



Full wwPDB EM Validation Report ⓘ

Aug 6, 2026 – 05:04 AM JST

PDB ID : 8J9I / pdb_00008j9i
EMDB ID : EMD-36108
Title : Cryo-EM structure of Euglena gracilis complex I, turnover 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 : 2.87 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.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
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) : 2.50

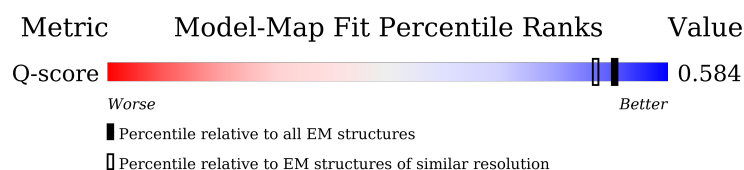
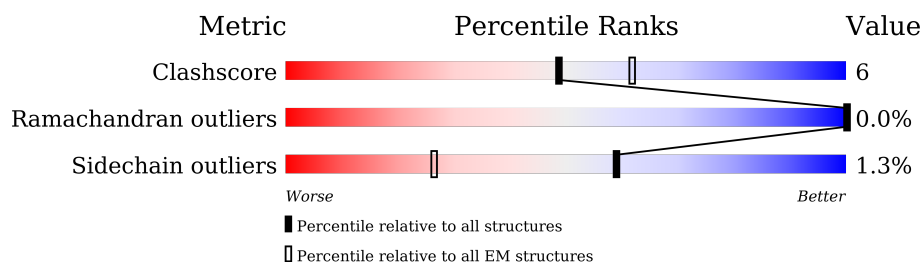
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.87 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.



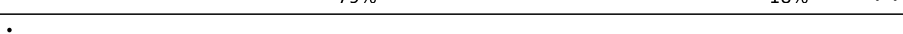
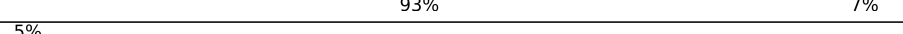
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12062 (2.37 - 3.37)

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	

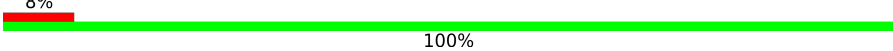
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Mol	Chain	Length	Quality of chain
30	E2	467	
31	E3	434	
32	E4	368	
33	E5	290	
34	E6	371	
35	E8	205	
36	EA	126	
37	EB	101	
38	EC	101	
39	ED	151	
40	FX	325	
41	G1	436	
42	G2	267	
43	G3	261	
44	N1	670	
45	N2	300	
46	N3	293	
46	N6	293	
47	N4	478	
48	N5	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 226854 atoms, of which 112888 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 NDUFC2.

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	342	Total	C	H	N	O	S	0	0
			5629	1839	2758	507	513	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 NDUFX.

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	418	Total	C	H	N	O	S	0	0
			6420	2072	3139	581	612	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 NDUF3.

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 NDUF4.

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 NDUF5.

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 NDUF6.

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 NDUF7.

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 NDUF8.

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		

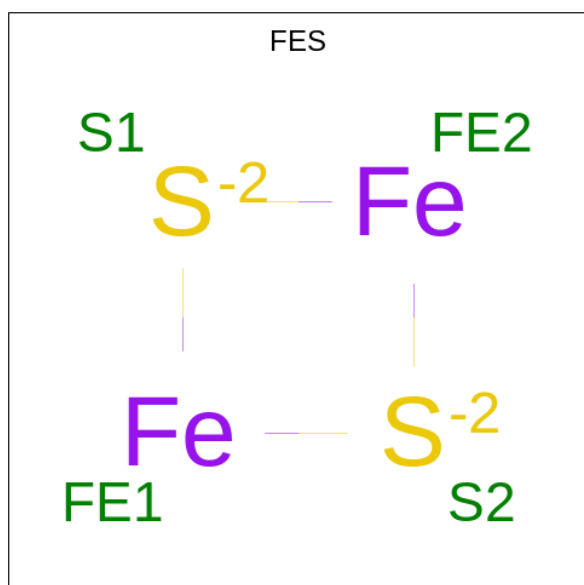
- Molecule 58 is a protein called NDUFV2.

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.

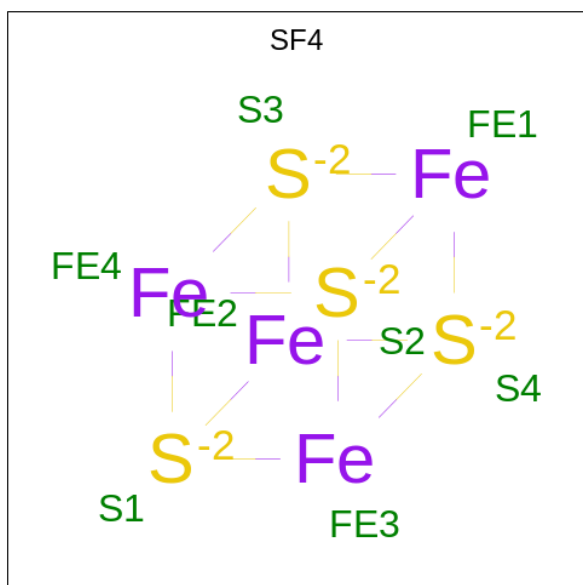
Mol	Chain	Residues	Atoms						AltConf	Trace
59	E7	246	Total	C	H	N	O	S	0	0
			3780	1205	1892	332	344	7		

- 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).

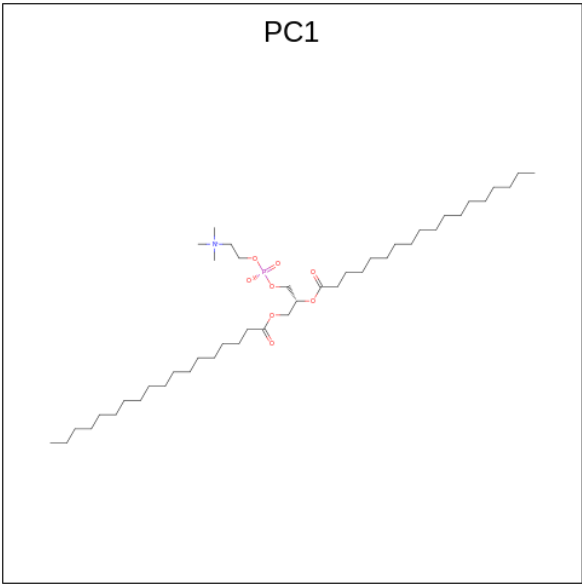


Mol	Chain	Residues	Atoms			AltConf
61	1A	1	Total	Fe	S	0
			8	4	4	
61	1A	1	Total	Fe	S	0
			8	4	4	
61	S7	1	Total	Fe	S	0
			8	4	4	
61	S8	1	Total	Fe	S	0
			8	4	4	
61	S8	1	Total	Fe	S	0
			8	4	4	
61	V1	1	Total	Fe	S	0
			8	4	4	

- 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).



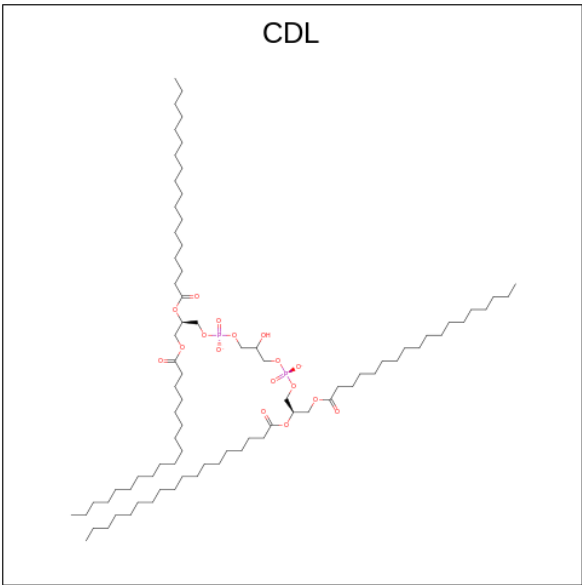
Mol	Chain	Residues	Atoms						AltConf
63	A1	1	Total	C	H	N	O	P	0
			124	39	75	1	8	1	
63	A1	1	Total	C	H	N	O	P	0
			67	21	36	1	8	1	
63	A9	1	Total	C	H	N	O	P	0
			73	23	40	1	8	1	
63	A9	1	Total	C	H	N	O	P	0
			73	23	40	1	8	1	
63	AL	1	Total	C	H	N	O	P	0
			127	40	77	1	8	1	
63	AM	1	Total	C	H	N	O	P	0
			124	39	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: $C_{81}H_{156}O_{17}P_2$).



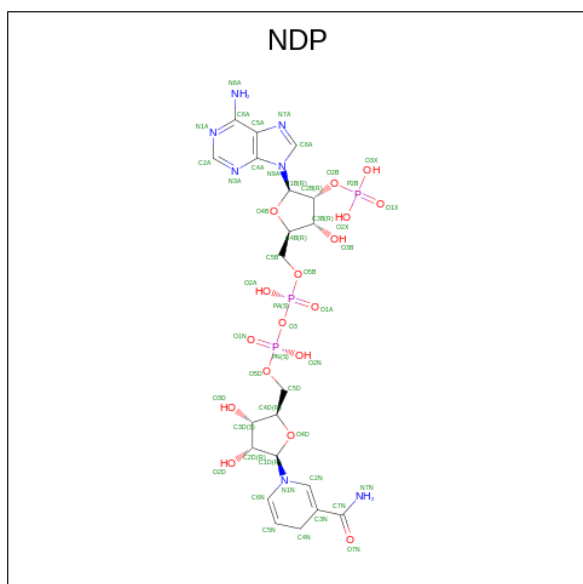
Mol	Chain	Residues	Atoms					AltConf
64	A3	1	Total	C	H	O	P	0
			118	39	60	17	2	
64	AL	1	Total	C	H	O	P	0
			148	49	80	17	2	
64	AL	1	Total	C	H	O	P	0
			136	45	72	17	2	
64	AL	1	Total	C	H	O	P	0
			154	51	84	17	2	
64	AM	1	Total	C	H	O	P	0
			163	53	91	17	2	
64	AM	1	Total	C	H	O	P	0
			163	53	91	17	2	
64	AM	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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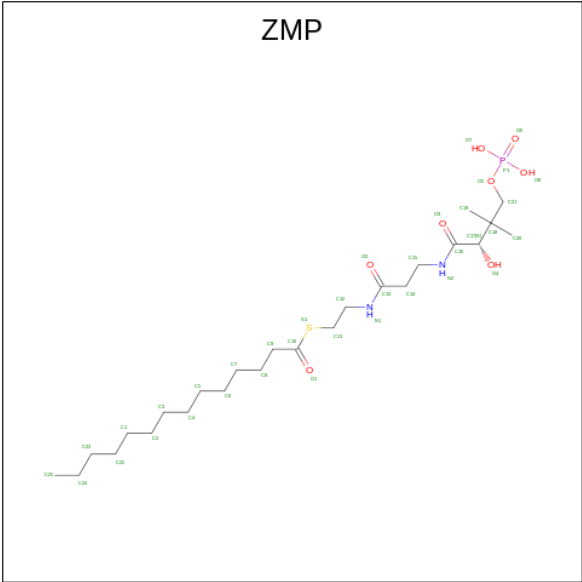
Mol	Chain	Residues	Atoms					AltConf
64	N4	1	Total	C	H	O	P	0
			247	79	149	17	2	
64	N5	1	Total	C	H	O	P	0
			157	51	87	17	2	
64	N5	1	Total	C	H	O	P	0
			229	74	136	17	2	
64	E7	1	Total	C	H	O	P	0
			148	49	80	17	2	

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



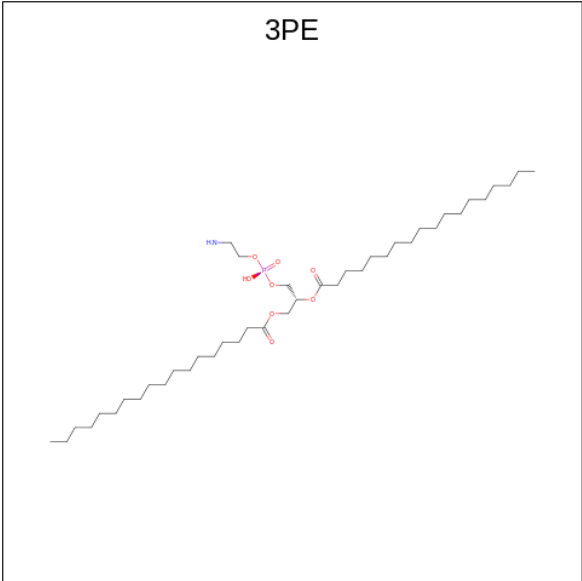
Mol	Chain	Residues	Atoms						AltConf
65	A9	1	Total	C	H	N	O	P	0
			74	21	26	7	17	3	

- 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).



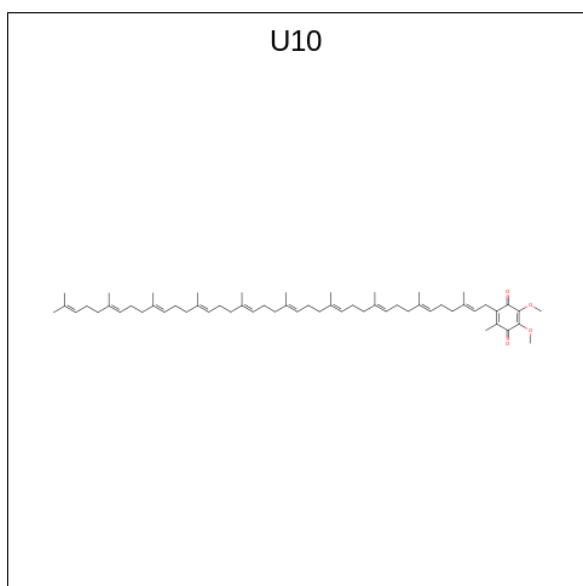
Mol	Chain	Residues	Atoms						AltConf
67	AN	1	Total	C	H	N	O	P	0
			132	41	81	1	8	1	

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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).

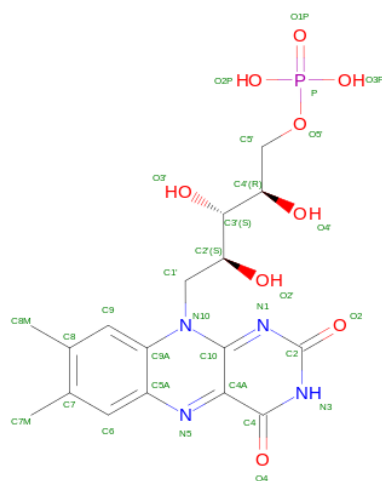


Mol	Chain	Residues	Atoms				AltConf
68	N4	1	Total	C	H	O	
			98	39	55	4	0

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

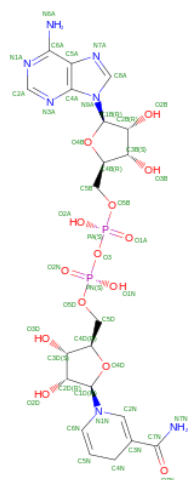
Mol	Chain	Residues	Atoms		AltConf
69	S6	1	Total	Zn	
			1	1	0
69	E7	1	Total	Zn	
			1	1	0

- 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: $\text{C}_{21}\text{H}_{29}\text{N}_7\text{O}_{14}\text{P}_2$).

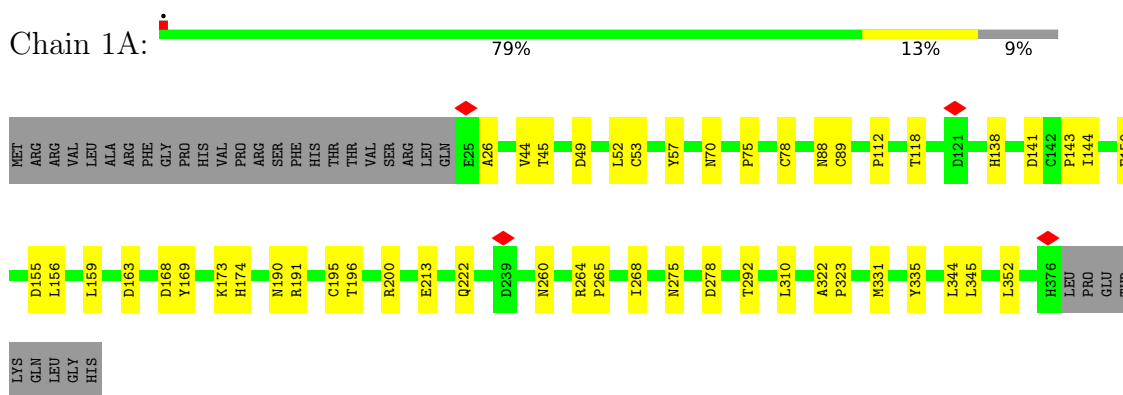


Mol	Chain	Residues	Atoms					AltConf
71	V1	1	Total 44	C 21	N 7	O 14	P 2	0

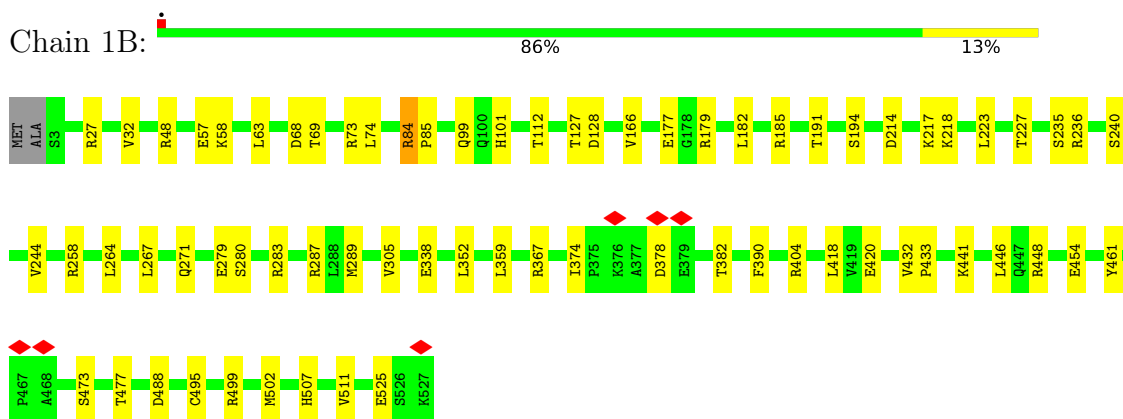
3 Residue-property plots

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.

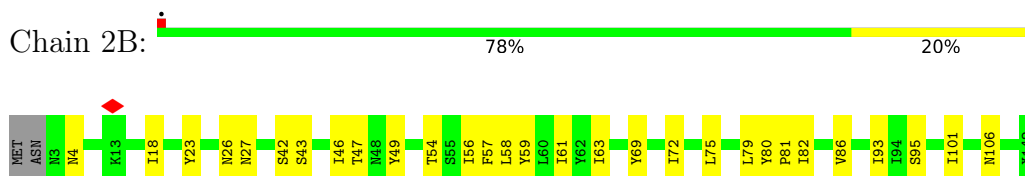
• Molecule 1: NDUFS1A



• Molecule 2: NDUFS1B

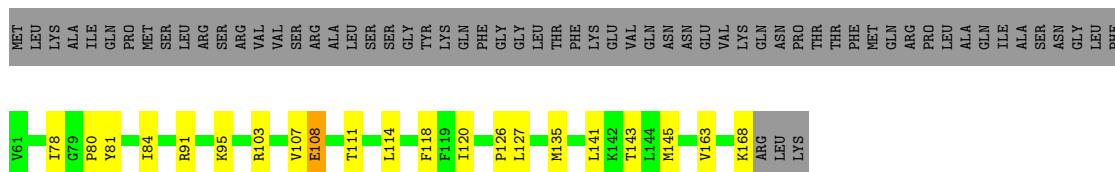


• Molecule 3: ND2B



• Molecule 4: ND4L

Chain 4L:  51% 12% 37%



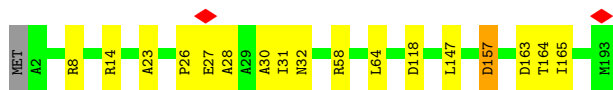
• Molecule 5: NDUFA1

Chain A1:  89% 8%



• Molecule 6: NDUFA2

Chain A2:  91% 8%



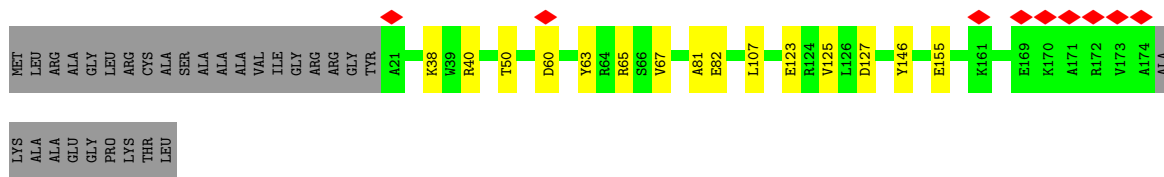
• Molecule 7: NDUFA3

Chain A3:  90% 10%



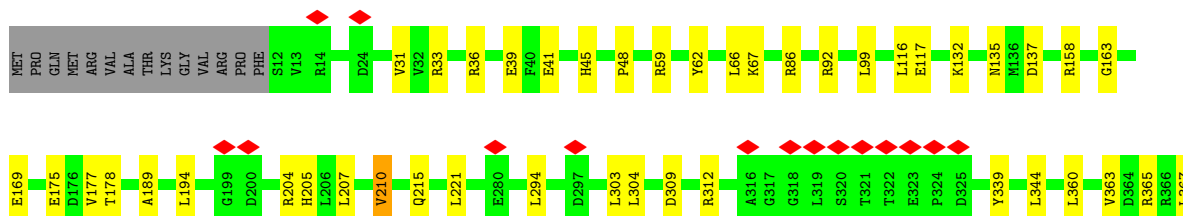
• Molecule 8: NDUFA5

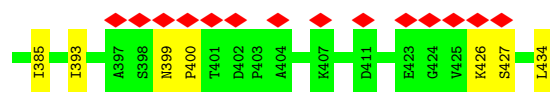
Chain A5:  5% 76% 8% 16%



• Molecule 9: NDUFA6

Chain A6:  7% 85% 11%

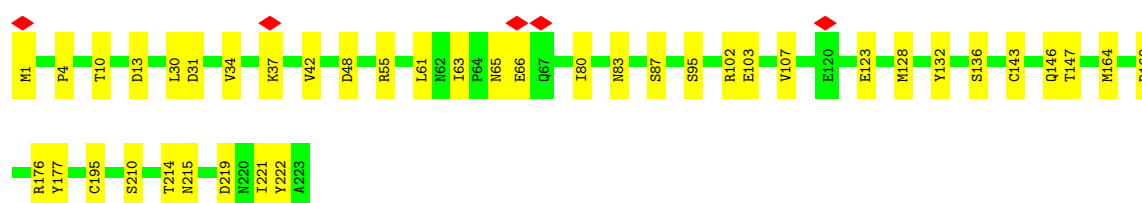
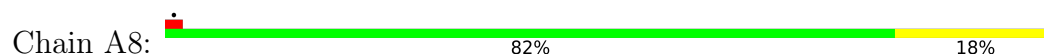




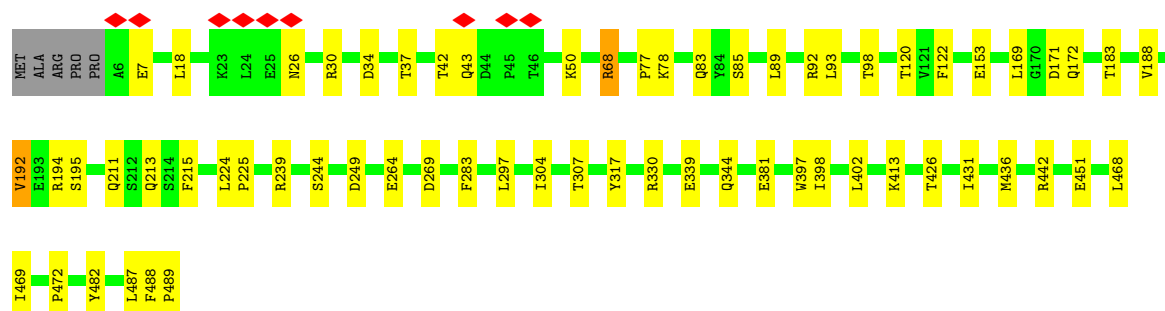
• Molecule 10: NDUFA7



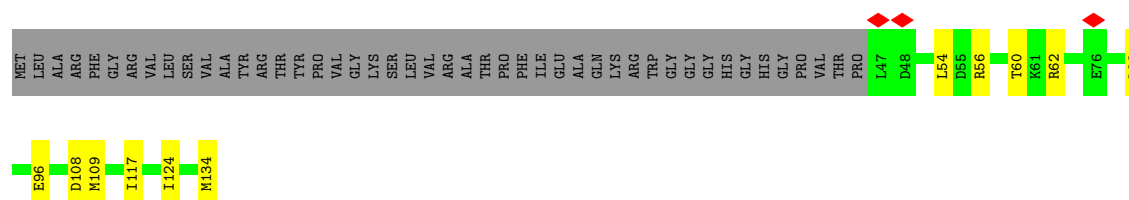
• Molecule 11: NDUFA8



• Molecule 12: NDUFA9

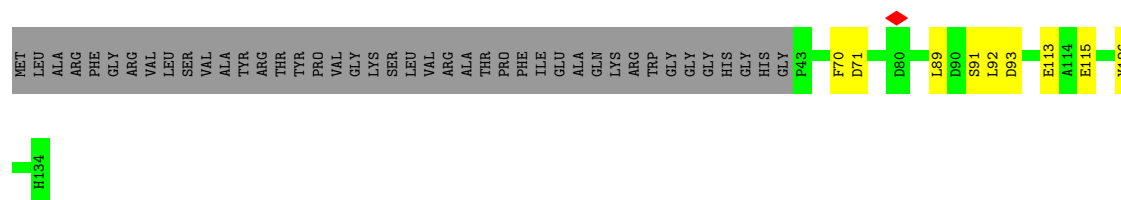


• Molecule 13: NDUFAB1-alpha

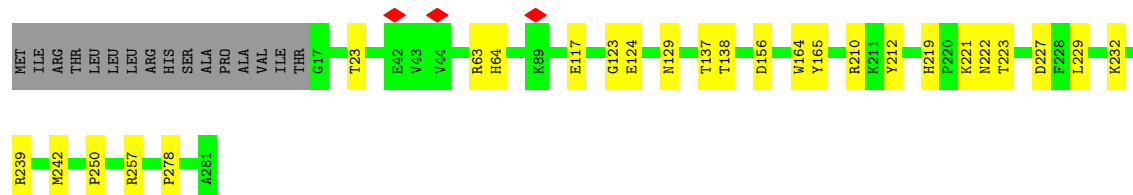


• Molecule 14: NDUFAB1-beta

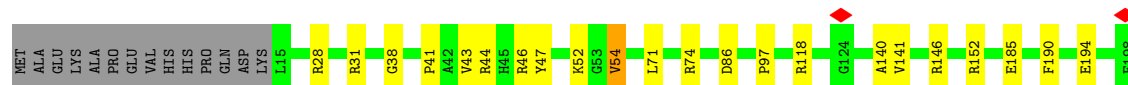
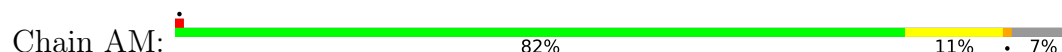




- Molecule 15: NDUFA12



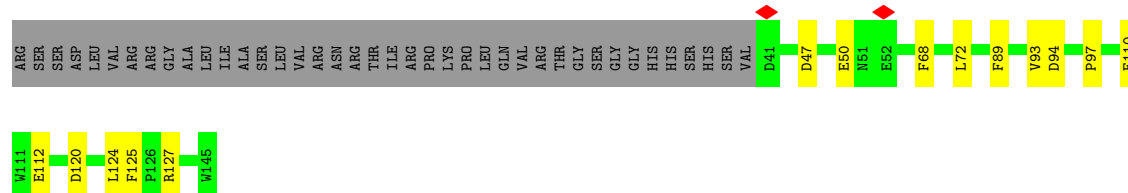
- Molecule 16: NDUFA13



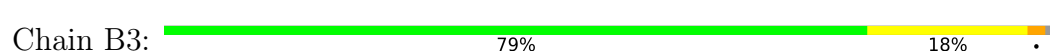
- Molecule 17: NDUFA11



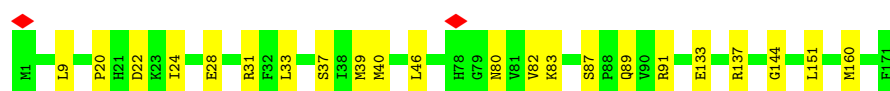
- Molecule 18: NDUFB2



- Molecule 19: NDUFB3



- Molecule 20: NDUFB4



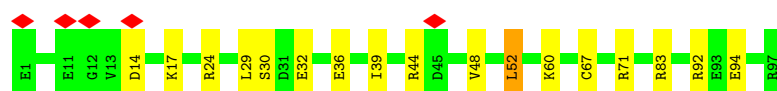
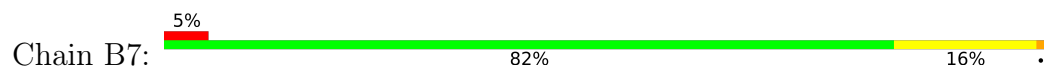
• Molecule 21: NDUFB5



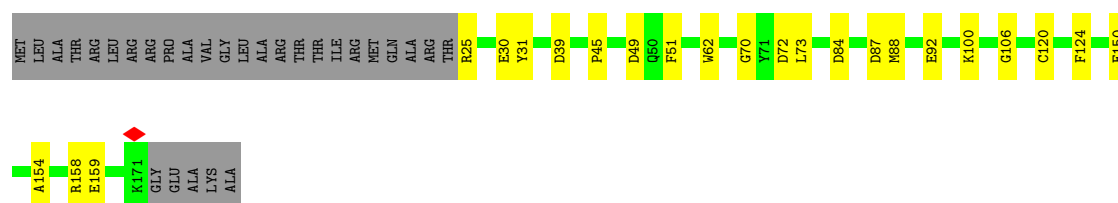
• Molecule 22: NDUFB6



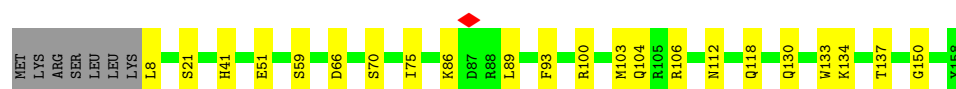
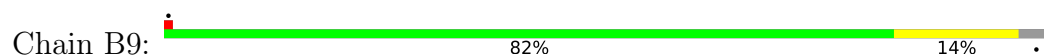
• Molecule 23: NDUFB7



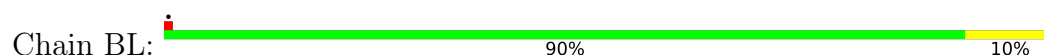
• Molecule 24: NDUFB8



• Molecule 25: NDUFB9



• Molecule 26: NDUFB10

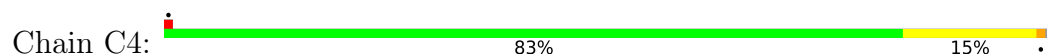




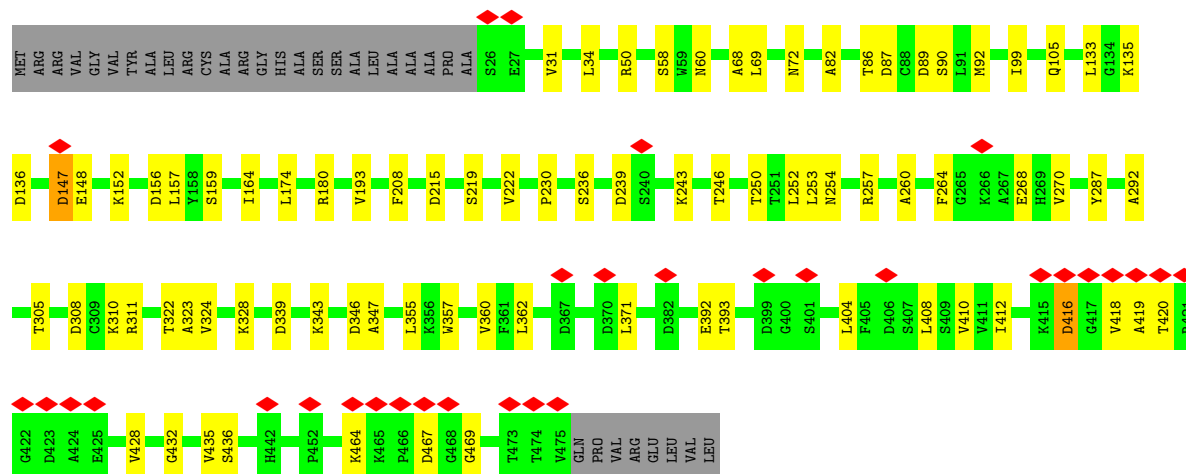
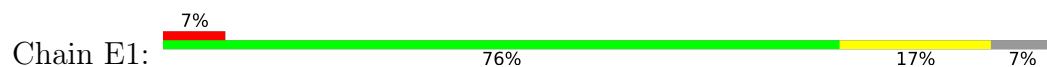
• Molecule 27: NDUFB1



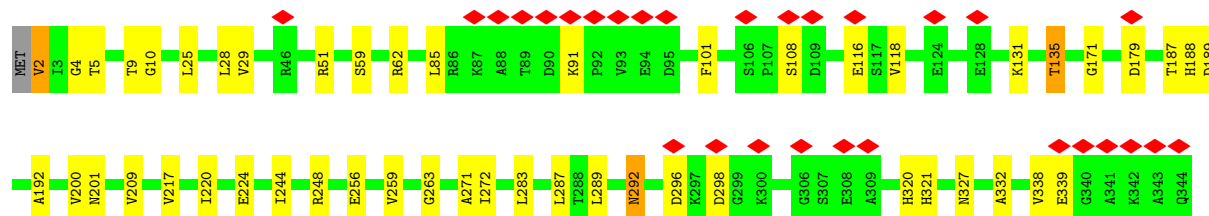
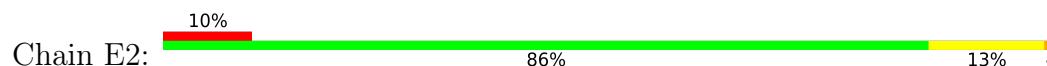
• Molecule 28: NDUFC2

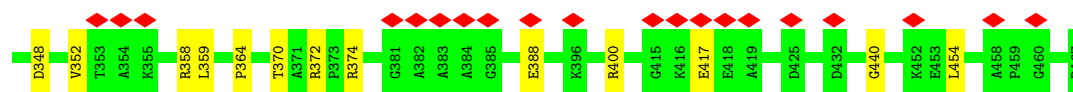


• Molecule 29: NDUEG1

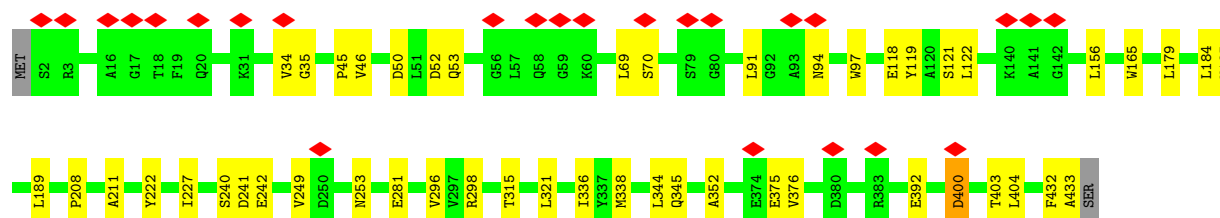


• Molecule 30: NDUEG2

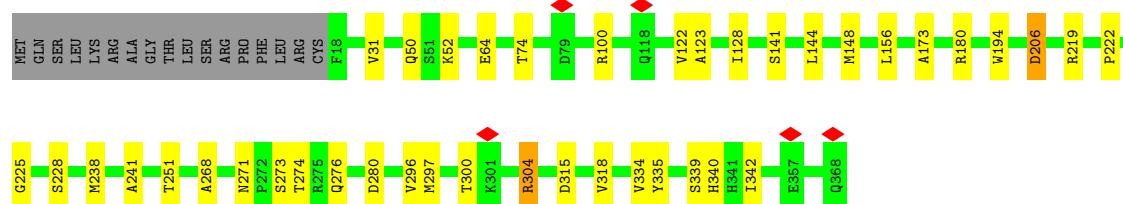
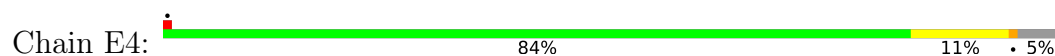




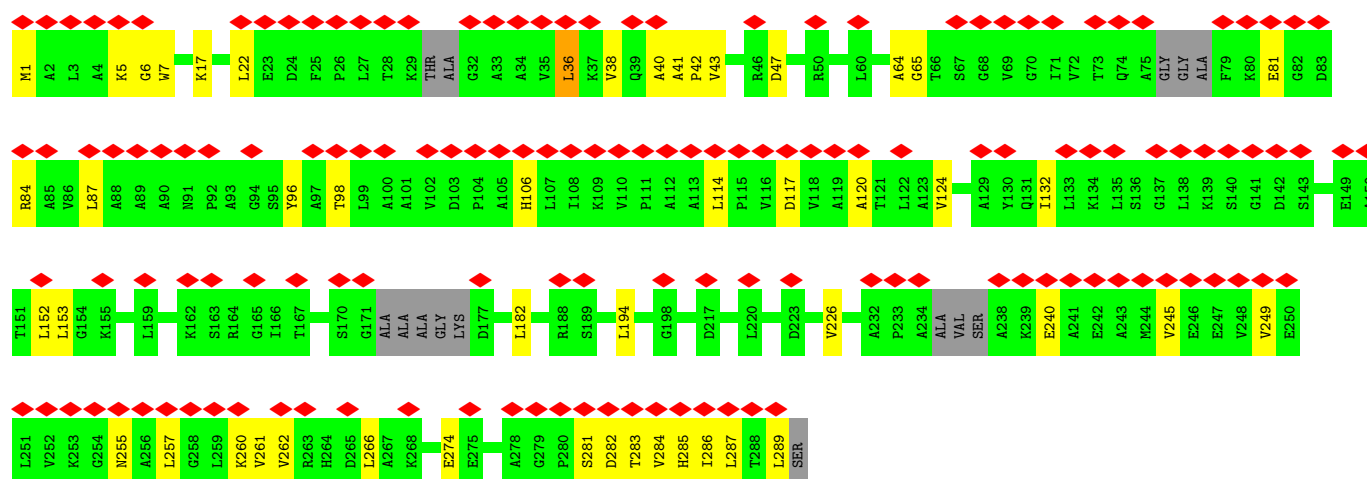
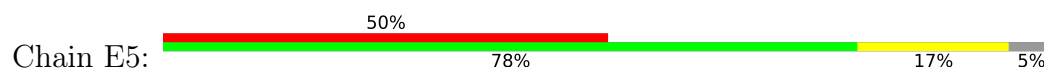
• Molecule 31: NDUEG3



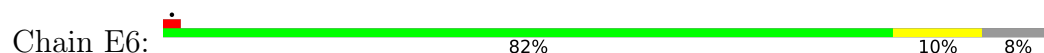
• Molecule 32: NDUEG4

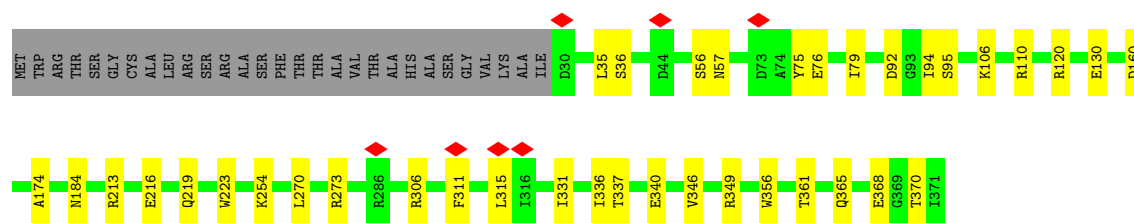


• Molecule 33: NDUEG5

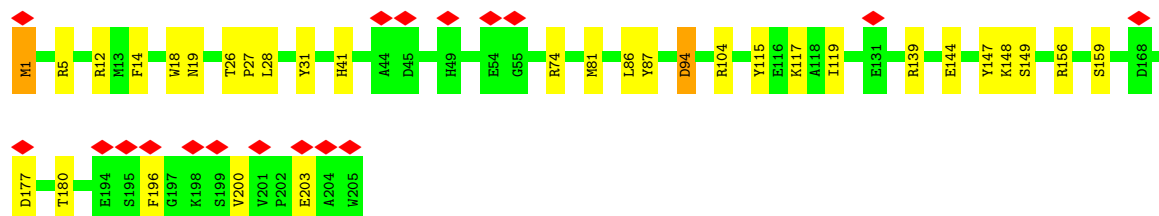
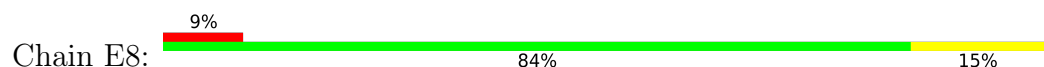


• Molecule 34: NDUEG6





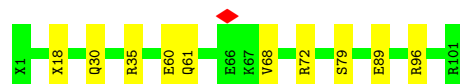
• Molecule 35: NDUEG8



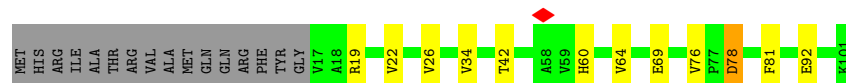
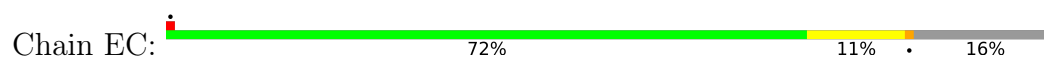
• Molecule 36: NDUEG10



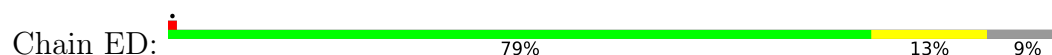
• Molecule 37: NDUEG11



• Molecule 38: NDUEG12

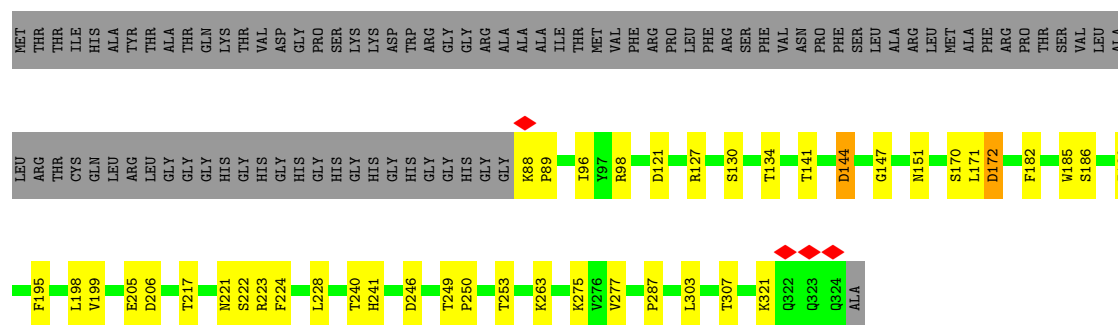


• Molecule 39: NDUEG13



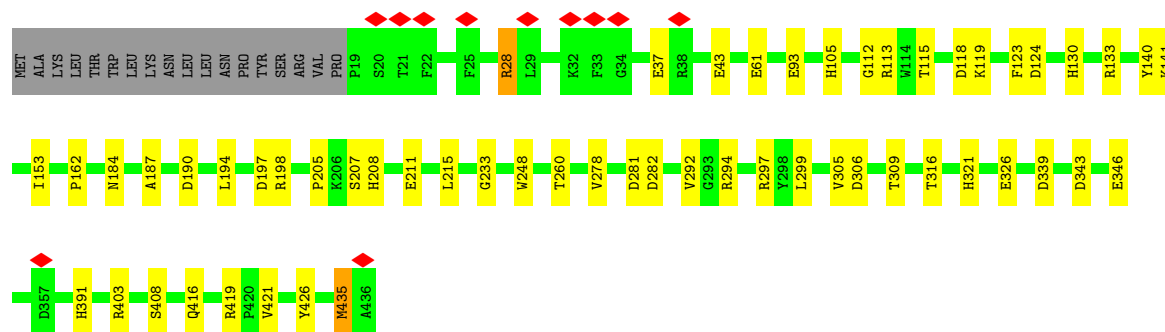
• Molecule 40: NDUFUX

Chain FX:  60% 13% 27%



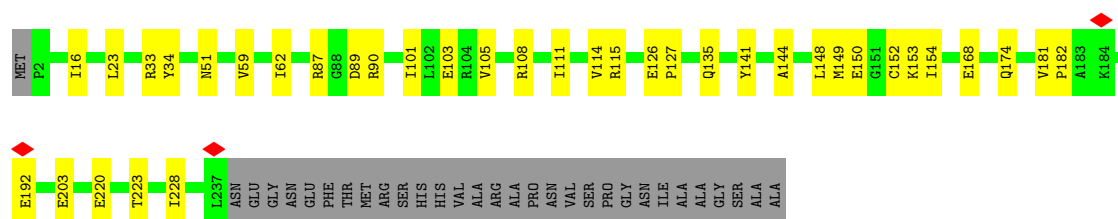
• Molecule 41: NDUCA1

Chain G1:  83% 13%



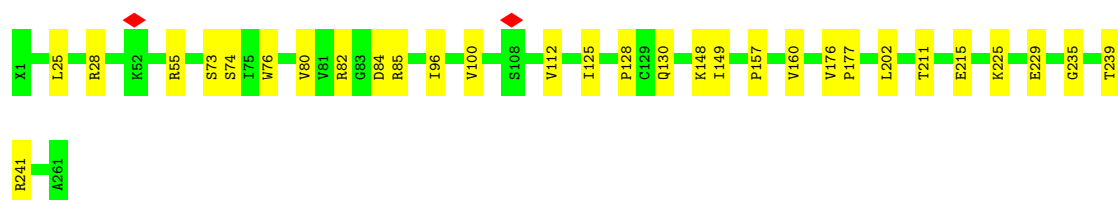
• Molecule 42: NDUCA2

Chain G2:  75% 14% 12%



• Molecule 43: NDUCA3

Chain G3:  88% 12%



• Molecule 44: ND1

- Molecule 45: ND2A

- Molecule 46: ND3

- Molecule 46: ND3

[illegible]

Response	Percentage
Yes, it is a crisis	78%
No, it is not a crisis	21%

L462	T317	K150	M1
P458	S318	I153	R9
L472	Y325	M157	L14
L478	I327	L162	M22
	F328	Y163	S33
	I329	S164	I34
	N330	M173	I35
	I331		S36
	M336	M177	I37
	I337	T184	I38
	Y352	S185	S39
	I353	N186	I40
	Y354	I187	I43
	D355		M44
	I356	N190	N59
	Y357	L211	I62
	N358		N67
	L362	G214	Y70
	I365	G228	I73
	N366	V232	G74
	I369	E233	I75
	I370	T236	L79
	V392	L242	I80
	F396	S246	Y91
	E397		E92
	S403	H254	Y95
	L404	Y255	N98
	S405	L256	N99
	I406	L269	M100
	F407	I273	Y108
	N408	Y274	I109
	S412		I110
	L415	I282	M111
	S419	Y283	M112
	C420	N284	I113
	S421	I287	F114
	N422		D119
	S426	T293	I120
		Y300	L125
	K432		I126
	I442	M305	T131
	F448	Y308	
		I346	

Category	Percentage
Satisfied	77%
Dissatisfied	23%

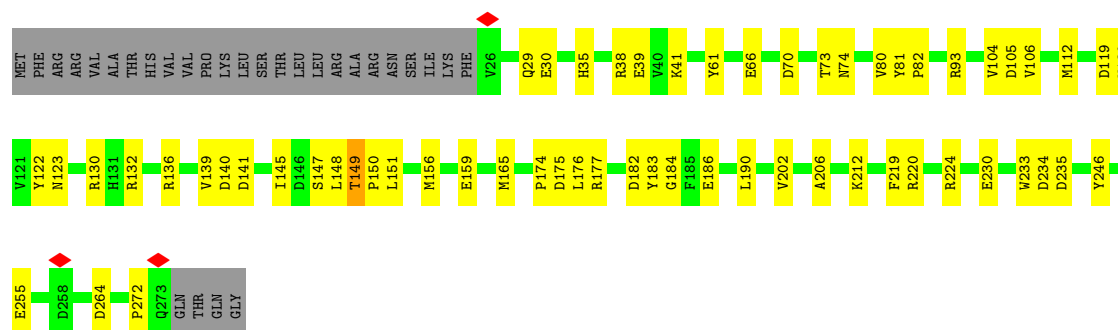
G417	L302	L152	M1
L430	L305	L153	L2
L431		N159	I6
Q432	I310	N160	I12
G433	V311	R161	
Y434	A312		I22
G435	Y313	K166	
L436	S314	K170	I32
G437	I315	K171	M33
L438		V172	L34
L439	I225		I38
S447	I328	R176	I42
Y448	D329		
	S335	V180	V46
L455	E336	I186	I52
F458	I337	I187	
M464	F343	I190	N67
Y465	K349	M194	Y71
L466		S195	
Y467	L355	M196	W75
L481	L481	Y209	L78
P482	Y358		
Y486	L363	M216	I82
L490	D367	T234	Y88
Y491	L368	Q239	L92
M492	R369	Q240	L93
M493		V241	I94
L494	L374	L242	
S495	H377	L243	S97
L496	I378	D244	
		A245	D111
H499	L381	M246	K112
I500		E247	
S501	I384	T250	R116
Y502		P251	F117
I503	I387		V118
L508	S388	L255	
Y528	L389	L256	I121
	L390	H257	M122
D540	I391	S258	T125
K541	I392	A259	
	L393	L260	I133
I555	L400	L261	S134
		V262	M135
I567	I406	T263	D136
	L407		L137
I577	L408	K271	I138
	E409		M139
I581		S280	L140
	I415		F141
Y594	L416	S291	

81% 18%



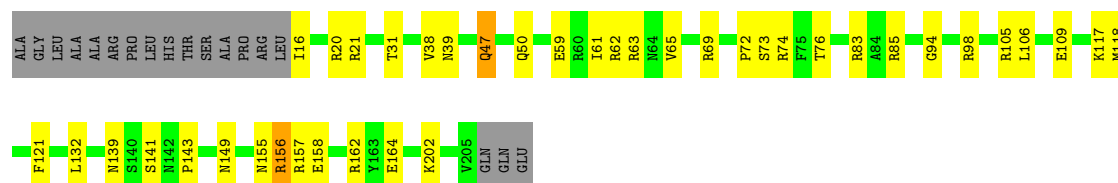
• Molecule 50: NDUFS3

Chain S3: 68% 22% 10%



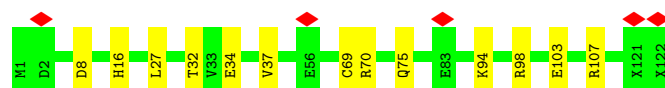
• Molecule 51: NDUFS4

Chain S4: 72% 18% 9%



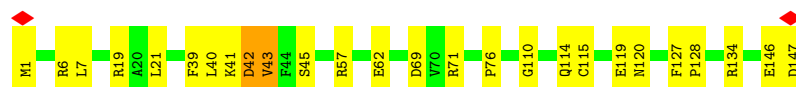
• Molecule 52: NDUFS5

Chain S5: 89% 11%



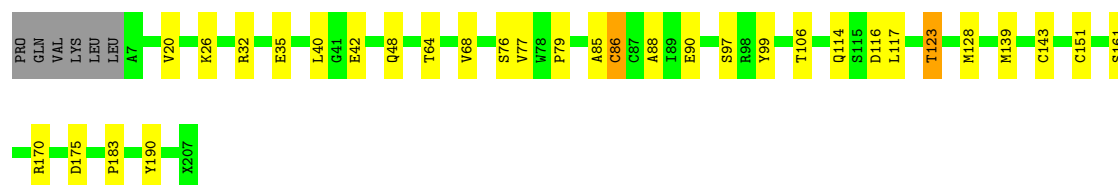
• Molecule 53: NDUFS6

Chain S6: 82% 16%



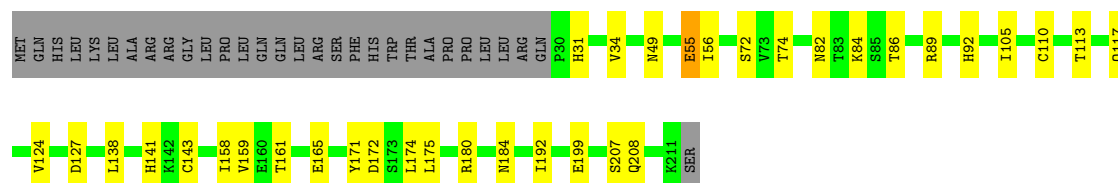
• Molecule 54: NDUFS7

Chain S7:  82% 14% . .

