



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 09:32 PM UTC

PDB ID : 8J9J / pdb_00008j9j
EMDB ID : EMD-36109
Title : Cryo-EM structure of Euglena gracilis complex I, NADH state
Authors : Wu, M.C.; He, Z.X.; Tian, H.T.; Hu, Y.Q.; Han, F.Z.; Zhou, L.
Deposited on : 2023-05-03
Resolution : 3.03 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

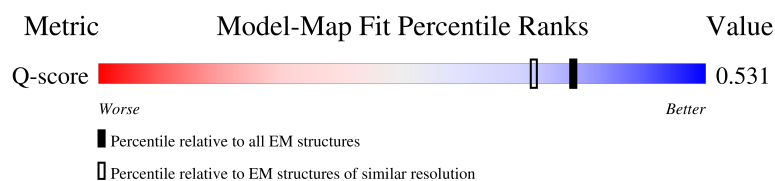
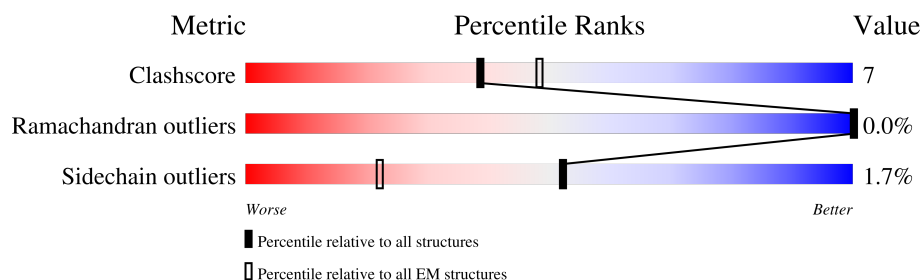
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.03 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13929 (2.53 - 3.53)

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

Mol	Chain	Length	Quality of chain
1	1A	385	
2	1B	527	
3	2B	142	
4	4L	171	

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Mol	Chain	Length	Quality of chain
5	A1	141	
6	A2	193	
7	A3	125	
8	A5	184	
9	A6	437	
10	A7	136	
11	A8	223	
12	A9	489	
13	AB	134	
14	AC	134	
15	AL	281	
16	AM	198	
17	AN	287	
18	B2	145	
19	B3	62	
20	B4	171	
21	B5	140	
22	B6	91	
23	B7	97	
24	B8	176	
25	B9	158	
26	BL	144	
27	BM	112	
28	C4	185	
29	E1	483	

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Mol	Chain	Length	Quality of chain
30	E2	467	
31	E3	434	
32	E4	368	
33	E5	290	
34	E6	371	
35	E8	205	
36	EA	126	
37	EB	101	
38	EC	101	
39	ED	151	
40	FX	325	
41	G1	436	
42	G2	267	
43	G3	261	
44	N1	670	
45	N2	300	
46	N3	293	
46	N6	293	
47	N4	478	
48	N5	584	
49	S2	395	
50	S3	277	
51	S4	208	
52	S5	122	
53	S6	147	

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Mol	Chain	Length	Quality of chain
54	S7	207	
55	S8	212	
56	U1	12	
56	U2	12	
57	V1	526	
58	V2	225	
59	E7	246	

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
61	SF4	S8	297	-	-	X	-

2 Entry composition [i](#)

There are 71 unique types of molecules in this entry. The entry contains 226179 atoms, of which 112544 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 NDUFS1A.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	1A	352	Total	C	H	N	O	S	0	0
			5501	1753	2700	488	537	23		

- Molecule 2 is a protein called NDUFS1B.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	1B	525	Total	C	H	N	O	S	1	0
			8357	2679	4159	743	765	11		

- Molecule 3 is a protein called ND2B.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	2B	140	Total	C	H	N	O	S	0	0
			2059	712	989	172	183	3		

- Molecule 4 is a protein called ND4L.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	4L	108	Total	C	H	N	O	S	0	0
			1768	606	878	133	145	6		

- Molecule 5 is a protein called NDUFA1.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	A1	137	Total	C	H	N	O	S	0	0
			2097	684	1026	192	192	3		

- Molecule 6 is a protein called NDUFA2.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	A2	192	Total	C	H	N	O	S	0	0
			2967	942	1474	267	280	4		

- Molecule 7 is a protein called NDUFA3.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	A3	124	Total	C	H	N	O	S	0	0
			2089	678	1039	191	175	6		

- Molecule 8 is a protein called NDUFA5.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	A5	154	Total	C	H	N	O	S	0	0
			2509	794	1248	221	244	2		

- Molecule 9 is a protein called NDUFA6.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	A6	423	Total	C	H	N	O	S	0	0
			6608	2091	3280	601	632	4		

- Molecule 10 is a protein called NDUFA7.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	A7	136	Total	C	H	N	O	S	0	0
			2272	735	1118	219	194	6		

- Molecule 11 is a protein called NDUFA8.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	A8	223	Total	C	H	N	O	S	0	0
			3548	1160	1726	315	334	13		

- Molecule 12 is a protein called NDUFA9.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	A9	484	Total	C	H	N	O	S	0	0
			7679	2449	3850	662	700	18		

- Molecule 13 is a protein called NDUFAB1-alpha.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	AB	88	Total	C	H	N	O	S	0	0
			1367	437	673	114	139	4		

- Molecule 14 is a protein called NDUFAB1-beta.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	AC	92	Total	C	H	N	O	S	0	0
			1418	461	697	116	140	4		

- Molecule 15 is a protein called NDUFA12.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	AL	265	Total	C	H	N	O	S	0	0
			4409	1439	2172	414	379	5		

- Molecule 16 is a protein called NDUFA13.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	AM	184	Total	C	H	N	O	S	0	0
			2935	953	1448	264	263	7		

- Molecule 17 is a protein called NDUFA11.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	AN	287	Total	C	H	N	O	S	0	0
			4573	1501	2267	396	399	10		

- Molecule 18 is a protein called NDUFB2.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	B2	105	Total	C	H	N	O	S	0	0
			1770	604	857	142	166	1		

- Molecule 19 is a protein called NDUFB3.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	B3	61	Total	C	H	N	O	S	0	0
			758	292	309	88	68	1		

- Molecule 20 is a protein called NDUFB4.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	B4	171	Total	C	H	N	O	S	0	0
			2735	885	1358	250	236	6		

- Molecule 21 is a protein called NDUFB5.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	B5	140	Total	C	H	N	O	S	0	0
			2181	708	1069	207	195	2		

- Molecule 22 is a protein called NDUFB6.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	B6	91	Total	C	H	N	O	S	0	0
			1520	509	747	132	128	4		

- Molecule 23 is a protein called NDUFB7.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	B7	97	Total	C	H	N	O	S	0	0
			1692	536	835	165	149	7		

- Molecule 24 is a protein called NDUFB8.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	B8	147	Total	C	H	N	O	S	0	0
			2351	804	1127	199	213	8		

- Molecule 25 is a protein called NDUFB9.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	B9	151	Total	C	H	N	O	S	0	0
			2443	795	1207	216	222	3		

- Molecule 26 is a protein called NDUFB10.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	BL	144	Total	C	H	N	O	S	0	0
			2406	786	1179	215	216	10		

- Molecule 27 is a protein called NDUFB11.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	BM	112	Total	C	H	N	O	S	0	0
			1737	577	827	164	167	2		

- Molecule 28 is a protein called NDUF2.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	C4	183	Total	C	H	N	O	S	0	0
			3062	1000	1517	268	271	6		

- Molecule 29 is a protein called NDUEG1.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	E1	450	Total	C	H	N	O	S	0	0
			7008	2244	3496	601	654	13		

- Molecule 30 is a protein called NDUEG2.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	E2	466	Total	C	H	N	O	S	0	0
			7103	2286	3540	618	655	4		

- Molecule 31 is a protein called NDUEG3.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	E3	432	Total	C	H	N	O	S	0	0
			6518	2071	3263	565	612	7		

- Molecule 32 is a protein called NDUEG4.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	E4	351	Total	C	H	N	O	S	0	0
			5502	1774	2732	477	504	15		

- Molecule 33 is a protein called NDUEG5.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	E5	276	Total	C	H	N	O	S	0	0
			4046	1265	2069	341	369	2		

- Molecule 34 is a protein called NDUEG6.

Mol	Chain	Residues	Atoms						AltConf	Trace
34	E6	318	Total	C	H	N	O	S	0	0
			5228	1703	2554	477	482	12		

- Molecule 35 is a protein called NDUEG8.

Mol	Chain	Residues	Atoms						AltConf	Trace
35	E8	205	Total	C	H	N	O	S	0	0
			3354	1100	1663	288	292	11		

- Molecule 36 is a protein called NDUEG10.

Mol	Chain	Residues	Atoms						AltConf	Trace
36	EA	124	Total	C	H	N	O	S	0	0
			1793	630	832	172	156	3		

- Molecule 37 is a protein called NDUEG11.

Mol	Chain	Residues	Atoms						AltConf	Trace
37	EB	101	Total	C	H	N	O	S	0	0
			1405	473	631	150	144	7		

- Molecule 38 is a protein called NDUEG12.

Mol	Chain	Residues	Atoms						AltConf	Trace
38	EC	85	Total	C	H	N	O	S	0	0
			1323	424	663	116	118	2		

- Molecule 39 is a protein called NDUEG13.

Mol	Chain	Residues	Atoms						AltConf	Trace
39	ED	138	Total	C	H	N	O	S	0	0
			2273	736	1131	205	196	5		

- Molecule 40 is a protein called NDUFEX.

Mol	Chain	Residues	Atoms						AltConf	Trace
40	FX	237	Total	C	H	N	O	S	0	0
			3816	1263	1849	338	359	7		

- Molecule 41 is a protein called NDUCA1.

Mol	Chain	Residues	Atoms						AltConf	Trace
41	G1	403	Total	C	H	N	O	S	0	0
			6146	1979	2999	558	594	16		

- Molecule 42 is a protein called NDUCA2.

Mol	Chain	Residues	Atoms						AltConf	Trace
42	G2	236	Total	C	H	N	O	S	0	0
			3650	1138	1846	323	338	5		

- Molecule 43 is a protein called NDUCA3.

Mol	Chain	Residues	Atoms						AltConf	Trace
43	G3	261	Total	C	H	N	O	S	0	0
			3905	1226	1944	356	373	6		

- Molecule 44 is a protein called ND1.

Mol	Chain	Residues	Atoms						AltConf	Trace
44	N1	310	Total	C	H	N	O	S	0	0
			5331	1783	2726	380	435	7		

- Molecule 45 is a protein called ND2A.

Mol	Chain	Residues	Atoms						AltConf	Trace
45	N2	296	Total	C	H	N	O	S	0	0
			5101	1725	2589	362	418	7		

- Molecule 46 is a protein called ND3.

Mol	Chain	Residues	Atoms						AltConf	Trace
46	N3	121	Total	C	H	N	O	S	0	0
			2094	720	1057	143	172	2		
46	N6	154	Total	C	H	N	O	S	0	0
			2642	857	1385	187	210	3		

- Molecule 47 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms						AltConf	Trace
47	N4	478	Total	C	H	N	O	S	0	0
			8215	2743	4214	582	663	13		

- Molecule 48 is a protein called ND5.

Mol	Chain	Residues	Atoms						AltConf	Trace
48	N5	584	Total	C	H	N	O	S	0	0
			9869	3293	5032	711	808	25		

- Molecule 49 is a protein called NDUFS2.

Mol	Chain	Residues	Atoms						AltConf	Trace
49	S2	394	Total	C	H	N	O	S	0	0
			6274	2041	3101	541	569	22		

- Molecule 50 is a protein called NDUFS3.

Mol	Chain	Residues	Atoms						AltConf	Trace
50	S3	248	Total	C	H	N	O	S	0	0
			3978	1307	1928	346	384	13		

- Molecule 51 is a protein called NDUFS4.

Mol	Chain	Residues	Atoms						AltConf	Trace
51	S4	190	Total	C	H	N	O	S	0	0
			3038	956	1502	300	273	7		

- Molecule 52 is a protein called NDUFS5.

Mol	Chain	Residues	Atoms						AltConf	Trace
52	S5	122	Total	C	H	N	O	S	0	0
			1886	625	895	173	188	5		

- Molecule 53 is a protein called NDUFS6.

Mol	Chain	Residues	Atoms						AltConf	Trace
53	S6	147	Total	C	H	N	O	S	0	0
			2392	759	1192	225	208	8		

- Molecule 54 is a protein called NDUFS7.

Mol	Chain	Residues	Atoms						AltConf	Trace
54	S7	201	Total	C	H	N	O	S	0	0
			3045	975	1500	272	284	14		

- Molecule 55 is a protein called NDUFS8.

Mol	Chain	Residues	Atoms						AltConf	Trace
55	S8	182	Total	C	H	N	O	S	0	0
			2843	915	1392	245	275	16		

- Molecule 56 is a protein called UNK-UNK-UNK-UNK-UNK-UNK-UNK-UNK-UNK-UNK-UNK-UNK.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	U1	12	Total	C	H	N	O	0	0
			76	36	16	12	12		
56	U2	12	Total	C	H	N	O	0	0
			76	36	16	12	12		

- Molecule 57 is a protein called NDUFV1.

Mol	Chain	Residues	Atoms						AltConf	Trace
57	V1	504	Total	C	H	N	O	S	0	0
			7724	2463	3827	680	727	27		

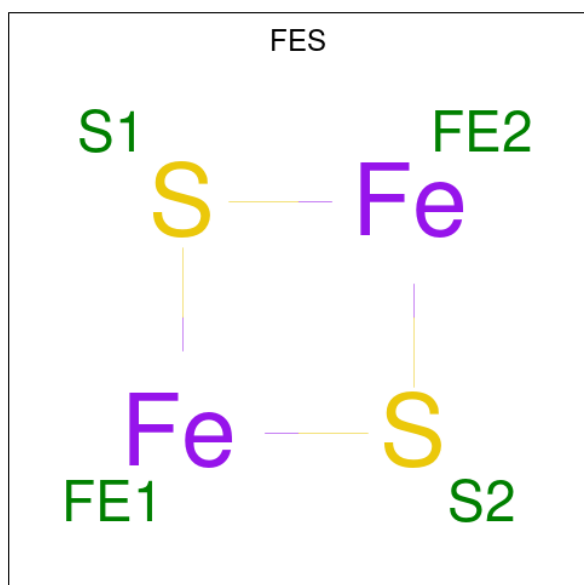
- Molecule 58 is a protein called NDUFV2.

Mol	Chain	Residues	Atoms						AltConf	Trace
58	V2	225	Total	C	H	N	O	S	0	0
			3460	1124	1701	299	319	17		

- Molecule 59 is a protein called NDUEG7.

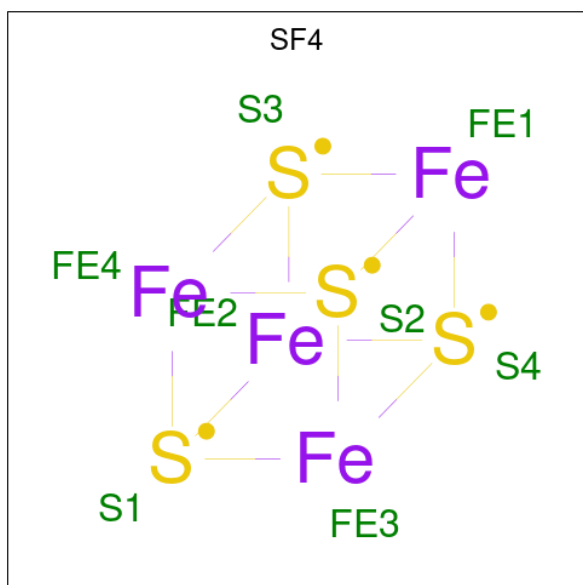
Mol	Chain	Residues	Atoms						AltConf	Trace
59	E7	246	Total	C	H	N	O	S	0	0
			3780	1205	1892	332	344	7		

- Molecule 60 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



Mol	Chain	Residues	Atoms			AltConf
60	1A	1	Total	Fe	S	0
			4	2	2	
60	V2	1	Total	Fe	S	0
			4	2	2	

- Molecule 61 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).

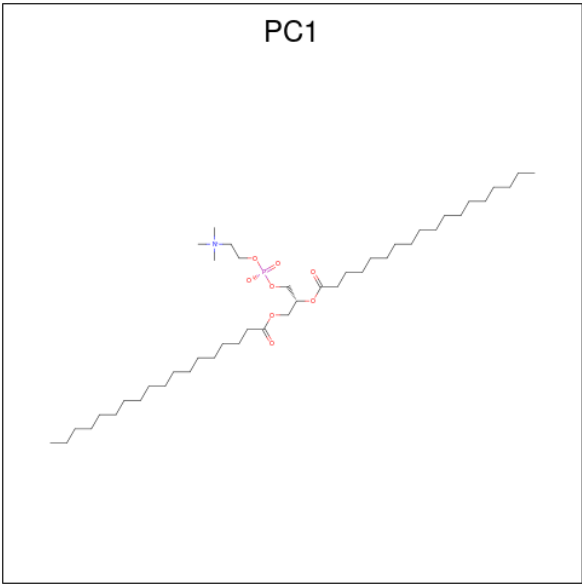


Mol	Chain	Residues	Atoms			AltConf
61	1A	1	Total	Fe	S	0
			8	4	4	
61	1A	1	Total	Fe	S	0
			8	4	4	
61	S7	1	Total	Fe	S	0
			8	4	4	
61	S8	1	Total	Fe	S	0
			8	4	4	
61	S8	1	Total	Fe	S	0
			8	4	4	
61	V1	1	Total	Fe	S	0
			8	4	4	

- Molecule 62 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
62	1A	1	Total	K	0
			1	1	

- Molecule 63 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: C₄₄H₈₈NO₈P).



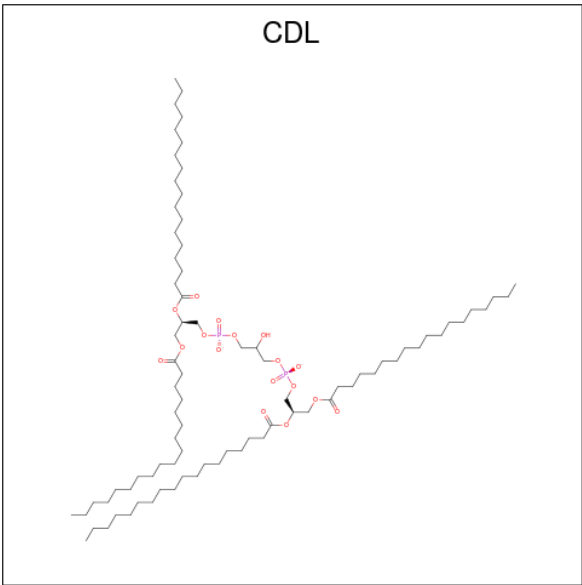
Mol	Chain	Residues	Atoms						AltConf
63	A1	1	Total	C	H	N	O	P	0
			124	39	75	1	8	1	
63	A1	1	Total	C	H	N	O	P	0
			67	21	36	1	8	1	
63	A9	1	Total	C	H	N	O	P	0
			73	23	40	1	8	1	
63	A9	1	Total	C	H	N	O	P	0
			73	23	40	1	8	1	
63	AL	1	Total	C	H	N	O	P	0
			127	40	77	1	8	1	
63	AM	1	Total	C	H	N	O	P	0
			124	39	75	1	8	1	
63	AM	1	Total	C	H	N	O	P	0
			121	38	73	1	8	1	
63	AN	1	Total	C	H	N	O	P	0
			121	38	73	1	8	1	
63	B5	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
63	B5	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
63	C4	1	Total	C	H	N	O	P	0
			88	28	50	1	8	1	
63	E4	1	Total	C	H	N	O	P	0
			130	41	79	1	8	1	

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Mol	Chain	Residues	Atoms						AltConf
63	E8	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
63	E8	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
63	E8	1	Total 73	C 23	H 40	N 1	O 8	P 1	0
63	E8	1	Total 64	C 20	H 34	N 1	O 8	P 1	0
63	ED	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
63	N1	1	Total 124	C 39	H 75	N 1	O 8	P 1	0
63	N1	1	Total 94	C 30	H 54	N 1	O 8	P 1	0
63	N2	1	Total 85	C 27	H 48	N 1	O 8	P 1	0
63	N3	1	Total 103	C 32	H 61	N 1	O 8	P 1	0
63	N4	1	Total 91	C 29	H 52	N 1	O 8	P 1	0
63	N4	1	Total 73	C 23	H 40	N 1	O 8	P 1	0
63	N5	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
63	N5	1	Total 97	C 31	H 56	N 1	O 8	P 1	0
63	N5	1	Total 82	C 26	H 46	N 1	O 8	P 1	0

- Molecule 64 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



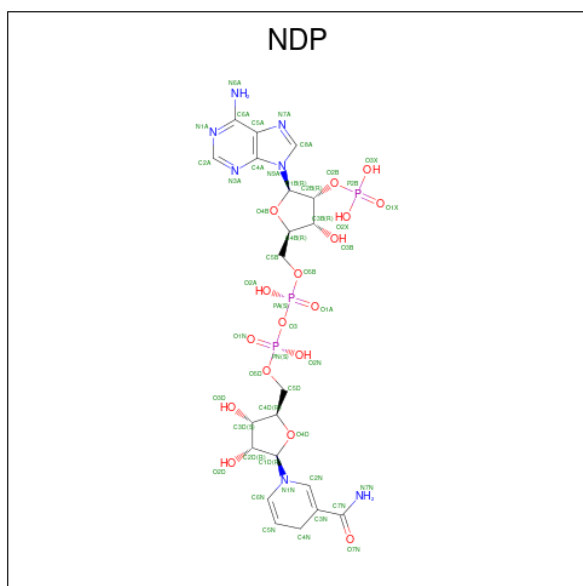
Mol	Chain	Residues	Atoms					AltConf
64	A3	1	Total	C	H	O	P	0
			118	39	60	17	2	
64	AL	1	Total	C	H	O	P	0
			148	49	80	17	2	
64	AL	1	Total	C	H	O	P	0
			136	45	72	17	2	
64	AL	1	Total	C	H	O	P	0
			154	51	84	17	2	
64	AM	1	Total	C	H	O	P	0
			163	53	91	17	2	
64	AM	1	Total	C	H	O	P	0
			163	53	91	17	2	
64	AM	1	Total	C	H	O	P	0
			163	53	91	17	2	
64	B3	1	Total	C	H	O	P	0
			139	46	74	17	2	
64	B5	1	Total	C	H	O	P	0
			118	39	60	17	2	
64	C4	1	Total	C	H	O	P	0
			235	75	141	17	2	
64	C4	1	Total	C	H	O	P	0
			151	50	82	17	2	
64	E6	1	Total	C	H	O	P	0
			136	45	72	17	2	
64	EA	1	Total	C	H	O	P	0
			121	40	62	17	2	
64	EA	1	Total	C	H	O	P	0
			109	36	54	17	2	

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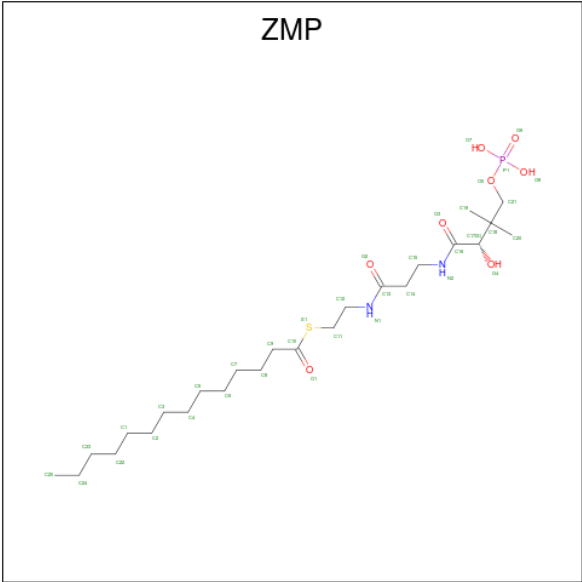
Mol	Chain	Residues	Atoms					AltConf
64	N4	1	Total	C	H	O	P	0
			247	79	149	17	2	
64	N5	1	Total	C	H	O	P	0
			157	51	87	17	2	
64	N5	1	Total	C	H	O	P	0
			229	74	136	17	2	
64	E7	1	Total	C	H	O	P	0
			148	49	80	17	2	

- Molecule 65 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



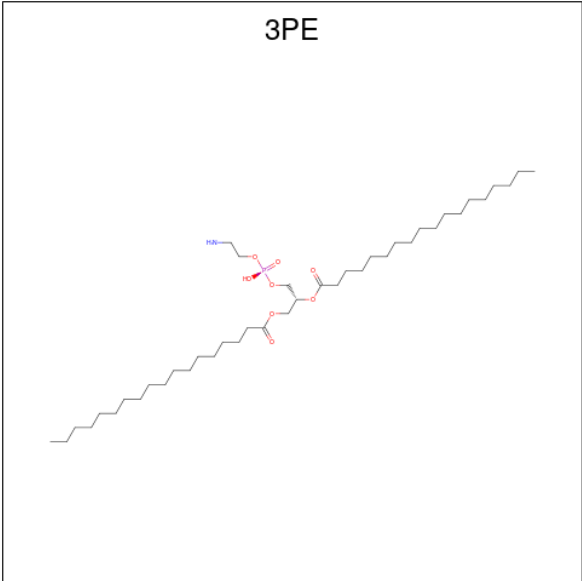
Mol	Chain	Residues	Atoms					AltConf	
65	A9	1	Total	C	H	N	O	P	0
			74	21	26	7	17	3	

- Molecule 66 is S-[2-(N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (CCD ID: ZMP) (formula: $C_{25}H_{49}N_2O_8PS$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 67 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: C₄₁H₈₂NO₈P).



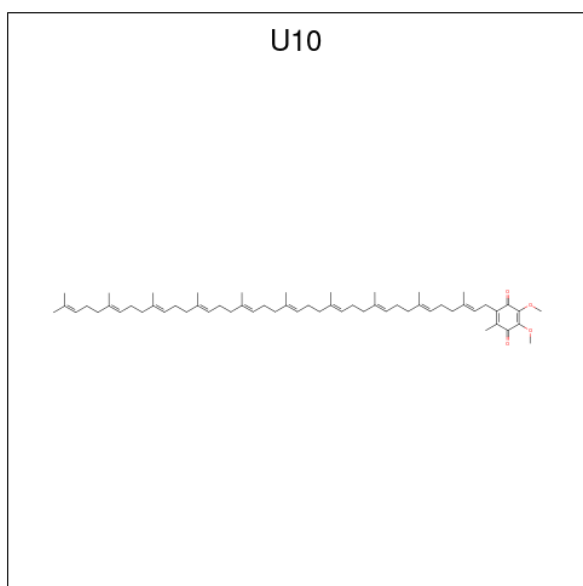
Mol	Chain	Residues	Atoms						AltConf
67	AN	1	Total	C	H	N	O	P	0
			132	41	81	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
67	G1	1	Total	C	H	N	O	P
			96	30	56	1	8	1
67	N4	1	Total	C	H	N	O	P
			96	31	55	1	8	1
67	N5	1	Total	C	H	N	O	P
			132	41	81	1	8	1

- Molecule 68 is UBIQUINONE-10 (CCD ID: U10) (formula: $C_{59}H_{90}O_4$) (labeled as "Ligand of Interest" by depositor).

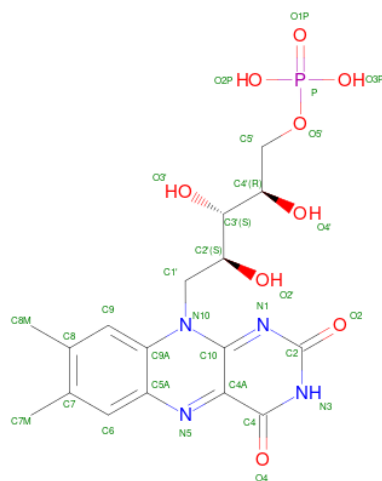


Mol	Chain	Residues	Atoms				AltConf
68	N4	1	Total	C	H	O	
			98	39	55	4	0

- Molecule 69 is ZINC ION (CCD ID: ZN) (formula: Zn).

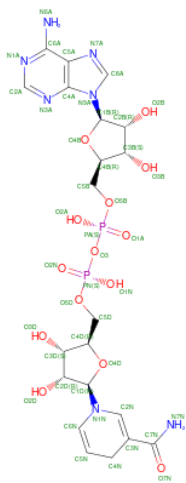
Mol	Chain	Residues	Atoms		AltConf
69	S6	1	Total	Zn	
			1	1	0
69	E7	1	Total	Zn	
			1	1	0

- Molecule 70 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



Mol	Chain	Residues	Atoms					AltConf	
70	V1	1	Total	C	H	N	O	P	0
			50	17	19	4	9	1	

- Molecule 71 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$).

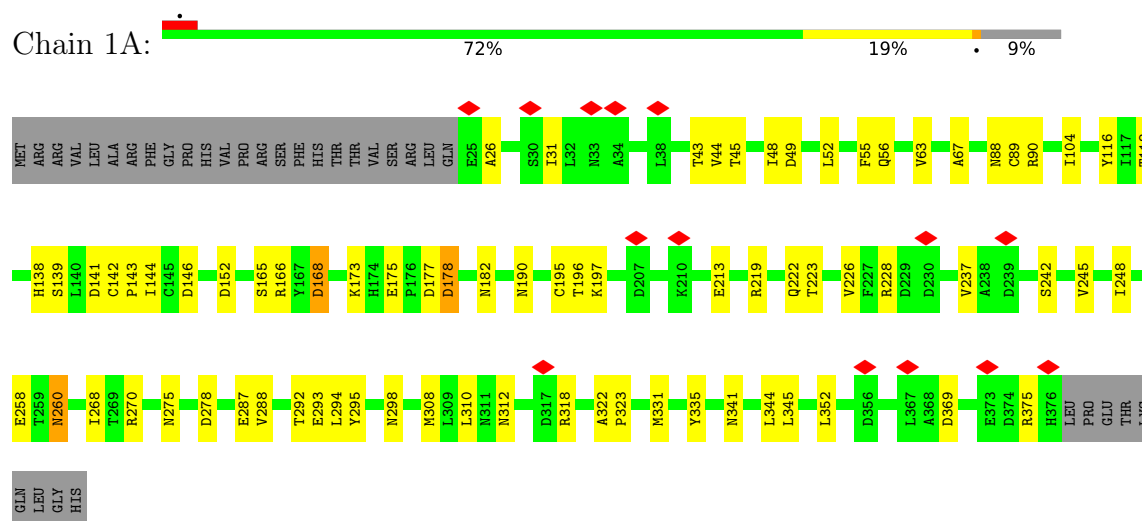


Mol	Chain	Residues	Atoms					AltConf
71	V1	1	Total 44	C 21	N 7	O 14	P 2	0

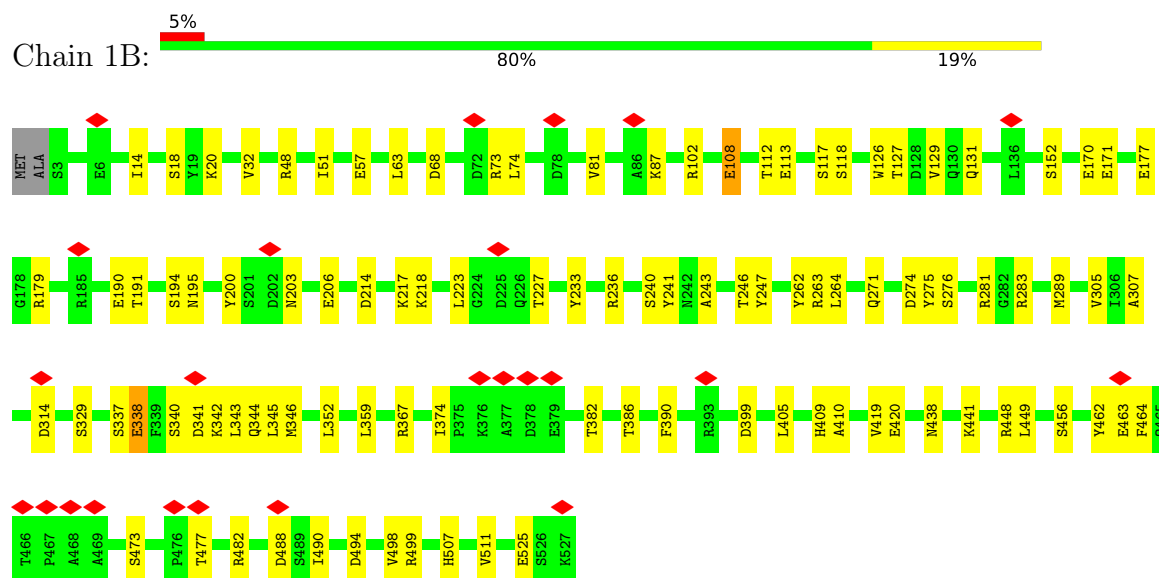
3 Residue-property plots

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.

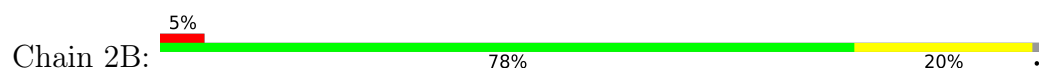
• Molecule 1: NDUFS1A



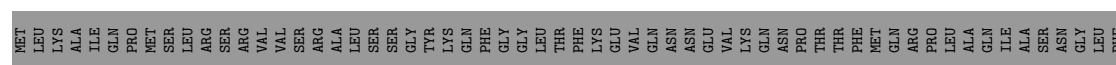
• Molecule 2: NDUFS1B



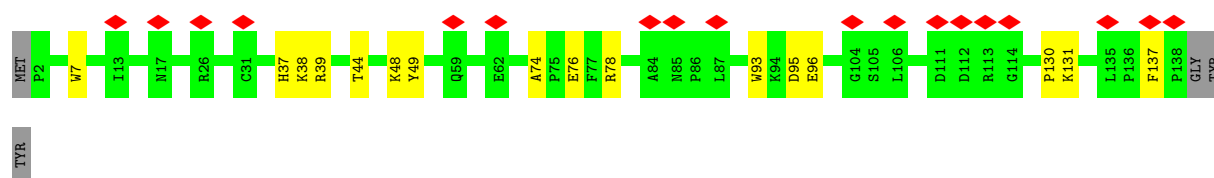
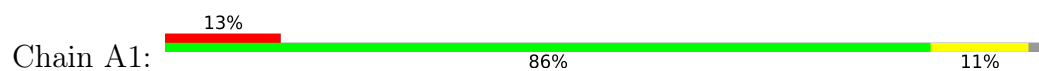
• Molecule 3: ND2B



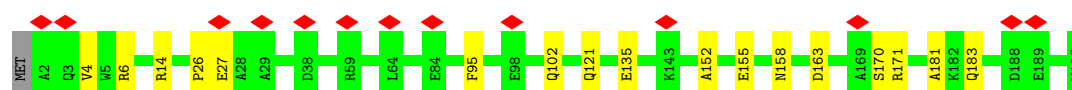
- Molecule 4: ND4L



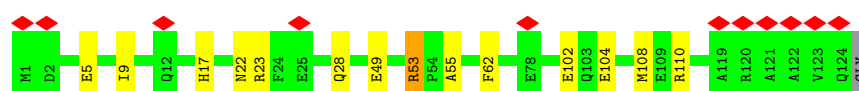
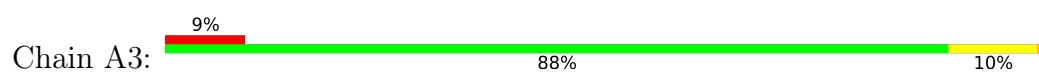
- Molecule 5: NDUFA1



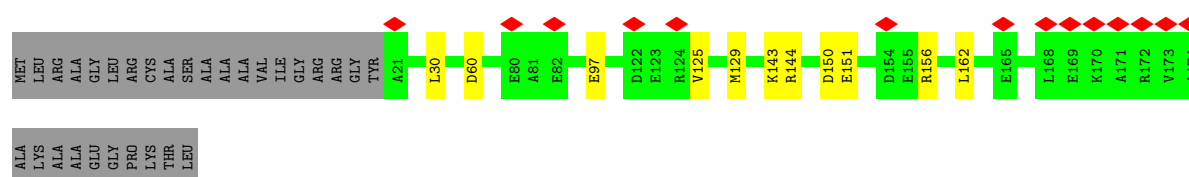
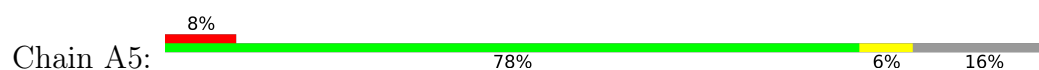
- Molecule 6: NDUFA2



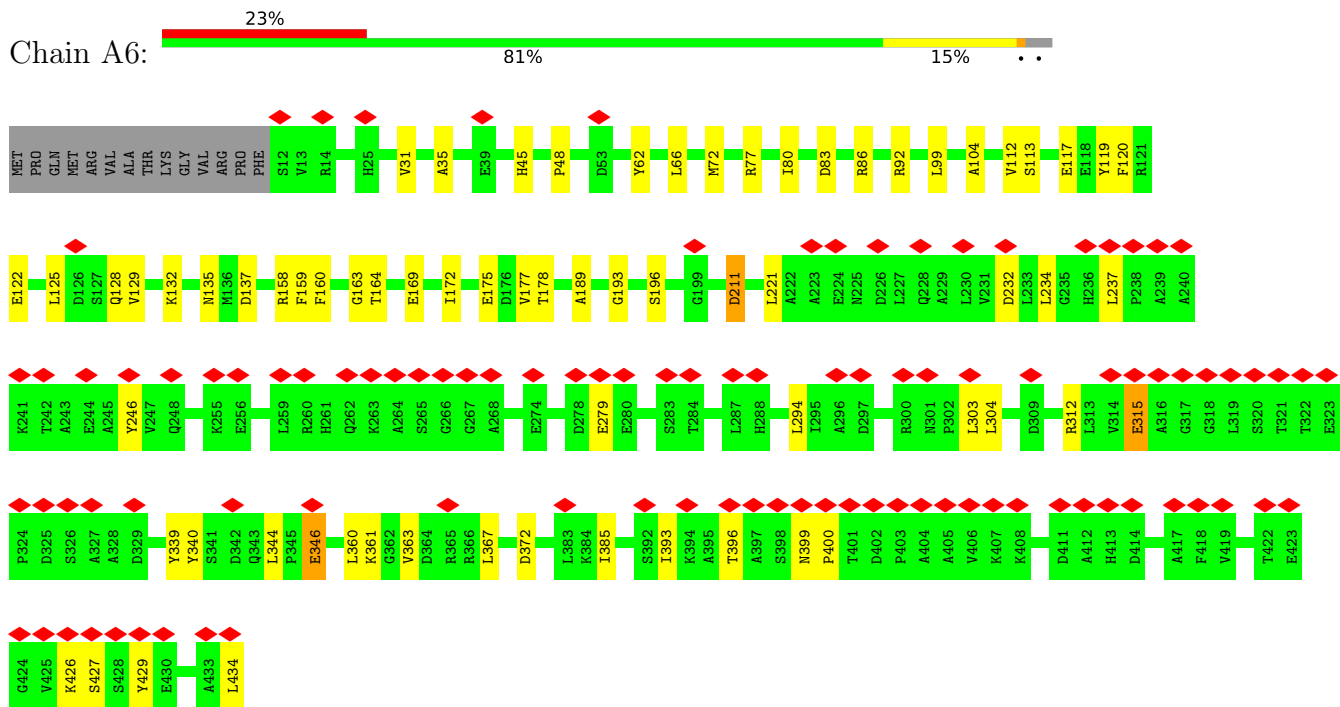
- Molecule 7: NDUFA3



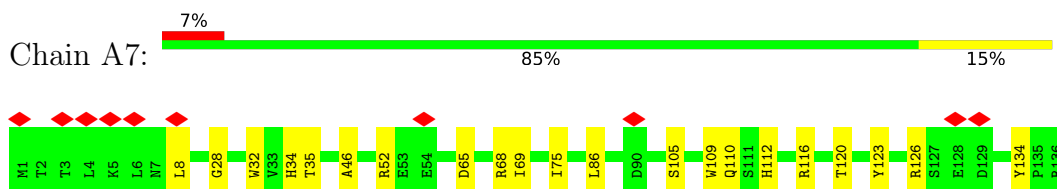
- Molecule 8: NDUFA5



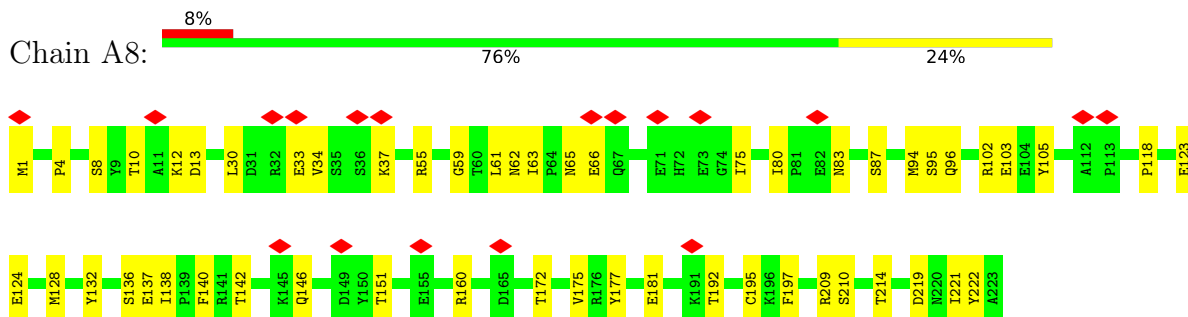
- Molecule 9: NDUFA6



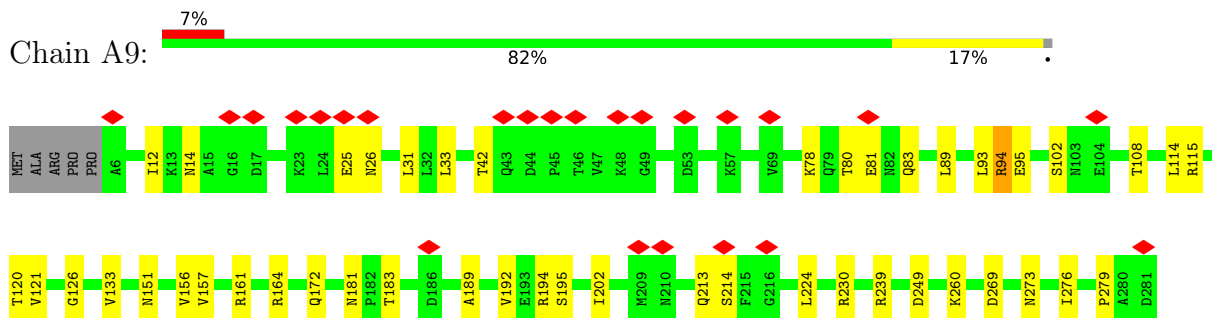
- Molecule 10: NDUFA7

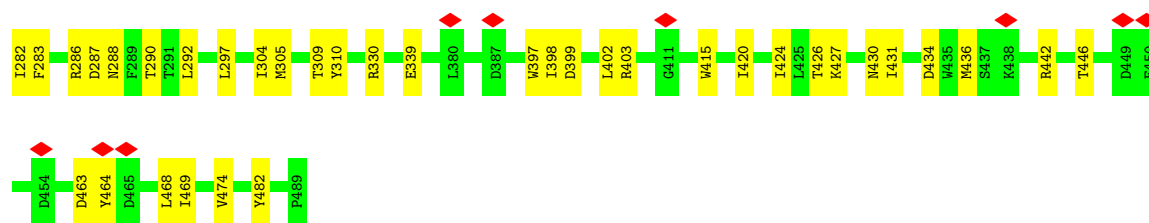


- Molecule 11: NDUFA8

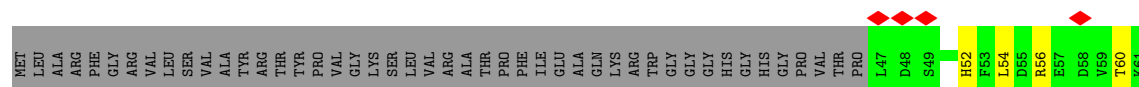


- Molecule 12: NDUFA9

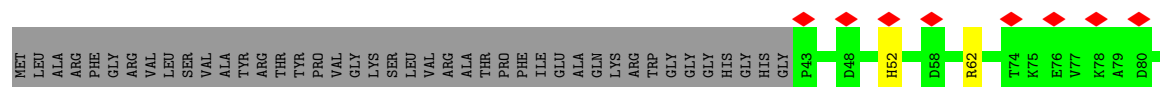




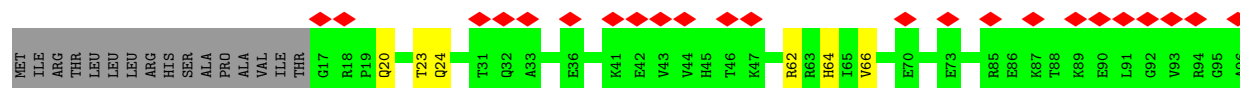
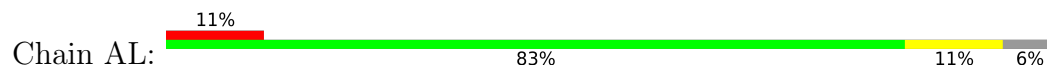
• Molecule 13: NDUFAB1-alpha



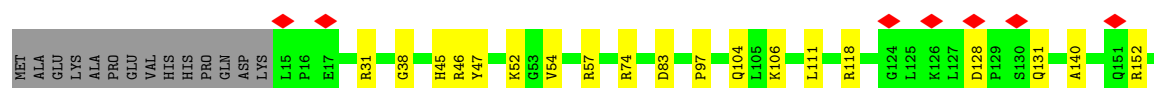
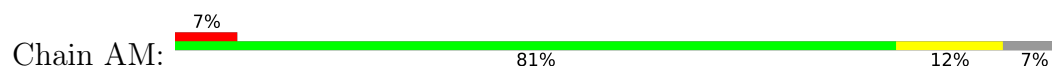
• Molecule 14: NDUFAB1-beta

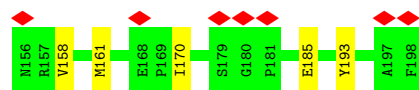


• Molecule 15: NDUFA12



• Molecule 16: NDUFA13

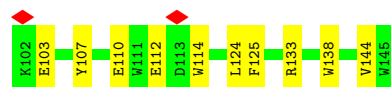
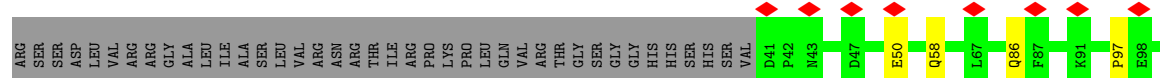




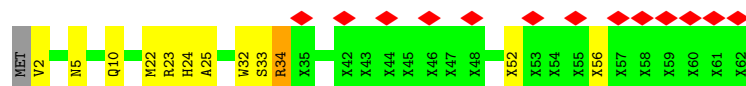
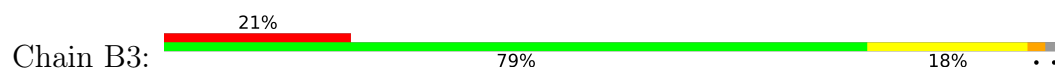
• Molecule 17: NDUFA11



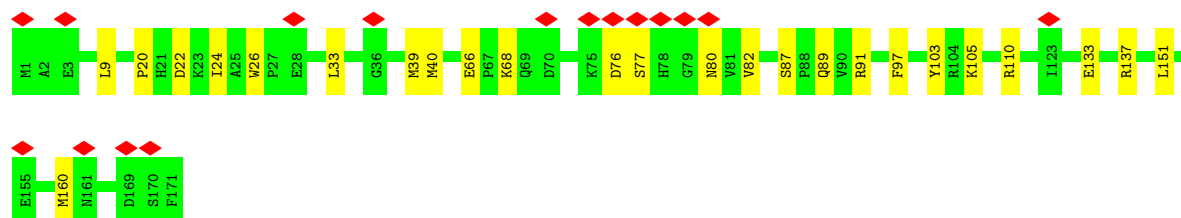
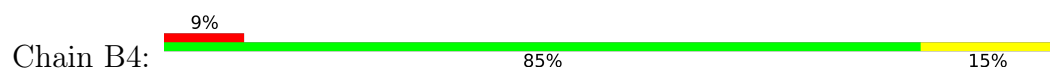
• Molecule 18: NDUFB2



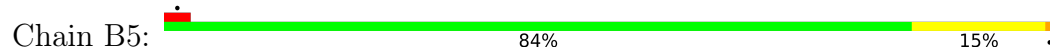
• Molecule 19: NDUFB3



• Molecule 20: NDUFB4



• Molecule 21: NDUFB5

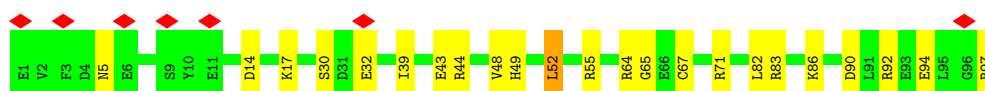
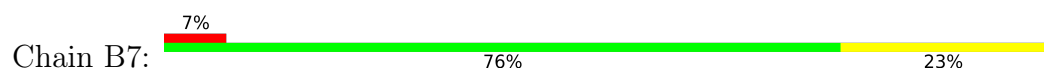




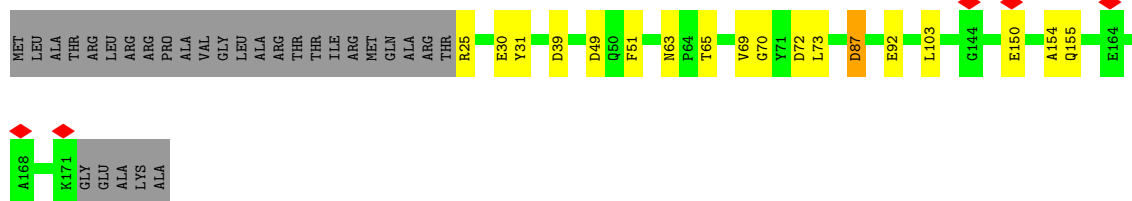
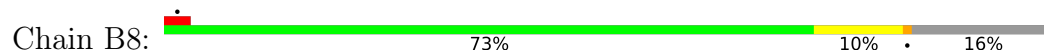
- Molecule 22: NDUFB6



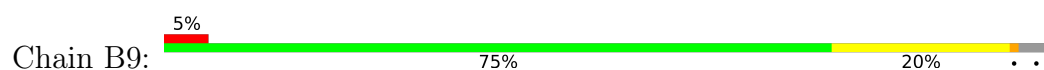
- Molecule 23: NDUFB7



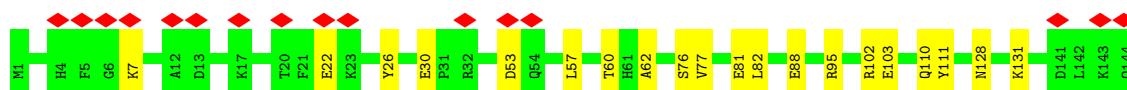
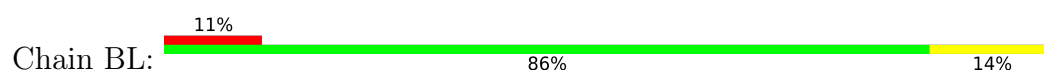
- Molecule 24: NDUFB8



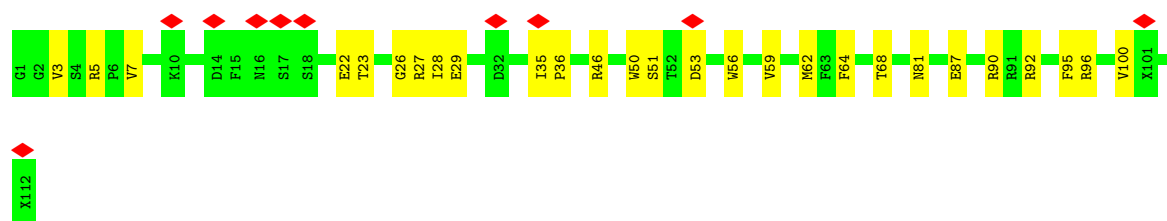
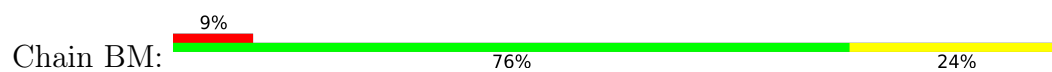
- Molecule 25: NDUFB9



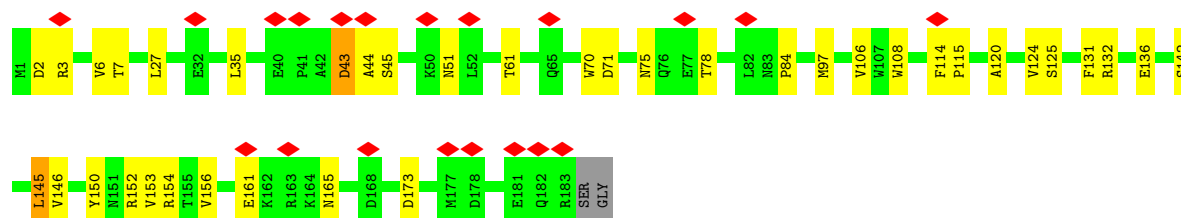
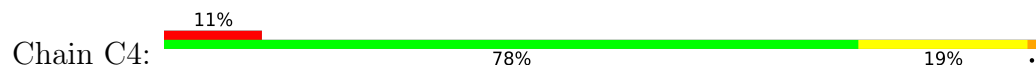
- Molecule 26: NDUFB10



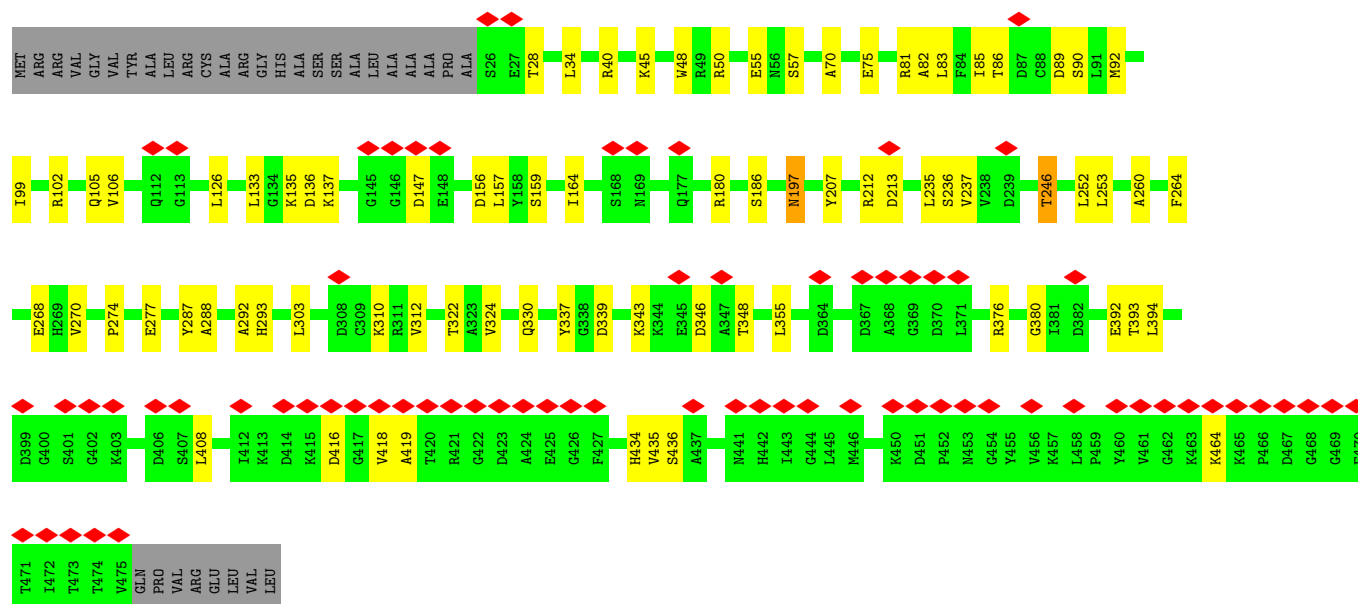
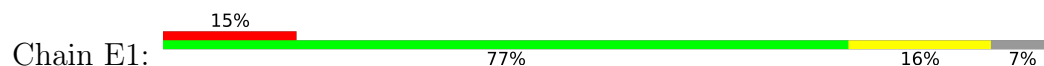
- Molecule 27: NDUFB11



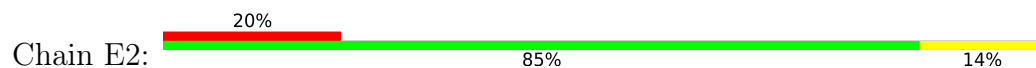
• Molecule 28: NDUFC2

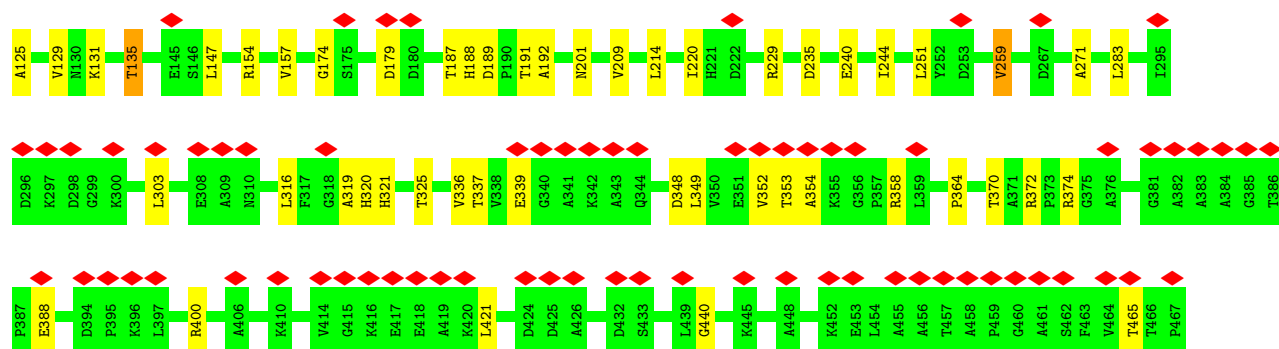


• Molecule 29: NDUEG1

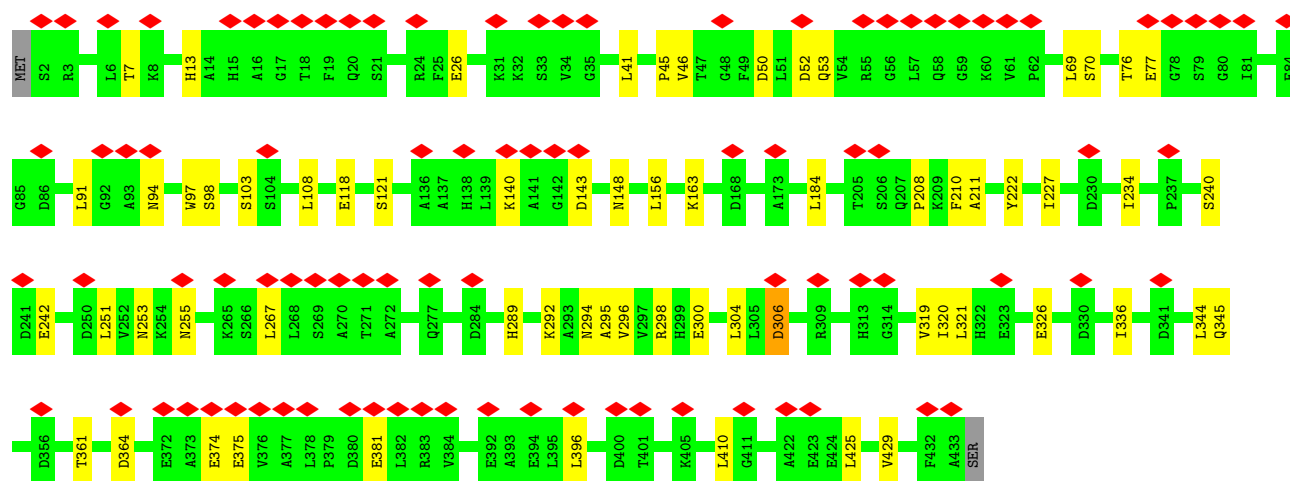
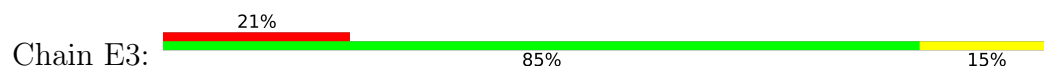


• Molecule 30: NDUEG2

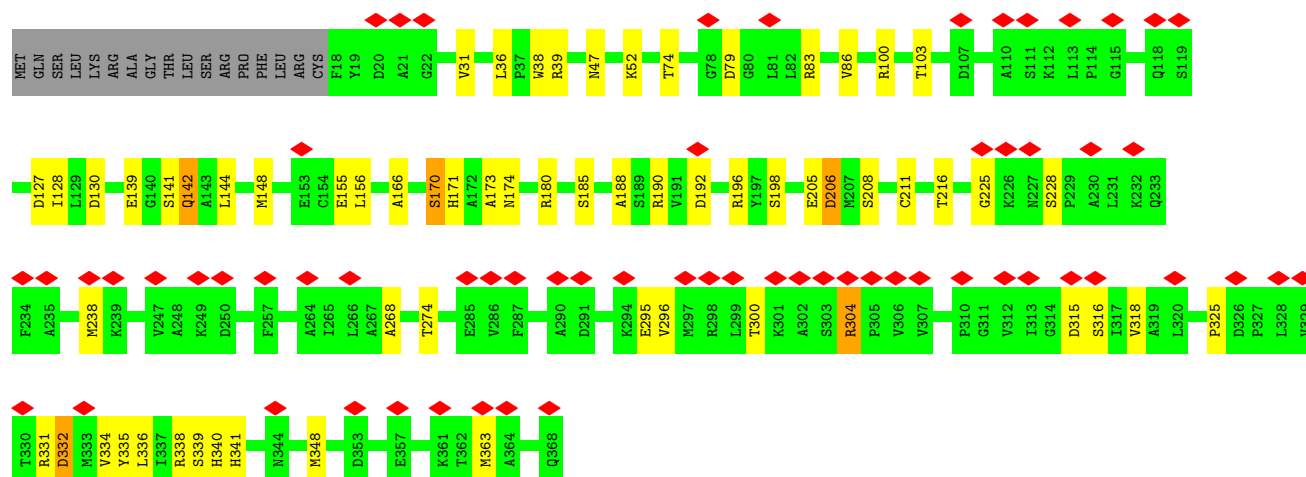
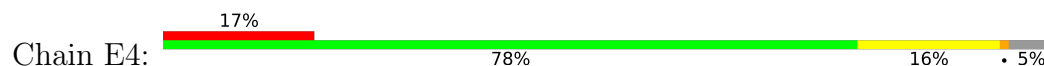




