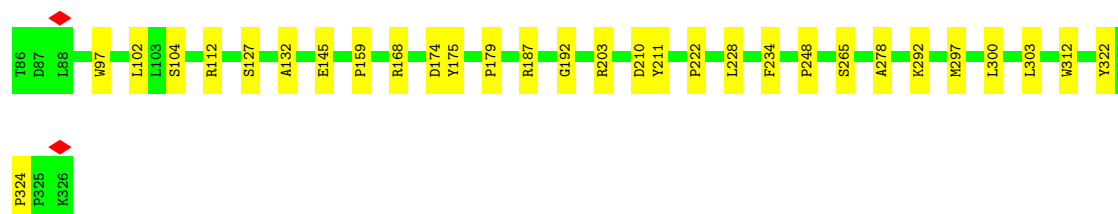
- Molecule 49: Cytochrome b

Chain Qc: 86% 13%

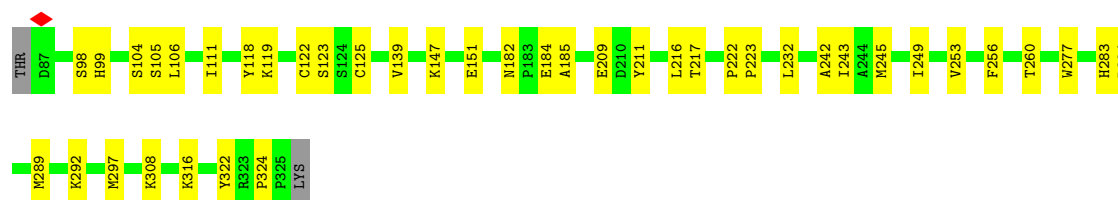
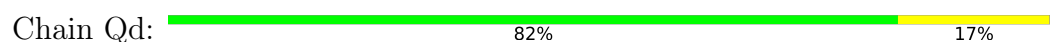




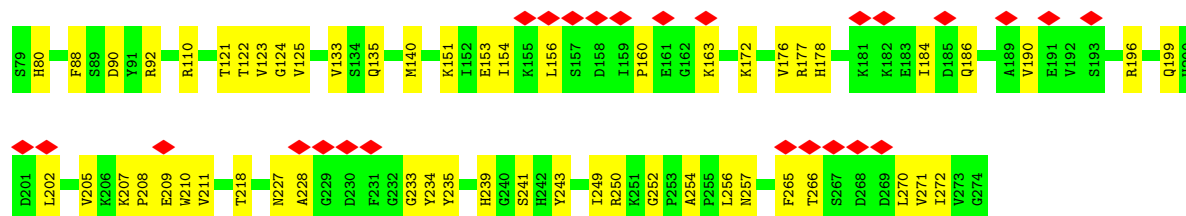
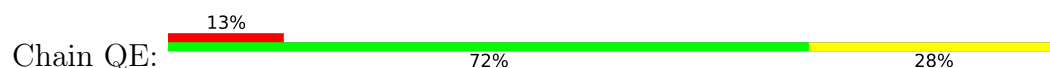
- Molecule 50: Cytochrome c domain-containing protein



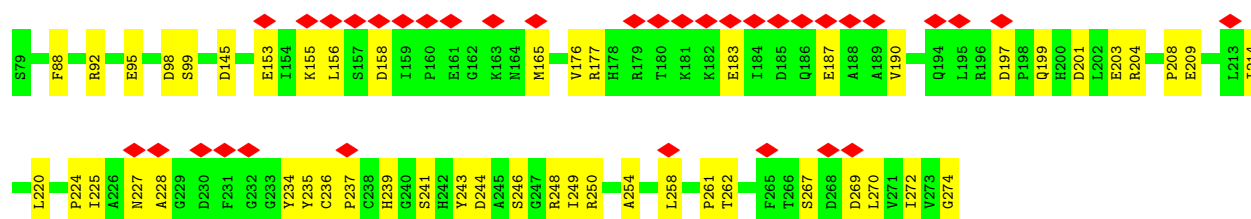
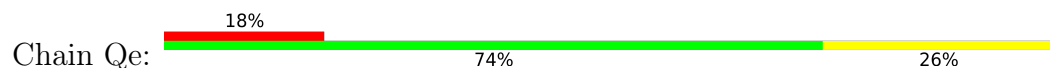
- Molecule 50: Cytochrome c domain-containing protein




- Molecule 51: Rieske domain-containing protein



- Molecule 51: Rieske domain-containing protein



- Molecule 52: Cytochrome b-c1 complex subunit 6

Chain QF:  88% 12%




- Molecule 52: Cytochrome b-c1 complex subunit 6

Chain Qf:  70% 25%




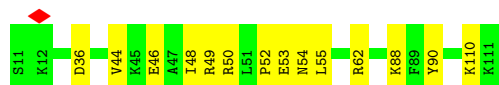
- Molecule 53: Cytochrome b-c1 complex subunit 7

Chain QG:  84% 15%




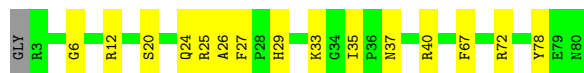
- Molecule 53: Cytochrome b-c1 complex subunit 7

Chain Qg:  86% 14%




- Molecule 54: Cytochrome b-c1 complex subunit 8

Chain QH:  80% 19%




- Molecule 54: Cytochrome b-c1 complex subunit 8

Chain Qh:  81% 19%



- Molecule 55: Ubiquinol-cytochrome c reductase complex

Chain QI:  84% 12%



- Molecule 55: Ubiquinol-cytochrome c reductase complex

Chain Qi: 83% 11% 6%



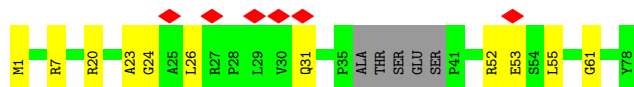
- Molecule 56: Cytochrome b-c1 complex subunit 10

Chain QJ: 94% 6%



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

Chain QK: 8% 79% 14% 6%



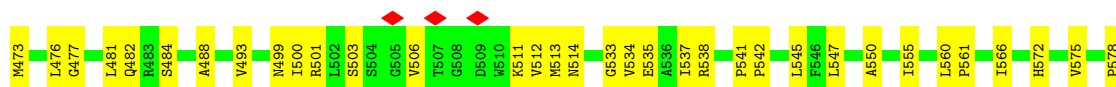
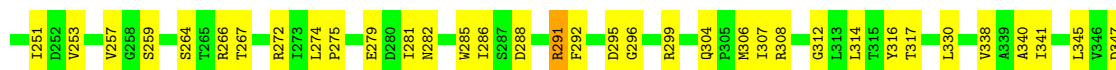
- Molecule 58: Cytochrome b-c1 complex subunit 10

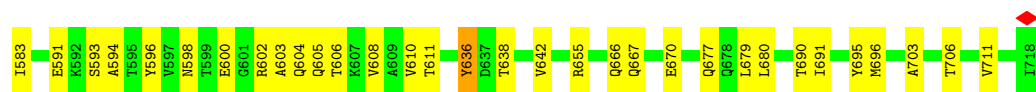
Chain Qj: 86% 14%



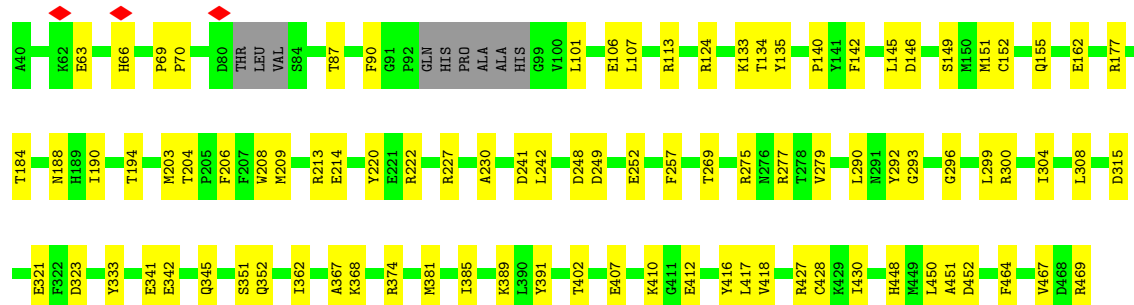
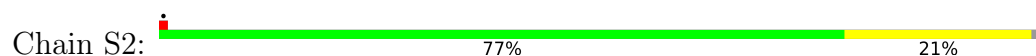
- Molecule 59: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain S1: 76% 24%

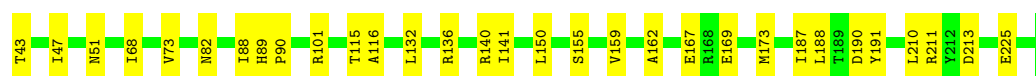
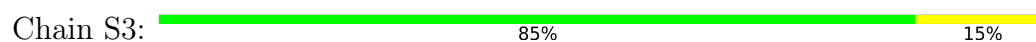




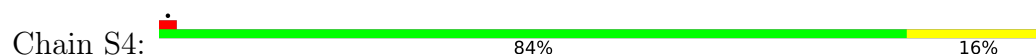
- Molecule 60: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial



- Molecule 61: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial



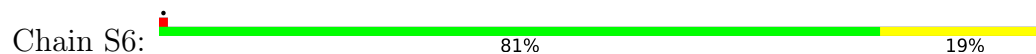
- Molecule 62: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



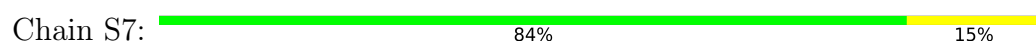
- Molecule 63: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



- Molecule 64: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



- Molecule 65: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial





- Molecule 66: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain S8: 83% 17%



- Molecule 67: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain V1: 77% 22%



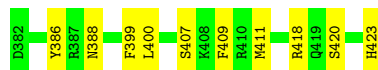
- Molecule 68: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain V2: 88% 12%



- Molecule 69: NADH:ubiquinone oxidoreductase subunit V3

Chain V3: 76% 24%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	181922	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 ( $e^-/\text{\AA}^2$ )	51.9	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	105000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	47.701	Depositor
Minimum map value	-16.089	Depositor
Average map value	-0.009	Depositor
Map value standard deviation	1.062	Depositor
Recommended contour level	4	Depositor
Map size ( $\text{\AA}$ )	576.0, 576.0, 576.0	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.2, 1.2, 1.2	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NDP, HEA, PC1, HEC, SF4, MG, ZN, PEE, ZMP, CU, 2MR, FES, 3PE, PLX, FMN, HEM, 6F6, ADP, CDL

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	4L	0.20	0/759	0.28	0/1029
2	5A	0.16	0/843	0.28	0/1145
3	5B	0.18	0/739	0.33	0/1002
4	6A	0.13	0/648	0.25	0/888
5	6B	0.19	0/704	0.39	0/951
6	6C	0.16	0/587	0.25	0/781
7	7A	0.15	0/457	0.28	0/620
8	7B	0.12	0/405	0.22	0/555
9	7C	0.17	0/400	0.24	0/536
10	8B	0.15	0/349	0.32	0/477
11	A1	0.17	0/577	0.27	0/777
12	A2	0.15	0/697	0.27	0/938
13	A3	0.15	0/664	0.24	0/912
14	A5	0.16	0/929	0.24	0/1258
15	A6	0.17	0/991	0.28	0/1335
16	A7	0.16	0/798	0.25	0/1079
17	A8	0.17	0/1436	0.26	0/1938
18	A9	0.17	0/2777	0.31	2/3762 (0.1%)
19	AB	0.10	0/633	0.22	0/851
19	AC	0.18	0/714	0.25	0/965
20	AK	0.16	0/2650	0.34	2/3588 (0.1%)
21	AL	0.14	0/1042	0.23	0/1411
22	AM	0.15	0/1236	0.24	0/1683
23	AN	0.18	0/1204	0.27	0/1624
24	B1	0.16	0/491	0.26	0/663
25	B2	0.18	0/610	0.28	0/836
26	B3	0.16	0/651	0.27	0/880
27	B4	0.18	0/1092	0.26	0/1481
28	B5	0.19	0/1184	0.27	0/1603
29	B6	0.19	0/888	0.32	0/1208
30	B7	0.17	0/1092	0.26	0/1459

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
31	B8	0.17	0/1371	0.25	0/1875
32	B9	0.19	0/1590	0.30	0/2155
33	BK	0.18	0/1489	0.26	0/2008
34	BL	0.19	0/851	0.30	0/1155
35	C1	0.21	0/4164	0.34	0/5689
36	C2	0.18	0/1880	0.32	0/2564
37	C3	0.19	0/2186	0.30	0/2991
38	C4	0.16	0/1187	0.26	0/1606
39	CA	0.15	0/430	0.24	0/581
40	CB	0.19	0/1031	0.28	0/1394
41	N1	0.20	0/2528	0.33	0/3455
42	N2	0.22	0/2773	0.34	0/3768
43	N3	0.18	0/804	0.27	0/1097
44	N4	0.23	0/3723	0.34	0/5078
45	N5	0.21	0/4914	0.35	0/6683
46	N6	0.18	0/1266	0.32	0/1712
47	QA	0.18	0/3200	0.29	0/4333
47	Qa	0.17	0/3200	0.28	0/4333
48	QB	0.19	0/3531	0.30	0/4793
48	Qb	0.18	0/3436	0.28	0/4659
49	QC	0.20	0/3123	0.32	0/4269
49	Qc	0.21	0/3123	0.31	0/4269
50	QD	0.18	0/1979	0.27	0/2684
50	Qd	0.18	0/1962	0.28	0/2663
51	QE	0.13	0/1550	0.25	0/2098
51	Qe	0.13	0/1550	0.27	0/2098
52	QF	0.14	0/558	0.22	0/747
52	Qf	0.16	0/534	0.25	0/714
53	QG	0.17	0/913	0.27	0/1223
53	Qg	0.18	0/913	0.26	0/1223
54	QH	0.17	0/684	0.30	0/926
54	Qh	0.17	0/688	0.29	0/931
55	QI	0.15	0/520	0.19	0/701
55	Qi	0.18	0/506	0.24	0/683
56	QJ	0.13	0/420	0.21	0/576
57	QK	0.12	0/528	0.26	0/716
58	Qj	0.16	0/437	0.29	0/598
59	S1	0.21	0/5378	0.32	0/7287
60	S2	0.23	0/3465	0.31	0/4691
61	S3	0.22	0/1780	0.29	0/2424
62	S4	0.20	0/1030	0.29	0/1391
63	S5	0.18	0/845	0.25	0/1129
64	S6	0.17	0/755	0.27	0/1018



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
65	S7	0.22	0/1279	0.29	0/1730
66	S8	0.22	0/1443	0.28	0/1952
67	V1	0.20	0/3391	0.31	0/4583
68	V2	0.17	0/1711	0.30	0/2328
69	V3	0.15	0/365	0.29	0/493
All	All	0.19	0/115231	0.30	4/156309 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A9	369	VAL	CA-C-N	7.40	135.01	120.94
18	A9	369	VAL	C-N-CA	7.40	135.01	120.94
20	AK	204	HIS	CA-C-N	-5.49	116.29	122.93
20	AK	204	HIS	C-N-CA	-5.49	116.29	122.93

There are no chirality outliers.

There are no planarity outliers.

## 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	4L	748	0	799	19	0
2	5A	825	0	823	19	0
3	5B	724	0	705	17	0
4	6A	620	0	589	19	0
5	6B	684	0	649	20	0
6	6C	574	0	590	14	0
7	7A	447	0	443	10	0
8	7B	392	0	372	7	0
9	7C	387	0	385	6	0
10	8B	338	0	342	9	0
11	A1	562	0	557	6	0
12	A2	686	0	699	6	0
13	A3	643	0	642	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	A5	910	0	950	5	0
15	A6	967	0	972	13	0
16	A7	780	0	808	6	0
17	A8	1398	0	1372	22	0
18	A9	2703	0	2720	33	0
19	AB	624	0	625	10	0
19	AC	702	0	694	14	0
20	AK	2590	0	2551	43	0
21	AL	1021	0	1025	9	0
22	AM	1195	0	1149	12	0
23	AN	1173	0	1166	21	0
24	B1	479	0	486	4	0
25	B2	584	0	529	7	0
26	B3	632	0	612	8	0
27	B4	1062	0	1072	13	0
28	B5	1151	0	1164	17	0
29	B6	861	0	877	20	0
30	B7	1068	0	1041	15	0
31	B8	1315	0	1208	14	0
32	B9	1534	0	1470	29	0
33	BK	1456	0	1424	15	0
34	BL	828	0	788	11	0
35	C1	4024	0	4005	114	0
36	C2	1833	0	1843	44	0
37	C3	2103	0	2034	48	0
38	C4	1153	0	1130	25	0
39	CA	417	0	422	6	0
40	CB	1000	0	994	19	0
41	N1	2457	0	2554	52	0
42	N2	2710	0	2874	59	0
43	N3	786	0	836	14	0
44	N4	3631	0	3839	74	0
45	N5	4785	0	4933	96	0
46	N6	1236	0	1241	30	0
47	QA	3147	0	3129	48	0
47	Qa	3147	0	3129	62	0
48	QB	3459	0	3350	46	0
48	Qb	3367	0	3262	52	0
49	QC	3025	0	3090	50	0
49	Qc	3025	0	3090	37	0
50	QD	1921	0	1867	24	0
50	Qd	1904	0	1849	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	QE	1517	0	1500	45	0
51	Qe	1517	0	1500	33	0
52	QF	552	0	536	7	0
52	Qf	528	0	510	11	0
53	QG	893	0	888	10	0
53	Qg	893	0	888	10	0
54	QH	662	0	660	13	0
54	Qh	666	0	663	14	0
55	QI	507	0	509	6	0
55	Qi	493	0	491	6	0
56	QJ	405	0	405	2	0
57	QK	520	0	554	10	0
58	Qj	421	0	418	5	0
59	S1	5290	0	5321	105	0
60	S2	3391	0	3328	67	0
61	S3	1729	0	1687	18	0
62	S4	1007	0	1008	15	0
63	S5	825	0	834	13	0
64	S6	741	0	701	13	0
65	S7	1248	0	1254	17	0
66	S8	1412	0	1363	25	0
67	V1	3316	0	3272	68	0
68	V2	1671	0	1673	17	0
69	V3	355	0	329	10	0
70	5B	1	0	0	0	0
70	S6	1	0	0	0	0
71	6A	45	0	64	16	0
71	7B	54	0	88	4	0
71	AL	54	0	88	2	0
71	C1	100	0	157	4	0
71	C3	92	0	138	8	0
71	N5	54	0	88	1	0
71	N6	54	0	88	0	0
71	QC	108	0	176	6	0
71	QH	54	0	88	5	0
71	Qb	29	0	32	1	0
71	Qj	54	0	88	0	0
72	6A	69	0	85	4	0
72	A8	83	0	113	4	0
72	AL	257	0	361	7	0
72	AM	51	0	46	1	0
72	B5	100	0	156	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
72	CB	100	0	156	11	0
72	N2	68	0	80	2	0
72	N5	189	0	284	15	0
72	QB	64	0	72	0	0
72	QC	149	0	192	10	0
72	QH	61	0	66	3	0
72	Qb	64	0	72	2	0
72	Qd	64	0	72	6	0
72	Qh	64	0	72	3	0
73	A9	48	0	26	2	0
74	AB	36	0	47	1	0
74	AC	36	0	47	4	0
75	AK	27	0	12	4	0
76	AL	51	0	82	2	0
76	C1	95	0	147	2	0
76	CA	51	0	82	2	0
76	CB	46	0	69	2	0
76	N4	51	0	82	4	0
76	QE	44	0	65	3	0
76	S7	51	0	82	4	0
77	AL	47	0	75	5	0
77	AM	104	0	176	9	0
77	B5	52	0	88	5	0
77	C2	43	0	67	1	0
77	CB	52	0	88	4	0
77	N4	52	0	88	1	0
77	QE	46	0	73	6	0
77	QI	52	0	88	5	0
78	B5	54	0	0	0	0
78	QJ	54	0	0	0	0
78	Qc	54	0	0	1	0
79	C1	120	0	108	23	0
80	C1	1	0	0	0	0
80	C2	2	0	0	0	0
81	C1	1	0	0	0	0
81	S1	1	0	0	0	0
82	C1	51	0	82	3	0
82	N1	38	0	50	1	0
82	N3	51	0	82	2	0
82	N5	46	0	69	5	0
82	QB	78	0	110	2	0
82	QC	89	0	132	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
82	QE	47	0	71	5	0
82	Qc	42	0	61	0	0
82	Qd	51	0	82	4	0
82	Qh	92	0	138	8	0
82	S2	48	0	73	3	0
82	S8	51	0	82	1	0
83	QC	86	0	60	10	0
83	Qc	86	0	60	7	0
84	QD	43	0	30	2	0
84	Qd	43	0	32	3	0
85	QE	4	0	0	2	0
85	Qe	4	0	0	1	0
85	S1	4	0	0	0	0
85	V2	4	0	0	0	0
86	S1	16	0	0	0	0
86	S7	8	0	0	1	0
86	S8	16	0	0	2	0
86	V1	8	0	0	1	0
87	V1	31	0	19	1	0
All	All	116743	0	117808	1761	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 8.