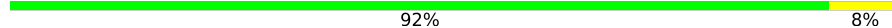


• Molecule 55: NDUFS8

Chain S8:  69% 16% 14%

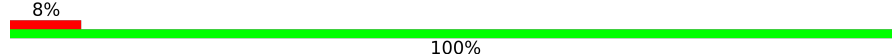


• Molecule 56: UNK-UNK-UNK-UNK-UNK-UNK-UNK-UNK-UNK-UNK-UNK-UNK

Chain U1:  92% 8%



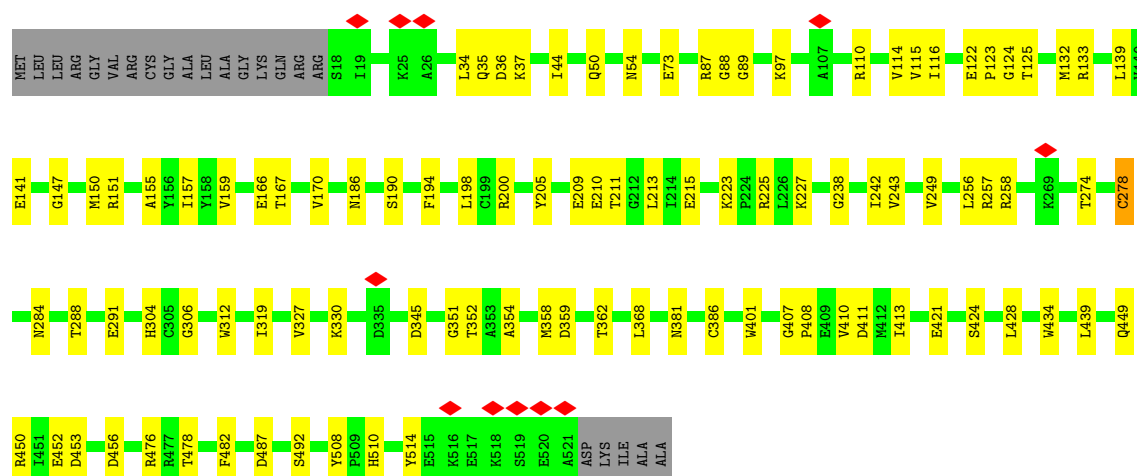
• Molecule 56: UNK-UNK-UNK-UNK-UNK-UNK-UNK-UNK-UNK-UNK-UNK-UNK

Chain U2:  8% 100%



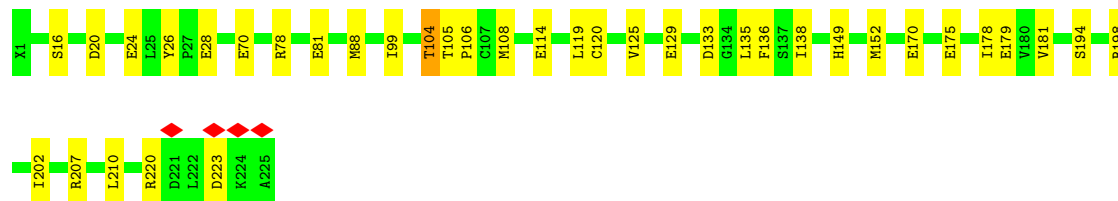
• Molecule 57: NDUFV1

Chain V1:  77% 19% .



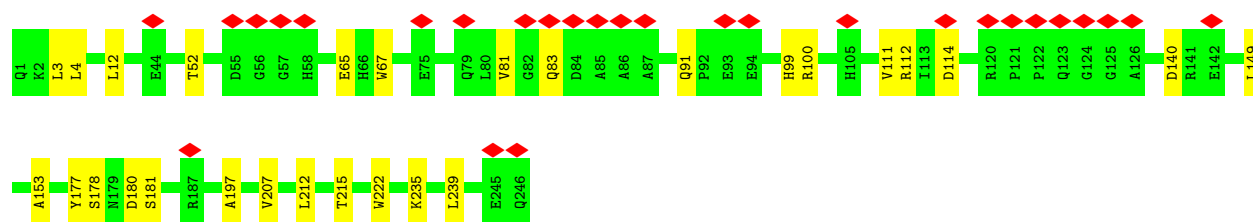
- Molecule 58: NDUFV2

Chain V2:  84% 16%



- Molecule 59: NDUEG7

Chain E7:  11% 89% 11%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	86599	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	33.507	Depositor
Minimum map value	-20.416	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.993	Depositor
Recommended contour level	4.5	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, K, ZN, FES, SF4, CDL, PC1, U10, NDP, NAI, 3PE, ZMP, FMN

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	0.19	0/2858	0.33	0/3878
2	1B	0.17	0/4306	0.27	0/5854
3	2B	0.20	0/958	0.33	0/1306
4	4L	0.18	0/924	0.26	0/1261
5	A1	0.15	0/1108	0.27	0/1511
6	A2	0.15	0/1530	0.28	0/2089
7	A3	0.17	0/1079	0.28	0/1453
8	A5	0.16	0/1282	0.25	0/1737
9	A6	0.16	0/3395	0.26	0/4608
10	A7	0.17	0/1194	0.30	0/1619
11	A8	0.15	0/1879	0.25	0/2543
12	A9	0.17	0/3920	0.29	0/5335
13	AB	0.15	0/704	0.23	0/951
14	AC	0.15	0/736	0.22	0/1000
15	AL	0.17	0/2317	0.29	0/3136
16	AM	0.16	0/1533	0.23	0/2079
17	AN	0.15	0/2382	0.24	0/3249
18	B2	0.15	0/947	0.22	0/1291
19	B3	0.16	0/326	0.30	0/441
20	B4	0.17	0/1419	0.27	0/1922
21	B5	0.18	0/1111	0.27	0/1505
22	B6	0.17	0/803	0.26	0/1087
23	B7	0.14	0/877	0.24	0/1172
24	B8	0.17	0/1273	0.26	0/1733
25	B9	0.17	0/1274	0.28	0/1728
26	BL	0.17	0/1266	0.27	0/1710
27	BM	0.18	0/876	0.27	0/1192
28	C4	0.17	0/1592	0.29	0/2158
29	E1	0.15	0/3596	0.26	0/4879
30	E2	0.14	0/3658	0.25	0/4983
31	E3	0.14	0/3320	0.26	0/4520
32	E4	0.16	0/2850	0.25	0/3884

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	E5	0.12	0/2004	0.34	0/2721
34	E6	0.15	0/2954	0.26	0/4004
35	E8	0.15	0/1747	0.28	0/2367
36	EA	0.19	0/858	0.27	0/1163
37	EB	0.13	0/650	0.22	0/863
38	EC	0.16	0/676	0.28	0/925
39	ED	0.14	0/1176	0.24	0/1590
40	FX	0.20	0/2035	0.33	0/2763
41	G1	0.18	0/3374	0.29	0/4589
42	G2	0.17	0/1832	0.29	0/2476
43	G3	0.16	0/1957	0.30	0/2646
44	N1	0.18	0/2672	0.32	0/3639
45	N2	0.20	0/2582	0.32	0/3530
46	N3	0.20	0/1068	0.36	0/1456
46	N6	0.16	0/1275	0.31	0/1730
47	N4	0.20	0/4105	0.33	0/5594
48	N5	0.19	0/4963	0.33	0/6758
49	S2	0.20	0/3244	0.32	0/4403
50	S3	0.19	0/2112	0.32	0/2874
51	S4	0.16	0/1573	0.29	0/2107
52	S5	0.13	0/960	0.23	0/1291
53	S6	0.17	0/1232	0.30	0/1659
54	S7	0.19	0/1558	0.29	0/2120
55	S8	0.19	0/1485	0.29	0/2010
57	V1	0.17	0/3990	0.30	0/5394
58	V2	0.16	0/1787	0.29	0/2428
59	E7	0.14	0/1931	0.27	0/2618
All	All	0.17	0/113093	0.29	0/153532