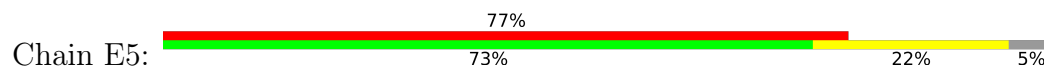
• Molecule 31: NDUEG3

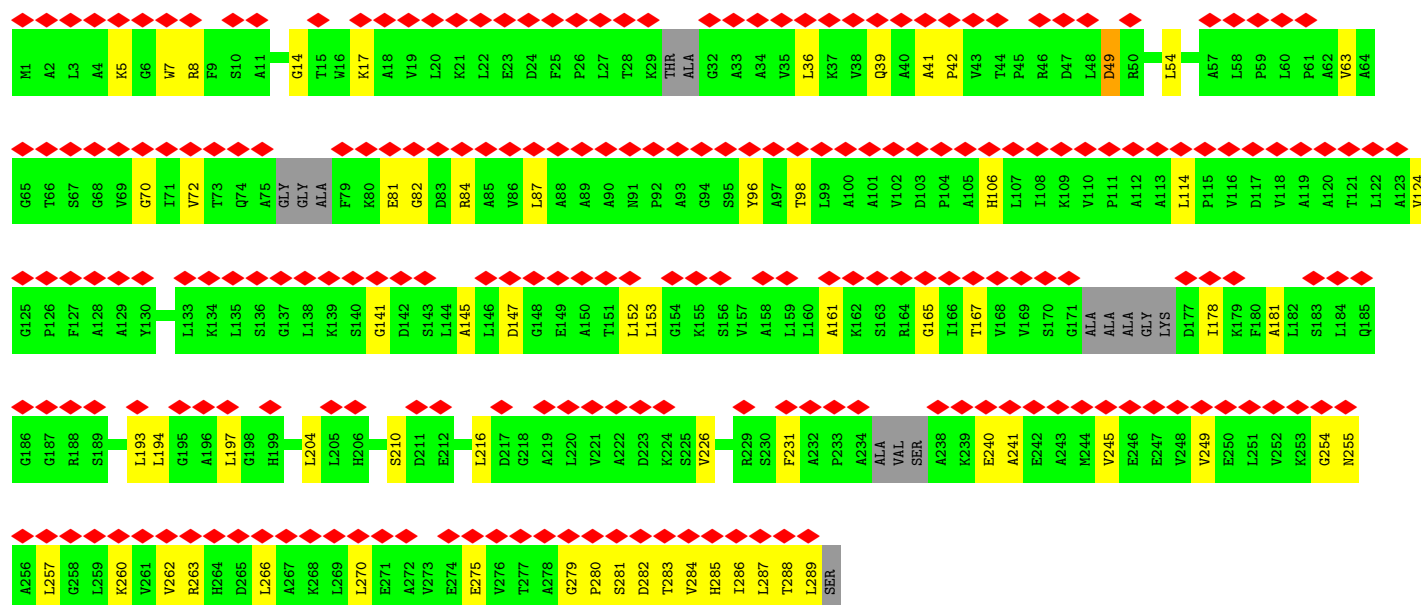


• Molecule 32: NDUEG4

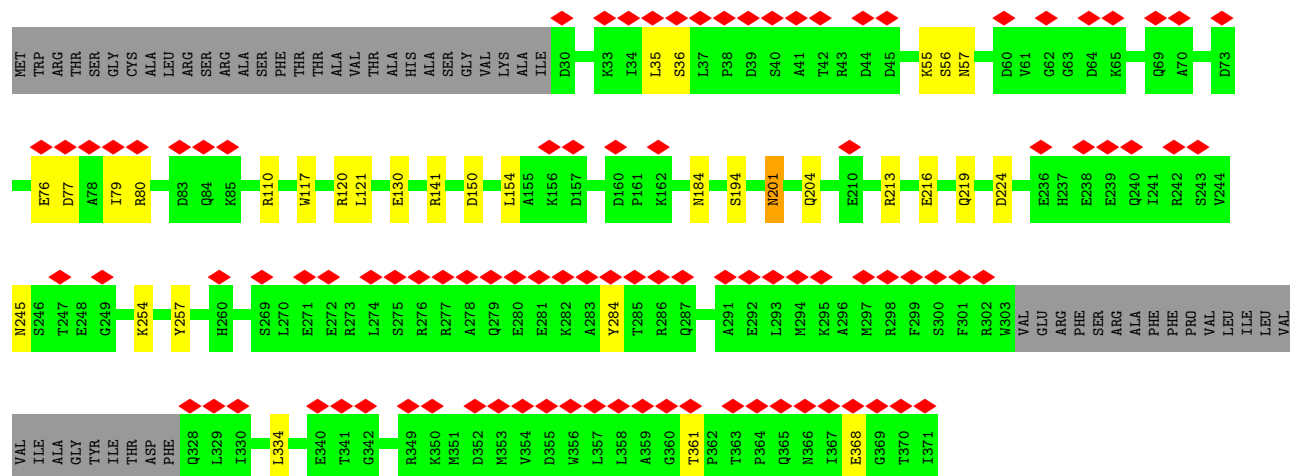
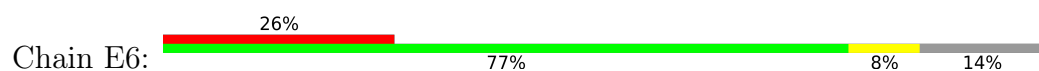


• Molecule 33: NDUEG5

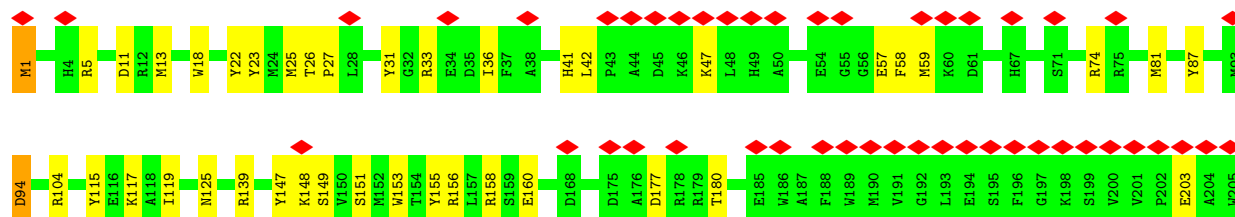
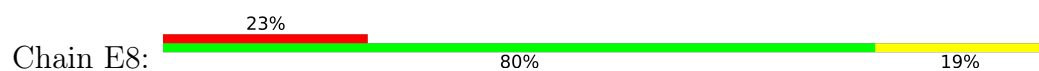




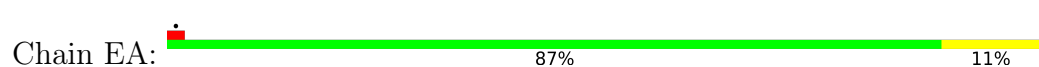
• Molecule 34: NDUEG6

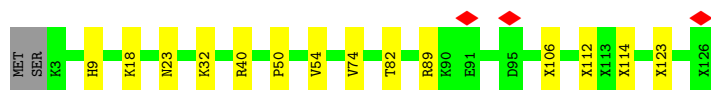


• Molecule 35: NDUEG8

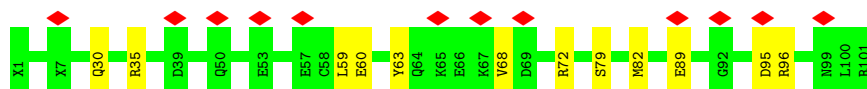


• Molecule 36: NDUEG10

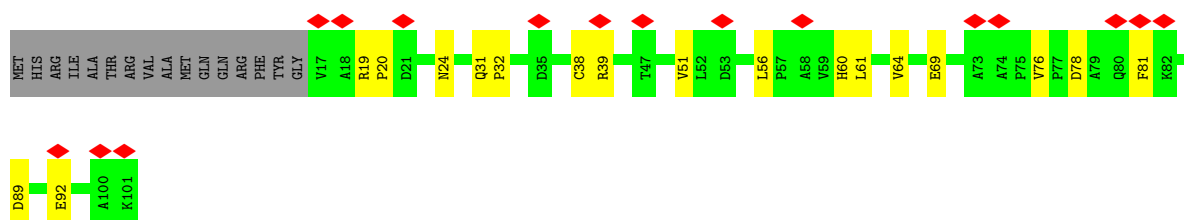




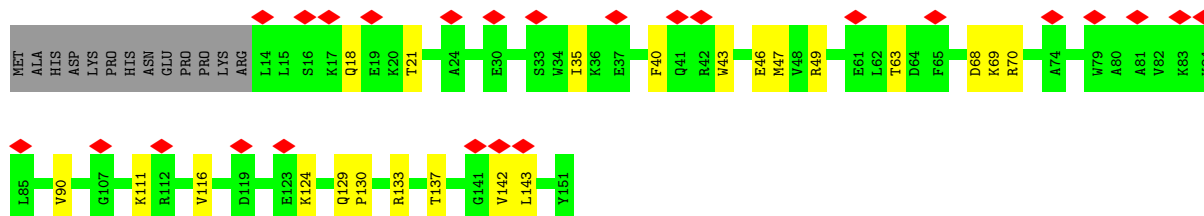
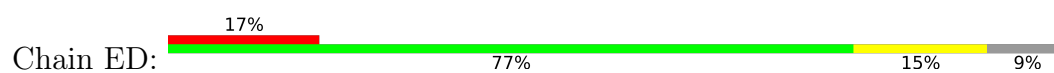
• Molecule 37: NDUEG11



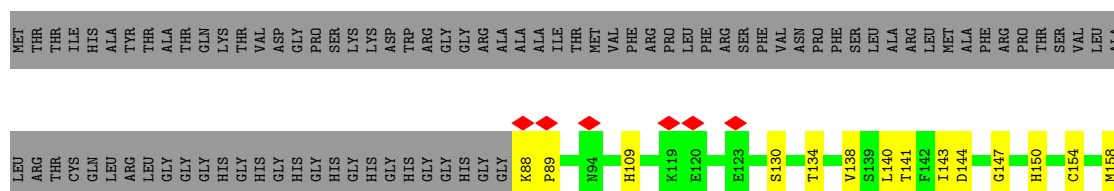
• Molecule 38: NDUEG12



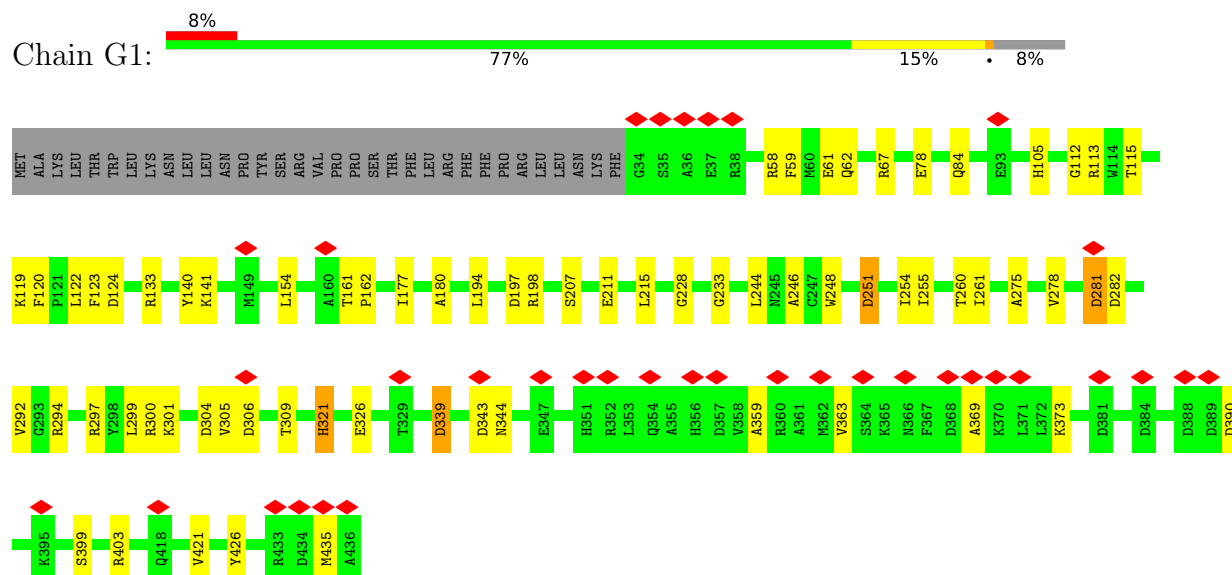
• Molecule 39: NDUEG13



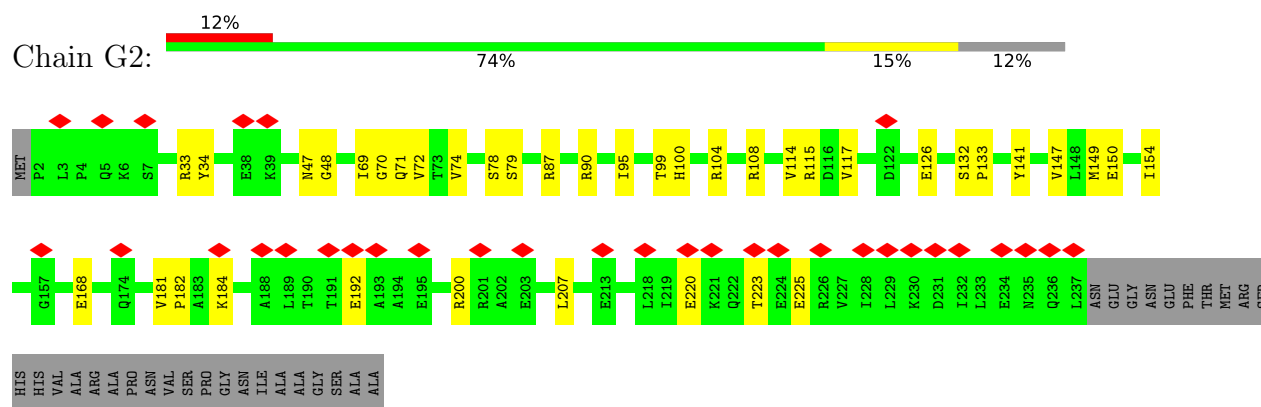
• Molecule 40: NDUFX



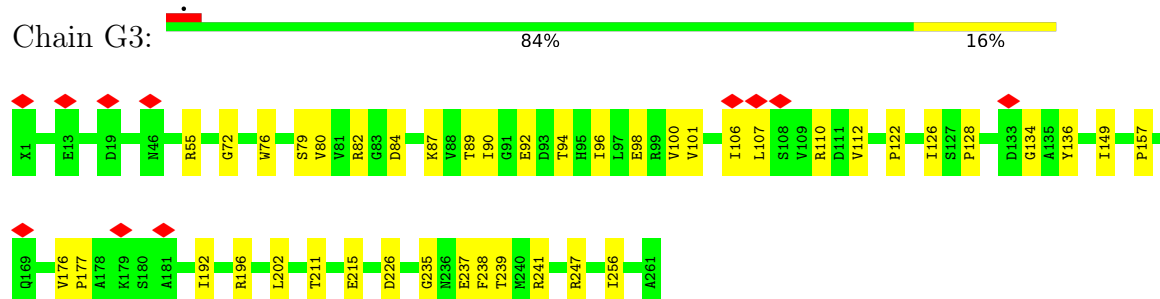
- Molecule 41: NDUCA1



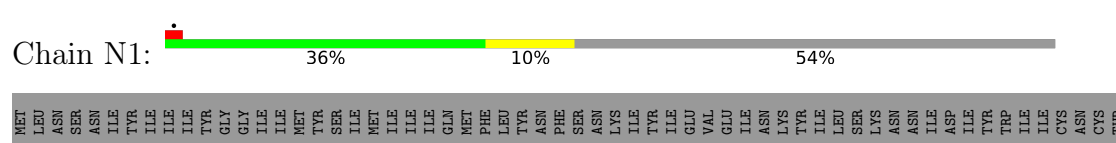
- Molecule 42: NDUCA2

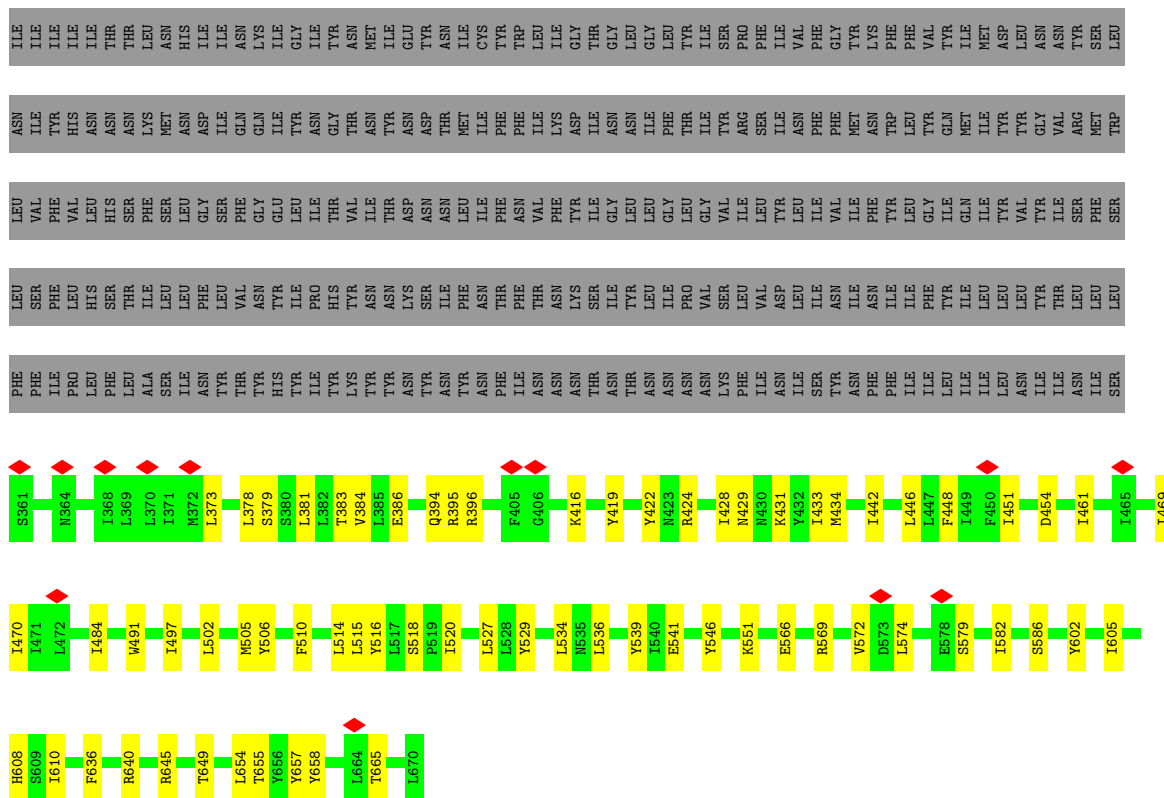


- Molecule 43: NDUCA3

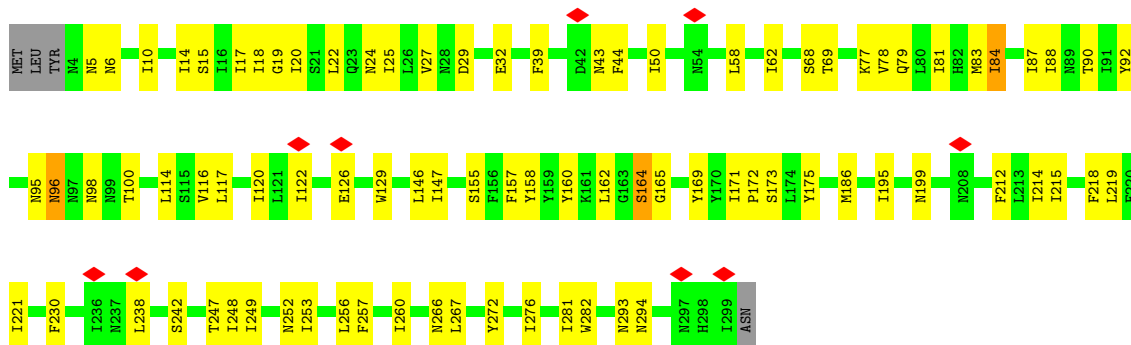


- Molecule 44: ND1

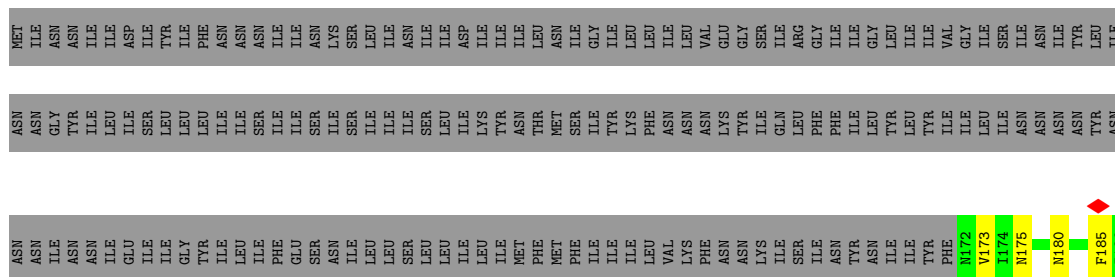




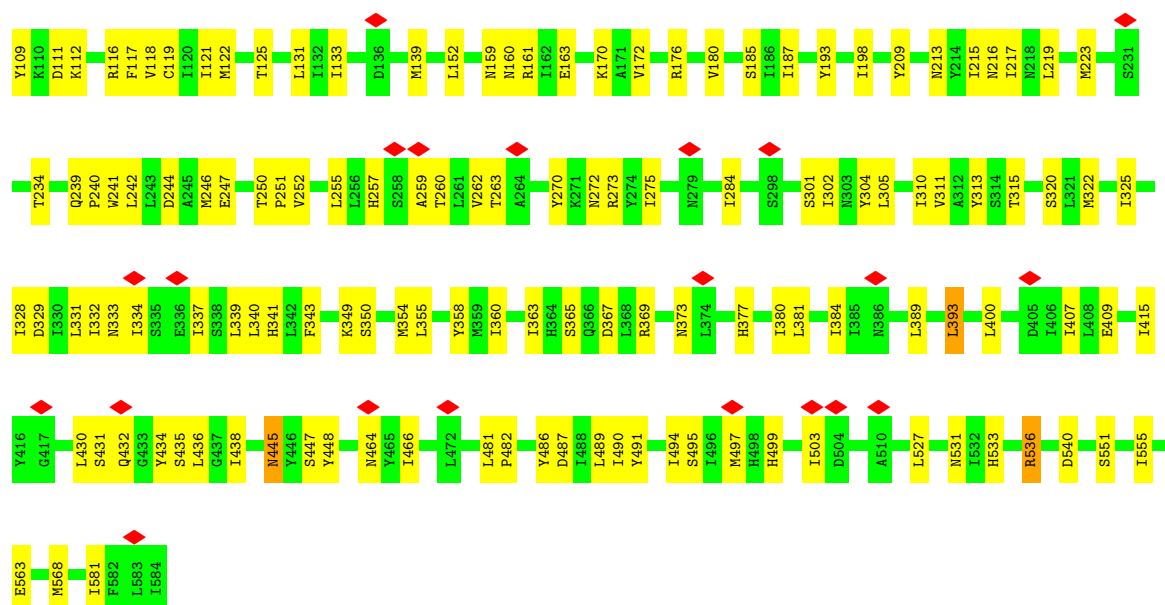
- Molecule 45: ND2A



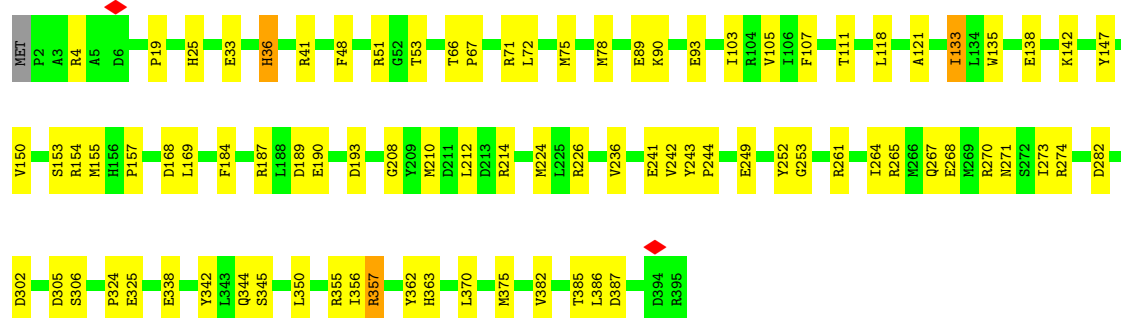
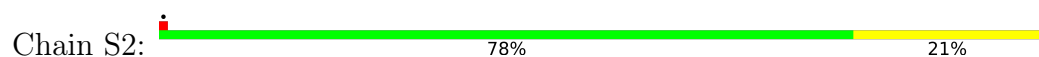
- Molecule 46: ND3



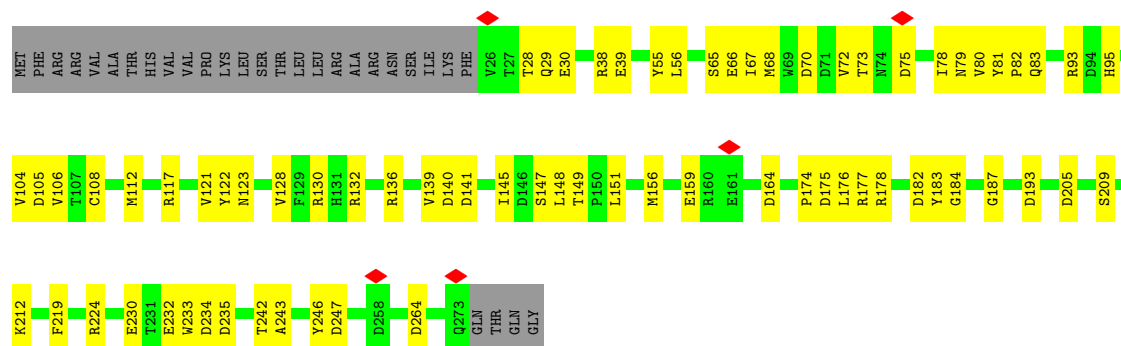




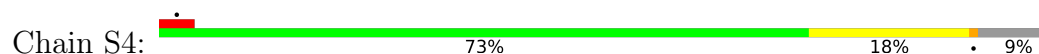
• Molecule 49: NDUF2S2

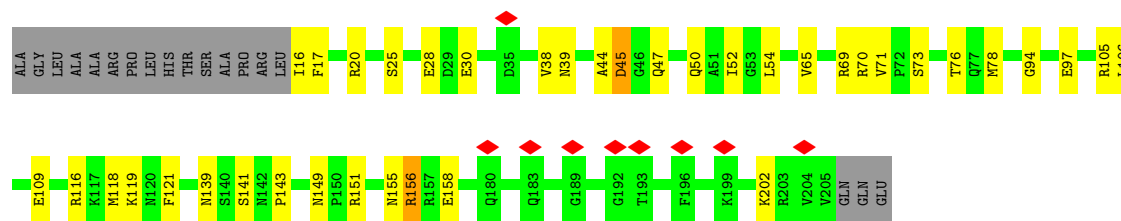


• Molecule 50: NDUF2S3

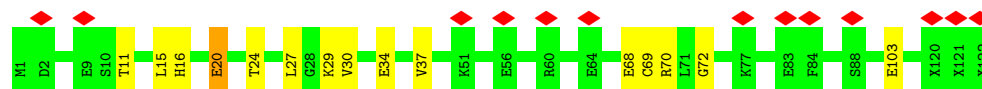
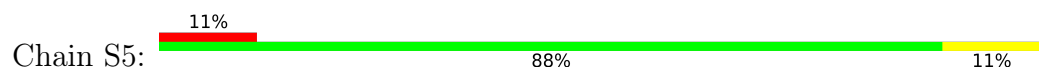


• Molecule 51: NDUF2S4

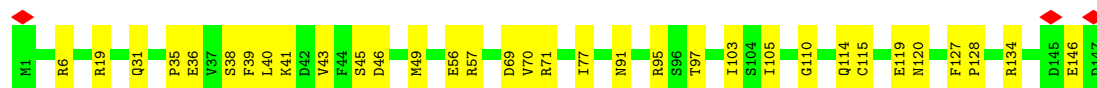
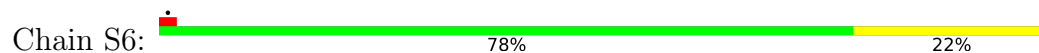




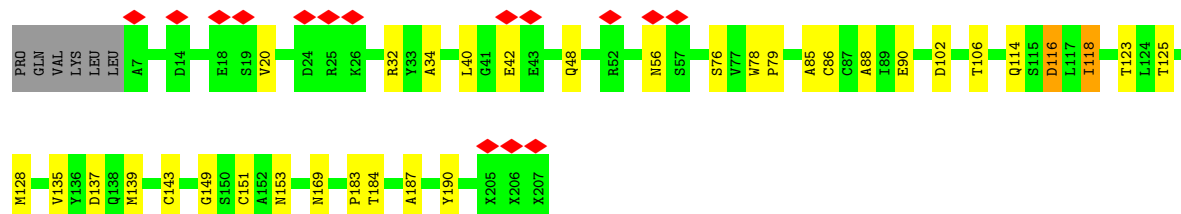
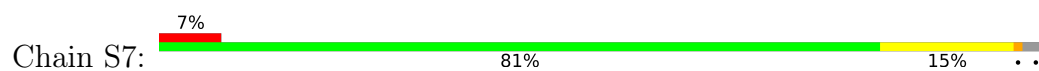
• Molecule 52: NDUFS5



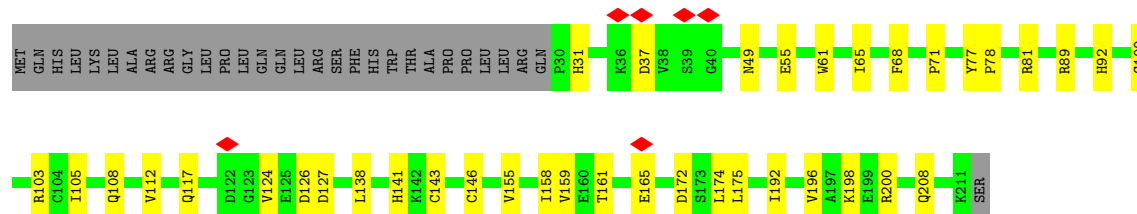
• Molecule 53: NDUFS6



• Molecule 54: NDUFS7

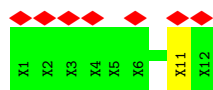


• Molecule 55: NDUFS8

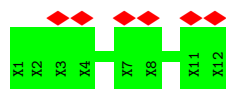


• Molecule 56: UNK-UNK-UNK-UNK-UNK-UNK-UNK-UNK-UNK-UNK-UNK

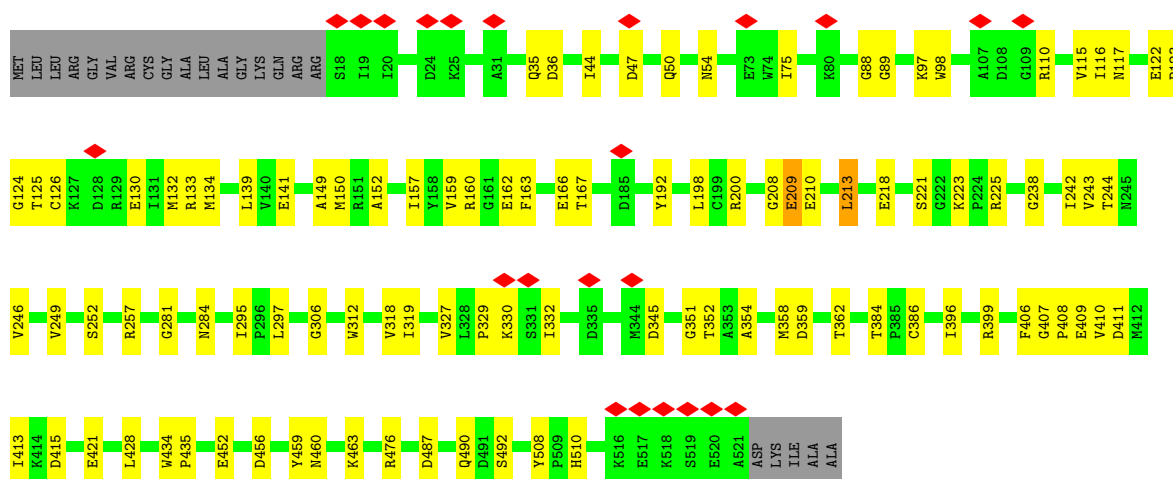
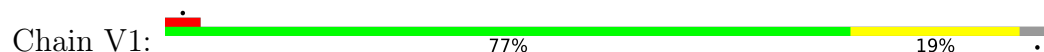




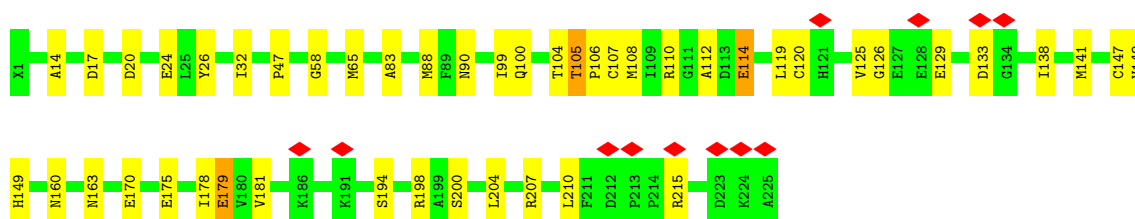
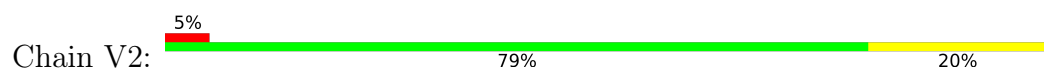
- Molecule 56: UNK-UNK-UNK-UNK-UNK-UNK-UNK-UNK-UNK-UNK-UNK-UNK



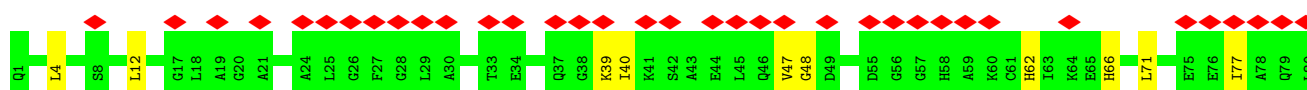
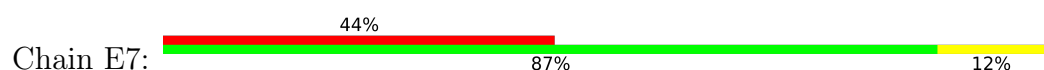
- Molecule 57: NDUFV1

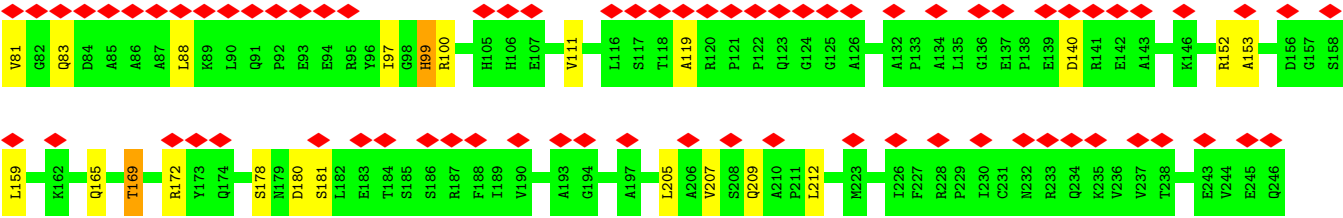


- Molecule 58: NDUFV2



- Molecule 59: NDUEG7





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	76643	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 ($e^-/\text{\AA}^2$)	61.5	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	130000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	41.632	Depositor
Minimum map value	-19.553	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.993	Depositor
Recommended contour level	5	Depositor
Map size (Å)	446.4, 446.4, 446.4	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.93, 0.93, 0.93	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 2MR, ZMP, NDP, K, CDL, SF4, PC1, FMN, 3PE, FES, NAI, ZN, U10

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	1A	0.16	0/2858	0.34	0/3878
2	1B	0.15	0/4306	0.28	0/5854
3	2B	0.17	0/958	0.35	0/1306
4	4L	0.15	0/924	0.29	0/1261
5	A1	0.13	0/1108	0.27	0/1511
6	A2	0.13	0/1530	0.28	0/2089
7	A3	0.14	0/1079	0.30	0/1453
8	A5	0.14	0/1282	0.25	0/1737
9	A6	0.13	0/3395	0.27	0/4608
10	A7	0.14	0/1194	0.31	0/1619
11	A8	0.13	0/1879	0.27	0/2543
12	A9	0.14	0/3920	0.29	0/5335
13	AB	0.13	0/704	0.24	0/951
14	AC	0.14	0/736	0.26	0/1000
15	AL	0.13	0/2317	0.27	0/3136
16	AM	0.13	0/1533	0.23	0/2079
17	AN	0.13	0/2382	0.26	0/3249
18	B2	0.12	0/947	0.23	0/1291
19	B3	0.14	0/326	0.24	0/441
20	B4	0.15	0/1419	0.31	0/1922
21	B5	0.16	0/1111	0.29	0/1505
22	B6	0.14	0/803	0.26	0/1087
23	B7	0.12	0/877	0.24	0/1172
24	B8	0.15	0/1273	0.27	0/1733
25	B9	0.15	0/1274	0.31	0/1728
26	BL	0.16	0/1266	0.30	0/1710
27	BM	0.16	0/876	0.27	0/1192
28	C4	0.14	0/1592	0.28	0/2158
29	E1	0.12	0/3596	0.27	0/4879
30	E2	0.12	0/3658	0.27	0/4983
31	E3	0.12	0/3320	0.27	0/4520
32	E4	0.13	0/2850	0.27	0/3884

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	E5	0.15	0/2004	0.35	0/2721
34	E6	0.12	0/2750	0.24	0/3724
35	E8	0.12	0/1747	0.28	0/2367
36	EA	0.16	0/858	0.28	0/1163
37	EB	0.11	0/650	0.23	0/863
38	EC	0.13	0/676	0.27	0/925
39	ED	0.12	0/1176	0.27	0/1590
40	FX	0.15	0/2035	0.30	0/2763
41	G1	0.15	0/3234	0.31	0/4401
42	G2	0.15	0/1832	0.31	0/2476
43	G3	0.15	0/1957	0.31	0/2646
44	N1	0.15	0/2672	0.32	0/3639
45	N2	0.18	0/2582	0.32	0/3530
46	N3	0.18	0/1068	0.37	0/1456
46	N6	0.14	0/1275	0.31	0/1730
47	N4	0.18	0/4105	0.34	0/5594
48	N5	0.17	0/4963	0.34	0/6758
49	S2	0.18	0/3244	0.32	0/4403
50	S3	0.17	0/2112	0.31	0/2874
51	S4	0.14	0/1573	0.30	0/2107
52	S5	0.11	0/960	0.24	0/1291
53	S6	0.14	0/1232	0.28	0/1659
54	S7	0.15	0/1558	0.29	0/2120
55	S8	0.16	0/1485	0.31	0/2010
57	V1	0.15	0/3990	0.31	0/5394
58	V2	0.14	0/1787	0.29	0/2428
59	E7	0.13	0/1931	0.28	0/2618
All	All	0.15	0/112749	0.29	0/153064

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

Mol	Chain	#Chirality outliers	#Planarity outliers
12	A9	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	A9	286	ARG	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	2801	2700	2710	56	0
2	1B	4198	4159	4175	74	0
3	2B	1070	989	1009	23	0
4	4L	890	878	880	19	0
5	A1	1071	1026	1030	12	0
6	A2	1493	1474	1478	14	0
7	A3	1050	1039	1041	15	0
8	A5	1261	1248	1251	8	0
9	A6	3328	3280	3293	62	0
10	A7	1154	1118	1123	23	0
11	A8	1822	1726	1736	48	0
12	A9	3829	3850	3857	61	0
13	AB	694	673	677	9	0
14	AC	721	697	702	10	0
15	AL	2237	2172	2180	25	0
16	AM	1487	1448	1452	25	0
17	AN	2306	2267	2275	14	0
18	B2	913	857	858	15	0
19	B3	449	309	312	10	0
20	B4	1377	1358	1364	24	0
21	B5	1112	1069	1075	20	0
22	B6	773	747	751	15	0
23	B7	857	835	841	13	0
24	B8	1224	1127	1136	22	0
25	B9	1236	1207	1212	31	0
26	BL	1227	1179	1185	14	0
27	BM	910	827	830	24	0
28	C4	1545	1517	1519	29	0
29	E1	3512	3496	3510	48	0
30	E2	3563	3540	3554	42	0
31	E3	3255	3263	3279	44	0
32	E4	2770	2732	2742	51	0
33	E5	1977	2069	2075	46	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	E6	2674	2554	2562	20	0
35	E8	1691	1663	1668	37	0
36	EA	961	832	836	11	0
37	EB	774	631	636	11	0
38	EC	660	663	666	12	0
39	ED	1142	1131	1134	19	0
40	FX	1967	1849	1858	42	0
41	G1	3147	2999	3015	53	0
42	G2	1804	1846	1850	34	0
43	G3	1961	1944	1950	33	0
44	N1	2605	2726	2729	55	0
45	N2	2512	2589	2592	80	0
46	N3	1037	1057	1057	30	0
46	N6	1257	1385	1385	42	0
47	N4	4001	4214	4224	112	0
48	N5	4837	5032	5046	130	0
49	S2	3173	3101	3114	69	0
50	S3	2050	1928	1936	61	0
51	S4	1536	1502	1505	34	0
52	S5	991	895	898	10	0
53	S6	1200	1192	1198	26	0
54	S7	1545	1500	1503	25	0
55	S8	1451	1392	1397	34	0
56	U1	60	16	18	1	0
56	U2	60	16	17	0	0
57	V1	3897	3827	3837	77	0
58	V2	1759	1701	1711	32	0
59	E7	1888	1892	1903	23	0
60	1A	4	0	0	0	0
60	V2	4	0	0	0	0
61	1A	16	0	0	1	0
61	S7	8	0	0	0	0
61	S8	16	0	0	4	0
61	V1	8	0	0	0	0
62	1A	1	0	0	0	0
63	A1	80	111	111	3	0
63	A9	66	80	80	2	0
63	AL	50	77	77	0	0
63	AM	97	148	148	1	0
63	AN	48	73	73	0	0
63	B5	108	176	176	2	0
63	C4	38	50	50	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
63	E4	51	79	79	0	0
63	E8	171	250	250	3	0
63	ED	54	88	88	0	0
63	N1	89	129	129	0	0
63	N2	37	48	48	0	0
63	N3	42	61	61	1	0
63	N4	72	92	92	0	0
63	N5	131	190	190	3	0
64	A3	58	60	60	2	0
64	AL	202	236	236	2	0
64	AM	216	273	273	10	0
64	B3	65	74	74	4	0
64	B5	58	60	60	1	0
64	C4	163	223	223	1	0
64	E6	64	72	72	0	0
64	E7	68	80	80	0	0
64	EA	114	116	116	0	0
64	N4	98	149	149	5	0
64	N5	163	223	223	2	0
65	A9	48	26	26	2	0
66	AB	36	0	47	8	0
66	AC	36	0	47	7	0
67	AN	51	81	82	0	0
67	G1	40	56	57	3	0
67	N4	41	55	56	0	0
67	N5	51	81	82	1	0
68	N4	43	55	55	10	0
69	E7	1	0	0	0	0
69	S6	1	0	0	0	0
70	V1	31	19	19	5	0
71	V1	44	0	27	11	0
All	All	113635	112544	113073	1649	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 7.