All (1761) 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)
33:BK:140:GLN:O	33:BK:144:SER:HB2	1.72	0.89
71:7B:101:PC1:H2D1	71:7B:101:PC1:H3E1	1.57	0.84
36:C2:196:CYS:HB3	36:C2:207:MET:SD	2.18	0.82
66:S8:205:ILE:O	66:S8:209:TYR:HB3	1.80	0.81
36:C2:196:CYS:CB	36:C2:207:MET:SD	2.69	0.80
18:A9:198:ALA:O	18:A9:260:GLY:HA2	1.81	0.80
29:B6:88:LEU:HD22	29:B6:92:GLU:HG2	1.67	0.77
44:N4:306:PRO:HA	44:N4:458:LEU:HD23	1.67	0.76
47:Qa:155:GLN:HE22	47:Qa:200:VAL:HB	1.50	0.75
67:V1:110:PRO:HB3	67:V1:152:ARG:HD3	1.69	0.75
59:S1:124:HIS:HD2	60:S2:381:MET:HE2	1.52	0.75
44:N4:371:PRO:HD2	72:N5:702:CDL:H391	1.67	0.74
74:AC:201:ZMP:H5	32:B9:109:ALA:HB1	1.68	0.73
45:N5:3:PRO:HB2	45:N5:53:MET:HE1	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:N1:62:ARG:HH11	41:N1:63:PRO:HD2	1.53	0.73
51:QE:177:ARG:HH12	51:QE:233:GLY:HA2	1.54	0.73
42:N2:108:LEU:HD11	42:N2:191:THR:HG21	1.70	0.73
59:S1:251:ILE:HG12	59:S1:606:THR:HG22	1.69	0.73
41:N1:65:THR:HG21	41:N1:71:PHE:HB2	1.69	0.72
49:QC:237:LEU:HB2	50:QD:297:MET:HE2	1.70	0.72
41:N1:100:LEU:HD23	41:N1:103:LEU:HD12	1.72	0.72
47:Qa:81:HIS:HD2	47:Qa:192:CYS:H	1.36	0.72
72:CB:203:CDL:HA21	72:CB:203:CDL:HB61	1.71	0.72
4:6A:83:HIS:HA	71:6A:101:PC1:H132	1.73	0.70
47:Qa:90:THR:HG23	47:Qa:95:SER:HA	1.73	0.70
77:AM:203:PLX:H111	77:AM:203:PLX:H271	1.72	0.70
7:7A:77:PRO:HG3	9:7C:62:LYS:HG3	1.72	0.70
51:Qe:153:GLU:HG2	51:Qe:272:ILE:HG12	1.72	0.70
12:A2:24:CYS:N	12:A2:58:CYS:SG	2.65	0.70
51:Qe:190:VAL:HG21	51:Qe:250:ARG:HH22	1.55	0.70
48:QB:100:GLY:HA2	48:QB:106:GLY:H	1.57	0.69
5:6B:35:LEU:HA	5:6B:86:ILE:HD11	1.74	0.69
5:6B:38:HIS:HB2	5:6B:86:ILE:HD13	1.74	0.69
76:C1:601:3PE:H2F1	38:C4:109:PHE:HB3	1.73	0.69
49:QC:98:VAL:HG22	83:QC:403:HEM:HBC2	1.75	0.69
67:V1:235:VAL:HG12	67:V1:240:THR:HG21	1.75	0.69
59:S1:456:ALA:O	59:S1:499:ASN:ND2	2.26	0.69
47:QA:116:ARG:NH1	47:QA:188:ASN:O	2.25	0.68
10:8B:28:LYS:HG3	35:C1:483:SER:HB3	1.76	0.68
68:V2:38:LEU:O	68:V2:124:ARG:NH2	2.25	0.68
72:6A:102:CDL:H231	72:6A:102:CDL:H122	1.76	0.68
60:S2:290:LEU:O	60:S2:293:GLY:N	2.26	0.68
45:N5:5:ALA:HB2	45:N5:61:MET:HE1	1.76	0.68
60:S2:162:GLU:OE2	60:S2:177:ARG:NH2	2.24	0.67
77:B5:201:PLX:H91	44:N4:40:SER:HB3	1.76	0.67
42:N2:88:LYS:HG3	42:N2:148:SER:HB3	1.77	0.67
49:QC:2:THR:O	82:QC:401:PEE:N	2.28	0.67
51:Qe:177:ARG:HH12	51:Qe:227:ASN:HD21	1.42	0.67
26:B3:27:THR:HG22	26:B3:29:LEU:H	1.57	0.67
3:5B:105:VAL:HA	3:5B:111:GLN:HG3	1.77	0.67
51:Qe:204:ARG:NH2	51:Qe:258:LEU:O	2.27	0.67
54:QH:27:PHE:H	71:QH:102:PC1:H143	1.60	0.67
60:S2:300:ARG:NH2	60:S2:407:GLU:OE2	2.28	0.67
41:N1:200:LEU:HD11	41:N1:285:LEU:HD21	1.77	0.66
67:V1:111:LYS:HB2	67:V1:151:ALA:HA	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5A:143:THR:HB	2:5A:146:GLU:HG3	1.78	0.66
71:6A:101:PC1:H322	37:C3:202:GLY:HA3	1.76	0.66
67:V1:40:ARG:NH1	67:V1:289:GLU:O	2.29	0.66
36:C2:132:GLU:HB3	36:C2:137:GLU:HG3	1.76	0.66
72:Qd:401:CDL:H721	72:Qd:401:CDL:H312	1.78	0.66
45:N5:530:PRO:O	45:N5:534:HIS:HB2	1.96	0.66
49:Qc:300:ILE:HD11	49:Qc:363:LEU:HD21	1.78	0.66
47:Qa:123:VAL:HB	47:Qa:133:LEU:HD23	1.78	0.66
59:S1:356:ASP:OD2	59:S1:636:TYR:OH	2.14	0.66
68:V2:182:ASN:HB3	68:V2:194:GLU:HB3	1.76	0.66
27:B4:71:ALA:HB2	31:B8:38:PRO:HG2	1.78	0.66
20:AK:64:VAL:HA	20:AK:205:VAL:O	1.96	0.65
50:Qd:125:CYS:SG	84:Qd:402:HEC:HAC	2.36	0.65
67:V1:112:TYR:HB2	67:V1:240:THR:HG22	1.77	0.65
37:C3:151:LEU:HD13	37:C3:159:MET:HG2	1.77	0.65
53:Qg:53:GLU:OE2	54:Qh:12:ARG:NH1	2.29	0.65
59:S1:149:ASP:HB2	60:S2:367:ALA:HB3	1.77	0.65
47:Qa:313:VAL:HG21	47:Qa:323:VAL:HG11	1.78	0.65
3:5B:86:LYS:NZ	38:C4:33:TYR:OH	2.29	0.65
72:AL:204:CDL:H852	45:N5:558:LEU:HD21	1.77	0.65
40:CB:2:THR:HB	40:CB:5:SER:HB3	1.78	0.65
35:C1:304:TYR:HB2	82:C1:609:PEE:H61	1.79	0.65
41:N1:180:PRO:HB3	82:S8:303:PEE:H21	1.78	0.65
29:B6:132:VAL:O	29:B6:136:LEU:HB3	1.97	0.65
47:Qa:51:SER:HB3	47:Qa:230:LEU:HD12	1.78	0.65
6:6C:53:TYR:OH	36:C2:188:ARG:NH1	2.29	0.64
35:C1:424:THR:HA	35:C1:454:SER:HA	1.80	0.64
54:QH:37:ASN:ND2	72:Qd:401:CDL:OB4	2.30	0.64
59:S1:405:THR:HB	59:S1:477:GLY:HA3	1.79	0.64
16:A7:32:SER:OG	16:A7:36:GLN:NE2	2.31	0.64
20:AK:182:ARG:NH1	20:AK:184:GLN:OE1	2.30	0.64
50:Qd:289:MET:HG2	82:Qd:403:PEE:H2	1.77	0.64
51:Qe:244:ASP:OD2	51:Qe:250:ARG:NH2	2.29	0.64
37:C3:221:ARG:HH22	71:C3:301:PC1:H111	1.62	0.64
59:S1:338:VAL:O	59:S1:365:SER:HB2	1.97	0.64
59:S1:387:LEU:HD12	59:S1:514:ASN:HB3	1.80	0.64
60:S2:412:GLU:OE2	61:S3:140:ARG:NH2	2.30	0.64
22:AM:34:ARG:NH2	66:S8:89:GLU:OE2	2.31	0.64
51:Qe:234:TYR:HB2	51:Qe:243:TYR:HB2	1.78	0.64
8:7B:53:TRP:HE1	38:C4:111:ILE:HG22	1.63	0.64
59:S1:266:ARG:HD2	59:S1:267:THR:HG23	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
71:6A:101:PC1:H392	71:6A:101:PC1:H281	1.80	0.64
20:AK:64:VAL:HG13	20:AK:207:VAL:HB	1.79	0.64
52:Qf:60:ARG:NH1	54:Qh:78:TYR:O	2.31	0.64
35:C1:124:THR:HG21	35:C1:133:ALA:HB2	1.79	0.63
67:V1:281:HIS:ND1	67:V1:358:ASP:OD1	2.31	0.63
77:QE:301:PLX:H291	76:QE:303:3PE:H2I3	1.80	0.63
51:Qe:187:GLU:OE1	51:Qe:248:ARG:NH2	2.32	0.63
72:CB:203:CDL:H231	72:CB:203:CDL:H401	1.81	0.63
59:S1:484:SER:HB2	59:S1:680:LEU:HD11	1.80	0.63
47:QA:77:LEU:O	47:QA:196:ARG:NH1	2.25	0.63
47:Qa:51:SER:HG	47:Qa:227:HIS:HD1	1.47	0.63
59:S1:246:ARG:HH22	62:S4:123:ASN:HD21	1.47	0.63
59:S1:299:ARG:NH1	59:S1:703:ALA:O	2.31	0.63
60:S2:308:LEU:HB2	60:S2:407:GLU:HB2	1.81	0.63
67:V1:280:GLY:O	68:V2:143:ARG:NH1	2.32	0.63
48:QB:301:ASN:ND2	48:QB:347:CYS:SG	2.68	0.63
51:QE:140:MET:O	49:Qc:177:ARG:NH2	2.32	0.63
51:Qe:262:THR:HB	51:Qe:274:GLY:O	1.99	0.63
65:S7:51:ASP:OD1	65:S7:55:ASN:ND2	2.31	0.63
11:A1:46:ASN:ND2	46:N6:132:ASP:OD2	2.32	0.62
20:AK:62:ILE:O	20:AK:160:VAL:HA	1.98	0.62
35:C1:96:ARG:HD2	37:C3:57:TRP:HE1	1.63	0.62
40:CB:13:LEU:HD21	63:S5:4:PHE:HB3	1.81	0.62
47:QA:90:THR:HG23	47:QA:95:SER:HA	1.81	0.62
49:QC:165:TRP:O	49:QC:174:THR:OG1	2.17	0.62
49:QC:233:LEU:HG	50:QD:297:MET:HE1	1.80	0.62
35:C1:169:ILE:O	35:C1:172:LYS:NZ	2.33	0.62
60:S2:155:GLN:NE2	60:S2:315:ASP:OD2	2.32	0.62
47:QA:70:ARG:HD2	47:QA:185:ALA:HB1	1.82	0.62
53:QG:72:ARG:NH1	53:QG:74:GLN:OE1	2.32	0.62
72:AL:204:CDL:HA32	72:AL:204:CDL:H521	1.81	0.62
42:N2:289:ASN:HA	42:N2:292:PHE:CE2	2.34	0.62
17:A8:219:TYR:OH	28:B5:189:ASN:ND2	2.32	0.62
38:C4:155:GLY:H	38:C4:158:ALA:HB3	1.64	0.62
31:B8:110:ASP:HB3	44:N4:278:ARG:HH11	1.65	0.62
33:BK:60:ARG:NH1	33:BK:62:TYR:OH	2.32	0.62
42:N2:252:GLY:HA3	42:N2:290:LEU:HD13	1.81	0.62
45:N5:387:THR:HG22	45:N5:465:GLY:H	1.65	0.62
60:S2:222:ARG:NH1	60:S2:249:ASP:OD2	2.28	0.62
18:A9:50:SER:OG	61:S3:225:GLU:OE2	2.17	0.62
1:4L:23:ARG:HH21	46:N6:86:ASN:HD22	1.48	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:B2:87:PRO:HD2	30:B7:99:MET:HE1	1.82	0.62
72:CB:203:CDL:H421	72:CB:203:CDL:H822	1.82	0.62
41:N1:24:GLU:OE2	41:N1:274:ARG:NH1	2.33	0.62
48:Qb:87:ASN:HD22	48:Qb:204:PRO:HD3	1.64	0.62
59:S1:308:ARG:NH1	59:S1:312:GLY:O	2.33	0.62
34:BL:89:VAL:HG21	44:N4:25:ILE:HG23	1.81	0.61
62:S4:62:THR:HG23	62:S4:72:ILE:HD13	1.80	0.61
15:A6:66:TYR:O	15:A6:86:ARG:NH1	2.32	0.61
41:N1:231:ILE:O	41:N1:235:ASN:ND2	2.34	0.61
43:N3:31:SER:O	43:N3:33:LYS:NZ	2.33	0.61
27:B4:15:PRO:HG2	27:B4:18:LEU:HB2	1.82	0.61
67:V1:128:ARG:NH2	68:V2:194:GLU:OE2	2.32	0.61
49:QC:81:TYR:OH	50:QD:203:ARG:NH1	2.34	0.61
59:S1:433:GLY:O	59:S1:444:HIS:NE2	2.31	0.61
48:QB:280:ASP:HA	48:QB:461:PRO:HB3	1.83	0.61
64:S6:104:LYS:HE3	64:S6:107:LYS:HD3	1.81	0.61
68:V2:108:PRO:HB2	68:V2:111:ARG:HG2	1.82	0.61
20:AK:94:HIS:HA	20:AK:97:ASP:HB2	1.81	0.61
59:S1:224:ASP:OD2	59:S1:291:ARG:NH2	2.33	0.61
48:Qb:388:VAL:HG21	48:Qb:438:ALA:HA	1.83	0.61
59:S1:433:GLY:HA2	59:S1:447:ASP:HA	1.82	0.61
60:S2:214:GLU:OE2	60:S2:227:ARG:NH2	2.33	0.61
2:5A:98:CYS:SG	2:5A:106:SER:OG	2.52	0.61
45:N5:100:ILE:HG21	45:N5:246:LEU:HB2	1.83	0.61
47:QA:92:LYS:HD2	47:QA:143:ALA:HB1	1.83	0.61
67:V1:140:GLU:OE2	67:V1:256:ARG:NH1	2.32	0.61
3:5B:41:GLU:HG2	3:5B:56:ARG:HH22	1.66	0.61
71:QC:407:PC1:H3E2	77:QI:301:PLX:H381	1.81	0.61
68:V2:68:LYS:NZ	69:V3:407:SER:OG	2.31	0.61
71:6A:101:PC1:H112	37:C3:187:THR:HA	1.82	0.60
19:AB:116:VAL:HG12	19:AB:120:MET:HE2	1.83	0.60
59:S1:426:ASP:OD2	69:V3:418:ARG:NH2	2.34	0.60
66:S8:144:ARG:NH1	66:S8:146:ASP:OD2	2.31	0.60
18:A9:129:LEU:HD23	18:A9:167:ILE:HG13	1.82	0.60
40:CB:13:LEU:HD11	63:S5:6:VAL:HG12	1.83	0.60
51:QE:227:ASN:N	51:QE:233:GLY:O	2.32	0.60
67:V1:113:LEU:HD13	67:V1:149:MET:HE1	1.84	0.60
22:AM:106:ARG:HB2	22:AM:109:ILE:HG13	1.82	0.60
37:C3:156:ARG:NH1	37:C3:222:GLN:O	2.33	0.60
53:QG:19:LYS:NZ	53:QG:85:GLU:OE2	2.33	0.60
47:Qa:66:LYS:HB2	47:Qa:217:ARG:HB3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
76:S7:302:3PE:H391	76:S7:302:3PE:H3E1	1.83	0.60
9:7C:62:LYS:NZ	35:C1:117:MET:O	2.35	0.60
72:CB:203:CDL:H401	72:CB:203:CDL:H262	1.83	0.60
51:QE:196:ARG:NH1	51:QE:254:ALA:O	2.35	0.60
48:Qb:195:THR:HG21	48:Qb:269:ARG:H	1.67	0.60
71:C1:606:PC1:H11	71:C1:606:PC1:H132	1.83	0.60
60:S2:145:LEU:HD13	60:S2:430:ILE:HG21	1.84	0.60
11:A1:66:LEU:HB3	17:A8:152:LYS:HE2	1.84	0.60
49:QC:47:THR:HG22	49:QC:79:ILE:HG23	1.83	0.60
62:S4:171:ARG:NH1	67:V1:217:GLU:OE1	2.27	0.60
21:AL:17:GLU:HG3	21:AL:20:ARG:HH21	1.66	0.60
59:S1:282:ASN:ND2	59:S1:285:TRP:O	2.35	0.60
17:A8:174:PHE:HB3	17:A8:178:ARG:HH12	1.66	0.60
57:QK:1:MET:O	57:QK:7:ARG:NH1	2.35	0.60
48:Qb:104:ARG:NH2	48:Qb:145:GLU:OE2	2.34	0.60
60:S2:63:GLU:HA	60:S2:66:HIS:CD2	2.36	0.60
48:QB:156:LEU:O	48:QB:213:ARG:NH1	2.34	0.59
51:QE:110:ARG:NH1	54:Qh:22:PHE:O	2.34	0.59
36:C2:173:ASP:O	36:C2:180:ASN:ND2	2.34	0.59
49:QC:229:ILE:HG23	77:QE:301:PLX:H151	1.83	0.59
35:C1:178:GLN:H	71:C1:607:PC1:H142	1.68	0.59
48:QB:467:ASP:OD2	49:QC:223:TYR:OH	2.20	0.59
52:Qf:38:GLU:OE1	52:Qf:47:ARG:NH2	2.34	0.59
52:Qf:53:CYS:SG	52:Qf:56:ARG:NH2	2.74	0.59
60:S2:188:ASN:OD1	60:S2:410:LYS:NZ	2.36	0.59
60:S2:374:ARG:NH2	66:S8:165:ASP:OD1	2.36	0.59
2:5A:130:GLN:HG3	6:6C:6:LEU:HD23	1.84	0.59
18:A9:279:TYR:HB2	18:A9:372:ALA:HB2	1.84	0.59
20:AK:241:ASN:HB3	20:AK:245:LYS:HE2	1.84	0.59
44:N4:122:PHE:HZ	44:N4:206:LYS:HG3	1.67	0.59
33:BK:99:ASP:OD2	33:BK:142:ARG:NH1	2.34	0.59
35:C1:62:ALA:HB2	79:C1:602:HEA:HBD1	1.84	0.59
2:5A:68:ASP:HA	2:5A:101:LEU:HD21	1.83	0.59
48:QB:181:ASP:OD1	48:QB:181:ASP:N	2.36	0.59
59:S1:666:GLN:NE2	59:S1:670:GLU:OE2	2.35	0.59
77:AM:201:PLX:H72	77:AM:203:PLX:H91	1.85	0.58
31:B8:83:GLN:HA	31:B8:86:ARG:HG3	1.84	0.58
35:C1:349:THR:HG21	36:C2:38:VAL:HG11	1.85	0.58
46:N6:103:MET:HA	46:N6:106:TYR:CZ	2.37	0.58
18:A9:204:SER:HB2	18:A9:266:VAL:HG12	1.84	0.58
20:AK:72:LYS:NZ	75:AK:401:ADP:O1A	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:AN:51:MET:HE2	41:N1:311:THR:HB	1.84	0.58
35:C1:438:ARG:NH1	79:C1:603:HEA:O1D	2.35	0.58
49:QC:100:ARG:NH2	83:QC:403:HEM:O1A	2.36	0.58
67:V1:118:ASP:HB3	67:V1:207:GLY:HA2	1.85	0.58
2:5A:143:THR:HG22	2:5A:145:GLU:H	1.69	0.58
13:A3:151:VAL:O	17:A8:207:LYS:NZ	2.30	0.58
47:QA:148:ARG:NH2	53:QG:50:ARG:O	2.35	0.58
48:QB:204:PRO:HG2	48:QB:207:ASN:HB2	1.84	0.58
14:A5:20:PRO:HB3	14:A5:77:ILE:HG21	1.86	0.58
28:B5:92:PHE:O	33:BK:59:ASN:ND2	2.36	0.58
35:C1:51:ASP:OD1	35:C1:55:ASN:ND2	2.37	0.58
36:C2:110:TYR:HB2	36:C2:116:LEU:HD12	1.86	0.58
36:C2:111:THR:O	36:C2:111:THR:OG1	2.21	0.58
45:N5:295:GLN:O	45:N5:425:ARG:NH1	2.36	0.58
55:QI:48:ASN:HD21	50:Qd:104:SER:HA	1.69	0.58
44:N4:392:THR:O	44:N4:396:MET:HG2	2.03	0.58
47:QA:116:ARG:HH12	47:QA:189:SER:HA	1.67	0.58
20:AK:67:ASN:OD1	20:AK:68:ILE:N	2.26	0.58
43:N3:68:GLU:HG3	43:N3:98:LEU:HD13	1.84	0.58
44:N4:369:LEU:HD21	45:N5:149:ILE:HD13	1.85	0.58
50:QD:292:LYS:NZ	55:Qi:37:ASP:OD1	2.30	0.58
54:QH:26:ALA:H	71:QH:102:PC1:H132	1.68	0.58
49:Qc:200:LEU:HD23	49:Qc:201:HIS:HD2	1.68	0.58
17:A8:196:ARG:NH2	23:AN:63:GLU:OE2	2.36	0.58
51:QE:125:VAL:HG21	77:QE:301:PLX:H111	1.85	0.58
48:Qb:42:LEU:HD22	48:Qb:426:LEU:HB3	1.85	0.58
8:7B:53:TRP:CE2	38:C4:115:ALA:HB2	2.39	0.58
35:C1:38:ARG:NH2	35:C1:451:ASN:O	2.36	0.58
67:V1:113:LEU:O	67:V1:154:ALA:HA	2.02	0.58
2:5A:104:PHE:N	38:C4:66:GLU:OE2	2.33	0.58
9:7C:59:GLN:NE2	35:C1:116:SER:O	2.36	0.58
20:AK:255:CYS:SG	20:AK:256:GLU:N	2.71	0.58
49:Qc:237:LEU:HD13	50:Qd:297:MET:HG2	1.85	0.58
49:QC:138:MET:HE1	49:QC:268:ILE:HA	1.86	0.58
49:Qc:213:SER:OG	49:Qc:217:LYS:NZ	2.37	0.58
53:Qg:36:ASP:OD2	53:Qg:62:ARG:NH1	2.37	0.58
59:S1:251:ILE:HG21	59:S1:604:GLN:HB3	1.85	0.58
59:S1:593:SER:HA	59:S1:606:THR:O	2.04	0.58
20:AK:134:GLN:HE22	75:AK:401:ADP:HN62	1.52	0.57
42:N2:26:TRP:HB3	42:N2:74:ILE:HD13	1.86	0.57
47:QA:70:ARG:NH2	47:QA:332:ASP:OD2	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:QE:205:VAL:HG11	51:QE:211:VAL:HG22	1.85	0.57
20:AK:92:GLY:H	20:AK:95:TYR:HB3	1.68	0.57
35:C1:347:LEU:HD13	35:C1:383:MET:HB3	1.85	0.57
44:N4:445:LEU:HB3	72:N5:702:CDL:H452	1.85	0.57
5:6B:33:ASN:HB2	5:6B:61:TYR:CE2	2.40	0.57
35:C1:101:SER:O	35:C1:156:SER:OG	2.20	0.57
36:C2:161:HIS:CE1	36:C2:207:MET:HE1	2.39	0.57
51:QE:172:LYS:NZ	49:Qc:168:PHE:O	2.37	0.57
52:Qf:40:ILE:HG13	52:Qf:43:CYS:H	1.69	0.57
59:S1:419:ARG:NH1	59:S1:439:THR:O	2.37	0.57
2:5A:55:ASP:HA	2:5A:90:ILE:HD11	1.87	0.57
20:AK:317:PRO:HB3	34:BL:54:ARG:HA	1.85	0.57
25:B2:54:GLN:NE2	45:N5:367:PRO:HD2	2.19	0.57
47:QA:151:VAL:O	47:QA:155:GLN:HG2	2.04	0.57
5:6B:7:THR:O	5:6B:11:ASN:ND2	2.38	0.57
17:A8:84:LEU:O	23:AN:88:ARG:NH1	2.38	0.57
41:N1:173:TRP:HB3	41:N1:175:ILE:HG22	1.86	0.57
60:S2:146:ASP:OD2	60:S2:149:SER:OG	2.22	0.57
5:6B:39:ARG:NH2	5:6B:85:LYS:O	2.36	0.57
72:CB:203:CDL:H722	72:CB:203:CDL:H321	1.85	0.57
42:N2:95:MET:HE2	42:N2:149:ILE:HA	1.87	0.57
42:N2:170:LEU:HD11	42:N2:288:LEU:HD22	1.86	0.57
67:V1:288:VAL:HG21	67:V1:303:HIS:CD2	2.40	0.57
2:5A:114:VAL:HG11	2:5A:128:VAL:HG11	1.86	0.57
41:N1:24:GLU:HA	41:N1:271:LEU:HD13	1.86	0.57
42:N2:42:PRO:HG2	46:N6:167:VAL:HG22	1.86	0.57
48:QB:126:ARG:NH1	48:QB:199:GLN:O	2.38	0.57
36:C2:102:HIS:CD2	36:C2:157:GLU:HG3	2.40	0.57
72:CB:203:CDL:HA62	42:N2:239:VAL:HG22	1.87	0.57
50:QD:112:ARG:NH2	50:QD:145:GLU:OE1	2.37	0.57
48:Qb:274:GLU:OE2	48:Qb:276:ARG:NE	2.29	0.57
49:Qc:126:THR:HG21	83:Qc:402:HEM:HBB2	1.85	0.57
22:AM:76:ASP:OD1	65:S7:185:LYS:NZ	2.37	0.57
42:N2:131:LEU:O	42:N2:135:LYS:HG2	2.05	0.57
50:QD:127:SER:HB3	50:QD:179:PRO:HD2	1.87	0.57
50:Qd:232:LEU:HD13	50:Qd:242:ALA:HB1	1.87	0.57
59:S1:219:SER:OG	59:S1:288:ASP:OD2	2.22	0.57
60:S2:469:ARG:NH2	61:S3:169:GLU:OE2	2.38	0.57
47:Qa:301:ARG:NH2	48:Qb:94:GLU:OE2	2.38	0.57
51:QE:234:TYR:HB2	51:QE:243:TYR:HB2	1.87	0.56
52:Qf:33:VAL:HG12	52:Qf:82:VAL:HG22	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:A9:61:ALA:HB3	18:A9:82:VAL:HG13	1.87	0.56
18:A9:211:ASP:O	18:A9:215:ASN:ND2	2.36	0.56
72:AL:201:CDL:H122	76:AL:202:3PE:H242	1.87	0.56
42:N2:323:MET:N	42:N2:323:MET:SD	2.77	0.56
6:6C:63:GLU:OE1	6:6C:66:ARG:NH2	2.37	0.56
29:B6:85:ASP:O	32:B9:163:LYS:NZ	2.37	0.56
35:C1:107:PRO:HB3	37:C3:25:LEU:HB2	1.87	0.56
47:QA:69:SER:HB3	47:QA:188:ASN:HB2	1.88	0.56
47:Qa:151:VAL:O	47:Qa:155:GLN:HG2	2.05	0.56
60:S2:275:ARG:O	60:S2:279:VAL:HB	2.05	0.56
1:4L:6:MET:HE3	46:N6:103:MET:HE3	1.87	0.56
3:5B:84:THR:OG1	3:5B:85:ASN:N	2.38	0.56
71:6A:101:PC1:H152	37:C3:187:THR:HA	1.86	0.56
35:C1:352:GLY:C	79:C1:603:HEA:H162	2.30	0.56
35:C1:406:ASN:HB3	35:C1:409:TRP:HB2	1.87	0.56
44:N4:403:THR:HA	44:N4:406:TYR:CE2	2.41	0.56
49:QC:71:ARG:NH2	50:QD:278:ALA:O	2.33	0.56
61:S3:132:LEU:HB2	61:S3:141:ILE:HG22	1.86	0.56
17:A8:198:ASP:N	17:A8:201:GLU:OE1	2.38	0.56
17:A8:243:ARG:NH2	40:CB:89:ASP:OD1	2.31	0.56
33:BK:142:ARG:NH1	33:BK:143:TYR:OH	2.39	0.56
5:6B:65:CYS:O	36:C2:98:LYS:NZ	2.37	0.56
35:C1:347:LEU:HD13	35:C1:383:MET:HE2	1.88	0.56
35:C1:443:TYR:O	36:C2:134:ARG:NH2	2.38	0.56
52:QF:60:ARG:HD3	52:QF:63:THR:HG21	1.87	0.56
54:Qh:57:TYR:HD1	82:Qh:101:PEE:H11	1.71	0.56
59:S1:279:GLU:OE2	62:S4:156:LYS:NZ	2.38	0.56
1:4L:73:LEU:HD21	42:N2:41:ILE:HG13	1.88	0.56
36:C2:200:CYS:SG	36:C2:207:MET:CE	2.93	0.56
76:CA:101:3PE:H3E1	42:N2:325:LEU:HD11	1.88	0.56
45:N5:97:THR:HG21	45:N5:125:LEU:HD22	1.87	0.56
48:QB:388:VAL:HG21	48:QB:438:ALA:HA	1.88	0.56
20:AK:94:HIS:HB3	20:AK:105:PRO:HB3	1.86	0.56
47:Qa:379:LYS:HG2	47:Qa:413:LEU:HD22	1.87	0.56
3:5B:109:GLU:OE1	3:5B:110:THR:N	2.38	0.56
6:6C:47:LYS:NZ	6:6C:51:ASP:OD2	2.38	0.56
77:AM:201:PLX:H291	77:AM:201:PLX:H102	1.88	0.56
35:C1:374:VAL:HA	35:C1:377:PHE:CE2	2.40	0.56
44:N4:70:THR:HA	44:N4:103:GLN:HE21	1.70	0.56
51:Qe:153:GLU:HB3	51:Qe:270:LEU:HD11	1.88	0.56
72:Qh:102:CDL:H311	72:Qh:102:CDL:H721	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:B1:50:ARG:NH2	28:B5:106:VAL:O	2.39	0.56
41:N1:149:ILE:HG21	41:N1:185:TRP:HB2	1.88	0.56
42:N2:36:ASN:OD1	42:N2:134:GLN:NE2	2.37	0.56
50:Qd:211:TYR:OH	84:Qd:402:HEC:O1A	2.20	0.56
59:S1:43:VAL:HG12	59:S1:55:LYS:HD2	1.88	0.56
59:S1:244:GLU:OE1	59:S1:266:ARG:NH1	2.37	0.56
5:6B:30:CYS:HA	5:6B:61:TYR:CE1	2.41	0.55
35:C1:184:PHE:H	35:C1:256:HIS:HE1	1.53	0.55
51:QE:209:GLU:HG3	51:QE:210:TRP:CD1	2.41	0.55
67:V1:88:ARG:O	67:V1:244:ASN:ND2	2.39	0.55
1:4L:98:CYS:HB3	45:N5:580:GLN:HB2	1.87	0.55
35:C1:135:ASN:ND2	35:C1:213:ARG:O	2.40	0.55
50:QD:159:PRO:HB2	50:Qd:184:GLU:HG3	1.88	0.55
19:AB:115:GLN:NE2	19:AB:135:ALA:O	2.37	0.55
19:AC:156:GLU:OE1	28:B5:52:LYS:NZ	2.39	0.55
45:N5:11:THR:HG22	45:N5:46:LEU:HB3	1.89	0.55
45:N5:23:ASN:HD22	72:N5:702:CDL:HB4	1.70	0.55
49:QC:43:LEU:O	49:QC:47:THR:OG1	2.25	0.55
72:QH:101:CDL:H711	72:Qd:401:CDL:H152	1.88	0.55
14:A5:44:TYR:O	14:A5:48:THR:HG22	2.06	0.55
22:AM:88:ARG:HD3	66:S8:200:GLU:HG3	1.88	0.55
35:C1:265:LYS:HD2	35:C1:490:THR:HG21	1.87	0.55
45:N5:375:ILE:HD12	45:N5:458:LEU:HD11	1.89	0.55
5:6B:62:LYS:O	36:C2:111:THR:OG1	2.23	0.55
18:A9:173:ASP:HB3	18:A9:176:SER:HB2	1.88	0.55
77:CB:201:PLX:H1B3	63:S5:2:PRO:HD2	1.89	0.55
45:N5:249:SER:HA	45:N5:306:THR:HG21	1.87	0.55
49:Qc:106:SER:OG	83:Qc:403:HEM:O1D	2.19	0.55
50:Qd:216:LEU:HB3	50:Qd:249:ILE:HD11	1.87	0.55
68:V2:187:GLN:HE21	68:V2:190:ASP:HA	1.70	0.55
18:A9:188:GLU:HG3	18:A9:200:ILE:HD13	1.87	0.55
19:AC:119:ILE:HG21	19:AC:135:ALA:HB1	1.89	0.55
59:S1:144:MET:HG3	60:S2:389:LYS:HG3	1.89	0.55
46:N6:34:ILE:HD13	46:N6:61:LEU:HD22	1.89	0.55
47:QA:180:ALA:HB2	47:QA:258:ILE:HG13	1.87	0.55
34:BL:77:ASP:OD1	34:BL:78:LYS:N	2.39	0.55
49:QC:126:THR:HG21	83:QC:402:HEM:HBB2	1.89	0.55
48:Qb:165:ARG:NH1	48:Qb:208:VAL:O	2.39	0.55
72:Qh:102:CDL:H362	72:Qh:102:CDL:H762	1.88	0.55
59:S1:667:GLN:OE1	59:S1:667:GLN:N	2.38	0.55
39:CA:72:ARG:NH2	40:CB:18:ASN:OD1	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:N4:1:MET:HE2	44:N4:111:THR:HG21	1.89	0.55
47:QA:313:VAL:HG11	47:QA:350:VAL:HG13	1.89	0.55
51:QE:199:GLN:NE2	51:QE:257:ASN:OD1	2.40	0.55
52:QF:38:GLU:OE1	52:QF:47:ARG:NH2	2.40	0.55
59:S1:476:LEU:HD21	59:S1:481:LEU:HD21	1.88	0.55
36:C2:98:LYS:HG2	36:C2:153:LEU:HB2	1.89	0.54
44:N4:282:LEU:HD13	44:N4:342:MET:HG3	1.88	0.54
2:5A:73:ARG:HA	38:C4:46:LEU:HD12	1.90	0.54
45:N5:103:PHE:HB2	45:N5:341:MET:HE3	1.89	0.54
82:N5:701:PEE:H33	72:N5:702:CDL:H231	1.89	0.54
49:QC:25:SER:OG	49:QC:216:ASP:OD2	2.24	0.54
49:QC:197:LEU:HD11	83:QC:403:HEM:HMA3	1.88	0.54
51:Qe:244:ASP:HB3	51:Qe:250:ARG:HE	1.71	0.54
1:4L:37:MET:HE3	1:4L:67:ALA:HB2	1.87	0.54
6:6C:49:TYR:CE1	38:C4:153:ILE:HD13	2.43	0.54
18:A9:238:GLN:OE1	18:A9:270:ARG:NH1	2.41	0.54
35:C1:184:PHE:H	35:C1:256:HIS:CE1	2.25	0.54
49:QC:100:ARG:NH1	83:QC:403:HEM:HBD1	2.21	0.54
47:Qa:84:ARG:NH1	47:Qa:114:SER:OG	2.40	0.54
28:B5:152:LYS:HD3	40:CB:96:VAL:HG21	1.88	0.54
35:C1:74:MET:HE3	35:C1:389:ILE:HG13	1.88	0.54
35:C1:316:THR:HG22	79:C1:603:HEA:H18	1.89	0.54
45:N5:253:VAL:HG23	45:N5:310:LEU:HD21	1.89	0.54
72:QH:101:CDL:H722	72:Qd:401:CDL:H172	1.89	0.54
51:Qe:204:ARG:NE	51:Qe:246:SER:O	2.35	0.54
22:AM:55:PHE:CZ	22:AM:58:ARG:HG3	2.42	0.54
35:C1:37:ILE:HD11	35:C1:58:VAL:HA	1.89	0.54
44:N4:211:GLY:H	44:N4:213:HIS:CD2	2.25	0.54
47:QA:178:HIS:NE2	47:QA:330:TYR:OH	2.34	0.54
47:QA:207:TYR:O	47:QA:211:ASN:ND2	2.30	0.54
48:Qb:276:ARG:NH2	48:Qb:466:PRO:O	2.41	0.54
8:7B:71:ARG:HG3	8:7B:72:VAL:HG23	1.89	0.54
47:Qa:177:LEU:HD11	47:Qa:272:VAL:HG22	1.89	0.54
47:Qa:319:GLN:HE21	47:Qa:320:PRO:HD2	1.72	0.54
5:6B:33:ASN:HB2	5:6B:61:TYR:OH	2.07	0.54
6:6C:60:LYS:NZ	6:6C:64:GLU:OE2	2.34	0.54
27:B4:14:LEU:HD12	27:B4:15:PRO:HD2	1.90	0.54
44:N4:122:PHE:CZ	44:N4:206:LYS:HG3	2.43	0.54
44:N4:391:ILE:HG23	44:N4:394:ILE:HD12	1.88	0.54
52:QF:71:LEU:HD22	50:Qd:223:PRO:HG3	1.89	0.54
47:Qa:214:THR:HG22	47:Qa:241:ARG:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:Qb:370:PHE:HE1	72:Qb:501:CDL:HA21	1.73	0.54
5:6B:9:ILE:HG12	5:6B:56:TRP:HB2	1.90	0.54
25:B2:44:TYR:HB2	26:B3:14:MET:HE1	1.90	0.54
44:N4:373:ILE:HD11	44:N4:444:LEU:HD23	1.90	0.54
47:Qa:81:HIS:CD2	47:Qa:192:CYS:H	2.20	0.54
51:Qe:95:GLU:N	51:Qe:95:GLU:OE1	2.39	0.54
53:Qg:36:ASP:OD1	53:Qg:90:TYR:OH	2.16	0.54
59:S1:388:ASN:ND2	59:S1:513:MET:O	2.32	0.54
6:6C:49:TYR:HE1	38:C4:153:ILE:HD13	1.71	0.54
47:Qa:65:ILE:HG12	47:Qa:218:MET:HG2	1.89	0.54
44:N4:361:VAL:HG22	72:N5:702:CDL:H311	1.90	0.54
61:S3:155:SER:OG	61:S3:167:GLU:OE1	2.26	0.54
6:6C:38:LYS:HE2	36:C2:29:MET:HE1	1.88	0.53
35:C1:233:HIS:CD2	35:C1:292:MET:HE1	2.44	0.53
37:C3:112:LEU:HD13	37:C3:118:PRO:HG3	1.90	0.53
40:CB:37:GLY:HA3	76:CB:202:3PE:H271	1.90	0.53
41:N1:25:ARG:NH1	65:S7:87:ASP:OD1	2.41	0.53
45:N5:274:GLN:NE2	45:N5:320:ASN:OD1	2.41	0.53
49:QC:92:ILE:HD11	72:QC:406:CDL:H742	1.90	0.53
59:S1:394:VAL:HA	59:S1:473:MET:HE1	1.90	0.53
64:S6:74:GLN:HG3	66:S8:108:SER:HB2	1.90	0.53
19:AC:94:ASP:HB3	19:AC:97:LYS:HG2	1.90	0.53
23:AN:98:MET:HE3	23:AN:101:VAL:HG21	1.89	0.53
35:C1:447:TYR:O	35:C1:451:ASN:ND2	2.42	0.53
45:N5:362:LEU:HA	45:N5:365:ALA:HB3	1.89	0.53
48:QB:195:THR:HG21	48:QB:268:CYS:HB3	1.89	0.53
77:QI:301:PLX:H192	49:Qc:232:ALA:HB1	1.89	0.53
37:C3:2:THR:OG1	37:C3:3:HIS:N	2.37	0.53
48:QB:165:ARG:HD3	48:QB:209:ARG:HA	1.90	0.53
63:S5:15:ASP:N	63:S5:15:ASP:OD1	2.39	0.53
69:V3:399:PHE:HD2	69:V3:400:LEU:HD12	1.74	0.53
20:AK:141:ARG:NH2	75:AK:401:ADP:N7	2.55	0.53
35:C1:352:GLY:HA3	79:C1:603:HEA:H14	1.91	0.53
44:N4:446:LEU:HB3	77:N4:501:PLX:H272	1.90	0.53
50:QD:187:ARG:HB3	50:QD:192:GLY:HA2	1.90	0.53
59:S1:274:LEU:HD21	62:S4:87:MET:HE2	1.88	0.53
3:5B:45:THR:OG1	3:5B:46:GLY:N	2.40	0.53
30:B7:29:TYR:OH	30:B7:111:ARG:NH2	2.42	0.53
72:QC:406:CDL:H792	82:Qh:101:PEE:H23	1.91	0.53
49:Qc:137:GLN:NE2	49:Qc:263:ASN:O	2.42	0.53
16:A7:34:ARG:NH2	66:S8:93:LEU:O	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:B1:47:ARG:NH2	24:B1:53:GLU:OE2	2.42	0.53
28:B5:163:ARG:NH1	40:CB:102:ASP:OD2	2.26	0.53
42:N2:128:LEU:HD12	42:N2:216:PHE:HB3	1.91	0.53
51:QE:196:ARG:NH2	51:QE:252:GLY:O	2.36	0.53
21:AL:43:LEU:HD12	72:AL:201:CDL:H522	1.90	0.53
30:B7:44:GLN:NE2	30:B7:48:ASP:OD1	2.42	0.53
43:N3:73:LEU:HD13	46:N6:55:MET:HE1	1.90	0.53
45:N5:76:LEU:HD21	45:N5:196:TRP:HE3	1.74	0.53
65:S7:62:LEU:O	65:S7:91:VAL:HA	2.09	0.53
22:AM:42:ASP:OD2	22:AM:46:ASN:ND2	2.40	0.53
35:C1:173:PRO:HD2	35:C1:176:MET:HE2	1.90	0.53
37:C3:187:THR:N	37:C3:190:ASP:OD2	2.34	0.53
48:QB:460:GLY:HA2	48:QB:462:ILE:HG12	1.91	0.53
74:AC:201:ZMP:H19	32:B9:58:VAL:HG11	1.91	0.53
35:C1:65:MET:HB3	79:C1:602:HEA:CAC	2.39	0.53
41:N1:99:ASN:N	82:N1:401:PEE:O2P	2.32	0.53
44:N4:408:LEU:HD12	45:N5:172:ILE:HG21	1.90	0.53
50:Qd:118:TYR:HA	50:Qd:122:CYS:SG	2.48	0.53
54:Qh:37:ASN:ND2	72:Qh:102:CDL:OB4	2.37	0.53
68:V2:59:ASN:ND2	68:V2:89:GLN:OE1	2.41	0.53
18:A9:171:ASN:ND2	18:A9:327:MET:H	2.07	0.53
41:N1:37:PRO:HA	65:S7:88:ARG:HA	1.91	0.53
46:N6:112:GLU:HB3	46:N6:119:PHE:HD2	1.74	0.53
48:QB:195:THR:HG22	48:QB:197:LEU:H	1.73	0.53
49:Qc:311:LYS:NZ	49:Qc:379:TRP:OXT	2.41	0.53
59:S1:512:VAL:O	59:S1:514:ASN:ND2	2.41	0.53
61:S3:187:ILE:HG23	61:S3:188:LEU:HG	1.90	0.53
4:6A:88:ASN:ND2	71:6A:101:PC1:H151	2.24	0.52
17:A8:202:LEU:HD13	23:AN:70:ALA:HB2	1.90	0.52
48:QB:121:ASN:ND2	48:QB:132:TYR:OH	2.42	0.52
48:Qb:278:ARG:NH2	48:Qb:463:GLU:OE1	2.43	0.52
48:QB:54:ASP:OD1	48:QB:54:ASP:N	2.41	0.52
72:QC:408:CDL:H512	72:QC:408:CDL:HA61	1.90	0.52
50:Qd:243:ILE:HG12	50:Qd:245:MET:H	1.74	0.52
35:C1:229:ILE:HD11	36:C2:175:ILE:HG12	1.91	0.52
46:N6:33:LEU:HG	46:N6:65:LEU:HD11	1.90	0.52
59:S1:591:GLU:HG2	59:S1:610:VAL:HG23	1.90	0.52
60:S2:101:LEU:HD13	60:S2:464:PHE:HZ	1.74	0.52
29:B6:147:LYS:HE3	29:B6:148:TYR:CZ	2.44	0.52
32:B9:218:GLU:HG2	32:B9:219:ARG:HG2	1.91	0.52
35:C1:352:GLY:HA3	79:C1:603:HEA:H162	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:N5:421:ALA:O	45:N5:424:THR:OG1	2.26	0.52
48:QB:87:ASN:HD21	48:QB:199:GLN:HB3	1.74	0.52
72:QC:406:CDL:H141	72:QC:406:CDL:H182	1.91	0.52
47:Qa:92:LYS:HD3	47:Qa:143:ALA:HB1	1.92	0.52
53:Qg:46:GLU:OE2	53:Qg:49:ARG:NH1	2.43	0.52
59:S1:452:LEU:HD21	59:S1:493:VAL:HG13	1.92	0.52
60:S2:464:PHE:HA	60:S2:467:VAL:HB	1.91	0.52
1:4L:56:ALA:HA	63:S5:18:MET:HE3	1.92	0.52
18:A9:357:ARG:NH1	18:A9:365:GLU:OE1	2.40	0.52
19:AC:112:SER:HB3	32:B9:59:LEU:HD11	1.92	0.52
35:C1:334:TRP:HZ3	71:C1:606:PC1:H332	1.74	0.52
44:N4:232:ALA:O	44:N4:237:LYS:NZ	2.43	0.52
45:N5:419:THR:HA	45:N5:422:TYR:CE2	2.45	0.52
45:N5:536:LEU:HB3	45:N5:537:PRO:HD3	1.92	0.52
59:S1:488:ALA:HB2	59:S1:677:GLN:HG3	1.90	0.52
3:5B:87:ARG:NH2	35:C1:508:PRO:O	2.43	0.52
6:6C:69:GLY:HA3	8:7B:79:GLU:HG3	1.92	0.52
35:C1:3:VAL:HG13	35:C1:7:LEU:HD12	1.91	0.52
37:C3:204:HIS:O	37:C3:208:VAL:HG13	2.10	0.52
72:CB:203:CDL:H661	44:N4:13:PRO:HG3	1.90	0.52
42:N2:337:LEU:O	42:N2:340:THR:OG1	2.27	0.52
49:QC:51:LEU:HD13	83:QC:402:HEM:HBD1	1.92	0.52
52:QF:34:ARG:O	52:QF:38:GLU:HG2	2.09	0.52
49:Qc:8:HIS:HB3	49:Qc:11:MET:HB2	1.91	0.52
19:AC:134:ASP:OD2	32:B9:44:ALA:N	2.42	0.52
36:C2:91:ASN:OD1	36:C2:92:ASN:N	2.39	0.52
51:QE:154:ILE:HB	51:QE:271:VAL:HG23	1.92	0.52
51:QE:184:ILE:HD11	51:QE:209:GLU:HA	1.92	0.52
64:S6:36:GLU:OE2	64:S6:60:LYS:NZ	2.34	0.52
67:V1:43:THR:HG21	67:V1:59:ARG:HG2	1.92	0.52
19:AC:128:PHE:HE2	19:AC:151:LYS:HD3	1.75	0.52
33:BK:107:GLN:HE22	45:N5:194:ASN:ND2	2.08	0.52
35:C1:316:THR:HB	79:C1:603:HEA:H262	1.91	0.52
47:QA:298:HIS:HB2	48:QB:114:GLU:HG2	1.91	0.52
59:S1:356:ASP:O	59:S1:360:ARG:HG2	2.10	0.52
61:S3:89:HIS:CG	61:S3:90:PRO:HD2	2.44	0.52
37:C3:204:HIS:CE1	37:C3:249:TRP:HB2	2.45	0.51
47:QA:326:PHE:HA	57:QK:61:GLY:HA2	1.91	0.51
50:Qd:122:CYS:SG	84:Qd:402:HEC:HAB	2.50	0.51
51:Qe:190:VAL:HG21	51:Qe:250:ARG:NH2	2.25	0.51
51:Qe:241:SER:OG	85:Qe:301:FES:S2	2.63	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:S2:300:ARG:NH1	60:S2:342:GLU:OE2	2.43	0.51
4:6A:69:THR:N	35:C1:216:ASN:OD1	2.42	0.51
4:6A:82:PHE:O	71:6A:101:PC1:H143	2.11	0.51
20:AK:210:ASP:OD1	20:AK:244:LYS:NZ	2.29	0.51
72:AM:202:CDL:H521	72:AM:202:CDL:HA61	1.93	0.51
36:C2:162:SER:HB3	36:C2:197:SER:H	1.76	0.51
38:C4:39:VAL:HG22	38:C4:41:ARG:HG3	1.91	0.51
44:N4:211:GLY:H	44:N4:213:HIS:HD2	1.58	0.51
72:QC:406:CDL:H522	82:Qh:101:PEE:H15	1.92	0.51
71:QC:407:PC1:H133	71:QC:407:PC1:H32	1.93	0.51
54:QH:25:ARG:HD2	71:QH:102:PC1:H141	1.91	0.51
33:BK:107:GLN:HE22	45:N5:194:ASN:HD22	1.57	0.51
49:QC:141:TRP:CD1	49:QC:265:PRO:HD3	2.46	0.51
67:V1:380:GLY:O	67:V1:386:ARG:NH1	2.40	0.51
34:BL:95:PHE:O	34:BL:99:LEU:HB2	2.10	0.51
44:N4:383:THR:HG21	45:N5:190:LEU:HD22	1.92	0.51
59:S1:197:THR:HG22	59:S1:206:VAL:HG22	1.93	0.51
6:6C:73:SER:HB2	36:C2:222:TRP:HB2	1.92	0.51
12:A2:18:GLU:HG2	12:A2:68:ARG:HB3	1.93	0.51
22:AM:12:GLN:O	22:AM:16:GLY:N	2.44	0.51
47:QA:60:ARG:NH1	47:QA:124:GLU:OE1	2.43	0.51
49:QC:112:THR:HG22	49:QC:196:HIS:CE1	2.46	0.51
52:Qf:38:GLU:OE2	52:Qf:78:ARG:NH1	2.43	0.51
59:S1:306:MET:HB2	59:S1:583:ILE:HB	1.92	0.51
67:V1:162:PHE:HB3	67:V1:165:GLU:HB2	1.92	0.51
10:8B:55:GLY:O	10:8B:59:SER:N	2.44	0.51
32:B9:137:GLU:OE2	32:B9:140:LYS:NZ	2.43	0.51
44:N4:216:LEU:HB3	44:N4:217:PRO:HD3	1.93	0.51
45:N5:248:HIS:O	45:N5:253:VAL:HG22	2.10	0.51
46:N6:122:LEU:HD23	46:N6:126:VAL:HG11	1.91	0.51
17:A8:121:MET:HE2	23:AN:73:PRO:HA	1.92	0.51
30:B7:107:ARG:HA	30:B7:110:GLN:HG2	1.93	0.51
36:C2:129:LYS:N	36:C2:132:GLU:OE1	2.43	0.51
51:QE:156:LEU:HD11	51:QE:271:VAL:HG13	1.92	0.51
59:S1:185:PHE:CZ	59:S1:221:ASN:HB2	2.45	0.51
67:V1:112:TYR:O	67:V1:240:THR:HA	2.11	0.51
33:BK:115:GLN:HG2	45:N5:62:ILE:HG12	1.92	0.51
42:N2:342:ALA:O	42:N2:345:SER:OG	2.23	0.51
49:QC:344:GLU:HG3	54:Qh:67:PHE:HE1	1.76	0.51
47:Qa:162:LYS:NZ	47:Qa:194:ASP:OD1	2.31	0.51
67:V1:217:GLU:OE2	67:V1:224:ARG:NH2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:B1:29:ARG:NH2	77:B5:201:PLX:O3	2.44	0.51
37:C3:163:LEU:HD21	37:C3:235:PHE:HE1	1.76	0.51
44:N4:233:ALA:HA	44:N4:320:GLY:HA2	1.92	0.51
48:QB:80:ARG:NH2	48:QB:350:GLU:OE1	2.44	0.51
67:V1:270:ASN:OD1	67:V1:270:ASN:N	2.43	0.51
3:5B:98:SER:OG	35:C1:266:GLU:OE1	2.23	0.51
4:6A:63:HIS:HB2	5:6B:76:ARG:HH21	1.76	0.51
28:B5:74:TYR:O	34:BL:96:SER:OG	2.26	0.51
72:B5:202:CDL:H822	72:N5:702:CDL:H473	1.91	0.51
39:CA:43:LYS:O	39:CA:47:THR:OG1	2.29	0.51
47:QA:66:LYS:HB2	47:QA:217:ARG:HB3	1.92	0.51
47:QA:123:VAL:HB	47:QA:133:LEU:HD23	1.93	0.51
48:Qb:396:ARG:NE	48:Qb:430:GLU:OE2	2.44	0.51
67:V1:94:PRO:HB2	67:V1:97:LEU:HB2	1.93	0.51
47:QA:138:LEU:O	47:QA:142:ALA:HB3	2.11	0.50
54:Qh:37:ASN:OD1	54:Qh:40:ARG:NH2	2.34	0.50
59:S1:389:THR:HG21	59:S1:473:MET:HE2	1.94	0.50
77:AM:203:PLX:H391	76:S7:302:3PE:H2E2	1.93	0.50
34:BL:151:GLU:OE1	34:BL:151:GLU:N	2.44	0.50
35:C1:236:TRP:HH2	79:C1:603:HEA:HBD1	1.76	0.50
35:C1:406:ASN:HD22	35:C1:409:TRP:H	1.60	0.50
47:QA:399:GLN:HA	47:QA:402:VAL:HG22	1.93	0.50
67:V1:204:TYR:HB3	67:V1:377:GLU:HB3	1.93	0.50
23:AN:16:TYR:OH	60:S2:248:ASP:OD1	2.25	0.50
23:AN:93:GLU:HG3	63:S5:98:HIS:CD2	2.46	0.50
42:N2:100:MET:HE1	45:N5:595:ILE:HG23	1.93	0.50
42:N2:112:HIS:O	42:N2:116:PRO:HD2	2.11	0.50
47:Qa:63:LEU:HD23	47:Qa:141:THR:HG21	1.93	0.50
48:Qb:393:ASN:OD1	48:Qb:396:ARG:NH1	2.44	0.50
50:Qd:147:LYS:NZ	50:Qd:151:GLU:OE2	2.30	0.50
59:S1:251:ILE:HD11	59:S1:596:TYR:HB2	1.92	0.50
59:S1:306:MET:HE2	59:S1:314:LEU:HB3	1.93	0.50
60:S2:194:THR:HB	60:S2:206:PHE:HA	1.92	0.50
5:6B:33:ASN:C	5:6B:61:TYR:HE2	2.19	0.50
14:A5:93:LYS:HG2	14:A5:96:ARG:HH22	1.75	0.50
31:B8:48:ARG:NH2	31:B8:62:TYR:O	2.44	0.50
79:C1:603:HEA:HBA2	79:C1:603:HEA:HMA	1.92	0.50
44:N4:445:LEU:HD22	72:N5:702:CDL:H401	1.92	0.50
45:N5:327:LEU:O	45:N5:331:MET:HG2	2.12	0.50
20:AK:206:VAL:HG13	20:AK:257:VAL:HG13	1.94	0.50
35:C1:27:GLY:HA3	79:C1:602:HEA:H273	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:C1:244:TYR:HA	35:C1:247:ILE:HG22	1.94	0.50
49:QC:137:GLN:NE2	49:QC:263:ASN:O	2.44	0.50
51:QE:151:LYS:HB3	51:QE:272:ILE:HD11	1.94	0.50
48:Qb:102:LYS:HG2	48:Qb:153:ASN:HB3	1.93	0.50
60:S2:107:LEU:HD21	60:S2:450:LEU:HD11	1.94	0.50
60:S2:133:LYS:HE2	66:S8:124:PRO:O	2.12	0.50
60:S2:321:GLU:O	60:S2:352:GLN:NE2	2.44	0.50
67:V1:311:TRP:NE1	67:V1:333:GLU:OE1	2.37	0.50
72:AL:204:CDL:H111	54:Qh:39:LEU:HD13	1.94	0.50
29:B6:165:PHE:O	29:B6:168:ASP:HB2	2.12	0.50
36:C2:200:CYS:SG	36:C2:207:MET:HE1	2.51	0.50
38:C4:90:PHE:HA	38:C4:93:MET:HG2	1.93	0.50
44:N4:133:ILE:HD11	44:N4:231:LEU:HD11	1.94	0.50
44:N4:412:ILE:HG12	44:N4:416:ARG:HD2	1.93	0.50
45:N5:559:GLU:O	45:N5:564:LYS:HB2	2.12	0.50
76:QE:303:3PE:H232	76:QE:303:3PE:H272	1.94	0.50
1:4L:68:ALA:HB2	46:N6:64:MET:HE2	1.93	0.50
21:AL:4:THR:HG22	21:AL:8:LYS:HE3	1.93	0.50
44:N4:82:SER:HB2	44:N4:432:ARG:CZ	2.42	0.50
45:N5:15:LEU:HD11	45:N5:94:LEU:HD21	1.94	0.50
45:N5:566:THR:O	45:N5:570:GLN:HG2	2.12	0.50
55:Ql:51:LYS:NZ	50:Qd:98:SER:O	2.45	0.50
59:S1:307:ILE:HG23	59:S1:317:THR:HG21	1.94	0.50
59:S1:455:ILE:O	59:S1:463:SER:OG	2.27	0.50
1:4L:73:LEU:HD22	42:N2:38:LEU:HD12	1.93	0.50
5:6B:12:TYR:CE2	5:6B:59:ARG:HB3	2.46	0.50
71:AL:206:PC1:H262	71:AL:206:PC1:H321	1.93	0.50
35:C1:251:PHE:HB3	35:C1:319:LYS:HE2	1.94	0.50
36:C2:160:LEU:O	36:C2:161:HIS:ND1	2.45	0.50
44:N4:76:MET:SD	44:N4:230:VAL:HB	2.52	0.50
71:QH:102:PC1:H2B1	71:QH:102:PC1:H382	1.94	0.50
47:Qa:164:VAL:HG21	48:Qb:317:THR:HG21	1.93	0.50
51:Qe:183:GLU:O	51:Qe:187:GLU:HG2	2.12	0.50
59:S1:49:VAL:HG13	59:S1:102:ILE:HD13	1.93	0.50
35:C1:300:ASP:OD1	35:C1:301:THR:N	2.45	0.50
36:C2:28:LEU:HA	36:C2:31:VAL:HG22	1.94	0.50
46:N6:17:PHE:HA	46:N6:20:PHE:CD2	2.47	0.50
47:Qa:91:THR:HG21	47:Qa:140:VAL:HA	1.94	0.50
60:S2:135:TYR:HE1	60:S2:417:LEU:HD21	1.77	0.50
3:5B:97:ASN:O	35:C1:180:GLN:NE2	2.35	0.49
37:C3:66:THR:HB	71:C3:301:PC1:H142	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:CA:68:GLU:HG2	40:CB:21:ARG:HB3	1.93	0.49
41:N1:195:ARG:HH12	41:N1:274:ARG:HD2	1.77	0.49
18:A9:126:VAL:HG23	18:A9:161:VAL:HG11	1.94	0.49
35:C1:183:LEU:HD13	35:C1:273:MET:HG2	1.94	0.49
51:QE:123:VAL:HG13	55:Qi:29:ALA:HA	1.94	0.49
57:QK:31:GLN:HE22	48:Qb:342:GLN:HB3	1.77	0.49
29:B6:141:ILE:HG23	82:N5:701:PEE:H60	1.94	0.49
37:C3:253:TYR:HA	37:C3:257:TYR:HD1	1.76	0.49
41:N1:110:SER:HB3	46:N6:62:GLY:HA3	1.94	0.49
41:N1:145:THR:OG1	41:N1:289:LEU:HD11	2.12	0.49
42:N2:132:THR:HG21	72:N2:401:CDL:H372	1.94	0.49
60:S2:296:GLY:HA2	60:S2:300:ARG:HH21	1.78	0.49
17:A8:228:ASN:OD1	63:S5:51:ARG:NH1	2.44	0.49
72:AL:204:CDL:H522	27:B4:84:PRO:HG3	1.94	0.49
35:C1:466:MET:O	35:C1:469:ILE:HG22	2.13	0.49
45:N5:383:MET:O	45:N5:389:PHE:HB2	2.12	0.49
48:QB:192:PHE:O	48:QB:198:ALA:HB2	2.12	0.49
48:QB:275:ILE:HG22	54:Qh:17:TYR:CD1	2.48	0.49
59:S1:347:ASP:OD1	59:S1:347:ASP:N	2.43	0.49
65:S7:108:THR:HA	65:S7:136:CYS:HB3	1.93	0.49
48:QB:120:LEU:HD13	48:QB:133:ILE:HG12	1.94	0.49
59:S1:603:ALA:O	59:S1:604:GLN:HG3	2.12	0.49
45:N5:562:LEU:HB3	45:N5:563:PRO:HD3	1.95	0.49
47:QA:82:LEU:HD23	47:QA:205:LEU:HD11	1.94	0.49
48:Qb:194:GLY:O	51:Qe:99:SER:OG	2.30	0.49
60:S2:269:THR:O	60:S2:333:TYR:OH	2.28	0.49
66:S8:153:ILE:HG12	86:S8:302:SF4:S1	2.53	0.49
14:A5:48:THR:HA	14:A5:51:ILE:HG12	1.95	0.49
71:QC:405:PC1:H3D1	71:QC:405:PC1:H392	1.94	0.49
51:Qe:224:PRO:HA	51:Qe:236:CYS:HA	1.94	0.49
55:Qi:34:ARG:HH21	58:Qj:50:GLY:HA3	1.78	0.49
71:6A:101:PC1:H321	71:C3:302:PC1:H271	1.93	0.49
18:A9:109:ASN:HB3	18:A9:112:ASP:HB2	1.94	0.49
18:A9:206:ILE:HG13	73:A9:401:NDP:H42N	1.95	0.49
48:QB:366:ASP:HB2	48:QB:464:GLN:HG2	1.92	0.49
7:7A:75:SER:HA	35:C1:118:VAL:HG12	1.94	0.49
42:N2:42:PRO:HG3	46:N6:167:VAL:HG13	1.95	0.49
42:N2:324:LYS:HB2	72:N2:401:CDL:H112	1.93	0.49
51:QE:160:PRO:HD2	51:QE:163:LYS:HG2	1.95	0.49
47:Qa:253:TYR:OH	47:Qa:435:ARG:O	2.19	0.49
53:Qg:52:PRO:HD2	53:Qg:55:LEU:HD12	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:S1:64:CYS:O	59:S1:184:ARG:NH2	2.30	0.49
67:V1:112:TYR:CD1	67:V1:153:ALA:HB3	2.48	0.49
5:6B:30:CYS:SG	5:6B:31:TRP:N	2.86	0.49
23:AN:124:LEU:HD12	46:N6:130:THR:HG21	1.95	0.49
32:B9:143:GLU:O	32:B9:164:ARG:NH2	2.46	0.49
44:N4:375:LEU:HD11	45:N5:141:PHE:HE2	1.77	0.49
47:QA:65:ILE:HG23	47:QA:218:MET:HG2	1.95	0.49
83:QC:402:HEM:HBC2	83:QC:402:HEM:HMC1	1.94	0.49
48:Qb:302:VAL:HB	48:Qb:303:PRO:HD3	1.94	0.49
59:S1:466:LEU:HD13	59:S1:500:ILE:HD11	1.93	0.49
64:S6:100:ILE:HD11	64:S6:111:CYS:HB2	1.94	0.49
47:Qa:371:VAL:HG12	47:Qa:375:LYS:HE3	1.94	0.48
49:Qc:116:GLY:HA3	83:Qc:403:HEM:HBC2	1.94	0.48
49:Qc:227:LYS:HG2	50:Qd:308:LYS:HE2	1.94	0.48
60:S2:190:ILE:HD11	60:S2:257:PHE:HZ	1.78	0.48
23:AN:57:ARG:NH1	41:N1:168:THR:OG1	2.46	0.48
29:B6:140:TRP:HD1	33:BK:41:VAL:HG13	1.78	0.48
35:C1:321:PHE:HB3	36:C2:65:TRP:CZ2	2.48	0.48
51:QE:178:HIS:CE1	51:QE:209:GLU:HB2	2.47	0.48
59:S1:163:LYS:HD3	59:S1:173:MET:HG3	1.94	0.48
59:S1:264:SER:HB2	59:S1:272:ARG:HB3	1.96	0.48
20:AK:142:LEU:HA	20:AK:165:ILE:HD11	1.94	0.48
43:N3:79:SER:HA	43:N3:87:MET:HE2	1.95	0.48
45:N5:7:LEU:O	45:N5:11:THR:HG23	2.12	0.48
76:QE:303:3PE:H271	58:Qj:35:ALA:HB1	1.94	0.48
47:Qa:155:GLN:HB3	47:Qa:198:GLY:HA2	1.96	0.48
50:Qd:292:LYS:HD2	82:Qd:403:PEE:H3	1.95	0.48
77:AM:203:PLX:H191	77:AM:203:PLX:H393	1.94	0.48
77:AM:203:PLX:H201	76:S7:302:3PE:H2F2	1.96	0.48
40:CB:35:TYR:OH	42:N2:335:LEU:O	2.29	0.48
43:N3:28:ASN:ND2	76:S7:302:3PE:H251	2.28	0.48
47:QA:214:THR:HA	47:QA:241:ARG:HB3	1.94	0.48
62:S4:109:ASN:ND2	62:S4:111:LEU:O	2.47	0.48
28:B5:175:ASP:HA	63:S5:45:HIS:HD2	1.78	0.48
37:C3:54:MET:HB3	37:C3:58:TRP:CZ3	2.49	0.48
37:C3:125:ASN:HD22	37:C3:128:GLU:HG3	1.78	0.48
45:N5:567:SER:OG	82:S2:501:PEE:O3	2.31	0.48
48:QB:190:THR:HG22	48:QB:275:ILE:HG23	1.94	0.48
71:QC:405:PC1:H2G2	82:Qh:103:PEE:H76	1.94	0.48
71:QC:407:PC1:H2I1	77:QI:301:PLX:H362	1.96	0.48
50:QD:104:SER:HA	55:Qi:48:ASN:HD21	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:Qa:63:LEU:HD21	47:Qa:218:MET:HE3	1.96	0.48
48:Qb:104:ARG:NH1	48:Qb:149:ASP:OD2	2.45	0.48
59:S1:224:ASP:CG	59:S1:291:ARG:HH12	2.20	0.48
17:A8:95:VAL:HG12	17:A8:97:VAL:HG22	1.95	0.48
29:B6:181:LYS:HG3	30:B7:40:VAL:HG13	1.95	0.48
30:B7:29:TYR:O	30:B7:104:ARG:NH2	2.47	0.48
41:N1:200:LEU:O	41:N1:204:GLU:N	2.46	0.48
48:QB:279:ASP:H	48:QB:460:GLY:HA3	1.77	0.48
51:QE:190:VAL:HG21	51:QE:250:ARG:HH22	1.79	0.48
47:Qa:70:ARG:HD2	47:Qa:117:GLU:HG2	1.95	0.48
65:S7:130:VAL:HB	65:S7:159:VAL:HA	1.96	0.48
68:V2:92:TRP:CE2	68:V2:126:PRO:HG3	2.49	0.48
5:6B:5:ILE:HG13	5:6B:7:THR:H	1.79	0.48
37:C3:66:THR:HB	71:C3:301:PC1:H153	1.95	0.48
45:N5:49:VAL:HB	45:N5:50:PRO:HD3	1.96	0.48
47:QA:153:ALA:O	47:QA:156:SER:OG	2.25	0.48
51:QE:207:LYS:HE3	51:QE:210:TRP:CD1	2.48	0.48
51:QE:234:TYR:N	51:QE:243:TYR:O	2.38	0.48
10:8B:52:ILE:HB	10:8B:53:PRO:HD3	1.96	0.48
29:B6:157:VAL:HG13	45:N5:61:MET:HE3	1.95	0.48
35:C1:18:LEU:HB3	35:C1:102:PHE:CZ	2.49	0.48
42:N2:49:ASN:OD1	42:N2:49:ASN:N	2.47	0.48
82:N3:201:PEE:H22	82:N3:201:PEE:H27	1.65	0.48
45:N5:8:THR:O	45:N5:11:THR:OG1	2.26	0.48
46:N6:150:GLY:HA2	63:S5:17:TRP:CZ2	2.49	0.48
59:S1:535:GLU:OE2	59:S1:538:ARG:NH1	2.46	0.48
60:S2:194:THR:HG21	60:S2:209:MET:HB2	1.94	0.48
60:S2:248:ASP:O	60:S2:252:GLU:HG2	2.14	0.48
68:V2:85:LEU:HD13	69:V3:400:LEU:HD22	1.94	0.48
4:6A:65:LEU:HD22	37:C3:190:ASP:HB3	1.96	0.48
5:6B:62:LYS:HD3	5:6B:62:LYS:HA	1.72	0.48
42:N2:139:LEU:HD13	42:N2:190:MET:HE1	1.96	0.48
49:Qc:200:LEU:HD23	49:Qc:201:HIS:CD2	2.48	0.48
66:S8:49:ASP:N	66:S8:49:ASP:OD1	2.40	0.48
10:8B:46:THR:O	10:8B:49:SER:OG	2.31	0.48
66:S8:75:SER:O	66:S8:79:ARG:HG3	2.14	0.48
35:C1:360:ASN:O	35:C1:364:ASP:N	2.41	0.47
35:C1:462:LEU:HG	35:C1:466:MET:HE2	1.96	0.47
41:N1:65:THR:HG23	41:N1:122:ALA:HB1	1.96	0.47
57:QK:20:ARG:HH11	57:QK:23:ALA:HA	1.79	0.47
51:Qe:267:SER:HB3	51:Qe:270:LEU:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:S1:338:VAL:HB	59:S1:363:SER:HB2	1.96	0.47
18:A9:198:ALA:O	18:A9:260:GLY:CA	2.59	0.47
18:A9:268:PRO:HG2	18:A9:269:ASN:HD22	1.78	0.47
18:A9:293:LEU:HD12	18:A9:294:PRO:HD2	1.96	0.47
20:AK:93:ILE:HA	20:AK:136:TRP:HE1	1.79	0.47
49:QC:300:ILE:HD11	49:QC:363:LEU:HD21	1.95	0.47
48:Qb:465:LEU:HD12	48:Qb:466:PRO:HD2	1.96	0.47
67:V1:138:LEU:HD13	67:V1:245:VAL:HG13	1.95	0.47
2:5A:126:PRO:O	2:5A:130:GLN:HG2	2.13	0.47
5:6B:30:CYS:HA	5:6B:61:TYR:CZ	2.49	0.47
35:C1:12:HIS:HD2	35:C1:81:TRP:HA	1.79	0.47
47:Qa:408:GLN:HE21	47:Qa:409:PRO:HD2	1.78	0.47
60:S2:241:ASP:OD1	60:S2:242:LEU:N	2.46	0.47
2:5A:66:ASP:OD1	2:5A:66:ASP:N	2.44	0.47
43:N3:64:LEU:HD13	46:N6:165:VAL:HG22	1.95	0.47
47:Qa:71:TYR:HB3	47:Qa:212:HIS:CE1	2.50	0.47
47:Qa:85:LEU:HD13	47:Qa:157:GLN:HG3	1.96	0.47
47:Qa:421:ASP:N	47:Qa:421:ASP:OD1	2.47	0.47
59:S1:340:ALA:HB3	59:S1:366:LEU:HD23	1.95	0.47
59:S1:476:LEU:HD22	59:S1:493:VAL:HG21	1.96	0.47
67:V1:302:LYS:HE3	67:V1:303:HIS:CE1	2.49	0.47
7:7A:23:GLU:H	7:7A:25:ARG:CZ	2.27	0.47
17:A8:235:LEU:HB3	40:CB:23:LEU:HD21	1.95	0.47
20:AK:131:TYR:OH	20:AK:188:HIS:ND1	2.40	0.47
35:C1:68:PHE:HA	35:C1:72:PRO:HG2	1.96	0.47
41:N1:59:GLU:HB2	43:N3:30:TYR:CD2	2.49	0.47
45:N5:14:ILE:HD11	45:N5:43:ALA:HA	1.96	0.47
45:N5:293:ILE:HD12	72:N5:703:CDL:H521	1.96	0.47
46:N6:124:ASP:N	46:N6:124:ASP:OD1	2.47	0.47
65:S7:65:MET:HE2	65:S7:103:MET:HG3	1.97	0.47
65:S7:67:PHE:HE2	65:S7:117:LEU:HA	1.80	0.47
67:V1:71:LYS:HE3	68:V2:249:LEU:HD23	1.95	0.47
2:5A:142:SER:HB2	2:5A:147:LEU:HD21	1.97	0.47
4:6A:81:LEU:HD11	72:6A:102:CDL:H321	1.96	0.47
24:B1:32:ASP:OD2	28:B5:131:LYS:NZ	2.36	0.47
28:B5:126:TYR:OH	44:N4:40:SER:O	2.33	0.47
32:B9:177:ARG:HH12	32:B9:204:ASP:HA	1.80	0.47
33:BK:144:SER:HB3	33:BK:158:LYS:NZ	2.29	0.47
34:BL:106:VAL:HA	34:BL:109:LEU:HG	1.97	0.47
35:C1:80:ASN:ND2	35:C1:98:ASN:HD21	2.11	0.47
36:C2:161:HIS:CE1	36:C2:200:CYS:SG	3.06	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:CB:46:ILE:HG12	72:CB:203:CDL:H741	1.97	0.47
41:N1:216:ALA:HB3	41:N1:219:PRO:HD2	1.96	0.47
42:N2:112:HIS:HB2	42:N2:184:ILE:HD13	1.97	0.47
47:QA:304:ASN:HB3	47:QA:307:SER:HB3	1.95	0.47
50:QD:265:SER:OG	52:Qf:30:LEU:HB2	2.15	0.47
50:QD:300:LEU:HD21	51:QE:124:GLY:HA3	1.95	0.47
49:Qc:234:PHE:CZ	72:Qd:401:CDL:H321	2.49	0.47
51:Qe:201:ASP:C	51:Qe:203:GLU:H	2.23	0.47
51:Qe:214:ILE:HG13	51:Qe:261:PRO:HD3	1.96	0.47
59:S1:222:ILE:HA	59:S1:225:ILE:HG12	1.96	0.47
60:S2:140:PRO:HB2	65:S7:142:TYR:CE2	2.50	0.47
5:6B:33:ASN:HB2	5:6B:61:TYR:CZ	2.50	0.47
35:C1:35:LEU:HD22	35:C1:462:LEU:HD22	1.95	0.47
35:C1:124:THR:HG23	35:C1:132:LEU:HG	1.97	0.47
35:C1:357:VAL:HG22	36:C2:27:THR:HG22	1.97	0.47
37:C3:126:PRO:HB3	37:C3:257:TYR:HB3	1.96	0.47
41:N1:173:TRP:NE1	41:N1:244:GLY:O	2.48	0.47
42:N2:231:SER:O	42:N2:234:TRP:HD1	1.97	0.47
45:N5:241:THR:HG21	45:N5:344:GLY:HA3	1.97	0.47
48:QB:413:ILE:HG12	48:QB:423:ARG:HD2	1.97	0.47
49:QC:246:SER:HB2	49:QC:249:LEU:HB2	1.95	0.47
50:QD:132:ALA:HA	50:QD:175:TYR:HA	1.96	0.47
77:QE:301:PLX:H233	82:QE:302:PEE:H28	1.97	0.47
82:Qh:103:PEE:H25	82:Qh:103:PEE:H50	1.97	0.47
61:S3:101:ARG:NH1	61:S3:159:VAL:O	2.47	0.47
67:V1:88:ARG:C	67:V1:244:ASN:HD22	2.23	0.47
4:6A:28:TRP:HB3	37:C3:146:TRP:HB2	1.96	0.47
31:B8:114:ARG:HB2	45:N5:162:THR:HG21	1.96	0.47
35:C1:148:PHE:CE2	37:C3:32:THR:HG23	2.49	0.47
50:Qd:182:ASN:OD1	50:Qd:185:ALA:N	2.43	0.47
59:S1:401:LEU:HD11	59:S1:432:ILE:HG13	1.96	0.47
59:S1:575:VAL:C	59:S1:578:PRO:HD2	2.40	0.47
20:AK:256:GLU:HG3	20:AK:278:LEU:HG	1.97	0.47
51:Qe:145:ASP:OD1	51:Qe:145:ASP:N	2.48	0.47
60:S2:299:LEU:HD22	60:S2:304:ILE:HD12	1.97	0.47
1:4L:20:LEU:HD23	45:N5:588:PHE:HD2	1.80	0.47
18:A9:64:PHE:O	18:A9:67:ARG:HG2	2.15	0.47
18:A9:168:SER:OG	18:A9:169:HIS:N	2.47	0.47
23:AN:56:GLU:OE1	23:AN:59:ARG:NH2	2.37	0.47
47:QA:293:LEU:HD21	47:QA:361:ILE:HD12	1.97	0.47
48:QB:113:VAL:HG12	48:QB:146:LEU:HD23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:QC:159:ASP:OD1	49:QC:160:LEU:N	2.48	0.47
48:Qb:126:ARG:NH1	48:Qb:199:GLN:O	2.48	0.47
49:Qc:97:HIS:HD1	49:Qc:100:ARG:NH2	2.13	0.47
51:Qe:225:ILE:HG12	51:Qe:237:PRO:HD3	1.97	0.47
4:6A:81:LEU:HB3	71:6A:101:PC1:H12	1.97	0.46
17:A8:160:THR:HA	17:A8:163:TRP:CD1	2.49	0.46
29:B6:132:VAL:O	29:B6:136:LEU:CB	2.62	0.46
34:BL:90:VAL:HG22	44:N4:28:THR:HG21	1.97	0.46
50:QD:248:PRO:HB2	84:QD:401:HEC:HBB2	1.97	0.46
48:Qb:74:TRP:CZ2	48:Qb:411:GLU:HA	2.51	0.46
48:Qb:315:ASP:OD1	48:Qb:316:SER:N	2.48	0.46
51:Qe:155:LYS:HB3	51:Qe:158:ASP:HB2	1.98	0.46
21:AL:118:MET:HA	21:AL:121:THR:HG22	1.98	0.46
23:AN:49:SER:HB2	41:N1:172:ILE:HD13	1.97	0.46
30:B7:103:GLU:O	30:B7:107:ARG:HG2	2.15	0.46
31:B8:62:TYR:OH	31:B8:74:ASP:O	2.29	0.46
32:B9:119:PRO:HB3	45:N5:525:MET:HE2	1.96	0.46
35:C1:436:MET:HE3	35:C1:443:TYR:HB3	1.96	0.46
71:C1:606:PC1:H222	38:C4:100:TRP:HB3	1.96	0.46
45:N5:293:ILE:HD13	45:N5:418:LEU:HD22	1.96	0.46
47:QA:138:LEU:HD13	47:QA:237:PHE:HB2	1.97	0.46
47:Qa:272:VAL:HA	47:Qa:337:GLY:HA3	1.98	0.46
49:Qc:3:ASN:HD22	49:Qc:6:LYS:HE2	1.80	0.46
59:S1:382:ARG:C	59:S1:384:ASN:H	2.23	0.46
2:5A:67:ILE:HG13	2:5A:71:GLU:HB2	1.96	0.46
3:5B:61:PRO:HG2	3:5B:62:TYR:CD1	2.51	0.46
6:6C:49:TYR:CE1	38:C4:153:ILE:HG21	2.51	0.46
37:C3:112:LEU:HD22	37:C3:118:PRO:HB3	1.98	0.46
41:N1:10:ILE:HD11	43:N3:10:ASN:HD21	1.79	0.46
53:QG:110:LYS:HB2	58:Qj:7:GLY:HA3	1.97	0.46
48:Qb:310:ILE:HD11	48:Qb:388:VAL:HA	1.97	0.46
59:S1:594:ALA:O	59:S1:605:GLN:HA	2.14	0.46
1:4L:1:MET:SD	42:N2:80:TYR:OH	2.72	0.46
71:6A:101:PC1:H31	71:6A:101:PC1:O12	2.15	0.46
16:A7:27:ARG:HD2	16:A7:31:ILE:HD11	1.98	0.46
20:AK:62:ILE:HG23	20:AK:205:VAL:CG2	2.46	0.46
21:AL:120:LEU:HD11	76:N4:502:3PE:H342	1.96	0.46
34:BL:119:ARG:NH2	45:N5:75:GLU:OE2	2.48	0.46
44:N4:278:ARG:HG3	45:N5:545:SER:HB2	1.98	0.46
44:N4:324:SER:OG	44:N4:440:HIS:NE2	2.39	0.46
52:Qf:47:ARG:O	52:Qf:51:GLU:HG2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:S1:281:ILE:HD11	59:S1:602:ARG:HD2	1.97	0.46
59:S1:389:THR:OG1	59:S1:511:LYS:O	2.34	0.46
60:S2:203:MET:O	60:S2:206:PHE:HB3	2.16	0.46
60:S2:341:GLU:O	60:S2:345:GLN:HG2	2.15	0.46
64:S6:29:VAL:HG21	64:S6:37:LYS:HD2	1.98	0.46
67:V1:203:ALA:HB3	67:V1:206:CYS:HB2	1.97	0.46
5:6B:56:TRP:O	5:6B:60:VAL:HG23	2.16	0.46
11:A1:66:LEU:O	11:A1:69:ILE:HG13	2.16	0.46
13:A3:121:SER:OG	41:N1:310:MET:O	2.28	0.46
72:A8:301:CDL:H542	72:A8:301:CDL:H162	1.95	0.46
19:AB:104:PHE:HD1	19:AB:108:LEU:HD12	1.81	0.46
23:AN:144:THR:HB	41:N1:96:ILE:HG23	1.97	0.46
41:N1:66:SER:OG	41:N1:124:ASN:ND2	2.35	0.46
76:N4:502:3PE:H2D2	45:N5:562:LEU:HD13	1.97	0.46
51:QE:186:GLN:O	51:QE:190:VAL:HG23	2.15	0.46
52:QF:65:GLU:HB2	54:QH:78:TYR:CD1	2.51	0.46
52:Qf:28:ASP:HB3	52:Qf:29:PRO:HD3	1.97	0.46
67:V1:119:GLU:HA	87:V1:502:FMN:HM71	1.96	0.46
2:5A:79:LEU:HD21	2:5A:86:PRO:HB3	1.97	0.46
32:B9:182:LEU:HD11	32:B9:208:LEU:HG	1.96	0.46
37:C3:253:TYR:HA	37:C3:257:TYR:CD1	2.50	0.46
53:QG:71:MET:HE2	50:Qd:316:LYS:HD3	1.98	0.46
50:Qd:119:LYS:O	50:Qd:123:SER:OG	2.27	0.46
60:S2:227:ARG:NH1	65:S7:75:GLU:OE1	2.48	0.46
35:C1:144:ASP:OD1	35:C1:213:ARG:NE	2.36	0.46
35:C1:501:PRO:O	35:C1:504:THR:HG23	2.16	0.46
39:CA:60:LYS:O	39:CA:64:GLU:HG2	2.16	0.46
48:Qb:304:LEU:HD13	48:Qb:354:LEU:HD22	1.98	0.46
59:S1:291:ARG:HG2	59:S1:292:PHE:CE2	2.51	0.46
61:S3:115:THR:OG1	61:S3:116:ALA:N	2.48	0.46
7:7A:33:PHE:HB2	37:C3:67:PHE:HB3	1.97	0.46
12:A2:59:SER:HB2	59:S1:655:ARG:HD3	1.97	0.46
15:A6:42:SER:HB2	62:S4:52:LEU:N	2.31	0.46
19:AC:110:LEU:HB3	19:AC:114:ASP:HB2	1.97	0.46
74:AC:201:ZMP:H8	32:B9:109:ALA:HB2	1.98	0.46
22:AM:8:ARG:HD3	22:AM:8:ARG:HA	1.76	0.46
27:B4:56:ARG:NH1	27:B4:58:GLY:O	2.48	0.46
30:B7:103:GLU:OE2	30:B7:106:ARG:NH2	2.49	0.46
35:C1:230:LEU:HD21	37:C3:100:ALA:HA	1.98	0.46
35:C1:412:ILE:HD13	38:C4:106:THR:HG21	1.97	0.46
76:CA:101:3PE:H231	40:CB:65:LEU:HD23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:N1:31:MET:HG2	66:S8:77:LEU:HB2	1.98	0.46
46:N6:19:GLY:O	46:N6:22:SER:OG	2.28	0.46
53:QG:44:VAL:O	53:QG:48:ILE:HG12	2.16	0.46
67:V1:283:ASN:ND2	67:V1:305:GLY:O	2.33	0.46
7:7A:72:GLY:O	7:7A:75:SER:OG	2.32	0.46
35:C1:378:HIS:O	35:C1:382:SER:OG	2.25	0.46
48:QB:80:ARG:HH22	48:QB:350:GLU:CD	2.24	0.46
51:QE:135:GLN:HE22	82:QE:302:PEE:H16	1.80	0.46
51:QE:207:LYS:HE3	51:QE:210:TRP:HD1	1.80	0.46
47:Qa:59:SER:HB2	47:Qa:130:ILE:HG21	1.97	0.46
66:S8:74:LEU:HD12	66:S8:77:LEU:HD23	1.98	0.46
12:A2:60:ASP:N	12:A2:60:ASP:OD1	2.49	0.46
18:A9:168:SER:O	18:A9:203:PRO:HD2	2.16	0.46
48:Qb:70:THR:HG21	48:Qb:407:THR:HA	1.98	0.46
50:Qd:106:LEU:HD13	50:Qd:111:ILE:HD11	1.97	0.46
50:Qd:322:TYR:CZ	50:Qd:324:PRO:HG3	2.51	0.46
59:S1:246:ARG:HH22	62:S4:123:ASN:ND2	2.14	0.46
9:7C:42:THR:HG23	10:8B:49:SER:HB3	1.98	0.45
9:7C:44:TYR:OH	35:C1:25:TRP:HB2	2.16	0.45
28:B5:147:ALA:HB2	44:N4:173:SER:HB2	1.98	0.45
76:N4:502:3PE:H3A2	76:N4:502:3PE:H2D1	1.98	0.45
47:QA:271:LEU:HD22	47:QA:453:LEU:HD13	1.98	0.45
49:QC:29:SER:OG	72:QC:408:CDL:HB61	2.15	0.45
77:QE:301:PLX:H152	77:QE:301:PLX:H182	1.77	0.45
61:S3:73:VAL:HA	61:S3:88:ILE:HG22	1.97	0.45
20:AK:131:TYR:CD1	20:AK:185:CYS:HB3	2.51	0.45
22:AM:93:MET:HE1	66:S8:171:PRO:HB2	1.98	0.45
36:C2:139:ASP:OD1	36:C2:139:ASP:N	2.49	0.45
44:N4:369:LEU:HD23	72:N5:702:CDL:H362	1.98	0.45
48:QB:110:GLU:HA	48:QB:113:VAL:HG22	1.97	0.45
53:QG:36:ASP:OD2	53:QG:62:ARG:NH1	2.47	0.45
61:S3:211:ARG:NH2	61:S3:213:ASP:OD1	2.44	0.45
4:6A:53:HIS:O	4:6A:54:HIS:ND1	2.48	0.45
4:6A:88:ASN:OD1	71:6A:101:PC1:H141	2.17	0.45
71:6A:101:PC1:H142	37:C3:181:TYR:O	2.16	0.45
72:A8:301:CDL:H261	44:N4:10:MET:HE3	1.99	0.45
28:B5:146:LYS:O	28:B5:150:ARG:HG3	2.16	0.45
77:B5:201:PLX:H371	77:B5:201:PLX:H342	1.81	0.45
41:N1:281:ARG:HB2	41:N1:284:GLN:HG3	1.99	0.45
42:N2:137:ALA:HB3	42:N2:138:PRO:HD3	1.97	0.45
50:QD:168:ARG:NH1	50:QD:174:ASP:OD2	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:Qd:256:PHE:HD2	50:Qd:260:THR:HB	1.82	0.45
60:S2:190:ILE:HG23	60:S2:209:MET:HB3	1.98	0.45
67:V1:55:GLY:O	67:V1:58:SER:OG	2.27	0.45
7:7A:40:PRO:HG2	7:7A:43:LEU:HB2	1.98	0.45
26:B3:24:ILE:O	26:B3:30:GLU:HB3	2.17	0.45
31:B8:111:MET:SD	44:N4:278:ARG:NH2	2.89	0.45
37:C3:137:LEU:HD12	37:C3:249:TRP:CD1	2.51	0.45
82:N5:701:PEE:H36	82:N5:701:PEE:H29	1.57	0.45
82:QE:302:PEE:H23	82:QE:302:PEE:H30	1.59	0.45
35:C1:328:HIS:HD2	36:C2:56:MET:HE1	1.81	0.45
44:N4:127:VAL:HB	44:N4:128:PRO:HD3	1.98	0.45
48:QB:445:CYS:O	48:QB:449:PHE:HB2	2.15	0.45
49:QC:116:GLY:HA3	83:QC:403:HEM:C3C	2.52	0.45
49:QC:236:MET:HG2	82:QE:302:PEE:H61	1.98	0.45
50:QD:322:TYR:CE2	50:QD:324:PRO:HG3	2.51	0.45
77:QI:301:PLX:H22	77:QI:301:PLX:H1C3	1.56	0.45
54:Qh:19:LEU:HD23	54:Qh:24:GLN:HB3	1.97	0.45
59:S1:36:VAL:HG11	59:S1:56:VAL:HG21	1.99	0.45
59:S1:541:PRO:HB3	59:S1:561:PRO:HD3	1.99	0.45
66:S8:98:ARG:NH1	66:S8:154:TYR:O	2.49	0.45
67:V1:177:TYR:CD1	69:V3:409:PHE:HB3	2.52	0.45
36:C2:154:VAL:HG12	36:C2:174:ALA:HB2	1.99	0.45
41:N1:66:SER:HG	41:N1:124:ASN:HD21	1.60	0.45
44:N4:79:ALA:O	44:N4:82:SER:HB3	2.17	0.45
57:QK:24:GLY:HA3	47:Qa:109:LYS:HB3	1.98	0.45
47:Qa:183:ARG:CG	47:Qa:254:ARG:HB2	2.46	0.45
48:Qb:121:ASN:ND2	48:Qb:132:TYR:OH	2.50	0.45
49:Qc:186:PRO:HG2	83:Qc:402:HEM:HMC3	1.98	0.45
60:S2:134:THR:HG22	60:S2:135:TYR:H	1.82	0.45
69:V3:386:TYR:CZ	69:V3:388:ASN:HB3	2.52	0.45
3:5B:70:ALA:N	3:5B:78:ASN:OD1	2.30	0.45
72:6A:102:CDL:H121	72:6A:102:CDL:H152	1.85	0.45
71:7B:101:PC1:H2B1	35:C1:423:MET:HE1	1.98	0.45
29:B6:91:ARG:NH2	32:B9:159:ASP:OD1	2.50	0.45
35:C1:445:ASP:OD1	36:C2:134:ARG:NE	2.34	0.45
79:C1:603:HEA:HBA2	79:C1:603:HEA:CMA	2.47	0.45
37:C3:49:THR:O	37:C3:53:THR:OG1	2.33	0.45
37:C3:204:HIS:NE2	37:C3:249:TRP:HB2	2.32	0.45
45:N5:584:ILE:O	45:N5:588:PHE:HB2	2.16	0.45
48:QB:176:ASP:OD1	51:QE:80:HIS:ND1	2.37	0.45
51:Qe:165:MET:HB3	51:Qe:176:VAL:HG23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:V1:364:VAL:HG12	67:V1:400:VAL:HG12	1.98	0.45
17:A8:239:LYS:O	17:A8:243:ARG:NH1	2.49	0.45
20:AK:316:LEU:HB2	20:AK:319:ILE:HG12	1.98	0.45
21:AL:14:GLU:HA	21:AL:21:LYS:HE3	1.99	0.45
77:AL:205:PLX:H101	77:AL:205:PLX:H292	1.99	0.45
26:B3:49:GLU:HG3	32:B9:80:ARG:HD2	1.99	0.45
35:C1:409:TRP:HB3	35:C1:471:ILE:HG12	1.98	0.45
41:N1:58:LYS:NZ	65:S7:125:PRO:O	2.50	0.45
48:Qb:356:ALA:HB3	48:Qb:372:LEU:HD21	1.99	0.45
59:S1:259:SER:HB3	59:S1:282:ASN:HD22	1.81	0.45
60:S2:190:ILE:HD11	60:S2:257:PHE:CZ	2.52	0.45
6:6C:72:GLN:N	36:C2:212:GLU:OE2	2.50	0.45
17:A8:246:PHE:HE1	72:A8:301:CDL:H341	1.82	0.45
18:A9:54:ILE:HD12	18:A9:76:MET:HE1	1.99	0.45
31:B8:173:ASP:OD1	31:B8:175:THR:OG1	2.35	0.45
44:N4:201:MET:HE1	44:N4:212:LEU:HD11	1.99	0.45
49:QC:207:ASN:ND2	49:QC:211:ILE:O	2.37	0.45
49:QC:336:THR:HG21	72:QC:406:CDL:H512	1.98	0.45
50:QD:211:TYR:OH	84:QD:401:HEC:O2A	2.32	0.45
55:QI:58:HIS:CE1	55:QI:59:LYS:HG3	2.52	0.45
47:Qa:115:THR:HG23	47:Qa:117:GLU:H	1.82	0.45
47:Qa:180:ALA:HB2	47:Qa:258:ILE:HG13	1.98	0.45
50:Qd:99:HIS:HB2	50:Qd:283:HIS:HE1	1.82	0.45
64:S6:38:VAL:HG22	64:S6:44:ALA:HB2	1.98	0.45
4:6A:64:HIS:ND1	4:6A:65:LEU:HG	2.32	0.45
20:AK:138:TYR:CE1	20:AK:165:ILE:HG23	2.52	0.45
71:AL:206:PC1:H271	44:N4:159:PRO:HB3	1.99	0.45
31:B8:39:GLY:N	31:B8:74:ASP:OD1	2.38	0.45
35:C1:413:HIS:CE1	35:C1:468:MET:HB2	2.51	0.45
35:C1:442:ASP:OD1	35:C1:443:TYR:N	2.49	0.45
41:N1:293:PHE:O	41:N1:297:THR:OG1	2.32	0.45
44:N4:225:ILE:HD13	44:N4:331:ASN:HB2	1.99	0.45
66:S8:155:CYS:N	86:S8:302:SF4:S4	2.88	0.45
23:AN:43:LEU:HG	41:N1:179:TRP:HE1	1.81	0.44
27:B4:70:TYR:HD2	31:B8:38:PRO:HD2	1.80	0.44
32:B9:77:ASP:OD1	32:B9:77:ASP:N	2.50	0.44
44:N4:82:SER:HB2	44:N4:432:ARG:NH1	2.32	0.44
45:N5:346:ILE:HD11	45:N5:431:PHE:CZ	2.52	0.44
51:QE:266:THR:OG1	51:QE:270:LEU:O	2.32	0.44
59:S1:296:GLY:O	59:S1:572:HIS:NE2	2.45	0.44
60:S2:142:PHE:HZ	60:S2:428:CYS:SG	2.41	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:6A:28:TRP:O	4:6A:32:THR:N	2.46	0.44
21:AL:139:PRO:HA	42:N2:273:ASN:HD22	1.82	0.44
72:AL:203:CDL:H432	72:AL:203:CDL:H671	1.99	0.44
35:C1:377:PHE:HA	35:C1:380:VAL:HG22	1.99	0.44
35:C1:492:LEU:HD12	35:C1:495:LEU:HD12	1.99	0.44
41:N1:283:ASP:OD1	41:N1:283:ASP:N	2.48	0.44
48:QB:270:PHE:CG	48:QB:292:GLU:HB2	2.52	0.44
49:QC:131:TYR:O	49:QC:134:PRO:HD2	2.16	0.44
49:QC:186:PRO:HG2	83:QC:402:HEM:HMC3	1.99	0.44
59:S1:119:PHE:HB3	67:V1:387:GLU:HB2	1.99	0.44
2:5A:109:ARG:O	2:5A:113:VAL:HG23	2.18	0.44
4:6A:88:ASN:CG	71:6A:101:PC1:H131	2.42	0.44
21:AL:22:ALA:O	21:AL:26:THR:OG1	2.33	0.44
35:C1:313:ALA:HB3	36:C2:73:LEU:HD11	1.98	0.44
35:C1:316:THR:HG21	79:C1:603:HEA:C14	2.46	0.44
35:C1:352:GLY:CA	79:C1:603:HEA:H162	2.48	0.44
37:C3:79:LEU:HB3	37:C3:233:PHE:CZ	2.52	0.44
44:N4:196:TRP:CD1	44:N4:250:LEU:HB3	2.52	0.44
44:N4:266:MET:HA	44:N4:269:MET:HE2	1.99	0.44
47:QA:125:CYS:HB3	47:QA:133:LEU:HD22	2.00	0.44
47:QA:306:THR:HG22	48:QB:114:GLU:OE1	2.18	0.44
48:Qb:324:MET:O	48:Qb:330:SER:OG	2.36	0.44
67:V1:205:ILE:HG12	67:V1:379:CYS:SG	2.56	0.44
67:V1:412:LEU:HD12	67:V1:415:ILE:HD11	1.98	0.44
26:B3:52:ARG:HD3	45:N5:435:PRO:O	2.17	0.44
41:N1:309:ILE:HD12	43:N3:88:LEU:HD13	2.00	0.44
44:N4:78:MET:O	44:N4:81:GLN:HG2	2.18	0.44
44:N4:168:GLN:HB2	44:N4:174:LEU:HG	1.99	0.44
44:N4:318:ALA:HB2	44:N4:373:ILE:HG13	1.99	0.44
45:N5:526:LEU:HD12	45:N5:530:PRO:HG3	2.00	0.44
67:V1:99:TRP:CD1	67:V1:149:MET:HE2	2.53	0.44
67:V1:151:ALA:O	67:V1:191:TYR:OH	2.23	0.44
15:A6:66:TYR:CE2	15:A6:86:ARG:HD3	2.52	0.44
20:AK:297:ARG:HA	20:AK:300:VAL:HG22	1.99	0.44
77:AM:201:PLX:H22	77:AM:201:PLX:H1A2	1.78	0.44
29:B6:164:ILE:HD12	29:B6:170:ILE:HD11	1.99	0.44
76:CB:202:3PE:H2C2	72:CB:203:CDL:H642	2.00	0.44
47:QA:82:LEU:HD11	47:QA:154:LEU:HB3	1.98	0.44
54:QH:29:HIS:O	54:QH:33:LYS:HG2	2.17	0.44
47:Qa:217:ARG:HD2	47:Qa:244:LEU:O	2.18	0.44
50:Qd:139:VAL:HG21	50:Qd:277:TRP:CZ2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:Qe:208:PRO:O	51:Qe:209:GLU:HG2	2.17	0.44
53:Qg:54:ASN:OD1	53:Qg:55:LEU:N	2.50	0.44
59:S1:152:ARG:NH1	67:V1:414:GLU:OE1	2.48	0.44
64:S6:63:ASN:OD1	66:S8:105:ARG:NH2	2.50	0.44
18:A9:163:LYS:NZ	18:A9:253:ILE:O	2.33	0.44
40:CB:38:PHE:HZ	72:CB:203:CDL:H812	1.83	0.44
41:N1:25:ARG:NH2	65:S7:92:VAL:HG22	2.33	0.44
72:N5:702:CDL:H161	72:N5:702:CDL:H192	1.78	0.44
46:N6:169:MET:HE2	46:N6:169:MET:HB3	1.80	0.44
47:Qa:262:ASN:OD1	47:Qa:442:GLY:N	2.51	0.44
48:Qb:76:ASP:O	48:Qb:228:ARG:NH1	2.50	0.44
59:S1:140:GLN:HG2	60:S2:385:ILE:HG23	1.99	0.44
60:S2:391:TYR:HD1	66:S8:122:VAL:HG21	1.82	0.44
60:S2:402:THR:O	60:S2:416:TYR:HA	2.18	0.44
60:S2:430:ILE:HB	60:S2:469:ARG:HD2	2.00	0.44
61:S3:51:ASN:HB3	61:S3:82:ASN:HD21	1.82	0.44
67:V1:270:ASN:HD22	67:V1:339:PHE:HB2	1.83	0.44
29:B6:85:ASP:OD2	32:B9:167:TRP:NE1	2.40	0.44
32:B9:70:GLU:OE2	32:B9:76:ARG:NH1	2.34	0.44
36:C2:164:ALA:HB2	36:C2:171:LYS:HG3	1.99	0.44
41:N1:32:GLN:HG2	60:S2:204:THR:HG22	2.00	0.44
49:QC:96:ILE:HD11	72:QC:408:CDL:H771	1.99	0.44
49:QC:200:LEU:HD23	49:QC:201:HIS:CD2	2.53	0.44
57:QK:26:LEU:HD23	57:QK:26:LEU:HA	1.90	0.44
47:Qa:89:LEU:HD22	47:Qa:150:GLU:HB3	1.98	0.44
67:V1:385:CYS:CB	86:V1:501:SF4:S2	3.05	0.44
19:AB:115:GLN:O	19:AB:119:ILE:HG12	2.17	0.44
20:AK:283:GLY:O	20:AK:286:PRO:HD2	2.18	0.44
77:AM:201:PLX:H341	77:AM:201:PLX:H372	1.73	0.44
29:B6:136:LEU:HD12	29:B6:136:LEU:HA	1.85	0.44
79:C1:602:HEA:HBA2	79:C1:602:HEA:HMA	2.00	0.44
37:C3:178:ALA:HB2	71:C3:302:PC1:H2B2	1.99	0.44
51:Qe:98:ASP:OD1	51:Qe:99:SER:N	2.51	0.44
67:V1:168:ASN:ND2	69:V3:388:ASN:HD21	2.15	0.44
67:V1:211:ALA:HB2	67:V1:223:PRO:HG3	1.99	0.44
1:4L:21:MET:HG2	45:N5:589:LEU:HD13	2.00	0.44
3:5B:82:SER:HB2	3:5B:122:LEU:HD11	2.00	0.44
17:A8:244:LEU:HD23	42:N2:341:PRO:HG3	2.00	0.44
73:A9:401:NDP:N7N	73:A9:401:NDP:O2N	2.50	0.44
20:AK:93:ILE:HG23	20:AK:136:TRP:NE1	2.32	0.44
35:C1:308:ALA:O	35:C1:311:ILE:HG12	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:C1:383:MET:HE3	35:C1:421:VAL:HG23	2.00	0.44
37:C3:86:PHE:HZ	71:C3:301:PC1:H3A1	1.82	0.44
37:C3:217:VAL:O	37:C3:221:ARG:HG3	2.18	0.44
45:N5:286:LEU:HD22	45:N5:411:MET:SD	2.58	0.44
49:QC:102:LEU:HD22	49:QC:304:MET:HE2	1.99	0.44
51:QE:241:SER:OG	85:QE:304:FES:S1	2.73	0.44
48:Qb:341:PHE:HB2	48:Qb:358:PHE:HB3	1.99	0.44
60:S2:418:VAL:HB	60:S2:427:ARG:HB3	1.99	0.44
82:S2:501:PEE:H49	82:S2:501:PEE:H54	1.81	0.44
66:S8:150:THR:HG21	66:S8:180:HIS:NE2	2.33	0.44
17:A8:157:GLU:HB2	17:A8:158:PRO:HD3	2.00	0.43
19:AB:138:LEU:HD23	19:AB:144:ILE:HD13	2.00	0.43
77:AL:205:PLX:H141	27:B4:99:PHE:HZ	1.82	0.43
26:B3:85:GLU:O	26:B3:89:GLU:HG2	2.18	0.43
27:B4:71:ALA:HA	27:B4:75:ASN:HB3	2.00	0.43
72:B5:202:CDL:H1	82:N5:701:PEE:H49	2.00	0.43
42:N2:211:MET:HG2	42:N2:333:SER:HB2	2.00	0.43
47:Qa:148:ARG:NH2	53:Qg:50:ARG:O	2.50	0.43
48:Qb:38:TYR:CZ	48:Qb:42:LEU:HD11	2.53	0.43
8:7B:69:VAL:HG12	38:C4:167:TRP:CZ3	2.53	0.43
77:CB:201:PLX:H1C3	77:CB:201:PLX:H22	1.78	0.43
42:N2:132:THR:HG23	42:N2:209:ILE:HG12	1.99	0.43
44:N4:328:CYS:HB3	44:N4:437:MET:HE1	2.00	0.43
44:N4:361:VAL:HG13	72:N5:702:CDL:H332	1.99	0.43
47:QA:70:ARG:NH1	47:QA:249:ALA:O	2.51	0.43
51:QE:90:ASP:OD1	51:QE:90:ASP:N	2.42	0.43
57:QK:24:GLY:HA3	47:Qa:109:LYS:HE3	2.00	0.43
49:Qc:132:VAL:HG22	49:Qc:143:ALA:HB2	2.00	0.43
49:Qc:233:LEU:HD23	49:Qc:233:LEU:HA	1.80	0.43
49:Qc:361:ILE:HG12	49:Qc:365:LEU:HD12	1.99	0.43
82:Qh:101:PEE:H19	82:Qh:101:PEE:H25	1.61	0.43
59:S1:217:GLU:HG2	59:S1:218:LEU:HG	2.00	0.43
67:V1:222:LYS:HG2	67:V1:379:CYS:HB3	2.00	0.43
2:5A:136:LEU:HD22	2:5A:141:ILE:HB	1.99	0.43
4:6A:67:ILE:HD13	35:C1:218:THR:HG21	2.00	0.43
19:AC:114:ASP:OD1	32:B9:87:ARG:NH2	2.50	0.43
20:AK:148:ALA:HB1	20:AK:159:VAL:HG21	1.99	0.43
20:AK:237:GLN:HG3	20:AK:241:ASN:HD21	1.82	0.43
20:AK:244:LYS:HA	20:AK:248:LEU:HD12	2.01	0.43
35:C1:427:PRO:HB3	35:C1:450:TRP:HB3	2.01	0.43
82:N3:201:PEE:H56	82:N3:201:PEE:H50	1.69	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:N4:260:PRO:HG3	76:N4:502:3PE:H221	2.00	0.43
47:QA:154:LEU:HD12	47:QA:154:LEU:HA	1.85	0.43
82:QB:502:PEE:H49	77:QE:301:PLX:H6	2.00	0.43
53:QG:99:ILE:O	53:QG:103:LYS:HG2	2.18	0.43
54:QH:72:ARG:HA	54:QH:72:ARG:HD3	1.88	0.43
47:Qa:378:LEU:HG	47:Qa:416:ILE:HD13	2.00	0.43
48:Qb:121:ASN:HB3	48:Qb:132:TYR:CE1	2.54	0.43
10:8B:47:PHE:O	10:8B:51:LEU:HG	2.19	0.43
20:AK:112:GLY:HA2	20:AK:136:TRP:CD2	2.53	0.43
20:AK:342:SER:HB3	20:AK:345:TYR:HD1	1.84	0.43
33:BK:114:GLN:HG3	45:N5:203:MET:HG2	1.99	0.43
35:C1:30:GLY:C	35:C1:65:MET:HE2	2.42	0.43
35:C1:368:HIS:HD1	79:C1:603:HEA:CGA	2.31	0.43
35:C1:409:TRP:CZ3	35:C1:467:LEU:HD11	2.53	0.43
82:C1:609:PEE:H60	82:C1:609:PEE:H66	1.58	0.43
37:C3:141:GLY:O	37:C3:144:ILE:HG22	2.19	0.43
38:C4:65:LYS:HB3	38:C4:65:LYS:HE2	1.72	0.43
42:N2:250:SER:O	42:N2:259:GLY:HA3	2.19	0.43
45:N5:289:ALA:O	45:N5:293:ILE:HG23	2.19	0.43
47:QA:230:LEU:HD23	47:QA:230:LEU:HA	1.87	0.43
48:QB:310:ILE:HD11	48:QB:388:VAL:HA	1.99	0.43
48:Qb:109:LEU:HD12	48:Qb:146:LEU:HD22	2.00	0.43
54:Qh:20:SER:O	54:Qh:24:GLN:HG2	2.19	0.43
82:Qh:101:PEE:H19	82:Qh:101:PEE:H13	1.49	0.43
59:S1:186:ALA:HB2	59:S1:195:LEU:HD12	1.99	0.43
17:A8:160:THR:HA	17:A8:163:TRP:NE1	2.34	0.43
34:BL:150:PRO:HG3	40:CB:115:LEU:HD22	2.01	0.43
35:C1:254:ILE:HG13	35:C1:344:PHE:CD2	2.53	0.43
79:C1:602:HEA:HBD2	79:C1:602:HEA:HA	2.00	0.43
42:N2:2:ASN:HD22	42:N2:4:ILE:H	1.66	0.43
44:N4:12:LEU:HB2	44:N4:13:PRO:HD3	1.99	0.43
44:N4:449:LEU:HG	72:N5:702:CDL:H441	2.00	0.43
44:N4:458:LEU:O	45:N5:72:GLN:NE2	2.51	0.43
46:N6:124:ASP:O	46:N6:127:ILE:HG12	2.18	0.43
50:QD:228:LEU:HD11	50:QD:234:PHE:HB2	2.00	0.43
53:QG:34:ARG:O	53:QG:37:THR:HG22	2.18	0.43
48:Qb:152:GLN:NE2	48:Qb:250:PHE:HA	2.33	0.43
66:S8:153:ILE:HG13	66:S8:155:CYS:HB3	2.00	0.43
67:V1:39:ASP:HB3	67:V1:265:PHE:CE2	2.54	0.43
67:V1:65:THR:O	67:V1:69:LEU:HG	2.19	0.43
67:V1:396:MET:O	67:V1:400:VAL:HG13	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:V2:83:LEU:HD21	68:V2:116:ALA:HB2	2.01	0.43
35:C1:94:PHE:CZ	35:C1:166:THR:HG21	2.53	0.43
35:C1:236:TRP:CH2	79:C1:603:HEA:HBD1	2.54	0.43
40:CB:4:MET:O	40:CB:10:ARG:NH1	2.52	0.43
54:QH:12:ARG:NH1	48:Qb:279:ASP:OD1	2.50	0.43
71:QH:102:PC1:H142	71:QH:102:PC1:H111	1.82	0.43
48:Qb:314:TYR:HB3	48:Qb:341:PHE:CD2	2.54	0.43
48:Qb:360:CYS:SG	48:Qb:368:MET:HG3	2.59	0.43
49:Qc:47:THR:HG23	49:Qc:79:ILE:HG23	1.99	0.43
58:Qj:23:MET:O	58:Qj:27:VAL:HG23	2.19	0.43
59:S1:338:VAL:HB	59:S1:363:SER:CB	2.48	0.43
60:S2:149:SER:HA	60:S2:184:THR:HG22	2.01	0.43
61:S3:190:ASP:OD1	61:S3:191:TYR:N	2.51	0.43
67:V1:69:LEU:HD22	67:V1:147:ARG:HG2	2.01	0.43
67:V1:79:GLU:OE2	68:V2:246:GLN:NE2	2.48	0.43
67:V1:141:GLY:HA2	67:V1:252:PRO:HD3	1.99	0.43
11:A1:50:ARG:NH1	17:A8:97:VAL:O	2.40	0.43
21:AL:81:ARG:HH11	21:AL:89:ASN:HD21	1.64	0.43
35:C1:104:LEU:HD23	35:C1:104:LEU:HA	1.85	0.43
71:C3:301:PC1:H132	71:C3:301:PC1:H112	1.89	0.43
42:N2:276:ILE:C	42:N2:279:PRO:HD2	2.43	0.43
43:N3:64:LEU:O	43:N3:68:GLU:HG2	2.18	0.43
47:Qa:409:PRO:O	47:Qa:413:LEU:HG	2.19	0.43
54:Qh:7:HIS:ND1	54:Qh:7:HIS:O	2.51	0.43
3:5B:112:ARG:HA	3:5B:118:THR:O	2.18	0.43
8:7B:34:HIS:NE2	76:C1:601:3PE:O22	2.52	0.43
19:AB:78:ALA:HA	19:AB:81:ASP:OD2	2.19	0.43
20:AK:72:LYS:HG3	20:AK:73:GLY:N	2.34	0.43
41:N1:160:TYR:OH	43:N3:73:LEU:O	2.35	0.43
47:Qa:154:LEU:HD23	47:Qa:154:LEU:HA	1.89	0.43
47:Qa:221:ILE:HG12	47:Qa:396:VAL:HG12	2.01	0.43
47:Qa:408:GLN:NE2	47:Qa:409:PRO:HD2	2.34	0.43
49:Qc:131:TYR:O	49:Qc:134:PRO:HD2	2.19	0.43
67:V1:44:ASN:ND2	67:V1:49:HIS:H	2.15	0.43
3:5B:38:PRO:HG3	7:7A:24:ASN:HD21	1.83	0.43
8:7B:60:ILE:HD12	38:C4:122:LYS:HG2	2.01	0.43
29:B6:92:GLU:HB3	29:B6:93:PRO:HD3	1.99	0.43
29:B6:148:TYR:CE1	33:BK:49:ARG:HG2	2.54	0.43
29:B6:164:ILE:HB	30:B7:48:ASP:HB3	2.01	0.43
29:B6:166:PRO:HG2	29:B6:180:MET:HG3	2.00	0.43
41:N1:179:TRP:CG	41:N1:180:PRO:HD3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:N4:207:MET:HB3	44:N4:298:ILE:HD11	2.01	0.43
44:N4:210:TYR:CG	44:N4:268:GLY:HA3	2.54	0.43
45:N5:172:ILE:O	45:N5:176:ARG:HG2	2.19	0.43
45:N5:233:LEU:HB3	45:N5:234:PRO:HD3	2.00	0.43
45:N5:399:VAL:HG12	45:N5:409:LEU:HD13	2.00	0.43
47:QA:348:GLY:HA2	47:QA:448:PRO:HD3	2.00	0.43
49:QC:223:TYR:O	50:QD:312:TRP:NE1	2.39	0.43
54:QH:35:ILE:HG12	72:Qd:401:CDL:H542	2.00	0.43
47:Qa:270:ALA:O	47:Qa:438:MET:HA	2.19	0.43
48:Qb:126:ARG:HH12	48:Qb:200:SER:HA	1.84	0.43
51:Qe:228:ALA:HB3	51:Qe:235:TYR:HB3	2.01	0.43
53:Qg:44:VAL:O	53:Qg:48:ILE:HG12	2.19	0.43
63:S5:95:PRO:HG2	63:S5:98:HIS:HB2	2.01	0.43
64:S6:79:VAL:O	64:S6:121:PRO:HD3	2.18	0.43
19:AB:77:GLU:CD	19:AB:77:GLU:H	2.27	0.43
74:AC:201:ZMP:H14	32:B9:102:ALA:HB1	2.00	0.43
20:AK:327:ASP:O	20:AK:331:GLN:HG2	2.19	0.43
22:AM:85:GLU:HG2	22:AM:86:TRP:H	1.84	0.43
39:CA:55:TRP:O	39:CA:59:ILE:HG12	2.19	0.43
41:N1:24:GLU:HG3	41:N1:271:LEU:HD22	2.00	0.43
42:N2:142:LEU:HB3	42:N2:194:LEU:HD21	2.00	0.43
42:N2:172:GLN:OE1	45:N5:578:SER:OG	2.22	0.43
45:N5:292:ALA:HB2	45:N5:304:PHE:HB3	2.01	0.43
47:QA:51:SER:OG	47:QA:230:LEU:HD12	2.19	0.43
47:QA:319:GLN:O	57:QK:52:ARG:NH2	2.40	0.43
51:QE:249:ILE:HG12	51:QE:254:ALA:HB3	2.00	0.43
48:Qb:113:VAL:HA	48:Qb:116:MET:HE2	2.01	0.43
48:Qb:393:ASN:O	48:Qb:397:ASN:ND2	2.39	0.43
3:5B:54:ALA:O	3:5B:58:GLY:N	2.51	0.42
36:C2:186:SER:OG	36:C2:213:LEU:HD13	2.19	0.42
72:CB:203:CDL:H792	72:CB:203:CDL:H432	2.01	0.42
45:N5:190:LEU:HB2	45:N5:196:TRP:NE1	2.34	0.42
48:QB:225:LYS:HD2	48:QB:257:TYR:CE2	2.54	0.42
56:QJ:6:LEU:O	53:Qg:110:LYS:HD2	2.19	0.42
52:Qf:40:ILE:HD13	52:Qf:81:CYS:SG	2.59	0.42
59:S1:253:VAL:HG12	59:S1:345:LEU:HD22	2.01	0.42
59:S1:467:LYS:HE3	59:S1:503:SER:HB3	2.00	0.42
60:S2:190:ILE:HG21	60:S2:213:ARG:HG3	2.00	0.42
64:S6:84:ILE:HD12	64:S6:84:ILE:HA	1.87	0.42
17:A8:124:ARG:NE	23:AN:80:ASP:OD2	2.43	0.42
18:A9:344:PRO:HG2	18:A9:347:LEU:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:AN:95:ALA:HA	23:AN:106:VAL:HG11	2.01	0.42
37:C3:156:ARG:HH22	37:C3:223:LEU:HA	1.84	0.42
42:N2:221:HIS:CD2	42:N2:240:ILE:HG13	2.54	0.42
43:N3:105:GLU:HG2	43:N3:110:GLY:HA3	2.00	0.42
45:N5:420:ALA:O	45:N5:424:THR:HG23	2.19	0.42
48:QB:271:THR:OG1	51:QE:92:ARG:NH2	2.44	0.42
49:QC:130:GLY:O	49:QC:134:PRO:HD3	2.19	0.42
49:Qc:296:ALA:HB1	78:Qc:404:6F6:O14	2.19	0.42
82:Qd:403:PEE:H21	82:Qd:403:PEE:H15	1.58	0.42
67:V1:62:TRP:CD2	67:V1:181:LEU:HD13	2.55	0.42
67:V1:115:VAL:HG21	67:V1:142:CYS:SG	2.59	0.42
67:V1:209:GLU:HG3	67:V1:210:THR:H	1.83	0.42
1:4L:35:GLY:HA3	46:N6:20:PHE:HZ	1.84	0.42
7:7A:60:CYS:SG	37:C3:19:THR:HG23	2.59	0.42
71:7B:101:PC1:H222	71:7B:101:PC1:H361	2.01	0.42
9:7C:19:TYR:CE2	35:C1:5:ARG:HG3	2.53	0.42
20:AK:97:ASP:OD1	42:N2:316:GLN:NE2	2.33	0.42
40:CB:15:PHE:HE1	77:CB:201:PLX:H261	1.85	0.42
44:N4:203:PHE:CE1	44:N4:242:GLY:HA3	2.54	0.42
47:QA:290:GLN:HB2	47:QA:336:PHE:HE1	1.84	0.42
48:QB:400:VAL:HG22	48:QB:426:LEU:HD21	2.00	0.42
51:QE:228:ALA:HB3	51:QE:235:TYR:HB3	2.01	0.42
55:QI:11:TYR:CZ	55:QI:16:ARG:HG3	2.53	0.42
48:Qb:152:GLN:HE22	48:Qb:250:PHE:HA	1.84	0.42
59:S1:124:HIS:CD2	60:S2:381:MET:HE2	2.42	0.42
66:S8:150:THR:HG21	66:S8:180:HIS:CD2	2.54	0.42
67:V1:63:TYR:CE2	67:V1:64:LYS:HE3	2.54	0.42
2:5A:107:ALA:HB1	2:5A:141:ILE:HD13	2.02	0.42
71:6A:101:PC1:H153	37:C3:184:ALA:HB3	2.00	0.42
18:A9:303:ARG:HB2	18:A9:316:ARG:HD3	2.00	0.42
19:AC:128:PHE:CE2	19:AC:151:LYS:HD3	2.54	0.42
20:AK:207:VAL:HA	20:AK:258:LEU:O	2.20	0.42
32:B9:150:HIS:CD2	32:B9:151:PRO:HD2	2.54	0.42
35:C1:352:GLY:HA3	79:C1:603:HEA:C14	2.48	0.42
41:N1:9:LEU:O	41:N1:13:ILE:HG12	2.19	0.42
45:N5:162:THR:O	45:N5:166:THR:HG23	2.20	0.42
45:N5:230:HIS:H	45:N5:230:HIS:CD2	2.36	0.42
45:N5:504:LEU:HD12	72:N5:703:CDL:H511	2.01	0.42
45:N5:563:PRO:HA	82:S2:501:PEE:H29	2.00	0.42
47:QA:177:LEU:HD11	47:QA:272:VAL:HG22	2.00	0.42
48:QB:92:PHE:HD2	48:QB:211:LEU:HD12	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:QC:139:SER:OG	49:QC:255:ASN:ND2	2.48	0.42
72:QC:406:CDL:H151	72:QC:406:CDL:H382	2.02	0.42
52:QF:56:ARG:NH1	52:QF:65:GLU:OE2	2.53	0.42
47:Qa:391:GLY:HA2	47:Qa:394:ASP:OD2	2.19	0.42
49:Qc:119:LEU:HD22	83:Qc:403:HEM:HBB2	2.00	0.42
50:Qd:222:PRO:HA	50:Qd:223:PRO:HD3	1.94	0.42
59:S1:76:ARG:NH2	59:S1:90:ALA:HB2	2.34	0.42
62:S4:102:ASP:OD1	62:S4:102:ASP:N	2.53	0.42
67:V1:64:LYS:HE2	67:V1:64:LYS:HB3	1.83	0.42
68:V2:237:PRO:HA	68:V2:238:PRO:HD3	1.91	0.42
6:C4:49:TYR:CD1	38:C4:153:ILE:HG21	2.55	0.42
18:A9:262:THR:O	18:A9:333:PRO:HD2	2.20	0.42
77:AL:205:PLX:H341	77:AL:205:PLX:H311	1.92	0.42
22:AM:28:PHE:HE1	77:AM:201:PLX:H112	1.84	0.42
26:B3:32:VAL:HG21	32:B9:77:ASP:HB2	2.02	0.42
27:B4:59:VAL:HG22	44:N4:423:ILE:HG12	1.99	0.42
30:B7:92:HIS:ND1	45:N5:481:THR:OG1	2.37	0.42
32:B9:161:PHE:O	32:B9:165:GLU:HG2	2.20	0.42
42:N2:2:ASN:ND2	42:N2:4:ILE:H	2.18	0.42
42:N2:17:THR:HG23	42:N2:137:ALA:HB2	2.00	0.42
49:QC:316:MET:HE3	82:QC:404:PEE:H10	2.01	0.42
50:QD:187:ARG:NH1	50:QD:192:GLY:O	2.53	0.42
50:QD:222:PRO:HG3	50:QD:234:PHE:HB2	2.02	0.42
47:Qa:49:ILE:HG22	47:Qa:227:HIS:CE1	2.55	0.42
50:Qd:105:SER:HB2	50:Qd:284:ASP:CG	2.45	0.42
52:Qf:31:THR:O	52:Qf:35:GLU:HG2	2.19	0.42
66:S8:63:TRP:HB3	66:S8:66:LEU:HD12	2.00	0.42
67:V1:44:ASN:C	67:V1:46:TYR:H	2.27	0.42
2:5A:143:THR:O	2:5A:147:LEU:HG	2.19	0.42
15:A6:48:SER:HB3	15:A6:53:GLU:HB2	2.00	0.42
20:AK:340:LYS:HE3	20:AK:341:TYR:CZ	2.55	0.42
35:C1:304:TYR:HB2	82:C1:609:PEE:H57	2.00	0.42
36:C2:104:TRP:CG	36:C2:203:ASN:HB2	2.55	0.42
38:C4:74:SER:O	38:C4:78:LYS:HG3	2.20	0.42
39:CA:72:ARG:HH11	40:CB:22:SER:HB3	1.84	0.42
42:N2:186:HIS:O	42:N2:190:MET:HG3	2.19	0.42
42:N2:267:ILE:HD11	42:N2:283:ALA:HB2	2.00	0.42
46:N6:117:PHE:HB2	46:N6:119:PHE:CZ	2.54	0.42
55:QI:11:TYR:OH	48:Qb:451:ASP:OD2	2.30	0.42
49:Qc:113:TRP:HE3	83:Qc:403:HEM:HMD1	1.83	0.42
59:S1:370:GLU:O	59:S1:533:GLY:N	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:S1:537:ILE:HG23	59:S1:542:PRO:HD3	2.01	0.42
60:S2:113:ARG:HD2	60:S2:113:ARG:HA	1.82	0.42
62:S4:71:HIS:CE1	62:S4:120:PRO:HD2	2.54	0.42
65:S7:107:GLY:HA2	86:S7:301:SF4:S4	2.59	0.42
67:V1:137:LYS:HE2	67:V1:137:LYS:HB2	1.86	0.42
1:4L:55:LEU:HD23	1:4L:55:LEU:HA	1.87	0.42
3:5B:83:ILE:HD11	37:C3:2:THR:N	2.34	0.42
18:A9:303:ARG:HD3	18:A9:316:ARG:CZ	2.50	0.42
18:A9:346:GLU:HG2	18:A9:371:PRO:HB3	2.01	0.42
19:AC:133:ILE:HG13	32:B9:46:SER:HB2	2.01	0.42
25:B2:76:ASP:OD1	25:B2:76:ASP:N	2.53	0.42
31:B8:139:PHE:CD2	72:N5:703:CDL:H851	2.54	0.42
33:BK:98:VAL:HG11	34:BL:125:LEU:HD12	2.01	0.42
36:C2:161:HIS:HB2	36:C2:174:ALA:HB3	2.00	0.42
38:C4:146:LEU:HD23	38:C4:146:LEU:HA	1.82	0.42
42:N2:25:HIS:HB2	63:S5:15:ASP:HB2	2.02	0.42
42:N2:168:GLY:O	42:N2:172:GLN:HG2	2.19	0.42
48:QB:165:ARG:NH1	48:QB:208:VAL:O	2.52	0.42
51:QE:88:PHE:O	51:QE:92:ARG:HG3	2.19	0.42
51:QE:207:LYS:HG3	51:QE:208:PRO:HD2	2.02	0.42
47:Qa:220:LEU:HD12	47:Qa:234:ALA:HB2	2.01	0.42
47:Qa:230:LEU:HD23	47:Qa:230:LEU:HA	1.84	0.42
59:S1:432:ILE:HD11	59:S1:455:ILE:HD12	2.02	0.42
69:V3:420:SER:HB3	69:V3:423:HIS:ND1	2.35	0.42
11:A1:1:MET:HE2	11:A1:1:MET:HB3	1.88	0.42
15:A6:78:LEU:HD22	15:A6:130:MET:HE3	2.01	0.42
20:AK:211:VAL:HB	20:AK:216:ILE:HD11	2.01	0.42
31:B8:94:HIS:O	31:B8:98:ARG:N	2.48	0.42
33:BK:130:GLU:OE2	33:BK:134:GLN:NE2	2.52	0.42
36:C2:165:VAL:HG22	36:C2:194:GLY:HA3	2.01	0.42
44:N4:73:LEU:HA	44:N4:76:MET:HE2	2.01	0.42
71:N5:704:PC1:H262	71:N5:704:PC1:H391	2.02	0.42
49:QC:27:ILE:HG12	49:QC:224:TYR:OH	2.20	0.42
48:Qb:172:LEU:HD21	48:Qb:202:GLU:HB3	2.02	0.42
48:Qb:388:VAL:O	48:Qb:392:LYS:HG3	2.19	0.42
60:S2:87:THR:OG1	60:S2:106:GLU:OE1	2.23	0.42
67:V1:43:THR:OG1	67:V1:44:ASN:N	2.51	0.42
68:V2:137:THR:HG22	68:V2:138:THR:H	1.84	0.42
11:A1:4:GLU:OE1	41:N1:26:LYS:NZ	2.47	0.42
13:A3:127:ALA:HB2	41:N1:312:ALA:HA	2.01	0.42
14:A5:76:GLN:O	14:A5:80:VAL:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
77:AL:205:PLX:H362	77:AL:205:PLX:H392	1.84	0.42
27:B4:77:TYR:CZ	45:N5:564:LYS:HG2	2.55	0.42
28:B5:110:TRP:O	28:B5:119:ARG:HG2	2.20	0.42
42:N2:169:GLY:HA3	42:N2:292:PHE:CE2	2.55	0.42
44:N4:10:MET:HE2	44:N4:10:MET:HA	2.02	0.42
45:N5:208:CYS:HA	45:N5:209:PRO:HD3	1.78	0.42
48:QB:121:ASN:OD1	48:QB:122:ALA:N	2.52	0.42
48:QB:223:HIS:HA	48:QB:228:ARG:HH21	1.85	0.42
49:QC:130:GLY:O	49:QC:133:LEU:HB2	2.20	0.42
72:QC:408:CDL:OB4	54:Qh:41:ARG:NH2	2.53	0.42
50:QD:303:LEU:HB3	51:QE:121:THR:OG1	2.20	0.42
49:Qc:332:LEU:HD21	49:Qc:358:TYR:CE2	2.55	0.42
59:S1:68:ARG:HH12	59:S1:279:GLU:HG2	1.85	0.42
59:S1:501:ARG:NE	59:S1:506:VAL:HG23	2.35	0.42
64:S6:67:ALA:HB1	66:S8:110:GLU:HA	2.02	0.42
69:V3:411:MET:HE2	69:V3:411:MET:HB3	1.92	0.42
69:V3:418:ARG:NH1	69:V3:423:HIS:O	2.51	0.42
12:A2:89:ARG:HA	12:A2:92:GLU:HG2	2.02	0.42
15:A6:45:PRO:HB3	62:S4:53:ILE:HD13	2.02	0.42
17:A8:117:ASN:HB3	23:AN:73:PRO:HG2	2.02	0.42
19:AB:112:SER:H	74:AB:201:ZMP:P1	2.42	0.42
19:AC:113:LEU:HB2	32:B9:87:ARG:HH21	1.84	0.42
20:AK:172:LEU:HD22	20:AK:189:TYR:CD1	2.54	0.42
29:B6:183:PHE:CE1	30:B7:40:VAL:HG11	2.55	0.42
31:B8:48:ARG:HE	31:B8:48:ARG:HB3	1.71	0.42
35:C1:91:ASP:OD1	35:C1:92:MET:N	2.41	0.42
35:C1:143:VAL:HB	35:C1:213:ARG:CZ	2.50	0.42
79:C1:603:HEA:HA	79:C1:603:HEA:HAD2	1.92	0.42
42:N2:14:MET:O	42:N2:18:MET:HG2	2.19	0.42
42:N2:88:LYS:HE3	42:N2:88:LYS:HB3	1.87	0.42
42:N2:111:PHE:HA	45:N5:591:PHE:CE1	2.55	0.42
42:N2:178:ILE:HG23	42:N2:292:PHE:CE1	2.55	0.42
45:N5:149:ILE:HD11	72:N5:702:CDL:H171	2.01	0.42
47:QA:438:MET:HB3	47:QA:450:VAL:HG22	2.02	0.42
49:QC:327:MET:HA	54:Qh:52:PRO:HB3	2.01	0.42
54:QH:37:ASN:OD1	54:QH:40:ARG:NH2	2.41	0.42
47:Qa:183:ARG:HG3	47:Qa:254:ARG:HB2	2.02	0.42
59:S1:330:LEU:HD23	59:S1:330:LEU:HA	1.93	0.42
61:S3:173:MET:HE2	61:S3:188:LEU:HB2	2.01	0.42
67:V1:384:PRO:HG2	67:V1:422:HIS:O	2.19	0.42
72:6A:102:CDL:H152	72:6A:102:CDL:H182	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:C1:71:MET:HB2	35:C1:72:PRO:HD3	2.02	0.41
44:N4:400:MET:HE1	45:N5:183:VAL:HG21	2.02	0.41
45:N5:297:ASP:O	45:N5:301:ILE:HG13	2.21	0.41
47:QA:239:ASN:OD1	47:QA:239:ASN:N	2.53	0.41
47:QA:272:VAL:HA	47:QA:337:GLY:HA3	2.02	0.41
48:QB:304:LEU:HD13	48:QB:354:LEU:HD22	2.00	0.41
51:QE:133:VAL:HG22	82:QE:302:PEE:H38	2.02	0.41
51:QE:239:HIS:HB2	85:QE:304:FES:S1	2.60	0.41
53:QG:41:ASP:OD1	53:QG:41:ASP:N	2.45	0.41
72:QH:101:CDL:HB62	49:Qc:29:SER:HB2	2.02	0.41
47:Qa:72:GLU:O	47:Qa:188:ASN:ND2	2.53	0.41
49:Qc:165:TRP:O	49:Qc:174:THR:OG1	2.29	0.41
65:S7:154:ASP:OD1	65:S7:154:ASP:N	2.48	0.41
4:6A:81:LEU:HD22	71:6A:101:PC1:H221	2.01	0.41
7:7A:53:TYR:CE1	37:C3:15:PRO:HG3	2.55	0.41
15:A6:140:ARG:HA	15:A6:140:ARG:HE	1.85	0.41
16:A7:54:TYR:CZ	60:S2:368:LYS:HD2	2.55	0.41
19:AC:117:GLU:OE2	32:B9:62:TYR:OH	2.38	0.41
23:AN:120:MET:HE2	23:AN:120:MET:HB3	1.88	0.41
28:B5:139:ILE:O	28:B5:143:GLU:HG2	2.20	0.41
41:N1:73:ILE:HD13	41:N1:73:ILE:HA	1.91	0.41
46:N6:170:GLU:CD	46:N6:173:ARG:HH21	2.28	0.41
82:QB:503:PEE:H39	82:QB:503:PEE:H72	2.02	0.41
47:Qa:125:CYS:SG	47:Qa:133:LEU:HD22	2.60	0.41
47:Qa:297:PRO:HB3	47:Qa:304:ASN:HD21	1.85	0.41
51:Qe:156:LEU:HB2	51:Qe:269:ASP:HA	2.02	0.41
59:S1:304:GLN:HB2	59:S1:316:TYR:HD1	1.85	0.41
67:V1:347:THR:HG22	67:V1:348:GLY:H	1.85	0.41
4:6A:79:HIS:HD2	4:6A:83:HIS:CD2	2.38	0.41
15:A6:127:THR:O	15:A6:131:ARG:HG3	2.20	0.41
18:A9:168:SER:HA	18:A9:184:LYS:NZ	2.35	0.41
20:AK:145:TYR:OH	20:AK:201:LEU:O	2.21	0.41
77:AL:205:PLX:H1C3	77:AL:205:PLX:H21	1.84	0.41
27:B4:63:PRO:O	27:B4:67:ARG:HG3	2.20	0.41
35:C1:372:TYR:N	35:C1:432:GLY:HA3	2.35	0.41
36:C2:93:PRO:HG2	36:C2:151:ARG:CZ	2.50	0.41
37:C3:205:GLY:O	37:C3:208:VAL:HG22	2.20	0.41
77:CB:201:PLX:H112	77:CB:201:PLX:H81	1.76	0.41
47:QA:301:ARG:HG2	57:QK:53:GLU:HB3	2.03	0.41
48:QB:363:MET:O	48:QB:464:GLN:NE2	2.54	0.41
50:QD:97:TRP:NE1	50:QD:210:ASP:OD1	2.42	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:QF:34:ARG:NH2	50:Qd:217:THR:O	2.51	0.41
47:Qa:68:GLY:H	47:Qa:71:TYR:HD2	1.68	0.41
51:Qe:249:ILE:HG12	51:Qe:254:ALA:O	2.20	0.41
6:6C:70:ILE:HD11	38:C4:147:ASP:HB3	2.02	0.41
16:A7:31:ILE:HD12	22:AM:56:PHE:CG	2.55	0.41
35:C1:438:ARG:NH2	79:C1:603:HEA:O2D	2.53	0.41
36:C2:158:ASP:OD1	36:C2:159:VAL:HG22	2.21	0.41
44:N4:368:ALA:HB1	44:N4:375:LEU:HA	2.02	0.41
59:S1:449:PRO:HB2	59:S1:679:LEU:HD13	2.02	0.41
1:4L:3:LEU:HG	46:N6:121:GLY:HA3	2.01	0.41
1:4L:23:ARG:NH2	46:N6:86:ASN:HD22	2.16	0.41
10:8B:43:LEU:HD23	10:8B:43:LEU:HA	1.90	0.41
18:A9:221:ARG:HD2	18:A9:286:ARG:NH1	2.35	0.41
79:C1:602:HEA:HBA2	79:C1:602:HEA:CMA	2.51	0.41
37:C3:208:VAL:HG12	37:C3:245:VAL:CG1	2.51	0.41
43:N3:65:PHE:CD2	43:N3:98:LEU:HD11	2.55	0.41
45:N5:176:ARG:HA	45:N5:176:ARG:HD2	1.85	0.41
45:N5:213:LEU:HB3	45:N5:273:VAL:HG11	2.03	0.41
46:N6:65:LEU:HA	46:N6:65:LEU:HD23	1.76	0.41
47:QA:68:GLY:N	47:QA:208:TYR:OH	2.50	0.41
48:QB:57:LEU:HD12	48:QB:229:MET:O	2.21	0.41
47:Qa:66:LYS:O	47:Qa:217:ARG:NH2	2.48	0.41
49:Qc:46:LEU:HD21	82:Qd:403:PEE:H35	2.03	0.41
82:Qh:103:PEE:H26	82:Qh:103:PEE:H32	1.84	0.41
59:S1:534:VAL:HG22	59:S1:537:ILE:HB	2.02	0.41
60:S2:230:ALA:O	66:S8:98:ARG:NH2	2.54	0.41
61:S3:150:LEU:HD12	62:S4:59:LEU:HD11	2.03	0.41
15:A6:145:LEU:HD12	15:A6:145:LEU:HA	1.87	0.41
27:B4:77:TYR:OH	45:N5:564:LYS:HG2	2.21	0.41
35:C1:96:ARG:H	35:C1:96:ARG:HG3	1.51	0.41
35:C1:331:ASN:HD21	38:C4:42:ARG:HB2	1.85	0.41
35:C1:417:MET:O	35:C1:421:VAL:HG22	2.21	0.41
41:N1:102:VAL:HG21	41:N1:154:LEU:HD11	2.02	0.41
45:N5:420:ALA:HB1	45:N5:498:PHE:CD1	2.56	0.41
49:QC:318:ARG:NH1	49:QC:321:SER:OG	2.53	0.41
51:QE:153:GLU:HB3	51:QE:270:LEU:HD11	2.03	0.41
54:QH:20:SER:O	54:QH:24:GLN:HG2	2.20	0.41
48:Qb:156:LEU:HB2	48:Qb:213:ARG:NH1	2.35	0.41
59:S1:295:ASP:OD2	59:S1:706:THR:OG1	2.29	0.41
59:S1:547:LEU:HB3	59:S1:550:ALA:HB3	2.02	0.41
68:V2:66:ILE:HG21	68:V2:81:PRO:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:A9:216:TYR:HE1	18:A9:314:THR:HB	1.86	0.41
19:AC:79:ILE:O	19:AC:83:VAL:HG13	2.21	0.41
20:AK:134:GLN:NE2	75:AK:401:ADP:HN62	2.16	0.41
72:B5:202:CDL:H191	72:B5:202:CDL:H731	2.01	0.41
29:B6:72:LEU:HD23	29:B6:72:LEU:HA	1.88	0.41
32:B9:69:LEU:HD21	32:B9:82:PHE:HB3	2.02	0.41
35:C1:115:SER:OG	35:C1:142:SER:O	2.38	0.41
35:C1:307:SER:O	35:C1:311:ILE:HG23	2.20	0.41
41:N1:289:LEU:HA	41:N1:293:PHE:HB2	2.03	0.41
45:N5:10:THR:O	45:N5:14:ILE:HG23	2.20	0.41
45:N5:67:HIS:O	82:N5:701:PEE:H11	2.21	0.41
46:N6:116:ILE:H	46:N6:116:ILE:HD12	1.86	0.41
46:N6:123:GLY:O	46:N6:127:ILE:HG23	2.21	0.41
49:QC:200:LEU:HD23	49:QC:201:HIS:HD2	1.85	0.41
57:QK:55:LEU:HA	57:QK:55:LEU:HD23	1.84	0.41
51:Qe:88:PHE:O	51:Qe:92:ARG:HG3	2.21	0.41
60:S2:69:PRO:HA	60:S2:70:PRO:HD3	1.96	0.41
60:S2:151:MET:HG3	60:S2:220:TYR:CZ	2.56	0.41
60:S2:290:LEU:O	60:S2:293:GLY:CA	2.69	0.41
64:S6:116:LEU:HD23	64:S6:116:LEU:HA	1.93	0.41
65:S7:140:GLY:HA3	65:S7:144:HIS:CD2	2.56	0.41
1:4L:38:LEU:HD21	46:N6:37:GLY:HA2	2.02	0.41
4:6A:60:ILE:O	4:6A:62:TYR:N	2.50	0.41
15:A6:107:LEU:HD23	15:A6:107:LEU:HA	1.94	0.41
15:A6:131:ARG:NH2	61:S3:210:LEU:HD21	2.36	0.41
18:A9:118:LYS:HE2	18:A9:118:LYS:HB3	1.86	0.41
28:B5:181:HIS:HE1	63:S5:38:LYS:HE2	1.86	0.41
77:B5:201:PLX:H21	77:B5:201:PLX:H1B3	1.89	0.41
30:B7:16:GLU:HA	30:B7:17:PRO:HD3	1.95	0.41
37:C3:63:ARG:HA	37:C3:67:PHE:CD2	2.56	0.41
44:N4:200:ILE:O	44:N4:204:MET:HG2	2.21	0.41
45:N5:102:GLU:OE1	45:N5:456:ARG:NH2	2.29	0.41
45:N5:260:LEU:HD23	45:N5:260:LEU:HA	1.88	0.41
49:QC:133:LEU:HD23	49:QC:133:LEU:HA	1.78	0.41
47:Qa:60:ARG:HD3	47:Qa:393:LEU:HD22	2.03	0.41
48:Qb:157:GLU:O	48:Qb:161:ILE:HG12	2.20	0.41
48:Qb:418:LEU:HD23	48:Qb:418:LEU:HA	1.92	0.41
49:Qc:237:LEU:HB2	50:Qd:297:MET:HG2	2.03	0.41
59:S1:555:ILE:HD13	59:S1:555:ILE:HA	1.94	0.41
59:S1:638:THR:O	59:S1:642:VAL:HG23	2.21	0.41
67:V1:235:VAL:H	67:V1:240:THR:HG21	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4L:9:ILE:HG12	42:N2:72:MET:HE1	2.03	0.41
10:8B:31:ARG:HD2	35:C1:481:GLU:CD	2.46	0.41
12:A2:69:TYR:HE2	12:A2:75:LYS:HD3	1.85	0.41
19:AB:93:ILE:HD12	19:AB:108:LEU:HD13	2.03	0.41
19:AC:140:CYS:HB3	19:AC:143:GLU:HG3	2.03	0.41
20:AK:41:GLY:HA2	20:AK:298:MET:SD	2.61	0.41
20:AK:256:GLU:HG2	20:AK:280:CYS:SG	2.61	0.41
76:AL:202:3PE:H3B1	76:AL:202:3PE:H382	1.92	0.41
23:AN:88:ARG:O	23:AN:92:GLU:HG2	2.21	0.41
23:AN:119:PRO:HB3	23:AN:123:GLU:HB2	2.02	0.41
27:B4:129:TYR:O	44:N4:307:TRP:HB2	2.21	0.41
77:B5:201:PLX:H271	77:B5:201:PLX:H24	1.83	0.41
32:B9:47:ALA:HB1	32:B9:194:GLU:HB2	2.03	0.41
35:C1:12:HIS:CG	35:C1:84:PRO:HG2	2.55	0.41
35:C1:202:LEU:HD22	35:C1:238:PHE:CE2	2.55	0.41
36:C2:143:VAL:HG12	36:C2:219:PHE:HD1	1.86	0.41
36:C2:145:PRO:HG3	36:C2:219:PHE:CD2	2.56	0.41
37:C3:86:PHE:CZ	71:C3:301:PC1:H3A1	2.56	0.41
37:C3:144:ILE:HD12	37:C3:144:ILE:HA	1.84	0.41
37:C3:148:HIS:HB2	37:C3:235:PHE:HE2	1.85	0.41
38:C4:130:PRO:HG2	38:C4:133:PHE:CE1	2.56	0.41
42:N2:218:LEU:HB3	42:N2:244:MET:HE2	2.03	0.41
42:N2:291:TYR:HA	44:N4:151:PHE:HZ	1.85	0.41
47:QA:183:ARG:HG3	47:QA:254:ARG:HB2	2.03	0.41
49:QC:277:ALA:HB1	49:QC:294:LEU:HG	2.03	0.41
51:QE:122:THR:HG21	55:Qi:25:ILE:HD13	2.03	0.41
54:QH:6:GLY:HA3	48:Qb:363:MET:SD	2.61	0.41
47:Qa:125:CYS:HB3	47:Qa:133:LEU:HD22	2.03	0.41
48:Qb:190:THR:HB	48:Qb:275:ILE:HG13	2.03	0.41
48:Qb:407:THR:HB	48:Qb:408:PRO:HD3	2.03	0.41
51:Qe:156:LEU:N	51:Qe:269:ASP:O	2.45	0.41
51:Qe:197:ASP:O	51:Qe:199:GLN:N	2.53	0.41
51:Qe:220:LEU:HD12	51:Qe:239:HIS:HE1	1.86	0.41
53:Qg:88:LYS:HD3	53:Qg:88:LYS:HA	1.89	0.41
59:S1:371:VAL:O	59:S1:482:GLN:NE2	2.54	0.41
10:8B:50:PHE:O	10:8B:53:PRO:HD2	2.21	0.41
25:B2:76:ASP:O	45:N5:385:TYR:OH	2.27	0.41
36:C2:11:ASP:OD1	36:C2:11:ASP:N	2.54	0.41
47:QA:214:THR:O	47:QA:218:MET:HG3	2.21	0.41
49:QC:119:LEU:HD22	83:QC:403:HEM:HBB2	2.03	0.41
51:QE:218:THR:HG21	51:QE:256:LEU:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:Qb:501:CDL:HA32	71:Qb:502:PC1:H151	2.02	0.41
59:S1:436:VAL:O	59:S1:442:TYR:OH	2.26	0.41
60:S2:277:ARG:NH2	60:S2:451:ALA:HB1	2.36	0.41
62:S4:168:LYS:HA	62:S4:168:LYS:HD3	1.92	0.41
3:5B:33:SER:OG	3:5B:34:GLY:N	2.54	0.40
7:7A:52:LEU:HD23	7:7A:52:LEU:HA	1.93	0.40
15:A6:88:LYS:O	15:A6:92:MET:HG2	2.21	0.40
72:A8:301:CDL:H221	72:A8:301:CDL:H252	1.90	0.40
28:B5:176:LYS:H	63:S5:45:HIS:CD2	2.39	0.40
31:B8:109:LEU:O	31:B8:113:ILE:HG23	2.22	0.40
35:C1:38:ARG:HG3	35:C1:458:SER:CB	2.51	0.40
35:C1:195:LEU:HD23	35:C1:245:ILE:HD13	2.02	0.40
44:N4:9:THR:O	44:N4:13:PRO:HD3	2.21	0.40
45:N5:200:GLN:HE21	45:N5:204:LEU:HD11	1.85	0.40
45:N5:504:LEU:HD23	45:N5:504:LEU:HA	1.90	0.40
71:QC:405:PC1:H242	50:QD:102:LEU:HD21	2.03	0.40
51:QE:202:LEU:HD11	51:QE:208:PRO:HB3	2.03	0.40
54:QH:67:PHE:HE1	49:Qc:344:GLU:HG3	1.86	0.40
55:QI:63:LYS:HE2	55:QI:63:LYS:HB2	1.94	0.40
47:Qa:115:THR:HG23	47:Qa:118:SER:H	1.86	0.40
49:Qc:32:ASN:ND2	49:Qc:228:ASP:HA	2.36	0.40
59:S1:691:ILE:HG12	59:S1:695:TYR:CE2	2.56	0.40
60:S2:149:SER:HA	60:S2:184:THR:CG2	2.51	0.40
60:S2:204:THR:HB	60:S2:208:TRP:CZ2	2.55	0.40
62:S4:56:ASP:OD1	62:S4:56:ASP:N	2.54	0.40
65:S7:190:LEU:HD23	65:S7:190:LEU:HA	1.86	0.40
71:6A:101:PC1:H241	35:C1:215:LEU:HD21	2.03	0.40
71:7B:101:PC1:H152	71:7B:101:PC1:H111	1.85	0.40
16:A7:101:ILE:HG22	61:S3:136:ARG:O	2.21	0.40
18:A9:246:SER:O	18:A9:250:ILE:HG12	2.22	0.40
30:B7:15:LYS:HD2	30:B7:113:LYS:HG3	2.03	0.40
30:B7:76:ASN:ND2	30:B7:79:ALA:HB2	2.36	0.40
38:C4:62:LEU:HG	38:C4:81:LEU:HD21	2.03	0.40
41:N1:170:GLU:HG2	41:N1:171:HIS:HD2	1.86	0.40
41:N1:290:TRP:HB3	43:N3:111:LEU:HD13	2.03	0.40
44:N4:231:LEU:HD23	44:N4:235:LEU:HD12	2.02	0.40
44:N4:398:MET:O	44:N4:402:ILE:HG13	2.21	0.40
51:QE:190:VAL:HG21	51:QE:250:ARG:NH2	2.36	0.40
56:QJ:14:ALA:O	56:QJ:18:ILE:HG12	2.22	0.40
49:Qc:24:PRO:HB2	49:Qc:27:ILE:HG23	2.01	0.40
49:Qc:197:LEU:HD11	83:Qc:403:HEM:HMA3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:Qj:42:LEU:HA	58:Qj:45:VAL:HG22	2.03	0.40
59:S1:696:MET:HG2	59:S1:711:VAL:HG21	2.03	0.40
60:S2:149:SER:HB2	60:S2:152:CYS:HB2	2.04	0.40
60:S2:323:ASP:OD1	66:S8:37:THR:OG1	2.30	0.40
64:S6:74:GLN:NE2	64:S6:75:PRO:HD2	2.36	0.40
1:4L:37:MET:HE1	1:4L:63:LEU:HD11	2.04	0.40
1:4L:62:ILE:HG21	42:N2:31:ILE:HD11	2.03	0.40
2:5A:134:PRO:O	2:5A:138:GLU:HG2	2.21	0.40
30:B7:22:MET:HE1	30:B7:102:PHE:CD2	2.56	0.40
32:B9:99:MET:HA	32:B9:99:MET:HE2	2.04	0.40
32:B9:178:GLU:OE2	32:B9:209:TRP:NE1	2.52	0.40
35:C1:390:MET:HE2	79:C1:602:HEA:H202	2.03	0.40
35:C1:469:ILE:HD12	35:C1:469:ILE:HA	1.93	0.40
36:C2:130:PRO:HA	38:C4:137:TRP:CH2	2.57	0.40
41:N1:206:GLU:HB2	60:S2:90:PHE:CE2	2.56	0.40
42:N2:277:ILE:H	42:N2:277:ILE:HD12	1.86	0.40
44:N4:1:MET:HG2	44:N4:52:PHE:CD2	2.56	0.40
45:N5:176:ARG:O	45:N5:180:ILE:HG13	2.21	0.40
45:N5:290:LEU:O	45:N5:293:ILE:HG12	2.22	0.40
48:QB:341:PHE:HB2	48:QB:358:PHE:HB3	2.02	0.40
49:QC:310:SER:HB2	49:QC:370:SER:HB3	2.02	0.40
51:QE:154:ILE:HD13	51:QE:176:VAL:HG21	2.03	0.40
51:QE:207:LYS:HE2	51:QE:265:PHE:CE1	2.56	0.40
77:QI:301:PLX:H122	77:QI:301:PLX:H91	1.98	0.40
59:S1:257:VAL:HG11	59:S1:413:LEU:HB2	2.03	0.40
59:S1:341:ILE:HG13	59:S1:545:LEU:HD11	2.02	0.40
59:S1:372:PHE:CZ	59:S1:385:TYR:HB3	2.57	0.40
59:S1:598:ASN:HD21	59:S1:600:GLU:HG2	1.86	0.40
60:S2:292:TYR:O	61:S3:162:ALA:HB2	2.20	0.40
64:S6:104:LYS:HG2	64:S6:107:LYS:HG2	2.04	0.40
4:6A:29:ARG:HB2	37:C3:146:TRP:CE2	2.56	0.40
5:6B:37:PHE:CE1	5:6B:58:ARG:HB2	2.57	0.40
15:A6:63:ARG:HG2	19:AB:120:MET:SD	2.62	0.40
26:B3:47:ARG:HA	26:B3:50:ALA:HB3	2.03	0.40
28:B5:163:ARG:HH22	40:CB:102:ASP:CG	2.28	0.40
35:C1:240:HIS:O	35:C1:243:VAL:HG22	2.21	0.40
77:C2:301:PLX:H21	77:C2:301:PLX:H1C3	1.65	0.40
41:N1:245:ALA:HB3	41:N1:255:TYR:CE2	2.56	0.40
42:N2:190:MET:HG2	42:N2:204:ASN:HB3	2.03	0.40
45:N5:572:LYS:HD3	45:N5:572:LYS:HA	1.93	0.40
47:QA:257:GLU:OE2	47:QA:259:ARG:HD3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:QB:56:GLY:HA3	48:QB:227:PRO:HB3	2.03	0.40
47:Qa:195:TYR:CZ	47:Qa:196:ARG:HG2	2.56	0.40
48:Qb:172:LEU:HD23	48:Qb:172:LEU:HA	1.91	0.40
49:Qc:33:PHE:HA	49:Qc:36:LEU:HB2	2.04	0.40
59:S1:560:LEU:HD12	59:S1:566:ILE:HD11	2.04	0.40
67:V1:244:ASN:OD1	67:V1:245:VAL:N	2.53	0.40
23:AN:19:ILE:HD12	60:S2:351:SER:HB2	2.04	0.40
25:B2:53:SER:HA	25:B2:56:ILE:HG12	2.04	0.40
25:B2:65:MET:SD	45:N5:375:ILE:HG12	2.61	0.40
33:BK:97:LYS:HE3	33:BK:97:LYS:HB3	1.89	0.40
41:N1:2:PHE:CE2	41:N1:6:ILE:HD11	2.56	0.40
42:N2:43:VAL:HG11	42:N2:129:LEU:HD23	2.04	0.40
44:N4:282:LEU:O	44:N4:286:ILE:HG13	2.21	0.40
44:N4:302:MET:HE2	44:N4:302:MET:HA	2.03	0.40
45:N5:389:PHE:O	45:N5:393:ASP:HB3	2.22	0.40
45:N5:504:LEU:O	45:N5:507:THR:OG1	2.38	0.40
48:QB:274:GLU:CD	48:QB:276:ARG:HH21	2.30	0.40
49:QC:103:TYR:CG	82:QC:404:PEE:H16	2.56	0.40
55:Qi:3:ALA:HA	55:Qi:4:PRO:HD3	1.98	0.40
59:S1:267:THR:HB	62:S4:115:SER:HB2	2.03	0.40
59:S1:275:PRO:HG3	59:S1:286:ILE:HG12	2.04	0.40
60:S2:448:HIS:HB3	60:S2:452:ASP:HB2	2.04	0.40
67:V1:99:TRP:CD1	67:V1:99:TRP:N	2.88	0.40
67:V1:258:GLY:HA2	68:V2:246:GLN:CD	2.47	0.40
67:V1:270:ASN:ND2	67:V1:338:ASP:OD2	2.54	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	4L	96/98 (98%)	94 (98%)	2 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	5A	100/102 (98%)	99 (99%)	1 (1%)	0	100	100
3	5B	93/95 (98%)	88 (95%)	5 (5%)	0	100	100
4	6A	73/75 (97%)	70 (96%)	3 (4%)	0	100	100
5	6B	80/82 (98%)	76 (95%)	4 (5%)	0	100	100
6	6C	68/70 (97%)	66 (97%)	2 (3%)	0	100	100
7	7A	55/57 (96%)	55 (100%)	0	0	100	100
8	7B	48/50 (96%)	46 (96%)	2 (4%)	0	100	100
9	7C	45/47 (96%)	44 (98%)	1 (2%)	0	100	100
10	8B	41/43 (95%)	41 (100%)	0	0	100	100
11	A1	68/70 (97%)	68 (100%)	0	0	100	100
12	A2	83/85 (98%)	79 (95%)	4 (5%)	0	100	100
13	A3	81/83 (98%)	78 (96%)	3 (4%)	0	100	100
14	A5	110/112 (98%)	105 (96%)	5 (4%)	0	100	100
15	A6	112/114 (98%)	107 (96%)	5 (4%)	0	100	100
16	A7	93/112 (83%)	89 (96%)	4 (4%)	0	100	100
17	A8	169/171 (99%)	166 (98%)	3 (2%)	0	100	100
18	A9	333/341 (98%)	322 (97%)	11 (3%)	0	100	100
19	AB	75/156 (48%)	74 (99%)	1 (1%)	0	100	100
19	AC	85/156 (54%)	85 (100%)	0	0	100	100
20	AK	318/320 (99%)	306 (96%)	12 (4%)	0	100	100
21	AL	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
22	AM	141/143 (99%)	138 (98%)	3 (2%)	0	100	100
23	AN	140/142 (99%)	132 (94%)	8 (6%)	0	100	100
24	B1	54/56 (96%)	54 (100%)	0	0	100	100
25	B2	65/67 (97%)	65 (100%)	0	0	100	100
26	B3	77/79 (98%)	75 (97%)	2 (3%)	0	100	100
27	B4	126/128 (98%)	124 (98%)	2 (2%)	0	100	100
28	B5	136/138 (99%)	131 (96%)	5 (4%)	0	100	100
29	B6	97/126 (77%)	93 (96%)	4 (4%)	0	100	100
30	B7	123/125 (98%)	118 (96%)	5 (4%)	0	100	100
31	B8	154/156 (99%)	149 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	B9	176/178 (99%)	172 (98%)	4 (2%)	0	100	100
33	BK	172/176 (98%)	171 (99%)	1 (1%)	0	100	100
34	BL	97/102 (95%)	90 (93%)	7 (7%)	0	100	100
35	C1	512/514 (100%)	495 (97%)	17 (3%)	0	100	100
36	C2	226/228 (99%)	221 (98%)	5 (2%)	0	100	100
37	C3	258/260 (99%)	246 (95%)	12 (5%)	0	100	100
38	C4	136/138 (99%)	127 (93%)	9 (7%)	0	100	100
39	CA	47/49 (96%)	46 (98%)	1 (2%)	0	100	100
40	CB	119/121 (98%)	118 (99%)	1 (1%)	0	100	100
41	N1	307/318 (96%)	295 (96%)	12 (4%)	0	100	100
42	N2	345/347 (99%)	337 (98%)	8 (2%)	0	100	100
43	N3	94/115 (82%)	91 (97%)	3 (3%)	0	100	100
44	N4	457/459 (100%)	451 (99%)	6 (1%)	0	100	100
45	N5	601/603 (100%)	568 (94%)	33 (6%)	0	100	100
46	N6	159/173 (92%)	146 (92%)	13 (8%)	0	100	100
47	QA	417/419 (100%)	404 (97%)	13 (3%)	0	100	100
47	Qa	417/419 (100%)	403 (97%)	14 (3%)	0	100	100
48	QB	444/446 (100%)	430 (97%)	14 (3%)	0	100	100
48	Qb	429/446 (96%)	421 (98%)	8 (2%)	0	100	100
49	QC	377/379 (100%)	368 (98%)	9 (2%)	0	100	100
49	Qc	377/379 (100%)	368 (98%)	9 (2%)	0	100	100
50	QD	239/241 (99%)	231 (97%)	8 (3%)	0	100	100
50	Qd	237/241 (98%)	234 (99%)	3 (1%)	0	100	100
51	QE	194/196 (99%)	188 (97%)	6 (3%)	0	100	100
51	Qe	194/196 (99%)	187 (96%)	7 (4%)	0	100	100
52	QF	65/67 (97%)	65 (100%)	0	0	100	100
52	Qf	62/67 (92%)	61 (98%)	1 (2%)	0	100	100
53	QG	99/101 (98%)	97 (98%)	2 (2%)	0	100	100
53	Qg	99/101 (98%)	96 (97%)	3 (3%)	0	100	100
54	QH	76/79 (96%)	74 (97%)	2 (3%)	0	100	100
54	Qh	77/79 (98%)	76 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
55	QI	60/64 (94%)	59 (98%)	1 (2%)	0	100	100
55	Qi	58/64 (91%)	58 (100%)	0	0	100	100
56	QJ	47/49 (96%)	44 (94%)	3 (6%)	0	100	100
57	QK	69/78 (88%)	68 (99%)	1 (1%)	0	100	100
58	Qj	49/51 (96%)	47 (96%)	2 (4%)	0	100	100
59	S1	687/689 (100%)	653 (95%)	34 (5%)	0	100	100
60	S2	414/430 (96%)	392 (95%)	22 (5%)	0	100	100
61	S3	205/207 (99%)	192 (94%)	13 (6%)	0	100	100
62	S4	122/124 (98%)	118 (97%)	4 (3%)	0	100	100
63	S5	98/100 (98%)	95 (97%)	3 (3%)	0	100	100
64	S6	94/96 (98%)	93 (99%)	1 (1%)	0	100	100
65	S7	154/156 (99%)	148 (96%)	6 (4%)	0	100	100
66	S8	174/176 (99%)	169 (97%)	5 (3%)	0	100	100
67	V1	429/431 (100%)	404 (94%)	25 (6%)	0	100	100
68	V2	215/217 (99%)	208 (97%)	7 (3%)	0	100	100
69	V3	40/42 (95%)	36 (90%)	4 (10%)	0	100	100
All	All	13901/14350 (97%)	13434 (97%)	467 (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	4L	85/85 (100%)	85 (100%)	0	100	100
2	5A	89/89 (100%)	88 (99%)	1 (1%)	70	84
3	5B	80/80 (100%)	80 (100%)	0	100	100
4	6A	66/66 (100%)	64 (97%)	2 (3%)	36	63
5	6B	73/73 (100%)	73 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	6C	57/57 (100%)	56 (98%)	1 (2%)	54	75
7	7A	48/48 (100%)	44 (92%)	4 (8%)	9	33
8	7B	39/39 (100%)	39 (100%)	0	100	100
9	7C	40/40 (100%)	40 (100%)	0	100	100
10	8B	37/37 (100%)	37 (100%)	0	100	100
11	A1	58/58 (100%)	58 (100%)	0	100	100
12	A2	76/76 (100%)	76 (100%)	0	100	100
13	A3	69/69 (100%)	69 (100%)	0	100	100
14	A5	99/99 (100%)	98 (99%)	1 (1%)	73	85
15	A6	107/107 (100%)	106 (99%)	1 (1%)	75	87
16	A7	87/97 (90%)	86 (99%)	1 (1%)	70	84
17	A8	153/153 (100%)	152 (99%)	1 (1%)	81	90
18	A9	291/295 (99%)	290 (100%)	1 (0%)	91	95
19	AB	71/132 (54%)	71 (100%)	0	100	100
19	AC	80/132 (61%)	79 (99%)	1 (1%)	65	81
20	AK	283/283 (100%)	278 (98%)	5 (2%)	54	75
21	AL	101/101 (100%)	99 (98%)	2 (2%)	50	73
22	AM	129/129 (100%)	129 (100%)	0	100	100
23	AN	123/123 (100%)	121 (98%)	2 (2%)	58	77
24	B1	53/53 (100%)	53 (100%)	0	100	100
25	B2	62/62 (100%)	62 (100%)	0	100	100
26	B3	61/61 (100%)	61 (100%)	0	100	100
27	B4	113/113 (100%)	113 (100%)	0	100	100
28	B5	121/121 (100%)	121 (100%)	0	100	100
29	B6	96/119 (81%)	96 (100%)	0	100	100
30	B7	112/112 (100%)	112 (100%)	0	100	100
31	B8	141/141 (100%)	141 (100%)	0	100	100
32	B9	159/159 (100%)	159 (100%)	0	100	100
33	BK	155/156 (99%)	155 (100%)	0	100	100
34	BL	91/94 (97%)	91 (100%)	0	100	100
35	C1	425/425 (100%)	415 (98%)	10 (2%)	44	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	C2	212/212 (100%)	209 (99%)	3 (1%)	62	80
37	C3	224/224 (100%)	222 (99%)	2 (1%)	75	87
38	C4	123/123 (100%)	122 (99%)	1 (1%)	79	88
39	CA	45/45 (100%)	43 (96%)	2 (4%)	24	54
40	CB	108/108 (100%)	108 (100%)	0	100	100
41	N1	269/275 (98%)	268 (100%)	1 (0%)	89	93
42	N2	311/311 (100%)	310 (100%)	1 (0%)	91	95
43	N3	86/100 (86%)	86 (100%)	0	100	100
44	N4	410/410 (100%)	409 (100%)	1 (0%)	92	96
45	N5	537/537 (100%)	533 (99%)	4 (1%)	81	90
46	N6	129/139 (93%)	127 (98%)	2 (2%)	58	77
47	QA	330/330 (100%)	329 (100%)	1 (0%)	91	95
47	Qa	330/330 (100%)	324 (98%)	6 (2%)	54	75
48	QB	372/372 (100%)	367 (99%)	5 (1%)	65	81
48	Qb	362/372 (97%)	357 (99%)	5 (1%)	62	80
49	QC	332/332 (100%)	325 (98%)	7 (2%)	48	72
49	Qc	332/332 (100%)	331 (100%)	1 (0%)	91	95
50	QD	206/206 (100%)	206 (100%)	0	100	100
50	Qd	204/206 (99%)	202 (99%)	2 (1%)	73	85
51	QE	166/166 (100%)	166 (100%)	0	100	100
51	Qe	166/166 (100%)	166 (100%)	0	100	100
52	QF	64/64 (100%)	64 (100%)	0	100	100
52	Qf	61/64 (95%)	61 (100%)	0	100	100
53	QG	93/93 (100%)	92 (99%)	1 (1%)	70	84
53	Qg	93/93 (100%)	93 (100%)	0	100	100
54	QH	70/70 (100%)	70 (100%)	0	100	100
54	Qh	70/70 (100%)	70 (100%)	0	100	100
55	QI	50/52 (96%)	49 (98%)	1 (2%)	50	73
55	Qi	49/52 (94%)	49 (100%)	0	100	100
56	QJ	40/40 (100%)	40 (100%)	0	100	100
57	QK	55/59 (93%)	55 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
58	Qj	41/41 (100%)	41 (100%)	0	100	100
59	S1	579/579 (100%)	574 (99%)	5 (1%)	75	87
60	S2	363/370 (98%)	362 (100%)	1 (0%)	91	95
61	S3	189/189 (100%)	186 (98%)	3 (2%)	58	77
62	S4	112/112 (100%)	109 (97%)	3 (3%)	40	66
63	S5	88/88 (100%)	88 (100%)	0	100	100
64	S6	79/79 (100%)	79 (100%)	0	100	100
65	S7	132/132 (100%)	130 (98%)	2 (2%)	60	78
66	S8	151/151 (100%)	149 (99%)	2 (1%)	65	81
67	V1	344/344 (100%)	337 (98%)	7 (2%)	50	73
68	V2	183/183 (100%)	181 (99%)	2 (1%)	70	84
69	V3	41/41 (100%)	41 (100%)	0	100	100
All	All	12131/12346 (98%)	12027 (99%)	104 (1%)	74	87