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	2801	2700	2710	34	0
2	1B	4198	4159	4175	54	0
3	2B	1070	989	1009	23	0
4	4L	890	878	880	19	0
5	A1	1071	1026	1030	7	0
6	A2	1493	1474	1478	16	0
7	A3	1050	1039	1041	9	0
8	A5	1261	1248	1251	10	0
9	A6	3328	3280	3293	40	0
10	A7	1154	1118	1123	15	0
11	A8	1822	1726	1736	34	0
12	A9	3829	3850	3857	48	0
13	AB	694	673	677	10	0
14	AC	721	697	702	9	0
15	AL	2237	2172	2180	18	0
16	AM	1487	1448	1452	24	0
17	AN	2306	2267	2275	18	0
18	B2	913	857	858	11	0
19	B3	449	309	313	9	0
20	B4	1377	1358	1364	16	0
21	B5	1112	1069	1075	14	0
22	B6	773	747	751	6	0
23	B7	857	835	841	13	0
24	B8	1224	1127	1136	23	0
25	B9	1236	1207	1212	19	0
26	BL	1227	1179	1185	10	0
27	BM	910	827	830	13	0
28	C4	1545	1517	1519	21	0
29	E1	3512	3496	3510	50	0
30	E2	3563	3540	3554	37	0
31	E3	3255	3263	3279	37	0
32	E4	2770	2732	2742	32	0
33	E5	1977	2069	2075	41	0
34	E6	2871	2758	2767	27	0
35	E8	1691	1663	1668	26	0
36	EA	961	832	835	10	0
37	EB	774	631	636	7	0
38	EC	660	663	666	10	0
39	ED	1142	1131	1134	18	0
40	FX	1967	1849	1858	32	0
41	G1	3281	3139	3156	51	0
42	G2	1804	1846	1850	30	0
43	G3	1961	1944	1950	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	N1	2605	2726	2729	50	0
45	N2	2512	2589	2592	50	0
46	N3	1037	1057	1057	26	0
46	N6	1257	1385	1385	35	0
47	N4	4001	4214	4224	77	0
48	N5	4837	5032	5046	96	0
49	S2	3173	3101	3114	60	0
50	S3	2050	1928	1936	45	0
51	S4	1536	1502	1505	32	0
52	S5	991	895	898	10	0
53	S6	1200	1192	1198	24	0
54	S7	1545	1500	1503	25	0
55	S8	1451	1392	1397	30	0
56	U1	60	16	18	1	0
56	U2	60	16	17	0	0
57	V1	3897	3827	3837	70	0
58	V2	1759	1701	1710	27	0
59	E7	1888	1892	1903	19	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	2	0
61	V1	8	0	0	1	0
62	1A	1	0	0	0	0
63	A1	80	111	111	2	0
63	A9	66	80	80	1	0
63	AL	50	77	77	0	0
63	AM	97	148	148	3	0
63	AN	48	73	73	0	0
63	B5	108	176	176	2	0
63	C4	38	50	50	1	0
63	E4	51	79	79	0	0
63	E8	171	250	250	1	0
63	ED	54	88	88	2	0
63	N1	89	129	129	0	0
63	N2	37	48	48	1	0
63	N3	42	61	61	0	0
63	N4	72	92	92	1	0
63	N5	131	190	190	3	0
64	A3	58	60	60	1	0
64	AL	202	236	236	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
64	AM	216	273	273	7	0
64	B3	65	74	74	3	0
64	B5	58	60	60	0	0
64	C4	163	223	223	2	0
64	E6	64	72	72	0	0
64	E7	68	80	80	0	0
64	EA	114	116	116	2	0
64	N4	98	149	149	2	0
64	N5	163	223	223	1	0
65	A9	48	26	26	0	0
66	AB	36	0	47	5	0
66	AC	36	0	47	4	0
67	AN	51	81	82	0	0
67	G1	40	56	57	2	0
67	N4	41	55	56	0	0
67	N5	51	81	82	0	0
68	N4	43	55	55	4	0
69	E7	1	0	0	0	0
69	S6	1	0	0	0	0
70	V1	31	19	19	2	0
71	V1	44	0	27	6	0
All	All	113966	112888	113418	1321	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (1321) 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)
47:N4:43:ILE:HD13	47:N4:472:LEU:HD21	1.39	1.04
33:E5:287:LEU:O	33:E5:289:LEU:N	1.98	0.96
47:N4:293:THR:HG21	47:N4:365:ILE:HD11	1.47	0.96
31:E3:222:TYR:HH	38:EC:60:HIS:HE2	0.98	0.91
9:A6:45:HIS:NE2	9:A6:117:GLU:OE1	2.03	0.91
48:N5:255:LEU:O	48:N5:260:THR:OG1	1.90	0.90
57:V1:452:GLU:OE2	57:V1:508:TYR:OH	1.90	0.90
30:E2:364:PRO:O	30:E2:400:ARG:NH1	2.04	0.89
40:FX:130:SER:OG	41:G1:297:ARG:NH2	2.06	0.88
9:A6:33:ARG:NH2	9:A6:41:GLU:OE2	2.07	0.88
11:A8:214:THR:OG1	11:A8:219:ASP:OD2	1.92	0.86
41:G1:113:ARG:NH1	41:G1:115:THR:OG1	2.08	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A3:22:ASN:OD1	7:A3:23:ARG:NH1	2.10	0.85
41:G1:28:ARG:NH2	41:G1:37:GLU:OE2	2.10	0.85
12:A9:442:ARG:NH2	44:N1:484:ILE:O	2.10	0.84
32:E4:31:VAL:HG21	49:S2:236:VAL:HG11	1.58	0.84
23:B7:14:ASP:OD2	23:B7:17:LYS:NZ	2.12	0.83
41:G1:294:ARG:HG2	42:G2:181:VAL:HG21	1.58	0.83
35:E8:74:ARG:NH2	59:E7:207:VAL:O	2.12	0.83
49:S2:210:MET:SD	49:S2:214:ARG:NH1	2.52	0.82
29:E1:58:SER:OG	58:V2:70:GLU:OE2	1.98	0.82
41:G1:133:ARG:NH1	43:G3:215:GLU:OE2	2.12	0.82
43:G3:235:GLY:O	46:N6:161:LYS:NZ	2.13	0.81
17:AN:248:ILE:O	28:C4:154:ARG:NH2	2.12	0.81
29:E1:105:GLN:NE2	29:E1:236:SER:OG	2.13	0.81
32:E4:219:ARG:NH1	32:E4:280:ASP:OD2	2.14	0.81
53:S6:41:LYS:O	53:S6:45:SER:OG	1.98	0.81
25:B9:100:ARG:NH2	35:E8:31:TYR:O	2.13	0.81
20:B4:133:GLU:OE1	47:N4:274:TYR:OH	1.98	0.81
16:AM:74:ARG:NH2	44:N1:516:TYR:O	2.13	0.81
2:1B:58:LYS:NZ	2:1B:495:CYS:SG	2.52	0.80
34:E6:120:ARG:NH1	53:S6:69:ASP:OD2	2.14	0.80
24:B8:25:ARG:NH1	24:B8:30:GLU:OE2	2.15	0.80
8:A5:40:ARG:NH2	8:A5:81:ALA:O	2.15	0.80
64:AM:215:CDL:OA4	32:E4:335:TYR:OH	1.99	0.80
34:E6:184:ASN:ND2	34:E6:216:GLU:OE2	2.14	0.80
47:N4:67:ASN:N	47:N4:119:ASP:OD2	2.15	0.79
28:C4:132:ARG:NH1	28:C4:136:GLU:OE1	2.15	0.79
28:C4:160:ARG:NH1	28:C4:161:GLU:OE2	2.16	0.79
57:V1:411:ASP:OD2	57:V1:510:HIS:NE2	2.16	0.79
41:G1:133:ARG:NH2	42:G2:34:TYR:O	2.17	0.78
51:S4:156:ARG:NH1	51:S4:158:GLU:OE2	2.17	0.78
53:S6:57:ARG:NH2	55:S8:127:ASP:OD1	2.17	0.77
11:A8:102:ARG:NH1	11:A8:221:ILE:O	2.17	0.77
23:B7:67:CYS:SG	23:B7:71:ARG:NH1	2.57	0.77
43:G3:82:ARG:NH1	43:G3:84:ASP:OD2	2.18	0.77
49:S2:111:THR:HG22	49:S2:147:TYR:OH	1.85	0.77
52:S5:103:GLU:O	52:S5:107:ARG:NH2	2.18	0.77
33:E5:41:ALA:O	33:E5:287:LEU:O	2.04	0.76
25:B9:137:THR:HG22	27:BM:23:THR:HG21	1.65	0.76
28:C4:71:ASP:O	28:C4:75:ASN:ND2	2.18	0.76
2:1B:214:ASP:OD2	2:1B:218:LYS:NZ	2.18	0.76
4:4L:95:LYS:O	4:4L:103:ARG:NH2	2.18	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:E2:374:ARG:NH2	38:EC:76:VAL:O	2.19	0.76
44:N1:367:GLN:OE1	46:N3:176:TYR:OH	2.02	0.76
9:A6:135:ASN:OD1	50:S3:212:LYS:NZ	2.19	0.76
12:A9:18:LEU:O	12:A9:50:LYS:NZ	2.19	0.75
31:E3:53:GLN:NE2	31:E3:94:ASN:OD1	2.19	0.75
45:N2:40:ASN:ND2	45:N2:69:THR:OG1	2.19	0.75
12:A9:344:GLN:OE1	12:A9:413:LYS:NZ	2.19	0.75
57:V1:449:GLN:NE2	57:V1:453:ASP:OD1	2.20	0.75
26:BL:81:GLU:OE2	27:BM:92:ARG:NH1	2.19	0.75
49:S2:107:PHE:O	49:S2:111:THR:HG23	1.86	0.75
47:N4:80:ILE:HD11	47:N4:337:ILE:HG23	1.69	0.75
49:S2:116:HIS:NE2	49:S2:268:GLU:OE1	2.19	0.75
49:S2:394:ASP:OD1	49:S2:394:ASP:N	2.15	0.75
2:1B:441:LYS:HG2	30:E2:25:LEU:HD11	1.69	0.74
12:A9:239:ARG:NH2	12:A9:339:GLU:OE2	2.20	0.74
43:G3:130:GLN:OE1	43:G3:148:LYS:NZ	2.18	0.74
45:N2:175:TYR:OH	45:N2:247:THR:HG21	1.87	0.74
2:1B:454:GLU:OE2	6:A2:58:ARG:NH1	2.20	0.74
25:B9:21:SER:OG	25:B9:118:GLN:OE1	2.05	0.74
2:1B:177:GLU:OE1	2:1B:179:ARG:NH1	2.20	0.74
41:G1:118:ASP:O	41:G1:408:SER:OG	2.04	0.74
7:A3:17:HIS:ND1	32:E4:206:ASP:OD1	2.20	0.74
10:A7:105:SER:O	50:S3:130:ARG:NH1	2.21	0.74
48:N5:409:GLU:OE1	48:N5:495:SER:OG	2.04	0.74
49:S2:19:PRO:HB3	54:S7:128:MET:HE1	1.68	0.74
32:E4:64:GLU:N	32:E4:64:GLU:OE1	2.20	0.74
57:V1:421:GLU:OE2	57:V1:434:TRP:NE1	2.21	0.74
14:AC:115:GLU:OE2	25:B9:41:HIS:NE2	2.18	0.73
48:N5:97:SER:OG	48:N5:125:THR:HG21	1.87	0.73
48:N5:355:LEU:HD11	48:N5:384:ILE:HG22	1.68	0.73
1:1A:163:ASP:OD1	10:A7:55:ARG:NH2	2.21	0.73
41:G1:124:ASP:OD1	41:G1:403:ARG:NH2	2.20	0.73
49:S2:89:GLU:O	49:S2:93:GLU:N	2.21	0.73
30:E2:339:GLU:OE2	30:E2:358:ARG:NH1	2.21	0.73
26:BL:128:ASN:O	26:BL:131:LYS:NZ	2.21	0.73
9:A6:426:LYS:O	9:A6:427:SER:OG	2.06	0.73
37:EB:60:GLU:OE2	37:EB:72:ARG:NH1	2.22	0.73
45:N2:126:GLU:N	45:N2:126:GLU:OE1	2.21	0.73
6:A2:164:THR:HG1	31:E3:119:TYR:HH	1.17	0.73
5:A1:38:LYS:NZ	5:A1:96:GLU:OE1	2.19	0.72
37:EB:30:GLN:O	37:EB:35:ARG:NH2	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A5:127:ASP:OD1	10:A7:78:ARG:NH2	2.22	0.72
50:S3:147:SER:OG	50:S3:159:GLU:OE1	2.05	0.72
57:V1:359:ASP:O	57:V1:362:THR:HG22	1.88	0.72
47:N4:242:LEU:O	47:N4:246:SER:OG	2.08	0.72
2:1B:48:ARG:NH1	6:A2:163:ASP:OD1	2.23	0.72
17:AN:36:SER:OG	17:AN:66:GLU:OE2	2.03	0.72
25:B9:70:SER:OG	35:E8:5:ARG:NH2	2.23	0.72
32:E4:225:GLY:O	32:E4:228:SER:OG	2.07	0.72
64:B3:102:CDL:HB22	39:ED:47:MET:HE1	1.72	0.71
25:B9:150:GLY:O	42:G2:115:ARG:NH1	2.23	0.71
12:A9:34:ASP:OD1	12:A9:37:THR:OG1	2.06	0.71
57:V1:284:ASN:ND2	57:V1:306:GLY:O	2.23	0.71
2:1B:271:GLN:O	2:1B:499:ARG:NH2	2.24	0.71
57:V1:215:GLU:OE2	57:V1:225:ARG:NE	2.21	0.71
1:1A:169:TYR:OH	49:S2:309:ASN:ND2	2.23	0.71
40:FX:185:TRP:O	40:FX:186:SER:OG	2.08	0.71
2:1B:217:LYS:NZ	2:1B:473:SER:OG	2.24	0.70
32:E4:241:ALA:O	32:E4:304:ARG:NH1	2.25	0.70
58:V2:20:ASP:OD1	58:V2:26:TYR:OH	2.09	0.70
18:B2:110:GLU:O	23:B7:92:ARG:NH1	2.24	0.70
29:E1:346:ASP:OD1	29:E1:347:ALA:N	2.25	0.70
47:N4:92:GLU:OE2	47:N4:100:ASN:ND2	2.23	0.70
2:1B:525:GLU:OE1	2:1B:525:GLU:N	2.24	0.70
9:A6:163:GLY:N	9:A6:169:GLU:OE1	2.24	0.70
1:1A:138:HIS:O	1:1A:173:LYS:NZ	2.24	0.70
48:N5:170:LYS:NZ	48:N5:540:ASP:OD2	2.24	0.70
29:E1:310:LYS:NZ	53:S6:146:GLU:OE1	2.19	0.70
2:1B:63:LEU:HD11	2:1B:352:LEU:HD12	1.73	0.70
24:B8:84:ASP:OD1	48:N5:166:LYS:NZ	2.24	0.69
24:B8:150:GLU:N	24:B8:150:GLU:OE1	2.24	0.69
1:1A:141:ASP:OD2	1:1A:190:ASN:ND2	2.25	0.69
47:N4:91:TYR:OH	47:N4:355:ASP:OD2	2.10	0.69
32:E4:128:ILE:HD11	32:E4:156:LEU:HD13	1.74	0.69
44:N1:461:ILE:HD11	46:N3:173:VAL:HG11	1.73	0.69
32:E4:50:GLN:O	32:E4:52:LYS:NZ	2.25	0.69
34:E6:340:GLU:OE1	34:E6:340:GLU:N	2.25	0.69
40:FX:144:ASP:O	40:FX:147:GLY:N	2.25	0.69
23:B7:30:SER:OG	23:B7:32:GLU:OE1	2.11	0.69
49:S2:338:GLU:OE2	50:S3:132:ARG:NH2	2.26	0.69
30:E2:187:THR:HG22	30:E2:189:ASP:H	1.58	0.69
2:1B:185:ARG:NH1	29:E1:215:ASP:OD2	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:N3:275:LEU:HD23	46:N6:148:MET:SD	2.33	0.68
57:V1:97:LYS:NZ	57:V1:243:VAL:O	2.20	0.68
4:4L:91:ARG:NH2	46:N6:96:ASN:OD1	2.26	0.68
33:E5:81:GLU:OE1	33:E5:81:GLU:N	2.25	0.68
50:S3:30:GLU:OE1	50:S3:246:TYR:OH	2.09	0.68
57:V1:35:GLN:N	57:V1:35:GLN:OE1	2.26	0.68
35:E8:156:ARG:NH2	35:E8:180:THR:O	2.25	0.68
47:N4:43:ILE:HG12	47:N4:79:LEU:HD22	1.76	0.68
15:AL:232:LYS:O	15:AL:239:ARG:NH1	2.27	0.68
16:AM:152:ARG:NH2	16:AM:185:GLU:OE2	2.26	0.68
44:N1:586:SER:O	54:S7:114:GLN:NE2	2.27	0.68
70:V1:579:FMN:N5	71:V1:581:NAI:H4N	2.09	0.68
1:1A:275:ASN:ND2	1:1A:278:ASP:OD1	2.27	0.68
44:N1:386:GLU:OE2	44:N1:640:ARG:NH1	2.26	0.68
49:S2:153:SER:OG	49:S2:155:MET:O	2.09	0.68
12:A9:78:LYS:NZ	12:A9:83:GLN:O	2.22	0.67
13:AB:56:ARG:O	13:AB:60:THR:HG23	1.95	0.67
47:N4:408:ASN:O	47:N4:412:SER:OG	2.11	0.67
68:N4:505:U10:C18	68:N4:505:U10:H151	2.24	0.67
57:V1:312:TRP:O	57:V1:330:LYS:NZ	2.28	0.67
9:A6:175:GLU:OE2	9:A6:178:THR:OG1	2.13	0.67
31:E3:375:GLU:N	31:E3:375:GLU:OE1	2.27	0.67
50:S3:264:ASP:OD1	51:S4:149:ASN:ND2	2.27	0.67
16:AM:47:TYR:OH	49:S2:193:ASP:OD1	2.13	0.67
29:E1:392:GLU:N	29:E1:392:GLU:OE1	2.27	0.67
35:E8:203:GLU:OE1	35:E8:203:GLU:N	2.28	0.67
2:1B:32:VAL:HG21	2:1B:359:LEU:HD23	1.76	0.67
13:AB:109:MET:HE1	13:AB:117:ILE:HD12	1.76	0.67
19:B3:22:MET:HE1	19:B3:34:ARG:HD2	1.75	0.67
57:V1:186:ASN:ND2	57:V1:190:SER:O	2.28	0.67
17:AN:180:ARG:NH1	40:FX:206:ASP:OD1	2.28	0.67
18:B2:50:GLU:O	39:ED:70:ARG:NH2	2.28	0.67
1:1A:222:GLN:NE2	57:V1:381:ASN:O	2.27	0.67
32:E4:31:VAL:HG21	49:S2:236:VAL:CG1	2.25	0.67
64:AM:217:CDL:OB3	55:S8:49:ASN:ND2	2.26	0.67
18:B2:97:PRO:O	23:B7:83:ARG:NH2	2.28	0.67
30:E2:187:THR:HG21	30:E2:192:ALA:HB3	1.77	0.67
36:EA:74:VAL:HG21	45:N2:15:SER:HA	1.76	0.66
10:A7:28:GLY:O	15:AL:64:HIS:NE2	2.26	0.66
27:BM:51:SER:OG	27:BM:53:ASP:OD1	2.11	0.66
17:AN:256:CYS:SG	26:BL:57:LEU:HD21	2.35	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:N4:284:ASN:O	47:N4:287:ILE:HG22	1.95	0.66
49:S2:51:ARG:O	54:S7:161:SER:OG	2.12	0.66
2:1B:84:ARG:NH2	2:1B:279:GLU:OE2	2.28	0.66
2:1B:112:THR:O	51:S4:155:ASN:ND2	2.29	0.66
26:BL:88:GLU:OE1	37:EB:79:SER:OG	2.13	0.66
47:N4:403:SER:O	47:N4:406:ILE:HG22	1.96	0.66
17:AN:91:VAL:O	45:N2:169:TYR:OH	2.10	0.66
38:EC:60:HIS:O	38:EC:64:VAL:HG23	1.95	0.66
41:G1:211:GLU:OE2	42:G2:87:ARG:NH1	2.29	0.66
53:S6:62:GLU:N	53:S6:62:GLU:OE1	2.28	0.66
57:V1:456:ASP:OD1	57:V1:476:ARG:NH1	2.27	0.65
31:E3:52:ASP:OD1	31:E3:240:SER:OG	2.11	0.65
33:E5:64:ALA:O	33:E5:96:TYR:N	2.28	0.65
40:FX:170:SER:OG	40:FX:172:ASP:OD1	2.14	0.65
45:N2:221:ILE:HD11	45:N2:252:ASN:CG	2.21	0.65
57:V1:110:ARG:NH1	57:V1:238:GLY:O	2.28	0.65
27:BM:64:PHE:O	27:BM:68:THR:HG23	1.95	0.65
63:AM:220:PC1:O14	41:G1:426:TYR:OH	2.10	0.65
25:B9:51:GLU:OE1	48:N5:448:TYR:OH	2.09	0.65
58:V2:114:GLU:OE1	58:V2:114:GLU:N	2.29	0.65
2:1B:68:ASP:OD1	6:A2:14:ARG:NH2	2.28	0.65
11:A8:55:ARG:NH2	11:A8:210:SER:O	2.30	0.65
54:S7:42:GLU:N	54:S7:42:GLU:OE1	2.30	0.65
44:N1:566:GLU:OE1	44:N1:608:HIS:NE2	2.30	0.65
31:E3:392:GLU:OE1	31:E3:392:GLU:N	2.28	0.65
34:E6:56:SER:OG	34:E6:57:ASN:ND2	2.29	0.65
58:V2:28:GLU:N	58:V2:28:GLU:OE1	2.30	0.65
1:1A:196:THR:N	61:1A:403:SF4:S4	2.70	0.64
57:V1:36:ASP:OD2	58:V2:210:LEU:N	2.28	0.64
29:E1:268:GLU:OE1	29:E1:322:THR:OG1	2.10	0.64
45:N2:175:TYR:CG	45:N2:186:MET:HE1	2.33	0.64
57:V1:428:LEU:HD23	57:V1:428:LEU:O	1.97	0.64
32:E4:180:ARG:NH2	32:E4:274:THR:OG1	2.30	0.64
41:G1:416:GLN:OE1	41:G1:419:ARG:NH1	2.30	0.64
46:N3:251:ILE:CD1	46:N3:279:ILE:HD11	2.27	0.64
48:N5:170:LYS:NZ	48:N5:244:ASP:OD2	2.24	0.64
1:1A:345:LEU:CD2	9:A6:367:LEU:HD22	2.28	0.64
11:A8:103:GLU:OE2	11:A8:222:TYR:OH	2.14	0.64
23:B7:94:GLU:OE2	59:E7:100:ARG:NH2	2.30	0.64
48:N5:259:ALA:O	48:N5:260:THR:HG23	1.97	0.64
20:B4:28:GLU:OE1	20:B4:31:ARG:NH2	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:G2:126:GLU:OE2	42:G2:141:TYR:OH	2.16	0.64
44:N1:394:GLN:OE1	44:N1:396:ARG:NH1	2.31	0.64
12:A9:26:ASN:O	12:A9:26:ASN:ND2	2.31	0.63
12:A9:468:LEU:HB3	63:A9:560:PC1:H142	1.80	0.63
59:E7:91:GLN:OE1	59:E7:91:GLN:N	2.32	0.63
9:A6:99:LEU:O	51:S4:47:GLN:NE2	2.30	0.63
35:E8:115:TYR:CZ	35:E8:119:ILE:HD11	2.32	0.63
41:G1:113:ARG:NH2	41:G1:119:LYS:O	2.31	0.63
41:G1:194:LEU:HD22	41:G1:215:LEU:HD12	1.80	0.63
35:E8:144:GLU:OE2	35:E8:159:SER:OG	2.17	0.63
48:N5:311:VAL:O	48:N5:315:THR:HG23	1.99	0.63
48:N5:337:ILE:HD11	48:N5:491:TYR:CG	2.34	0.63
2:1B:264:LEU:HD21	31:E3:344:LEU:HD13	1.80	0.63
8:A5:38:LYS:NZ	41:G1:391:HIS:O	2.30	0.63
48:N5:92:LEU:HD22	48:N5:343:PHE:HA	1.80	0.63
48:N5:118:VAL:HG12	48:N5:122:MET:HE2	1.81	0.63
9:A6:48:PRO:HG2	50:S3:176:LEU:HD22	1.81	0.63
42:G2:192:GLU:OE1	42:G2:192:GLU:N	2.31	0.63
44:N1:422:TYR:OH	46:N3:192:CYS:O	2.17	0.63
50:S3:112:MET:HE1	51:S4:118:MET:SD	2.39	0.63
6:A2:28:ALA:O	6:A2:32:ASN:ND2	2.32	0.62
57:V1:116:ILE:HG21	57:V1:139:LEU:HD11	1.81	0.62
11:A8:177:TYR:OH	44:N1:541:GLU:OE2	2.17	0.62
40:FX:275:LYS:O	40:FX:277:VAL:N	2.32	0.62
55:S8:92:HIS:CE1	61:S8:297:SF4:S4	2.93	0.62
15:AL:221:LYS:NZ	54:S7:20:VAL:O	2.24	0.62
48:N5:2:LEU:HD21	48:N5:133:ILE:HD12	1.80	0.62
9:A6:31:VAL:HG11	40:FX:141:THR:HG21	1.82	0.62
35:E8:14:PHE:O	35:E8:19:ASN:ND2	2.32	0.62
45:N2:88:ILE:HG21	46:N6:143:LEU:HD21	1.81	0.62
41:G1:112:GLY:HA3	45:N2:27:VAL:HG11	1.82	0.62
47:N4:328:PHE:HA	47:N4:331:ILE:HD12	1.82	0.62
54:S7:139:MET:HE3	54:S7:143:CYS:HB2	1.81	0.62
32:E4:318:VAL:HG21	32:E4:334:VAL:HG21	1.81	0.62
50:S3:174:PRO:O	51:S4:20:ARG:NH1	2.32	0.62
17:AN:227:SER:OG	28:C4:173:ASP:OD2	2.09	0.61
44:N1:424:ARG:NH1	46:N3:202:SER:OG	2.32	0.61
28:C4:78:THR:HG22	47:N4:59:ASN:HB3	1.82	0.61
6:A2:8:ARG:NH1	31:E3:189:LEU:O	2.33	0.61
17:AN:11:MET:HE1	48:N5:581:ILE:HG22	1.80	0.61
22:B6:12:ASP:OD2	48:N5:116:ARG:NH2	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:V1:73:GLU:OE2	57:V1:151:ARG:NH2	2.34	0.61
22:B6:77:ASP:OD2	39:ED:125:TYR:OH	2.06	0.61
49:S2:265:ARG:NE	49:S2:387:ASP:OD2	2.34	0.61
20:B4:20:PRO:O	20:B4:22:ASP:N	2.33	0.61
49:S2:362:TYR:OH	50:S3:105:ASP:OD1	2.16	0.61
51:S4:31:THR:HG22	51:S4:31:THR:O	1.99	0.61
64:AM:215:CDL:O1	32:E4:315:ASP:OD2	2.08	0.61
29:E1:239:ASP:OD1	29:E1:243:LYS:N	2.33	0.61
40:FX:221:ASN:O	40:FX:223:ARG:N	2.34	0.61
50:S3:175:ASP:OD2	50:S3:177:ARG:NH1	2.33	0.61
25:B9:103:MET:HE1	48:N5:305:LEU:HD11	1.83	0.61
49:S2:75:MET:SD	49:S2:118:LEU:HD22	2.41	0.61
21:B5:43:TRP:O	21:B5:47:THR:HG23	2.01	0.60
7:A3:116:ARG:NH2	11:A8:31:ASP:OD2	2.33	0.60
12:A9:183:THR:OG1	54:S7:32:ARG:NH2	2.34	0.60
49:S2:75:MET:HE2	49:S2:75:MET:HA	1.83	0.60
32:E4:100:ARG:NH2	32:E4:141:SER:OG	2.35	0.60
4:4L:108:GLU:OE2	4:4L:143:THR:OG1	2.19	0.60
25:B9:134:LYS:O	25:B9:137:THR:HG23	2.00	0.60
12:A9:7:GLU:OE2	12:A9:30:ARG:NH2	2.34	0.60
48:N5:358:TYR:OH	48:N5:464:ASN:OD1	2.19	0.60
27:BM:93:ARG:NH2	37:EB:18:UNK:O	2.35	0.60
21:B5:21:GLY:O	42:G2:90:ARG:NH2	2.34	0.60
48:N5:2:LEU:HD22	48:N5:82:ILE:HG13	1.82	0.60
50:S3:38:ARG:NE	50:S3:39:GLU:OE2	2.33	0.60
13:AB:92:LEU:CD1	66:AB:150:ZMP:H20A	2.31	0.60
16:AM:41:PRO:O	49:S2:277:HIS:NE2	2.31	0.60
21:B5:47:THR:HG22	63:B5:203:PC1:H2E1	1.82	0.60
24:B8:25:ARG:NH2	40:FX:172:ASP:OD2	2.35	0.60
57:V1:115:VAL:HG11	57:V1:213:LEU:HD22	1.83	0.60
48:N5:486:TYR:CZ	48:N5:490:ILE:HD12	2.37	0.60
1:1A:143:PRO:O	1:1A:264:ARG:NH2	2.35	0.59
44:N1:419:TYR:O	46:N3:199:ARG:NH2	2.33	0.59
47:N4:354:TYR:O	47:N4:358:ASN:N	2.35	0.59
57:V1:88:GLY:O	71:V1:581:NAI:H2N	2.02	0.59
1:1A:26:ALA:O	2:1B:448:ARG:NE	2.35	0.59
28:C4:6:VAL:HG22	45:N2:100:THR:OG1	2.01	0.59
41:G1:207:SER:OG	41:G1:233:GLY:O	2.20	0.59
50:S3:70:ASP:OD2	50:S3:73:THR:OG1	2.13	0.59
12:A9:381:GLU:OE2	41:G1:28:ARG:NH1	2.35	0.59
14:AC:92:LEU:HG	66:AC:201:ZMP:H19B	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:S8:141:HIS:CE1	55:S8:174:LEU:HD12	2.37	0.59
59:E7:111:VAL:O	59:E7:153:ALA:N	2.35	0.59
2:1B:507:HIS:O	2:1B:511:VAL:HG23	2.03	0.59
19:B3:32:TRP:O	19:B3:33:SER:OG	2.20	0.59
49:S2:107:PHE:CZ	49:S2:150:VAL:HG11	2.37	0.59
35:E8:87:TYR:OH	64:N5:603:CDL:OA4	2.18	0.59
38:EC:69:GLU:OE2	38:EC:76:VAL:N	2.34	0.59
39:ED:46:GLU:OE1	39:ED:49:ARG:NH1	2.35	0.59
46:N6:52:GLY:HA3	46:N6:75:ILE:HD13	1.85	0.59
3:2B:101:ILE:HD11	41:G1:248:TRP:CH2	2.38	0.59
7:A3:28:GLN:O	55:S8:31:HIS:NE2	2.35	0.59
11:A8:128:MET:HE1	16:AM:97:PRO:HB3	1.85	0.59
30:E2:135:THR:HG23	30:E2:440:GLY:N	2.18	0.59
40:FX:199:VAL:O	40:FX:223:ARG:NH2	2.30	0.59
1:1A:331:MET:HE2	2:1B:305:VAL:CG1	2.33	0.59
45:N2:186:MET:HE3	45:N2:282:TRP:CZ2	2.38	0.59
58:V2:202:ILE:HD11	58:V2:207:ARG:HB3	1.85	0.58
29:E1:136:ASP:CG	29:E1:193:VAL:HG11	2.28	0.58
35:E8:196:PHE:O	35:E8:200:VAL:HG22	2.03	0.58
12:A9:120:THR:OG1	12:A9:195:SER:OG	2.13	0.58
49:S2:187:ARG:NH1	49:S2:190:GLU:OE2	2.37	0.58
3:2B:56:ILE:HD12	45:N2:257:PHE:CZ	2.39	0.58
8:A5:146:TYR:OH	50:S3:66:GLU:OE1	2.17	0.58
39:ED:43:TRP:CZ2	39:ED:47:MET:HE3	2.38	0.58
57:V1:291:GLU:OE2	57:V1:304:HIS:NE2	2.23	0.58
27:BM:62:MET:HA	27:BM:62:MET:HE2	1.85	0.58
28:C4:43:ASP:OD1	28:C4:43:ASP:N	2.36	0.58
48:N5:260:THR:O	48:N5:263:THR:N	2.35	0.58
59:E7:4:LEU:HD12	59:E7:4:LEU:O	2.04	0.58
27:BM:62:MET:HE1	47:N4:458:PRO:HD3	1.84	0.58
7:A3:49:GLU:OE1	46:N3:291:ASN:ND2	2.34	0.58
15:AL:117:GLU:OE1	15:AL:117:GLU:N	2.35	0.58
47:N4:43:ILE:HD12	47:N4:44:MET:N	2.19	0.58
2:1B:420:GLU:HG2	12:A9:89:LEU:HD13	1.86	0.58
29:E1:254:ASN:OD1	29:E1:257:ARG:NH2	2.37	0.58
36:EA:112:UNK:O	36:EA:114:UNK:N	2.36	0.58
51:S4:69:ARG:NH1	51:S4:143:PRO:O	2.36	0.58
13:AB:92:LEU:HD13	66:AB:150:ZMP:H20A	1.84	0.58
39:ED:125:TYR:O	39:ED:136:ARG:NH1	2.37	0.58
29:E1:68:ALA:O	29:E1:72:ASN:ND2	2.37	0.58
32:E4:238:MET:HA	32:E4:238:MET:HE2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:E6:365:GLN:OE1	34:E6:365:GLN:N	2.35	0.57
42:G2:16:ILE:HD12	43:G3:25:LEU:HD12	1.85	0.57
46:N3:261:ILE:HD13	46:N6:128:ILE:HB	1.86	0.57
57:V1:125:THR:HG22	57:V1:354:ALA:HB2	1.85	0.57
57:V1:319:ILE:HG12	57:V1:327:VAL:HG12	1.85	0.57
57:V1:478:THR:O	57:V1:514:TYR:OH	2.19	0.57
2:1B:99:GLN:OE1	2:1B:101:HIS:NE2	2.34	0.57
3:2B:18:ILE:HD11	3:2B:23:TYR:OH	2.03	0.57
26:BL:30:GLU:OE1	26:BL:30:GLU:N	2.37	0.57
29:E1:418:VAL:HG22	29:E1:419:ALA:H	1.68	0.57
31:E3:50:ASP:OD2	31:E3:69:LEU:N	2.34	0.57
32:E4:296:VAL:O	32:E4:300:THR:HG22	2.04	0.57
50:S3:202:VAL:O	54:S7:170:ARG:NH1	2.37	0.57
50:S3:224:ARG:O	55:S8:117:GLN:NE2	2.37	0.57
20:B4:80:ASN:O	20:B4:82:VAL:HG23	2.04	0.57
40:FX:172:ASP:OD1	40:FX:172:ASP:N	2.38	0.57
57:V1:116:ILE:HD12	57:V1:249:VAL:HG11	1.86	0.57
57:V1:401:TRP:O	57:V1:450:ARG:NH1	2.37	0.57
41:G1:93:GLU:OE2	51:S4:21:ARG:NH1	2.37	0.57
8:A5:65:ARG:NH1	10:A7:88:LEU:O	2.38	0.57
44:N1:461:ILE:CD1	46:N3:173:VAL:HG11	2.33	0.57
48:N5:329:ASP:OD2	48:N5:335:SER:OG	2.21	0.57
18:B2:125:PHE:CE2	48:N5:415:ILE:HG22	2.39	0.57
29:E1:156:ASP:OD2	29:E1:159:SER:OG	2.15	0.57
30:E2:59:SER:O	30:E2:62:ARG:NH1	2.38	0.57
50:S3:255:GLU:OE1	51:S4:85:ARG:NH2	2.36	0.57
4:4L:95:LYS:NZ	46:N6:39:GLU:OE2	2.38	0.57
44:N1:379:SER:O	44:N1:383:THR:HG23	2.05	0.57
47:N4:43:ILE:HG22	47:N4:75:ILE:HG23	1.87	0.57
31:E3:156:LEU:HD13	31:E3:184:LEU:HD22	1.86	0.57
49:S2:48:PHE:HB3	54:S7:128:MET:HE2	1.86	0.57
11:A8:1:MET:HE1	45:N2:58:LEU:CD2	2.35	0.57
11:A8:30:LEU:O	11:A8:34:VAL:HG13	2.05	0.57
13:AB:54:LEU:HD21	13:AB:62:ARG:NH2	2.19	0.57
30:E2:116:GLU:OE1	30:E2:116:GLU:N	2.38	0.57
37:EB:60:GLU:HG3	37:EB:68:VAL:HG11	1.87	0.57
22:B6:74:ASN:ND2	39:ED:130:PRO:O	2.37	0.57
30:E2:101:PHE:CZ	30:E2:244:ILE:HG22	2.39	0.57
66:AC:201:ZMP:H14A	25:B9:86:LYS:HE3	1.87	0.56
19:B3:24:HIS:NE2	64:B3:102:CDL:OA7	2.37	0.56
44:N1:395:ARG:NH2	49:S2:190:GLU:OE1	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:N5:328:ILE:HG22	48:N5:328:ILE:O	2.05	0.56
55:S8:165:GLU:N	55:S8:165:GLU:OE1	2.39	0.56
4:4L:114:LEU:HD21	45:N2:143:TRP:HB3	1.86	0.56
33:E5:5:LYS:O	33:E5:98:THR:N	2.38	0.56
33:E5:117:ASP:OD1	33:E5:261:VAL:HG11	2.05	0.56
34:E6:160:ASP:N	34:E6:160:ASP:OD1	2.39	0.56
46:N3:249:ASP:O	46:N3:252:ILE:HG22	2.05	0.56
47:N4:95:TYR:OH	47:N4:448:PHE:O	2.09	0.56
3:2B:4:ASN:ND2	4:4L:168:LYS:O	2.37	0.56
15:AL:212:TYR:OH	55:S8:175:LEU:O	2.18	0.56
54:S7:85:ALA:O	54:S7:88:ALA:N	2.35	0.56
16:AM:54:VAL:HG13	64:AM:216:CDL:H532	1.88	0.56
33:E5:7:TRP:O	33:E5:96:TYR:HB2	2.06	0.56
50:S3:112:MET:HE2	51:S4:121:PHE:CZ	2.40	0.56
5:A1:137:PHE:O	16:AM:118:ARG:NH2	2.38	0.56
10:A7:6:LEU:O	10:A7:11:ARG:NH1	2.39	0.56
49:S2:249:GLU:OE1	49:S2:274:ARG:NH1	2.38	0.56
34:E6:368:GLU:OE1	34:E6:368:GLU:N	2.36	0.56
49:S2:241:GLU:O	57:V1:492:SER:OG	2.19	0.56
3:2B:80:TYR:HB3	3:2B:81:PRO:HD3	1.87	0.56
4:4L:141:LEU:HB3	45:N2:116:VAL:HG11	1.87	0.56
17:AN:263:LYS:NZ	26:BL:53:ASP:OD2	2.39	0.56
23:B7:36:GLU:OE1	39:ED:133:ARG:NH2	2.38	0.56
29:E1:308:ASP:OD1	29:E1:311:ARG:NH2	2.39	0.56
44:N1:657:TYR:OH	46:N3:286:SER:OG	2.19	0.56
10:A7:26:VAL:HG12	16:AM:52:LYS:HD2	1.88	0.56
10:A7:126:ARG:NH2	16:AM:38:GLY:O	2.39	0.56
12:A9:194:ARG:NH2	15:AL:222:ASN:O	2.37	0.56
43:G3:239:THR:OG1	46:N6:161:LYS:NZ	2.38	0.56
49:S2:157:PRO:O	55:S8:89:ARG:NH2	2.28	0.56
59:E7:212:LEU:O	59:E7:215:THR:OG1	2.22	0.56
2:1B:235:SER:HG	2:1B:240:SER:CB	2.17	0.55
63:A1:202:PC1:C1	63:A1:202:PC1:H152	2.36	0.55
7:A3:31:ARG:NH2	7:A3:33:GLU:OE2	2.39	0.55
11:A8:128:MET:HE2	11:A8:132:TYR:HE2	1.71	0.55
16:AM:28:ARG:NH2	53:S6:21:LEU:O	2.38	0.55
40:FX:205:GLU:OE2	40:FX:223:ARG:NE	2.33	0.55
48:N5:159:ASN:HB2	63:N5:601:PC1:H141	1.88	0.55
55:S8:86:THR:OG1	55:S8:199:GLU:OE2	2.12	0.55
48:N5:121:ILE:O	48:N5:125:THR:HG23	2.06	0.55
11:A8:1:MET:HE2	45:N2:195:ILE:HG21	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:B8:72:ASP:O	47:N4:432:LYS:NZ	2.39	0.55
48:N5:12:ILE:HG22	48:N5:122:MET:HE1	1.87	0.55
48:N5:136:ASP:OD2	48:N5:196:ASN:ND2	2.39	0.55
57:V1:205:TYR:OH	71:V1:581:NAI:H5N	2.06	0.55
20:B4:160:MET:HE1	24:B8:154:ALA:HB1	1.89	0.55
2:1B:236:ARG:NH2	2:1B:488:ASP:O	2.37	0.55
11:A8:164:MET:O	11:A8:169:ARG:NH2	2.40	0.55
32:E4:128:ILE:HD13	32:E4:148:MET:HE2	1.88	0.55
49:S2:59:MET:SD	51:S4:117:LYS:NZ	2.70	0.55
6:A2:157:ASP:OD1	6:A2:157:ASP:N	2.37	0.55
21:B5:119:LYS:NZ	21:B5:123:GLU:OE2	2.29	0.55
30:E2:4:GLY:O	30:E2:5:THR:OG1	2.22	0.55
68:N4:505:U10:H151	68:N4:505:U10:H18	1.88	0.55
20:B4:24:ILE:O	20:B4:24:ILE:HG22	2.07	0.55
33:E5:41:ALA:HB3	33:E5:289:LEU:HB3	1.89	0.55
54:S7:79:PRO:HD3	54:S7:106:THR:HG23	1.89	0.55
70:V1:579:FMN:C5A	71:V1:581:NAI:H4N	2.37	0.55
17:AN:56:ARG:NH2	17:AN:141:GLY:O	2.39	0.55
41:G1:113:ARG:NH2	46:N6:166:TYR:OH	2.36	0.55
57:V1:368:LEU:HD22	57:V1:439:LEU:HB2	1.88	0.55
30:E2:118:VAL:HG13	30:E2:283:LEU:HD13	1.88	0.55
39:ED:91:ILE:N	63:ED:201:PC1:O14	2.40	0.55
44:N1:500:ILE:HG21	46:N6:84:LEU:HB2	1.87	0.55
50:S3:139:VAL:HG11	50:S3:145:ILE:HB	1.89	0.55
21:B5:26:GLY:O	21:B5:30:ASN:ND2	2.36	0.55
29:E1:164:ILE:O	29:E1:180:ARG:NH1	2.40	0.55
12:A9:244:SER:OG	12:A9:264:GLU:OE2	2.19	0.54
14:AC:92:LEU:CG	66:AC:201:ZMP:H19B	2.36	0.54
52:S5:8:ASP:OD2	52:S5:16:HIS:NE2	2.37	0.54
41:G1:130:HIS:NE2	41:G1:346:GLU:OE1	2.38	0.54
46:N6:45:ILE:HD11	46:N6:82:ILE:HG22	1.89	0.54
2:1B:223:LEU:O	2:1B:227:THR:OG1	2.23	0.54
2:1B:267:LEU:HD11	2:1B:280:SER:HB3	1.88	0.54
4:4L:80:PRO:HD3	46:N6:112:ILE:HD11	1.88	0.54
9:A6:67:LYS:NZ	13:AB:108:ASP:OD1	2.28	0.54
23:B7:24:ARG:NH2	24:B8:159:GLU:OE1	2.39	0.54
41:G1:140:TYR:CE2	43:G3:211:THR:HG22	2.43	0.54
43:G3:84:ASP:OD1	43:G3:85:ARG:N	2.41	0.54
48:N5:392:ILE:HA	48:N5:400:LEU:HD23	1.89	0.54
15:AL:210:ARG:NH2	55:S8:172:ASP:OD1	2.33	0.54
50:S3:234:ASP:OD1	50:S3:235:ASP:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:B8:49:ASP:OD1	47:N4:150:LYS:NZ	2.19	0.54
26:BL:60:THR:HG22	26:BL:62:ALA:H	1.72	0.54
44:N1:380:SER:O	44:N1:383:THR:OG1	2.23	0.54
47:N4:325:TYR:CE2	47:N4:329:ILE:HD11	2.43	0.54
1:1A:222:GLN:OE1	57:V1:223:LYS:NZ	2.39	0.54
29:E1:50:ARG:NH2	29:E1:89:ASP:OD2	2.40	0.54
43:G3:112:VAL:HG22	43:G3:128:PRO:HA	1.90	0.54
47:N4:9:ARG:NH2	47:N4:70:TYR:OH	2.40	0.54
47:N4:80:ILE:CD1	47:N4:337:ILE:HG23	2.37	0.54
50:S3:112:MET:HE2	51:S4:121:PHE:HZ	1.73	0.54
11:A8:103:GLU:O	11:A8:107:VAL:HG23	2.08	0.54
30:E2:259:VAL:HG21	30:E2:271:ALA:HB1	1.88	0.54
6:A2:147:LEU:HD13	31:E3:432:PHE:HA	1.90	0.54
18:B2:112:GLU:OE2	24:B8:158:ARG:NH1	2.41	0.54
34:E6:106:LYS:NZ	53:S6:76:PRO:O	2.37	0.54
39:ED:68:ASP:OD1	39:ED:69:LYS:N	2.41	0.54
40:FX:223:ARG:NH2	40:FX:228:LEU:HD21	2.23	0.54
7:A3:55:ALA:HB3	44:N1:658:TYR:HA	1.90	0.54
12:A9:42:THR:OG1	12:A9:43:GLN:OE1	2.19	0.54
21:B5:100:GLN:HG3	28:C4:146:VAL:HG21	1.89	0.54
63:C4:203:PC1:H141	47:N4:22:MET:O	2.06	0.54
48:N5:367:ASP:OD2	48:N5:369:ARG:NH1	2.41	0.54
53:S6:1:MET:SD	53:S6:1:MET:N	2.81	0.54
2:1B:404:ARG:NH2	12:A9:98:THR:O	2.36	0.54
8:A5:63:TYR:O	8:A5:67:VAL:HG23	2.08	0.54
19:B3:5:ASN:ND2	39:ED:21:THR:OG1	2.41	0.54
47:N4:173:ASN:O	47:N4:177:ASN:ND2	2.39	0.54
50:S3:119:ASP:OD2	50:S3:136:ARG:NH1	2.41	0.54
57:V1:278:CYS:HB3	57:V1:288:THR:HG22	1.89	0.54
8:A5:155:GLU:OE2	12:A9:68:ARG:NH2	2.40	0.53
11:A8:128:MET:HE1	16:AM:97:PRO:CB	2.38	0.53
63:AM:220:PC1:H143	32:E4:194:TRP:CE3	2.42	0.53
32:E4:128:ILE:HD11	32:E4:156:LEU:CD1	2.38	0.53
48:N5:67:ASN:ND2	48:N5:75:ASN:OD1	2.41	0.53
49:S2:107:PHE:HZ	49:S2:150:VAL:HG11	1.71	0.53
47:N4:173:ASN:OD1	47:N4:177:ASN:ND2	2.42	0.53
48:N5:161:ARG:NH1	48:N5:247:GLU:OE1	2.40	0.53
53:S6:1:MET:N	55:S8:207:SER:OG	2.41	0.53
58:V2:194:SER:OG	58:V2:198:ARG:O	2.26	0.53
33:E5:240:GLU:OE1	33:E5:240:GLU:N	2.40	0.53
14:AC:70:PHE:O	39:ED:17:LYS:NZ	2.31	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:E1:260:ALA:HB1	29:E1:292:ALA:HB2	1.89	0.53
9:A6:132:LYS:NZ	50:S3:184:GLY:O	2.42	0.53
57:V1:410:VAL:O	57:V1:413:ILE:HG22	2.08	0.53
68:N4:505:U10:H303	68:N4:505:U10:H261	1.90	0.53
4:4L:141:LEU:HD11	46:N6:150:MET:HE1	1.91	0.53
64:AL:304:CDL:H151	54:S7:68:VAL:HG22	1.91	0.53
26:BL:96:GLU:O	26:BL:100:ALA:N	2.42	0.53
30:E2:224:GLU:N	30:E2:224:GLU:OE1	2.42	0.53
57:V1:50:GLN:O	57:V1:54:ASN:ND2	2.41	0.53
30:E2:287:LEU:HD12	30:E2:454:LEU:HD12	1.91	0.53
49:S2:98:LEU:HD12	57:V1:482:PHE:HB3	1.91	0.53
49:S2:104:ARG:NH2	49:S2:161:ARG:O	2.42	0.53
1:1A:49:ASP:OD2	1:1A:118:THR:OG1	2.27	0.53
1:1A:344:LEU:HD23	9:A6:363:VAL:HG13	1.91	0.53
1:1A:352:LEU:HD11	9:A6:360:LEU:CD1	2.38	0.53
36:EA:68:GLU:O	36:EA:69:THR:HG23	2.09	0.53
44:N1:506:TYR:HB2	44:N1:562:ILE:HG23	1.90	0.53
59:E7:67:TRP:CZ2	59:E7:239:LEU:HD11	2.44	0.53
12:A9:451:GLU:OE2	46:N6:43:ARG:NH1	2.40	0.53
18:B2:120:ASP:OD1	18:B2:127:ARG:NE	2.38	0.53
33:E5:84:ARG:NH1	33:E5:114:LEU:O	2.37	0.53
44:N1:476:HIS:CD2	44:N1:506:TYR:HH	2.22	0.53
55:S8:92:HIS:CD2	55:S8:143:CYS:SG	3.02	0.53
41:G1:278:VAL:HG23	41:G1:294:ARG:HD3	1.91	0.52
49:S2:105:VAL:HG21	49:S2:242:VAL:HG22	1.91	0.52
12:A9:436:MET:HE2	12:A9:436:MET:HA	1.91	0.52
27:BM:60:LEU:HD13	47:N4:33:SER:OG	2.08	0.52
33:E5:1:MET:SD	33:E5:1:MET:N	2.79	0.52
58:V2:78:ARG:NH1	58:V2:81:GLU:OE1	2.42	0.52
1:1A:213:GLU:N	1:1A:213:GLU:OE1	2.43	0.52
2:1B:283:ARG:NH2	31:E3:345:GLN:OE1	2.42	0.52
48:N5:190:ILE:O	48:N5:194:ASN:N	2.41	0.52
57:V1:89:GLY:HA3	71:V1:581:NAI:H1D	1.92	0.52
10:A7:26:VAL:HG12	16:AM:52:LYS:CD	2.39	0.52
10:A7:46:ALA:O	16:AM:31:ARG:NH1	2.41	0.52
11:A8:66:GLU:OE1	11:A8:66:GLU:N	2.40	0.52
48:N5:42:ILE:O	48:N5:46:VAL:HG23	2.09	0.52
48:N5:246:MET:SD	48:N5:257:HIS:NE2	2.82	0.52
3:2B:42:SER:O	3:2B:43:SER:OG	2.21	0.52
3:2B:54:THR:HG21	64:N4:501:CDL:H792	1.92	0.52
46:N3:248:LEU:HD23	46:N3:251:ILE:HD11	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:S6:39:PHE:O	53:S6:43:VAL:HG13	2.10	0.52
1:1A:331:MET:HE1	1:1A:335:TYR:CD2	2.44	0.52
17:AN:258:PRO:HG2	21:B5:91:ILE:HG21	1.90	0.52
29:E1:328:LYS:HD2	29:E1:371:LEU:HD22	1.91	0.52
35:E8:18:TRP:CZ3	48:N5:436:LEU:HD12	2.45	0.52
40:FX:190:ILE:HG21	40:FX:198:LEU:HD11	1.90	0.52
42:G2:135:GLN:OE1	42:G2:153:LYS:NZ	2.37	0.52
8:A5:123:GLU:OE2	50:S3:61:TYR:OH	2.18	0.52
12:A9:153:GLU:O	12:A9:211:GLN:NE2	2.41	0.52
53:S6:115:CYS:O	53:S6:119:GLU:N	2.43	0.52
64:A3:201:CDL:OA3	64:A3:201:CDL:O1	2.23	0.52
9:A6:303:LEU:HD21	9:A6:434:LEU:HD21	1.90	0.52
28:C4:45:SER:O	28:C4:51:ASN:ND2	2.43	0.52
31:E3:432:PHE:O	31:E3:433:ALA:HB2	2.08	0.52
2:1B:127:THR:O	2:1B:127:THR:HG23	2.09	0.52
9:A6:210:VAL:O	9:A6:215:GLN:NE2	2.42	0.52
33:E5:152:LEU:HB2	33:E5:284:VAL:HG11	1.92	0.52
38:EC:69:GLU:HG2	38:EC:76:VAL:HG23	1.91	0.52
45:N2:32:GLU:N	45:N2:32:GLU:OE1	2.42	0.52
51:S4:72:PRO:O	51:S4:74:ARG:NH1	2.43	0.52
12:A9:442:ARG:NH1	44:N1:429:ASN:O	2.43	0.51
32:E4:318:VAL:HG21	32:E4:334:VAL:CG2	2.39	0.51
37:EB:89:GLU:N	37:EB:89:GLU:OE1	2.40	0.51
44:N1:582:ILE:HD11	46:N3:214:VAL:CG1	2.40	0.51
48:N5:310:ILE:HG21	48:N5:438:ILE:CG2	2.40	0.51
49:S2:208:GLY:O	49:S2:261:ARG:NH2	2.35	0.51
4:4L:84:ILE:CG2	46:N6:33:ILE:HD11	2.40	0.51
5:A1:65:ALA:O	5:A1:69:VAL:HG23	2.11	0.51
6:A2:31:ILE:HG21	50:S3:272:PRO:HB3	1.91	0.51
16:AM:190:PHE:O	52:S5:98:ARG:NH1	2.40	0.51
1:1A:331:MET:HE2	2:1B:305:VAL:HG11	1.91	0.51
11:A8:13:ASP:OD1	21:B5:115:ASN:ND2	2.38	0.51
45:N2:81:ILE:HD12	46:N6:153:ILE:HD12	1.92	0.51
11:A8:63:ILE:O	11:A8:95:SER:OG	2.14	0.51
30:E2:9:THR:HG22	30:E2:10:GLY:N	2.25	0.51
32:E4:339:SER:O	32:E4:340:HIS:ND1	2.43	0.51
38:EC:19:ARG:NH1	38:EC:92:GLU:OE1	2.40	0.51
48:N5:337:ILE:HD11	48:N5:491:TYR:CD1	2.45	0.51
51:S4:38:VAL:HG23	51:S4:39:ASN:N	2.26	0.51
29:E1:34:LEU:HD22	29:E1:253:LEU:HD22	1.93	0.51
30:E2:135:THR:OG1	30:E2:440:GLY:O	2.20	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A6:99:LEU:HD21	51:S4:50:GLN:HG3	1.92	0.51
43:G3:176:VAL:HB	43:G3:177:PRO:HD3	1.93	0.51
4:4L:118:PHE:CD1	4:4L:135:MET:HE1	2.45	0.51
28:C4:142:SER:O	28:C4:146:VAL:HG22	2.11	0.51
33:E5:266:LEU:HG	33:E5:289:LEU:HD13	1.93	0.51
44:N1:413:ASP:OD1	54:S7:76:SER:OG	2.21	0.51
49:S2:75:MET:HE1	49:S2:118:LEU:HD13	1.92	0.51
1:1A:265:PRO:HA	1:1A:268:ILE:HD12	1.92	0.51
28:C4:2:ASP:OD1	28:C4:3:ARG:N	2.43	0.51
30:E2:417:GLU:N	30:E2:417:GLU:OE1	2.44	0.51
34:E6:331:ILE:HD11	56:U1:8:UNK:CB	2.41	0.51
35:E8:104:ARG:O	35:E8:139:ARG:NH2	2.43	0.51
40:FX:240:THR:HG22	40:FX:241:HIS:O	2.11	0.51
57:V1:358:MET:HB3	57:V1:362:THR:HG21	1.92	0.51
11:A8:102:ARG:HA	11:A8:128:MET:HE3	1.93	0.51
28:C4:84:PRO:O	28:C4:125:SER:OG	2.28	0.51
41:G1:141:LYS:NZ	43:G3:211:THR:HG21	2.26	0.51
54:S7:32:ARG:NH1	54:S7:35:GLU:OE1	2.44	0.51
55:S8:92:HIS:HE1	61:S8:297:SF4:S4	2.31	0.51
3:2B:75:LEU:HD13	45:N2:221:ILE:HG21	1.93	0.51
42:G2:220:GLU:O	42:G2:223:THR:HG22	2.11	0.51
48:N5:503:ILE:HD12	48:N5:508:LEU:HD11	1.93	0.51
9:A6:39:GLU:OE2	49:S2:8:ARG:NH2	2.41	0.50
34:E6:35:LEU:O	34:E6:36:SER:OG	2.23	0.50
35:E8:148:LYS:O	35:E8:149:SER:OG	2.16	0.50
46:N3:245:PHE:HD2	46:N6:81:ILE:HD11	1.76	0.50
47:N4:14:LEU:HD11	63:N4:502:PC1:H362	1.92	0.50
48:N5:239:GLN:N	48:N5:240:PRO:CD	2.74	0.50
51:S4:73:SER:O	51:S4:76:THR:HG22	2.11	0.50
57:V1:167:THR:HG23	57:V1:198:LEU:CD2	2.41	0.50
46:N6:45:ILE:HD11	46:N6:82:ILE:CG2	2.41	0.50
57:V1:157:ILE:HB	57:V1:198:LEU:HD12	1.92	0.50
3:2B:82:ILE:O	3:2B:86:VAL:HG23	2.10	0.50
29:E1:412:ILE:O	29:E1:420:THR:HG23	2.11	0.50
31:E3:118:GLU:HB3	31:E3:296:VAL:HG11	1.93	0.50
2:1B:473:SER:O	30:E2:51:ARG:NH2	2.44	0.50
4:4L:81:TYR:OH	46:N6:25:ASP:OD2	2.28	0.50
27:BM:68:THR:HG22	47:N4:40:ILE:HG12	1.93	0.50
30:E2:2:VAL:N	51:S4:157:ARG:O	2.44	0.50
32:E4:74:THR:OG1	32:E4:141:SER:OG	2.25	0.50
41:G1:343:ASP:OD1	42:G2:33:ARG:NH2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:S3:140:ASP:OD1	50:S3:141:ASP:N	2.36	0.50
9:A6:309:ASP:OD1	9:A6:312:ARG:NH2	2.44	0.50
16:AM:54:VAL:HG12	64:AM:215:CDL:HA31	1.93	0.50
47:N4:300:TYR:OH	47:N4:426:SER:N	2.44	0.50
57:V1:123:PRO:O	58:V2:106:PRO:HG2	2.11	0.50
4:4L:163:VAL:HG13	43:G3:240:MET:HE1	1.92	0.50
40:FX:263:LYS:NZ	41:G1:61:GLU:O	2.43	0.50
16:AM:71:LEU:HD13	63:AM:218:PC1:H342	1.93	0.50
16:AM:141:VAL:O	16:AM:146:ARG:NH1	2.45	0.50
30:E2:201:ASN:ND2	30:E2:332:ALA:O	2.45	0.50
47:N4:352:TYR:CG	47:N4:452:LEU:HD22	2.47	0.50
5:A1:31:CYS:SG	44:N1:370:LEU:HD12	2.51	0.50
24:B8:70:GLY:HA2	48:N5:555:ILE:HG21	1.94	0.50
45:N2:167:GLY:O	45:N2:171:ILE:HG23	2.11	0.50
32:E4:144:LEU:HD12	32:E4:173:ALA:HB2	1.94	0.50
41:G1:292:VAL:HG21	67:G1:516:3PE:H332	1.93	0.50
46:N3:251:ILE:HD11	46:N3:279:ILE:HD11	1.94	0.50
29:E1:246:THR:O	29:E1:436:SER:OG	2.26	0.49
33:E5:283:THR:HG23	33:E5:283:THR:O	2.13	0.49
34:E6:94:ILE:HD11	53:S6:7:LEU:HB2	1.93	0.49
34:E6:130:GLU:OE2	34:E6:213:ARG:NH2	2.45	0.49
40:FX:246:ASP:OD2	40:FX:249:THR:OG1	2.30	0.49
49:S2:241:GLU:N	57:V1:492:SER:OG	2.45	0.49
12:A9:482:TYR:OH	46:N3:175:ASN:ND2	2.45	0.49
45:N2:186:MET:HE3	45:N2:282:TRP:HZ2	1.76	0.49
46:N6:65:ILE:HG23	46:N6:66:LEU:N	2.27	0.49
57:V1:256:LEU:O	58:V2:220:ARG:NH2	2.45	0.49
12:A9:398:ILE:HG12	12:A9:402:LEU:HD12	1.95	0.49
12:A9:469:ILE:HG22	12:A9:472:PRO:HG2	1.94	0.49
33:E5:260:LYS:C	33:E5:284:VAL:O	2.55	0.49
34:E6:361:THR:O	34:E6:361:THR:HG22	2.12	0.49
47:N4:420:CYS:SG	48:N5:180:VAL:HG22	2.52	0.49
44:N1:527:LEU:C	44:N1:527:LEU:HD12	2.36	0.49
44:N1:602:TYR:HA	44:N1:605:ILE:HG22	1.94	0.49
45:N2:175:TYR:CD2	45:N2:186:MET:HE1	2.47	0.49
2:1B:84:ARG:NH1	2:1B:85:PRO:O	2.45	0.49
3:2B:57:PHE:CE2	3:2B:61:ILE:HD11	2.46	0.49
19:B3:10:GLN:NE2	48:N5:447:SER:O	2.45	0.49
40:FX:303:LEU:O	40:FX:307:THR:HG23	2.11	0.49
41:G1:153:ILE:HG23	41:G1:162:PRO:HD2	1.93	0.49
3:2B:63:ILE:C	3:2B:63:ILE:HD12	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:B9:8:LEU:HD23	40:FX:96:ILE:HA	1.95	0.49
64:C4:204:CDL:H342	42:G2:23:LEU:HD11	1.94	0.49
59:E7:12:LEU:HD21	59:E7:212:LEU:HB3	1.95	0.49
21:B5:111:ARG:O	21:B5:116:LYS:NZ	2.37	0.49
31:E3:249:VAL:O	31:E3:253:ASN:ND2	2.41	0.49
47:N4:98:ASN:N	47:N4:98:ASN:OD1	2.46	0.49
59:E7:12:LEU:HD21	59:E7:212:LEU:CB	2.42	0.49
39:ED:91:ILE:HD11	48:N5:34:LEU:HD21	1.95	0.49
40:FX:182:PHE:O	40:FX:217:THR:OG1	2.29	0.49
47:N4:357:THR:CG2	47:N4:369:ILE:HD13	2.43	0.49
46:N6:147:ILE:O	46:N6:150:MET:HG3	2.13	0.49
57:V1:37:LYS:O	57:V1:258:ARG:NH2	2.45	0.49
9:A6:48:PRO:CG	50:S3:176:LEU:HD22	2.43	0.49
20:B4:33:LEU:HD21	20:B4:39:MET:HB2	1.95	0.49
33:E5:7:TRP:NE1	33:E5:266:LEU:O	2.45	0.49
28:C4:9:ARG:NH2	45:N2:147:ILE:O	2.37	0.49
29:E1:148:GLU:OE1	29:E1:148:GLU:N	2.37	0.49
30:E2:188:HIS:CD2	30:E2:220:ILE:HG22	2.48	0.49
46:N6:33:ILE:HA	46:N6:36:ILE:HG22	1.95	0.49
57:V1:351:GLY:O	57:V1:352:THR:OG1	2.26	0.49
27:BM:5:ARG:HG3	41:G1:305:VAL:HG11	1.95	0.48
43:G3:225:LYS:NZ	43:G3:229:GLU:OE1	2.46	0.48
53:S6:127:PHE:N	53:S6:128:PRO:CD	2.76	0.48
14:AC:113:GLU:OE1	14:AC:126:TYR:OH	2.30	0.48
32:E4:238:MET:O	32:E4:304:ARG:NH1	2.47	0.48
34:E6:315:LEU:C	34:E6:315:LEU:HD23	2.39	0.48
59:E7:112:ARG:NH2	59:E7:114:ASP:OD1	2.46	0.48
5:A1:49:TYR:OH	11:A8:83:ASN:ND2	2.45	0.48
24:B8:87:ASP:CG	48:N5:541:LYS:HZ2	2.21	0.48
43:G3:235:GLY:O	43:G3:239:THR:OG1	2.31	0.48
21:B5:35:LEU:HD22	63:B5:203:PC1:C31	2.43	0.48
36:EA:18:LYS:O	36:EA:23:ASN:ND2	2.41	0.48
31:E3:45:PRO:HB2	31:E3:70:SER:HB2	1.95	0.48
49:S2:78:MET:HB2	49:S2:111:THR:HG21	1.95	0.48
57:V1:210:GLU:OE2	57:V1:227:LYS:NZ	2.34	0.48
18:B2:68:PHE:CE2	18:B2:72:LEU:HD11	2.49	0.48
44:N1:536:LEU:O	44:N1:540:ILE:HD13	2.12	0.48
46:N3:219:ASN:ND2	46:N3:221:SER:OG	2.42	0.48
48:N5:152:LEU:C	48:N5:152:LEU:HD23	2.38	0.48
54:S7:97:SER:O	55:S8:74:THR:OG1	2.27	0.48
2:1B:367:ARG:HD2	31:E3:376:VAL:HG11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A6:339:TYR:HB2	9:A6:344:LEU:HD12	1.95	0.48
12:A9:297:LEU:HD11	12:A9:397:TRP:CZ2	2.49	0.48
22:B6:4:LEU:HD13	27:BM:36:PRO:HD2	1.95	0.48
29:E1:136:ASP:OD1	29:E1:193:VAL:HG11	2.13	0.48
33:E5:114:LEU:HD11	33:E5:249:VAL:HG22	1.95	0.48
3:2B:26:ASN:ND2	3:2B:27:ASN:OD1	2.46	0.48
33:E5:42:PRO:HB3	33:E5:286:ILE:HG22	1.94	0.48
47:N4:114:PHE:HB2	47:N4:126:ILE:HG21	1.95	0.48
48:N5:32:ILE:HD11	48:N5:118:VAL:HG11	1.96	0.48
59:E7:177:TYR:OH	59:E7:235:LYS:O	2.31	0.48
15:AL:257:ARG:HD2	55:S8:124:VAL:HG11	1.95	0.48
29:E1:339:ASP:OD2	29:E1:343:LYS:NZ	2.47	0.48
40:FX:134:THR:OG1	41:G1:282:ASP:OD1	2.17	0.48
3:2B:79:LEU:HD11	63:N2:301:PC1:H2A1	1.95	0.48
13:AB:60:THR:HG22	13:AB:124:ILE:HD13	1.95	0.48
29:E1:360:VAL:HG11	29:E1:371:LEU:HD23	1.95	0.48
42:G2:144:ALA:HB1	43:G3:125:ILE:HD13	1.96	0.48
47:N4:35:ILE:HG21	47:N4:108:TYR:OH	2.13	0.48
2:1B:374:ILE:HG21	2:1B:382:THR:HG21	1.95	0.47
18:B2:47:ASP:OD1	19:B3:8:ARG:NH1	2.47	0.47
45:N2:81:ILE:CD1	46:N6:153:ILE:HD12	2.43	0.47
45:N2:171:ILE:N	45:N2:172:PRO:CD	2.77	0.47
1:1A:75:PRO:HB3	1:1A:156:LEU:HD22	1.96	0.47
9:A6:294:LEU:HD12	9:A6:393:ILE:HD11	1.96	0.47
41:G1:105:HIS:CE1	43:G3:241:ARG:HE	2.32	0.47
57:V1:424:SER:HB3	61:V1:580:SF4:S2	2.54	0.47
2:1B:289:MET:SD	2:1B:305:VAL:HG13	2.54	0.47
2:1B:382:THR:HG22	31:E3:392:GLU:HB3	1.96	0.47
12:A9:426:THR:HG21	12:A9:431:ILE:HD13	1.96	0.47
31:E3:242:GLU:N	31:E3:242:GLU:OE1	2.47	0.47
33:E5:87:LEU:HD12	33:E5:87:LEU:H	1.79	0.47
33:E5:124:VAL:HG22	33:E5:124:VAL:O	2.12	0.47
38:EC:78:ASP:OD1	38:EC:78:ASP:N	2.47	0.47
41:G1:305:VAL:O	41:G1:309:THR:HG23	2.15	0.47
44:N1:469:ILE:HD11	44:N1:514:LEU:HD12	1.95	0.47
53:S6:114:GLN:N	53:S6:114:GLN:OE1	2.47	0.47
10:A7:32:TRP:O	49:S2:187:ARG:NH2	2.33	0.47
20:B4:160:MET:HE1	24:B8:154:ALA:CB	2.44	0.47
29:E1:264:PHE:CE2	29:E1:270:VAL:HG21	2.49	0.47
41:G1:294:ARG:CG	42:G2:181:VAL:HG21	2.38	0.47
44:N1:534:LEU:HD11	46:N3:260:PHE:CE1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A6:66:LEU:HD22	9:A6:86:ARG:HG3	1.97	0.47
12:A9:487:LEU:HD21	46:N3:179:LEU:HD11	1.96	0.47
20:B4:89:GLN:NE2	20:B4:91:ARG:O	2.47	0.47
35:E8:26:THR:N	35:E8:27:PRO:CD	2.77	0.47
42:G2:181:VAL:HG23	43:G3:176:VAL:CG2	2.45	0.47
45:N2:5:ASN:OD1	45:N2:6:ASN:ND2	2.48	0.47
47:N4:404:LEU:HD21	47:N4:415:LEU:HD12	1.97	0.47
53:S6:42:ASP:N	53:S6:42:ASP:OD1	2.46	0.47
6:A2:27:GLU:HA	6:A2:30:ALA:HB3	1.97	0.47
33:E5:194:LEU:HD12	33:E5:226:VAL:HG11	1.97	0.47
47:N4:110:ILE:CG2	47:N4:126:ILE:HG23	2.45	0.47
54:S7:99:TYR:OH	55:S8:82:ASN:ND2	2.48	0.47
3:2B:82:ILE:HD11	47:N4:162:LEU:HD13	1.95	0.47
4:4L:145:MET:HE1	45:N2:120:ILE:HG13	1.97	0.47
13:AB:54:LEU:HD21	13:AB:62:ARG:HH21	1.80	0.47
18:B2:124:LEU:HD12	48:N5:280:SER:HB2	1.97	0.47
29:E1:89:ASP:OD1	29:E1:90:SER:N	2.46	0.47
29:E1:135:LYS:O	29:E1:157:LEU:HD12	2.15	0.47
29:E1:328:LYS:HB2	29:E1:362:LEU:HD23	1.96	0.47
33:E5:17:LYS:NZ	33:E5:274:GLU:OE2	2.46	0.47
35:E8:94:ASP:OD1	35:E8:117:LYS:NZ	2.32	0.47
45:N2:68:SER:OG	45:N2:79:GLN:NE2	2.43	0.47
45:N2:248:ILE:O	45:N2:252:ASN:ND2	2.45	0.47
49:S2:121:ALA:HB1	49:S2:133:ILE:HA	1.97	0.47
50:S3:80:VAL:HG12	50:S3:81:TYR:O	2.15	0.47
50:S3:82:PRO:HB3	50:S3:139:VAL:HG12	1.97	0.47
51:S4:162:ARG:NE	51:S4:164:GLU:OE1	2.37	0.47
55:S8:110:CYS:HA	55:S8:113:THR:HG22	1.96	0.47
33:E5:261:VAL:HA	33:E5:285:HIS:HA	1.97	0.47
51:S4:65:VAL:O	51:S4:139:ASN:N	2.47	0.47
53:S6:40:LEU:HA	53:S6:43:VAL:HG22	1.97	0.47
57:V1:209:GLU:OE1	57:V1:211:THR:N	2.45	0.47
58:V2:104:THR:HG22	58:V2:105:THR:H	1.79	0.47
1:1A:345:LEU:HD23	9:A6:367:LEU:HD22	1.95	0.47
3:2B:95:SER:OG	24:B8:31:TYR:O	2.30	0.47
8:A5:50:THR:HA	8:A5:107:LEU:HD13	1.96	0.47
9:A6:189:ALA:HB2	34:E6:219:GLN:HG3	1.96	0.47
9:A6:304:LEU:HD21	9:A6:385:ILE:HG21	1.95	0.47
66:AC:201:ZMP:H9A	25:B9:89:LEU:HB3	1.96	0.47
33:E5:7:TRP:HB2	33:E5:96:TYR:HB3	1.97	0.47
57:V1:167:THR:HG23	57:V1:198:LEU:HD21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:331:MET:HE2	2:1B:305:VAL:HG12	1.96	0.47
10:A7:71:ARG:NH1	49:S2:93:GLU:OE2	2.44	0.47
16:AM:54:VAL:HG12	64:AM:215:CDL:CA3	2.45	0.47
48:N5:393:LEU:HD11	48:N5:432:GLN:HG2	1.95	0.47
22:B6:26:ASN:HB3	48:N5:22:ILE:HG22	1.96	0.46
47:N4:228:GLY:O	47:N4:232:VAL:HG13	2.15	0.46
55:S8:31:HIS:HB3	55:S8:34:VAL:HG23	1.97	0.46
17:AN:247:TYR:O	17:AN:271:TYR:OH	2.14	0.46
29:E1:416:ASP:OD1	29:E1:416:ASP:N	2.47	0.46
45:N2:42:ASP:OD1	45:N2:42:ASP:N	2.41	0.46
57:V1:200:ARG:HH21	58:V2:88:MET:HE1	1.80	0.46
58:V2:119:LEU:HD22	58:V2:181:VAL:HG11	1.97	0.46
2:1B:267:LEU:HD12	2:1B:287:ARG:NH1	2.30	0.46
11:A8:1:MET:HE1	45:N2:58:LEU:HD21	1.96	0.46
64:AL:304:CDL:OB4	44:N1:403:GLY:N	2.45	0.46
44:N1:514:LEU:O	44:N1:539:TYR:OH	2.23	0.46
45:N2:157:PHE:HA	45:N2:160:TYR:HB2	1.97	0.46
47:N4:80:ILE:HD11	47:N4:337:ILE:CG2	2.43	0.46
46:N6:35:LEU:HD13	46:N6:46:ILE:HG22	1.97	0.46
1:1A:45:THR:O	1:1A:112:PRO:O	2.32	0.46
9:A6:137:ASP:OD2	12:A9:330:ARG:NH2	2.44	0.46
17:AN:9:ILE:HA	45:N2:219:LEU:HD22	1.97	0.46
23:B7:60:LYS:O	39:ED:115:THR:HG22	2.15	0.46
25:B9:59:SER:OG	35:E8:12:ARG:NH1	2.48	0.46
35:E8:18:TRP:CE3	48:N5:436:LEU:HD12	2.50	0.46
44:N1:424:ARG:NH2	46:N3:203:LYS:O	2.47	0.46
47:N4:352:TYR:CD2	47:N4:452:LEU:HD22	2.50	0.46
48:N5:491:TYR:OH	48:N5:493:ASN:ND2	2.48	0.46
57:V1:124:GLY:O	57:V1:354:ALA:HB1	2.16	0.46
1:1A:144:ILE:HG23	55:S8:105:ILE:HD12	1.97	0.46
2:1B:338:GLU:OE2	51:S4:98:ARG:NE	2.40	0.46
20:B4:83:LYS:NZ	67:G1:516:3PE:O12	2.36	0.46
30:E2:296:ASP:OD1	30:E2:298:ASP:N	2.49	0.46
44:N1:579:SER:OG	44:N1:645:ARG:NH1	2.49	0.46
59:E7:178:SER:OG	59:E7:180:ASP:OD1	2.33	0.46
9:A6:92:ARG:HB3	66:AB:150:ZMP:H7A	1.97	0.46
16:AM:44:ARG:NH1	16:AM:46:ARG:O	2.48	0.46
31:E3:165:TRP:NE1	31:E3:281:GLU:OE2	2.45	0.46
33:E5:43:VAL:HG23	33:E5:287:LEU:HB2	1.97	0.46
34:E6:254:LYS:NZ	54:S7:40:LEU:O	2.41	0.46
35:E8:147:TYR:CE2	63:E8:301:PC1:H151	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:ED:201:PC1:H132	63:ED:201:PC1:O13	2.16	0.46
42:G2:154:ILE:HD12	42:G2:154:ILE:N	2.31	0.46
44:N1:562:ILE:HD13	44:N1:565:ILE:HD12	1.96	0.46
44:N1:660:LEU:HB3	44:N1:661:PRO:HD3	1.98	0.46
48:N5:363:ILE:O	48:N5:363:ILE:HG22	2.15	0.46
57:V1:159:VAL:CG2	57:V1:198:LEU:HD11	2.45	0.46
24:B8:88:MET:SD	25:B9:104:GLN:NE2	2.89	0.46
45:N2:58:LEU:HD22	45:N2:87:ILE:HG12	1.97	0.46
57:V1:487:ASP:O	57:V1:492:SER:HA	2.16	0.46
17:AN:11:MET:HE1	48:N5:581:ILE:CG2	2.45	0.46
23:B7:44:ARG:HA	23:B7:48:VAL:CG1	2.45	0.46
29:E1:147:ASP:N	29:E1:147:ASP:OD1	2.49	0.46
48:N5:481:LEU:N	48:N5:482:PRO:CD	2.79	0.46
57:V1:122:GLU:HG2	71:V1:581:NAI:H42N	1.98	0.46
4:4L:78:ILE:HG21	4:4L:120:ILE:HG21	1.98	0.46
11:A8:146:GLN:OE1	11:A8:146:GLN:N	2.42	0.46
14:AC:71:ASP:N	35:E8:1:MET:O	2.48	0.46
21:B5:23:ILE:HG13	42:G2:114:VAL:HG21	1.97	0.46
48:N5:153:LEU:HD13	63:N5:601:PC1:H321	1.97	0.46
49:S2:342:TYR:OH	49:S2:344:GLN:NE2	2.47	0.46
50:S3:35:HIS:ND1	50:S3:39:GLU:OE1	2.44	0.46
18:B2:94:ASP:OD2	48:N5:502:TYR:OH	2.14	0.46
64:B3:102:CDL:CB2	39:ED:47:MET:HE1	2.43	0.46
30:E2:348:ASP:HB3	30:E2:359:LEU:HD11	1.98	0.46
39:ED:140:ASP:OD1	39:ED:140:ASP:N	2.49	0.46
40:FX:224:PHE:O	40:FX:228:LEU:HD12	2.16	0.46
41:G1:278:VAL:HB	41:G1:294:ARG:O	2.16	0.46
48:N5:431:SER:HA	48:N5:434:TYR:CE2	2.51	0.46
9:A6:221:LEU:HD23	9:A6:221:LEU:C	2.41	0.45
12:A9:469:ILE:HG22	12:A9:472:PRO:CG	2.46	0.45
33:E5:132:ILE:HG21	33:E5:182:LEU:HD22	1.97	0.45
45:N2:50:ILE:HD12	45:N2:62:ILE:HG21	1.98	0.45
50:S3:220:ARG:NH2	55:S8:171:TYR:OH	2.49	0.45
1:1A:78:CYS:O	1:1A:200:ARG:NH2	2.40	0.45
15:AL:124:GLU:HA	15:AL:129:ASN:O	2.17	0.45
19:B3:58:UNK:O	19:B3:59:UNK:C	2.63	0.45
24:B8:124:PHE:HE2	48:N5:500:ILE:HG23	1.81	0.45
33:E5:245:VAL:O	33:E5:249:VAL:HG23	2.16	0.45
43:G3:149:ILE:N	43:G3:149:ILE:HD12	2.30	0.45
50:S3:148:LEU:HD22	50:S3:151:LEU:HD12	1.97	0.45
58:V2:125:VAL:HG22	58:V2:129:GLU:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A5:125:VAL:HG13	51:S4:38:VAL:HG11	1.98	0.45
11:A8:1:MET:HE3	45:N2:90:THR:CB	2.46	0.45
20:B4:9:LEU:HD11	40:FX:253:THR:HG21	1.97	0.45
29:E1:86:THR:HG21	29:E1:92:MET:HE2	1.98	0.45
29:E1:404:LEU:HD13	29:E1:469:GLY:HA2	1.97	0.45
30:E2:28:LEU:HD12	30:E2:29:VAL:HG23	1.98	0.45
31:E3:400:ASP:OD1	31:E3:400:ASP:N	2.49	0.45
42:G2:103:GLU:HG2	43:G3:80:VAL:HG11	1.99	0.45
53:S6:115:CYS:O	53:S6:119:GLU:HA	2.15	0.45
9:A6:399:ASN:HB2	9:A6:400:PRO:HD3	1.99	0.45
31:E3:46:VAL:HG13	31:E3:97:TRP:HZ2	1.81	0.45
47:N4:186:ASN:O	47:N4:190:ASN:ND2	2.44	0.45
58:V2:24:GLU:N	58:V2:24:GLU:OE1	2.49	0.45
30:E2:348:ASP:OD1	30:E2:372:ARG:NH2	2.42	0.45
44:N1:527:LEU:HD11	46:N6:128:ILE:HD13	1.99	0.45
47:N4:305:MET:HE3	47:N4:305:MET:HA	1.99	0.45
53:S6:71:ARG:NH1	53:S6:120:ASN:OD1	2.50	0.45
1:1A:53:CYS:SG	1:1A:70:ASN:ND2	2.90	0.45
2:1B:191:THR:O	2:1B:194:SER:OG	2.34	0.45
3:2B:69:TYR:HA	3:2B:72:ILE:HG22	1.99	0.45
11:A8:1:MET:HE2	45:N2:195:ILE:CG2	2.46	0.45
25:B9:51:GLU:O	25:B9:106:ARG:NH2	2.50	0.45
30:E2:292:ASN:OD1	30:E2:292:ASN:N	2.48	0.45
41:G1:194:LEU:HD22	41:G1:215:LEU:CD1	2.47	0.45
48:N5:111:ASP:OD1	48:N5:112:LYS:N	2.50	0.45
1:1A:45:THR:HB	1:1A:52:LEU:HD11	1.99	0.45
29:E1:410:VAL:HG13	29:E1:428:VAL:HG13	1.99	0.45
41:G1:190:ASP:OD1	42:G2:87:ARG:NH2	2.43	0.45
47:N4:327:ILE:O	48:N5:71:TYR:OH	2.34	0.45
48:N5:12:ILE:HD11	48:N5:35:ILE:HG22	1.98	0.45
48:N5:494:ILE:HD13	48:N5:499:HIS:CE1	2.51	0.45
9:A6:177:VAL:HG12	9:A6:177:VAL:O	2.16	0.45
34:E6:174:ALA:HB2	34:E6:223:TRP:CZ3	2.52	0.45
41:G1:187:ALA:HB3	41:G1:208:HIS:ND1	2.31	0.45
41:G1:292:VAL:HG22	41:G1:299:LEU:HB2	1.98	0.45
45:N2:171:ILE:HD11	45:N2:248:ILE:HG13	1.99	0.45
52:S5:69:CYS:SG	52:S5:70:ARG:N	2.90	0.45
57:V1:155:ALA:HB2	57:V1:194:PHE:HZ	1.82	0.45
2:1B:418:LEU:HD22	2:1B:446:LEU:HD22	1.98	0.45
35:E8:115:TYR:CE1	35:E8:119:ILE:HD11	2.52	0.45
49:S2:155:MET:HE1	54:S7:86:CYS:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:S4:94:GLY:N	51:S4:109:GLU:OE2	2.49	0.45
15:AL:23:THR:O	15:AL:23:THR:HG22	2.17	0.45
36:EA:56:LYS:NZ	64:EA:201:CDL:OB3	2.33	0.45
48:N5:134:SER:O	48:N5:271:LYS:NZ	2.46	0.45
48:N5:387:ILE:O	48:N5:391:THR:HG23	2.18	0.45
50:S3:156:MET:HE1	50:S3:174:PRO:CG	2.46	0.45
50:S3:219:PHE:O	51:S4:106:LEU:HD23	2.16	0.45
3:2B:46:ILE:O	3:2B:47:THR:HG23	2.16	0.44
24:B8:120:CYS:O	48:N5:417:GLY:O	2.35	0.44
29:E1:305:THR:OG1	53:S6:147:ASP:O	2.27	0.44
38:EC:22:VAL:O	38:EC:26:VAL:HG23	2.17	0.44
41:G1:140:TYR:HE2	43:G3:211:THR:HG22	1.81	0.44
47:N4:37:ILE:O	47:N4:40:ILE:HG22	2.18	0.44
48:N5:52:ILE:HG22	48:N5:52:ILE:O	2.17	0.44
50:S3:93:ARG:NH1	50:S3:151:LEU:O	2.50	0.44
54:S7:64:THR:O	54:S7:68:VAL:HG23	2.17	0.44
1:1A:292:THR:OG1	51:S4:105:ARG:NH2	2.51	0.44
2:1B:258:ARG:NH2	6:A2:165:ILE:O	2.50	0.44
11:A8:42:VAL:HG21	36:EA:113:UNK:N	2.32	0.44
12:A9:283:PHE:CE2	12:A9:431:ILE:HD11	2.52	0.44
22:B6:10:ARG:NH2	47:N4:370:ILE:O	2.50	0.44
24:B8:92:GLU:OE1	24:B8:100:LYS:NZ	2.49	0.44
30:E2:179:ASP:OD1	30:E2:327:ASN:ND2	2.50	0.44
30:E2:338:VAL:HG12	30:E2:339:GLU:N	2.32	0.44
45:N2:175:TYR:CD1	45:N2:186:MET:HE1	2.51	0.44
48:N5:302:ILE:HG21	48:N5:430:LEU:HD22	1.98	0.44
50:S3:104:VAL:N	50:S3:123:ASN:O	2.50	0.44
51:S4:38:VAL:HG23	51:S4:39:ASN:H	1.81	0.44
11:A8:107:VAL:HG21	36:EA:114:UNK:HA	1.99	0.44
40:FX:249:THR:N	40:FX:250:PRO:HD2	2.33	0.44
44:N1:397:ILE:HG23	55:S8:72:SER:OG	2.16	0.44
47:N4:357:THR:HG23	47:N4:369:ILE:HD13	1.99	0.44
12:A9:77:PRO:HB3	51:S4:132:LEU:HD11	1.99	0.44
21:B5:114:LEU:HD13	28:C4:145:LEU:HD13	1.99	0.44
31:E3:403:THR:OG1	31:E3:404:LEU:N	2.50	0.44
38:EC:34:VAL:HG11	38:EC:42:THR:O	2.17	0.44
41:G1:197:ASP:OD1	41:G1:198:ARG:N	2.51	0.44
47:N4:62:ILE:HG23	47:N4:62:ILE:O	2.18	0.44
47:N4:282:ILE:HD13	48:N5:567:ILE:HD11	2.00	0.44
48:N5:234:THR:HG21	48:N5:242:LEU:HB2	1.99	0.44
49:S2:324:PRO:O	49:S2:345:SER:OG	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:S6:115:CYS:O	53:S6:119:GLU:CA	2.65	0.44
58:V2:178:ILE:HD12	58:V2:179:GLU:N	2.33	0.44
11:A8:83:ASN:O	11:A8:87:SER:OG	2.21	0.44
17:AN:266:TYR:OH	21:B5:89:THR:OG1	2.25	0.44
34:E6:336:ILE:HD12	34:E6:346:VAL:HG22	1.99	0.44
47:N4:305:MET:HE1	47:N4:336:MET:SD	2.58	0.44
50:S3:73:THR:O	50:S3:74:ASN:HB2	2.17	0.44
55:S8:158:ILE:HG23	55:S8:158:ILE:O	2.17	0.44
57:V1:34:LEU:HD11	57:V1:274:THR:HG22	1.99	0.44
1:1A:352:LEU:HD11	9:A6:360:LEU:HD12	1.99	0.44
11:A8:4:PRO:O	11:A8:10:THR:OG1	2.22	0.44
33:E5:124:VAL:O	33:E5:153:LEU:HD21	2.18	0.44
42:G2:51:ASN:O	43:G3:28:ARG:NH2	2.51	0.44
48:N5:325:ILE:HD13	48:N5:407:ILE:HA	2.00	0.44
46:N6:42:ILE:HD12	46:N6:42:ILE:C	2.43	0.44
9:A6:158:ARG:NE	9:A6:169:GLU:OE2	2.51	0.44
24:B8:39:ASP:OD1	24:B8:39:ASP:N	2.50	0.44
30:E2:135:THR:HG23	30:E2:440:GLY:H	1.80	0.44
42:G2:150:GLU:OE1	42:G2:150:GLU:N	2.46	0.44
46:N3:228:ILE:O	46:N3:228:ILE:HG22	2.17	0.44
46:N3:255:ILE:HA	46:N3:258:ILE:HG22	1.99	0.44
7:A3:10:ARG:NH2	7:A3:25:GLU:OE2	2.49	0.44
16:AM:141:VAL:HG13	52:S5:75:GLN:NE2	2.33	0.44
28:C4:161:GLU:OE2	28:C4:164:LYS:NZ	2.51	0.44
29:E1:174:LEU:HD21	31:E3:179:LEU:HB2	2.00	0.44
40:FX:185:TRP:C	40:FX:186:SER:HG	2.16	0.44
45:N2:122:ILE:HD13	45:N2:178:ILE:HG12	1.99	0.44
47:N4:131:THR:HG21	47:N4:164:SER:HB2	2.00	0.44
55:S8:161:THR:HG22	55:S8:192:ILE:HD11	2.00	0.44
11:A8:37:LYS:O	36:EA:106:UNK:N	2.51	0.44
34:E6:75:TYR:CZ	34:E6:79:ILE:HD11	2.52	0.44
46:N6:25:ASP:OD1	46:N6:25:ASP:N	2.50	0.44
49:S2:197:GLN:HB3	55:S8:55:GLU:HG2	1.99	0.44
9:A6:36:ARG:NH1	49:S2:6:ASP:OD2	2.51	0.43
20:B4:133:GLU:OE2	20:B4:137:ARG:NE	2.38	0.43
31:E3:321:LEU:HD12	31:E3:321:LEU:N	2.33	0.43
32:E4:128:ILE:HD13	32:E4:148:MET:CE	2.48	0.43
47:N4:153:ILE:HG22	47:N4:157:ASN:HD21	1.83	0.43
47:N4:293:THR:HG22	47:N4:362:LEU:CD2	2.48	0.43
48:N5:528:TYR:CB	59:E7:3:LEU:HD13	2.48	0.43
50:S3:165:MET:HB3	50:S3:190:LEU:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:S6:110:GLY:O	53:S6:134:ARG:NH2	2.51	0.43
2:1B:48:ARG:HE	31:E3:336:ILE:HD13	1.83	0.43
2:1B:461:TYR:O	6:A2:23:ALA:O	2.36	0.43
12:A9:93:LEU:HB3	51:S4:141:SER:HB3	1.99	0.43
12:A9:249:ASP:N	12:A9:249:ASP:OD1	2.51	0.43
13:AB:62:ARG:NH2	13:AB:134:MET:O	2.48	0.43
23:B7:39:ILE:HD11	23:B7:52:LEU:HD13	1.99	0.43
26:BL:22:GLU:OE1	26:BL:22:GLU:N	2.40	0.43
30:E2:108:SER:OG	30:E2:256:GLU:OE2	2.26	0.43
31:E3:298:ARG:HB3	31:E3:321:LEU:HD13	2.00	0.43
34:E6:76:GLU:OE1	34:E6:110:ARG:NH2	2.51	0.43
36:EA:106:UNK:O	36:EA:107:UNK:CB	2.66	0.43
40:FX:121:ASP:OD1	40:FX:127:ARG:NH2	2.47	0.43
48:N5:141:PHE:HB2	48:N5:186:ILE:HD11	2.00	0.43
51:S4:61:ILE:O	51:S4:61:ILE:HG23	2.18	0.43
57:V1:407:GLY:N	57:V1:408:PRO:HD2	2.33	0.43
10:A7:119:ARG:NH1	32:E4:276:GLN:OE1	2.51	0.43
15:AL:227:ASP:OD1	15:AL:227:ASP:N	2.51	0.43
20:B4:37:SER:OG	20:B4:46:LEU:O	2.36	0.43
25:B9:134:LYS:NZ	27:BM:20:PRO:O	2.41	0.43
26:BL:82:LEU:C	26:BL:82:LEU:HD23	2.43	0.43
30:E2:320:HIS:O	30:E2:321:HIS:CG	2.71	0.43
33:E5:36:LEU:HD22	33:E5:87:LEU:HD11	2.00	0.43
41:G1:184:ASN:O	41:G1:205:PRO:HA	2.18	0.43
44:N1:480:ILE:O	46:N6:87:TYR:OH	2.30	0.43
49:S2:210:MET:HE2	49:S2:370:LEU:HD21	1.99	0.43
49:S2:224:MET:SD	49:S2:386:LEU:HD23	2.58	0.43
9:A6:59:ARG:NH1	66:AB:150:ZMP:O7	2.51	0.43
66:AB:150:ZMP:H14	66:AB:150:ZMP:H12A	1.76	0.43
17:AN:105:MET:SD	17:AN:113:LEU:HD12	2.59	0.43
44:N1:525:ILE:HG22	44:N1:525:ILE:O	2.18	0.43
47:N4:99:ASN:ND2	68:N4:505:U10:O3	2.43	0.43
49:S2:103:ILE:HG23	49:S2:169:LEU:HD21	2.01	0.43
58:V2:135:LEU:HD23	58:V2:136:PHE:CE2	2.54	0.43
2:1B:177:GLU:HG3	2:1B:477:THR:HG21	1.99	0.43
12:A9:171:ASP:OD1	12:A9:172:GLN:N	2.45	0.43
12:A9:317:TYR:HH	41:G1:43:GLU:CD	2.26	0.43
12:A9:488:PHE:HB2	12:A9:489:PRO:HD3	2.00	0.43
44:N1:506:TYR:C	44:N1:506:TYR:CD1	2.96	0.43
47:N4:73:ILE:N	47:N4:73:ILE:HD12	2.33	0.43
49:S2:105:VAL:HG21	49:S2:242:VAL:CG2	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:V1:123:PRO:HB3	58:V2:104:THR:HG21	2.00	0.43
63:A1:203:PC1:H152	63:A1:203:PC1:O13	2.18	0.43
25:B9:66:ASP:CG	35:E8:41:HIS:HE2	2.27	0.43
31:E3:45:PRO:HD3	31:E3:121:SER:HB2	1.99	0.43
43:G3:96:ILE:HG23	43:G3:100:VAL:HG11	1.99	0.43
58:V2:105:THR:HA	58:V2:108:MET:HG2	1.99	0.43
25:B9:75:ILE:HD11	25:B9:93:PHE:CE2	2.53	0.43
47:N4:43:ILE:HD12	47:N4:43:ILE:C	2.44	0.43
6:A2:23:ALA:HA	6:A2:64:LEU:HD21	2.01	0.43
29:E1:82:ALA:HB3	29:E1:99:ILE:HD13	2.01	0.43
31:E3:208:PRO:O	31:E3:227:ILE:HD12	2.18	0.43
41:G1:316:THR:HG21	42:G2:111:ILE:O	2.19	0.43
50:S3:230:GLU:O	51:S4:83:ARG:NH2	2.47	0.43
54:S7:77:VAL:HG11	54:S7:117:LEU:HD22	2.00	0.43
55:S8:159:VAL:CG1	55:S8:192:ILE:HD12	2.48	0.43
3:2B:93:ILE:HD13	24:B8:51:PHE:CD1	2.54	0.43
11:A8:80:ILE:HD13	11:A8:136:SER:OG	2.18	0.43
17:AN:245:MET:O	28:C4:152:ARG:NH1	2.42	0.43
23:B7:39:ILE:HD11	23:B7:52:LEU:CD1	2.49	0.43
30:E2:91:LYS:HD3	30:E2:352:VAL:HG21	2.00	0.43
41:G1:260:THR:HG21	43:G3:157:PRO:HB2	2.01	0.43
46:N3:267:THR:O	46:N3:271:THR:HG22	2.19	0.43
47:N4:419:SER:O	47:N4:422:ASN:HB2	2.19	0.43
48:N5:315:THR:HG22	48:N5:349:LYS:HG2	2.00	0.43
46:N6:124:ASN:ND2	52:S5:34:GLU:OE2	2.51	0.43
2:1B:57:GLU:OE1	2:1B:57:GLU:N	2.49	0.43
6:A2:118:ASP:OD1	6:A2:118:ASP:N	2.52	0.43
17:AN:44:GLN:O	17:AN:46:ARG:NH2	2.52	0.43
41:G1:133:ARG:NH2	41:G1:339:ASP:OD1	2.52	0.43
41:G1:306:ASP:O	41:G1:309:THR:OG1	2.29	0.43
43:G3:74:SER:OG	43:G3:76:TRP:NE1	2.50	0.43
47:N4:273:ILE:HD12	47:N4:317:ILE:HD13	2.01	0.43
1:1A:155:ASP:HB3	50:S3:233:TRP:HB2	2.01	0.42
5:A1:124:ASN:N	16:AM:194:GLU:OE2	2.42	0.42
7:A3:99:GLY:O	11:A8:215:ASN:ND2	2.44	0.42
12:A9:122:PHE:HE2	12:A9:192:VAL:HG12	1.84	0.42
34:E6:356:TRP:CZ2	34:E6:361:THR:HG23	2.53	0.42
47:N4:316:LEU:HD21	47:N4:325:TYR:CZ	2.54	0.42
48:N5:6:ILE:HG22	48:N5:94:ILE:HD11	2.01	0.42
46:N6:118:ASN:OD1	46:N6:120:ASN:ND2	2.51	0.42
49:S2:62:VAL:CG2	49:S2:323:ILE:HD11	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:S3:182:ASP:OD1	50:S3:183:TYR:N	2.50	0.42
54:S7:90:GLU:HG2	54:S7:183:PRO:O	2.19	0.42
11:A8:61:LEU:HD11	11:A8:195:CYS:SG	2.59	0.42
12:A9:215:PHE:O	54:S7:48:GLN:NE2	2.45	0.42
18:B2:89:PHE:O	18:B2:93:VAL:HG23	2.19	0.42
57:V1:200:ARG:NH2	58:V2:88:MET:HE1	2.34	0.42
1:1A:322:ALA:N	1:1A:323:PRO:HD2	2.34	0.42
5:A1:127:VAL:HG21	52:S5:94:LYS:HB2	2.01	0.42
9:A6:62:TYR:CZ	9:A6:66:LEU:HD11	2.54	0.42
21:B5:44:ALA:HB3	21:B5:45:PRO:HD3	2.01	0.42
33:E5:7:TRP:HB2	33:E5:96:TYR:CB	2.50	0.42
64:EA:202:CDL:OA3	64:EA:202:CDL:O1	2.29	0.42
42:G2:59:VAL:HG21	42:G2:62:ILE:HG13	2.01	0.42
43:G3:55:ARG:N	43:G3:73:SER:O	2.52	0.42
43:G3:241:ARG:HD3	49:S2:10:MET:HE3	2.00	0.42
49:S2:75:MET:SD	49:S2:118:LEU:HD13	2.59	0.42
51:S4:62:ARG:O	51:S4:63:ARG:NH1	2.48	0.42
28:C4:145:LEU:C	28:C4:145:LEU:HD12	2.43	0.42
29:E1:252:LEU:HD21	29:E1:287:TYR:CZ	2.54	0.42
33:E5:255:ASN:HB2	33:E5:257:LEU:HD23	2.01	0.42
37:EB:96:ARG:NH1	47:N4:319:ASN:O	2.52	0.42
40:FX:141:THR:HG23	40:FX:151:ASN:OD1	2.19	0.42
44:N1:447:LEU:HD11	44:N1:472:LEU:HD23	2.00	0.42
46:N3:258:ILE:HD13	46:N3:271:THR:HG21	2.01	0.42
4:4L:127:LEU:HD12	52:S5:27:LEU:O	2.20	0.42
14:AC:89:LEU:HD13	35:E8:1:MET:SD	2.60	0.42
20:B4:40:MET:HE3	24:B8:73:LEU:HD12	2.01	0.42
29:E1:230:PRO:HB2	29:E1:250:THR:HG23	2.02	0.42
30:E2:217:VAL:HG21	30:E2:272:ILE:HG12	2.02	0.42
34:E6:94:ILE:HG23	34:E6:95:SER:N	2.33	0.42
40:FX:171:LEU:HB3	40:FX:186:SER:HA	2.01	0.42
47:N4:293:THR:HG22	47:N4:362:LEU:HD23	2.01	0.42
48:N5:78:LEU:HD13	48:N5:139:MET:CE	2.50	0.42
48:N5:260:THR:O	48:N5:261:LEU:C	2.63	0.42
51:S4:59:GLU:OE2	51:S4:62:ARG:NH2	2.51	0.42
57:V1:114:VAL:O	57:V1:155:ALA:HA	2.19	0.42
29:E1:323:ALA:HB2	29:E1:357:TRP:CE2	2.55	0.42
32:E4:122:VAL:HG12	32:E4:123:ALA:N	2.34	0.42
33:E5:282:ASP:O	33:E5:284:VAL:HG13	2.18	0.42
34:E6:349:ARG:NH2	34:E6:365:GLN:O	2.45	0.42
41:G1:141:LYS:HZ3	43:G3:211:THR:HG21	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:N2:122:ILE:HD11	45:N2:185:LEU:HD23	2.01	0.42
47:N4:236:THR:OG1	47:N4:355:ASP:OD2	2.36	0.42
48:N5:337:ILE:HG12	48:N5:406:ILE:HG21	2.02	0.42
50:S3:149:THR:N	50:S3:150:PRO:HD2	2.35	0.42
50:S3:186:GLU:OE1	50:S3:186:GLU:N	2.50	0.42
57:V1:150:MET:SD	57:V1:242:ILE:HG21	2.59	0.42
58:V2:149:HIS:HB3	58:V2:170:GLU:HB3	2.01	0.42
58:V2:175:GLU:O	58:V2:178:ILE:HG13	2.19	0.42
58:V2:178:ILE:HA	58:V2:181:VAL:HG22	2.01	0.42
58:V2:223:ASP:OD1	58:V2:223:ASP:N	2.48	0.42
14:AC:113:GLU:OE2	40:FX:98:ARG:N	2.48	0.42
41:G1:281:ASP:N	41:G1:281:ASP:OD1	2.53	0.42
48:N5:374:LEU:HD21	48:N5:455:ILE:HD11	2.01	0.42
49:S2:305:ASP:OD2	53:S6:19:ARG:NH2	2.52	0.42
57:V1:87:ARG:NH1	57:V1:274:THR:O	2.52	0.42
9:A6:365:ARG:HG2	31:E3:338:MET:HB3	2.02	0.42
19:B3:39:UNK:O	19:B3:40:UNK:CB	2.68	0.42
29:E1:324:VAL:HG23	29:E1:355:LEU:HD11	2.01	0.42
32:E4:271:ASN:ND2	32:E4:273:SER:OG	2.52	0.42
34:E6:92:ASP:OD1	34:E6:92:ASP:N	2.53	0.42
41:G1:197:ASP:OD2	43:G3:202:LEU:HD22	2.19	0.42
47:N4:269:LEU:HB2	47:N4:317:ILE:HG22	2.02	0.42
47:N4:404:LEU:O	47:N4:408:ASN:N	2.48	0.42
48:N5:78:LEU:HD13	48:N5:139:MET:HE2	2.02	0.42
48:N5:250:THR:N	48:N5:251:PRO:HD2	2.35	0.42
63:N5:601:PC1:O13	63:N5:601:PC1:H143	2.19	0.42
50:S3:106:VAL:HG22	50:S3:122:TYR:CD2	2.55	0.42
2:1B:378:ASP:O	2:1B:382:THR:HG23	2.20	0.42
3:2B:23:TYR:OH	3:2B:106:ASN:HB2	2.20	0.42
33:E5:40:ALA:HA	33:E5:289:LEU:N	2.34	0.42
33:E5:266:LEU:O	33:E5:266:LEU:HD23	2.20	0.42
39:ED:86:GLU:OE1	39:ED:86:GLU:N	2.47	0.42
44:N1:381:LEU:HA	44:N1:384:VAL:HG12	2.01	0.42
48:N5:466:ILE:HG23	48:N5:467:TYR:N	2.35	0.42
57:V1:150:MET:CE	57:V1:242:ILE:HG21	2.50	0.42
59:E7:12:LEU:HD21	59:E7:212:LEU:HA	2.01	0.42
15:AL:156:ASP:OD2	54:S7:190:TYR:OH	2.36	0.42
24:B8:106:GLY:HA3	35:E8:81:MET:O	2.19	0.42
28:C4:3:ARG:NH2	28:C4:17:GLU:OE2	2.53	0.42
30:E2:135:THR:N	30:E2:440:GLY:O	2.52	0.42
33:E5:38:VAL:HG11	33:E5:41:ALA:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:G2:148:LEU:HB3	42:G2:152:CYS:SG	2.59	0.42
48:N5:577:ILE:O	48:N5:581:ILE:HG13	2.19	0.42
57:V1:114:VAL:HG21	57:V1:147:GLY:HA2	2.00	0.42
1:1A:44:VAL:HG21	1:1A:57:TYR:HB2	2.02	0.41
1:1A:195:CYS:O	1:1A:196:THR:OG1	2.35	0.41
4:4L:118:PHE:CE1	4:4L:135:MET:HE1	2.55	0.41
10:A7:78:ARG:HB3	10:A7:79:PRO:HD3	2.02	0.41
12:A9:122:PHE:CE2	12:A9:192:VAL:HG12	2.55	0.41
12:A9:224:LEU:HB3	12:A9:225:PRO:HD3	2.02	0.41
15:AL:123:GLY:HA3	15:AL:164:TRP:CZ2	2.55	0.41
31:E3:211:ALA:HB2	31:E3:227:ILE:HD13	2.01	0.41
40:FX:195:PHE:HE1	40:FX:223:ARG:HB2	1.85	0.41
45:N2:17:ILE:HD11	46:N6:146:LEU:HA	2.02	0.41
46:N3:251:ILE:HD13	46:N3:279:ILE:HD11	2.01	0.41
48:N5:137:LEU:HB3	48:N5:186:ILE:HG12	2.02	0.41
57:V1:141:GLU:OE2	57:V1:257:ARG:NH1	2.47	0.41
58:V2:99:ILE:HB	58:V2:138:ILE:HD13	2.02	0.41
59:E7:81:VAL:HG23	59:E7:83:GLN:H	1.85	0.41
6:A2:8:ARG:NH2	31:E3:185:LYS:O	2.50	0.41
9:A6:204:ARG:HD2	9:A6:207:LEU:HD12	2.01	0.41
17:AN:242:VAL:O	17:AN:242:VAL:HG12	2.20	0.41
24:B8:45:PRO:HB3	24:B8:62:TRP:CE2	2.55	0.41
24:B8:124:PHE:CZ	48:N5:496:ILE:HB	2.55	0.41
28:C4:47:PHE:O	28:C4:133:ARG:NH1	2.53	0.41
29:E1:69:LEU:HD12	29:E1:208:PHE:O	2.20	0.41
44:N1:453:ILE:HG21	44:N1:461:ILE:HD12	2.01	0.41
47:N4:125:LEU:HD21	64:N4:501:CDL:H802	2.02	0.41
47:N4:420:CYS:HB3	48:N5:176:ARG:HG3	2.01	0.41
2:1B:69:THR:O	2:1B:73:ARG:HG2	2.20	0.41
23:B7:29:LEU:HD12	23:B7:48:VAL:HB	2.02	0.41
47:N4:232:VAL:HG23	47:N4:233:GLU:HG2	2.02	0.41
48:N5:241:TRP:CH2	48:N5:261:LEU:HD23	2.55	0.41
6:A2:26:PRO:O	6:A2:27:GLU:HB3	2.20	0.41
33:E5:47:ASP:OD2	33:E5:65:GLY:N	2.54	0.41
47:N4:405:SER:OG	48:N5:187:ILE:HD12	2.20	0.41
48:N5:377:HIS:O	48:N5:378:ILE:C	2.64	0.41
57:V1:132:MET:HE1	57:V1:159:VAL:HG13	2.02	0.41
2:1B:240:SER:O	2:1B:244:VAL:HG23	2.21	0.41
15:AL:137:THR:OG1	15:AL:138:THR:N	2.53	0.41
15:AL:242:MET:HE1	15:AL:250:PRO:O	2.20	0.41
29:E1:31:VAL:HG12	29:E1:253:LEU:HD21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:E1:270:VAL:HG22	29:E1:323:ALA:HB3	2.03	0.41
34:E6:94:ILE:HD11	53:S6:7:LEU:CB	2.51	0.41
42:G2:203:GLU:OE1	43:G3:85:ARG:NH1	2.53	0.41
47:N4:366:ASN:ND2	47:N4:442:ILE:O	2.53	0.41
49:S2:131:THR:N	49:S2:132:PRO:CD	2.83	0.41
59:E7:52:THR:OG1	59:E7:65:GLU:OE2	2.35	0.41
12:A9:297:LEU:HD11	12:A9:397:TRP:CE2	2.55	0.41
29:E1:152:LYS:HG3	29:E1:305:THR:HG23	2.02	0.41
45:N2:263:ILE:HA	45:N2:267:LEU:HD23	2.02	0.41
48:N5:301:SER:HB3	48:N5:313:TYR:HB3	2.03	0.41
55:S8:180:ARG:NH1	55:S8:184:ASN:OD1	2.53	0.41
2:1B:432:VAL:HB	2:1B:433:PRO:HD3	2.03	0.41
11:A8:143:CYS:O	11:A8:147:THR:OG1	2.31	0.41
29:E1:87:ASP:OD1	29:E1:87:ASP:N	2.51	0.41
32:E4:238:MET:SD	32:E4:297:MET:HE2	2.61	0.41
41:G1:421:VAL:HG21	49:S2:206:LYS:HD3	2.02	0.41
48:N5:328:ILE:O	48:N5:328:ILE:CG2	2.67	0.41
46:N6:126:ILE:O	46:N6:129:ILE:HG12	2.21	0.41
49:S2:10:MET:HE2	49:S2:10:MET:HA	2.03	0.41
2:1B:128:ASP:OD1	2:1B:128:ASP:N	2.54	0.41
2:1B:166:VAL:HG21	2:1B:182:LEU:HD12	2.03	0.41
2:1B:502:MET:HE1	15:AL:278:PRO:HD2	2.03	0.41
3:2B:49:TYR:CG	45:N2:281:ILE:HG13	2.55	0.41
28:C4:114:PHE:CZ	64:C4:202:CDL:OA7	2.74	0.41
33:E5:6:GLY:HA2	33:E5:22:LEU:HD12	2.02	0.41
33:E5:281:SER:OG	33:E5:283:THR:HG22	2.21	0.41
47:N4:211:LEU:HA	47:N4:254:HIS:CE1	2.56	0.41
48:N5:381:LEU:HD11	48:N5:458:PHE:CE2	2.55	0.41
2:1B:74:LEU:HD22	2:1B:390:PHE:HZ	1.86	0.41
4:4L:107:VAL:O	4:4L:111:THR:HG23	2.21	0.41
9:A6:86:ARG:NE	13:AB:96:GLU:OE2	2.41	0.41
12:A9:85:SER:HA	12:A9:92:ARG:O	2.21	0.41
16:AM:140:ALA:HA	52:S5:37:VAL:HG21	2.02	0.41
29:E1:219:SER:HB2	29:E1:222:VAL:HG23	2.03	0.41
30:E2:171:GLY:HA3	30:E2:200:VAL:HG11	2.02	0.41
31:E3:34:VAL:HG23	31:E3:35:GLY:N	2.36	0.41
33:E5:261:VAL:HG12	33:E5:285:HIS:HA	2.02	0.41
34:E6:337:THR:HG22	34:E6:370:THR:HA	2.02	0.41
36:EA:68:GLU:OE1	45:N2:80:LEU:HD11	2.21	0.41
38:EC:78:ASP:O	38:EC:81:PHE:HB2	2.21	0.41
44:N1:527:LEU:HD12	44:N1:528:LEU:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:N2:139:THR:HG23	45:N2:161:LYS:HZ3	1.86	0.41
48:N5:262:VAL:HG23	48:N5:263:THR:HG23	2.03	0.41
48:N5:389:LEU:HD13	48:N5:439:LEU:HB2	2.03	0.41
54:S7:123:THR:HA	54:S7:151:CYS:HB3	2.02	0.41
57:V1:150:MET:HE1	57:V1:242:ILE:HG21	2.03	0.41
58:V2:105:THR:HB	58:V2:106:PRO:HD3	2.01	0.41
10:A7:52:ARG:NH1	49:S2:302:ASP:OD2	2.46	0.41
16:AM:52:LYS:NZ	64:AM:216:CDL:OB4	2.23	0.41
27:BM:56:TRP:HA	27:BM:59:VAL:HG22	2.02	0.41
29:E1:174:LEU:HD13	31:E3:315:THR:CG2	2.51	0.41
30:E2:248:ARG:HD3	30:E2:263:GLY:HA2	2.03	0.41
32:E4:180:ARG:NH2	32:E4:268:ALA:O	2.54	0.41
33:E5:120:ALA:HB3	33:E5:286:ILE:HG21	2.03	0.41
43:G3:160:VAL:HB	43:G3:176:VAL:O	2.21	0.41
44:N1:643:LEU:HD21	55:S8:56:ILE:HG23	2.02	0.41
47:N4:9:ARG:HB2	47:N4:38:ILE:HG21	2.03	0.41
57:V1:133:ARG:HB3	57:V1:166:GLU:HG3	2.02	0.41
4:4L:126:PRO:HG3	52:S5:32:THR:HG21	2.02	0.40
12:A9:169:LEU:HD22	50:S3:206:ALA:HB2	2.02	0.40
15:AL:165:TYR:OH	55:S8:84:LYS:NZ	2.54	0.40
20:B4:151:LEU:HD22	48:N5:209:TYR:OH	2.20	0.40
25:B9:133:TRP:HB3	25:B9:137:THR:HG21	2.02	0.40
32:E4:251:THR:HB	41:G1:435:MET:HE1	2.02	0.40
33:E5:262:VAL:H	33:E5:285:HIS:HB2	1.86	0.40
40:FX:88:LYS:N	40:FX:89:PRO:HD2	2.36	0.40
42:G2:126:GLU:HB3	42:G2:127:PRO:HD2	2.03	0.40
44:N1:626:PHE:O	44:N1:629:ILE:HG13	2.20	0.40
47:N4:110:ILE:HG23	47:N4:126:ILE:HG23	2.03	0.40
47:N4:214:GLY:HA3	47:N4:254:HIS:CE1	2.56	0.40
46:N6:126:ILE:HG22	46:N6:128:ILE:HG13	2.02	0.40
46:N6:155:LEU:C	46:N6:155:LEU:HD23	2.47	0.40
49:S2:135:TRP:O	49:S2:138:GLU:HG3	2.21	0.40
1:1A:88:ASN:OD1	1:1A:89:CYS:N	2.54	0.40
2:1B:27:ARG:HH22	31:E3:352:ALA:HB2	1.85	0.40
3:2B:54:THR:O	3:2B:58:LEU:HG	2.20	0.40
3:2B:59:TYR:CE1	45:N2:267:LEU:HD22	2.57	0.40
29:E1:408:LEU:HD23	29:E1:432:GLY:HA3	2.03	0.40
31:E3:45:PRO:HB3	31:E3:122:LEU:HD23	2.03	0.40
31:E3:91:LEU:HD12	31:E3:91:LEU:N	2.37	0.40
44:N1:446:LEU:O	44:N1:449:ILE:HG22	2.22	0.40
44:N1:459:ILE:HG22	44:N1:461:ILE:HG13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:N2:199:ASN:HB2	45:N2:200:PRO:HD3	2.03	0.40
49:S2:174:LEU:HD11	49:S2:283:ILE:HG21	2.04	0.40
49:S2:253:GLY:H	49:S2:264:ILE:HD11	1.86	0.40
12:A9:42:THR:HG1	12:A9:43:GLN:CD	2.24	0.40
29:E1:393:THR:HG22	29:E1:435:VAL:HG22	2.02	0.40
32:E4:222:PRO:HD3	32:E4:342:ILE:HG21	2.02	0.40
35:E8:177:ASP:OD1	35:E8:177:ASP:N	2.54	0.40
42:G2:181:VAL:HB	42:G2:182:PRO:CD	2.51	0.40
47:N4:308:TYR:CE1	47:N4:396:PHE:CE2	3.09	0.40
53:S6:6:ARG:NH2	55:S8:208:GLN:O	2.55	0.40
57:V1:159:VAL:HG23	57:V1:198:LEU:HD11	2.02	0.40
57:V1:291:GLU:CD	57:V1:304:HIS:HE2	2.22	0.40
59:E7:180:ASP:OD1	59:E7:181:SER:N	2.54	0.40
3:2B:63:ILE:HD13	45:N2:260:ILE:HG21	2.03	0.40
11:A8:210:SER:N	16:AM:86:ASP:OD2	2.54	0.40
12:A9:188:VAL:O	12:A9:192:VAL:HG13	2.21	0.40
12:A9:304:ILE:H	12:A9:304:ILE:HD12	1.86	0.40
20:B4:144:GLY:O	48:N5:216:ASN:ND2	2.54	0.40
34:E6:273:ARG:NH1	54:S7:26:LYS:O	2.50	0.40
35:E8:28:LEU:HA	35:E8:31:TYR:HB2	2.04	0.40
44:N1:587:ILE:HG23	44:N1:588:GLU:HG2	2.04	0.40
45:N2:18:ILE:O	45:N2:19:GLY:C	2.63	0.40
57:V1:170:VAL:HG11	57:V1:198:LEU:HD13	2.03	0.40
59:E7:140:ASP:OD1	59:E7:140:ASP:N	2.47	0.40
9:A6:194:LEU:HD13	9:A6:205:HIS:CE1	2.57	0.40
11:A8:65:ASN:OD1	11:A8:65:ASN:N	2.51	0.40
12:A9:194:ARG:NH1	15:AL:219:HIS:O	2.55	0.40
14:AC:93:ASP:HB3	35:E8:1:MET:SD	2.62	0.40
19:B3:34:ARG:NH2	39:ED:53:ARG:O	2.55	0.40
40:FX:287:PRO:CD	40:FX:307:THR:HG22	2.51	0.40
42:G2:101:ILE:HG23	42:G2:105:VAL:HG11	2.03	0.40
42:G2:149:MET:HE2	42:G2:168:GLU:HG3	2.03	0.40
42:G2:181:VAL:HG23	43:G3:176:VAL:HG21	2.03	0.40
47:N4:187:ILE:HG21	47:N4:256:LEU:HD13	2.04	0.40
46:N6:139:ILE:HG23	46:N6:140:LEU:N	2.37	0.40
49:S2:357:ARG:O	49:S2:357:ARG:HG3	2.20	0.40
57:V1:44:ILE:HG22	58:V2:210:LEU:HD11	2.04	0.40
59:E7:197:ALA:HB2	59:E7:222:TRP:HB2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1A	350/385 (91%)	337 (96%)	13 (4%)	0	100	100
2	1B	523/527 (99%)	507 (97%)	16 (3%)	0	100	100
3	2B	112/142 (79%)	106 (95%)	6 (5%)	0	100	100
4	4L	106/171 (62%)	104 (98%)	2 (2%)	0	100	100
5	A1	135/141 (96%)	125 (93%)	10 (7%)	0	100	100
6	A2	190/193 (98%)	186 (98%)	4 (2%)	0	100	100
7	A3	122/125 (98%)	118 (97%)	4 (3%)	0	100	100
8	A5	152/184 (83%)	148 (97%)	4 (3%)	0	100	100
9	A6	421/437 (96%)	404 (96%)	17 (4%)	0	100	100
10	A7	134/136 (98%)	124 (92%)	10 (8%)	0	100	100
11	A8	221/223 (99%)	215 (97%)	6 (3%)	0	100	100
12	A9	482/489 (99%)	466 (97%)	16 (3%)	0	100	100
13	AB	86/134 (64%)	86 (100%)	0	0	100	100
14	AC	90/134 (67%)	90 (100%)	0	0	100	100
15	AL	263/281 (94%)	248 (94%)	15 (6%)	0	100	100
16	AM	182/198 (92%)	177 (97%)	5 (3%)	0	100	100
17	AN	285/287 (99%)	281 (99%)	4 (1%)	0	100	100
18	B2	103/145 (71%)	102 (99%)	1 (1%)	0	100	100
19	B3	32/62 (52%)	31 (97%)	0	1 (3%)	3	12
20	B4	169/171 (99%)	159 (94%)	10 (6%)	0	100	100
21	B5	132/140 (94%)	129 (98%)	3 (2%)	0	100	100
22	B6	89/91 (98%)	87 (98%)	2 (2%)	0	100	100
23	B7	95/97 (98%)	94 (99%)	1 (1%)	0	100	100
24	B8	145/176 (82%)	143 (99%)	2 (1%)	0	100	100
25	B9	149/158 (94%)	140 (94%)	9 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	BL	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
27	BM	99/112 (88%)	96 (97%)	3 (3%)	0	100	100
28	C4	181/185 (98%)	177 (98%)	4 (2%)	0	100	100
29	E1	448/483 (93%)	432 (96%)	16 (4%)	0	100	100
30	E2	464/467 (99%)	450 (97%)	13 (3%)	1 (0%)	43	70
31	E3	430/434 (99%)	423 (98%)	7 (2%)	0	100	100
32	E4	349/368 (95%)	340 (97%)	9 (3%)	0	100	100
33	E5	266/290 (92%)	245 (92%)	21 (8%)	0	100	100
34	E6	340/371 (92%)	334 (98%)	6 (2%)	0	100	100
35	E8	203/205 (99%)	194 (96%)	9 (4%)	0	100	100
36	EA	96/126 (76%)	91 (95%)	5 (5%)	0	100	100
37	EB	73/101 (72%)	73 (100%)	0	0	100	100
38	EC	83/101 (82%)	76 (92%)	7 (8%)	0	100	100
39	ED	136/151 (90%)	132 (97%)	4 (3%)	0	100	100
40	FX	235/325 (72%)	224 (95%)	11 (5%)	0	100	100
41	G1	416/436 (95%)	405 (97%)	11 (3%)	0	100	100
42	G2	234/267 (88%)	222 (95%)	12 (5%)	0	100	100
43	G3	253/261 (97%)	239 (94%)	14 (6%)	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
46	N3	119/293 (41%)	116 (98%)	3 (2%)	0	100	100
46	N6	152/293 (52%)	149 (98%)	3 (2%)	0	100	100
47	N4	476/478 (100%)	464 (98%)	12 (2%)	0	100	100
48	N5	582/584 (100%)	562 (97%)	20 (3%)	0	100	100
49	S2	391/395 (99%)	373 (95%)	18 (5%)	0	100	100
50	S3	246/277 (89%)	238 (97%)	8 (3%)	0	100	100
51	S4	188/208 (90%)	178 (95%)	10 (5%)	0	100	100
52	S5	110/122 (90%)	106 (96%)	4 (4%)	0	100	100
53	S6	145/147 (99%)	142 (98%)	3 (2%)	0	100	100
54	S7	195/207 (94%)	188 (96%)	7 (4%)	0	100	100
55	S8	180/212 (85%)	176 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
57	V1	502/526 (95%)	481 (96%)	21 (4%)	0	100	100
58	V2	220/225 (98%)	215 (98%)	5 (2%)	0	100	100
59	E7	244/246 (99%)	236 (97%)	8 (3%)	0	100	100
All	All	13568/15237 (89%)	13090 (96%)	476 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
19	B3	34	ARG
30	E2	370	THR

