



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 05:39 AM UTC

PDB ID : 6Y79 / pdb_00006y79
EMDB ID : EMD-10711
Title : Cryo-EM structure of a respiratory complex I F89A mutant
Authors : Parey, K.
Deposited on : 2020-02-28
Resolution : 2.96 Å(reported)
Based on initial model : 6RFR

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

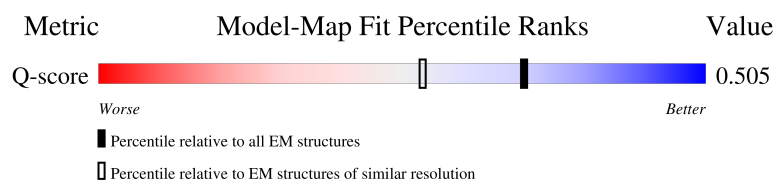
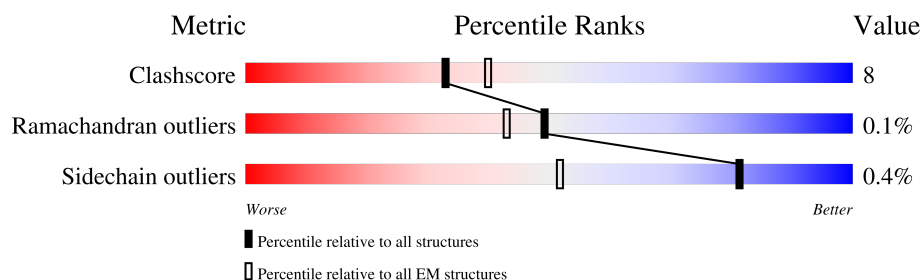
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

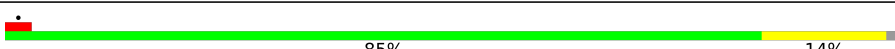
The reported resolution of this entry is 2.96 Å.

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	13155 (2.46 - 3.46)

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

Mol	Chain	Length	Quality of chain
1	A	728	
2	B	488	
3	C	466	
4	D	87	

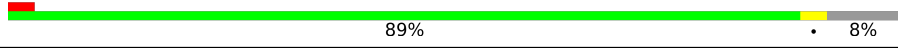
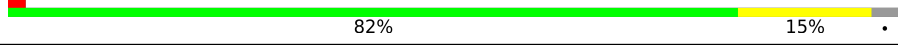
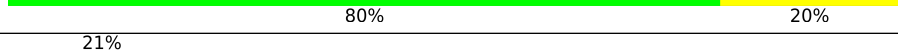
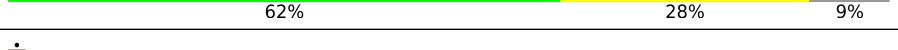
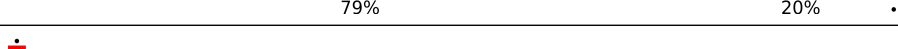
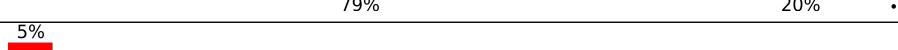
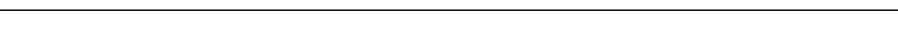
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	E	375	
6	F	144	
7	G	281	
8	H	243	
9	I	229	
10	J	198	
11	K	210	
12	L	89	
13	M	136	
14	O	109	
15	P	124	
16	Q	132	
17	R	109	
18	S	249	
19	U	172	
20	W	123	
21	X	169	
22	Y	161	
23	Z	182	
24	a	149	
25	b	74	
26	c	60	
27	d	92	
28	e	67	
29	f	87	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
30	g	78	
31	h	138	
32	i	90	
33	j	93	
34	n	120	
35	1	341	
36	2	469	
37	3	128	
38	4	486	
39	5	655	
40	6	185	
41	8	99	
42	9	89	

2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 65173 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Subunit NUAM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	692	Total	C	N	O	S	0	0
			5258	3263	926	1040	29		

- Molecule 2 is a protein called Subunit NUBM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	456	Total	C	N	O	S	0	0
			3528	2229	621	654	24		

- Molecule 3 is a protein called Subunit NUCM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	433	Total	C	N	O	S	0	0
			3426	2177	586	641	22		

- Molecule 4 is a protein called Subunit NIMM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	86	Total	C	N	O	S	0	0
			681	432	127	119	3		

- Molecule 5 is a protein called Subunit NUEM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	317	Total	C	N	O	S	0	0
			2527	1606	435	478	8		

- Molecule 6 is a protein called Subunit NUFM of NADH:Ubiquinone Oxidoreductase (Com-

plex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	121	Total	C	N	O	S	0	0
			990	629	166	193	2		

- Molecule 7 is a protein called Subunit NUGM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	239	Total	C	N	O	S	0	0
			1978	1272	336	366	4		

- Molecule 8 is a protein called Subunit NUHM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	216	Total	C	N	O	S	0	0
			1688	1060	284	326	18		

- Molecule 9 is a protein called Subunit NUIM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	190	Total	C	N	O	S	0	0
			1519	966	254	289	10		

- Molecule 10 is a protein called Subunit NUJM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	179	Total	C	N	O	S	0	0
			1329	844	241	239	5		

- Molecule 11 is a protein called Subunit NUKM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	175	Total	C	N	O	S	0	0
			1377	874	241	247	15		

- Molecule 12 is a protein called Subunit NULM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	89	Total	C	N	O	S	0	0
			691	464	109	115	3		

- Molecule 13 is a protein called Subunit NUMM of protein NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	117	Total	C	N	O	S	0	0
			912	568	163	176	5		

- Molecule 14 is a protein called Acyl carrier protein ACPM1 of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms				AltConf	Trace
14	O	77	Total	C	N	O	0	0
			591	373	93	125		

- Molecule 15 is a protein called Subunit NB4M of protein NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	123	Total	C	N	O	S	0	0
			1030	661	182	185	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	89	ALA	PHE	conflict	UNP A0A1D8N3C8

- Molecule 16 is a protein called Acyl carrier protein ACPM2 of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	85	Total	C	N	O	S	0	0
			648	405	103	138	2		

- Molecule 17 is a protein called Subunit NI2M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	106	Total	C	N	O	S	0	0
			884	562	168	151	3		

- Molecule 18 is a protein called Subunit NESM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	174	Total	C	N	O	S	0	0
			1430	920	245	263	2		

- Molecule 19 is a protein called Subunit NUPM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	171	Total	C	N	O	S	0	0
			1345	847	236	252	10		

- Molecule 20 is a protein called Subunit NB6M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
20	W	121	Total	C	N	O	S	0	0
			974	623	178	168	5		

- Molecule 21 is a protein called Subunit NUXM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
21	X	167	Total	C	N	O	S	0	0
			1296	839	221	232	4		

- Molecule 22 is a protein called Subunit NUYM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Y	123	Total	C	N	O	S	0	0
			1021	651	187	181	2		

- Molecule 23 is a protein called Subunit NUZM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Z	181	Total	C	N	O	S	0	0
			1389	893	240	255	1		

- Molecule 24 is a protein called Subunit NIAM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
24	a	124	Total	C	N	O	S	0	0
			1030	669	165	194	2		

- Molecule 25 is a protein called Subunit NEBM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
25	b	64	Total	C	N	O	S	0	0
			490	326	83	81			

- Molecule 26 is a protein called Subunit NB2M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
26	c	44	Total	C	N	O	S	0	0
			353	229	67	57			

- Molecule 27 is a protein called Subunit NIDM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
27	d	90	Total	C	N	O	S	0	0
			760	472	137	148	3		

- Molecule 28 is a protein called Subunit NUVM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
28	e	52	Total	C	N	O	S	0	0
			436	293	75	65	3		

- Molecule 29 is a protein called Subunit NI8M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
29	f	80	Total	C	N	O	S	0	0
			629	394	119	115	1		

- Molecule 30 is a protein called Subunit NI9M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms				AltConf	Trace
30	g	76	Total	C	N	O	0	0
			617	405	112	100		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
g	71	GLY	GLN	conflict	UNP A0A1D8NJR0

- Molecule 31 is a protein called Subunit N7BM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
31	h	136	Total	C	N	O	S	0	0
			1130	727	193	208	2		

- Molecule 32 is a protein called Subunit NUUM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
32	i	83	Total	C	N	O	S	0	0
			646	413	117	115	1		

- Molecule 33 is a protein called Subunit NB5M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms				AltConf	Trace
33	j	90	Total	C	N	O	0	0
			724	465	132	127		

- Molecule 34 is a protein called Subunit NUNM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
34	n	114	Total	C	N	O	S	0	0
			914	588	156	169	1		

- Molecule 35 is a protein called Subunit NU1M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
35	1	329	Total	C	N	O	S	0	0
			2627	1793	382	445	7		

- Molecule 36 is a protein called Subunit NU2M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
36	2	469	Total	C	N	O	S	0	0
			3774	2557	550	655	12		

- Molecule 37 is a protein called Subunit NU3M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
37	3	116	Total	C	N	O	S	0	0
			933	641	137	153	2		

- Molecule 38 is a protein called Subunit NU4M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
38	4	485	Total	C	N	O	S	0	0
			3847	2595	585	653	14		

- Molecule 39 is a protein called Subunit NU5M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
39	5	654	Total	C	N	O	S	0	0
			5197	3479	785	905	28		

- Molecule 40 is a protein called Subunit NU6M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
40	6	180	Total	C	N	O	S	0	0
			1415	959	204	245	7		

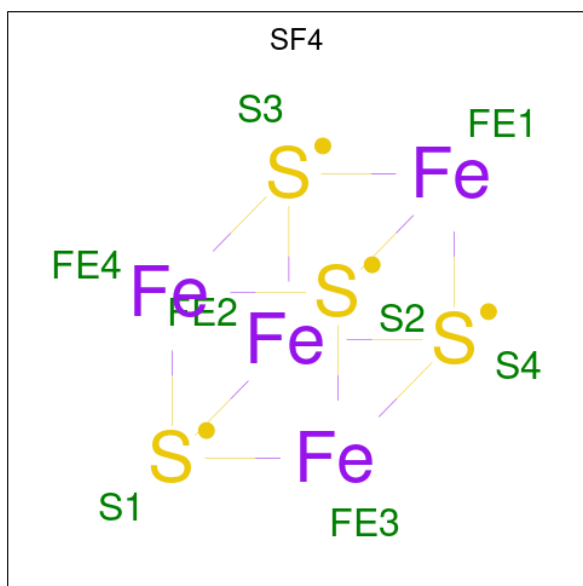
- Molecule 41 is a protein called Subunit NB8M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
41	8	77	Total	C	N	O	S	0	0
			643	408	116	111	8		

- Molecule 42 is a protein called Subunit NIPM of NADH:Ubiquinone Oxidoreductase (Complex I).

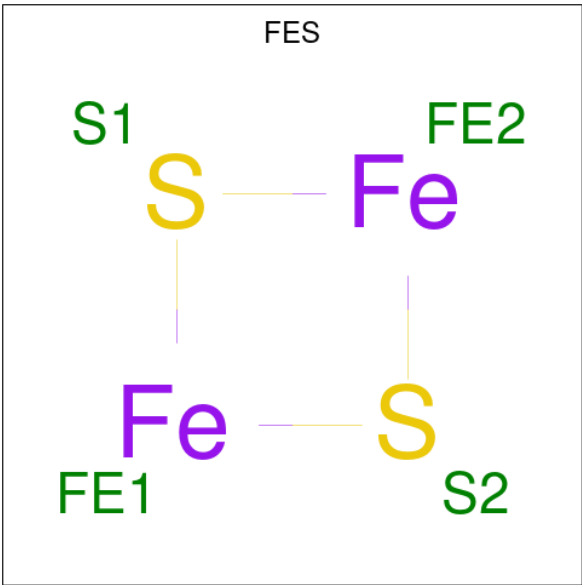
Mol	Chain	Residues	Atoms					AltConf	Trace
42	9	86	Total	C	N	O	S	0	0
			672	422	122	122	6		

- Molecule 43 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



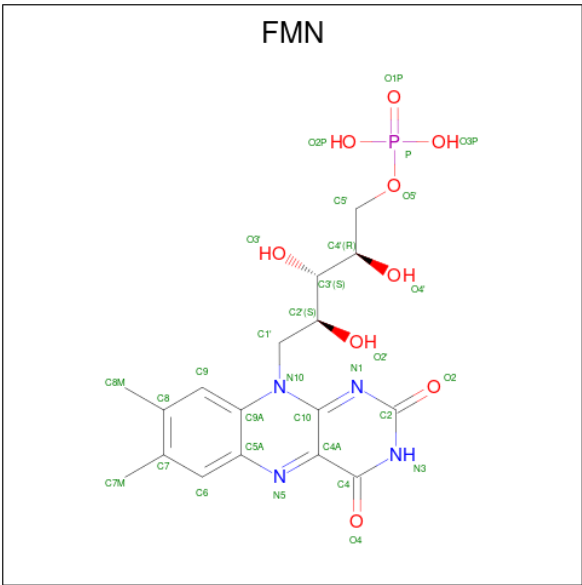
Mol	Chain	Residues	Atoms			AltConf
43	A	1	Total	Fe	S	0
			8	4	4	
43	A	1	Total	Fe	S	0
			8	4	4	
43	B	1	Total	Fe	S	0
			8	4	4	
43	I	1	Total	Fe	S	0
			8	4	4	
43	I	1	Total	Fe	S	0
			8	4	4	
43	K	1	Total	Fe	S	0
			8	4	4	

- Molecule 44 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			AltConf
44	A	1	Total	Fe	S	0
			4	2	2	
44	H	1	Total	Fe	S	0
			4	2	2	

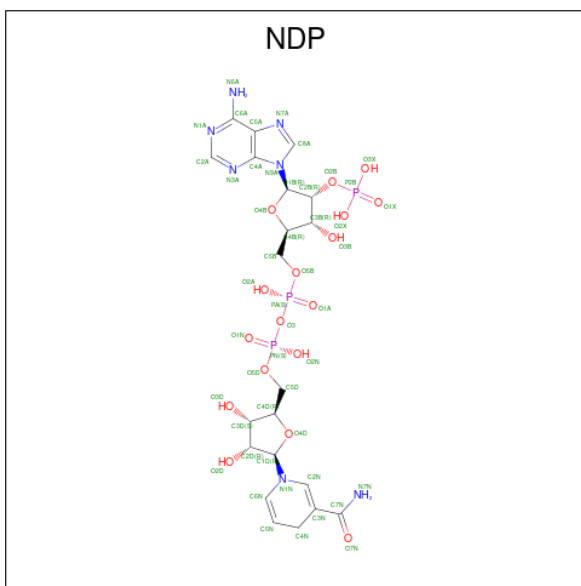
- Molecule 45 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



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

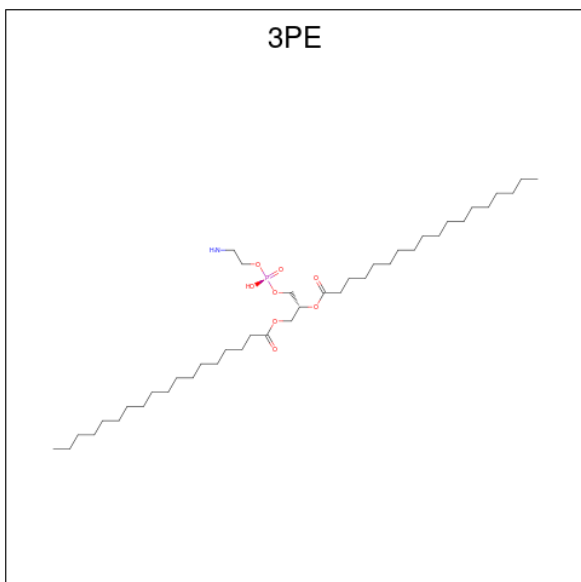
- Molecule 46 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE

PHOSPHATE (CCD ID: NDP) (formula: $\text{C}_{21}\text{H}_{30}\text{N}_7\text{O}_{17}\text{P}_3$).



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

- Molecule 47 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



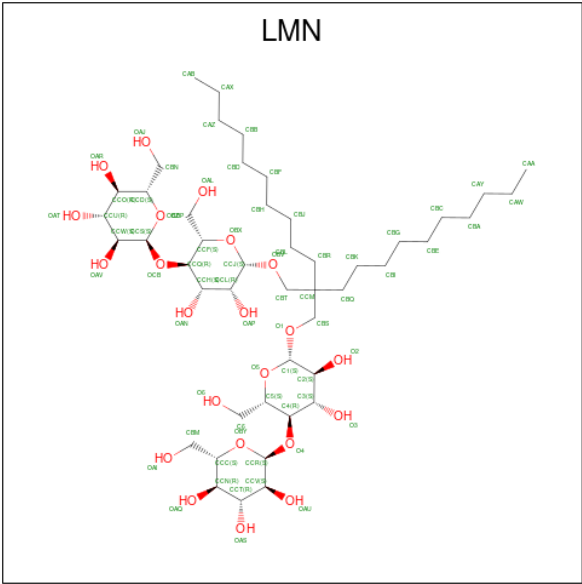
Mol	Chain	Residues	Atoms					AltConf
47	I	1	Total 51	C 41	N 1	O 8	P 1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
47	J	1	Total	C	N	O	P	0
			41	31	1	8	1	
47	J	1	Total	C	N	O	P	0
			44	34	1	8	1	
47	S	1	Total	C	N	O	P	0
			42	32	1	8	1	
47	a	1	Total	C	N	O	P	0
			51	41	1	8	1	
47	b	1	Total	C	N	O	P	0
			42	32	1	8	1	
47	i	1	Total	C	N	O	P	0
			42	32	1	8	1	
47	3	1	Total	C	N	O	P	0
			43	33	1	8	1	
47	4	1	Total	C	N	O	P	0
			43	33	1	8	1	
47	4	1	Total	C	N	O	P	0
			42	32	1	8	1	
47	4	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 48 is Lauryl Maltose Neopentyl Glycol (CCD ID: LMN) (formula: C₄₇H₈₈O₂₂).