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	5A	84	LEU
4	6A	23	THR
4	6A	50	HIS
6	6C	23	ILE
7	7A	25	ARG
7	7A	30	GLN
7	7A	41	VAL
7	7A	50	ASN
14	A5	33	ASP
15	A6	41	THR
16	A7	43	VAL
17	A8	151	ILE
18	A9	129	LEU
19	AC	112	SER
20	AK	38	LEU
20	AK	68	ILE
20	AK	152	LEU
20	AK	205	VAL
20	AK	206	VAL
21	AL	106	ARG
21	AL	115	CYS

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Mol	Chain	Res	Type
23	AN	5	LYS
23	AN	7	LYS
35	C1	53	ILE
35	C1	96	ARG
35	C1	97	MET
35	C1	109	PHE
35	C1	124	THR
35	C1	127	THR
35	C1	128	VAL
35	C1	370	THR
35	C1	426	PHE
35	C1	448	THR
36	C2	48	THR
36	C2	111	THR
36	C2	207	MET
37	C3	32	THR
37	C3	66	THR
38	C4	76	ASP
39	CA	28	LYS
39	CA	47	THR
41	N1	251	THR
42	N2	303	THR
44	N4	375	LEU
45	N5	286	LEU
45	N5	340	PHE
45	N5	419	THR
45	N5	450	LEU
46	N6	57	PHE
46	N6	66	VAL
47	QA	238	LEU
48	QB	71	VAL
48	QB	125	THR
48	QB	195	THR
48	QB	258	VAL
48	QB	289	ILE
49	QC	47	THR
49	QC	112	THR
49	QC	158	THR
49	QC	171	ASP
49	QC	200	LEU
49	QC	281	LEU
49	QC	343	VAL

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Mol	Chain	Res	Type
53	QG	37	THR
55	QI	5	THR
47	Qa	231	LYS
47	Qa	237	PHE
47	Qa	238	LEU
47	Qa	252	LYS
47	Qa	369	THR
47	Qa	421	ASP
48	Qb	92	PHE
48	Qb	101	THR
48	Qb	181	ASP
48	Qb	289	ILE
48	Qb	341	PHE
49	Qc	200	LEU
50	Qd	209	GLU
50	Qd	253	VAL
59	S1	291	ARG
59	S1	608	VAL
59	S1	611	THR
59	S1	636	TYR
59	S1	690	THR
60	S2	362	ILE
61	S3	43	THR
61	S3	47	ILE
61	S3	68	ILE
62	S4	58	LYS
62	S4	77	VAL
62	S4	152	VAL
65	S7	67	PHE
65	S7	71	CYS
66	S8	76	TYR
66	S8	114	ILE
67	V1	270	ASN
67	V1	294	VAL
67	V1	307	VAL
67	V1	334	THR
67	V1	347	THR
67	V1	379	CYS
67	V1	385	CYS
68	V2	137	THR
68	V2	150	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (268)



such sidechains are listed below:

Mol	Chain	Res	Type
1	4L	7	ASN
2	5A	77	ASN
2	5A	102	ASN
3	5B	43	GLN
3	5B	119	HIS
4	6A	50	HIS
4	6A	83	HIS
5	6B	11	ASN
5	6B	25	ASN
5	6B	26	GLN
5	6B	33	ASN
6	6C	22	HIS
6	6C	55	ASN
7	7A	24	ASN
7	7A	50	ASN
8	7B	59	GLN
12	A2	25	GLN
13	A3	156	GLN
13	A3	159	GLN
13	A3	168	ASN
14	A5	71	GLN
14	A5	86	ASN
15	A6	74	HIS
15	A6	84	GLN
15	A6	96	ASN
16	A7	9	GLN
16	A7	21	GLN
16	A7	36	GLN
16	A7	73	GLN
17	A8	108	HIS
18	A9	38	HIS
18	A9	122	HIS
18	A9	138	ASN
18	A9	150	HIS
18	A9	171	ASN
18	A9	269	ASN
18	A9	278	GLN
19	AC	101	ASN
19	AC	103	HIS
19	AC	142	GLN
20	AK	87	HIS
20	AK	134	GLN

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Mol	Chain	Res	Type
20	AK	178	GLN
20	AK	221	GLN
20	AK	227	HIS
20	AK	259	GLN
21	AL	7	HIS
21	AL	89	ASN
22	AM	5	GLN
22	AM	31	ASN
22	AM	113	HIS
23	AN	61	GLN
24	B1	3	ASN
24	B1	6	GLN
24	B1	14	HIS
25	B2	49	GLN
25	B2	54	GLN
25	B2	57	GLN
26	B3	21	GLN
26	B3	33	GLN
27	B4	50	GLN
27	B4	123	GLN
28	B5	181	HIS
28	B5	189	ASN
29	B6	143	HIS
30	B7	110	GLN
31	B8	94	HIS
31	B8	115	ASN
31	B8	154	GLN
32	B9	104	GLN
32	B9	108	GLN
32	B9	117	GLN
32	B9	211	HIS
33	BK	107	GLN
35	C1	11	ASN
35	C1	12	HIS
35	C1	43	GLN
35	C1	55	ASN
35	C1	80	ASN
35	C1	98	ASN
35	C1	138	HIS
35	C1	233	HIS
35	C1	291	HIS
35	C1	328	HIS

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Mol	Chain	Res	Type
35	C1	407	GLN
35	C1	422	ASN
35	C1	491	ASN
35	C1	496	HIS
36	C2	26	HIS
36	C2	59	GLN
36	C2	102	HIS
37	C3	38	ASN
37	C3	70	HIS
37	C3	71	HIS
37	C3	125	ASN
37	C3	161	GLN
37	C3	204	HIS
37	C3	231	HIS
38	C4	123	HIS
38	C4	141	GLN
38	C4	154	GLN
41	N1	124	ASN
41	N1	138	GLN
41	N1	169	GLN
41	N1	171	HIS
41	N1	317	GLN
42	N2	83	GLN
42	N2	171	ASN
42	N2	186	HIS
42	N2	221	HIS
42	N2	273	ASN
42	N2	310	ASN
42	N2	322	GLN
42	N2	347	ASN
43	N3	10	ASN
44	N4	30	HIS
44	N4	44	GLN
44	N4	81	GLN
44	N4	103	GLN
44	N4	213	HIS
44	N4	251	ASN
44	N4	304	GLN
44	N4	399	ASN
44	N4	415	GLN
45	N5	136	ASN
45	N5	139	GLN

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Mol	Chain	Res	Type
45	N5	230	HIS
45	N5	248	HIS
45	N5	518	GLN
45	N5	524	ASN
45	N5	546	GLN
45	N5	580	GLN
47	QA	168	ASN
47	QA	176	ASN
47	QA	184	ASN
47	QA	284	ASN
47	QA	291	HIS
47	QA	298	HIS
47	QA	365	ASN
47	QA	368	ASN
47	QA	399	GLN
47	QA	415	GLN
47	QA	426	ASN
48	QB	66	GLN
48	QB	173	GLN
48	QB	239	HIS
48	QB	301	ASN
48	QB	357	HIS
48	QB	464	GLN
49	QC	32	ASN
49	QC	68	HIS
49	QC	201	HIS
49	QC	267	HIS
49	QC	312	GLN
49	QC	322	GLN
49	QC	345	HIS
49	QC	374	ASN
50	QD	206	HIS
50	QD	266	GLN
50	QD	310	HIS
51	QE	135	GLN
51	QE	164	ASN
51	QE	186	GLN
51	QE	199	GLN
51	QE	257	ASN
52	QF	88	ASN
53	QG	80	GLN
54	QH	7	HIS