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	74
2	1B	453/454 (100%)	452 (100%)	1 (0%)	87	96
3	2B	109/111 (98%)	109 (100%)	0	100	100
4	4L	96/151 (64%)	95 (99%)	1 (1%)	68	87
5	A1	115/118 (98%)	113 (98%)	2 (2%)	53	80
6	A2	159/160 (99%)	158 (99%)	1 (1%)	78	92
7	A3	104/104 (100%)	104 (100%)	0	100	100
8	A5	134/152 (88%)	132 (98%)	2 (2%)	57	82
9	A6	346/358 (97%)	344 (99%)	2 (1%)	78	92
10	A7	119/119 (100%)	119 (100%)	0	100	100
11	A8	196/196 (100%)	193 (98%)	3 (2%)	57	82
12	A9	420/424 (99%)	415 (99%)	5 (1%)	63	84
13	AB	79/114 (69%)	79 (100%)	0	100	100
14	AC	80/111 (72%)	79 (99%)	1 (1%)	61	84
15	AL	228/242 (94%)	225 (99%)	3 (1%)	61	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	AM	156/168 (93%)	154 (99%)	2 (1%)	61	84
17	AN	241/241 (100%)	239 (99%)	2 (1%)	73	89
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%)	143 (99%)	1 (1%)	76	90
21	B5	108/108 (100%)	108 (100%)	0	100	100
22	B6	82/82 (100%)	82 (100%)	0	100	100
23	B7	93/93 (100%)	92 (99%)	1 (1%)	65	86
24	B8	127/148 (86%)	127 (100%)	0	100	100
25	B9	132/139 (95%)	130 (98%)	2 (2%)	57	82
26	BL	132/132 (100%)	130 (98%)	2 (2%)	57	82
27	BM	93/93 (100%)	93 (100%)	0	100	100
28	C4	166/167 (99%)	162 (98%)	4 (2%)	43	73
29	E1	381/404 (94%)	375 (98%)	6 (2%)	55	81
30	E2	379/380 (100%)	371 (98%)	8 (2%)	47	75
31	E3	339/341 (99%)	337 (99%)	2 (1%)	78	92
32	E4	302/317 (95%)	300 (99%)	2 (1%)	76	90
33	E5	200/205 (98%)	198 (99%)	2 (1%)	68	87
34	E6	293/314 (93%)	290 (99%)	3 (1%)	68	87
35	E8	179/179 (100%)	176 (98%)	3 (2%)	53	80
36	EA	84/86 (98%)	84 (100%)	0	100	100
37	EB	70/70 (100%)	69 (99%)	1 (1%)	59	83
38	EC	73/86 (85%)	72 (99%)	1 (1%)	59	83
39	ED	121/133 (91%)	120 (99%)	1 (1%)	73	89
40	FX	212/276 (77%)	208 (98%)	4 (2%)	50	77
41	G1	348/365 (95%)	343 (99%)	5 (1%)	59	83
42	G2	192/214 (90%)	188 (98%)	4 (2%)	47	75
43	G3	202/202 (100%)	202 (100%)	0	100	100
44	N1	295/639 (46%)	291 (99%)	4 (1%)	59	83
45	N2	285/289 (99%)	281 (99%)	4 (1%)	59	83
46	N3	116/281 (41%)	112 (97%)	4 (3%)	32	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	N6	147/281 (52%)	144 (98%)	3 (2%)	48	76
47	N4	455/455 (100%)	447 (98%)	8 (2%)	51	78
48	N5	546/546 (100%)	539 (99%)	7 (1%)	61	84
49	S2	335/336 (100%)	327 (98%)	8 (2%)	43	73
50	S3	224/250 (90%)	220 (98%)	4 (2%)	51	78
51	S4	159/172 (92%)	155 (98%)	4 (2%)	42	72
52	S5	102/102 (100%)	102 (100%)	0	100	100
53	S6	130/130 (100%)	128 (98%)	2 (2%)	57	82
54	S7	165/171 (96%)	161 (98%)	4 (2%)	43	73
55	S8	160/187 (86%)	158 (99%)	2 (1%)	61	84
57	V1	412/427 (96%)	409 (99%)	3 (1%)	76	90
58	V2	190/190 (100%)	185 (97%)	5 (3%)	40	71
59	E7	192/192 (100%)	190 (99%)	2 (1%)	68	87
All	All	11837/13051 (91%)	11689 (99%)	148 (1%)	59	84

All (148) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1A	150	GLU
1	1A	159	LEU
1	1A	168	ASP
1	1A	174	HIS
1	1A	191	ARG
1	1A	260	ASN
1	1A	310	LEU
2	1B	84	ARG
4	4L	108	GLU
5	A1	37	HIS
5	A1	43	ASP
6	A2	157	ASP
8	A5	60	ASP
8	A5	82	GLU
9	A6	116	LEU
9	A6	210	VAL
11	A8	48	ASP
11	A8	123	GLU
11	A8	176	ARG

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Mol	Chain	Res	Type
12	A9	68	ARG
12	A9	192	VAL
12	A9	213	GLN
12	A9	269	ASP
12	A9	307	THR
14	AC	91	SER
15	AL	63	ARG
15	AL	223	THR
15	AL	229	LEU
16	AM	43	VAL
16	AM	54	VAL
17	AN	20	HIS
17	AN	256	CYS
20	B4	87	SER
23	B7	52	LEU
25	B9	112	ASN
25	B9	130	GLN
26	BL	7	LYS
26	BL	25	ASN
28	C4	43	ASP
28	C4	110	VAL
28	C4	131	PHE
28	C4	145	LEU
29	E1	60	ASN
29	E1	133	LEU
29	E1	147	ASP
29	E1	416	ASP
29	E1	464	LYS
29	E1	467	ASP
30	E2	2	VAL
30	E2	85	LEU
30	E2	131	LYS
30	E2	135	THR
30	E2	209	VAL
30	E2	289	LEU
30	E2	292	ASN
30	E2	388	GLU
31	E3	241	ASP
31	E3	400	ASP
32	E4	206	ASP
32	E4	304	ARG
33	E5	36	LEU

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Mol	Chain	Res	Type
33	E5	106	HIS
34	E6	270	LEU
34	E6	306	ARG
34	E6	311	PHE
35	E8	1	MET
35	E8	86	LEU
35	E8	94	ASP
37	EB	61	GLN
38	EC	78	ASP
39	ED	129	GLN
40	FX	144	ASP
40	FX	172	ASP
40	FX	222	SER
40	FX	321	LYS
41	G1	28	ARG
41	G1	123	PHE
41	G1	321	HIS
41	G1	326	GLU
41	G1	435	MET
42	G2	89	ASP
42	G2	108	ARG
42	G2	174	GLN
42	G2	228	ILE
44	N1	373	LEU
44	N1	376	LEU
44	N1	378	LEU
44	N1	515	LEU
45	N2	44	PHE
45	N2	90	THR
45	N2	155	SER
45	N2	253	ILE
46	N3	233	ILE
46	N3	258	ILE
46	N3	264	ASN
46	N3	292	ASN
47	N4	70	TYR
47	N4	75	ILE
47	N4	98	ASN
47	N4	112	ASN
47	N4	120	ILE
47	N4	184	THR
47	N4	392	VAL

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Mol	Chain	Res	Type
47	N4	397	GLU
48	N5	85	TYR
48	N5	172	VAL
48	N5	367	ASP
48	N5	369	ARG
48	N5	377	HIS
48	N5	393	LEU
48	N5	503	ILE
46	N6	101	ILE
46	N6	108	TYR
46	N6	127	GLU
49	S2	33	GLU
49	S2	133	ILE
49	S2	147	TYR
49	S2	194	LEU
49	S2	260	ASP
49	S2	357	ARG
49	S2	385	THR
49	S2	394	ASP
50	S3	29	GLN
50	S3	41	LYS
50	S3	120	VAL
50	S3	149	THR
51	S4	16	ILE
51	S4	47	GLN
51	S4	156	ARG
51	S4	202	LYS
53	S6	42	ASP
53	S6	43	VAL
54	S7	86	CYS
54	S7	116	ASP
54	S7	123	THR
54	S7	175	ASP
55	S8	55	GLU
55	S8	138	LEU
57	V1	278	CYS
57	V1	345	ASP
57	V1	386	CYS
58	V2	16	SER
58	V2	104	THR
58	V2	120	CYS
58	V2	133	ASP

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Mol	Chain	Res	Type
58	V2	152	MET
59	E7	99	HIS
59	E7	149	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (257) such sidechains are listed below:

Mol	Chain	Res	Type
1	1A	70	ASN
1	1A	76	HIS
1	1A	80	ASN
1	1A	82	ASN
1	1A	113	ASN
1	1A	128	GLN
1	1A	260	ASN
1	1A	261	HIS
1	1A	275	ASN
2	1B	17	ASN
2	1B	33	ASN
2	1B	36	ASN
2	1B	149	ASN
2	1B	155	HIS
2	1B	242	ASN
2	1B	271	GLN
2	1B	278	ASN
2	1B	315	ASN
2	1B	344	GLN
2	1B	438	ASN
2	1B	465	GLN
2	1B	500	HIS
2	1B	507	HIS
3	2B	3	ASN
3	2B	9	ASN
3	2B	26	ASN
3	2B	97	ASN
3	2B	98	ASN
3	2B	99	HIS
3	2B	102	ASN
4	4L	106	HIS
5	A1	60	ASN
5	A1	108	GLN
5	A1	121	HIS
5	A1	132	HIS

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Mol	Chain	Res	Type
5	A1	133	ASN
6	A2	12	HIS
6	A2	75	GLN
6	A2	113	HIS
6	A2	123	ASN
6	A2	183	GLN
7	A3	28	GLN
9	A6	107	HIS
9	A6	128	GLN
9	A6	161	ASN
9	A6	205	HIS
9	A6	336	GLN
9	A6	350	GLN
9	A6	409	HIS
10	A7	7	ASN
10	A7	17	HIS
10	A7	56	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	182	GLN
11	A8	203	HIS
11	A8	208	GLN
12	A9	165	GLN
12	A9	213	GLN
12	A9	242	HIS
12	A9	288	ASN
12	A9	394	HIS
13	AB	52	HIS
14	AC	110	HIS
15	AL	20	GLN
15	AL	39	GLN
15	AL	219	HIS
16	AM	25	GLN
16	AM	73	GLN
16	AM	89	HIS
16	AM	104	GLN
16	AM	172	GLN
17	AN	20	HIS

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Mol	Chain	Res	Type
17	AN	90	HIS
17	AN	154	GLN
17	AN	221	HIS
18	B2	119	HIS
19	B3	5	ASN
20	B4	49	ASN
20	B4	51	HIS
20	B4	69	GLN
21	B5	98	HIS
21	B5	100	GLN
22	B6	19	ASN
22	B6	62	GLN
23	B7	70	HIS
23	B7	75	HIS
24	B8	61	HIS
24	B8	91	GLN
24	B8	113	ASN
24	B8	121	HIS
24	B8	156	GLN
24	B8	165	HIS
25	B9	20	GLN
25	B9	104	GLN
25	B9	112	ASN
26	BL	128	ASN
26	BL	129	HIS
26	BL	144	GLN
27	BM	71	GLN
28	C4	76	GLN
28	C4	95	ASN
29	E1	44	HIS
29	E1	61	GLN
29	E1	105	GLN
29	E1	169	ASN
29	E1	177	GLN
29	E1	192	GLN
29	E1	197	ASN
29	E1	198	GLN
29	E1	223	HIS
29	E1	291	HIS
29	E1	293	HIS
29	E1	302	GLN
29	E1	395	ASN

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Mol	Chain	Res	Type
30	E2	20	GLN
30	E2	58	ASN
30	E2	219	HIS
30	E2	266	GLN
30	E2	321	HIS
30	E2	344	GLN
30	E2	366	GLN
31	E3	20	GLN
31	E3	99	GLN
31	E3	106	ASN
31	E3	160	GLN
31	E3	207	GLN
31	E3	225	HIS
31	E3	303	ASN
31	E3	355	GLN
32	E4	25	GLN
32	E4	59	HIS
32	E4	162	HIS
32	E4	233	GLN
32	E4	358	HIS
33	E5	264	HIS
34	E6	57	ASN
34	E6	147	GLN
34	E6	197	ASN
34	E6	209	HIS
34	E6	222	GLN
34	E6	328	GLN
35	E8	39	ASN
35	E8	67	HIS
35	E8	89	HIS
35	E8	127	ASN
36	EA	4	GLN
36	EA	43	GLN
36	EA	49	HIS
37	EB	99	ASN
38	EC	97	HIS
39	ED	122	GLN
39	ED	139	HIS
40	FX	124	HIS
40	FX	133	GLN
40	FX	180	GLN
40	FX	203	HIS

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Mol	Chain	Res	Type
40	FX	324	GLN
41	G1	105	HIS
41	G1	117	ASN
41	G1	191	HIS
41	G1	252	HIS
41	G1	404	GLN
41	G1	418	GLN
42	G2	36	HIS
42	G2	50	HIS
42	G2	71	GLN
43	G3	36	GLN
43	G3	206	HIS
43	G3	210	ASN
43	G3	231	GLN
44	N1	440	ASN
44	N1	475	ASN
44	N1	526	ASN
45	N2	23	GLN
45	N2	40	ASN
45	N2	75	ASN
45	N2	76	ASN
45	N2	82	HIS
45	N2	89	ASN
45	N2	135	GLN
45	N2	184	ASN
45	N2	208	ASN
45	N2	209	HIS
45	N2	210	ASN
46	N3	172	ASN
46	N3	175	ASN
46	N3	219	ASN
46	N3	264	ASN
46	N3	292	ASN
47	N4	26	ASN
47	N4	48	GLN
47	N4	54	ASN
47	N4	59	ASN
47	N4	112	ASN
47	N4	139	ASN
47	N4	186	ASN
47	N4	200	HIS
47	N4	209	ASN

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Mol	Chain	Res	Type
47	N4	254	HIS
47	N4	262	GLN
47	N4	283	ASN
47	N4	322	ASN
47	N4	339	HIS
47	N4	359	ASN
47	N4	385	ASN
48	N5	21	ASN
48	N5	49	ASN
48	N5	95	ASN
48	N5	101	ASN
48	N5	159	ASN
48	N5	202	ASN
48	N5	366	GLN
48	N5	492	ASN
48	N5	520	ASN
48	N5	533	HIS
48	N5	572	HIS
48	N5	575	ASN
46	N6	124	ASN
49	S2	16	ASN
49	S2	36	HIS
49	S2	45	HIS
49	S2	278	GLN
49	S2	309	ASN
49	S2	344	GLN
49	S2	372	GLN
50	S3	97	GLN
50	S3	99	GLN
50	S3	153	HIS
50	S3	173	HIS
50	S3	208	ASN
50	S3	238	HIS
50	S3	273	GLN
51	S4	47	GLN
52	S5	75	GLN
53	S6	31	GLN
53	S6	85	HIS
54	S7	50	HIS
54	S7	93	GLN
55	S8	70	GLN
55	S8	82	ASN

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Mol	Chain	Res	Type
57	V1	245	ASN
57	V1	282	HIS
57	V1	442	HIS
58	V2	42	GLN
58	V2	122	HIS
58	V2	149	HIS
58	V2	176	GLN
58	V2	183	ASN
59	E7	1	GLN
59	E7	83	GLN
59	E7	99	HIS
59	E7	209	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	2.42	2 (20%)	5,13,15	0.89	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	-	2/10/13/15	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	S2	154	2MR	CZ-NH2	5.11	1.44	1.33
49	S2	154	2MR	CZ-NE	5.09	1.45	1.34

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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	$\# Z > 2$
61	SF4	V1	580	57	0,12,12	-	-	-		
60	FES	V2	301	58	0,4,4	-	-	-		
66	ZMP	AC	201	14	29,35,36	0.67	1 (3%)	34,42,45	0.87	1 (2%)
68	U10	N4	505	-	43,43,63	2.43	15 (34%)	52,55,79	1.74	15 (28%)
61	SF4	S8	298	55	0,12,12	-	-	-		
63	PC1	N1	701	-	48,48,53	0.30	0	54,56,61	0.29	0
63	PC1	A9	560	-	32,32,53	0.38	0	38,40,61	0.33	0
64	CDL	B5	201	-	57,57,99	0.39	0	63,69,111	0.34	0
63	PC1	C4	203	-	37,37,53	0.35	0	43,45,61	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
61	SF4	S8	297	55	0,12,12	-	-	-		
64	CDL	AM	216	-	71,71,99	0.35	0	77,83,111	0.37	0
63	PC1	N4	502	-	38,38,53	0.34	0	44,46,61	0.31	0
64	CDL	AM	215	-	71,71,99	0.35	0	77,83,111	0.30	0
66	ZMP	AB	150	13	29,35,36	0.71	1 (3%)	34,42,45	0.92	1 (2%)
64	CDL	N5	608	-	92,92,99	0.31	0	98,104,111	0.29	0
67	3PE	AN	302	-	50,50,50	0.30	0	53,55,55	0.30	0
67	3PE	G1	516	-	39,39,50	0.34	0	42,44,55	0.31	0
60	FES	1A	401	1	0,4,4	-	-	-		
64	CDL	E7	301	-	67,67,99	0.36	0	73,79,111	0.30	0
64	CDL	N5	603	-	69,69,99	0.35	0	75,81,111	0.32	0
63	PC1	AN	301	-	47,47,53	0.32	0	53,55,61	0.28	0
65	NDP	A9	559	-	49,52,52	0.38	0	66,80,80	0.39	0
64	CDL	AM	217	-	71,71,99	0.36	0	77,83,111	0.33	0
63	PC1	N5	601	-	53,53,53	0.30	0	59,61,61	0.28	0
63	PC1	N5	606	-	35,35,53	0.35	0	41,43,61	0.31	0
61	SF4	1A	402	1	0,12,12	-	-	-		
63	PC1	N4	503	-	32,32,53	0.37	0	38,40,61	0.34	0
64	CDL	A3	201	-	57,57,99	0.39	0	63,69,111	0.34	0
64	CDL	AL	302	-	67,67,99	0.36	0	73,79,111	0.31	0
64	CDL	C4	202	-	93,93,99	0.31	0	99,105,111	0.30	0
63	PC1	B5	202	-	53,53,53	0.29	0	59,61,61	0.32	0
71	NAI	V1	581	-	45,48,48	0.30	0	60,73,73	0.39	0
63	PC1	N3	301	-	41,41,53	0.34	0	47,49,61	0.39	0
63	PC1	N5	605	-	40,40,53	0.33	0	46,48,61	0.30	0
64	CDL	C4	204	-	68,68,99	0.36	0	74,80,111	0.34	0
64	CDL	E6	431	-	63,63,99	0.37	0	69,75,111	0.33	0
67	3PE	N5	607	-	50,50,50	0.31	0	53,55,55	0.31	0
63	PC1	AM	220	-	47,47,53	0.31	0	53,55,61	0.25	0
64	CDL	AL	303	-	63,63,99	0.37	0	69,75,111	0.32	0
64	CDL	AL	304	-	69,69,99	0.36	0	75,81,111	0.31	0
63	PC1	E8	302	-	53,53,53	0.30	0	59,61,61	0.28	0
61	SF4	1A	403	1	0,12,12	-	-	-		
64	CDL	EA	202	-	54,54,99	0.39	0	60,66,111	0.35	0
63	PC1	A1	203	-	30,30,53	0.37	0	36,38,61	0.35	0
61	SF4	S7	301	54	0,12,12	-	-	-		
64	CDL	EA	201	-	58,58,99	0.39	0	64,70,111	0.36	0
64	CDL	N4	501	-	97,97,99	0.31	0	103,109,111	0.28	0
63	PC1	E8	301	-	53,53,53	0.30	0	59,61,61	0.31	0
63	PC1	A1	202	-	48,48,53	0.31	0	54,56,61	0.31	0
63	PC1	AM	218	-	48,48,53	0.31	0	54,56,61	0.28	0
63	PC1	N1	702	-	39,39,53	0.34	0	45,47,61	0.29	0
70	FMN	V1	579	-	33,33,33	0.32	0	48,50,50	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
63	PC1	ED	201	-	53,53,53	0.30	0	59,61,61	0.30	0
64	CDL	B3	102	-	64,64,99	0.37	0	70,76,111	0.34	0
63	PC1	AL	301	-	49,49,53	0.31	0	55,57,61	0.28	0
63	PC1	A9	561	-	32,32,53	0.36	0	38,40,61	0.34	0
63	PC1	B5	203	-	53,53,53	0.30	0	59,61,61	0.32	0
67	3PE	N4	504	-	40,40,50	0.34	0	43,45,55	0.31	0
63	PC1	E4	401	-	50,50,53	0.30	0	56,58,61	0.28	0
63	PC1	E8	303	-	32,32,53	0.36	0	38,40,61	0.37	0
63	PC1	E8	304	-	29,29,53	0.38	0	35,37,61	0.32	0
63	PC1	N2	301	-	36,36,53	0.35	0	42,44,61	0.34	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
68	U10	N4	505	-	-	8/39/63/87	0/1/1/1
66	ZMP	AC	201	14	-	24/40/42/43	-
60	FES	V2	301	58	-	-	0/1/1/1
61	SF4	V1	580	57	-	-	0/6/5/5
61	SF4	S8	298	55	-	-	0/6/5/5
63	PC1	A9	560	-	-	10/36/36/57	-
64	CDL	B5	201	-	-	8/68/68/110	-
63	PC1	C4	203	-	-	9/41/41/57	-
64	CDL	AM	216	-	-	16/82/82/110	-
61	SF4	S8	297	55	-	-	0/6/5/5
63	PC1	N4	502	-	-	12/42/42/57	-
64	CDL	AM	215	-	-	23/82/82/110	-
66	ZMP	AB	150	13	-	16/40/42/43	-
64	CDL	N5	608	-	-	20/103/103/110	-
67	3PE	AN	302	-	-	9/54/54/54	-
67	3PE	G1	516	-	-	11/43/43/54	-
60	FES	1A	401	1	-	-	0/1/1/1
64	CDL	E7	301	-	-	19/78/78/110	-
64	CDL	N5	603	-	-	11/80/80/110	-
63	PC1	AN	301	-	-	12/51/51/57	-
65	NDP	A9	559	-	-	3/34/77/77	0/5/5/5
64	CDL	AM	217	-	-	20/82/82/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
63	PC1	N5	601	-	-	10/57/57/57	-
63	PC1	N5	606	-	-	7/39/39/57	-
64	CDL	A3	201	-	-	7/68/68/110	-
63	PC1	N4	503	-	-	6/36/36/57	-
64	CDL	AL	302	-	-	14/78/78/110	-
64	CDL	C4	202	-	-	22/104/104/110	-
71	NAI	V1	581	-	-	7/29/72/72	0/5/5/5
63	PC1	B5	202	-	-	19/57/57/57	-
61	SF4	1A	402	1	-	-	0/6/5/5
63	PC1	N3	301	-	-	11/45/45/57	-
63	PC1	N5	605	-	-	13/44/44/57	-
64	CDL	C4	204	-	-	9/79/79/110	-
64	CDL	E6	431	-	-	24/74/74/110	-
67	3PE	N5	607	-	-	10/54/54/54	-
63	PC1	AM	220	-	-	9/51/51/57	-
64	CDL	AL	303	-	-	22/74/74/110	-
64	CDL	AL	304	-	-	29/80/80/110	-
63	PC1	E8	302	-	-	19/57/57/57	-
64	CDL	EA	202	-	-	18/65/65/110	-
61	SF4	1A	403	1	-	-	0/6/5/5
63	PC1	A1	203	-	-	6/34/34/57	-
64	CDL	EA	201	-	-	12/69/69/110	-
64	CDL	N4	501	-	-	20/108/108/110	-
61	SF4	S7	301	54	-	-	0/6/5/5
63	PC1	E8	301	-	-	8/57/57/57	-
63	PC1	A1	202	-	-	17/52/52/57	-
63	PC1	AM	218	-	-	17/52/52/57	-
63	PC1	N1	702	-	-	10/43/43/57	-
70	FMN	V1	579	-	-	2/18/18/18	0/3/3/3
63	PC1	ED	201	-	-	11/57/57/57	-
64	CDL	B3	102	-	-	17/75/75/110	-
63	PC1	AL	301	-	-	11/53/53/57	-
63	PC1	A9	561	-	-	5/36/36/57	-
63	PC1	N1	701	-	-	16/52/52/57	-
63	PC1	B5	203	-	-	20/57/57/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
67	3PE	N4	504	-	-	9/44/44/54	-
63	PC1	E4	401	-	-	13/54/54/57	-
63	PC1	E8	303	-	-	5/36/36/57	-
63	PC1	E8	304	-	-	11/33/33/57	-
63	PC1	N2	301	-	-	14/40/40/57	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
68	N4	505	U10	C6-C1	10.21	1.53	1.35
68	N4	505	U10	C4-C3	4.27	1.53	1.36
68	N4	505	U10	C7-C8	3.02	1.55	1.50
68	N4	505	U10	C7-C6	2.95	1.56	1.51
68	N4	505	U10	C31-C29	2.73	1.57	1.51
68	N4	505	U10	C16-C14	2.66	1.56	1.51
66	AB	150	ZMP	C9-C10	-2.62	1.48	1.50
68	N4	505	U10	C6-C5	2.52	1.53	1.46
68	N4	505	U10	C21-C19	2.52	1.56	1.51
68	N4	505	U10	C26-C24	2.47	1.56	1.51
68	N4	505	U10	O5-C5	-2.47	1.18	1.23
66	AC	201	ZMP	C9-C10	-2.46	1.48	1.50
68	N4	505	U10	C11-C9	2.39	1.56	1.51
68	N4	505	U10	O2-C2	-2.26	1.18	1.23
68	N4	505	U10	C27-C28	2.19	1.57	1.50
68	N4	505	U10	O3-C3M	-2.09	1.40	1.45
68	N4	505	U10	C36-C34	2.04	1.55	1.50

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
68	N4	505	U10	C30-C29-C31	4.40	122.67	115.27
68	N4	505	U10	C7-C8-C9	-4.12	119.94	126.79
68	N4	505	U10	C7-C6-C5	3.47	122.66	118.48
68	N4	505	U10	C15-C14-C16	3.27	120.77	115.27
68	N4	505	U10	C22-C23-C24	-2.95	120.56	127.66
66	AB	150	ZMP	C15-C14-C13	-2.89	107.55	112.36
68	N4	505	U10	C17-C18-C19	-2.73	121.08	127.66
68	N4	505	U10	C20-C19-C21	2.65	119.73	115.27
68	N4	505	U10	C25-C24-C26	2.64	119.71	115.27
68	N4	505	U10	C15-C14-C13	-2.59	117.03	123.68
68	N4	505	U10	C1M-C1-C6	-2.54	120.25	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
66	AC	201	ZMP	C15-C14-C13	-2.42	108.33	112.36
68	N4	505	U10	C10-C9-C11	2.35	119.23	115.27
68	N4	505	U10	C27-C28-C29	-2.21	122.34	127.66
68	N4	505	U10	C12-C13-C14	-2.13	122.53	127.66
68	N4	505	U10	C32-C33-C34	-2.12	120.52	127.75
68	N4	505	U10	C36-C34-C35	2.03	119.09	114.60

There are no chirality outliers.