Mol	Chain	Residues	Atoms			AltConf
48	J	1	Total	C	O	0
			69	47	22	

Continued on next page...

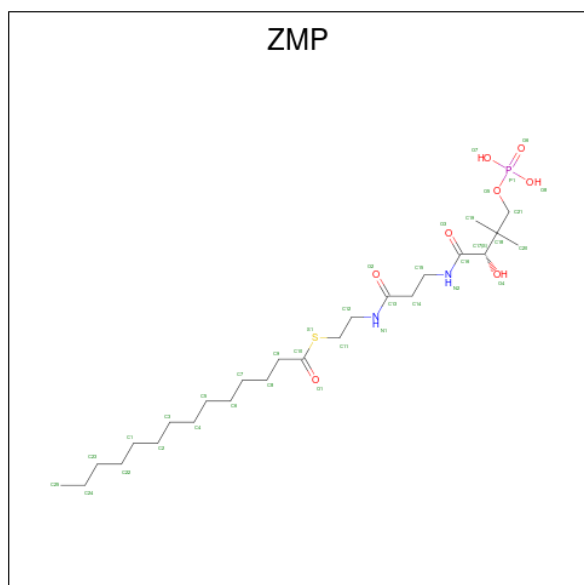
Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
48	J	1	Total	C	O	0
			65	43	22	
48	j	1	Total	C	O	0
			69	47	22	

- Molecule 49 is ZINC ION (CCD ID: ZN) (formula: Zn).

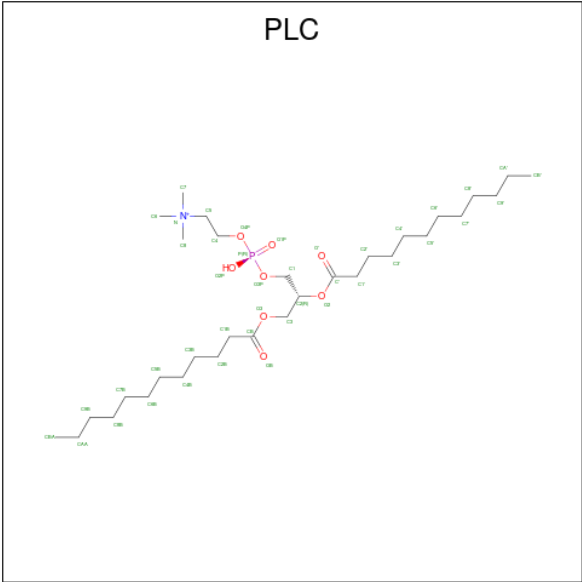
Mol	Chain	Residues	Atoms		AltConf
49	M	1	Total	Zn	0
			1	1	

- Molecule 50 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (CCD ID: ZMP) (formula: C₂₅H₄₉N₂O₈PS).



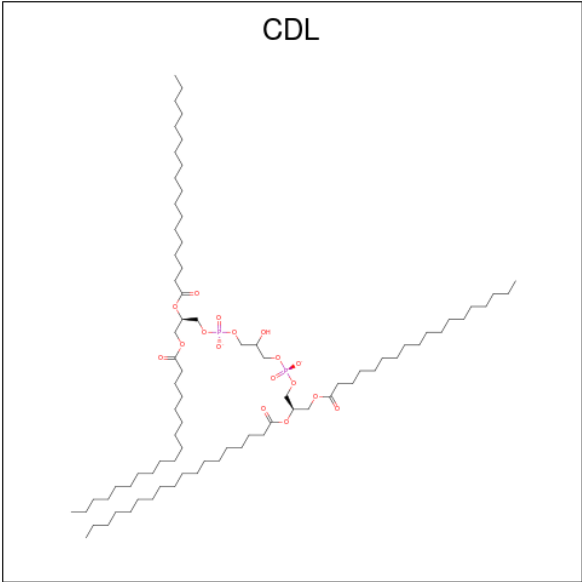
Mol	Chain	Residues	Atoms						AltConf
50	O	1	Total	C	N	O	P	S	0
			33	22	2	7	1	1	
50	Q	1	Total	C	N	O	P	S	0
			33	22	2	7	1	1	

- Molecule 51 is DIUNDECYL PHOSPHATIDYL CHOLINE (CCD ID: PLC) (formula: C₃₂H₆₅NO₈P).



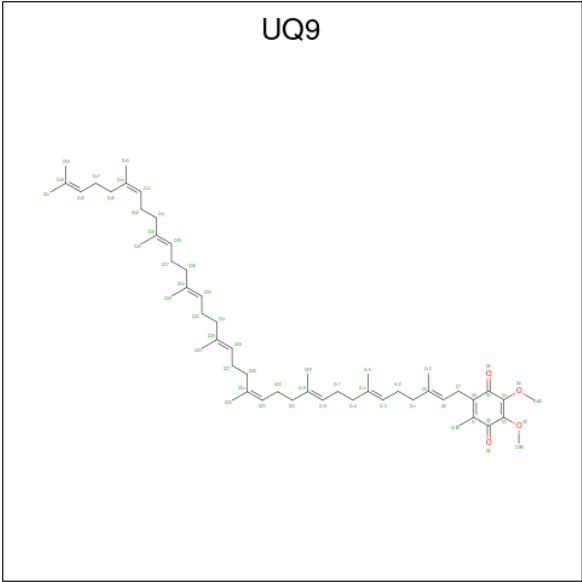
Mol	Chain	Residues	Atoms					AltConf
51	W	1	Total	C	N	O	P	0
			41	31	1	8	1	
51	W	1	Total	C	N	O	P	0
			42	32	1	8	1	
51	1	1	Total	C	N	O	P	0
			42	32	1	8	1	
51	1	1	Total	C	N	O	P	0
			35	25	1	8	1	
51	5	1	Total	C	N	O	P	0
			42	32	1	8	1	
51	5	1	Total	C	N	O	P	0
			31	21	1	8	1	

- Molecule 52 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



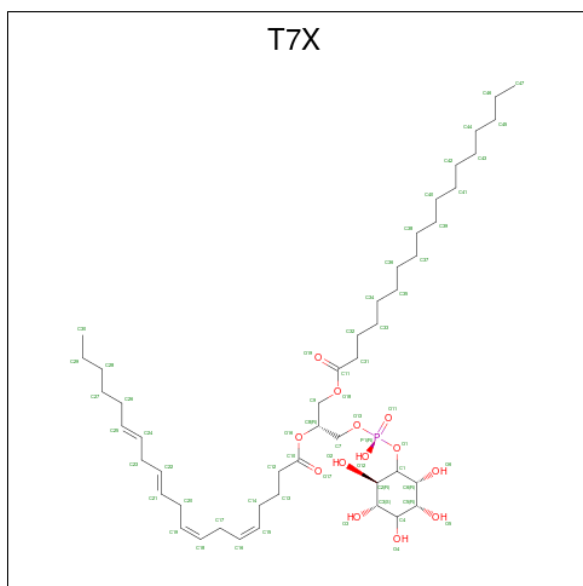
Mol	Chain	Residues	Atoms				AltConf
52	X	1	Total	C	O	P	0
			86	67	17	2	
52	Z	1	Total	C	O	P	0
			76	57	17	2	
52	2	1	Total	C	O	P	0
			83	64	17	2	
52	4	1	Total	C	O	P	0
			92	73	17	2	
52	5	1	Total	C	O	P	0
			78	59	17	2	

- Molecule 53 is Ubiquinone-9 (CCD ID: UQ9) (formula: C₅₄H₈₂O₄).



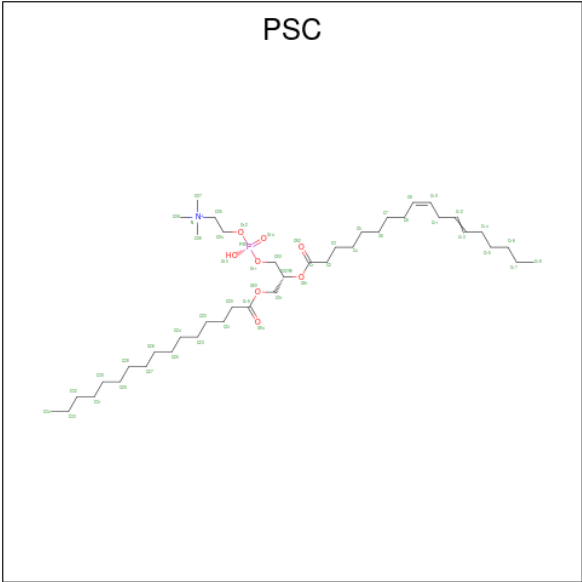
Mol	Chain	Residues	Atoms			AltConf
53	1	1	Total	C	O	0
			35	31	4	

- Molecule 54 is Phosphatidylinositol (CCD ID: T7X) (formula: $C_{47}H_{83}O_{13}P$).



Mol	Chain	Residues	Atoms				AltConf
54	2	1	Total	C	O	P	0
			48	34	13	1	
54	2	1	Total	C	O	P	0
			52	38	13	1	
54	3	1	Total	C	O	P	0
			49	35	13	1	
54	4	1	Total	C	O	P	0
			43	29	13	1	

- Molecule 55 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (CCD ID: PSC) (formula: $C_{42}H_{81}NO_8P$).

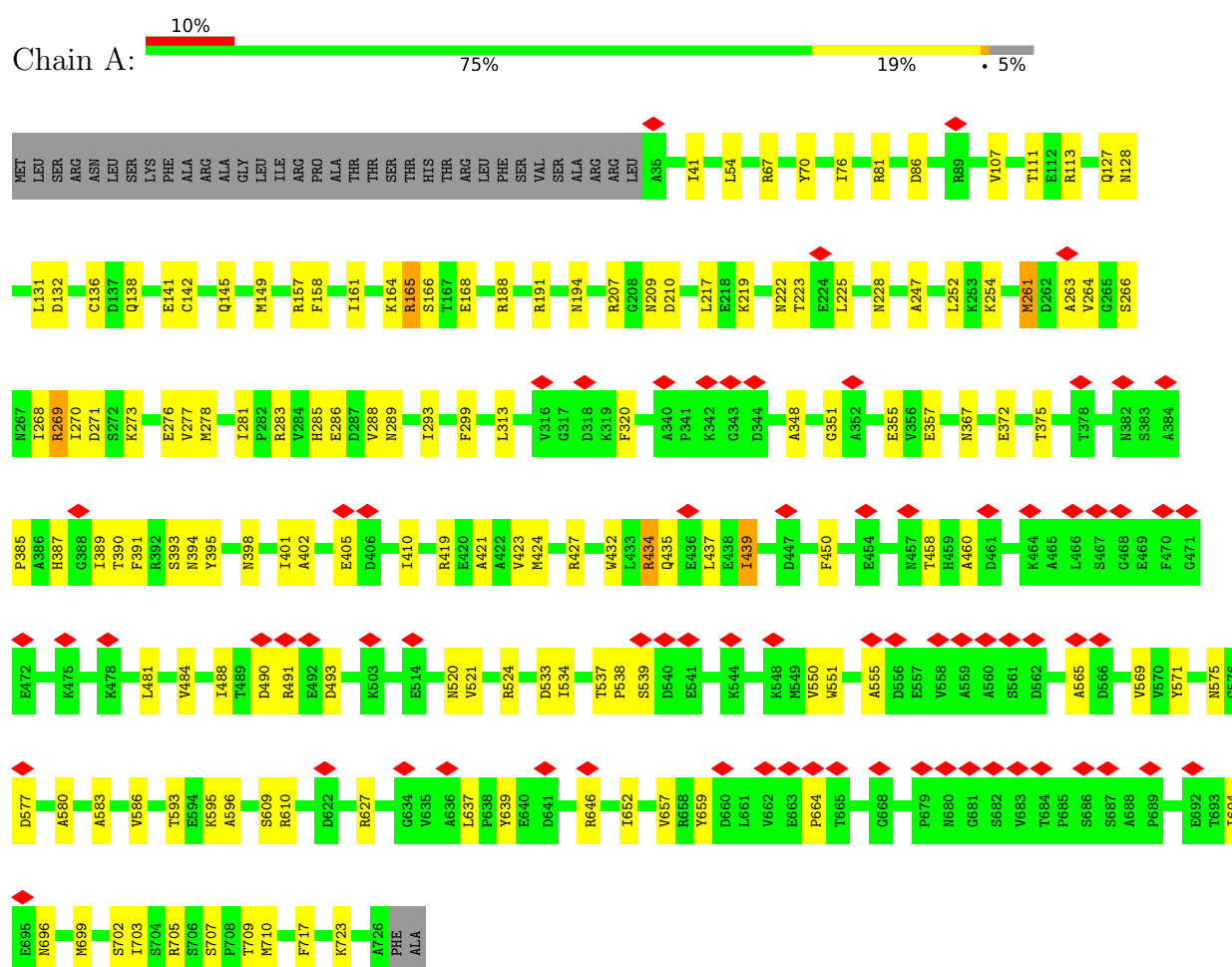


Mol	Chain	Residues	Atoms					AltConf
55	2	1	Total	C	N	O	P	0
			52	42	1	8	1	

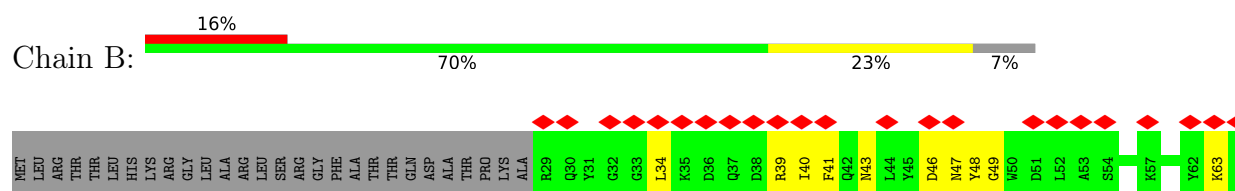
3 Residue-property plots

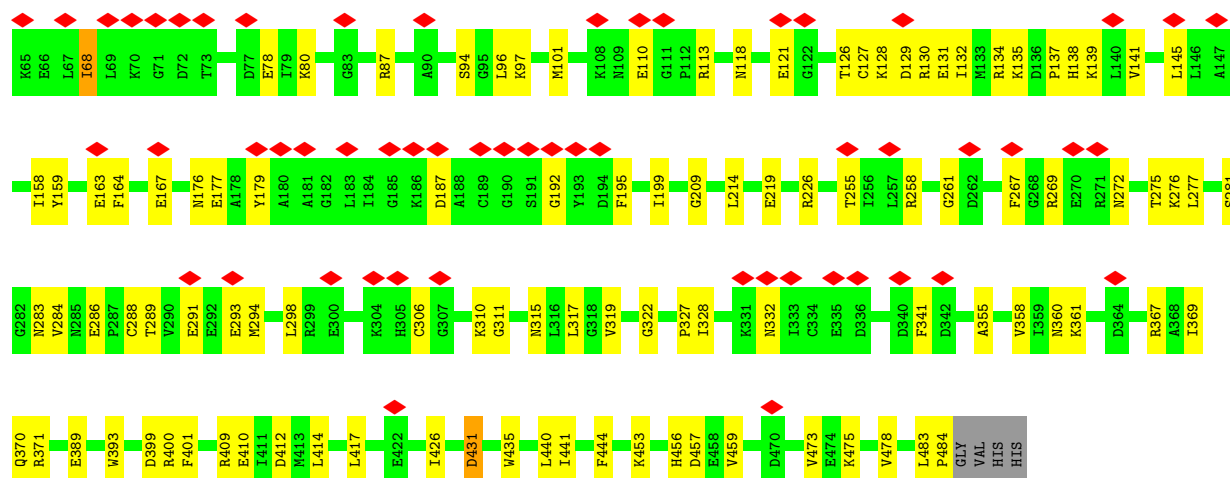
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Subunit NUAM of NADH:Ubiquinone Oxidoreductase (Complex I)



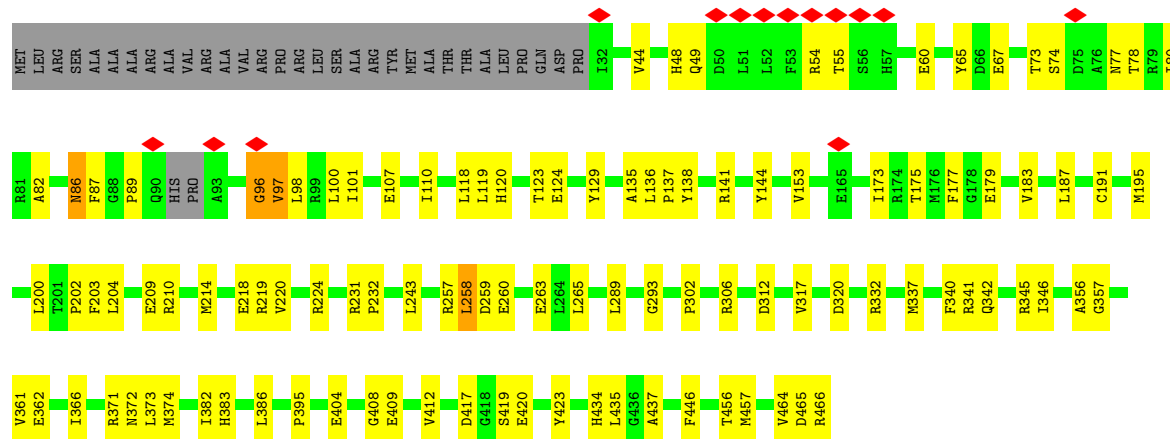
- Molecule 2: Subunit NUBM of NADH:Ubiquinone Oxidoreductase (Complex I)





• Molecule 3: Subunit NUCM of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain C: 70% 23% 7%