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Mol	Chain	Res	Type
55	QI	38	GLN
55	QI	46	HIS
55	QI	48	ASN
55	QI	55	HIS
57	QK	31	GLN
57	QK	58	GLN
47	Qa	36	GLN
47	Qa	81	HIS
47	Qa	139	ASN
47	Qa	155	GLN
47	Qa	167	GLN
47	Qa	172	GLN
47	Qa	212	HIS
47	Qa	290	GLN
47	Qa	304	ASN
47	Qa	319	GLN
47	Qa	376	ASN
47	Qa	408	GLN
48	Qb	43	GLN
48	Qb	87	ASN
48	Qb	95	HIS
48	Qb	152	GLN
48	Qb	153	ASN
48	Qb	160	GLN
48	Qb	170	GLN
48	Qb	188	HIS
48	Qb	223	HIS
48	Qb	239	HIS
48	Qb	249	HIS
48	Qb	357	HIS
49	Qc	3	ASN
49	Qc	201	HIS
49	Qc	260	ASN
49	Qc	341	GLN
50	Qd	116	GLN
50	Qd	190	ASN
50	Qd	206	HIS
50	Qd	251	ASN
50	Qd	283	HIS
51	Qe	135	GLN
51	Qe	186	GLN
51	Qe	199	GLN

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Mol	Chain	Res	Type
51	Qe	227	ASN
52	Qf	36	GLN
52	Qf	55	GLN
53	Qg	23	ASN
55	Qi	38	GLN
55	Qi	48	ASN
58	Qj	16	ASN
59	S1	39	GLN
59	S1	51	GLN
59	S1	123	ASN
59	S1	202	ASN
59	S1	282	ASN
59	S1	331	GLN
59	S1	336	ASN
59	S1	424	HIS
59	S1	425	ASN
59	S1	453	GLN
59	S1	498	GLN
59	S1	652	ASN
59	S1	677	GLN
59	S1	688	GLN
60	S2	66	HIS
60	S2	239	HIS
60	S2	240	GLN
61	S3	51	ASN
61	S3	75	GLN
61	S3	82	ASN
61	S3	107	GLN
61	S3	123	GLN
61	S3	131	ASN
61	S3	247	GLN
62	S4	92	ASN
62	S4	93	ASN
62	S4	123	ASN
62	S4	163	ASN
63	S5	25	GLN
63	S5	34	HIS
63	S5	45	HIS
64	S6	43	GLN
64	S6	74	GLN
64	S6	120	GLN
67	V1	44	ASN

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Mol	Chain	Res	Type
67	V1	133	HIS
67	V1	136	HIS
67	V1	170	GLN
67	V1	303	HIS
67	V1	344	GLN
67	V1	381	GLN
67	V1	456	GLN
67	V1	458	GLN
68	V2	41	HIS
68	V2	87	GLN
68	V2	90	ASN
68	V2	133	GLN
68	V2	153	GLN
68	V2	187	GLN
69	V3	388	ASN
69	V3	419	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z  > 2$
60	2MR	S2	124	60	10,12,13	2.41	3 (30%)	5,13,15	0.90	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	2MR	S2	124	60	-	3/10/13/15	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	S2	124	2MR	CZ-NE	5.08	1.45	1.34
60	S2	124	2MR	CZ-NH2	4.94	1.44	1.33
60	S2	124	2MR	CQ1-NH1	-2.06	1.42	1.46

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
60	S2	124	2MR	NE-CD-CG-CB
60	S2	124	2MR	CA-CB-CG-CD
60	S2	124	2MR	C-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 97 ligands modelled in this entry, 7 are monoatomic - leaving 90 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	$\# Z  > 2$
86	SF4	S8	301	66	0,12,12	-	-	-		
72	CDL	Qh	102	-	63,63,99	0.37	0	69,75,111	0.37	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
82	PEE	Qc	401	-	41,41,50	1.27	4 (9%)	44,46,55	1.21	4 (9%)
82	PEE	QB	502	-	26,26,50	1.36	3 (11%)	29,31,55	1.22	2 (6%)
82	PEE	C1	609	-	50,50,50	1.32	5 (10%)	53,55,55	1.16	3 (5%)
77	PLX	C2	301	-	42,42,51	1.17	4 (9%)	46,50,59	0.85	1 (2%)
77	PLX	AM	201	-	51,51,51	1.11	4 (7%)	55,59,59	0.88	1 (1%)
71	PC1	C3	301	-	48,48,53	0.31	0	54,56,61	0.38	0
72	CDL	Qb	501	-	63,63,99	0.37	0	69,75,111	0.38	0
75	ADP	AK	401	-	24,29,29	0.95	1 (4%)	29,45,45	1.47	4 (13%)
72	CDL	QC	408	-	54,54,99	0.39	0	60,66,111	0.38	0
86	SF4	S8	302	66	0,12,12	-	-	-		
73	NDP	A9	401	-	45,52,52	0.55	0	53,80,80	0.53	1 (1%)
71	PC1	Qj	101	-	53,53,53	0.30	0	59,61,61	0.34	0
78	6F6	B5	203	-	53,53,53	0.29	0	59,61,61	0.33	0
76	3PE	S7	302	-	50,50,50	0.31	0	53,55,55	0.34	0
72	CDL	6A	102	-	68,68,99	0.35	0	74,80,111	0.35	0
76	3PE	C1	601	-	50,50,50	0.30	0	53,55,55	0.30	0
71	PC1	QC	405	-	53,53,53	0.30	0	59,61,61	0.30	0
71	PC1	N5	704	-	53,53,53	0.29	0	59,61,61	0.28	0
76	3PE	N4	502	-	50,50,50	0.31	0	53,55,55	0.33	0
77	PLX	AM	203	-	51,51,51	1.10	3 (5%)	55,59,59	0.89	1 (1%)
72	CDL	N5	702	-	88,88,99	0.31	0	94,100,111	0.32	0
86	SF4	S1	802	59	0,12,12	-	-	-		
71	PC1	C1	607	-	45,45,53	0.31	0	51,53,61	0.35	0
76	3PE	QE	303	-	43,43,50	0.32	0	46,48,55	0.31	0
82	PEE	QB	503	-	50,50,50	1.31	5 (10%)	53,55,55	1.16	3 (5%)
72	CDL	QB	501	-	63,63,99	0.37	0	69,75,111	0.41	0
84	HEC	Qd	402	50	32,50,50	2.07	4 (12%)	24,82,82	2.23	12 (50%)
76	3PE	CB	202	-	45,45,50	0.31	0	48,50,55	0.29	0
77	PLX	AL	205	-	46,46,51	1.13	4 (8%)	50,54,59	0.93	2 (4%)
72	CDL	AM	202	-	50,50,99	0.40	0	56,62,111	0.34	0
72	CDL	AL	203	-	92,92,99	0.31	0	98,104,111	0.29	0
77	PLX	CB	201	-	51,51,51	1.11	3 (5%)	55,59,59	0.92	1 (1%)
82	PEE	S2	501	-	47,47,50	1.35	5 (10%)	50,52,55	1.18	3 (6%)
71	PC1	AL	206	-	53,53,53	0.29	0	59,61,61	0.31	0
74	ZMP	AC	201	19	29,35,36	0.73	1 (3%)	34,42,45	0.76	0
83	HEM	QC	403	49	41,50,50	1.27	3 (7%)	45,82,82	1.69	7 (15%)
82	PEE	Qd	403	-	50,50,50	1.31	5 (10%)	53,55,55	1.20	4 (7%)
71	PC1	N6	201	-	53,53,53	0.30	0	59,61,61	0.26	0
72	CDL	B5	202	-	99,99,99	0.31	0	105,111,111	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
82	PEE	N3	201	-	50,50,50	1.30	5 (10%)	53,55,55	1.19	5 (9%)
83	HEM	QC	402	49	41,50,50	1.24	4 (9%)	45,82,82	1.72	9 (20%)
72	CDL	CB	203	-	99,99,99	0.30	0	105,111,111	0.29	0
71	PC1	QH	102	-	53,53,53	0.29	0	59,61,61	0.32	0
87	FMN	V1	502	-	33,33,33	0.31	0	48,50,50	0.44	0
85	FES	Qe	301	51	0,4,4	-	-	-	-	-
72	CDL	AL	204	-	79,79,99	0.33	0	85,91,111	0.42	0
82	PEE	N1	401	-	37,37,50	1.47	5 (13%)	39,42,55	1.27	4 (10%)
77	PLX	N4	501	-	51,51,51	1.11	3 (5%)	55,59,59	0.92	2 (3%)
76	3PE	C1	608	-	43,43,50	0.33	0	46,48,55	0.41	0
82	PEE	Qh	103	-	50,50,50	1.32	5 (10%)	53,55,55	1.18	4 (7%)
78	6F6	QJ	101	-	53,53,53	0.29	0	59,61,61	0.30	0
78	6F6	Qc	404	-	53,53,53	0.29	0	59,61,61	0.38	0
86	SF4	S1	801	59	0,12,12	-	-	-	-	-
77	PLX	B5	201	-	51,51,51	1.11	3 (5%)	55,59,59	0.91	1 (1%)
72	CDL	AL	201	-	83,83,99	0.32	0	89,95,111	0.34	0
82	PEE	QC	401	-	50,50,50	1.32	5 (10%)	53,55,55	1.22	3 (5%)
74	ZMP	AB	201	19	29,35,36	0.70	1 (3%)	34,42,45	0.90	2 (5%)
72	CDL	QC	406	-	93,93,99	0.31	0	99,105,111	0.33	0
77	PLX	QE	301	-	45,45,51	1.18	3 (6%)	49,53,59	0.92	1 (2%)
72	CDL	N2	401	-	67,67,99	0.35	0	73,79,111	0.30	0
77	PLX	QI	301	-	51,51,51	1.12	3 (5%)	55,59,59	0.89	1 (1%)
86	SF4	V1	501	67	0,12,12	-	-	-	-	-
84	HEC	QD	401	50	32,50,50	2.06	4 (12%)	24,82,82	2.37	13 (54%)
71	PC1	C1	606	-	53,53,53	0.28	0	59,61,61	0.27	0
71	PC1	6A	101	-	44,44,53	0.32	0	50,52,61	0.33	0
76	3PE	CA	101	-	50,50,50	0.30	0	53,55,55	0.33	0
82	PEE	QC	404	-	37,37,50	1.34	4 (10%)	40,42,55	1.15	2 (5%)
85	FES	QE	304	51	0,4,4	-	-	-	-	-
82	PEE	S8	303	-	50,50,50	1.30	5 (10%)	53,55,55	1.20	4 (7%)
76	3PE	AL	202	-	50,50,50	0.31	0	53,55,55	0.32	0
82	PEE	QE	302	-	46,46,50	1.35	5 (10%)	49,51,55	1.28	4 (8%)
71	PC1	QC	407	-	53,53,53	0.29	0	59,61,61	0.32	0
72	CDL	N5	703	-	99,99,99	0.30	0	105,111,111	0.30	0
71	PC1	Qb	502	-	28,28,53	0.39	0	34,36,61	0.40	0
85	FES	S1	803	59	0,4,4	-	-	-	-	-
72	CDL	A8	301	-	82,82,99	0.33	0	88,94,111	0.33	0
85	FES	V2	301	68	0,4,4	-	-	-	-	-
83	HEM	Qc	402	49	41,50,50	1.24	3 (7%)	45,82,82	1.72	8 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
72	CDL	QH	101	-	60,60,99	0.38	0	66,72,111	0.37	0
79	HEA	C1	603	35	57,67,67	2.01	16 (28%)	61,103,103	2.70	26 (42%)
86	SF4	S7	301	65	0,12,12	-	-	-	-	-
82	PEE	N5	701	-	45,45,50	1.38	5 (11%)	48,50,55	1.18	2 (4%)
71	PC1	C3	302	-	42,42,53	0.33	0	48,50,61	0.31	0
82	PEE	Qh	101	-	40,40,50	1.47	5 (12%)	42,45,55	1.14	3 (7%)
79	HEA	C1	602	35	57,67,67	2.02	15 (26%)	61,103,103	2.70	28 (45%)
83	HEM	Qc	403	49	41,50,50	1.25	3 (7%)	45,82,82	1.71	8 (17%)
72	CDL	Qd	401	-	63,63,99	0.37	0	69,75,111	0.36	0
71	PC1	7B	101	-	53,53,53	0.29	0	59,61,61	0.27	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	SF4	S8	301	66	-	-	0/6/5/5
72	CDL	Qh	102	-	-	27/74/74/110	-
82	PEE	Qc	401	-	-	26/45/45/54	-
82	PEE	QB	502	-	-	13/30/30/54	-
82	PEE	C1	609	-	-	25/54/54/54	-
77	PLX	C2	301	-	-	21/46/46/55	-
77	PLX	AM	201	-	-	19/55/55/55	-
71	PC1	C3	301	-	-	17/52/52/57	-
72	CDL	Qb	501	-	-	18/74/74/110	-
75	ADP	AK	401	-	-	2/12/32/32	0/3/3/3
72	CDL	QC	408	-	-	18/65/65/110	-
86	SF4	S8	302	66	-	-	0/6/5/5
73	NDP	A9	401	-	-	6/30/77/77	0/5/5/5
71	PC1	Qj	101	-	-	18/57/57/57	-
78	6F6	B5	203	-	-	11/57/57/57	-
76	3PE	S7	302	-	-	15/54/54/54	-
72	CDL	6A	102	-	-	28/79/79/110	-
76	3PE	C1	601	-	-	11/54/54/54	-
71	PC1	QC	405	-	-	16/57/57/57	-
71	PC1	N5	704	-	-	11/57/57/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
76	3PE	N4	502	-	-	12/54/54/54	-
77	PLX	AM	203	-	-	24/55/55/55	-
72	CDL	N5	702	-	-	22/99/99/110	-
86	SF4	S1	802	59	-	-	0/6/5/5
71	PC1	C1	607	-	-	10/49/49/57	-
76	3PE	QE	303	-	-	7/47/47/54	-
82	PEE	QB	503	-	-	23/54/54/54	-
72	CDL	QB	501	-	-	21/74/74/110	-
84	HEC	Qd	402	50	-	1/10/54/54	-
76	3PE	CB	202	-	-	8/49/49/54	-
77	PLX	AL	205	-	-	21/50/50/55	-
72	CDL	AM	202	-	-	9/61/61/110	-
72	CDL	AL	203	-	-	22/103/103/110	-
77	PLX	CB	201	-	-	27/55/55/55	-
82	PEE	S2	501	-	-	30/51/51/54	-
71	PC1	AL	206	-	-	15/57/57/57	-
74	ZMP	AC	201	19	-	18/40/42/43	-
83	HEM	QC	403	49	-	4/12/54/54	-
82	PEE	Qd	403	-	-	24/54/54/54	-
71	PC1	N6	201	-	-	6/57/57/57	-
72	CDL	B5	202	-	-	17/110/110/110	-
82	PEE	N3	201	-	-	24/54/54/54	-
83	HEM	QC	402	49	-	7/12/54/54	-
72	CDL	CB	203	-	-	31/110/110/110	-
71	PC1	QH	102	-	-	9/57/57/57	-
87	FMN	V1	502	-	-	6/18/18/18	0/3/3/3
85	FES	Qe	301	51	-	-	0/1/1/1
72	CDL	AL	204	-	-	25/90/90/110	-
82	PEE	N1	401	-	-	19/41/41/54	-
77	PLX	N4	501	-	-	17/55/55/55	-
76	3PE	C1	608	-	-	12/47/47/54	-
82	PEE	Qh	103	-	-	17/54/54/54	-
78	6F6	QJ	101	-	-	18/57/57/57	-
78	6F6	Qc	404	-	-	13/57/57/57	-
86	SF4	S1	801	59	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
77	PLX	B5	201	-	-	23/55/55/55	-
72	CDL	AL	201	-	-	28/94/94/110	-
82	PEE	QC	401	-	-	26/54/54/54	-
74	ZMP	AB	201	19	-	16/40/42/43	-
72	CDL	QC	406	-	-	23/104/104/110	-
77	PLX	QE	301	-	-	19/49/49/55	-
72	CDL	N2	401	-	-	25/78/78/110	-
77	PLX	QI	301	-	-	19/55/55/55	-
86	SF4	V1	501	67	-	-	0/6/5/5
84	HEC	QD	401	50	-	2/10/54/54	-
71	PC1	C1	606	-	-	11/57/57/57	-
71	PC1	6A	101	-	-	15/48/48/57	-
76	3PE	CA	101	-	-	11/54/54/54	-
82	PEE	QC	404	-	-	12/41/41/54	-
85	FES	QE	304	51	-	-	0/1/1/1
82	PEE	S8	303	-	-	22/54/54/54	-
76	3PE	AL	202	-	-	10/54/54/54	-
82	PEE	QE	302	-	-	20/50/50/54	-
71	PC1	QC	407	-	-	10/57/57/57	-
72	CDL	N5	703	-	-	21/110/110/110	-
71	PC1	Qb	502	-	-	11/32/32/57	-
85	FES	S1	803	59	-	-	0/1/1/1
72	CDL	A8	301	-	-	24/93/93/110	-
85	FES	V2	301	68	-	-	0/1/1/1
83	HEM	Qc	402	49	-	7/12/54/54	-
72	CDL	QH	101	-	-	12/71/71/110	-
79	HEA	C1	603	35	-	10/32/76/76	-
86	SF4	S7	301	65	-	-	0/6/5/5
82	PEE	N5	701	-	-	15/49/49/54	-
71	PC1	C3	302	-	-	9/46/46/57	-
82	PEE	Qh	101	-	-	25/44/44/54	-
79	HEA	C1	602	35	-	11/32/76/76	-
83	HEM	Qc	403	49	-	7/12/54/54	-
72	CDL	Qd	401	-	-	17/74/74/110	-
71	PC1	7B	101	-	-	16/57/57/57	-

All (156) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	Qd	402	HEC	C3C-C2C	-6.77	1.33	1.40
84	QD	401	HEC	C3C-C2C	-6.67	1.33	1.40
84	Qd	402	HEC	C2B-C3B	-6.46	1.34	1.40
84	QD	401	HEC	C2B-C3B	-6.31	1.34	1.40
79	C1	602	HEA	C3B-C2B	5.25	1.46	1.34
79	C1	603	HEA	C3B-C2B	5.10	1.46	1.34
79	C1	602	HEA	CHC-C4B	4.60	1.46	1.35
79	C1	603	HEA	CHC-C4B	4.51	1.46	1.35
79	C1	603	HEA	C3A-C2A	4.34	1.46	1.40
79	C1	602	HEA	C3C-C2C	4.19	1.46	1.40
79	C1	603	HEA	C4B-NB	-4.17	1.33	1.40
79	C1	602	HEA	C1D-ND	-4.10	1.33	1.40
82	Qh	101	PEE	C18-C19	4.08	1.55	1.31
82	C1	609	PEE	C18-C19	4.06	1.55	1.31
82	QE	302	PEE	C18-C19	4.06	1.55	1.31
79	C1	602	HEA	CHD-C1D	4.05	1.45	1.35
82	QC	404	PEE	C18-C19	4.04	1.55	1.31
82	N5	701	PEE	C18-C19	4.04	1.55	1.31
82	QC	401	PEE	C18-C19	4.04	1.55	1.31
82	S2	501	PEE	C18-C19	4.03	1.55	1.31
82	Qd	403	PEE	C18-C19	4.03	1.55	1.31
82	QB	503	PEE	C18-C19	4.02	1.55	1.31
82	Qh	103	PEE	C18-C19	4.01	1.55	1.31
79	C1	603	HEA	C1D-ND	-4.01	1.33	1.40
82	S8	303	PEE	C18-C19	3.99	1.54	1.31
82	Qc	401	PEE	C18-C19	3.99	1.54	1.31
82	N3	201	PEE	C18-C19	3.98	1.54	1.31
82	C1	609	PEE	C39-C38	3.96	1.54	1.31
82	Qh	101	PEE	C39-C38	3.95	1.54	1.31
82	Qh	103	PEE	C39-C38	3.95	1.54	1.31
82	N5	701	PEE	C39-C38	3.94	1.54	1.31
79	C1	602	HEA	C3A-C2A	3.94	1.45	1.40
82	QC	401	PEE	C39-C38	3.94	1.54	1.31
82	QB	503	PEE	C39-C38	3.94	1.54	1.31
82	S2	501	PEE	C39-C38	3.93	1.54	1.31
82	N1	401	PEE	C39-C38	3.93	1.54	1.31
79	C1	603	HEA	CHD-C1D	3.93	1.45	1.35
82	S8	303	PEE	C39-C38	3.92	1.54	1.31
82	Qd	403	PEE	C39-C38	3.91	1.54	1.31
82	QE	302	PEE	C39-C38	3.91	1.54	1.31
83	QC	403	HEM	C4D-ND	-3.91	1.33	1.40
82	N3	201	PEE	C39-C38	3.90	1.54	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
79	C1	603	HEA	C3C-C2C	3.89	1.45	1.40
83	Qc	403	HEM	C4D-ND	-3.84	1.33	1.40
83	QC	402	HEM	C4D-ND	-3.83	1.33	1.40
79	C1	603	HEA	C3D-C2D	3.81	1.44	1.36
79	C1	602	HEA	C4B-NB	-3.79	1.33	1.40
79	C1	602	HEA	C3D-C2D	3.74	1.44	1.36
83	Qc	402	HEM	C4D-ND	-3.68	1.34	1.40
84	Qd	402	HEC	CBC-CAC	-3.43	1.36	1.49
84	QD	401	HEC	CBC-CAC	-3.43	1.36	1.49
82	N1	401	PEE	C18-C19	3.41	1.55	1.29
79	C1	602	HEA	CAA-C2A	-3.40	1.46	1.52
77	QE	301	PLX	O6-C4	-3.32	1.40	1.44
82	Qh	101	PEE	O3-C30	3.25	1.42	1.33
82	QC	401	PEE	O3-C30	3.24	1.42	1.33
82	Qh	103	PEE	O3-C30	3.24	1.42	1.33
83	QC	403	HEM	C1B-NB	-3.24	1.34	1.40
82	QB	502	PEE	O3-C30	3.23	1.42	1.33
82	Qc	401	PEE	O3-C30	3.23	1.42	1.33
82	QB	503	PEE	O3-C30	3.21	1.42	1.33
82	C1	609	PEE	O3-C30	3.21	1.42	1.33
83	Qc	403	HEM	C1B-NB	-3.20	1.34	1.40
82	QC	404	PEE	O3-C30	3.20	1.42	1.33
77	CB	201	PLX	O6-C4	-3.19	1.40	1.44
82	S2	501	PEE	O3-C30	3.18	1.42	1.33
82	S8	303	PEE	O3-C30	3.14	1.42	1.33
82	N3	201	PEE	O3-C30	3.14	1.42	1.33
83	Qc	402	HEM	C1B-NB	-3.13	1.34	1.40
82	N5	701	PEE	O3-C30	3.13	1.42	1.33
82	Qd	403	PEE	O3-C30	3.12	1.42	1.33
77	QI	301	PLX	O6-C4	-3.11	1.40	1.44
82	QE	302	PEE	O3-C30	3.11	1.42	1.33
83	QC	402	HEM	C1B-NB	-3.10	1.35	1.40
77	N4	501	PLX	O6-C4	-3.09	1.40	1.44
82	N1	401	PEE	O3-C30	3.08	1.42	1.33
77	B5	201	PLX	O6-C4	-3.05	1.40	1.44
79	C1	603	HEA	C1B-NB	-3.03	1.32	1.38
79	C1	602	HEA	C1B-NB	-2.98	1.32	1.38
77	AM	203	PLX	O6-C4	-2.97	1.40	1.44
77	AM	201	PLX	O6-C4	-2.95	1.40	1.44
79	C1	602	HEA	C4D-ND	-2.94	1.32	1.38
77	C2	301	PLX	O6-C4	-2.87	1.40	1.44
79	C1	603	HEA	CAA-C2A	-2.85	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
74	AC	201	ZMP	C9-C10	-2.79	1.48	1.50
83	QC	403	HEM	C1D-ND	-2.79	1.33	1.38
82	N1	401	PEE	O2-C10	2.73	1.42	1.34
82	S8	303	PEE	O2-C10	2.73	1.42	1.34
83	Qc	403	HEM	C1D-ND	-2.66	1.33	1.38
82	N5	701	PEE	O2-C10	2.66	1.41	1.34
82	Qd	403	PEE	O2-C10	2.65	1.41	1.34
82	Qh	101	PEE	O2-C10	2.64	1.41	1.34
83	Qc	402	HEM	C1D-ND	-2.64	1.33	1.38
82	S2	501	PEE	O2-C10	2.63	1.41	1.34
74	AB	201	ZMP	C9-C10	-2.63	1.48	1.50
82	Qh	103	PEE	O2-C2	-2.63	1.40	1.46
79	C1	603	HEA	C4D-ND	-2.62	1.33	1.38
82	C1	609	PEE	O2-C10	2.62	1.41	1.34
82	QB	503	PEE	O2-C2	-2.62	1.40	1.46
82	Qc	401	PEE	O2-C2	-2.61	1.40	1.46
82	QB	502	PEE	O2-C10	2.61	1.41	1.34
83	QC	402	HEM	C1D-ND	-2.61	1.33	1.38
82	N3	201	PEE	O2-C10	2.60	1.41	1.34
82	QB	502	PEE	O2-C2	-2.60	1.40	1.46
82	QC	401	PEE	O2-C10	2.59	1.41	1.34
82	QC	401	PEE	O2-C2	-2.59	1.40	1.46
82	QC	404	PEE	O2-C2	-2.58	1.40	1.46
82	QE	302	PEE	O2-C10	2.57	1.41	1.34
82	QC	404	PEE	O2-C10	2.56	1.41	1.34
79	C1	602	HEA	FE-ND	2.53	2.09	1.96
82	Qh	103	PEE	O2-C10	2.52	1.41	1.34
79	C1	603	HEA	FE-ND	2.51	2.09	1.96
82	Qc	401	PEE	O2-C10	2.51	1.41	1.34
82	N3	201	PEE	O2-C2	-2.51	1.40	1.46
82	QB	503	PEE	O2-C10	2.51	1.41	1.34
82	Qd	403	PEE	O2-C2	-2.50	1.40	1.46
82	QE	302	PEE	O2-C2	-2.49	1.40	1.46
77	AL	205	PLX	O6-C4	-2.48	1.41	1.44
79	C1	602	HEA	O2D-CGD	-2.46	1.22	1.30
82	C1	609	PEE	O2-C2	-2.46	1.40	1.46
82	Qh	101	PEE	O2-C2	-2.45	1.40	1.46
79	C1	603	HEA	FE-NB	2.45	2.09	1.96
82	N5	701	PEE	O2-C2	-2.45	1.40	1.46
82	S2	501	PEE	O2-C2	-2.44	1.40	1.46
79	C1	603	HEA	O2D-CGD	-2.42	1.22	1.30
75	AK	401	ADP	C5-C4	2.41	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	Qd	402	HEC	CBB-CAB	-2.41	1.40	1.49
79	C1	603	HEA	O2A-CGA	-2.40	1.22	1.30
79	C1	602	HEA	FE-NB	2.37	2.08	1.96
84	QD	401	HEC	CBB-CAB	-2.37	1.40	1.49
79	C1	602	HEA	O2A-CGA	-2.34	1.22	1.30
77	N4	501	PLX	C1B-N1	-2.34	1.43	1.50
82	N1	401	PEE	O2-C2	-2.30	1.40	1.46
77	QE	301	PLX	C1B-N1	-2.30	1.43	1.50
79	C1	603	HEA	C4B-C3B	2.28	1.48	1.44
82	S8	303	PEE	O2-C2	-2.26	1.40	1.46
77	B5	201	PLX	C1B-N1	-2.25	1.43	1.50
77	CB	201	PLX	C1B-N1	-2.23	1.43	1.50
77	QI	301	PLX	C1B-N1	-2.23	1.43	1.50
77	AL	205	PLX	C1B-N1	-2.21	1.43	1.50
77	AM	203	PLX	C1B-N1	-2.20	1.43	1.50
77	C2	301	PLX	C1B-N1	-2.17	1.43	1.50
77	QE	301	PLX	C1C-N1	-2.17	1.43	1.50
77	AM	201	PLX	C1B-N1	-2.14	1.43	1.50
77	QI	301	PLX	C1C-N1	-2.12	1.43	1.50
77	AM	203	PLX	C1C-N1	-2.10	1.43	1.50
77	AL	205	PLX	C1C-N1	-2.10	1.43	1.50
77	N4	501	PLX	C1C-N1	-2.10	1.43	1.50
77	CB	201	PLX	C1C-N1	-2.09	1.43	1.50
77	B5	201	PLX	C1C-N1	-2.06	1.44	1.50
77	AM	201	PLX	P1-O4	2.05	1.67	1.59
77	C2	301	PLX	C1C-N1	-2.04	1.44	1.50
77	C2	301	PLX	P1-O4	2.04	1.67	1.59
83	QC	402	HEM	C4B-NB	-2.03	1.34	1.38
77	AM	201	PLX	C1C-N1	-2.02	1.44	1.50
77	AL	205	PLX	P1-O4	2.01	1.67	1.59

All (179) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
79	C1	603	HEA	CAD-CBD-CGD	-8.30	95.74	113.60
79	C1	602	HEA	CAD-CBD-CGD	-7.80	96.81	113.60
79	C1	603	HEA	C3D-C4D-ND	6.02	116.18	110.36
79	C1	602	HEA	C3D-C4D-ND	5.65	115.83	110.36
79	C1	602	HEA	C13-C12-C11	-5.51	106.07	114.35
79	C1	603	HEA	C13-C12-C11	-5.08	106.72	114.35
79	C1	603	HEA	C2B-C1B-NB	5.07	115.96	109.88
79	C1	603	HEA	CAA-CBA-CGA	-5.02	99.68	113.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
79	C1	602	HEA	C1D-C2D-C3D	-4.95	101.75	106.96
79	C1	602	HEA	C2B-C1B-NB	4.90	115.75	109.88
79	C1	602	HEA	CAA-CBA-CGA	-4.81	100.27	113.76
83	QC	402	HEM	CHC-C4B-NB	4.78	129.62	124.43
83	Qc	403	HEM	CHC-C4B-NB	4.75	129.59	124.43
79	C1	603	HEA	CHB-C1B-C2B	-4.73	117.59	124.98
79	C1	602	HEA	CHB-C1B-C2B	-4.69	117.65	124.98
79	C1	602	HEA	C2D-C1D-ND	4.68	115.38	109.84
83	Qc	402	HEM	CHC-C4B-NB	4.63	129.47	124.43
82	QC	401	PEE	O2-C10-C11	4.61	121.45	111.50
79	C1	603	HEA	C2D-C1D-ND	4.57	115.25	109.84
79	C1	602	HEA	C3C-C4C-NC	4.52	115.05	109.21
79	C1	603	HEA	C1D-C2D-C3D	-4.49	102.23	106.96
82	QE	302	PEE	O2-C10-C11	4.41	121.01	111.50
84	QD	401	HEC	CMD-C2D-C1D	-4.37	121.75	128.46
83	QC	403	HEM	CHC-C4B-NB	4.36	129.17	124.43
82	Qd	403	PEE	O2-C10-C11	4.26	120.67	111.50
82	QB	502	PEE	O2-C10-C11	4.25	120.66	111.50
79	C1	602	HEA	CHA-C4D-C3D	-4.15	118.73	124.84
84	Qd	402	HEC	CMD-C2D-C1D	-4.14	122.11	128.46
83	QC	403	HEM	C4D-ND-C1D	4.12	109.32	105.07
79	C1	603	HEA	C3B-C4B-NB	4.04	114.63	109.84
82	S2	501	PEE	O2-C10-C11	4.02	120.17	111.50
82	C1	609	PEE	O2-C10-C11	4.02	120.16	111.50
82	N1	401	PEE	O2-C10-C11	4.00	120.13	111.50
79	C1	602	HEA	C3B-C4B-NB	3.99	114.56	109.84
83	QC	402	HEM	CHB-C1B-NB	3.99	129.31	124.38
82	N3	201	PEE	O2-C10-C11	3.98	120.07	111.50
83	Qc	402	HEM	CHB-C1B-NB	3.94	129.25	124.38
82	Qc	401	PEE	O2-C10-C11	3.93	119.98	111.50
82	S8	303	PEE	O2-C10-C11	3.92	119.96	111.50
82	Qh	101	PEE	O2-C10-C11	3.92	119.94	111.50
83	Qc	403	HEM	CHB-C1B-NB	3.90	129.20	124.38
79	C1	603	HEA	C3C-C4C-NC	3.88	114.23	109.21
82	QB	503	PEE	O2-C10-C11	3.88	119.86	111.50
75	AK	401	ADP	PA-O3A-PB	-3.86	119.57	132.83
82	QC	404	PEE	O2-C10-C11	3.84	119.77	111.50
79	C1	603	HEA	CHA-C4D-C3D	-3.81	119.25	124.84
82	N5	701	PEE	O2-C10-C11	3.78	119.65	111.50
82	Qh	103	PEE	O2-C10-C11	3.75	119.59	111.50
83	QC	403	HEM	CHB-C1B-NB	3.68	128.92	124.38
79	C1	603	HEA	C4B-C3B-C2B	-3.63	101.21	107.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
79	C1	602	HEA	C4B-C3B-C2B	-3.55	101.34	107.41
84	QD	401	HEC	CMC-C2C-C3C	3.50	129.94	125.82
83	QC	403	HEM	C1B-NB-C4B	3.49	108.68	105.07
83	Qc	403	HEM	C4D-ND-C1D	3.46	108.65	105.07
84	QD	401	HEC	CBD-CAD-C3D	3.45	118.51	112.62
84	Qd	402	HEC	CMB-C2B-C1B	-3.45	123.17	128.46
84	QD	401	HEC	CMB-C2B-C1B	-3.37	123.29	128.46
79	C1	602	HEA	CMC-C2C-C3C	3.34	130.93	124.68
84	QD	401	HEC	CMB-C2B-C3B	3.34	129.74	125.82
79	C1	603	HEA	CMC-C2C-C3C	3.25	130.76	124.68
83	Qc	402	HEM	C4D-ND-C1D	3.25	108.43	105.07
83	QC	402	HEM	C4D-ND-C1D	3.24	108.42	105.07
79	C1	603	HEA	C17-C18-C19	-3.17	120.03	127.66
84	Qd	402	HEC	CMB-C2B-C3B	3.16	129.54	125.82
83	QC	402	HEM	C1B-NB-C4B	3.16	108.33	105.07
75	AK	401	ADP	N3-C2-N1	-3.15	123.75	128.68
83	Qc	403	HEM	C1B-NB-C4B	3.12	108.29	105.07
83	Qc	402	HEM	C1B-NB-C4B	3.04	108.22	105.07
84	Qd	402	HEC	CMC-C2C-C3C	3.04	129.39	125.82
83	Qc	403	HEM	CHA-C4D-ND	2.98	128.07	124.38
83	Qc	402	HEM	CHA-C4D-ND	2.96	128.04	124.38
83	QC	402	HEM	CHA-C4D-ND	2.96	128.03	124.38
75	AK	401	ADP	C3'-C2'-C1'	2.95	105.42	100.98
84	QD	401	HEC	O1D-CGD-CBD	-2.94	113.63	123.08
84	Qd	402	HEC	C4C-C3C-C2C	2.92	109.50	106.35
82	QE	302	PEE	O3-C30-C31	2.88	120.95	111.91
84	Qd	402	HEC	CBD-CAD-C3D	2.87	117.53	112.62
79	C1	603	HEA	C27-C19-C20	2.86	120.08	115.27
82	Qc	401	PEE	O3-C30-C31	2.85	120.86	111.91
79	C1	602	HEA	C27-C19-C20	2.82	120.01	115.27
84	QD	401	HEC	C4C-C3C-C2C	2.80	109.38	106.35
79	C1	602	HEA	C17-C18-C19	-2.80	120.92	127.66
83	Qc	402	HEM	CHD-C1D-ND	2.80	127.47	124.43
79	C1	603	HEA	C13-C14-C15	-2.79	120.94	127.66
83	Qc	403	HEM	CAD-CBD-CGD	-2.79	107.60	113.60
82	Qh	103	PEE	O3-C30-C31	2.79	120.65	111.91
82	S8	303	PEE	O3-C30-C31	2.78	120.63	111.91
84	Qd	402	HEC	O1D-CGD-CBD	-2.77	114.17	123.08
83	Qc	403	HEM	CHD-C1D-ND	2.72	127.38	124.43
79	C1	602	HEA	C13-C14-C15	-2.71	121.15	127.66
84	QD	401	HEC	CMC-C2C-C1C	-2.68	124.35	128.46
83	QC	402	HEM	CHD-C1D-ND	2.67	127.33	124.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
83	QC	403	HEM	CHA-C4D-ND	2.67	127.67	124.38
82	N1	401	PEE	C17-C18-C19	-2.66	109.90	131.07
82	S2	501	PEE	O3-C30-C31	2.66	120.25	111.91
84	QD	401	HEC	CMD-C2D-C3D	2.64	129.93	124.94
82	Qd	403	PEE	O3-C30-C31	2.61	120.11	111.91
82	QB	502	PEE	O3-C30-C31	2.61	120.10	111.91
82	C1	609	PEE	O3-C30-C31	2.59	120.04	111.91
82	QC	404	PEE	O3-C30-C31	2.59	120.02	111.91
79	C1	602	HEA	CBA-CAA-C2A	-2.55	108.31	112.60
75	AK	401	ADP	C4-C5-N7	-2.53	106.76	109.40
79	C1	603	HEA	C4D-C3D-C2D	-2.51	103.24	106.90
79	C1	602	HEA	CMB-C2B-C1B	-2.49	121.24	125.04
84	Qd	402	HEC	CMD-C2D-C3D	2.48	129.62	124.94
82	N1	401	PEE	O3-C30-C31	2.48	119.70	111.91
79	C1	603	HEA	CMB-C2B-C1B	-2.45	121.31	125.04
82	N3	201	PEE	O3-C30-C31	2.43	119.54	111.91
82	Qh	101	PEE	O3-C30-C31	2.43	119.52	111.91
84	Qd	402	HEC	CMC-C2C-C1C	-2.43	124.73	128.46
84	QD	401	HEC	O1A-CGA-CBA	-2.42	115.29	123.08
82	N5	701	PEE	O3-C30-C31	2.41	119.48	111.91
83	QC	403	HEM	CHD-C1D-ND	2.40	127.04	124.43
82	QC	401	PEE	O3-C30-C31	2.40	119.45	111.91
79	C1	603	HEA	C1B-C2B-C3B	-2.37	103.96	106.80
84	QD	401	HEC	CMA-C3A-C2A	2.37	129.41	124.94
82	QB	503	PEE	O3-C30-C31	2.36	119.32	111.91
83	Qc	402	HEM	CHB-C1B-C2B	-2.36	120.20	126.72
74	AB	201	ZMP	C15-C14-C13	-2.34	108.46	112.36
83	QC	402	HEM	CHB-C1B-C2B	-2.32	120.29	126.72
79	C1	602	HEA	C27-C19-C18	-2.32	117.72	123.68
79	C1	603	HEA	CAA-C2A-C3A	2.32	132.59	126.86
77	AL	205	PLX	C8-C7-C6	-2.31	108.03	113.38
84	Qd	402	HEC	O2A-CGA-O1A	2.31	129.06	123.30
79	C1	602	HEA	CHC-C4B-NB	-2.30	121.53	124.38
79	C1	603	HEA	CMB-C2B-C3B	2.30	134.73	130.34
79	C1	602	HEA	C1B-C2B-C3B	-2.29	104.06	106.80
83	Qc	403	HEM	CHB-C1B-C2B	-2.29	120.39	126.72
84	QD	401	HEC	O2A-CGA-O1A	2.29	129.00	123.30
84	Qd	402	HEC	CMA-C3A-C2A	2.29	129.25	124.94
79	C1	602	HEA	CMB-C2B-C3B	2.28	134.69	130.34
83	Qc	402	HEM	CAD-CBD-CGD	-2.28	108.70	113.60
73	A9	401	NDP	C5A-C6A-N6A	2.27	123.81	120.35
79	C1	603	HEA	C27-C19-C18	-2.26	117.87	123.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
77	QI	301	PLX	O3-P1-O2	-2.26	101.08	112.24
79	C1	603	HEA	CHC-C4B-NB	-2.25	121.59	124.38
77	B5	201	PLX	O3-P1-O2	-2.25	101.12	112.24
77	AM	201	PLX	O3-P1-O2	-2.24	101.17	112.24
79	C1	603	HEA	C26-C15-C16	2.24	119.03	115.27
77	QE	301	PLX	O3-P1-O2	-2.21	101.30	112.24
84	Qd	402	HEC	O1A-CGA-CBA	-2.20	116.01	123.08
79	C1	602	HEA	C4D-C3D-C2D	-2.20	103.69	106.90
77	AM	203	PLX	O3-P1-O2	-2.20	101.38	112.24
79	C1	602	HEA	C26-C15-C16	2.18	118.94	115.27
77	AL	205	PLX	O3-P1-O2	-2.17	101.51	112.24
77	CB	201	PLX	O3-P1-O2	-2.17	101.51	112.24
79	C1	603	HEA	O1D-CGD-CBD	-2.17	116.11	123.08
77	C2	301	PLX	O3-P1-O2	-2.17	101.53	112.24
77	N4	501	PLX	O3-P1-O2	-2.16	101.56	112.24
83	QC	403	HEM	CHB-C1B-C2B	-2.15	120.78	126.72
77	N4	501	PLX	C2-C1-N1	-2.15	108.61	115.78
83	QC	402	HEM	CBA-CAA-C2A	-2.13	108.98	112.62
74	AB	201	ZMP	C14-C13-N1	2.11	119.97	116.42
79	C1	603	HEA	OMA-CMA-C3A	-2.11	120.32	124.91
82	S8	303	PEE	C17-C18-C19	-2.10	108.60	124.73
84	QD	401	HEC	C2B-C3B-C4B	2.10	108.62	106.35
79	C1	602	HEA	CMD-C2D-C1D	2.09	128.23	125.04
82	N1	401	PEE	C20-C19-C18	-2.09	109.11	126.37
82	Qc	401	PEE	C17-C18-C19	-2.06	108.92	124.73
82	N3	201	PEE	C37-C38-C39	-2.05	108.98	124.73
82	Qd	403	PEE	C37-C38-C39	-2.05	109.02	124.73
82	S8	303	PEE	C37-C38-C39	-2.04	109.03	124.73
82	QC	401	PEE	C37-C38-C39	-2.04	109.05	124.73
79	C1	602	HEA	O1D-CGD-CBD	-2.04	116.52	123.08
82	N3	201	PEE	C40-C39-C38	-2.04	109.07	124.73
82	Qd	403	PEE	C20-C19-C18	-2.04	109.11	124.73
82	QE	302	PEE	C40-C39-C38	-2.03	109.11	124.73
82	Qh	103	PEE	C17-C18-C19	-2.03	109.12	124.73
79	C1	602	HEA	OMA-CMA-C3A	-2.02	120.50	124.91
82	Qh	103	PEE	C20-C19-C18	-2.02	109.20	124.73
82	N3	201	PEE	C17-C18-C19	-2.02	109.20	124.73
82	QE	302	PEE	C2-O2-C10	-2.02	112.81	117.79
82	S2	501	PEE	C37-C38-C39	-2.02	109.22	124.73
82	C1	609	PEE	C20-C19-C18	-2.02	109.26	124.73
82	Qh	101	PEE	C37-C38-C39	-2.01	109.29	124.73
82	QB	503	PEE	C37-C38-C39	-2.01	109.30	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
83	QC	402	HEM	CAD-CBD-CGD	-2.01	109.29	113.60
82	Qc	401	PEE	C20-C19-C18	-2.00	109.35	124.73
79	C1	602	HEA	O1A-CGA-CBA	-2.00	116.64	123.08

There are no chirality outliers.

All (1298) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
71	6A	101	PC1	C11-O13-P-O14
71	7B	101	PC1	C1-O11-P-O12
71	7B	101	PC1	C1-O11-P-O14
71	7B	101	PC1	O13-C11-C12-N
71	AL	206	PC1	C11-O13-P-O14
71	AL	206	PC1	C1-O11-P-O12
71	AL	206	PC1	C1-O11-P-O14
71	AL	206	PC1	C1-O11-P-O13
71	C1	606	PC1	C11-O13-P-O12
71	C1	606	PC1	C11-O13-P-O14
71	C1	607	PC1	O13-C11-C12-N
71	C3	301	PC1	C1-O11-P-O14
71	C3	301	PC1	O13-C11-C12-N
71	C3	302	PC1	C11-O13-P-O11
71	N5	704	PC1	C11-O13-P-O12
71	N5	704	PC1	C11-O13-P-O14
71	N5	704	PC1	C11-O13-P-O11
71	N6	201	PC1	C11-O13-P-O12
71	N6	201	PC1	C11-O13-P-O11
71	QC	407	PC1	C11-O13-P-O14
71	QC	407	PC1	O13-C11-C12-N
71	QH	102	PC1	C1-O11-P-O12
71	Qj	101	PC1	C1-O11-P-O14
71	Qj	101	PC1	C1-O11-P-O13
72	6A	102	CDL	CA2-OA2-PA1-OA3
72	6A	102	CDL	CA3-OA5-PA1-OA3
72	6A	102	CDL	CB2-OB2-PB2-OB3
72	6A	102	CDL	CB2-OB2-PB2-OB4
72	6A	102	CDL	CB2-OB2-PB2-OB5
72	6A	102	CDL	CB3-OB5-PB2-OB3
72	A8	301	CDL	CA2-OA2-PA1-OA3
72	A8	301	CDL	CA2-OA2-PA1-OA4
72	A8	301	CDL	CA2-OA2-PA1-OA5
72	A8	301	CDL	CB3-OB5-PB2-OB3

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Mol	Chain	Res	Type	Atoms
72	AL	201	CDL	CA2-OA2-PA1-OA3
72	AL	201	CDL	CA3-OA5-PA1-OA2
72	AL	201	CDL	CA3-OA5-PA1-OA4
72	AL	201	CDL	CB3-OB5-PB2-OB4
72	AL	203	CDL	CA2-OA2-PA1-OA4
72	AL	203	CDL	CB2-OB2-PB2-OB3
72	AL	203	CDL	CB2-OB2-PB2-OB4
72	AL	203	CDL	CB2-OB2-PB2-OB5
72	AL	203	CDL	CB3-OB5-PB2-OB3
72	AL	204	CDL	CA3-OA5-PA1-OA4
72	AL	204	CDL	CB2-OB2-PB2-OB3
72	AL	204	CDL	CB2-OB2-PB2-OB4
72	AL	204	CDL	CB2-OB2-PB2-OB5
72	AL	204	CDL	OB5-CB3-CB4-OB6
72	AM	202	CDL	CB3-OB5-PB2-OB4
72	B5	202	CDL	CB2-OB2-PB2-OB3
72	B5	202	CDL	CB2-OB2-PB2-OB4
72	B5	202	CDL	CB2-OB2-PB2-OB5
72	CB	203	CDL	CA3-OA5-PA1-OA2
72	CB	203	CDL	CB2-OB2-PB2-OB4
72	CB	203	CDL	CB3-OB5-PB2-OB3
72	N2	401	CDL	CA3-OA5-PA1-OA2
72	N2	401	CDL	CA3-OA5-PA1-OA3
72	N2	401	CDL	CA3-OA5-PA1-OA4
72	N5	702	CDL	CA3-OA5-PA1-OA3
72	N5	702	CDL	CB2-OB2-PB2-OB3
72	N5	702	CDL	CB2-OB2-PB2-OB5
72	N5	702	CDL	CB3-OB5-PB2-OB2
72	N5	702	CDL	CB3-OB5-PB2-OB3
72	N5	702	CDL	CB3-OB5-PB2-OB4
72	N5	703	CDL	CA2-OA2-PA1-OA3
72	QB	501	CDL	CA2-OA2-PA1-OA3
72	QB	501	CDL	CB2-OB2-PB2-OB4
72	QB	501	CDL	CB3-OB5-PB2-OB3
72	QC	406	CDL	CA2-OA2-PA1-OA3
72	QC	406	CDL	CA2-OA2-PA1-OA4
72	QC	406	CDL	CA2-OA2-PA1-OA5
72	QC	406	CDL	CB2-OB2-PB2-OB3
72	QC	406	CDL	CB2-OB2-PB2-OB5
72	QC	406	CDL	CB3-OB5-PB2-OB4
72	QC	408	CDL	CA3-OA5-PA1-OA3
72	QC	408	CDL	CA3-OA5-PA1-OA4

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Mol	Chain	Res	Type	Atoms
72	QC	408	CDL	CB3-OB5-PB2-OB4
72	QH	101	CDL	CB2-OB2-PB2-OB3
72	QH	101	CDL	CB2-OB2-PB2-OB4
72	QH	101	CDL	CB2-OB2-PB2-OB5
72	Qb	501	CDL	CA2-OA2-PA1-OA4
72	Qb	501	CDL	CA3-OA5-PA1-OA4
72	Qb	501	CDL	CB2-OB2-PB2-OB3
72	Qb	501	CDL	CB2-OB2-PB2-OB4
72	Qb	501	CDL	CB2-OB2-PB2-OB5
72	Qb	501	CDL	CB3-OB5-PB2-OB3
72	Qd	401	CDL	CA2-OA2-PA1-OA4
72	Qd	401	CDL	CA3-OA5-PA1-OA3
72	Qd	401	CDL	OB5-CB3-CB4-OB6
72	Qh	102	CDL	CA2-OA2-PA1-OA3
72	Qh	102	CDL	CA3-OA5-PA1-OA3
73	A9	401	NDP	C5D-O5D-PN-O1N
74	AB	201	ZMP	S1-C11-C12-N1
74	AB	201	ZMP	C9-C10-S1-C11
74	AB	201	ZMP	C7-C8-C9-C10
74	AC	201	ZMP	C17-C18-C21-O5
74	AC	201	ZMP	C9-C10-S1-C11
74	AC	201	ZMP	O1-C10-C9-C8
75	AK	401	ADP	C3'-C4'-C5'-O5'
76	AL	202	3PE	C1-O11-P-O12
76	AL	202	3PE	C11-O13-P-O14
76	AL	202	3PE	O13-C11-C12-N
76	C1	601	3PE	C11-O13-P-O12
76	C1	601	3PE	O13-C11-C12-N
76	C1	608	3PE	O13-C11-C12-N
76	CA	101	3PE	C1-O11-P-O12
76	CB	202	3PE	C1-O11-P-O12
76	CB	202	3PE	C1-O11-P-O14
76	CB	202	3PE	C11-O13-P-O14
76	CB	202	3PE	O13-C11-C12-N
76	N4	502	3PE	C1-O11-P-O12
76	N4	502	3PE	C1-O11-P-O13
76	N4	502	3PE	C1-O11-P-O14
76	N4	502	3PE	C11-O13-P-O12
76	N4	502	3PE	C11-O13-P-O14
76	N4	502	3PE	O13-C11-C12-N
76	QE	303	3PE	C11-O13-P-O12
76	S7	302	3PE	C1-O11-P-O12

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Mol	Chain	Res	Type	Atoms
76	S7	302	3PE	C11-O13-P-O12
76	S7	302	3PE	O13-C11-C12-N
77	AL	205	PLX	C3-C4-O6-C6
77	AL	205	PLX	C2-O1-P1-O4
77	AL	205	PLX	C2-O1-P1-O3
77	AL	205	PLX	C25-C24-O8-C5
77	AM	201	PLX	O7-C6-C7-C8
77	AM	201	PLX	C3-O4-P1-O1
77	AM	201	PLX	C3-O4-P1-O2
77	AM	201	PLX	C3-O4-P1-O3
77	AM	201	PLX	N1-C1-C2-O1
77	AM	201	PLX	O9-C24-O8-C5
77	AM	201	PLX	O9-C24-C25-C26
77	AM	203	PLX	O7-C6-O6-C4
77	AM	203	PLX	C3-O4-P1-O2
77	AM	203	PLX	C3-O4-P1-O3
77	AM	203	PLX	O9-C24-O8-C5
77	B5	201	PLX	O7-C6-O6-C4
77	B5	201	PLX	C3-O4-P1-O1
77	B5	201	PLX	C3-O4-P1-O2
77	B5	201	PLX	C3-O4-P1-O3
77	B5	201	PLX	C2-O1-P1-O2
77	B5	201	PLX	C2-O1-P1-O3
77	C2	301	PLX	O7-C6-C7-C8
77	C2	301	PLX	N1-C1-C2-O1
77	C2	301	PLX	O9-C24-O8-C5
77	C2	301	PLX	O9-C24-C25-C26
77	CB	201	PLX	O7-C6-C7-C8
77	CB	201	PLX	O7-C6-O6-C4
77	CB	201	PLX	C2-O1-P1-O2
77	CB	201	PLX	C2-O1-P1-O3
77	N4	501	PLX	O7-C6-O6-C4
77	N4	501	PLX	C2-O1-P1-O4
77	N4	501	PLX	C25-C24-O8-C5
77	QE	301	PLX	O7-C6-C7-C8
77	QE	301	PLX	O7-C6-O6-C4
77	QE	301	PLX	C2-O1-P1-O2
77	QE	301	PLX	C2-O1-P1-O3
77	QE	301	PLX	O9-C24-C25-C26
77	QI	301	PLX	C2-O1-P1-O2
77	QI	301	PLX	C2-O1-P1-O3
77	QI	301	PLX	O9-C24-O8-C5

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Mol	Chain	Res	Type	Atoms
78	B5	203	6F6	C1-O11-P-O12
78	B5	203	6F6	C1-O11-P-O13
78	QJ	101	6F6	C1-O11-P-O12
78	QJ	101	6F6	C1-O11-P-O14
78	QJ	101	6F6	C1-O11-P-O13
78	QJ	101	6F6	O13-C11-C12-N
79	C1	602	HEA	C1A-C2A-CAA-CBA
79	C1	602	HEA	C3A-C2A-CAA-CBA
79	C1	603	HEA	C1A-C2A-CAA-CBA
79	C1	603	HEA	C3A-C2A-CAA-CBA
79	C1	603	HEA	C17-C18-C19-C27
79	C1	603	HEA	C19-C20-C21-C22
82	C1	609	PEE	C4-O4P-P-O3P
82	C1	609	PEE	C4-O4P-P-O2P
82	N1	401	PEE	C1-O3P-P-O1P
82	N3	201	PEE	C17-C18-C19-C20
82	N3	201	PEE	O2-C2-C3-O3
82	N3	201	PEE	C1-O3P-P-O1P
82	N3	201	PEE	C4-O4P-P-O3P
82	N3	201	PEE	C4-O4P-P-O2P
82	N3	201	PEE	C4-O4P-P-O1P
82	N5	701	PEE	C4-O4P-P-O2P
82	N5	701	PEE	O4P-C4-C5-N
82	QB	502	PEE	C11-C10-O2-C2
82	QB	502	PEE	O4-C10-O2-C2
82	QB	502	PEE	C4-O4P-P-O2P
82	QB	503	PEE	C1-O3P-P-O2P
82	QB	503	PEE	C1-O3P-P-O1P
82	QB	503	PEE	C1-O3P-P-O4P
82	QB	503	PEE	C4-O4P-P-O2P
82	QB	503	PEE	C37-C38-C39-C40
82	QC	401	PEE	C11-C10-O2-C2
82	QC	401	PEE	O4-C10-O2-C2
82	QC	401	PEE	O4P-C4-C5-N
82	QC	404	PEE	C4-O4P-P-O2P
82	QC	404	PEE	C4-O4P-P-O1P
82	QE	302	PEE	C1-O3P-P-O2P
82	QE	302	PEE	C1-O3P-P-O1P
82	QE	302	PEE	C1-O3P-P-O4P
82	Qd	403	PEE	C1-O3P-P-O2P
82	Qd	403	PEE	C1-O3P-P-O1P
82	Qd	403	PEE	C1-O3P-P-O4P

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Mol	Chain	Res	Type	Atoms
82	Qd	403	PEE	O4P-C4-C5-N
82	Qh	101	PEE	C1-O3P-P-O4P
82	Qh	101	PEE	C4-O4P-P-O2P
82	Qh	101	PEE	O4P-C4-C5-N
82	Qh	103	PEE	C1-O3P-P-O2P
82	Qh	103	PEE	C1-O3P-P-O1P
82	Qh	103	PEE	C37-C38-C39-C40
82	S2	501	PEE	C1-O3P-P-O2P
82	S2	501	PEE	O4P-C4-C5-N
82	S8	303	PEE	O4P-C4-C5-N
83	QC	402	HEM	C2B-C3B-CAB-CBB
83	QC	402	HEM	C4B-C3B-CAB-CBB
83	QC	403	HEM	C2B-C3B-CAB-CBB
83	QC	403	HEM	C4B-C3B-CAB-CBB
83	Qc	402	HEM	C2B-C3B-CAB-CBB
83	Qc	402	HEM	C4B-C3B-CAB-CBB
83	Qc	403	HEM	C2B-C3B-CAB-CBB
83	Qc	403	HEM	C4B-C3B-CAB-CBB
87	V1	502	FMN	C3'-C4'-C5'-O5'
87	V1	502	FMN	O4'-C4'-C5'-O5'
87	V1	502	FMN	C5'-O5'-P-O1P
87	V1	502	FMN	C5'-O5'-P-O2P
87	V1	502	FMN	C5'-O5'-P-O3P
82	Qc	401	PEE	O5-C30-O3-C3
82	N1	401	PEE	O5-C30-O3-C3
82	QB	502	PEE	O5-C30-O3-C3
82	Qc	401	PEE	C31-C30-O3-C3
79	C1	602	HEA	C27-C19-C20-C21
82	N1	401	PEE	C31-C30-O3-C3
82	QB	502	PEE	C31-C30-O3-C3
82	Qd	403	PEE	C31-C30-O3-C3
82	QB	503	PEE	C17-C18-C19-C20
82	QC	401	PEE	C17-C18-C19-C20
82	S8	303	PEE	C37-C38-C39-C40
79	C1	602	HEA	C17-C18-C19-C27
79	C1	602	HEA	C17-C18-C19-C20
79	C1	603	HEA	C17-C18-C19-C20
72	QC	408	CDL	O1-C1-CB2-OB2
82	N1	401	PEE	C11-C10-O2-C2
82	S8	303	PEE	C11-C10-O2-C2
82	Qd	403	PEE	O5-C30-O3-C3
74	AC	201	ZMP	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
82	C1	609	PEE	C11-C12-C13-C14
82	S2	501	PEE	C2-C1-O3P-P
83	QC	402	HEM	C3D-CAD-CBD-CGD
79	C1	602	HEA	C19-C20-C21-C22
82	Qc	401	PEE	C17-C18-C19-C20
72	Qb	501	CDL	CA2-C1-CB2-OB2
82	N1	401	PEE	O4-C10-O2-C2
82	S8	303	PEE	O4-C10-O2-C2
82	S8	303	PEE	C31-C30-O3-C3
82	QE	302	PEE	C33-C34-C35-C36
77	QE	301	PLX	O4-C3-C4-O6
72	Qb	501	CDL	O1-C1-CB2-OB2
78	B5	203	6F6	C31-C32-C33-C34
71	7B	101	PC1	O21-C2-C3-O31
72	6A	102	CDL	OB6-CB4-CB6-OB8
77	CB	201	PLX	O6-C4-C5-O8
72	AL	201	CDL	CA5-C11-C12-C13
72	CB	203	CDL	CB7-C71-C72-C73
82	QB	503	PEE	C30-C31-C32-C33
83	Qc	403	HEM	C2A-CAA-CBA-CGA
82	QC	401	PEE	C30-C31-C32-C33
82	Qd	403	PEE	C10-C11-C12-C13
82	QC	401	PEE	C37-C38-C39-C40
72	AL	201	CDL	CA7-C31-C32-C33
72	AL	203	CDL	CB7-C71-C72-C73
72	QC	408	CDL	CB7-C71-C72-C73
78	B5	203	6F6	C21-C22-C23-C24
82	QC	404	PEE	C10-C11-C12-C13
82	QE	302	PEE	C10-C11-C12-C13
82	N3	201	PEE	C11-C12-C13-C14
82	Qc	401	PEE	C11-C12-C13-C14
78	B5	203	6F6	C11-C12-N-C15
82	Qh	103	PEE	C10-C11-C12-C13
74	AC	201	ZMP	C14-C15-N2-C16
82	S8	303	PEE	O5-C30-O3-C3
76	AL	202	3PE	C31-C32-C33-C34
72	CB	203	CDL	O1-C1-CA2-OA2
82	QB	503	PEE	C10-C11-C12-C13
82	Qh	101	PEE	C14-C15-C16-C17
82	Qh	103	PEE	C17-C18-C19-C20
82	Qh	101	PEE	C11-C10-O2-C2
77	AL	205	PLX	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
71	6A	101	PC1	C11-O13-P-O11
71	7B	101	PC1	C1-O11-P-O13
71	AL	206	PC1	C11-O13-P-O11
71	C1	606	PC1	C11-O13-P-O11
71	QH	102	PC1	C1-O11-P-O13
71	Qb	502	PC1	C11-O13-P-O11
72	6A	102	CDL	CA2-OA2-PA1-OA5
72	AL	201	CDL	CA2-OA2-PA1-OA5
72	AL	201	CDL	CB2-OB2-PB2-OB5
72	AL	201	CDL	CB3-OB5-PB2-OB2
72	AL	203	CDL	CA2-OA2-PA1-OA5
72	AL	203	CDL	CB3-OB5-PB2-OB2
72	AL	204	CDL	CA2-OA2-PA1-OA5
72	AM	202	CDL	CB3-OB5-PB2-OB2
72	B5	202	CDL	CA3-OA5-PA1-OA2
72	CB	203	CDL	CB2-OB2-PB2-OB5
72	N2	401	CDL	CA2-OA2-PA1-OA5
72	N2	401	CDL	CB2-OB2-PB2-OB5
72	N5	702	CDL	CA2-OA2-PA1-OA5
72	N5	702	CDL	CA3-OA5-PA1-OA2
72	QB	501	CDL	CA2-OA2-PA1-OA5
72	QB	501	CDL	CA3-OA5-PA1-OA2
72	QB	501	CDL	CB2-OB2-PB2-OB5
72	QC	406	CDL	CA3-OA5-PA1-OA2
72	QC	406	CDL	CB3-OB5-PB2-OB2
72	QC	408	CDL	CA3-OA5-PA1-OA2
72	QC	408	CDL	CB3-OB5-PB2-OB2
72	QH	101	CDL	CA2-OA2-PA1-OA5
72	Qb	501	CDL	CA2-OA2-PA1-OA5
72	Qb	501	CDL	CA3-OA5-PA1-OA2
72	Qd	401	CDL	CA2-OA2-PA1-OA5
72	Qd	401	CDL	CB3-OB5-PB2-OB2
72	Qh	102	CDL	CA2-OA2-PA1-OA5
72	Qh	102	CDL	CA3-OA5-PA1-OA2
72	Qh	102	CDL	CB2-OB2-PB2-OB5
72	Qh	102	CDL	CB3-OB5-PB2-OB2
76	AL	202	3PE	C1-O11-P-O13
76	C1	608	3PE	C1-O11-P-O13
76	CA	101	3PE	C1-O11-P-O13
76	CB	202	3PE	C1-O11-P-O13
76	CB	202	3PE	C11-O13-P-O11
76	N4	502	3PE	C11-O13-P-O11