All (1649) 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)
25:B9:137:THR:HG22	27:BM:23:THR:HG21	1.48	0.95
33:E5:287:LEU:O	33:E5:289:LEU:N	1.98	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:B2:50:GLU:O	39:ED:70:ARG:NH2	2.04	0.91
44:N1:657:TYR:HH	46:N3:286:SER:HG	1.09	0.91
10:A7:34:HIS:O	49:S2:142:LYS:NZ	2.05	0.87
16:AM:74:ARG:NH2	44:N1:516:TYR:O	2.07	0.87
9:A6:45:HIS:NE2	9:A6:117:GLU:OE1	2.08	0.86
28:C4:132:ARG:NH1	28:C4:136:GLU:OE1	2.08	0.86
57:V1:97:LYS:NZ	57:V1:243:VAL:O	2.08	0.86
11:A8:102:ARG:NH1	11:A8:221:ILE:O	2.08	0.86
17:AN:248:ILE:O	28:C4:154:ARG:NH2	2.08	0.86
2:1B:223:LEU:O	2:1B:227:THR:OG1	1.94	0.86
16:AM:52:LYS:NZ	64:AM:216:CDL:OB4	2.09	0.85
35:E8:87:TYR:OH	64:N5:603:CDL:OA4	1.94	0.85
44:N1:514:LEU:O	44:N1:539:TYR:OH	1.92	0.85
29:E1:86:THR:HG21	29:E1:92:MET:HE2	1.57	0.85
13:AB:92:LEU:HD13	66:AB:150:ZMP:H20A	1.60	0.84
29:E1:268:GLU:OE1	29:E1:322:THR:OG1	1.96	0.83
2:1B:206:GLU:OE1	2:1B:482:ARG:NH1	2.12	0.83
7:A3:17:HIS:ND1	32:E4:206:ASP:OD1	2.11	0.83
9:A6:132:LYS:NZ	50:S3:184:GLY:O	2.11	0.83
11:A8:214:THR:OG1	11:A8:219:ASP:OD2	1.96	0.83
48:N5:255:LEU:O	48:N5:260:THR:OG1	1.97	0.83
9:A6:315:GLU:OE2	9:A6:340:TYR:OH	1.96	0.82
41:G1:294:ARG:HG2	42:G2:181:VAL:HG21	1.59	0.82
49:S2:111:THR:HG22	49:S2:147:TYR:OH	1.78	0.82
47:N4:80:ILE:HD11	47:N4:337:ILE:HG23	1.61	0.82
25:B9:100:ARG:NH2	35:E8:31:TYR:O	2.13	0.82
15:AL:193:GLY:O	15:AL:198:ARG:NH1	2.12	0.81
10:A7:134:TYR:OH	32:E4:174:ASN:OD1	1.98	0.81
1:1A:26:ALA:O	2:1B:448:ARG:NE	2.14	0.81
32:E4:74:THR:OG1	32:E4:141:SER:OG	1.97	0.81
2:1B:399:ASP:OD2	12:A9:102:SER:OG	1.99	0.80
10:A7:105:SER:O	50:S3:130:ARG:NH1	2.14	0.80
30:E2:339:GLU:OE2	30:E2:358:ARG:NH1	2.15	0.80
41:G1:133:ARG:NH1	43:G3:215:GLU:OE2	2.14	0.80
43:G3:107:LEU:O	43:G3:110:ARG:NH1	2.14	0.80
34:E6:120:ARG:NH1	53:S6:69:ASP:OD2	2.14	0.80
16:AM:47:TYR:OH	49:S2:193:ASP:OD1	2.00	0.80
2:1B:102:ARG:O	2:1B:200:TYR:OH	1.99	0.80
35:E8:156:ARG:NH2	35:E8:180:THR:O	2.14	0.80
49:S2:107:PHE:O	49:S2:111:THR:HG23	1.80	0.80
26:BL:88:GLU:OE1	37:EB:79:SER:OG	1.99	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:E3:118:GLU:OE1	31:E3:118:GLU:N	2.15	0.79
34:E6:55:LYS:NZ	53:S6:46:ASP:OD1	2.15	0.79
47:N4:67:ASN:N	47:N4:119:ASP:OD2	2.15	0.79
57:V1:36:ASP:O	58:V2:215:ARG:NH1	2.15	0.79
51:S4:25:SER:OG	51:S4:30:GLU:OE2	1.99	0.79
10:A7:120:THR:OG1	10:A7:123:TYR:O	2.00	0.79
12:A9:230:ARG:NH1	34:E6:150:ASP:OD1	2.15	0.79
53:S6:41:LYS:O	53:S6:45:SER:OG	2.01	0.79
34:E6:254:LYS:NZ	54:S7:40:LEU:O	2.16	0.79
41:G1:133:ARG:NH2	42:G2:34:TYR:O	2.15	0.79
47:N4:368:ASN:ND2	47:N4:444:THR:O	2.16	0.79
2:1B:217:LYS:NZ	2:1B:473:SER:OG	2.15	0.78
18:B2:112:GLU:O	18:B2:133:ARG:NH2	2.17	0.78
47:N4:408:ASN:O	47:N4:412:SER:OG	2.01	0.78
43:G3:87:LYS:NZ	43:G3:89:THR:OG1	2.15	0.78
49:S2:53:THR:HG21	49:S2:72:LEU:HD21	1.65	0.78
32:E4:166:ALA:O	32:E4:170:SER:OG	2.02	0.78
47:N4:9:ARG:NH2	47:N4:70:TYR:OH	2.17	0.78
32:E4:225:GLY:O	32:E4:228:SER:OG	2.01	0.78
36:EA:18:LYS:O	36:EA:23:ASN:ND2	2.17	0.78
7:A3:22:ASN:OD1	7:A3:23:ARG:NH1	2.16	0.77
40:FX:196:GLU:N	40:FX:196:GLU:OE1	2.16	0.77
43:G3:235:GLY:O	46:N6:161:LYS:NZ	2.17	0.77
50:S3:70:ASP:OD1	50:S3:73:THR:OG1	2.01	0.77
1:1A:138:HIS:O	1:1A:173:LYS:NZ	2.17	0.77
1:1A:222:GLN:OE1	57:V1:223:LYS:NZ	2.18	0.77
48:N5:97:SER:OG	48:N5:125:THR:HG21	1.84	0.77
37:EB:95:ASP:OD1	37:EB:96:ARG:N	2.18	0.77
33:E5:41:ALA:O	33:E5:287:LEU:O	2.03	0.77
4:4L:98:MET:O	4:4L:103:ARG:NH1	2.18	0.76
57:V1:411:ASP:OD2	57:V1:510:HIS:NE2	2.18	0.76
7:A3:104:GLU:N	7:A3:104:GLU:OE1	2.17	0.76
26:BL:81:GLU:OE2	27:BM:92:ARG:NH1	2.19	0.76
15:AL:212:TYR:OH	55:S8:175:LEU:O	2.02	0.76
48:N5:170:LYS:NZ	48:N5:540:ASP:OD2	2.18	0.76
49:S2:153:SER:OG	49:S2:155:MET:O	2.01	0.76
32:E4:128:ILE:HD11	32:E4:156:LEU:HD13	1.68	0.76
33:E5:81:GLU:OE1	33:E5:81:GLU:N	2.18	0.76
33:E5:240:GLU:OE1	33:E5:240:GLU:N	2.18	0.76
57:V1:35:GLN:N	57:V1:35:GLN:OE1	2.19	0.76
26:BL:22:GLU:OE1	26:BL:22:GLU:N	2.19	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:E1:392:GLU:N	29:E1:392:GLU:OE1	2.19	0.76
35:E8:94:ASP:OD1	35:E8:117:LYS:NZ	2.16	0.76
47:N4:43:ILE:HD13	47:N4:472:LEU:HD21	1.68	0.75
1:1A:49:ASP:OD2	1:1A:118:THR:OG1	2.04	0.75
2:1B:214:ASP:OD2	2:1B:218:LYS:NZ	2.20	0.75
3:2B:4:ASN:ND2	4:4L:168:LYS:O	2.20	0.75
57:V1:284:ASN:ND2	57:V1:306:GLY:O	2.19	0.75
32:E4:31:VAL:HG21	49:S2:236:VAL:HG11	1.69	0.75
5:A1:49:TYR:OH	11:A8:83:ASN:ND2	2.19	0.75
6:A2:170:SER:OG	31:E3:326:GLU:OE2	2.03	0.75
32:E4:74:THR:HG1	32:E4:141:SER:HG	1.27	0.75
45:N2:32:GLU:N	45:N2:32:GLU:OE1	2.20	0.75
57:V1:452:GLU:OE2	57:V1:508:TYR:OH	2.02	0.75
31:E3:222:TYR:OH	38:EC:60:HIS:NE2	2.20	0.75
49:S2:338:GLU:OE2	50:S3:132:ARG:NH2	2.20	0.74
20:B4:24:ILE:O	20:B4:110:ARG:NH1	2.20	0.74
49:S2:19:PRO:HB3	54:S7:128:MET:HE1	1.69	0.74
28:C4:71:ASP:O	28:C4:75:ASN:ND2	2.20	0.74
2:1B:177:GLU:OE1	2:1B:179:ARG:NH1	2.21	0.74
25:B9:63:GLU:OE1	35:E8:22:TYR:OH	2.05	0.74
9:A6:31:VAL:HG11	40:FX:141:THR:HG21	1.68	0.74
27:BM:23:THR:OG1	27:BM:26:GLY:O	2.06	0.74
28:C4:161:GLU:OE1	28:C4:165:ASN:ND2	2.21	0.74
1:1A:141:ASP:OD2	1:1A:190:ASN:ND2	2.21	0.73
20:B4:68:LYS:NZ	25:B9:129:GLN:O	2.19	0.73
40:FX:161:ALA:N	40:FX:225:VAL:O	2.20	0.73
48:N5:67:ASN:ND2	48:N5:75:ASN:OD1	2.21	0.73
40:FX:185:TRP:O	40:FX:186:SER:OG	2.06	0.73
57:V1:50:GLN:O	57:V1:54:ASN:ND2	2.22	0.73
45:N2:77:LYS:NZ	46:N3:281:TYR:OH	2.15	0.73
29:E1:34:LEU:HD22	29:E1:253:LEU:HD22	1.71	0.73
42:G2:150:GLU:OE1	42:G2:150:GLU:N	2.22	0.73
2:1B:449:LEU:O	2:1B:456:SER:OG	2.07	0.72
15:AL:151:SER:OG	64:AL:303:CDL:OB3	2.07	0.72
51:S4:69:ARG:NH1	51:S4:143:PRO:O	2.22	0.72
11:A8:209:ARG:NH1	16:AM:83:ASP:OD1	2.23	0.72
55:S8:165:GLU:N	55:S8:165:GLU:OE1	2.21	0.72
29:E1:75:GLU:OE2	29:E1:186:SER:OG	2.05	0.72
35:E8:203:GLU:OE1	35:E8:203:GLU:N	2.22	0.72
2:1B:113:GLU:OE2	51:S4:151:ARG:NH2	2.23	0.72
64:AM:215:CDL:O1	32:E4:338:ARG:NH2	2.23	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:N4:293:THR:HG21	47:N4:365:ILE:HD11	1.70	0.72
9:A6:135:ASN:OD1	50:S3:212:LYS:NZ	2.24	0.71
14:AC:115:GLU:OE2	25:B9:41:HIS:NE2	2.22	0.71
9:A6:92:ARG:HB3	66:AB:150:ZMP:H7A	1.70	0.71
45:N2:221:ILE:HD11	45:N2:252:ASN:CG	2.16	0.71
6:A2:6:ARG:NH2	6:A2:135:GLU:OE1	2.22	0.71
37:EB:89:GLU:N	37:EB:89:GLU:OE1	2.23	0.71
3:2B:95:SER:OG	24:B8:31:TYR:O	2.09	0.71
9:A6:163:GLY:N	9:A6:169:GLU:OE1	2.22	0.71
40:FX:199:VAL:O	40:FX:223:ARG:NH2	2.22	0.71
49:S2:265:ARG:NE	49:S2:387:ASP:OD2	2.24	0.71
57:V1:116:ILE:HD12	57:V1:249:VAL:HG11	1.73	0.71
11:A8:63:ILE:O	11:A8:95:SER:OG	2.06	0.71
33:E5:49:ASP:OD2	33:E5:210:SER:N	2.24	0.71
24:B8:25:ARG:NH2	40:FX:172:ASP:OD2	2.24	0.71
45:N2:88:ILE:HG21	46:N6:143:LEU:HD21	1.71	0.71
2:1B:507:HIS:O	2:1B:511:VAL:HG23	1.90	0.70
47:N4:284:ASN:O	47:N4:287:ILE:HG22	1.90	0.70
11:A8:55:ARG:NH2	11:A8:210:SER:O	2.24	0.70
53:S6:71:ARG:NH1	53:S6:120:ASN:OD1	2.24	0.70
57:V1:116:ILE:HG21	57:V1:139:LEU:HD11	1.72	0.70
26:BL:26:TYR:OH	27:BM:90:ARG:NH2	2.24	0.70
32:E4:339:SER:O	32:E4:340:HIS:ND1	2.25	0.70
57:V1:36:ASP:OD2	58:V2:210:LEU:N	2.25	0.70
4:4L:141:LEU:HB3	45:N2:116:VAL:HG11	1.74	0.70
13:AB:52:HIS:ND1	13:AB:54:LEU:O	2.20	0.70
26:BL:53:ASP:OD1	26:BL:57:LEU:N	2.23	0.70
30:E2:4:GLY:O	30:E2:5:THR:OG1	2.10	0.70
12:A9:239:ARG:NH2	12:A9:339:GLU:OE2	2.24	0.69
34:E6:56:SER:OG	34:E6:57:ASN:ND2	2.24	0.69
35:E8:13:MET:O	35:E8:23:TYR:OH	2.08	0.69
39:ED:46:GLU:OE1	39:ED:49:ARG:NH1	2.24	0.69
41:G1:211:GLU:OE2	42:G2:87:ARG:NH1	2.24	0.69
44:N1:379:SER:O	44:N1:383:THR:HG23	1.92	0.69
49:S2:362:TYR:OH	50:S3:105:ASP:OD1	2.09	0.69
10:A7:126:ARG:NH2	16:AM:38:GLY:O	2.26	0.69
12:A9:463:ASP:OD1	12:A9:464:TYR:N	2.24	0.69
2:1B:441:LYS:HG2	30:E2:25:LEU:HD11	1.75	0.69
68:N4:505:U10:C18	68:N4:505:U10:H151	2.22	0.69
21:B5:94:ARG:NH1	47:N4:63:GLY:O	2.25	0.69
12:A9:468:LEU:HB3	63:A9:560:PC1:H142	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:AM:128:ASP:OD2	16:AM:131:GLN:N	2.26	0.69
64:AM:215:CDL:O1	32:E4:315:ASP:OD2	2.03	0.69
19:B3:22:MET:SD	19:B3:34:ARG:NH1	2.66	0.69
9:A6:48:PRO:HG2	50:S3:176:LEU:HD22	1.75	0.69
15:AL:257:ARG:NH2	53:S6:56:GLU:OE2	2.26	0.69
37:EB:60:GLU:HG3	37:EB:68:VAL:HG11	1.74	0.69
8:A5:144:ARG:NH1	50:S3:66:GLU:OE2	2.26	0.68
30:E2:316:LEU:O	30:E2:400:ARG:NH2	2.26	0.68
57:V1:47:ASP:OD2	58:V2:207:ARG:NH2	2.27	0.68
23:B7:30:SER:OG	23:B7:32:GLU:OE1	2.10	0.68
27:BM:64:PHE:O	27:BM:68:THR:HG23	1.93	0.68
48:N5:358:TYR:OH	48:N5:464:ASN:OD1	2.10	0.68
29:E1:105:GLN:NE2	29:E1:236:SER:OG	2.26	0.68
9:A6:361:LYS:NZ	9:A6:372:ASP:OD1	2.25	0.68
10:A7:52:ARG:NH1	49:S2:302:ASP:OD2	2.26	0.68
11:A8:66:GLU:N	11:A8:66:GLU:OE1	2.26	0.68
31:E3:211:ALA:HB2	31:E3:227:ILE:HD13	1.75	0.68
32:E4:128:ILE:HD13	32:E4:148:MET:HE2	1.74	0.68
34:E6:334:LEU:O	56:U1:11:UNK:N	2.27	0.68
29:E1:310:LYS:NZ	53:S6:146:GLU:OE1	2.16	0.68
44:N1:386:GLU:OE2	44:N1:640:ARG:NH1	2.26	0.68
57:V1:312:TRP:O	57:V1:330:LYS:NZ	2.27	0.68
41:G1:133:ARG:NH2	41:G1:339:ASP:OD1	2.27	0.68
47:N4:295:ARG:NH1	48:N5:563:GLU:OE2	2.26	0.68
11:A8:62:ASN:ND2	11:A8:62:ASN:O	2.27	0.67
12:A9:26:ASN:O	12:A9:26:ASN:ND2	2.27	0.67
50:S3:164:ASP:OD1	50:S3:178:ARG:NH1	2.27	0.67
12:A9:442:ARG:NH2	44:N1:484:ILE:O	2.27	0.67
26:BL:128:ASN:O	26:BL:131:LYS:NZ	2.25	0.67
46:N3:251:ILE:CD1	46:N3:279:ILE:HD11	2.23	0.67
2:1B:118:SER:OG	2:1B:438:ASN:ND2	2.28	0.67
64:A3:201:CDL:OA3	64:A3:201:CDL:O1	2.11	0.67
22:B6:71:ASP:OD1	26:BL:95:ARG:NH2	2.27	0.67
30:E2:364:PRO:O	30:E2:400:ARG:NH1	2.28	0.67
42:G2:126:GLU:OE2	42:G2:141:TYR:OH	2.11	0.67
47:N4:354:TYR:O	47:N4:358:ASN:N	2.28	0.67
48:N5:409:GLU:OE1	48:N5:495:SER:OG	2.07	0.67
18:B2:110:GLU:O	23:B7:92:ARG:NH1	2.28	0.67
49:S2:89:GLU:O	49:S2:93:GLU:N	2.26	0.67
41:G1:211:GLU:OE1	41:G1:211:GLU:N	2.28	0.67
2:1B:20:LYS:NZ	31:E3:364:ASP:OD1	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1B:18:SER:O	2:1B:343:LEU:N	2.27	0.66
2:1B:405:LEU:O	2:1B:409:HIS:ND1	2.28	0.66
33:E5:114:LEU:HD11	33:E5:249:VAL:HG22	1.75	0.66
44:N1:424:ARG:NH1	46:N3:202:SER:OG	2.28	0.66
30:E2:374:ARG:NH2	38:EC:69:GLU:OE2	2.27	0.66
1:1A:287:GLU:OE2	1:1A:298:ASN:ND2	2.28	0.66
12:A9:120:THR:HG1	12:A9:195:SER:HG	1.17	0.66
26:BL:102:ARG:NH2	26:BL:103:GLU:OE2	2.29	0.66
44:N1:502:LEU:HD21	44:N1:574:LEU:HD12	1.76	0.66
50:S3:174:PRO:O	51:S4:20:ARG:NH1	2.28	0.66
9:A6:279:GLU:OE2	9:A6:429:TYR:OH	2.14	0.66
48:N5:494:ILE:HD13	48:N5:499:HIS:HE1	1.61	0.66
2:1B:68:ASP:OD1	6:A2:14:ARG:NH2	2.28	0.66
22:B6:12:ASP:OD1	22:B6:13:PHE:N	2.29	0.66
34:E6:284:TYR:OH	54:S7:56:ASN:OD1	2.09	0.66
40:FX:172:ASP:OD1	40:FX:172:ASP:N	2.25	0.66
49:S2:48:PHE:O	54:S7:125:THR:OG1	2.11	0.66
70:V1:579:FMN:O2'	71:V1:581:NAI:O2N	2.14	0.66
7:A3:28:GLN:O	55:S8:31:HIS:NE2	2.28	0.66
57:V1:456:ASP:O	57:V1:460:ASN:ND2	2.29	0.66
13:AB:56:ARG:O	13:AB:60:THR:HG23	1.96	0.65
15:AL:206:TYR:OH	54:S7:190:TYR:OH	2.06	0.65
25:B9:51:GLU:OE1	48:N5:448:TYR:OH	2.07	0.65
48:N5:325:ILE:HD11	48:N5:334:ILE:HG12	1.75	0.65
49:S2:210:MET:HE2	49:S2:370:LEU:HD21	1.79	0.65
8:A5:97:GLU:N	8:A5:97:GLU:OE1	2.28	0.65
45:N2:126:GLU:N	45:N2:126:GLU:OE1	2.29	0.65
41:G1:113:ARG:NH1	41:G1:115:THR:OG1	2.29	0.65
31:E3:375:GLU:N	31:E3:375:GLU:OE1	2.28	0.65
59:E7:4:LEU:HD12	59:E7:4:LEU:O	1.97	0.65
22:B6:45:GLU:CG	48:N5:64:LEU:HD11	2.27	0.65
27:BM:62:MET:HA	27:BM:62:MET:HE2	1.79	0.65
37:EB:96:ARG:NH1	47:N4:319:ASN:O	2.29	0.65
48:N5:92:LEU:HD22	48:N5:343:PHE:HA	1.79	0.65
31:E3:52:ASP:OD1	31:E3:240:SER:OG	2.13	0.65
18:B2:97:PRO:O	23:B7:83:ARG:NH2	2.30	0.65
38:EC:60:HIS:O	38:EC:64:VAL:HG23	1.96	0.65
20:B4:76:ASP:OD1	20:B4:77:SER:N	2.29	0.64
38:EC:20:PRO:O	38:EC:24:ASN:ND2	2.30	0.64
55:S8:92:HIS:CE1	61:S8:297:SF4:S4	2.90	0.64
6:A2:183:GLN:O	29:E1:197:ASN:ND2	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A9:151:ASN:O	12:A9:161:ARG:NH1	2.30	0.64
28:C4:2:ASP:OD1	28:C4:3:ARG:N	2.30	0.64
29:E1:274:PRO:O	29:E1:330:GLN:NE2	2.29	0.64
40:FX:130:SER:OG	41:G1:297:ARG:NH2	2.28	0.64
43:G3:239:THR:OG1	46:N6:161:LYS:NZ	2.29	0.64
48:N5:272:ASN:O	48:N5:275:ILE:HG22	1.96	0.64
49:S2:157:PRO:O	55:S8:89:ARG:NH2	2.30	0.64
2:1B:236:ARG:NH2	2:1B:488:ASP:O	2.29	0.64
33:E5:266:LEU:HG	33:E5:289:LEU:HD13	1.80	0.64
13:AB:92:LEU:CD1	66:AB:150:ZMP:H20A	2.28	0.64
16:AM:193:TYR:OH	52:S5:103:GLU:OE2	2.14	0.64
29:E1:81:ARG:NE	29:E1:126:LEU:O	2.29	0.64
49:S2:90:LYS:NZ	50:S3:75:ASP:OD2	2.19	0.64
11:A8:1:MET:HE2	45:N2:195:ILE:HG21	1.80	0.64
48:N5:121:ILE:O	48:N5:125:THR:HG23	1.98	0.64
48:N5:234:THR:HG21	48:N5:242:LEU:HB2	1.79	0.64
48:N5:315:THR:HG22	48:N5:349:LYS:HG2	1.78	0.64
53:S6:70:VAL:HG11	55:S8:100:GLY:O	1.98	0.64
29:E1:89:ASP:OD1	29:E1:90:SER:N	2.31	0.64
40:FX:275:LYS:O	40:FX:277:VAL:N	2.29	0.64
41:G1:113:ARG:NH2	46:N6:166:TYR:OH	2.29	0.64
40:FX:219:HIS:H	40:FX:222:SER:HG	1.46	0.64
18:B2:125:PHE:CE2	48:N5:415:ILE:HG22	2.32	0.64
35:E8:115:TYR:CZ	35:E8:119:ILE:HD11	2.32	0.64
12:A9:120:THR:OG1	12:A9:195:SER:OG	1.98	0.63
44:N1:586:SER:O	54:S7:114:GLN:NE2	2.31	0.63
32:E4:31:VAL:HG21	49:S2:236:VAL:CG1	2.27	0.63
12:A9:260:LYS:NZ	65:A9:559:NDP:O2D	2.20	0.63
23:B7:86:LYS:NZ	23:B7:90:ASP:OD2	2.29	0.63
42:G2:47:ASN:OD1	42:G2:48:GLY:N	2.30	0.63
57:V1:428:LEU:HD23	57:V1:428:LEU:O	1.98	0.63
6:A2:102:GLN:O	12:A9:78:LYS:NZ	2.30	0.63
32:E4:318:VAL:HG21	32:E4:334:VAL:HG21	1.78	0.63
47:N4:43:ILE:HD12	47:N4:44:MET:N	2.13	0.63
49:S2:226:ARG:NH2	49:S2:268:GLU:OE2	2.31	0.63
37:EB:30:GLN:O	37:EB:35:ARG:NH2	2.31	0.63
45:N2:272:TYR:CZ	45:N2:276:ILE:HD11	2.33	0.63
1:1A:165:SER:CB	49:S2:306:SER:HG	2.12	0.63
5:A1:137:PHE:O	16:AM:118:ARG:NH2	2.31	0.63
45:N2:5:ASN:OD1	45:N2:6:ASN:ND2	2.32	0.63
52:S5:20:GLU:OE1	52:S5:24:THR:OG1	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1B:262:TYR:O	2:1B:263:ARG:NH1	2.31	0.63
17:AN:180:ARG:NH1	40:FX:206:ASP:OD1	2.31	0.63
37:EB:60:GLU:OE2	37:EB:72:ARG:NH1	2.31	0.63
49:S2:105:VAL:HG21	49:S2:242:VAL:HG22	1.80	0.63
17:AN:91:VAL:O	45:N2:169:TYR:OH	2.16	0.63
30:E2:19:GLU:N	30:E2:19:GLU:OE1	2.32	0.62
30:E2:187:THR:HG22	30:E2:189:ASP:H	1.63	0.62
28:C4:45:SER:O	28:C4:51:ASN:ND2	2.32	0.62
29:E1:70:ALA:O	29:E1:102:ARG:NH1	2.32	0.62
49:S2:342:TYR:OH	49:S2:344:GLN:NE2	2.32	0.62
25:B9:134:LYS:O	25:B9:137:THR:HG23	1.98	0.62
41:G1:198:ARG:HD3	43:G3:202:LEU:HD21	1.81	0.62
41:G1:207:SER:OG	41:G1:233:GLY:O	2.17	0.62
48:N5:355:LEU:HD11	48:N5:384:ILE:HG22	1.80	0.62
29:E1:50:ARG:NH1	29:E1:55:GLU:OE1	2.32	0.62
43:G3:112:VAL:HG22	43:G3:128:PRO:HA	1.81	0.62
4:4L:84:ILE:CG2	46:N6:33:ILE:HD11	2.29	0.62
44:N1:396:ARG:NH2	54:S7:102:ASP:OD2	2.33	0.62
51:S4:73:SER:O	51:S4:76:THR:HG22	1.99	0.62
48:N5:244:ASP:OD1	48:N5:536:ARG:NH2	2.33	0.62
50:S3:230:GLU:OE1	51:S4:70:ARG:NH2	2.32	0.62
48:N5:111:ASP:OD1	48:N5:112:LYS:N	2.33	0.62
6:A2:155:GLU:OE2	31:E3:163:LYS:NZ	2.30	0.62
44:N1:546:TYR:O	44:N1:551:LYS:NZ	2.31	0.62
57:V1:359:ASP:O	57:V1:362:THR:HG22	1.98	0.62
1:1A:331:MET:HE1	1:1A:335:TYR:HD2	1.65	0.62
27:BM:51:SER:OG	27:BM:53:ASP:OD1	2.14	0.62
39:ED:116:VAL:HG12	39:ED:116:VAL:O	2.00	0.62
44:N1:419:TYR:O	46:N3:199:ARG:NH2	2.32	0.61
1:1A:195:CYS:O	1:1A:196:THR:OG1	2.18	0.61
66:AC:201:ZMP:H12A	66:AC:201:ZMP:HN2	1.65	0.61
32:E4:238:MET:HA	32:E4:238:MET:HE2	1.82	0.61
45:N2:20:ILE:O	45:N2:24:ASN:ND2	2.33	0.61
24:B8:63:ASN:ND2	24:B8:65:THR:OG1	2.32	0.61
32:E4:180:ARG:NH2	32:E4:268:ALA:O	2.33	0.61
43:G3:82:ARG:NH1	43:G3:84:ASP:OD2	2.33	0.61
34:E6:368:GLU:OE1	34:E6:368:GLU:N	2.34	0.61
10:A7:35:THR:O	15:AL:62:ARG:NH2	2.34	0.61
10:A7:46:ALA:O	16:AM:31:ARG:NH1	2.31	0.61
11:A8:4:PRO:O	11:A8:10:THR:OG1	2.10	0.61
25:B9:18:GLN:NE2	25:B9:22:SER:O	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:E1:164:ILE:O	29:E1:180:ARG:NH1	2.33	0.61
32:E4:128:ILE:HD11	32:E4:156:LEU:CD1	2.30	0.61
48:N5:2:LEU:HD22	48:N5:82:ILE:HG13	1.82	0.61
1:1A:165:SER:OG	1:1A:168:ASP:OD1	2.08	0.61
45:N2:175:TYR:CG	45:N2:186:MET:HE1	2.35	0.61
1:1A:146:ASP:OD1	1:1A:260:ASN:ND2	2.34	0.61
9:A6:72:MET:HE3	9:A6:120:PHE:HD1	1.65	0.61
48:N5:259:ALA:O	48:N5:260:THR:HG23	2.01	0.61
50:S3:230:GLU:OE2	51:S4:119:LYS:NZ	2.32	0.61
50:S3:234:ASP:OD1	50:S3:235:ASP:N	2.33	0.61
49:S2:48:PHE:HB3	54:S7:128:MET:HE2	1.83	0.60
58:V2:194:SER:OG	58:V2:198:ARG:O	2.19	0.60
29:E1:264:PHE:CE2	29:E1:270:VAL:HG21	2.36	0.60
3:2B:54:THR:HG21	64:N4:501:CDL:H792	1.84	0.60
9:A6:211:ASP:OD1	9:A6:211:ASP:N	2.35	0.60
25:B9:21:SER:OG	25:B9:118:GLN:OE1	2.19	0.60
19:B3:22:MET:HE1	19:B3:34:ARG:HD2	1.83	0.60
28:C4:142:SER:O	28:C4:146:VAL:HG22	2.02	0.60
32:E4:185:SER:OG	32:E4:205:GLU:OE2	2.10	0.60
46:N3:275:LEU:HD23	46:N6:148:MET:SD	2.41	0.60
22:B6:12:ASP:OD2	48:N5:116:ARG:NH2	2.34	0.60
30:E2:374:ARG:NH2	38:EC:76:VAL:O	2.34	0.60
39:ED:43:TRP:CZ2	39:ED:47:MET:HE3	2.36	0.60
57:V1:351:GLY:O	57:V1:352:THR:OG1	2.18	0.60
59:E7:178:SER:OG	59:E7:180:ASP:OD1	2.20	0.60
13:AB:109:MET:HE1	13:AB:117:ILE:HD12	1.84	0.60
14:AC:113:GLU:OE1	14:AC:126:TYR:OH	2.18	0.60
43:G3:98:GLU:OE1	43:G3:98:GLU:N	2.34	0.60
44:N1:461:ILE:HD11	46:N3:173:VAL:HG11	1.83	0.60
9:A6:125:LEU:N	9:A6:128:GLN:OE1	2.34	0.60
21:B5:29:HIS:NE2	27:BM:50:TRP:O	2.24	0.60
44:N1:395:ARG:NH2	49:S2:190:GLU:OE1	2.35	0.60
50:S3:30:GLU:OE1	50:S3:246:TYR:OH	2.17	0.60
32:E4:174:ASN:ND2	32:E4:211:CYS:O	2.31	0.60
49:S2:189:ASP:OD1	49:S2:270:ARG:NH2	2.35	0.60
58:V2:14:ALA:N	58:V2:17:ASP:OD2	2.33	0.60
2:1B:63:LEU:HD11	2:1B:352:LEU:HD12	1.84	0.59
2:1B:264:LEU:HD21	31:E3:344:LEU:HD13	1.84	0.59
24:B8:150:GLU:N	24:B8:150:GLU:OE1	2.35	0.59
30:E2:101:PHE:CZ	30:E2:244:ILE:HG22	2.37	0.59
47:N4:352:TYR:CG	47:N4:452:LEU:HD22	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:N5:170:LYS:NZ	48:N5:244:ASP:OD2	2.27	0.59
48:N5:367:ASP:OD2	48:N5:369:ARG:NH1	2.35	0.59
14:AC:109:MET:HE1	14:AC:117:ILE:HD12	1.84	0.59
11:A8:37:LYS:O	36:EA:106:UNK:N	2.35	0.59
44:N1:461:ILE:CD1	46:N3:173:VAL:HG11	2.31	0.59
51:S4:156:ARG:NH1	51:S4:158:GLU:OE2	2.35	0.59
54:S7:42:GLU:N	54:S7:42:GLU:OE1	2.35	0.59
9:A6:99:LEU:O	51:S4:47:GLN:NE2	2.34	0.59
29:E1:303:LEU:HD21	29:E1:312:VAL:HG21	1.83	0.59
33:E5:245:VAL:O	33:E5:249:VAL:HG23	2.02	0.59
57:V1:329:PRO:HD2	57:V1:332:ILE:HD12	1.84	0.59
66:AC:201:ZMP:H24	25:B9:46:ALA:HB1	1.84	0.59
54:S7:149:GLY:O	54:S7:153:ASN:ND2	2.35	0.59
2:1B:420:GLU:HG2	12:A9:89:LEU:HD13	1.84	0.59
9:A6:426:LYS:O	9:A6:427:SER:OG	2.14	0.59
10:A7:65:ASP:O	10:A7:68:ARG:NH1	2.34	0.59
17:AN:247:TYR:O	17:AN:271:TYR:OH	2.19	0.59
47:N4:403:SER:O	47:N4:406:ILE:HG22	2.01	0.59
66:AC:201:ZMP:H25A	25:B9:100:ARG:CD	2.33	0.59
9:A6:175:GLU:OE2	9:A6:178:THR:OG1	2.20	0.59
29:E1:277:GLU:OE1	29:E1:277:GLU:N	2.32	0.59
37:EB:82:MET:HA	37:EB:82:MET:HE2	1.84	0.59
49:S2:75:MET:SD	49:S2:118:LEU:HD22	2.42	0.59
20:B4:20:PRO:O	20:B4:22:ASP:N	2.35	0.59
21:B5:21:GLY:O	42:G2:90:ARG:NH2	2.35	0.59
48:N5:360:ILE:HG23	48:N5:365:SER:O	2.03	0.59
50:S3:38:ARG:NE	50:S3:39:GLU:OE2	2.32	0.59
2:1B:171:GLU:OE1	2:1B:171:GLU:N	2.36	0.58
4:4L:154:TYR:OH	45:N2:129:TRP:NE1	2.35	0.58
7:A3:5:GLU:OE1	10:A7:116:ARG:NH1	2.36	0.58
9:A6:119:TYR:CZ	66:AB:150:ZMP:H25A	2.38	0.58
21:B5:11:PRO:O	68:N4:505:U10:H302	2.03	0.58
26:BL:30:GLU:OE1	26:BL:30:GLU:N	2.34	0.58
33:E5:254:GLY:O	33:E5:255:ASN:ND2	2.36	0.58
50:S3:224:ARG:O	55:S8:117:GLN:NE2	2.35	0.58
16:AM:140:ALA:HA	52:S5:37:VAL:HG21	1.84	0.58
27:BM:3:VAL:O	42:G2:115:ARG:NH2	2.36	0.58
40:FX:263:LYS:NZ	41:G1:61:GLU:O	2.27	0.58
50:S3:264:ASP:OD1	51:S4:149:ASN:ND2	2.33	0.58
63:AM:220:PC1:O14	41:G1:426:TYR:OH	2.08	0.58
64:C4:202:CDL:OB3	47:N4:23:LYS:NZ	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:E2:125:ALA:O	30:E2:129:VAL:HG23	2.03	0.58
44:N1:394:GLN:OE1	44:N1:396:ARG:NH1	2.37	0.58
48:N5:12:ILE:HG22	48:N5:122:MET:HE1	1.85	0.58
49:S2:324:PRO:O	49:S2:345:SER:OG	2.21	0.58
8:A5:30:LEU:HD22	49:S2:212:LEU:HD22	1.86	0.58
19:B3:32:TRP:O	19:B3:33:SER:OG	2.17	0.58
33:E5:84:ARG:NH1	33:E5:114:LEU:O	2.36	0.58
48:N5:209:TYR:O	48:N5:213:ASN:ND2	2.37	0.58
49:S2:208:GLY:O	49:S2:261:ARG:NH1	2.31	0.58
16:AM:152:ARG:NH2	16:AM:185:GLU:OE2	2.36	0.58
20:B4:105:LYS:NZ	47:N4:292:ASP:OD2	2.34	0.58
44:N1:579:SER:OG	44:N1:645:ARG:NH1	2.37	0.58
48:N5:118:VAL:HG12	48:N5:122:MET:HE2	1.85	0.58
48:N5:494:ILE:HD13	48:N5:499:HIS:CE1	2.39	0.58
20:B4:9:LEU:HD11	40:FX:253:THR:HG21	1.86	0.57
22:B6:74:ASN:ND2	39:ED:130:PRO:O	2.37	0.57
33:E5:275:GLU:O	33:E5:279:GLY:N	2.36	0.57
49:S2:168:ASP:OD1	49:S2:169:LEU:N	2.36	0.57
57:V1:44:ILE:HG22	58:V2:210:LEU:HD11	1.86	0.57
16:AM:54:VAL:HG13	64:AM:216:CDL:H532	1.85	0.57
17:AN:108:TRP:HZ3	40:FX:307:THR:HG21	1.69	0.57
23:B7:94:GLU:OE2	59:E7:100:ARG:NH2	2.37	0.57
53:S6:40:LEU:HA	53:S6:43:VAL:HG22	1.85	0.57
5:A1:78:ARG:NH2	63:A1:203:PC1:O12	2.37	0.57
15:AL:66:VAL:HG11	55:S8:65:ILE:HG22	1.87	0.57
47:N4:316:LEU:HD21	47:N4:325:TYR:CZ	2.39	0.57
1:1A:331:MET:HE2	2:1B:305:VAL:CG1	2.35	0.57
8:A5:143:LYS:NZ	8:A5:151:GLU:OE2	2.17	0.57
44:N1:582:ILE:HD11	46:N3:214:VAL:HG12	1.85	0.57
49:S2:241:GLU:O	57:V1:492:SER:OG	2.17	0.57
1:1A:352:LEU:HD11	9:A6:360:LEU:CD1	2.35	0.57
11:A8:146:GLN:OE1	11:A8:146:GLN:N	2.35	0.57
54:S7:139:MET:HE3	54:S7:143:CYS:HB2	1.85	0.57
29:E1:147:ASP:O	29:E1:337:TYR:OH	2.18	0.57
32:E4:348:MET:HE2	32:E4:348:MET:HA	1.87	0.57
2:1B:374:ILE:HG21	2:1B:382:THR:HG21	1.87	0.57
5:A1:76:GLU:OE1	5:A1:93:TRP:NE1	2.36	0.57
8:A5:156:ARG:NH1	50:S3:28:THR:OG1	2.35	0.57
35:E8:1:MET:HE3	35:E8:1:MET:HA	1.86	0.57
48:N5:161:ARG:NH1	48:N5:247:GLU:OE1	2.38	0.57
55:S8:103:ARG:O	55:S8:155:VAL:HG21	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1B:367:ARG:NH1	31:E3:374:GLU:OE1	2.38	0.57
19:B3:5:ASN:ND2	39:ED:21:THR:OG1	2.38	0.57
24:B8:103:LEU:HD12	35:E8:81:MET:HB2	1.85	0.57
41:G1:197:ASP:OD1	41:G1:198:ARG:N	2.38	0.57
47:N4:327:ILE:HG22	48:N5:72:TYR:CE2	2.40	0.57
58:V2:114:GLU:OE1	58:V2:114:GLU:N	2.37	0.57
66:AC:201:ZMP:H12A	66:AC:201:ZMP:N2	2.20	0.56
53:S6:31:GLN:OE1	53:S6:31:GLN:N	2.38	0.56
1:1A:152:ASP:OD1	50:S3:233:TRP:NE1	2.37	0.56
18:B2:138:TRP:NE1	24:B8:155:GLN:OE1	2.34	0.56
29:E1:212:ARG:NH1	29:E1:213:ASP:OD2	2.36	0.56
33:E5:7:TRP:O	33:E5:96:TYR:HB2	2.05	0.56
40:FX:144:ASP:OD2	40:FX:150:HIS:NE2	2.29	0.56
41:G1:124:ASP:OD1	41:G1:403:ARG:NH2	2.36	0.56
48:N5:393:LEU:HD11	48:N5:432:GLN:HG2	1.87	0.56
57:V1:456:ASP:OD1	57:V1:476:ARG:NH1	2.38	0.56
59:E7:165:GLN:O	59:E7:169:THR:OG1	2.22	0.56
2:1B:525:GLU:OE1	2:1B:525:GLU:N	2.33	0.56
40:FX:205:GLU:OE2	40:FX:223:ARG:NE	2.34	0.56
48:N5:152:LEU:C	48:N5:152:LEU:HD23	2.31	0.56
53:S6:91:ASN:ND2	53:S6:95:ARG:O	2.38	0.56
3:2B:80:TYR:HB3	3:2B:81:PRO:HD3	1.86	0.56
20:B4:133:GLU:OE2	20:B4:137:ARG:NE	2.39	0.56
42:G2:114:VAL:HG22	42:G2:114:VAL:O	2.06	0.56
32:E4:47:ASN:O	32:E4:52:LYS:NZ	2.31	0.56
48:N5:260:THR:O	48:N5:263:THR:N	2.38	0.56
57:V1:152:ALA:O	57:V1:192:TYR:OH	2.16	0.56
35:E8:148:LYS:O	35:E8:149:SER:OG	2.17	0.56
1:1A:345:LEU:CD2	9:A6:367:LEU:HD22	2.36	0.56
3:2B:18:ILE:HD11	3:2B:23:TYR:OH	2.05	0.56
11:A8:83:ASN:O	11:A8:87:SER:OG	2.16	0.56
31:E3:13:HIS:NE2	31:E3:26:GLU:OE2	2.32	0.56
41:G1:343:ASP:OD1	42:G2:33:ARG:NH2	2.39	0.56
53:S6:115:CYS:O	53:S6:119:GLU:N	2.38	0.56
30:E2:187:THR:HG21	30:E2:192:ALA:HB3	1.88	0.56
31:E3:118:GLU:HB3	31:E3:296:VAL:HG11	1.88	0.56
25:B9:66:ASP:CG	35:E8:41:HIS:HE2	2.13	0.56
32:E4:190:ARG:NH2	32:E4:341:HIS:O	2.38	0.56
46:N6:52:GLY:HA3	46:N6:75:ILE:HD13	1.88	0.56
49:S2:249:GLU:OE1	49:S2:274:ARG:NH1	2.39	0.56
1:1A:88:ASN:OD1	1:1A:89:CYS:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:G1:62:GLN:OE1	49:S2:4:ARG:NE	2.38	0.55
48:N5:2:LEU:HD21	48:N5:133:ILE:HD12	1.87	0.55
70:V1:579:FMN:C5A	71:V1:581:NAI:H4N	2.36	0.55
9:A6:83:ASP:OD1	9:A6:86:ARG:NH1	2.38	0.55
5:A1:7:TRP:N	55:S8:68:PHE:O	2.38	0.55
11:A8:105:TYR:OH	16:AM:104:GLN:NE2	2.39	0.55
41:G1:344:ASN:ND2	42:G2:225:GLU:OE2	2.37	0.55
46:N6:45:ILE:HD11	46:N6:82:ILE:CG2	2.36	0.55
55:S8:172:ASP:OD1	55:S8:172:ASP:N	2.40	0.55
3:2B:87:LEU:HD11	45:N2:242:SER:CB	2.36	0.55
11:A8:8:SER:OG	45:N2:95:ASN:O	2.23	0.55
22:B6:45:GLU:HG3	48:N5:64:LEU:HD11	1.88	0.55
26:BL:111:TYR:OH	48:N5:193:TYR:O	2.17	0.55
30:E2:118:VAL:HG11	30:E2:214:LEU:CD2	2.37	0.55
55:S8:78:PRO:O	55:S8:81:ARG:NE	2.35	0.55
1:1A:258:GLU:OE2	15:AL:238:ARG:NH1	2.37	0.55
2:1B:48:ARG:NH1	6:A2:163:ASP:OD1	2.39	0.55
40:FX:253:THR:HG23	40:FX:304:TRP:HE1	1.71	0.55
48:N5:393:LEU:HD11	48:N5:432:GLN:CG	2.37	0.55
3:2B:59:TYR:CE1	45:N2:267:LEU:HD22	2.42	0.55
47:N4:173:ASN:OD1	47:N4:177:ASN:ND2	2.39	0.55
59:E7:77:ILE:O	59:E7:81:VAL:HG22	2.07	0.55
2:1B:281:ARG:NH1	6:A2:181:ALA:O	2.39	0.55
7:A3:53:ARG:NH2	45:N2:25:ILE:O	2.36	0.55
9:A6:304:LEU:HD21	9:A6:385:ILE:HG21	1.88	0.55
11:A8:1:MET:HE1	45:N2:58:LEU:CD2	2.37	0.55
47:N4:35:ILE:HG21	47:N4:108:TYR:OH	2.07	0.55
29:E1:418:VAL:HG22	29:E1:419:ALA:H	1.71	0.55
44:N1:416:LYS:NZ	54:S7:116:ASP:OD2	2.37	0.55
5:A1:95:ASP:OD1	11:A8:160:ARG:NH2	2.38	0.55
30:E2:118:VAL:HG13	30:E2:283:LEU:HD13	1.89	0.55
35:E8:18:TRP:CZ3	48:N5:436:LEU:HD12	2.42	0.55
32:E4:39:ARG:NH2	49:S2:282:ASP:OD1	2.40	0.55
44:N1:510:PHE:CE2	44:N1:514:LEU:HD11	2.42	0.55
57:V1:157:ILE:HB	57:V1:198:LEU:HD12	1.88	0.55
47:N4:189:HIS:CD2	47:N4:193:ILE:HD11	2.42	0.54
54:S7:184:THR:O	54:S7:187:ALA:N	2.40	0.54
47:N4:302:ILE:O	47:N4:306:ASN:ND2	2.36	0.54
48:N5:322:MET:O	48:N5:325:ILE:HG22	2.06	0.54
50:S3:29:GLN:OE1	50:S3:29:GLN:N	2.41	0.54
1:1A:318:ARG:NH2	2:1B:494:ASP:OD1	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4L:154:TYR:HH	45:N2:129:TRP:NE1	2.05	0.54
63:A1:202:PC1:C1	63:A1:202:PC1:H152	2.37	0.54
12:A9:121:VAL:HG11	12:A9:133:VAL:HG23	1.88	0.54
30:E2:154:ARG:O	30:E2:157:VAL:HG23	2.06	0.54
46:N6:45:ILE:HD11	46:N6:82:ILE:HG22	1.89	0.54
31:E3:289:HIS:O	31:E3:292:LYS:NZ	2.38	0.54
35:E8:18:TRP:CE3	48:N5:436:LEU:HD12	2.43	0.54
1:1A:331:MET:HE1	1:1A:335:TYR:CD2	2.41	0.54
53:S6:35:PRO:HD3	53:S6:77:ILE:HD11	1.90	0.54
12:A9:474:VAL:HG21	63:A9:560:PC1:H232	1.88	0.54
17:AN:133:PHE:O	17:AN:137:ASN:ND2	2.39	0.54
47:N4:43:ILE:HD13	47:N4:472:LEU:CD2	2.37	0.54
1:1A:375:ARG:NH1	9:A6:232:ASP:OD1	2.38	0.54
11:A8:124:GLU:N	11:A8:124:GLU:OE1	2.40	0.54
15:AL:257:ARG:CD	55:S8:124:VAL:HG11	2.37	0.54
17:AN:108:TRP:CZ3	40:FX:307:THR:HG21	2.43	0.54
46:N6:163:SER:O	46:N6:165:ASN:ND2	2.40	0.54
57:V1:88:GLY:O	71:V1:581:NAI:H2N	2.08	0.54
6:A2:152:ALA:O	6:A2:158:ASN:ND2	2.40	0.54
31:E3:253:ASN:ND2	33:E5:54:LEU:O	2.40	0.54
41:G1:254:ILE:C	41:G1:255:ILE:HD12	2.32	0.54
47:N4:176:TYR:CE2	47:N4:180:LEU:HD11	2.42	0.54
48:N5:311:VAL:O	48:N5:315:THR:HG23	2.08	0.54
9:A6:31:VAL:HG12	40:FX:143:ILE:HD11	1.89	0.54
45:N2:25:ILE:HA	46:N3:284:LEU:HD22	1.89	0.54
45:N2:81:ILE:CD1	46:N6:153:ILE:HD12	2.38	0.54
46:N3:261:ILE:HD13	46:N6:128:ILE:HB	1.89	0.54
51:S4:65:VAL:O	51:S4:139:ASN:N	2.41	0.54
57:V1:117:ASN:ND2	57:V1:208:GLY:O	2.33	0.54
4:4L:84:ILE:HG23	46:N6:33:ILE:HD11	1.91	0.54
14:AC:52:HIS:NE2	22:B6:3:ASP:OD2	2.40	0.54
42:G2:181:VAL:HG23	43:G3:176:VAL:CG2	2.38	0.53
44:N1:491:TRP:NE1	46:N3:213:GLU:OE1	2.39	0.53
47:N4:175:MET:HE1	47:N4:257:PHE:CZ	2.43	0.53
59:E7:81:VAL:HG23	59:E7:83:GLN:H	1.73	0.53
11:A8:140:PHE:CZ	11:A8:151:THR:HG21	2.42	0.53
64:B3:102:CDL:HB22	39:ED:47:MET:HE1	1.89	0.53
31:E3:306:ASP:OD1	31:E3:306:ASP:N	2.40	0.53
42:G2:220:GLU:O	42:G2:223:THR:HG22	2.08	0.53
68:N4:505:U10:C33	68:N4:505:U10:H301	2.39	0.53
50:S3:117:ARG:NH2	50:S3:193:ASP:OD1	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:V1:125:THR:HG22	57:V1:354:ALA:HB2	1.89	0.53
12:A9:181:ASN:OD1	12:A9:183:THR:OG1	2.14	0.53
12:A9:297:LEU:HD11	12:A9:397:TRP:CZ2	2.43	0.53
29:E1:45:LYS:NZ	29:E1:293:HIS:O	2.40	0.53
32:E4:341:HIS:NE2	41:G1:435:MET:SD	2.82	0.53
41:G1:305:VAL:O	41:G1:309:THR:HG23	2.09	0.53
35:E8:22:TYR:O	35:E8:26:THR:OG1	2.25	0.53
35:E8:148:LYS:O	35:E8:158:ARG:NH1	2.40	0.53
59:E7:180:ASP:OD1	59:E7:181:SER:N	2.42	0.53
30:E2:118:VAL:HG11	30:E2:214:LEU:HD21	1.89	0.53
32:E4:180:ARG:NH2	32:E4:274:THR:OG1	2.41	0.53
48:N5:102:ILE:HG23	48:N5:466:ILE:HD11	1.91	0.53
41:G1:58:ARG:NE	41:G1:61:GLU:OE1	2.35	0.53
50:S3:156:MET:HE2	51:S4:17:PHE:CE1	2.44	0.53
2:1B:170:GLU:N	2:1B:170:GLU:OE1	2.42	0.53
2:1B:203:ASN:OD1	2:1B:482:ARG:NH2	2.40	0.53
9:A6:393:ILE:O	9:A6:396:THR:OG1	2.27	0.53
13:AB:90:ASP:OD1	13:AB:91:SER:N	2.39	0.53
36:EA:40:ARG:NH1	45:N2:29:ASP:OD1	2.41	0.53
45:N2:78:VAL:HG13	45:N2:117:LEU:HD22	1.91	0.53
46:N3:245:PHE:HD2	46:N6:81:ILE:HD11	1.74	0.53
48:N5:304:TYR:O	48:N5:310:ILE:HD11	2.09	0.53
49:S2:253:GLY:H	49:S2:264:ILE:HD11	1.74	0.53
57:V1:410:VAL:O	57:V1:413:ILE:HG22	2.08	0.53
11:A8:172:THR:OG1	44:N1:529:TYR:O	2.14	0.53
30:E2:421:LEU:HD11	30:E2:465:THR:OG1	2.09	0.53
41:G1:113:ARG:NH2	41:G1:119:LYS:O	2.42	0.53
57:V1:209:GLU:OE1	57:V1:210:GLU:N	2.42	0.53
59:E7:140:ASP:OD1	59:E7:140:ASP:N	2.41	0.53
29:E1:408:LEU:HD21	29:E1:434:HIS:CE1	2.44	0.53
35:E8:74:ARG:NH2	59:E7:207:VAL:O	2.41	0.53
46:N6:42:ILE:HD12	46:N6:43:ARG:N	2.24	0.53
7:A3:102:GLU:OE2	36:EA:89:ARG:NH2	2.42	0.52
28:C4:43:ASP:O	28:C4:44:ALA:HB3	2.09	0.52
40:FX:144:ASP:O	40:FX:147:GLY:N	2.42	0.52
41:G1:78:GLU:O	41:G1:84:GLN:NE2	2.41	0.52
47:N4:299:LEU:HD23	47:N4:302:ILE:HD12	1.91	0.52
49:S2:267:GLN:NE2	49:S2:271:ASN:OD1	2.41	0.52
50:S3:122:TYR:CE1	50:S3:148:LEU:HD12	2.45	0.52
52:S5:27:LEU:O	52:S5:30:VAL:HG23	2.09	0.52
2:1B:131:GLN:OE1	2:1B:490:ILE:N	2.35	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:E4:318:VAL:HG21	32:E4:334:VAL:CG2	2.38	0.52
33:E5:152:LEU:HB2	33:E5:284:VAL:HG11	1.91	0.52
47:N4:405:SER:OG	48:N5:187:ILE:HD12	2.08	0.52
2:1B:32:VAL:HG21	2:1B:359:LEU:HD23	1.90	0.52
40:FX:134:THR:OG1	41:G1:282:ASP:OD1	2.18	0.52
5:A1:44:THR:HG23	16:AM:106:LYS:HZ3	1.74	0.52
11:A8:102:ARG:HA	11:A8:128:MET:HE3	1.91	0.52
15:AL:20:GLN:NE2	15:AL:24:GLN:OE1	2.42	0.52
21:B5:47:THR:HG22	63:B5:203:PC1:H2E1	1.91	0.52
23:B7:67:CYS:SG	23:B7:71:ARG:NH1	2.83	0.52
27:BM:35:ILE:HD11	48:N5:109:TYR:OH	2.10	0.52
28:C4:6:VAL:HG22	45:N2:100:THR:OG1	2.08	0.52
31:E3:242:GLU:N	31:E3:242:GLU:OE1	2.39	0.52
36:EA:9:HIS:ND1	43:G3:226:ASP:OD2	2.29	0.52
20:B4:160:MET:HE1	24:B8:154:ALA:CB	2.39	0.52
42:G2:149:MET:HE2	42:G2:168:GLU:HG3	1.91	0.52
48:N5:328:ILE:HG22	48:N5:328:ILE:O	2.10	0.52
4:4L:141:LEU:HD11	46:N6:150:MET:HE1	1.92	0.52
15:AL:232:LYS:O	15:AL:239:ARG:NH1	2.43	0.52
33:E5:161:ALA:O	33:E5:165:GLY:N	2.43	0.52
45:N2:58:LEU:HD22	45:N2:87:ILE:HG12	1.91	0.52
45:N2:214:ILE:HG23	45:N2:256:LEU:HD21	1.90	0.52
49:S2:67:PRO:O	49:S2:71:ARG:NH1	2.43	0.52
58:V2:204:LEU:O	58:V2:204:LEU:HD23	2.09	0.52
17:AN:104:THR:HG22	40:FX:248:VAL:HG13	1.92	0.52
25:B9:158:TYR:O	47:N4:446:THR:HG22	2.09	0.52
47:N4:110:ILE:CG2	47:N4:126:ILE:HG23	2.40	0.52
48:N5:54:ASN:OD1	48:N5:55:ILE:N	2.42	0.52
63:N5:601:PC1:O13	63:N5:601:PC1:H143	2.09	0.52
4:4L:81:TYR:OH	46:N6:25:ASP:OD2	2.24	0.52
22:B6:57:ARG:NH1	22:B6:82:MET:SD	2.80	0.52
40:FX:138:VAL:HG22	40:FX:232:PRO:HA	1.90	0.52
40:FX:158:MET:HE1	40:FX:166:GLN:NE2	2.24	0.52
48:N5:239:GLN:N	48:N5:240:PRO:CD	2.73	0.52
48:N5:340:LEU:HD13	48:N5:489:LEU:HD22	1.92	0.52
50:S3:232:GLU:HG2	51:S4:76:THR:HG21	1.90	0.52
57:V1:124:GLY:O	57:V1:354:ALA:HB1	2.10	0.52
2:1B:108:GLU:CG	2:1B:419:VAL:HG21	2.40	0.52
16:AM:54:VAL:HG13	64:AM:216:CDL:C53	2.40	0.52
18:B2:107:TYR:N	18:B2:110:GLU:OE1	2.40	0.52
23:B7:14:ASP:OD2	23:B7:17:LYS:NZ	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:ED:18:GLN:OE1	39:ED:18:GLN:N	2.38	0.52
48:N5:329:ASP:HA	48:N5:334:ILE:HG22	1.92	0.52
46:N6:124:ASN:ND2	52:S5:34:GLU:OE2	2.43	0.52
46:N6:147:ILE:O	46:N6:150:MET:HG3	2.10	0.52
2:1B:112:THR:O	51:S4:155:ASN:ND2	2.38	0.52
11:A8:128:MET:HE2	11:A8:132:TYR:HE2	1.74	0.52
20:B4:160:MET:HE1	24:B8:154:ALA:HB3	1.92	0.52
25:B9:54:PRO:HG3	35:E8:25:MET:HE3	1.92	0.52
42:G2:95:ILE:HG23	42:G2:99:THR:HG21	1.92	0.52
45:N2:293:ASN:OD1	45:N2:294:ASN:N	2.43	0.52
47:N4:92:GLU:OE2	47:N4:100:ASN:ND2	2.42	0.52
3:2B:56:ILE:HD12	45:N2:257:PHE:CZ	2.45	0.51
9:A6:122:GLU:OE2	46:N3:220:MET:N	2.44	0.51
12:A9:288:ASN:O	12:A9:292:LEU:HD12	2.10	0.51
32:E4:100:ARG:NH2	32:E4:141:SER:OG	2.37	0.51
41:G1:141:LYS:NZ	43:G3:211:THR:HG21	2.25	0.51
47:N4:289:TYR:OH	48:N5:551:SER:OG	2.12	0.51
48:N5:42:ILE:O	48:N5:46:VAL:HG23	2.09	0.51
48:N5:389:LEU:HD21	48:N5:438:ILE:HD11	1.93	0.51
50:S3:156:MET:HE1	50:S3:174:PRO:HG2	1.91	0.51
58:V2:104:THR:HG22	58:V2:105:THR:H	1.74	0.51
2:1B:341:ASP:OD1	2:1B:341:ASP:N	2.44	0.51
12:A9:12:ILE:HD11	12:A9:31:LEU:HD11	1.92	0.51
14:AC:62:ARG:NE	14:AC:104:GLU:OE2	2.35	0.51
24:B8:87:ASP:N	24:B8:87:ASP:OD1	2.42	0.51
29:E1:252:LEU:HD12	29:E1:394:LEU:HD11	1.92	0.51
34:E6:141:ARG:NH2	34:E6:224:ASP:OD2	2.43	0.51
40:FX:140:LEU:HD22	40:FX:237:MET:HE2	1.92	0.51
40:FX:190:ILE:HD13	40:FX:239:VAL:HG13	1.92	0.51
46:N6:33:ILE:HA	46:N6:36:ILE:HG22	1.92	0.51
57:V1:97:LYS:NZ	70:V1:579:FMN:O2P	2.37	0.51
30:E2:28:LEU:HD12	30:E2:29:VAL:HG23	1.91	0.51
45:N2:186:MET:HE3	45:N2:282:TRP:CZ2	2.45	0.51
48:N5:131:LEU:C	48:N5:131:LEU:HD23	2.35	0.51
55:S8:92:HIS:CD2	55:S8:143:CYS:SG	3.03	0.51
4:4L:132:TRP:CH2	4:4L:136:LEU:HD11	2.46	0.51
32:E4:196:ARG:N	32:E4:332:ASP:OD2	2.43	0.51
33:E5:283:THR:HG23	33:E5:283:THR:O	2.10	0.51
44:N1:442:ILE:HD11	46:N3:185:PHE:HA	1.92	0.51
50:S3:56:LEU:HD21	50:S3:78:ILE:HD11	1.92	0.51
3:2B:42:SER:O	3:2B:43:SER:OG	2.20	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A3:49:GLU:OE1	46:N3:291:ASN:ND2	2.43	0.51
29:E1:82:ALA:HB3	29:E1:99:ILE:HD13	1.93	0.51
30:E2:91:LYS:HD3	30:E2:352:VAL:HG21	1.92	0.51
45:N2:84:ILE:CG2	46:N6:146:LEU:HD21	2.41	0.51
9:A6:129:VAL:HG12	9:A6:129:VAL:O	2.10	0.51
10:A7:28:GLY:O	15:AL:64:HIS:NE2	2.40	0.51
21:B5:23:ILE:HG13	42:G2:114:VAL:HG21	1.91	0.51
40:FX:221:ASN:O	40:FX:223:ARG:N	2.44	0.51
47:N4:43:ILE:HG12	47:N4:79:LEU:HD22	1.92	0.51
2:1B:48:ARG:HE	31:E3:336:ILE:HD13	1.75	0.51
15:AL:154:THR:OG1	64:AL:303:CDL:OB4	2.20	0.51
64:B3:102:CDL:CB2	39:ED:47:MET:HE1	2.41	0.51
29:E1:260:ALA:HB1	29:E1:292:ALA:HB2	1.93	0.51
47:N4:449:ASP:OD1	47:N4:449:ASP:N	2.44	0.51
10:A7:109:TRP:HZ2	50:S3:128:VAL:HG22	1.75	0.51
12:A9:420:ILE:HG23	12:A9:424:ILE:HD11	1.93	0.51
64:AM:217:CDL:OB3	55:S8:49:ASN:ND2	2.43	0.51
30:E2:259:VAL:HG21	30:E2:271:ALA:HB1	1.93	0.51
44:N1:572:VAL:HG12	44:N1:572:VAL:O	2.10	0.51
50:S3:178:ARG:NH2	50:S3:187:GLY:O	2.43	0.51
2:1B:129:VAL:HG12	2:1B:129:VAL:O	2.11	0.51
2:1B:233:TYR:O	2:1B:241:TYR:OH	2.10	0.51
66:AC:201:ZMP:H14	25:B9:86:LYS:HD2	1.92	0.51
44:N1:451:ILE:HD13	44:N1:536:LEU:HD11	1.93	0.51
46:N3:255:ILE:HA	46:N3:258:ILE:HG22	1.91	0.51
11:A8:118:PRO:HG2	16:AM:111:LEU:HD12	1.93	0.51
32:E4:295:GLU:HB3	32:E4:363:MET:HE3	1.92	0.51
9:A6:137:ASP:OD2	12:A9:330:ARG:NH2	2.41	0.50
12:A9:115:ARG:NH1	51:S4:97:GLU:OE2	2.45	0.50
43:G3:176:VAL:HB	43:G3:177:PRO:HD3	1.93	0.50
70:V1:579:FMN:H1'1	71:V1:581:NAI:H52N	1.92	0.50
11:A8:65:ASN:N	11:A8:65:ASN:OD1	2.41	0.50
55:S8:161:THR:HG22	55:S8:192:ILE:HD11	1.93	0.50
1:1A:242:SER:O	1:1A:245:VAL:HG22	2.11	0.50
8:A5:125:VAL:HG13	51:S4:38:VAL:HG11	1.92	0.50
9:A6:112:VAL:HG21	66:AB:150:ZMP:H9	1.93	0.50
22:B6:45:GLU:HG2	48:N5:64:LEU:HD11	1.93	0.50
45:N2:171:ILE:HD11	45:N2:248:ILE:HG13	1.92	0.50
48:N5:217:ILE:N	48:N5:217:ILE:HD12	2.27	0.50
51:S4:38:VAL:HG23	51:S4:39:ASN:N	2.26	0.50
52:S5:69:CYS:SG	52:S5:70:ARG:N	2.85	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1B:177:GLU:HG3	2:1B:477:THR:HG21	1.94	0.50
19:B3:10:GLN:NE2	48:N5:447:SER:O	2.44	0.50
33:E5:17:LYS:HE3	33:E5:270:LEU:HD13	1.93	0.50
53:S6:57:ARG:NH2	55:S8:127:ASP:OD1	2.44	0.50
23:B7:64:ARG:NH1	39:ED:111:LYS:O	2.42	0.50
32:E4:127:ASP:O	32:E4:130:ASP:N	2.42	0.50
49:S2:350:LEU:HD11	51:S4:116:ARG:NE	2.26	0.50
55:S8:92:HIS:HE1	61:S8:297:SF4:S4	2.31	0.50
12:A9:297:LEU:HD11	12:A9:397:TRP:CE2	2.47	0.50
64:AM:215:CDL:OA4	32:E4:335:TYR:OH	2.29	0.50
44:N1:582:ILE:HD11	46:N3:214:VAL:CG1	2.41	0.50
47:N4:181:LEU:HD21	47:N4:200:HIS:CD2	2.47	0.50
50:S3:72:VAL:O	57:V1:490:GLN:NE2	2.44	0.50
2:1B:87:LYS:NZ	2:1B:240:SER:OG	2.44	0.50
11:A8:1:MET:HE2	45:N2:195:ILE:CG2	2.41	0.50
24:B8:49:ASP:OD1	47:N4:150:LYS:NZ	2.32	0.50
31:E3:76:THR:OG1	31:E3:77:GLU:OE1	2.10	0.50
42:G2:181:VAL:HG23	43:G3:176:VAL:HG21	1.93	0.50
47:N4:91:TYR:OH	47:N4:355:ASP:OD2	2.29	0.50
46:N6:35:LEU:HD13	46:N6:46:ILE:HG22	1.93	0.50
29:E1:83:LEU:HD13	29:E1:126:LEU:HD12	1.94	0.50
47:N4:175:MET:HE2	47:N4:178:ILE:HD12	1.93	0.50
47:N4:319:ASN:ND2	47:N4:321:ASN:O	2.45	0.50
47:N4:334:TYR:CE2	47:N4:392:VAL:HG23	2.47	0.50
1:1A:352:LEU:HD11	9:A6:360:LEU:HD13	1.94	0.50
2:1B:190:GLU:OE2	30:E2:22:VAL:HG11	2.12	0.50
14:AC:103:TRP:NE1	48:N5:448:TYR:O	2.32	0.50
19:B3:52:UNK:O	19:B3:56:UNK:N	2.44	0.50
28:C4:150:TYR:HA	28:C4:153:VAL:HG12	1.92	0.50
29:E1:346:ASP:OD1	29:E1:348:THR:N	2.44	0.50
44:N1:469:ILE:HD11	44:N1:514:LEU:HD12	1.94	0.50
45:N2:158:TYR:CE2	45:N2:162:LEU:HD12	2.47	0.50
49:S2:107:PHE:CZ	49:S2:150:VAL:HG11	2.47	0.50
55:S8:192:ILE:O	55:S8:196:VAL:HG23	2.12	0.50
2:1B:57:GLU:N	2:1B:57:GLU:OE1	2.43	0.49
32:E4:36:LEU:HD12	32:E4:36:LEU:N	2.27	0.49
33:E5:72:VAL:O	33:E5:82:GLY:N	2.44	0.49
44:N1:602:TYR:HA	44:N1:605:ILE:HG22	1.93	0.49
49:S2:355:ARG:NH1	50:S3:105:ASP:OD1	2.45	0.49
50:S3:182:ASP:OD1	50:S3:183:TYR:N	2.42	0.49
50:S3:219:PHE:O	51:S4:106:LEU:HD23	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:V1:319:ILE:HG12	57:V1:327:VAL:HG12	1.94	0.49
3:2B:63:ILE:HD13	45:N2:260:ILE:HD13	1.94	0.49
4:4L:95:LYS:O	4:4L:103:ARG:NH2	2.45	0.49
9:A6:339:TYR:HB2	9:A6:344:LEU:HD12	1.94	0.49
15:AL:143:ARG:NH2	15:AL:173:ASP:OD1	2.43	0.49
31:E3:156:LEU:HD13	31:E3:184:LEU:HD22	1.94	0.49
33:E5:281:SER:OG	33:E5:283:THR:HG22	2.11	0.49
36:EA:74:VAL:HG21	45:N2:15:SER:HA	1.93	0.49
40:FX:219:HIS:N	40:FX:222:SER:OG	2.31	0.49
44:N1:520:ILE:HD11	44:N1:534:LEU:CD1	2.42	0.49
33:E5:194:LEU:CD1	33:E5:226:VAL:HG11	2.43	0.49
39:ED:35:ILE:HD11	39:ED:40:PHE:HA	1.95	0.49
40:FX:280:GLU:OE2	40:FX:319:ARG:NH2	2.45	0.49
45:N2:114:LEU:HD23	45:N2:117:LEU:HD12	1.95	0.49
45:N2:171:ILE:HD12	45:N2:247:THR:OG1	2.13	0.49
45:N2:186:MET:HE3	45:N2:282:TRP:HZ2	1.77	0.49
48:N5:363:ILE:O	48:N5:363:ILE:HG22	2.12	0.49
51:S4:38:VAL:HG23	51:S4:39:ASN:H	1.77	0.49
2:1B:283:ARG:NH2	31:E3:345:GLN:OE1	2.44	0.49
5:A1:44:THR:HG23	16:AM:106:LYS:NZ	2.27	0.49
9:A6:45:HIS:ND1	9:A6:113:SER:OG	2.20	0.49
20:B4:91:ARG:NH1	47:N4:358:ASN:OD1	2.45	0.49
25:B9:133:TRP:HB3	25:B9:137:THR:HG21	1.93	0.49
46:N3:276:ILE:O	46:N3:280:SER:OG	2.30	0.49
48:N5:393:LEU:HD13	48:N5:393:LEU:O	2.12	0.49
11:A8:142:THR:CG2	11:A8:192:THR:HG21	2.43	0.49
19:B3:24:HIS:NE2	64:B3:102:CDL:OA7	2.42	0.49
32:E4:144:LEU:HD12	32:E4:173:ALA:HB2	1.94	0.49
33:E5:145:ALA:HB2	33:E5:178:ILE:HG21	1.94	0.49
47:N4:420:CYS:SG	48:N5:180:VAL:HG22	2.52	0.49
48:N5:373:ASN:N	48:N5:445:ASN:O	2.38	0.49
11:A8:142:THR:HG21	11:A8:192:THR:HG21	1.95	0.49
29:E1:40:ARG:NH2	30:E2:235:ASP:OD2	2.46	0.49
31:E3:41:LEU:HD12	31:E3:98:SER:O	2.12	0.49
33:E5:42:PRO:HB3	33:E5:286:ILE:HG22	1.93	0.49
48:N5:486:TYR:CZ	48:N5:490:ILE:HD12	2.48	0.49
50:S3:93:ARG:NH1	50:S3:151:LEU:O	2.45	0.49
55:S8:141:HIS:CE1	55:S8:174:LEU:HD12	2.46	0.49
55:S8:61:TRP:CZ2	55:S8:65:ILE:HD11	2.48	0.49
57:V1:159:VAL:HG21	57:V1:198:LEU:HD11	1.95	0.49
10:A7:86:LEU:HD23	50:S3:55:TYR:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:N5:131:LEU:HD23	48:N5:131:LEU:O	2.13	0.49
22:B6:13:PHE:O	48:N5:21:ASN:ND2	2.46	0.49
40:FX:185:TRP:C	40:FX:186:SER:HG	2.15	0.49
47:N4:323:LEU:O	47:N4:327:ILE:HG23	2.13	0.49
48:N5:78:LEU:HB3	48:N5:139:MET:HE2	1.94	0.49
50:S3:70:ASP:OD1	50:S3:70:ASP:N	2.44	0.49
55:S8:126:ASP:OD1	55:S8:127:ASP:N	2.41	0.49
57:V1:396:ILE:HB	57:V1:413:ILE:HD13	1.95	0.49
9:A6:80:ILE:HG22	12:A9:430:ASN:O	2.13	0.49
33:E5:7:TRP:HB2	33:E5:96:TYR:HB3	1.95	0.49
42:G2:69:ILE:O	42:G2:72:VAL:HG23	2.13	0.49
44:N1:422:TYR:OH	46:N3:192:CYS:O	2.21	0.49
45:N2:10:ILE:HG22	45:N2:14:ILE:HD12	1.95	0.49
57:V1:358:MET:HB3	57:V1:362:THR:HG21	1.95	0.49
64:A3:201:CDL:OB3	36:EA:32:LYS:N	2.43	0.48
9:A6:303:LEU:HD21	9:A6:434:LEU:HD21	1.94	0.48
10:A7:46:ALA:HB1	55:S8:198:LYS:HE2	1.95	0.48
18:B2:86:GLN:NE2	48:N5:497:MET:O	2.46	0.48
20:B4:151:LEU:HD22	48:N5:209:TYR:OH	2.13	0.48
41:G1:194:LEU:HD22	41:G1:215:LEU:HD12	1.95	0.48
41:G1:292:VAL:HG21	67:G1:516:3PE:H332	1.93	0.48
47:N4:125:LEU:HD21	64:N4:501:CDL:H802	1.94	0.48
47:N4:423:LEU:HD23	48:N5:176:ARG:CZ	2.43	0.48
48:N5:159:ASN:HB2	63:N5:601:PC1:H141	1.95	0.48
48:N5:163:GLU:OE2	67:N5:607:3PE:N	2.24	0.48
11:A8:94:MET:HE1	11:A8:197:PHE:CD1	2.47	0.48
20:B4:80:ASN:O	20:B4:82:VAL:HG23	2.13	0.48
45:N2:171:ILE:N	45:N2:172:PRO:CD	2.77	0.48
57:V1:487:ASP:O	57:V1:492:SER:HA	2.13	0.48
10:A7:110:GLN:O	49:S2:252:TYR:OH	2.27	0.48
12:A9:283:PHE:CE2	12:A9:431:ILE:HD11	2.48	0.48
12:A9:398:ILE:HG12	12:A9:402:LEU:HD12	1.96	0.48
29:E1:252:LEU:HD21	29:E1:287:TYR:CZ	2.48	0.48
40:FX:140:LEU:HD12	40:FX:154:CYS:SG	2.54	0.48
41:G1:112:GLY:HA3	45:N2:27:VAL:HG11	1.95	0.48