All (711) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
63	A1	202	PC1	C11-O13-P-O14
63	A1	202	PC1	C11-O13-P-O11
63	A1	202	PC1	C1-O11-P-O12
63	A1	203	PC1	C1-O11-P-O13
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	C1-O11-P-O12
63	A9	561	PC1	O13-C11-C12-N
63	AL	301	PC1	C11-O13-P-O12
63	AM	220	PC1	C1-O11-P-O14
63	AN	301	PC1	C1-O11-P-O14
63	B5	202	PC1	C11-O13-P-O12
63	B5	202	PC1	C1-O11-P-O13
63	E4	401	PC1	C11-O13-P-O12
63	E8	301	PC1	C11-O13-P-O14
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	C11-O13-P-O14
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	702	PC1	C1-O11-P-O12
63	N1	702	PC1	O21-C2-C3-O31
63	N2	301	PC1	C1-O11-P-O14
63	N4	503	PC1	C1-O11-P-O14
63	N4	503	PC1	C1-O11-P-O13
63	N5	601	PC1	C11-O13-P-O12
63	N5	601	PC1	C11-O13-P-O14

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Mol	Chain	Res	Type	Atoms
63	N5	601	PC1	C11-O13-P-O11
63	N5	605	PC1	C11-O13-P-O12
63	N5	605	PC1	C1-O11-P-O14
63	N5	605	PC1	C1-O11-P-O13
63	N5	606	PC1	C1-O11-P-O14
64	A3	201	CDL	C1-CA2-OA2-PA1
64	AL	303	CDL	CA2-OA2-PA1-OA3
64	AL	303	CDL	CA2-OA2-PA1-OA5
64	AL	303	CDL	CA3-OA5-PA1-OA3
64	AL	303	CDL	CB2-OB2-PB2-OB3
64	AL	304	CDL	CA2-OA2-PA1-OA3
64	AL	304	CDL	CA2-OA2-PA1-OA4
64	AL	304	CDL	CA2-OA2-PA1-OA5
64	AM	215	CDL	CA2-OA2-PA1-OA3
64	AM	215	CDL	CA2-OA2-PA1-OA4
64	AM	215	CDL	CA3-OA5-PA1-OA3
64	AM	215	CDL	CB3-OB5-PB2-OB4
64	AM	216	CDL	CB2-OB2-PB2-OB4
64	AM	216	CDL	CB3-OB5-PB2-OB3
64	AM	216	CDL	CB3-OB5-PB2-OB4
64	AM	217	CDL	CA2-OA2-PA1-OA4
64	AM	217	CDL	CA3-OA5-PA1-OA4
64	B3	102	CDL	CA2-OA2-PA1-OA3
64	B3	102	CDL	CA3-OA5-PA1-OA3
64	B3	102	CDL	CA3-OA5-PA1-OA4
64	C4	202	CDL	CA2-OA2-PA1-OA3
64	C4	202	CDL	CA2-OA2-PA1-OA4
64	C4	202	CDL	CA2-OA2-PA1-OA5
64	C4	202	CDL	CA3-OA5-PA1-OA3
64	C4	202	CDL	CA3-OA5-PA1-OA4
64	C4	202	CDL	CB3-OB5-PB2-OB4
64	C4	204	CDL	CA3-OA5-PA1-OA2
64	C4	204	CDL	CA3-OA5-PA1-OA3
64	C4	204	CDL	CA3-OA5-PA1-OA4
64	C4	204	CDL	CB2-OB2-PB2-OB4
64	E6	431	CDL	CA2-OA2-PA1-OA4
64	E6	431	CDL	CA3-OA5-PA1-OA4
64	E6	431	CDL	CB2-OB2-PB2-OB4
64	E6	431	CDL	CB3-OB5-PB2-OB3
64	E6	431	CDL	CB3-OB5-PB2-OB4
64	EA	201	CDL	CA3-OA5-PA1-OA3
64	EA	201	CDL	CA3-OA5-PA1-OA4

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Mol	Chain	Res	Type	Atoms
64	EA	202	CDL	CB3-OB5-PB2-OB3
64	N4	501	CDL	CA2-OA2-PA1-OA3
64	N4	501	CDL	CA2-OA2-PA1-OA4
64	N5	603	CDL	CA2-OA2-PA1-OA5
64	N5	603	CDL	CB2-OB2-PB2-OB4
64	N5	603	CDL	CB3-OB5-PB2-OB3
64	N5	608	CDL	CA2-OA2-PA1-OA3
64	N5	608	CDL	CA2-OA2-PA1-OA4
64	E7	301	CDL	C1-CA2-OA2-PA1
64	E7	301	CDL	CA3-OA5-PA1-OA2
64	E7	301	CDL	CA3-OA5-PA1-OA3
64	E7	301	CDL	OB5-CB3-CB4-OB6
66	AB	150	ZMP	O4-C17-C18-C21
66	AB	150	ZMP	C16-C17-C18-C21
66	AB	150	ZMP	O4-C17-C18-C19
66	AB	150	ZMP	C16-C17-C18-C19
66	AB	150	ZMP	O4-C17-C18-C20
66	AB	150	ZMP	C16-C17-C18-C20
66	AB	150	ZMP	N2-C16-C17-O4
66	AB	150	ZMP	C7-C8-C9-C10
66	AC	201	ZMP	C19-C18-C21-O5
66	AC	201	ZMP	C17-C18-C21-O5
66	AC	201	ZMP	O4-C17-C18-C21
66	AC	201	ZMP	C16-C17-C18-C21
66	AC	201	ZMP	O4-C17-C18-C19
66	AC	201	ZMP	C16-C17-C18-C19
66	AC	201	ZMP	O4-C17-C18-C20
66	AC	201	ZMP	C16-C17-C18-C20
66	AC	201	ZMP	C13-C14-C15-N2
66	AC	201	ZMP	C12-C11-S1-C10
66	AC	201	ZMP	C7-C8-C9-C10
67	AN	302	3PE	O13-C11-C12-N
67	N4	504	3PE	C11-O13-P-O14
67	N5	607	3PE	C11-O13-P-O11
67	N5	607	3PE	C11-O13-P-O12
67	N5	607	3PE	C11-O13-P-O14
67	N5	607	3PE	O13-C11-C12-N
68	N4	505	U10	C1-C6-C7-C8
68	N4	505	U10	C5-C6-C7-C8
70	V1	579	FMN	N10-C1'-C2'-O2'
71	V1	581	NAI	C5B-O5B-PA-O1A
71	V1	581	NAI	C5B-O5B-PA-O2A

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Mol	Chain	Res	Type	Atoms
71	V1	581	NAI	PN-O3-PA-O5B
71	V1	581	NAI	O4B-C4B-C5B-O5B
66	AB	150	ZMP	C14-C13-N1-C12
66	AC	201	ZMP	C14-C13-N1-C12
66	AC	201	ZMP	C3-C4-C5-C6
68	N4	505	U10	C30-C29-C31-C32
68	N4	505	U10	C28-C29-C31-C32
66	AB	150	ZMP	O2-C13-N1-C12
66	AC	201	ZMP	O2-C13-N1-C12
64	B3	102	CDL	CA7-C31-C32-C33
63	N3	301	PC1	C11-C12-N-C15
64	AL	304	CDL	O1-C1-CA2-OA2
64	AM	217	CDL	O1-C1-CB2-OB2
64	EA	201	CDL	O1-C1-CA2-OA2
63	N5	605	PC1	C21-C22-C23-C24
64	C4	202	CDL	CB7-C71-C72-C73
63	B5	202	PC1	C21-C22-C23-C24
64	AL	302	CDL	CB5-C51-C52-C53
64	AM	217	CDL	CB5-C51-C52-C53
64	N4	501	CDL	CA5-C11-C12-C13
64	N5	608	CDL	CA7-C31-C32-C33
71	V1	581	NAI	C3B-C4B-C5B-O5B
63	E4	401	PC1	C11-C12-N-C13
64	A3	201	CDL	CA5-C11-C12-C13
63	B5	202	PC1	C26-C27-C28-C29
63	A1	202	PC1	C1-O11-P-O13
63	A9	561	PC1	C1-O11-P-O13
63	AM	220	PC1	C1-O11-P-O13
63	AN	301	PC1	C1-O11-P-O13
63	B5	202	PC1	C11-O13-P-O11
63	B5	203	PC1	C1-O11-P-O13
63	C4	203	PC1	C11-O13-P-O11
63	E4	401	PC1	C11-O13-P-O11
63	E8	303	PC1	C1-O11-P-O13
63	N1	701	PC1	C1-O11-P-O13
63	N1	702	PC1	C1-O11-P-O13
63	N2	301	PC1	C1-O11-P-O13
63	N5	606	PC1	C1-O11-P-O13
64	AL	303	CDL	CA3-OA5-PA1-OA2
64	AL	303	CDL	CB2-OB2-PB2-OB5
64	AL	304	CDL	CB2-OB2-PB2-OB5
64	AL	304	CDL	CB3-OB5-PB2-OB2

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Mol	Chain	Res	Type	Atoms
64	AM	215	CDL	CA2-OA2-PA1-OA5
64	AM	215	CDL	CA3-OA5-PA1-OA2
64	AM	215	CDL	CB2-OB2-PB2-OB5
64	AM	215	CDL	CB3-OB5-PB2-OB2
64	AM	216	CDL	CB2-OB2-PB2-OB5
64	AM	216	CDL	CB3-OB5-PB2-OB2
64	AM	217	CDL	CA2-OA2-PA1-OA5
64	AM	217	CDL	CA3-OA5-PA1-OA2
64	B3	102	CDL	CA3-OA5-PA1-OA2
64	B5	201	CDL	CA3-OA5-PA1-OA2
64	C4	202	CDL	CA3-OA5-PA1-OA2
64	C4	204	CDL	CB2-OB2-PB2-OB5
64	E6	431	CDL	CA2-OA2-PA1-OA5
64	E6	431	CDL	CB2-OB2-PB2-OB5
64	E6	431	CDL	CB3-OB5-PB2-OB2
64	EA	201	CDL	CA3-OA5-PA1-OA2
64	N4	501	CDL	CA2-OA2-PA1-OA5
64	N5	603	CDL	CA3-OA5-PA1-OA2
64	N5	603	CDL	CB2-OB2-PB2-OB5
64	N5	608	CDL	CA2-OA2-PA1-OA5
64	N5	608	CDL	CA3-OA5-PA1-OA2
64	E7	301	CDL	CA2-OA2-PA1-OA5
67	AN	302	3PE	C11-O13-P-O11
67	G1	516	3PE	C21-C22-C23-C24
64	AL	304	CDL	CB2-C1-CA2-OA2
63	N3	301	PC1	C11-C12-N-C13
63	N3	301	PC1	C11-C12-N-C14
64	N5	608	CDL	CB5-C51-C52-C53
66	AB	150	ZMP	C3-C4-C5-C6
63	N2	301	PC1	C24-C25-C26-C27
63	N5	601	PC1	C22-C23-C24-C25
66	AC	201	ZMP	C2-C3-C4-C5
66	AC	201	ZMP	C20-C18-C21-O5
63	AM	218	PC1	C24-C25-C26-C27
64	N4	501	CDL	C34-C35-C36-C37
64	N4	501	CDL	C78-C79-C80-C81
67	N4	504	3PE	C22-C23-C24-C25
63	A9	561	PC1	C32-C33-C34-C35
63	AM	218	PC1	C25-C26-C27-C28
63	B5	203	PC1	C2E-C2F-C2G-C2H
64	AL	304	CDL	CA7-C31-C32-C33
64	AL	304	CDL	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
64	AL	304	CDL	C14-C15-C16-C17
66	AB	150	ZMP	C2-C3-C4-C5
64	EA	202	CDL	CB7-C71-C72-C73
64	AL	302	CDL	C32-C33-C34-C35
64	AM	216	CDL	C37-C38-C39-C40
67	G1	516	3PE	O13-C11-C12-N
63	AM	220	PC1	C23-C24-C25-C26
63	N1	701	PC1	C37-C38-C39-C3A
66	AB	150	ZMP	S1-C11-C12-N1
63	E4	401	PC1	C33-C34-C35-C36
64	AL	303	CDL	C51-C52-C53-C54
64	N4	501	CDL	C19-C20-C21-C22
66	AC	201	ZMP	C1-C2-C3-C4
63	AM	220	PC1	C2C-C2D-C2E-C2F
63	N5	601	PC1	C23-C24-C25-C26
63	N5	601	PC1	C32-C33-C34-C35
63	N5	605	PC1	C23-C24-C25-C26
63	N2	301	PC1	C27-C28-C29-C2A
64	B3	102	CDL	C51-C52-C53-C54
63	N1	701	PC1	C2B-C2C-C2D-C2E
64	AL	302	CDL	CB4-CB3-OB5-PB2
66	AB	150	ZMP	C6-C7-C8-C9
63	E8	304	PC1	C11-C12-N-C15
63	N1	701	PC1	C11-C12-N-C15
63	N5	605	PC1	C11-C12-N-C13
63	AM	218	PC1	C35-C36-C37-C38
63	AM	218	PC1	C37-C38-C39-C3A
64	N5	608	CDL	CA5-C11-C12-C13
66	AC	201	ZMP	C1-C22-C23-C24
67	G1	516	3PE	C29-C2A-C2B-C2C
63	AL	301	PC1	C2A-C2B-C2C-C2D
64	N5	608	CDL	C42-C43-C44-C45
63	A1	202	PC1	C31-C32-C33-C34
63	A1	203	PC1	C21-C22-C23-C24
63	ED	201	PC1	C24-C25-C26-C27
64	AM	216	CDL	C34-C35-C36-C37
64	AL	302	CDL	C35-C36-C37-C38
63	N1	702	PC1	C27-C28-C29-C2A
63	E8	304	PC1	O11-C1-C2-O21
64	AM	215	CDL	OB5-CB3-CB4-OB6
66	AC	201	ZMP	C5-C6-C7-C8
64	AM	217	CDL	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
64	EA	202	CDL	C53-C54-C55-C56
64	AL	303	CDL	OB6-CB4-CB6-OB8
63	B5	203	PC1	C11-C12-N-C13
63	E4	401	PC1	C11-C12-N-C14
63	E4	401	PC1	C11-C12-N-C15
63	E8	301	PC1	C29-C2A-C2B-C2C
63	A1	203	PC1	C11-O13-P-O11
63	AL	301	PC1	C11-O13-P-O11
64	AL	303	CDL	CB3-OB5-PB2-OB2
64	B3	102	CDL	CA2-OA2-PA1-OA5
64	EA	202	CDL	CB3-OB5-PB2-OB2
67	N4	504	3PE	C11-O13-P-O11
63	AN	301	PC1	C35-C36-C37-C38
63	B5	202	PC1	C31-C32-C33-C34
63	A9	560	PC1	C2-C1-O11-P
63	B5	202	PC1	C2-C1-O11-P
63	N1	702	PC1	C2-C1-O11-P
64	AM	217	CDL	OA5-CA3-CA4-CA6
64	C4	202	CDL	OA5-CA3-CA4-CA6
67	G1	516	3PE	C25-C26-C27-C28
63	AM	220	PC1	C27-C28-C29-C2A
64	A3	201	CDL	C52-C53-C54-C55
64	C4	202	CDL	C61-C62-C63-C64
63	B5	203	PC1	C2C-C2D-C2E-C2F
64	C4	202	CDL	C59-C60-C61-C62
63	E4	401	PC1	C1-C2-C3-O31
63	N1	702	PC1	C1-C2-C3-O31
64	AL	302	CDL	CA3-CA4-CA6-OA8
64	E6	431	CDL	CA3-CA4-CA6-OA8
64	EA	201	CDL	CB3-CB4-CB6-OB8
64	E7	301	CDL	CA3-CA4-CA6-OA8
64	E7	301	CDL	CB3-CB4-CB6-OB8
64	AM	215	CDL	C56-C57-C58-C59
64	B5	201	CDL	C71-C72-C73-C74
66	AB	150	ZMP	O3-C16-C17-O4
64	N5	603	CDL	C58-C59-C60-C61
63	E8	301	PC1	C31-C32-C33-C34
63	ED	201	PC1	C25-C26-C27-C28
63	B5	202	PC1	C3B-C3C-C3D-C3E
63	A1	202	PC1	C11-C12-N-C13
63	AN	301	PC1	C11-C12-N-C13
63	E8	304	PC1	C11-C12-N-C13

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Mol	Chain	Res	Type	Atoms
63	N1	701	PC1	C11-C12-N-C13
64	B3	102	CDL	O1-C1-CB2-OB2
63	AM	218	PC1	C39-C3A-C3B-C3C
63	ED	201	PC1	C3B-C3C-C3D-C3E
63	N1	701	PC1	C2C-C2D-C2E-C2F
63	E4	401	PC1	O21-C2-C3-O31
64	AL	303	CDL	C32-C31-CA7-OA8
64	E6	431	CDL	C15-C16-C17-C18
64	A3	201	CDL	C71-C72-C73-C74
63	N4	502	PC1	C31-C32-C33-C34
63	B5	203	PC1	C27-C28-C29-C2A
63	B5	203	PC1	C11-C12-N-C15
63	N5	605	PC1	C11-C12-N-C15
63	ED	201	PC1	O11-C1-C2-C3
64	AM	215	CDL	OB5-CB3-CB4-CB6
64	E7	301	CDL	OA5-CA3-CA4-CA6
63	A1	202	PC1	C25-C26-C27-C28
63	E8	301	PC1	C24-C25-C26-C27
63	B5	203	PC1	C21-C22-C23-C24
63	B5	203	PC1	C31-C32-C33-C34
63	N3	301	PC1	C2-C1-O11-P
64	E6	431	CDL	CA4-CA3-OA5-PA1
66	AC	201	ZMP	S1-C11-C12-N1
63	B5	203	PC1	C24-C25-C26-C27
63	B5	203	PC1	C38-C39-C3A-C3B
66	AC	201	ZMP	C6-C7-C8-C9
63	A9	560	PC1	C1-C2-C3-O31
63	B5	203	PC1	C1-C2-C3-O31
63	N3	301	PC1	C1-C2-C3-O31
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	EA	202	CDL	CA3-CA4-CA6-OA8
63	A9	560	PC1	C2-C3-O31-C31
67	AN	302	3PE	C27-C28-C29-C2A
63	A1	202	PC1	C11-C12-N-C14
63	E4	401	PC1	C28-C29-C2A-C2B
63	E8	303	PC1	C11-O13-P-O11
63	N5	605	PC1	C11-O13-P-O11
64	N5	603	CDL	CB3-OB5-PB2-OB2
67	G1	516	3PE	C1-O11-P-O13
64	AL	302	CDL	C32-C31-CA7-OA8

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Mol	Chain	Res	Type	Atoms
63	B5	202	PC1	O11-C1-C2-O21
64	C4	202	CDL	OA5-CA3-CA4-OA6
63	B5	203	PC1	O21-C2-C3-O31
64	E6	431	CDL	OA6-CA4-CA6-OA8
64	E6	431	CDL	OB6-CB4-CB6-OB8
64	E7	301	CDL	OB6-CB4-CB6-OB8
67	N4	504	3PE	O31-C31-C32-C33
64	B3	102	CDL	CA2-C1-CB2-OB2
63	B5	203	PC1	C3B-C3C-C3D-C3E
63	ED	201	PC1	C28-C29-C2A-C2B
64	EA	202	CDL	C1-CA2-OA2-PA1
63	AN	301	PC1	C3A-C3B-C3C-C3D
63	N2	301	PC1	C25-C26-C27-C28
64	B5	201	CDL	CA5-C11-C12-C13
68	N4	505	U10	C26-C27-C28-C29
64	C4	202	CDL	C51-C52-C53-C54
64	N4	501	CDL	C54-C55-C56-C57
63	B5	202	PC1	O11-C1-C2-C3
64	AL	304	CDL	OB5-CB3-CB4-CB6
64	C4	204	CDL	OB5-CB3-CB4-CB6
64	E7	301	CDL	OB5-CB3-CB4-CB6
64	E6	431	CDL	O1-C1-CA2-OA2
64	EA	202	CDL	O1-C1-CA2-OA2
63	N3	301	PC1	C26-C27-C28-C29
64	N5	608	CDL	C17-C18-C19-C20
63	N1	701	PC1	C11-C12-N-C14
64	A3	201	CDL	CB7-C71-C72-C73
63	N4	502	PC1	C34-C35-C36-C37
63	AM	218	PC1	C2-C1-O11-P
63	AM	218	PC1	C1-C2-C3-O31
63	N4	502	PC1	C1-C2-C3-O31
64	AL	303	CDL	CB4-CB3-OB5-PB2
63	E8	302	PC1	O11-C1-C2-O21
63	N1	701	PC1	O11-C1-C2-O21
64	AM	217	CDL	OA5-CA3-CA4-OA6
64	C4	202	CDL	OB5-CB3-CB4-OB6
64	B5	201	CDL	C32-C31-CA7-OA8
63	E8	302	PC1	C3D-C3E-C3F-C3G
63	B5	203	PC1	C25-C26-C27-C28
63	AL	301	PC1	O21-C2-C3-O31
63	AM	218	PC1	O21-C2-C3-O31
63	N3	301	PC1	O21-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
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	EA	202	CDL	OA6-CA4-CA6-OA8
64	E7	301	CDL	OA6-CA4-CA6-OA8
63	AN	301	PC1	C24-C25-C26-C27
63	B5	203	PC1	C36-C37-C38-C39
65	A9	559	NDP	PA-O3-PN-O2N
64	C4	202	CDL	C38-C39-C40-C41
64	AL	304	CDL	C13-C14-C15-C16
63	AM	220	PC1	C25-C26-C27-C28
63	N5	601	PC1	C34-C35-C36-C37
63	E8	301	PC1	C11-O13-P-O11
63	ED	201	PC1	C11-O13-P-O11
63	N3	301	PC1	C1-O11-P-O13
64	B3	102	CDL	CB3-OB5-PB2-OB2
64	E6	431	CDL	CA3-OA5-PA1-OA2
64	EA	202	CDL	CA2-OA2-PA1-OA5
63	B5	202	PC1	C24-C25-C26-C27
63	C4	203	PC1	C2-C1-O11-P
64	AL	303	CDL	C1-CA2-OA2-PA1
64	AL	304	CDL	C1-CA2-OA2-PA1
64	N4	501	CDL	CA4-CA3-OA5-PA1
67	N5	607	3PE	C2-C1-O11-P
63	ED	201	PC1	C27-C28-C29-C2A
66	AC	201	ZMP	C22-C23-C24-C25
63	A1	202	PC1	C1-O11-P-O14
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	AL	301	PC1	C11-O13-P-O14
63	AM	220	PC1	C1-O11-P-O12
63	AN	301	PC1	C1-O11-P-O12
63	AN	301	PC1	C11-C12-N-C15
63	B5	202	PC1	C11-O13-P-O14
63	B5	202	PC1	C1-O11-P-O12
63	B5	203	PC1	C1-O11-P-O14
63	C4	203	PC1	C11-O13-P-O14
63	E8	302	PC1	C11-C12-N-C14
63	E8	303	PC1	C1-O11-P-O14
63	N2	301	PC1	C1-O11-P-O12
63	N2	301	PC1	C11-C12-N-C13

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Mol	Chain	Res	Type	Atoms
63	N5	605	PC1	C11-O13-P-O14
63	N5	606	PC1	C1-O11-P-O12
64	AL	302	CDL	CB3-OB5-PB2-OB4
64	AL	303	CDL	CA3-OA5-PA1-OA4
64	AL	303	CDL	CB2-OB2-PB2-OB4
64	AL	303	CDL	CB3-OB5-PB2-OB3
64	AL	304	CDL	CB2-OB2-PB2-OB3
64	AL	304	CDL	CB2-OB2-PB2-OB4
64	AL	304	CDL	CB3-OB5-PB2-OB4
64	AM	215	CDL	CA3-OA5-PA1-OA4
64	AM	215	CDL	CB2-OB2-PB2-OB3
64	AM	215	CDL	CB2-OB2-PB2-OB4
64	AM	215	CDL	CB3-OB5-PB2-OB3
64	B5	201	CDL	CA3-OA5-PA1-OA3
64	C4	204	CDL	CA2-OA2-PA1-OA3
64	E6	431	CDL	CA3-OA5-PA1-OA3
64	EA	202	CDL	CB3-OB5-PB2-OB4
64	N5	603	CDL	CA2-OA2-PA1-OA4
64	N5	603	CDL	CA3-OA5-PA1-OA3
64	N5	603	CDL	CA3-OA5-PA1-OA4
64	N5	608	CDL	CA3-OA5-PA1-OA3
64	E7	301	CDL	CA2-OA2-PA1-OA3
67	AN	302	3PE	C11-O13-P-O14
67	G1	516	3PE	C1-O11-P-O12
67	N4	504	3PE	C11-O13-P-O12
63	E8	304	PC1	O11-C1-C2-C3
63	N1	701	PC1	O11-C1-C2-C3
64	EA	202	CDL	OB5-CB3-CB4-CB6
64	AM	217	CDL	C31-C32-C33-C34
67	N5	607	3PE	C2C-C2D-C2E-C2F
63	B5	202	PC1	C12-C11-O13-P
64	AL	302	CDL	C14-C15-C16-C17
63	AM	218	PC1	C3C-C3D-C3E-C3F
64	EA	201	CDL	CB2-C1-CA2-OA2
63	E8	302	PC1	C2A-C2B-C2C-C2D
63	ED	201	PC1	O11-C1-C2-O21
64	AL	304	CDL	OB5-CB3-CB4-OB6
64	C4	204	CDL	OB5-CB3-CB4-OB6
64	EA	202	CDL	OB5-CB3-CB4-OB6
64	E7	301	CDL	OA5-CA3-CA4-OA6
67	N5	607	3PE	O11-C1-C2-O21
70	V1	579	FMN	N10-C1'-C2'-C3'

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Mol	Chain	Res	Type	Atoms
65	A9	559	NDP	O4D-C1D-N1N-C6N
63	C4	203	PC1	C11-C12-N-C15
63	E8	304	PC1	C11-C12-N-C14
63	N4	502	PC1	C11-C12-N-C13
63	N5	605	PC1	C11-C12-N-C14
63	ED	201	PC1	C21-C22-C23-C24
63	A9	560	PC1	O13-C11-C12-N
63	AN	301	PC1	O13-C11-C12-N
63	B5	202	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
63	N5	606	PC1	C22-C23-C24-C25
63	A9	560	PC1	O21-C2-C3-O31
63	N4	502	PC1	O21-C2-C3-O31
63	E8	302	PC1	C22-C23-C24-C25
63	N1	701	PC1	C23-C24-C25-C26
66	AC	201	ZMP	O3-C16-C17-O4
64	AM	215	CDL	C15-C16-C17-C18
64	AM	217	CDL	C36-C37-C38-C39
63	A1	202	PC1	C22-C23-C24-C25
63	A1	202	PC1	C11-C12-N-C15
63	AM	218	PC1	C11-C12-N-C13
63	B5	203	PC1	C11-C12-N-C14
63	E8	302	PC1	C11-C12-N-C13
63	N2	301	PC1	C11-C12-N-C14
64	C4	202	CDL	C72-C71-CB7-OB8
64	E6	431	CDL	O1-C1-CB2-OB2
68	N4	505	U10	C2-C3-O3-C3M
63	N5	605	PC1	C35-C36-C37-C38
63	E8	302	PC1	C24-C25-C26-C27
63	B5	203	PC1	C35-C36-C37-C38
64	C4	204	CDL	C11-C12-C13-C14
64	N4	501	CDL	C38-C39-C40-C41
67	N5	607	3PE	O11-C1-C2-C3
64	AM	216	CDL	C35-C36-C37-C38
63	N5	606	PC1	O31-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
64	EA	201	CDL	C1-CB2-OB2-PB2
63	E8	302	PC1	C3A-C3B-C3C-C3D
64	AL	302	CDL	OA6-CA4-CA6-OA8
63	AM	218	PC1	C11-O13-P-O11
63	AN	301	PC1	C11-O13-P-O11
63	N4	502	PC1	C1-O11-P-O13
64	AL	304	CDL	CA3-OA5-PA1-OA2
64	EA	202	CDL	CB2-OB2-PB2-OB5
64	N4	501	CDL	CB2-OB2-PB2-OB5
67	AN	302	3PE	C2B-C2C-C2D-C2E
64	AL	304	CDL	C12-C13-C14-C15
63	AL	301	PC1	C1-C2-C3-O31
64	AL	302	CDL	CB3-CB4-CB6-OB8
64	E6	431	CDL	CB3-CB4-CB6-OB8
67	AN	302	3PE	C34-C35-C36-C37
63	AN	301	PC1	C11-C12-N-C14
63	E8	302	PC1	C35-C36-C37-C38
63	AL	301	PC1	C2-C1-O11-P
64	AM	217	CDL	CA4-CA3-OA5-PA1
64	EA	201	CDL	CB4-CB3-OB5-PB2
63	A1	202	PC1	C33-C34-C35-C36
63	B5	202	PC1	C2B-C2C-C2D-C2E
64	B5	201	CDL	C55-C56-C57-C58
63	C4	203	PC1	C11-C12-N-C13
64	C4	202	CDL	OB5-CB3-CB4-CB6
71	V1	581	NAI	O4D-C1D-N1N-C2N
67	N5	607	3PE	C35-C36-C37-C38
64	B3	102	CDL	C34-C35-C36-C37
64	E6	431	CDL	C56-C57-C58-C59
67	AN	302	3PE	C38-C39-C3A-C3B
64	AM	216	CDL	OB6-CB4-CB6-OB8
63	N4	503	PC1	C2-C1-O11-P
66	AB	150	ZMP	C1-C2-C3-C4
67	G1	516	3PE	C24-C25-C26-C27
65	A9	559	NDP	O4B-C4B-C5B-O5B
63	AL	301	PC1	C31-C32-C33-C34
63	A1	202	PC1	C3-C2-O21-C21
63	A9	560	PC1	C1-C2-O21-C21
63	AL	301	PC1	C1-C2-O21-C21
63	AN	301	PC1	C1-C2-O21-C21
63	N2	301	PC1	C3-C2-O21-C21
63	N3	301	PC1	C1-C2-O21-C21

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Mol	Chain	Res	Type	Atoms
63	N3	301	PC1	C3-C2-O21-C21
63	N4	502	PC1	C1-C2-O21-C21
64	AM	217	CDL	CA3-CA4-OA6-CA5
64	AM	217	CDL	CB6-CB4-OB6-CB5
64	E6	431	CDL	CA6-CA4-OA6-CA5
64	E6	431	CDL	CB6-CB4-OB6-CB5
63	C4	203	PC1	C11-C12-N-C14
63	E8	302	PC1	C11-C12-N-C15
63	N2	301	PC1	C11-C12-N-C15
63	N4	502	PC1	C32-C33-C34-C35
63	C4	203	PC1	C21-C22-C23-C24
64	N5	608	CDL	CB2-OB2-PB2-OB5
68	N4	505	U10	C4-C3-O3-C3M
63	N1	701	PC1	O31-C31-C32-C33
64	N5	608	CDL	C58-C59-C60-C61
63	E4	401	PC1	C21-C22-C23-C24
64	AL	302	CDL	OB6-CB4-CB6-OB8
63	A9	560	PC1	C32-C33-C34-C35
68	N4	505	U10	C24-C26-C27-C28
63	E8	302	PC1	C39-C3A-C3B-C3C
63	E4	401	PC1	C22-C23-C24-C25
63	N1	701	PC1	C2A-C2B-C2C-C2D
64	C4	202	CDL	C14-C15-C16-C17
63	AM	218	PC1	C22-C23-C24-C25
67	G1	516	3PE	C34-C35-C36-C37
64	AM	216	CDL	C31-C32-C33-C34
67	N5	607	3PE	C3B-C3C-C3D-C3E
63	B5	203	PC1	C34-C35-C36-C37
63	E8	304	PC1	O31-C31-C32-C33
64	AM	217	CDL	CA2-C1-CB2-OB2
64	N4	501	CDL	C73-C74-C75-C76
64	E6	431	CDL	C52-C51-CB5-OB6
66	AC	201	ZMP	N2-C16-C17-O4
63	N1	702	PC1	O21-C21-C22-C23
64	AL	303	CDL	C72-C71-CB7-OB8
64	AL	302	CDL	C32-C31-CA7-OA9
63	E8	302	PC1	C2C-C2D-C2E-C2F
64	EA	201	CDL	CB2-OB2-PB2-OB5
63	AM	218	PC1	C11-C12-N-C14
63	N4	502	PC1	C11-C12-N-C14
63	N4	502	PC1	C11-C12-N-C15
64	N4	501	CDL	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
64	B3	102	CDL	C35-C36-C37-C38
67	G1	516	3PE	C33-C34-C35-C36
63	AL	301	PC1	C28-C29-C2A-C2B
64	C4	202	CDL	C39-C40-C41-C42
63	A1	202	PC1	C1-C2-O21-C21
64	AM	217	CDL	CB3-CB4-OB6-CB5
64	E7	301	CDL	CA3-CA4-OA6-CA5
64	E7	301	CDL	CA6-CA4-OA6-CA5
63	N4	503	PC1	O31-C31-C32-C33
64	AL	303	CDL	C12-C11-CA5-OA6
64	AL	304	CDL	C72-C71-CB7-OB8
64	AM	217	CDL	C72-C71-CB7-OB8
63	E8	302	PC1	C2D-C2E-C2F-C2G
63	B5	202	PC1	O31-C31-C32-C33
64	B3	102	CDL	C12-C11-CA5-OA6
64	N5	608	CDL	C12-C11-CA5-OA6
63	E8	301	PC1	C35-C36-C37-C38
67	AN	302	3PE	C2-C1-O11-P
67	G1	516	3PE	C2-C1-O11-P
64	N4	501	CDL	C41-C42-C43-C44
64	N4	501	CDL	C80-C81-C82-C83
67	N4	504	3PE	O32-C31-C32-C33
63	E4	401	PC1	O11-C1-C2-O21
64	EA	202	CDL	OA5-CA3-CA4-OA6
63	C4	203	PC1	O31-C31-C32-C33
63	N1	701	PC1	O21-C21-C22-C23
64	E7	301	CDL	C32-C31-CA7-OA8
63	AM	218	PC1	C11-C12-N-C15
63	ED	201	PC1	C11-C12-N-C14
64	AM	216	CDL	C41-C42-C43-C44
63	N2	301	PC1	C32-C33-C34-C35
64	EA	202	CDL	C52-C51-CB5-OB6
63	N1	702	PC1	C33-C34-C35-C36
63	E8	302	PC1	O11-C1-C2-C3
64	AL	304	CDL	C12-C11-CA5-OA6
64	N5	608	CDL	C52-C51-CB5-OB6
63	N5	601	PC1	C11-C12-N-C13
71	V1	581	NAI	C5B-O5B-PA-O3
63	N2	301	PC1	O21-C21-C22-C23
64	N4	501	CDL	C52-C51-CB5-OB6
63	B5	202	PC1	C3E-C3F-C3G-C3H
64	AM	216	CDL	C71-C72-C73-C74

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Mol	Chain	Res	Type	Atoms
64	B5	201	CDL	C1-CA2-OA2-PA1
64	AM	215	CDL	C12-C11-CA5-OA6
64	EA	201	CDL	C72-C71-CB7-OB8
63	AM	220	PC1	C31-C32-C33-C34
64	N4	501	CDL	C32-C31-CA7-OA8
64	AL	304	CDL	C31-C32-C33-C34
63	N1	701	PC1	O22-C21-C22-C23
63	N4	503	PC1	O32-C31-C32-C33
64	N4	501	CDL	C22-C23-C24-C25
64	N5	608	CDL	C32-C31-CA7-OA8
63	N1	702	PC1	O22-C21-C22-C23
64	AM	217	CDL	C72-C71-CB7-OB9
64	E6	431	CDL	C52-C51-CB5-OB7
63	A1	202	PC1	O31-C31-C32-C33
64	N5	608	CDL	C34-C35-C36-C37
63	E8	302	PC1	C27-C28-C29-C2A
64	AL	303	CDL	C72-C71-CB7-OB9
64	B3	102	CDL	C12-C11-CA5-OA7
64	N4	501	CDL	C32-C31-CA7-OA9
64	AL	304	CDL	C52-C51-CB5-OB6
63	N3	301	PC1	C2D-C2E-C2F-C2G
64	AL	302	CDL	CB3-OB5-PB2-OB2
64	C4	202	CDL	CB3-OB5-PB2-OB2
64	AM	215	CDL	C12-C11-CA5-OA7
64	EA	202	CDL	C52-C51-CB5-OB7
64	N5	608	CDL	C12-C11-CA5-OA7
63	N5	605	PC1	O21-C21-C22-C23
64	AM	215	CDL	C72-C71-CB7-OB8
67	N4	504	3PE	C2-C1-O11-P
63	C4	203	PC1	O32-C31-C32-C33
64	N5	608	CDL	C81-C82-C83-C84
64	B3	102	CDL	C32-C33-C34-C35
63	AM	218	PC1	C1-O11-P-O14
63	ED	201	PC1	C11-O13-P-O12
64	A3	201	CDL	CA2-OA2-PA1-OA3
64	A3	201	CDL	CB2-OB2-PB2-OB3
64	AL	302	CDL	CB3-OB5-PB2-OB3
64	AL	303	CDL	CB3-OB5-PB2-OB4
64	AL	304	CDL	CA3-OA5-PA1-OA3
64	B3	102	CDL	CA2-OA2-PA1-OA4
64	C4	202	CDL	CB3-OB5-PB2-OB3
64	EA	201	CDL	CB2-OB2-PB2-OB3

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Mol	Chain	Res	Type	Atoms
64	EA	202	CDL	CB2-OB2-PB2-OB3
63	B5	202	PC1	O32-C31-C32-C33
64	E6	431	CDL	OB5-CB3-CB4-CB6
63	N5	601	PC1	C37-C38-C39-C3A
64	E7	301	CDL	C72-C73-C74-C75
64	AL	304	CDL	C72-C71-CB7-OB9
63	N1	701	PC1	C29-C2A-C2B-C2C
63	A9	561	PC1	O21-C21-C22-C23
63	A1	202	PC1	C28-C29-C2A-C2B
63	AM	218	PC1	C3D-C3E-C3F-C3G
67	N4	504	3PE	C37-C38-C39-C3A
64	AL	303	CDL	C12-C11-CA5-OA7
64	E7	301	CDL	C32-C31-CA7-OA9
64	E7	301	CDL	C32-C33-C34-C35
67	N4	504	3PE	C35-C36-C37-C38
63	AL	301	PC1	C3-C2-O21-C21
63	AM	218	PC1	C3-C2-O21-C21
63	E8	301	PC1	C12-C11-O13-P
63	E8	304	PC1	C12-C11-O13-P
63	N2	301	PC1	C1-C2-O21-C21
63	N4	502	PC1	C3-C2-O21-C21
64	AM	216	CDL	CA3-CA4-OA6-CA5
64	AM	216	CDL	CA6-CA4-OA6-CA5
64	AM	217	CDL	CA6-CA4-OA6-CA5
67	AN	302	3PE	C12-C11-O13-P
67	G1	516	3PE	C12-C11-O13-P
64	EA	202	CDL	C32-C31-CA7-OA8
64	AM	215	CDL	C63-C64-C65-C66
63	E8	302	PC1	O31-C31-C32-C33
64	AL	303	CDL	C52-C51-CB5-OB6
64	B3	102	CDL	C16-C17-C18-C19
64	N5	603	CDL	C1-CA2-OA2-PA1
64	AM	215	CDL	C52-C51-CB5-OB6
63	N5	605	PC1	O22-C21-C22-C23
64	AL	304	CDL	C12-C11-CA5-OA7
64	N4	501	CDL	C52-C51-CB5-OB7
64	N5	608	CDL	C52-C51-CB5-OB7
63	B5	203	PC1	C32-C33-C34-C35
64	B5	201	CDL	C52-C51-CB5-OB6
64	AM	215	CDL	C72-C71-CB7-OB9
64	N5	608	CDL	C32-C31-CA7-OA9
63	N5	606	PC1	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
64	C4	202	CDL	C17-C18-C19-C20
63	AM	220	PC1	O31-C31-C32-C33
64	AM	217	CDL	C52-C51-CB5-OB6
64	AL	304	CDL	C52-C51-CB5-OB7
63	E4	401	PC1	C36-C37-C38-C39
64	AM	215	CDL	CB5-C51-C52-C53
63	A1	202	PC1	O32-C31-C32-C33
63	N5	601	PC1	O21-C21-C22-C23

There are no ring outliers.

33 monomers are involved in 62 short contacts:

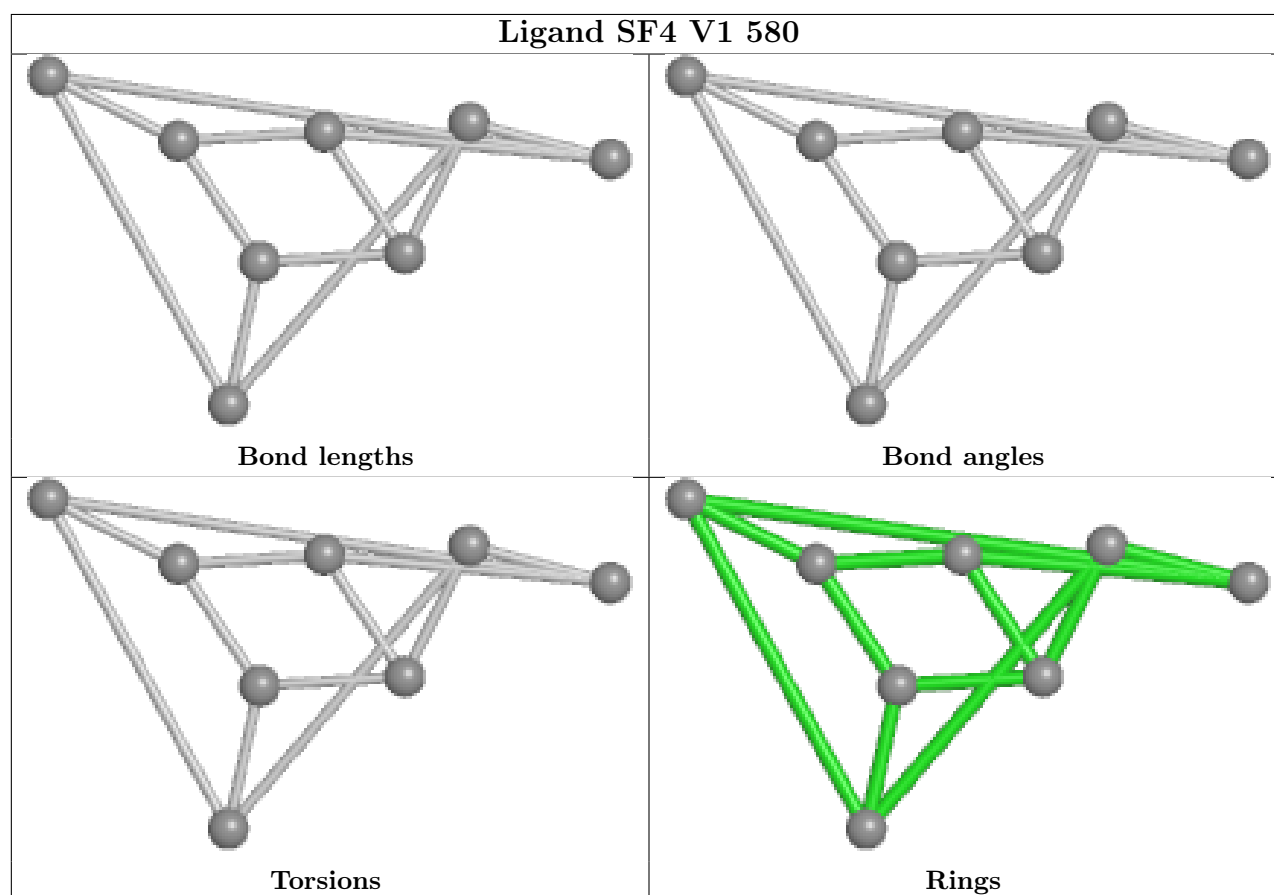
Mol	Chain	Res	Type	Clashes	Symm-Clashes
61	V1	580	SF4	1	0
66	AC	201	ZMP	4	0
68	N4	505	U10	4	0
63	A9	560	PC1	1	0
63	C4	203	PC1	1	0
61	S8	297	SF4	2	0
64	AM	216	CDL	2	0
63	N4	502	PC1	1	0
64	AM	215	CDL	4	0
66	AB	150	ZMP	5	0
67	G1	516	3PE	2	0
64	N5	603	CDL	1	0
64	AM	217	CDL	1	0
63	N5	601	PC1	3	0
64	A3	201	CDL	1	0
64	C4	202	CDL	1	0
71	V1	581	NAI	6	0
64	C4	204	CDL	1	0
63	AM	220	PC1	2	0
64	AL	304	CDL	2	0
61	1A	403	SF4	1	0
64	EA	202	CDL	1	0
63	A1	203	PC1	1	0
64	EA	201	CDL	1	0
64	N4	501	CDL	2	0
63	E8	301	PC1	1	0
63	A1	202	PC1	1	0
63	AM	218	PC1	1	0
70	V1	579	FMN	2	0

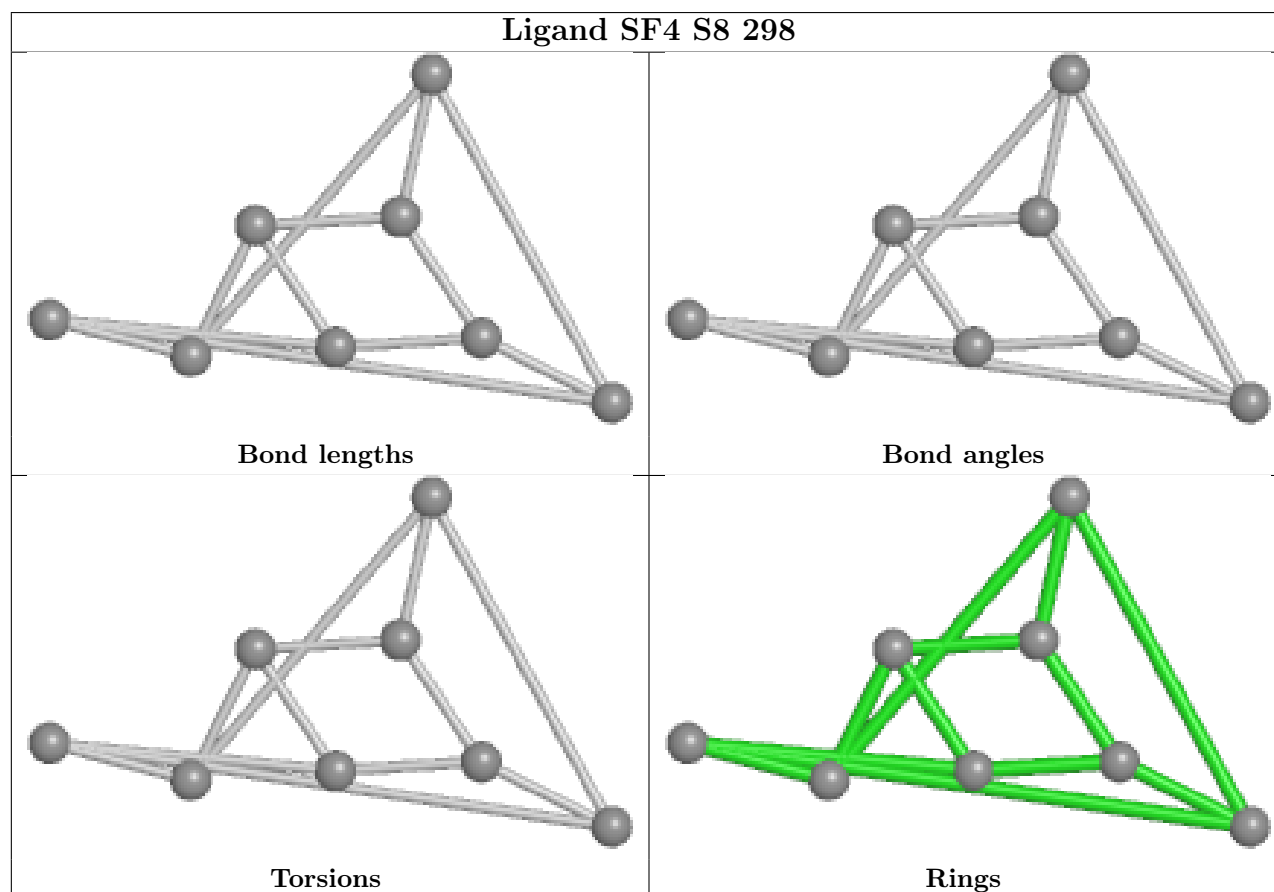
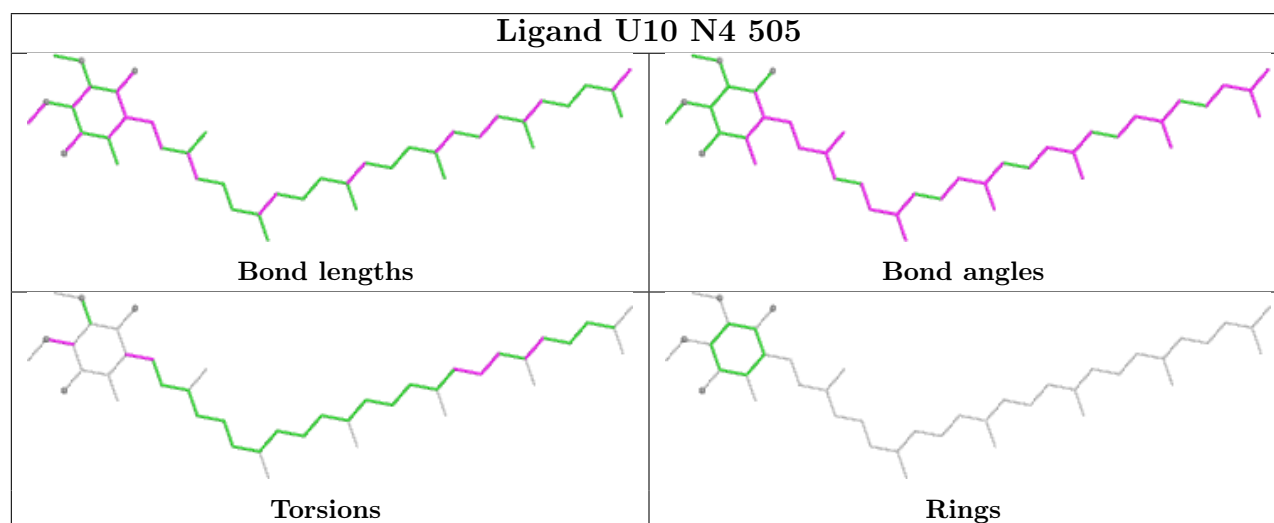
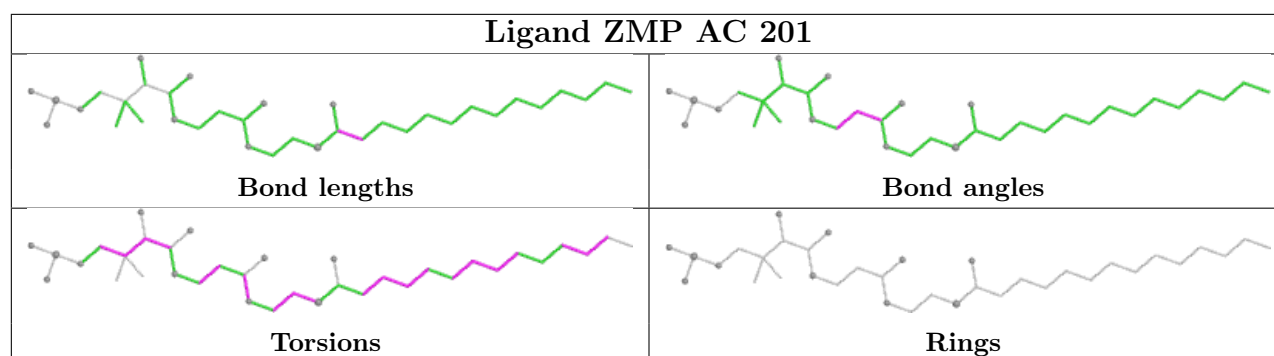
Continued on next page...

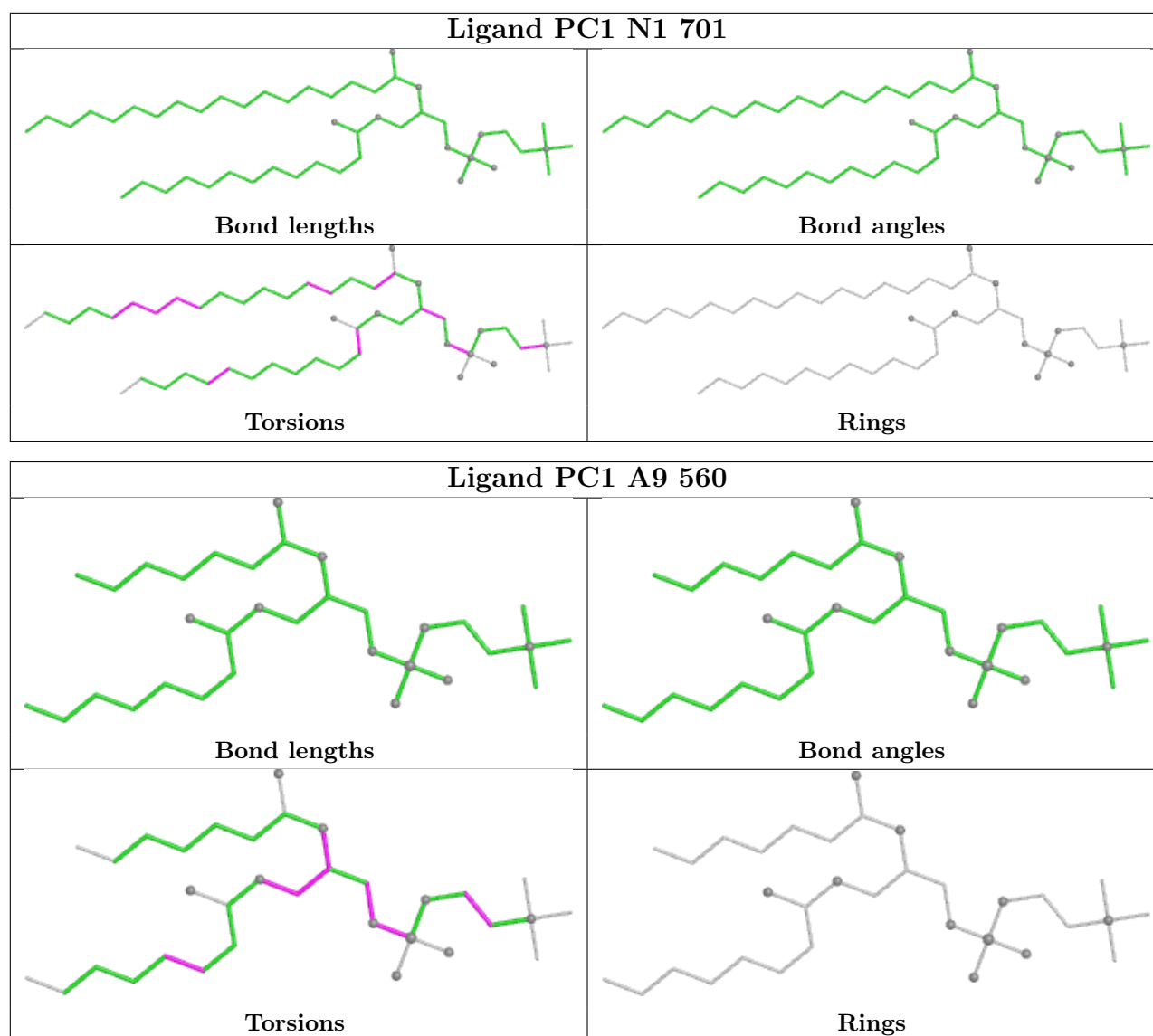
Continued from previous page...