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Mol	Chain	Res	Type	Atoms
76	QE	303	3PE	C1-O11-P-O13
77	AL	205	PLX	C3-O4-P1-O1
77	AM	203	PLX	C3-O4-P1-O1
77	B5	201	PLX	C2-O1-P1-O4
77	C2	301	PLX	C2-O1-P1-O4
77	CB	201	PLX	C3-O4-P1-O1
77	CB	201	PLX	C2-O1-P1-O4
77	QE	301	PLX	C2-O1-P1-O4
77	QI	301	PLX	C2-O1-P1-O4
78	Qc	404	6F6	C11-O13-P-O11
82	C1	609	PEE	C1-O3P-P-O4P
82	N3	201	PEE	C1-O3P-P-O4P
82	N5	701	PEE	C4-O4P-P-O3P
82	QB	502	PEE	C4-O4P-P-O3P
82	QC	401	PEE	C4-O4P-P-O3P
82	QC	404	PEE	C4-O4P-P-O3P
82	Qh	101	PEE	C4-O4P-P-O3P
82	Qh	103	PEE	C1-O3P-P-O4P
82	S2	501	PEE	C1-O3P-P-O4P
82	S2	501	PEE	C4-O4P-P-O3P
71	AL	206	PC1	C29-C2A-C2B-C2C
72	CB	203	CDL	CB2-C1-CA2-OA2
82	Qh	101	PEE	O4-C10-O2-C2
71	C1	607	PC1	C11-C12-N-C13
71	C1	607	PC1	C11-C12-N-C14
71	C1	607	PC1	C11-C12-N-C15
78	B5	203	6F6	C11-C12-N-C14
78	QJ	101	6F6	C11-C12-N-C13
78	QJ	101	6F6	C11-C12-N-C14
78	Qc	404	6F6	C11-C12-N-C14
71	AL	206	PC1	C36-C37-C38-C39
82	Qh	101	PEE	C30-C31-C32-C33
77	AM	201	PLX	O6-C6-C7-C8
77	CB	201	PLX	O6-C6-C7-C8
77	CB	201	PLX	O8-C24-C25-C26
77	QE	301	PLX	O6-C6-C7-C8
77	AL	205	PLX	C30-C31-C32-C33
82	C1	609	PEE	C12-C13-C14-C15
82	QB	503	PEE	C33-C34-C35-C36
82	QB	503	PEE	C42-C43-C44-C45
76	C1	608	3PE	C2B-C2C-C2D-C2E
77	AL	205	PLX	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
82	Qh	101	PEE	C11-C12-C13-C14
82	S8	303	PEE	C13-C14-C15-C16
82	QC	401	PEE	C11-C12-C13-C14
72	N5	702	CDL	C58-C59-C60-C61
76	S7	302	3PE	C3B-C3C-C3D-C3E
82	Qh	103	PEE	C12-C13-C14-C15
77	AM	201	PLX	C10-C11-C12-C13
82	N5	701	PEE	C11-C12-C13-C14
82	Qd	403	PEE	C40-C41-C42-C43
72	AM	202	CDL	O1-C1-CA2-OA2
83	Qc	402	HEM	C3D-CAD-CBD-CGD
72	AL	203	CDL	C36-C37-C38-C39
72	AL	204	CDL	C35-C36-C37-C38
77	AL	205	PLX	C12-C13-C14-C15
82	Qd	403	PEE	C20-C21-C22-C23
82	Qd	403	PEE	C12-C13-C14-C15
72	AL	201	CDL	CB7-C71-C72-C73
82	Qd	403	PEE	C30-C31-C32-C33
82	N1	401	PEE	C12-C13-C14-C15
82	Qd	403	PEE	C11-C12-C13-C14
82	Qc	401	PEE	C22-C23-C24-C25
72	AL	203	CDL	C58-C59-C60-C61
82	QE	302	PEE	C32-C33-C34-C35
82	Qd	403	PEE	C31-C32-C33-C34
77	CB	201	PLX	C7-C8-C9-C10
77	QE	301	PLX	C28-C29-C30-C31
82	C1	609	PEE	C40-C41-C42-C43
82	N3	201	PEE	C22-C23-C24-C25
71	QC	405	PC1	C28-C29-C2A-C2B
72	CB	203	CDL	C59-C60-C61-C62
77	AM	201	PLX	C26-C27-C28-C29
77	CB	201	PLX	C19-C20-C21-C22
82	Qc	401	PEE	C31-C32-C33-C34
82	S2	501	PEE	C14-C15-C16-C17
82	Qh	101	PEE	C19-C20-C21-C22
82	Qh	101	PEE	C15-C16-C17-C18
82	S2	501	PEE	C35-C36-C37-C38
71	QC	405	PC1	C21-C22-C23-C24
72	6A	102	CDL	CB7-C71-C72-C73
72	QC	406	CDL	CB5-C51-C52-C53
82	N1	401	PEE	C30-C31-C32-C33
71	Qb	502	PC1	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
74	AC	201	ZMP	C2-C3-C4-C5
82	QC	401	PEE	C33-C34-C35-C36
71	N5	704	PC1	C11-C12-N-C15
78	QJ	101	6F6	C11-C12-N-C15
78	Qc	404	6F6	C11-C12-N-C13
78	Qc	404	6F6	C11-C12-N-C15
71	6A	101	PC1	C33-C34-C35-C36
72	A8	301	CDL	C55-C56-C57-C58
77	AM	203	PLX	C34-C35-C36-C37
82	QB	503	PEE	C22-C23-C24-C25
82	QC	401	PEE	C42-C43-C44-C45
82	S2	501	PEE	C40-C41-C42-C43
82	QE	302	PEE	O4P-C4-C5-N
76	CA	101	3PE	C2B-C2C-C2D-C2E
77	B5	201	PLX	C13-C14-C15-C16
77	QE	301	PLX	C11-C10-C9-C8
82	N3	201	PEE	C30-C31-C32-C33
71	C3	301	PC1	C39-C3A-C3B-C3C
77	N4	501	PLX	C11-C10-C9-C8
82	N5	701	PEE	C33-C34-C35-C36
82	S2	501	PEE	C43-C44-C45-C46
82	S8	303	PEE	C21-C22-C23-C24
71	N6	201	PC1	C23-C24-C25-C26
77	QI	301	PLX	C7-C8-C9-C10
82	C1	609	PEE	C42-C43-C44-C45
82	N3	201	PEE	C33-C34-C35-C36
72	A8	301	CDL	C33-C34-C35-C36
77	CB	201	PLX	C34-C35-C36-C37
77	QE	301	PLX	C16-C17-C18-C19
71	AL	206	PC1	C3A-C3B-C3C-C3D
77	C2	301	PLX	C12-C13-C14-C15
82	C1	609	PEE	C32-C33-C34-C35
72	CB	203	CDL	C16-C17-C18-C19
77	B5	201	PLX	C17-C18-C19-C20
82	Qc	401	PEE	C11-C10-O2-C2
72	N5	702	CDL	C16-C17-C18-C19
77	AL	205	PLX	O9-C24-C25-C26
77	B5	201	PLX	O9-C24-C25-C26
77	CB	201	PLX	O9-C24-C25-C26
72	CB	203	CDL	C38-C39-C40-C41
76	C1	608	3PE	C32-C33-C34-C35
82	C1	609	PEE	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
82	C1	609	PEE	C39-C40-C41-C42
82	QE	302	PEE	C35-C36-C37-C38
82	QB	502	PEE	C12-C13-C14-C15
77	N4	501	PLX	C32-C33-C34-C35
77	QI	301	PLX	C34-C35-C36-C37
82	N3	201	PEE	C34-C35-C36-C37
77	C2	301	PLX	C25-C26-C27-C28
78	B5	203	6F6	C38-C39-C3A-C3B
79	C1	603	HEA	C13-C14-C15-C16
82	S8	303	PEE	C12-C13-C14-C15
71	QC	405	PC1	C11-C12-N-C13
71	Qj	101	PC1	C11-C12-N-C15
71	7B	101	PC1	C21-C22-C23-C24
82	S2	501	PEE	C31-C30-O3-C3
71	C3	302	PC1	C2B-C2C-C2D-C2E
77	AL	205	PLX	C26-C27-C28-C29
82	N5	701	PEE	C12-C13-C14-C15
82	Qh	101	PEE	C10-C11-C12-C13
72	B5	202	CDL	C35-C36-C37-C38
77	C2	301	PLX	C11-C12-C13-C14
82	S2	501	PEE	C33-C34-C35-C36
82	Qc	401	PEE	O4-C10-O2-C2
72	QH	101	CDL	CA7-C31-C32-C33
72	Qb	501	CDL	CA7-C31-C32-C33
71	Qj	101	PC1	C3C-C3D-C3E-C3F
72	N2	401	CDL	C31-C32-C33-C34
74	AC	201	ZMP	C6-C7-C8-C9
74	AC	201	ZMP	C22-C23-C24-C25
71	Qj	101	PC1	C21-C22-C23-C24
82	Qc	401	PEE	C30-C31-C32-C33
71	7B	101	PC1	C22-C23-C24-C25
76	C1	601	3PE	C2D-C2E-C2F-C2G
82	C1	609	PEE	C21-C22-C23-C24
82	S8	303	PEE	C33-C34-C35-C36
77	CB	201	PLX	C16-C17-C18-C19
82	C1	609	PEE	C41-C42-C43-C44
82	QB	503	PEE	C41-C42-C43-C44
82	QB	503	PEE	C11-C10-O2-C2
71	QH	102	PC1	O11-C1-C2-O21
77	QI	301	PLX	O4-C3-C4-O6
72	N2	401	CDL	C12-C13-C14-C15
82	Qd	403	PEE	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
72	N5	702	CDL	O1-C1-CA2-OA2
77	AL	205	PLX	O6-C4-C5-O8
82	QB	502	PEE	O2-C2-C3-O3
82	Qh	101	PEE	O2-C2-C3-O3
72	QC	406	CDL	C14-C15-C16-C17
82	C1	609	PEE	C33-C34-C35-C36
78	B5	203	6F6	C11-C12-N-C13
71	C1	607	PC1	C2C-C2D-C2E-C2F
82	QC	401	PEE	C31-C32-C33-C34
82	N3	201	PEE	C35-C36-C37-C38
82	Qh	101	PEE	C35-C36-C37-C38
78	QJ	101	6F6	C31-C32-C33-C34
77	QI	301	PLX	C26-C27-C28-C29
75	AK	401	ADP	O4'-C4'-C5'-O5'
77	AM	203	PLX	C7-C8-C9-C10
74	AC	201	ZMP	C4-C5-C6-C7
82	N3	201	PEE	C10-C11-C12-C13
77	N4	501	PLX	C27-C28-C29-C30
82	S2	501	PEE	O5-C30-O3-C3
82	QB	503	PEE	O4-C10-O2-C2
82	QE	302	PEE	C16-C17-C18-C19
71	C3	301	PC1	C1-O11-P-O13
71	QC	407	PC1	C11-O13-P-O11
71	Qj	101	PC1	C11-O13-P-O11
72	AL	204	CDL	CA3-OA5-PA1-OA2
72	CB	203	CDL	CB3-OB5-PB2-OB2
72	N5	703	CDL	CA2-OA2-PA1-OA5
72	QB	501	CDL	CB3-OB5-PB2-OB2
76	C1	601	3PE	C11-O13-P-O11
74	AB	201	ZMP	C3-C4-C5-C6
76	N4	502	3PE	C2-C1-O11-P
72	AL	204	CDL	OB5-CB3-CB4-CB6
72	Qb	501	CDL	OB5-CB3-CB4-CB6
77	QE	301	PLX	O4-C3-C4-C5
76	S7	302	3PE	C3A-C3B-C3C-C3D
71	C3	301	PC1	C3A-C3B-C3C-C3D
72	AL	204	CDL	C52-C53-C54-C55
72	B5	202	CDL	C83-C84-C85-C86
77	CB	201	PLX	C32-C33-C34-C35
82	Qc	401	PEE	C32-C33-C34-C35
82	Qc	401	PEE	C33-C34-C35-C36
71	C1	606	PC1	C29-C2A-C2B-C2C

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Mol	Chain	Res	Type	Atoms
72	Qd	401	CDL	C73-C74-C75-C76
77	B5	201	PLX	C30-C31-C32-C33
82	QE	302	PEE	C21-C22-C23-C24
71	N5	704	PC1	C11-C12-N-C14
71	Qb	502	PC1	C1-C2-C3-O31
72	A8	301	CDL	CB3-CB4-CB6-OB8
72	QB	501	CDL	CB3-CB4-CB6-OB8
72	Qb	501	CDL	CB3-CB4-CB6-OB8
72	Qd	401	CDL	CA3-CA4-CA6-OA8
76	C1	601	3PE	C1-C2-C3-O31
77	B5	201	PLX	C3-C4-C5-O8
77	N4	501	PLX	C3-C4-C5-O8
82	QC	401	PEE	C1-C2-C3-O3
82	QE	302	PEE	C1-C2-C3-O3
82	Qc	401	PEE	C1-C2-C3-O3
82	Qh	101	PEE	C17-C18-C19-C20
71	C1	607	PC1	C36-C37-C38-C39
71	C3	302	PC1	C29-C2A-C2B-C2C
78	Qc	404	6F6	C39-C3A-C3B-C4
82	QC	401	PEE	C24-C25-C26-C27
82	QE	302	PEE	C12-C13-C14-C15
78	B5	203	6F6	C29-C2A-C2B-C2C
78	QJ	101	6F6	C2F-C2G-C2H-C2I
77	AM	203	PLX	O8-C24-C25-C26
77	C2	301	PLX	O6-C6-C7-C8
77	C2	301	PLX	O8-C24-C25-C26
74	AB	201	ZMP	O3-C16-C17-O4
72	AL	201	CDL	C17-C18-C19-C20
82	Qh	103	PEE	C41-C42-C43-C44
77	QI	301	PLX	C27-C28-C29-C30
82	C1	609	PEE	C35-C36-C37-C38
82	N1	401	PEE	C35-C36-C37-C38
82	Qc	401	PEE	C15-C16-C17-C18
82	Qd	403	PEE	C15-C16-C17-C18
82	Qh	103	PEE	C19-C20-C21-C22
82	S8	303	PEE	C35-C36-C37-C38
72	QC	406	CDL	C75-C76-C77-C78
71	Qj	101	PC1	C24-C25-C26-C27
77	C2	301	PLX	C16-C17-C18-C19
82	Qh	103	PEE	C20-C21-C22-C23
74	AB	201	ZMP	C22-C23-C24-C25
77	QE	301	PLX	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
82	S8	303	PEE	C3-C2-O2-C10
72	AL	204	CDL	C53-C54-C55-C56
72	CB	203	CDL	C80-C81-C82-C83
82	N1	401	PEE	C14-C15-C16-C17
82	QC	404	PEE	C16-C17-C18-C19
82	QC	404	PEE	C21-C22-C23-C24
82	Qh	101	PEE	C37-C38-C39-C40
71	N5	704	PC1	C11-C12-N-C13
71	QC	405	PC1	C11-C12-N-C14
71	Qj	101	PC1	C11-C12-N-C14
82	QC	404	PEE	C33-C34-C35-C36
77	AM	203	PLX	C36-C37-C38-C39
82	QE	302	PEE	C40-C41-C42-C43
82	Qc	401	PEE	C19-C20-C21-C22
71	6A	101	PC1	O21-C2-C3-O31
77	AM	201	PLX	O6-C4-C5-O8
77	AM	203	PLX	O6-C4-C5-O8
72	CB	203	CDL	C72-C73-C74-C75
71	7B	101	PC1	C25-C26-C27-C28
82	QB	503	PEE	C21-C22-C23-C24
82	S2	501	PEE	C16-C17-C18-C19
78	Qc	404	6F6	O31-C31-C32-C33
72	B5	202	CDL	C21-C22-C23-C24
72	N2	401	CDL	C73-C74-C75-C76
77	AM	203	PLX	C18-C19-C20-C21
77	AM	203	PLX	C14-C15-C16-C17
82	N3	201	PEE	C31-C32-C33-C34
82	N1	401	PEE	C32-C33-C34-C35
82	QE	302	PEE	C11-C12-C13-C14
82	Qc	401	PEE	C12-C13-C14-C15
72	N5	703	CDL	CA7-C31-C32-C33
82	S8	303	PEE	C11-C12-C13-C14
72	CB	203	CDL	OB5-CB3-CB4-CB6
72	QC	408	CDL	OA5-CA3-CA4-CA6
72	Qd	401	CDL	OB5-CB3-CB4-CB6
77	AM	203	PLX	O4-C3-C4-C5
77	QI	301	PLX	O4-C3-C4-C5
82	Qc	401	PEE	O3P-C1-C2-C3
82	Qc	401	PEE	C35-C36-C37-C38
82	S2	501	PEE	C32-C33-C34-C35
71	Qj	101	PC1	C23-C24-C25-C26
82	S2	501	PEE	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
72	QB	501	CDL	CA5-C11-C12-C13
82	Qc	401	PEE	C10-C11-C12-C13
72	AL	201	CDL	C21-C22-C23-C24
82	N5	701	PEE	C39-C40-C41-C42
72	QC	406	CDL	C16-C17-C18-C19
82	Qh	103	PEE	C31-C32-C33-C34
82	S2	501	PEE	C41-C42-C43-C44
71	Qb	502	PC1	C21-C22-C23-C24
72	N5	703	CDL	C17-C18-C19-C20
82	QE	302	PEE	C22-C23-C24-C25
72	N5	703	CDL	CA4-CA3-OA5-PA1
72	QH	101	CDL	CB4-CB3-OB5-PB2
72	Qh	102	CDL	C1-CA2-OA2-PA1
72	AL	201	CDL	C13-C14-C15-C16
72	N5	703	CDL	C43-C44-C45-C46
71	6A	101	PC1	C1-C2-C3-O31
72	6A	102	CDL	CB3-CB4-CB6-OB8
72	N2	401	CDL	CA3-CA4-CA6-OA8
76	C1	608	3PE	C1-C2-C3-O31
77	AL	205	PLX	C3-C4-C5-O8
77	CB	201	PLX	C3-C4-C5-O8
82	C1	609	PEE	C1-C2-C3-O3
82	N3	201	PEE	C1-C2-C3-O3
82	Qh	101	PEE	C1-C2-C3-O3
72	A8	301	CDL	C19-C20-C21-C22
76	C1	601	3PE	C29-C2A-C2B-C2C
82	N1	401	PEE	C33-C34-C35-C36
82	QC	404	PEE	C11-C12-C13-C14
82	C1	609	PEE	C37-C38-C39-C40
82	N5	701	PEE	C24-C25-C26-C27
72	Qd	401	CDL	C51-C52-C53-C54
77	N4	501	PLX	C12-C13-C14-C15
74	AB	201	ZMP	N2-C16-C17-C18
79	C1	603	HEA	C27-C19-C20-C21
82	S2	501	PEE	C11-C12-C13-C14
72	A8	301	CDL	C56-C57-C58-C59
82	S8	303	PEE	C22-C23-C24-C25
76	S7	302	3PE	C11-O13-P-O11
77	B5	201	PLX	C3-C4-O6-C6
77	B5	201	PLX	C5-C4-O6-C6
77	C2	301	PLX	C3-C4-O6-C6
77	C2	301	PLX	C5-C4-O6-C6

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Mol	Chain	Res	Type	Atoms
77	CB	201	PLX	C3-C4-O6-C6
77	CB	201	PLX	C5-C4-O6-C6
77	N4	501	PLX	C5-C4-O6-C6
82	N1	401	PEE	C1-O3P-P-O4P
82	QB	503	PEE	C4-O4P-P-O3P
71	QC	405	PC1	O11-C1-C2-O21
72	AL	201	CDL	OB5-CB3-CB4-OB6
72	AL	203	CDL	OB5-CB3-CB4-OB6
72	QB	501	CDL	OA5-CA3-CA4-OA6
72	QC	408	CDL	OA5-CA3-CA4-OA6
72	Qb	501	CDL	OB5-CB3-CB4-OB6
76	AL	202	3PE	O11-C1-C2-O21
82	C1	609	PEE	O3P-C1-C2-O2
82	Qh	101	PEE	O3P-C1-C2-O2
72	N5	703	CDL	C52-C53-C54-C55
76	S7	302	3PE	C21-C22-C23-C24
72	N5	703	CDL	C31-C32-C33-C34
82	S2	501	PEE	C13-C14-C15-C16
72	N5	703	CDL	C32-C31-CA7-OA8
82	S8	303	PEE	C32-C33-C34-C35
77	QE	301	PLX	C12-C13-C14-C15
72	A8	301	CDL	OB6-CB4-CB6-OB8
72	Qb	501	CDL	OB6-CB4-CB6-OB8
76	C1	601	3PE	O21-C2-C3-O31
77	B5	201	PLX	O6-C4-C5-O8
82	C1	609	PEE	O2-C2-C3-O3
82	QC	401	PEE	O2-C2-C3-O3
72	N2	401	CDL	C32-C33-C34-C35
72	AM	202	CDL	CB2-C1-CA2-OA2
72	QC	408	CDL	CA2-C1-CB2-OB2
79	C1	602	HEA	C15-C16-C17-C18
72	A8	301	CDL	C23-C24-C25-C26
76	CA	101	3PE	C24-C25-C26-C27
77	QI	301	PLX	C11-C10-C9-C8
71	C3	301	PC1	C3B-C3C-C3D-C3E
72	6A	102	CDL	C1-CB2-OB2-PB2
72	A8	301	CDL	C1-CA2-OA2-PA1
72	AL	203	CDL	C1-CB2-OB2-PB2
72	CB	203	CDL	CB4-CB3-OB5-PB2
72	QC	408	CDL	CA4-CA3-OA5-PA1
72	QC	408	CDL	C1-CB2-OB2-PB2
72	Qd	401	CDL	C1-CA2-OA2-PA1

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Mol	Chain	Res	Type	Atoms
72	Qh	102	CDL	CA4-CA3-OA5-PA1
76	QE	303	3PE	C2-C1-O11-P
82	S8	303	PEE	C2-C1-O3P-P
71	QC	405	PC1	C3B-C3C-C3D-C3E
71	C3	301	PC1	O21-C21-C22-C23
82	S2	501	PEE	C18-C19-C20-C21
74	AB	201	ZMP	O1-C10-S1-C11
74	AC	201	ZMP	O1-C10-S1-C11
77	CB	201	PLX	C33-C34-C35-C36
71	C1	606	PC1	C31-C32-C33-C34
74	AC	201	ZMP	S1-C10-C9-C8
82	Qh	101	PEE	C38-C39-C40-C41
72	6A	102	CDL	OB5-CB3-CB4-CB6
72	AL	201	CDL	OB5-CB3-CB4-CB6
72	Qh	102	CDL	OB5-CB3-CB4-CB6
76	AL	202	3PE	O11-C1-C2-C3
76	C1	608	3PE	O11-C1-C2-C3
77	N4	501	PLX	O4-C3-C4-C5
82	N1	401	PEE	O3P-C1-C2-C3
82	N5	701	PEE	O3P-C1-C2-C3
82	QB	502	PEE	O3P-C1-C2-C3
74	AB	201	ZMP	C1-C2-C3-C4
82	Qh	101	PEE	C34-C35-C36-C37
72	AL	201	CDL	C52-C53-C54-C55
72	N2	401	CDL	C13-C14-C15-C16
82	S8	303	PEE	C14-C15-C16-C17
82	QC	404	PEE	C20-C21-C22-C23
77	C2	301	PLX	C26-C27-C28-C29
72	AL	201	CDL	C62-C63-C64-C65
82	N1	401	PEE	C3-C2-O2-C10
71	C1	606	PC1	C27-C28-C29-C2A
82	Qh	103	PEE	C21-C22-C23-C24
71	C1	607	PC1	C24-C25-C26-C27
82	Qh	103	PEE	C23-C24-C25-C26
71	7B	101	PC1	C1-C2-C3-O31
78	Qc	404	6F6	C1-C2-C3-O31
82	QB	502	PEE	C1-C2-C3-O3
82	QB	503	PEE	C1-C2-C3-O3
82	Qc	401	PEE	C2-C1-O3P-P
71	Qj	101	PC1	O11-C1-C2-O21
72	6A	102	CDL	OA5-CA3-CA4-OA6
72	6A	102	CDL	OB5-CB3-CB4-OB6

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Mol	Chain	Res	Type	Atoms
72	CB	203	CDL	OB5-CB3-CB4-OB6
76	C1	608	3PE	O11-C1-C2-O21
77	AM	201	PLX	O4-C3-C4-O6
77	AM	203	PLX	O4-C3-C4-O6
77	CB	201	PLX	O4-C3-C4-O6
82	N5	701	PEE	O3P-C1-C2-O2
72	QB	501	CDL	C72-C71-CB7-OB8
76	CA	101	3PE	C37-C38-C39-C3A
76	C1	601	3PE	C3C-C3D-C3E-C3F
72	CB	203	CDL	CA5-C11-C12-C13
72	AL	203	CDL	C71-C72-C73-C74
82	S8	303	PEE	C34-C35-C36-C37
72	N5	703	CDL	C36-C37-C38-C39
72	QB	501	CDL	OB6-CB4-CB6-OB8
72	QH	101	CDL	OA6-CA4-CA6-OA8
72	Qh	102	CDL	OA6-CA4-CA6-OA8
82	QB	503	PEE	O2-C2-C3-O3
82	Qd	403	PEE	O2-C2-C3-O3
72	B5	202	CDL	C53-C54-C55-C56
71	QH	102	PC1	C23-C24-C25-C26
71	QC	405	PC1	C11-C12-N-C15
73	A9	401	NDP	C5D-O5D-PN-O3
82	QB	503	PEE	C32-C33-C34-C35
82	S2	501	PEE	C39-C40-C41-C42
71	N6	201	PC1	C35-C36-C37-C38
77	N4	501	PLX	C9-C10-C11-C12
72	A8	301	CDL	C22-C23-C24-C25
76	CA	101	3PE	C25-C26-C27-C28
82	N5	701	PEE	C22-C23-C24-C25
72	N2	401	CDL	C52-C51-CB5-OB6
82	Qc	401	PEE	C13-C14-C15-C16
72	B5	202	CDL	C17-C18-C19-C20
82	N1	401	PEE	C10-C11-C12-C13
82	S2	501	PEE	C34-C35-C36-C37
71	QC	407	PC1	C1-O11-P-O13
71	Qb	502	PC1	C1-O11-P-O13
72	6A	102	CDL	CA3-OA5-PA1-OA2
72	N5	703	CDL	CA3-OA5-PA1-OA2
77	AM	203	PLX	C2-O1-P1-O4
72	AL	204	CDL	C82-C83-C84-C85
72	N2	401	CDL	C1-CA2-OA2-PA1
72	QC	408	CDL	C1-CA2-OA2-PA1

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Mol	Chain	Res	Type	Atoms
72	Qd	401	CDL	CA4-CA3-OA5-PA1
77	B5	201	PLX	C33-C34-C35-C36
71	6A	101	PC1	C11-O13-P-O12
71	AL	206	PC1	C11-O13-P-O12
71	AL	206	PC1	C11-C12-N-C14
71	C3	301	PC1	C1-O11-P-O12
71	C3	302	PC1	C11-O13-P-O12
71	N6	201	PC1	C11-O13-P-O14
71	Qb	502	PC1	C11-O13-P-O12
71	Qb	502	PC1	C11-O13-P-O14
71	Qj	101	PC1	C11-O13-P-O12
71	Qj	101	PC1	C11-O13-P-O14
72	6A	102	CDL	CA2-OA2-PA1-OA4
72	A8	301	CDL	CB3-OB5-PB2-OB4
72	AL	201	CDL	CA2-OA2-PA1-OA4
72	AL	201	CDL	CA3-OA5-PA1-OA3
72	AL	201	CDL	CB2-OB2-PB2-OB3
72	AL	201	CDL	CB2-OB2-PB2-OB4
72	AL	203	CDL	CB3-OB5-PB2-OB4
72	AL	204	CDL	CA2-OA2-PA1-OA3
72	AL	204	CDL	CA3-OA5-PA1-OA3
72	B5	202	CDL	CA3-OA5-PA1-OA3
72	CB	203	CDL	CA3-OA5-PA1-OA4
72	CB	203	CDL	CB2-OB2-PB2-OB3
72	CB	203	CDL	CB3-OB5-PB2-OB4
72	N2	401	CDL	CA2-OA2-PA1-OA3
72	N2	401	CDL	CA2-OA2-PA1-OA4
72	N2	401	CDL	CB2-OB2-PB2-OB3
72	N5	702	CDL	CA2-OA2-PA1-OA3
72	N5	702	CDL	CA3-OA5-PA1-OA4
72	N5	703	CDL	CA2-OA2-PA1-OA4
72	QB	501	CDL	CA2-OA2-PA1-OA4
72	QB	501	CDL	CA3-OA5-PA1-OA4
72	QB	501	CDL	CB3-OB5-PB2-OB4
72	QC	406	CDL	CA3-OA5-PA1-OA3
72	QC	406	CDL	CA3-OA5-PA1-OA4
72	QC	408	CDL	CB3-OB5-PB2-OB3
72	QH	101	CDL	CA2-OA2-PA1-OA3
72	Qb	501	CDL	CA3-OA5-PA1-OA3
72	Qd	401	CDL	CA2-OA2-PA1-OA3
72	Qd	401	CDL	CB3-OB5-PB2-OB3
72	Qd	401	CDL	CB3-OB5-PB2-OB4

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Mol	Chain	Res	Type	Atoms
72	Qh	102	CDL	CA2-OA2-PA1-OA4
72	Qh	102	CDL	CA3-OA5-PA1-OA4
72	Qh	102	CDL	CB2-OB2-PB2-OB3
72	Qh	102	CDL	CB2-OB2-PB2-OB4
72	Qh	102	CDL	CB3-OB5-PB2-OB3
73	A9	401	NDP	C5D-O5D-PN-O2N
76	C1	601	3PE	C11-O13-P-O14
76	C1	608	3PE	C1-O11-P-O14
76	CB	202	3PE	C11-O13-P-O12
76	QE	303	3PE	C1-O11-P-O14
76	S7	302	3PE	C11-O13-P-O14
77	AL	205	PLX	C3-O4-P1-O2
77	AL	205	PLX	C3-O4-P1-O3
77	AL	205	PLX	C2-O1-P1-O2
77	C2	301	PLX	C2-O1-P1-O2
77	C2	301	PLX	C2-O1-P1-O3
77	CB	201	PLX	C3-O4-P1-O3
78	Qc	404	6F6	C11-O13-P-O14
82	C1	609	PEE	C1-O3P-P-O2P
82	C1	609	PEE	C4-O4P-P-O1P
82	N1	401	PEE	C1-O3P-P-O2P
82	N3	201	PEE	C1-O3P-P-O2P
82	N5	701	PEE	C4-O4P-P-O1P
82	QB	502	PEE	C4-O4P-P-O1P
82	QB	503	PEE	C4-O4P-P-O1P
82	QC	401	PEE	C4-O4P-P-O2P
82	Qh	101	PEE	C4-O4P-P-O1P
82	S2	501	PEE	C1-O3P-P-O1P
82	S2	501	PEE	C4-O4P-P-O2P
82	S2	501	PEE	C4-O4P-P-O1P
82	S8	303	PEE	C1-O3P-P-O2P
72	6A	102	CDL	CB5-C51-C52-C53
72	6A	102	CDL	OA5-CA3-CA4-CA6
72	AL	203	CDL	OB5-CB3-CB4-CB6
77	AM	201	PLX	O4-C3-C4-C5
82	Qh	101	PEE	O3P-C1-C2-C3
77	CB	201	PLX	C26-C27-C28-C29
77	QI	301	PLX	C30-C31-C32-C33
78	B5	203	6F6	C22-C23-C24-C25
82	S8	303	PEE	C17-C18-C19-C20
82	Qc	401	PEE	C14-C15-C16-C17
76	AL	202	3PE	C12-C11-O13-P

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Mol	Chain	Res	Type	Atoms
77	AL	205	PLX	C1-C2-O1-P1
77	B5	201	PLX	C1-C2-O1-P1
77	CB	201	PLX	C1-C2-O1-P1
78	Qc	404	6F6	C12-C11-O13-P
82	N3	201	PEE	C5-C4-O4P-P
71	6A	101	PC1	C21-C22-C23-C24
72	QC	408	CDL	CA7-C31-C32-C33
77	C2	301	PLX	C7-C8-C9-C10
72	N5	703	CDL	OA5-CA3-CA4-OA6
72	Qh	102	CDL	CA7-C31-C32-C33
77	N4	501	PLX	O4-C3-C4-O6
78	QJ	101	6F6	O11-C1-C2-O21
82	N1	401	PEE	O3P-C1-C2-O2
82	QB	502	PEE	O3P-C1-C2-O2
82	Qc	401	PEE	O3P-C1-C2-O2
72	AL	201	CDL	C58-C59-C60-C61
82	S2	501	PEE	C38-C39-C40-C41
72	QC	406	CDL	C36-C37-C38-C39
72	N5	702	CDL	C72-C73-C74-C75
74	AB	201	ZMP	C1-C22-C23-C24
71	Qj	101	PC1	C11-C12-N-C13
72	QC	406	CDL	C72-C71-CB7-OB8
72	Qh	102	CDL	C52-C51-CB5-OB6
71	6A	101	PC1	O13-C11-C12-N
71	C3	302	PC1	O13-C11-C12-N
71	QC	405	PC1	O13-C11-C12-N
72	Qh	102	CDL	CA3-CA4-CA6-OA8
74	AC	201	ZMP	C2-C1-C22-C23
77	AL	205	PLX	N1-C1-C2-O1
77	AM	201	PLX	C3-C4-C5-O8
77	AM	203	PLX	C3-C4-C5-O8
77	B5	201	PLX	N1-C1-C2-O1
77	N4	501	PLX	N1-C1-C2-O1
77	QE	301	PLX	N1-C1-C2-O1
78	Qc	404	6F6	O13-C11-C12-N
82	QC	401	PEE	C12-C13-C14-C15
72	Qd	401	CDL	OA6-CA4-CA6-OA8
72	Qh	102	CDL	OB6-CB4-CB6-OB8
76	C1	608	3PE	O21-C2-C3-O31
77	N4	501	PLX	O6-C4-C5-O8
82	QE	302	PEE	O2-C2-C3-O3
82	Qc	401	PEE	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
77	AM	203	PLX	C26-C27-C28-C29
72	B5	202	CDL	C59-C60-C61-C62
82	QC	401	PEE	C20-C21-C22-C23
82	Qd	403	PEE	C14-C15-C16-C17
82	Qh	101	PEE	C12-C13-C14-C15
72	AL	203	CDL	CA4-CA3-OA5-PA1
74	AB	201	ZMP	C2-C3-C4-C5
82	Qh	103	PEE	C24-C25-C26-C27
77	AM	201	PLX	O8-C24-C25-C26
72	6A	102	CDL	C16-C17-C18-C19
72	CB	203	CDL	C53-C54-C55-C56
74	AC	201	ZMP	O3-C16-C17-O4
77	N4	501	PLX	O9-C24-C25-C26
71	N5	704	PC1	C3A-C3B-C3C-C3D
82	QC	404	PEE	C14-C15-C16-C17
71	AL	206	PC1	C11-C12-N-C15
71	N5	704	PC1	C33-C34-C35-C36
82	N3	201	PEE	C12-C13-C14-C15
72	AL	203	CDL	C13-C14-C15-C16
74	AC	201	ZMP	C22-C1-C2-C3
72	CB	203	CDL	C74-C75-C76-C77
74	AB	201	ZMP	C19-C18-C21-O5
82	Qc	401	PEE	C20-C21-C22-C23
82	QC	401	PEE	C34-C35-C36-C37
71	C1	607	PC1	C29-C2A-C2B-C2C
71	C3	302	PC1	O31-C31-C32-C33
71	Qj	101	PC1	O11-C1-C2-C3
72	A8	301	CDL	OB5-CB3-CB4-CB6
82	C1	609	PEE	O3P-C1-C2-C3
79	C1	602	HEA	C11-C12-C13-C14
71	QC	405	PC1	C32-C33-C34-C35
72	CB	203	CDL	C22-C23-C24-C25
82	Qh	103	PEE	C16-C17-C18-C19
72	AL	204	CDL	CB4-CB3-OB5-PB2
71	Qj	101	PC1	C22-C23-C24-C25
72	Qh	102	CDL	OB5-CB3-CB4-OB6
77	B5	201	PLX	O4-C3-C4-O6
82	S2	501	PEE	C17-C18-C19-C20
72	AL	201	CDL	C34-C35-C36-C37
77	AL	205	PLX	C28-C29-C30-C31
82	Qh	101	PEE	O2-C10-C11-C12
72	AL	201	CDL	C55-C56-C57-C58

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Mol	Chain	Res	Type	Atoms
82	QB	503	PEE	C34-C35-C36-C37
77	B5	201	PLX	C11-C10-C9-C8
82	C1	609	PEE	O2-C10-C11-C12
72	AL	203	CDL	C40-C41-C42-C43
71	Qb	502	PC1	O21-C2-C3-O31
72	N2	401	CDL	OA6-CA4-CA6-OA8
72	N5	703	CDL	OB6-CB4-CB6-OB8
71	6A	101	PC1	C1-O11-P-O13
71	7B	101	PC1	C11-O13-P-O11
71	C1	607	PC1	C11-O13-P-O11
71	C3	302	PC1	C1-O11-P-O13
71	QC	405	PC1	C11-O13-P-O11
72	6A	102	CDL	CB3-OB5-PB2-OB2
72	A8	301	CDL	CB3-OB5-PB2-OB2
72	AM	202	CDL	CA2-OA2-PA1-OA5
72	AM	202	CDL	CB2-OB2-PB2-OB5
72	Qd	401	CDL	CA3-OA5-PA1-OA2
76	CA	101	3PE	C11-O13-P-O11
77	AM	201	PLX	C2-O1-P1-O4
77	C2	301	PLX	C3-O4-P1-O1
82	QC	401	PEE	C1-O3P-P-O4P
82	Qc	401	PEE	C1-O3P-P-O4P
77	QI	301	PLX	C29-C30-C31-C32
72	N5	703	CDL	CB3-CB4-CB6-OB8
77	QI	301	PLX	C3-C4-C5-O8
77	AM	203	PLX	C2-C1-N1-C1A
72	Qh	102	CDL	CB7-C71-C72-C73
77	AM	201	PLX	C4-C3-O4-P1
87	V1	502	FMN	C4'-C5'-O5'-P
77	AL	205	PLX	C27-C28-C29-C30
77	QE	301	PLX	C25-C26-C27-C28
78	B5	203	6F6	C25-C26-C27-C28
72	B5	202	CDL	C37-C38-C39-C40
82	C1	609	PEE	C14-C15-C16-C17
82	S8	303	PEE	C15-C16-C17-C18
77	CB	201	PLX	C11-C10-C9-C8
79	C1	602	HEA	CAD-CBD-CGD-O2D
72	AL	204	CDL	C13-C14-C15-C16
77	QI	301	PLX	C12-C13-C14-C15
71	6A	101	PC1	O31-C31-C32-C33
72	B5	202	CDL	C80-C81-C82-C83
72	QC	406	CDL	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
78	QJ	101	6F6	O11-C1-C2-C3
73	A9	401	NDP	O4D-C1D-N1N-C6N
72	QB	501	CDL	C53-C54-C55-C56
72	A8	301	CDL	OB5-CB3-CB4-OB6
72	CB	203	CDL	C19-C20-C21-C22
76	S7	302	3PE	O31-C31-C32-C33
74	AC	201	ZMP	C5-C6-C7-C8
82	QE	302	PEE	C34-C35-C36-C37
74	AB	201	ZMP	O3-C16-C17-C18
83	QC	403	HEM	CAA-CBA-CGA-O1A
71	N5	704	PC1	C2E-C2F-C2G-C2H
83	QC	402	HEM	CAD-CBD-CGD-O1D
83	Qc	402	HEM	CAA-CBA-CGA-O2A
83	Qc	403	HEM	CAD-CBD-CGD-O1D
77	B5	201	PLX	O6-C6-C7-C8
77	N4	501	PLX	O8-C24-C25-C26
78	Qc	404	6F6	C2-C1-O11-P
71	7B	101	PC1	C2D-C2E-C2F-C2G
83	QC	402	HEM	CAA-CBA-CGA-O1A
72	6A	102	CDL	C21-C22-C23-C24
72	AL	204	CDL	C72-C73-C74-C75
72	CB	203	CDL	C36-C37-C38-C39
82	QC	401	PEE	C35-C36-C37-C38
72	QC	406	CDL	C35-C36-C37-C38
72	A8	301	CDL	C74-C75-C76-C77
78	QJ	101	6F6	C26-C27-C28-C29
83	QC	403	HEM	CAA-CBA-CGA-O2A
82	S2	501	PEE	C21-C22-C23-C24
71	QC	407	PC1	C27-C28-C29-C2A
71	C3	301	PC1	C1-C2-C3-O31
72	N5	702	CDL	CA3-CA4-CA6-OA8
76	N4	502	3PE	C1-C2-C3-O31
82	Qd	403	PEE	C1-C2-C3-O3
83	Qc	402	HEM	CAA-CBA-CGA-O1A
72	CB	203	CDL	C84-C85-C86-C87
74	AB	201	ZMP	C20-C18-C21-O5
74	AC	201	ZMP	C20-C18-C21-O5
71	C3	301	PC1	C32-C33-C34-C35
77	AL	205	PLX	C15-C16-C17-C18
77	QE	301	PLX	C7-C8-C9-C10
82	Qd	403	PEE	C21-C22-C23-C24
71	C3	301	PC1	C27-C28-C29-C2A

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Mol	Chain	Res	Type	Atoms
72	QC	406	CDL	C17-C18-C19-C20
71	Qb	502	PC1	C3-C2-O21-C21
71	Qj	101	PC1	C3-C2-O21-C21
72	Qb	501	CDL	CA3-CA4-OA6-CA5
72	Qd	401	CDL	CA3-CA4-OA6-CA5
76	C1	608	3PE	C3-C2-O21-C21
71	AL	206	PC1	C11-C12-N-C13
83	Qc	403	HEM	CAA-CBA-CGA-O1A
78	QJ	101	6F6	C11-O13-P-O11
79	C1	603	HEA	CAD-CBD-CGD-O1D
82	QC	401	PEE	C40-C41-C42-C43
77	C2	301	PLX	C6-C7-C8-C9
72	AL	204	CDL	OA5-CA3-CA4-CA6
72	Qh	102	CDL	OA5-CA3-CA4-CA6
77	B5	201	PLX	O4-C3-C4-C5
77	CB	201	PLX	O4-C3-C4-C5
76	S7	302	3PE	C25-C26-C27-C28
83	Qc	403	HEM	CAD-CBD-CGD-O2D
72	QC	406	CDL	C13-C14-C15-C16
76	S7	302	3PE	C2A-C2B-C2C-C2D
72	AL	201	CDL	CB5-C51-C52-C53
83	QC	402	HEM	CAD-CBD-CGD-O2D
83	Qc	402	HEM	CAD-CBD-CGD-O1D
82	QC	401	PEE	C14-C15-C16-C17
74	AB	201	ZMP	C12-C11-S1-C10
72	N5	702	CDL	OA6-CA4-CA6-OA8
76	N4	502	3PE	O21-C2-C3-O31
77	QE	301	PLX	O6-C4-C5-O8
82	S2	501	PEE	O2-C2-C3-O3
76	C1	601	3PE	O21-C21-C22-C23
77	QI	301	PLX	C36-C37-C38-C39
83	Qc	402	HEM	CAD-CBD-CGD-O2D
82	S2	501	PEE	C37-C38-C39-C40
82	C1	609	PEE	C38-C39-C40-C41
72	AL	201	CDL	C35-C36-C37-C38
82	QB	503	PEE	C43-C44-C45-C46
83	QC	402	HEM	CAA-CBA-CGA-O2A
83	Qc	403	HEM	CAA-CBA-CGA-O2A
71	QH	102	PC1	O21-C21-C22-C23
72	N5	703	CDL	C12-C11-CA5-OA6
77	QE	301	PLX	C3-C4-C5-O8
82	Qh	103	PEE	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
84	QD	401	HEC	CAD-CBD-CGD-O2D
77	QI	301	PLX	C6-C7-C8-C9
71	Qb	502	PC1	C32-C33-C34-C35
78	Qc	404	6F6	O32-C31-C32-C33
82	C1	609	PEE	C20-C21-C22-C23
72	QC	406	CDL	C12-C13-C14-C15
77	C2	301	PLX	C15-C16-C17-C18
82	Qd	403	PEE	C33-C34-C35-C36
72	N5	702	CDL	C14-C15-C16-C17
72	AL	204	CDL	OA5-CA3-CA4-OA6
72	Qh	102	CDL	OA5-CA3-CA4-OA6
76	N4	502	3PE	O11-C1-C2-O21
77	QI	301	PLX	C15-C16-C17-C18
82	QC	401	PEE	C32-C33-C34-C35
79	C1	602	HEA	CAD-CBD-CGD-O1D
71	7B	101	PC1	C26-C27-C28-C29
82	QB	503	PEE	C14-C15-C16-C17
71	QC	405	PC1	O11-C1-C2-C3
72	QB	501	CDL	OA5-CA3-CA4-CA6
72	N5	703	CDL	C1-CB2-OB2-PB2
72	N5	702	CDL	C71-C72-C73-C74
71	C1	606	PC1	C33-C34-C35-C36
82	N3	201	PEE	C32-C33-C34-C35
79	C1	603	HEA	CAD-CBD-CGD-O2D
82	S8	303	PEE	C16-C17-C18-C19
74	AC	201	ZMP	N2-C16-C17-O4
78	QJ	101	6F6	C38-C39-C3A-C3B
74	AC	201	ZMP	C19-C18-C21-O5
71	C3	301	PC1	C38-C39-C3A-C3B
72	N5	703	CDL	C32-C31-CA7-OA9
77	CB	201	PLX	C31-C32-C33-C34
82	QE	302	PEE	C18-C19-C20-C21
71	C3	301	PC1	C3-C2-O21-C21
72	QB	501	CDL	CA6-CA4-OA6-CA5
72	QH	101	CDL	CA6-CA4-OA6-CA5
72	Qh	102	CDL	CB6-CB4-OB6-CB5
76	S7	302	3PE	C1-C2-O21-C21
82	QB	502	PEE	C30-C31-C32-C33
72	B5	202	CDL	C72-C73-C74-C75
82	QC	401	PEE	C41-C42-C43-C44
84	QD	401	HEC	CAD-CBD-CGD-O1D
72	A8	301	CDL	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
72	QB	501	CDL	C74-C75-C76-C77
71	C1	606	PC1	O21-C21-C22-C23
72	A8	301	CDL	C32-C31-CA7-OA8
72	A8	301	CDL	C72-C71-CB7-OB8
82	N3	201	PEE	O3-C30-C31-C32
72	N5	702	CDL	C12-C11-CA5-OA6
72	QH	101	CDL	C52-C51-CB5-OB6
72	6A	102	CDL	C13-C14-C15-C16
82	N1	401	PEE	C16-C17-C18-C19
82	QE	302	PEE	C15-C16-C17-C18
76	C1	608	3PE	C2-C1-O11-P
77	CB	201	PLX	C7-C6-O6-C4
71	6A	101	PC1	O11-C1-C2-O21
82	N1	401	PEE	C37-C38-C39-C40
72	6A	102	CDL	C52-C51-CB5-OB6
72	N2	401	CDL	C32-C31-CA7-OA8
77	AM	203	PLX	C2-C1-N1-C1B
77	QI	301	PLX	C32-C33-C34-C35
72	N5	703	CDL	C33-C34-C35-C36
72	CB	203	CDL	C12-C13-C14-C15
72	AM	202	CDL	C72-C71-CB7-OB8
78	QJ	101	6F6	O21-C21-C22-C23
71	C3	301	PC1	C28-C29-C2A-C2B
77	AM	203	PLX	C11-C12-C13-C14
71	AL	206	PC1	O21-C21-C22-C23
71	Qj	101	PC1	O21-C21-C22-C23
76	C1	608	3PE	C34-C35-C36-C37
71	QH	102	PC1	O11-C1-C2-C3
71	C3	302	PC1	O21-C21-C22-C23
72	AL	201	CDL	C52-C51-CB5-OB6
72	QC	406	CDL	C32-C31-CA7-OA8
72	QC	408	CDL	C72-C71-CB7-OB8
72	6A	102	CDL	C17-C18-C19-C20
72	CB	203	CDL	OB6-CB4-CB6-OB8
72	AL	204	CDL	CB7-C71-C72-C73
71	C3	301	PC1	O22-C21-C22-C23
82	N3	201	PEE	C36-C37-C38-C39
71	7B	101	PC1	O31-C31-C32-C33
71	QC	405	PC1	O31-C31-C32-C33
72	CB	203	CDL	C32-C31-CA7-OA8
77	N4	501	PLX	C16-C17-C18-C19
73	A9	401	NDP	C2B-O2B-P2B-O2X

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Mol	Chain	Res	Type	Atoms
77	AM	203	PLX	O7-C6-C7-C8
72	AL	204	CDL	C11-CA5-OA6-CA4
72	Qh	102	CDL	C12-C11-CA5-OA6
82	Qd	403	PEE	O3-C30-C31-C32
79	C1	603	HEA	C26-C15-C16-C17
72	AL	204	CDL	CA7-C31-C32-C33
72	QC	406	CDL	CB4-CB3-OB5-PB2
82	Qd	403	PEE	C16-C17-C18-C19
71	N5	704	PC1	O21-C21-C22-C23
76	QE	303	3PE	O31-C31-C32-C33
82	Qh	103	PEE	C11-C12-C13-C14
72	AL	203	CDL	C37-C38-C39-C40
73	A9	401	NDP	O4B-C4B-C5B-O5B
82	QC	401	PEE	O3-C30-C31-C32
71	QC	405	PC1	C39-C3A-C3B-C3C
72	A8	301	CDL	C72-C71-CB7-OB9
78	QJ	101	6F6	O22-C21-C22-C23
72	QC	408	CDL	C31-C32-C33-C34
72	AL	204	CDL	C36-C37-C38-C39
77	AM	203	PLX	C2-C1-N1-C1C
77	B5	201	PLX	C34-C35-C36-C37
72	6A	102	CDL	C15-C16-C17-C18
72	AL	203	CDL	C21-C22-C23-C24
76	CA	101	3PE	C39-C3A-C3B-C3C
72	N2	401	CDL	C32-C31-CA7-OA9
72	N5	702	CDL	C12-C11-CA5-OA7
77	C2	301	PLX	C9-C10-C11-C12
71	AL	206	PC1	O22-C21-C22-C23
71	C1	606	PC1	O22-C21-C22-C23
71	C3	302	PC1	O22-C21-C22-C23
72	Qh	102	CDL	C12-C11-CA5-OA7
72	N2	401	CDL	C72-C71-CB7-OB8
78	QJ	101	6F6	C27-C28-C29-C2A
71	QC	405	PC1	C33-C34-C35-C36
71	QC	407	PC1	O31-C31-C32-C33
71	7B	101	PC1	C2-C1-O11-P
72	AL	204	CDL	CA4-CA3-OA5-PA1
76	CA	101	3PE	C2-C1-O11-P
71	Qj	101	PC1	O22-C21-C22-C23
72	A8	301	CDL	C32-C31-CA7-OA9
82	QE	302	PEE	C31-C32-C33-C34
72	CB	203	CDL	C56-C57-C58-C59

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Mol	Chain	Res	Type	Atoms
77	AM	203	PLX	C25-C26-C27-C28
71	7B	101	PC1	C11-O13-P-O14
71	C1	607	PC1	C11-O13-P-O14
71	QC	405	PC1	C11-O13-P-O14
71	QC	407	PC1	C11-O13-P-O12
72	AM	202	CDL	CA2-OA2-PA1-OA3
72	N5	703	CDL	CA3-OA5-PA1-OA4
72	Qb	501	CDL	CB3-OB5-PB2-OB4
76	C1	601	3PE	C1-O11-P-O14
76	QE	303	3PE	C11-O13-P-O14
76	S7	302	3PE	C1-O11-P-O14
78	QJ	101	6F6	C11-O13-P-O12
82	Qd	403	PEE	C4-O4P-P-O1P
72	CB	203	CDL	C32-C31-CA7-OA9
82	QC	404	PEE	C12-C13-C14-C15
71	7B	101	PC1	O32-C31-C32-C33
72	AM	202	CDL	C72-C71-CB7-OB9
72	6A	102	CDL	C18-C19-C20-C21
76	S7	302	3PE	C26-C27-C28-C29
82	N3	201	PEE	C40-C41-C42-C43
76	N4	502	3PE	C31-C32-C33-C34
72	AL	201	CDL	C52-C51-CB5-OB7
72	AL	204	CDL	C33-C34-C35-C36
71	N6	201	PC1	O31-C31-C32-C33
72	B5	202	CDL	C12-C11-CA5-OA6
71	C3	301	PC1	C3D-C3E-C3F-C3G
72	N2	401	CDL	C72-C71-CB7-OB9
71	6A	101	PC1	C34-C35-C36-C37
71	6A	101	PC1	C12-C11-O13-P
71	AL	206	PC1	C12-C11-O13-P
71	C3	301	PC1	C1-C2-O21-C21
71	QC	407	PC1	C12-C11-O13-P
72	QB	501	CDL	CA3-CA4-OA6-CA5
72	QH	101	CDL	CA3-CA4-OA6-CA5
72	Qh	102	CDL	CB3-CB4-OB6-CB5
76	S7	302	3PE	C3-C2-O21-C21
77	AM	201	PLX	C1-C2-O1-P1
77	AM	201	PLX	C25-C24-O8-C5
77	AM	203	PLX	C1-C2-O1-P1
72	6A	102	CDL	C52-C51-CB5-OB7
72	QH	101	CDL	C52-C51-CB5-OB7
71	6A	101	PC1	C28-C29-C2A-C2B

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Mol	Chain	Res	Type	Atoms
72	N2	401	CDL	C12-C11-CA5-OA6
82	N3	201	PEE	O2-C10-C11-C12
82	N5	701	PEE	O2-C10-C11-C12
72	N2	401	CDL	C37-C38-C39-C40
79	C1	602	HEA	CAA-CBA-CGA-O1A
72	N2	401	CDL	C12-C11-CA5-OA7
72	QC	408	CDL	C72-C71-CB7-OB9
82	Qd	403	PEE	O5-C30-C31-C32
71	C1	606	PC1	C2E-C2F-C2G-C2H
71	QH	102	PC1	C38-C39-C3A-C3B
71	QC	407	PC1	C11-C12-N-C15
71	C1	606	PC1	O31-C31-C32-C33
76	CA	101	3PE	O31-C31-C32-C33
76	AL	202	3PE	C2A-C2B-C2C-C2D
71	N5	704	PC1	O22-C21-C22-C23
71	QH	102	PC1	C39-C3A-C3B-C3C
82	QC	404	PEE	O2-C10-C11-C12
71	QH	102	PC1	C22-C23-C24-C25
76	AL	202	3PE	C32-C33-C34-C35
71	6A	101	PC1	C2-C1-O11-P
72	AL	203	CDL	C52-C51-CB5-OB7
82	QC	401	PEE	O5-C30-C31-C32
72	N2	401	CDL	C74-C75-C76-C77
72	A8	301	CDL	C52-C51-CB5-OB6
72	AL	203	CDL	C52-C51-CB5-OB6
76	CB	202	3PE	O31-C31-C32-C33
82	Qc	401	PEE	C18-C19-C20-C21
82	S2	501	PEE	C31-C32-C33-C34
72	B5	202	CDL	C36-C37-C38-C39
72	N5	703	CDL	C12-C13-C14-C15
72	QB	501	CDL	C13-C14-C15-C16
82	N5	701	PEE	C14-C15-C16-C17
71	QC	407	PC1	O32-C31-C32-C33
84	Qd	402	HEC	CAA-CBA-CGA-O2A
72	B5	202	CDL	C77-C78-C79-C80
78	Qc	404	6F6	C24-C25-C26-C27
76	QE	303	3PE	C24-C25-C26-C27
71	QC	405	PC1	O32-C31-C32-C33
76	CA	101	3PE	C33-C34-C35-C36
71	Qb	502	PC1	O31-C31-C32-C33
74	AB	201	ZMP	C11-C12-N1-C13
72	N5	702	CDL	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
82	N5	701	PEE	O4-C10-C11-C12
72	N5	702	CDL	C17-C18-C19-C20
82	Qh	101	PEE	C32-C33-C34-C35
72	6A	102	CDL	C32-C31-CA7-OA8

There are no ring outliers.

78 monomers are involved in 256 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
72	Qh	102	CDL	3	0
82	QB	502	PEE	1	0
82	C1	609	PEE	3	0
77	C2	301	PLX	1	0
77	AM	201	PLX	5	0
71	C3	301	PC1	6	0
72	Qb	501	CDL	2	0
75	AK	401	ADP	4	0
72	QC	408	CDL	4	0
86	S8	302	SF4	2	0
73	A9	401	NDP	2	0
76	S7	302	3PE	4	0
72	6A	102	CDL	4	0
76	C1	601	3PE	2	0
71	QC	405	PC1	3	0
71	N5	704	PC1	1	0
76	N4	502	3PE	4	0
77	AM	203	PLX	5	0
72	N5	702	CDL	12	0
71	C1	607	PC1	1	0
76	QE	303	3PE	3	0
82	QB	503	PEE	1	0
84	Qd	402	HEC	3	0
76	CB	202	3PE	2	0
77	AL	205	PLX	5	0
72	AM	202	CDL	1	0
72	AL	203	CDL	1	0
77	CB	201	PLX	4	0
82	S2	501	PEE	3	0
71	AL	206	PC1	2	0
74	AC	201	ZMP	4	0
83	QC	403	HEM	6	0
82	Qd	403	PEE	4	0

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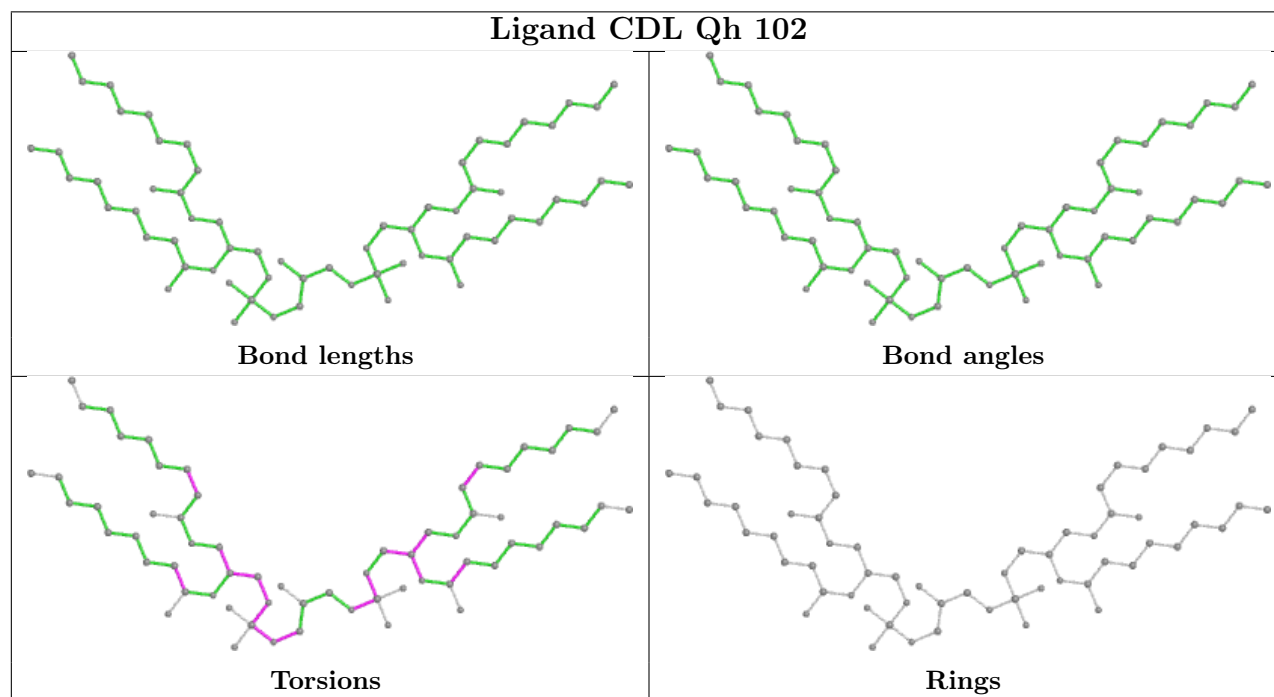
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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82	N3	201	PEE	2	0
83	QC	402	HEM	4	0
72	CB	203	CDL	11	0
71	QH	102	PC1	5	0
87	V1	502	FMN	1	0
85	Qe	301	FES	1	0
72	AL	204	CDL	4	0
82	N1	401	PEE	1	0
77	N4	501	PLX	1	0
82	Qh	103	PEE	3	0
78	Qc	404	6F6	1	0
77	B5	201	PLX	5	0
72	AL	201	CDL	2	0
82	QC	401	PEE	1	0
74	AB	201	ZMP	1	0
72	QC	406	CDL	6	0
77	QE	301	PLX	6	0
72	N2	401	CDL	2	0
77	QI	301	PLX	5	0
86	V1	501	SF4	1	0
84	QD	401	HEC	2	0
71	C1	606	PC1	3	0
71	6A	101	PC1	16	0
76	CA	101	3PE	2	0
82	QC	404	PEE	2	0
85	QE	304	FES	2	0
82	S8	303	PEE	1	0
76	AL	202	3PE	2	0
82	QE	302	PEE	5	0
71	QC	407	PC1	3	0
72	N5	703	CDL	3	0
71	Qb	502	PC1	1	0
72	A8	301	CDL	4	0
83	Qc	402	HEM	2	0
72	QH	101	CDL	3	0
79	C1	603	HEA	16	0
86	S7	301	SF4	1	0
82	N5	701	PEE	5	0
71	C3	302	PC1	2	0
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79	C1	602	HEA	7	0

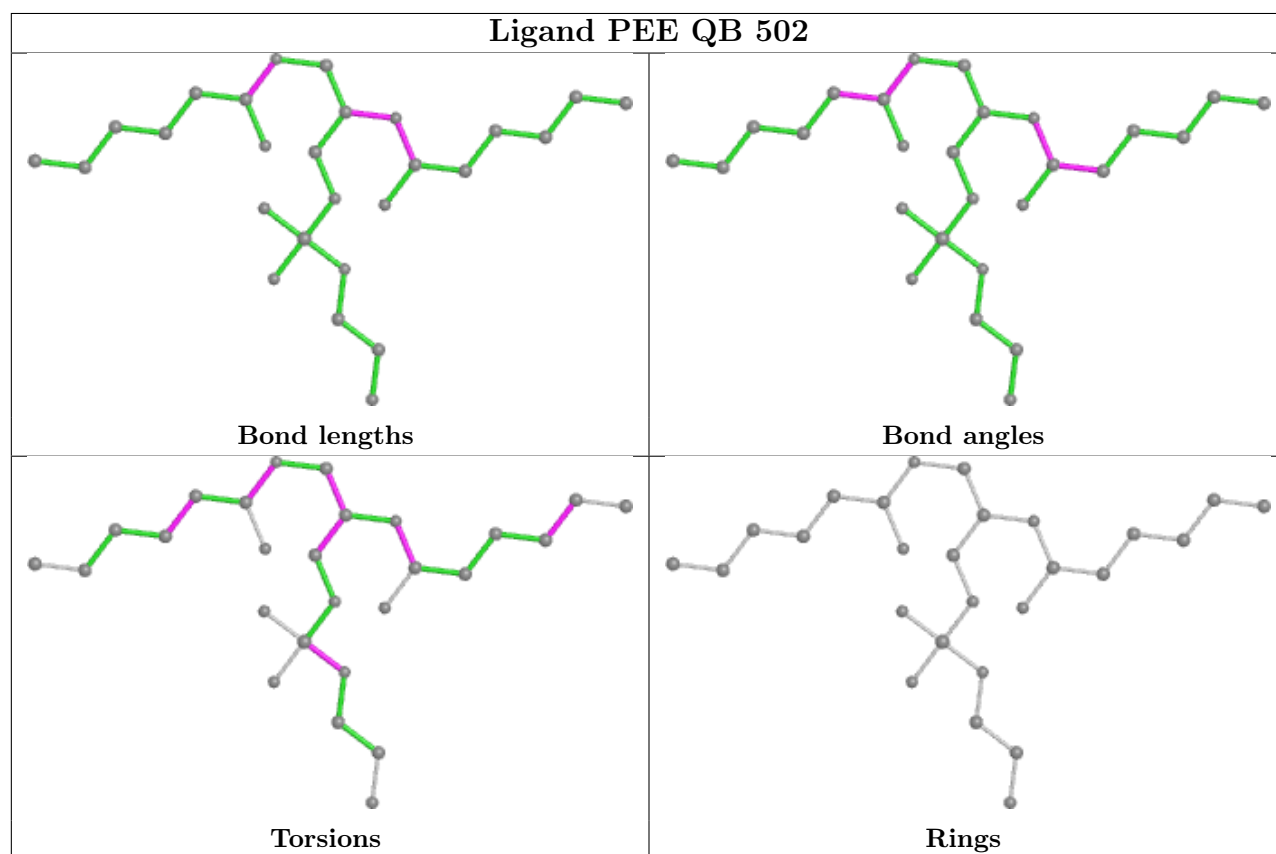
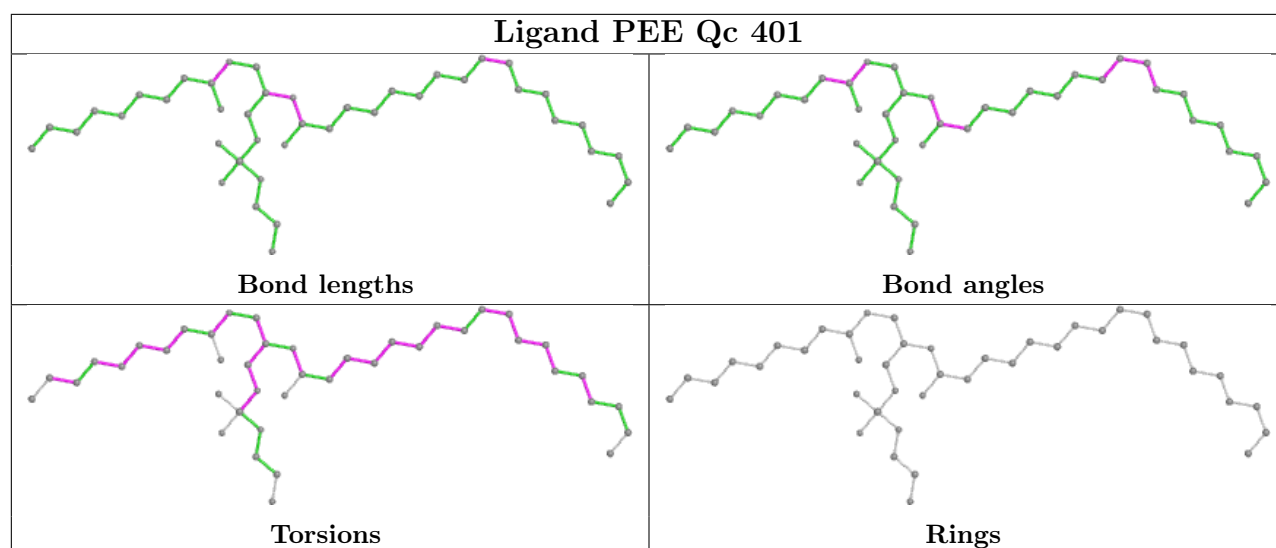
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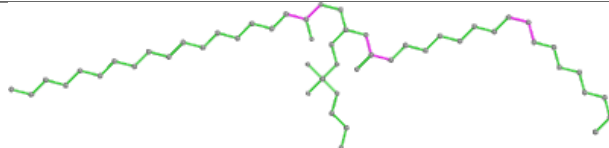
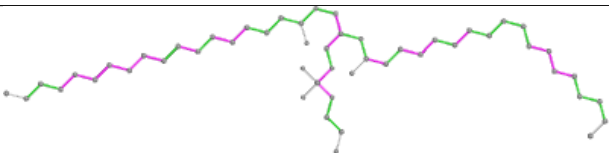
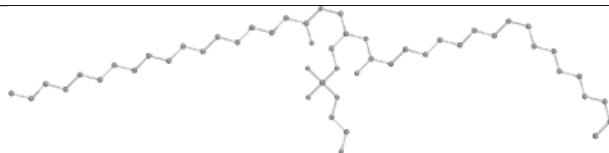
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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72	Qd	401	CDL	6	0
71	7B	101	PC1	4	0