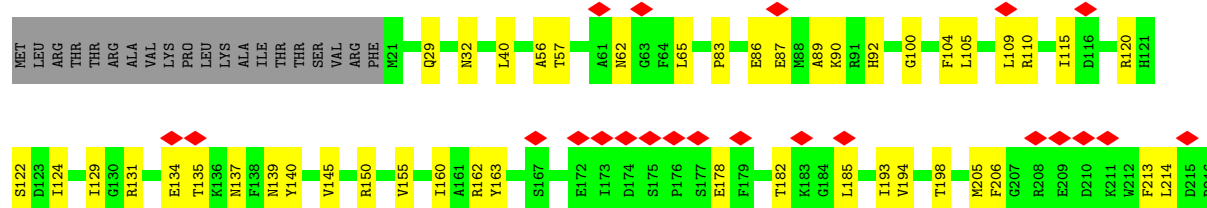
• Molecule 4: Subunit NIMM of NADH:Ubiquinone Oxidoreductase (Complex I)

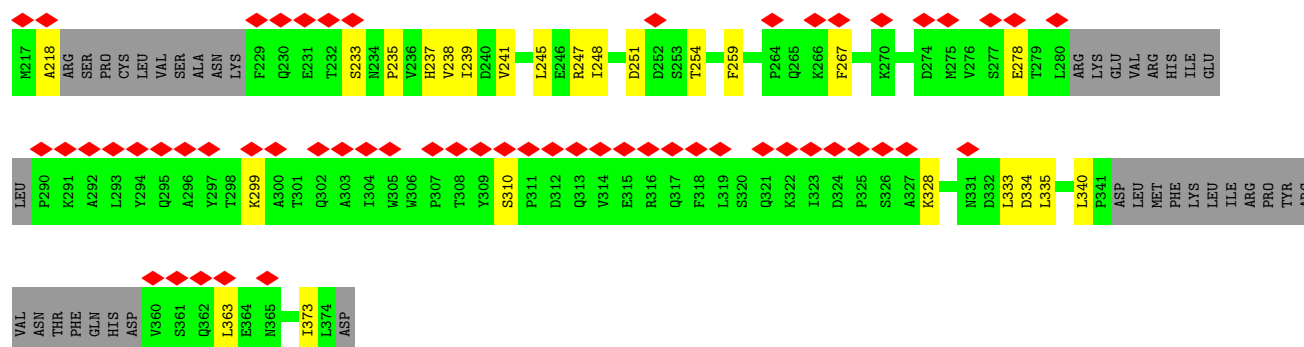
Chain D: 85% 14%



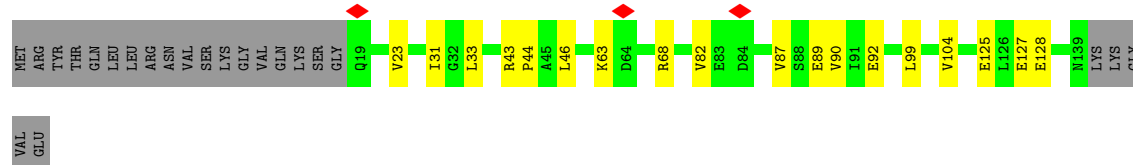
• Molecule 5: Subunit NUEM of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain E: 21% 66% 18% 15%

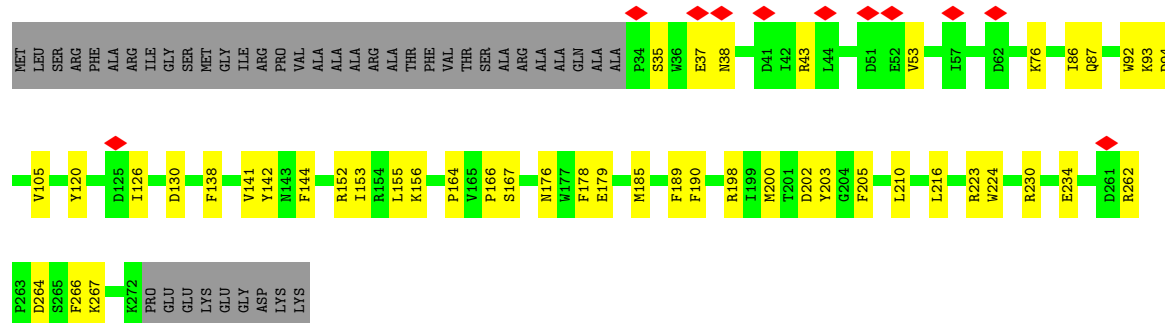




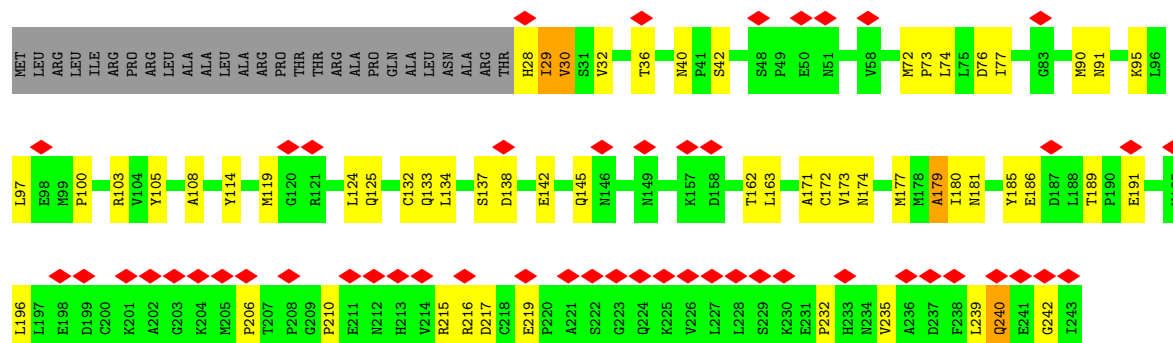
• Molecule 6: Subunit NUFM of NADH:Ubiquinone Oxidoreductase (Complex I)



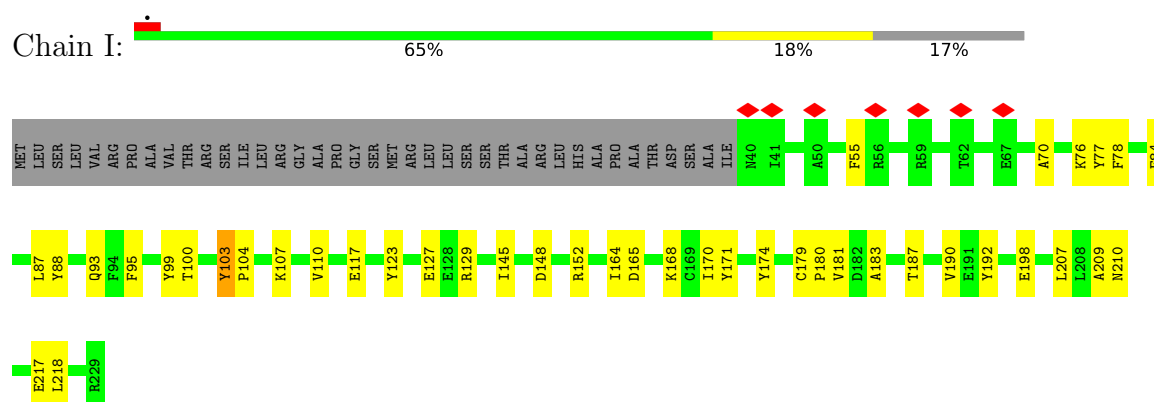
• Molecule 7: Subunit NUGM of NADH:Ubiquinone Oxidoreductase (Complex I)



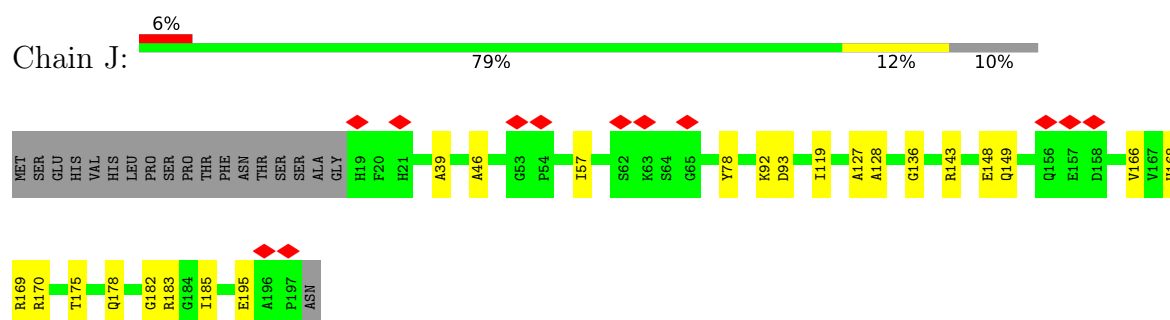
• Molecule 8: Subunit NUHM of NADH:Ubiquinone Oxidoreductase (Complex I)



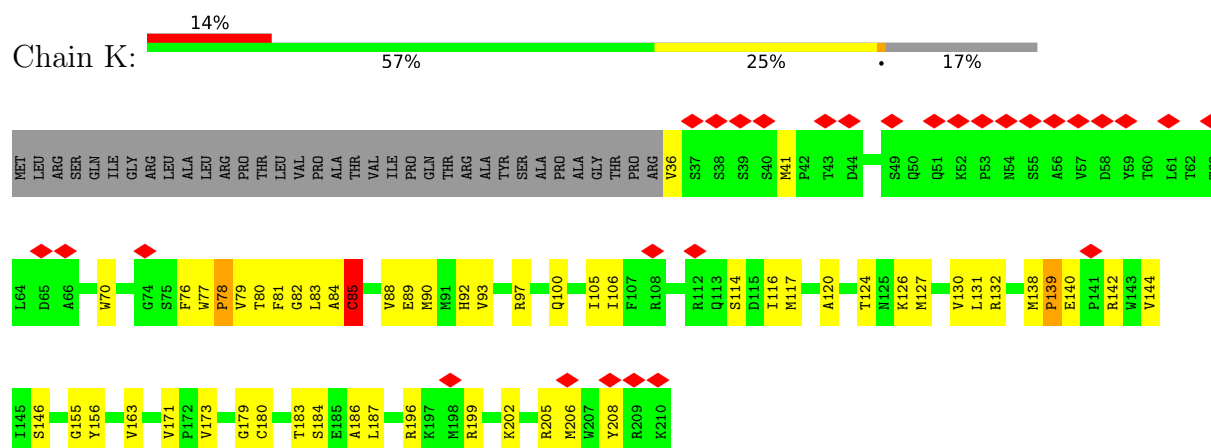
- Molecule 9: Subunit NUIM of NADH:Ubiquinone Oxidoreductase (Complex I)



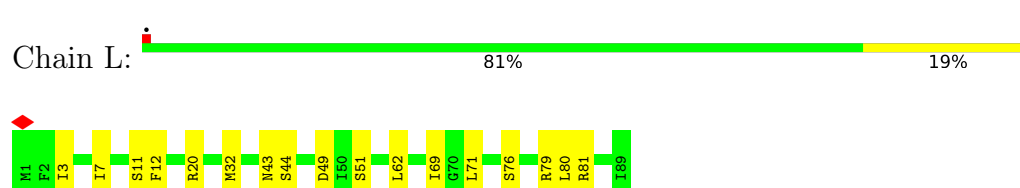
- Molecule 10: Subunit NUJM of NADH:Ubiquinone Oxidoreductase (Complex I)



- Molecule 11: Subunit NUKM of NADH:Ubiquinone Oxidoreductase (Complex I)

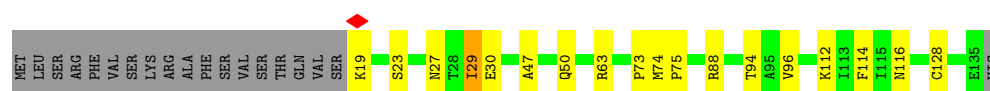


- Molecule 12: Subunit NULM of NADH:Ubiquinone Oxidoreductase (Complex I)



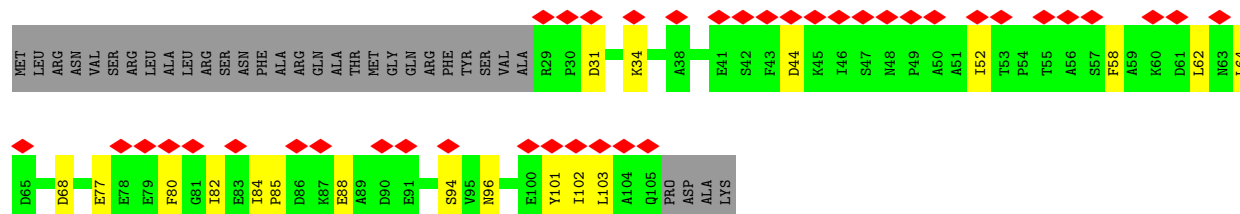
- Molecule 13: Subunit NUMM of protein NADH:Ubiquinone Oxidoreductase (Complex I)

Chain M: 



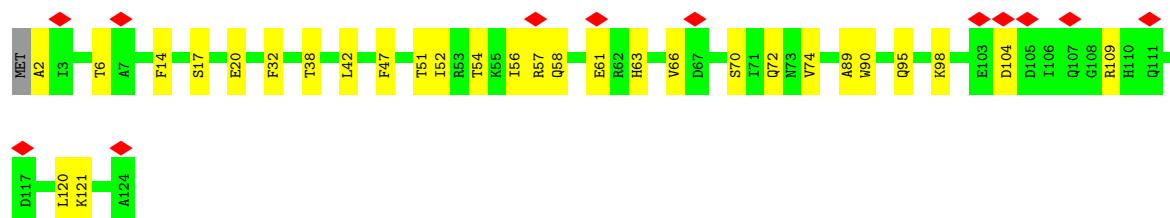
- Molecule 14: Acyl carrier protein ACPM1 of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain O: 



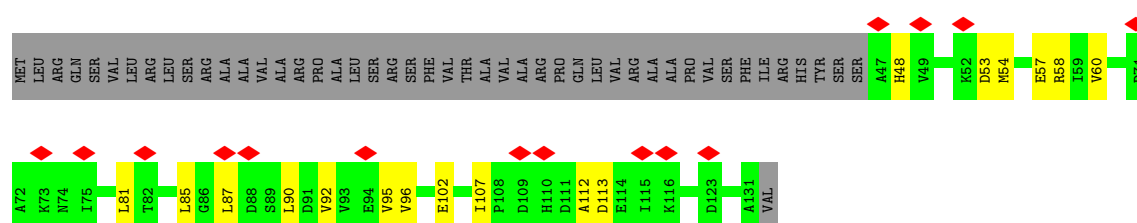
- Molecule 15: Subunit NB4M of protein NADH:Ubiquinone Oxidoreductase (Complex I)

Chain P: 



- Molecule 16: Acyl carrier protein ACPM2 of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain Q: 

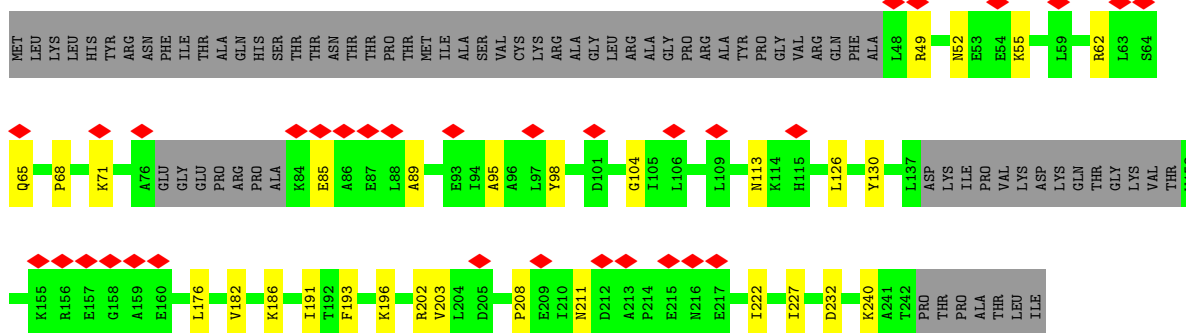


- Molecule 17: Subunit NI2M of NADH:Ubiquinone Oxidoreductase (Complex I)

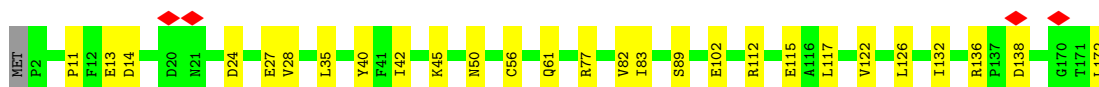
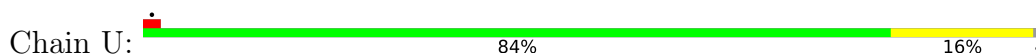
Chain R: 



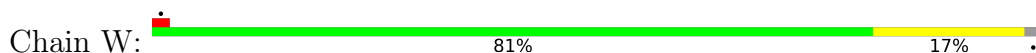
- Molecule 18: Subunit NESM of NADH:Ubiquinone Oxidoreductase (Complex I)



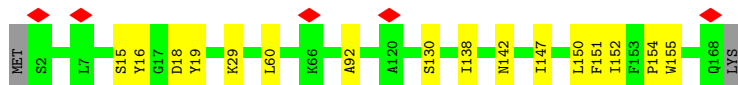
- Molecule 19: Subunit NUPM of NADH:Ubiquinone Oxidoreductase (Complex I)



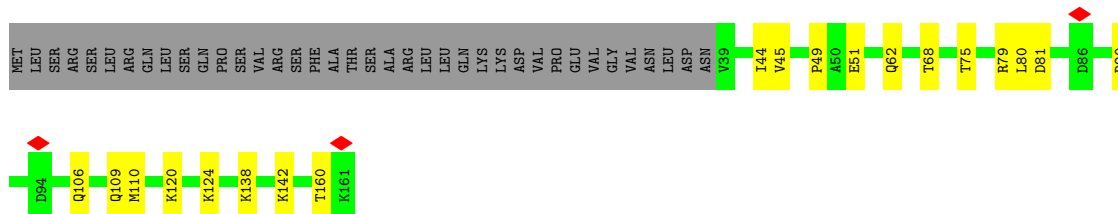
- Molecule 20: Subunit NB6M of NADH:Ubiquinone Oxidoreductase (Complex I)