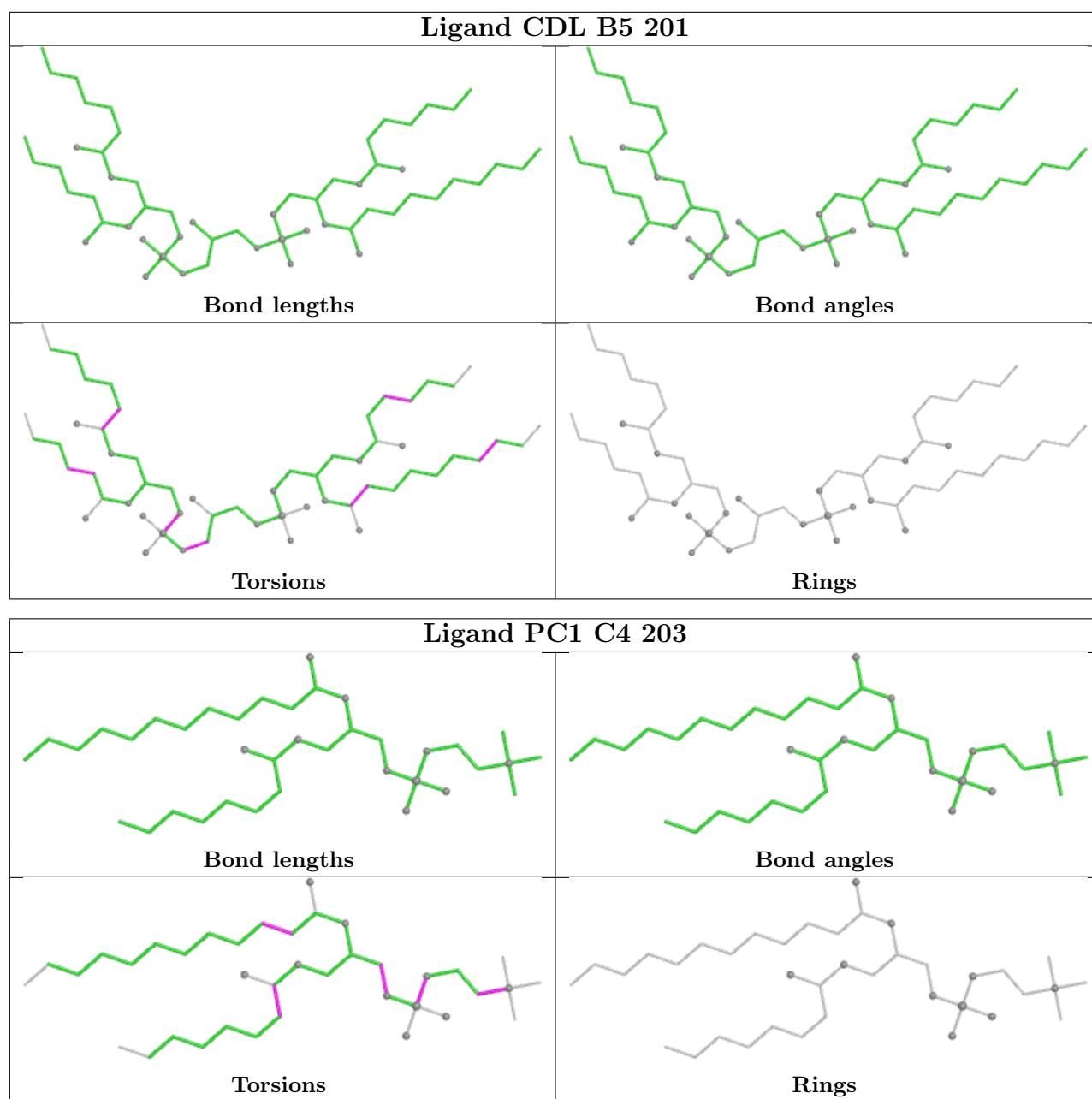
Mol	Chain	Res	Type	Clashes	Symm-Clashes
63	ED	201	PC1	2	0
64	B3	102	CDL	3	0
63	B5	203	PC1	2	0
63	N2	301	PC1	1	0

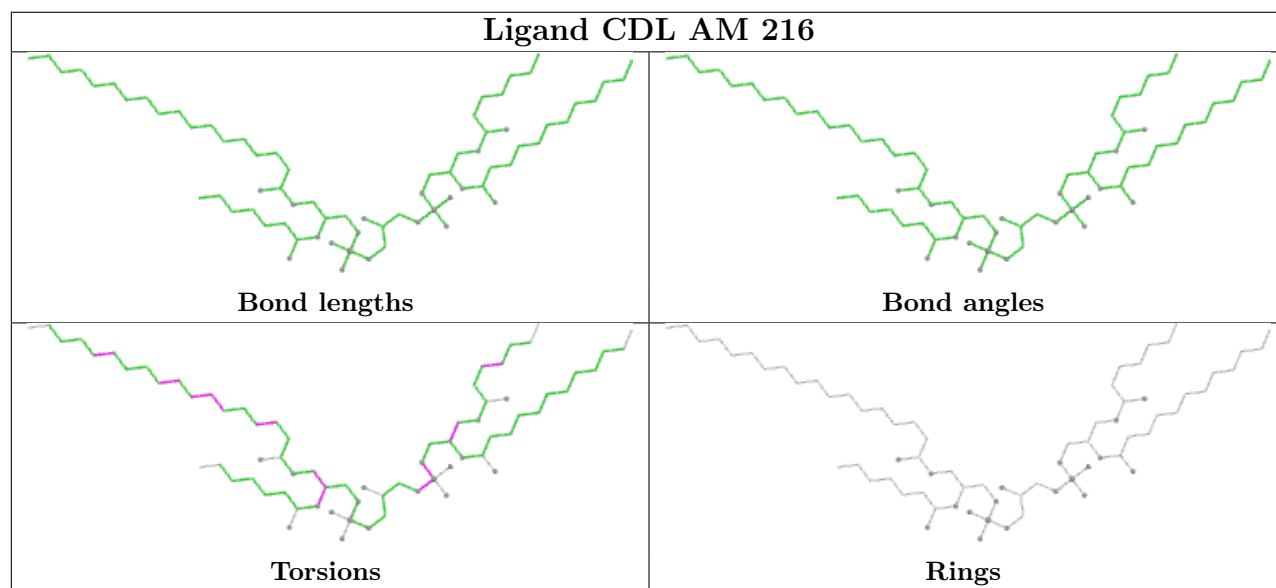
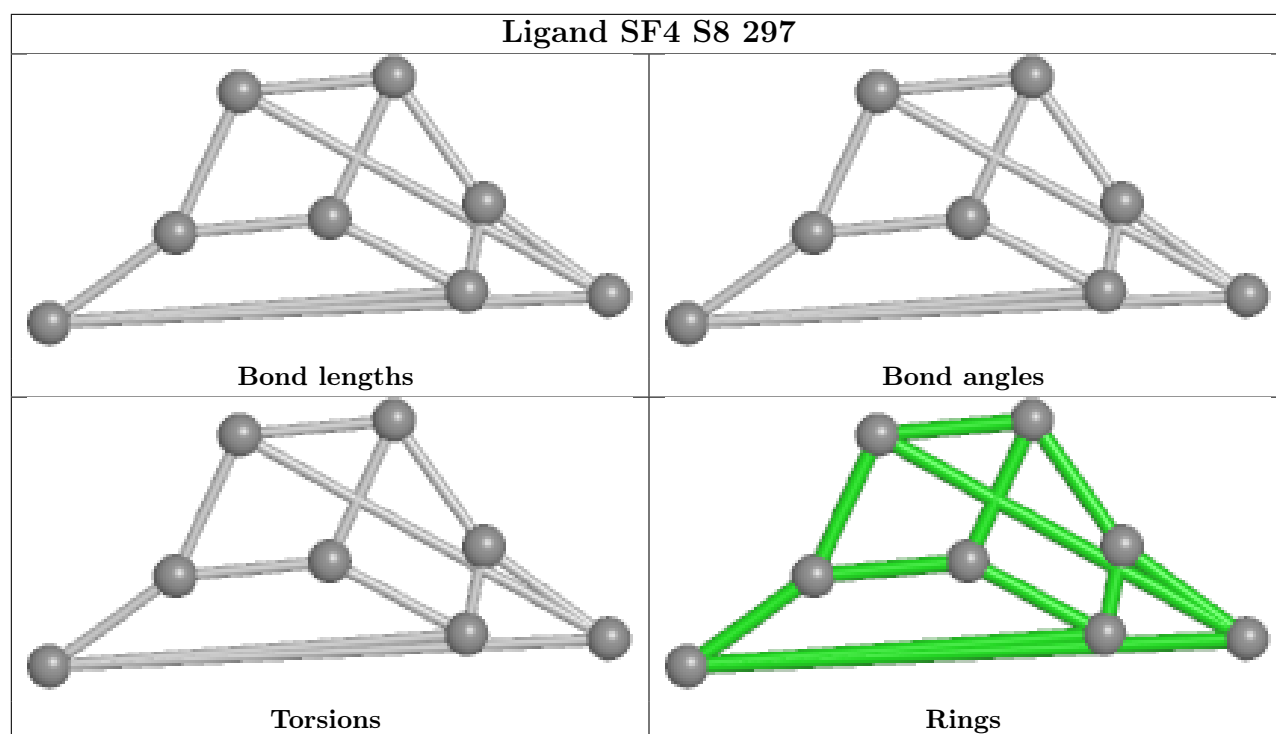
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

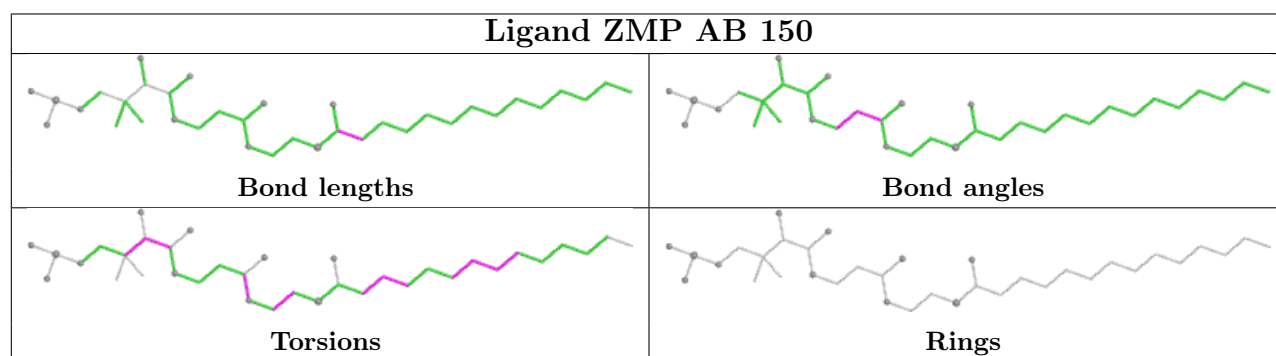
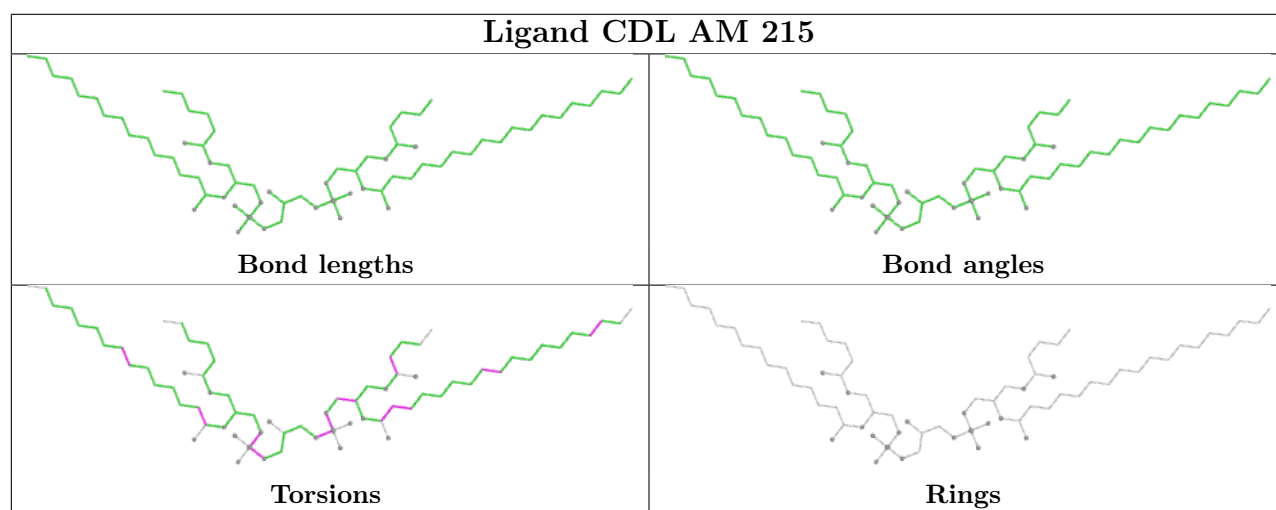
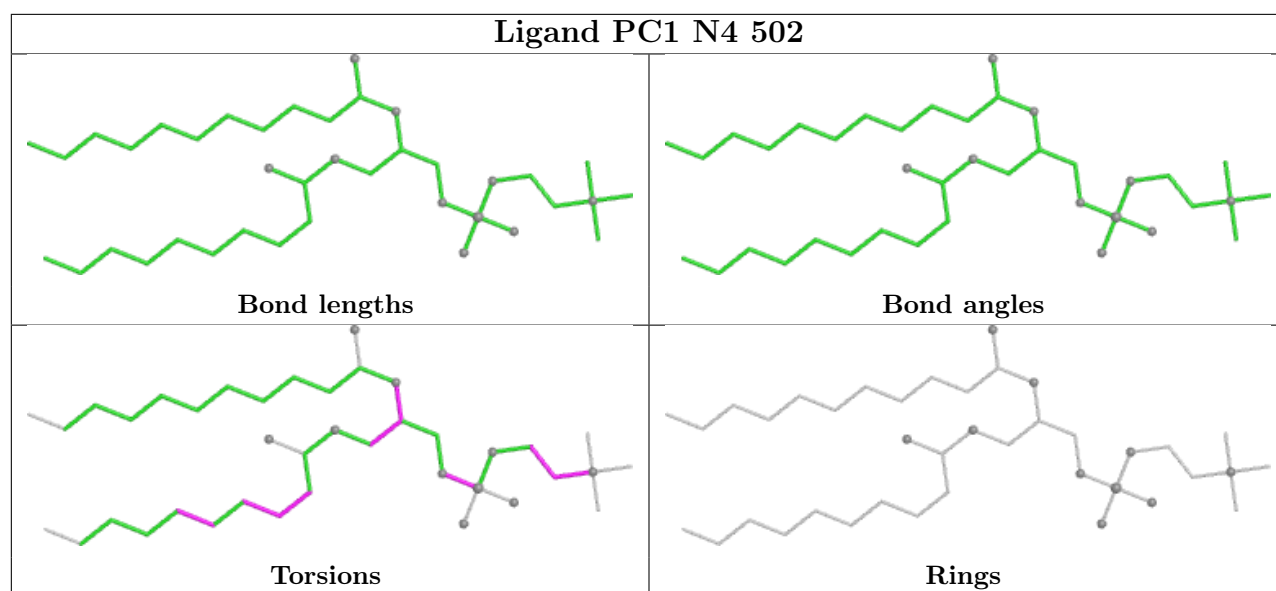


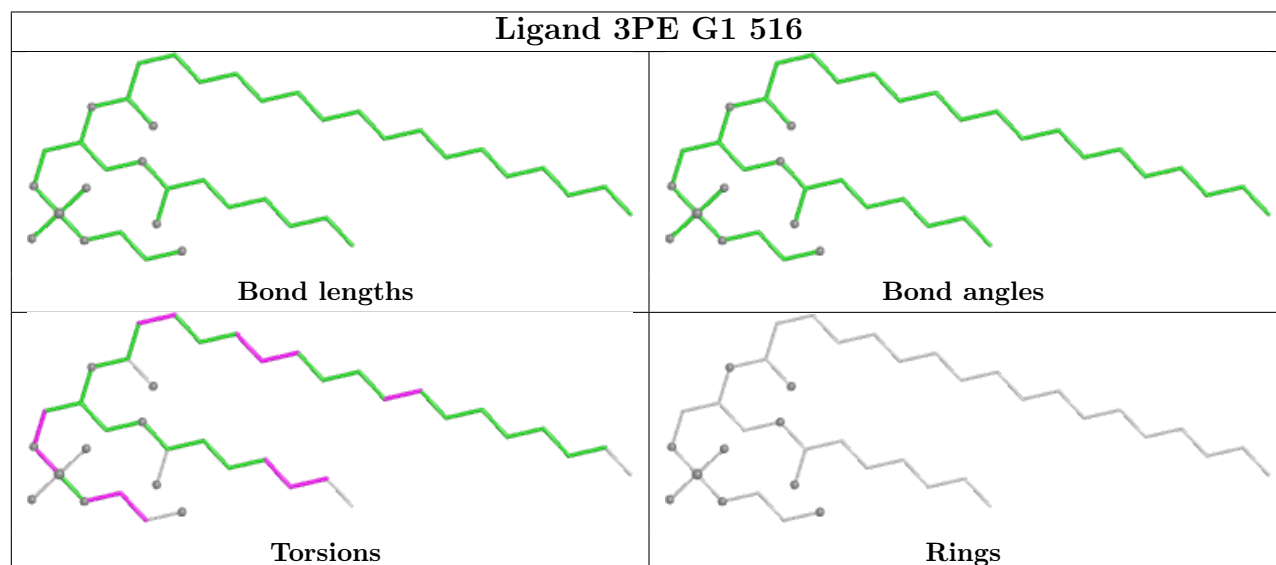
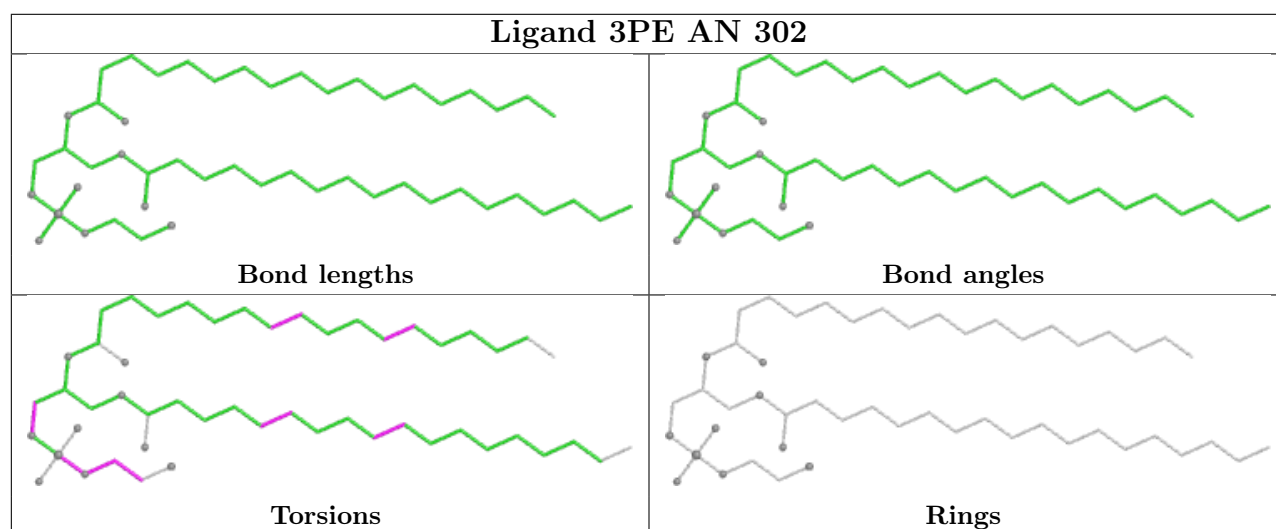
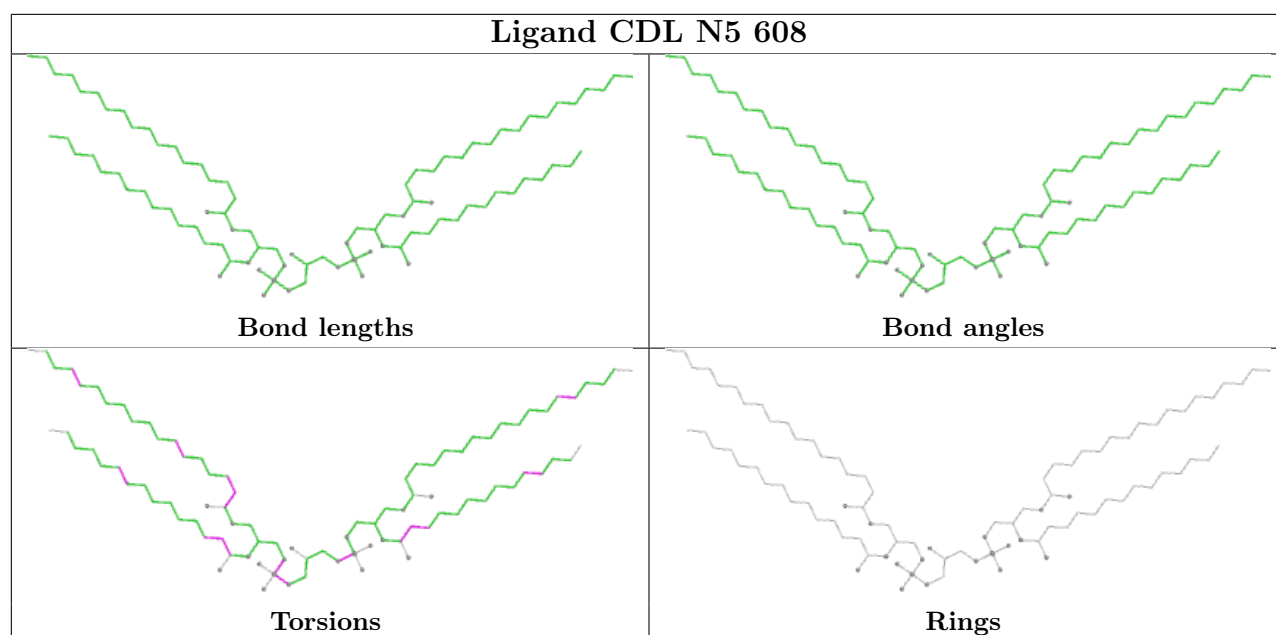


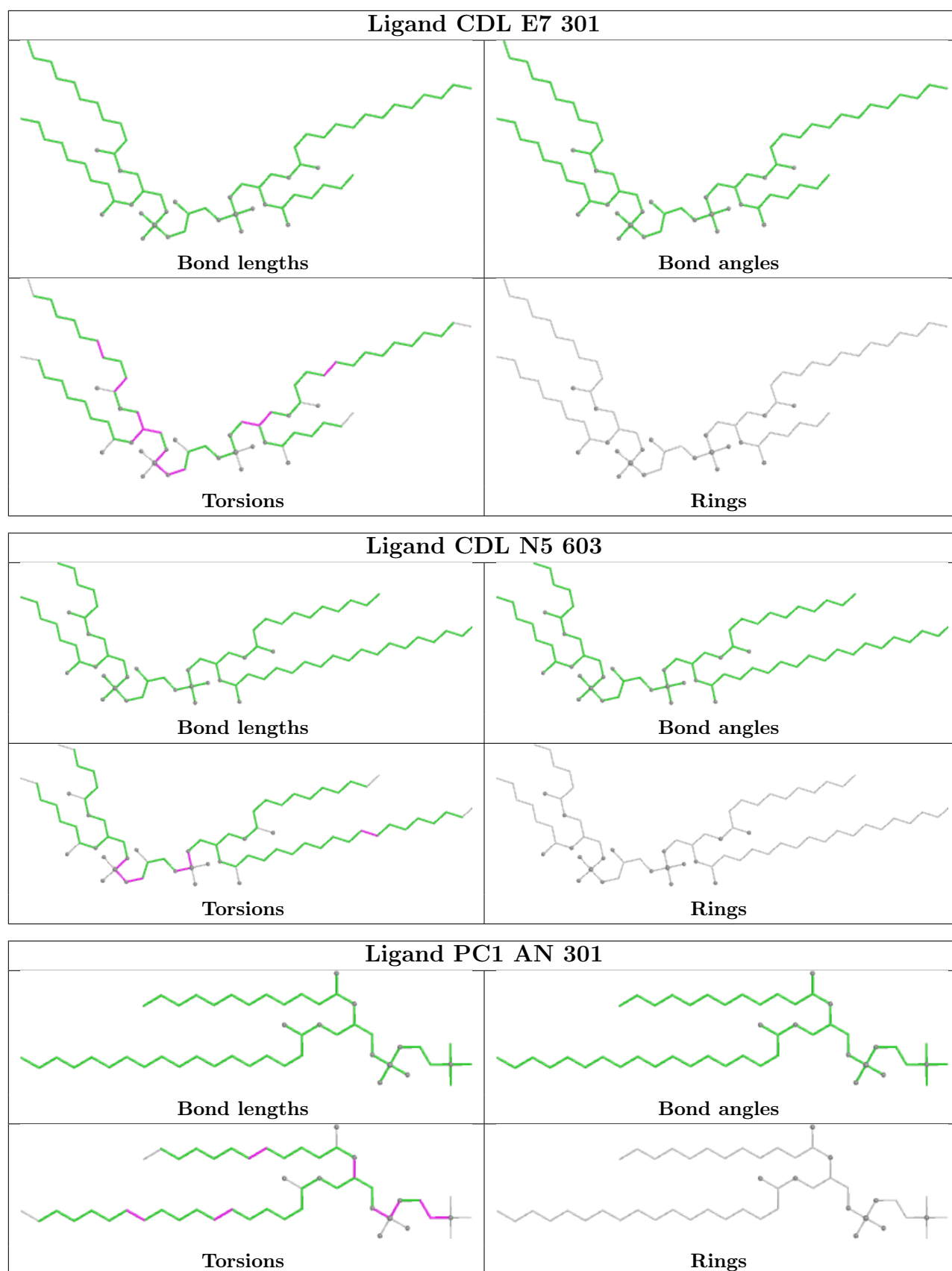


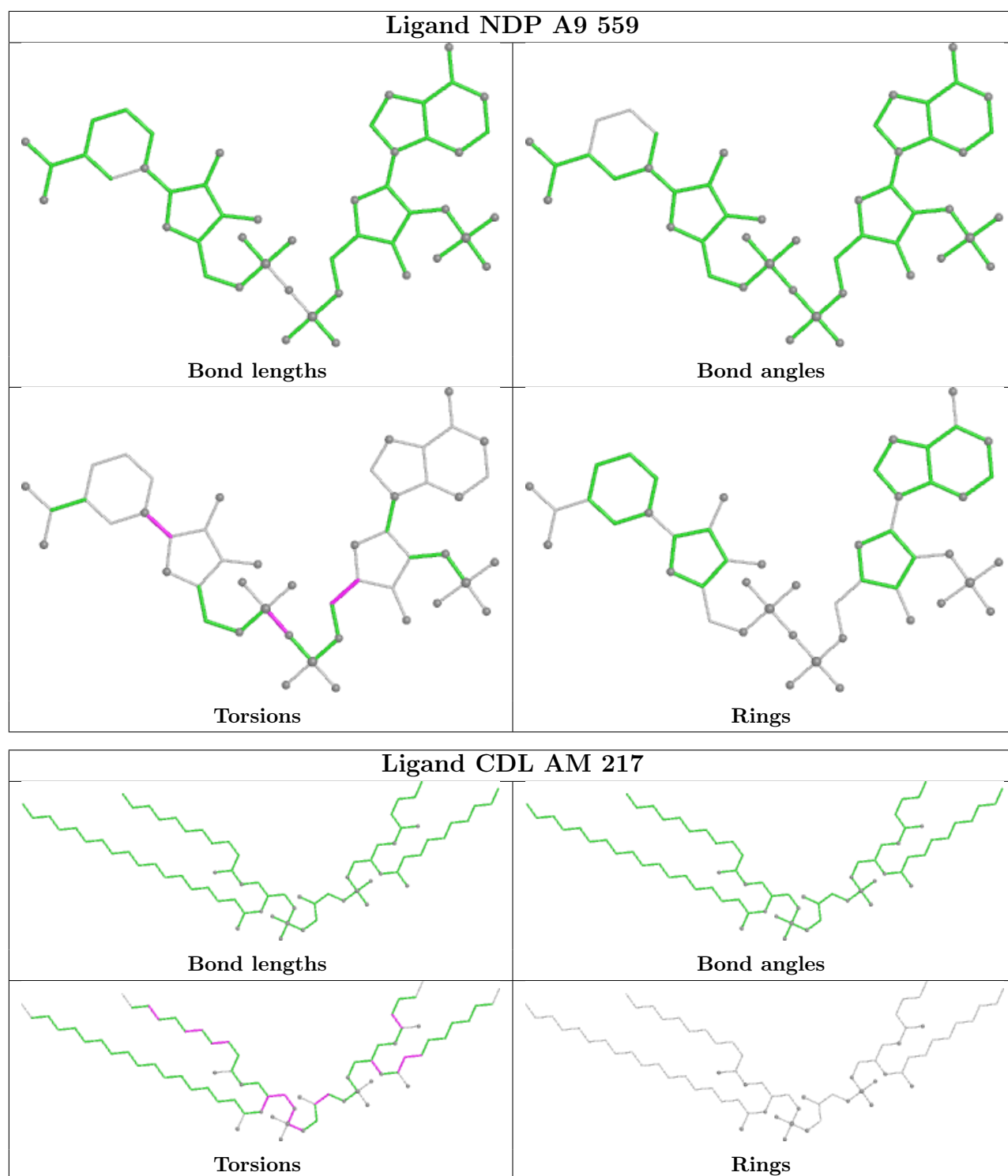


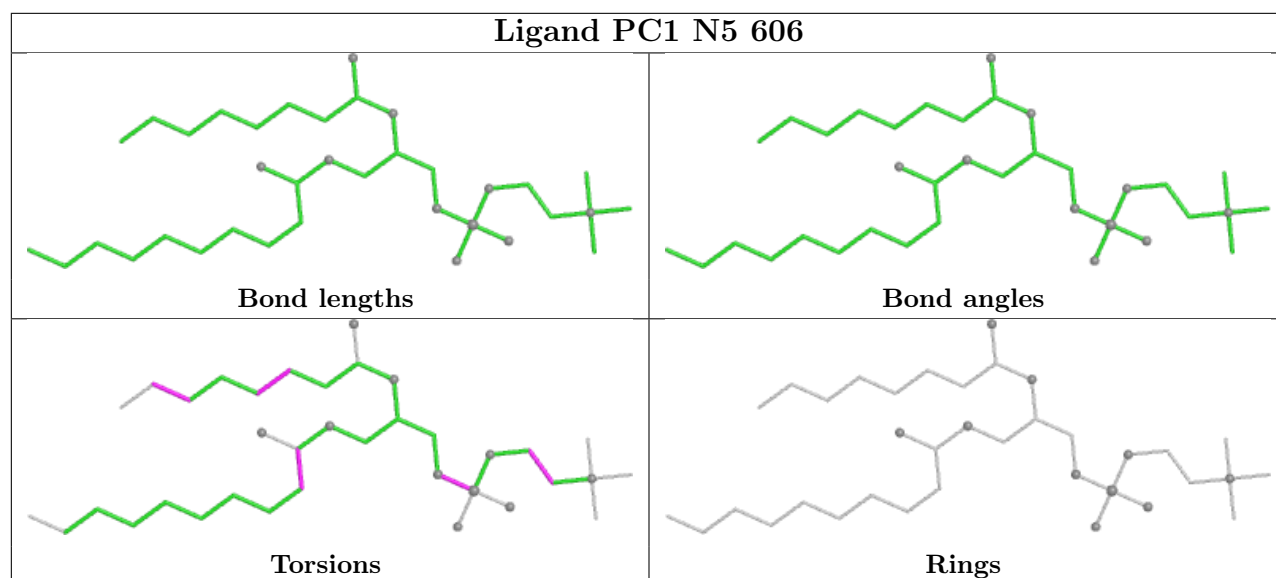
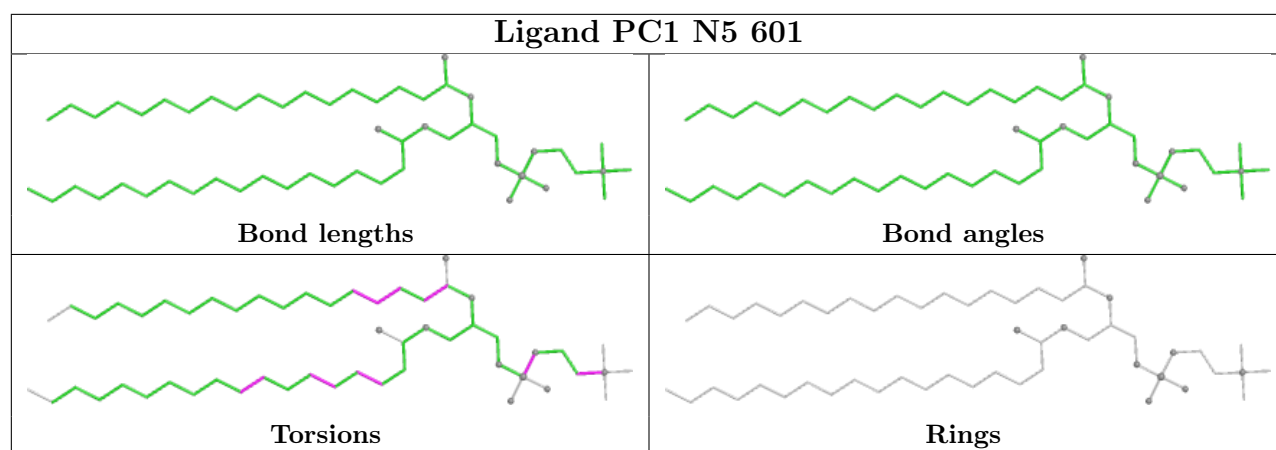


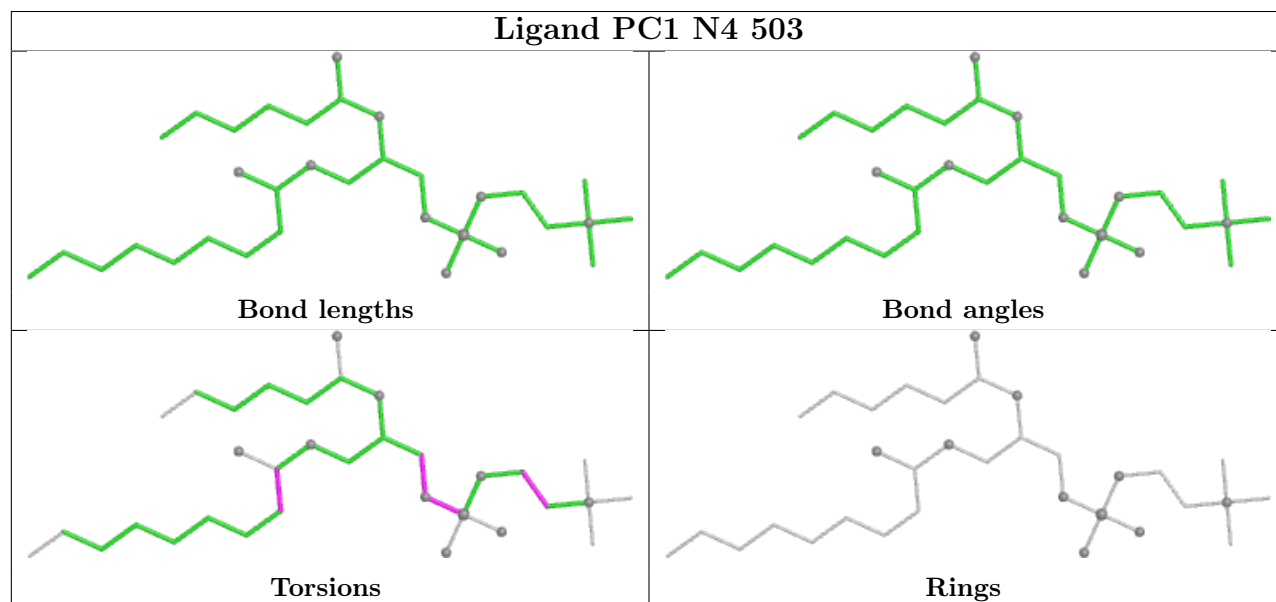
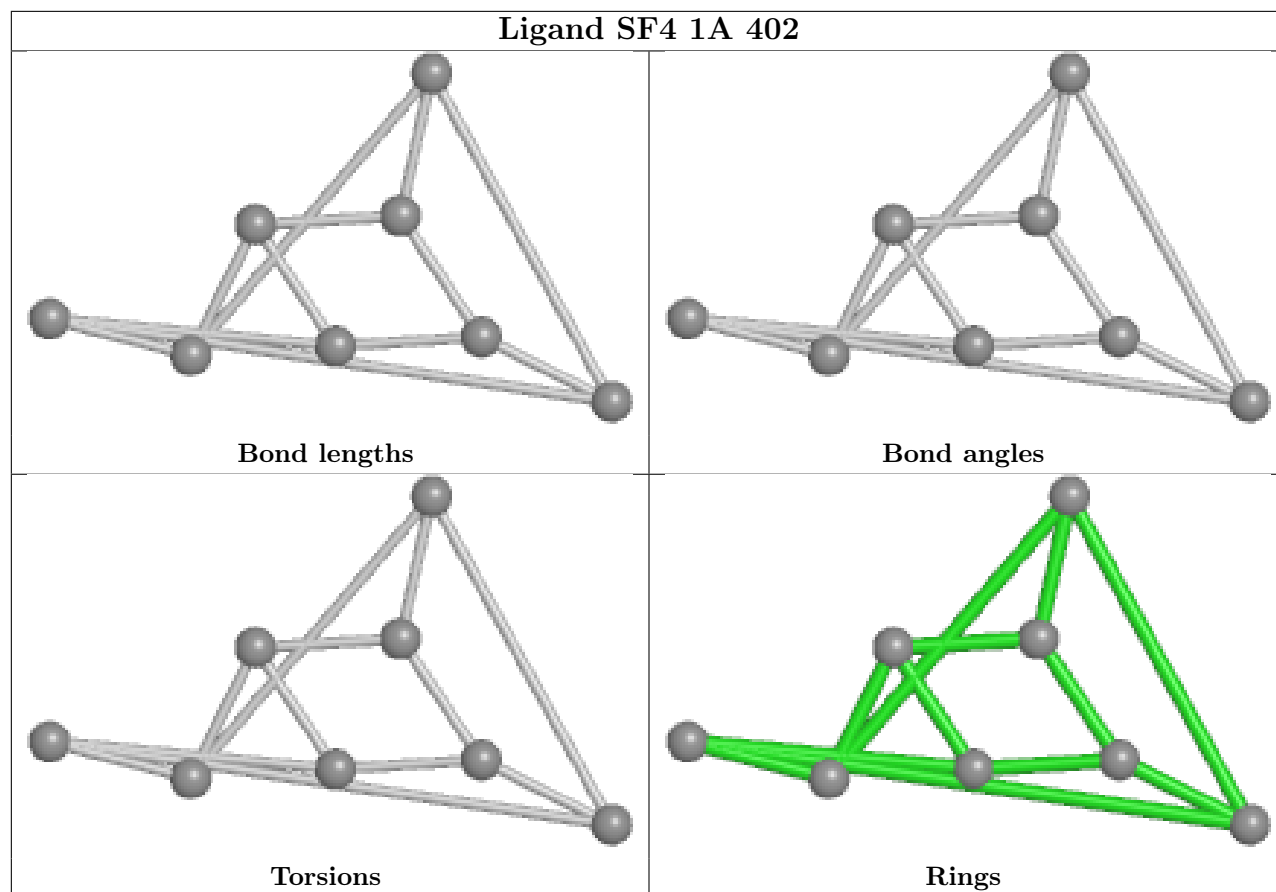


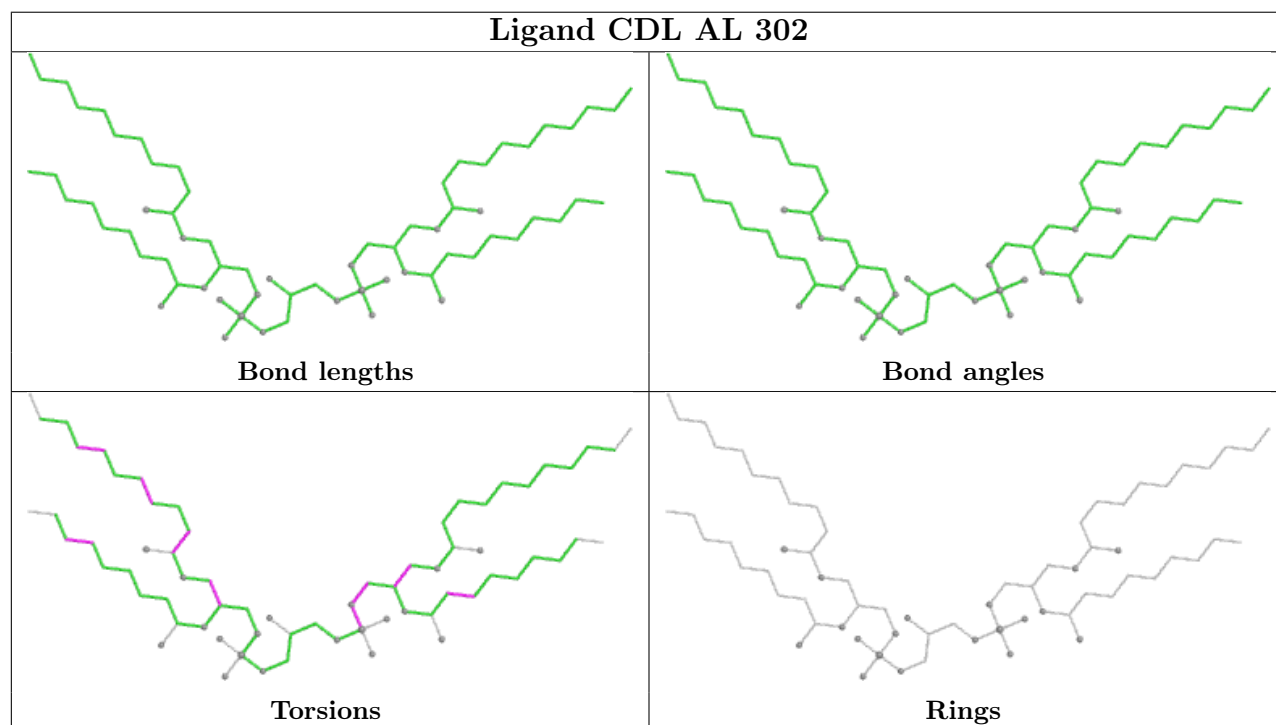
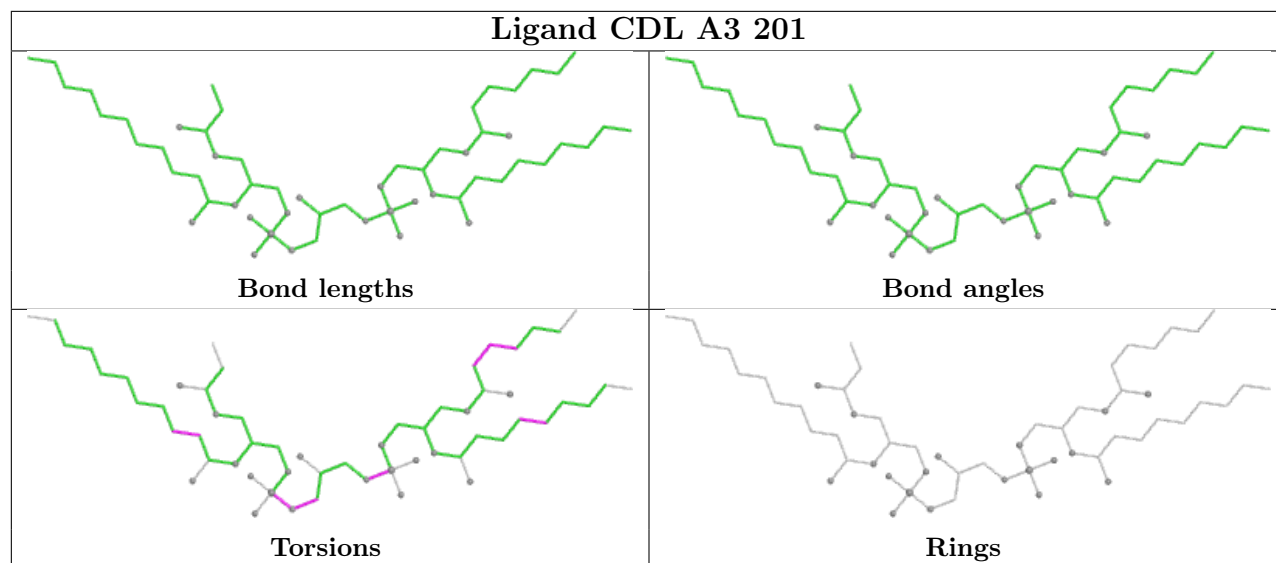


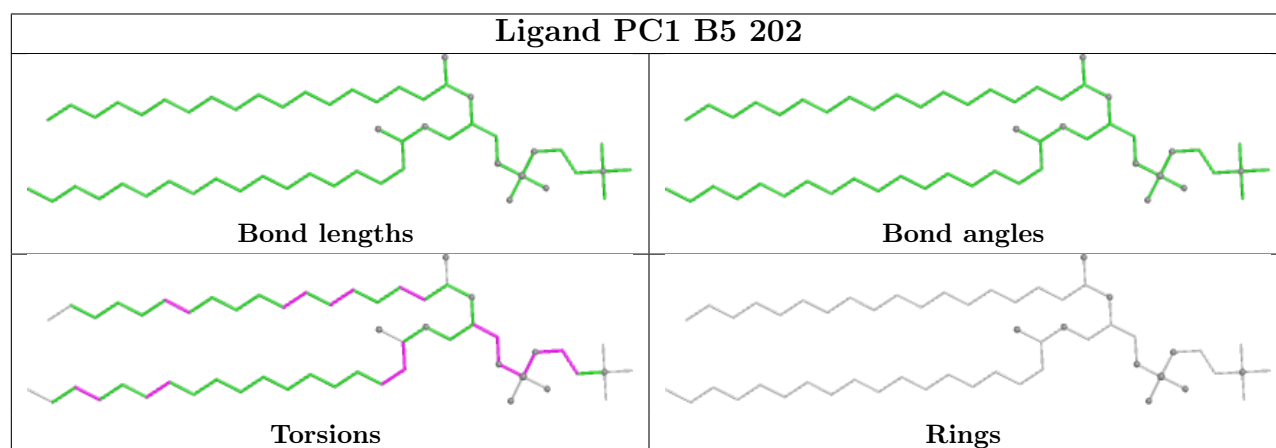
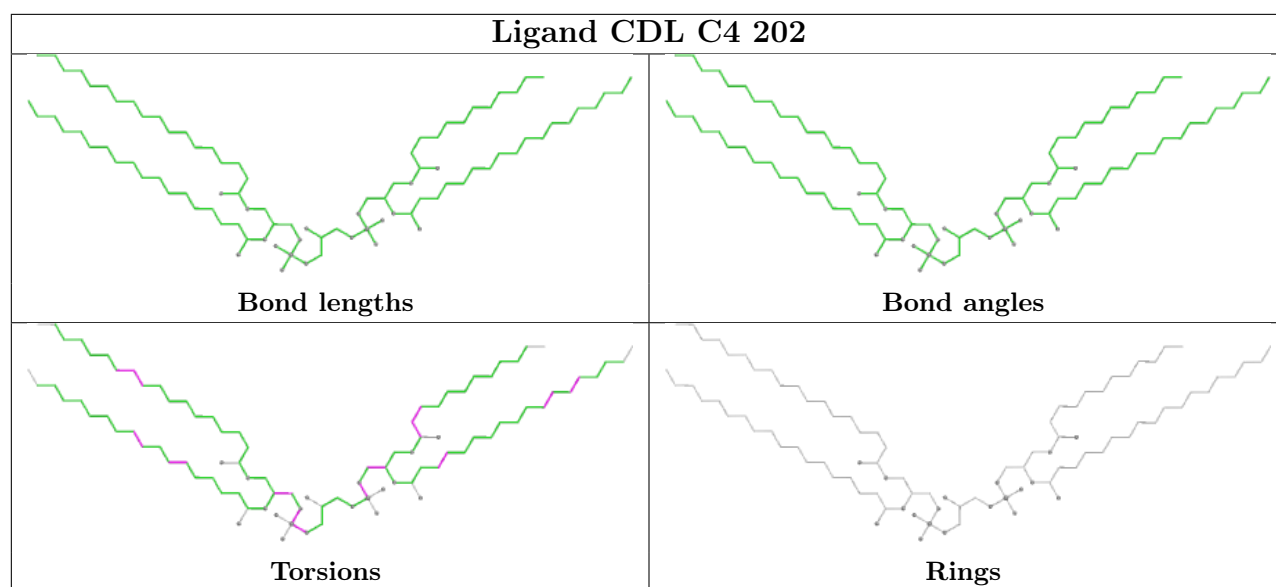