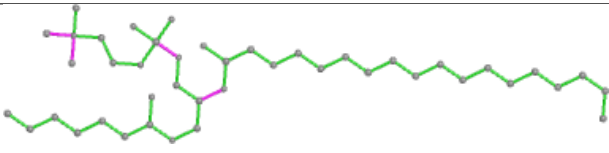
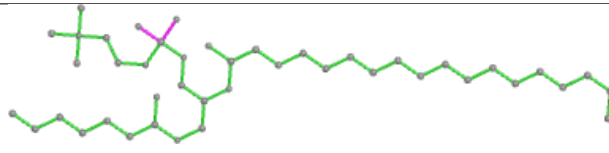
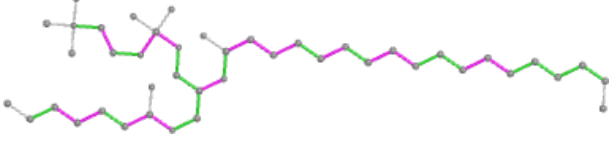
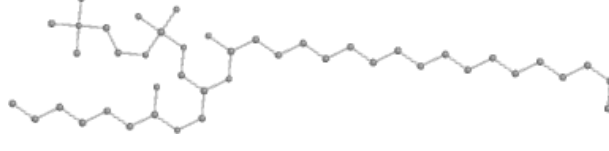
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

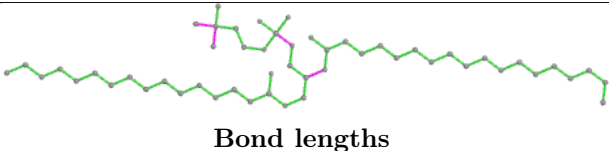
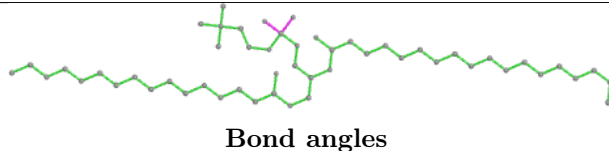
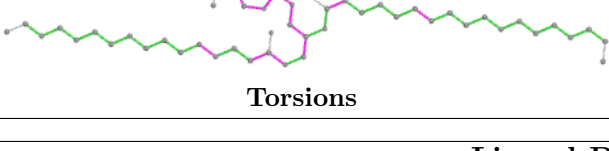



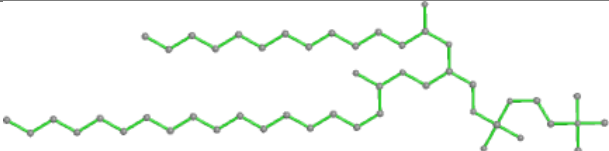
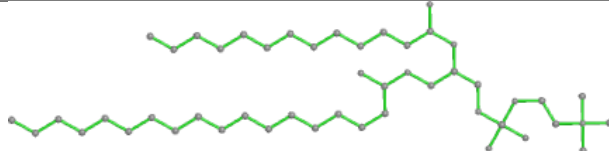
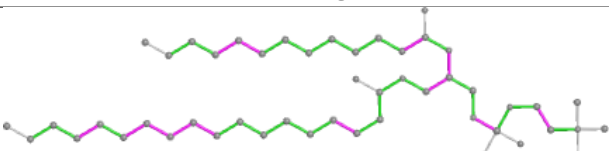
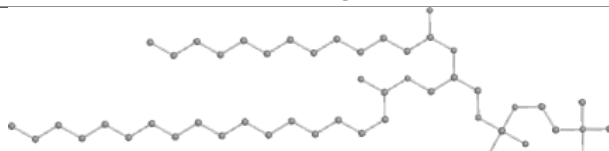


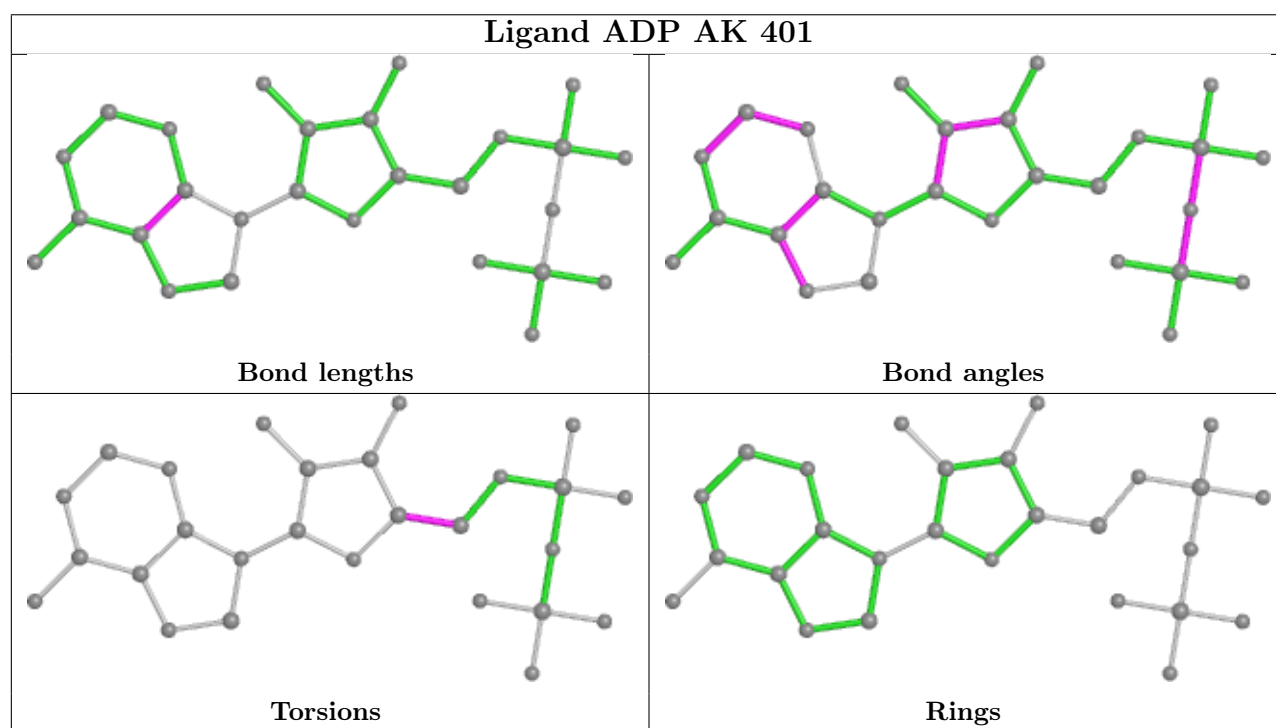
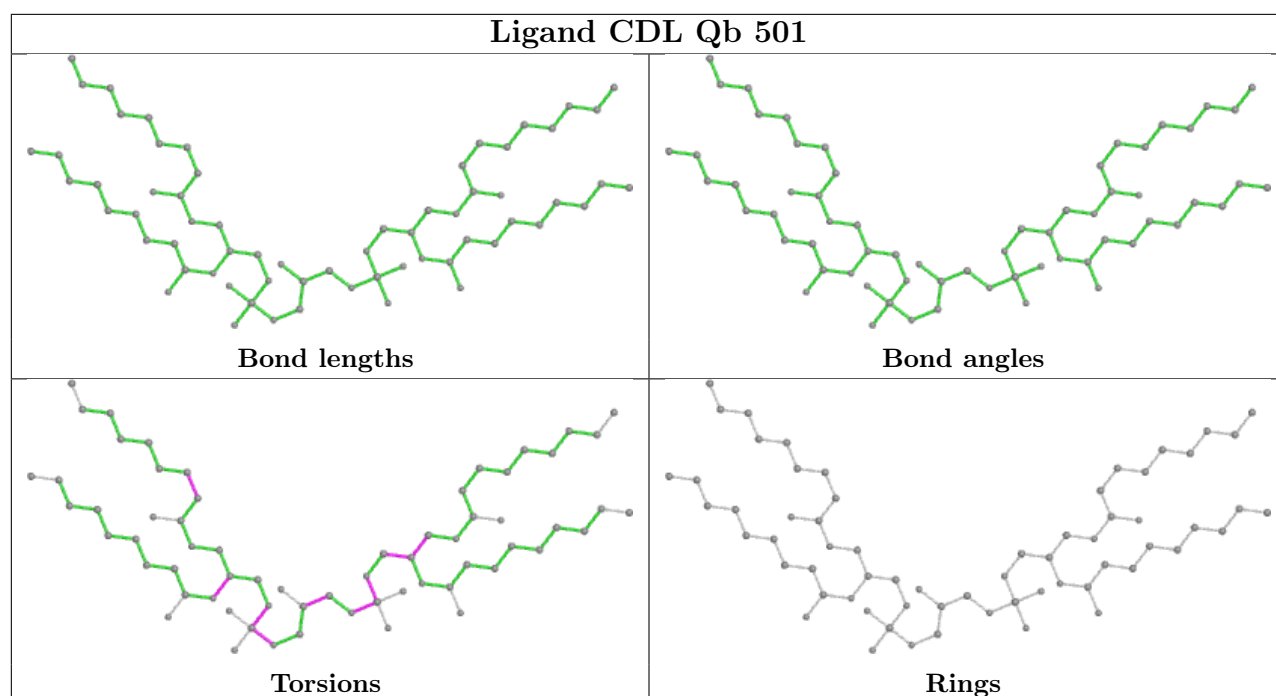


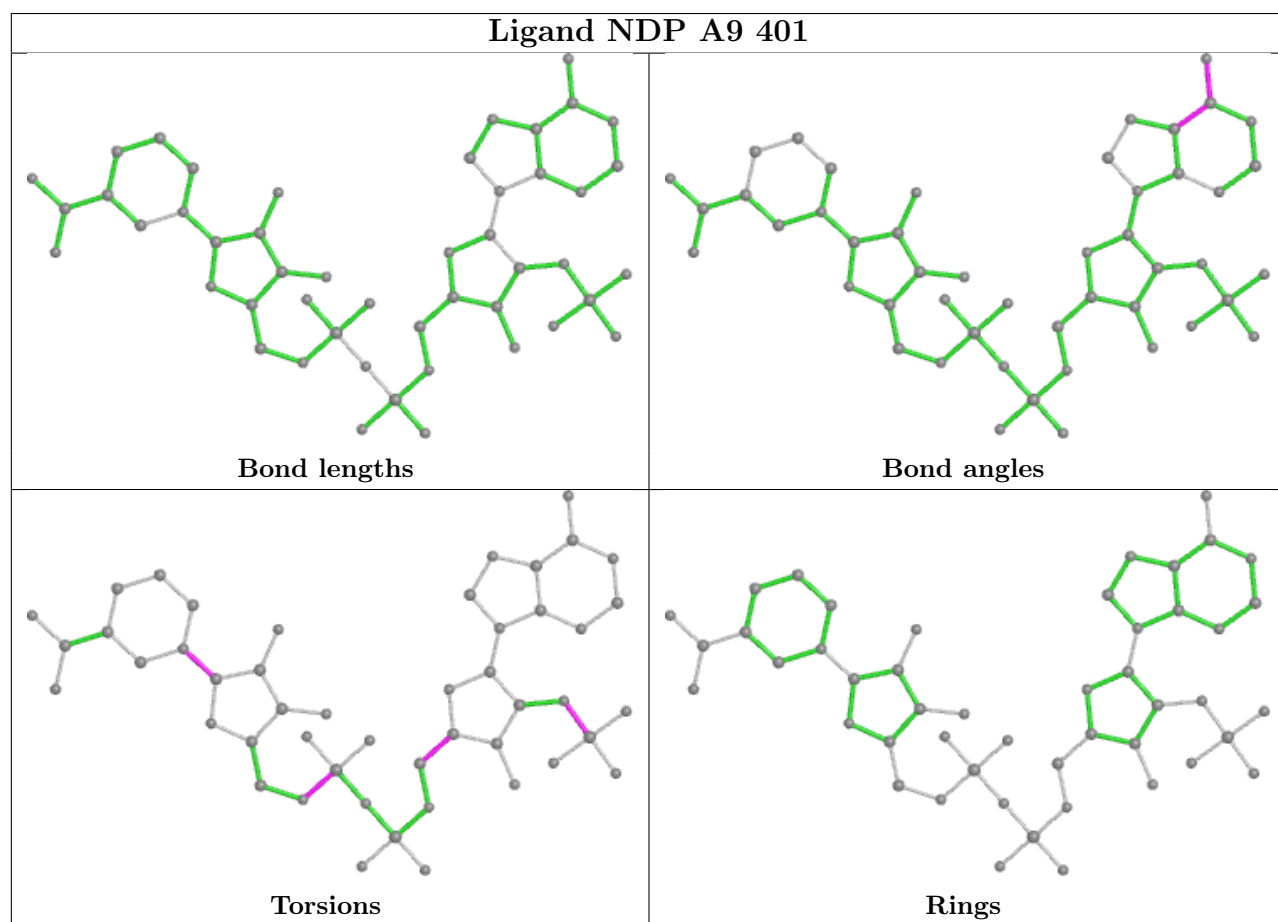
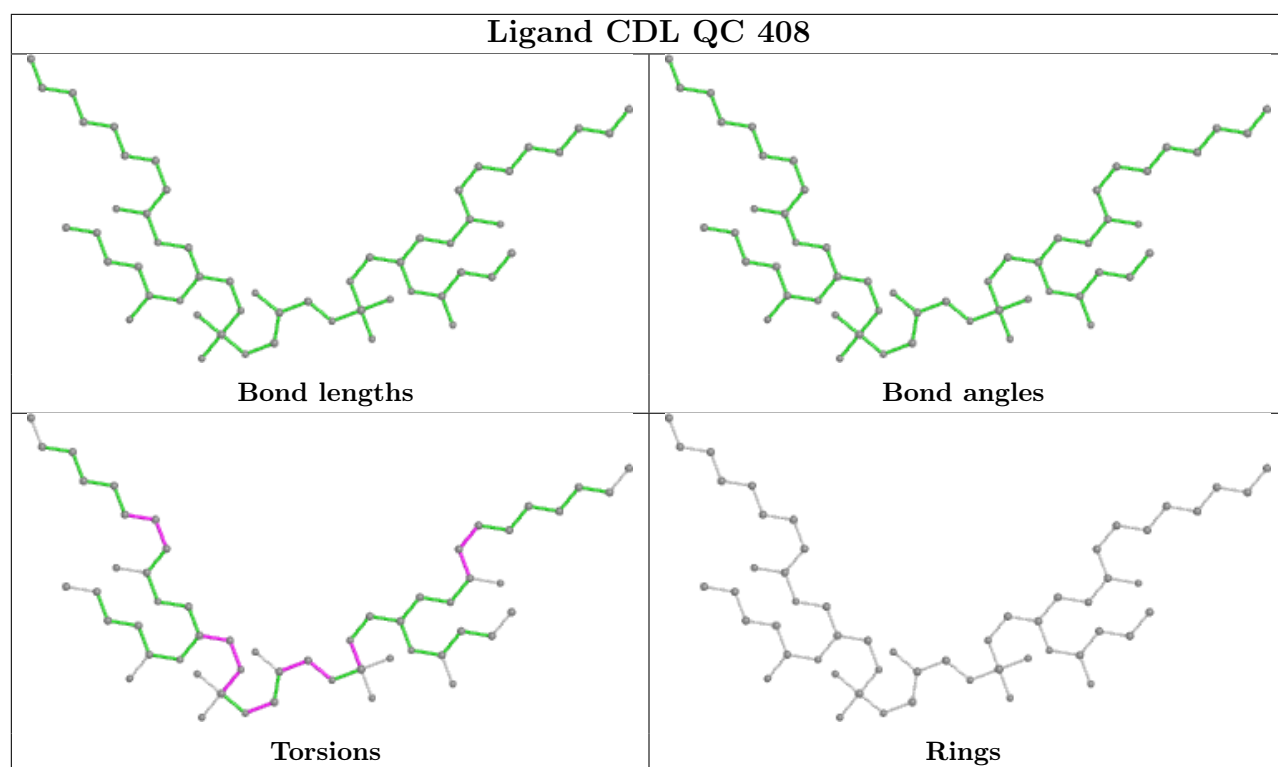
Ligand PEE C1 609	
	
Bond lengths	Bond angles
	
Torsions	Rings

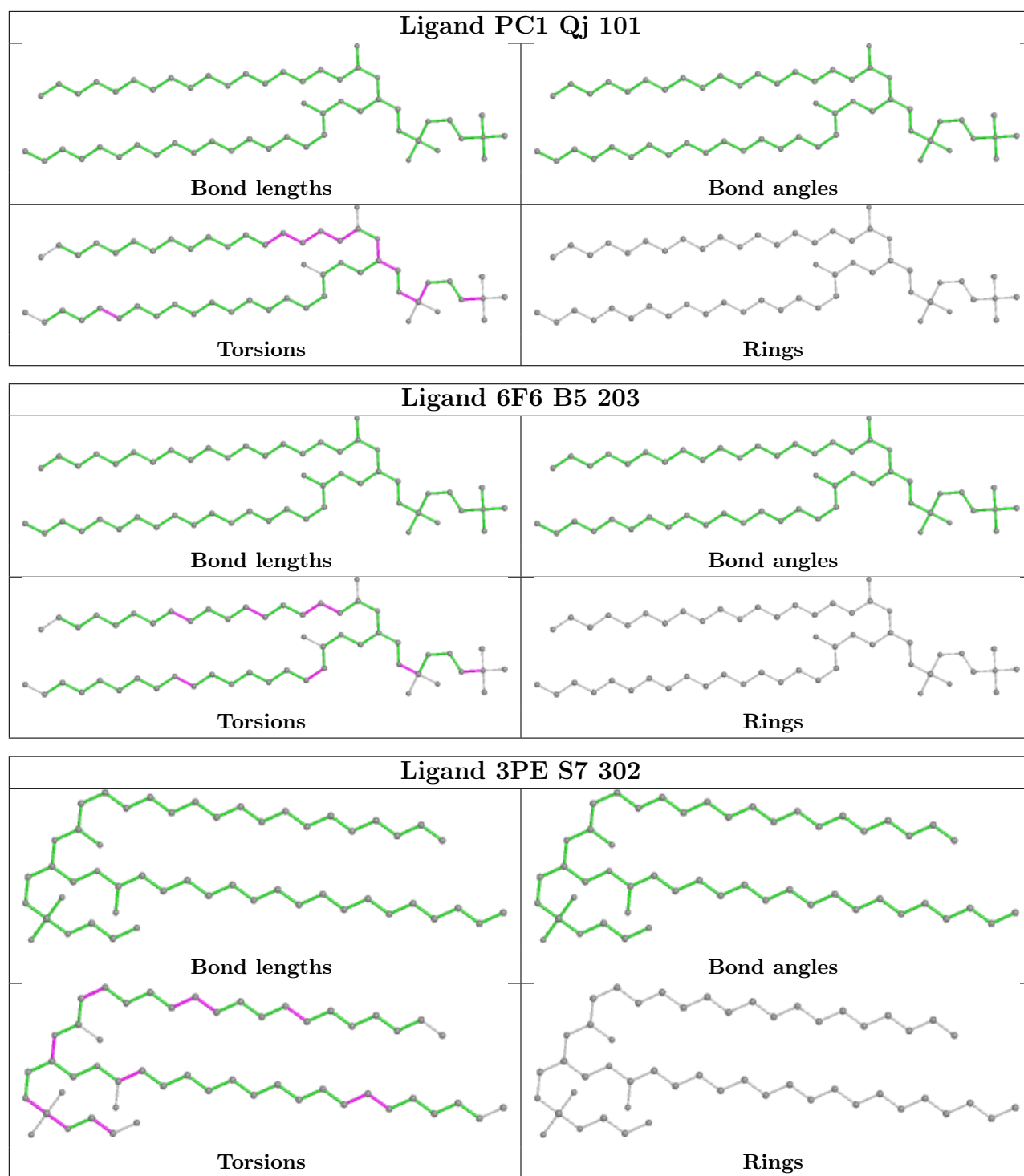
Ligand PLX C2 301	
	
Bond lengths	Bond angles
	
Torsions	Rings

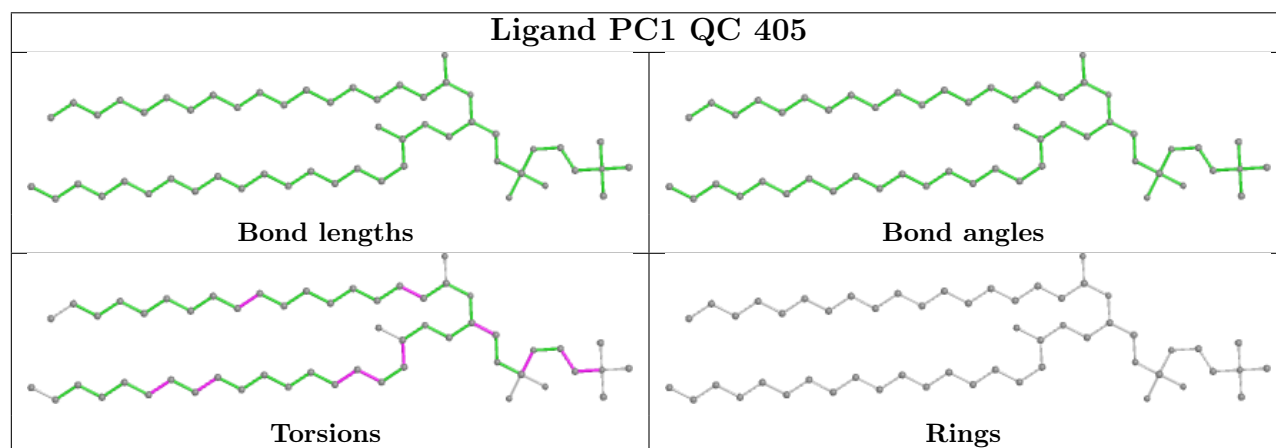
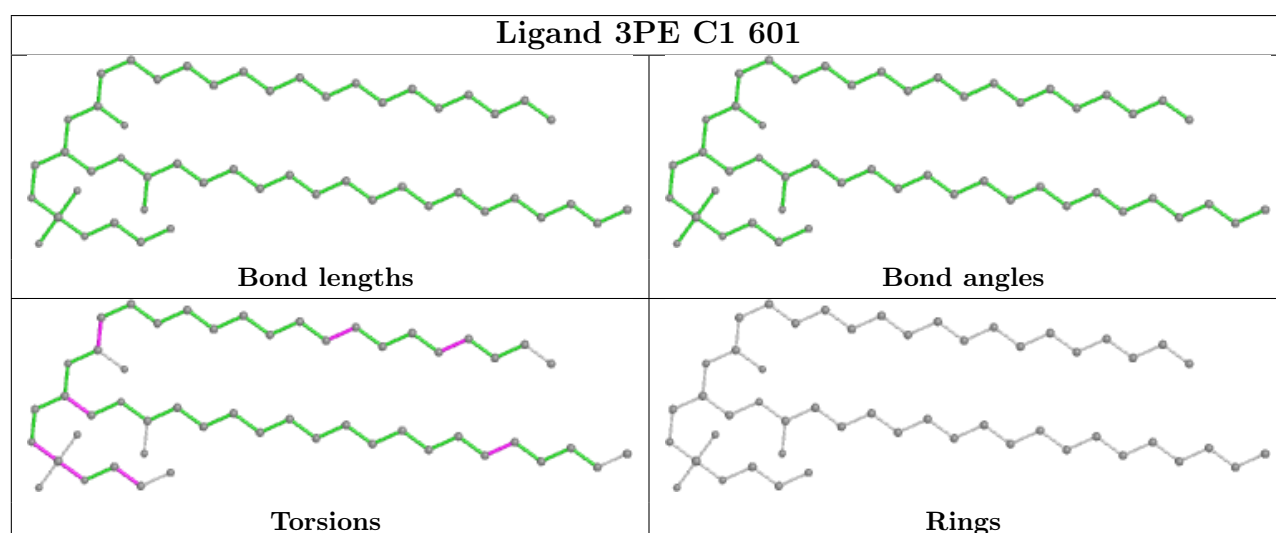
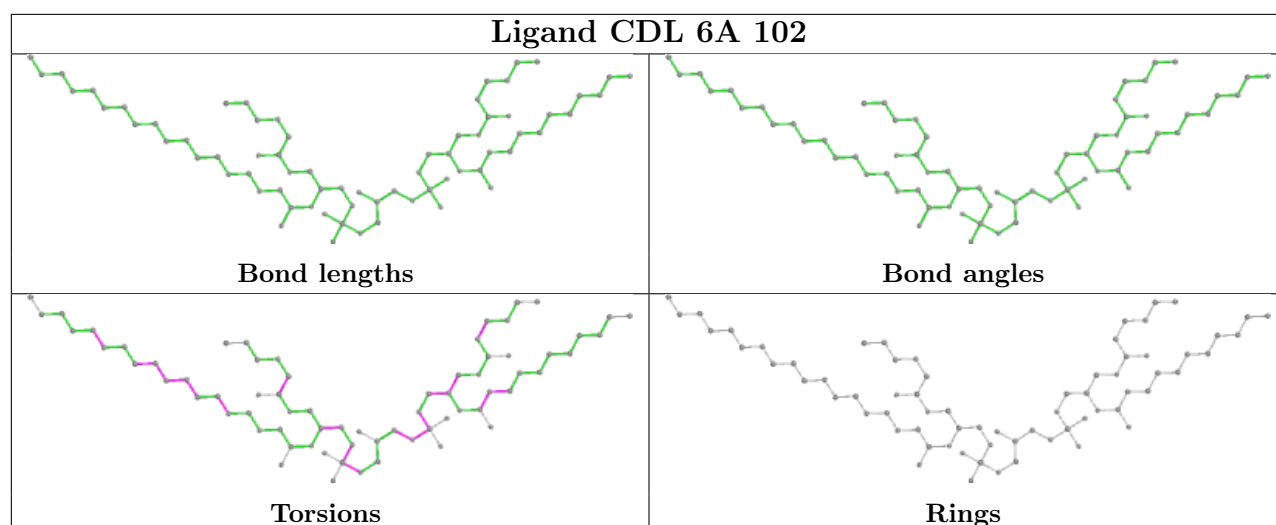
Ligand PLX AM 201	
	
Bond lengths	Bond angles
	
Torsions	Rings

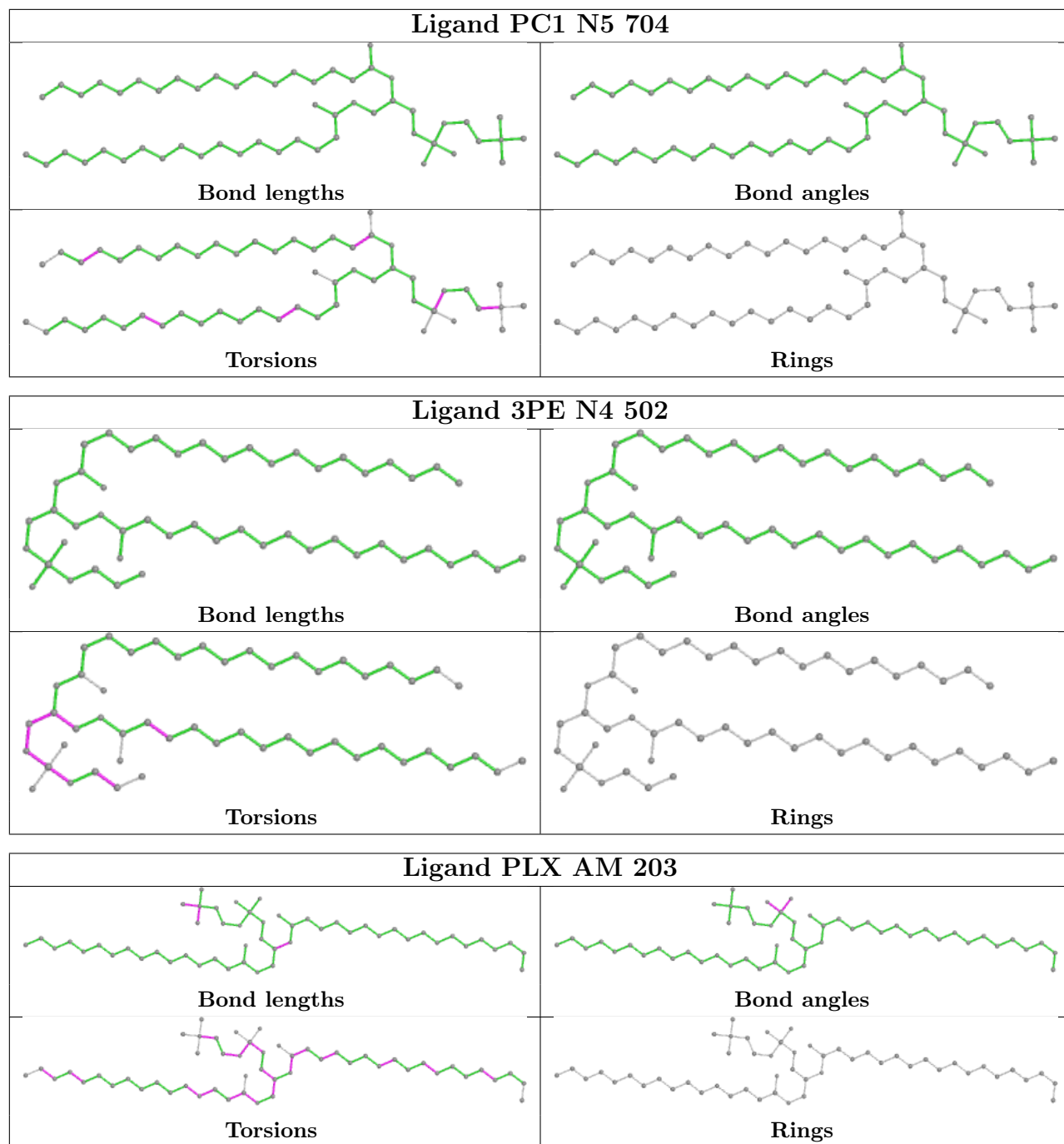
Ligand PC1 C3 301	
	
Bond lengths	Bond angles
	
Torsions	Rings

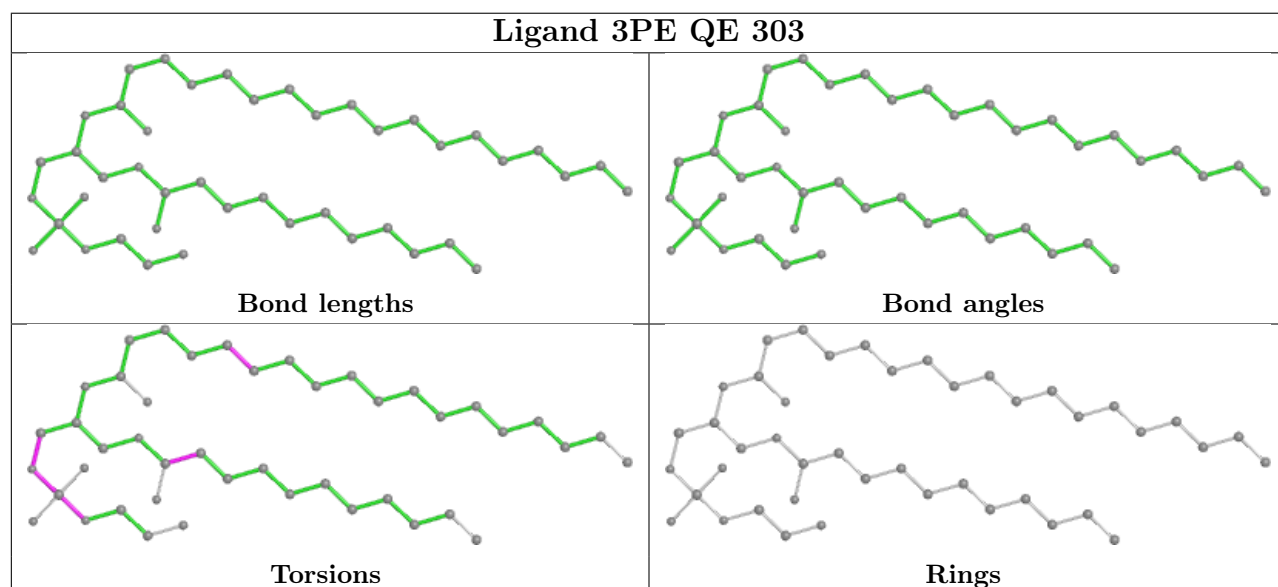
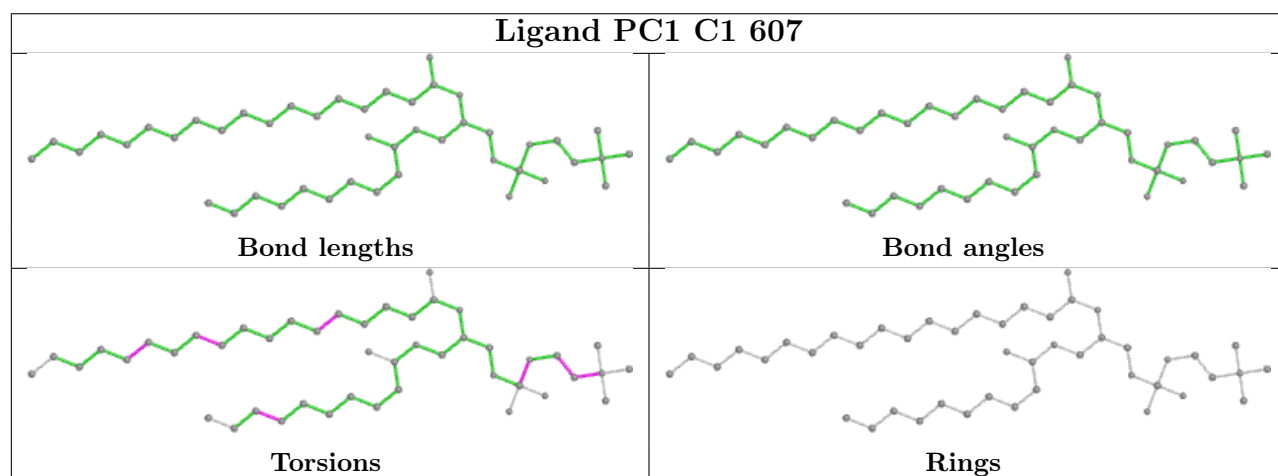
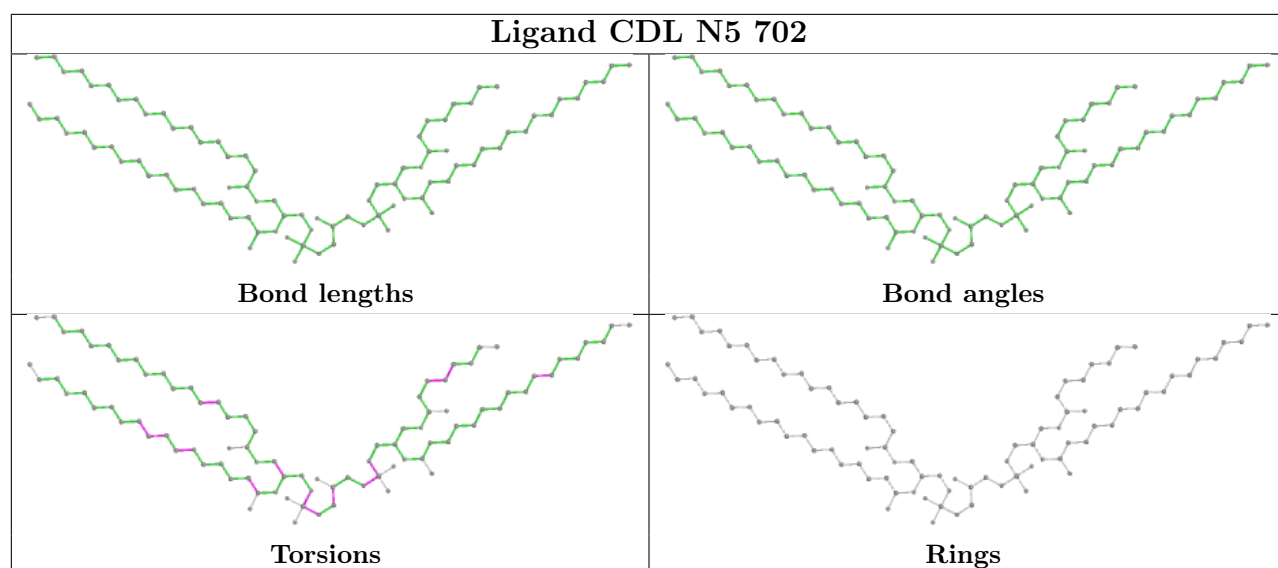


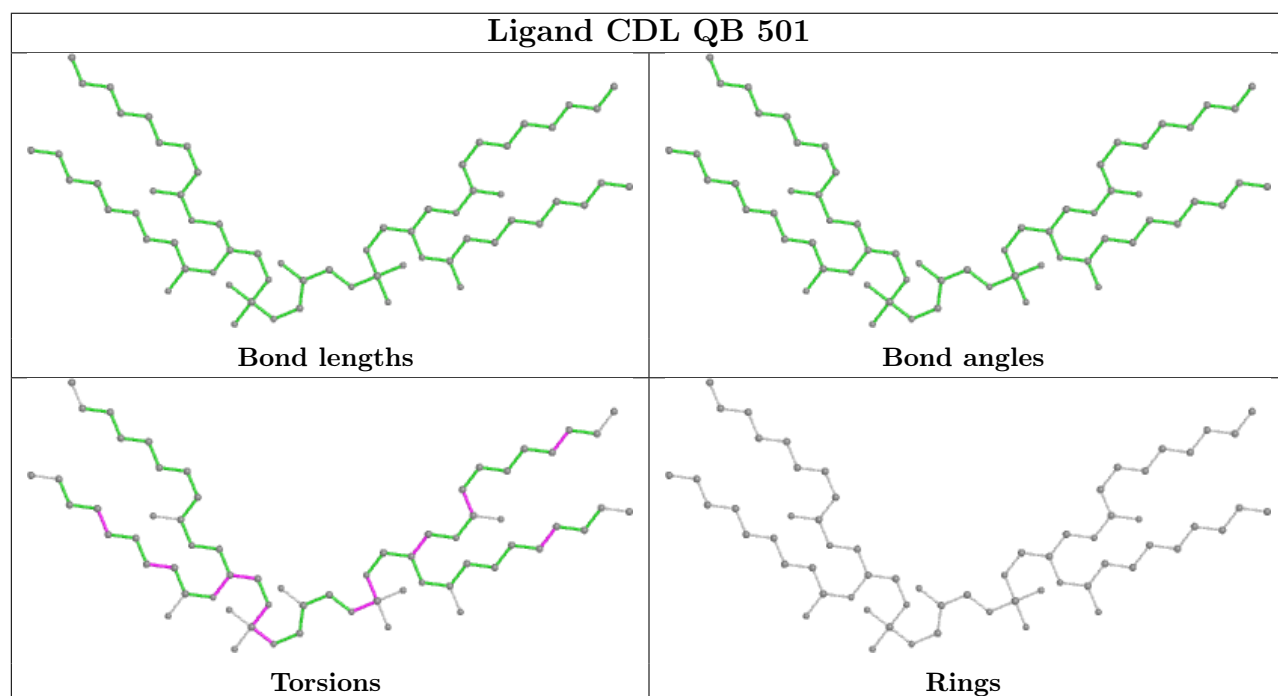
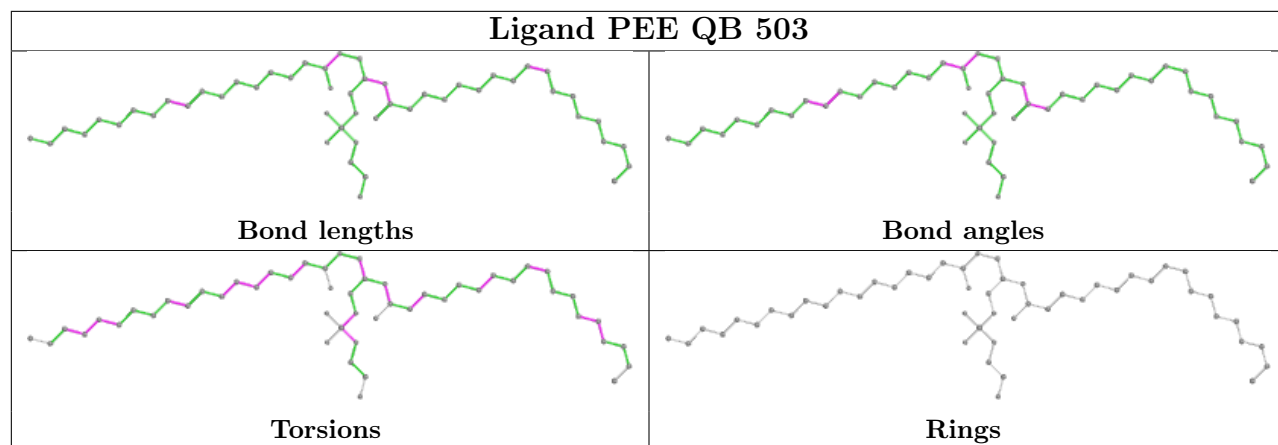




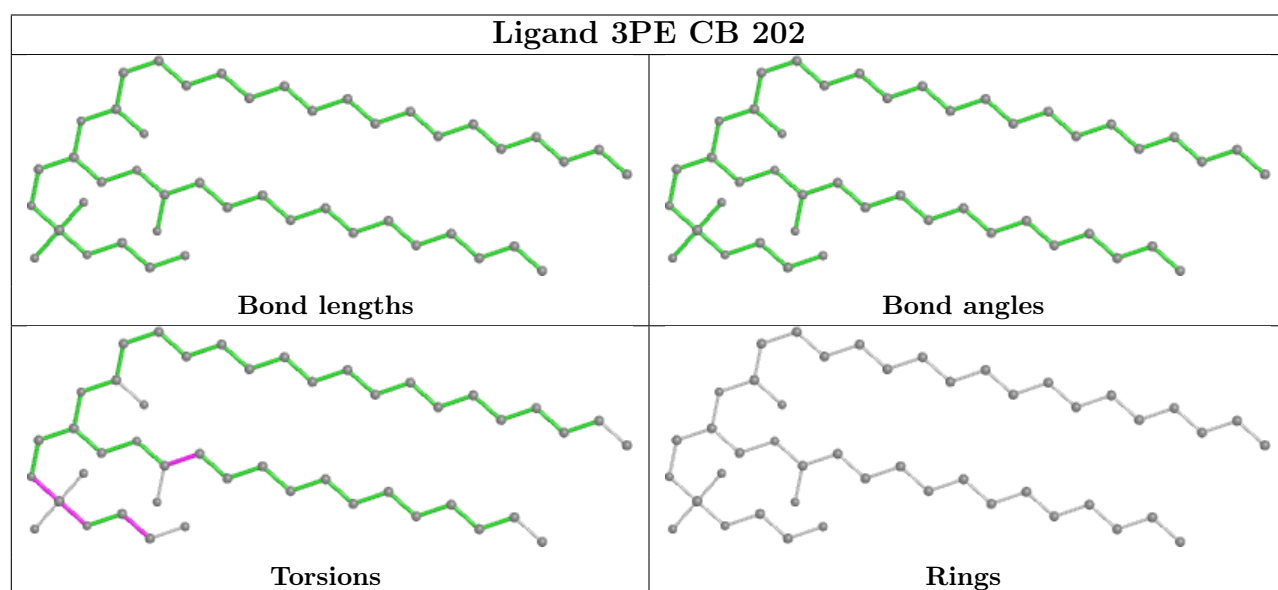
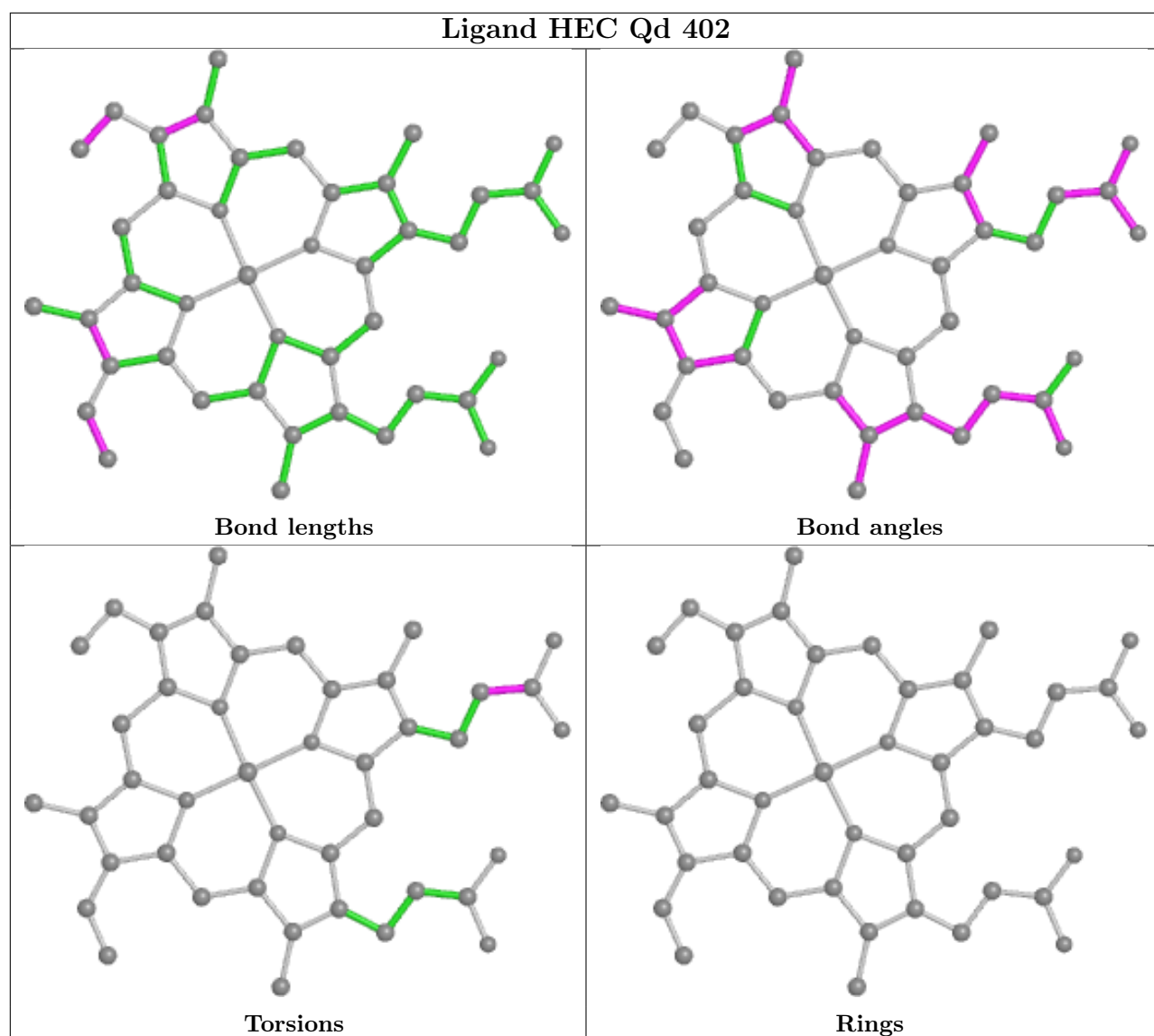


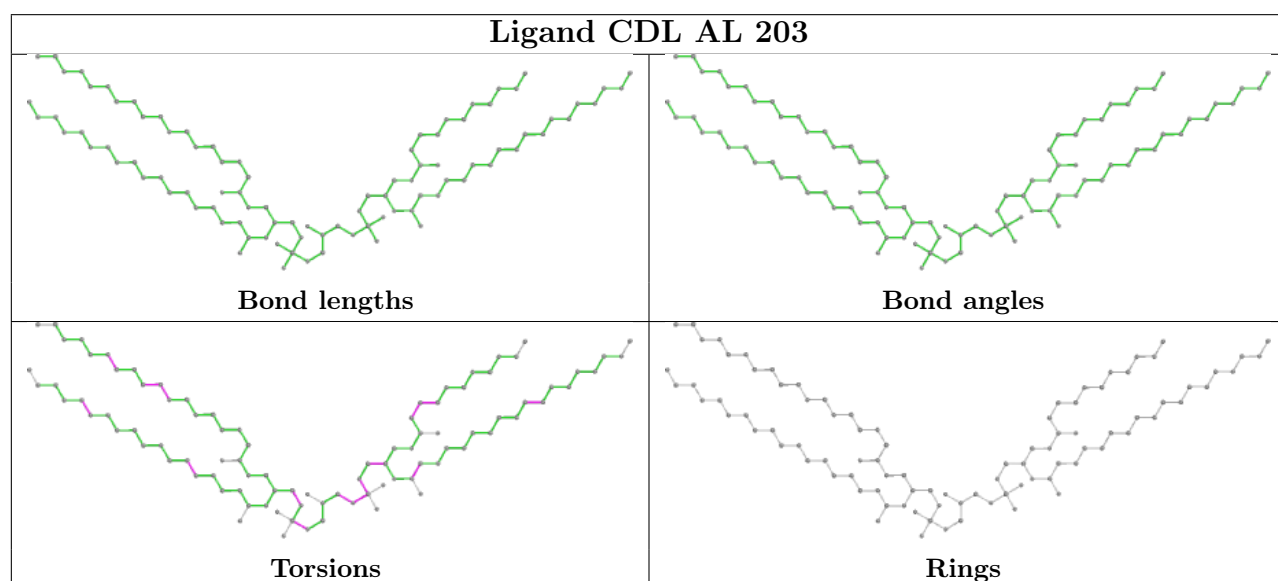
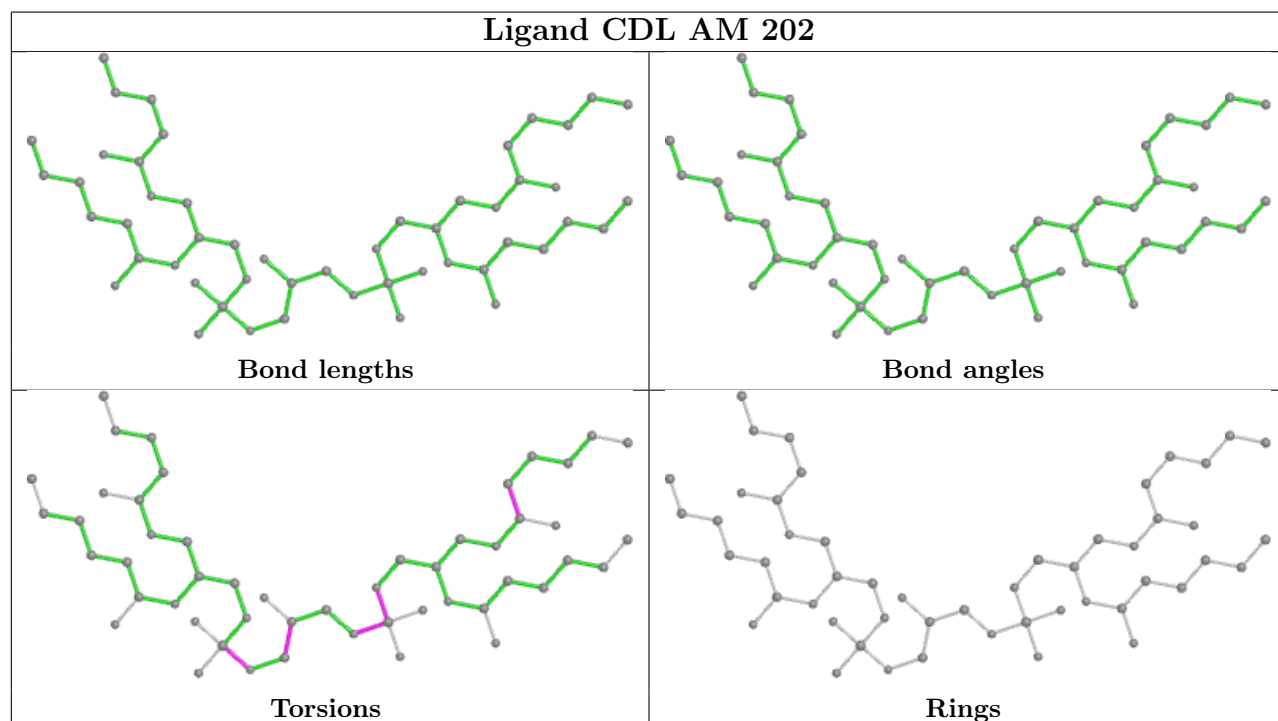
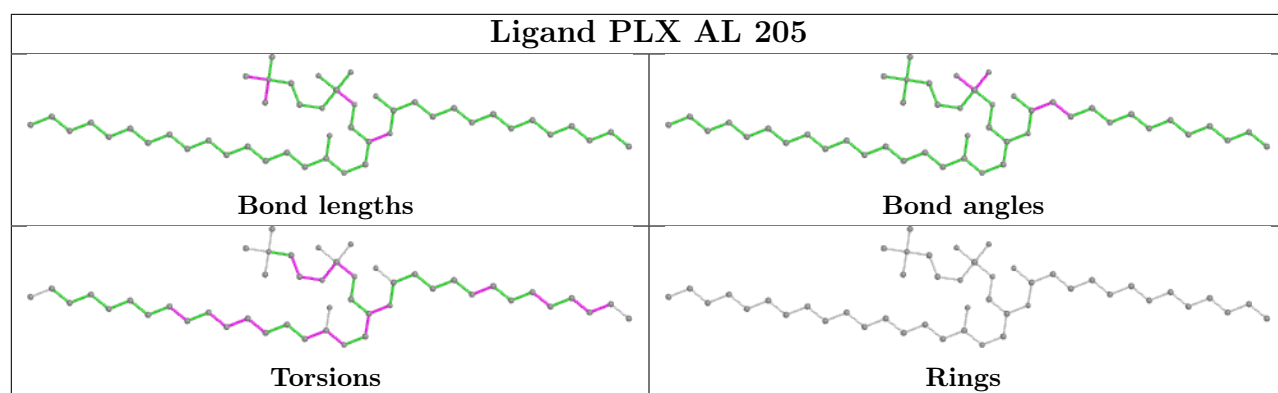


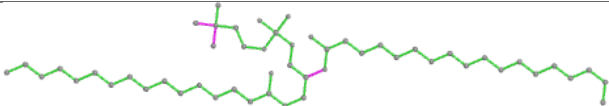
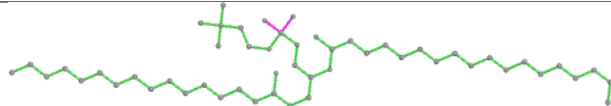
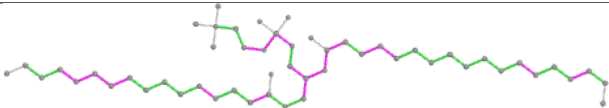
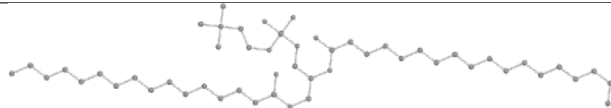
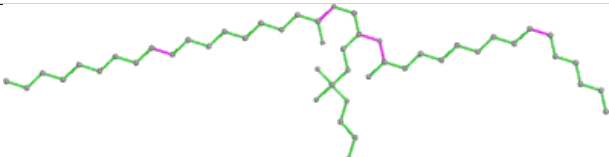
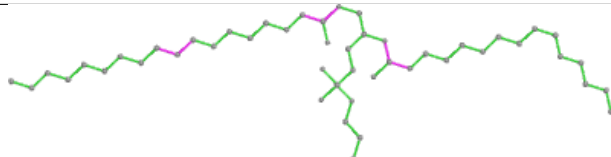
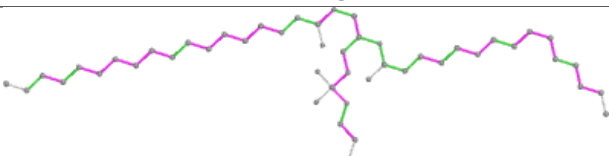
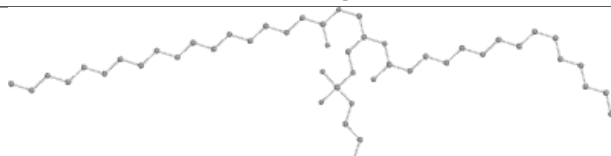
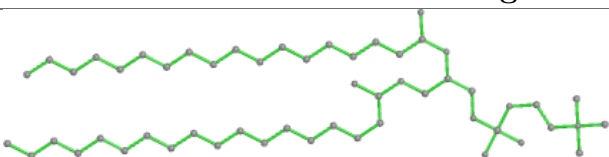
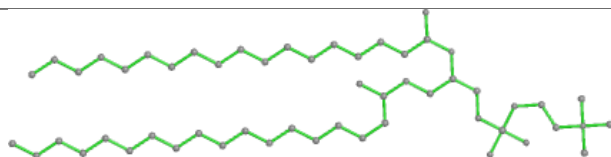
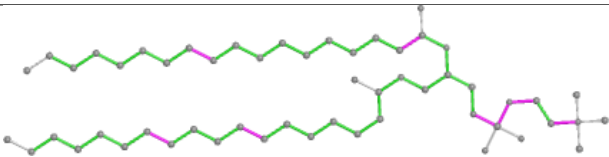
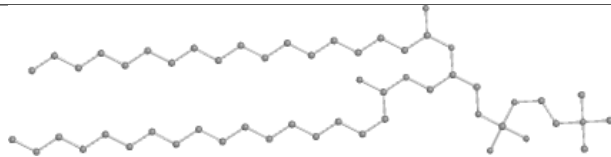
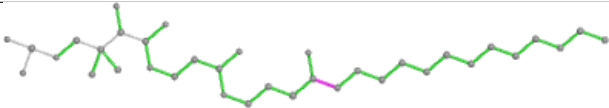

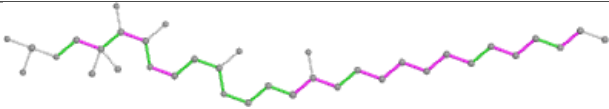
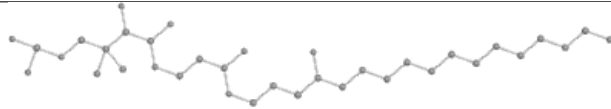




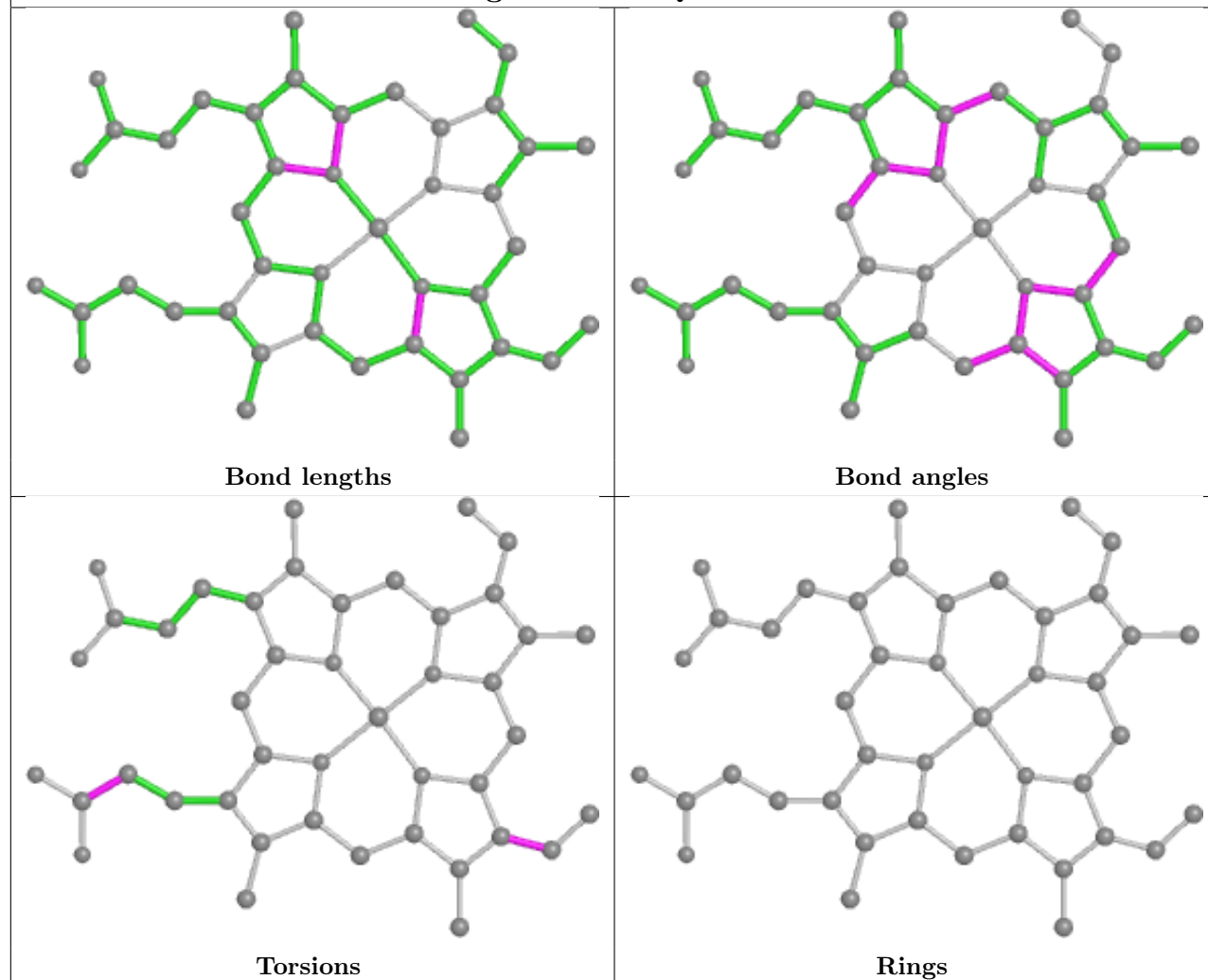




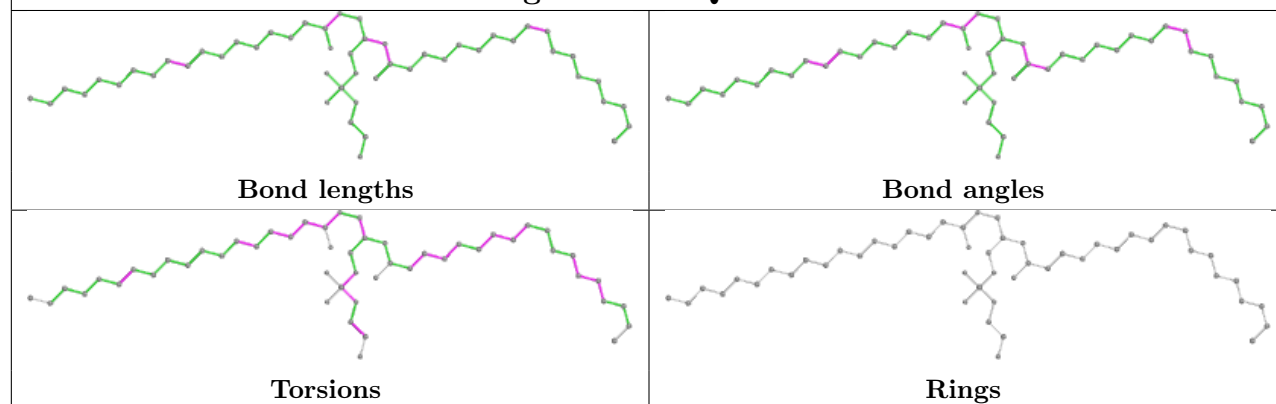


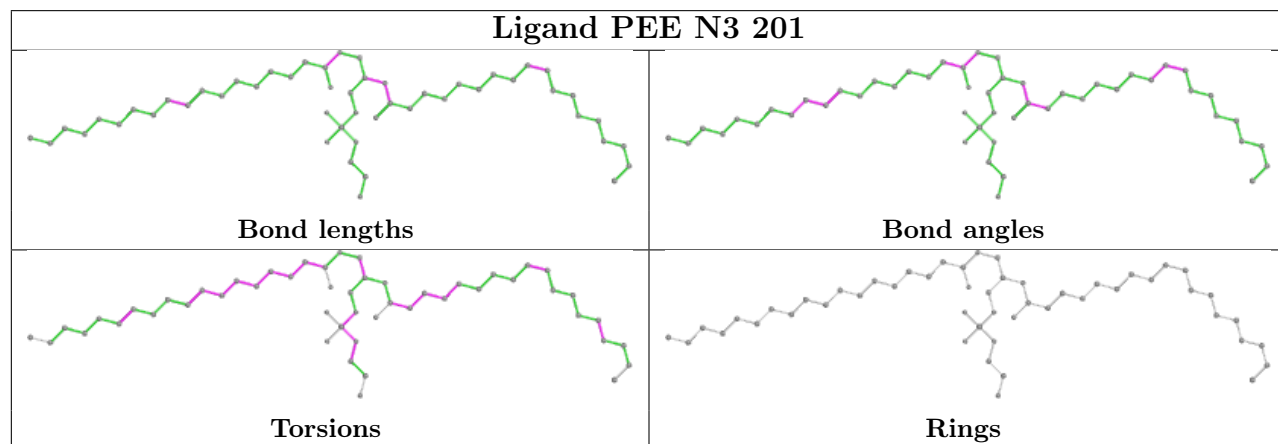
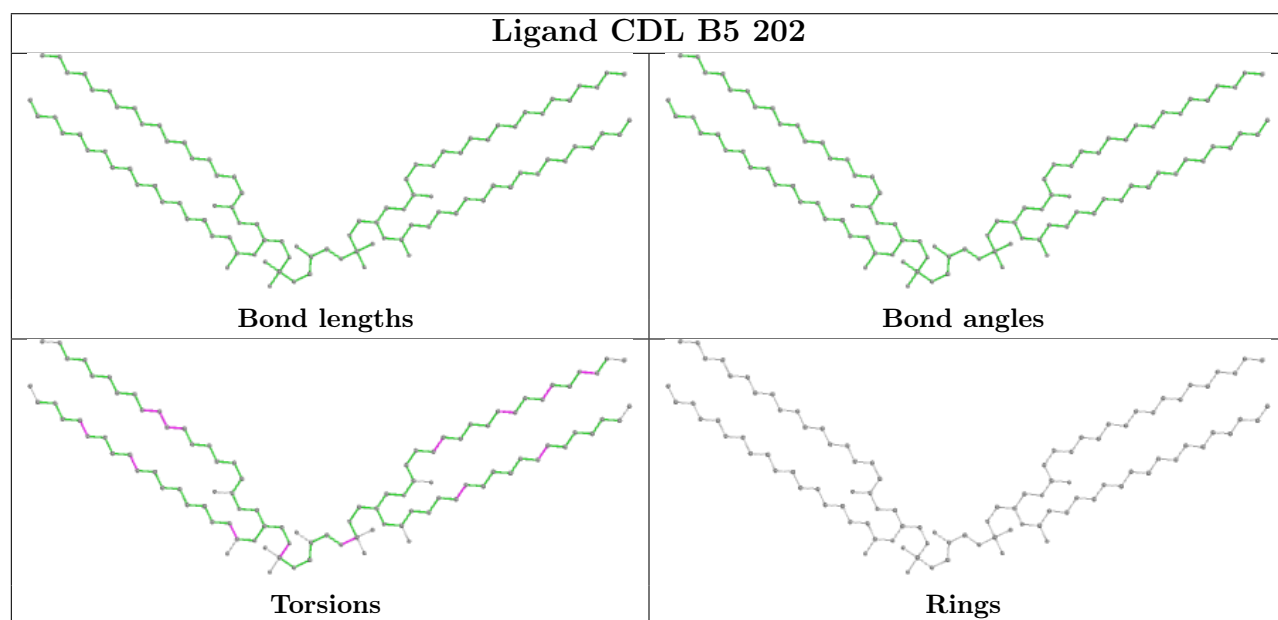
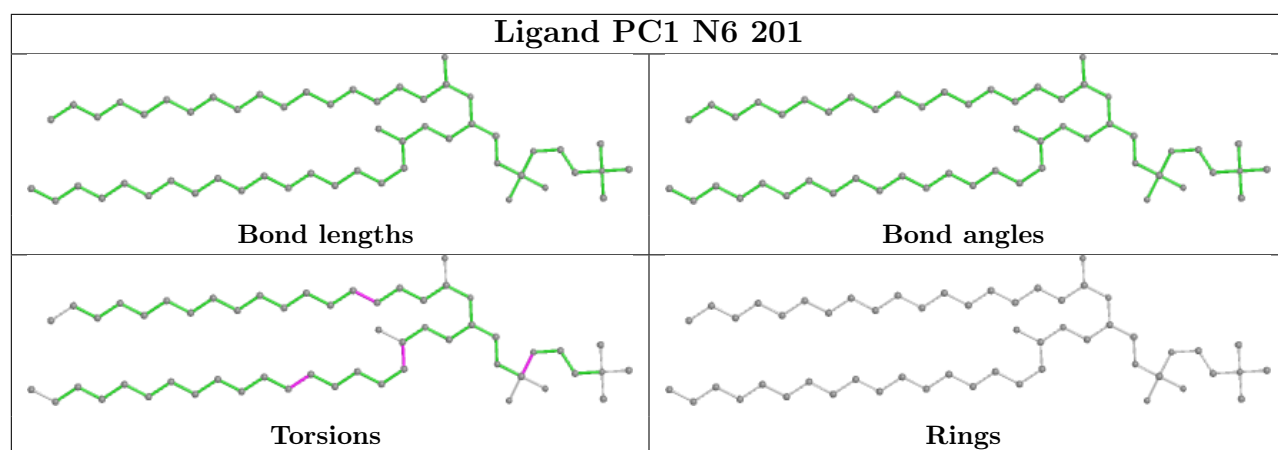
Ligand PLX CB 201	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand PEE S2 501	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand PC1 AL 206	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand ZMP AC 201	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