44:N1:497:ILE:HG21	49:S2:36:HIS:CE1	2.48	0.48
45:N2:81:ILE:HG21	46:N6:150:MET:CB	2.43	0.48
13:AB:60:THR:HG22	13:AB:124:ILE:HD13	1.95	0.48
64:B5:201:CDL:OA3	27:BM:46:ARG:NH2	2.47	0.48
27:BM:95:PHE:CD2	37:EB:82:MET:HE1	2.47	0.48
47:N4:290:GLN:O	47:N4:362:LEU:HD12	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:S6:49:MET:N	53:S6:49:MET:HE2	2.28	0.48
57:V1:281:GLY:O	58:V2:110:ARG:NH1	2.42	0.48
1:1A:43:THR:OG1	1:1A:56:GLN:NE2	2.46	0.48
3:2B:63:ILE:C	3:2B:63:ILE:HD12	2.39	0.48
6:A2:171:ARG:NH2	31:E3:300:GLU:OE1	2.47	0.48
7:A3:55:ALA:HB3	44:N1:658:TYR:HA	1.95	0.48
11:A8:177:TYR:OH	44:N1:541:GLU:OE2	2.29	0.48
18:B2:58:GLN:NE2	39:ED:63:THR:O	2.45	0.48
31:E3:77:GLU:OE1	31:E3:77:GLU:N	2.47	0.48
47:N4:264:ILE:HG22	47:N4:265:TYR:N	2.28	0.48
57:V1:123:PRO:HB3	58:V2:104:THR:HG21	1.96	0.48
5:A1:38:LYS:NZ	5:A1:96:GLU:OE1	2.39	0.48
23:B7:44:ARG:HA	23:B7:48:VAL:CG1	2.43	0.48
31:E3:53:GLN:NE2	31:E3:94:ASN:OD1	2.45	0.48
35:E8:42:LEU:O	35:E8:47:LYS:NZ	2.46	0.48
48:N5:246:MET:SD	48:N5:257:HIS:NE2	2.86	0.48
48:N5:270:TYR:CE2	48:N5:339:LEU:HD11	2.48	0.48
50:S3:112:MET:HE1	51:S4:118:MET:SD	2.54	0.48
59:E7:159:LEU:HD23	59:E7:159:LEU:C	2.38	0.48
1:1A:213:GLU:N	1:1A:213:GLU:OE1	2.47	0.48
26:BL:82:LEU:C	26:BL:82:LEU:HD23	2.38	0.48
29:E1:252:LEU:HD21	29:E1:287:TYR:CE2	2.48	0.48
29:E1:339:ASP:OD2	29:E1:343:LYS:NZ	2.46	0.48
31:E3:46:VAL:HG22	31:E3:97:TRP:CZ2	2.48	0.48
63:E8:301:PC1:H111	48:N5:284:ILE:HD13	1.95	0.48
50:S3:56:LEU:HD23	50:S3:67:ILE:HD11	1.96	0.48
53:S6:127:PHE:N	53:S6:128:PRO:CD	2.77	0.48
54:S7:85:ALA:O	54:S7:88:ALA:N	2.41	0.48
57:V1:200:ARG:NH2	58:V2:88:MET:HE1	2.29	0.48
59:E7:39:LYS:O	59:E7:40:ILE:HG23	2.14	0.48
12:A9:399:ASP:OD1	12:A9:403:ARG:NH1	2.46	0.48
30:E2:40:TYR:HA	30:E2:43:VAL:HG22	1.96	0.48
30:E2:147:LEU:HB2	30:E2:251:LEU:HD22	1.95	0.48
30:E2:191:THR:HG23	30:E2:349:LEU:HD11	1.95	0.48
49:S2:305:ASP:OD2	53:S6:19:ARG:NH2	2.46	0.48
2:1B:340:SER:O	2:1B:344:GLN:NE2	2.47	0.48
17:AN:245:MET:O	28:C4:152:ARG:NH1	2.39	0.48
29:E1:156:ASP:OD2	29:E1:159:SER:OG	2.26	0.48
29:E1:393:THR:CG2	29:E1:435:VAL:HG22	2.44	0.48
47:N4:43:ILE:HG22	47:N4:75:ILE:HG23	1.96	0.48
48:N5:310:ILE:HG21	48:N5:438:ILE:HG21	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:E7:111:VAL:O	59:E7:153:ALA:N	2.47	0.48
1:1A:31:ILE:HD13	30:E2:28:LEU:HD23	1.96	0.48
4:4L:80:PRO:HD3	46:N6:112:ILE:HD11	1.95	0.48
27:BM:53:ASP:OD2	47:N4:93:ARG:NH2	2.45	0.48
32:E4:180:ARG:NH1	32:E4:216:THR:OG1	2.45	0.48
45:N2:164:SER:OG	45:N2:165:GLY:N	2.47	0.48
50:S3:106:VAL:HG22	50:S3:122:TYR:HD1	1.77	0.48
11:A8:140:PHE:HZ	11:A8:151:THR:HG21	1.79	0.47
12:A9:249:ASP:N	12:A9:249:ASP:OD1	2.46	0.47
21:B5:100:GLN:HG3	28:C4:146:VAL:HG21	1.95	0.47
26:BL:110:GLN:NE2	37:EB:79:SER:O	2.47	0.47
30:E2:9:THR:HG22	30:E2:10:GLY:N	2.29	0.47
31:E3:210:PHE:HZ	31:E3:234:ILE:HD12	1.79	0.47
41:G1:140:TYR:CE1	43:G3:211:THR:HG22	2.49	0.47
9:A6:221:LEU:HD23	9:A6:221:LEU:C	2.39	0.47
32:E4:296:VAL:O	32:E4:300:THR:HG22	2.15	0.47
40:FX:303:LEU:O	40:FX:307:THR:HG23	2.13	0.47
44:N1:428:ILE:O	44:N1:431:LYS:NZ	2.45	0.47
48:N5:334:ILE:HG23	48:N5:334:ILE:O	2.13	0.47
49:S2:241:GLU:N	57:V1:492:SER:OG	2.48	0.47
2:1B:386:THR:HA	31:E3:396:LEU:HD21	1.96	0.47
25:B9:150:GLY:O	42:G2:115:ARG:NH1	2.48	0.47
41:G1:292:VAL:HG22	41:G1:299:LEU:HB2	1.95	0.47
42:G2:104:ARG:HD3	43:G3:101:VAL:HG23	1.95	0.47
43:G3:149:ILE:N	43:G3:149:ILE:HD12	2.29	0.47
45:N2:146:LEU:C	45:N2:146:LEU:HD23	2.39	0.47
47:N4:469:ASN:O	47:N4:469:ASN:ND2	2.47	0.47
48:N5:47:LEU:HB2	48:N5:91:ILE:HD11	1.97	0.47
53:S6:110:GLY:O	53:S6:134:ARG:NH2	2.46	0.47
58:V2:99:ILE:HB	58:V2:138:ILE:HD13	1.96	0.47
1:1A:331:MET:HE2	2:1B:305:VAL:HG12	1.96	0.47
4:4L:107:VAL:O	4:4L:111:THR:HG23	2.15	0.47
10:A7:109:TRP:CZ2	50:S3:128:VAL:HG22	2.50	0.47
40:FX:253:THR:HG23	40:FX:304:TRP:NE1	2.29	0.47
47:N4:99:ASN:ND2	68:N4:505:U10:O3	2.42	0.47
47:N4:366:ASN:ND2	47:N4:369:ILE:HG23	2.30	0.47
57:V1:459:TYR:O	57:V1:463:LYS:N	2.46	0.47
9:A6:189:ALA:HB2	34:E6:219:GLN:HG3	1.96	0.47
24:B8:70:GLY:HA2	48:N5:555:ILE:HG21	1.97	0.47
28:C4:61:THR:HG22	28:C4:61:THR:O	2.15	0.47
30:E2:135:THR:HG23	30:E2:440:GLY:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:N1:381:LEU:HA	44:N1:384:VAL:HG12	1.97	0.47
47:N4:357:THR:CG2	47:N4:369:ILE:HD13	2.45	0.47
48:N5:234:THR:HG22	48:N5:241:TRP:NE1	2.30	0.47
48:N5:302:ILE:HG21	48:N5:430:LEU:HD22	1.96	0.47
48:N5:310:ILE:HG21	48:N5:438:ILE:CG2	2.45	0.47
55:S8:112:VAL:O	55:S8:112:VAL:HG22	2.14	0.47
57:V1:406:PHE:O	57:V1:409:GLU:N	2.35	0.47
58:V2:178:ILE:HD12	58:V2:179:GLU:N	2.30	0.47
4:4L:99:ALA:HA	43:G3:256:ILE:HD11	1.97	0.47
12:A9:126:GLY:N	65:A9:559:NDP:O3B	2.48	0.47
29:E1:235:LEU:HD21	29:E1:237:VAL:HG13	1.96	0.47
30:E2:336:VAL:HG22	30:E2:337:THR:N	2.30	0.47
34:E6:361:THR:O	34:E6:361:THR:HG22	2.14	0.47
47:N4:314:ILE:HG21	47:N4:404:LEU:HD11	1.97	0.47
10:A7:69:ILE:O	10:A7:69:ILE:HG23	2.14	0.47
11:A8:103:GLU:OE2	11:A8:222:TYR:OH	2.25	0.47
12:A9:415:TRP:HE3	12:A9:420:ILE:HG21	1.79	0.47
35:E8:125:ASN:ND2	35:E8:153:TRP:O	2.40	0.47
45:N2:81:ILE:HD11	46:N6:153:ILE:HD12	1.95	0.47
46:N6:65:ILE:HG23	46:N6:66:LEU:N	2.29	0.47
46:N6:126:ILE:HG22	46:N6:128:ILE:HG13	1.97	0.47
50:S3:140:ASP:OD1	50:S3:141:ASP:N	2.38	0.47
57:V1:297:LEU:HD21	57:V1:318:VAL:HG11	1.95	0.47
17:AN:56:ARG:NH2	17:AN:141:GLY:O	2.47	0.47
35:E8:33:ARG:HG3	35:E8:36:ILE:HD12	1.96	0.47
39:ED:90:VAL:HG12	39:ED:90:VAL:O	2.15	0.47
49:S2:224:MET:HE2	49:S2:386:LEU:HD23	1.96	0.47
57:V1:396:ILE:HG21	57:V1:413:ILE:HB	1.96	0.47
1:1A:45:THR:HB	1:1A:52:LEU:HD11	1.97	0.47
3:2B:56:ILE:HD12	45:N2:257:PHE:HZ	1.80	0.47
9:A6:177:VAL:HG12	9:A6:177:VAL:O	2.15	0.47
32:E4:238:MET:O	32:E4:304:ARG:NH1	2.46	0.47
36:EA:50:PRO:O	36:EA:54:VAL:HG23	2.15	0.47
48:N5:93:LEU:HD13	48:N5:259:ALA:O	2.15	0.47
57:V1:160:ARG:NH2	57:V1:162:GLU:OE1	2.47	0.47
71:V1:581:NAI:H6N	71:V1:581:NAI:H3D	1.96	0.47
7:A3:53:ARG:HH22	45:N2:27:VAL:HG23	1.79	0.47
15:AL:245:ASP:O	15:AL:253:ARG:NH2	2.48	0.47
30:E2:135:THR:N	30:E2:440:GLY:O	2.46	0.47
30:E2:353:THR:HG22	30:E2:354:ALA:N	2.29	0.47
32:E4:188:ALA:HB1	32:E4:336:LEU:HD21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:E5:8:ARG:HB2	33:E5:63:VAL:HA	1.97	0.47
33:E5:141:GLY:O	33:E5:167:THR:OG1	2.28	0.47
48:N5:48:TYR:OH	63:N5:605:PC1:O12	2.28	0.47
49:S2:210:MET:SD	49:S2:214:ARG:NH1	2.88	0.47
9:A6:99:LEU:HD22	9:A6:104:ALA:HB1	1.96	0.46
20:B4:97:PHE:HD2	47:N4:364:LEU:HD21	1.80	0.46
32:E4:128:ILE:HD13	32:E4:148:MET:CE	2.43	0.46
43:G3:134:GLY:O	43:G3:196:ARG:NH2	2.48	0.46
57:V1:249:VAL:O	57:V1:252:SER:OG	2.32	0.46
1:1A:44:VAL:HG23	1:1A:55:PHE:CZ	2.51	0.46
12:A9:93:LEU:HB3	51:S4:141:SER:HB3	1.98	0.46
21:B5:101:GLN:NE2	64:N4:501:CDL:OA3	2.48	0.46
24:B8:72:ASP:O	47:N4:432:LYS:NZ	2.48	0.46
44:N1:506:TYR:C	44:N1:506:TYR:CD1	2.92	0.46
48:N5:527:LEU:N	48:N5:527:LEU:HD12	2.30	0.46
58:V2:65:MET:HE2	58:V2:83:ALA:HB1	1.96	0.46
58:V2:119:LEU:HD22	58:V2:181:VAL:HG11	1.98	0.46
58:V2:126:GLY:N	58:V2:129:GLU:OE2	2.47	0.46
9:A6:234:LEU:HD23	9:A6:237:LEU:HD12	1.97	0.46
28:C4:43:ASP:OD1	28:C4:43:ASP:N	2.48	0.46
30:E2:4:GLY:C	30:E2:5:THR:HG1	2.19	0.46
30:E2:62:ARG:HH12	30:E2:113:LEU:HD21	1.81	0.46
30:E2:240:GLU:N	30:E2:240:GLU:OE1	2.48	0.46
44:N1:510:PHE:CZ	44:N1:514:LEU:HD11	2.50	0.46
45:N2:175:TYR:CD1	45:N2:186:MET:HE1	2.50	0.46
47:N4:110:ILE:HG23	47:N4:126:ILE:HG23	1.97	0.46
49:S2:33:GLU:HB2	49:S2:41:ARG:HB3	1.97	0.46
49:S2:51:ARG:HG2	54:S7:123:THR:HG21	1.97	0.46
52:S5:68:GLU:O	52:S5:72:GLY:N	2.48	0.46
55:S8:159:VAL:HG13	55:S8:200:ARG:NH2	2.31	0.46
2:1B:274:ASP:OD1	2:1B:275:TYR:N	2.49	0.46
18:B2:124:LEU:HB3	48:N5:331:LEU:HD21	1.98	0.46
27:BM:62:MET:HE1	47:N4:457:ILE:CG2	2.45	0.46
2:1B:191:THR:O	2:1B:194:SER:OG	2.31	0.46
5:A1:39:ARG:NH1	5:A1:74:ALA:O	2.48	0.46
7:A3:110:ARG:NH2	11:A8:33:GLU:OE2	2.49	0.46
11:A8:30:LEU:O	11:A8:34:VAL:HG13	2.16	0.46
32:E4:170:SER:O	32:E4:173:ALA:HB3	2.15	0.46
49:S2:105:VAL:HG21	49:S2:242:VAL:CG2	2.43	0.46
57:V1:139:LEU:HD13	57:V1:246:VAL:HG13	1.97	0.46
2:1B:410:ALA:HB1	6:A2:95:PHE:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A5:162:LEU:HD11	12:A9:42:THR:HG22	1.97	0.46
12:A9:164:ARG:NH1	54:S7:143:CYS:O	2.45	0.46
32:E4:36:LEU:HD13	32:E4:39:ARG:NH1	2.31	0.46
47:N4:184:THR:HG22	47:N4:186:ASN:H	1.80	0.46
46:N6:46:ILE:HD12	46:N6:46:ILE:N	2.31	0.46
1:1A:144:ILE:HG23	55:S8:105:ILE:HD12	1.97	0.46
9:A6:48:PRO:CG	50:S3:176:LEU:HD22	2.44	0.46
33:E5:241:ALA:O	33:E5:245:VAL:HG23	2.15	0.46
44:N1:502:LEU:HD23	44:N1:505:MET:SD	2.56	0.46
44:N1:518:SER:O	46:N3:259:TYR:OH	2.34	0.46
44:N1:649:THR:HG23	49:S2:375:MET:HE1	1.98	0.46
47:N4:258:ILE:HD11	47:N4:312:MET:SD	2.56	0.46
57:V1:126:CYS:SG	58:V2:147:CYS:N	2.89	0.46
15:AL:124:GLU:HA	15:AL:129:ASN:O	2.16	0.46
29:E1:135:LYS:O	29:E1:157:LEU:HD12	2.16	0.46
33:E5:260:LYS:C	33:E5:284:VAL:O	2.59	0.46
44:N1:605:ILE:HD11	44:N1:636:PHE:CE2	2.51	0.46
47:N4:73:ILE:N	47:N4:73:ILE:HD12	2.31	0.46
48:N5:340:LEU:CD1	48:N5:489:LEU:HD22	2.45	0.46
49:S2:325:GLU:O	50:S3:242:THR:OG1	2.29	0.46
5:A1:130:PRO:O	5:A1:131:LYS:HB3	2.16	0.46
9:A6:112:VAL:CG2	66:AB:150:ZMP:H9	2.46	0.46
29:E1:376:ARG:O	29:E1:380:GLY:N	2.41	0.46
31:E3:50:ASP:OD2	31:E3:69:LEU:N	2.39	0.46
41:G1:228:GLY:HA2	41:G1:246:ALA:HB1	1.97	0.46
1:1A:182:ASN:OD1	1:1A:237:VAL:HB	2.16	0.46
11:A8:13:ASP:OD1	21:B5:115:ASN:ND2	2.45	0.46
16:AM:54:VAL:HG12	64:AM:215:CDL:CA3	2.46	0.46
23:B7:65:GLY:N	48:N5:487:ASP:OD2	2.41	0.46
31:E3:425:LEU:O	31:E3:429:VAL:HG23	2.16	0.46
33:E5:87:LEU:N	33:E5:87:LEU:HD12	2.31	0.46
45:N2:175:TYR:CD2	45:N2:186:MET:HE1	2.51	0.46
47:N4:232:VAL:HG23	47:N4:233:GLU:HG2	1.98	0.46
47:N4:309:TYR:HE1	47:N4:336:MET:HE1	1.81	0.46
48:N5:47:LEU:HB2	48:N5:91:ILE:CD1	2.45	0.46
48:N5:431:SER:HA	48:N5:434:TYR:CE2	2.50	0.46
57:V1:159:VAL:CG2	57:V1:198:LEU:HD11	2.46	0.46
1:1A:318:ARG:O	1:1A:322:ALA:HB2	2.17	0.45
1:1A:322:ALA:N	1:1A:323:PRO:HD2	2.30	0.45
28:C4:173:ASP:OD1	28:C4:173:ASP:N	2.50	0.45
32:E4:318:VAL:HG23	32:E4:331:ARG:HG2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:E5:282:ASP:O	33:E5:284:VAL:HG13	2.16	0.45
38:EC:51:VAL:HG22	38:EC:61:LEU:HD11	1.97	0.45
47:N4:89:ILE:HG22	47:N4:104:ILE:HG21	1.97	0.45
47:N4:395:ILE:HG23	48:N5:69:ILE:HD11	1.96	0.45
48:N5:337:ILE:N	48:N5:337:ILE:HD12	2.32	0.45
13:AB:62:ARG:NH2	13:AB:134:MET:O	2.48	0.45
30:E2:348:ASP:OD1	30:E2:372:ARG:NH2	2.42	0.45
33:E5:260:LYS:HB2	33:E5:284:VAL:H	1.80	0.45
34:E6:77:ASP:OD1	34:E6:80:ARG:NH2	2.47	0.45
49:S2:78:MET:HB2	49:S2:111:THR:HG21	1.97	0.45
53:S6:105:ILE:HD11	53:S6:115:CYS:HB2	1.98	0.45
54:S7:79:PRO:HD3	54:S7:106:THR:HG23	1.98	0.45
57:V1:89:GLY:HA3	71:V1:581:NAI:H1D	1.97	0.45
9:A6:62:TYR:CZ	9:A6:66:LEU:HD11	2.51	0.45
31:E3:45:PRO:HB2	31:E3:70:SER:HB2	1.98	0.45
68:N4:505:U10:H151	68:N4:505:U10:H18	1.95	0.45
4:4L:154:TYR:HH	45:N2:129:TRP:HZ2	1.59	0.45
11:A8:12:LYS:CB	28:C4:145:LEU:HD21	2.47	0.45
11:A8:94:MET:HE1	11:A8:197:PHE:CE1	2.52	0.45
25:B9:103:MET:HE1	48:N5:305:LEU:HD11	1.98	0.45
32:E4:336:LEU:HD23	32:E4:336:LEU:C	2.41	0.45
33:E5:41:ALA:HB3	33:E5:289:LEU:HB3	1.98	0.45
40:FX:249:THR:N	40:FX:250:PRO:HD2	2.32	0.45
67:G1:516:3PE:H291	42:G2:149:MET:HE1	1.97	0.45
45:N2:92:TYR:O	45:N2:96:ASN:ND2	2.50	0.45
47:N4:218:LEU:HD13	47:N4:309:TYR:CE1	2.50	0.45
48:N5:60:LEU:HD11	48:N5:81:GLY:HA3	1.98	0.45
49:S2:121:ALA:HB1	49:S2:133:ILE:HA	1.97	0.45
53:S6:6:ARG:NH2	55:S8:208:GLN:O	2.48	0.45
57:V1:200:ARG:HH21	58:V2:88:MET:HE1	1.82	0.45
9:A6:119:TYR:OH	66:AB:150:ZMP:H25A	2.16	0.45
15:AL:221:LYS:NZ	54:S7:20:VAL:O	2.40	0.45
45:N2:116:VAL:HG12	45:N2:120:ILE:HD12	1.99	0.45
47:N4:9:ARG:HB2	47:N4:38:ILE:HG21	1.97	0.45
47:N4:76:TYR:OH	47:N4:472:LEU:HD22	2.17	0.45
47:N4:91:TYR:CZ	47:N4:236:THR:HG21	2.51	0.45
50:S3:68:MET:HE1	50:S3:79:ASN:OD1	2.17	0.45
54:S7:76:SER:OG	54:S7:78:TRP:NE1	2.49	0.45
2:1B:177:GLU:CG	2:1B:477:THR:HG21	2.47	0.45
46:N3:238:ILE:HD12	46:N3:238:ILE:C	2.42	0.45
47:N4:62:ILE:O	64:N4:501:CDL:O1	2.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:N5:23:ILE:HD12	48:N5:31:ILE:HD12	1.98	0.45
50:S3:104:VAL:N	50:S3:123:ASN:O	2.50	0.45
57:V1:110:ARG:NH1	57:V1:238:GLY:O	2.50	0.45
57:V1:141:GLU:OE2	57:V1:257:ARG:NH1	2.40	0.45
2:1B:51:ILE:HB	2:1B:81:VAL:HG22	1.99	0.45
3:2B:69:TYR:HA	3:2B:72:ILE:HG22	1.99	0.45
11:A8:30:LEU:O	11:A8:34:VAL:HG22	2.17	0.45
12:A9:194:ARG:NH2	15:AL:222:ASN:O	2.47	0.45
24:B8:103:LEU:HD12	35:E8:81:MET:CB	2.46	0.45
33:E5:147:ASP:CG	33:E5:193:LEU:HD11	2.41	0.45
41:G1:359:ALA:O	41:G1:363:VAL:HG23	2.16	0.45
49:S2:107:PHE:HZ	49:S2:150:VAL:HG11	1.82	0.45
50:S3:139:VAL:HG11	50:S3:145:ILE:HB	1.99	0.45
57:V1:98:TRP:HE1	57:V1:244:THR:HG21	1.81	0.45
9:A6:172:ILE:HG23	12:A9:239:ARG:HD2	1.99	0.45
11:A8:59:GLY:O	36:EA:123:UNK:N	2.49	0.45
12:A9:446:THR:HG22	12:A9:446:THR:O	2.15	0.45
15:AL:257:ARG:HD2	55:S8:124:VAL:HG11	1.98	0.45
20:B4:103:TYR:HE2	24:B8:69:VAL:HG22	1.82	0.45
22:B6:52:LEU:HD11	48:N5:60:LEU:HD23	1.99	0.45
34:E6:201:ASN:N	34:E6:201:ASN:OD1	2.48	0.45
47:N4:273:ILE:HD12	47:N4:317:ILE:HD13	1.99	0.45
25:B9:89:LEU:HD23	35:E8:59:MET:HE1	1.99	0.45
28:C4:97:MET:HE1	47:N4:21:LEU:O	2.17	0.45
28:C4:120:ALA:O	28:C4:124:VAL:HG23	2.16	0.45
45:N2:215:ILE:O	45:N2:219:LEU:HG	2.17	0.45
50:S3:112:MET:HE2	51:S4:121:PHE:CZ	2.52	0.45
1:1A:177:ASP:OD1	1:1A:223:THR:HG21	2.16	0.45
15:AL:137:THR:OG1	15:AL:138:THR:N	2.50	0.45
25:B9:54:PRO:CG	35:E8:25:MET:HE3	2.47	0.45
29:E1:85:ILE:N	29:E1:85:ILE:HD12	2.32	0.45
36:EA:112:UNK:C	36:EA:114:UNK:H	2.29	0.45
42:G2:207:LEU:HD21	43:G3:84:ASP:OD2	2.17	0.45
45:N2:17:ILE:HD13	46:N6:145:ILE:HG22	1.98	0.45
46:N3:249:ASP:O	46:N3:252:ILE:HG22	2.16	0.45
47:N4:324:TYR:O	47:N4:327:ILE:HG12	2.17	0.45
57:V1:134:MET:HE3	58:V2:200:SER:CB	2.47	0.45
1:1A:268:ILE:HD11	1:1A:295:TYR:CD2	2.52	0.44
9:A6:77:ARG:NH1	12:A9:434:ASP:O	2.47	0.44
15:AL:23:THR:O	15:AL:23:THR:HG22	2.16	0.44
18:B2:114:TRP:NE1	18:B2:138:TRP:O	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:E5:262:VAL:H	33:E5:285:HIS:HB2	1.82	0.44
50:S3:106:VAL:HG22	50:S3:122:TYR:CD1	2.52	0.44
58:V2:58:GLY:O	58:V2:90:ASN:ND2	2.48	0.44
12:A9:276:ILE:N	12:A9:276:ILE:HD12	2.32	0.44
17:AN:11:MET:HE1	48:N5:581:ILE:HG22	1.99	0.44
24:B8:92:GLU:OE2	48:N5:533:HIS:NE2	2.50	0.44
30:E2:319:ALA:HB1	30:E2:336:VAL:HG23	2.00	0.44
48:N5:332:ILE:HG22	48:N5:333:ASN:N	2.32	0.44
3:2B:34:THR:HG21	3:2B:91:PHE:CZ	2.53	0.44
46:N3:219:ASN:ND2	46:N3:221:SER:OG	2.45	0.44
47:N4:225:ILE:HG23	48:N5:568:MET:SD	2.57	0.44
48:N5:262:VAL:HG23	48:N5:263:THR:HG23	1.99	0.44
48:N5:301:SER:HB3	48:N5:313:TYR:HB3	1.99	0.44
57:V1:132:MET:HE1	57:V1:159:VAL:HG13	1.99	0.44
1:1A:139:SER:HG	1:1A:141:ASP:CG	2.20	0.44
2:1B:126:TRP:NE1	29:E1:207:TYR:OH	2.48	0.44
41:G1:260:THR:HG21	43:G3:157:PRO:HB2	1.98	0.44
42:G2:69:ILE:HG22	42:G2:70:GLY:N	2.32	0.44
45:N2:212:PHE:HA	45:N2:215:ILE:HG22	1.99	0.44
1:1A:197:LYS:HB3	1:1A:248:ILE:CG2	2.47	0.44
11:A8:12:LYS:HB3	28:C4:145:LEU:HD21	2.00	0.44
14:AC:96:GLU:OE2	25:B9:43:TYR:OH	2.28	0.44
21:B5:58:ARG:HE	63:B5:202:PC1:H111	1.83	0.44
23:B7:39:ILE:HD11	23:B7:52:LEU:CD1	2.48	0.44
31:E3:91:LEU:HD12	31:E3:91:LEU:N	2.32	0.44
35:E8:177:ASP:OD1	35:E8:177:ASP:N	2.50	0.44
41:G1:300:ARG:NH1	41:G1:301:LYS:O	2.50	0.44
42:G2:154:ILE:HD12	42:G2:154:ILE:N	2.33	0.44
45:N2:218:PHE:CZ	45:N2:256:LEU:HD11	2.52	0.44
47:N4:73:ILE:HD13	47:N4:255:TYR:OH	2.17	0.44
48:N5:117:PHE:CZ	48:N5:252:VAL:HG23	2.52	0.44
53:S6:115:CYS:O	53:S6:119:GLU:CA	2.65	0.44
17:AN:258:PRO:HG2	21:B5:91:ILE:HG21	1.98	0.44
40:FX:171:LEU:HB3	40:FX:186:SER:HA	1.99	0.44
47:N4:217:LYS:O	47:N4:247:LEU:HD23	2.17	0.44
49:S2:382:VAL:HA	49:S2:385:THR:HG22	1.99	0.44
1:1A:308:MET:O	1:1A:312:ASN:ND2	2.50	0.44
1:1A:341:ASN:O	1:1A:345:LEU:HG	2.17	0.44
12:A9:194:ARG:NH1	15:AL:222:ASN:O	2.45	0.44
16:AM:57:ARG:NH2	64:AM:217:CDL:OA2	2.51	0.44
29:E1:28:THR:O	30:E2:229:ARG:NH1	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:E1:324:VAL:HG23	29:E1:355:LEU:CD1	2.48	0.44
31:E3:46:VAL:HG13	31:E3:97:TRP:HZ2	1.81	0.44
45:N2:81:ILE:HG21	46:N6:150:MET:HB3	1.99	0.44
47:N4:93:ARG:HH22	68:N4:505:U10:H152	1.83	0.44
58:V2:178:ILE:HA	58:V2:181:VAL:HG22	1.99	0.44
3:2B:86:VAL:HG12	45:N2:238:LEU:HD21	2.00	0.44
12:A9:156:VAL:HG12	12:A9:157:VAL:HG23	1.99	0.44
29:E1:106:VAL:HG13	29:E1:106:VAL:O	2.17	0.44
39:ED:133:ARG:O	39:ED:137:THR:HG23	2.18	0.44
40:FX:256:PHE:HB3	40:FX:282:PRO:HB3	1.99	0.44
47:N4:287:ILE:HD13	47:N4:299:LEU:HB2	2.00	0.44
12:A9:172:GLN:OE1	54:S7:169:ASN:ND2	2.51	0.44
21:B5:43:TRP:O	21:B5:47:THR:HG23	2.17	0.44
33:E5:204:LEU:HD21	33:E5:231:PHE:HB2	2.00	0.44
35:E8:26:THR:N	35:E8:27:PRO:CD	2.81	0.44
41:G1:306:ASP:O	41:G1:309:THR:OG1	2.28	0.44
48:N5:325:ILE:HD11	48:N5:334:ILE:CG1	2.45	0.44
12:A9:304:ILE:N	12:A9:304:ILE:HD12	2.32	0.43
13:AB:60:THR:HG22	13:AB:124:ILE:HG21	2.00	0.43
20:B4:26:TRP:CZ2	24:B8:69:VAL:HG21	2.52	0.43
31:E3:208:PRO:O	31:E3:227:ILE:HD12	2.17	0.43
45:N2:98:ASN:O	52:S5:29:LYS:NZ	2.37	0.43
57:V1:213:LEU:O	57:V1:213:LEU:HD23	2.18	0.43
57:V1:407:GLY:N	57:V1:408:PRO:HD2	2.32	0.43
58:V2:105:THR:HB	58:V2:106:PRO:HD3	1.99	0.43
1:1A:369:ASP:OD2	9:A6:246:TYR:OH	2.23	0.43
17:AN:227:SER:OG	28:C4:173:ASP:OD2	2.26	0.43
18:B2:138:TRP:CD1	20:B4:160:MET:HE2	2.53	0.43
20:B4:24:ILE:O	20:B4:24:ILE:HG22	2.17	0.43
25:B9:38:ARG:NH2	25:B9:94:GLU:OE1	2.48	0.43
33:E5:262:VAL:O	33:E5:263:ARG:C	2.60	0.43
35:E8:156:ARG:NH1	35:E8:160:GLU:OE2	2.51	0.43
40:FX:88:LYS:N	40:FX:89:PRO:HD2	2.34	0.43
67:G1:516:3PE:C29	42:G2:149:MET:HE1	2.48	0.43
49:S2:357:ARG:O	49:S2:357:ARG:HG3	2.18	0.43
57:V1:122:GLU:HG2	71:V1:581:NAI:H42N	2.00	0.43
7:A3:9:ILE:HD12	10:A7:116:ARG:HB2	1.99	0.43
9:A6:159:PHE:O	9:A6:160:PHE:HB2	2.18	0.43
9:A6:399:ASN:HB2	9:A6:400:PRO:HD3	1.99	0.43
11:A8:61:LEU:HD11	11:A8:195:CYS:SG	2.57	0.43
12:A9:12:ILE:HB	12:A9:33:LEU:HD23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A9:309:THR:OG1	12:A9:310:TYR:N	2.52	0.43
31:E3:294:ASN:O	31:E3:295:ALA:C	2.61	0.43
41:G1:251:ASP:N	41:G1:251:ASP:OD1	2.51	0.43
49:S2:107:PHE:CZ	49:S2:150:VAL:HG21	2.53	0.43
51:S4:44:ALA:HB3	51:S4:47:GLN:HG3	1.99	0.43
1:1A:318:ARG:CZ	2:1B:498:VAL:HG21	2.49	0.43
1:1A:331:MET:HE2	2:1B:305:VAL:HG11	2.00	0.43
6:A2:4:VAL:O	6:A2:4:VAL:HG22	2.18	0.43
6:A2:26:PRO:O	6:A2:27:GLU:HB3	2.19	0.43
21:B5:119:LYS:NZ	21:B5:123:GLU:OE2	2.37	0.43
26:BL:77:VAL:HG21	27:BM:87:GLU:HG2	2.00	0.43
27:BM:56:TRP:HA	27:BM:59:VAL:HG22	2.00	0.43
34:E6:257:TYR:HB2	54:S7:34:ALA:HB1	2.01	0.43
44:N1:566:GLU:OE1	44:N1:608:HIS:NE2	2.50	0.43
45:N2:175:TYR:OH	45:N2:247:THR:HG21	2.18	0.43
47:N4:89:ILE:CG2	47:N4:104:ILE:HG21	2.49	0.43
48:N5:325:ILE:HB	48:N5:407:ILE:HG23	2.01	0.43
50:S3:175:ASP:OD2	50:S3:177:ARG:NH1	2.52	0.43
71:V1:581:NAI:HO3A	71:V1:581:NAI:HO2A	1.58	0.43
58:V2:160:ASN:OD1	58:V2:163:ASN:ND2	2.42	0.43
2:1B:463:GLU:OE1	2:1B:463:GLU:N	2.48	0.43
27:BM:96:ARG:O	27:BM:100:VAL:HG23	2.18	0.43
30:E2:174:GLY:O	30:E2:201:ASN:ND2	2.51	0.43
31:E3:140:LYS:N	31:E3:143:ASP:OD2	2.45	0.43
31:E3:321:LEU:HD12	31:E3:321:LEU:N	2.33	0.43
38:EC:19:ARG:NH1	38:EC:92:GLU:OE1	2.45	0.43
41:G1:154:LEU:HD12	41:G1:177:ILE:HG12	1.99	0.43
43:G3:90:ILE:HG23	43:G3:94:THR:HG21	1.99	0.43
45:N2:5:ASN:OD1	45:N2:6:ASN:N	2.50	0.43
47:N4:114:PHE:HB2	47:N4:126:ILE:HG21	2.00	0.43
57:V1:123:PRO:O	58:V2:147:CYS:SG	2.77	0.43
2:1B:346:MET:HE2	9:A6:158:ARG:NE	2.34	0.43
3:2B:101:ILE:HD11	41:G1:248:TRP:CH2	2.54	0.43
4:4L:166:SER:O	4:4L:167:LEU:HD23	2.19	0.43
7:A3:53:ARG:NH2	45:N2:27:VAL:HG23	2.33	0.43
9:A6:99:LEU:HD21	51:S4:50:GLN:HG3	2.00	0.43
19:B3:2:VAL:HG12	19:B3:2:VAL:O	2.17	0.43
29:E1:48:TRP:CE2	29:E1:57:SER:HB3	2.54	0.43
35:E8:151:SER:O	35:E8:155:TYR:N	2.47	0.43
42:G2:117:VAL:HG22	42:G2:133:PRO:HA	2.00	0.43
46:N3:239:TYR:OH	46:N6:88:ASN:ND2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:N4:305:MET:HE3	47:N4:305:MET:HA	2.00	0.43
46:N6:47:GLY:O	46:N6:51:VAL:HG23	2.19	0.43
9:A6:294:LEU:CD1	9:A6:393:ILE:HD11	2.49	0.43
24:B8:103:LEU:HD11	64:N5:608:CDL:H312	1.99	0.43
32:E4:83:ARG:HA	32:E4:86:VAL:HG22	2.00	0.43
33:E5:14:GLY:N	38:EC:89:ASP:OD2	2.51	0.43
45:N2:18:ILE:O	45:N2:19:GLY:C	2.60	0.43
47:N4:220:ILE:CG2	47:N4:276:LEU:HD11	2.49	0.43
47:N4:314:ILE:HG21	47:N4:404:LEU:CD1	2.49	0.43
46:N6:126:ILE:O	46:N6:129:ILE:HG12	2.19	0.43
2:1B:289:MET:SD	2:1B:305:VAL:HG13	2.58	0.43
3:2B:59:TYR:CE1	3:2B:63:ILE:HG21	2.53	0.43
10:A7:32:TRP:O	49:S2:187:ARG:NH2	2.40	0.43
12:A9:78:LYS:NZ	12:A9:83:GLN:O	2.50	0.43
20:B4:66:GLU:HB2	47:N4:443:ILE:HG23	2.00	0.43
28:C4:106:VAL:HG21	28:C4:108:TRP:CE2	2.54	0.43
29:E1:136:ASP:OD1	29:E1:137:LYS:N	2.50	0.43
31:E3:91:LEU:HD23	31:E3:267:LEU:HD13	2.01	0.43
31:E3:251:LEU:O	31:E3:255:ASN:N	2.51	0.43
33:E5:194:LEU:HD12	33:E5:226:VAL:HG11	2.00	0.43
48:N5:198:ILE:HG22	48:N5:198:ILE:O	2.19	0.43
58:V2:148:VAL:HG23	58:V2:149:HIS:CD2	2.54	0.43
3:2B:49:TYR:CG	45:N2:281:ILE:HG13	2.54	0.43
63:A1:203:PC1:H152	63:A1:203:PC1:O13	2.19	0.43
12:A9:189:ALA:HA	12:A9:192:VAL:HG22	2.01	0.43
12:A9:273:ASN:ND2	31:E3:361:THR:O	2.45	0.43
15:AL:177:GLN:O	15:AL:180:ARG:NH1	2.43	0.43
20:B4:33:LEU:HD21	20:B4:39:MET:HB2	2.01	0.43
25:B9:23:ILE:HD13	48:N5:247:GLU:OE2	2.18	0.43
25:B9:70:SER:OG	35:E8:5:ARG:NH2	2.52	0.43
28:C4:114:PHE:HB2	28:C4:115:PRO:HD3	2.01	0.43
29:E1:393:THR:HG22	29:E1:435:VAL:HG22	2.01	0.43
30:E2:116:GLU:OE1	30:E2:116:GLU:N	2.45	0.43
33:E5:49:ASP:OD1	33:E5:210:SER:OG	2.37	0.43
33:E5:255:ASN:HB2	33:E5:257:LEU:HD23	2.00	0.43
41:G1:281:ASP:OD1	41:G1:281:ASP:N	2.52	0.43
42:G2:74:VAL:HG12	42:G2:78:SER:HB2	2.00	0.43
42:G2:79:SER:OG	42:G2:100:HIS:ND1	2.41	0.43
43:G3:96:ILE:HG23	43:G3:100:VAL:HG11	2.01	0.43
45:N2:50:ILE:CD1	45:N2:62:ILE:HG21	2.48	0.43
45:N2:266:ASN:OD1	45:N2:267:LEU:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:N4:122:THR:HG23	64:N4:501:CDL:H602	2.00	0.43
47:N4:227:LEU:HD13	47:N4:227:LEU:C	2.44	0.43
48:N5:380:ILE:HG23	48:N5:381:LEU:N	2.32	0.43
50:S3:70:ASP:CG	50:S3:73:THR:HG1	2.19	0.43
51:S4:52:ILE:HD11	51:S4:54:LEU:HD12	2.00	0.43
59:E7:48:GLY:O	59:E7:172:ARG:NH1	2.51	0.43
1:1A:226:VAL:O	1:1A:228:ARG:N	2.50	0.43
2:1B:243:ALA:O	2:1B:247:TYR:N	2.52	0.43
2:1B:314:ASP:OD2	2:1B:337:SER:OG	2.34	0.43
11:A8:1:MET:HE1	45:N2:58:LEU:HD21	2.00	0.43
11:A8:80:ILE:HD13	11:A8:136:SER:OG	2.19	0.43
18:B2:144:VAL:HG13	35:E8:139:ARG:NH2	2.33	0.43
30:E2:188:HIS:HD2	30:E2:220:ILE:HG22	1.84	0.43
32:E4:36:LEU:HD23	32:E4:38:TRP:CZ2	2.54	0.43
37:EB:59:LEU:O	37:EB:63:TYR:N	2.42	0.43
40:FX:143:ILE:HG21	40:FX:244:PHE:CD2	2.54	0.43
44:N1:654:LEU:O	44:N1:655:THR:C	2.61	0.43
48:N5:337:ILE:HD11	48:N5:491:TYR:CD1	2.54	0.43
49:S2:75:MET:HE2	49:S2:75:MET:HA	1.99	0.43
50:S3:55:TYR:OH	50:S3:95:HIS:NE2	2.40	0.43
53:S6:39:PHE:O	53:S6:43:VAL:HG13	2.18	0.43
55:S8:158:ILE:HG23	55:S8:158:ILE:O	2.17	0.43
57:V1:421:GLU:OE2	57:V1:434:TRP:NE1	2.40	0.43
58:V2:65:MET:HE2	58:V2:83:ALA:CB	2.48	0.43
59:E7:66:HIS:HE2	59:E7:99:HIS:HD2	1.66	0.43
2:1B:246:THR:HG22	2:1B:246:THR:O	2.19	0.42
2:1B:338:GLU:OE2	51:S4:105:ARG:NH1	2.53	0.42
11:A8:128:MET:HE1	16:AM:97:PRO:HB3	2.01	0.42
19:B3:25:ALA:O	39:ED:35:ILE:HG22	2.19	0.42
22:B6:45:GLU:OE2	48:N5:62:TYR:OH	2.21	0.42
34:E6:76:GLU:OE1	34:E6:110:ARG:NH2	2.48	0.42
44:N1:649:THR:HG23	49:S2:375:MET:CE	2.49	0.42
47:N4:227:LEU:HD22	47:N4:231:HIS:CE1	2.54	0.42
47:N4:419:SER:O	47:N4:422:ASN:HB2	2.19	0.42
49:S2:66:THR:N	49:S2:67:PRO:CD	2.82	0.42
57:V1:163:PHE:HB3	57:V1:166:GLU:HB2	2.00	0.42
58:V2:20:ASP:OD1	58:V2:26:TYR:OH	2.36	0.42
1:1A:344:LEU:HD23	9:A6:363:VAL:HG13	2.02	0.42
2:1B:367:ARG:NE	31:E3:410:LEU:O	2.52	0.42
9:A6:72:MET:HE3	9:A6:120:PHE:CD1	2.51	0.42
14:AC:90:ASP:O	14:AC:94:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B7:43:GLU:OE1	23:B7:55:ARG:NH1	2.49	0.42
29:E1:418:VAL:HG22	29:E1:419:ALA:N	2.34	0.42
41:G1:59:PHE:O	43:G3:247:ARG:NH1	2.52	0.42
42:G2:200:ARG:HG2	43:G3:106:ILE:HD11	2.01	0.42
45:N2:218:PHE:HZ	45:N2:256:LEU:HD11	1.84	0.42
45:N2:249:ILE:O	45:N2:253:ILE:HD13	2.19	0.42
9:A6:77:ARG:NH2	12:A9:434:ASP:O	2.49	0.42
9:A6:172:ILE:HD12	12:A9:114:LEU:HD22	2.00	0.42
11:A8:1:MET:N	45:N2:199:ASN:OD1	2.52	0.42
42:G2:192:GLU:OE1	42:G2:192:GLU:N	2.41	0.42
43:G3:126:ILE:N	43:G3:126:ILE:HD12	2.34	0.42
47:N4:411:LEU:O	47:N4:415:LEU:HG	2.19	0.42
50:S3:82:PRO:HB3	50:S3:139:VAL:HG12	2.02	0.42
58:V2:149:HIS:HB3	58:V2:170:GLU:HB3	2.00	0.42
10:A7:34:HIS:NE2	55:S8:71:PRO:O	2.52	0.42
11:A8:75:ILE:N	11:A8:137:GLU:OE2	2.48	0.42
20:B4:103:TYR:CE2	24:B8:69:VAL:HG22	2.54	0.42
21:B5:47:THR:O	21:B5:51:SER:OG	2.36	0.42
25:B9:154:LYS:N	27:BM:7:VAL:O	2.53	0.42
31:E3:108:LEU:HD12	31:E3:108:LEU:N	2.34	0.42
35:E8:104:ARG:NH2	48:N5:219:LEU:HD22	2.34	0.42
40:FX:177:GLU:OE1	40:FX:180:GLN:NE2	2.52	0.42
44:N1:386:GLU:OE2	44:N1:569:ARG:NH2	2.53	0.42
47:N4:73:ILE:HD13	47:N4:255:TYR:CZ	2.54	0.42
50:S3:264:ASP:OD2	51:S4:151:ARG:NH1	2.52	0.42
53:S6:36:GLU:CD	53:S6:38:SER:HG	2.27	0.42
54:S7:90:GLU:HG2	54:S7:183:PRO:O	2.20	0.42
3:2B:57:PHE:CE2	3:2B:61:ILE:HD11	2.54	0.42
9:A6:66:LEU:HD22	9:A6:86:ARG:HG3	2.00	0.42
64:B3:102:CDL:OB3	39:ED:43:TRP:NE1	2.48	0.42
24:B8:25:ARG:NH1	24:B8:30:GLU:OE2	2.52	0.42
33:E5:5:LYS:O	33:E5:98:THR:HG23	2.19	0.42
48:N5:215:ILE:HG23	48:N5:216:ASN:N	2.34	0.42
49:S2:363:HIS:HB3	49:S2:386:LEU:HD22	2.02	0.42
53:S6:115:CYS:O	53:S6:119:GLU:HA	2.19	0.42
55:S8:108:GLN:N	61:S8:298:SF4:S1	2.82	0.42
59:E7:205:LEU:O	59:E7:209:GLN:N	2.46	0.42
1:1A:270:ARG:NH1	51:S4:71:VAL:O	2.53	0.42
9:A6:315:GLU:N	9:A6:315:GLU:OE1	2.52	0.42
16:AM:46:ARG:NH2	32:E4:192:ASP:OD2	2.40	0.42
21:B5:89:THR:HG21	28:C4:70:TRP:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:G2:182:PRO:O	42:G2:184:LYS:HG2	2.20	0.42
43:G3:80:VAL:HG12	43:G3:101:VAL:HG22	2.01	0.42
45:N2:157:PHE:HA	45:N2:160:TYR:HB2	2.02	0.42
47:N4:186:ASN:O	47:N4:190:ASN:ND2	2.43	0.42
46:N6:42:ILE:HD12	46:N6:42:ILE:C	2.44	0.42
49:S2:75:MET:HE1	49:S2:118:LEU:HD13	2.02	0.42
57:V1:295:ILE:HG23	57:V1:295:ILE:O	2.19	0.42
57:V1:407:GLY:O	57:V1:410:VAL:N	2.53	0.42
2:1B:329:SER:O	12:A9:94:ARG:NH2	2.44	0.42
14:AC:89:LEU:HD13	35:E8:1:MET:SD	2.60	0.42
16:AM:54:VAL:HG12	64:AM:215:CDL:HA31	2.01	0.42
20:B4:87:SER:O	20:B4:89:GLN:N	2.45	0.42
22:B6:4:LEU:HD13	27:BM:36:PRO:HD2	2.02	0.42
29:E1:288:ALA:O	29:E1:292:ALA:N	2.37	0.42
43:G3:237:GLU:O	43:G3:238:PHE:CG	2.73	0.42
47:N4:83:ILE:N	47:N4:83:ILE:HD13	2.34	0.42
48:N5:17:ASN:N	48:N5:119:CYS:SG	2.92	0.42
58:V2:175:GLU:O	58:V2:178:ILE:HG13	2.19	0.42
4:4L:114:LEU:HD12	45:N2:147:ILE:HD13	2.02	0.42
11:A8:175:VAL:HG12	11:A8:175:VAL:O	2.19	0.42
21:B5:104:GLN:OE1	21:B5:104:GLN:N	2.50	0.42
32:E4:142:GLN:N	32:E4:142:GLN:OE1	2.52	0.42
44:N1:582:ILE:HD13	46:N3:212:TYR:HE2	1.85	0.42
47:N4:327:ILE:HG22	48:N5:72:TYR:CD2	2.55	0.42
48:N5:57:ASN:HB3	48:N5:85:TYR:HD2	1.85	0.42
48:N5:481:LEU:N	48:N5:482:PRO:CD	2.83	0.42
50:S3:80:VAL:HG12	50:S3:81:TYR:O	2.19	0.42
54:S7:118:ILE:HD11	54:S7:135:VAL:HG12	2.02	0.42
57:V1:75:ILE:HG21	57:V1:149:ALA:HB2	2.01	0.42
2:1B:307:ALA:HB1	2:1B:345:LEU:HD22	2.01	0.42
3:2B:82:ILE:O	3:2B:86:VAL:HG23	2.20	0.42
25:B9:107:VAL:HG22	25:B9:108:HIS:O	2.20	0.42
26:BL:60:THR:HG22	26:BL:62:ALA:H	1.84	0.42
29:E1:50:ARG:NH2	29:E1:89:ASP:OD2	2.48	0.42
38:EC:38:CYS:SG	38:EC:56:LEU:HD23	2.60	0.42
44:N1:454:ASP:HB3	44:N1:536:LEU:HD12	2.01	0.42
44:N1:470:ILE:HG23	46:N6:76:ILE:CD1	2.50	0.42
45:N2:17:ILE:HD11	46:N6:146:LEU:HA	2.02	0.42
45:N2:39:PHE:HA	45:N2:69:THR:HG21	2.02	0.42
57:V1:399:ARG:NH2	57:V1:409:GLU:OE1	2.47	0.42
59:E7:88:LEU:O	59:E7:152:ARG:NH1	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:177:ASP:O	1:1A:223:THR:HG21	2.20	0.42
2:1B:14:ILE:HD13	15:AL:246:PRO:HB2	2.02	0.42
2:1B:74:LEU:HD22	2:1B:390:PHE:HZ	1.85	0.42
2:1B:271:GLN:O	2:1B:499:ARG:NH2	2.53	0.42
11:A8:63:ILE:HD12	11:A8:138:ILE:HD13	2.02	0.42
12:A9:25:GLU:OE1	12:A9:25:GLU:N	2.42	0.42
12:A9:442:ARG:NH1	44:N1:429:ASN:O	2.52	0.42
22:B6:38:TYR:OH	48:N5:4:ILE:O	2.35	0.42
36:EA:82:THR:HG23	52:S5:15:LEU:HD12	2.01	0.42
41:G1:294:ARG:CG	42:G2:181:VAL:HG21	2.41	0.42
43:G3:55:ARG:NH1	43:G3:72:GLY:O	2.51	0.42
43:G3:136:TYR:HD2	43:G3:192:ILE:HG23	1.84	0.42
44:N1:383:THR:HG22	44:N1:602:TYR:CD2	2.54	0.42
46:N3:242:ILE:HG23	46:N6:81:ILE:HG23	2.01	0.42
47:N4:43:ILE:HD12	47:N4:43:ILE:C	2.45	0.42
68:N4:505:U10:O5	68:N4:505:U10:H8	2.19	0.42
48:N5:310:ILE:HD13	48:N5:438:ILE:HG22	2.02	0.42
49:S2:103:ILE:HG23	49:S2:169:LEU:HD21	2.01	0.42
57:V1:150:MET:SD	57:V1:242:ILE:HG21	2.60	0.42
1:1A:288:VAL:HG12	1:1A:294:LEU:HA	2.02	0.41
3:2B:82:ILE:HD11	47:N4:162:LEU:HD13	2.01	0.41
3:2B:85:ILE:O	3:2B:88:ILE:HB	2.20	0.41
66:AC:201:ZMP:H25A	25:B9:100:ARG:HD2	2.01	0.41
21:B5:71:VAL:HG21	47:N4:50:ILE:CD1	2.50	0.41
27:BM:62:MET:HE1	47:N4:457:ILE:HB	2.02	0.41
32:E4:79:ASP:OD1	32:E4:79:ASP:N	2.52	0.41
40:FX:234:MET:O	40:FX:235:GLU:C	2.62	0.41
43:G3:76:TRP:O	43:G3:79:SER:OG	2.32	0.41
50:S3:147:SER:OG	50:S3:159:GLU:OE1	2.25	0.41
55:S8:77:TYR:CG	55:S8:78:PRO:HA	2.55	0.41
59:E7:12:LEU:HD21	59:E7:212:LEU:HA	2.02	0.41
59:E7:159:LEU:HD23	59:E7:159:LEU:O	2.20	0.41
15:AL:123:GLY:HA3	15:AL:164:TRP:CZ2	2.55	0.41
16:AM:170:ILE:HD12	16:AM:185:GLU:OE1	2.20	0.41
19:B3:23:ARG:NH2	35:E8:11:ASP:OD2	2.50	0.41
68:N4:505:U10:H252	68:N4:505:U10:H211	2.02	0.41
48:N5:1:MET:H2	48:N5:4:ILE:HG12	1.85	0.41
46:N6:126:ILE:HG22	46:N6:128:ILE:CG1	2.50	0.41
51:S4:45:ASP:N	51:S4:45:ASP:OD1	2.52	0.41
4:4L:73:LEU:C	4:4L:73:LEU:HD23	2.45	0.41
18:B2:103:GLU:OE2	23:B7:97:ARG:NH2	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:C4:27:LEU:HB3	28:C4:35:LEU:HD21	2.01	0.41
41:G1:162:PRO:HA	41:G1:180:ALA:O	2.20	0.41
45:N2:50:ILE:HD12	45:N2:62:ILE:HG21	2.03	0.41
48:N5:103:TYR:HB2	48:N5:354:MET:HE3	2.03	0.41
48:N5:250:THR:N	48:N5:251:PRO:HD2	2.35	0.41
48:N5:341:HIS:HE1	48:N5:400:LEU:HD11	1.84	0.41
53:S6:103:ILE:HD11	53:S6:115:CYS:SG	2.60	0.41
59:E7:97:ILE:CD1	59:E7:119:ALA:HB2	2.51	0.41
1:1A:345:LEU:HD23	9:A6:367:LEU:HD22	2.02	0.41
12:A9:279:PRO:CG	12:A9:282:ILE:HD11	2.50	0.41
12:A9:305:MET:HE2	12:A9:469:ILE:HD11	2.03	0.41
14:AC:93:ASP:OD1	14:AC:93:ASP:N	2.54	0.41
28:C4:152:ARG:O	28:C4:156:VAL:HG23	2.20	0.41
40:FX:144:ASP:CG	40:FX:150:HIS:HE2	2.22	0.41
41:G1:120:PHE:O	41:G1:122:LEU:N	2.49	0.41
41:G1:260:THR:HB	41:G1:278:VAL:HG22	2.02	0.41
44:N1:433:ILE:HG23	44:N1:434:MET:N	2.35	0.41
45:N2:62:ILE:HG23	45:N2:83:MET:HE2	2.02	0.41
45:N2:81:ILE:HD12	46:N6:153:ILE:HD12	2.03	0.41
48:N5:67:ASN:ND2	48:N5:77:ASP:OD1	2.52	0.41
2:1B:117:SER:OG	2:1B:195:ASN:ND2	2.53	0.41
10:A7:8:LEU:HD11	32:E4:325:PRO:HB2	2.02	0.41
12:A9:202:ILE:HG21	12:A9:224:LEU:HD23	2.02	0.41
12:A9:213:GLN:O	54:S7:48:GLN:NE2	2.50	0.41
12:A9:287:ASP:OD2	12:A9:290:THR:OG1	2.29	0.41
17:AN:11:MET:HE1	48:N5:581:ILE:CG2	2.50	0.41
27:BM:28:ILE:HG22	27:BM:29:GLU:N	2.35	0.41
35:E8:57:GLU:O	35:E8:58:PHE:CG	2.74	0.41
40:FX:287:PRO:CD	40:FX:307:THR:HG22	2.51	0.41
47:N4:228:GLY:O	47:N4:232:VAL:HG13	2.20	0.41
59:E7:12:LEU:HD21	59:E7:212:LEU:HB3	2.02	0.41
1:1A:48:ILE:HD13	1:1A:67:ALA:HB2	2.02	0.41
5:A1:44:THR:HG22	5:A1:48:LYS:HE3	2.03	0.41
9:A6:158:ARG:NE	9:A6:169:GLU:OE2	2.54	0.41
12:A9:80:THR:HG22	12:A9:81:GLU:N	2.35	0.41
66:AB:150:ZMP:H14A	51:S4:50:GLN:HE21	1.86	0.41
30:E2:320:HIS:O	30:E2:321:HIS:CG	2.74	0.41
31:E3:103:SER:HB3	31:E3:108:LEU:HD11	2.01	0.41
34:E6:154:LEU:O	34:E6:245:ASN:ND2	2.49	0.41
44:N1:446:LEU:HD12	46:N3:180:ASN:ND2	2.36	0.41
45:N2:84:ILE:HG22	46:N6:146:LEU:HD21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
70:V1:579:FMN:C6	71:V1:581:NAI:H4N	2.50	0.41
59:E7:62:HIS:CE1	59:E7:66:HIS:HB2	2.55	0.41
1:1A:63:VAL:HG21	1:1A:116:TYR:CE2	2.56	0.41
1:1A:166:ARG:NH1	57:V1:415:ASP:OD2	2.45	0.41
4:4L:78:ILE:HG21	4:4L:120:ILE:HG21	2.02	0.41
20:B4:66:GLU:CB	47:N4:444:THR:HG22	2.51	0.41
25:B9:45:ARG:O	25:B9:49:VAL:HG23	2.20	0.41
29:E1:246:THR:O	29:E1:436:SER:OG	2.28	0.41
38:EC:78:ASP:O	38:EC:81:PHE:HB2	2.20	0.41
43:G3:98:GLU:O	43:G3:122:PRO:HA	2.21	0.41
48:N5:92:LEU:HD21	48:N5:259:ALA:HB2	2.03	0.41
58:V2:107:CYS:O	58:V2:112:ALA:HB2	2.20	0.41
2:1B:342:LYS:O	2:1B:343:LEU:C	2.63	0.41
9:A6:312:ARG:NH1	9:A6:346:GLU:OE2	2.53	0.41
10:A7:112:HIS:CD2	32:E4:31:VAL:HG13	2.55	0.41
27:BM:22:GLU:OE2	27:BM:27:ARG:NH1	2.49	0.41
31:E3:45:PRO:HD3	31:E3:121:SER:HB2	2.01	0.41
38:EC:31:GLN:N	38:EC:32:PRO:HD2	2.35	0.41
41:G1:275:ALA:HB1	42:G2:147:VAL:HG11	2.02	0.41
47:N4:2:ILE:HG23	47:N4:3:TYR:N	2.35	0.41
47:N4:25:TYR:CE1	68:N4:505:U10:H3M3	2.56	0.41
47:N4:94:TYR:CE1	68:N4:505:U10:H251	2.55	0.41
46:N6:67:ILE:HD11	46:N6:127:GLU:HB2	2.03	0.41
1:1A:196:THR:N	61:1A:403:SF4:S4	2.82	0.41
3:2B:93:ILE:HD13	24:B8:51:PHE:CD1	2.56	0.41
7:A3:108:MET:HE3	21:B5:135:VAL:HA	2.02	0.41
9:A6:35:ALA:O	41:G1:67:ARG:NH1	2.54	0.41
10:A7:75:ILE:HD11	50:S3:243:ALA:HB1	2.03	0.41
16:AM:45:HIS:O	16:AM:45:HIS:ND1	2.53	0.41
16:AM:158:VAL:CG1	16:AM:161:MET:HA	2.51	0.41
27:BM:5:ARG:HG3	41:G1:305:VAL:HG11	2.03	0.41
28:C4:7:THR:O	28:C4:7:THR:HG23	2.20	0.41
28:C4:84:PRO:O	28:C4:125:SER:OG	2.34	0.41
32:E4:171:HIS:O	32:E4:174:ASN:N	2.54	0.41
32:E4:188:ALA:O	32:E4:198:SER:OG	2.39	0.41
33:E5:279:GLY:N	33:E5:280:PRO:CD	2.83	0.41
39:ED:68:ASP:OD1	39:ED:69:LYS:N	2.54	0.41
41:G1:105:HIS:CE1	43:G3:241:ARG:HE	2.38	0.41
41:G1:321:HIS:ND1	41:G1:321:HIS:C	2.78	0.41
42:G2:132:SER:O	42:G2:133:PRO:C	2.63	0.41
47:N4:167:SER:OG	47:N4:217:LYS:NZ	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:N4:173:ASN:O	47:N4:177:ASN:ND2	2.42	0.41
47:N4:435:TYR:OH	48:N5:160:ASN:O	2.37	0.41
49:S2:184:PHE:CD2	49:S2:273:ILE:HG21	2.56	0.41
49:S2:243:TYR:N	49:S2:244:PRO:HD2	2.36	0.41
50:S3:205:ASP:O	50:S3:209:SER:N	2.53	0.41
50:S3:232:GLU:HG3	51:S4:78:MET:HB3	2.03	0.41
57:V1:133:ARG:HB3	57:V1:166:GLU:HG3	2.02	0.41
57:V1:428:LEU:HD23	57:V1:428:LEU:C	2.45	0.41
1:1A:142:CYS:HB2	1:1A:143:PRO:HD3	2.02	0.41
1:1A:275:ASN:ND2	1:1A:278:ASP:OD1	2.54	0.41
2:1B:127:THR:O	2:1B:127:THR:HG23	2.21	0.41
11:A8:181:GLU:OE1	11:A8:181:GLU:N	2.48	0.41
12:A9:482:TYR:OH	46:N3:175:ASN:ND2	2.53	0.41
20:B4:40:MET:HE3	24:B8:73:LEU:HD12	2.02	0.41
33:E5:39:GLN:H	33:E5:70:GLY:HA2	1.86	0.41
33:E5:124:VAL:O	33:E5:153:LEU:HD21	2.21	0.41
33:E5:216:LEU:C	33:E5:216:LEU:HD23	2.46	0.41
35:E8:148:LYS:C	35:E8:149:SER:HG	2.18	0.41
49:S2:356:ILE:HD12	49:S2:356:ILE:N	2.36	0.41
52:S5:11:THR:HG22	52:S5:16:HIS:CE1	2.55	0.41
1:1A:178:ASP:OD1	1:1A:178:ASP:N	2.54	0.40
21:B5:44:ALA:HB3	21:B5:45:PRO:HD3	2.04	0.40
21:B5:89:THR:HG21	28:C4:70:TRP:CB	2.51	0.40
22:B6:81:LEU:HD11	39:ED:124:LYS:HD3	2.03	0.40
31:E3:304:LEU:HD13	31:E3:320:ILE:HD13	2.03	0.40
34:E6:130:GLU:OE2	34:E6:213:ARG:NH2	2.50	0.40
45:N2:18:ILE:HG23	45:N2:22:LEU:HD12	2.03	0.40
50:S3:65:SER:N	50:S3:79:ASN:O	2.53	0.40
55:S8:159:VAL:HG11	55:S8:192:ILE:HD12	2.02	0.40
57:V1:218:GLU:OE2	57:V1:225:ARG:NH2	2.54	0.40
8:A5:129:MET:SD	50:S3:83:GLN:NE2	2.88	0.40
66:AC:201:ZMP:H25A	25:B9:100:ARG:HD3	2.02	0.40
20:B4:89:GLN:OE1	41:G1:304:ASP:N	2.43	0.40
30:E2:303:LEU:HD12	30:E2:303:LEU:N	2.36	0.40
33:E5:262:VAL:O	33:E5:262:VAL:HG12	2.21	0.40
63:E8:301:PC1:H332	48:N5:223:MET:HE2	2.02	0.40
50:S3:156:MET:HE1	50:S3:174:PRO:CG	2.51	0.40
54:S7:123:THR:HA	54:S7:151:CYS:HB3	2.04	0.40
57:V1:88:GLY:O	71:V1:581:NAI:N7N	2.42	0.40
57:V1:487:ASP:O	57:V1:492:SER:CA	2.69	0.40
27:BM:68:THR:HG22	47:N4:40:ILE:HG12	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:E6:35:LEU:O	34:E6:36:SER:OG	2.28	0.40
34:E6:184:ASN:ND2	34:E6:216:GLU:OE2	2.55	0.40
38:EC:39:ARG:HA	38:EC:39:ARG:CZ	2.51	0.40
39:ED:142:VAL:HG23	39:ED:143:LEU:N	2.37	0.40
45:N2:68:SER:OG	45:N2:79:GLN:NE2	2.54	0.40
46:N3:244:LEU:O	46:N3:248:LEU:HG	2.20	0.40
63:N3:301:PC1:H292	46:N6:28:ILE:HD11	2.02	0.40
47:N4:37:ILE:O	47:N4:40:ILE:HG22	2.22	0.40
47:N4:218:LEU:HD13	47:N4:309:TYR:CZ	2.56	0.40
47:N4:241:LEU:O	47:N4:242:LEU:C	2.62	0.40
47:N4:308:TYR:HD2	47:N4:336:MET:HE2	1.86	0.40
48:N5:242:LEU:HD11	48:N5:257:HIS:CE1	2.56	0.40
49:S2:135:TRP:O	49:S2:138:GLU:HG3	2.22	0.40
55:S8:146:CYS:N	61:S8:297:SF4:S4	2.92	0.40
57:V1:115:VAL:HG11	57:V1:213:LEU:HD22	2.03	0.40
59:E7:12:LEU:HD11	59:E7:212:LEU:HB3	2.03	0.40
59:E7:47:VAL:HG13	59:E7:71:LEU:O	2.22	0.40
1:1A:90:ARG:HD2	1:1A:104:ILE:HG21	2.03	0.40
1:1A:292:THR:OG1	51:S4:105:ARG:NH2	2.54	0.40
2:1B:462:TYR:C	2:1B:464:PHE:N	2.79	0.40
12:A9:415:TRP:CE3	12:A9:420:ILE:HG21	2.56	0.40
25:B9:16:VAL:HG12	25:B9:18:GLN:H	1.85	0.40
25:B9:99:ARG:NH2	48:N5:531:ASN:OD1	2.50	0.40
33:E5:181:ALA:HB2	33:E5:197:LEU:HD21	2.03	0.40
35:E8:147:TYR:CD2	63:E8:301:PC1:H151	2.57	0.40
41:G1:244:LEU:HD22	41:G1:261:ILE:HD12	2.03	0.40
41:G1:369:ALA:O	41:G1:373:LYS:N	2.55	0.40
44:N1:527:LEU:HD12	44:N1:527:LEU:C	2.46	0.40
49:S2:224:MET:CE	49:S2:386:LEU:HD23	2.51	0.40
51:S4:94:GLY:N	51:S4:109:GLU:OE2	2.55	0.40
53:S6:97:THR:O	53:S6:97:THR:HG22	2.20	0.40
53:S6:114:GLN:OE1	53:S6:114:GLN:N	2.55	0.40
58:V2:32:ILE:HG21	58:V2:47:PRO:HB2	2.03	0.40
2:1B:73:ARG:NH2	6:A2:121:GLN:OE1	2.51	0.40
7:A3:62:PHE:CD2	44:N1:665:THR:HG23	2.56	0.40
9:A6:164:THR:O	9:A6:164:THR:HG22	2.21	0.40
9:A6:193:GLY:O	9:A6:196:SER:OG	2.38	0.40
12:A9:426:THR:HG22	12:A9:427:LYS:N	2.37	0.40
18:B2:144:VAL:HG22	35:E8:139:ARG:NH1	2.36	0.40
24:B8:39:ASP:OD1	24:B8:39:ASP:N	2.52	0.40
28:C4:78:THR:HG22	47:N4:59:ASN:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:E6:117:TRP:NE1	34:E6:121:LEU:HD11	2.37	0.40
44:N1:448:PHE:HE1	44:N1:610:ILE:HD12	1.86	0.40
47:N4:305:MET:HE1	47:N4:336:MET:SD	2.62	0.40
57:V1:130:GLU:OE1	57:V1:133:ARG:NH2	2.53	0.40
57:V1:221:SER:O	57:V1:223:LYS:N	2.50	0.40
57:V1:434:TRP:N	57:V1:435:PRO:HD2	2.37	0.40
71:V1:581:NAI:H6N	71:V1:581:NAI:C3D	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1A	350/385 (91%)	340 (97%)	10 (3%)	0	100	100
2	1B	523/527 (99%)	506 (97%)	17 (3%)	0	100	100
3	2B	112/142 (79%)	105 (94%)	7 (6%)	0	100	100
4	4L	106/171 (62%)	103 (97%)	3 (3%)	0	100	100
5	A1	135/141 (96%)	126 (93%)	9 (7%)	0	100	100
6	A2	190/193 (98%)	184 (97%)	6 (3%)	0	100	100
7	A3	122/125 (98%)	118 (97%)	4 (3%)	0	100	100
8	A5	152/184 (83%)	147 (97%)	5 (3%)	0	100	100
9	A6	421/437 (96%)	409 (97%)	12 (3%)	0	100	100
10	A7	134/136 (98%)	129 (96%)	5 (4%)	0	100	100
11	A8	221/223 (99%)	215 (97%)	6 (3%)	0	100	100
12	A9	482/489 (99%)	465 (96%)	17 (4%)	0	100	100
13	AB	86/134 (64%)	84 (98%)	2 (2%)	0	100	100
14	AC	90/134 (67%)	89 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	AL	263/281 (94%)	243 (92%)	20 (8%)	0	100	100
16	AM	182/198 (92%)	175 (96%)	7 (4%)	0	100	100
17	AN	285/287 (99%)	282 (99%)	3 (1%)	0	100	100
18	B2	103/145 (71%)	103 (100%)	0	0	100	100
19	B3	32/62 (52%)	31 (97%)	0	1 (3%)	3	16
20	B4	169/171 (99%)	157 (93%)	12 (7%)	0	100	100
21	B5	132/140 (94%)	129 (98%)	3 (2%)	0	100	100
22	B6	89/91 (98%)	86 (97%)	3 (3%)	0	100	100
23	B7	95/97 (98%)	93 (98%)	2 (2%)	0	100	100
24	B8	145/176 (82%)	137 (94%)	8 (6%)	0	100	100
25	B9	149/158 (94%)	146 (98%)	3 (2%)	0	100	100
26	BL	142/144 (99%)	137 (96%)	5 (4%)	0	100	100
27	BM	99/112 (88%)	98 (99%)	1 (1%)	0	100	100
28	C4	181/185 (98%)	178 (98%)	3 (2%)	0	100	100
29	E1	448/483 (93%)	434 (97%)	14 (3%)	0	100	100
30	E2	464/467 (99%)	447 (96%)	16 (3%)	1 (0%)	43	73
31	E3	430/434 (99%)	423 (98%)	7 (2%)	0	100	100
32	E4	349/368 (95%)	343 (98%)	6 (2%)	0	100	100
33	E5	266/290 (92%)	242 (91%)	23 (9%)	1 (0%)	30	61
34	E6	314/371 (85%)	312 (99%)	2 (1%)	0	100	100
35	E8	203/205 (99%)	192 (95%)	11 (5%)	0	100	100
36	EA	96/126 (76%)	91 (95%)	5 (5%)	0	100	100
37	EB	73/101 (72%)	72 (99%)	1 (1%)	0	100	100
38	EC	83/101 (82%)	77 (93%)	6 (7%)	0	100	100
39	ED	136/151 (90%)	127 (93%)	9 (7%)	0	100	100
40	FX	235/325 (72%)	223 (95%)	11 (5%)	1 (0%)	30	61
41	G1	401/436 (92%)	387 (96%)	14 (4%)	0	100	100
42	G2	234/267 (88%)	218 (93%)	16 (7%)	0	100	100
43	G3	253/261 (97%)	234 (92%)	19 (8%)	0	100	100
44	N1	308/670 (46%)	290 (94%)	18 (6%)	0	100	100
45	N2	294/300 (98%)	278 (95%)	16 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
46	N3	119/293 (41%)	115 (97%)	4 (3%)	0	100	100
46	N6	152/293 (52%)	148 (97%)	4 (3%)	0	100	100
47	N4	476/478 (100%)	464 (98%)	12 (2%)	0	100	100
48	N5	582/584 (100%)	558 (96%)	24 (4%)	0	100	100
49	S2	391/395 (99%)	377 (96%)	13 (3%)	1 (0%)	36	67
50	S3	246/277 (89%)	237 (96%)	9 (4%)	0	100	100
51	S4	188/208 (90%)	180 (96%)	8 (4%)	0	100	100
52	S5	110/122 (90%)	108 (98%)	2 (2%)	0	100	100
53	S6	145/147 (99%)	141 (97%)	4 (3%)	0	100	100
54	S7	195/207 (94%)	188 (96%)	7 (4%)	0	100	100
55	S8	180/212 (85%)	174 (97%)	6 (3%)	0	100	100
57	V1	502/526 (95%)	480 (96%)	22 (4%)	0	100	100
58	V2	220/225 (98%)	214 (97%)	6 (3%)	0	100	100
59	E7	244/246 (99%)	235 (96%)	9 (4%)	0	100	100
All	All	13527/15237 (89%)	13024 (96%)	498 (4%)	5 (0%)	100	100