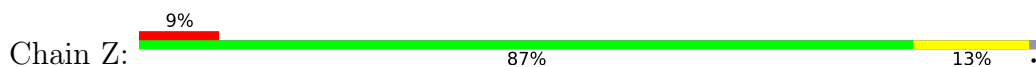
- Molecule 21: Subunit NUXM of NADH:Ubiquinone Oxidoreductase (Complex I)

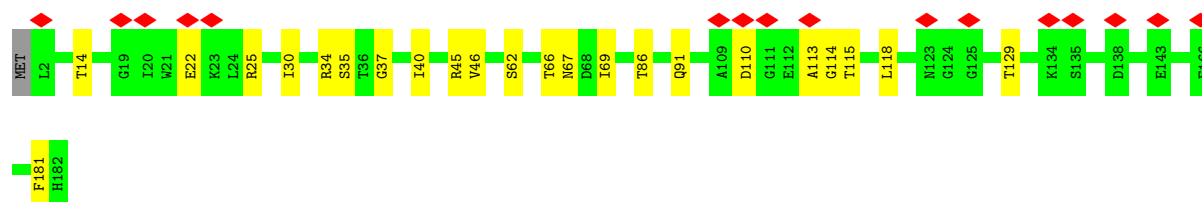


- Molecule 22: Subunit NUYM of NADH:Ubiquinone Oxidoreductase (Complex I)

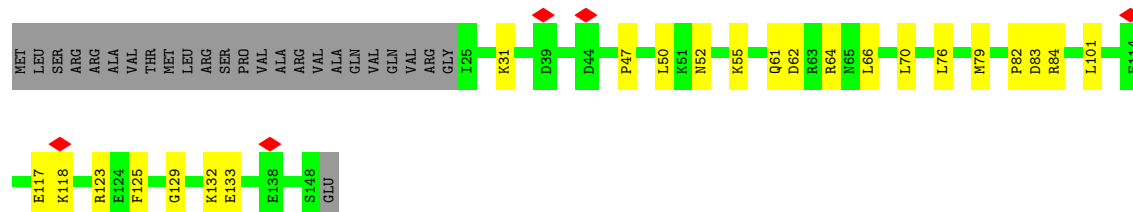


- Molecule 23: Subunit NUZM of NADH:Ubiquinone Oxidoreductase (Complex I)

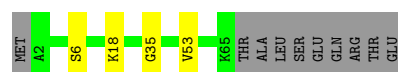
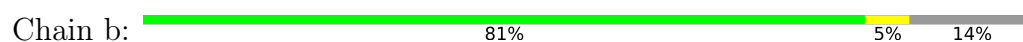




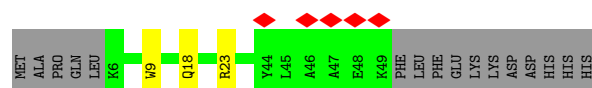
- Molecule 24: Subunit NIAM of NADH:Ubiquinone Oxidoreductase (Complex I)



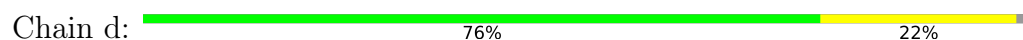
- Molecule 25: Subunit NEBM of NADH:Ubiquinone Oxidoreductase (Complex I)



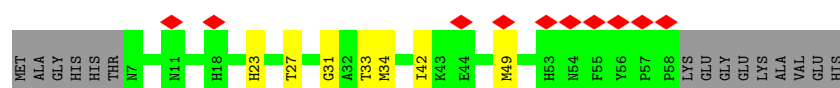
- Molecule 26: Subunit NB2M of NADH:Ubiquinone Oxidoreductase (Complex I)



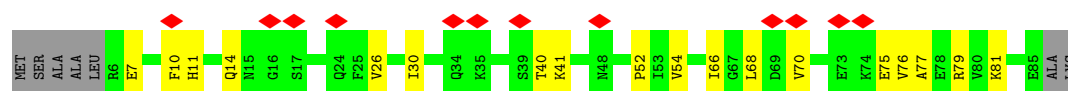
- Molecule 27: Subunit NIDM of NADH:Ubiquinone Oxidoreductase (Complex I)



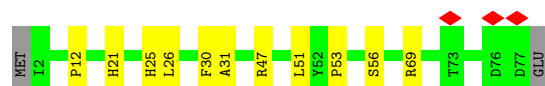
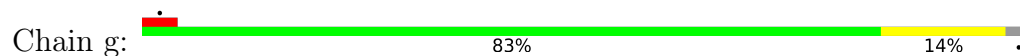
- Molecule 28: Subunit NUVN of NADH:Ubiquinone Oxidoreductase (Complex I)



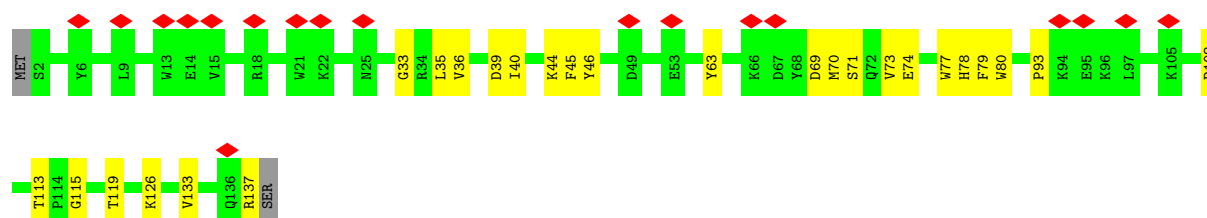
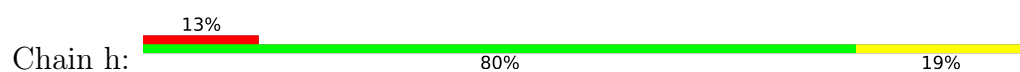
- Molecule 29: Subunit NI8M of NADH:Ubiquinone Oxidoreductase (Complex I)



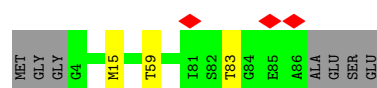
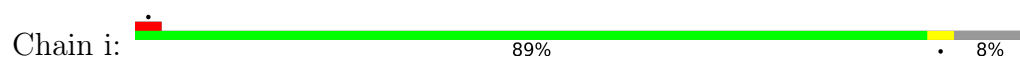
- Molecule 30: Subunit NI9M of NADH:Ubiquinone Oxidoreductase (Complex I)



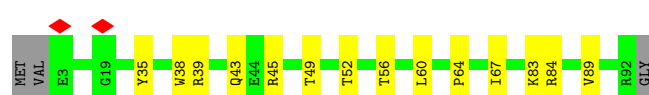
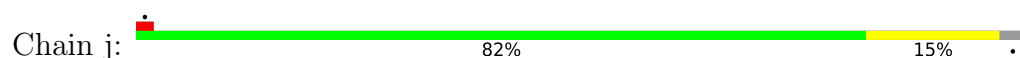
- Molecule 31: Subunit N7BM of NADH:Ubiquinone Oxidoreductase (Complex I)



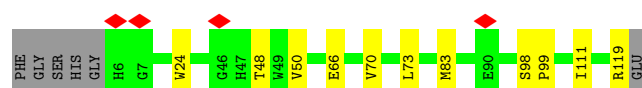
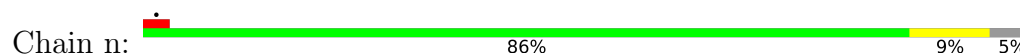
- Molecule 32: Subunit NUUM of NADH:Ubiquinone Oxidoreductase (Complex I)



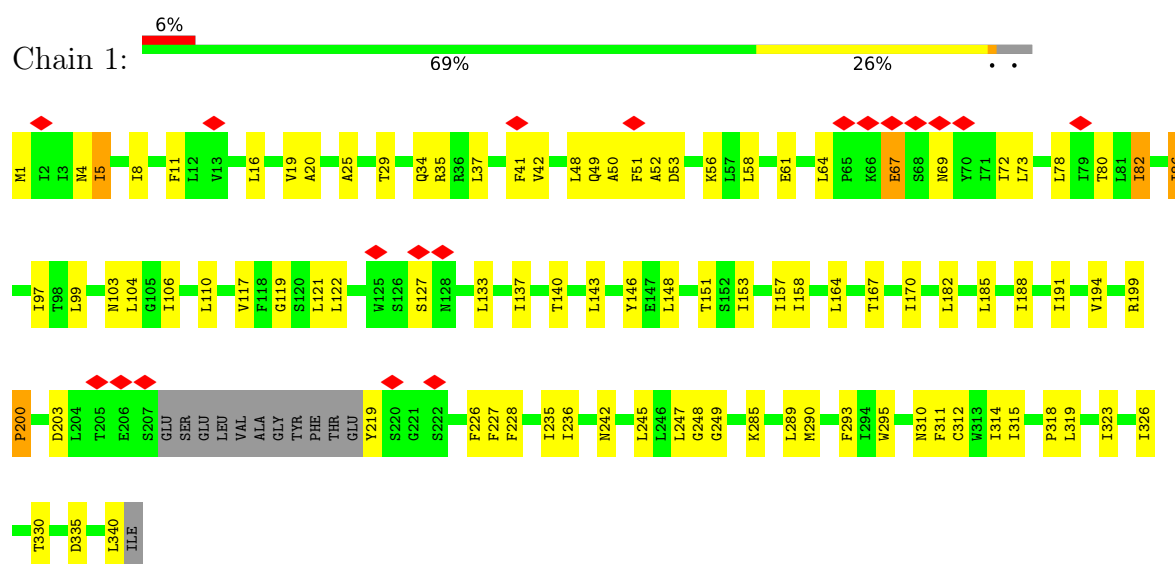
- Molecule 33: Subunit NB5M of NADH:Ubiquinone Oxidoreductase (Complex I)



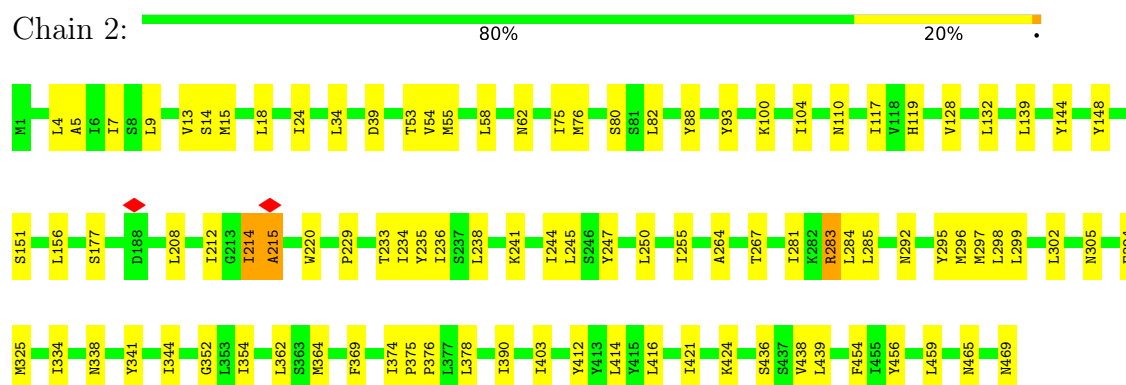
- Molecule 34: Subunit NUNM of NADH:Ubiquinone Oxidoreductase (Complex I)



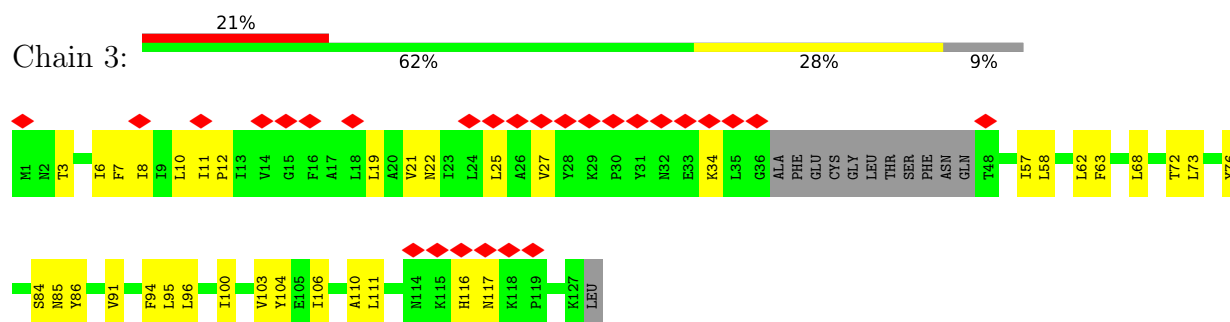
- Molecule 35: Subunit NU1M of NADH:Ubiquinone Oxidoreductase (Complex I)



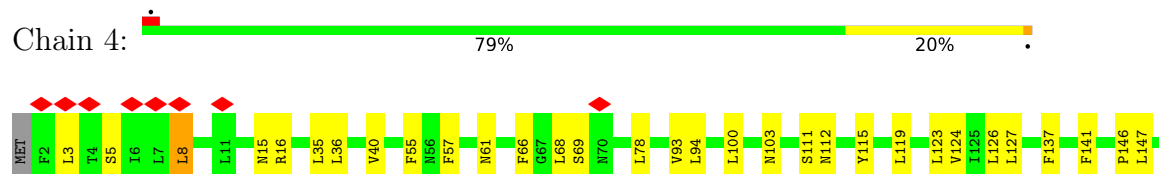
- Molecule 36: Subunit NU2M of NADH:Ubiquinone Oxidoreductase (Complex I)

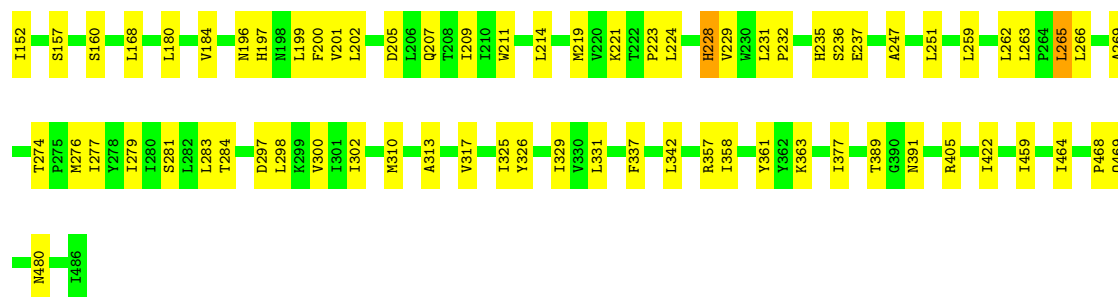


- Molecule 37: Subunit NU3M of NADH:Ubiquinone Oxidoreductase (Complex I)



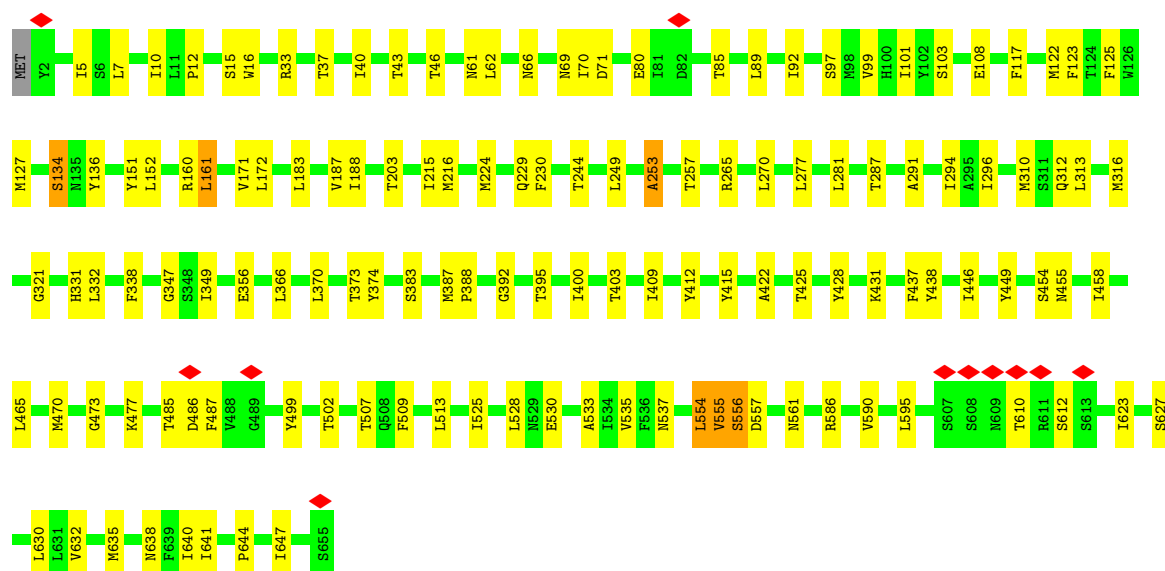
- Molecule 38: Subunit NU4M of NADH:Ubiquinone Oxidoreductase (Complex I)





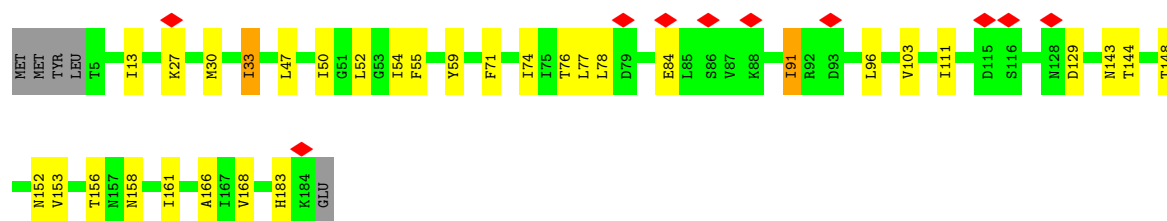
• Molecule 39: Subunit NU5M of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain 5: 79% 20%