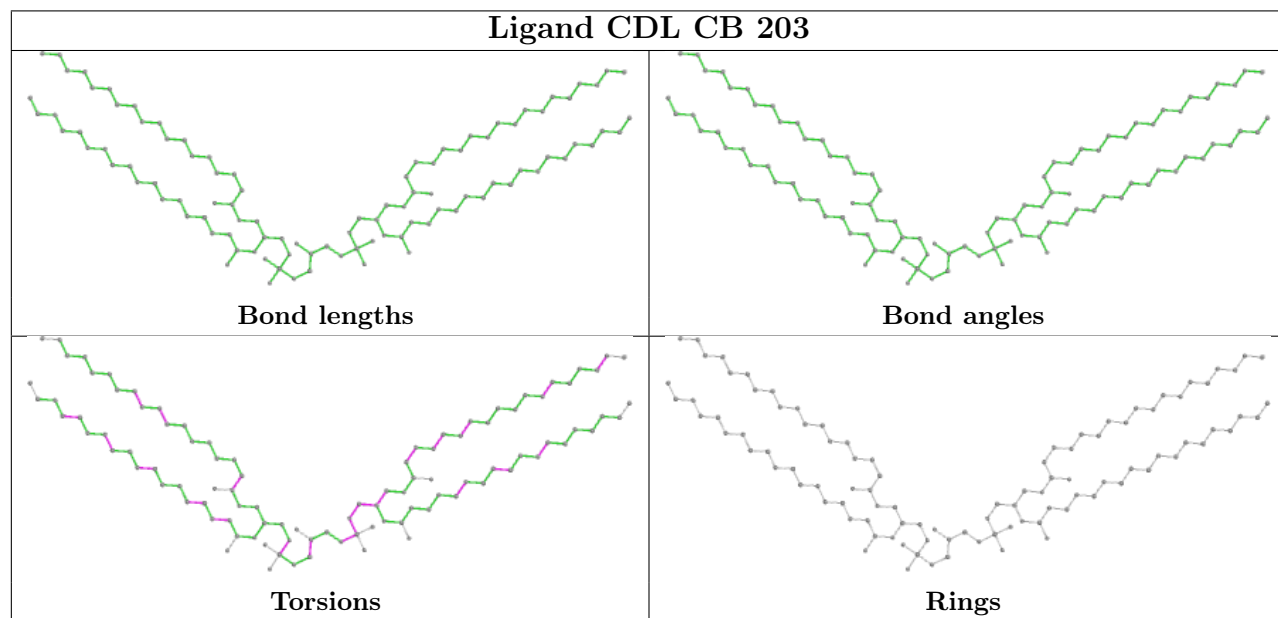
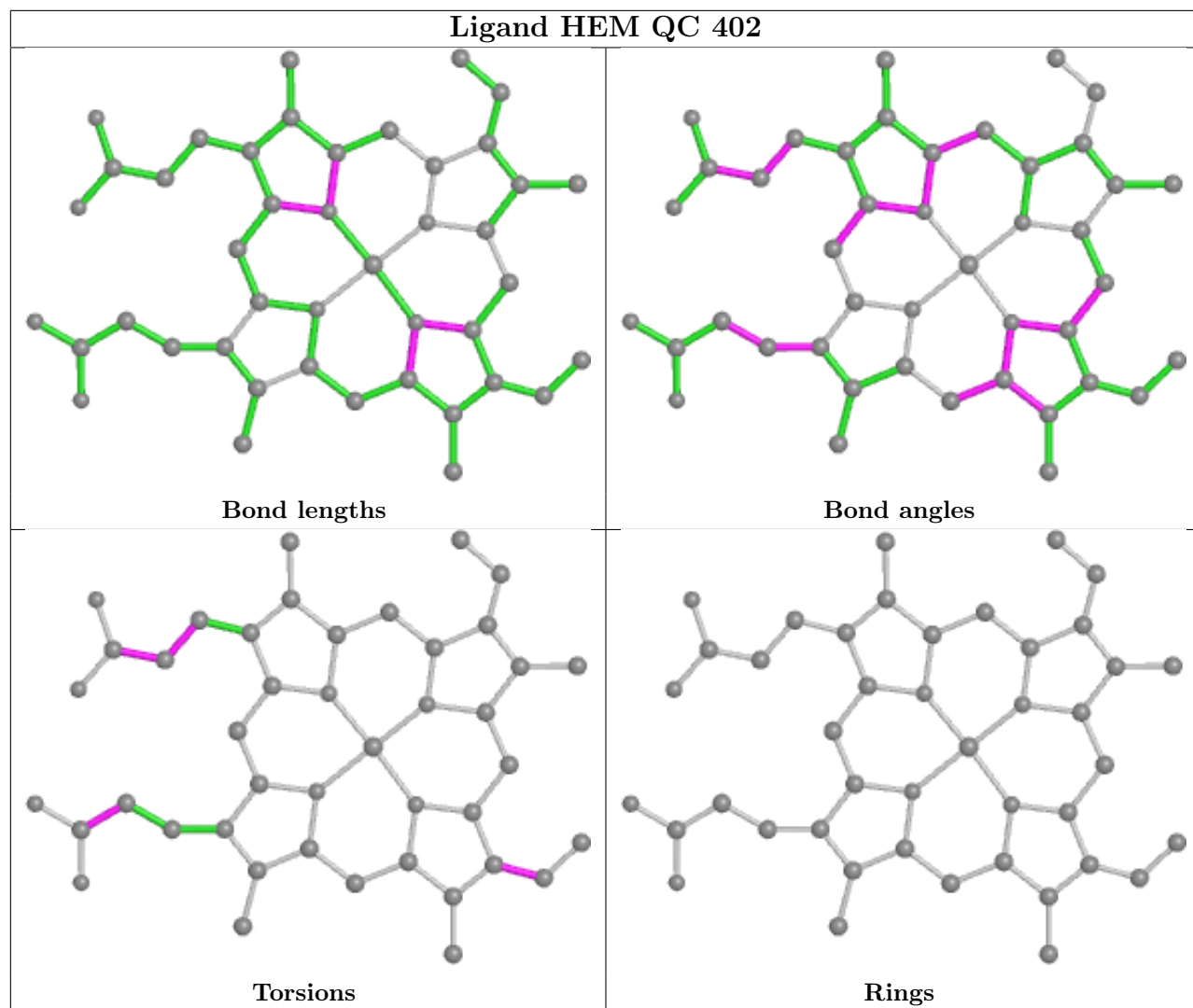
## Ligand HEM QC 403



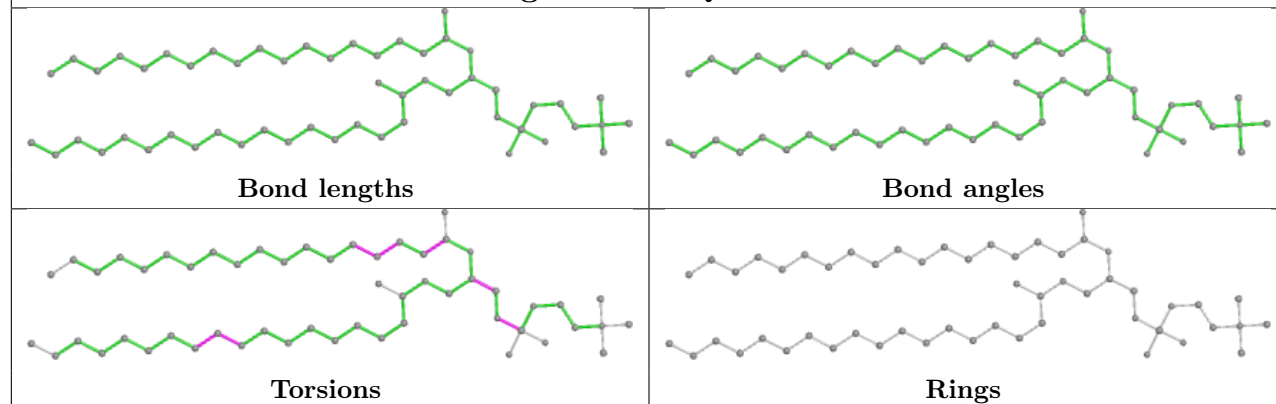
## Ligand PEE Qd 403



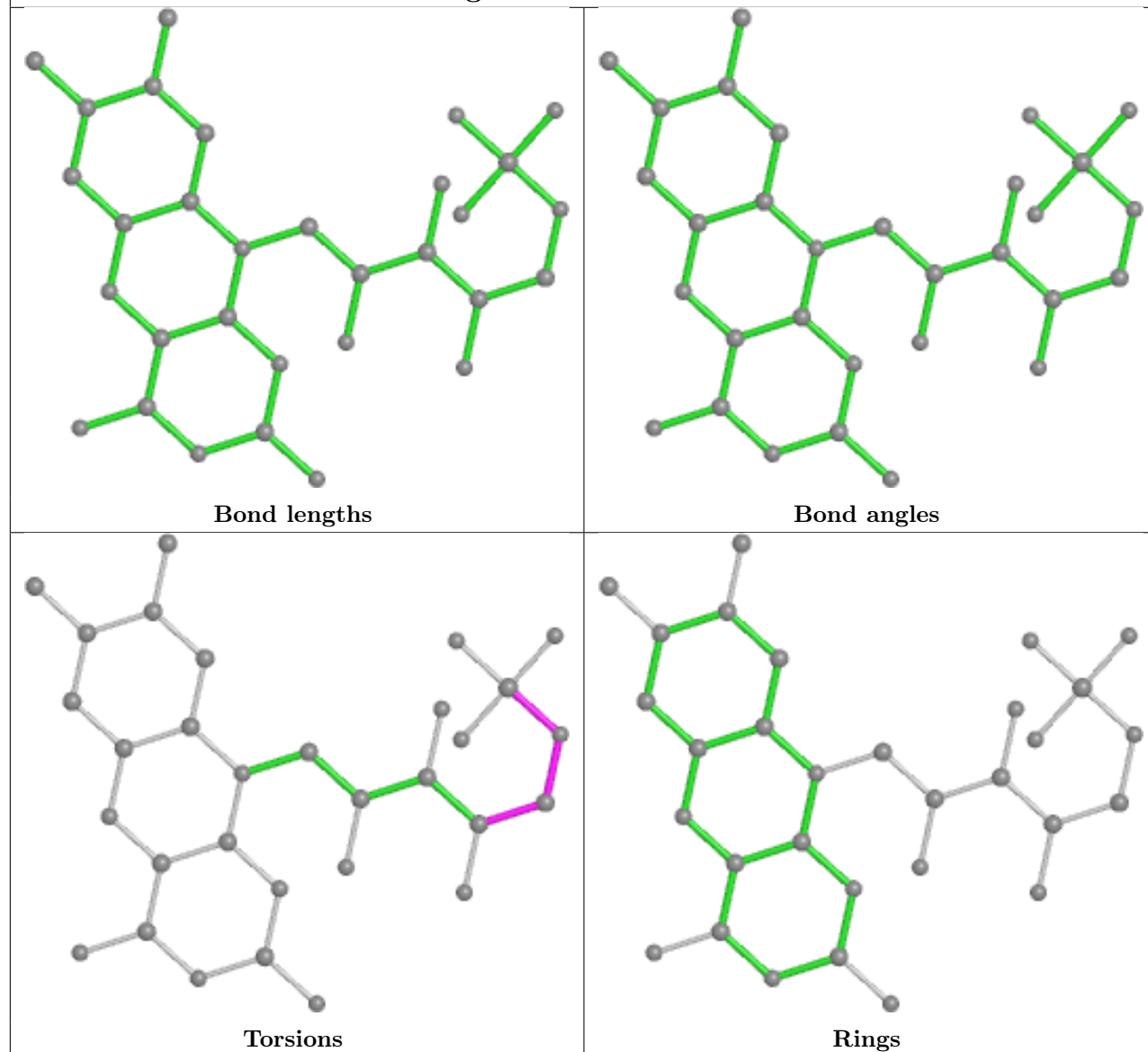


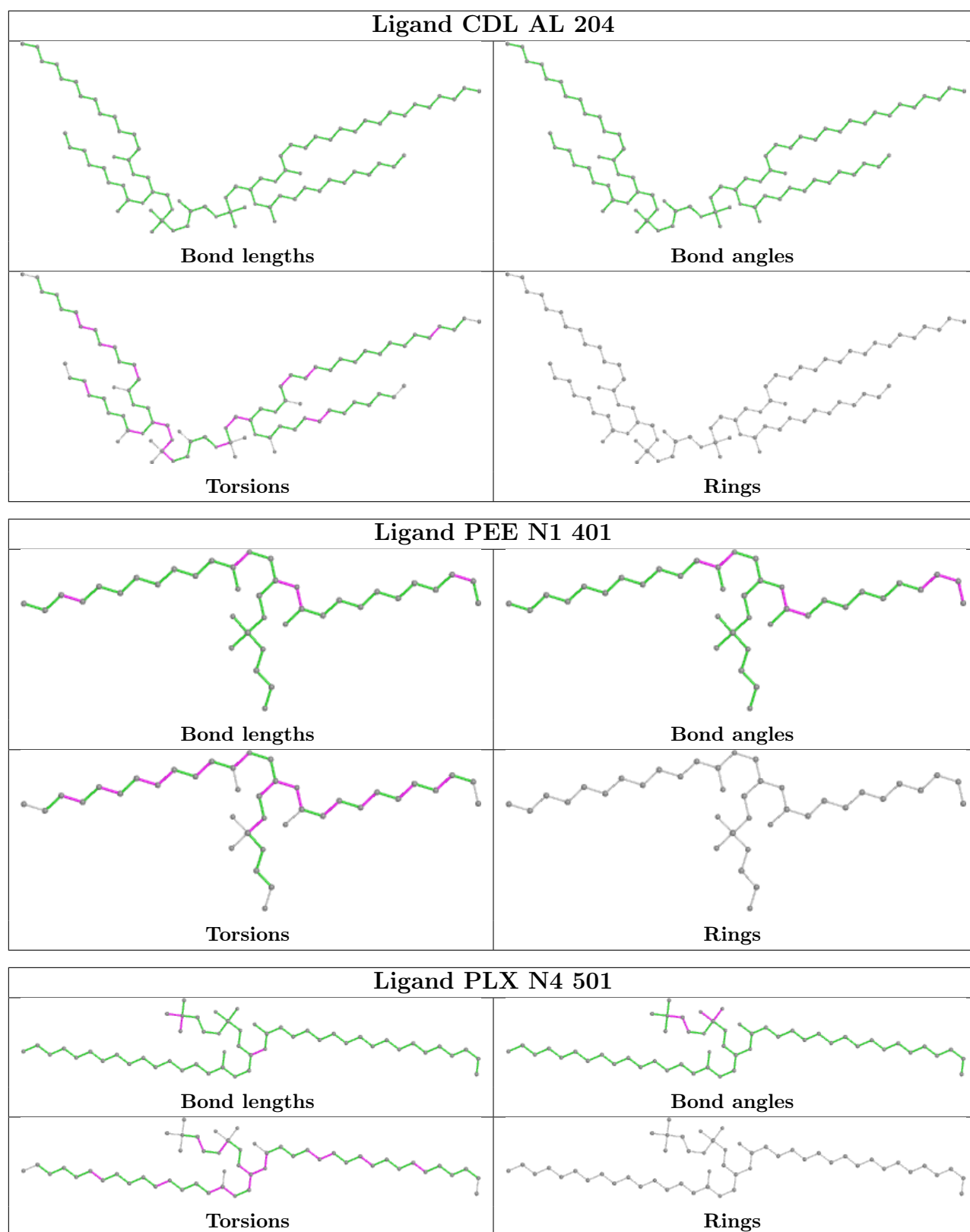


## Ligand PC1 QH 102

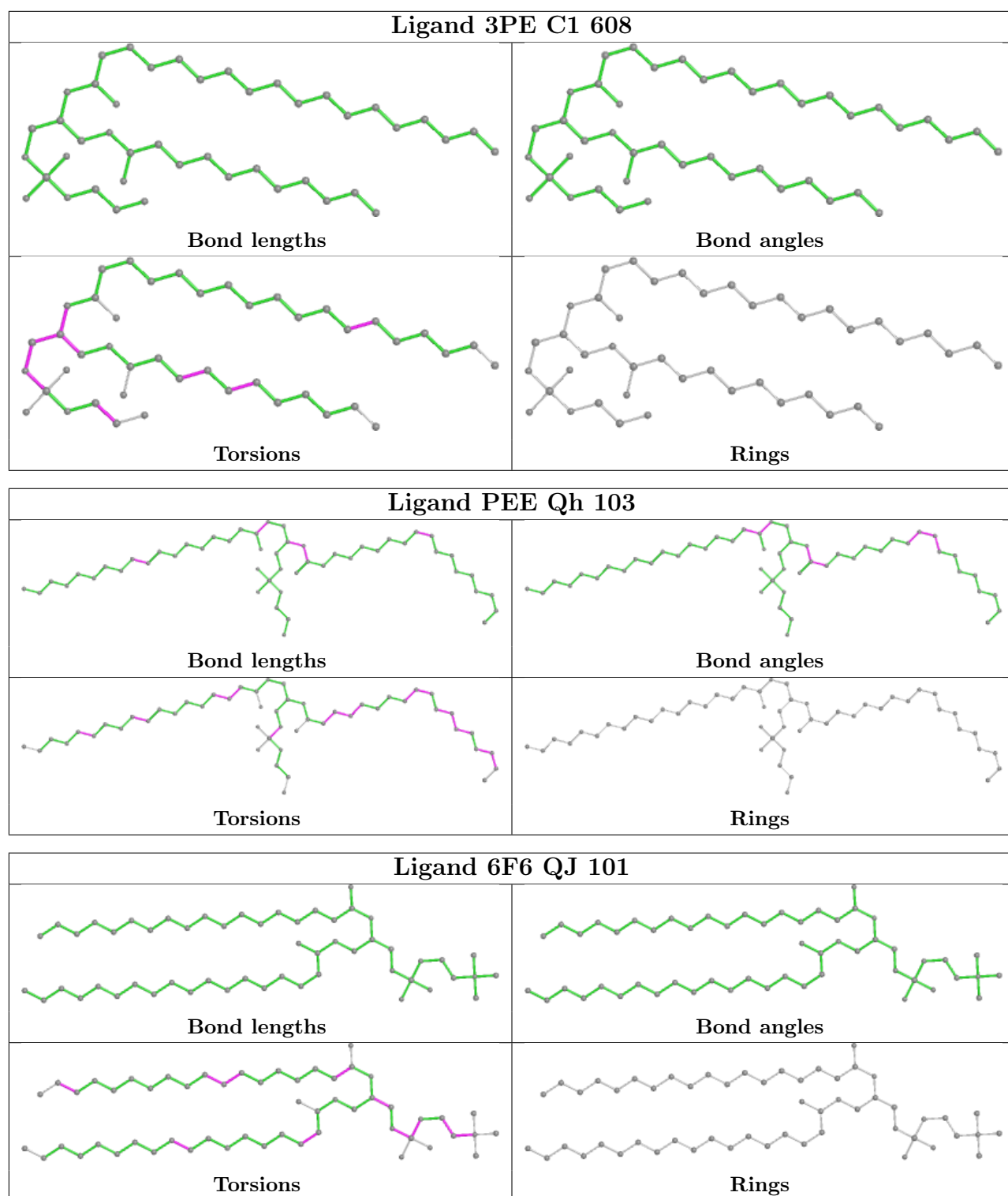


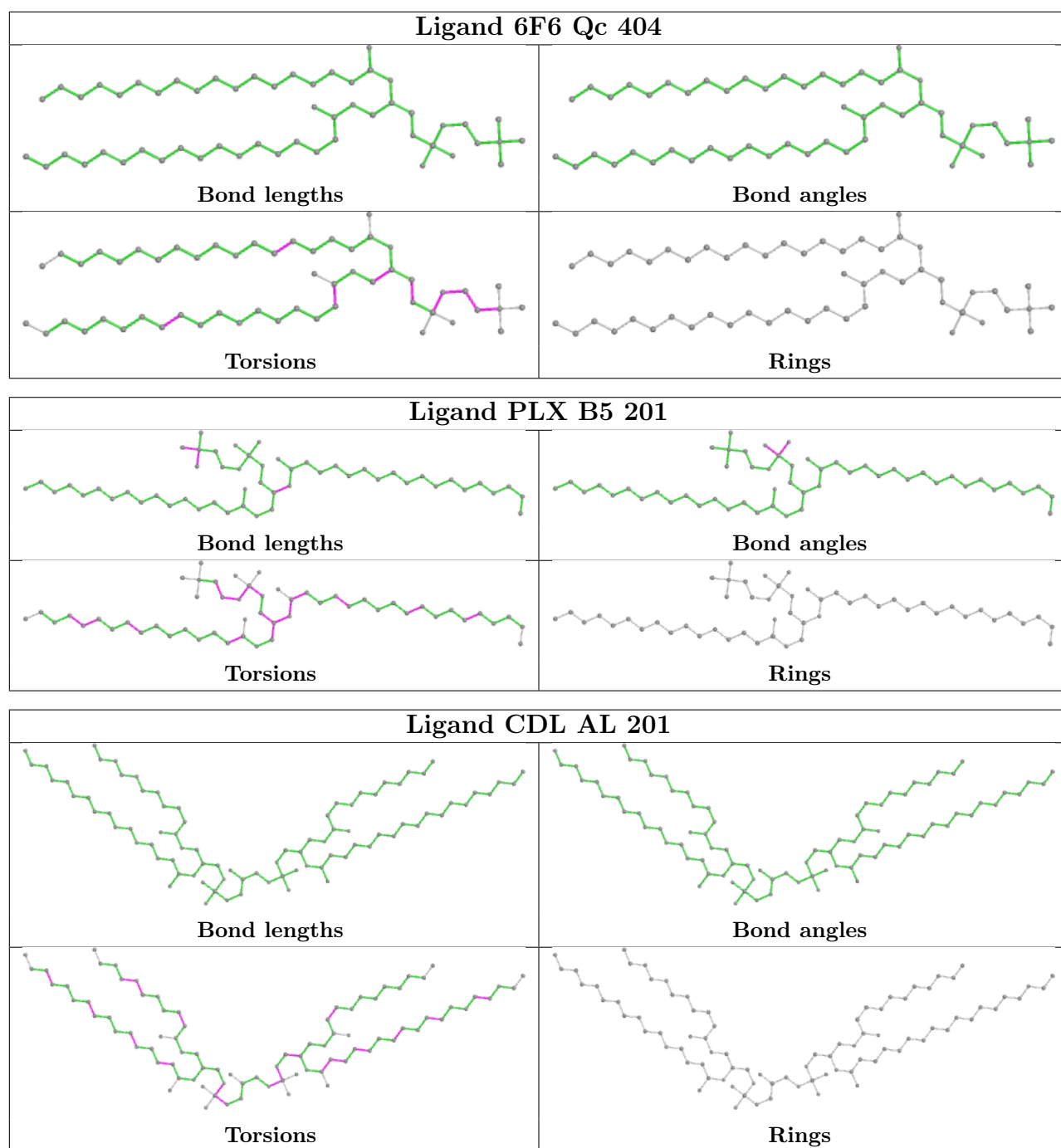
## Ligand FMN V1 502

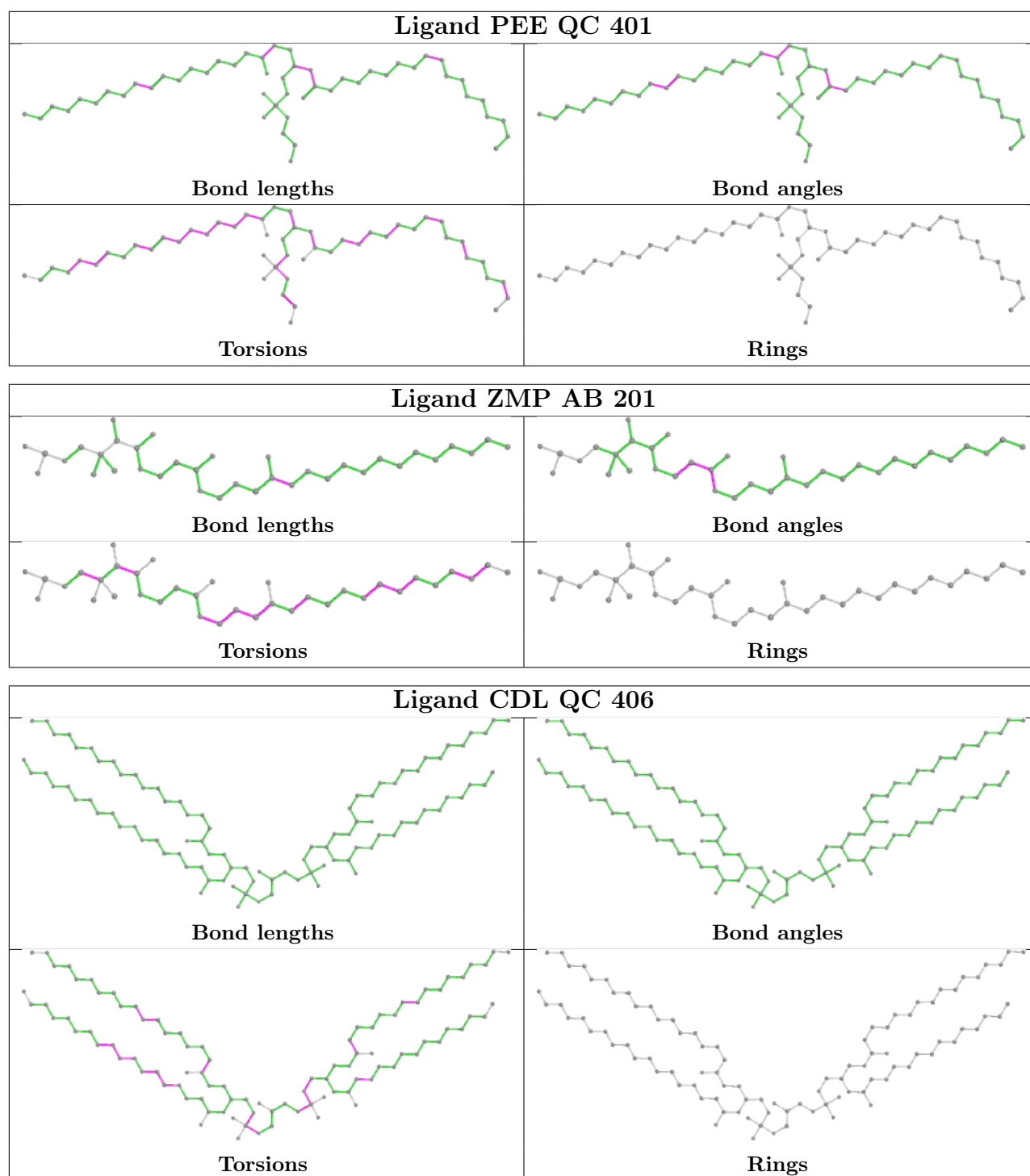


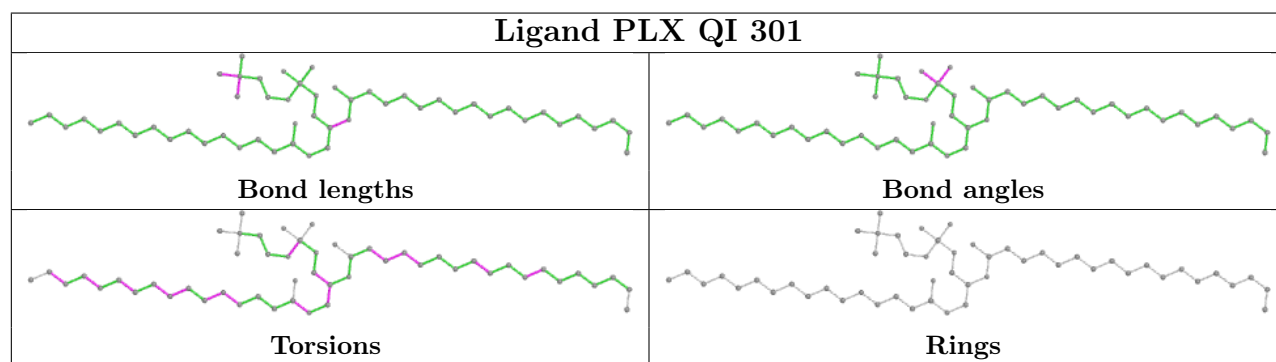
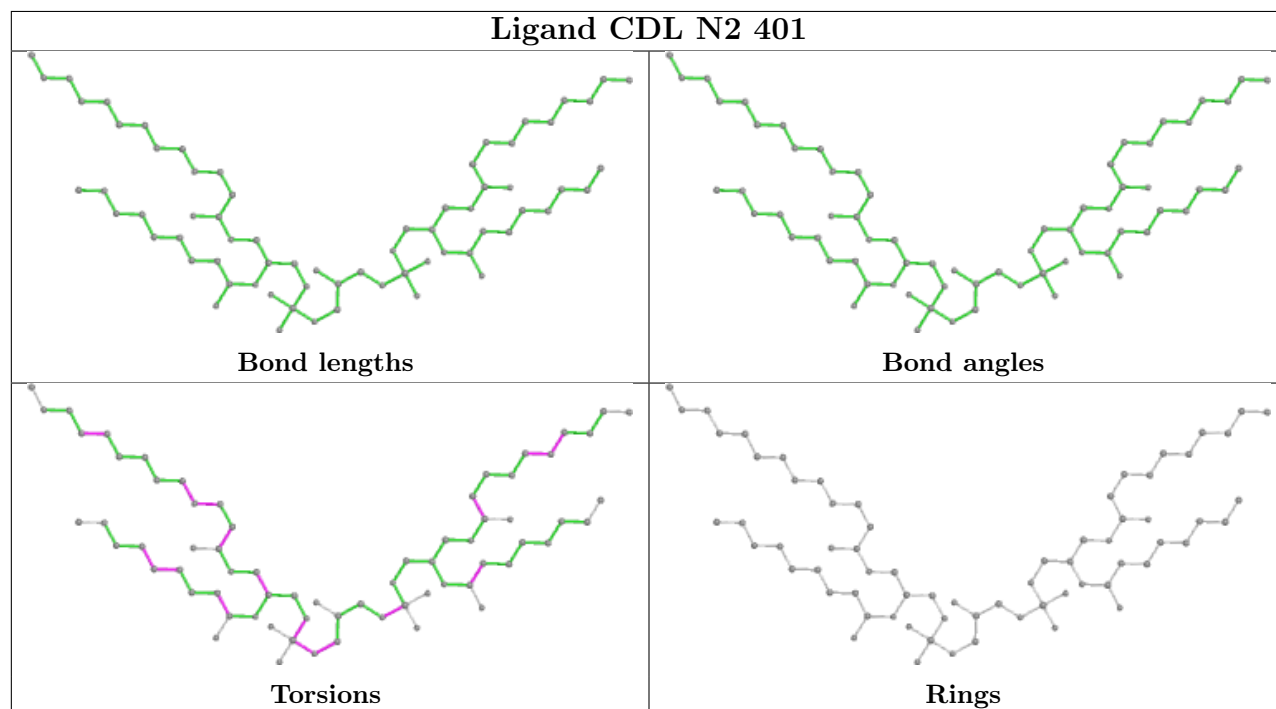
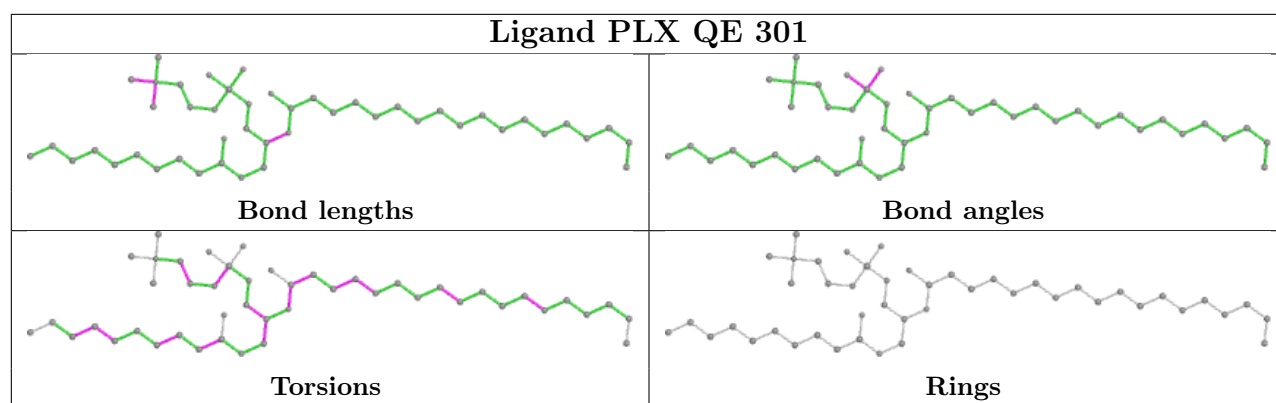




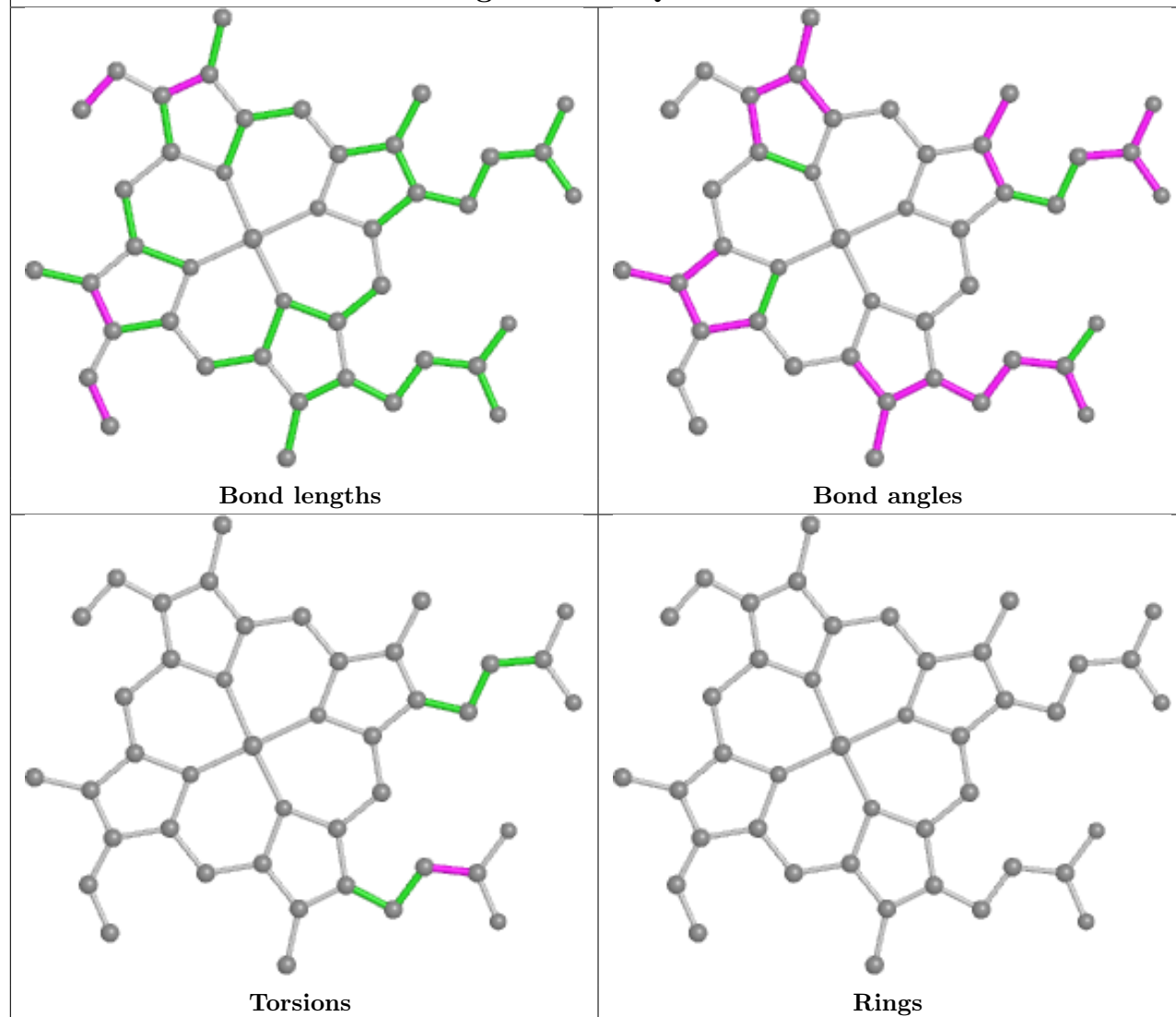




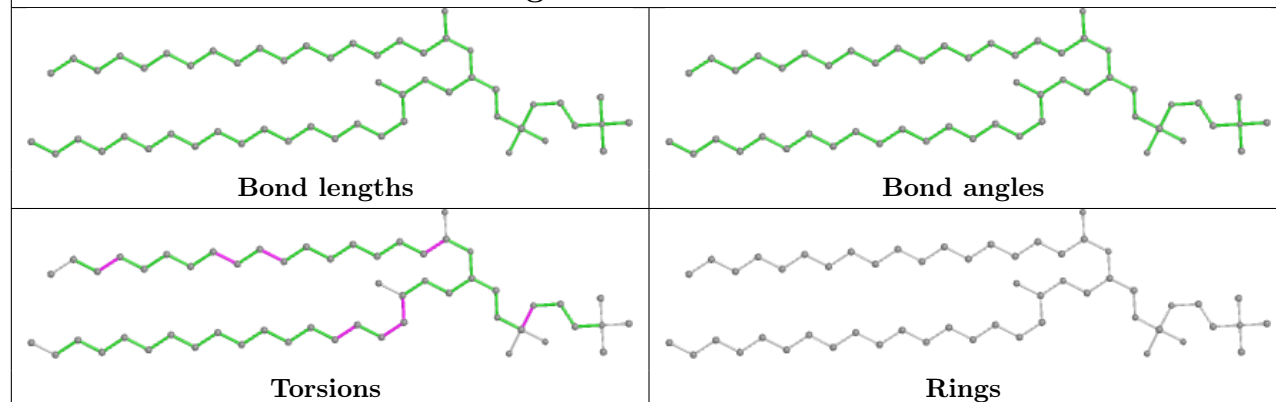


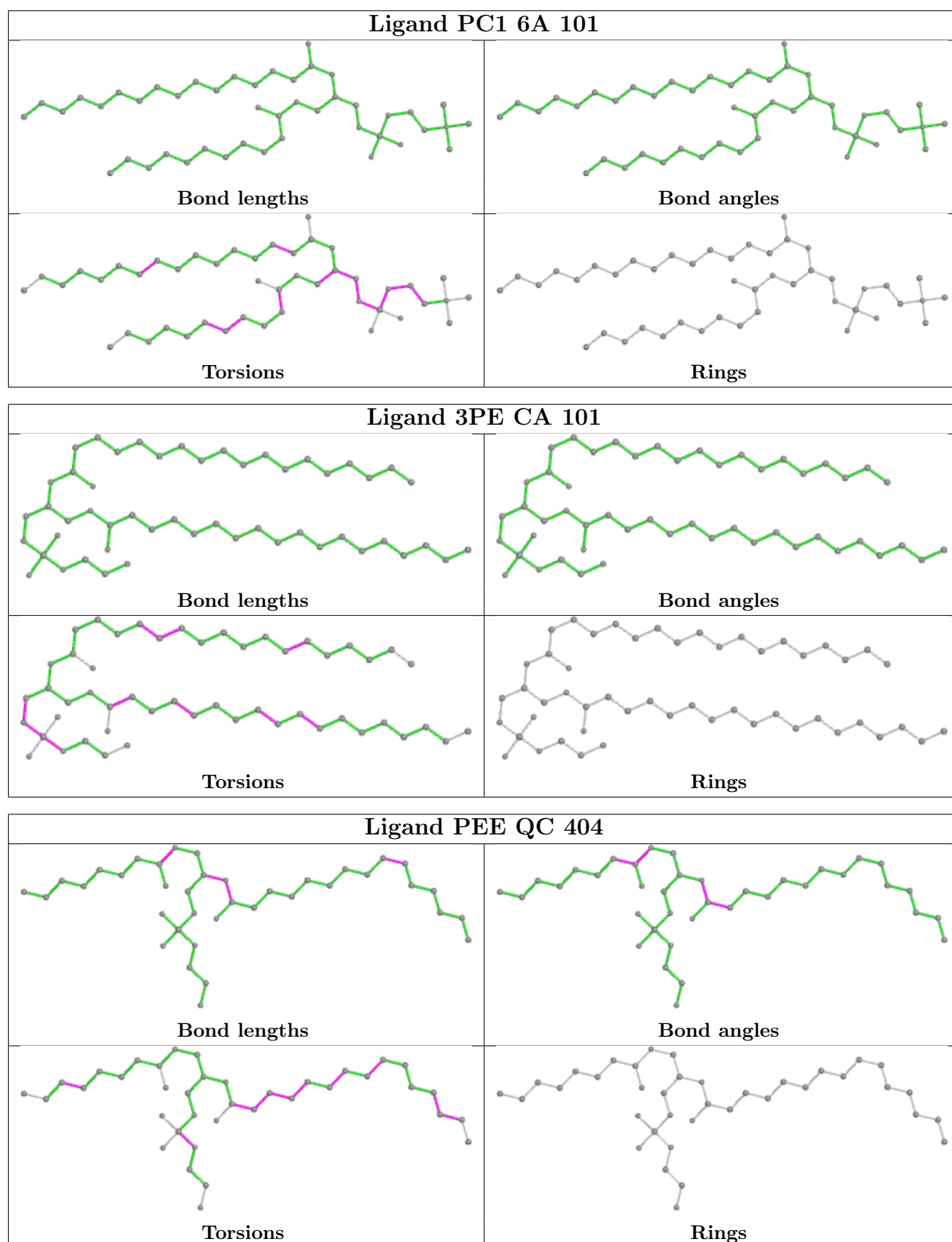


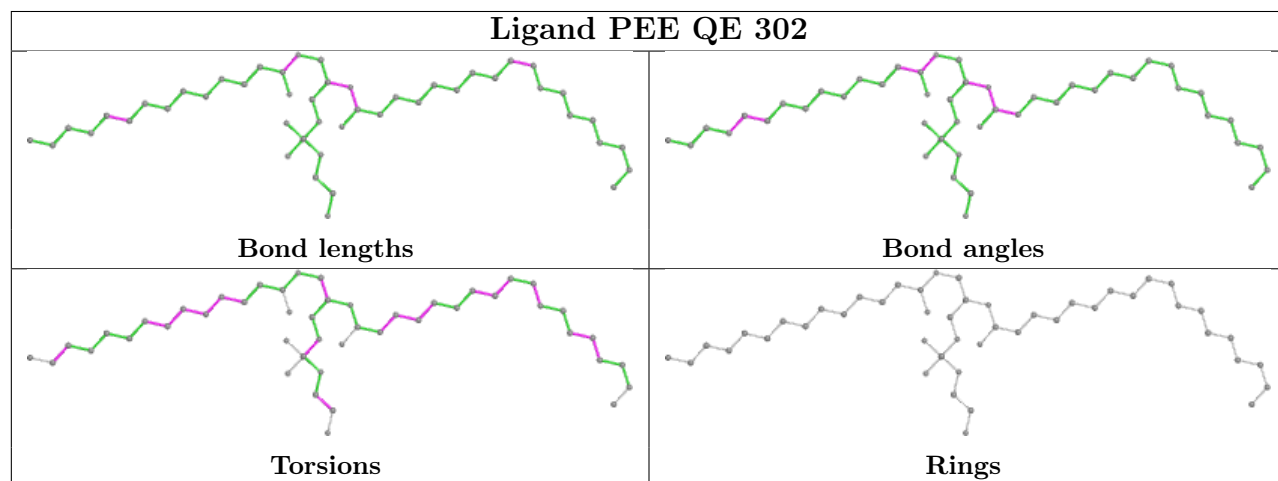
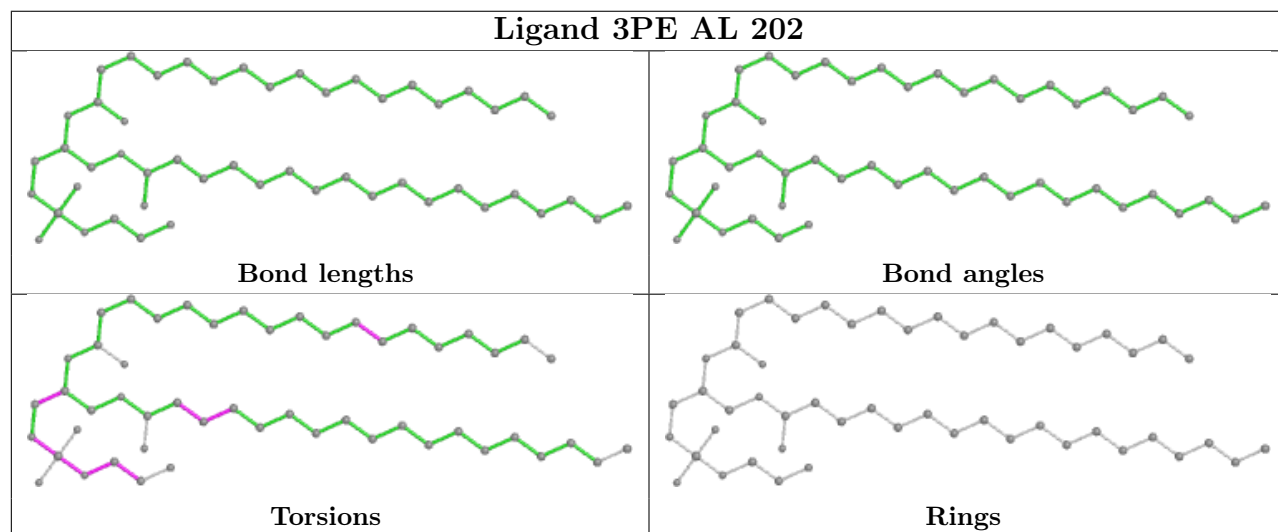
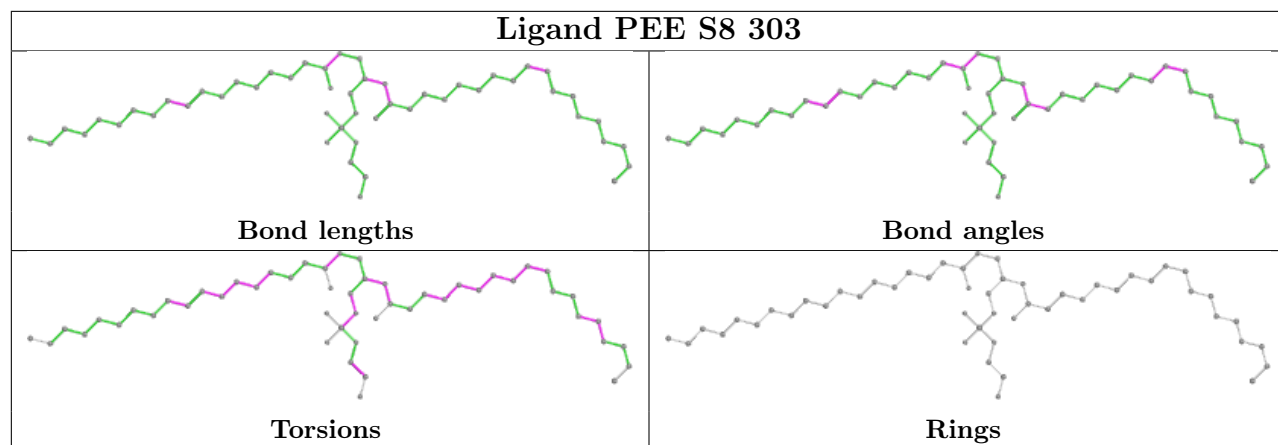
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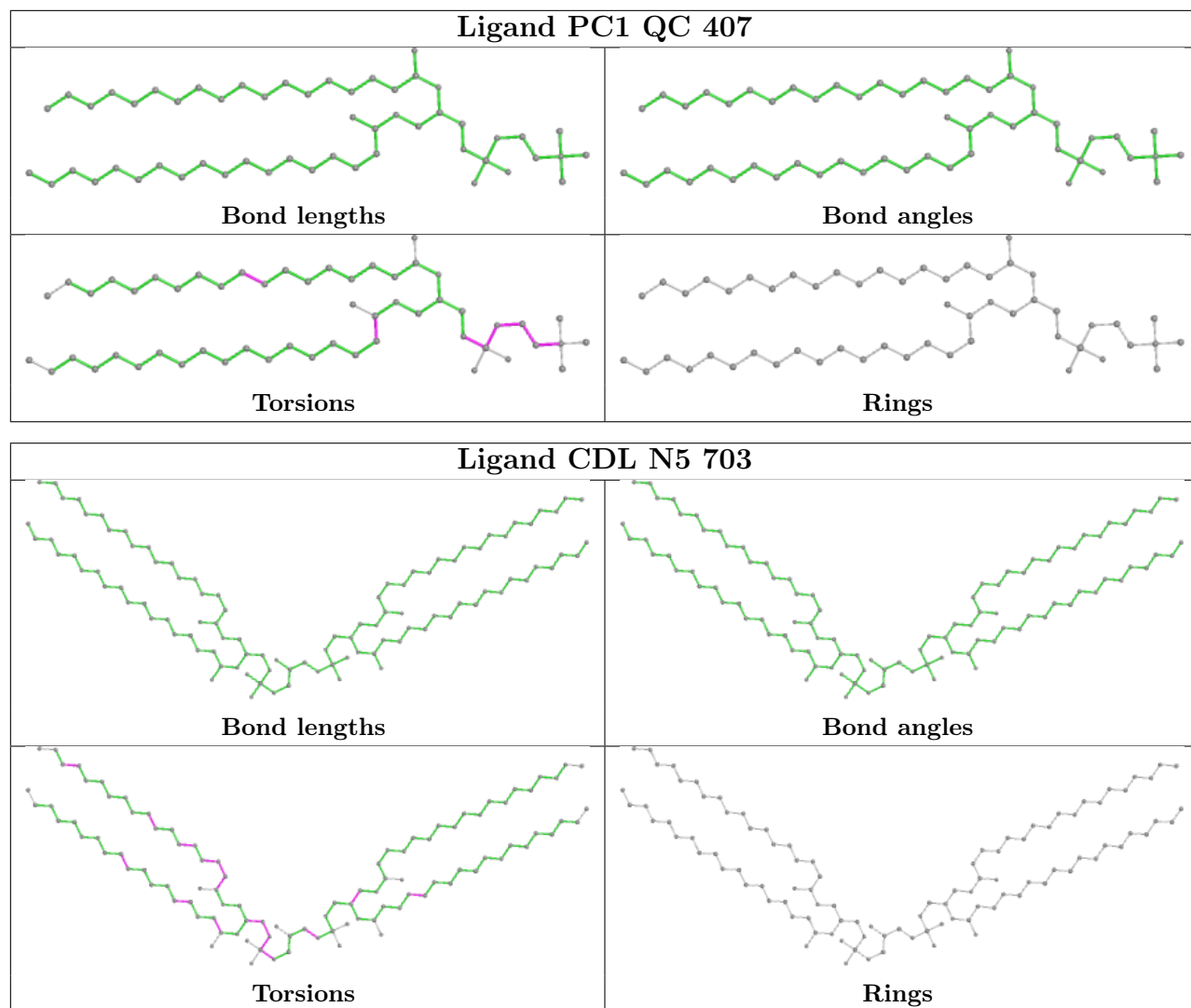


## Ligand PC1 C1 606

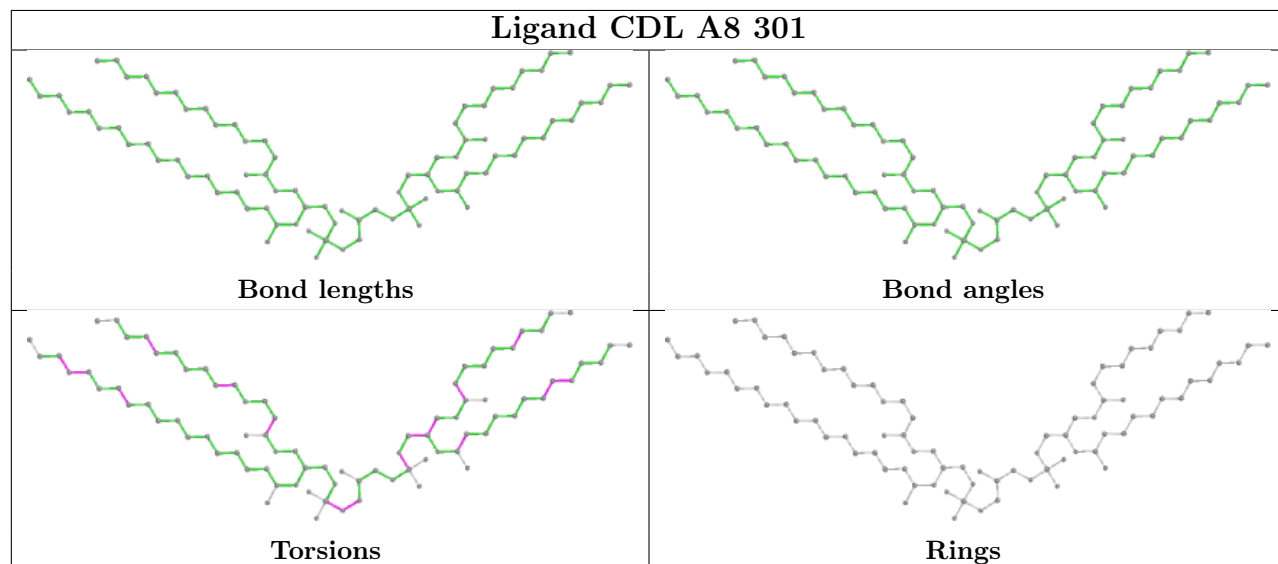
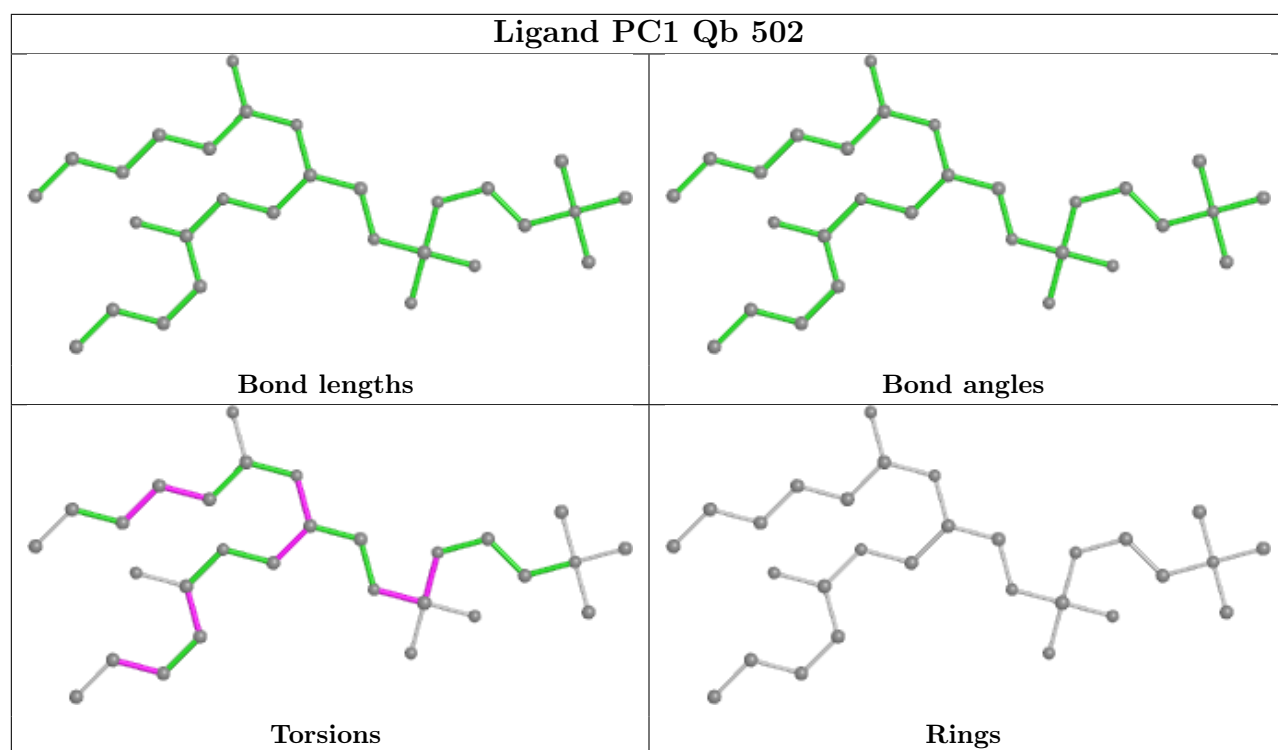