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
19	B3	34	ARG
30	E2	370	THR
33	E5	288	THR
49	S2	36	HIS
40	FX	276	VAL

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	1A	310/340 (91%)	303 (98%)	7 (2%)	44	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	1B	453/454 (100%)	449 (99%)	4 (1%)	70	82
3	2B	109/111 (98%)	106 (97%)	3 (3%)	38	67
4	4L	96/151 (64%)	93 (97%)	3 (3%)	35	65
5	A1	115/118 (98%)	114 (99%)	1 (1%)	70	82
6	A2	159/160 (99%)	159 (100%)	0	100	100
7	A3	104/104 (100%)	103 (99%)	1 (1%)	68	81
8	A5	134/152 (88%)	132 (98%)	2 (2%)	57	77
9	A6	346/358 (97%)	343 (99%)	3 (1%)	70	82
10	A7	119/119 (100%)	119 (100%)	0	100	100
11	A8	196/196 (100%)	194 (99%)	2 (1%)	68	81
12	A9	420/424 (99%)	413 (98%)	7 (2%)	53	75
13	AB	79/114 (69%)	79 (100%)	0	100	100
14	AC	80/111 (72%)	78 (98%)	2 (2%)	42	69
15	AL	228/242 (94%)	228 (100%)	0	100	100
16	AM	156/168 (93%)	156 (100%)	0	100	100
17	AN	241/241 (100%)	240 (100%)	1 (0%)	84	87
18	B2	97/131 (74%)	97 (100%)	0	100	100
19	B3	30/31 (97%)	30 (100%)	0	100	100
20	B4	144/144 (100%)	144 (100%)	0	100	100
21	B5	108/108 (100%)	106 (98%)	2 (2%)	50	73
22	B6	82/82 (100%)	82 (100%)	0	100	100
23	B7	93/93 (100%)	89 (96%)	4 (4%)	26	57
24	B8	127/148 (86%)	126 (99%)	1 (1%)	73	83
25	B9	132/139 (95%)	130 (98%)	2 (2%)	57	77
26	BL	132/132 (100%)	130 (98%)	2 (2%)	57	77
27	BM	93/93 (100%)	92 (99%)	1 (1%)	65	80
28	C4	166/167 (99%)	163 (98%)	3 (2%)	51	74
29	E1	381/404 (94%)	376 (99%)	5 (1%)	61	79
30	E2	379/380 (100%)	370 (98%)	9 (2%)	43	70
31	E3	339/341 (99%)	333 (98%)	6 (2%)	51	74
32	E4	302/317 (95%)	292 (97%)	10 (3%)	33	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	E5	200/205 (98%)	197 (98%)	3 (2%)	57	77
34	E6	272/314 (87%)	268 (98%)	4 (2%)	57	77
35	E8	179/179 (100%)	177 (99%)	2 (1%)	65	80
36	EA	84/86 (98%)	84 (100%)	0	100	100
37	EB	70/70 (100%)	70 (100%)	0	100	100
38	EC	73/86 (85%)	73 (100%)	0	100	100
39	ED	121/133 (91%)	120 (99%)	1 (1%)	73	83
40	FX	212/276 (77%)	207 (98%)	5 (2%)	43	70
41	G1	333/365 (91%)	323 (97%)	10 (3%)	36	66
42	G2	192/214 (90%)	190 (99%)	2 (1%)	68	81
43	G3	202/202 (100%)	201 (100%)	1 (0%)	81	86
44	N1	295/639 (46%)	292 (99%)	3 (1%)	68	81
45	N2	285/289 (99%)	275 (96%)	10 (4%)	32	62
46	N3	116/281 (41%)	112 (97%)	4 (3%)	32	63
46	N6	147/281 (52%)	145 (99%)	2 (1%)	59	78
47	N4	455/455 (100%)	442 (97%)	13 (3%)	37	67
48	N5	546/546 (100%)	532 (97%)	14 (3%)	40	69
49	S2	335/336 (100%)	332 (99%)	3 (1%)	70	82
50	S3	224/250 (90%)	219 (98%)	5 (2%)	45	71
51	S4	159/172 (92%)	154 (97%)	5 (3%)	35	65
52	S5	102/102 (100%)	101 (99%)	1 (1%)	68	81
53	S6	130/130 (100%)	130 (100%)	0	100	100
54	S7	165/171 (96%)	160 (97%)	5 (3%)	36	66
55	S8	160/187 (86%)	157 (98%)	3 (2%)	50	73
57	V1	412/427 (96%)	406 (98%)	6 (2%)	57	77
58	V2	190/190 (100%)	180 (95%)	10 (5%)	20	51
59	E7	192/192 (100%)	190 (99%)	2 (1%)	68	81
All	All	11801/13051 (90%)	11606 (98%)	195 (2%)	52	75

All (195) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1A	168	ASP

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Mol	Chain	Res	Type
1	1A	175	GLU
1	1A	178	ASP
1	1A	219	ARG
1	1A	260	ASN
1	1A	293	GLU
1	1A	310	LEU
2	1B	108	GLU
2	1B	152	SER
2	1B	276	SER
2	1B	338	GLU
3	2B	5	LEU
3	2B	45	LEU
3	2B	66	ASN
4	4L	61	VAL
4	4L	97	GLU
4	4L	108	GLU
5	A1	37	HIS
7	A3	53	ARG
8	A5	60	ASP
8	A5	150	ASP
9	A6	211	ASP
9	A6	315	GLU
9	A6	346	GLU
11	A8	96	GLN
11	A8	123	GLU
12	A9	14	ASN
12	A9	94	ARG
12	A9	95	GLU
12	A9	108	THR
12	A9	214	SER
12	A9	269	ASP
12	A9	436	MET
14	AC	91	SER
14	AC	93	ASP
17	AN	256	CYS
21	B5	25	THR
21	B5	51	SER
23	B7	5	ASN
23	B7	49	HIS
23	B7	52	LEU
23	B7	82	LEU
24	B8	87	ASP

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Mol	Chain	Res	Type
25	B9	107	VAL
25	B9	130	GLN
26	BL	7	LYS
26	BL	76	SER
27	BM	81	ASN
28	C4	43	ASP
28	C4	131	PHE
28	C4	145	LEU
29	E1	133	LEU
29	E1	197	ASN
29	E1	246	THR
29	E1	416	ASP
29	E1	464	LYS
30	E2	2	VAL
30	E2	115	ASN
30	E2	131	LYS
30	E2	135	THR
30	E2	179	ASP
30	E2	209	VAL
30	E2	259	VAL
30	E2	325	THR
30	E2	388	GLU
31	E3	7	THR
31	E3	148	ASN
31	E3	298	ARG
31	E3	306	ASP
31	E3	319	VAL
31	E3	381	GLU
32	E4	103	THR
32	E4	139	GLU
32	E4	142	GLN
32	E4	155	GLU
32	E4	170	SER
32	E4	206	ASP
32	E4	208	SER
32	E4	304	ARG
32	E4	316	SER
32	E4	332	ASP
33	E5	36	LEU
33	E5	49	ASP
33	E5	106	HIS
34	E6	79	ILE

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Mol	Chain	Res	Type
34	E6	194	SER
34	E6	201	ASN
34	E6	204	GLN
35	E8	1	MET
35	E8	94	ASP
39	ED	129	GLN
40	FX	109	HIS
40	FX	172	ASP
40	FX	180	GLN
40	FX	221	ASN
40	FX	321	LYS
41	G1	123	PHE
41	G1	161	THR
41	G1	251	ASP
41	G1	281	ASP
41	G1	321	HIS
41	G1	326	GLU
41	G1	339	ASP
41	G1	390	ASP
41	G1	399	SER
41	G1	421	VAL
42	G2	71	GLN
42	G2	108	ARG
43	G3	92	GLU
44	N1	373	LEU
44	N1	378	LEU
44	N1	515	LEU
45	N2	43	ASN
45	N2	44	PHE
45	N2	84	ILE
45	N2	90	THR
45	N2	96	ASN
45	N2	122	ILE
45	N2	155	SER
45	N2	164	SER
45	N2	173	SER
45	N2	230	PHE
46	N3	233	ILE
46	N3	264	ASN
46	N3	280	SER
46	N3	292	ASN
47	N4	76	TYR

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Mol	Chain	Res	Type
47	N4	98	ASN
47	N4	112	ASN
47	N4	124	SER
47	N4	156	SER
47	N4	174	SER
47	N4	187	ILE
47	N4	242	LEU
47	N4	365	ILE
47	N4	385	ASN
47	N4	390	LEU
47	N4	392	VAL
47	N4	449	ASP
48	N5	8	LYS
48	N5	13	SER
48	N5	85	TYR
48	N5	172	VAL
48	N5	185	SER
48	N5	273	ARG
48	N5	320	SER
48	N5	350	SER
48	N5	377	HIS
48	N5	393	LEU
48	N5	435	SER
48	N5	445	ASN
48	N5	503	ILE
48	N5	536	ARG
46	N6	90	MET
46	N6	128	ILE
49	S2	25	HIS
49	S2	133	ILE
49	S2	357	ARG
50	S3	108	CYS
50	S3	121	VAL
50	S3	136	ARG
50	S3	149	THR
50	S3	247	ASP
51	S4	16	ILE
51	S4	28	GLU
51	S4	45	ASP
51	S4	156	ARG
51	S4	202	LYS
52	S5	20	GLU

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Mol	Chain	Res	Type
54	S7	32	ARG
54	S7	86	CYS
54	S7	116	ASP
54	S7	118	ILE
54	S7	137	ASP
55	S8	37	ASP
55	S8	55	GLU
55	S8	138	LEU
57	V1	167	THR
57	V1	209	GLU
57	V1	213	LEU
57	V1	345	ASP
57	V1	384	THR
57	V1	386	CYS
58	V2	24	GLU
58	V2	100	GLN
58	V2	105	THR
58	V2	108	MET
58	V2	114	GLU
58	V2	120	CYS
58	V2	125	VAL
58	V2	133	ASP
58	V2	141	MET
58	V2	179	GLU
59	E7	99	HIS
59	E7	169	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (218) such sidechains are listed below:

Mol	Chain	Res	Type
1	1A	56	GLN
1	1A	80	ASN
1	1A	82	ASN
1	1A	128	GLN
1	1A	194	HIS
1	1A	260	ASN
1	1A	275	ASN
2	1B	33	ASN
2	1B	36	ASN
2	1B	137	HIS
2	1B	155	HIS
2	1B	195	ASN

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Mol	Chain	Res	Type
2	1B	242	ASN
2	1B	271	GLN
2	1B	315	ASN
2	1B	344	GLN
2	1B	465	GLN
2	1B	500	HIS
2	1B	507	HIS
2	1B	509	ASN
3	2B	4	ASN
3	2B	9	ASN
3	2B	98	ASN
3	2B	99	HIS
4	4L	106	HIS
4	4L	148	HIS
4	4L	162	GLN
5	A1	60	ASN
5	A1	121	HIS
6	A2	12	HIS
6	A2	75	GLN
6	A2	113	HIS
6	A2	128	ASN
8	A5	108	GLN
9	A6	46	GLN
9	A6	88	ASN
9	A6	107	HIS
9	A6	134	ASN
9	A6	205	HIS
9	A6	337	HIS
9	A6	343	GLN
9	A6	409	HIS
10	A7	92	GLN
10	A7	124	GLN
11	A8	23	HIS
11	A8	27	GLN
11	A8	54	HIS
11	A8	83	ASN
11	A8	96	GLN
11	A8	130	ASN
11	A8	159	HIS
11	A8	182	GLN
12	A9	79	GLN
12	A9	174	GLN

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Mol	Chain	Res	Type
12	A9	242	HIS
14	AC	110	HIS
15	AL	39	GLN
15	AL	107	GLN
15	AL	201	HIS
15	AL	217	ASN
16	AM	25	GLN
16	AM	104	GLN
17	AN	20	HIS
17	AN	90	HIS
17	AN	114	HIS
17	AN	115	GLN
17	AN	221	HIS
18	B2	119	HIS
19	B3	5	ASN
20	B4	69	GLN
20	B4	161	ASN
21	B5	100	GLN
22	B6	19	ASN
22	B6	22	HIS
23	B7	70	HIS
24	B8	63	ASN
24	B8	156	GLN
24	B8	165	HIS
25	B9	112	ASN
25	B9	125	HIS
26	BL	25	ASN
26	BL	61	HIS
27	BM	71	GLN
27	BM	81	ASN
27	BM	99	GLN
28	C4	51	ASN
29	E1	192	GLN
29	E1	198	GLN
29	E1	204	ASN
29	E1	223	HIS
29	E1	291	HIS
30	E2	18	HIS
30	E2	24	HIS
30	E2	58	ASN
30	E2	99	GLN
30	E2	114	HIS

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Mol	Chain	Res	Type
30	E2	119	HIS
30	E2	321	HIS
30	E2	344	GLN
31	E3	20	GLN
31	E3	29	GLN
31	E3	58	GLN
31	E3	99	GLN
31	E3	218	ASN
31	E3	225	HIS
31	E3	248	ASN
31	E3	303	ASN
31	E3	313	HIS
31	E3	333	ASN
31	E3	355	GLN
31	E3	365	GLN
32	E4	43	GLN
32	E4	146	ASN
32	E4	171	HIS
32	E4	358	HIS
33	E5	199	HIS
33	E5	255	ASN
34	E6	49	GLN
34	E6	57	ASN
34	E6	127	HIS
34	E6	147	GLN
34	E6	197	ASN
34	E6	240	GLN
35	E8	19	ASN
36	EA	49	HIS
37	EB	44	GLN
39	ED	38	ASN
39	ED	89	GLN
39	ED	139	HIS
40	FX	124	HIS
40	FX	133	GLN
40	FX	324	GLN
41	G1	87	HIS
41	G1	117	ASN
41	G1	333	ASN
42	G2	36	HIS
42	G2	50	HIS
42	G2	71	GLN

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Mol	Chain	Res	Type
42	G2	174	GLN
43	G3	36	GLN
43	G3	66	GLN
43	G3	210	ASN
44	N1	402	ASN
44	N1	409	GLN
44	N1	440	ASN
44	N1	476	HIS
44	N1	537	ASN
45	N2	4	ASN
45	N2	6	ASN
45	N2	23	GLN
45	N2	76	ASN
45	N2	82	HIS
45	N2	184	ASN
45	N2	209	HIS
45	N2	237	ASN
45	N2	294	ASN
46	N3	172	ASN
46	N3	180	ASN
46	N3	219	ASN
46	N3	226	ASN
46	N3	264	ASN
46	N3	292	ASN
47	N4	20	GLN
47	N4	48	GLN
47	N4	139	ASN
47	N4	143	ASN
47	N4	157	ASN
47	N4	189	HIS
47	N4	200	HIS
47	N4	209	ASN
47	N4	254	HIS
47	N4	267	ASN
47	N4	339	HIS
47	N4	368	ASN
47	N4	437	HIS
48	N5	21	ASN
48	N5	95	ASN
48	N5	159	ASN
48	N5	218	ASN
48	N5	333	ASN

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Mol	Chain	Res	Type
48	N5	341	HIS
48	N5	345	HIS
48	N5	499	HIS
48	N5	524	ASN
48	N5	525	HIS
48	N5	572	HIS
49	S2	36	HIS
49	S2	50	HIS
49	S2	158	ASN
49	S2	278	GLN
49	S2	309	ASN
49	S2	313	HIS
49	S2	344	GLN
49	S2	372	GLN
50	S3	97	GLN
50	S3	99	GLN
50	S3	153	HIS
50	S3	208	ASN
50	S3	273	GLN
51	S4	39	ASN
51	S4	47	GLN
52	S5	75	GLN
53	S6	85	HIS
53	S6	136	GLN
54	S7	27	GLN
54	S7	37	GLN
54	S7	50	HIS
54	S7	67	GLN
54	S7	93	GLN
54	S7	159	HIS
55	S8	70	GLN
55	S8	82	ASN
55	S8	108	GLN
57	V1	48	HIS
57	V1	382	GLN
58	V2	149	HIS
59	E7	1	GLN
59	E7	246	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	$\# Z > 2$
49	2MR	S2	154	49	10,12,13	2.52	2 (20%)	5,13,15	0.92	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
49	2MR	S2	154	49	-	1/10/13/15	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	S2	154	2MR	CZ-NH2	5.52	1.45	1.33
49	S2	154	2MR	CZ-NE	5.16	1.45	1.34

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
49	S2	154	2MR	CG-CD-NE-CZ

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 65 ligands modelled in this entry, 3 are monoatomic - leaving 62 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	$\# Z > 2$
63	PC1	E8	303	-	32,32,53	0.36	0	38,40,61	0.37	0
64	CDL	N5	603	-	69,69,99	0.35	0	75,81,111	0.30	0
70	FMN	V1	579	-	33,33,33	0.27	0	48,50,50	0.33	0
63	PC1	A9	560	-	32,32,53	0.37	0	38,40,61	0.35	0
64	CDL	A3	201	-	57,57,99	0.38	0	63,69,111	0.34	0
64	CDL	AM	217	-	71,71,99	0.35	0	77,83,111	0.33	0
63	PC1	E8	304	-	29,29,53	0.38	0	35,37,61	0.35	0
61	SF4	1A	402	1	0,12,12	-	-	-	-	-
66	ZMP	AB	150	13	30,35,36	0.69	1 (3%)	34,42,45	0.88	1 (2%)
64	CDL	N5	608	-	92,92,99	0.31	0	98,104,111	0.30	0
63	PC1	B5	202	-	53,53,53	0.29	0	59,61,61	0.32	0
63	PC1	N5	605	-	40,40,53	0.33	0	46,48,61	0.30	0
61	SF4	S8	298	55	0,12,12	-	-	-	-	-
64	CDL	C4	202	-	93,93,99	0.31	0	99,105,111	0.30	0
63	PC1	ED	201	-	53,53,53	0.29	0	59,61,61	0.30	0
67	3PE	G1	516	-	39,39,50	0.34	0	42,44,55	0.32	0
63	PC1	A1	203	-	30,30,53	0.37	0	36,38,61	0.36	0
71	NAI	V1	581	-	47,48,48	0.28	0	64,73,73	0.32	0
63	PC1	N2	301	-	36,36,53	0.34	0	42,44,61	0.38	0
63	PC1	E8	301	-	53,53,53	0.30	0	59,61,61	0.33	0
66	ZMP	AC	201	14	30,35,36	0.68	1 (3%)	34,42,45	0.76	0
61	SF4	S7	301	54	0,12,12	-	-	-	-	-
64	CDL	AL	304	-	69,69,99	0.35	0	75,81,111	0.32	0
63	PC1	N1	702	-	39,39,53	0.33	0	45,47,61	0.34	0
64	CDL	B3	102	-	64,64,99	0.37	0	70,76,111	0.34	0
63	PC1	N1	701	-	48,48,53	0.30	0	54,56,61	0.29	0
63	PC1	AN	301	-	47,47,53	0.31	0	53,55,61	0.31	0
63	PC1	N4	502	-	38,38,53	0.34	0	44,46,61	0.33	0
63	PC1	N4	503	-	32,32,53	0.36	0	38,40,61	0.37	0
64	CDL	EA	201	-	58,58,99	0.38	0	64,70,111	0.35	0
63	PC1	A1	202	-	48,48,53	0.31	0	54,56,61	0.33	0
64	CDL	EA	202	-	54,54,99	0.39	0	60,66,111	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
63	PC1	AM	220	-	47,47,53	0.31	0	53,55,61	0.27	0
60	FES	1A	401	1	0,4,4	-	-	-		
63	PC1	E4	401	-	50,50,53	0.30	0	56,58,61	0.33	0
63	PC1	AM	218	-	48,48,53	0.31	0	54,56,61	0.30	0
67	3PE	N4	504	-	40,40,50	0.34	0	43,45,55	0.32	0
63	PC1	N5	606	-	35,35,53	0.34	0	41,43,61	0.34	0
64	CDL	N4	501	-	97,97,99	0.30	0	103,109,111	0.28	0
63	PC1	B5	203	-	53,53,53	0.31	0	59,61,61	0.33	0
63	PC1	E8	302	-	53,53,53	0.30	0	59,61,61	0.29	0
61	SF4	V1	580	57	0,12,12	-	-	-		
64	CDL	B5	201	-	57,57,99	0.38	0	63,69,111	0.35	0
64	CDL	AL	302	-	67,67,99	0.36	0	73,79,111	0.34	0
63	PC1	C4	203	-	37,37,53	0.34	0	43,45,61	0.31	0
63	PC1	N3	301	-	41,41,53	0.33	0	47,49,61	0.33	0
61	SF4	S8	297	55	0,12,12	-	-	-		
64	CDL	AL	303	-	63,63,99	0.36	0	69,75,111	0.31	0
63	PC1	N5	601	-	53,53,53	0.29	0	59,61,61	0.30	0
64	CDL	C4	204	-	68,68,99	0.35	0	74,80,111	0.33	0
63	PC1	AL	301	-	49,49,53	0.31	0	55,57,61	0.31	0
65	NDP	A9	559	-	51,52,52	0.35	0	71,80,80	0.35	0
67	3PE	AN	302	-	50,50,50	0.30	0	53,55,55	0.29	0
63	PC1	A9	561	-	32,32,53	0.36	0	38,40,61	0.34	0
68	U10	N4	505	-	43,43,63	2.49	20 (46%)	54,55,79	1.73	16 (29%)
64	CDL	E7	301	-	67,67,99	0.36	0	73,79,111	0.31	0
67	3PE	N5	607	-	50,50,50	0.30	0	53,55,55	0.29	0
64	CDL	E6	431	-	63,63,99	0.37	0	69,75,111	0.31	0
64	CDL	AM	216	-	71,71,99	0.35	0	77,83,111	0.37	0
61	SF4	1A	403	1	0,12,12	-	-	-		
60	FES	V2	301	58,57	0,4,4	-	-	-		
64	CDL	AM	215	-	71,71,99	0.35	0	77,83,111	0.31	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
63	PC1	E8	303	-	-	4/36/36/57	-
64	CDL	N5	603	-	-	14/80/80/110	-
70	FMN	V1	579	-	-	2/18/18/18	0/3/3/3
63	PC1	A9	560	-	-	12/36/36/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
64	CDL	A3	201	-	-	11/68/68/110	-
64	CDL	AM	217	-	-	18/82/82/110	-
63	PC1	E8	304	-	-	10/33/33/57	-
61	SF4	1A	402	1	-	-	0/6/5/5
66	ZMP	AB	150	13	-	22/40/42/43	-
64	CDL	N5	608	-	-	18/103/103/110	-
63	PC1	B5	202	-	-	12/57/57/57	-
63	PC1	N5	605	-	-	11/44/44/57	-
64	CDL	C4	202	-	-	19/104/104/110	-
67	3PE	G1	516	-	-	8/43/43/54	-
63	PC1	ED	201	-	-	11/57/57/57	-
71	NAI	V1	581	-	-	8/29/72/72	0/5/5/5
63	PC1	A1	203	-	-	8/34/34/57	-
61	SF4	S8	298	55	-	-	0/6/5/5
63	PC1	N2	301	-	-	15/40/40/57	-
63	PC1	E8	301	-	-	11/57/57/57	-
66	ZMP	AC	201	14	-	19/40/42/43	-
61	SF4	S7	301	54	-	-	0/6/5/5
64	CDL	AL	304	-	-	28/80/80/110	-
63	PC1	N1	702	-	-	10/43/43/57	-
64	CDL	B3	102	-	-	11/75/75/110	-
63	PC1	N1	701	-	-	17/52/52/57	-
63	PC1	AN	301	-	-	11/51/51/57	-
63	PC1	N4	502	-	-	17/42/42/57	-
63	PC1	N4	503	-	-	5/36/36/57	-
64	CDL	EA	201	-	-	11/69/69/110	-
63	PC1	A1	202	-	-	16/52/52/57	-
64	CDL	EA	202	-	-	16/65/65/110	-
63	PC1	AM	220	-	-	8/51/51/57	-
63	PC1	E4	401	-	-	11/54/54/57	-
60	FES	1A	401	1	-	-	0/1/1/1
63	PC1	AM	218	-	-	17/52/52/57	-
67	3PE	N4	504	-	-	11/44/44/54	-
63	PC1	N5	606	-	-	7/39/39/57	-
64	CDL	N4	501	-	-	18/108/108/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
63	PC1	B5	203	-	-	21/57/57/57	-
63	PC1	E8	302	-	-	20/57/57/57	-
64	CDL	B5	201	-	-	12/68/68/110	-
61	SF4	V1	580	57	-	-	0/6/5/5
64	CDL	AL	302	-	-	9/78/78/110	-
63	PC1	C4	203	-	-	6/41/41/57	-
63	PC1	N3	301	-	-	9/45/45/57	-
64	CDL	AL	303	-	-	14/74/74/110	-
64	CDL	C4	204	-	-	11/79/79/110	-
63	PC1	N5	601	-	-	9/57/57/57	-
68	U10	N4	505	-	-	12/39/63/87	0/1/1/1
63	PC1	AL	301	-	-	12/53/53/57	-
65	NDP	A9	559	-	-	6/34/77/77	0/5/5/5
67	3PE	AN	302	-	-	9/54/54/54	-
63	PC1	A9	561	-	-	8/36/36/57	-
61	SF4	S8	297	55	-	-	0/6/5/5
64	CDL	E7	301	-	-	18/78/78/110	-
67	3PE	N5	607	-	-	6/54/54/54	-
64	CDL	E6	431	-	-	23/74/74/110	-
64	CDL	AM	216	-	-	13/82/82/110	-
61	SF4	1A	403	1	-	-	0/6/5/5
60	FES	V2	301	58,57	-	-	0/1/1/1
64	CDL	AM	215	-	-	14/82/82/110	-

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
68	N4	505	U10	C6-C1	10.54	1.54	1.35
68	N4	505	U10	C4-C3	4.73	1.53	1.36
68	N4	505	U10	C7-C8	2.91	1.55	1.50
68	N4	505	U10	C7-C6	2.72	1.56	1.51
68	N4	505	U10	C31-C29	2.64	1.56	1.51
68	N4	505	U10	C16-C14	2.63	1.56	1.51
68	N4	505	U10	C26-C24	2.63	1.56	1.51
68	N4	505	U10	C6-C5	2.63	1.53	1.46
66	AB	150	ZMP	C9-C10	-2.54	1.48	1.50
66	AC	201	ZMP	C9-C10	-2.50	1.48	1.50
68	N4	505	U10	C21-C19	2.44	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
68	N4	505	U10	O5-C5	-2.43	1.18	1.23
68	N4	505	U10	C11-C9	2.32	1.56	1.51
68	N4	505	U10	C27-C28	2.30	1.57	1.50
68	N4	505	U10	O2-C2	-2.21	1.18	1.23
68	N4	505	U10	O3-C3M	-2.15	1.40	1.45
68	N4	505	U10	C22-C23	2.14	1.56	1.50
68	N4	505	U10	C32-C33	2.11	1.56	1.50
68	N4	505	U10	C36-C34	2.10	1.56	1.50
68	N4	505	U10	C17-C18	2.06	1.56	1.50
68	N4	505	U10	O4-C4M	-2.05	1.40	1.45
68	N4	505	U10	C12-C13	2.01	1.56	1.50

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
68	N4	505	U10	C7-C6-C1	-3.87	118.25	124.89
68	N4	505	U10	C7-C8-C9	-3.54	120.73	126.83
68	N4	505	U10	C7-C6-C5	3.54	122.63	118.52
68	N4	505	U10	C15-C14-C16	3.34	121.03	115.23
68	N4	505	U10	C22-C23-C24	-3.04	120.67	127.62
68	N4	505	U10	C30-C29-C31	2.87	120.22	115.23
68	N4	505	U10	C20-C19-C21	2.81	120.10	115.23
68	N4	505	U10	C17-C18-C19	-2.78	121.26	127.62
68	N4	505	U10	C1M-C1-C6	-2.67	120.06	124.45
68	N4	505	U10	C12-C13-C14	-2.61	121.66	127.62
68	N4	505	U10	C25-C24-C26	2.51	119.59	115.23
68	N4	505	U10	C15-C14-C13	-2.45	117.32	123.63
66	AB	150	ZMP	C15-C14-C13	-2.38	108.43	112.39
68	N4	505	U10	C10-C9-C11	2.20	119.05	115.23
68	N4	505	U10	C27-C28-C29	-2.20	122.60	127.62
68	N4	505	U10	C36-C34-C35	2.13	119.48	114.59
68	N4	505	U10	C32-C33-C34	-2.12	120.57	127.64

There are no chirality outliers.

All (679) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
63	A1	202	PC1	C11-O13-P-O11
63	A1	203	PC1	C11-O13-P-O12
63	A1	203	PC1	C11-O13-P-O14
63	A1	203	PC1	C1-O11-P-O12
63	A1	203	PC1	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
63	A9	560	PC1	C1-O11-P-O12
63	A9	560	PC1	C1-O11-P-O14
63	A9	560	PC1	C1-O11-P-O13
63	A9	561	PC1	C11-O13-P-O14
63	A9	561	PC1	C1-O11-P-O12
63	A9	561	PC1	C1-O11-P-O13
63	AM	220	PC1	C1-O11-P-O14
63	AM	220	PC1	C1-O11-P-O13
63	AN	301	PC1	C1-O11-P-O12
63	AN	301	PC1	C1-O11-P-O14
63	AN	301	PC1	C1-O11-P-O13
63	B5	202	PC1	C11-O13-P-O12
63	B5	202	PC1	C11-O13-P-O11
63	B5	203	PC1	C1-O11-P-O12
63	B5	203	PC1	C1-O11-P-O14
63	B5	203	PC1	C1-O11-P-O13
63	C4	203	PC1	C11-O13-P-O11
63	E4	401	PC1	C11-O13-P-O12
63	E4	401	PC1	C11-O13-P-O11
63	E8	301	PC1	C11-O13-P-O11
63	E8	302	PC1	C1-O11-P-O12
63	E8	302	PC1	C1-O11-P-O14
63	E8	302	PC1	C1-O11-P-O13
63	E8	303	PC1	C1-O11-P-O14
63	E8	303	PC1	C1-O11-P-O13
63	E8	304	PC1	C11-O13-P-O14
63	E8	304	PC1	C11-O13-P-O11
63	E8	304	PC1	C1-O11-P-O14
63	E8	304	PC1	C1-O11-P-O13
63	E8	304	PC1	C2-C1-O11-P
63	N1	701	PC1	C1-O11-P-O12
63	N1	701	PC1	C1-O11-P-O14
63	N1	701	PC1	C1-O11-P-O13
63	N1	702	PC1	C1-O11-P-O12
63	N1	702	PC1	C1-O11-P-O14
63	N1	702	PC1	C1-O11-P-O13
63	N1	702	PC1	C2-C1-O11-P
63	N1	702	PC1	O21-C2-C3-O31
63	N2	301	PC1	C1-O11-P-O12
63	N2	301	PC1	C1-O11-P-O14
63	N2	301	PC1	C1-O11-P-O13
63	N3	301	PC1	C11-O13-P-O11

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Mol	Chain	Res	Type	Atoms
63	N4	502	PC1	C11-O13-P-O12
63	N4	502	PC1	C11-O13-P-O14
63	N4	502	PC1	C11-O13-P-O11
63	N4	502	PC1	C1-O11-P-O12
63	N4	502	PC1	C1-O11-P-O14
63	N4	502	PC1	C1-O11-P-O13
63	N5	601	PC1	C11-O13-P-O14
63	N5	601	PC1	C11-O13-P-O11
63	N5	605	PC1	C11-O13-P-O12
63	N5	605	PC1	C11-O13-P-O14
63	N5	605	PC1	C11-O13-P-O11
63	N5	605	PC1	C1-O11-P-O13
63	N5	606	PC1	C11-O13-P-O12
64	A3	201	CDL	CB2-OB2-PB2-OB4
64	A3	201	CDL	CB2-OB2-PB2-OB5
64	AL	303	CDL	CA2-OA2-PA1-OA5
64	AL	303	CDL	OB6-CB4-CB6-OB8
64	AL	304	CDL	CA2-OA2-PA1-OA4
64	AL	304	CDL	CA2-OA2-PA1-OA5
64	AL	304	CDL	CB2-OB2-PB2-OB4
64	AL	304	CDL	CB3-OB5-PB2-OB2
64	AL	304	CDL	CB3-OB5-PB2-OB4
64	AM	215	CDL	CA3-OA5-PA1-OA3
64	AM	215	CDL	CB2-OB2-PB2-OB5
64	AM	215	CDL	CB3-OB5-PB2-OB2
64	AM	215	CDL	CB3-OB5-PB2-OB4
64	AM	216	CDL	CB2-OB2-PB2-OB3
64	AM	216	CDL	CB2-OB2-PB2-OB4
64	AM	216	CDL	CB2-OB2-PB2-OB5
64	AM	217	CDL	CA2-OA2-PA1-OA4
64	AM	217	CDL	CA2-OA2-PA1-OA5
64	AM	217	CDL	CB2-OB2-PB2-OB5
64	B3	102	CDL	CA2-OA2-PA1-OA3
64	B3	102	CDL	CA3-OA5-PA1-OA2
64	B3	102	CDL	CA3-OA5-PA1-OA3
64	B3	102	CDL	CA3-OA5-PA1-OA4
64	B5	201	CDL	CA3-OA5-PA1-OA2
64	B5	201	CDL	CB3-OB5-PB2-OB2
64	B5	201	CDL	CB3-OB5-PB2-OB3
64	B5	201	CDL	CB3-OB5-PB2-OB4
64	C4	202	CDL	CA2-OA2-PA1-OA3
64	C4	202	CDL	CA2-OA2-PA1-OA4

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Mol	Chain	Res	Type	Atoms
64	C4	202	CDL	CA2-OA2-PA1-OA5
64	C4	202	CDL	CA3-OA5-PA1-OA2
64	C4	202	CDL	CA3-OA5-PA1-OA3
64	C4	202	CDL	CA3-OA5-PA1-OA4
64	C4	204	CDL	CA2-OA2-PA1-OA3
64	C4	204	CDL	CA2-OA2-PA1-OA4
64	C4	204	CDL	CA2-OA2-PA1-OA5
64	C4	204	CDL	CA3-OA5-PA1-OA2
64	E6	431	CDL	O1-C1-CA2-OA2
64	E6	431	CDL	CA2-OA2-PA1-OA3
64	E6	431	CDL	CA3-OA5-PA1-OA2
64	E6	431	CDL	CA3-OA5-PA1-OA3
64	E6	431	CDL	CA3-OA5-PA1-OA4
64	E6	431	CDL	CB2-OB2-PB2-OB4
64	E6	431	CDL	CB2-OB2-PB2-OB5
64	E6	431	CDL	CB3-OB5-PB2-OB2
64	E6	431	CDL	CB3-OB5-PB2-OB3
64	E6	431	CDL	CB3-OB5-PB2-OB4
64	EA	201	CDL	CA2-OA2-PA1-OA3
64	EA	201	CDL	CA2-OA2-PA1-OA5
64	EA	201	CDL	C1-CB2-OB2-PB2
64	EA	201	CDL	CB3-OB5-PB2-OB3
64	EA	201	CDL	CB3-OB5-PB2-OB4
64	EA	202	CDL	CB3-OB5-PB2-OB2
64	EA	202	CDL	CB3-OB5-PB2-OB3
64	EA	202	CDL	CB3-OB5-PB2-OB4
64	N4	501	CDL	CA2-OA2-PA1-OA3
64	N4	501	CDL	CA2-OA2-PA1-OA4
64	N4	501	CDL	CA2-OA2-PA1-OA5
64	N5	603	CDL	CA2-OA2-PA1-OA4
64	N5	603	CDL	CA2-OA2-PA1-OA5
64	N5	603	CDL	CA3-OA5-PA1-OA2
64	N5	603	CDL	CA3-OA5-PA1-OA3
64	N5	603	CDL	CA3-OA5-PA1-OA4
64	N5	603	CDL	CB2-OB2-PB2-OB3
64	N5	603	CDL	CB2-OB2-PB2-OB5
64	N5	608	CDL	CA2-OA2-PA1-OA4
64	N5	608	CDL	CA3-OA5-PA1-OA3
64	N5	608	CDL	CB2-OB2-PB2-OB3
64	N5	608	CDL	CB2-OB2-PB2-OB4
64	N5	608	CDL	CB3-OB5-PB2-OB4
64	E7	301	CDL	C1-CA2-OA2-PA1

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Mol	Chain	Res	Type	Atoms
64	E7	301	CDL	CA2-OA2-PA1-OA5
64	E7	301	CDL	CA3-OA5-PA1-OA2
64	E7	301	CDL	CA3-OA5-PA1-OA4
64	E7	301	CDL	OB5-CB3-CB4-OB6
65	A9	559	NDP	C5D-O5D-PN-O3
65	A9	559	NDP	C5D-O5D-PN-O1N
65	A9	559	NDP	C5D-O5D-PN-O2N
65	A9	559	NDP	C2N-C3N-C7N-N7N
66	AB	150	ZMP	O4-C17-C18-C21
66	AB	150	ZMP	C16-C17-C18-C21
66	AB	150	ZMP	C16-C17-C18-C19
66	AB	150	ZMP	C16-C17-C18-C20
66	AB	150	ZMP	S1-C11-C12-N1
66	AB	150	ZMP	O1-C10-S1-C11
66	AB	150	ZMP	C7-C8-C9-C10
66	AC	201	ZMP	C19-C18-C21-O5
66	AC	201	ZMP	C20-C18-C21-O5
66	AC	201	ZMP	C17-C18-C21-O5
67	AN	302	3PE	C11-O13-P-O11
67	AN	302	3PE	C11-O13-P-O14
67	AN	302	3PE	O13-C11-C12-N
67	G1	516	3PE	C1-O11-P-O12
67	G1	516	3PE	C1-O11-P-O13
67	N4	504	3PE	C11-O13-P-O11
67	N4	504	3PE	C11-O13-P-O12
67	N4	504	3PE	C11-O13-P-O14
67	N5	607	3PE	C1-O11-P-O12
67	N5	607	3PE	C1-O11-P-O13
67	N5	607	3PE	C1-O11-P-O14
68	N4	505	U10	C1-C6-C7-C8
68	N4	505	U10	C5-C6-C7-C8
70	V1	579	FMN	N10-C1'-C2'-O2'
70	V1	579	FMN	N10-C1'-C2'-C3'
71	V1	581	NAI	C5D-O5D-PN-O3
71	V1	581	NAI	C5D-O5D-PN-O1N
71	V1	581	NAI	O4D-C4D-C5D-O5D
71	V1	581	NAI	C3D-C4D-C5D-O5D
68	N4	505	U10	C30-C29-C31-C32
68	N4	505	U10	C28-C29-C31-C32
66	AB	150	ZMP	C14-C13-N1-C12
66	AC	201	ZMP	C14-C13-N1-C12
64	A3	201	CDL	C1-CA2-OA2-PA1

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Mol	Chain	Res	Type	Atoms
66	AB	150	ZMP	O2-C13-N1-C12
66	AC	201	ZMP	O2-C13-N1-C12
64	AL	304	CDL	CB2-C1-CA2-OA2
64	E6	431	CDL	CB2-C1-CA2-OA2
66	AC	201	ZMP	C3-C4-C5-C6
64	AL	304	CDL	O1-C1-CA2-OA2
66	AC	201	ZMP	C5-C6-C7-C8
64	A3	201	CDL	CA5-C11-C12-C13
64	B3	102	CDL	CA7-C31-C32-C33
64	AM	215	CDL	OB5-CB3-CB4-OB6
63	B5	202	PC1	C31-C32-C33-C34
63	B5	202	PC1	C21-C22-C23-C24
64	N4	501	CDL	CA5-C11-C12-C13
64	AM	217	CDL	CB5-C51-C52-C53
67	G1	516	3PE	C21-C22-C23-C24
71	V1	581	NAI	C2D-C1D-N1N-C2N
64	AL	302	CDL	CB5-C51-C52-C53
71	V1	581	NAI	C2D-C1D-N1N-C6N
66	AB	150	ZMP	C6-C7-C8-C9
63	AM	218	PC1	C25-C26-C27-C28
64	AL	304	CDL	C11-C12-C13-C14
66	AC	201	ZMP	C2-C1-C22-C23
66	AC	201	ZMP	S1-C11-C12-N1
63	AM	218	PC1	C24-C25-C26-C27
63	N3	301	PC1	C26-C27-C28-C29
66	AB	150	ZMP	C1-C22-C23-C24
64	B3	102	CDL	C51-C52-C53-C54
63	N5	601	PC1	C32-C33-C34-C35
64	AL	302	CDL	C32-C33-C34-C35
63	ED	201	PC1	C24-C25-C26-C27
66	AC	201	ZMP	C1-C22-C23-C24
67	G1	516	3PE	C29-C2A-C2B-C2C
66	AB	150	ZMP	C22-C1-C2-C3
63	ED	201	PC1	C11-C12-N-C14
63	AM	220	PC1	C23-C24-C25-C26
63	N5	605	PC1	C21-C22-C23-C24
64	N5	608	CDL	CB5-C51-C52-C53
63	B5	202	PC1	C2-C1-O11-P
63	AM	220	PC1	C2C-C2D-C2E-C2F
64	B5	201	CDL	CA5-C11-C12-C13
64	N4	501	CDL	C19-C20-C21-C22
64	N4	501	CDL	C78-C79-C80-C81

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Mol	Chain	Res	Type	Atoms
66	AB	150	ZMP	C3-C4-C5-C6
66	AC	201	ZMP	C2-C3-C4-C5
63	AM	218	PC1	C3C-C3D-C3E-C3F
63	A1	202	PC1	C31-C32-C33-C34
63	B5	203	PC1	C2C-C2D-C2E-C2F
64	AM	216	CDL	C37-C38-C39-C40
64	AL	302	CDL	O1-C1-CA2-OA2
63	E4	401	PC1	C33-C34-C35-C36
64	AL	302	CDL	C35-C36-C37-C38
66	AB	150	ZMP	C2-C3-C4-C5
63	N2	301	PC1	C27-C28-C29-C2A
64	AL	303	CDL	C51-C52-C53-C54
63	AL	301	PC1	C11-C12-N-C14
63	E4	401	PC1	C11-C12-N-C13
63	N3	301	PC1	C11-C12-N-C15
64	B5	201	CDL	C55-C56-C57-C58
64	A3	201	CDL	CB7-C71-C72-C73
64	C4	204	CDL	C11-C12-C13-C14
63	N1	701	PC1	C2B-C2C-C2D-C2E
64	AL	304	CDL	C13-C14-C15-C16
64	C4	204	CDL	CA5-C11-C12-C13
63	B5	203	PC1	O21-C2-C3-O31
63	N5	601	PC1	C22-C23-C24-C25
64	AL	302	CDL	CB4-CB3-OB5-PB2
63	N1	701	PC1	C37-C38-C39-C3A
64	B3	102	CDL	O1-C1-CB2-OB2
64	AL	304	CDL	C14-C15-C16-C17
64	N5	608	CDL	C42-C43-C44-C45
63	A9	561	PC1	C32-C33-C34-C35
64	AM	217	CDL	C33-C34-C35-C36
64	C4	202	CDL	C61-C62-C63-C64
67	N5	607	3PE	C22-C23-C24-C25
66	AC	201	ZMP	O3-C16-C17-O4
63	N5	601	PC1	C23-C24-C25-C26
67	N5	607	3PE	C35-C36-C37-C38
64	C4	202	CDL	OB5-CB3-CB4-CB6
64	E7	301	CDL	OA5-CA3-CA4-CA6
63	B5	203	PC1	C2E-C2F-C2G-C2H
63	AM	218	PC1	C39-C3A-C3B-C3C
64	N5	608	CDL	CA7-C31-C32-C33
63	AN	301	PC1	C35-C36-C37-C38
63	N1	701	PC1	C2C-C2D-C2E-C2F

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Mol	Chain	Res	Type	Atoms
64	A3	201	CDL	C52-C53-C54-C55
64	B5	201	CDL	C71-C72-C73-C74
63	A9	560	PC1	C1-C2-C3-O31
63	B5	203	PC1	C1-C2-C3-O31
63	E4	401	PC1	C1-C2-C3-O31
63	N1	702	PC1	C1-C2-C3-O31
63	N3	301	PC1	C1-C2-C3-O31
63	N4	502	PC1	C1-C2-C3-O31
64	E7	301	CDL	CB3-CB4-CB6-OB8
63	AM	220	PC1	C27-C28-C29-C2A
64	EA	202	CDL	C53-C54-C55-C56
63	B5	202	PC1	C26-C27-C28-C29
64	N4	501	CDL	C53-C54-C55-C56
66	AB	150	ZMP	C4-C5-C6-C7
63	ED	201	PC1	C11-C12-N-C15
63	N3	301	PC1	C11-C12-N-C14
63	A9	560	PC1	C2-C1-O11-P
63	N1	702	PC1	C27-C28-C29-C2A
67	N4	504	3PE	C22-C23-C24-C25
63	E8	301	PC1	C31-C32-C33-C34
63	A9	560	PC1	C2-C3-O31-C31
63	AM	220	PC1	C31-C32-C33-C34
63	E8	302	PC1	O11-C1-C2-O21
64	C4	202	CDL	OA5-CA3-CA4-OA6
64	C4	202	CDL	OB5-CB3-CB4-OB6
64	C4	202	CDL	C51-C52-C53-C54
64	C4	202	CDL	C59-C60-C61-C62
64	EA	202	CDL	O1-C1-CA2-OA2
63	E4	401	PC1	C11-C12-N-C14
63	ED	201	PC1	C11-C12-N-C13
64	C4	202	CDL	C72-C71-CB7-OB8
63	AM	218	PC1	C37-C38-C39-C3A
66	AB	150	ZMP	C22-C23-C24-C25
63	E8	302	PC1	C22-C23-C24-C25
63	N2	301	PC1	C24-C25-C26-C27
63	C4	203	PC1	C2-C1-O11-P
63	N3	301	PC1	C2-C1-O11-P
64	AM	216	CDL	C31-C32-C33-C34
64	E6	431	CDL	C15-C16-C17-C18
66	AC	201	ZMP	C22-C23-C24-C25
64	AL	304	CDL	OB5-CB3-CB4-CB6
64	AM	215	CDL	OB5-CB3-CB4-CB6

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Mol	Chain	Res	Type	Atoms
64	AM	217	CDL	OA5-CA3-CA4-CA6
63	N1	701	PC1	O31-C31-C32-C33
64	N4	501	CDL	C83-C84-C85-C86
63	ED	201	PC1	C28-C29-C2A-C2B
63	AL	301	PC1	C11-C12-N-C15
63	N5	605	PC1	C11-C12-N-C13
66	AB	150	ZMP	N2-C16-C17-C18
64	A3	201	CDL	C71-C72-C73-C74
63	E4	401	PC1	C28-C29-C2A-C2B
63	B5	203	PC1	C3B-C3C-C3D-C3E
67	AN	302	3PE	C27-C28-C29-C2A
63	ED	201	PC1	C21-C22-C23-C24
64	B3	102	CDL	CA2-C1-CB2-OB2
64	AL	302	CDL	CA3-CA4-CA6-OA8
64	AL	303	CDL	CB3-CB4-CB6-OB8
64	AL	304	CDL	CB3-CB4-CB6-OB8
64	AM	216	CDL	CA3-CA4-CA6-OA8
64	E6	431	CDL	CB3-CB4-CB6-OB8
64	EA	201	CDL	CB3-CB4-CB6-OB8
63	N5	601	PC1	C31-C32-C33-C34
63	B5	202	PC1	O11-C1-C2-O21
64	AM	217	CDL	OA5-CA3-CA4-OA6
64	C4	204	CDL	OB5-CB3-CB4-OB6
64	N4	501	CDL	C34-C35-C36-C37
63	E4	401	PC1	O21-C2-C3-O31
63	N4	502	PC1	O21-C2-C3-O31
64	AL	302	CDL	OA6-CA4-CA6-OA8
64	N4	501	CDL	CA7-C31-C32-C33
64	N5	608	CDL	C17-C18-C19-C20
64	C4	202	CDL	CB7-C71-C72-C73
64	EA	202	CDL	CB7-C71-C72-C73
63	N1	702	PC1	C22-C23-C24-C25
63	N4	502	PC1	C35-C36-C37-C38
63	B5	203	PC1	C27-C28-C29-C2A
63	B5	202	PC1	C24-C25-C26-C27
63	E8	302	PC1	C11-C12-N-C14
63	N3	301	PC1	C11-C12-N-C13
64	AL	304	CDL	CB5-C51-C52-C53
66	AB	150	ZMP	C9-C10-S1-C11
63	B5	202	PC1	O11-C1-C2-C3
64	EA	202	CDL	OB5-CB3-CB4-CB6
64	E7	301	CDL	OB5-CB3-CB4-CB6

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Mol	Chain	Res	Type	Atoms
63	E8	302	PC1	C39-C3A-C3B-C3C
63	A1	202	PC1	C22-C23-C24-C25
63	N5	605	PC1	C11-C12-N-C15
64	N5	603	CDL	C54-C55-C56-C57
64	AL	304	CDL	OB5-CB3-CB4-OB6
64	N5	603	CDL	OB5-CB3-CB4-OB6
64	AM	217	CDL	CA3-CA4-CA6-OA8
63	E8	304	PC1	C12-C11-O13-P
67	N4	504	3PE	C12-C11-O13-P
63	AM	218	PC1	O21-C2-C3-O31
63	N3	301	PC1	O21-C2-C3-O31
64	E6	431	CDL	OB6-CB4-CB6-OB8
63	E8	302	PC1	C11-C12-N-C13
63	ED	201	PC1	C25-C26-C27-C28
65	A9	559	NDP	O4D-C1D-N1N-C6N
63	AN	301	PC1	C24-C25-C26-C27
63	A9	560	PC1	O13-C11-C12-N
63	A9	561	PC1	O13-C11-C12-N
63	AN	301	PC1	O13-C11-C12-N
63	E8	301	PC1	O13-C11-C12-N
63	E8	303	PC1	O13-C11-C12-N
63	E8	304	PC1	O13-C11-C12-N
63	N1	702	PC1	O13-C11-C12-N
63	N2	301	PC1	O13-C11-C12-N
63	N4	502	PC1	O13-C11-C12-N
63	N4	503	PC1	O13-C11-C12-N
63	N5	606	PC1	O13-C11-C12-N
64	N4	501	CDL	C16-C17-C18-C19
67	AN	302	3PE	C38-C39-C3A-C3B
63	AL	301	PC1	C11-C12-N-C13
63	E4	401	PC1	C11-C12-N-C15
63	N1	701	PC1	C11-C12-N-C15
66	AB	150	ZMP	O3-C16-C17-O4
63	N2	301	PC1	C31-C32-C33-C34
71	V1	581	NAI	O4D-C1D-N1N-C2N
71	V1	581	NAI	O4D-C1D-N1N-C6N
64	N4	501	CDL	C38-C39-C40-C41
63	N1	701	PC1	O11-C1-C2-C3
64	C4	202	CDL	OA5-CA3-CA4-CA6
64	N5	603	CDL	OB5-CB3-CB4-CB6
64	C4	202	CDL	C38-C39-C40-C41
64	AM	215	CDL	C56-C57-C58-C59

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Mol	Chain	Res	Type	Atoms
63	AM	218	PC1	C31-C32-C33-C34
64	E7	301	CDL	C72-C73-C74-C75
63	AL	301	PC1	C2-C1-O11-P
63	N5	606	PC1	C2-C1-O11-P
64	EA	202	CDL	C1-CA2-OA2-PA1
63	N1	701	PC1	O11-C1-C2-O21
64	EA	202	CDL	OB5-CB3-CB4-OB6
64	E7	301	CDL	OA5-CA3-CA4-OA6
63	A1	202	PC1	C11-C12-N-C13
63	B5	203	PC1	C11-C12-N-C13
63	N1	701	PC1	C11-C12-N-C13
63	N2	301	PC1	C11-C12-N-C13
63	B5	203	PC1	C24-C25-C26-C27
63	N2	301	PC1	C25-C26-C27-C28
63	A9	560	PC1	O21-C2-C3-O31
63	AL	301	PC1	O21-C2-C3-O31
64	AL	304	CDL	OB6-CB4-CB6-OB8
64	AM	216	CDL	OA6-CA4-CA6-OA8
64	EA	201	CDL	OB6-CB4-CB6-OB8
64	E7	301	CDL	OB6-CB4-CB6-OB8
63	AL	301	PC1	C1-C2-C3-O31
63	A9	560	PC1	C32-C33-C34-C35
63	A1	203	PC1	C21-C22-C23-C24
68	N4	505	U10	C2-C3-O3-C3M
63	N1	702	PC1	C33-C34-C35-C36
63	A1	202	PC1	C11-O13-P-O14
63	A1	202	PC1	C1-O11-P-O12
63	A1	202	PC1	C1-O11-P-O14
63	A1	202	PC1	C1-O11-P-O13
63	A1	202	PC1	C11-C12-N-C14
63	A1	203	PC1	C11-O13-P-O11
63	A9	561	PC1	C11-O13-P-O11
63	AL	301	PC1	C1-O11-P-O14
63	AM	220	PC1	C1-O11-P-O12
63	B5	203	PC1	C11-C12-N-C15
63	C4	203	PC1	C11-O13-P-O14
63	E8	301	PC1	C11-O13-P-O14
63	E8	303	PC1	C11-O13-P-O14
63	E8	304	PC1	C11-O13-P-O12
63	N3	301	PC1	C11-O13-P-O14
63	N4	503	PC1	C1-O11-P-O14
63	N5	601	PC1	C11-O13-P-O12