• Molecule 40: Subunit NU6M of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain 6: 5% 80% 16%



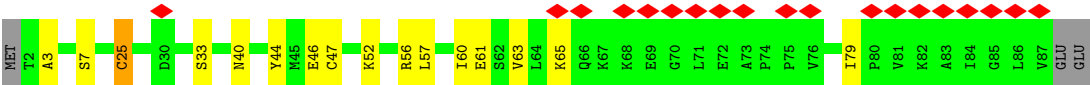
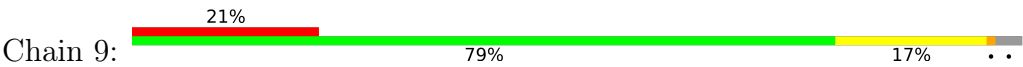
• Molecule 41: Subunit NB8M of NADH:Ubiquinone Oxidoreductase (Complex I)

Chain 8: 15% 65% 11% 22%



LYS

● Molecule 42: Subunit NIPM of NADH:Ubiquinone Oxidoreductase (Complex I)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	143203	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	51.8	Depositor
Minimum defocus (nm)	-1500	Depositor
Maximum defocus (nm)	-2500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.134	Depositor
Minimum map value	-0.070	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.013	Depositor
Map size (Å)	334.80002, 334.80002, 334.80002	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8370001, 0.8370001, 0.8370001	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PSC, 3PE, ZN, FMN, LMN, T7X, NDP, CDL, SF4, ZMP, PLC, FES, UQ9

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.35	0/5351	0.67	3/7262 (0.0%)
2	B	0.47	0/3605	0.84	1/4865 (0.0%)
3	C	0.52	1/3503 (0.0%)	0.80	2/4744 (0.0%)
4	D	0.45	0/697	0.73	0/940
5	E	0.54	0/2580	0.95	3/3493 (0.1%)
6	F	0.43	0/1011	0.81	0/1371
7	G	0.48	0/2040	0.78	1/2781 (0.0%)
8	H	0.46	0/1725	0.93	6/2343 (0.3%)
9	I	0.43	0/1557	0.78	1/2110 (0.0%)
10	J	0.38	0/1362	0.74	2/1855 (0.1%)
11	K	0.71	1/1415 (0.1%)	1.02	5/1925 (0.3%)
12	L	0.47	0/700	0.70	0/947
13	M	0.52	1/935 (0.1%)	0.73	0/1268
14	O	0.62	0/598	1.07	0/813
15	P	0.45	0/1054	0.84	2/1418 (0.1%)
16	Q	0.52	0/654	0.94	0/890
17	R	0.42	0/909	0.81	0/1229
18	S	0.40	0/1454	0.77	0/1960
19	U	0.48	0/1374	0.78	0/1856
20	W	0.45	0/998	0.64	0/1346
21	X	0.37	0/1335	0.64	0/1811
22	Y	0.43	0/1051	0.64	0/1420
23	Z	0.37	0/1430	0.77	2/1955 (0.1%)
24	a	0.41	0/1064	0.75	0/1439
25	b	0.32	0/503	0.56	0/679
26	c	0.34	0/364	0.66	0/491
27	d	0.42	0/776	0.70	0/1043
28	e	0.41	0/456	0.77	0/619
29	f	0.60	0/639	1.00	0/856
30	g	0.33	0/643	0.58	0/880
31	h	0.44	0/1168	0.81	2/1589 (0.1%)
32	i	0.50	0/666	0.80	0/907

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	j	0.34	0/745	0.65	0/1006
34	n	0.37	0/943	0.71	0/1279
35	1	0.48	0/2699	0.85	3/3684 (0.1%)
36	2	0.53	0/3854	0.79	6/5252 (0.1%)
37	3	0.51	0/954	0.98	2/1300 (0.2%)
38	4	0.48	0/3941	0.72	1/5382 (0.0%)
39	5	0.44	0/5327	0.75	4/7273 (0.1%)
40	6	0.48	1/1439 (0.1%)	0.90	3/1964 (0.2%)
41	8	0.53	0/657	0.99	2/879 (0.2%)
42	9	0.46	0/684	0.79	0/918
All	All	0.46	4/64860 (0.0%)	0.79	51/88042 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
2	B	0	1
3	C	0	2
8	H	0	3
10	J	0	1
11	K	0	3
13	M	0	1
14	O	0	1
24	a	0	1
26	c	0	1
35	1	0	2
36	2	0	2
38	4	0	1
39	5	0	4
All	All	0	28

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	K	78	PRO	N-CA	17.92	1.70	1.47
13	M	74	MET	C-O	-8.86	1.19	1.23
3	C	395	PRO	CA-C	-6.92	1.48	1.51
40	6	33	ILE	CG1-CD1	-5.05	1.32	1.51

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	77	TRP	CA-C-N	15.97	139.80	119.84
11	K	77	TRP	C-N-CA	15.97	139.80	119.84
40	6	27	LYS	CA-C-N	10.35	156.47	121.27
40	6	27	LYS	C-N-CA	10.35	156.47	121.27
11	K	78	PRO	CA-N-CD	-8.11	100.65	112.00
36	2	215	ALA	N-CA-C	6.95	123.03	113.16
10	J	195	GLU	CA-C-N	6.91	129.71	120.58
10	J	195	GLU	C-N-CA	6.91	129.71	120.58
41	8	15	LYS	CA-CB-CG	6.42	126.95	114.10
5	E	299	LYS	CA-CB-CG	6.29	126.68	114.10
7	G	93	LYS	N-CA-C	-6.26	97.47	110.80
36	2	375	PRO	N-CA-C	6.20	118.27	110.70
36	2	214	ILE	CA-C-N	5.98	127.56	120.09
36	2	214	ILE	C-N-CA	5.98	127.56	120.09
41	8	63	GLN	OE1-CD-NE2	-5.98	116.62	122.60
8	H	235	VAL	N-CA-CB	-5.94	103.42	112.15
8	H	235	VAL	CB-CA-C	5.88	119.93	111.88
9	I	103	TYR	CA-CB-CG	-5.77	103.51	113.90
3	C	258	LEU	CB-CG-CD2	-5.76	93.42	110.70
38	4	265	LEU	CA-CB-CG	5.65	136.06	116.30
3	C	395	PRO	O-C-N	-5.54	118.76	121.31
35	1	73	LEU	CA-C-N	-5.48	113.88	121.77
35	1	73	LEU	C-N-CA	-5.48	113.88	121.77
11	K	139	PRO	CA-C-N	5.42	126.86	120.09
11	K	139	PRO	C-N-CA	5.42	126.86	120.09
40	6	129	ASP	O-C-N	-5.36	115.31	122.43
36	2	283	ARG	CA-C-N	5.34	127.70	120.38
36	2	283	ARG	C-N-CA	5.34	127.70	120.38
23	Z	40	ILE	CA-C-N	5.30	124.57	120.33
23	Z	40	ILE	C-N-CA	5.30	124.57	120.33
37	3	84	SER	CA-C-N	5.30	131.66	121.54
37	3	84	SER	C-N-CA	5.30	131.66	121.54
8	H	179	ALA	CA-C-N	-5.29	117.78	122.97
8	H	179	ALA	C-N-CA	-5.29	117.78	122.97
39	5	338	PHE	CB-CA-C	-5.27	102.53	110.92
1	A	659	TYR	CA-C-N	5.21	131.49	121.54
1	A	659	TYR	C-N-CA	5.21	131.49	121.54
15	P	121	LYS	CA-C-N	5.21	131.48	121.54
15	P	121	LYS	C-N-CA	5.21	131.48	121.54
39	5	555	VAL	N-CA-C	5.17	120.08	109.34
2	B	110	GLU	CA-CB-CG	5.17	124.43	114.10
1	A	261	MET	CA-CB-CG	5.15	124.39	114.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	1	64	LEU	CA-CB-CG	5.12	134.20	116.30
39	5	161	LEU	CB-CG-CD1	-5.11	95.38	110.70
8	H	240	GLN	CA-C-N	5.05	135.40	126.45
8	H	240	GLN	C-N-CA	5.05	135.40	126.45
39	5	70	ILE	N-CA-C	-5.03	98.87	109.34
31	h	93	PRO	CA-C-N	5.03	127.72	120.38
31	h	93	PRO	C-N-CA	5.03	127.72	120.38
5	E	233	SER	CA-C-N	5.00	130.44	120.94
5	E	233	SER	C-N-CA	5.00	130.44	120.94

There are no chirality outliers.