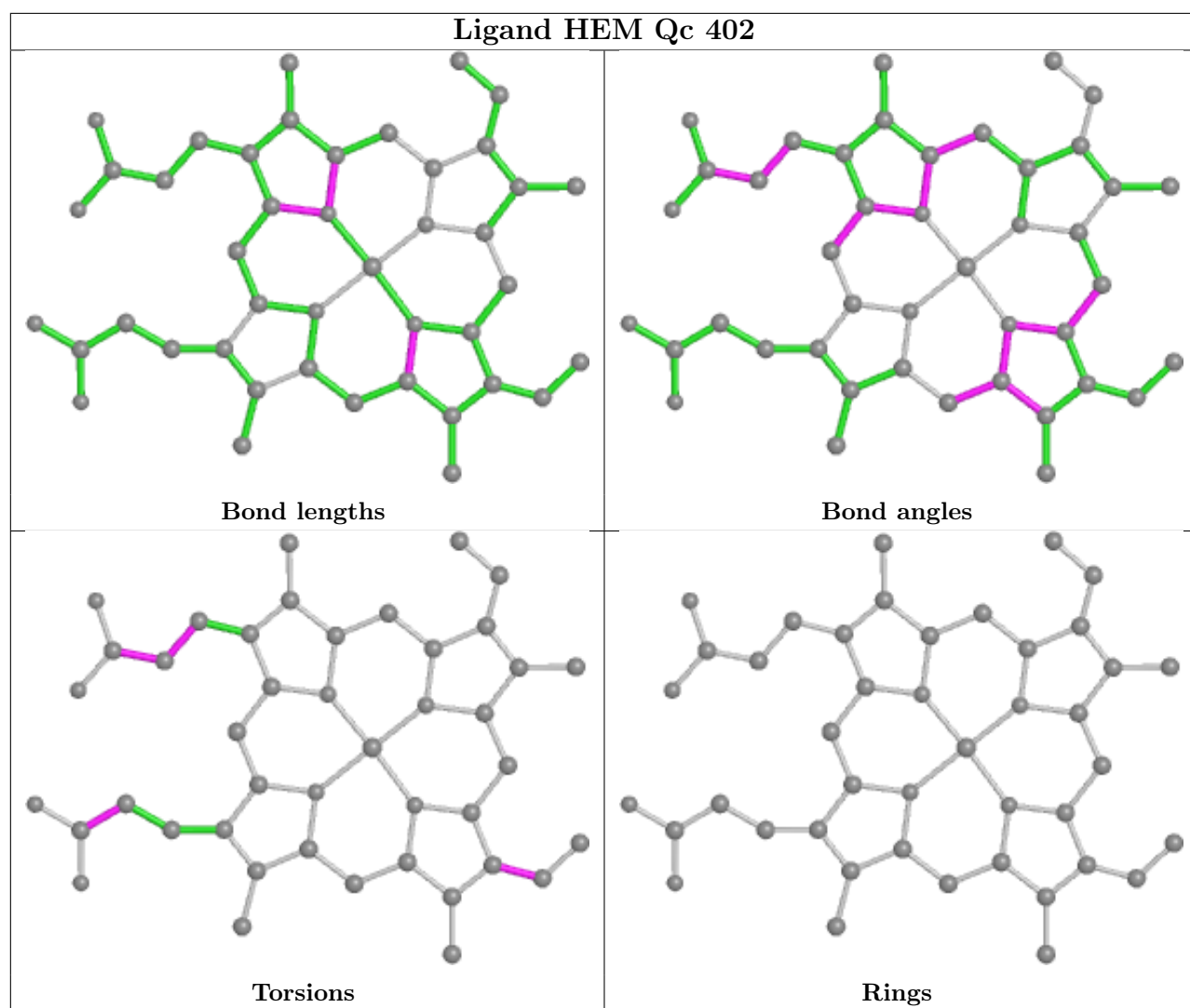


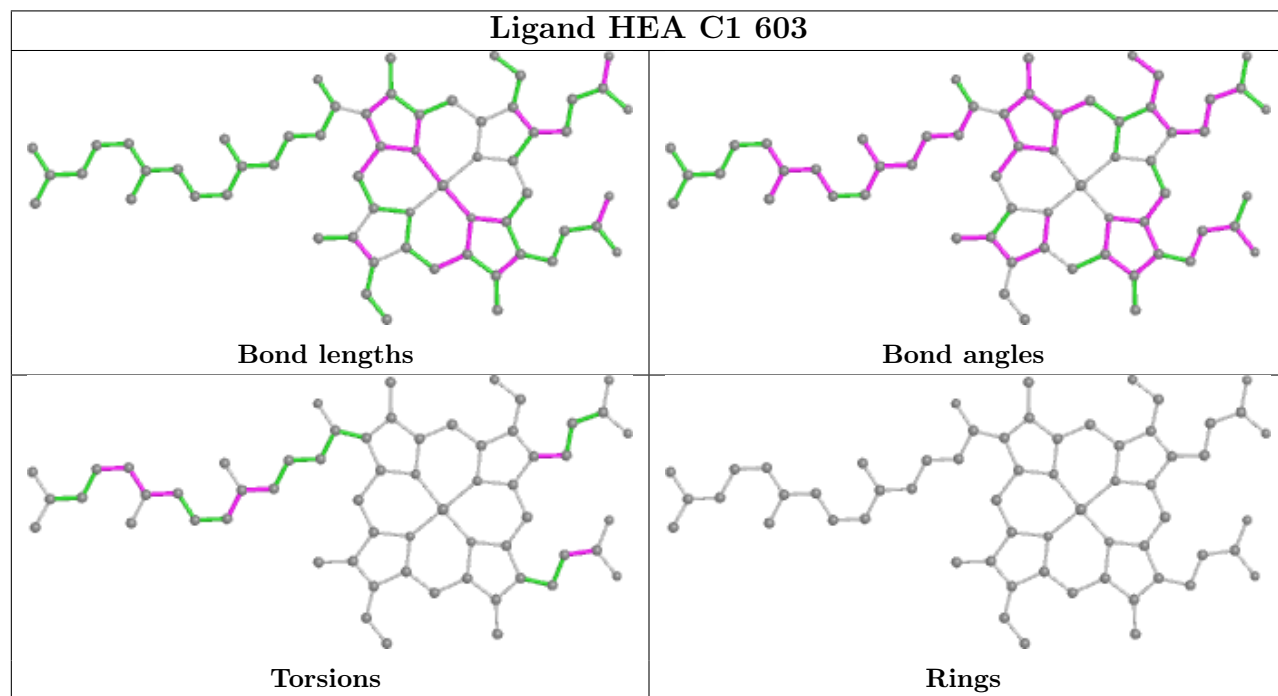
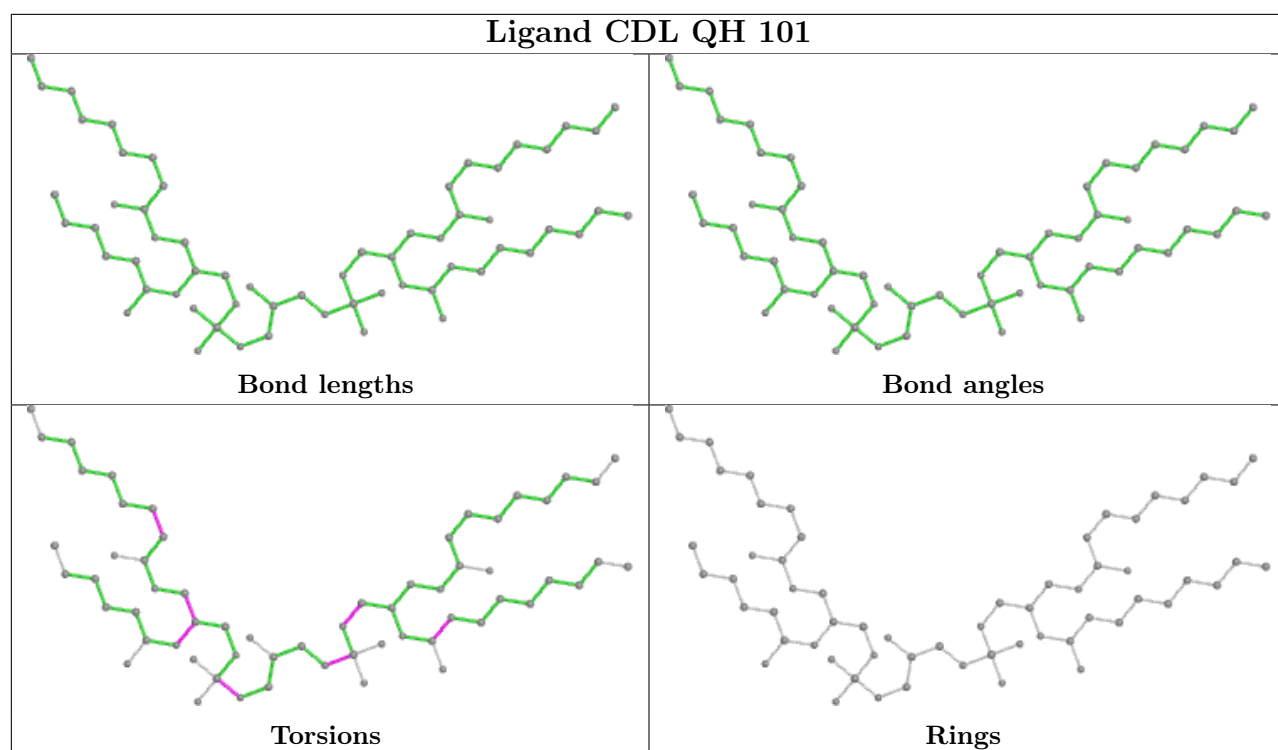


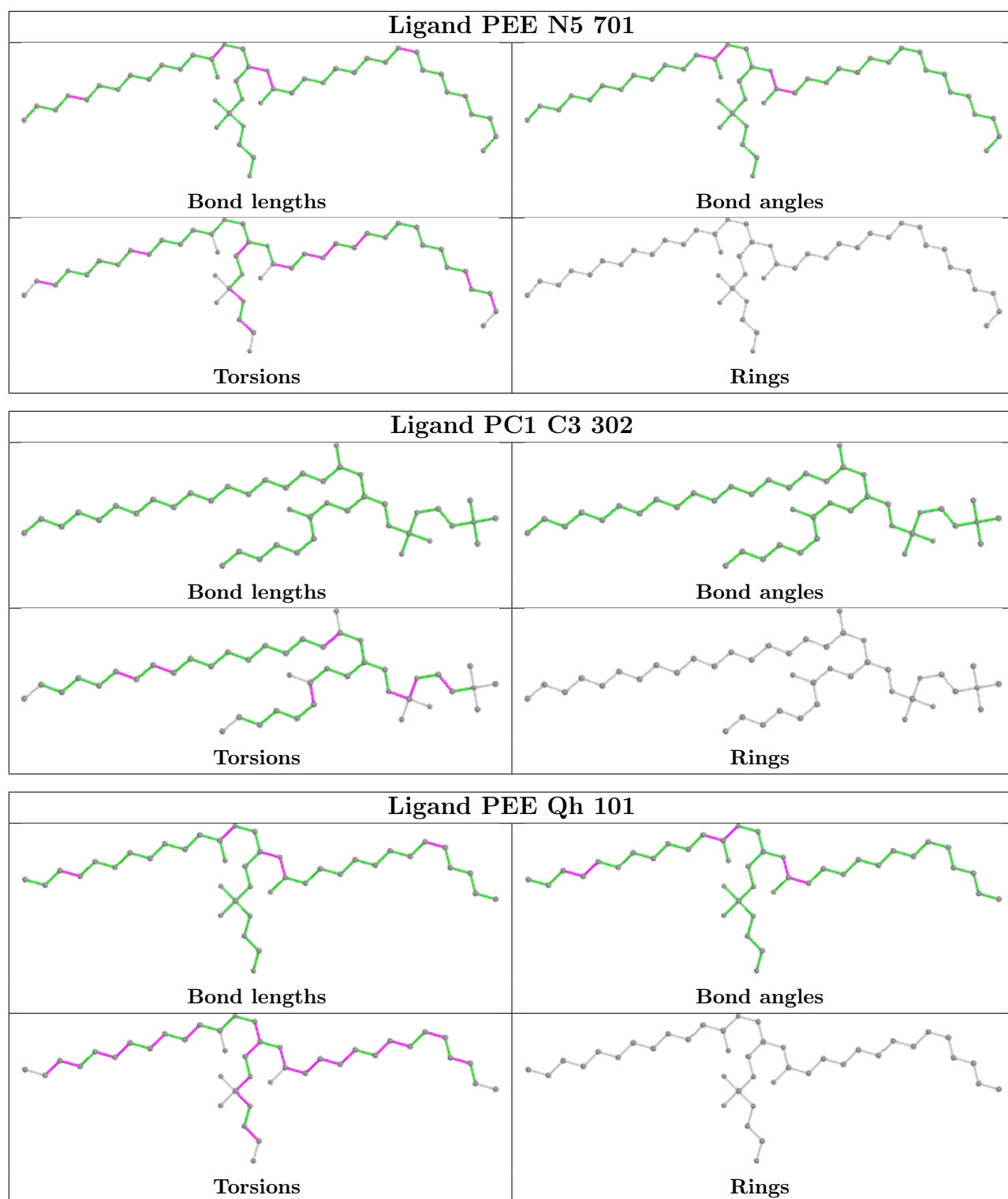




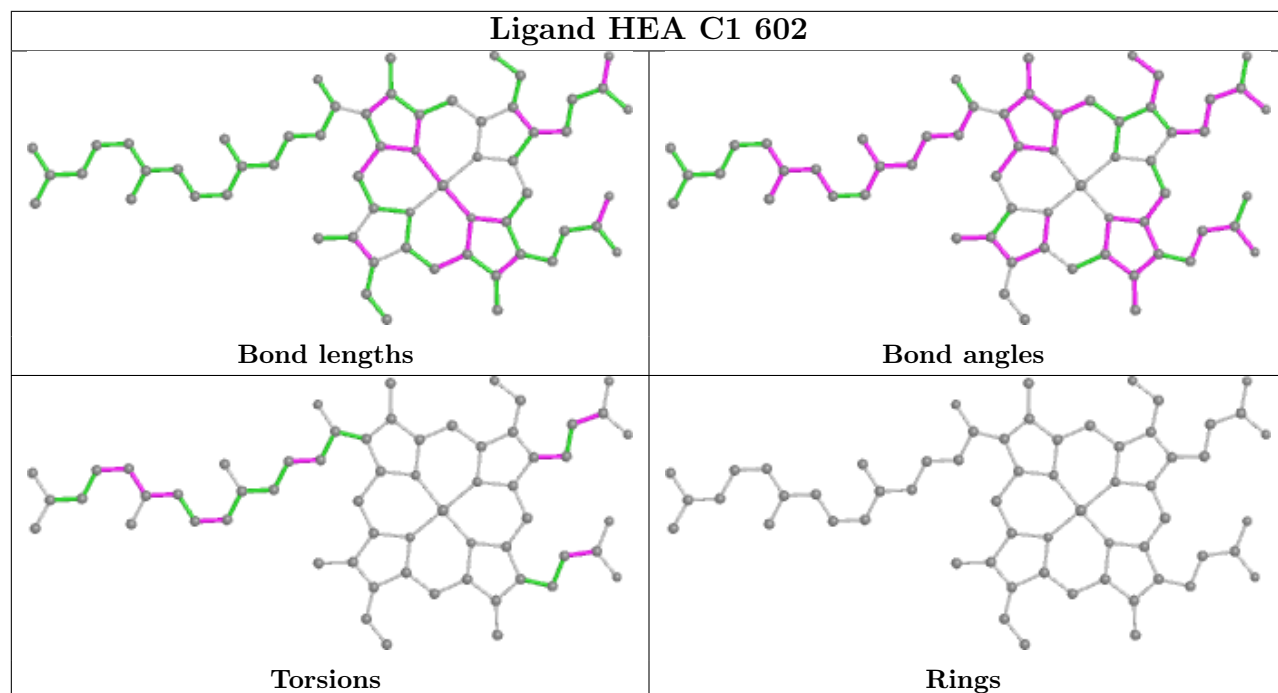




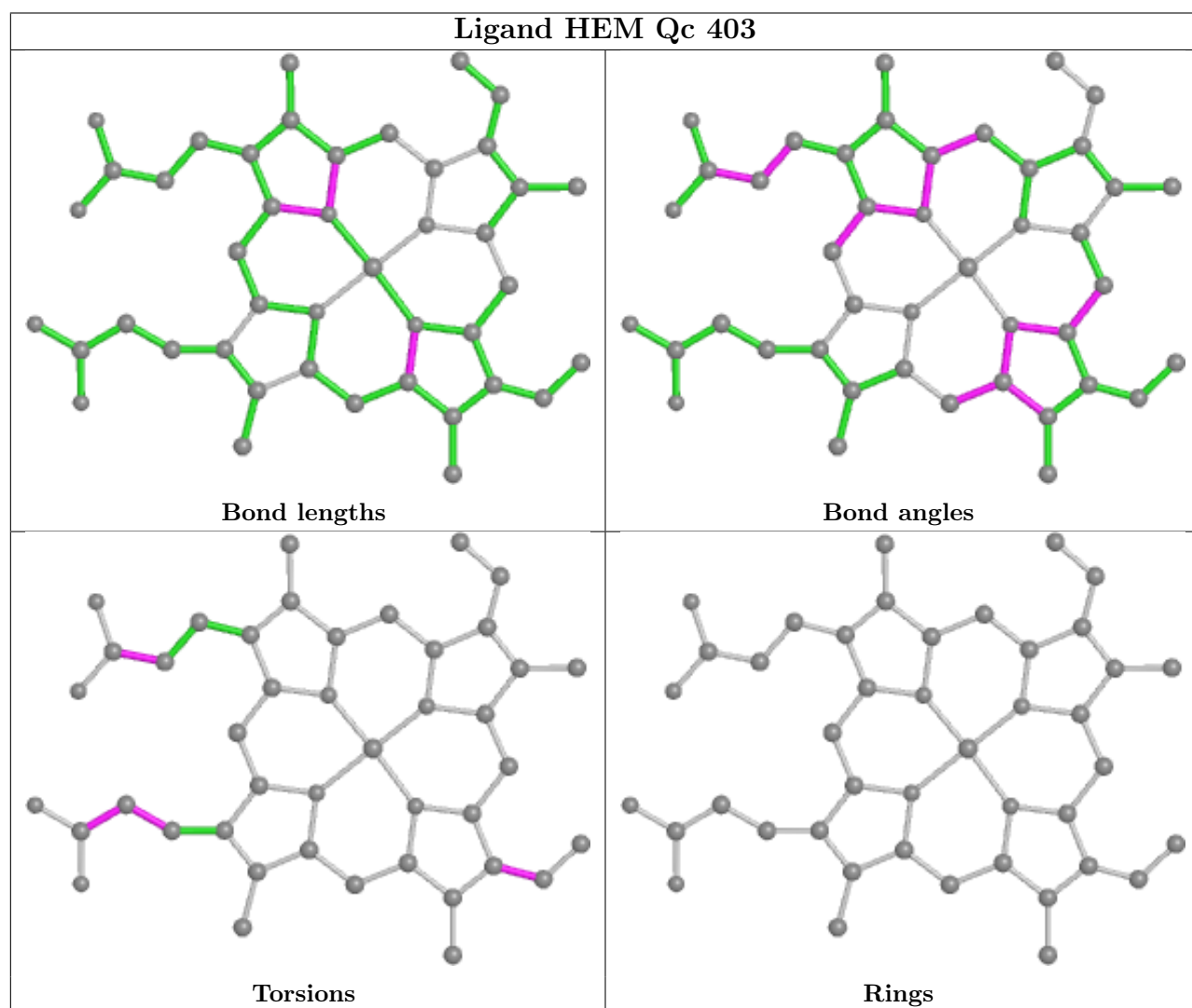


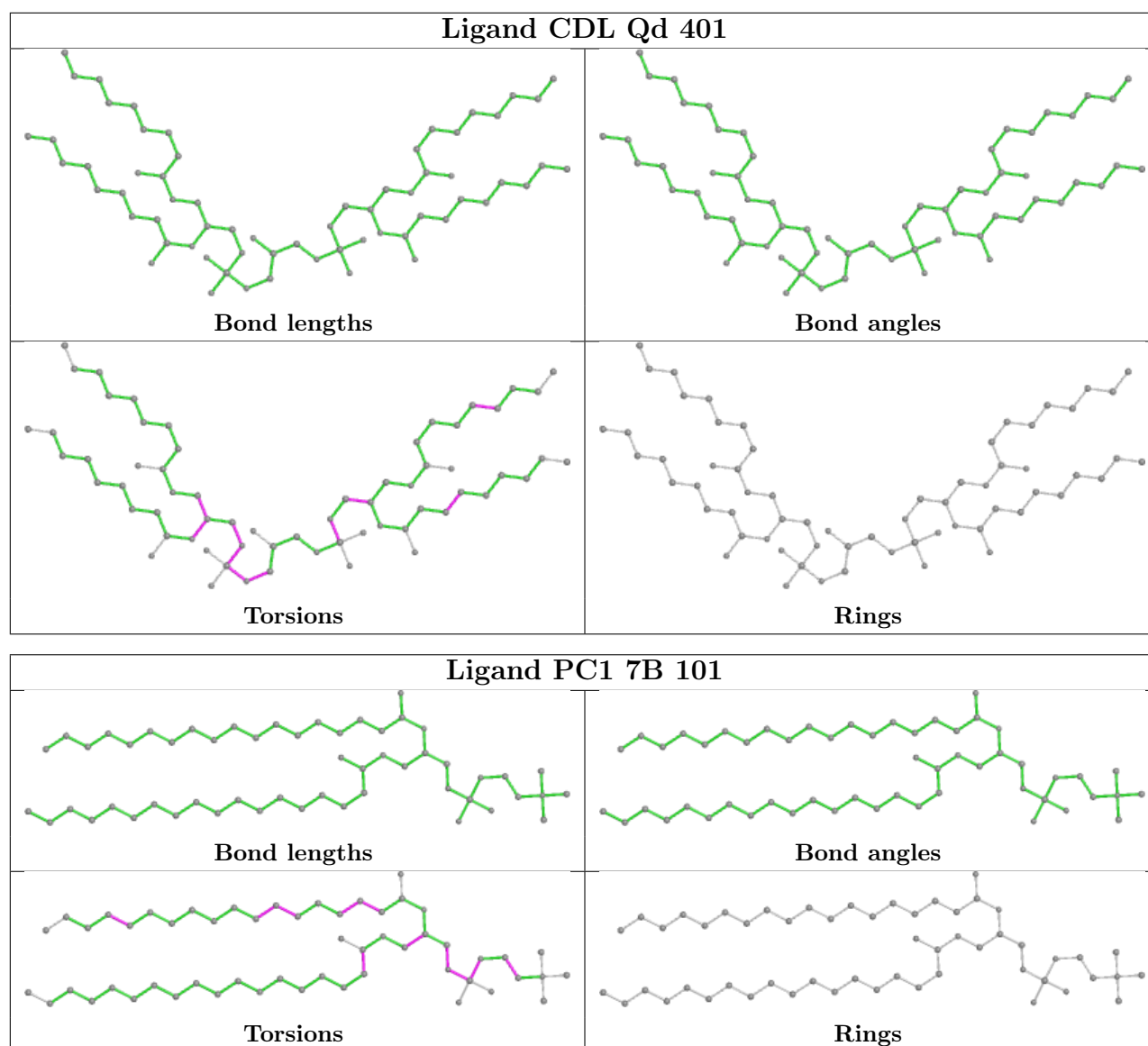


## Ligand HEA C1 602



## Ligand HEM Qc 403





## 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.

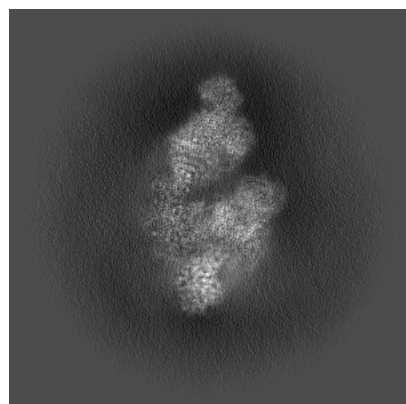
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60284. These allow visual inspection of the internal detail of the map and identification of artifacts.

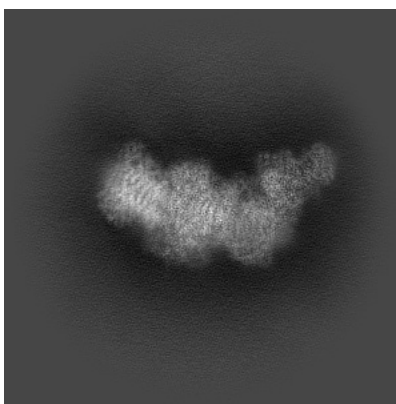
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

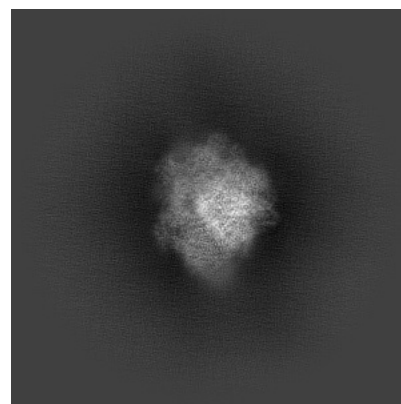
#### 6.1.1 Primary map



X

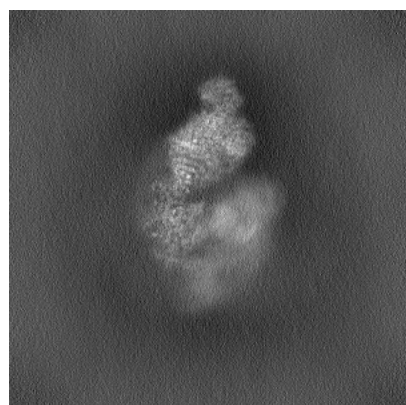


Y

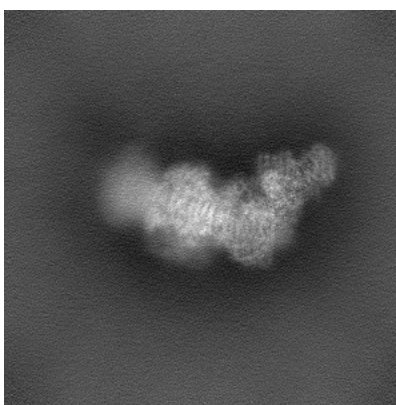


Z

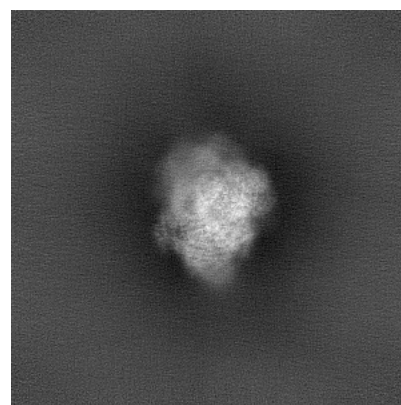
#### 6.1.2 Raw map



X



Y

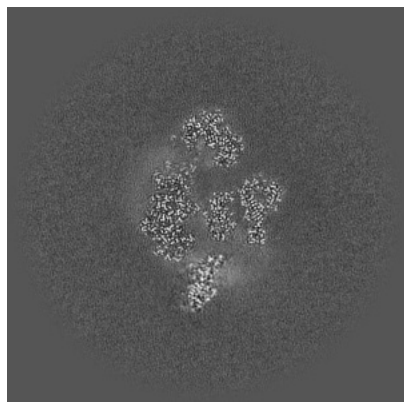


Z

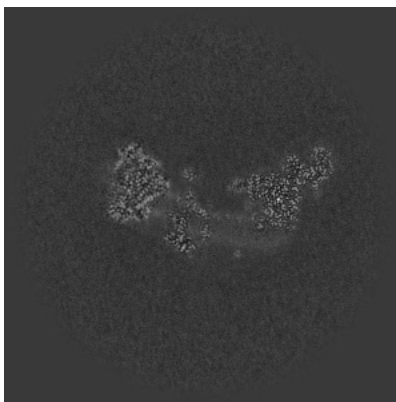
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

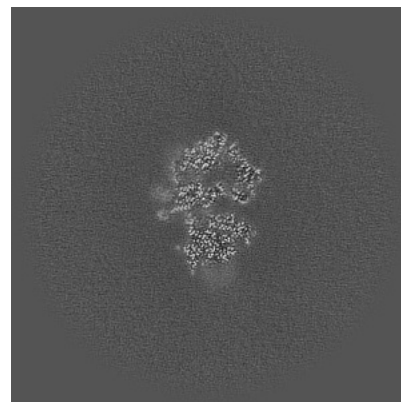
### 6.2.1 Primary map



X Index: 240

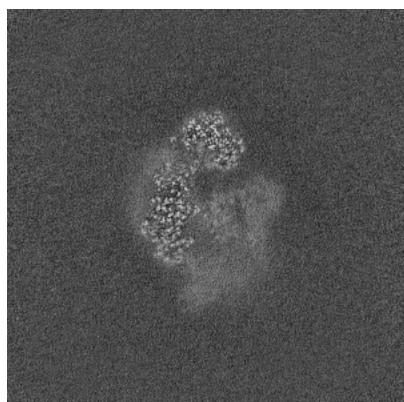


Y Index: 240

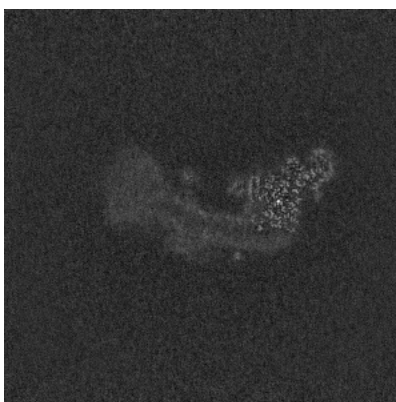


Z Index: 240

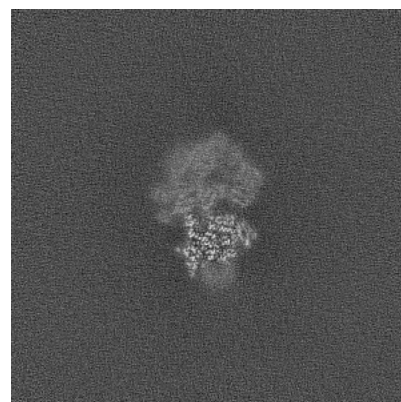
### 6.2.2 Raw map



X Index: 240



Y Index: 240



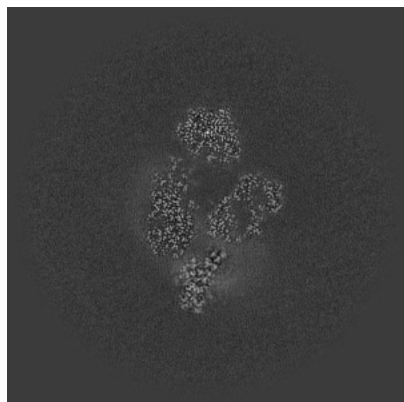
Z Index: 240

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

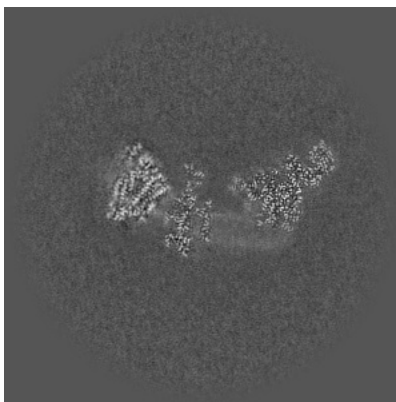


## 6.3 Largest variance slices [i](#)

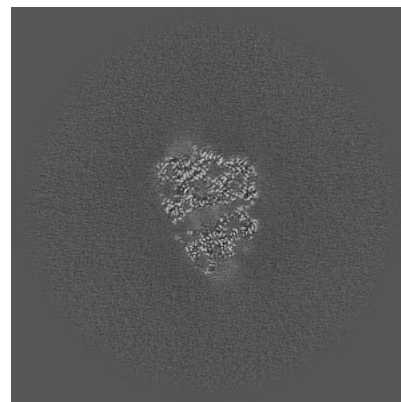
### 6.3.1 Primary map



X Index: 248

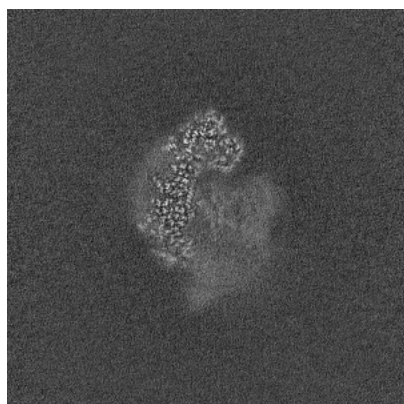


Y Index: 243

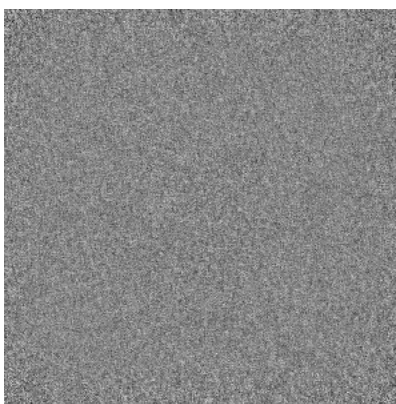


Z Index: 217

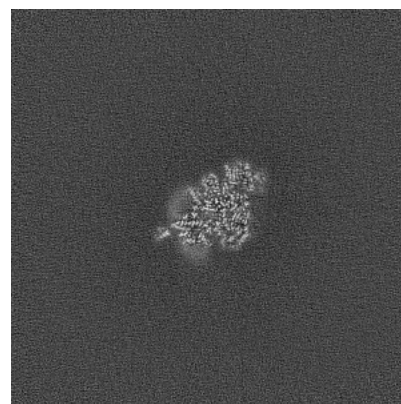
### 6.3.2 Raw map



X Index: 235



Y Index: 0

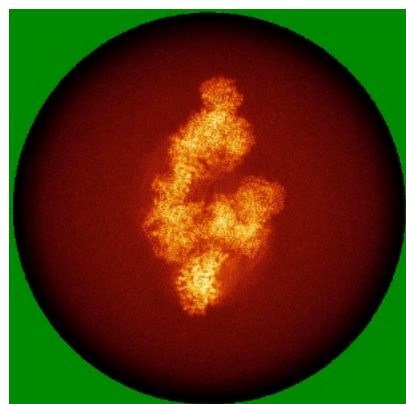


Z Index: 321

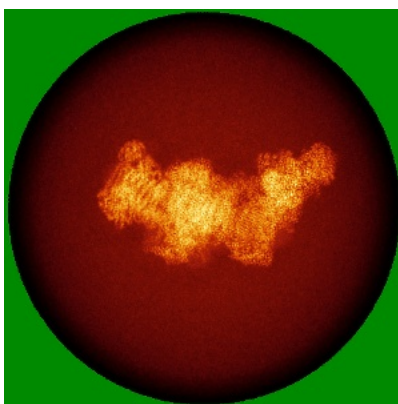
The images above show the largest variance slices of the map in three orthogonal directions.

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

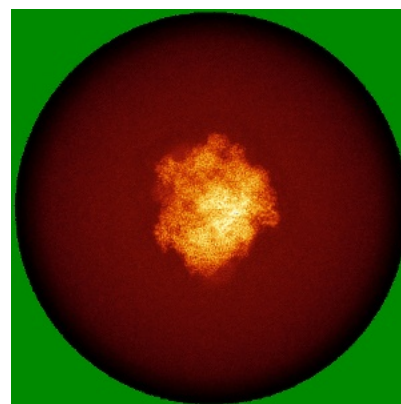
### 6.4.1 Primary map



X

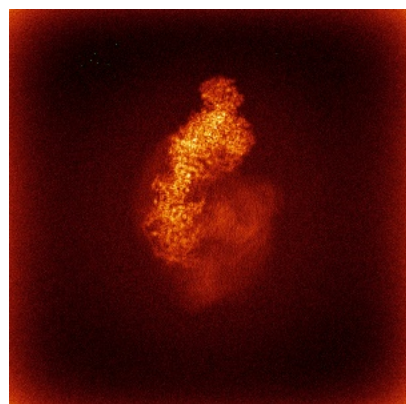


Y

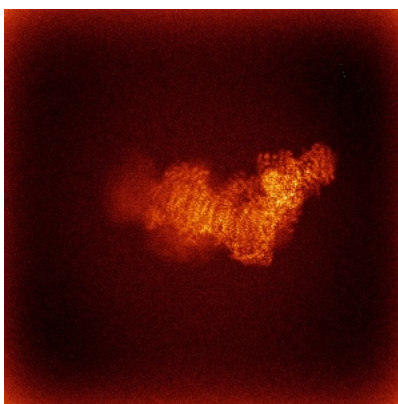


Z

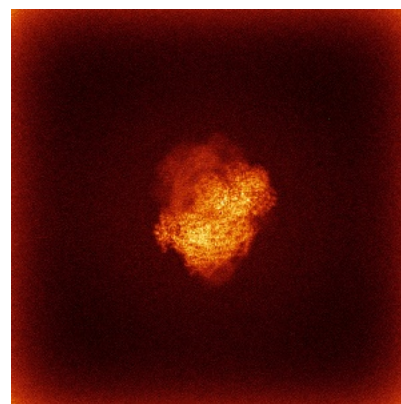
### 6.4.2 Raw map



X



Y

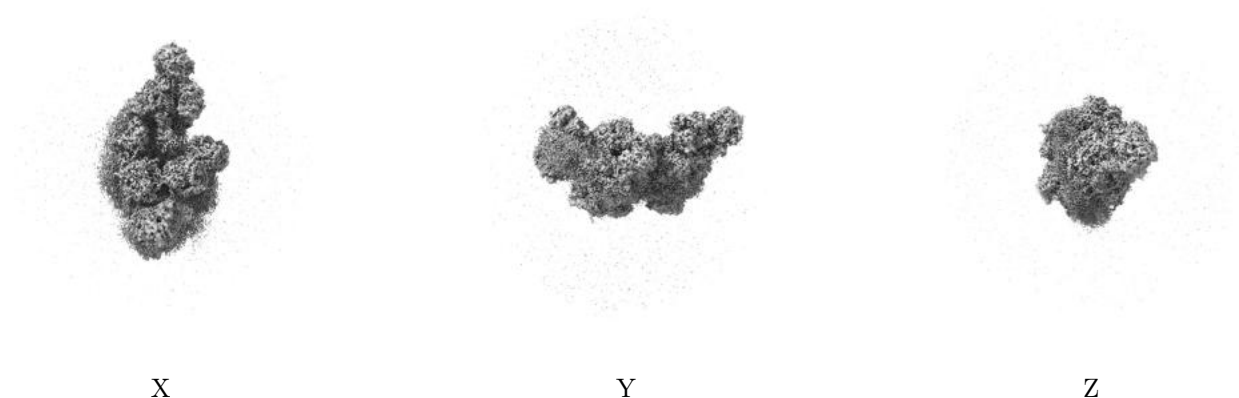


Z

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

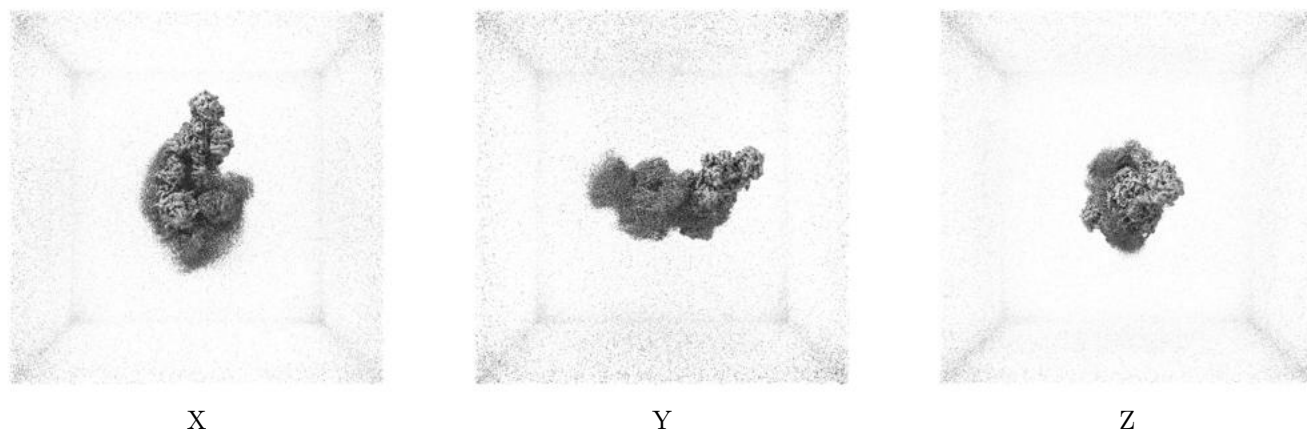
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 4.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

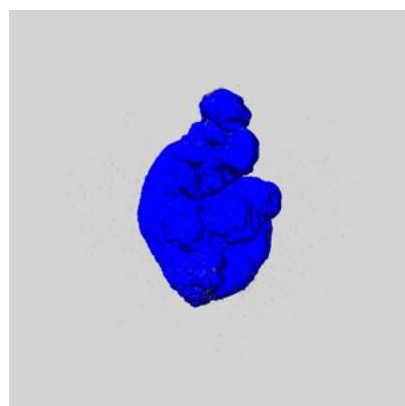
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

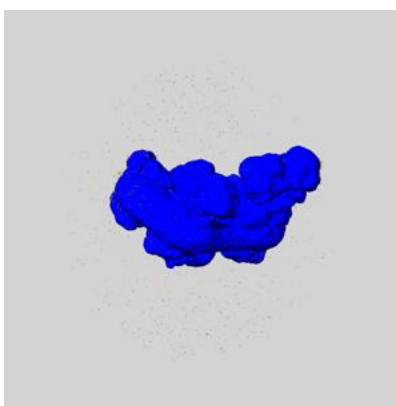
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

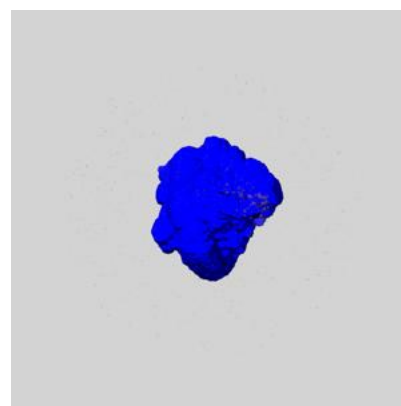
### 6.6.1 emd\_60284\_msk\_1.map [i](#)



X



Y

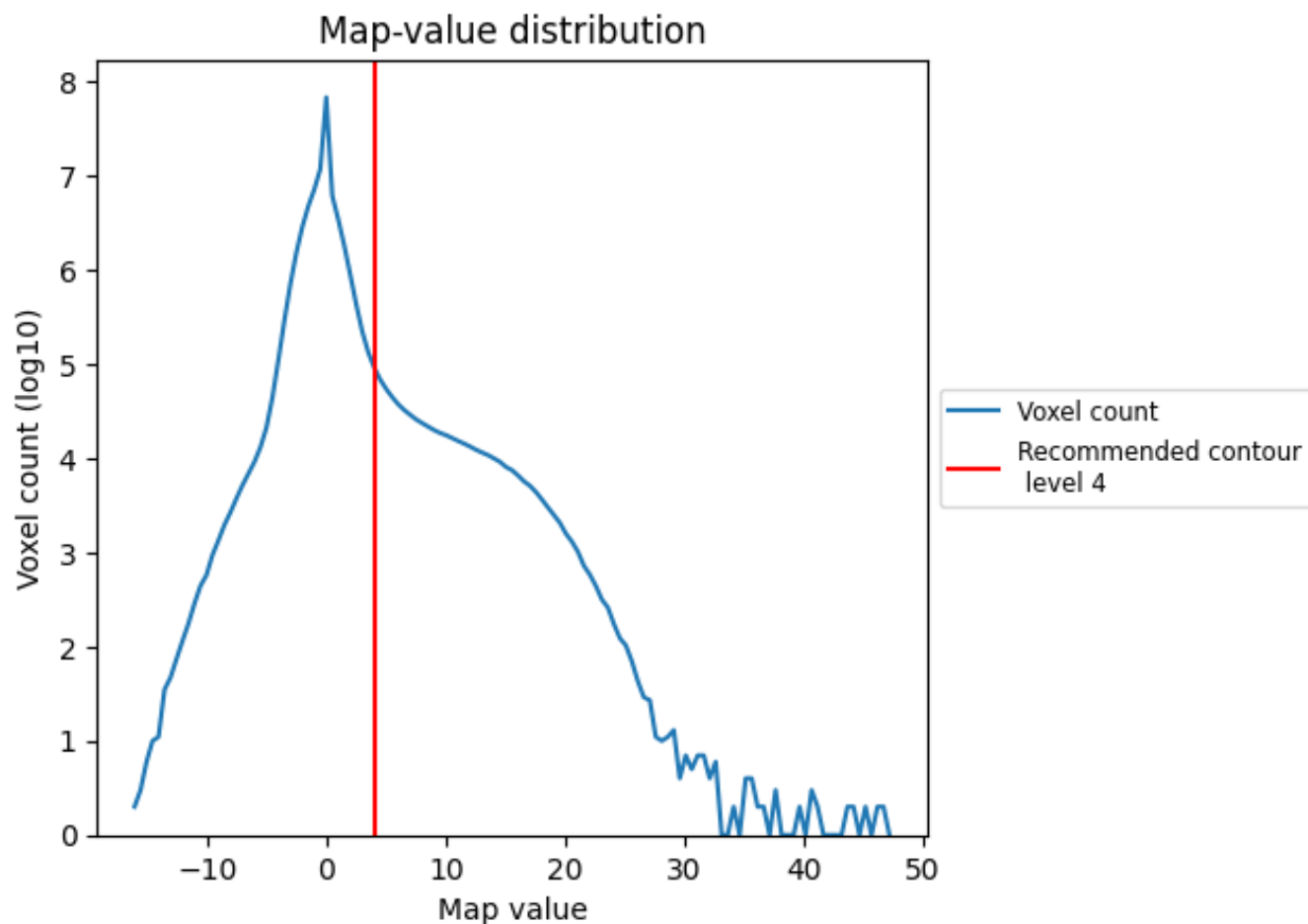


Z

## 7 Map analysis [i](#)

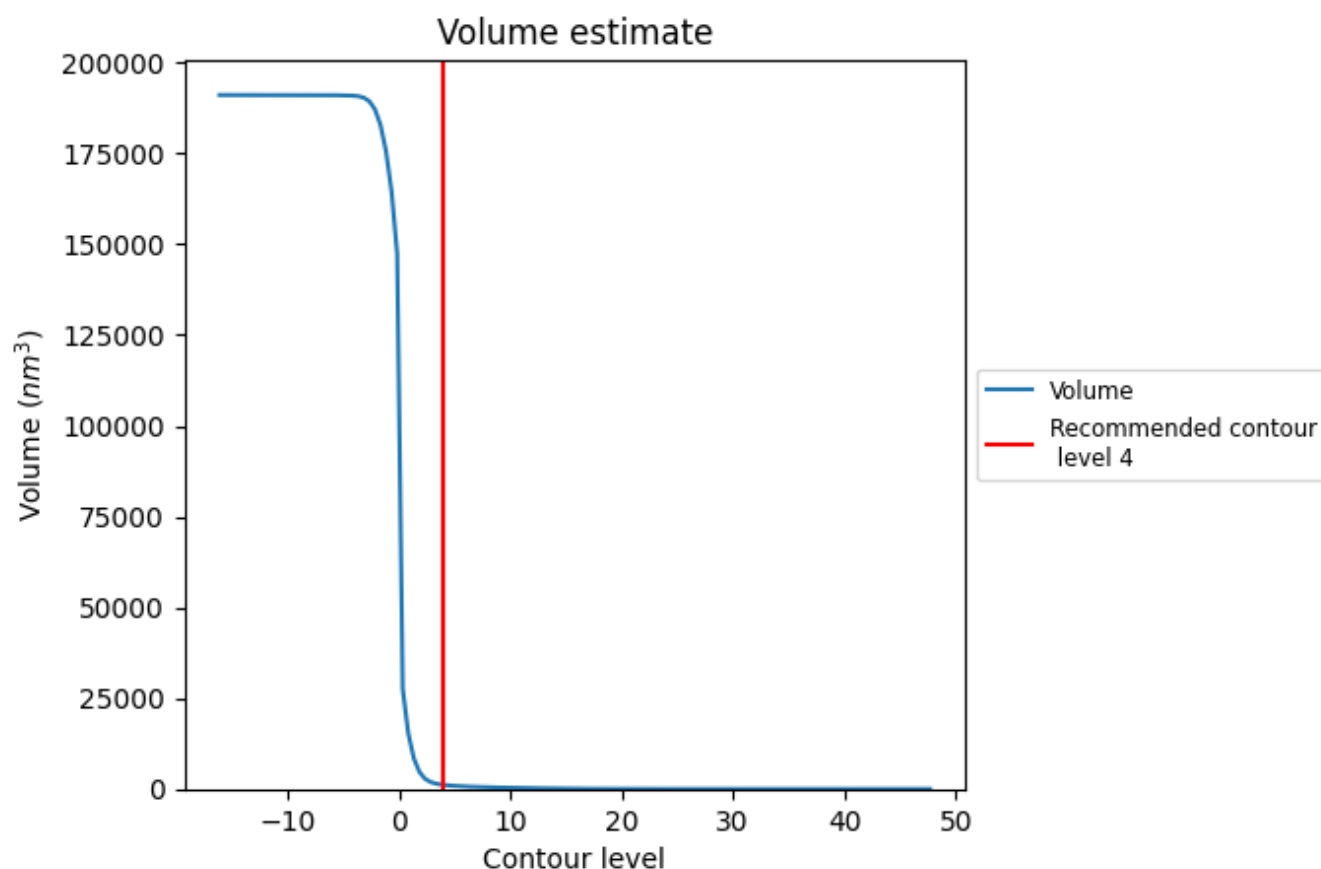
This section contains the results of statistical analysis of the map.

### 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.

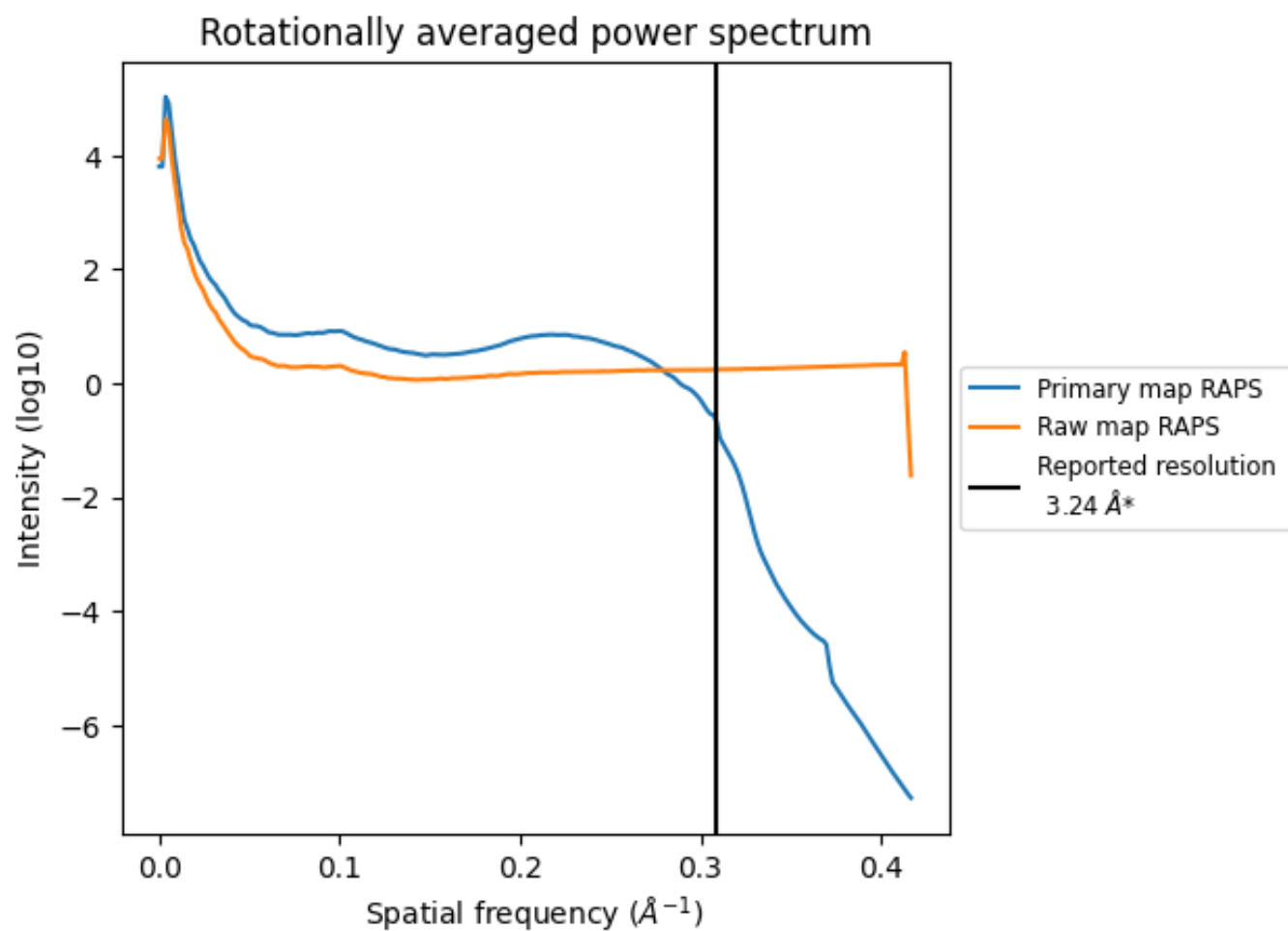
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1136 nm<sup>3</sup>; this corresponds to an approximate mass of 1026 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 ⓘ



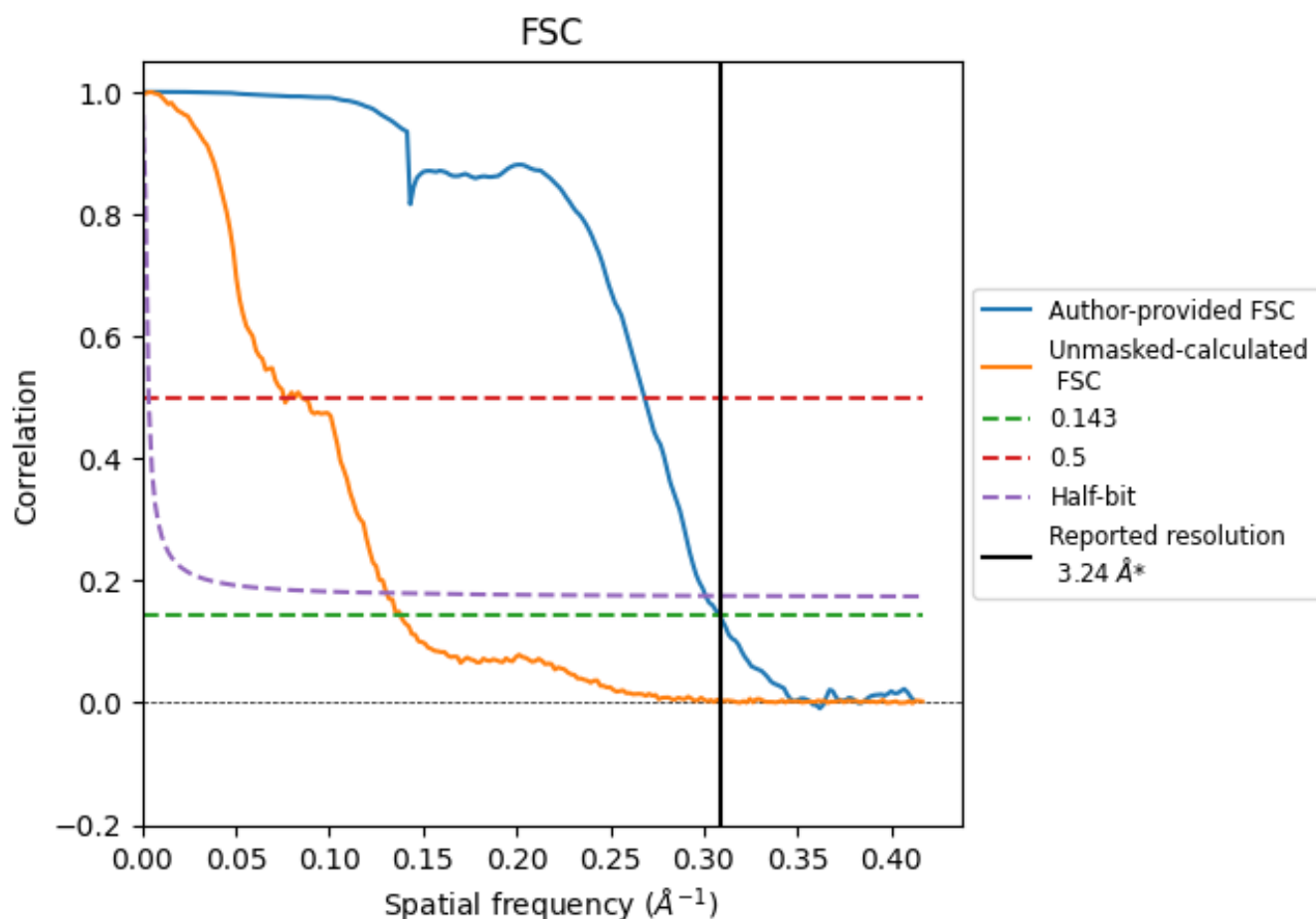
\*Reported resolution corresponds to spatial frequency of  $0.309 \text{ \AA}^{-1}$



## 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 0.309 Å<sup>-1</sup>



## 8.2 Resolution estimates [i](#)

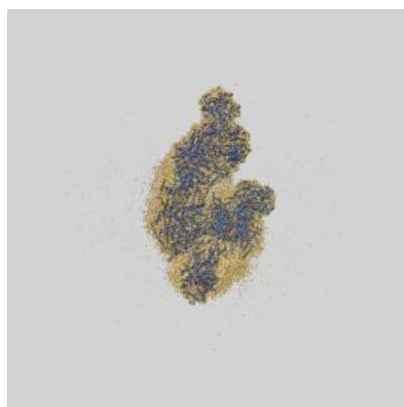
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.24	-	-
Author-provided FSC curve	3.24	3.72	3.32
Unmasked-calculated*	7.25	13.21	7.66

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.25 differs from the reported value 3.24 by more than 10 %

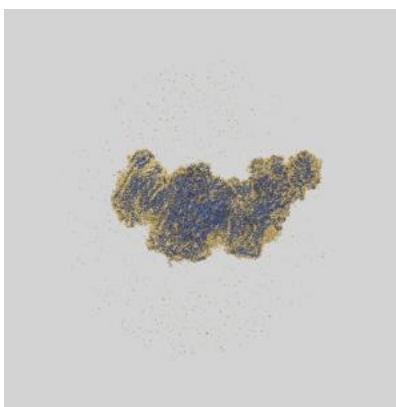
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-60284 and PDB model 8ZO8. Per-residue inclusion information can be found in section [3](#) on page [31](#).

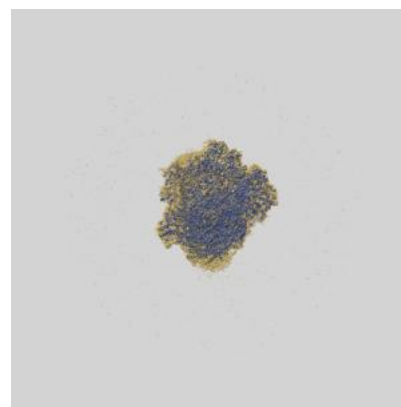
### 9.1 Map-model overlay [i](#)



X



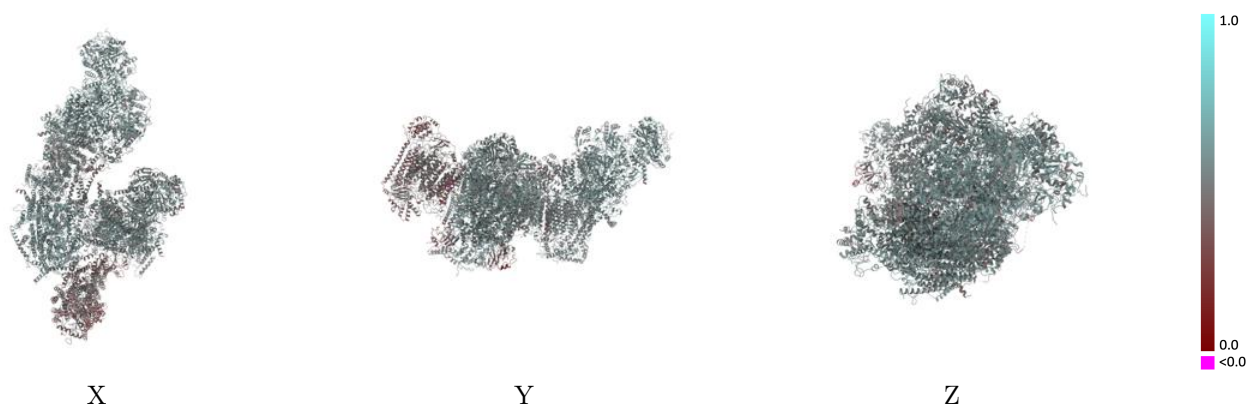
Y



Z

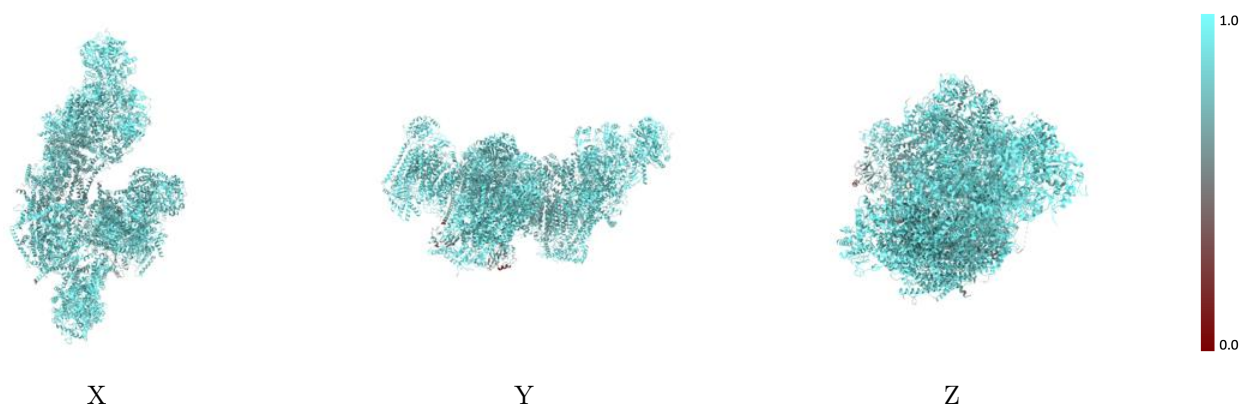
The images above show the 3D surface view of the map at the recommended contour level 4.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



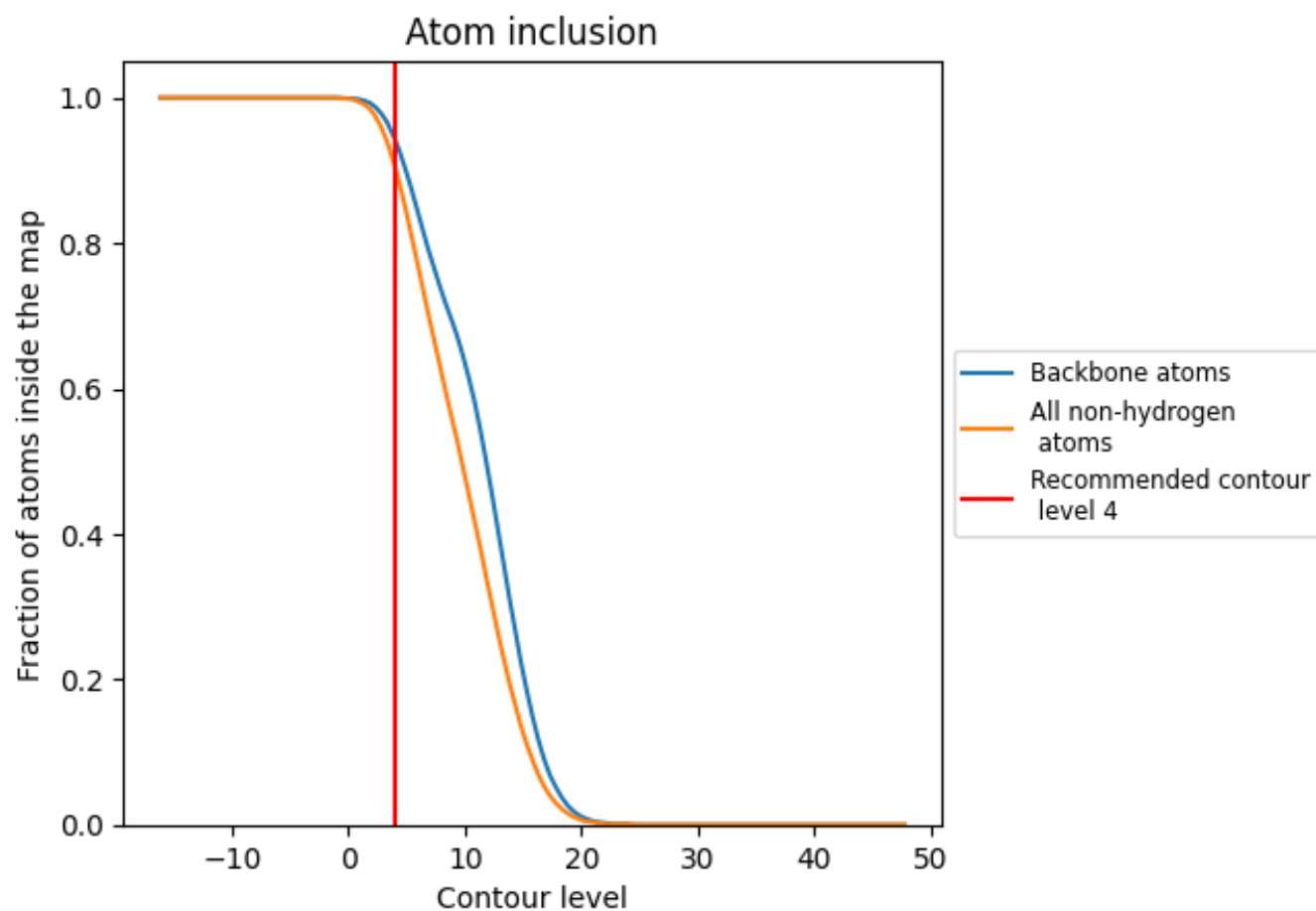
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (4).







































































## 9.4 Atom inclusion ⓘ



At the recommended contour level, 94% of all backbone atoms, 91% 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 (4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9060	 0.5230
4L	 0.8920	 0.5330
5A	 0.8780	 0.3720
5B	 0.9470	 0.3950
6A	 0.9500	 0.3820
6B	 0.9550	 0.4030
6C	 0.8530	 0.3780
7A	 0.9200	 0.3970
7B	 0.8800	 0.4190
7C	 0.9610	 0.4060
8B	 0.9550	 0.4040
A1	 0.9560	 0.5430
A2	 0.9040	 0.5270
A3	 0.9520	 0.5390
A5	 0.9130	 0.5320
A6	 0.9060	 0.5390
A7	 0.8810	 0.5380
A8	 0.9350	 0.5470
A9	 0.9270	 0.5480
AB	 0.7680	 0.4310
AC	 0.9130	 0.5590
AK	 0.8350	 0.5000
AL	 0.8060	 0.5060
AM	 0.8860	 0.5400
AN	 0.9410	 0.5390
B1	 0.8600	 0.5310
B2	 0.9260	 0.5520
B3	 0.8940	 0.5380
B4	 0.8830	 0.5500
B5	 0.9220	 0.5710
B6	 0.8690	 0.5350
B7	 0.9020	 0.5510
B8	 0.9040	 0.5610
B9	 0.9120	 0.5620
BK	 0.8910	 0.5490









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Chain	Atom inclusion	Q-score
BL	 0.8770	 0.5430
C1	 0.9430	 0.4490
C2	 0.9360	 0.4280
C3	 0.9370	 0.4070
C4	 0.9020	 0.3950
CA	 0.8680	 0.5190
CB	 0.9090	 0.5530
N1	 0.9280	 0.5420
N2	 0.9340	 0.5510
N3	 0.9110	 0.5370
N4	 0.9220	 0.5690
N5	 0.9150	 0.5680
N6	 0.8620	 0.4940
QA	 0.9000	 0.5270
QB	 0.9030	 0.5350
QC	 0.9190	 0.5400
QD	 0.9090	 0.5310
QE	 0.7200	 0.4260
QF	 0.8220	 0.4780
QG	 0.9140	 0.5330
QH	 0.9090	 0.5250
QI	 0.9090	 0.5260
QJ	 0.8890	 0.4980
QK	 0.7450	 0.4870
Qa	 0.8870	 0.5260
Qb	 0.9010	 0.5300
Qc	 0.9390	 0.5360
Qd	 0.9110	 0.5390
Qe	 0.6850	 0.4040
Qf	 0.8160	 0.4670
Qg	 0.8860	 0.5230
Qh	 0.8910	 0.5260
Qi	 0.9290	 0.5290
Qj	 0.8840	 0.5140
S1	 0.9300	 0.5560
S2	 0.9260	 0.5650
S3	 0.9660	 0.5800
S4	 0.9240	 0.5630
S5	 0.9210	 0.5370
S6	 0.9210	 0.5560
S7	 0.9440	 0.5670
S8	 0.9650	 0.5740

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Chain	Atom inclusion	Q-score
V1	 0.9330	 0.5460
V2	 0.9140	 0.5410
V3	 0.9450	 0.5440