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Mol	Chain	Res	Type	Atoms
63	N5	605	PC1	C1-O11-P-O14
63	N5	605	PC1	C11-C12-N-C14
63	N5	606	PC1	C11-O13-P-O14
63	N5	606	PC1	C11-O13-P-O11
64	A3	201	CDL	CB2-OB2-PB2-OB3
64	A3	201	CDL	CB3-OB5-PB2-OB3
64	AL	303	CDL	CA2-OA2-PA1-OA3
64	AL	303	CDL	CA3-OA5-PA1-OA3
64	AL	304	CDL	CA3-OA5-PA1-OA3
64	AL	304	CDL	CB2-OB2-PB2-OB3
64	AL	304	CDL	CB2-OB2-PB2-OB5
64	AM	215	CDL	CA3-OA5-PA1-OA2
64	AM	215	CDL	CB2-OB2-PB2-OB3
64	B5	201	CDL	CA3-OA5-PA1-OA3
64	C4	204	CDL	CA3-OA5-PA1-OA3
64	C4	204	CDL	CB2-OB2-PB2-OB3
64	EA	201	CDL	CB3-OB5-PB2-OB2
64	EA	202	CDL	CA2-OA2-PA1-OA4
64	N5	603	CDL	CB2-OB2-PB2-OB4
64	N5	608	CDL	CA2-OA2-PA1-OA3
64	N5	608	CDL	CA2-OA2-PA1-OA5
64	N5	608	CDL	CB2-OB2-PB2-OB5
64	N5	608	CDL	CB3-OB5-PB2-OB2
64	E7	301	CDL	CA2-OA2-PA1-OA3
65	A9	559	NDP	C5B-O5B-PA-O1A
67	G1	516	3PE	C11-O13-P-O14
64	AM	217	CDL	C36-C37-C38-C39
64	AL	302	CDL	C32-C31-CA7-OA8
67	N4	504	3PE	C36-C37-C38-C39
63	AM	218	PC1	C2-C1-O11-P
64	AL	303	CDL	CA4-CA3-OA5-PA1
64	AL	304	CDL	C1-CA2-OA2-PA1
64	E6	431	CDL	CA4-CA3-OA5-PA1
64	N4	501	CDL	CA4-CA3-OA5-PA1
67	N5	607	3PE	C2C-C2D-C2E-C2F
63	B5	203	PC1	C21-C22-C23-C24
63	B5	203	PC1	C38-C39-C3A-C3B
63	AL	301	PC1	C3-C2-O21-C21
63	AN	301	PC1	C1-C2-O21-C21
64	AM	217	CDL	CB6-CB4-OB6-CB5
68	N4	505	U10	C9-C11-C12-C13
63	N2	301	PC1	C11-C12-N-C14

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Mol	Chain	Res	Type	Atoms
64	C4	204	CDL	OB5-CB3-CB4-CB6
63	E8	302	PC1	C2D-C2E-C2F-C2G
64	AL	304	CDL	C31-C32-C33-C34
63	A1	202	PC1	C25-C26-C27-C28
64	AM	216	CDL	C71-C72-C73-C74
64	N5	608	CDL	CB4-CB3-OB5-PB2
64	AM	217	CDL	O1-C1-CB2-OB2
67	AN	302	3PE	C34-C35-C36-C37
64	AL	304	CDL	CA7-C31-C32-C33
63	AL	301	PC1	C28-C29-C2A-C2B
67	N4	504	3PE	O31-C31-C32-C33
66	AB	150	ZMP	O4-C17-C18-C20
63	N5	605	PC1	C24-C25-C26-C27
64	E7	301	CDL	C32-C33-C34-C35
63	E8	302	PC1	C2A-C2B-C2C-C2D
66	AC	201	ZMP	O3-C16-C17-C18
63	E4	401	PC1	C21-C22-C23-C24
63	E8	301	PC1	C27-C28-C29-C2A
63	E8	302	PC1	O11-C1-C2-C3
64	N4	501	CDL	C22-C23-C24-C25
64	N5	603	CDL	C58-C59-C60-C61
64	N5	608	CDL	C81-C82-C83-C84
63	N1	701	PC1	C23-C24-C25-C26
63	A1	202	PC1	C24-C25-C26-C27
66	AC	201	ZMP	N2-C16-C17-C18
64	C4	202	CDL	C72-C71-CB7-OB9
63	AM	218	PC1	C35-C36-C37-C38
63	A9	560	PC1	C22-C23-C24-C25
63	A1	202	PC1	C11-C12-N-C15
63	B5	203	PC1	C11-C12-N-C14
63	E8	302	PC1	C11-C12-N-C15
63	N1	701	PC1	C11-C12-N-C14
63	B5	203	PC1	C35-C36-C37-C38
64	N5	608	CDL	C58-C59-C60-C61
66	AB	150	ZMP	N2-C16-C17-O4
63	A9	560	PC1	C1-C2-O21-C21
63	AM	218	PC1	C3-C2-O21-C21
63	N4	502	PC1	C3-C2-O21-C21
64	AM	217	CDL	CA3-CA4-OA6-CA5
64	AM	217	CDL	CB3-CB4-OB6-CB5
64	E6	431	CDL	CA6-CA4-OA6-CA5
64	E6	431	CDL	CB6-CB4-OB6-CB5

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Mol	Chain	Res	Type	Atoms
64	E7	301	CDL	C75-C76-C77-C78
64	AL	303	CDL	C73-C74-C75-C76
63	N2	301	PC1	C11-C12-N-C15
68	N4	505	U10	C4-C3-O3-C3M
63	N4	503	PC1	C2-C1-O11-P
64	AL	303	CDL	C1-CA2-OA2-PA1
67	G1	516	3PE	C25-C26-C27-C28
63	N1	701	PC1	C2A-C2B-C2C-C2D
64	AM	216	CDL	OB6-CB4-CB6-OB8
64	AM	217	CDL	OA6-CA4-CA6-OA8
64	E6	431	CDL	OA6-CA4-CA6-OA8
64	AL	302	CDL	C72-C73-C74-C75
63	E8	301	PC1	C24-C25-C26-C27
68	N4	505	U10	C5-C4-O4-C4M
64	AM	217	CDL	C52-C51-CB5-OB6
67	AN	302	3PE	C29-C2A-C2B-C2C
64	AM	216	CDL	C1-CB2-OB2-PB2
64	E6	431	CDL	C1-CB2-OB2-PB2
64	C4	202	CDL	C19-C20-C21-C22
63	ED	201	PC1	C3B-C3C-C3D-C3E
63	B5	203	PC1	C2A-C2B-C2C-C2D
63	E8	301	PC1	C29-C2A-C2B-C2C
63	AM	218	PC1	C1-C2-C3-O31
68	N4	505	U10	C24-C26-C27-C28
63	E8	301	PC1	C39-C3A-C3B-C3C
63	AM	220	PC1	O31-C31-C32-C33
63	B5	202	PC1	C3B-C3C-C3D-C3E
64	AL	304	CDL	C12-C13-C14-C15
64	N4	501	CDL	C76-C77-C78-C79
64	N4	501	CDL	C54-C55-C56-C57
63	N1	701	PC1	O32-C31-C32-C33
63	ED	201	PC1	C22-C23-C24-C25
64	AM	216	CDL	OB5-CB3-CB4-CB6
64	C4	204	CDL	C1-CA2-OA2-PA1
67	AN	302	3PE	C2B-C2C-C2D-C2E
64	A3	201	CDL	C11-C12-C13-C14
63	N4	502	PC1	C33-C34-C35-C36
63	AN	301	PC1	C3A-C3B-C3C-C3D
67	AN	302	3PE	C2C-C2D-C2E-C2F
63	E8	302	PC1	C3C-C3D-C3E-C3F
64	N4	501	CDL	C80-C81-C82-C83
63	C4	203	PC1	C11-C12-N-C15

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Mol	Chain	Res	Type	Atoms
63	A1	202	PC1	C1-C2-O21-C21
63	N2	301	PC1	C1-C2-O21-C21
64	AL	304	CDL	CB6-CB4-OB6-CB5
68	N4	505	U10	C26-C27-C28-C29
64	E6	431	CDL	C1-CA2-OA2-PA1
64	EA	201	CDL	CB4-CB3-OB5-PB2
64	E6	431	CDL	OA5-CA3-CA4-OA6
64	N5	603	CDL	CA7-C31-C32-C33
64	AM	215	CDL	C63-C64-C65-C66
64	AL	303	CDL	C54-C55-C56-C57
66	AC	201	ZMP	C16-C17-C18-C20
63	B5	203	PC1	C34-C35-C36-C37
63	E8	302	PC1	C2C-C2D-C2E-C2F
63	ED	201	PC1	C34-C35-C36-C37
63	B5	203	PC1	C2B-C2C-C2D-C2E
64	B3	102	CDL	C32-C31-CA7-OA8
63	AN	301	PC1	O11-C1-C2-C3
63	N5	605	PC1	O11-C1-C2-C3
64	E6	431	CDL	OB5-CB3-CB4-CB6
63	ED	201	PC1	C2A-C2B-C2C-C2D
63	E8	304	PC1	C11-C12-N-C15
64	AM	217	CDL	C72-C71-CB7-OB8
64	AL	303	CDL	C12-C11-CA5-OA6
64	AL	303	CDL	C72-C73-C74-C75
64	EA	202	CDL	C12-C11-CA5-OA6
63	AM	218	PC1	O31-C31-C32-C33
63	C4	203	PC1	C11-C12-N-C13
67	G1	516	3PE	C24-C25-C26-C27
66	AC	201	ZMP	C1-C2-C3-C4
64	EA	202	CDL	C52-C51-CB5-OB6
64	E7	301	CDL	C12-C11-CA5-OA6
67	N4	504	3PE	O21-C21-C22-C23
66	AB	150	ZMP	O3-C16-C17-C18
63	E8	302	PC1	C35-C36-C37-C38
64	N5	608	CDL	C18-C19-C20-C21
63	B5	203	PC1	C25-C26-C27-C28
63	A1	203	PC1	O31-C31-C32-C33
63	A9	561	PC1	O31-C31-C32-C33
63	E8	302	PC1	O31-C31-C32-C33
63	N5	606	PC1	C35-C36-C37-C38
63	E8	301	PC1	O21-C21-C22-C23
63	N4	503	PC1	O31-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
63	N5	606	PC1	C22-C23-C24-C25
63	N1	701	PC1	O21-C21-C22-C23
63	N4	502	PC1	O31-C31-C32-C33
63	N5	601	PC1	O21-C21-C22-C23
64	AL	304	CDL	C72-C71-CB7-OB8
64	AM	215	CDL	C12-C11-CA5-OA6
64	B5	201	CDL	C32-C31-CA7-OA8
64	EA	201	CDL	C72-C71-CB7-OB8
64	E7	301	CDL	C32-C31-CA7-OA8
64	A3	201	CDL	OB6-CB4-CB6-OB8
63	B5	203	PC1	C36-C37-C38-C39
64	N5	603	CDL	C59-C60-C61-C62
66	AC	201	ZMP	C16-C17-C18-C21
63	E8	301	PC1	C35-C36-C37-C38
63	E8	302	PC1	C24-C25-C26-C27
63	A1	202	PC1	C3-C2-O21-C21
63	A9	560	PC1	C3-C2-O21-C21
63	AM	218	PC1	C1-C2-O21-C21
63	B5	202	PC1	C1-C2-O21-C21
63	N2	301	PC1	C3-C2-O21-C21
64	AL	304	CDL	CB3-CB4-OB6-CB5
64	AM	216	CDL	CA6-CA4-OA6-CA5
64	AM	217	CDL	CA6-CA4-OA6-CA5
63	AM	218	PC1	C11-C12-N-C13
68	N4	505	U10	C3-C4-O4-C4M
63	N4	502	PC1	O21-C21-C22-C23
64	AL	304	CDL	C12-C11-CA5-OA6
67	N4	504	3PE	C28-C29-C2A-C2B
63	N2	301	PC1	O21-C21-C22-C23
63	AM	218	PC1	O32-C31-C32-C33
63	E8	302	PC1	C3A-C3B-C3C-C3D
63	A1	202	PC1	C2-C1-O11-P
64	EA	202	CDL	C12-C11-CA5-OA7
64	AM	215	CDL	C52-C51-CB5-OB6
64	B5	201	CDL	C12-C11-CA5-OA6
63	E8	302	PC1	C3D-C3E-C3F-C3G
63	N2	301	PC1	C33-C34-C35-C36
63	AN	301	PC1	O11-C1-C2-O21
63	AL	301	PC1	C27-C28-C29-C2A
68	N4	505	U10	C11-C12-C13-C14
64	E7	301	CDL	C12-C11-CA5-OA7
63	E8	304	PC1	C11-C12-N-C13

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Mol	Chain	Res	Type	Atoms
63	E4	401	PC1	C22-C23-C24-C25
64	B3	102	CDL	C16-C17-C18-C19
63	A1	203	PC1	O32-C31-C32-C33
64	AL	303	CDL	C12-C11-CA5-OA7
64	B3	102	CDL	C32-C31-CA7-OA9
64	EA	202	CDL	C52-C51-CB5-OB7
63	AM	218	PC1	C3D-C3E-C3F-C3G
64	N4	501	CDL	C73-C74-C75-C76
63	N4	502	PC1	C31-C32-C33-C34
63	A9	561	PC1	O32-C31-C32-C33
63	AL	301	PC1	C2A-C2B-C2C-C2D
64	AM	216	CDL	C42-C43-C44-C45
64	AM	215	CDL	C72-C71-CB7-OB8
64	EA	202	CDL	C32-C31-CA7-OA8
63	N5	601	PC1	O22-C21-C22-C23
64	AM	217	CDL	C72-C71-CB7-OB9
67	N4	504	3PE	O22-C21-C22-C23
64	E6	431	CDL	C57-C58-C59-C60
67	G1	516	3PE	O31-C31-C32-C33
64	AL	303	CDL	CB7-C71-C72-C73
63	AL	301	PC1	C2D-C2E-C2F-C2G
63	B5	202	PC1	C3A-C3B-C3C-C3D
66	AC	201	ZMP	N2-C16-C17-O4
63	E8	301	PC1	O22-C21-C22-C23
63	E8	302	PC1	O32-C31-C32-C33
63	N1	701	PC1	O22-C21-C22-C23
63	N4	502	PC1	O22-C21-C22-C23
64	EA	201	CDL	C72-C71-CB7-OB9
64	B5	201	CDL	C1-CA2-OA2-PA1
63	AN	301	PC1	O31-C31-C32-C33
63	C4	203	PC1	C11-C12-N-C14
63	N4	502	PC1	O32-C31-C32-C33
64	AM	215	CDL	C12-C11-CA5-OA7
64	AL	304	CDL	C72-C71-CB7-OB9
63	A1	202	PC1	C21-C22-C23-C24
64	N5	608	CDL	C12-C11-CA5-OA6
64	C4	202	CDL	C17-C18-C19-C20
63	N4	503	PC1	O32-C31-C32-C33
64	EA	202	CDL	C32-C31-CA7-OA9
64	AL	304	CDL	C12-C11-CA5-OA7
64	B5	201	CDL	C12-C11-CA5-OA7
64	E7	301	CDL	C32-C31-CA7-OA9

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Mol	Chain	Res	Type	Atoms
63	AM	218	PC1	C27-C28-C29-C2A
67	N4	504	3PE	C35-C36-C37-C38

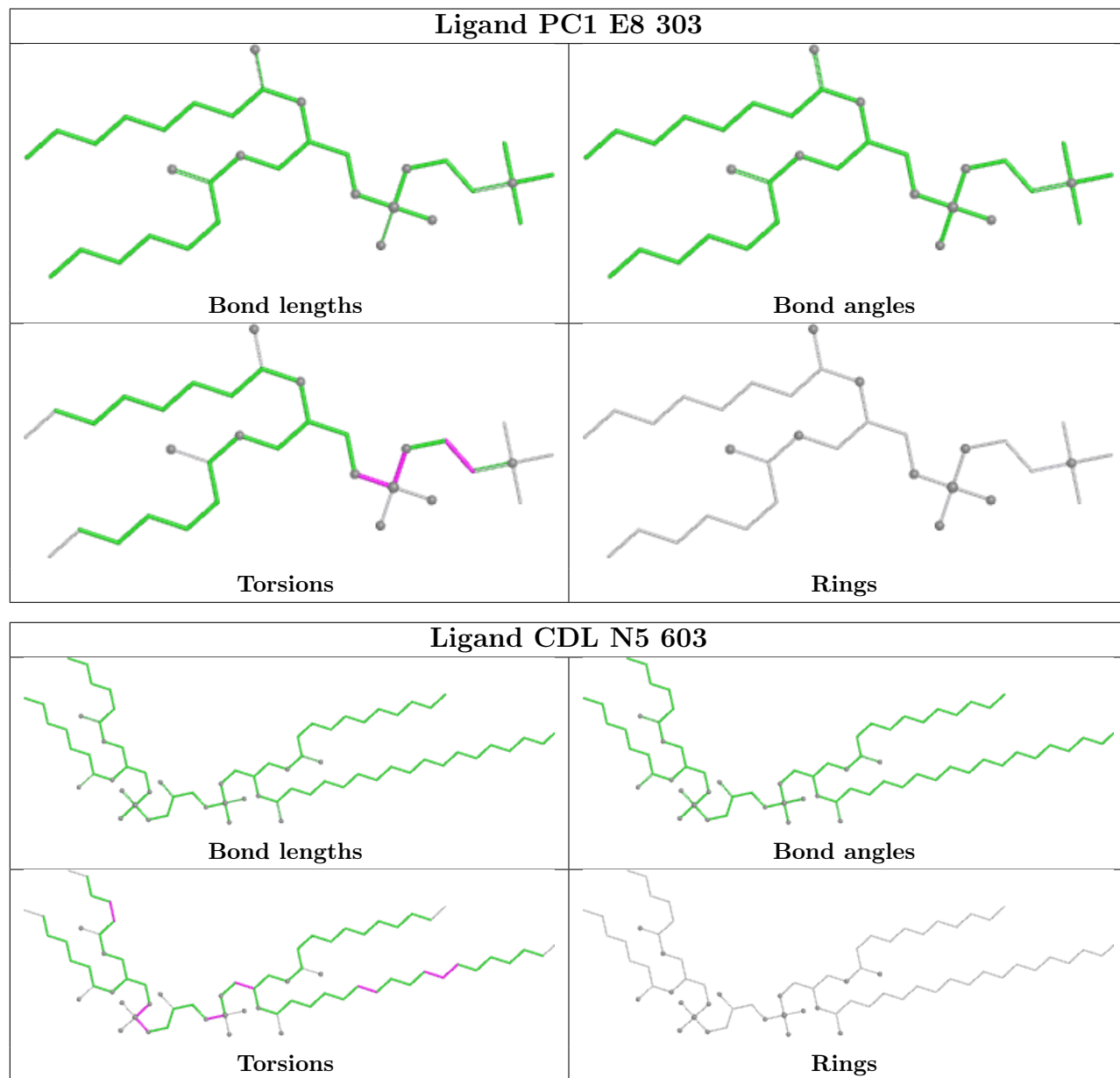
There are no ring outliers.

32 monomers are involved in 90 short contacts:

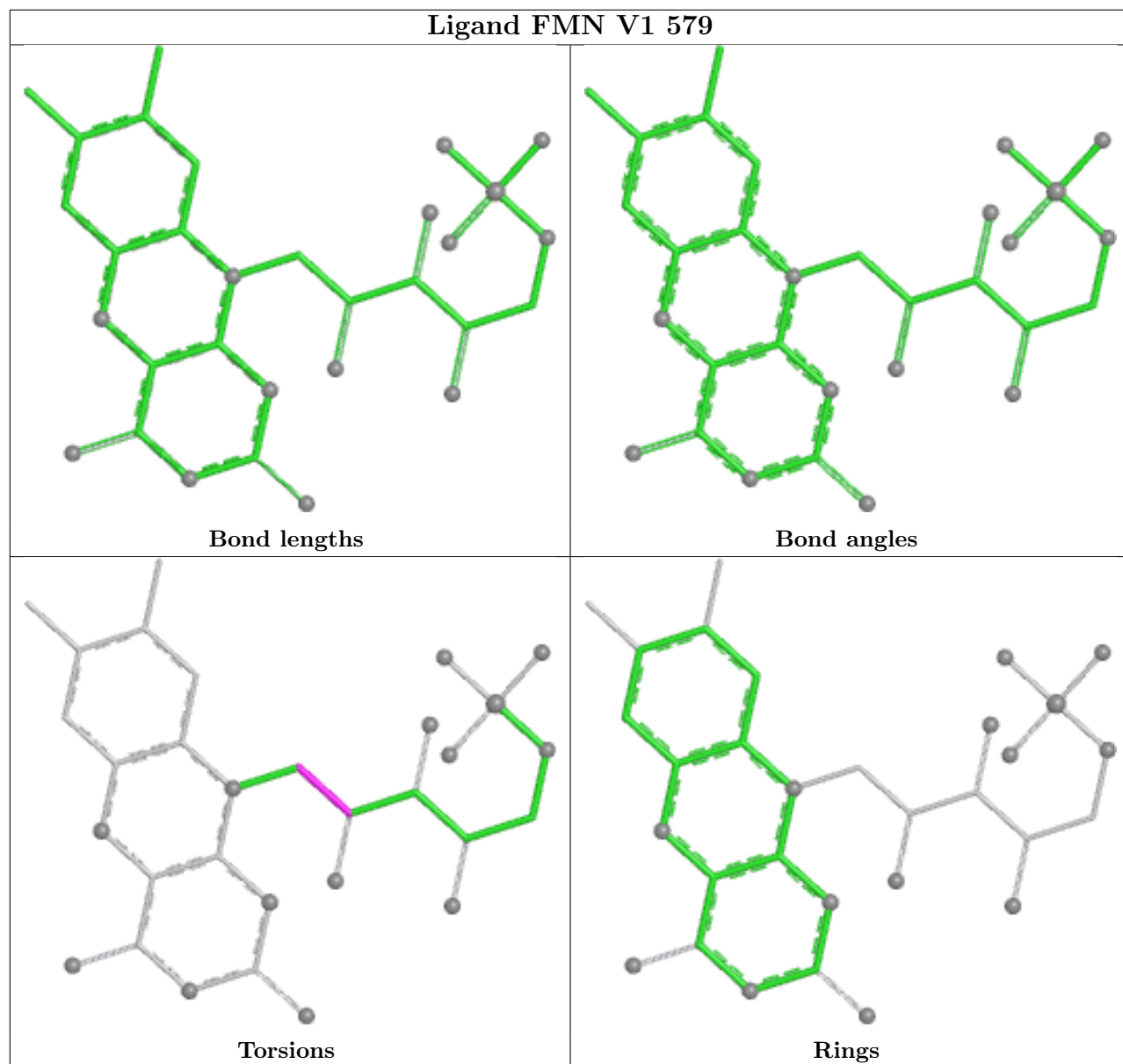
Mol	Chain	Res	Type	Clashes	Symm-Clashes
64	N5	603	CDL	1	0
70	V1	579	FMN	5	0
63	A9	560	PC1	2	0
64	A3	201	CDL	2	0
64	AM	217	CDL	2	0
66	AB	150	ZMP	8	0
64	N5	608	CDL	1	0
63	B5	202	PC1	1	0
63	N5	605	PC1	1	0
61	S8	298	SF4	1	0
64	C4	202	CDL	1	0
67	G1	516	3PE	3	0
63	A1	203	PC1	2	0
71	V1	581	NAI	11	0
63	E8	301	PC1	3	0
66	AC	201	ZMP	7	0
64	B3	102	CDL	4	0
63	A1	202	PC1	1	0
63	AM	220	PC1	1	0
64	N4	501	CDL	5	0
63	B5	203	PC1	1	0
64	B5	201	CDL	1	0
63	N3	301	PC1	1	0
61	S8	297	SF4	3	0
64	AL	303	CDL	2	0
63	N5	601	PC1	2	0
65	A9	559	NDP	2	0
68	N4	505	U10	10	0
67	N5	607	3PE	1	0
64	AM	216	CDL	3	0
61	1A	403	SF4	1	0
64	AM	215	CDL	5	0

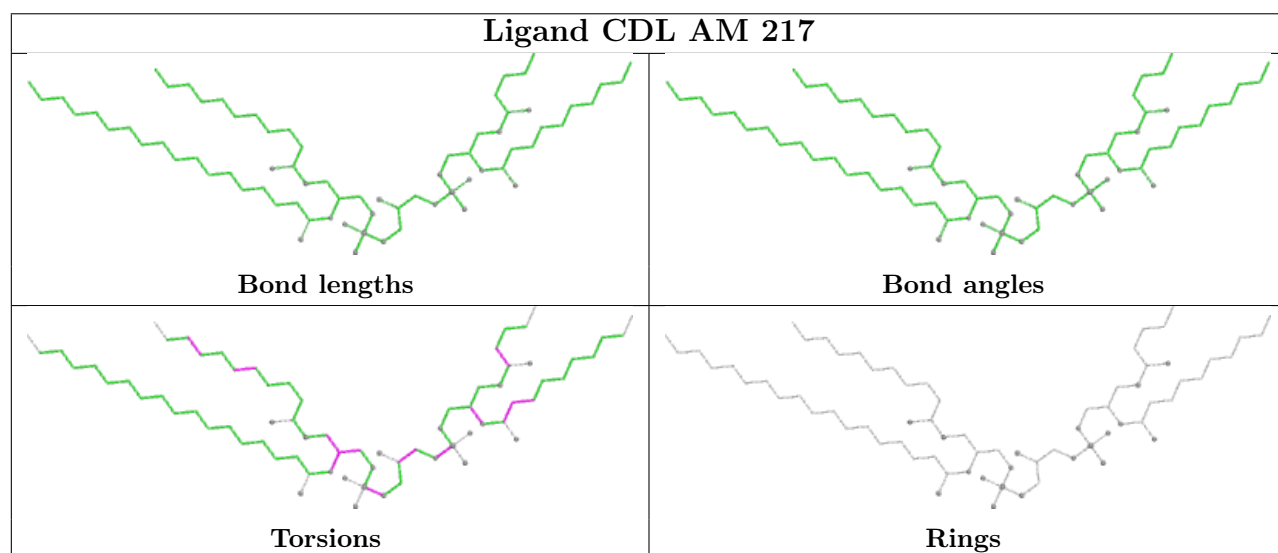
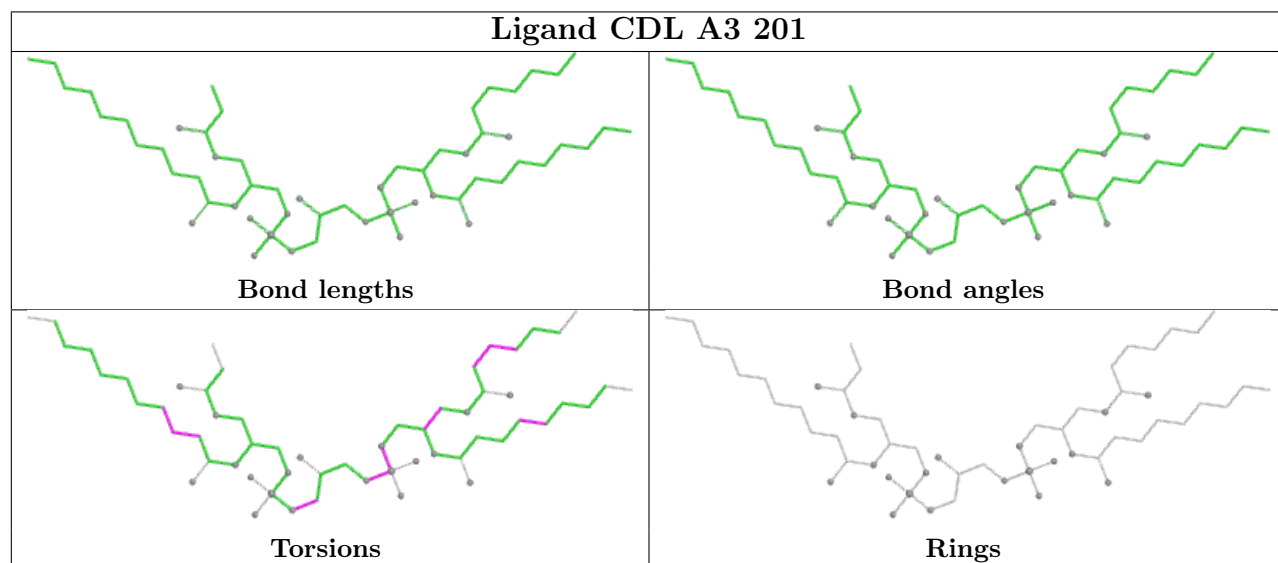
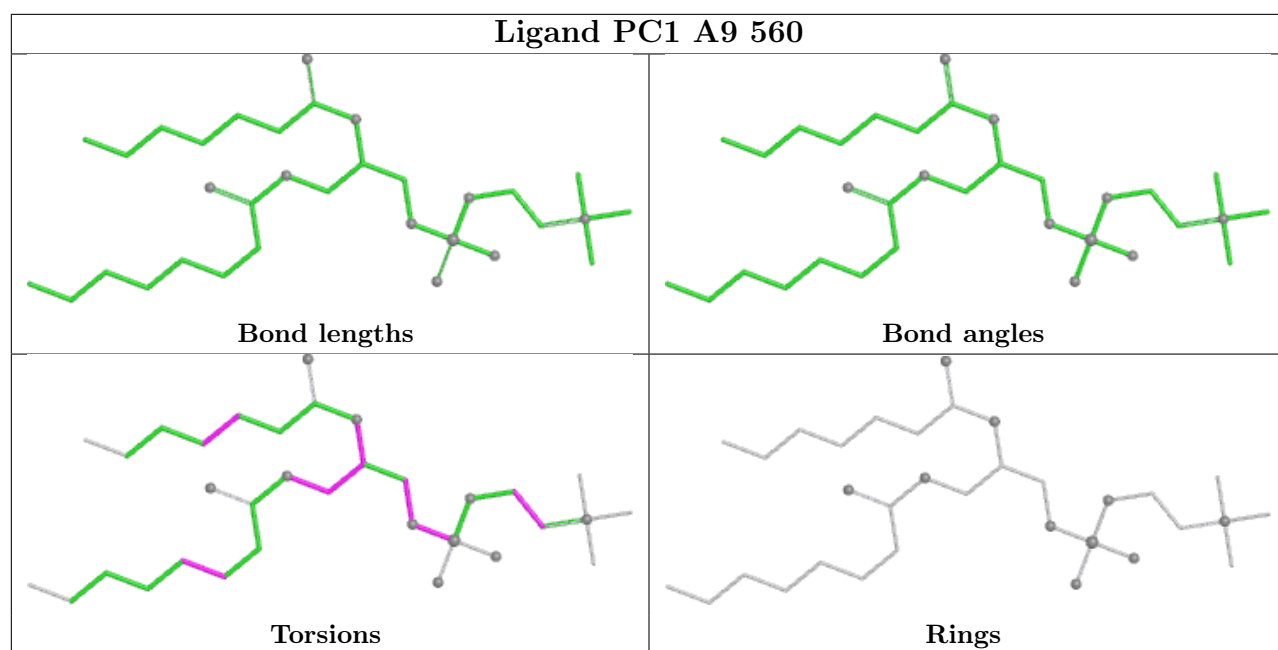
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

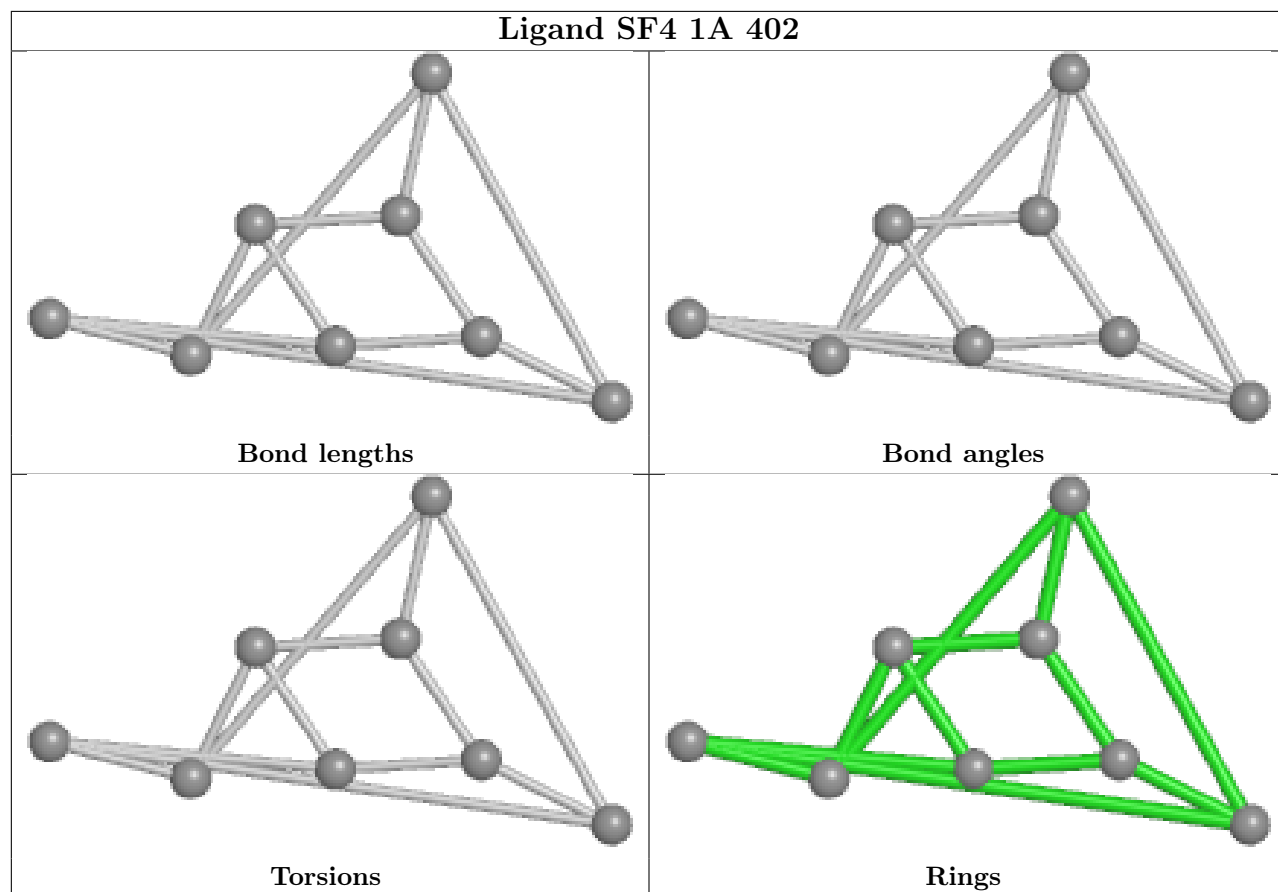
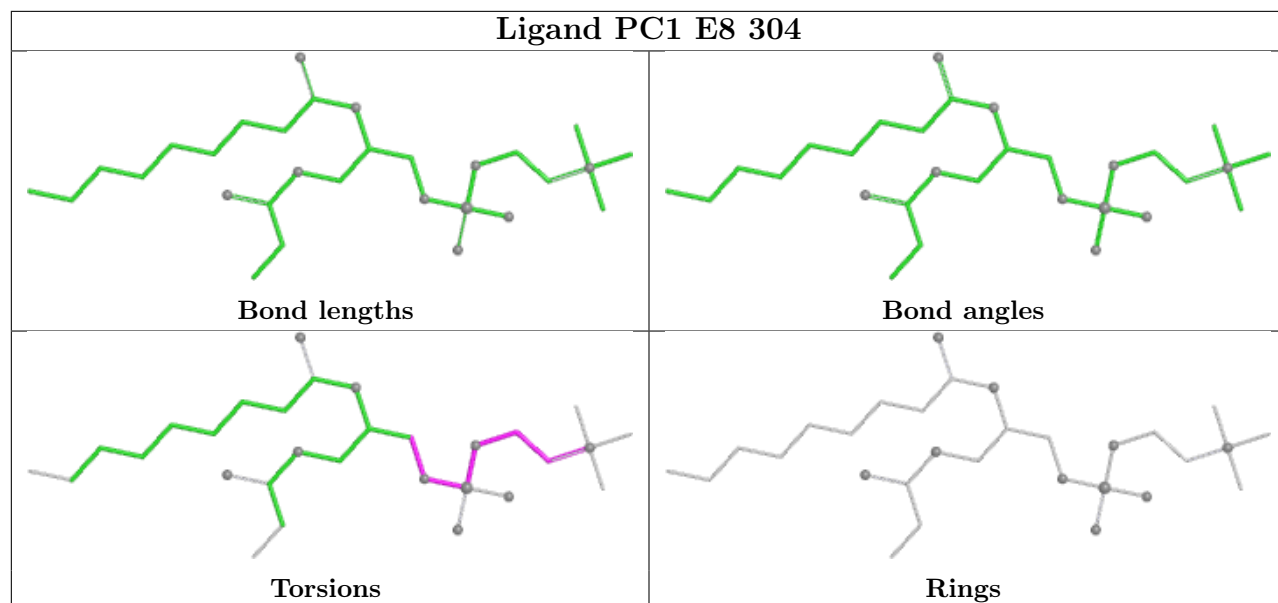
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.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

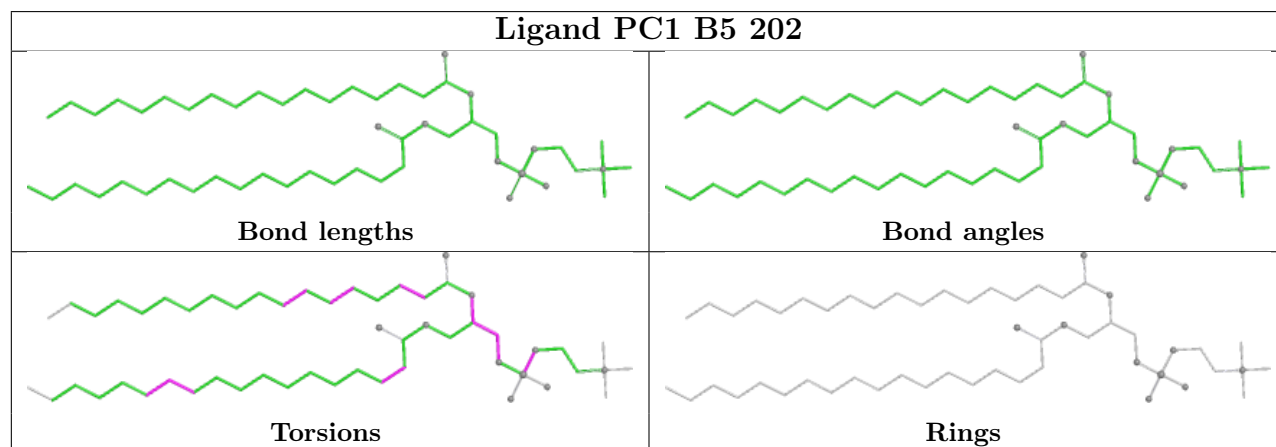
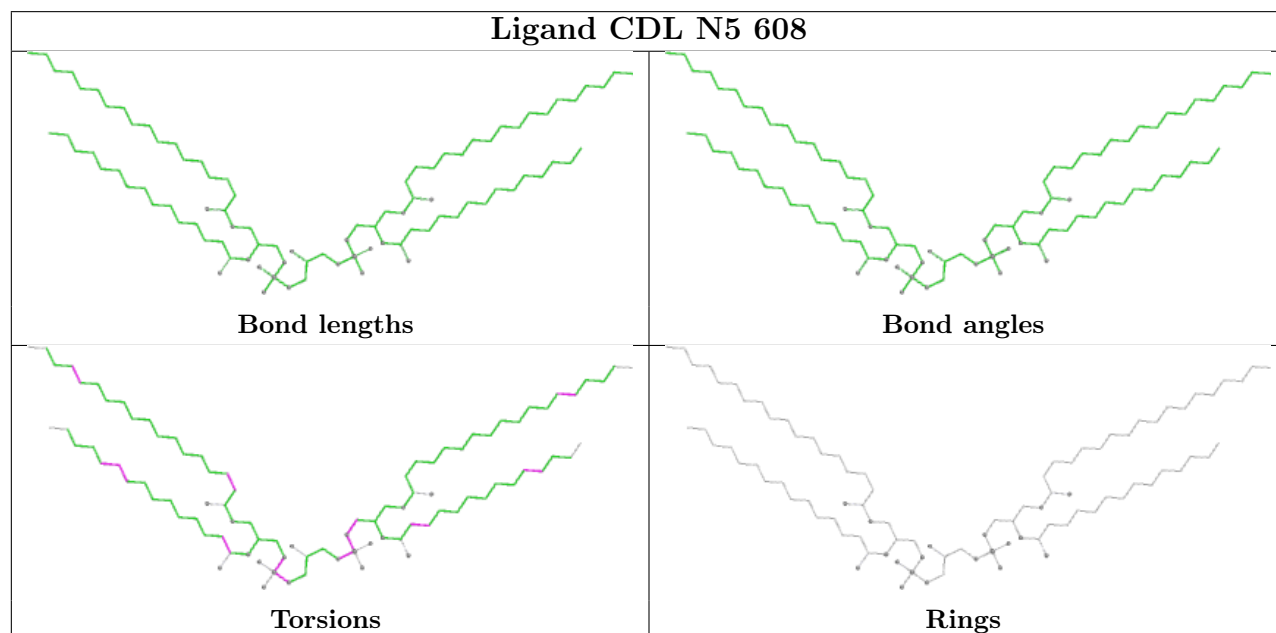
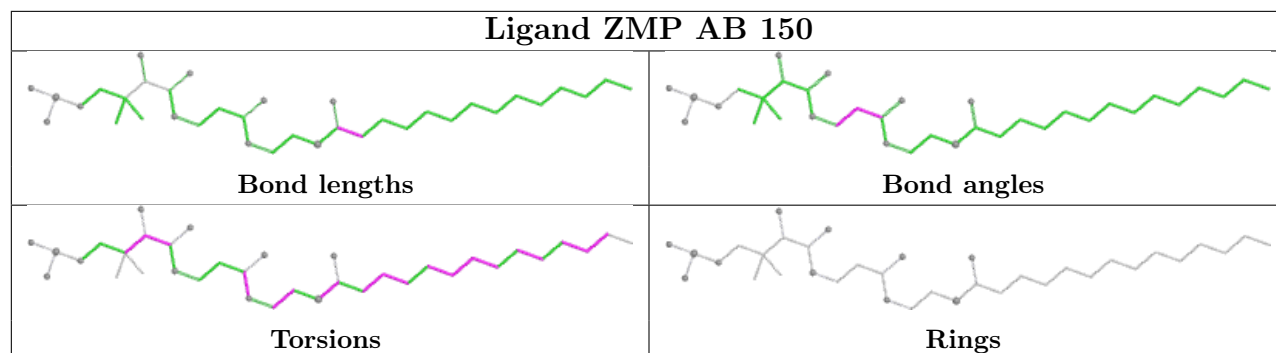


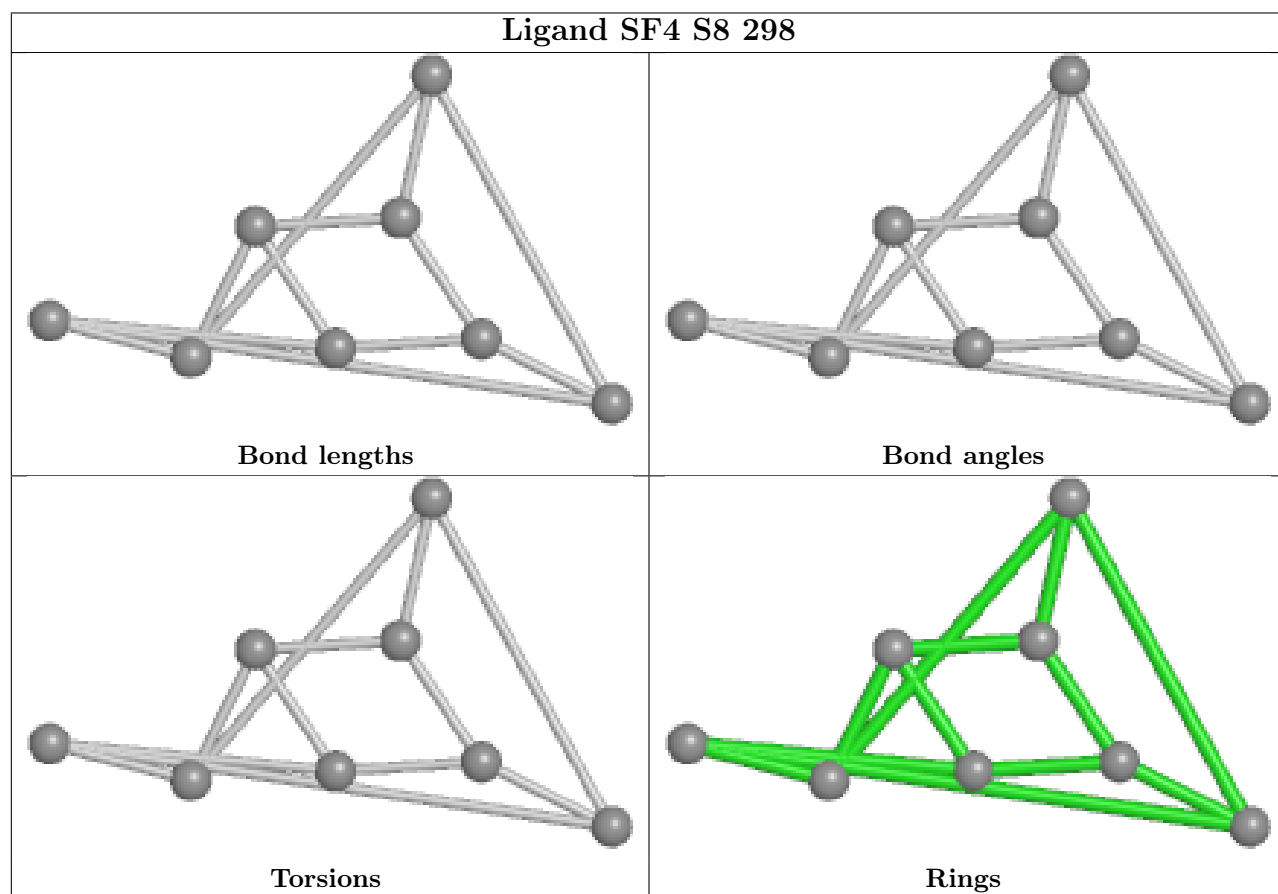
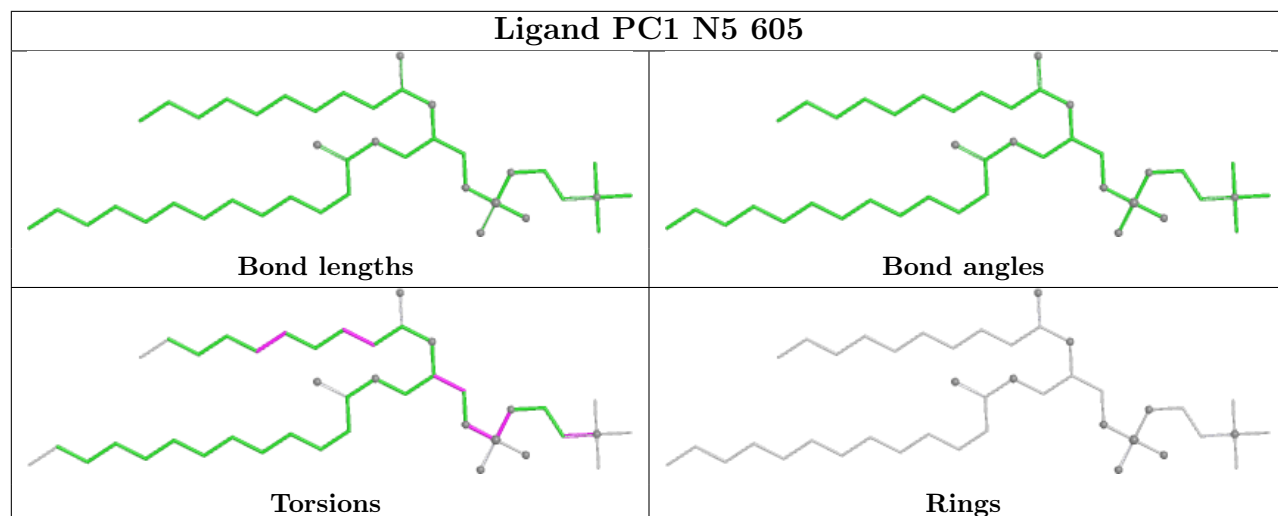
Ligand FMN V1 579

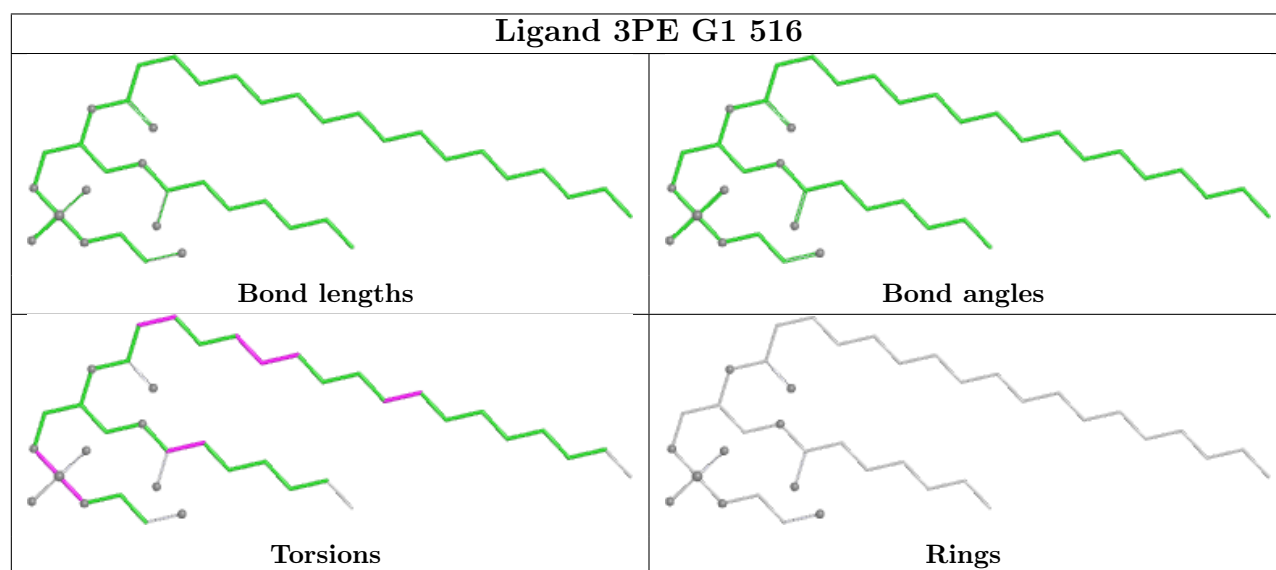
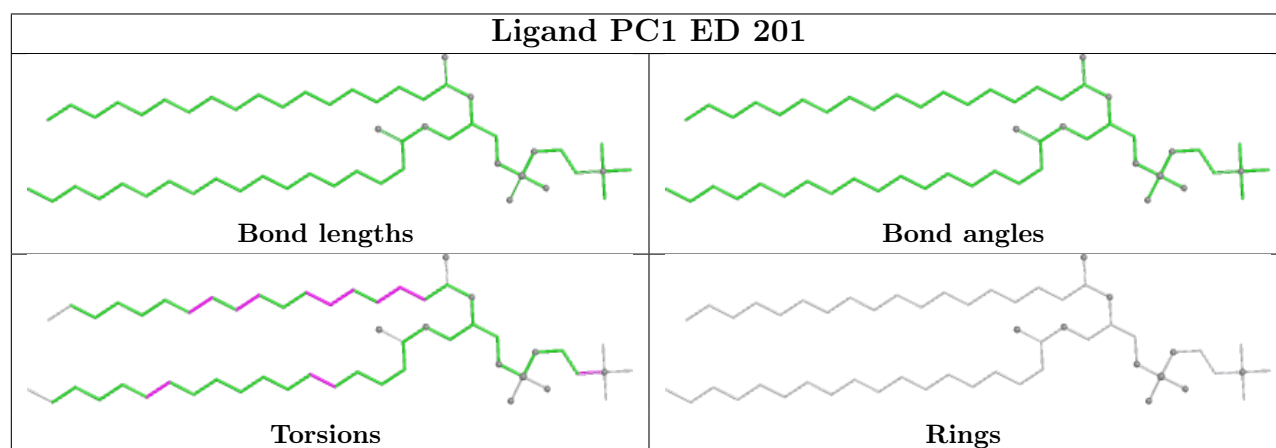
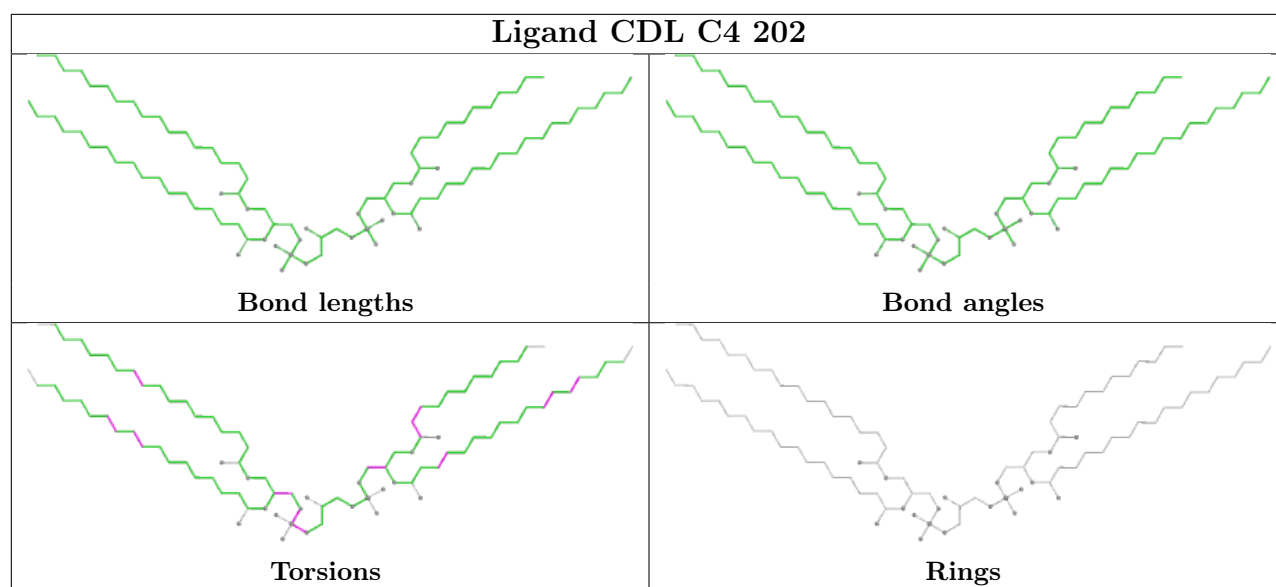


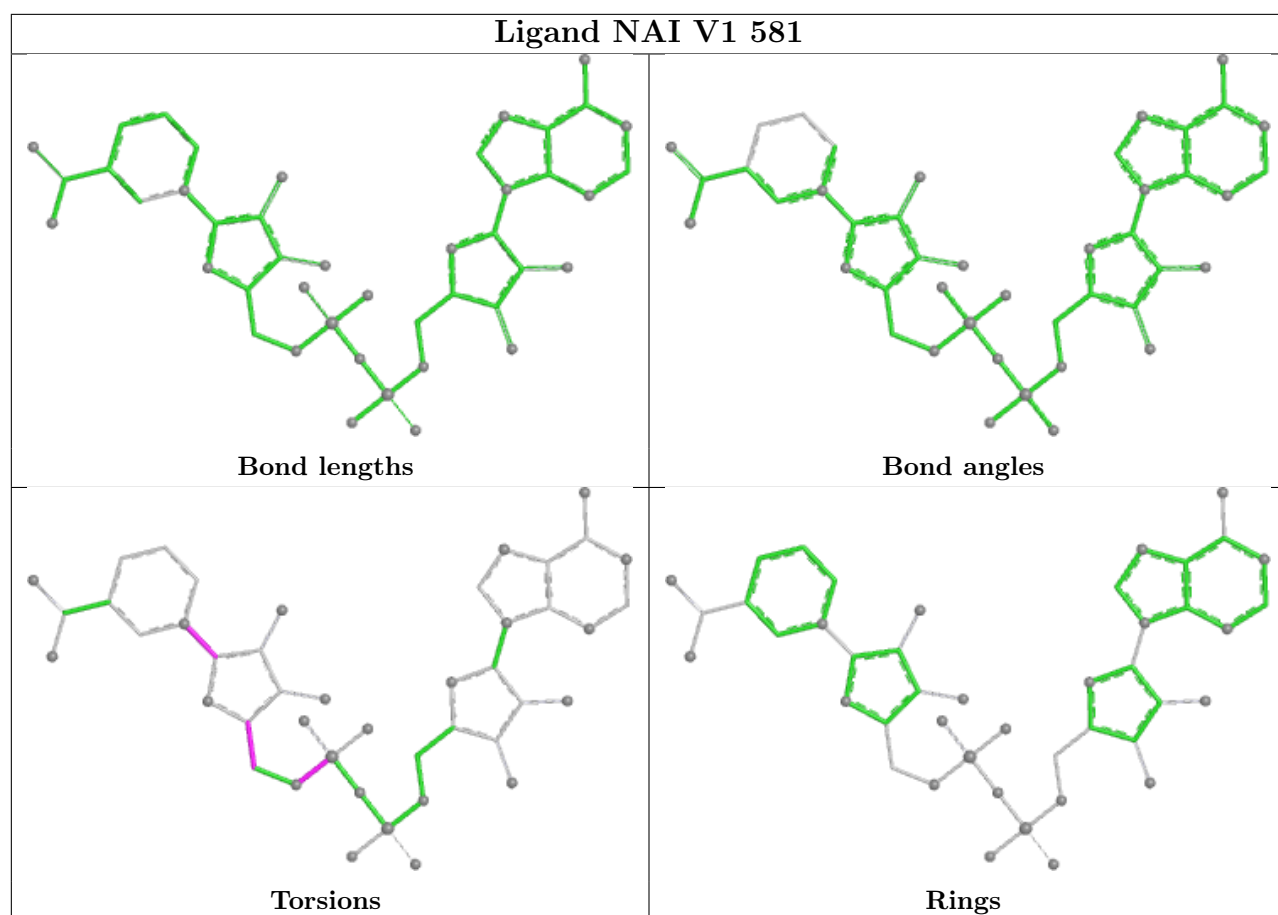
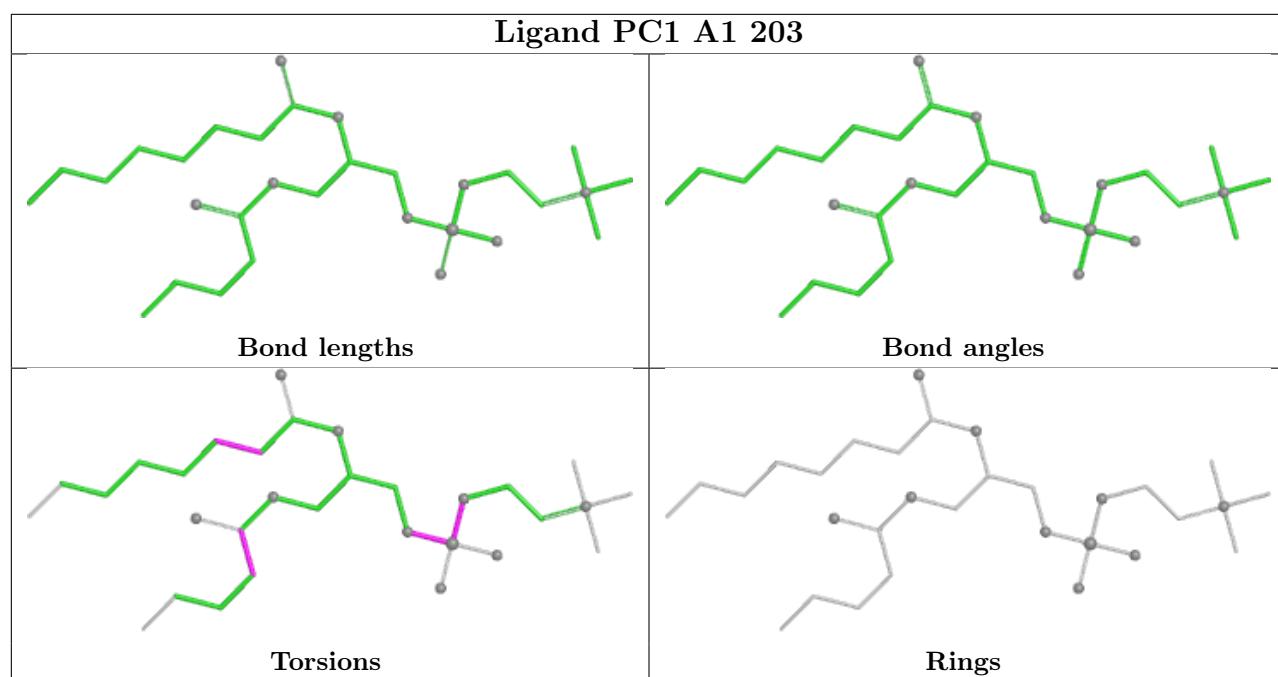