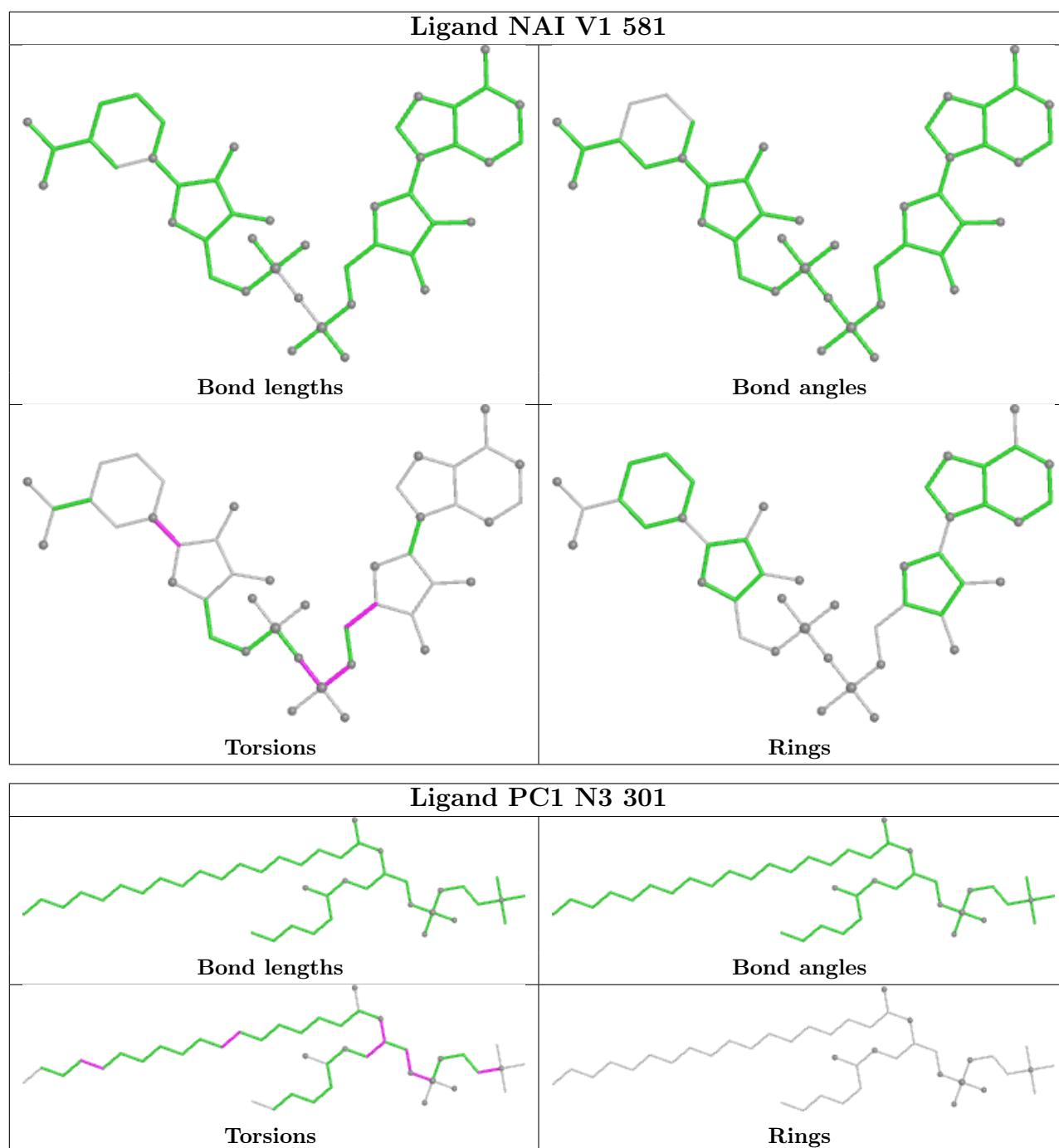


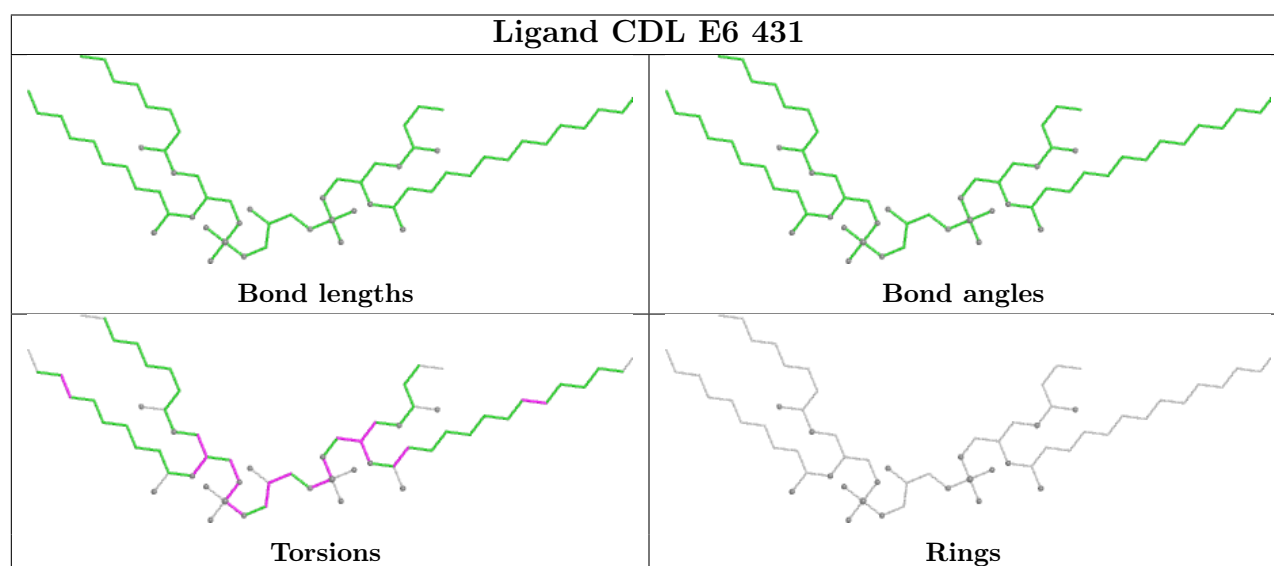
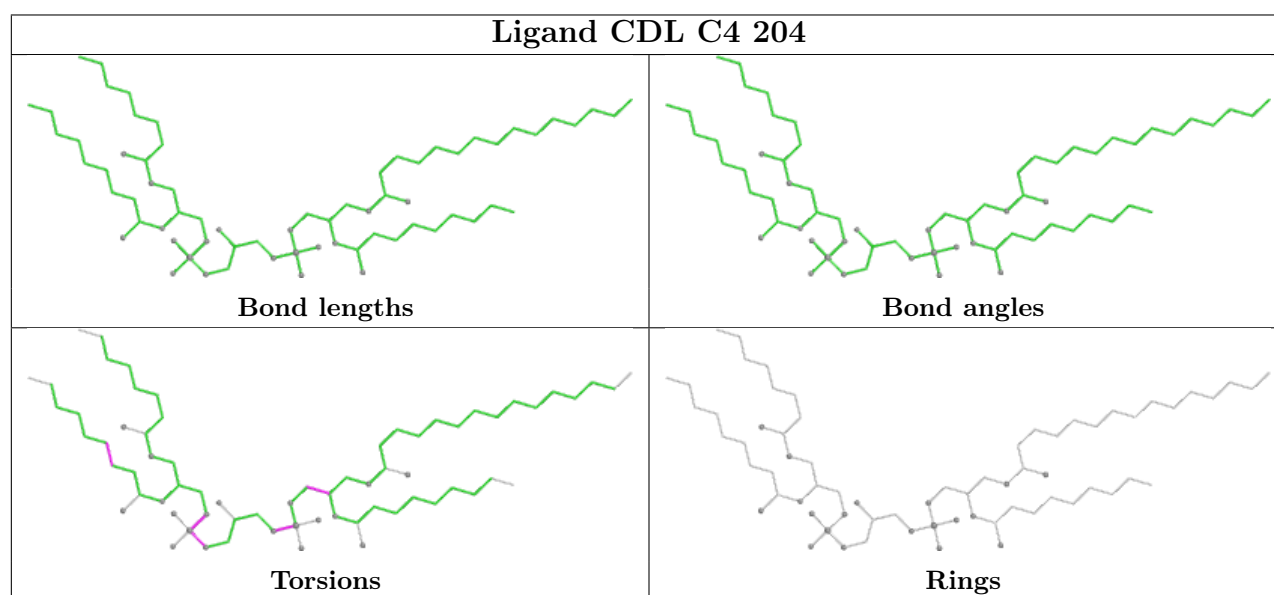
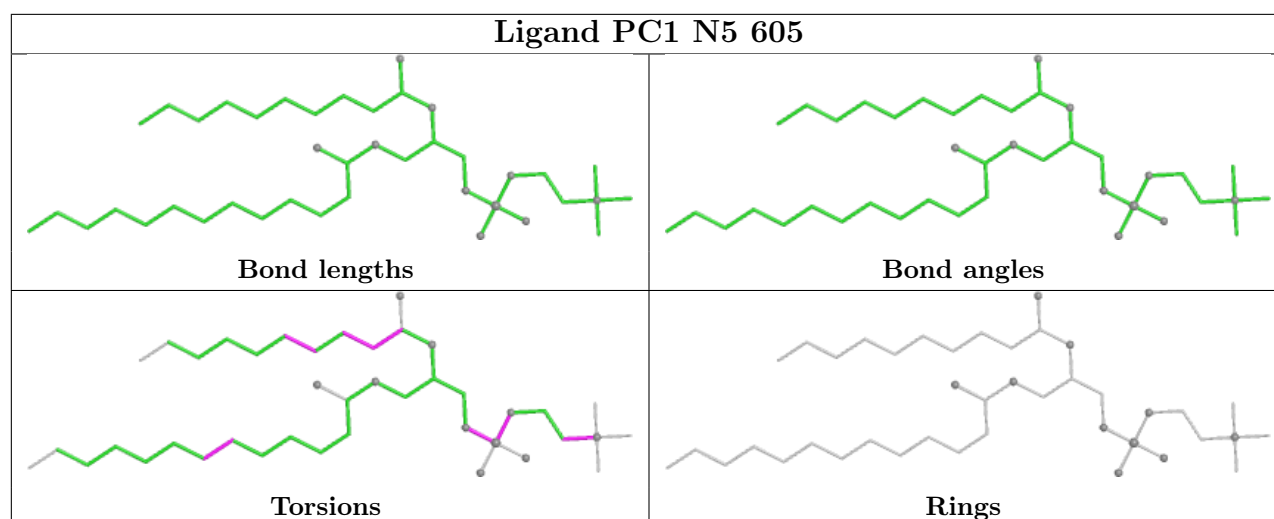


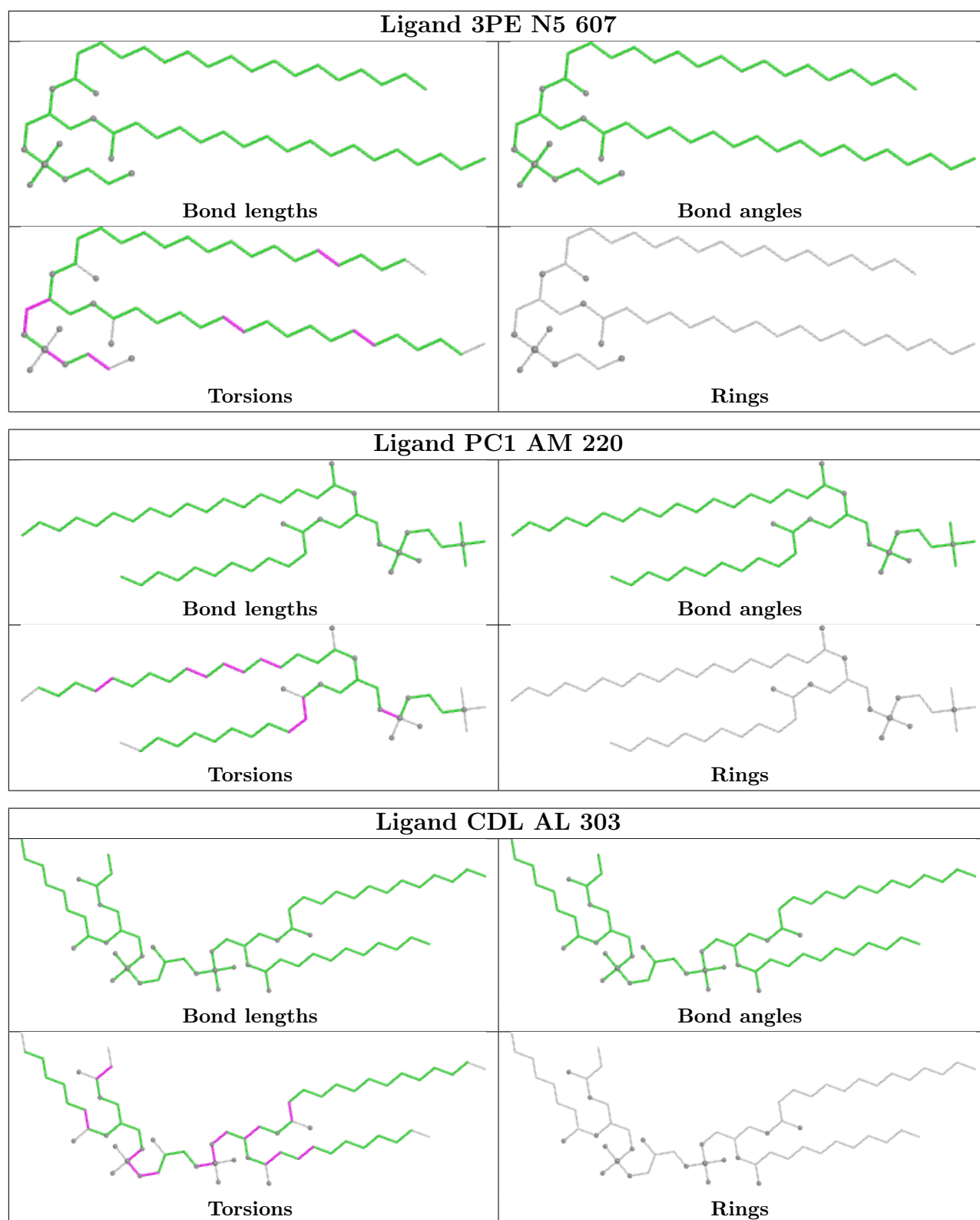


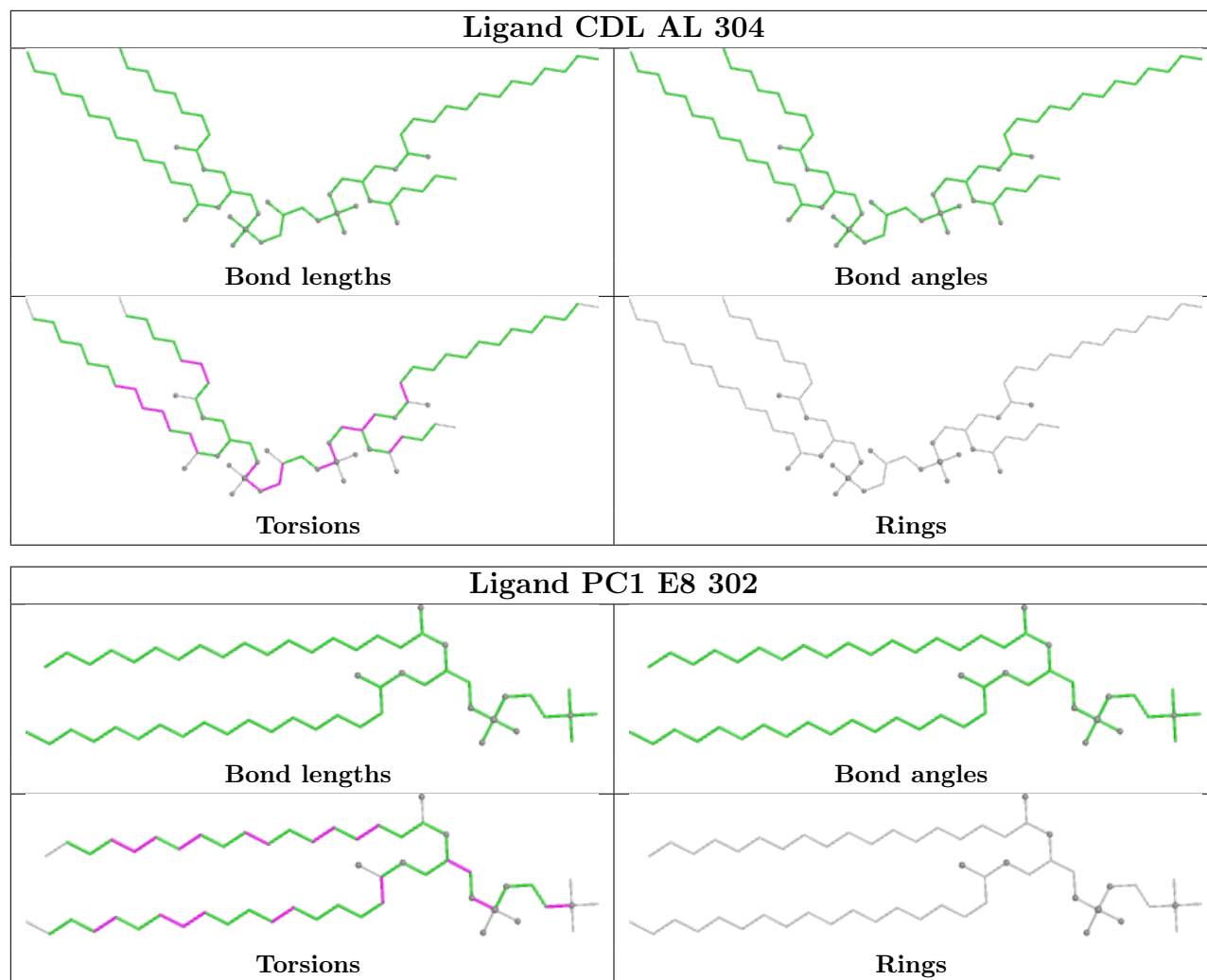


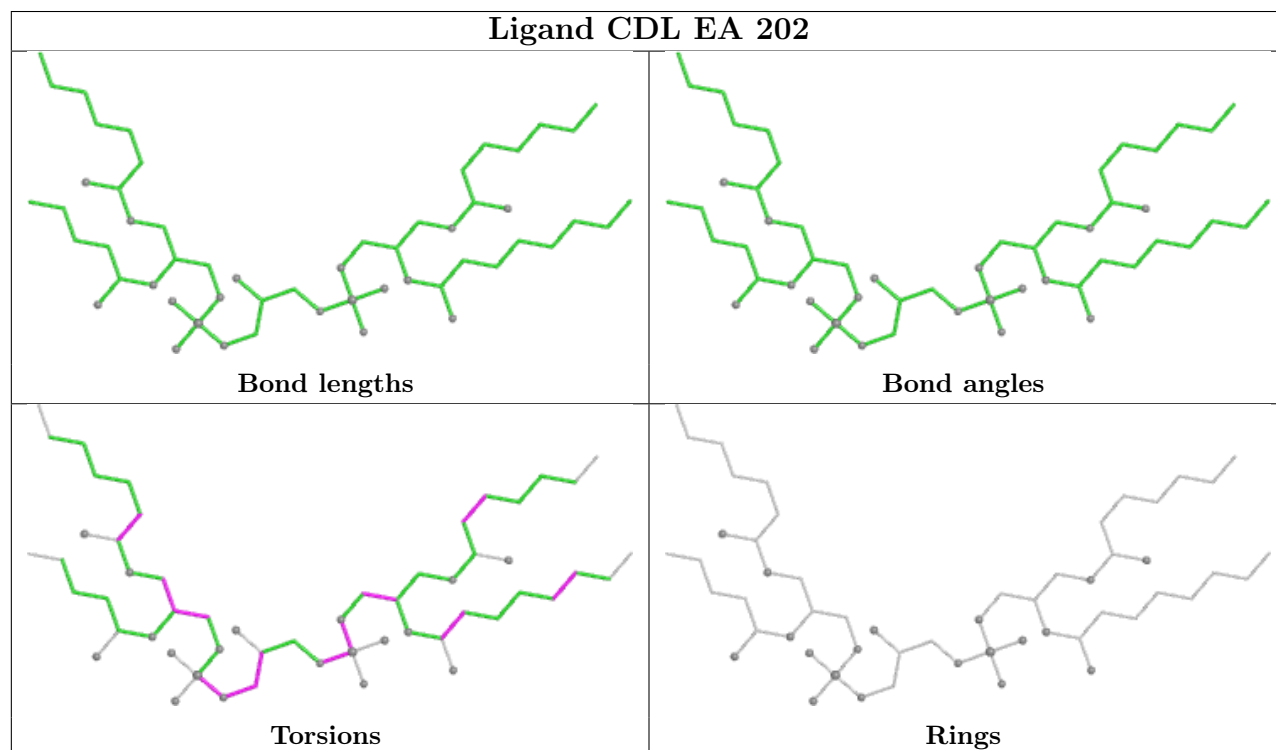
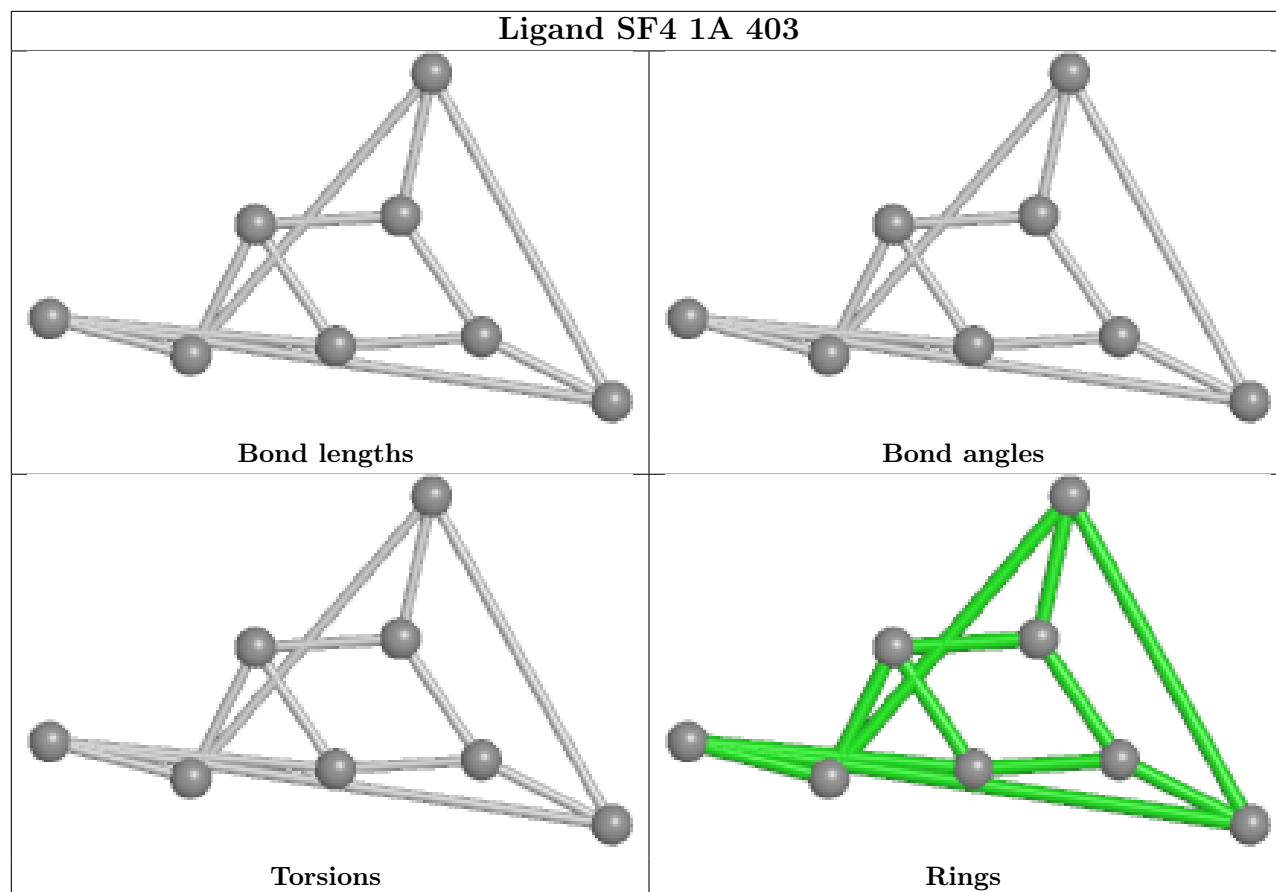


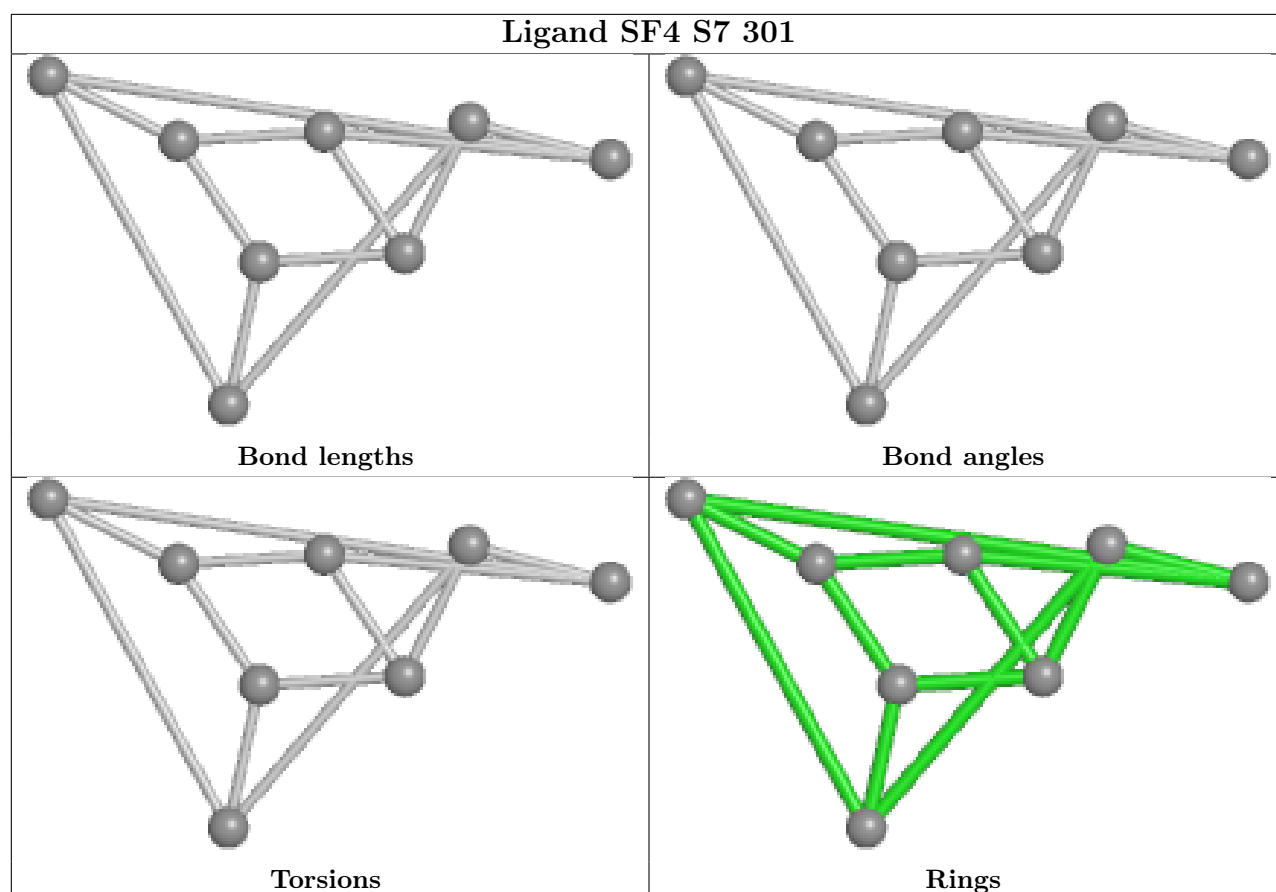
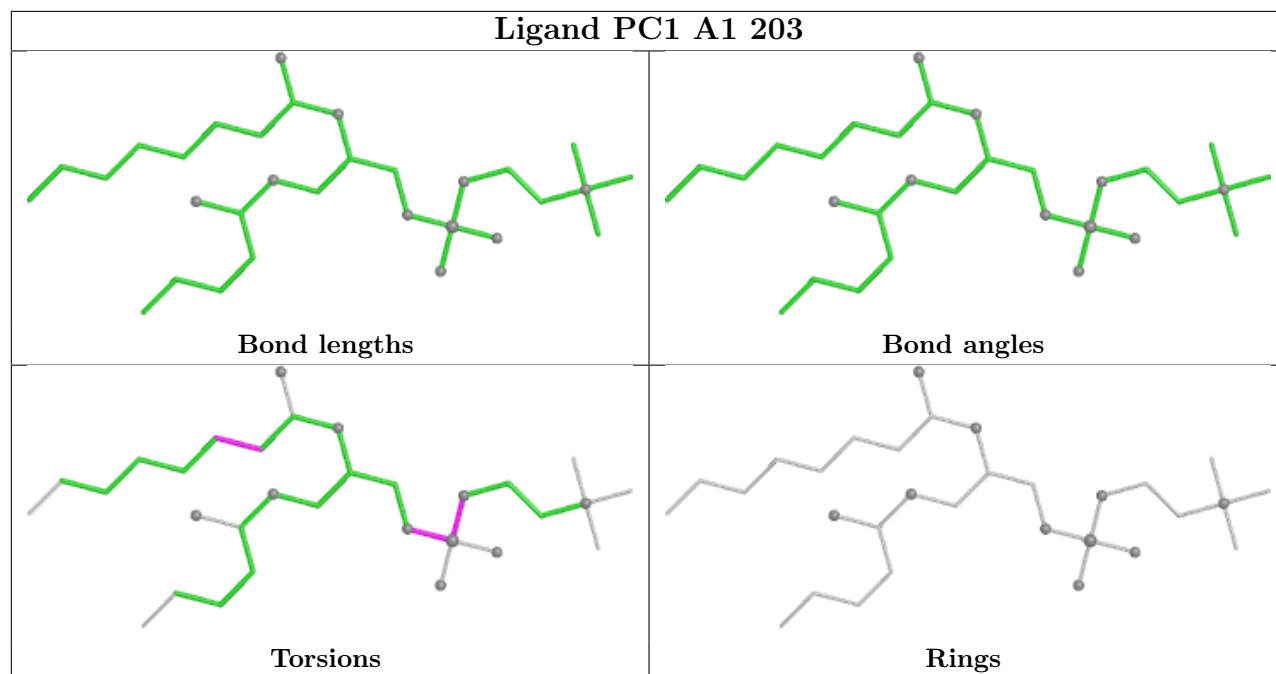


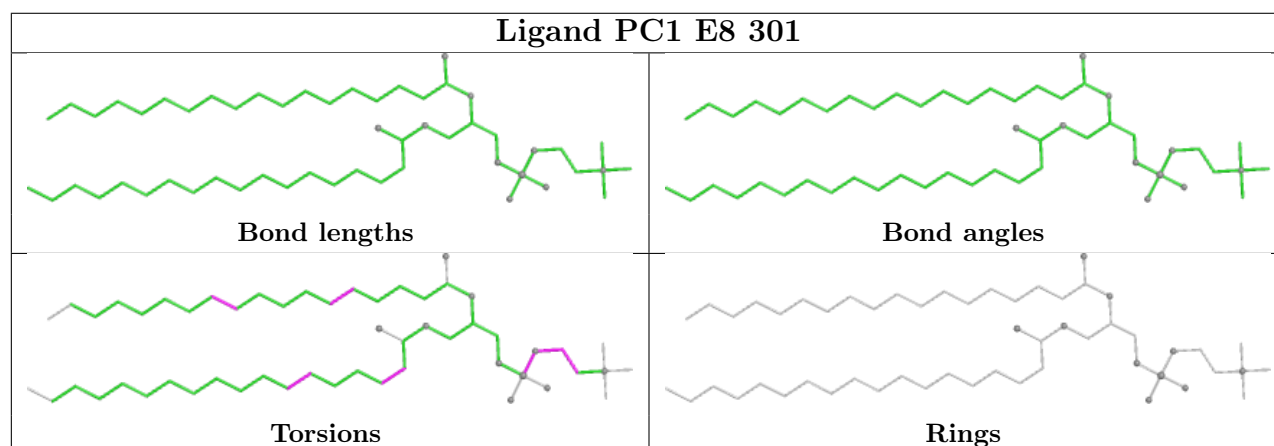
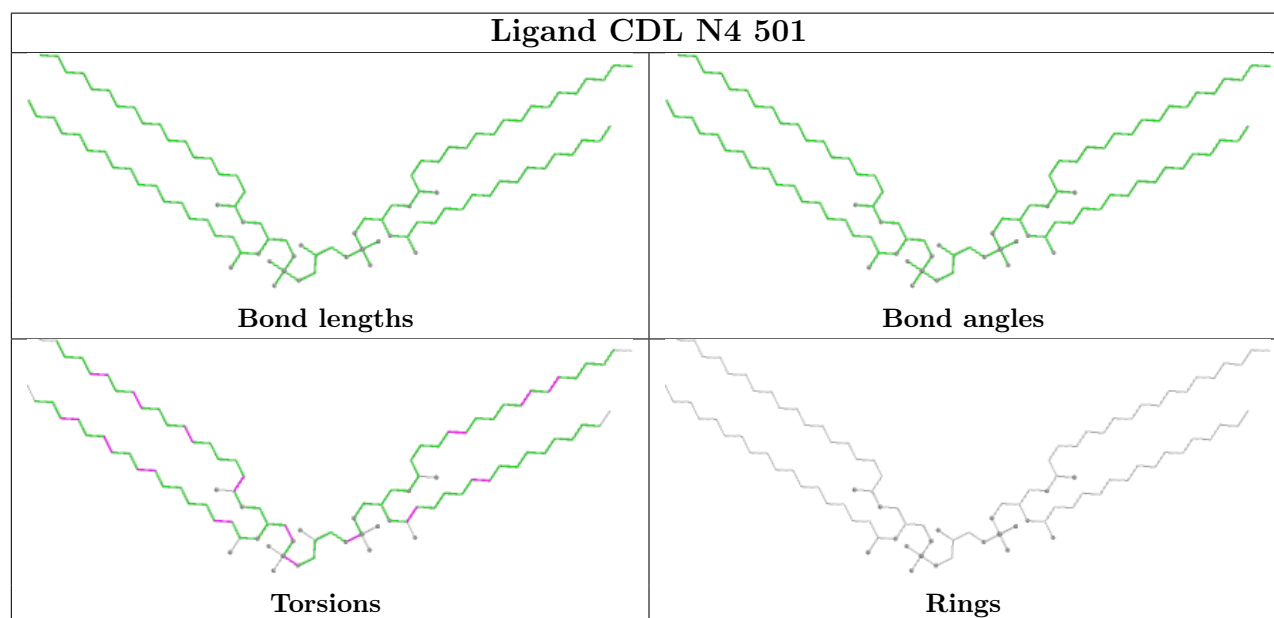
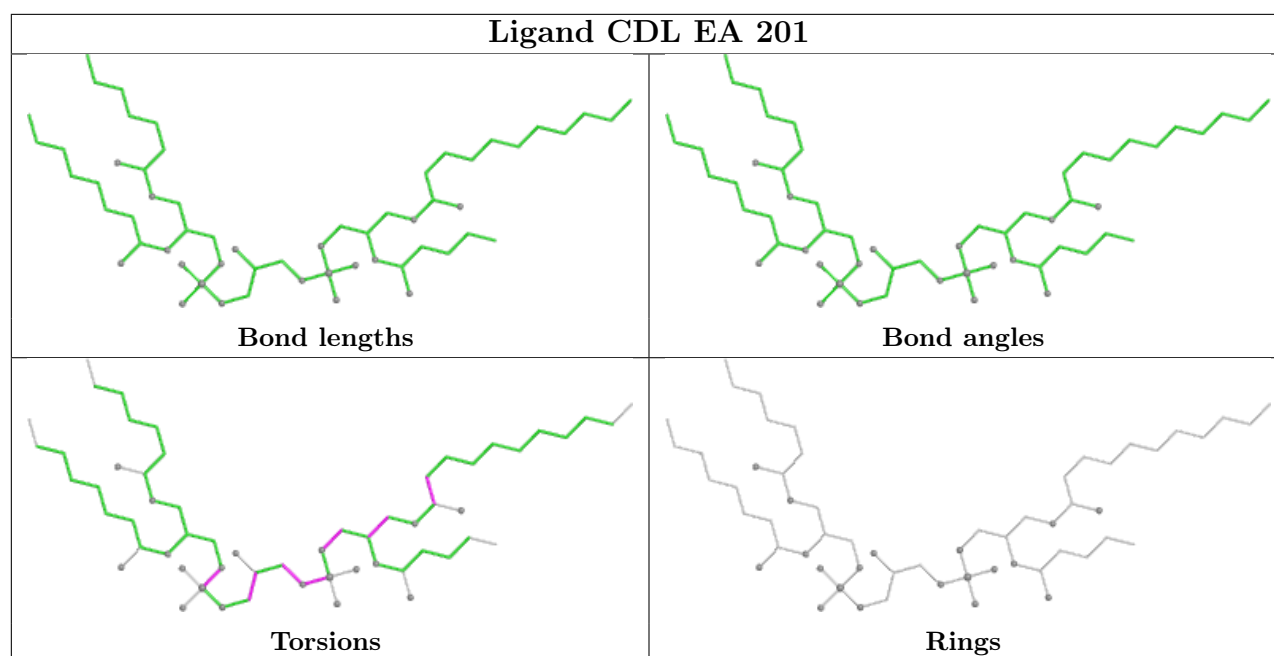


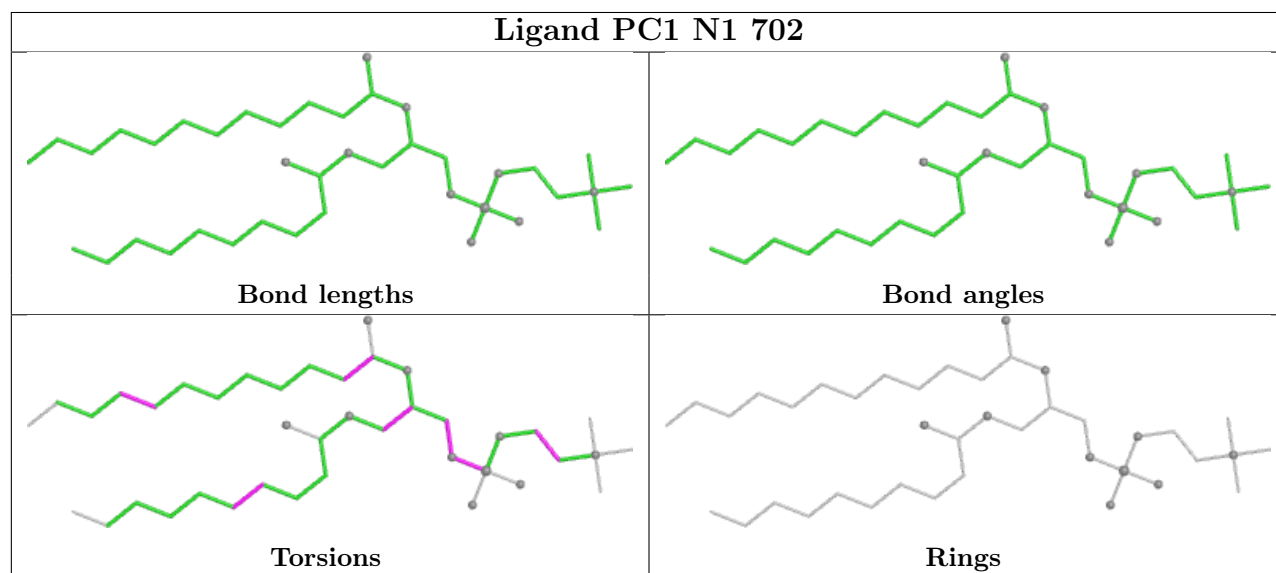
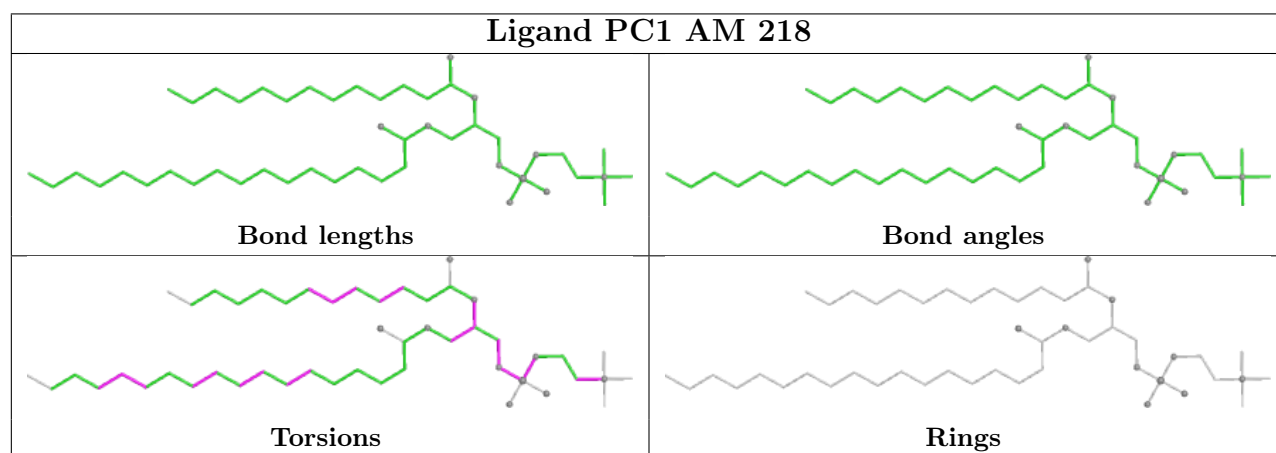
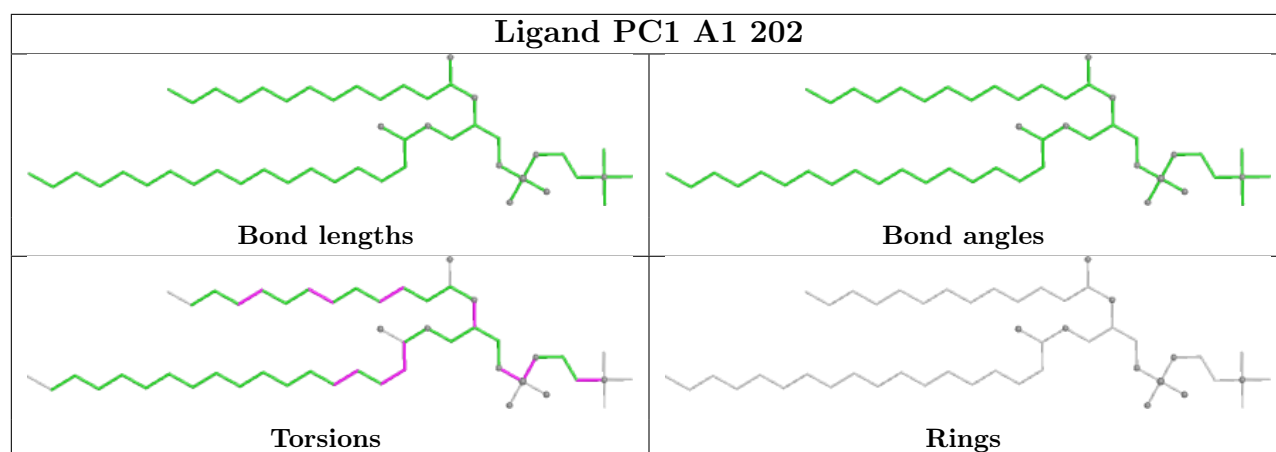




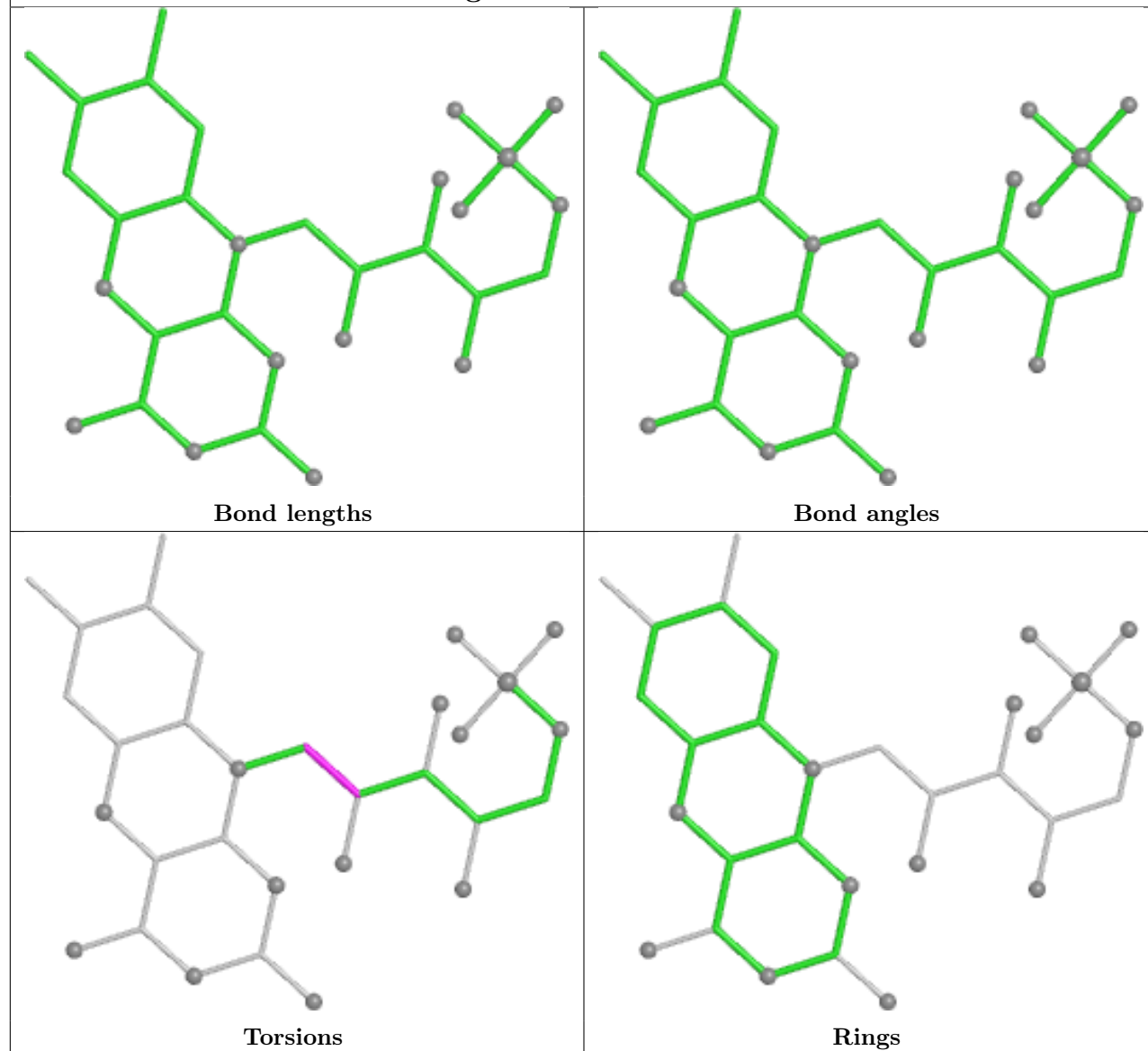




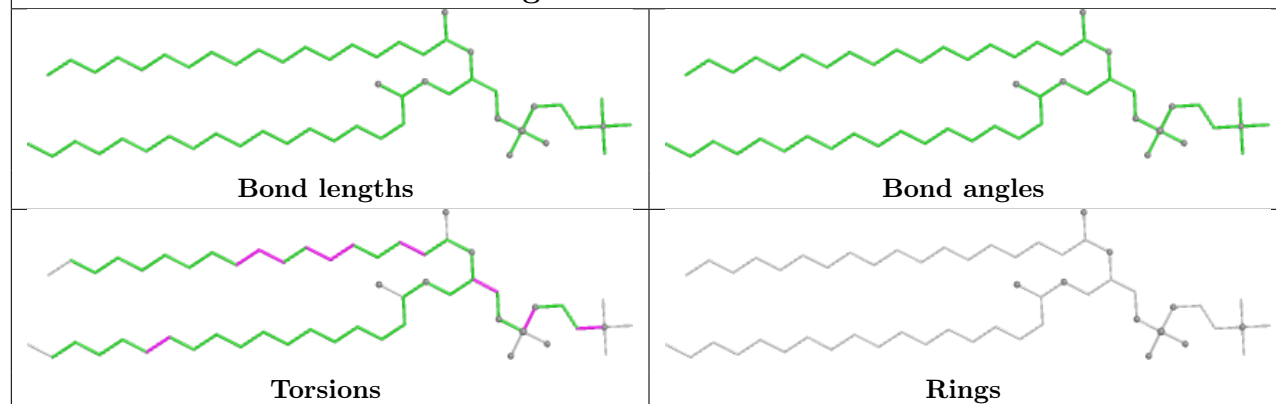


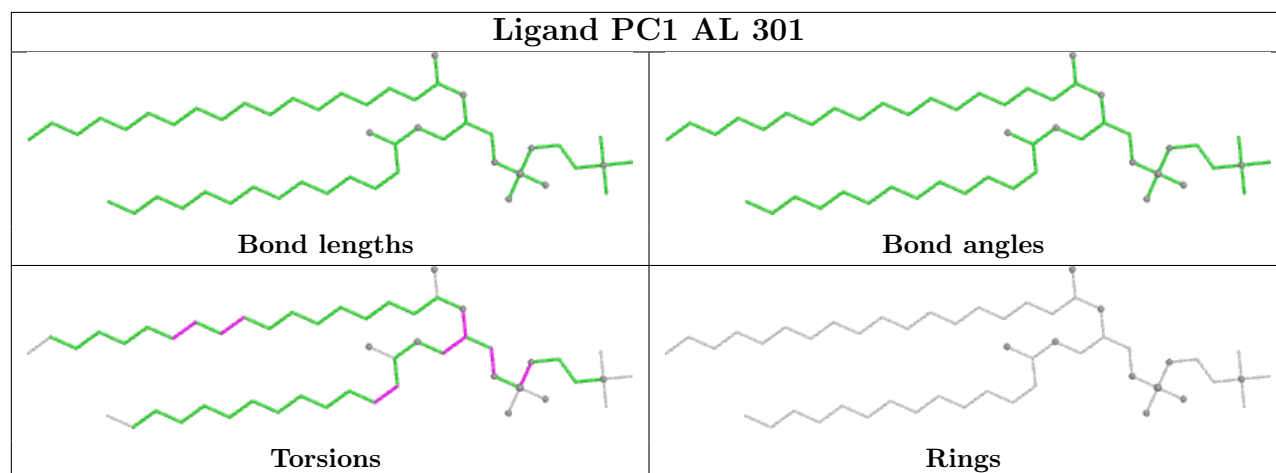
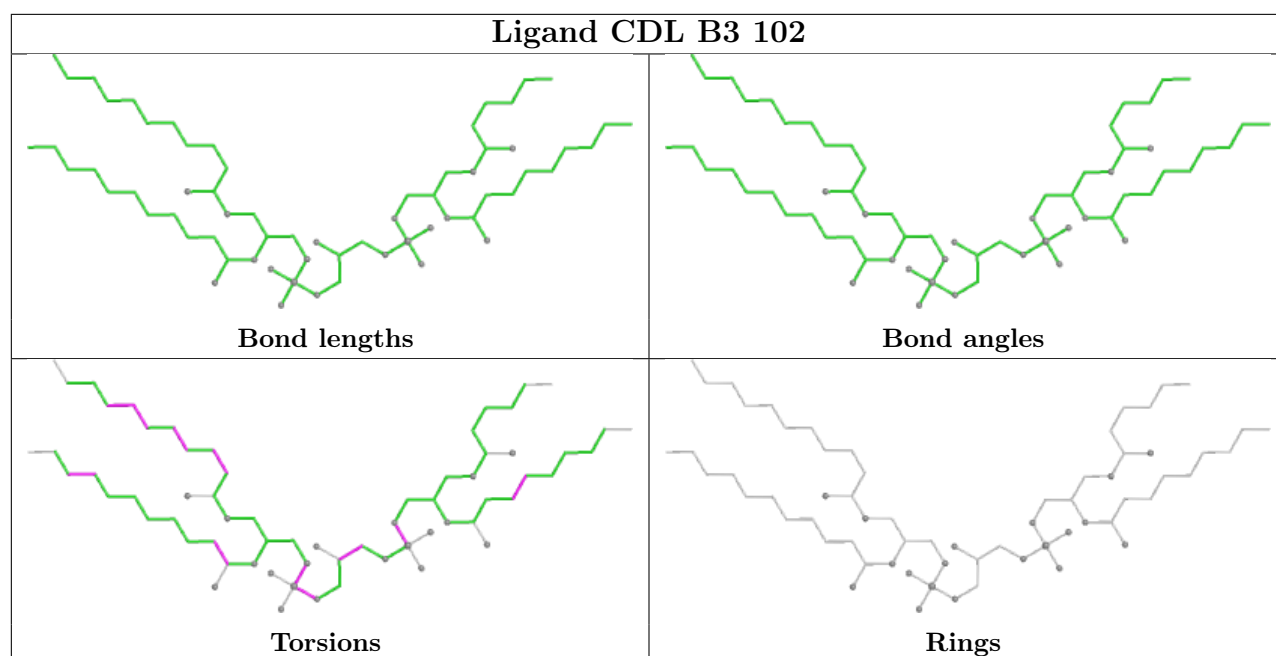