All (28) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
35	1	200	PRO	Peptide
35	1	67	GLU	Peptide
36	2	214	ILE	Peptide
36	2	338	ASN	Peptide
38	4	228	HIS	Peptide
39	5	134	SER	Peptide
39	5	253	ALA	Peptide
39	5	387	MET	Peptide
39	5	554	LEU	Peptide
1	A	165	ARG	Sidechain
1	A	247	ALA	Peptide
1	A	269	ARG	Sidechain
1	A	434	ARG	Sidechain
1	A	439	ILE	Peptide
2	B	457	ASP	Peptide
3	C	86	ASN	Peptide
3	C	96	GLY	Peptide
8	H	174	ASN	Peptide
8	H	239	LEU	Peptide
8	H	29	ILE	Peptide
10	J	182	GLY	Peptide
11	K	180	CYS	Peptide
11	K	199	ARG	Sidechain
11	K	97	ARG	Sidechain
13	M	75	PRO	Peptide
14	O	44	ASP	Peptide
24	a	117	GLU	Peptide
26	c	18	GLN	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5258	0	5159	132	0
2	B	3528	0	3489	78	0
3	C	3426	0	3364	80	0
4	D	681	0	671	11	0
5	E	2527	0	2494	45	0
6	F	990	0	977	14	0
7	G	1978	0	1908	36	0
8	H	1688	0	1660	38	0
9	I	1519	0	1460	49	0
10	J	1329	0	1311	19	0
11	K	1377	0	1354	75	0
12	L	691	0	754	15	0
13	M	912	0	869	17	0
14	O	591	0	585	10	0
15	P	1030	0	1014	21	0
16	Q	648	0	636	12	0
17	R	884	0	893	17	0
18	S	1430	0	1463	19	0
19	U	1345	0	1327	20	0
20	W	974	0	987	20	0
21	X	1296	0	1268	18	0
22	Y	1021	0	984	14	0
23	Z	1389	0	1395	20	0
24	a	1030	0	967	16	0
25	b	490	0	509	3	0
26	c	353	0	343	2	0
27	d	760	0	721	21	0
28	e	436	0	426	6	0
29	f	629	0	640	14	0
30	g	617	0	597	10	0
31	h	1130	0	1084	24	0
32	i	646	0	630	3	0
33	j	724	0	706	12	0
34	n	914	0	880	12	0
35	1	2627	0	2737	86	0
36	2	3774	0	4005	75	0
37	3	933	0	1006	40	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	4	3847	0	4042	76	0
39	5	5197	0	5353	86	0
40	6	1415	0	1535	28	0
41	8	643	0	644	8	0
42	9	672	0	683	11	0
43	A	16	0	0	1	0
43	B	8	0	0	0	0
43	I	16	0	0	0	0
43	K	8	0	0	0	0
44	A	4	0	0	0	0
44	H	4	0	0	0	0
45	B	31	0	19	1	0
46	E	48	0	26	1	0
47	3	43	0	63	10	0
47	4	136	0	203	14	0
47	I	51	0	82	3	0
47	J	85	0	118	4	0
47	S	42	0	61	2	0
47	a	51	0	82	3	0
47	b	42	0	58	2	0
47	i	42	0	58	2	0
48	J	134	0	165	7	0
48	j	69	0	88	3	0
49	M	1	0	0	0	0
50	O	33	0	38	1	0
50	Q	33	0	38	2	0
51	1	77	0	108	4	0
51	5	73	0	100	1	0
51	W	83	0	123	7	0
52	2	83	0	116	19	0
52	4	92	0	137	4	0
52	5	78	0	103	4	0
52	X	86	0	119	14	0
52	Z	76	0	96	2	0
53	1	35	0	43	11	0
54	2	100	0	0	0	0
54	3	49	0	0	0	0
54	4	43	0	0	3	0
55	2	52	0	80	1	0
All	All	65173	0	65654	1099	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (1099) 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)
11:K:78:PRO:N	11:K:78:PRO:CA	1.70	1.36
11:K:81:PHE:CD2	11:K:131:LEU:HD12	1.82	1.14
1:A:264:VAL:HG12	1:A:424:MET:HE2	1.37	1.03
1:A:264:VAL:CG1	1:A:424:MET:HE2	1.89	1.01
35:1:228:PHE:CE1	53:1:402:UQ9:H12	1.95	1.01
9:I:171:TYR:CE2	11:K:179:GLY:HA2	1.96	0.99
1:A:210:ASP:OD2	8:H:28:HIS:HB2	1.65	0.97
11:K:80:THR:HG21	11:K:90:MET:SD	2.05	0.96
52:2:501:CDL:HB62	52:2:501:CDL:HA62	1.47	0.95
11:K:81:PHE:CE2	11:K:131:LEU:HB2	2.02	0.94
1:A:141:GLU:HB2	22:Y:68:THR:HG21	1.48	0.94
52:X:201:CDL:H601	52:X:201:CDL:H671	1.51	0.92
9:I:171:TYR:HE2	11:K:179:GLY:HA2	1.32	0.92
11:K:81:PHE:CE2	11:K:131:LEU:HD12	2.04	0.90
36:2:4:LEU:HD11	52:2:501:CDL:H262	1.53	0.90
11:K:139:PRO:HB3	35:1:61:GLU:HB3	1.52	0.89
1:A:168:GLU:OE1	8:H:32:VAL:HG21	1.72	0.89
11:K:81:PHE:HD2	11:K:131:LEU:HD12	1.35	0.88
1:A:355:GLU:HB2	1:A:595:LYS:NZ	1.90	0.87
11:K:81:PHE:CZ	11:K:127:MET:HE2	2.11	0.86
1:A:276:GLU:CD	31:h:126:LYS:HE3	1.99	0.86
1:A:367:ASN:ND2	1:A:372:GLU:HG3	1.91	0.86
11:K:81:PHE:CE1	11:K:127:MET:HE2	2.12	0.85
11:K:79:VAL:HG12	11:K:117:MET:HA	1.58	0.84
1:A:276:GLU:OE2	31:h:126:LYS:HE3	1.79	0.82
11:K:81:PHE:CD2	11:K:131:LEU:CD1	2.63	0.82
1:A:405:GLU:HG3	1:A:427:ARG:HH11	1.46	0.81
37:3:21:VAL:O	37:3:25:LEU:HB2	1.81	0.81
52:2:501:CDL:HB62	52:2:501:CDL:CA6	2.10	0.80
5:E:86:GLU:HG3	11:K:206:MET:HE3	1.64	0.80
1:A:355:GLU:HB2	1:A:595:LYS:HZ1	1.47	0.80
30:g:30:PHE:CD2	47:3:201:3PE:H271	2.19	0.77
39:5:61:ASN:HB3	39:5:80:GLU:HB3	1.65	0.77
50:O:201:ZMP:H14	15:P:63:HIS:O	1.85	0.77
2:B:409:ARG:O	2:B:412:ASP:HB3	1.85	0.76
39:5:66:ASN:HD21	39:5:69:ASN:HB2	1.52	0.74
3:C:362:GLU:HB3	23:Z:66:THR:HG21	1.70	0.74
16:Q:90:LEU:HB3	17:R:44:ARG:HH22	1.53	0.73
36:2:15:MET:SD	52:2:501:CDL:HA32	2.29	0.73
36:2:5:ALA:O	36:2:9:LEU:HB2	1.89	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:g:26:LEU:HD13	47:3:201:3PE:H2	1.71	0.72
8:H:240:GLN:HG3	8:H:242:GLY:H	1.54	0.72
11:K:81:PHE:CE2	11:K:131:LEU:CB	2.72	0.72
19:U:61:GLN:HG3	34:n:119:ARG:HA	1.72	0.71
36:2:15:MET:HE1	52:2:501:CDL:HB61	1.72	0.71
1:A:67:ARG:HD2	1:A:70:TYR:HB3	1.72	0.71
9:I:76:LYS:HE2	51:W:201:PLC:O2P	1.89	0.71
39:5:151:TYR:HB2	39:5:171:VAL:HG21	1.70	0.71
1:A:264:VAL:HG12	1:A:424:MET:CE	2.16	0.71
35:1:228:PHE:HE1	53:1:402:UQ9:H12	1.52	0.71
3:C:258:LEU:HD21	3:C:340:PHE:HB3	1.72	0.71
37:3:103:VAL:HG12	47:3:201:3PE:H331	1.73	0.70
1:A:401:ILE:HD13	1:A:424:MET:HE1	1.74	0.70
10:J:92:LYS:HD2	48:J:202:LMN:OAQ	1.91	0.70
1:A:264:VAL:HG11	1:A:424:MET:HE2	1.72	0.70
1:A:149:MET:SD	3:C:383:HIS:ND1	2.65	0.69
3:C:144:TYR:HB2	11:K:85:CYS:HB3	1.74	0.69
35:1:78:LEU:HD11	37:3:19:LEU:CD2	2.22	0.69
2:B:132:ILE:HD11	2:B:277:LEU:HD11	1.74	0.69
3:C:119:LEU:HD11	11:K:84:ALA:HB2	1.75	0.69
5:E:373:ILE:HG13	12:L:79:ARG:HG2	1.74	0.69
1:A:217:LEU:HD23	1:A:219:LYS:HD3	1.74	0.69
1:A:484:VAL:HB	1:A:521:VAL:HG12	1.74	0.69
52:2:501:CDL:H532	47:3:201:3PE:H262	1.74	0.69
39:5:638:ASN:HD22	39:5:641:ILE:HG23	1.59	0.68
18:S:98:TYR:HB2	18:S:126:LEU:HB3	1.76	0.68
30:g:31:ALA:HA	47:3:201:3PE:H2B1	1.76	0.68
9:I:76:LYS:HE3	20:W:30:PRO:HG2	1.75	0.67
1:A:217:LEU:CD2	1:A:219:LYS:HD3	2.25	0.67
23:Z:110:ASP:O	23:Z:114:GLY:N	2.28	0.67
15:P:38:THR:O	15:P:42:LEU:HB2	1.94	0.67
1:A:434:ARG:HG3	1:A:435:GLN:HG3	1.76	0.66
36:2:414:LEU:HD11	38:4:168:LEU:HD23	1.77	0.66
36:2:7:ILE:HG22	52:2:501:CDL:H792	1.76	0.66
11:K:81:PHE:HE2	11:K:131:LEU:HB2	1.59	0.66
1:A:210:ASP:OD2	8:H:28:HIS:CB	2.43	0.66
38:4:302:ILE:HD13	38:4:342:LEU:HB3	1.78	0.66
8:H:142:GLU:HA	8:H:145:GLN:HG2	1.78	0.66
1:A:81:ARG:HH21	2:B:426:ILE:HG12	1.61	0.65
3:C:214:MET:SD	11:K:92:HIS:CE1	2.90	0.65
22:Y:44:ILE:HG13	22:Y:45:VAL:HG13	1.79	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:4:197:HIS:HB2	38:4:265:LEU:HD23	1.77	0.65
18:S:85:GLU:HB2	18:S:89:ALA:HB2	1.77	0.65
1:A:268:ILE:O	1:A:283:ARG:NH1	2.29	0.65
38:4:68:LEU:HD21	47:4:504:3PE:H32	1.78	0.65
9:I:129:ARG:NH1	9:I:181:VAL:O	2.31	0.64
14:O:80:PHE:HB2	14:O:82:ILE:HG22	1.80	0.64
52:X:201:CDL:C25	52:2:501:CDL:H791	2.26	0.64
11:K:79:VAL:HB	11:K:114:SER:OG	1.97	0.64
4:D:62:ARG:NH1	19:U:102:GLU:O	2.31	0.64
10:J:170:ARG:NH2	10:J:178:GLN:OE1	2.31	0.64
37:3:73:LEU:HD21	37:3:95:LEU:HD21	1.80	0.64
1:A:367:ASN:HD21	1:A:372:GLU:HG3	1.62	0.64
3:C:54:ARG:NH2	3:C:65:TYR:OH	2.30	0.64
21:X:29:LYS:HE3	52:X:201:CDL:HB31	1.80	0.64
6:F:99:LEU:HD11	9:I:55:PHE:CE2	2.33	0.63
39:5:610:THR:HG22	39:5:612:SER:H	1.63	0.63
3:C:60:GLU:HG3	36:2:283:ARG:HH12	1.62	0.63
1:A:273:LYS:CG	1:A:278:MET:HE3	2.29	0.63
52:2:501:CDL:H381	52:2:501:CDL:H191	1.79	0.63
1:A:263:ALA:HB3	1:A:421:ALA:HB2	1.80	0.63
1:A:596:ALA:HA	1:A:609:SER:O	1.99	0.63
7:G:189:PHE:HE2	15:P:74:VAL:HG12	1.64	0.63
27:d:63:CYS:HB2	27:d:66:LEU:HB2	1.80	0.62
1:A:401:ILE:CD1	1:A:424:MET:HE1	2.29	0.62
9:I:148:ASP:OD2	31:h:126:LYS:NZ	2.31	0.62
1:A:550:VAL:HB	1:A:569:VAL:HG12	1.82	0.62
1:A:537:THR:O	29:f:41:LYS:NZ	2.33	0.62
38:4:223:PRO:HG2	38:4:231:LEU:HD22	1.81	0.62
16:Q:81:LEU:HD21	16:Q:95:VAL:HG11	1.81	0.62
27:d:31:THR:HG23	38:4:480:ASN:HD22	1.64	0.62
38:4:127:LEU:HD11	47:4:504:3PE:H372	1.80	0.62
9:I:110:VAL:H	23:Z:45:ARG:HH22	1.46	0.62
13:M:63:ARG:NH2	31:h:119:THR:O	2.33	0.62
1:A:299:PHE:O	1:A:709:THR:HG21	1.99	0.62
1:A:439:ILE:HG21	1:A:450:PHE:HE2	1.64	0.62
2:B:367:ARG:NH1	8:H:138:ASP:OD2	2.33	0.62
35:1:20:ALA:HB2	53:1:402:UQ9:H23	1.81	0.61
17:R:92:ARG:NH1	39:5:356:GLU:OE2	2.33	0.61
11:K:80:THR:CG2	11:K:90:MET:SD	2.86	0.61
35:1:78:LEU:HD11	37:3:19:LEU:HD23	1.82	0.61
36:2:281:ILE:O	36:2:285:LEU:HB2	2.00	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:288:CYS:SG	2:B:289:THR:N	2.73	0.61
2:B:164:PHE:HB3	2:B:167:GLU:HB2	1.83	0.61
39:5:349:ILE:HG23	39:5:373:THR:HG21	1.82	0.61
2:B:310:LYS:O	2:B:315:ASN:ND2	2.32	0.61
3:C:263:GLU:OE2	23:Z:34:ARG:NH2	2.34	0.61
28:e:42:ILE:HD13	28:e:49:MET:HE3	1.83	0.61
11:K:140:GLU:HG2	37:3:27:VAL:HG11	1.82	0.61
24:a:61:GLN:HE21	39:5:161:LEU:HD12	1.66	0.61
2:B:267:PHE:HB3	2:B:293:GLU:HG3	1.82	0.61
16:Q:113:ASP:OD2	17:R:13:LYS:NZ	2.34	0.61
1:A:391:PHE:HZ	29:f:30:ILE:HG13	1.66	0.60
5:E:155:VAL:HG13	5:E:160:ILE:HB	1.82	0.60
7:G:167:SER:HB2	7:G:190:PHE:HB3	1.83	0.60
35:1:199:ARG:HD3	35:1:235:ILE:HD11	1.83	0.60
16:Q:107:ILE:O	17:R:20:ARG:NH2	2.33	0.60
1:A:254:LYS:HE2	1:A:269:ARG:HH22	1.66	0.60
8:H:119:MET:HB2	8:H:162:THR:HG21	1.82	0.60
8:H:215:ARG:NH1	8:H:219:GLU:O	2.35	0.60
16:Q:81:LEU:HD23	16:Q:92:VAL:HG23	1.82	0.60
9:I:107:LYS:HE3	31:h:78:HIS:CE1	2.36	0.60
20:W:60:ARG:NH1	30:g:56:SER:O	2.34	0.60
31:h:113:THR:HG22	31:h:115:GLY:H	1.66	0.60
36:2:75:ILE:HD13	36:2:238:LEU:HD21	1.82	0.60
38:4:3:LEU:HD11	47:4:504:3PE:H121	1.83	0.60
41:8:12:ASP:HA	41:8:15:LYS:HG2	1.82	0.60
1:A:458:THR:HG22	1:A:460:ALA:H	1.66	0.60
3:C:144:TYR:CB	11:K:85:CYS:HB3	2.32	0.60
4:D:70:ALA:HB3	19:U:27:GLU:HB2	1.84	0.60
6:F:31:ILE:HG23	6:F:33:LEU:H	1.67	0.60
40:6:33:ILE:HD11	40:6:71:PHE:HB3	1.83	0.60
2:B:414:LEU:HD12	2:B:417:LEU:HD11	1.84	0.60
1:A:355:GLU:HB2	1:A:595:LYS:HZ2	1.67	0.60
11:K:79:VAL:CG1	11:K:117:MET:HA	2.32	0.60
2:B:128:LYS:HB2	2:B:277:LEU:HD13	1.84	0.60
11:K:79:VAL:HB	11:K:114:SER:CB	2.32	0.60
35:1:182:LEU:HD23	35:1:185:LEU:HD22	1.83	0.60
35:1:228:PHE:CE1	53:1:402:UQ9:C12	2.80	0.60
35:1:318:PRO:HB3	47:3:201:3PE:H352	1.84	0.60
10:J:57:ILE:HB	40:6:91:ILE:HG22	1.84	0.59
51:W:201:PLC:HTA1	51:W:202:PLC:H7'2	1.84	0.59
33:j:64:PRO:HG3	38:4:283:LEU:HD11	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:79:VAL:O	11:K:117:MET:HA	2.02	0.59
39:5:331:HIS:HA	39:5:395:THR:HB	1.85	0.59
3:C:218:GLU:HB2	3:C:224:ARG:HG2	1.83	0.59
12:L:12:PHE:HA	12:L:32:MET:HE2	1.84	0.59
36:2:403:ILE:HG13	38:4:180:LEU:HD11	1.84	0.59
1:A:491:ARG:HG2	1:A:493:ASP:H	1.67	0.59
10:J:136:GLY:HA2	48:J:202:LMN:H3	1.85	0.59
2:B:322:GLY:N	2:B:355:ALA:O	2.35	0.59
24:a:133:GLU:OE1	41:8:23:ARG:NH1	2.36	0.59
3:C:435:LEU:HD23	3:C:464:VAL:HG11	1.84	0.59
39:5:632:VAL:HA	39:5:635:MET:HB3	1.84	0.59
6:F:43:ARG:NH2	6:F:82:VAL:O	2.35	0.59
19:U:13:GLU:HA	20:W:84:ARG:HH22	1.66	0.59
27:d:24:ARG:NH2	34:n:66:GLU:OE2	2.36	0.59
11:K:82:GLY:CA	11:K:120:ALA:O	2.50	0.59
29:f:68:LEU:HD23	29:f:76:VAL:HG22	1.84	0.59
35:1:137:ILE:HG13	40:6:77:LEU:HD23	1.85	0.59
1:A:285:HIS:HD2	1:A:288:VAL:H	1.51	0.58
29:f:11:HIS:O	29:f:52:PRO:HA	2.03	0.58
38:4:313:ALA:HB2	38:4:331:LEU:HD22	1.84	0.58
3:C:54:ARG:HG3	3:C:55:THR:HG22	1.85	0.58
14:O:58:PHE:HB3	14:O:64:LEU:HD12	1.85	0.58
15:P:66:VAL:O	15:P:72:GLN:NE2	2.36	0.58
35:1:104:LEU:HD11	40:6:54:ILE:HG13	1.85	0.58
2:B:475:LYS:HB2	13:M:88:ARG:HG2	1.86	0.58
8:H:124:LEU:HB2	8:H:163:LEU:HA	1.86	0.58
9:I:77:TYR:HE1	47:I:501:3PE:H111	1.68	0.58
1:A:269:ARG:HB3	1:A:281:ILE:HG23	1.85	0.58
5:E:109:LEU:HA	5:E:115:ILE:HD11	1.85	0.58
36:2:7:ILE:HG23	37:3:100:ILE:HD13	1.85	0.58
1:A:273:LYS:HG2	1:A:278:MET:HE3	1.84	0.58
29:f:70:VAL:HG21	29:f:76:VAL:HG23	1.86	0.58
52:2:501:CDL:OB9	52:2:501:CDL:H731	2.03	0.58
39:5:40:ILE:HD13	39:5:97:SER:HB2	1.86	0.58
3:C:317:VAL:HG11	3:C:346:ILE:HG23	1.85	0.57
11:K:81:PHE:HD2	11:K:131:LEU:CD1	2.11	0.57
31:h:74:GLU:HB3	31:h:77:TRP:HD1	1.67	0.57