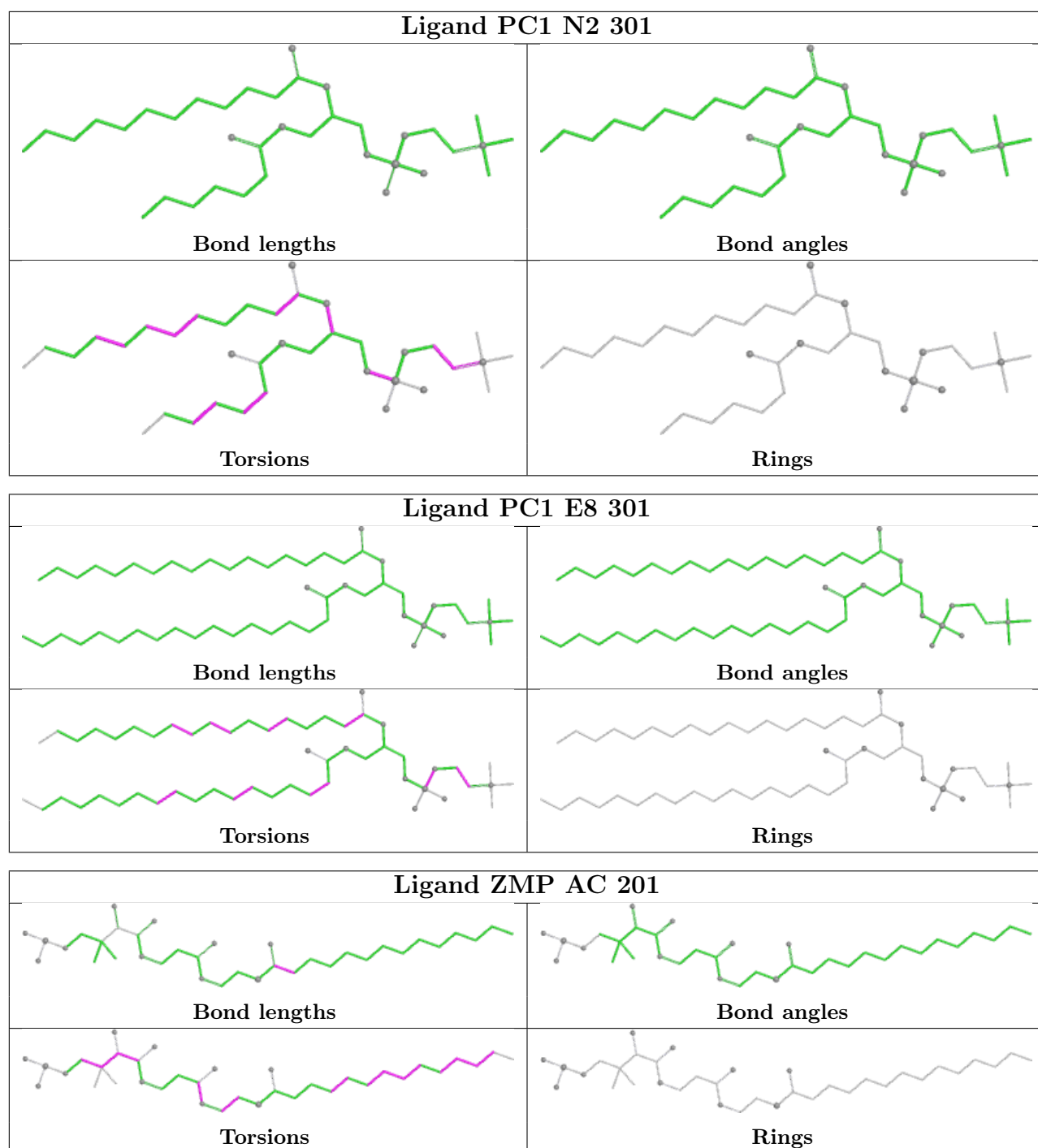


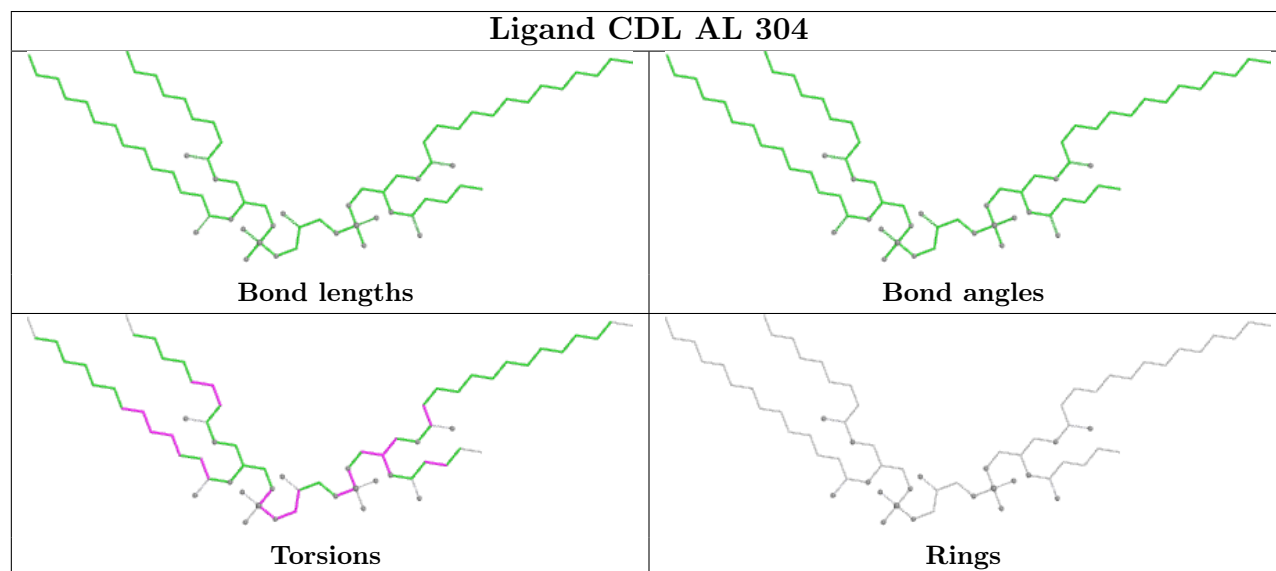
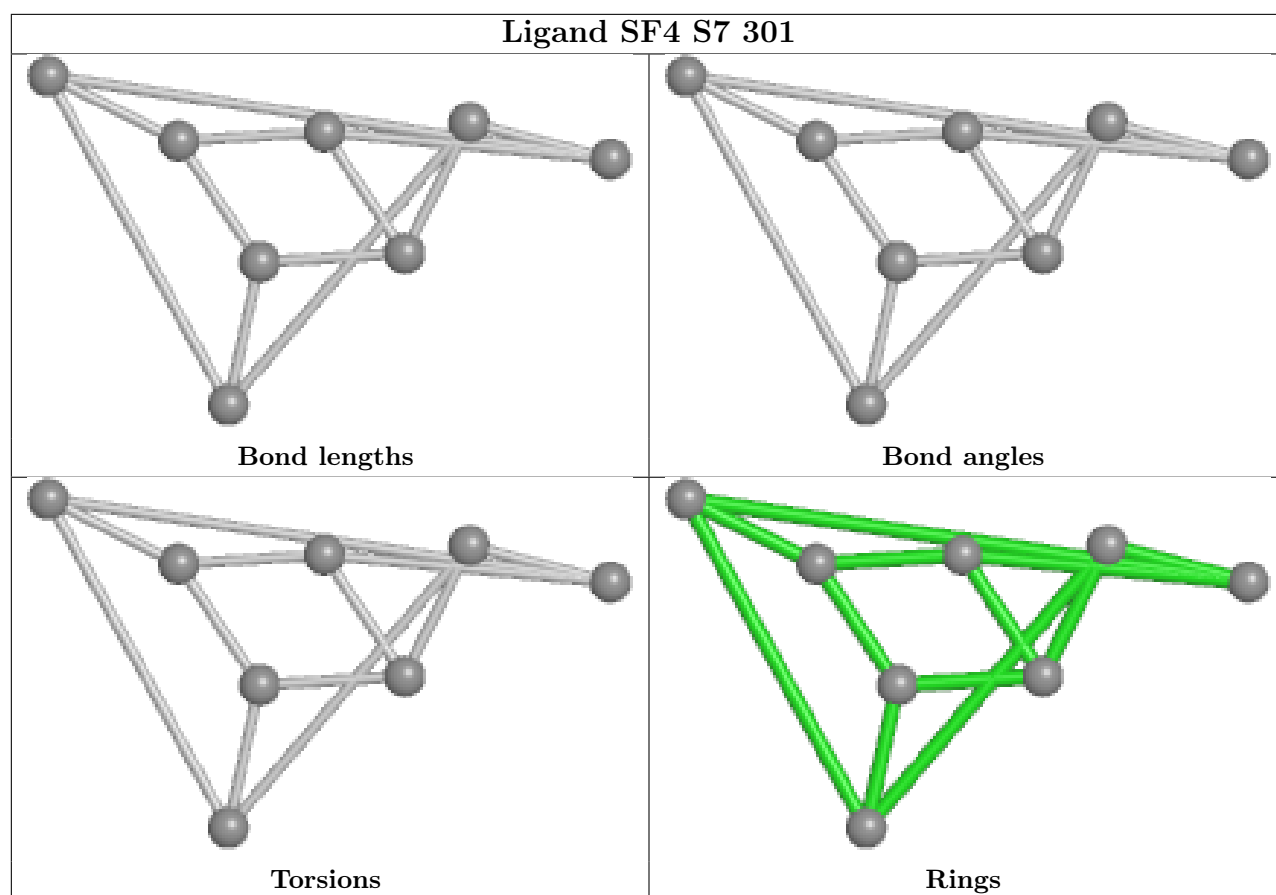


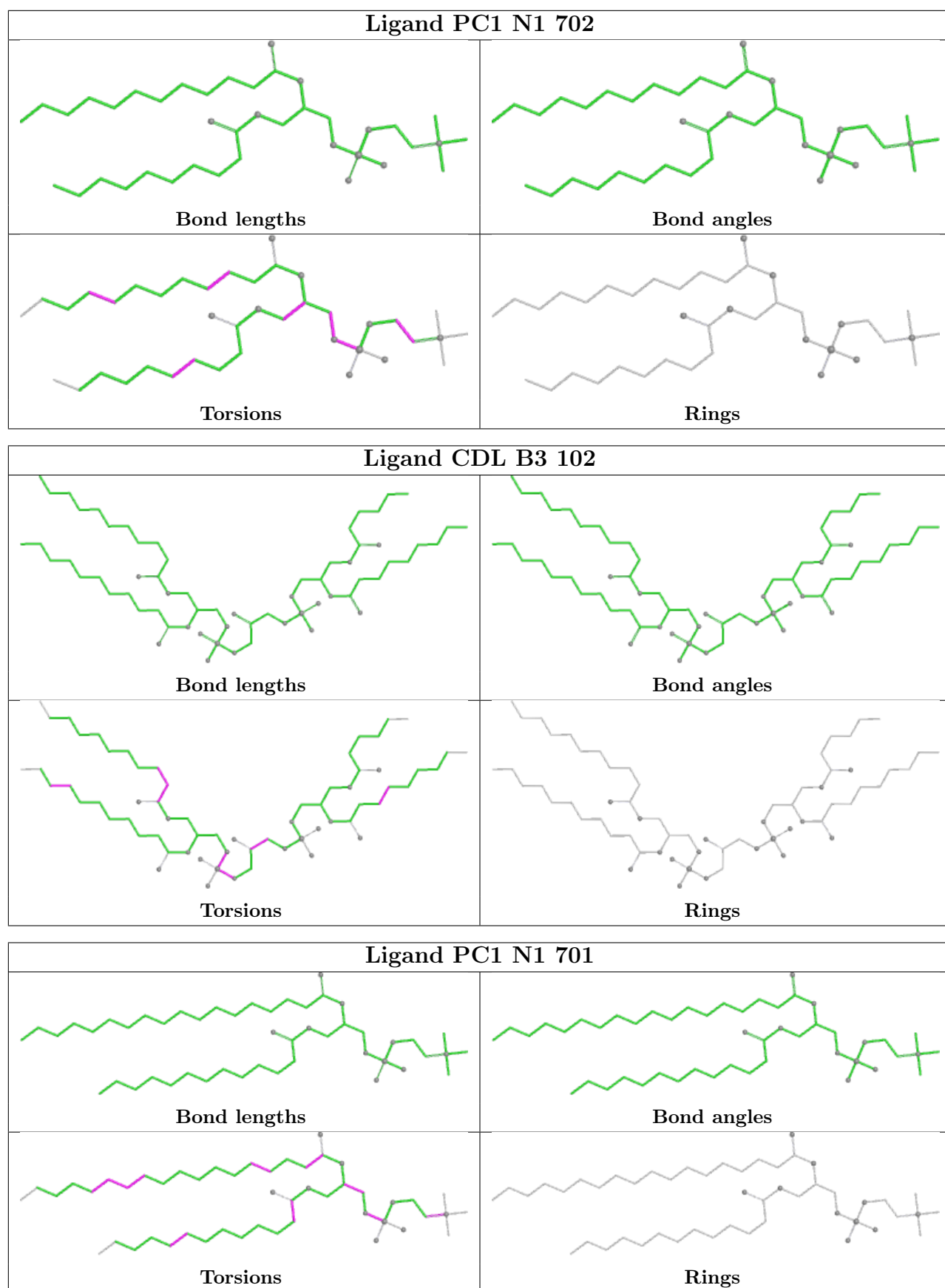


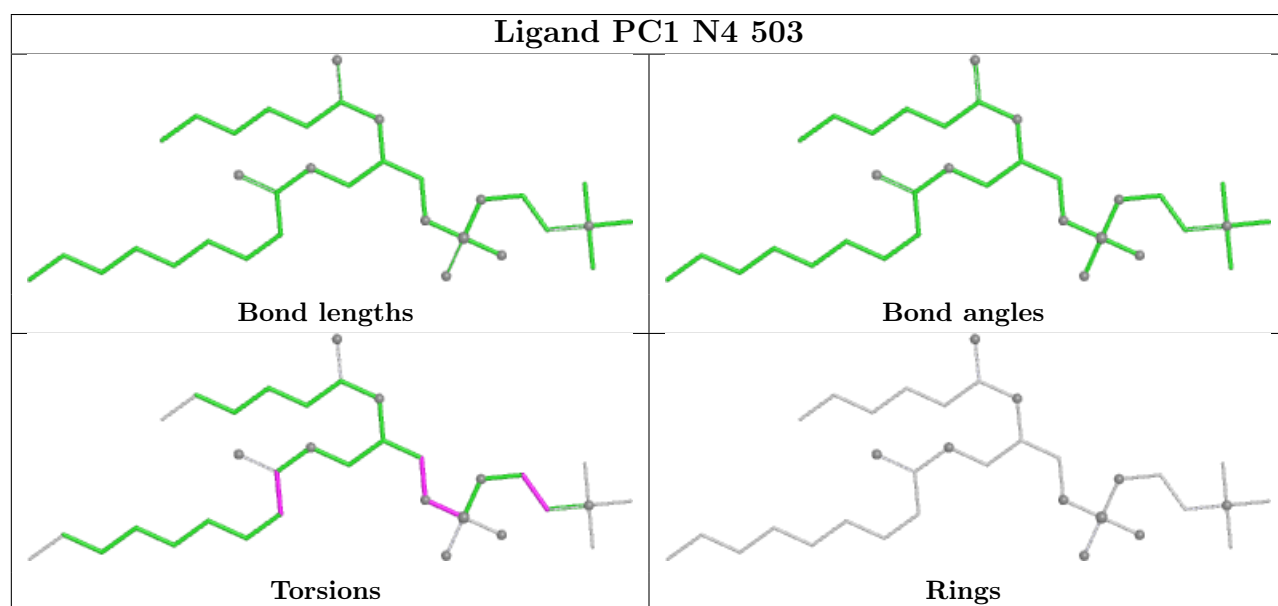
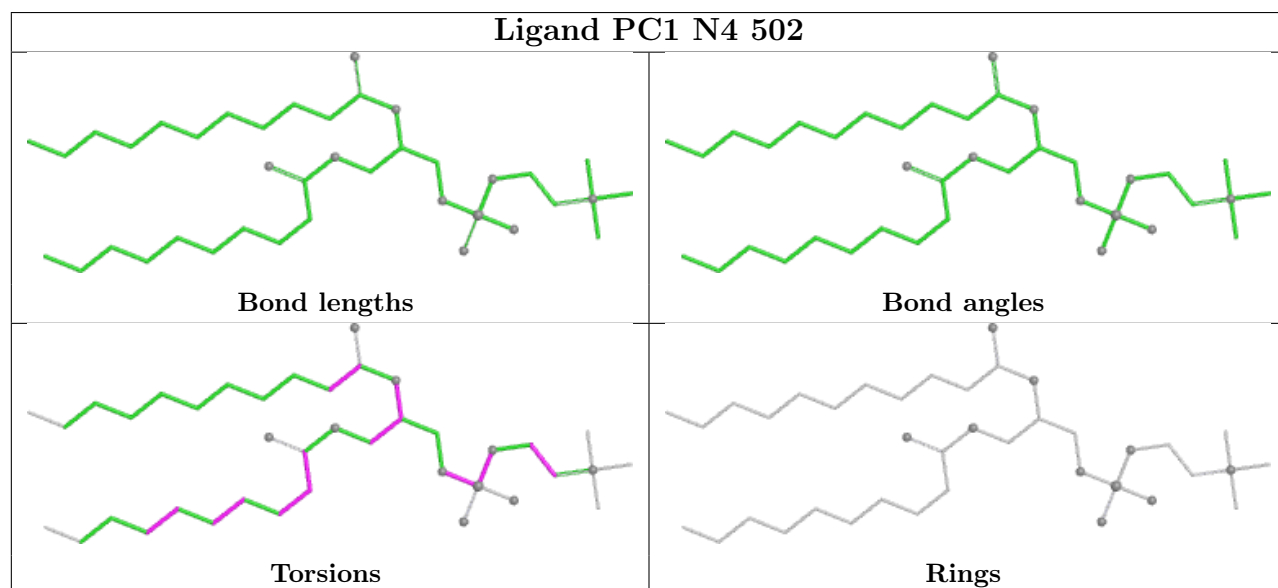
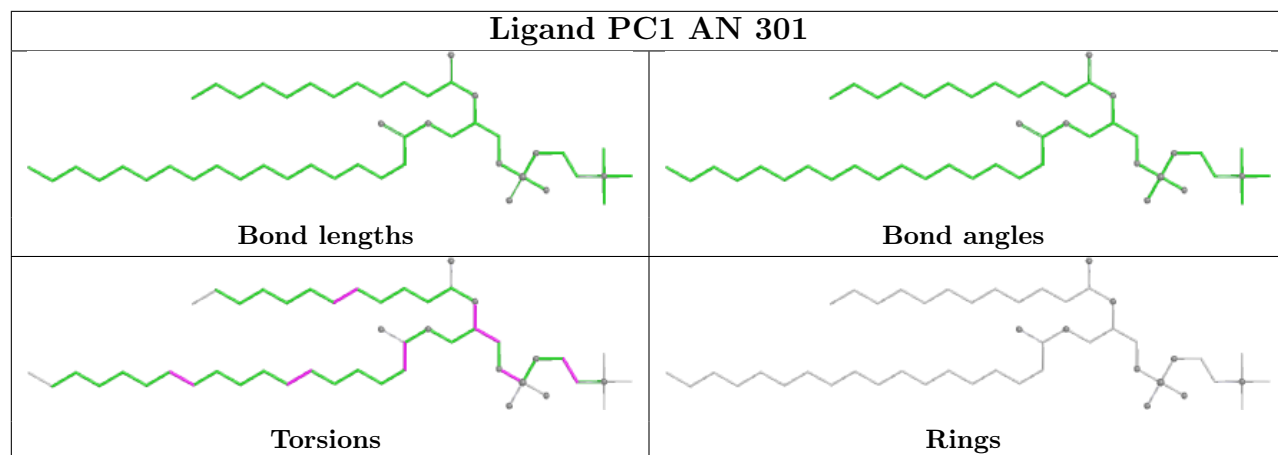


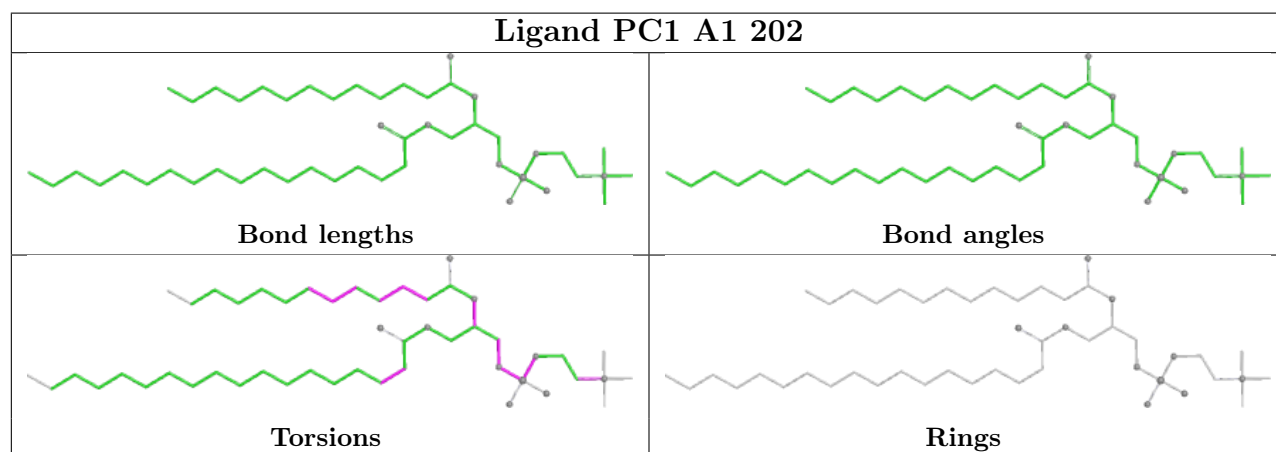
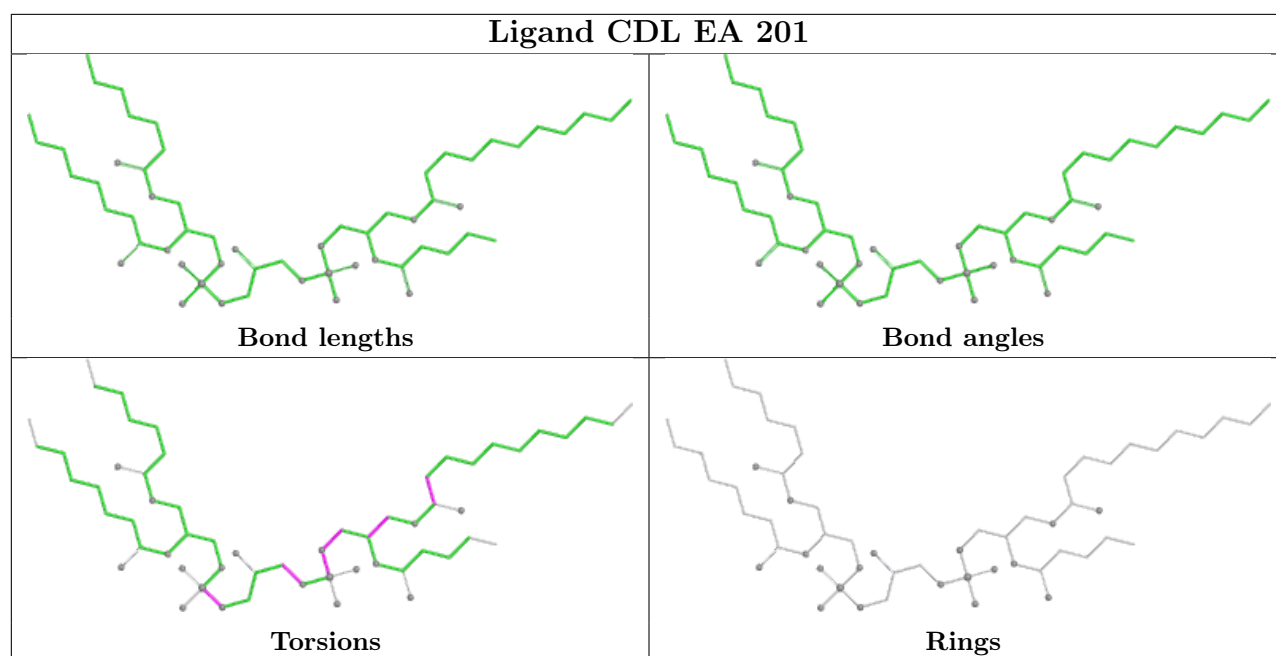


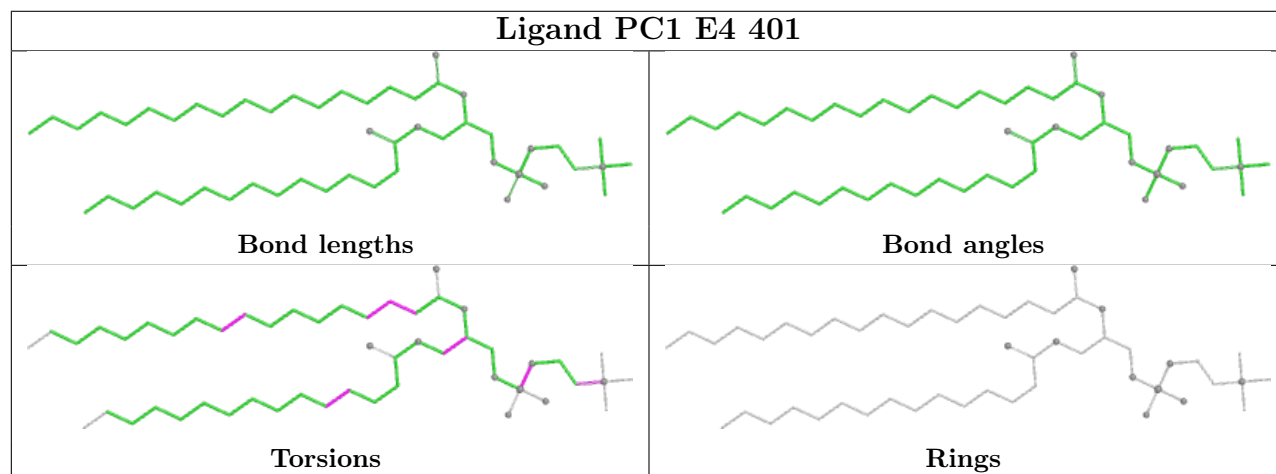
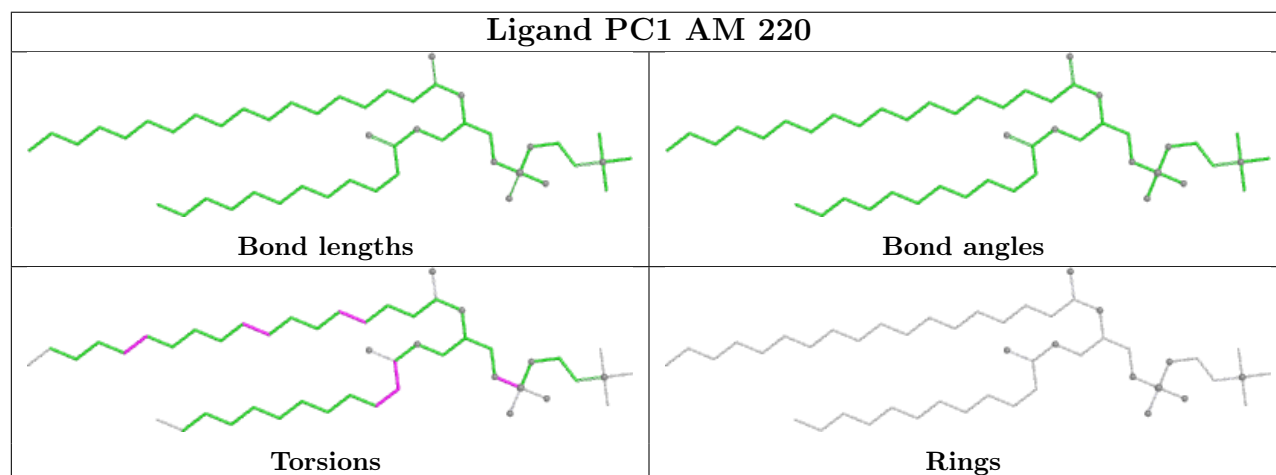
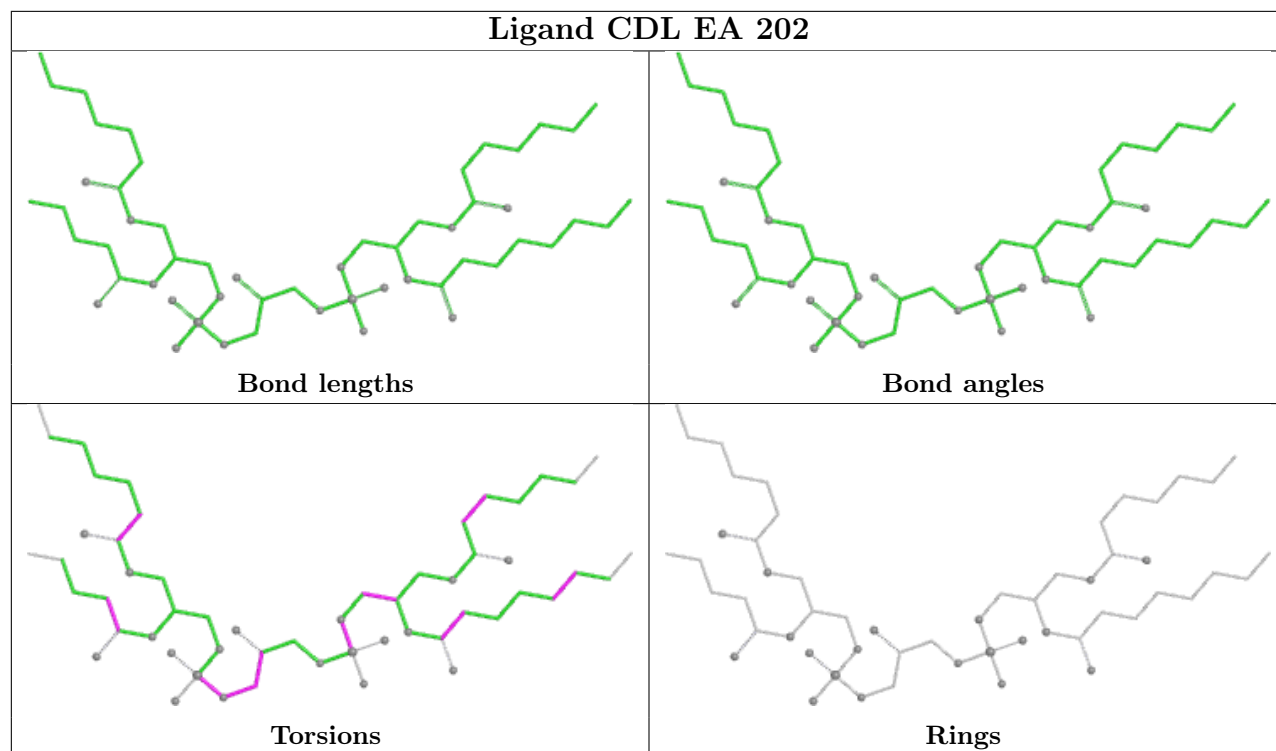


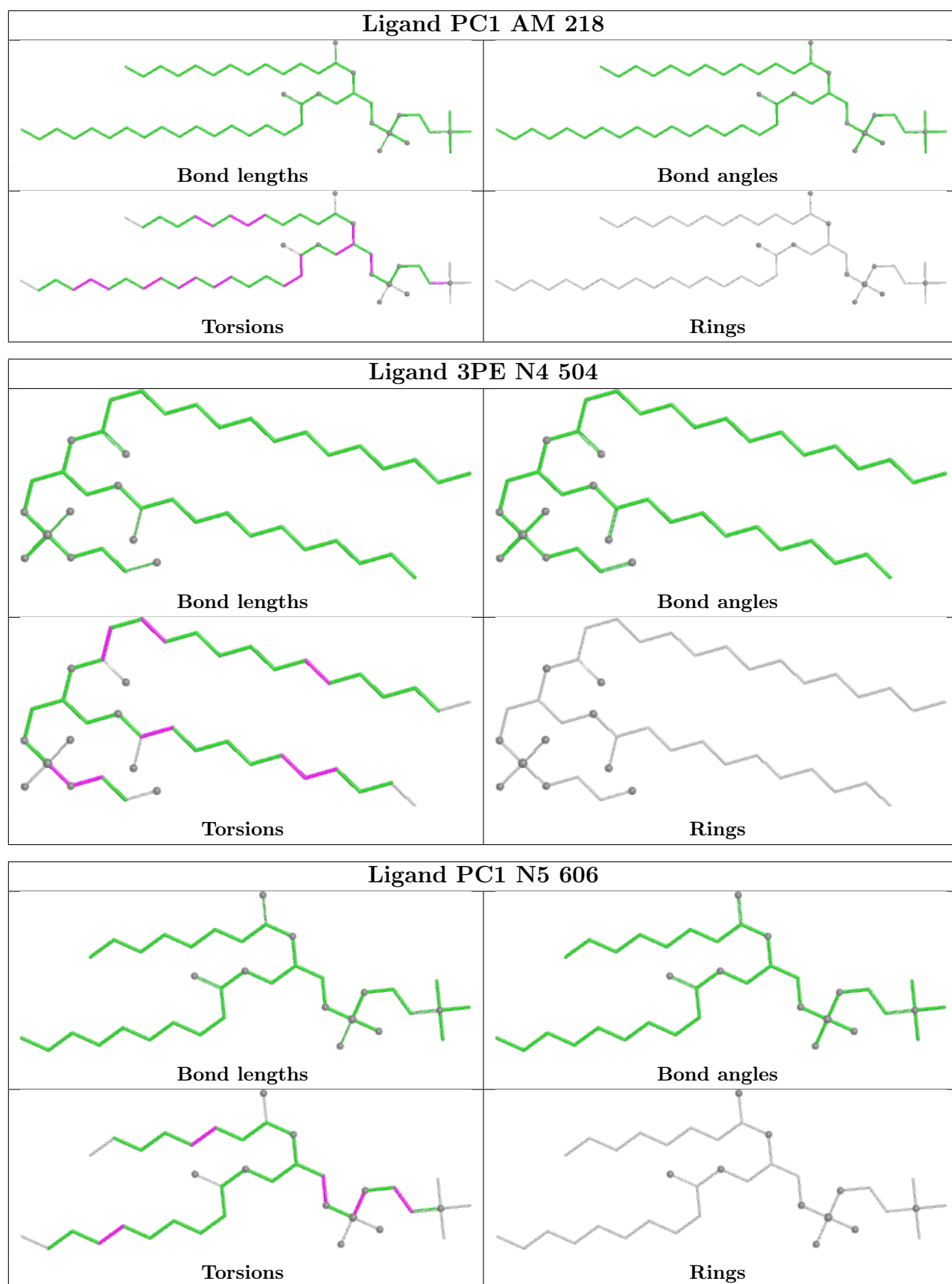


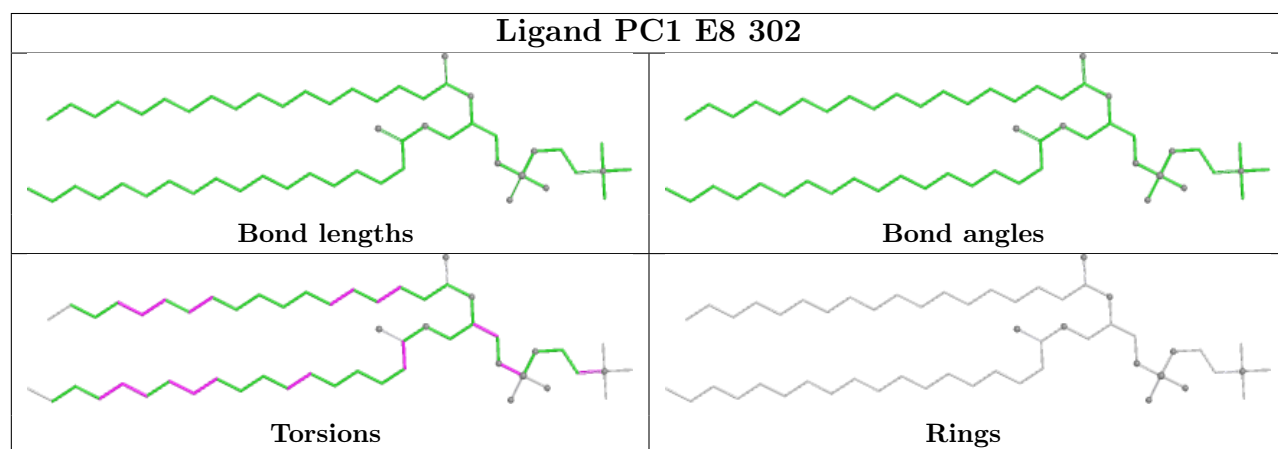
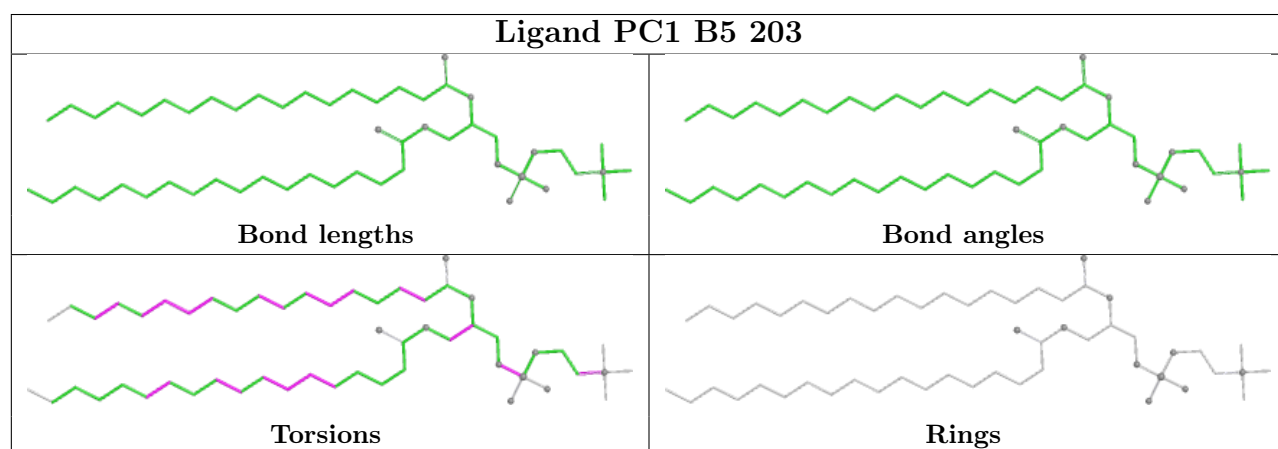
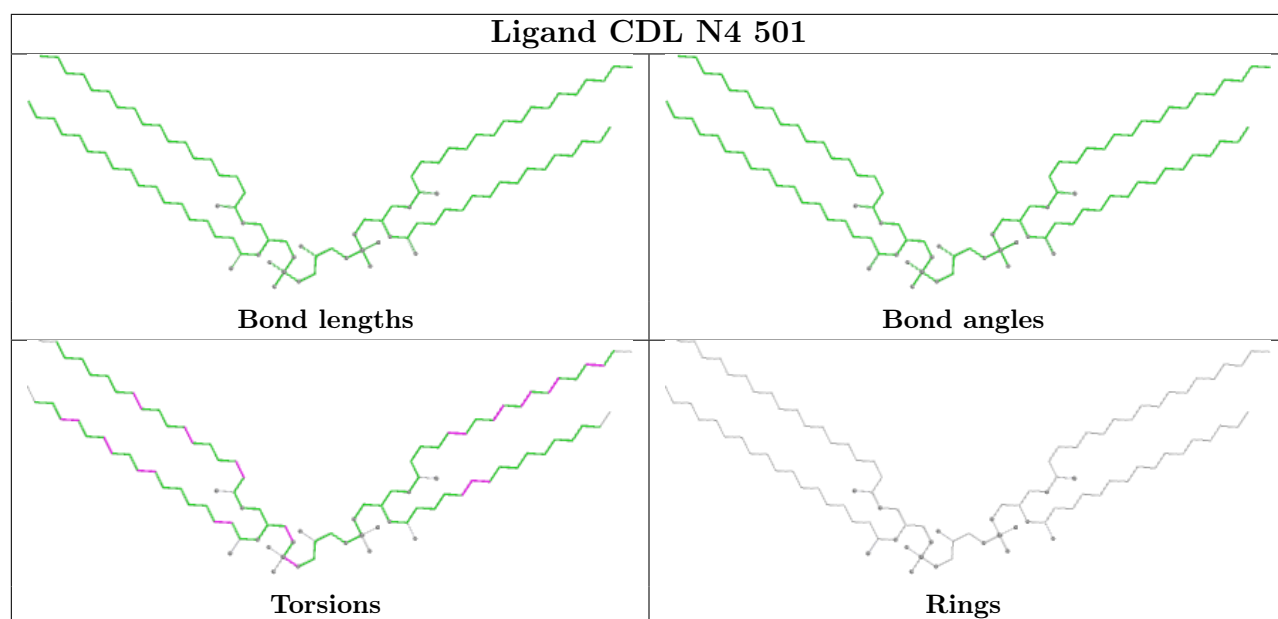


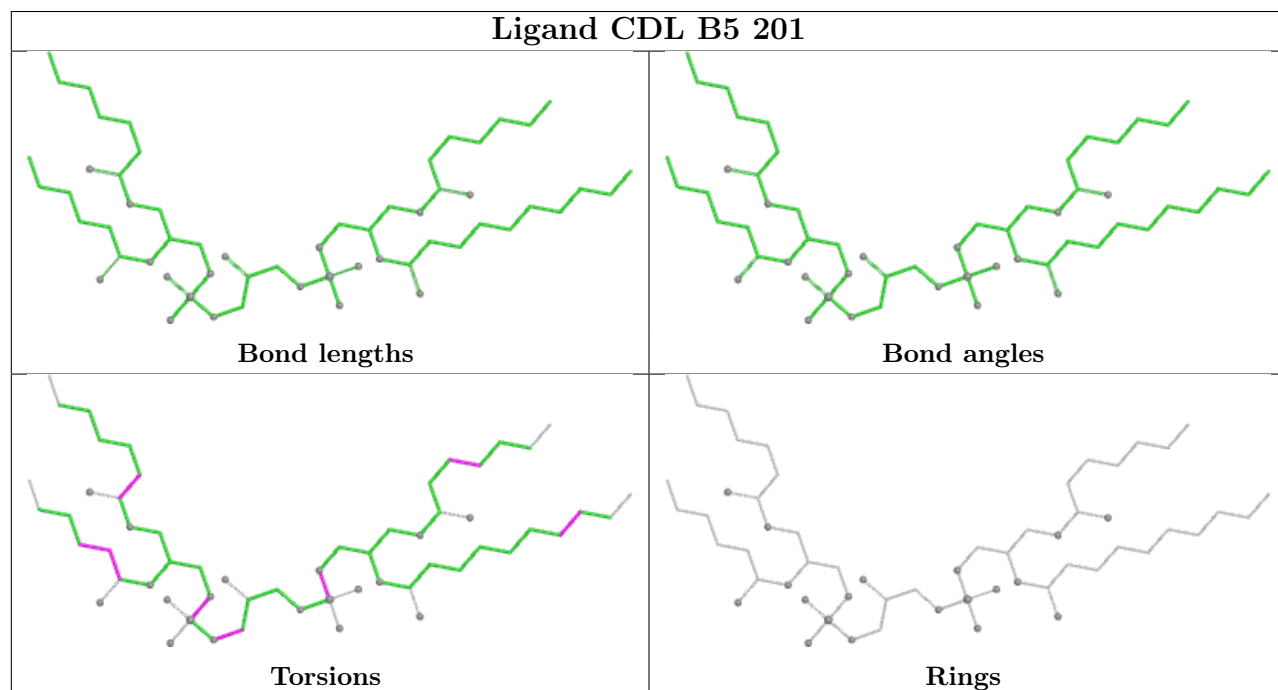
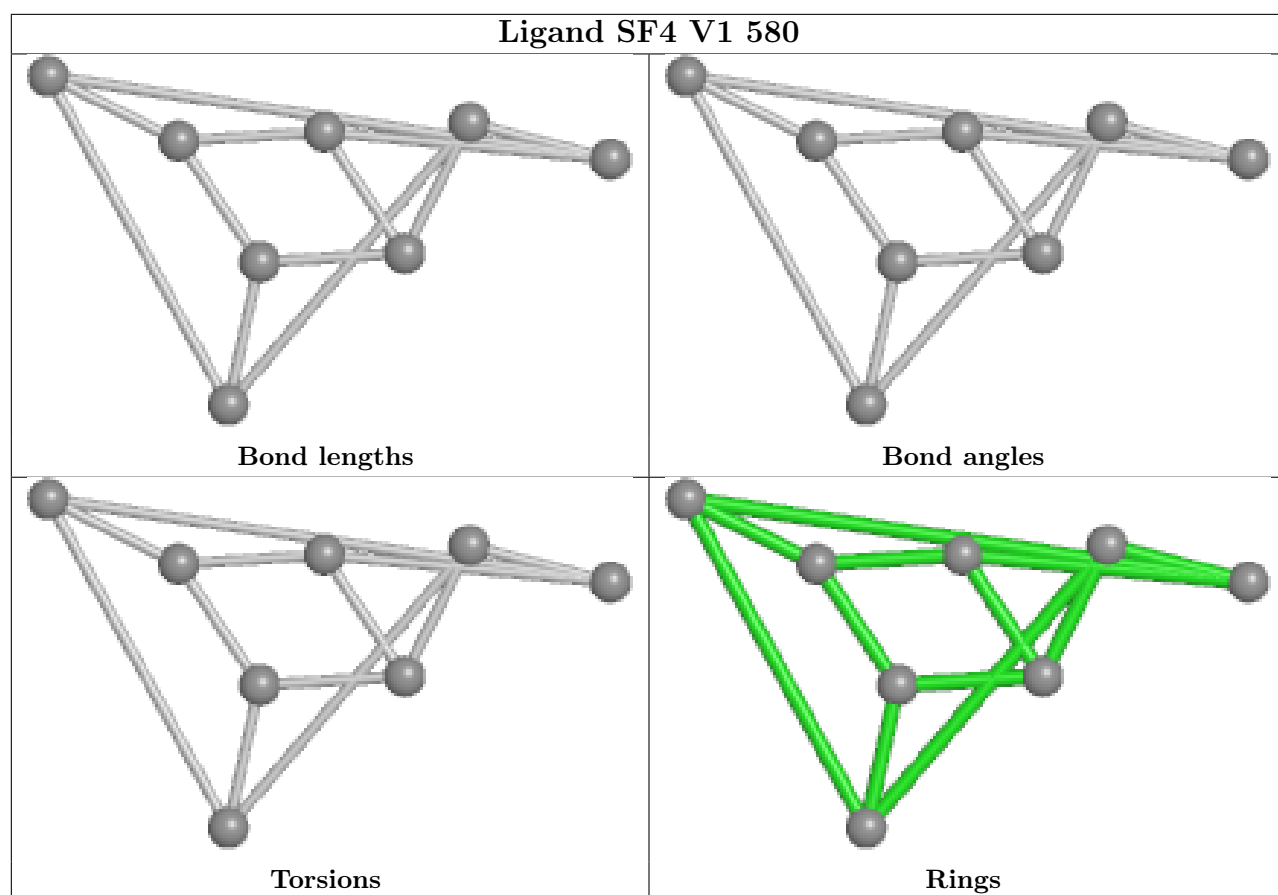


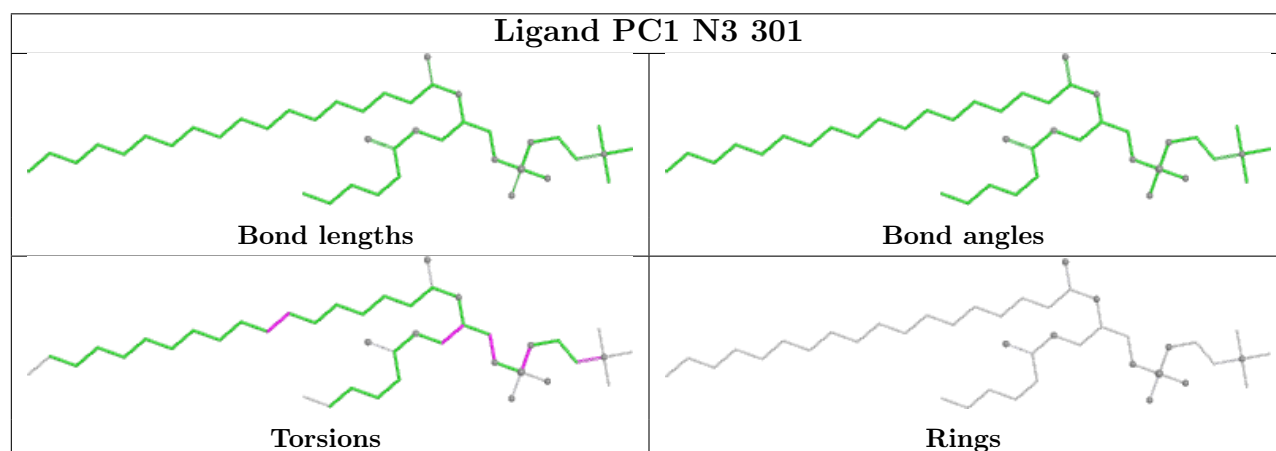
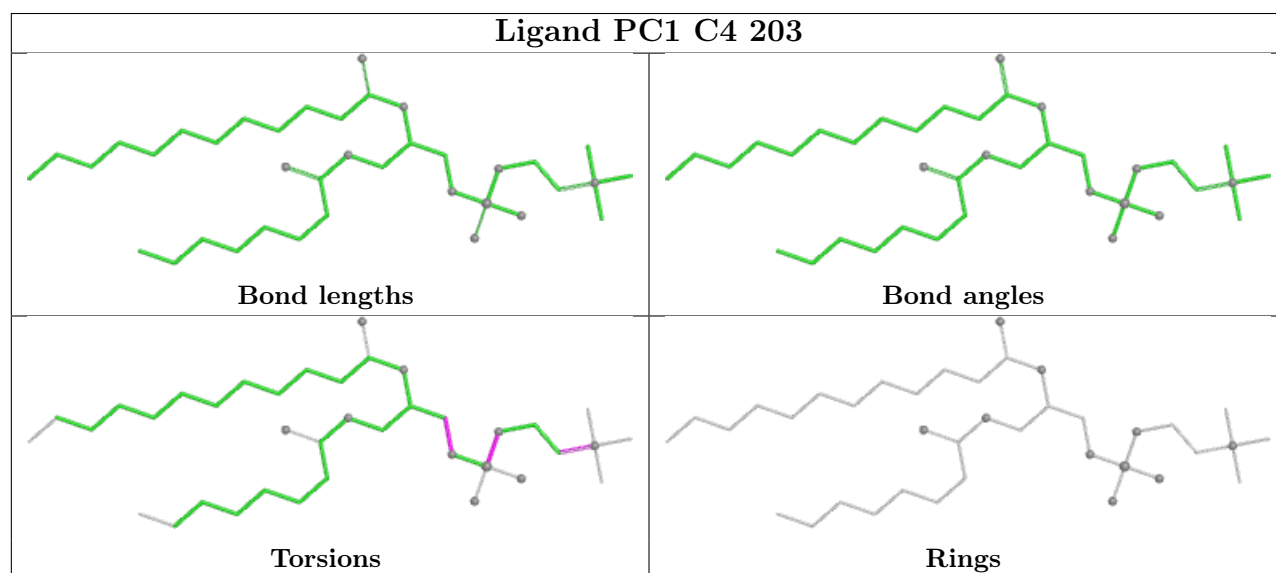
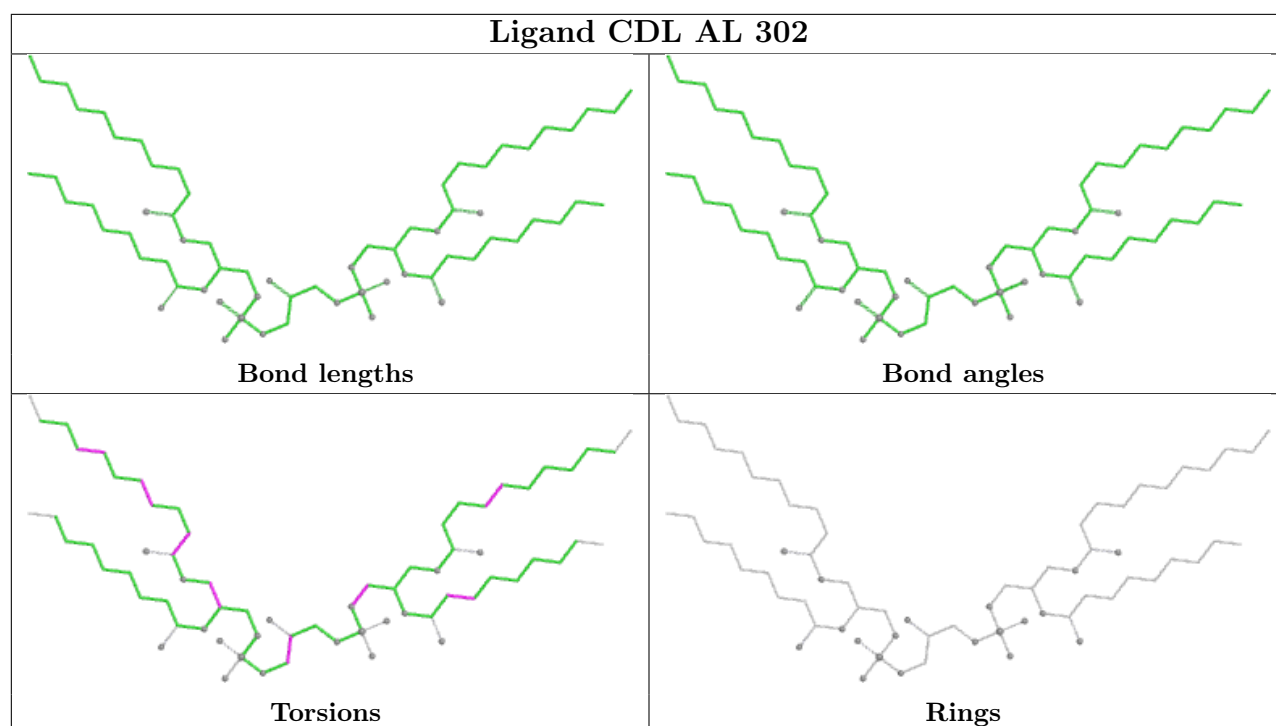


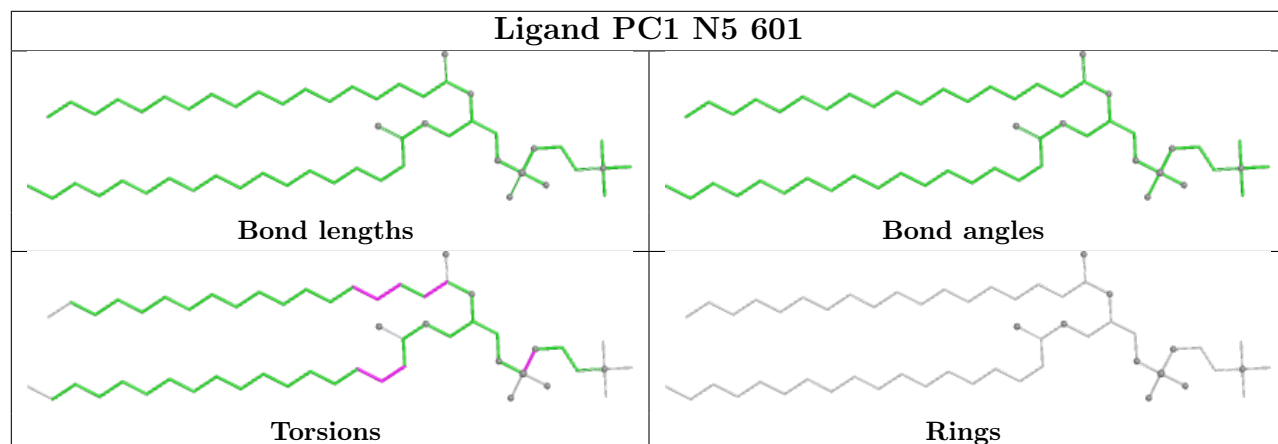
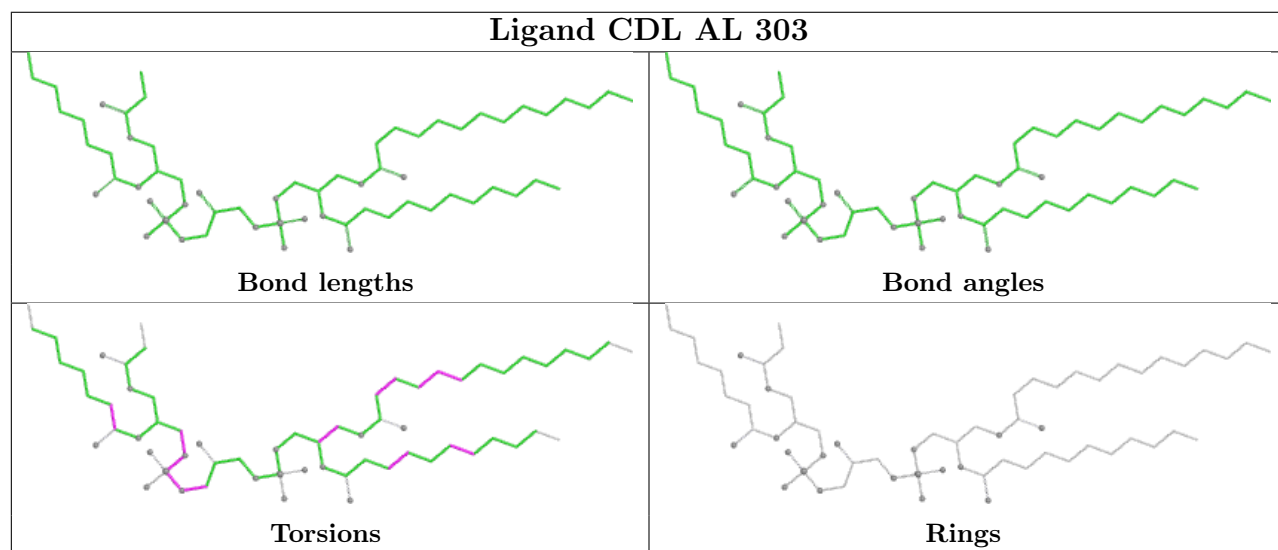
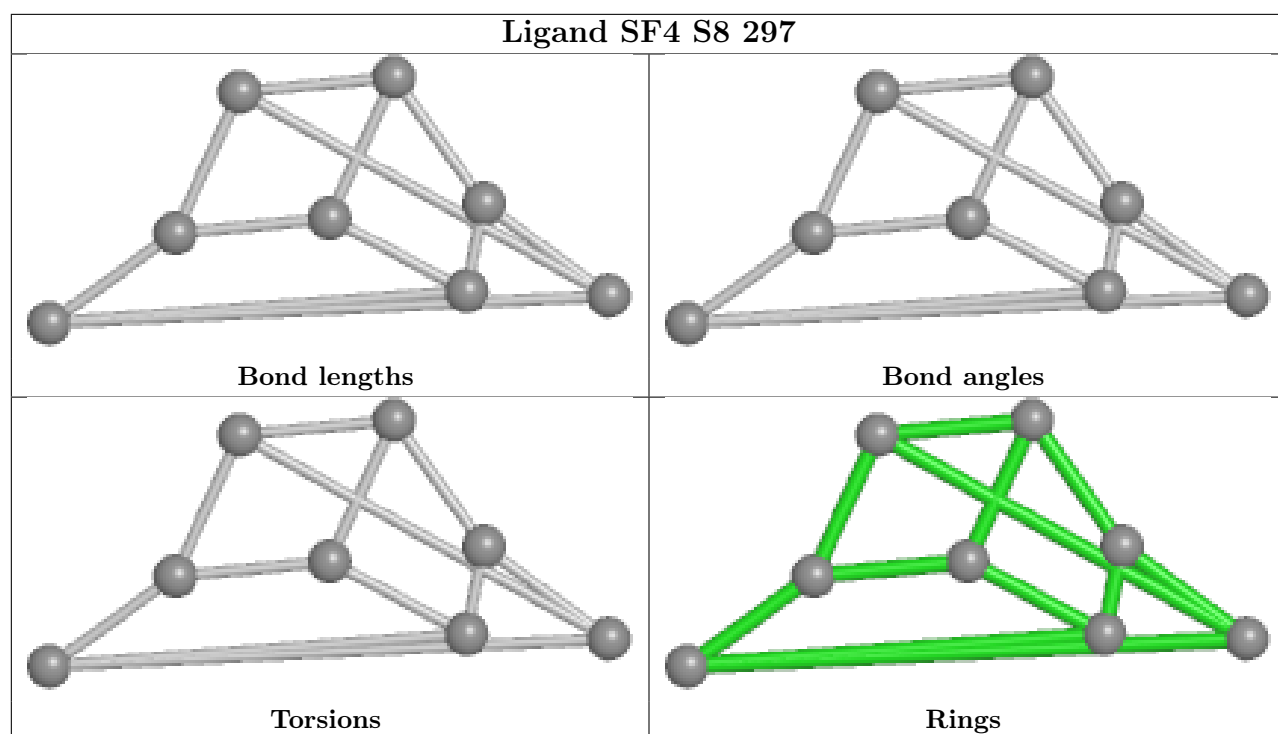