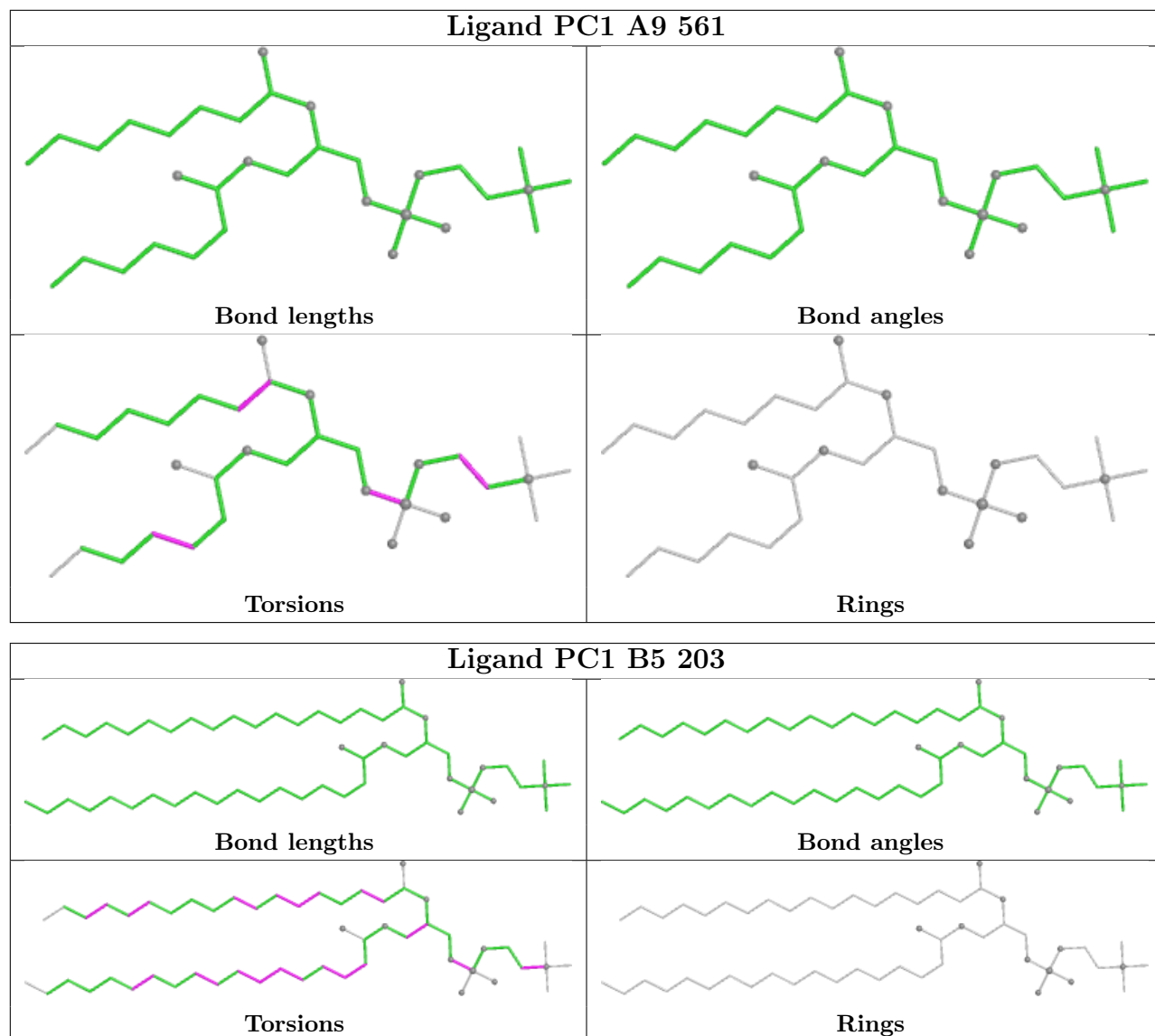
Ligand FMN V1 579

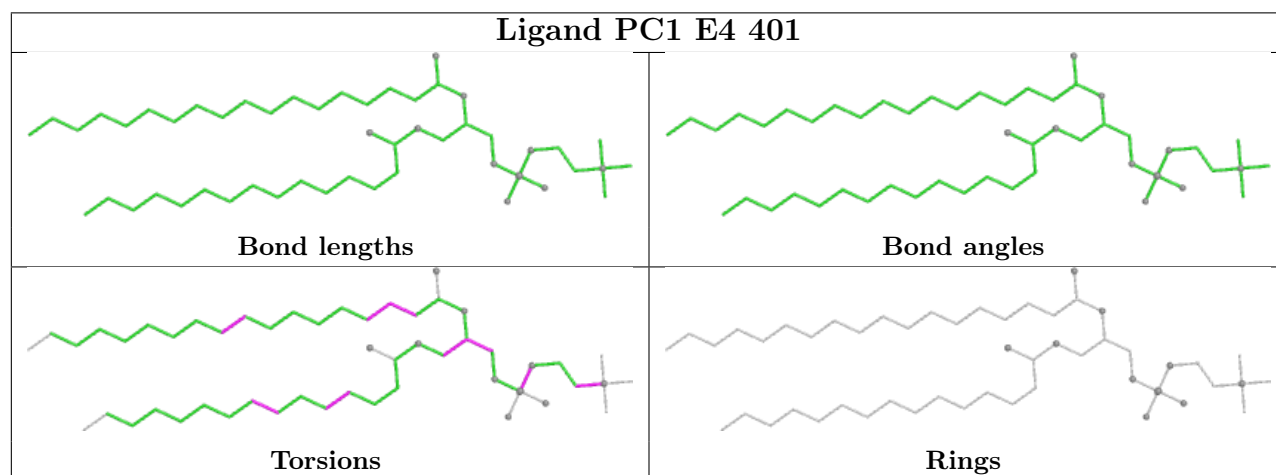
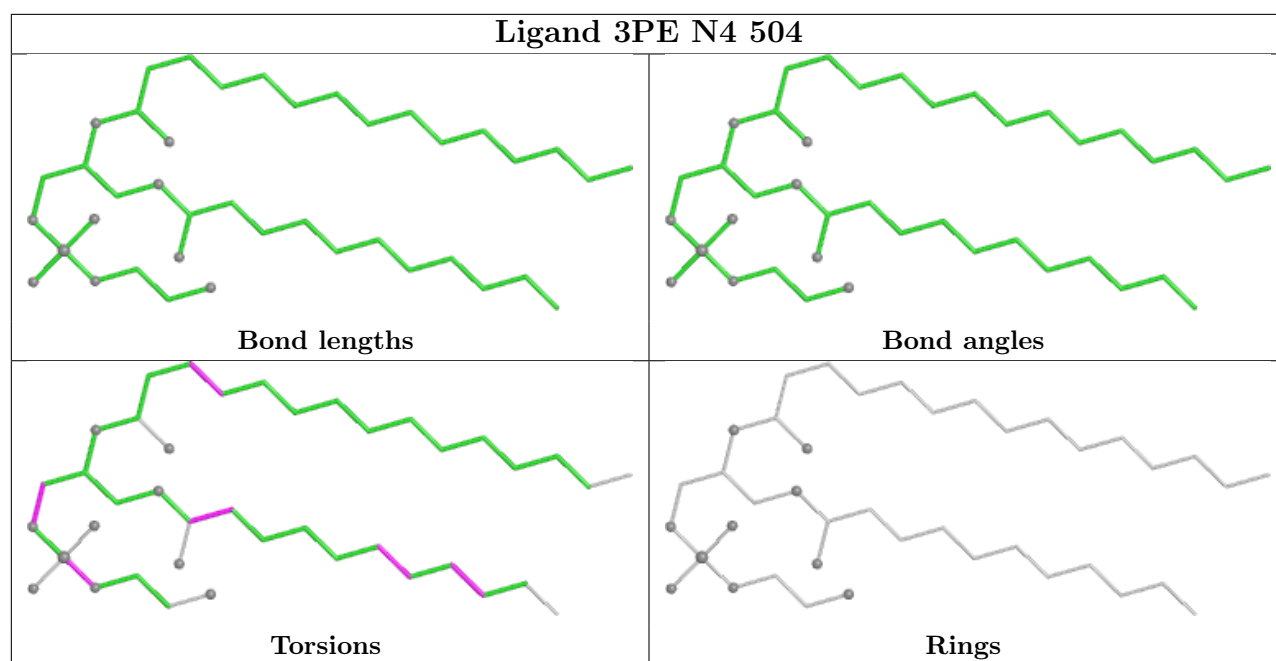


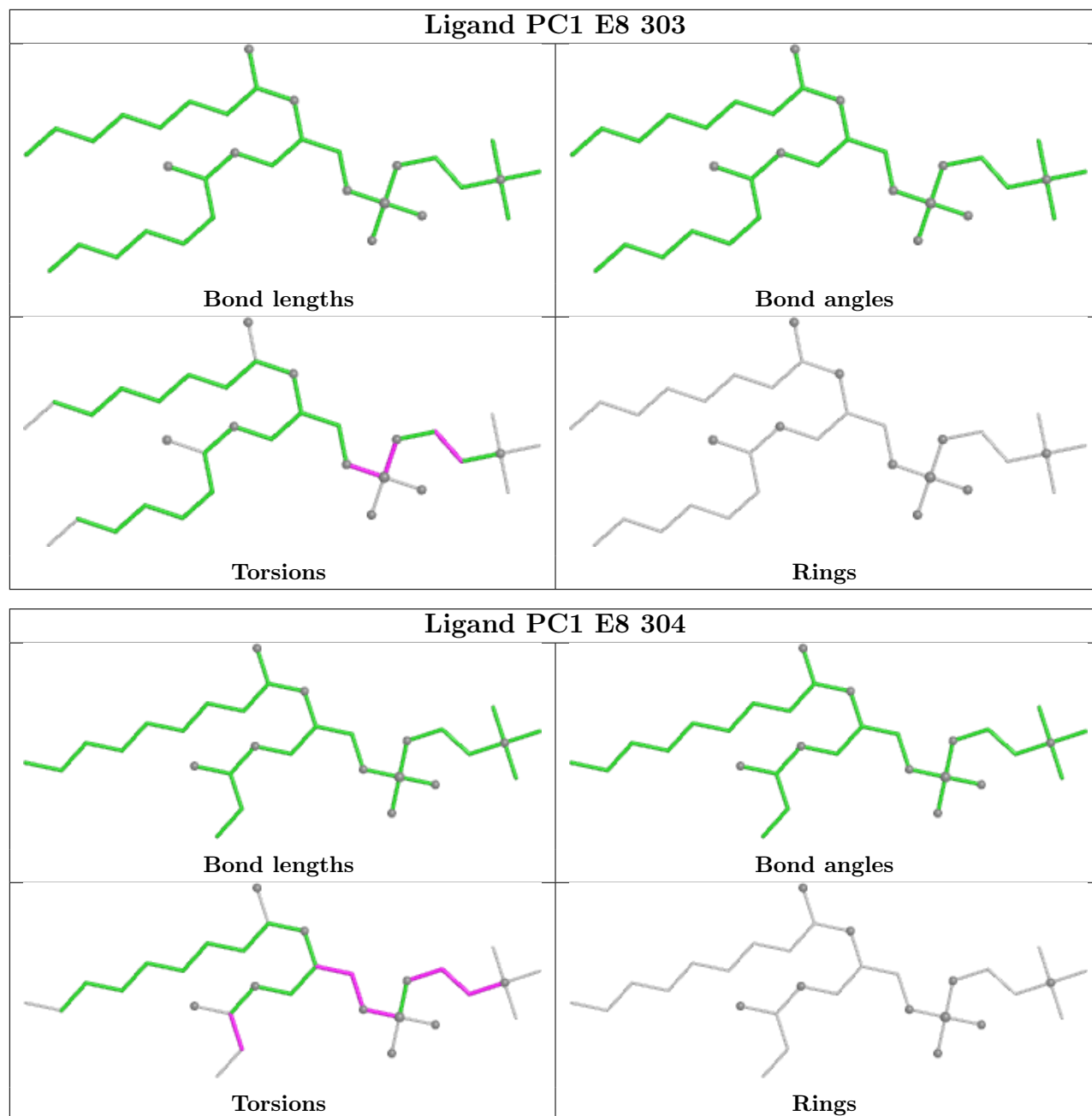
Ligand PC1 ED 201

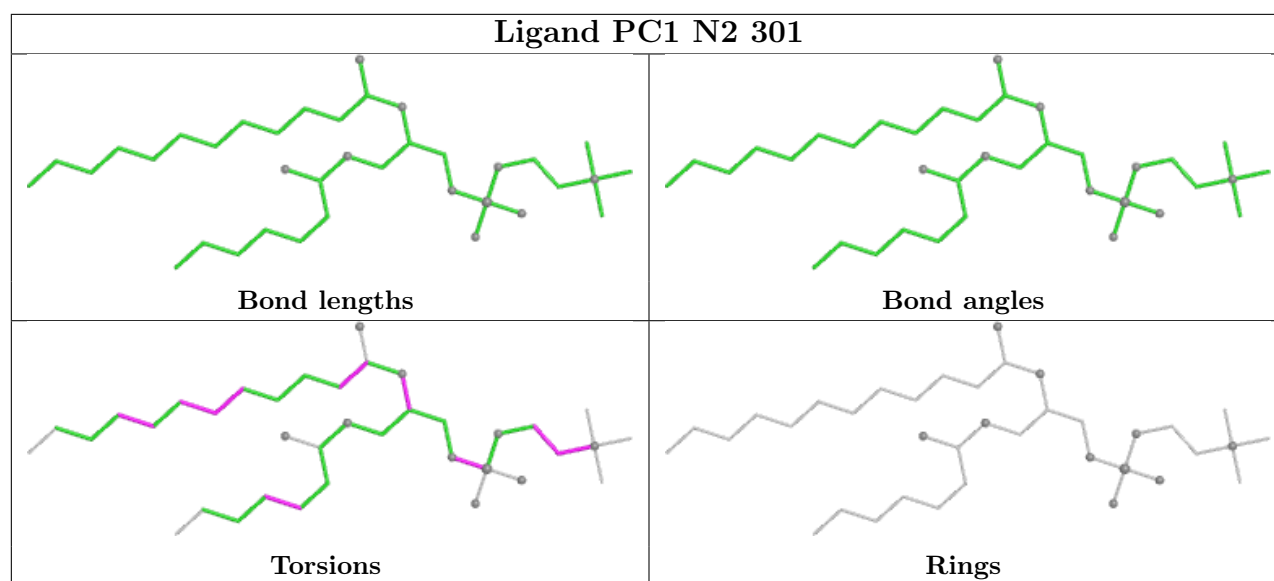












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

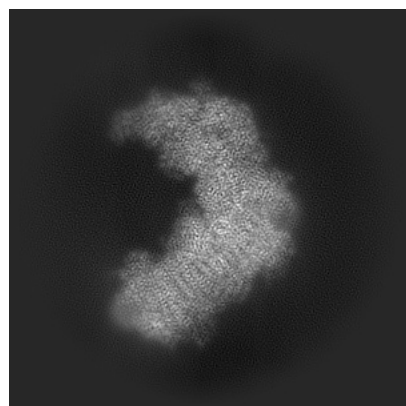
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36108. These allow visual inspection of the internal detail of the map and identification of artifacts.

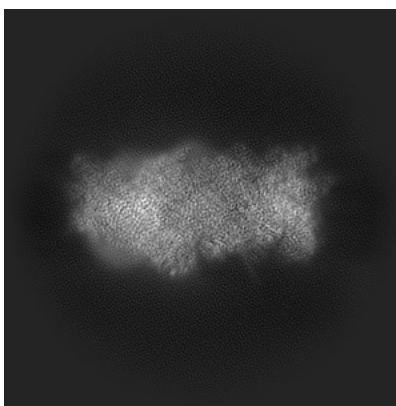
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

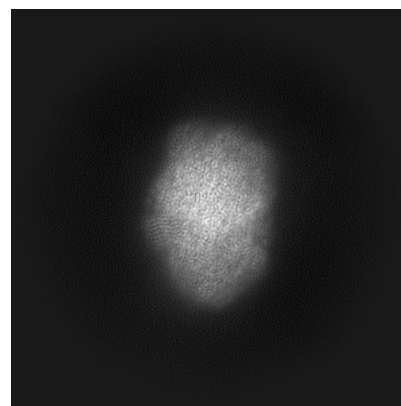
6.1.1 Primary map



X

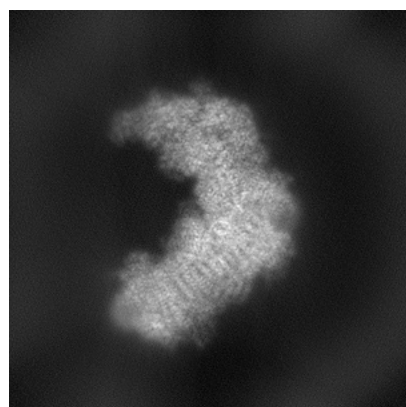


Y

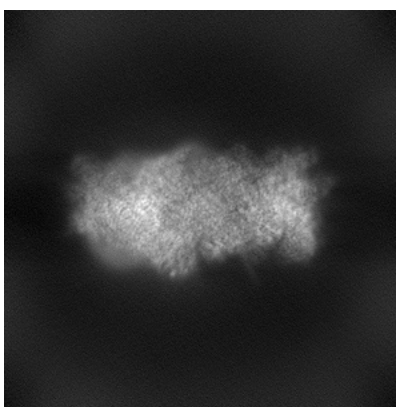


Z

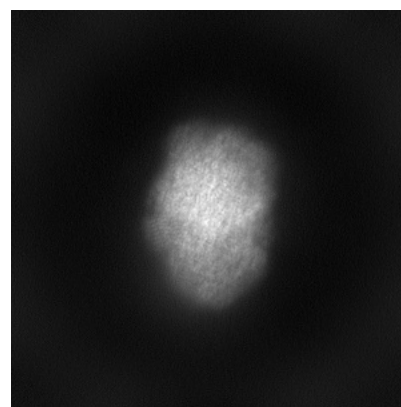
6.1.2 Raw map



X



Y

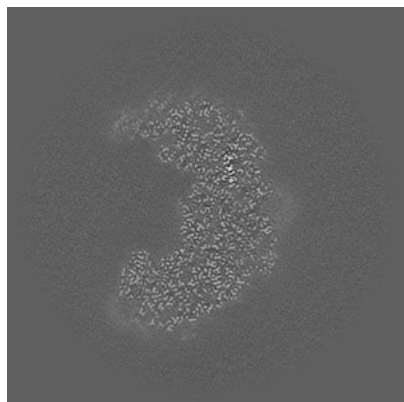


Z

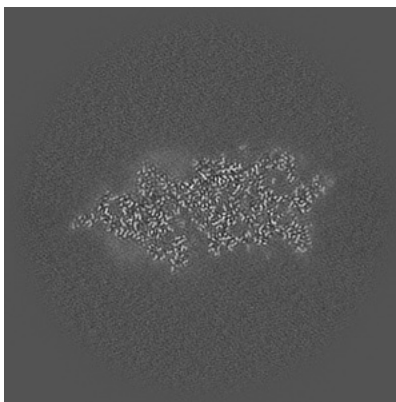
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

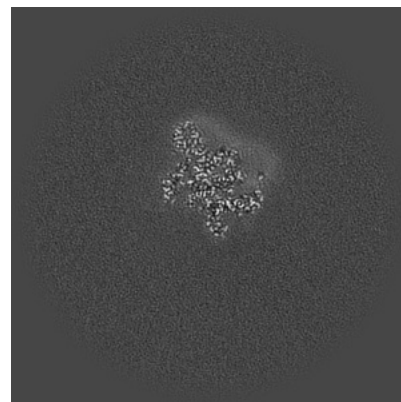
6.2.1 Primary map



X Index: 240

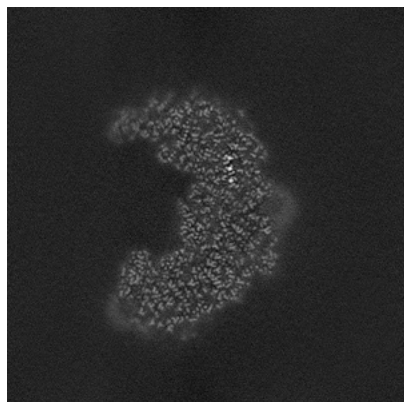


Y Index: 240

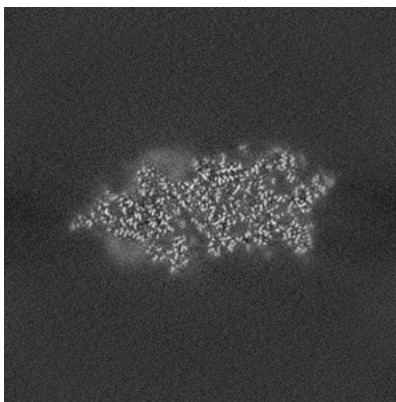


Z Index: 240

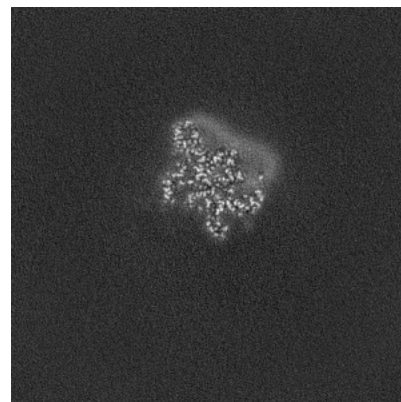
6.2.2 Raw map



X Index: 240



Y Index: 240

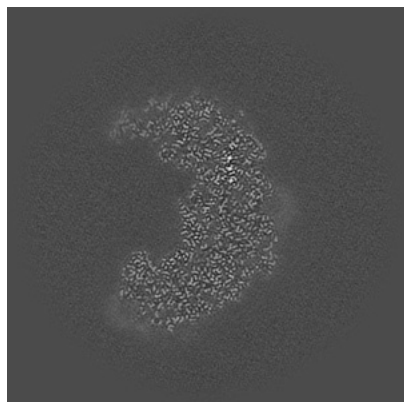


Z Index: 240

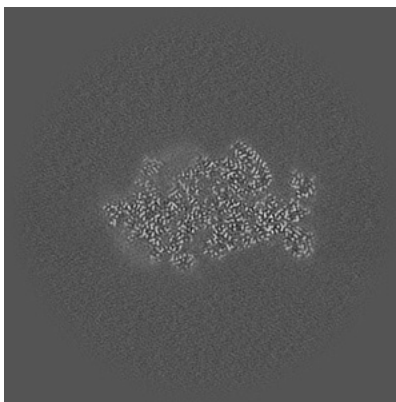
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

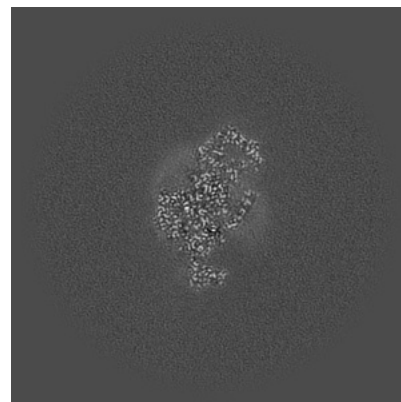
6.3.1 Primary map



X Index: 241

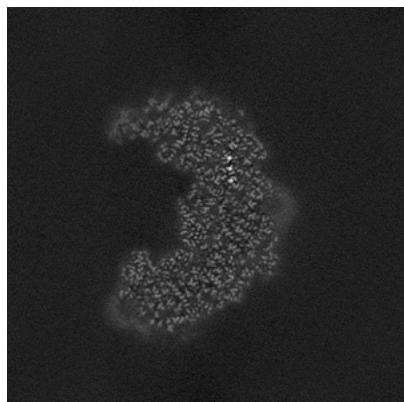


Y Index: 254

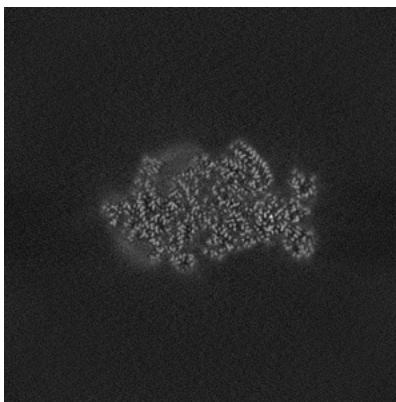


Z Index: 181

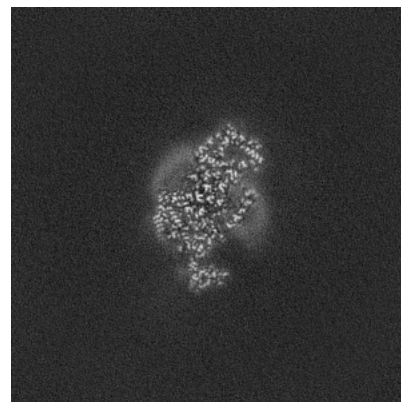
6.3.2 Raw map



X Index: 241



Y Index: 254

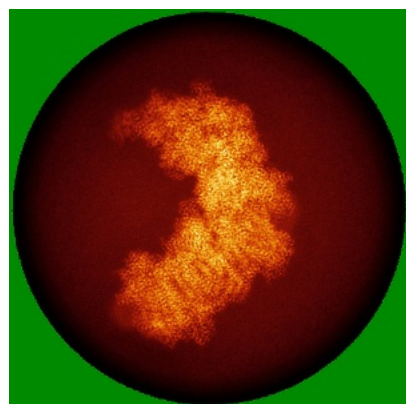


Z Index: 182

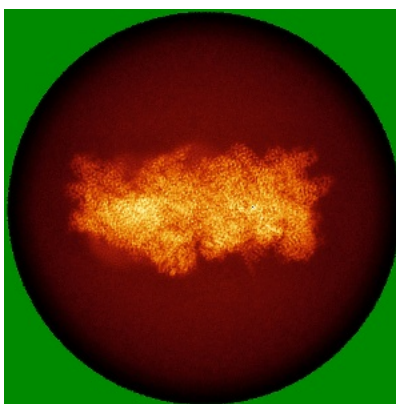
The images above show the largest variance slices of the map in three orthogonal directions.

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

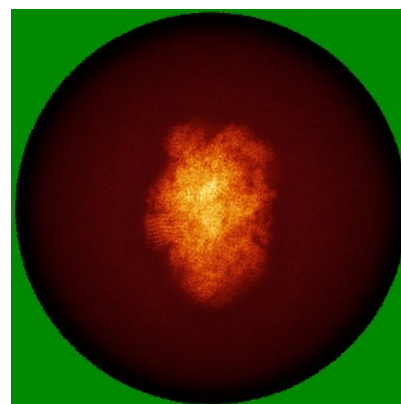
6.4.1 Primary map



X



Y

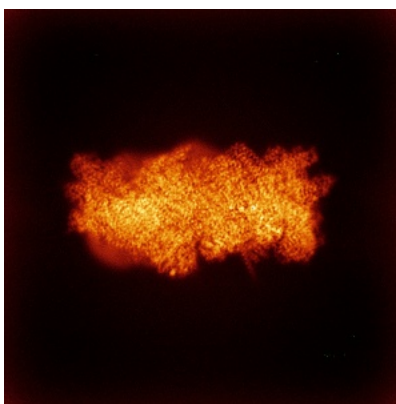


Z

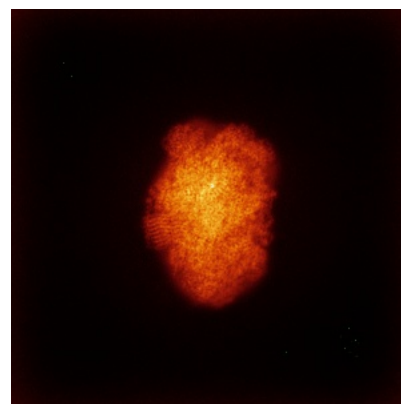
6.4.2 Raw map



X



Y

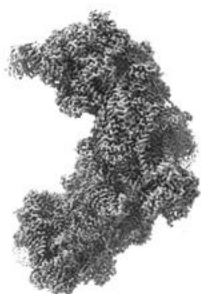


Z

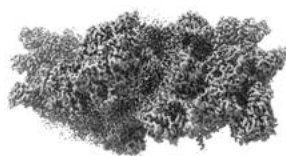
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



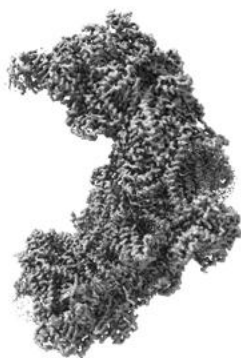
Y



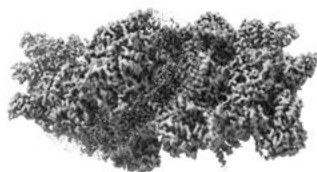
Z

The images above show the 3D surface view of the map at the recommended contour level 4.5. 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.

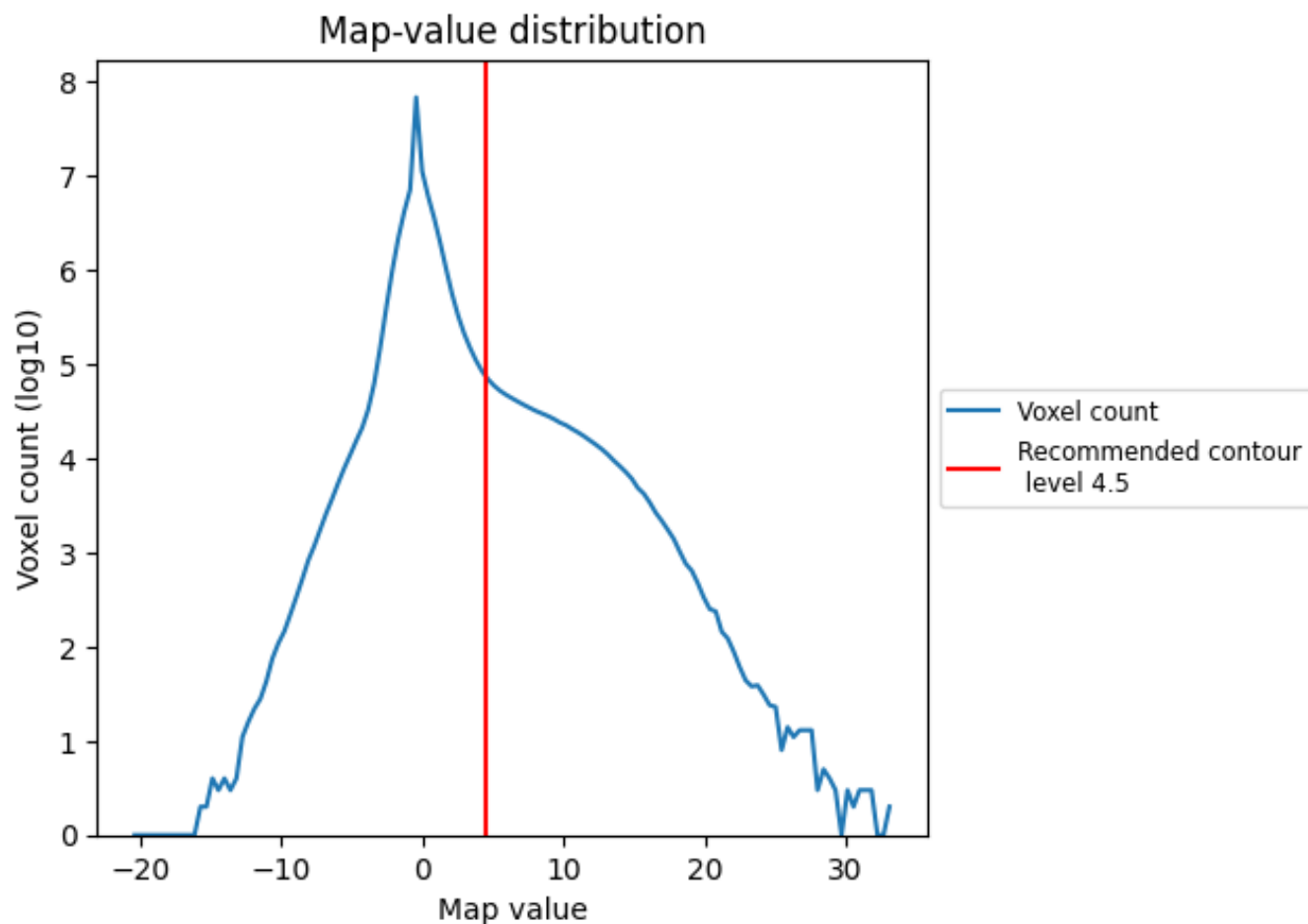
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

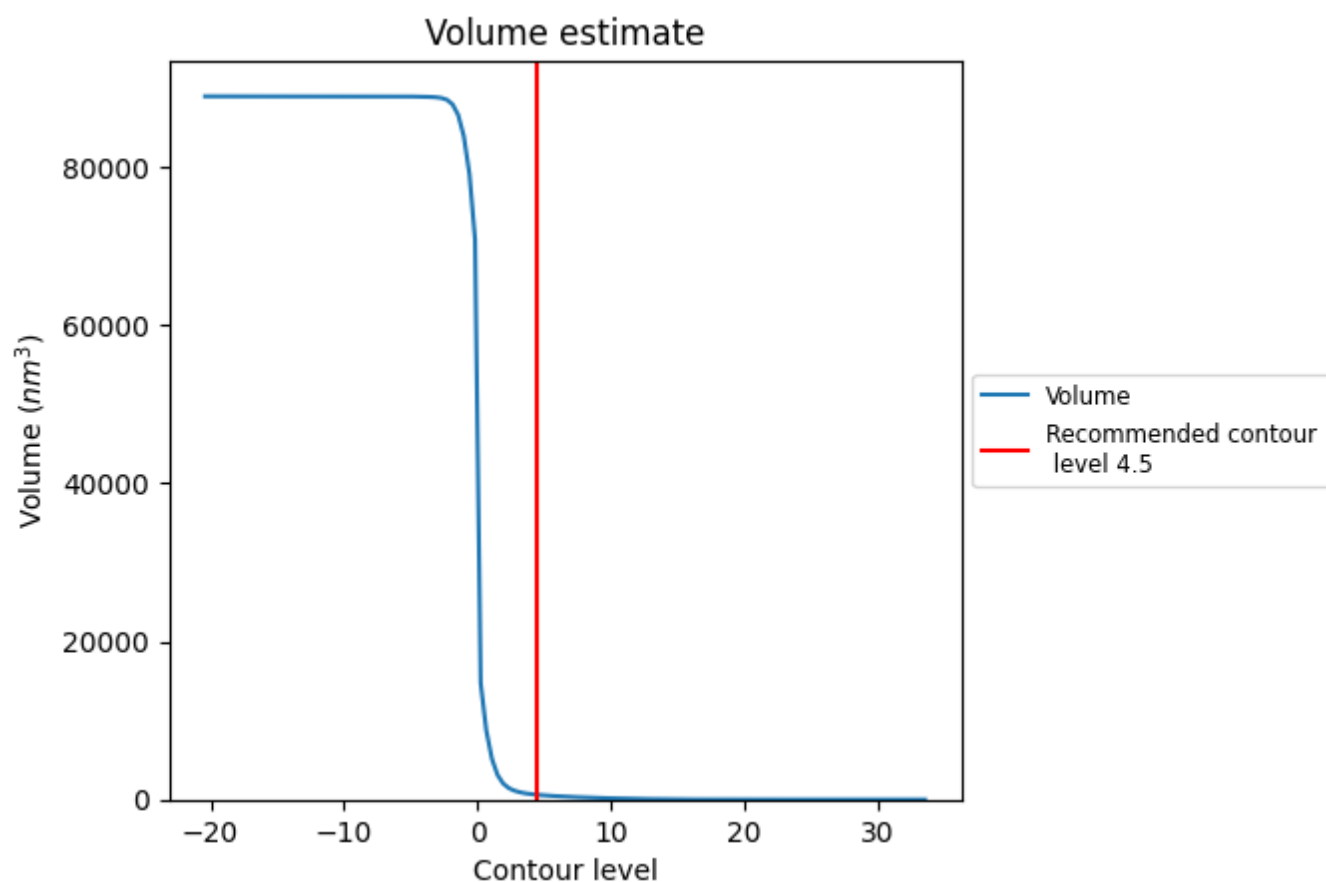
This section contains the results of statistical analysis of the map.

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.

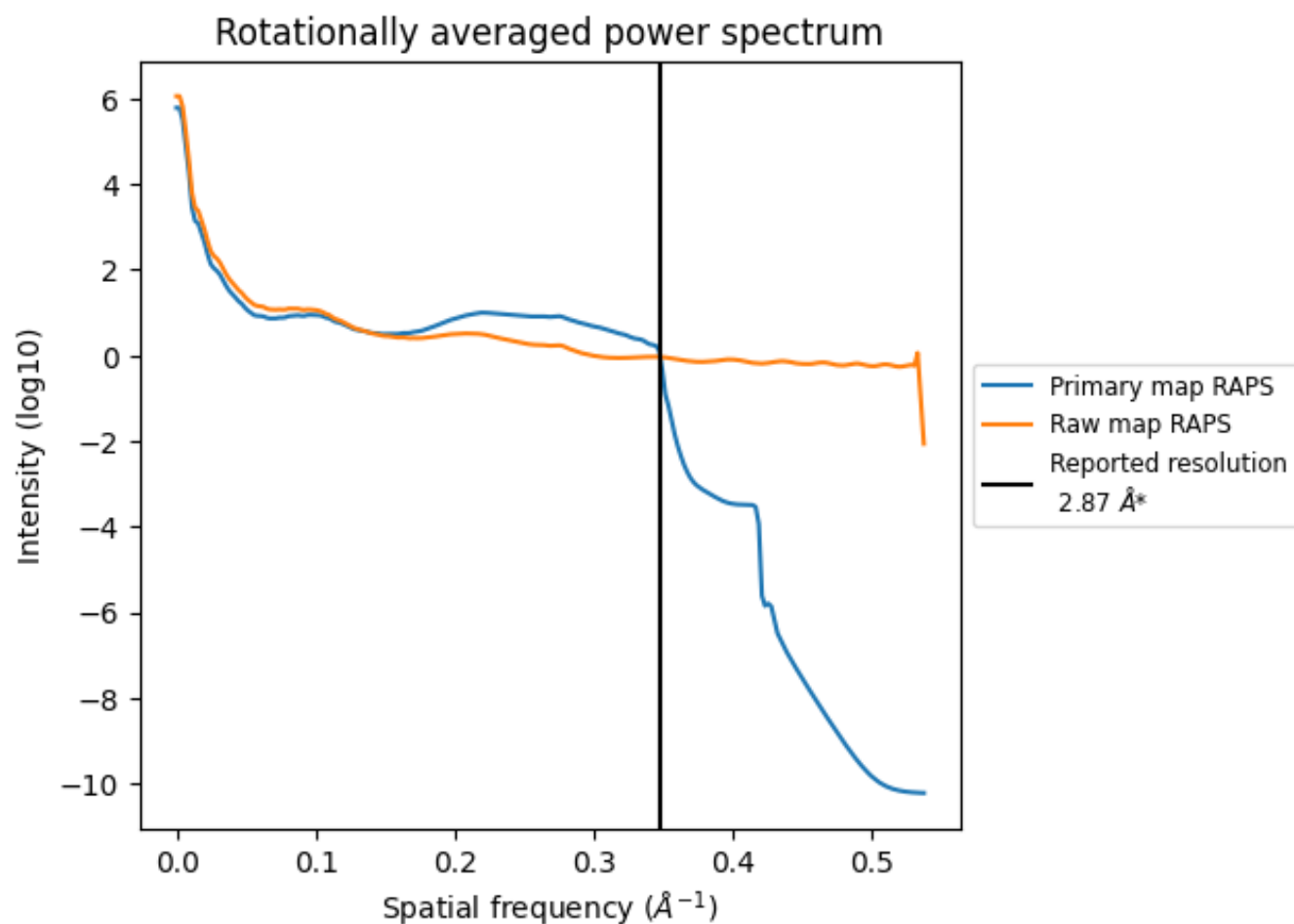
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 596 nm³; this corresponds to an approximate mass of 538 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 ⓘ

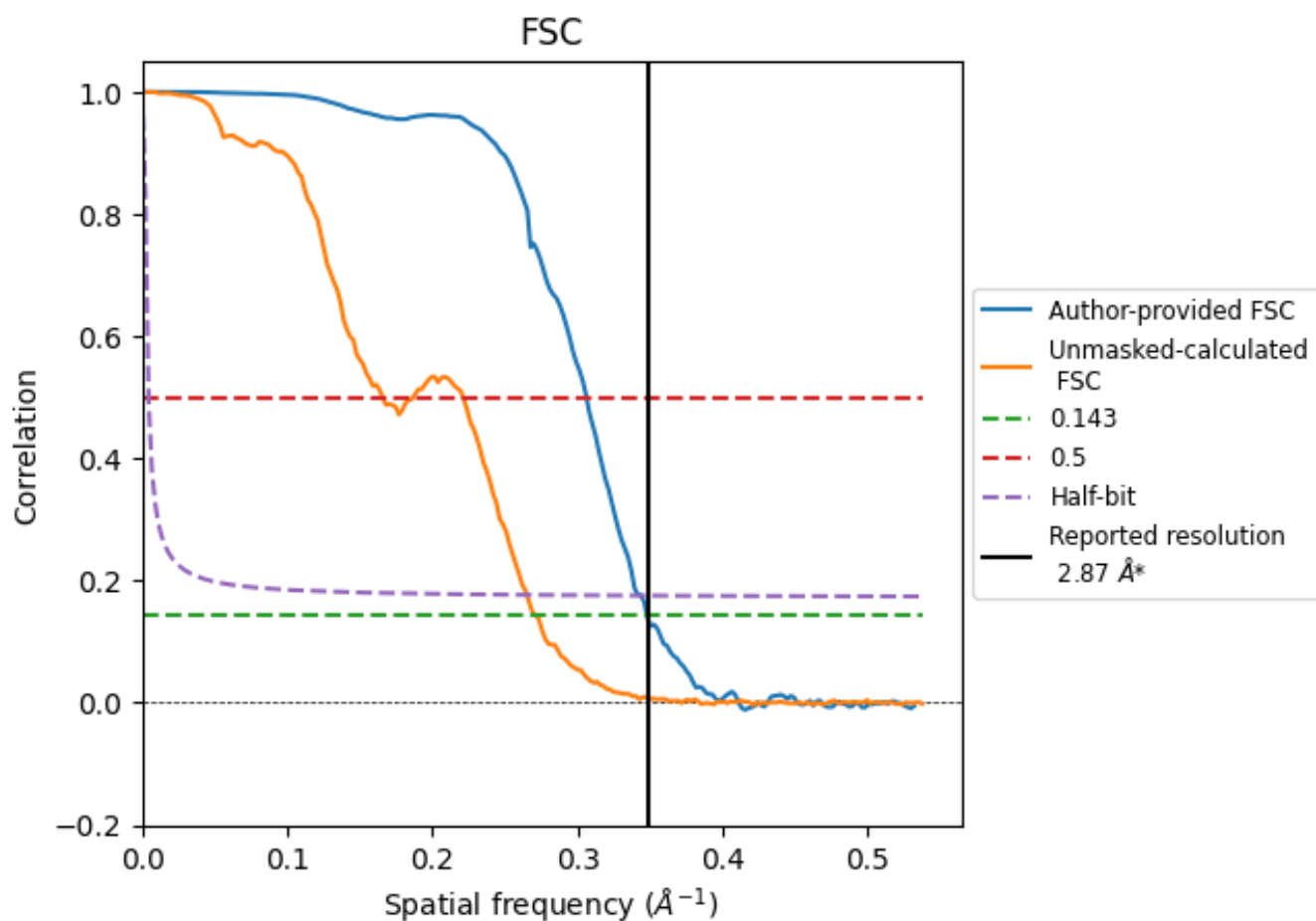


*Reported resolution corresponds to spatial frequency of 0.348 Å⁻¹

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 0.348 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

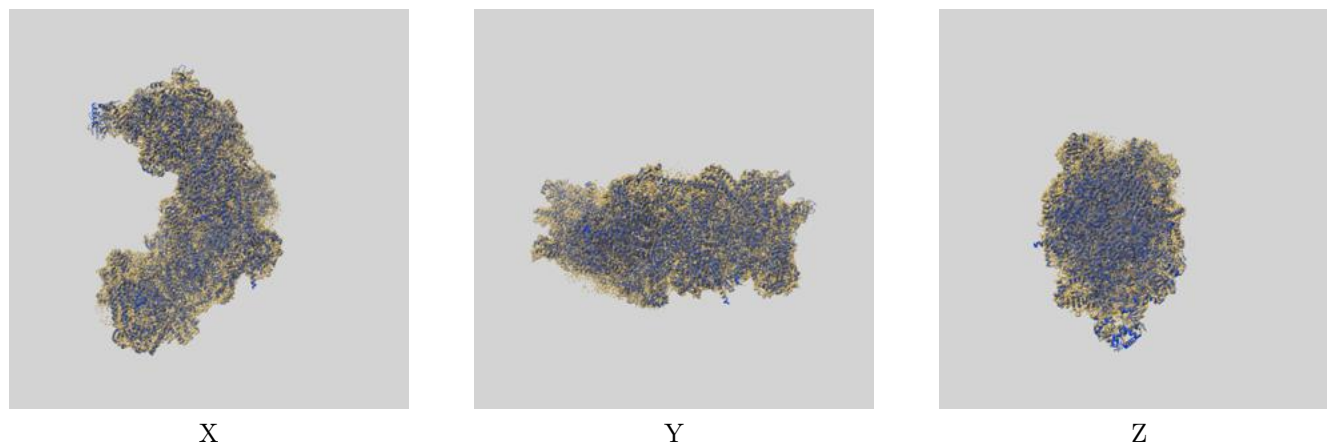
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.87	-	-
Author-provided FSC curve	2.87	3.27	2.91
Unmasked-calculated*	3.69	6.04	3.77

*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 3.69 differs from the reported value 2.87 by more than 10 %

9 Map-model fit [i](#)

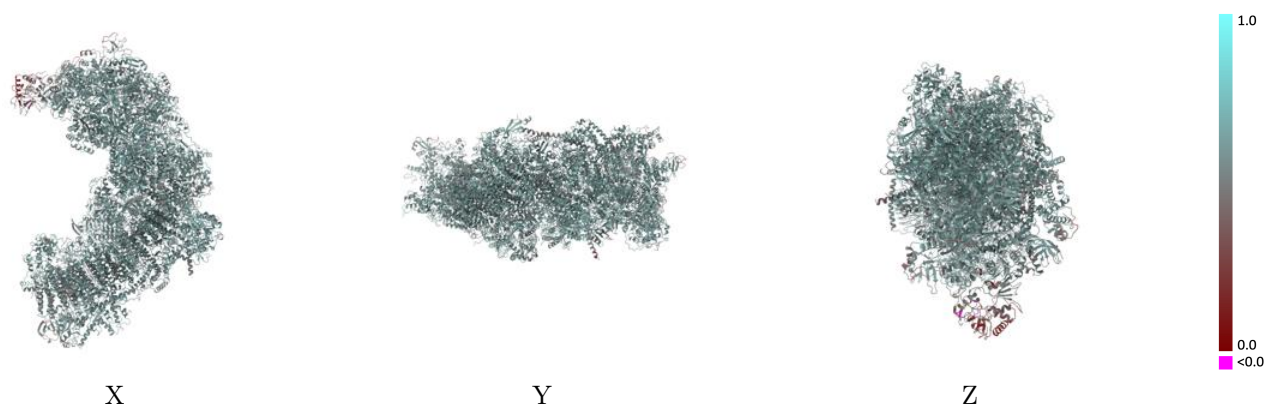
This section contains information regarding the fit between EMDB map EMD-36108 and PDB model 8J9I. Per-residue inclusion information can be found in section [3](#) on page [23](#).

9.1 Map-model overlay [i](#)



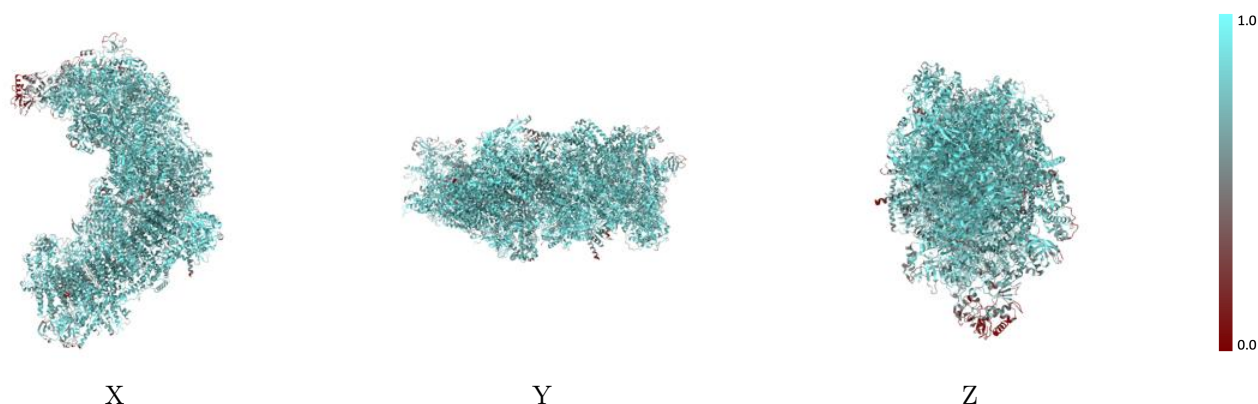
The images above show the 3D surface view of the map at the recommended contour level 4.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



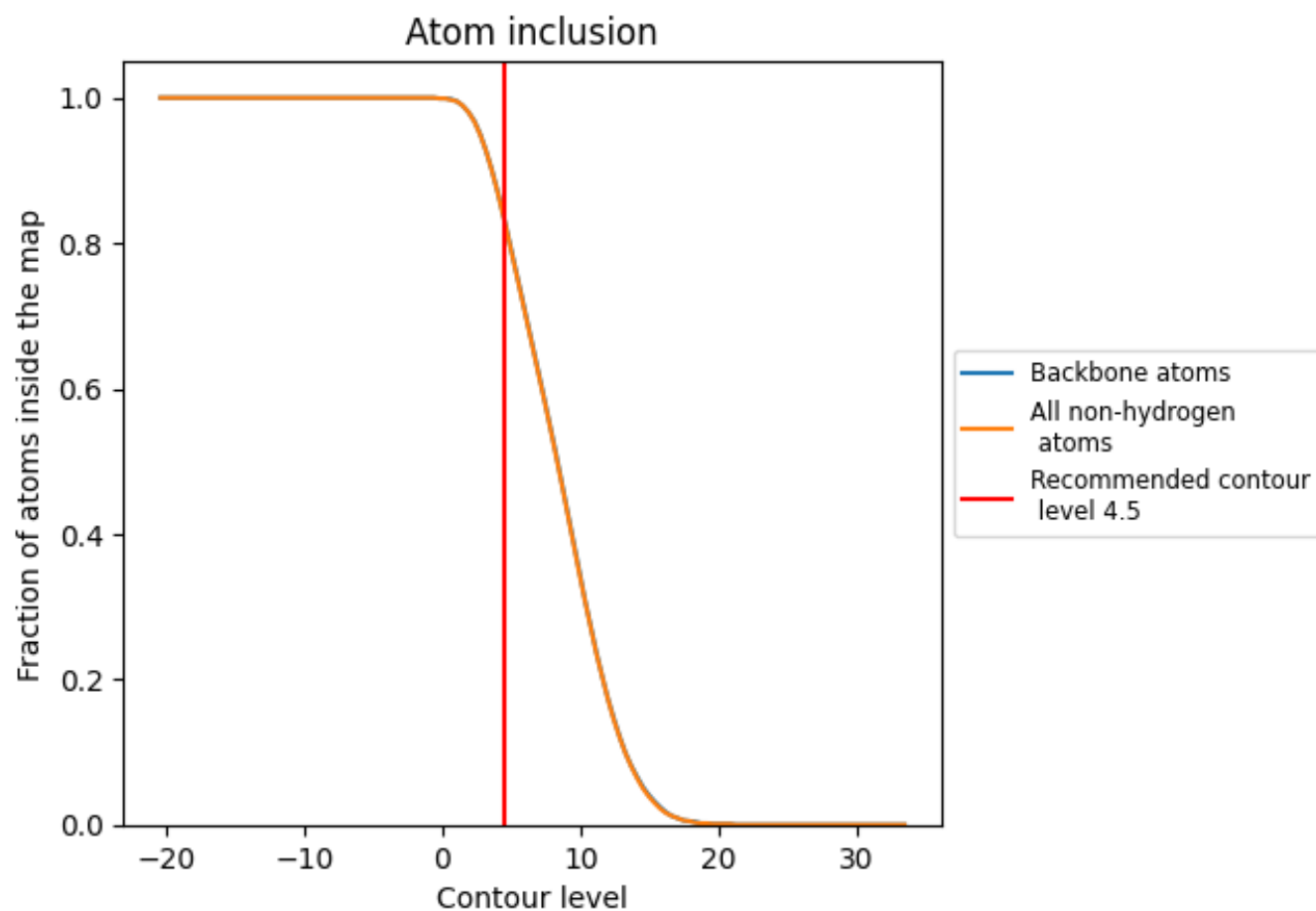
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (4.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 83% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (4.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8320	 0.5840
1A	 0.8850	 0.6050
1B	 0.8780	 0.6010
2B	 0.8970	 0.6010
4L	 0.8940	 0.6050
A1	 0.8480	 0.5840
A2	 0.8250	 0.5930
A3	 0.8540	 0.5910
A5	 0.8090	 0.5780
A6	 0.7810	 0.5720
A7	 0.8870	 0.6100
A8	 0.8570	 0.5850
A9	 0.8550	 0.5980
AB	 0.7880	 0.5790
AC	 0.8040	 0.5790
AL	 0.8630	 0.5990
AM	 0.8100	 0.5780
AN	 0.8380	 0.5800
B2	 0.8460	 0.5920
B3	 0.8530	 0.5760
B4	 0.8550	 0.5800
B5	 0.8360	 0.5770
B6	 0.8610	 0.5910
B7	 0.8300	 0.5830
B8	 0.8910	 0.6040
B9	 0.8590	 0.5990
BL	 0.8520	 0.5900
BM	 0.8460	 0.5910
C4	 0.8310	 0.5730
E1	 0.7900	 0.5690
E2	 0.7420	 0.5540
E3	 0.7540	 0.5640
E4	 0.8450	 0.5930
E5	 0.3800	 0.3750
E6	 0.7900	 0.5690



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Chain	Atom inclusion	Q-score
E7	 0.6840	 0.5290
E8	 0.7620	 0.5640
EA	 0.8770	 0.5980
EB	 0.8160	 0.5790
EC	 0.7800	 0.5610
ED	 0.7820	 0.5670
FX	 0.8710	 0.5990
G1	 0.8610	 0.6000
G2	 0.8310	 0.5840
G3	 0.8310	 0.5890
N1	 0.8780	 0.5960
N2	 0.8980	 0.6030
N3	 0.8840	 0.6000
N4	 0.8800	 0.5940
N5	 0.8580	 0.5880
N6	 0.8590	 0.5890
S2	 0.9040	 0.6120
S3	 0.8900	 0.6100
S4	 0.8630	 0.6040
S5	 0.8350	 0.5820
S6	 0.8910	 0.6100
S7	 0.9390	 0.6140
S8	 0.9200	 0.6160
U1	 0.9000	 0.5850
U2	 0.8000	 0.5230
V1	 0.8420	 0.5900
V2	 0.8580	 0.5890