23:Z:115:THR:HA	23:Z:118:LEU:HD12	1.86	0.57
2:B:46:ASP:O	8:H:216:ARG:NH2	2.38	0.57
52:X:201:CDL:H632	36:2:4:LEU:HD21	1.85	0.57
26:c:23:ARG:NH2	39:5:530:GLU:OE1	2.36	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:2:212:ILE:HD11	36:2:244:ILE:HB	1.86	0.57
9:I:168:LYS:HA	11:K:155:GLY:HA2	1.87	0.57
36:2:9:LEU:HD21	36:2:104:ILE:HG23	1.86	0.57
39:5:509:PHE:O	39:5:513:LEU:HB2	2.05	0.57
1:A:375:THR:HA	1:A:538:PRO:HD3	1.87	0.57
21:X:142:ASN:ND2	37:3:86:TYR:OH	2.37	0.57
39:5:151:TYR:HD2	39:5:152:LEU:HD12	1.70	0.57
30:g:47:ARG:HG3	30:g:51:LEU:HD12	1.87	0.57
35:1:242:ASN:HB3	35:1:289:LEU:HD21	1.87	0.57
39:5:400:ILE:O	39:5:403:THR:OG1	2.22	0.57
23:Z:110:ASP:HB3	23:Z:113:ALA:HB3	1.85	0.56
35:1:323:ILE:HA	35:1:326:ILE:HG22	1.87	0.56
36:2:229:PRO:HB3	36:2:341:TYR:HB3	1.86	0.56
1:A:707:SER:HB2	1:A:709:THR:HG22	1.87	0.56
11:K:146:SER:HB2	11:K:173:VAL:HG11	1.86	0.56
35:1:117:VAL:HG12	35:1:143:LEU:HG	1.87	0.56
1:A:86:ASP:OD1	1:A:113:ARG:NH2	2.39	0.56
1:A:664:PRO:O	29:f:14:GLN:NE2	2.37	0.56
7:G:126:ILE:HD11	7:G:179:GLU:HG3	1.86	0.56
7:G:262:ARG:HE	7:G:267:LYS:HB3	1.70	0.56
9:I:84:PHE:HA	9:I:87:LEU:HD12	1.86	0.56
40:6:153:VAL:HG11	42:9:3:ALA:HB2	1.87	0.56
21:X:16:TYR:HE1	34:n:99:PRO:HG2	1.70	0.56
1:A:223:THR:HG23	1:A:225:LEU:H	1.70	0.56
1:A:269:ARG:HH21	1:A:269:ARG:HG2	1.70	0.56
2:B:453:LYS:HD3	2:B:456:HIS:HB3	1.88	0.56
1:A:217:LEU:HB3	1:A:219:LYS:HG2	1.86	0.56
36:2:292:ASN:HA	36:2:295:TYR:HD2	1.71	0.56
11:K:79:VAL:HG12	11:K:117:MET:CA	2.33	0.56
20:W:27:GLY:HA3	51:W:201:PLC:H32	1.88	0.56
35:1:53:ASP:HB3	53:1:402:UQ9:H15A	1.87	0.56
12:L:81:ARG:HH22	36:2:151:SER:HB2	1.71	0.56
18:S:208:PRO:O	18:S:211:ASN:HB2	2.06	0.56
34:n:83:MET:HE3	36:2:469:ASN:HD22	1.71	0.56
36:2:18:LEU:HD11	40:6:183:HIS:HB3	1.88	0.56
29:f:26:VAL:HG13	29:f:30:ILE:HD11	1.87	0.55
39:5:291:ALA:HB2	39:5:310:MET:HE2	1.88	0.55
9:I:103:TYR:OH	31:h:70:MET:HG2	2.05	0.55
12:L:3:ILE:HB	40:6:13:ILE:HG12	1.89	0.55
38:4:276:MET:HA	38:4:279:ILE:HD12	1.87	0.55
1:A:389:ILE:HG13	1:A:537:THR:HG21	1.87	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:68:ASP:OD1	15:P:57:ARG:NH2	2.39	0.55
36:2:299:LEU:O	36:2:305:ASN:ND2	2.39	0.55
3:C:73:THR:OG1	3:C:74:SER:N	2.35	0.55
9:I:127:GLU:OE2	9:I:152:ARG:NH2	2.33	0.55
1:A:111:THR:HG22	1:A:113:ARG:H	1.71	0.55
5:E:89:ALA:O	5:E:92:HIS:ND1	2.35	0.55
19:U:40:TYR:OH	20:W:61:GLU:O	2.23	0.55
33:j:83:LYS:HG3	33:j:89:VAL:HG12	1.88	0.55
34:n:73:LEU:HD11	38:4:78:LEU:HD11	1.87	0.55
36:2:215:ALA:HB2	36:2:267:THR:HA	1.89	0.55
38:4:265:LEU:HD12	38:4:266:LEU:HD22	1.88	0.55
2:B:284:VAL:HG22	2:B:286:GLU:H	1.71	0.55
11:K:70:TRP:CH2	35:1:52:ALA:HB2	2.42	0.55
52:2:501:CDL:CA2	52:2:501:CDL:CA3	2.85	0.55
39:5:5:ILE:HG23	39:5:62:LEU:HD23	1.89	0.55
17:R:64:ASP:OD1	17:R:67:ARG:NH2	2.39	0.55
36:2:264:ALA:HB1	36:2:298:LEU:HD12	1.88	0.55
2:B:370:GLN:NE2	2:B:399:ASP:OD1	2.39	0.55
28:e:33:THR:HG22	39:5:470:MET:HE1	1.88	0.55
31:h:33:GLY:HA3	31:h:46:TYR:HB3	1.89	0.55
5:E:238:VAL:HA	5:E:241:VAL:HG12	1.89	0.55
35:1:61:GLU:OE1	37:3:34:LYS:NZ	2.40	0.55
35:1:310:ASN:HD22	35:1:314:ILE:HD12	1.71	0.55
37:3:103:VAL:HG12	47:3:201:3PE:C33	2.37	0.55
5:E:182:THR:HA	5:E:185:LEU:HB2	1.89	0.54
9:I:95:PHE:CE2	52:Z:201:CDL:H561	2.42	0.54
11:K:100:GLN:HB2	11:K:105:ILE:HB	1.89	0.54
33:j:49:THR:H	33:j:52:THR:HB	1.72	0.54
35:1:106:ILE:HG21	35:1:158:ILE:HD11	1.89	0.54
36:2:62:ASN:HD21	36:2:250:LEU:HD11	1.71	0.54
3:C:67:GLU:HB3	36:2:148:TYR:HD2	1.71	0.54
11:K:78:PRO:HA	11:K:116:ILE:HG13	1.89	0.54
11:K:79:VAL:HG12	11:K:116:ILE:O	2.07	0.54
1:A:261:MET:HE1	1:A:703:ILE:HB	1.89	0.54
3:C:224:ARG:NH1	11:K:89:GLU:OE2	2.41	0.54
5:E:83:PRO:HA	5:E:105:LEU:O	2.08	0.54
35:1:78:LEU:HD11	37:3:19:LEU:HD21	1.90	0.54
9:I:99:TYR:HE2	35:1:35:ARG:HE	1.54	0.54
9:I:107:LYS:HE3	31:h:78:HIS:NE2	2.23	0.54
3:C:82:ALA:HB2	3:C:110:ILE:HD11	1.90	0.54
8:H:72:MET:O	8:H:114:TYR:OH	2.26	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:132:CYS:HB3	8:H:137:SER:HB3	1.90	0.54
11:K:93:VAL:HG21	11:K:187:LEU:HD23	1.89	0.54
52:2:501:CDL:H171	52:2:501:CDL:H362	1.89	0.54
38:4:464:ILE:HD11	52:4:502:CDL:H632	1.90	0.54
21:X:138:ILE:HG21	40:6:156:THR:HB	1.90	0.54
34:n:48:THR:HG22	34:n:50:VAL:H	1.73	0.54
2:B:138:HIS:NE2	2:B:177:GLU:OE2	2.39	0.54
3:C:465:ASP:OD1	3:C:465:ASP:N	2.38	0.54
11:K:183:THR:O	11:K:186:ALA:N	2.41	0.54
1:A:432:TRP:HD1	1:A:437:LEU:HB3	1.72	0.54
7:G:185:MET:HB3	7:G:210:LEU:HB2	1.90	0.54
23:Z:22:GLU:HA	23:Z:25:ARG:HG2	1.90	0.54
35:1:228:PHE:CZ	53:1:402:UQ9:H12	2.43	0.54
52:2:501:CDL:CA3	52:2:501:CDL:HA21	2.37	0.54
39:5:374:TYR:OH	39:5:438:TYR:OH	2.23	0.54
7:G:202:ASP:OD1	15:P:95:GLN:NE2	2.41	0.54
8:H:74:LEU:HD23	8:H:77:ILE:HD12	1.90	0.54
11:K:81:PHE:O	11:K:83:LEU:CD2	2.56	0.54
19:U:24:ASP:O	19:U:77:ARG:NH2	2.41	0.54
36:2:212:ILE:HG23	36:2:241:LYS:HG2	1.89	0.54
11:K:76:PHE:HD2	11:K:105:ILE:HG12	1.74	0.53
13:M:19:LYS:N	13:M:30:GLU:OE2	2.41	0.53
14:O:31:ASP:HA	14:O:34:LYS:HB3	1.91	0.53
47:S:501:3PE:H252	47:b:201:3PE:H351	1.89	0.53
22:Y:79:ARG:HA	22:Y:110:MET:O	2.06	0.53
35:1:103:ASN:HD21	40:6:143:ASN:HD21	1.55	0.53
36:2:212:ILE:HD12	36:2:241:LYS:HA	1.89	0.53
39:5:257:THR:HG22	39:5:332:LEU:HD11	1.90	0.53
1:A:81:ARG:HH21	2:B:426:ILE:CG1	2.21	0.53
1:A:571:TYR:HB3	1:A:586:VAL:HG12	1.90	0.53
35:1:148:LEU:HB2	37:3:63:PHE:HE1	1.74	0.53
38:4:94:LEU:HD11	38:4:337:PHE:HE1	1.73	0.53
1:A:54:LEU:HD11	1:A:107:VAL:HG21	1.90	0.53
11:K:81:PHE:CE2	11:K:131:LEU:CD1	2.84	0.53
22:Y:80:LEU:HB3	22:Y:110:MET:HB2	1.89	0.53
35:1:226:PHE:HE2	37:3:19:LEU:HB3	1.74	0.53
39:5:244:THR:HG21	39:5:347:GLY:HA3	1.90	0.53
29:f:10:PHE:HB3	29:f:54:VAL:HG23	1.88	0.53
39:5:99:VAL:HG11	39:5:249:LEU:HG	1.90	0.53
1:A:610:ARG:HH12	22:Y:81:ASP:CG	2.17	0.53
2:B:43:ASN:ND2	2:B:49:GLY:O	2.38	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:332:ASN:N	2:B:332:ASN:OD1	2.42	0.53
17:R:4:PRO:HG2	17:R:5:VAL:HG23	1.90	0.53
35:1:86:ILE:HD12	37:3:8:ILE:HD13	1.90	0.53
15:P:58:GLN:HA	15:P:61:GLU:HG2	1.90	0.53
21:X:154:PRO:HG3	52:X:201:CDL:H641	1.89	0.53
35:1:153:ILE:HD11	35:1:188:ILE:HG22	1.89	0.53
38:4:389:THR:HG23	38:4:391:ASN:H	1.74	0.53
35:1:42:VAL:HG21	35:1:49:GLN:HG3	1.91	0.53
39:5:412:TYR:O	39:5:415:TYR:HB3	2.08	0.53
40:6:77:LEU:HD12	40:6:78:LEU:HD12	1.90	0.53
5:E:87:GLU:HB2	5:E:90:LYS:HE3	1.90	0.53
38:4:202:LEU:HB2	38:4:207:GLN:HG3	1.90	0.53
38:4:274:THR:OG1	38:4:405:ARG:NH1	2.42	0.53
1:A:128:ASN:ND2	2:B:389:GLU:OE1	2.41	0.53
2:B:41:PHE:CE1	2:B:139:LYS:HD2	2.44	0.53
9:I:123:TYR:HE2	13:M:128:CYS:HA	1.72	0.53
19:U:122:VAL:HG13	19:U:126:LEU:HD12	1.91	0.53
2:B:269:ARG:N	2:B:272:ASN:O	2.41	0.53
3:C:219:ARG:HD2	3:C:243:LEU:HD13	1.91	0.53
31:h:35:LEU:HD11	31:h:44:LYS:HE3	1.89	0.52
40:6:52:LEU:HB3	40:6:55:PHE:HD2	1.74	0.52
1:A:127:GLN:HG3	1:A:158:PHE:CD1	2.44	0.52
11:K:127:MET:HG3	11:K:130:VAL:HB	1.91	0.52
20:W:103:VAL:O	42:9:56:ARG:NH2	2.42	0.52
36:2:284:LEU:HD11	36:2:412:TYR:HB2	1.90	0.52
3:C:123:THR:HG22	3:C:466:ARG:HB3	1.91	0.52
15:P:51:THR:HA	15:P:54:THR:HG22	1.91	0.52
24:a:132:LYS:HD3	41:8:10:GLN:HE22	1.74	0.52
38:4:219:MET:HG3	38:4:224:LEU:HB2	1.91	0.52
11:K:93:VAL:HG12	11:K:100:GLN:HB3	1.90	0.52
17:R:58:LEU:HD13	17:R:61:ARG:HD3	1.92	0.52
35:1:1:MET:HE3	35:1:5:ILE:HD11	1.91	0.52
35:1:5:ILE:HA	35:1:8:ILE:HG22	1.91	0.52
39:5:485:THR:HG22	39:5:487:PHE:H	1.75	0.52
1:A:138:GLN:HA	1:A:141:GLU:HG3	1.92	0.52
6:F:87:VAL:HB	6:F:90:VAL:HG12	1.90	0.52
39:5:630:LEU:HD11	40:6:103:VAL:HG21	1.90	0.52
1:A:217:LEU:CG	1:A:219:LYS:HD3	2.39	0.52
1:A:419:ARG:HB3	1:A:694:ILE:HD11	1.91	0.52
5:E:237:HIS:HE1	5:E:239:ILE:HD12	1.75	0.52
8:H:215:ARG:HB2	8:H:219:GLU:HB2	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:S:49:ARG:HB2	18:S:104:GLY:HA3	1.90	0.52
19:U:11:PRO:HG2	42:9:79:ILE:HG13	1.91	0.52
38:4:236:SER:O	38:4:357:ARG:NH1	2.43	0.52
1:A:222:ASN:HB3	1:A:723:LYS:HE3	1.92	0.52
6:F:99:LEU:HD21	9:I:55:PHE:HD2	1.75	0.52
10:J:148:GLU:HG3	10:J:149:GLN:HG3	1.92	0.52
52:X:201:CDL:HA32	52:X:201:CDL:OA7	2.09	0.52
2:B:118:ASN:ND2	2:B:209:GLY:O	2.42	0.52
3:C:87:PHE:HB2	3:C:100:LEU:HB3	1.92	0.52
2:B:473:VAL:HG22	2:B:478:VAL:HG22	1.91	0.52
3:C:97:VAL:HG23	11:K:127:MET:SD	2.50	0.52
18:S:227:ILE:HG23	27:d:69:GLN:HE22	1.74	0.52
51:W:201:PLC:H8A1	51:W:202:PLC:H6'1	1.92	0.52
8:H:74:LEU:HD12	8:H:97:LEU:HD11	1.92	0.51
8:H:90:MET:HE3	8:H:108:ALA:HB3	1.92	0.51
41:8:33:LEU:HG	41:8:37:ARG:HE	1.74	0.51
1:A:539:SER:OG	29:f:41:LYS:HE3	2.10	0.51
1:A:569:VAL:HG23	1:A:583:ALA:HA	1.91	0.51
3:C:259:ASP:OD1	3:C:341:ARG:NH2	2.43	0.51
7:G:141:VAL:HG12	7:G:156:LYS:HG2	1.91	0.51
29:f:7:GLU:HA	29:f:40:THR:HG23	1.92	0.51
35:1:78:LEU:CD1	37:3:19:LEU:HD21	2.40	0.51
37:3:106:ILE:HD11	47:3:201:3PE:C33	2.40	0.51
1:A:166:SER:OG	13:M:94:THR:HG22	2.10	0.51
1:A:217:LEU:HG	1:A:219:LYS:HD3	1.92	0.51
7:G:264:ASP:OD1	7:G:267:LYS:NZ	2.43	0.51
25:b:18:LYS:HE3	25:b:35:GLY:HA3	1.92	0.51
9:I:123:TYR:CE2	13:M:128:CYS:HA	2.46	0.51
2:B:78:GLU:OE2	2:B:261:GLY:N	2.43	0.51
37:3:6:ILE:O	37:3:10:LEU:HB2	2.10	0.51
39:5:528:LEU:HD21	39:5:535:VAL:HB	1.92	0.51
7:G:223:ARG:NE	7:G:234:GLU:OE1	2.43	0.51
36:2:374:ILE:HG22	36:2:376:PRO:HD2	1.91	0.51
1:A:481:LEU:HD13	1:A:520:ASN:HD22	1.76	0.51
5:E:90:LYS:HD2	5:E:104:PHE:CD1	2.45	0.51
11:K:117:MET:HE1	11:K:171:VAL:HG11	1.93	0.51
14:O:77:GLU:HG2	14:O:84:ILE:HD11	1.92	0.51
27:d:71:LEU:HB3	33:j:84:ARG:HH12	1.76	0.51
40:6:152:ASN:O	40:6:156:THR:OG1	2.29	0.51
1:A:402:ALA:HA	1:A:427:ARG:HH12	1.76	0.51
15:P:32:PHE:HB3	15:P:56:ILE:HD13	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:646:ARG:HE	1:A:657:VAL:HG13	1.75	0.51
2:B:47:ASN:OD1	2:B:47:ASN:N	2.44	0.51
7:G:144:PHE:HB2	7:G:153:ILE:HG22	1.92	0.51
27:d:50:LYS:HD3	32:i:59:THR:HG21	1.93	0.51
1:A:228:ASN:ND2	1:A:293:ILE:O	2.30	0.51
11:K:106:ILE:HD11	53:l:402:UQ9:C4	2.40	0.51
24:a:118:LYS:HZ3	39:5:409:ILE:HG22	1.76	0.51
36:2:456:TYR:HD1	36:2:459:LEU:HD12	1.75	0.51
5:E:193:ILE:HG22	5:E:194:VAL:HG13	1.92	0.50
7:G:105:VAL:HG12	7:G:166:PRO:HG2	1.92	0.50
11:K:144:VAL:HG13	11:K:173:VAL:HA	1.93	0.50
12:L:43:ASN:ND2	36:2:177:SER:OG	2.44	0.50
13:M:47:ALA:HB3	13:M:50:GLN:HB2	1.92	0.50
20:W:64:TRP:CE3	20:W:67:ILE:HD11	2.45	0.50
35:1:247:LEU:HD23	35:1:285:LYS:HD2	1.92	0.50
52:2:501:CDL:HA62	52:2:501:CDL:CB6	2.30	0.50
39:5:313:LEU:HA	39:5:316:MET:HE3	1.93	0.50
1:A:390:THR:O	1:A:394:ASN:ND2	2.44	0.50
1:A:490:ASP:OD2	1:A:524:ARG:NH1	2.45	0.50
5:E:62:ASN:HD21	5:E:89:ALA:HB3	1.77	0.50
1:A:699:MET:HB3	1:A:705:ARG:HG2	1.93	0.50
3:C:96:GLY:O	3:C:98:LEU:N	2.41	0.50
8:H:171:ALA:HB3	8:H:177:MET:HE3	1.92	0.50
19:U:132:ILE:HD11	20:W:61:GLU:HG3	1.94	0.50
30:g:30:PHE:HD2	47:3:201:3PE:H271	1.73	0.50
36:2:156:LEU:HD21	36:2:220:TRP:HB2	1.92	0.50
38:4:214:LEU:HB3	38:4:262:LEU:HD11	1.93	0.50
38:4:232:PRO:HB3	38:4:300:VAL:HG23	1.93	0.50
5:E:155:VAL:HG11	5:E:163:TYR:HB2	1.93	0.50
5:E:206:PHE:HD1	5:E:235:PRO:HB2	1.77	0.50
5:E:259:PHE:HE1	5:E:328:LYS:HD3	1.77	0.50
2:B:187:ASP:OD1	2:B:192:GLY:N	2.45	0.50
31:h:36:VAL:HG21	31:h:80:TRP:CH2	2.46	0.50
33:j:35:TYR:OH	33:j:39:ARG:NH2	2.45	0.50
35:1:110:LEU:HD21	35:1:151:THR:HG23	1.93	0.50
36:2:364:MET:HE2	36:2:416:LEU:HB3	1.93	0.50
3:C:289:LEU:HD13	3:C:437:ALA:HB1	1.94	0.50
37:3:62:LEU:HD11	37:3:111:LEU:HD11	1.94	0.50
1:A:225:LEU:HB2	1:A:228:ASN:HD22	1.77	0.50
9:I:170:ILE:HG21	11:K:156:TYR:CD1	2.47	0.50
36:2:88:TYR:HB2	36:2:93:TYR:HD2	1.77	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:5:507:THR:HG22	39:5:509:PHE:H	1.76	0.50
6:F:127:GLU:HG3	6:F:128:GLU:HG3	1.94	0.49
19:U:112:ARG:HA	19:U:115:GLU:HG2	1.93	0.49
35:1:330:THR:HG21	51:1:401:PLC:H9'1	1.93	0.49
47:4:503:3PE:H221	47:4:503:3PE:H342	1.93	0.49
39:5:80:GLU:HG3	39:5:134:SER:HB3	1.94	0.49
31:h:39:ASP:OD1	31:h:40:ILE:N	2.44	0.49
33:j:67:ILE:HD11	38:4:283:LEU:HD12	1.94	0.49
35:1:200:PRO:HA	35:1:203:ASP:HB2	1.94	0.49
36:2:233:THR:HA	36:2:236:ILE:HG12	1.94	0.49
2:B:87:ARG:HB3	2:B:276:LYS:HZ3	1.77	0.49
37:3:6:ILE:O	37:3:10:LEU:CB	2.60	0.49
3:C:409:GLU:OE2	7:G:152:ARG:NH2	2.41	0.49
9:I:170:ILE:HG21	11:K:156:TYR:HD1	1.77	0.49
5:E:251:ASP:O	5:E:254:THR:OG1	2.30	0.49
10:J:168:HIS:HB3	27:d:17:TYR:HD2	1.77	0.49
17:R:82:PRO:HB2	17:R:89:LYS:HB2	1.95	0.49
19:U:28:VAL:HG21	20:W:72:LEU:HD11	1.94	0.49
20:W:26:ARG:HD2	51:W:202:PLC:H51	1.94	0.49
39:5:40:ILE:HD11	39:5:101:ILE:HD11	1.94	0.49
1:A:355:GLU:CB	1:A:595:LYS:NZ	2.71	0.49
2:B:393:TRP:HD1	2:B:417:LEU:HD13	1.76	0.49
14:O:52:ILE:HG13	14:O:62:LEU:HD21	1.94	0.49
35:1:82:ILE:HG13	37:3:11:ILE:HG22	1.94	0.49
38:4:326:TYR:OH	38:4:468:PRO:O	2.29	0.49
1:A:709:THR:HG23	1:A:710:MET:N	2.27	0.49
17:R:90:TYR:O	39:5:160:ARG:NH1	2.45	0.49
37:3:106:ILE:HD11	47:3:201:3PE:H331	1.95	0.49
3:C:434:HIS:HB3	3:C:457:MET:HB2	1.93	0.49
39:5:281:LEU:HB2	39:5:321:GLY:HA3	1.94	0.49
1:A:577:ASP:OD2	1:A:705:ARG:NH2	2.38	0.49
36:2:144:TYR:HD2	36:2:229:PRO:HG3	1.77	0.49
36:2:362:LEU:HB2	47:4:501:3PE:H262	1.94	0.49
37:3:57:ILE:HD11	40:6:74:ILE:HD13	1.95	0.49
39:5:270:LEU:HB3	39:5:277:LEU:HD11	1.95	0.49
5:E:247:ARG:NH1	5:E:334:ASP:O	2.46	0.49
11:K:36:VAL:HG23	11:K:36:VAL:O	2.13	0.48
35:1:106:ILE:HD12	35:1:164:LEU:HA	1.94	0.48
39:5:43:THR:HA	39:5:46:THR:HG22	1.95	0.48
1:A:401:ILE:HD13	1:A:424:MET:CE	2.43	0.48
9:I:100:THR:OG1	35:1:37:LEU:HD13	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:5:533:ALA:O	39:5:537:ASN:ND2	2.45	0.48
2:B:327:PRO:HD3	2:B:435:TRP:HB3	1.94	0.48
27:d:71:LEU:HD11	39:5:203:THR:HB	1.95	0.48
1:A:276:GLU:OE2	31:h:126:LYS:HB3	2.13	0.48
1:A:351:GLY:HA3	1:A:555:ALA:H	1.77	0.48
2:B:163:GLU:N	2:B:163:GLU:OE1	2.44	0.48
9:I:187:THR:HG22	9:I:218:LEU:HD21	1.94	0.48
48:J:204:LMN:HAWA	48:J:204:LMN:HBCA	1.60	0.48
18:S:113:ASN:HD21	38:4:16:ARG:HH22	1.61	0.48
29:f:66:ILE:HD12	29:f:79:ARG:HB3	1.95	0.48
15:P:47:PHE:HE2	15:P:52:ILE:HG13	1.77	0.48
28:e:42:ILE:HD11	39:5:388:PRO:HG2	1.94	0.48
29:f:77:ALA:O	29:f:81:LYS:HG2	2.13	0.48
37:3:116:HIS:NE2	37:3:117:ASN:OD1	2.47	0.48
2:B:328:ILE:HG21	2:B:444:PHE:HE2	1.78	0.48
3:C:153:VAL:HG22	3:C:412:VAL:HG12	1.96	0.48
5:E:120:ARG:HD3	13:M:29:ILE:HG22	1.96	0.48
9:I:207:LEU:HD23	9:I:210:ASN:HD22	1.78	0.48
12:L:71:LEU:HD12	40:6:74:ILE:HG13	1.95	0.48
39:5:224:MET:HG3	39:5:229:GLN:HB2	1.95	0.48
1:A:277:VAL:HG21	1:A:593:THR:HG21	1.94	0.48
2:B:311:GLY:HA3	2:B:315:ASN:HD22	1.77	0.48
10:J:169:ARG:HE	27:d:89:ASP:HB3	1.78	0.48
12:L:76:SER:HA	12:L:79:ARG:HG3	1.95	0.48
13:M:96:VAL:HG13	13:M:114:PHE:HE1	1.79	0.48
53:1:402:UQ9:H7A	53:1:402:UQ9:H10	1.68	0.48
3:C:183:VAL:O	3:C:187:LEU:HB2	2.13	0.48
5:E:245:LEU:HA	5:E:248:ILE:HD12	1.94	0.48
8:H:180:ILE:HG12	8:H:185:TYR:HE2	1.79	0.48
22:Y:62:GLN:NE2	22:Y:75:THR:O	2.41	0.48
3:C:374:MET:HE1	9:I:180:PRO:HB3	1.96	0.48
11:K:82:GLY:HA2	11:K:120:ALA:O	2.13	0.48
34:n:98:SER:HB2	36:2:53:THR:H	1.79	0.48
35:1:157:ILE:HG21	35:1:245:LEU:HB2	1.96	0.48
39:5:16:TRP:CD1	39:5:122:MET:HB3	2.48	0.48
1:A:165:ARG:HD3	1:A:209:ASN:HB3	1.96	0.48
1:A:194:ASN:ND2	22:Y:160:THR:HG23	2.29	0.48
1:A:313:LEU:HB2	1:A:586:VAL:HG22	1.95	0.48
1:A:432:TRP:HB2	1:A:437:LEU:HD23	1.95	0.48
3:C:356:ALA:HB2	20:W:8:LEU:HD11	1.94	0.48
36:2:7:ILE:HG22	52:2:501:CDL:C79	2.44	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:5:647:ILE:HG23	52:5:701:CDL:H602	1.95	0.48
24:a:62:ASP:OD2	38:4:363:LYS:NZ	2.41	0.47
24:a:123:ARG:HB3	41:8:65:ARG:HE	1.78	0.47
52:4:502:CDL:H782	51:5:702:PLC:H9'2	1.96	0.47
39:5:265:ARG:HD2	39:5:265:ARG:HA	1.68	0.47
2:B:298:LEU:HD21	2:B:319:VAL:HG21	1.96	0.47
8:H:180:ILE:HG13	8:H:181:ASN:H	1.79	0.47
23:Z:14:THR:HG21	23:Z:35:SER:HB3	1.95	0.47
1:A:207:ARG:H	8:H:29:ILE:HG21	1.79	0.47
27:d:23:VAL:HG11	38:4:199:LEU:HD21	1.97	0.47
48:j:101:LMN:HBFA	38:4:276:MET:HG2	1.96	0.47
38:4:5:SER:HA	38:4:8:LEU:HD23	1.95	0.47
1:A:145:GLN:HG2	3:C:386:LEU:HD11	1.95	0.47
47:I:501:3PE:H391	35:1:319:LEU:HD21	1.97	0.47
36:2:58:LEU:HD11	40:6:161:ILE:HD11	1.97	0.47
11:K:139:PRO:HA	35:1:61:GLU:OE2	2.15	0.47
35:1:19:VAL:HG12	35:1:236:ILE:HD12	1.97	0.47
36:2:14:SER:HB3	37:3:104:TYR:CD1	2.50	0.47
3:C:129:TYR:HE2	7:G:216:LEU:HB2	1.78	0.47
9:I:217:GLU:HG2	31:h:79:PHE:HB2	1.96	0.47
51:1:401:PLC:H2	51:1:401:PLC:H1'1	1.73	0.47
38:4:228:HIS:H	38:4:229:VAL:HG23	1.80	0.47
1:A:410:ILE:HG22	1:A:481:LEU:H	1.80	0.47
2:B:101:MET:HG2	2:B:113:ARG:HH11	1.80	0.47
2:B:121:GLU:OE1	2:B:126:THR:OG1	2.28	0.47
2:B:176:ASN:HA	2:B:179:TYR:HD2	1.78	0.47
2:B:409:ARG:O	2:B:412:ASP:CB	2.58	0.47
45:B:502:FMN:O4'	45:B:502:FMN:O2'	2.27	0.47
3:C:97:VAL:CG2	11:K:83:LEU:HB3	2.44	0.47
5:E:140:TYR:OH	5:E:310:SER:OG	2.28	0.47
6:F:89:GLU:HA	6:F:92:GLU:HG2	1.97	0.47
7:G:86:ILE:O	23:Z:91:GLN:NE2	2.48	0.47
12:L:44:SER:OG	12:L:49:ASP:O	2.29	0.47
22:Y:79:ARG:HB3	22:Y:109:GLN:HE21	1.80	0.47
25:b:6:SER:HA	38:4:66:PHE:HD2	1.79	0.47
28:e:23:HIS:O	28:e:27:THR:HG23	2.15	0.47
31:h:45:PHE:CE2	31:h:77:TRP:HB3	2.50	0.47
1:A:534:ILE:HG13	1:A:652:ILE:HD13	1.96	0.47
2:B:283:ASN:HD22	2:B:360:ASN:HB2	1.79	0.47
9:I:103:TYR:CD1	9:I:103:TYR:C	2.89	0.47
2:B:63:LYS:H	2:B:258:ARG:HH12	1.62	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:125:GLN:HB2	8:H:179:ALA:HB3	1.96	0.47
10:J:166:VAL:HG11	38:4:200:PHE:HD1	1.79	0.47
11:K:78:PRO:HD2	11:K:106:ILE:O	2.15	0.47
51:W:201:PLC:H9A1	35:1:295:TRP:HH2	1.80	0.47
35:1:78:LEU:CD1	37:3:19:LEU:CD2	2.93	0.47
36:2:354:ILE:HD12	36:2:421:ILE:HG22	1.97	0.47
2:B:431:ASP:OD1	2:B:431:ASP:N	2.41	0.47
3:C:361:VAL:HG11	3:C:366:ILE:HD11	1.97	0.47
6:F:23:VAL:HG13	6:F:104:VAL:HG12	1.96	0.47
6:F:63:LYS:HA	6:F:68:ARG:HD3	1.96	0.47
19:U:56:CYS:HA	30:g:69:ARG:HD2	1.97	0.47
23:Z:62:SER:HB3	23:Z:67:ASN:HB3	1.96	0.47
34:n:83:MET:HE2	36:2:465:ASN:HB3	1.97	0.47
38:4:123:LEU:HD13	47:4:504:3PE:H2F1	1.96	0.47
2:B:219:GLU:OE1	2:B:226:ARG:NH1	2.47	0.46
6:F:128:GLU:O	7:G:87:GLN:NE2	2.47	0.46
32:i:83:THR:HG23	33:j:84:ARG:HB3	1.97	0.46
35:1:170:ILE:HD13	35:1:249:GLY:HA3	1.97	0.46
36:2:54:VAL:HG12	36:2:55:MET:HG2	1.96	0.46
38:4:100:LEU:HD11	38:4:119:LEU:HD12	1.97	0.46
1:A:575:ASN:OD1	1:A:702:SER:OG	2.26	0.46
7:G:202:ASP:HB3	7:G:205:PHE:HB2	1.97	0.46
15:P:17:SER:HB3	15:P:20:GLU:HG2	1.97	0.46
36:2:76:MET:HE3	36:2:80:SER:HB3	1.97	0.46
36:2:376:PRO:HB3	47:4:504:3PE:H3G2	1.97	0.46
38:4:251:LEU:HD23	38:4:310:MET:HG3	1.97	0.46
11:K:202:LYS:HB2	11:K:205:ARG:HB2	1.97	0.46
15:P:70:SER:O	15:P:74:VAL:HG13	2.14	0.46
22:Y:49:PRO:HB2	22:Y:51:GLU:HG2	1.96	0.46
35:1:58:LEU:HD13	37:3:22:ASN:HB2	1.97	0.46
35:1:191:ILE:HD12	35:1:311:PHE:HZ	1.80	0.46
38:4:35:LEU:HD21	38:4:126:LEU:HD22	1.97	0.46
38:4:211:TRP:HZ2	38:4:277:ILE:HD11	1.79	0.46
39:5:366:LEU:H	39:5:437:PHE:HA	1.80	0.46
5:E:162:ARG:NH1	5:E:251:ASP:O	2.49	0.46
28:e:31:GLY:HA2	28:e:34:MET:HG2	1.97	0.46
38:4:112:ASN:HB3	47:4:501:3PE:H31	1.97	0.46
47:4:503:3PE:H3D2	47:4:504:3PE:H3G1	1.96	0.46
1:A:696:ASN:HD21	1:A:699:MET:HB2	1.81	0.46
2:B:94:SER:HA	2:B:97:LYS:HB3	1.97	0.46
5:E:247:ARG:HD2	5:E:335:LEU:HD23	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:W:26:ARG:NH2	23:Z:30:ILE:O	2.48	0.46
21:X:152:ILE:HD11	36:2:119:HIS:CD2	2.51	0.46
51:1:401:PLC:H3'1	51:1:401:PLC:H2A2	1.96	0.46
52:2:501:CDL:H191	52:2:501:CDL:C38	2.45	0.46
38:4:259:LEU:HD11	38:4:329:ILE:HD11	1.96	0.46
1:A:484:VAL:HG13	1:A:488:ILE:HD11	1.98	0.46
4:D:14:ILE:HG21	35:1:290:MET:HE1	1.98	0.46
10:J:169:ARG:HH21	27:d:89:ASP:HA	1.81	0.46
12:L:7:ILE:O	12:L:11:SER:HB2	2.14	0.46
24:a:83:ASP:H	39:5:561:ASN:HD21	1.63	0.46
36:2:13:VAL:HG22	36:2:24:ILE:HD13	1.97	0.46
36:2:110:ASN:HD22	36:2:235:TYR:HE2	1.64	0.46
38:4:358:ILE:HD12	38:4:361:TYR:HE2	1.81	0.46
1:A:225:LEU:HB2	1:A:228:ASN:ND2	2.30	0.46
4:D:43:ASP:HB3	4:D:46:ASP:H	1.81	0.46
8:H:100:PRO:HG2	8:H:103:ARG:HG2	1.98	0.46
18:S:240:LYS:HE2	27:d:13:ASP:HB3	1.98	0.46
48:j:101:LMN:HCD	38:4:205:ASP:HB3	1.98	0.46
35:1:56:LYS:HB3	35:1:56:LYS:HE3	1.79	0.46
35:1:248:GLY:O	35:1:285:LYS:NZ	2.49	0.46
36:2:376:PRO:HG2	47:4:501:3PE:H2I2	1.98	0.46
38:4:207:GLN:HB3	38:4:269:ALA:HB2	1.96	0.46
10:J:143:ARG:HH12	36:2:255:ILE:HG22	1.80	0.46
10:J:175:THR:HG22	10:J:185:ILE:HD11	1.97	0.46
48:J:202:LMN:HBA	38:4:184:VAL:HG21	1.98	0.46
19:U:45:LYS:HD3	19:U:82:VAL:HG22	1.96	0.46
36:2:245:LEU:HD13	36:2:296:MET:HG3	1.97	0.46
38:4:235:HIS:NE2	38:4:247:ALA:HB2	2.31	0.46
5:E:110:ARG:HH12	5:E:137:ASN:HB3	1.81	0.46
8:H:90:MET:HE2	8:H:105:TYR:HD1	1.81	0.46
21:X:154:PRO:HG2	52:X:201:CDL:H642	1.96	0.46
31:h:35:LEU:HD12	31:h:35:LEU:HA	1.84	0.46
1:A:401:ILE:CG1	1:A:424:MET:HE1	2.45	0.46
1:A:627:ARG:HA	1:A:637:LEU:HD12	1.98	0.46
2:B:272:ASN:HD21	2:B:341:PHE:HB2	1.80	0.46
5:E:198:THR:OG1	5:E:254:THR:O	2.23	0.46
13:M:23:SER:HB3	13:M:27:ASN:HB2	1.96	0.46
16:Q:53:ASP:OD1	16:Q:54:MET:N	2.49	0.46
24:a:79:MET:HG3	39:5:161:LEU:HD11	1.98	0.46
35:1:78:LEU:HD23	35:1:78:LEU:HA	1.65	0.46
36:2:369:PHE:CE2	38:4:146:PRO:HB3	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:3:68:LEU:O	37:3:72:THR:OG1	2.28	0.46
2:B:401:PHE:HE2	2:B:414:LEU:HD22	1.82	0.45
7:G:126:ILE:HG22	7:G:142:TYR:HA	1.96	0.45
9:I:110:VAL:O	23:Z:45:ARG:NH2	2.49	0.45
47:J:203:3PE:H382	39:5:630:LEU:HB3	1.98	0.45
11:K:89:GLU:OE2	11:K:184:SER:N	2.49	0.45
39:5:296:ILE:HA	39:5:428:TYR:HB3	1.98	0.45
3:C:86:ASN:HB3	3:C:101:ILE:HD13	1.98	0.45
12:L:49:ASP:HA	42:9:7:SER:HA	1.98	0.45
12:L:69:ILE:HD12	36:2:139:LEU:HD11	1.98	0.45
36:2:7:ILE:CG2	52:2:501:CDL:H792	2.44	0.45
36:2:297:MET:HB3	36:2:297:MET:HE2	1.76	0.45
39:5:7:LEU:HA	39:5:10:ILE:HG22	1.96	0.45
2:B:401:PHE:CE2	2:B:414:LEU:HD22	2.52	0.45
3:C:302:PRO:HB3	23:Z:181:PHE:CD2	2.51	0.45
7:G:230:ARG:NH1	15:P:104:ASP:OD2	2.49	0.45
8:H:196:LEU:HG	8:H:206:PRO:HG3	1.98	0.45
10:J:93:ASP:OD1	10:J:93:ASP:N	2.49	0.45
36:2:100:LYS:HG2	36:2:144:TYR:HE1	1.81	0.45
38:4:123:LEU:HD22	47:4:504:3PE:H2D1	1.99	0.45
38:4:152:ILE:O	38:4:160:SER:HB2	2.17	0.45
39:5:446:ILE:HA	39:5:449:TYR:HD2	1.81	0.45
7:G:76:LYS:HD2	7:G:266:PHE:HE1	1.81	0.45
16:Q:81:LEU:HD12	16:Q:85:LEU:HD22	1.98	0.45
20:W:96:MET:HE3	42:9:63:VAL:HG21	1.99	0.45
52:X:201:CDL:H632	36:2:4:LEU:CD2	2.45	0.45
29:f:70:VAL:HB	29:f:75:GLU:HG2	1.97	0.45
36:2:234:ILE:HG22	36:2:324:PHE:CD1	2.51	0.45
39:5:183:LEU:O	39:5:187:VAL:HG23	2.16	0.45
39:5:557:ASP:O	39:5:561:ASN:HB2	2.17	0.45
39:5:638:ASN:HD21	39:5:640:ILE:HB	1.80	0.45
7:G:35:SER:HB2	7:G:38:ASN:HD22	1.81	0.45
48:J:204:LMN:HBL	48:J:204:LMN:HBT	1.68	0.45
18:S:62:ARG:O	18:S:65:GLN:NE2	2.50	0.45
38:4:137:PHE:O	38:4:141:PHE:HB2	2.16	0.45
39:5:12:PRO:HA	39:5:15:SER:HB3	1.97	0.45
3:C:371:ARG:NH2	9:I:179:CYS:O	2.32	0.45
35:1:133:LEU:HD22	40:6:76:THR:HG23	1.98	0.45
3:C:231:ARG:HH12	9:I:174:TYR:HE1	1.65	0.45
3:C:293:GLY:HA3	3:C:408:GLY:HA2	1.98	0.45
35:1:4:ASN:HB2	37:3:3:THR:HB	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:5:108:GLU:OE2	39:5:455:ASN:ND2	2.49	0.45
1:A:401:ILE:O	1:A:427:ARG:NH1	2.49	0.45
1:A:723:LYS:HE2	1:A:723:LYS:HB3	1.71	0.45
3:C:120:HIS:HB2	3:C:465:ASP:HB2	1.99	0.45
7:G:126:ILE:HG12	7:G:178:PHE:HB3	1.98	0.45
7:G:200:MET:HE2	7:G:200:MET:HB3	1.88	0.45
22:Y:90:ARG:NH2	22:