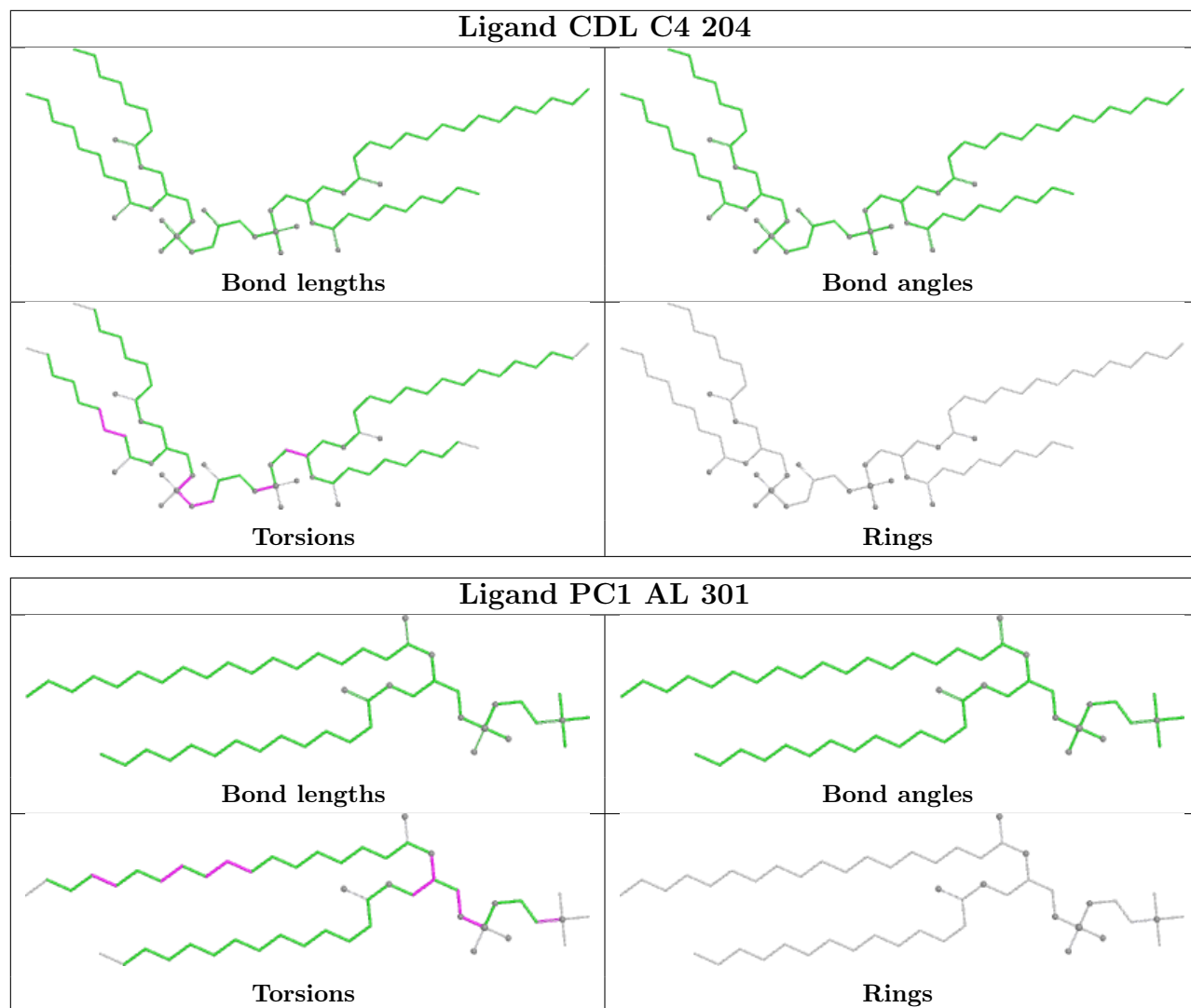


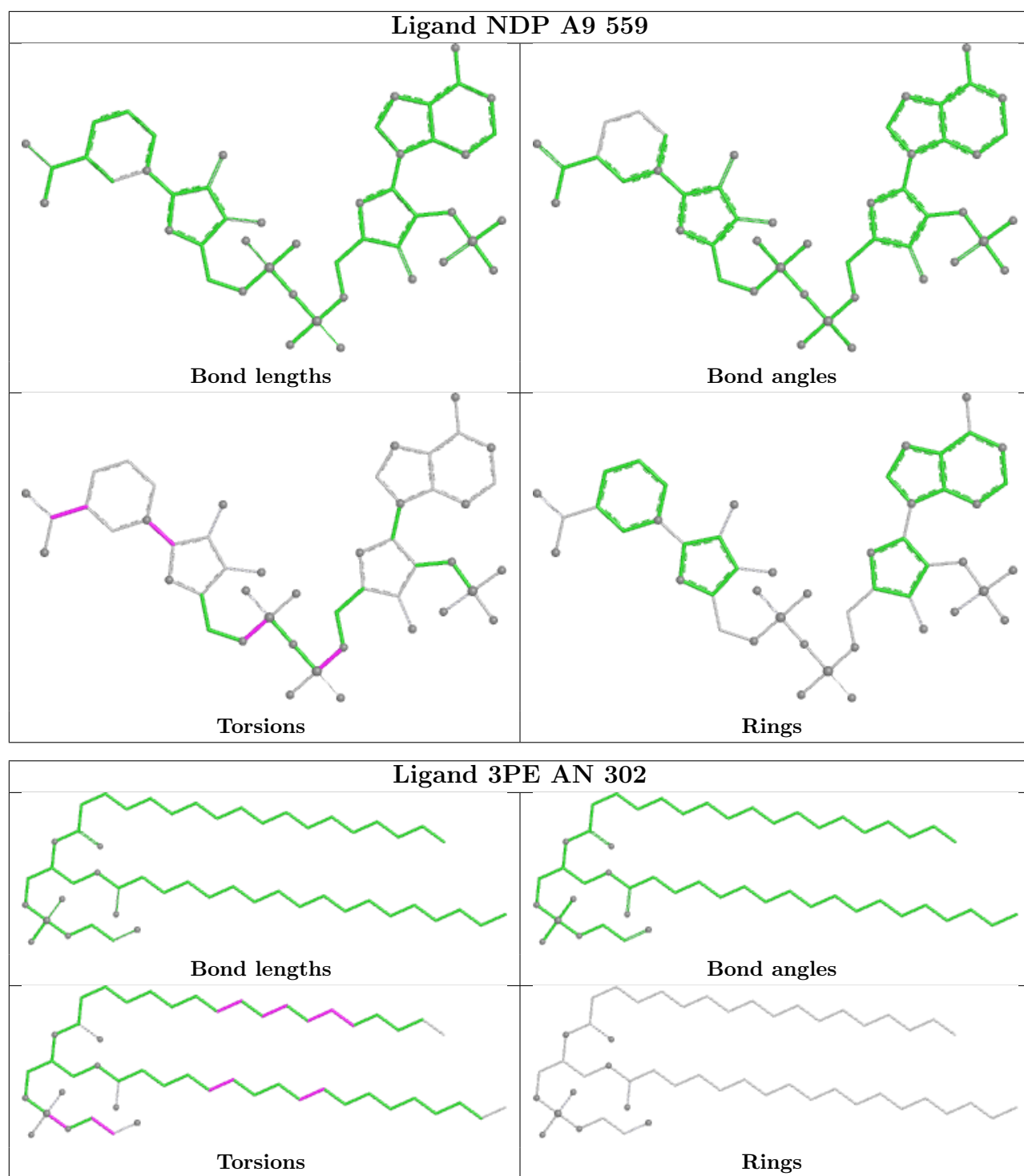


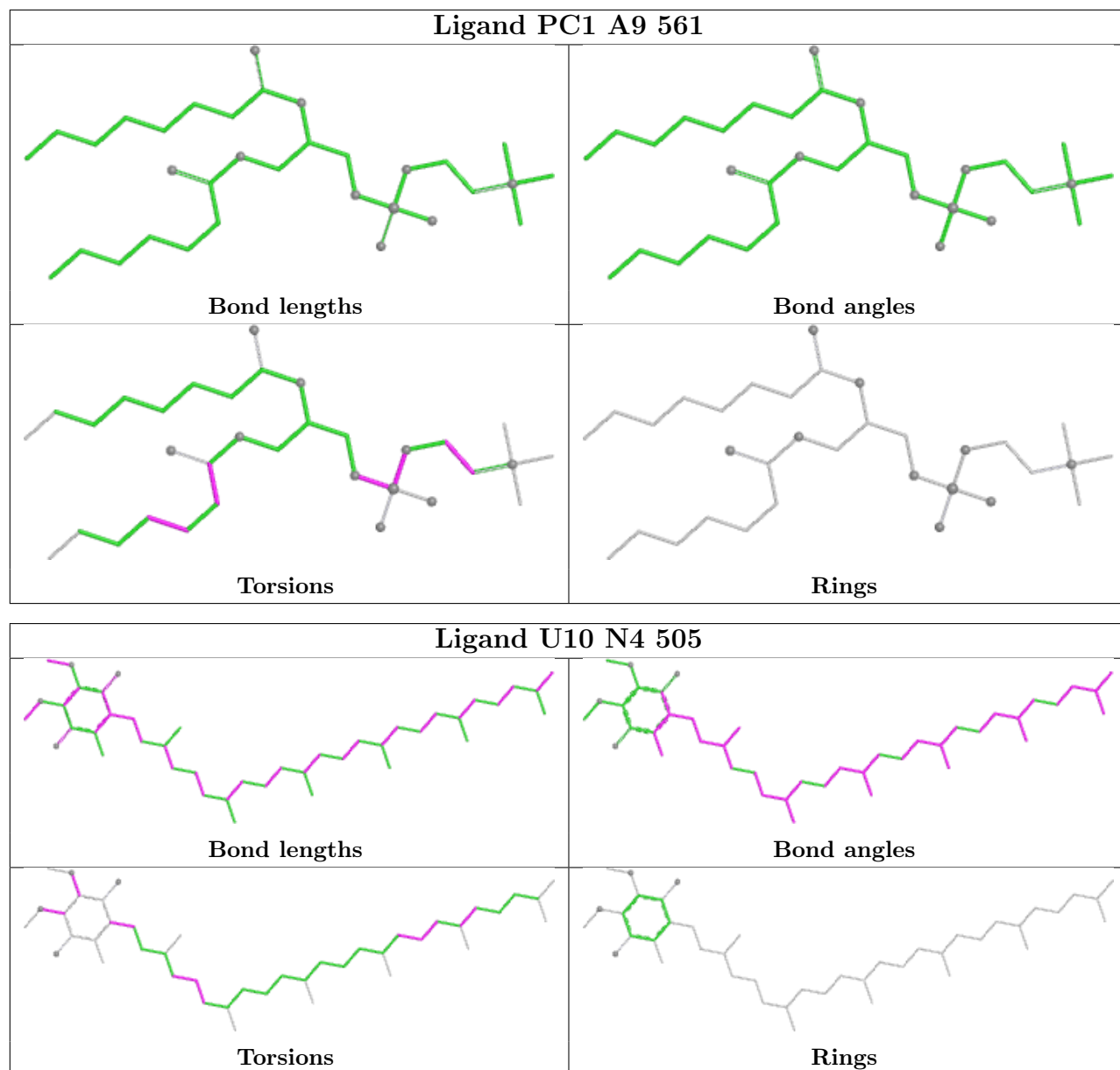


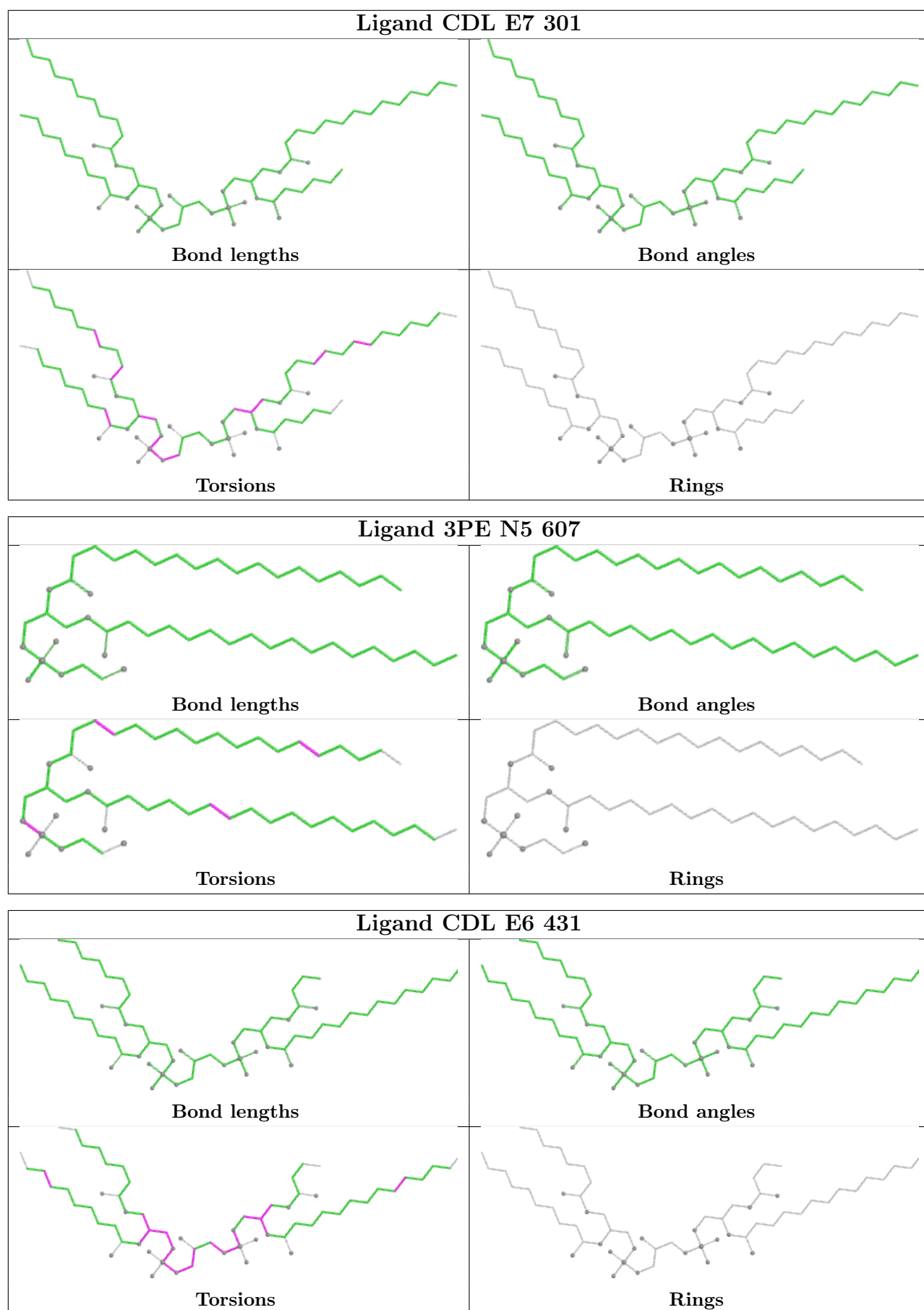


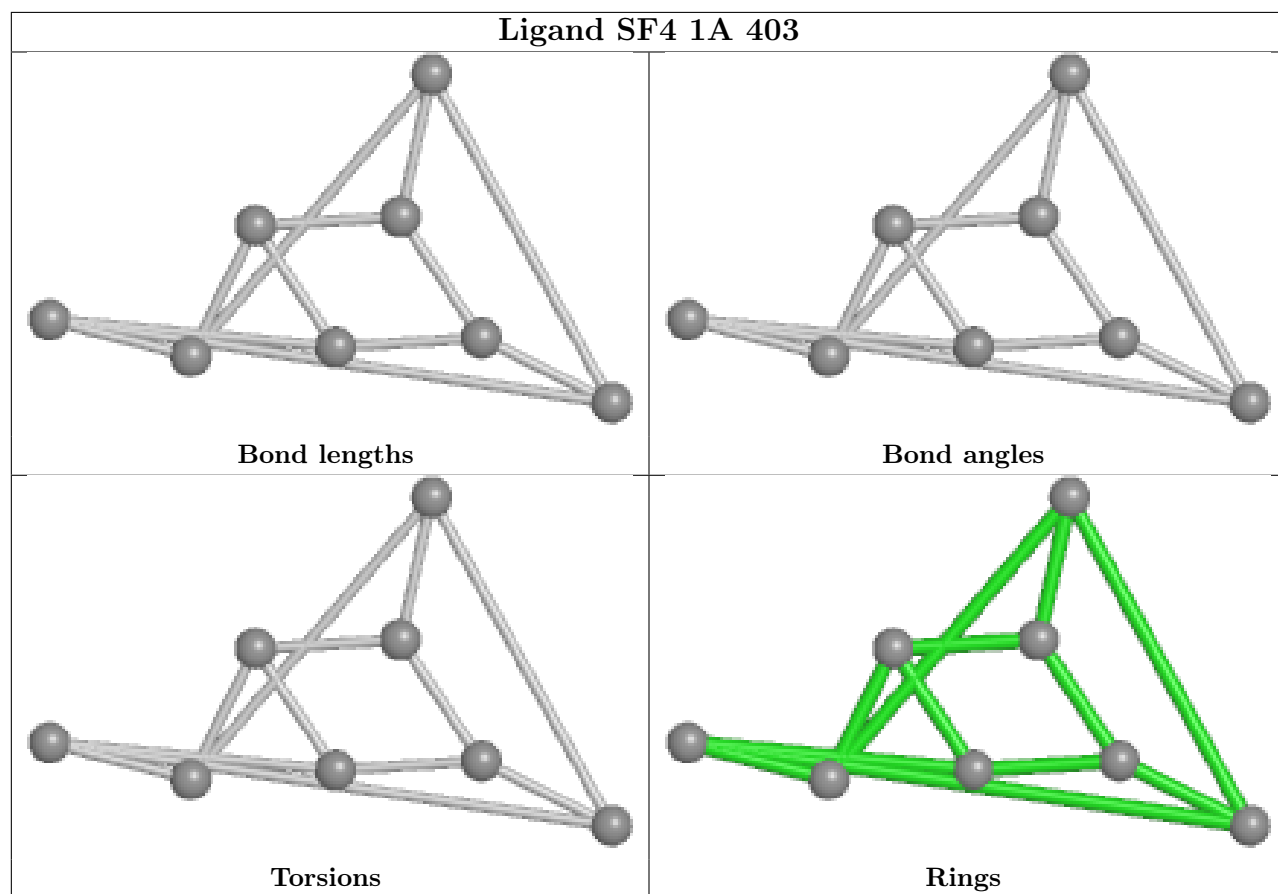
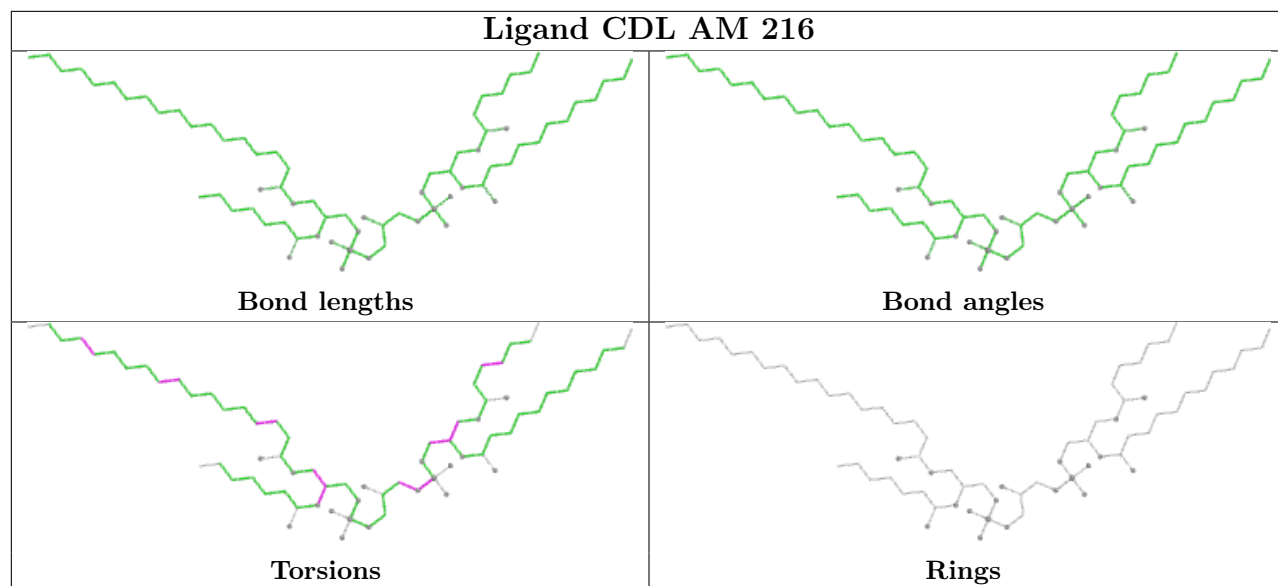


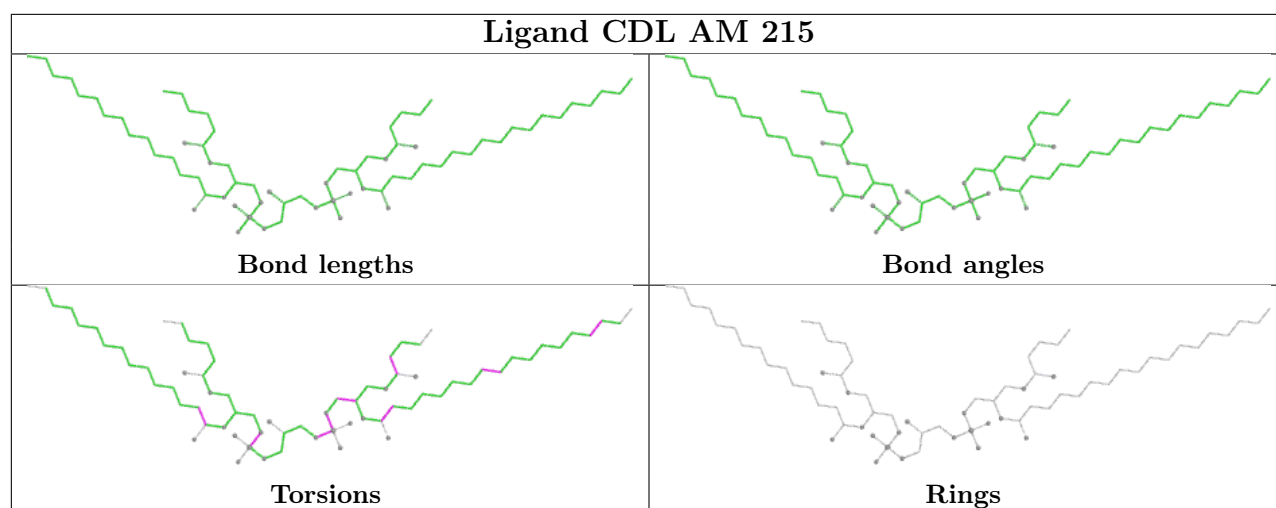












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

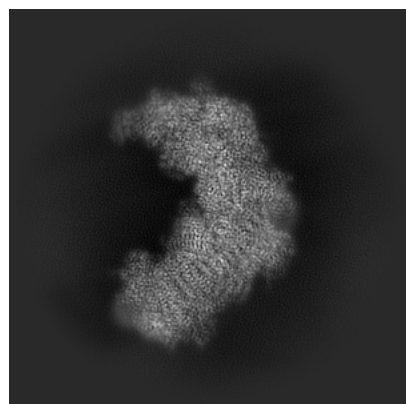
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36109. These allow visual inspection of the internal detail of the map and identification of artifacts.

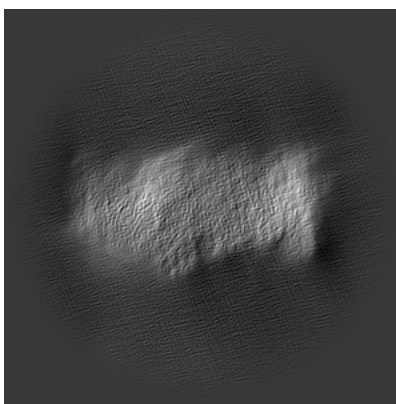
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

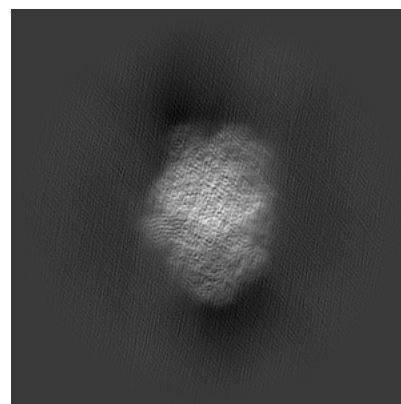
6.1.1 Primary map



X

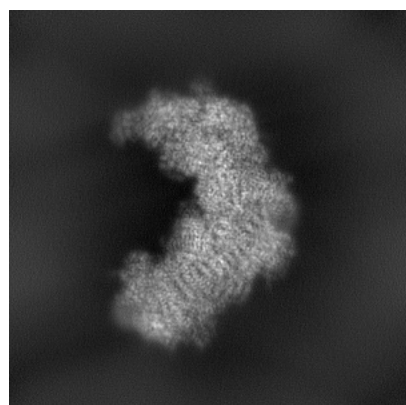


Y

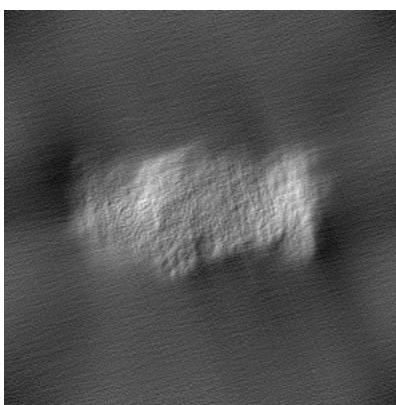


Z

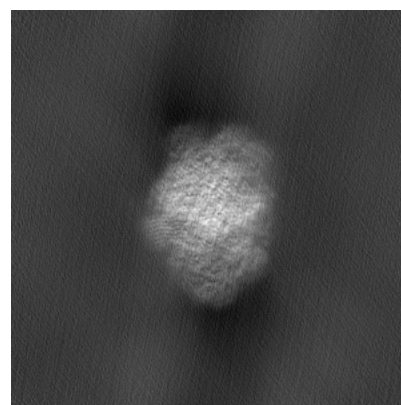
6.1.2 Raw map



X



Y

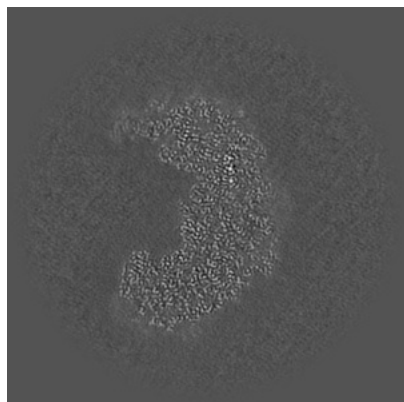


Z

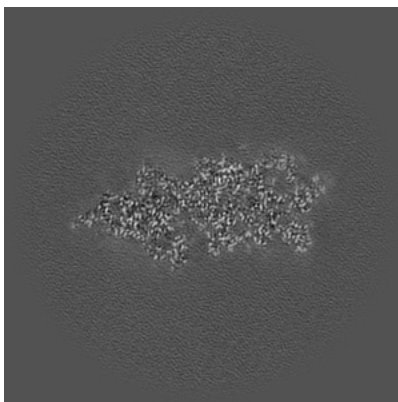
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

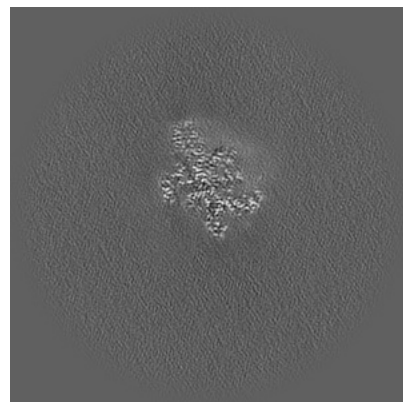
6.2.1 Primary map



X Index: 240

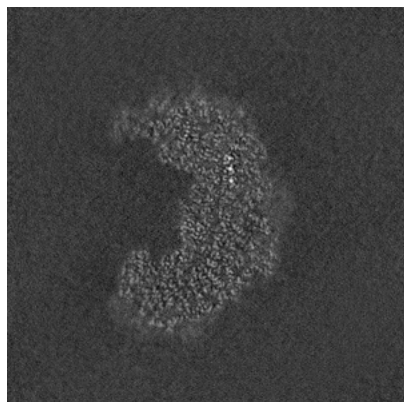


Y Index: 240

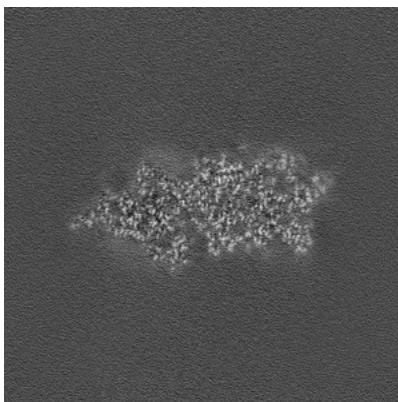


Z Index: 240

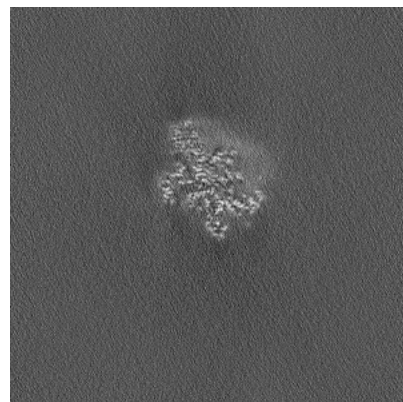
6.2.2 Raw map



X Index: 240



Y Index: 240

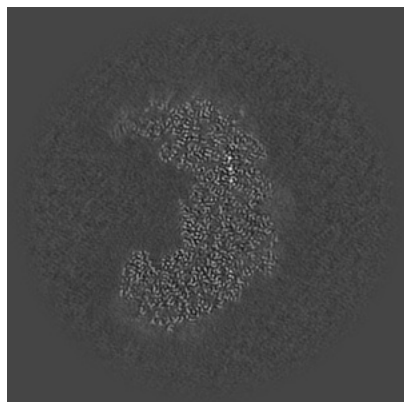


Z Index: 240

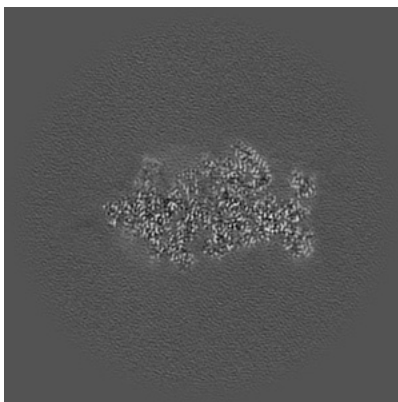
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

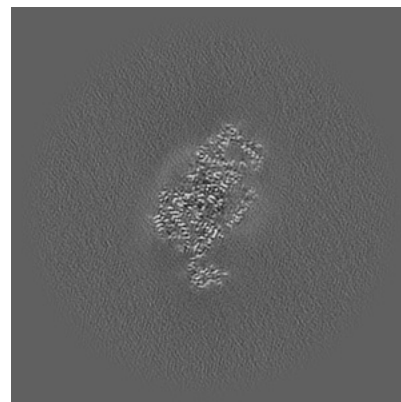
6.3.1 Primary map



X Index: 241

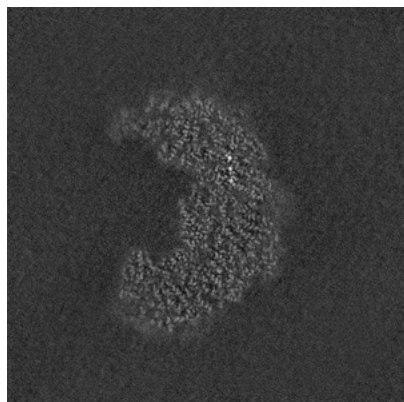


Y Index: 254

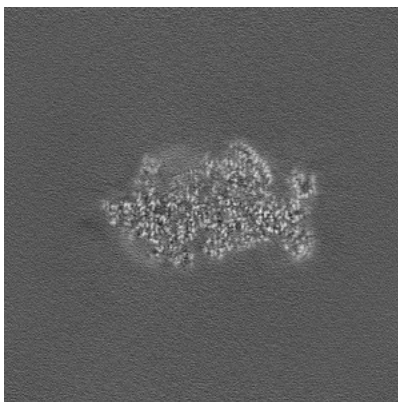


Z Index: 183

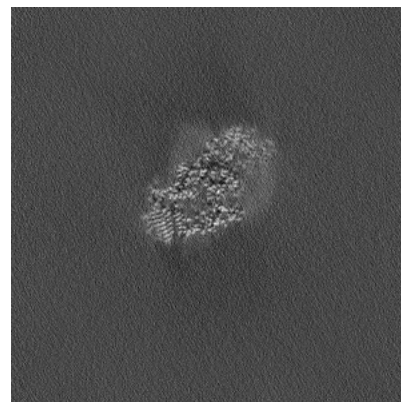
6.3.2 Raw map



X Index: 242



Y Index: 255

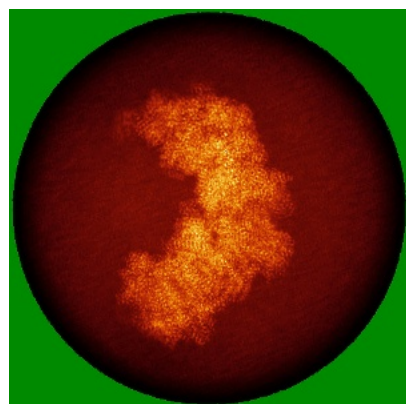


Z Index: 211

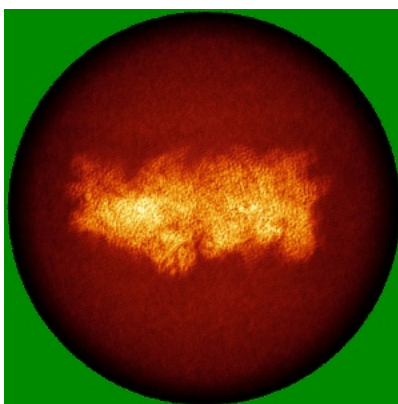
The images above show the largest variance slices of the map in three orthogonal directions.

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

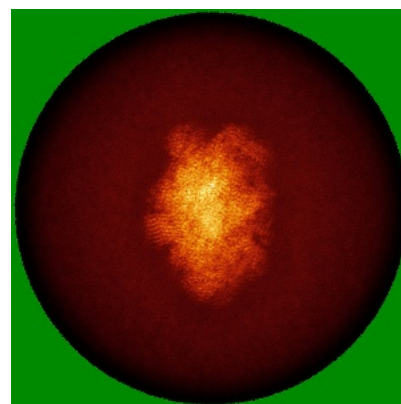
6.4.1 Primary map



X

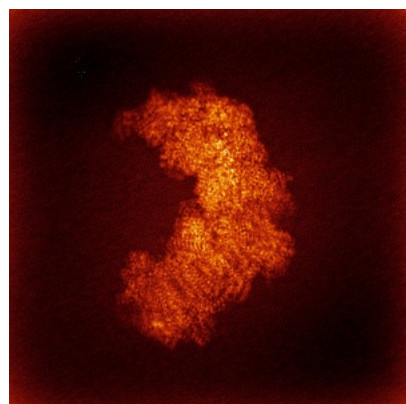


Y

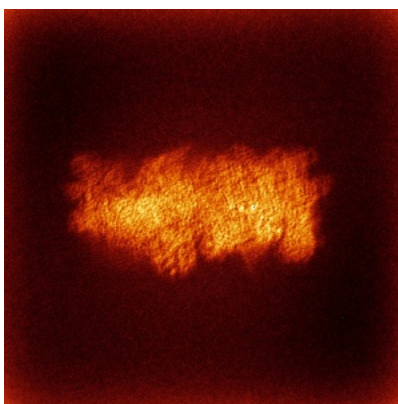


Z

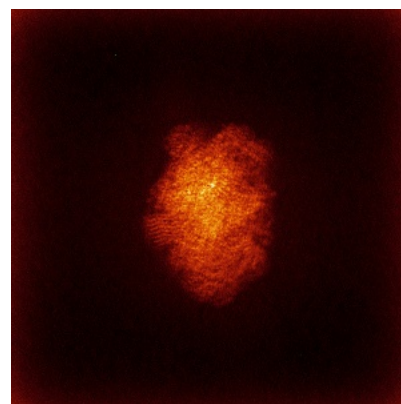
6.4.2 Raw map



X



Y

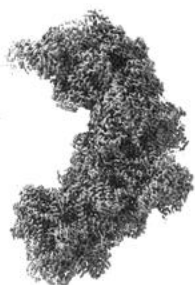


Z

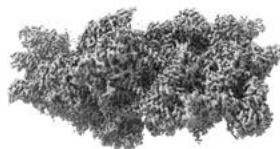
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 5.0. 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



X



Y



Z

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.

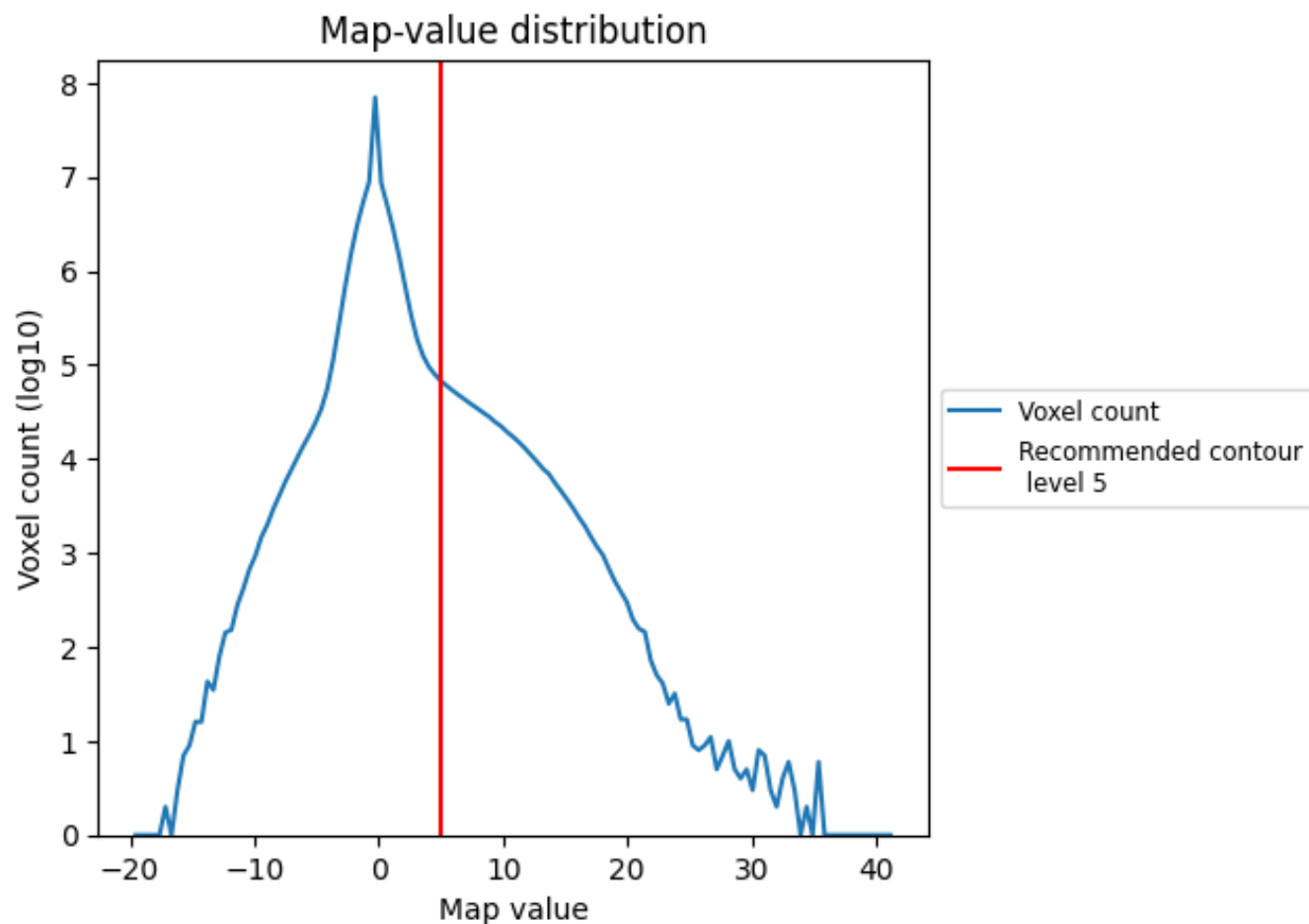
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

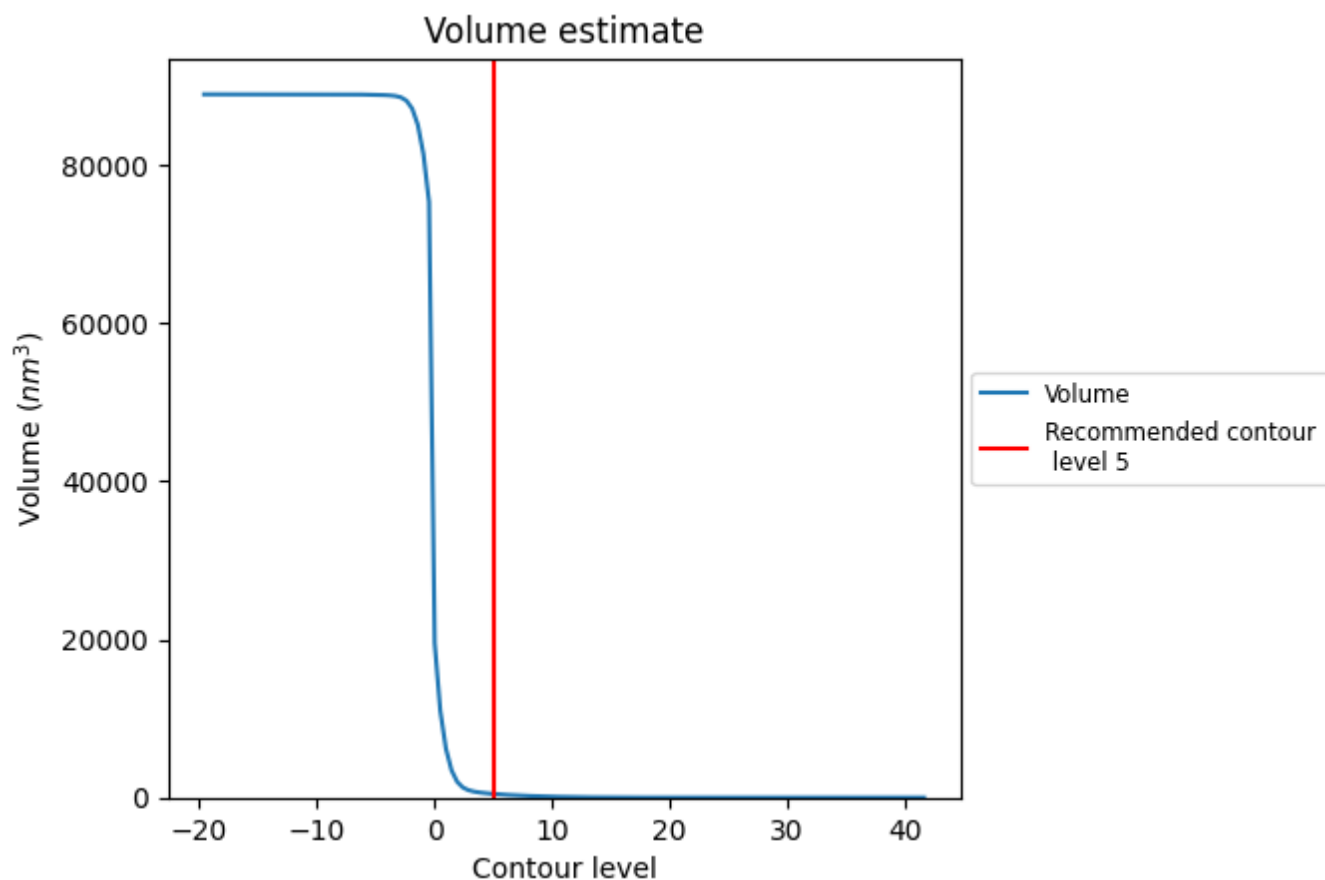
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

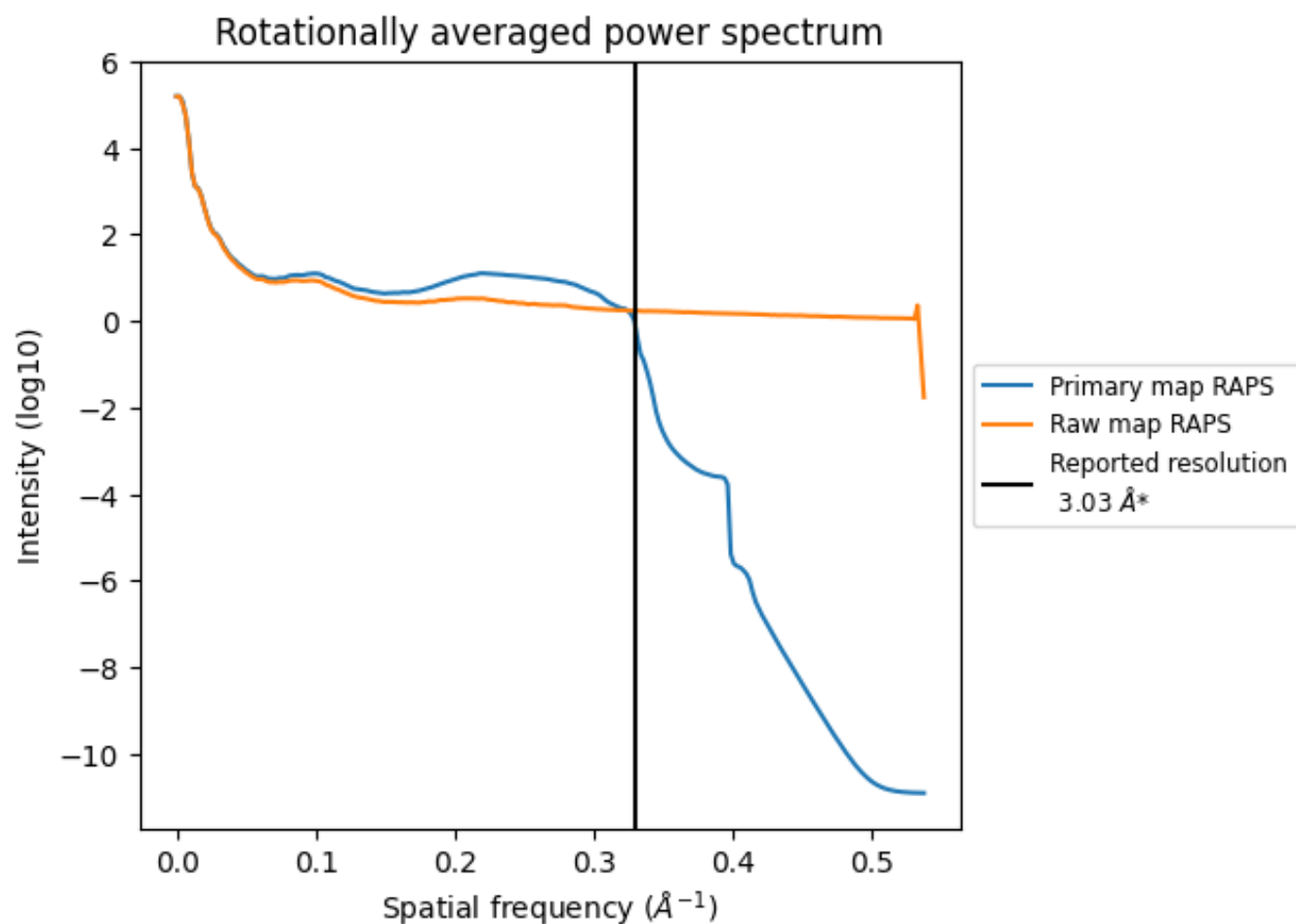
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 468 nm³; this corresponds to an approximate mass of 422 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 ⓘ

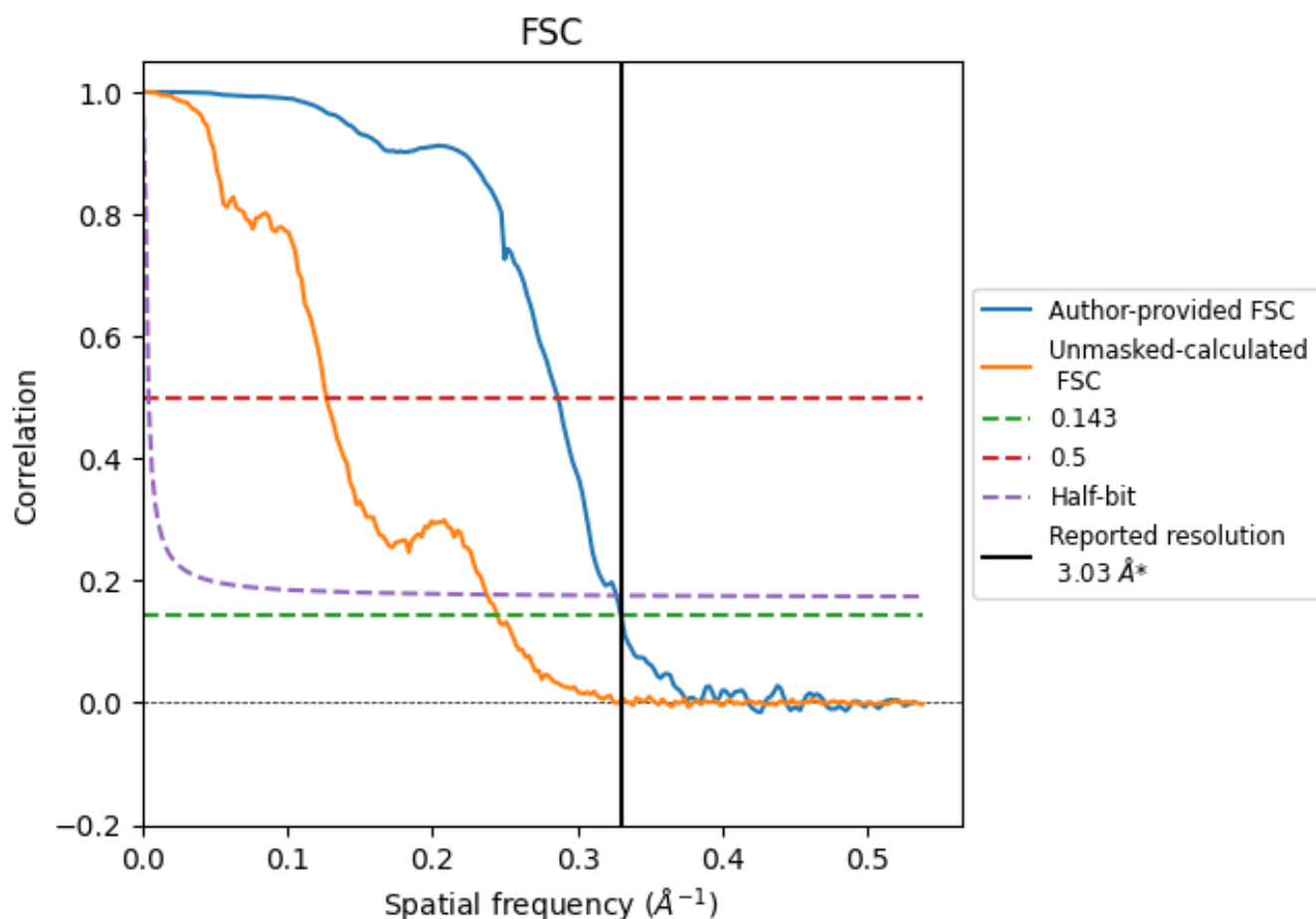


*Reported resolution corresponds to spatial frequency of 0.330 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.330 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

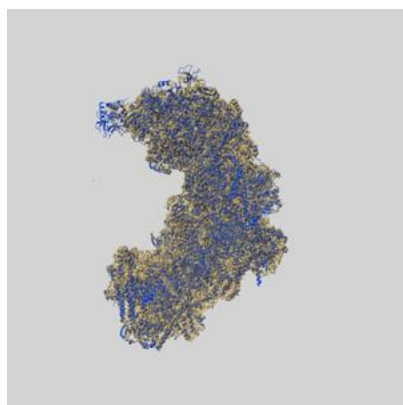
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.03	-	-
Author-provided FSC curve	3.03	3.49	3.06
Unmasked-calculated*	4.08	7.88	4.21

*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 4.08 differs from the reported value 3.03 by more than 10 %

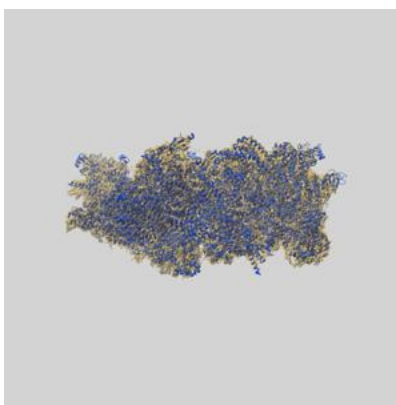
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-36109 and PDB model 8J9J. Per-residue inclusion information can be found in [section 3](#) on [page 23](#).

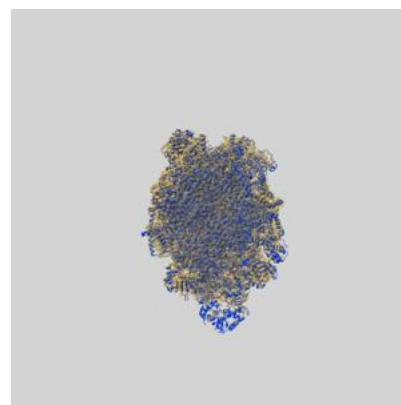
9.1 Map-model overlay [i](#)



X



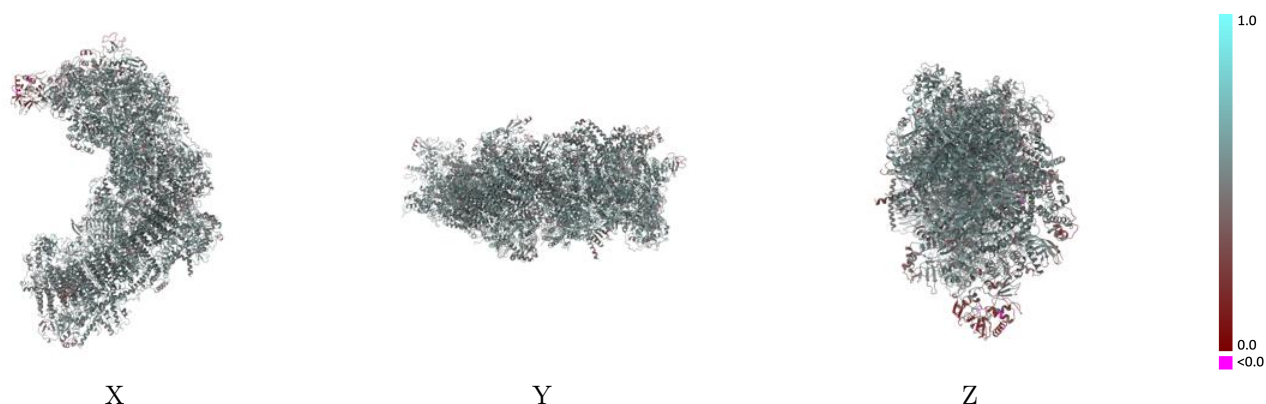
Y



Z

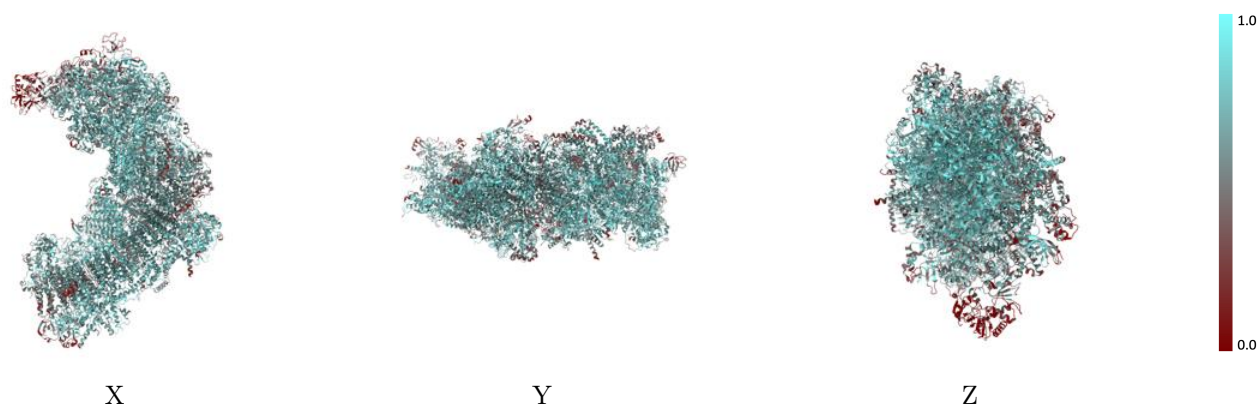
The images above show the 3D surface view of the map at the recommended contour level 5.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



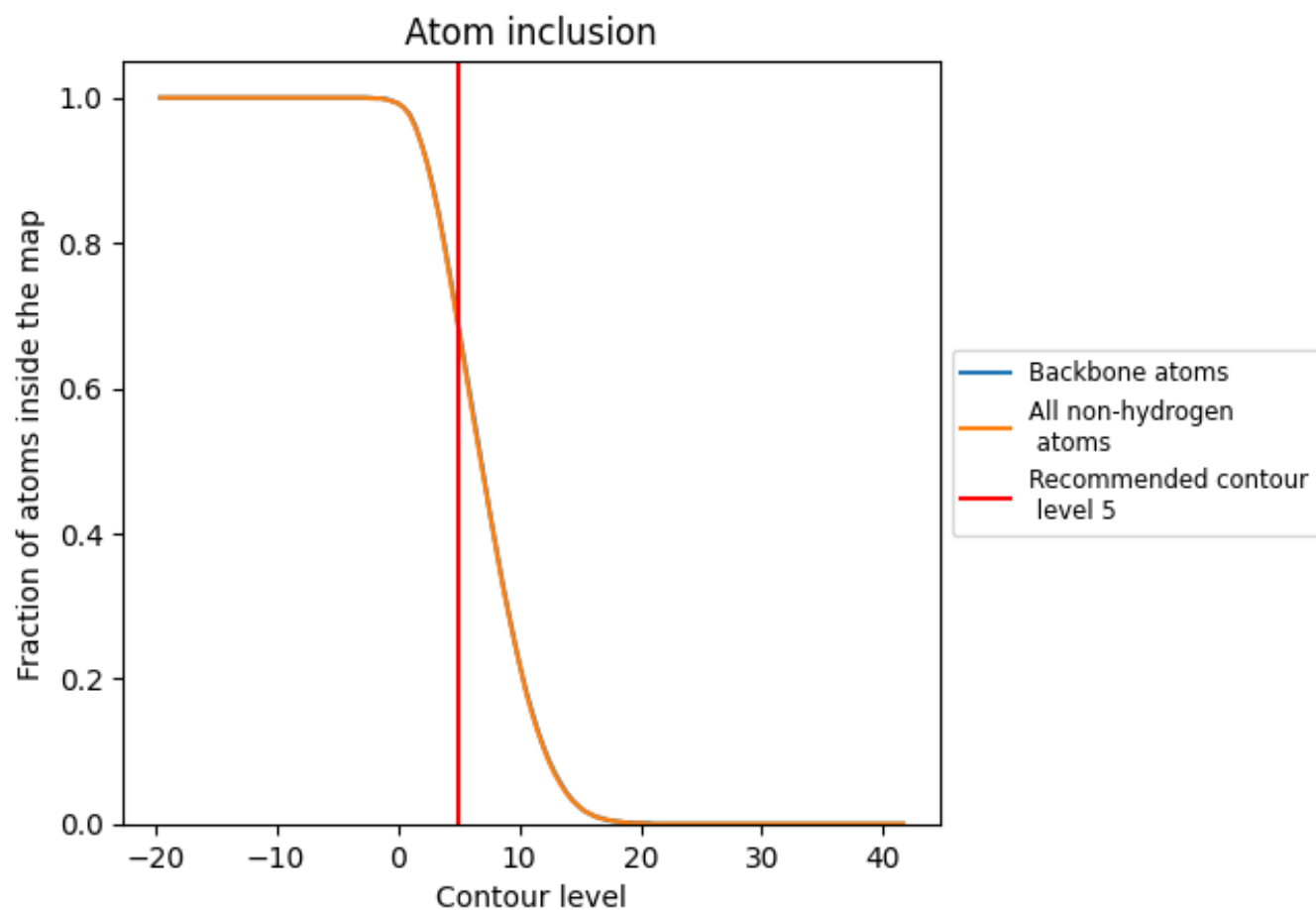
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (5).

9.4 Atom inclusion ⓘ



At the recommended contour level, 69% of all backbone atoms, 68% 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 (5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6830	 0.5310
1A	 0.7740	 0.5520
1B	 0.7650	 0.5520
2B	 0.7530	 0.5500
4L	 0.7580	 0.5550
A1	 0.6010	 0.5150
A2	 0.7160	 0.5450
A3	 0.7040	 0.5380
A5	 0.7070	 0.5240
A6	 0.6070	 0.5050
A7	 0.7800	 0.5580
A8	 0.7210	 0.5270
A9	 0.7230	 0.5360
AB	 0.6720	 0.5390
AC	 0.6660	 0.5430
AL	 0.6780	 0.5390
AM	 0.6390	 0.5220
AN	 0.6640	 0.5320
B2	 0.7130	 0.5450
B3	 0.6530	 0.5270
B4	 0.7300	 0.5410
B5	 0.7140	 0.5340
B6	 0.7120	 0.5420
B7	 0.7310	 0.5310
B8	 0.7680	 0.5540
B9	 0.7450	 0.5530
BL	 0.7280	 0.5310
BM	 0.7410	 0.5460
C4	 0.6710	 0.5330
E1	 0.6680	 0.5160
E2	 0.6130	 0.5020
E3	 0.5980	 0.5050
E4	 0.6400	 0.5360
E5	 0.1700	 0.3130
E6	 0.5780	 0.5030



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Chain	Atom inclusion	Q-score
E7	 0.4490	 0.4710
E8	 0.5760	 0.5010
EA	 0.7550	 0.5570
EB	 0.6830	 0.5350
EC	 0.5790	 0.5140
ED	 0.6060	 0.5130
FX	 0.7730	 0.5560
G1	 0.7360	 0.5520
G2	 0.6790	 0.5310
G3	 0.7150	 0.5390
N1	 0.6910	 0.5350
N2	 0.7650	 0.5540
N3	 0.6990	 0.5490
N4	 0.7490	 0.5480
N5	 0.7090	 0.5390
N6	 0.6400	 0.5200
S2	 0.8060	 0.5640
S3	 0.8000	 0.5580
S4	 0.7480	 0.5540
S5	 0.6870	 0.5320
S6	 0.7910	 0.5640
S7	 0.7590	 0.5510
S8	 0.7810	 0.5590
U1	 0.4330	 0.4740
U2	 0.4830	 0.4840
V1	 0.7460	 0.5390
V2	 0.7500	 0.5420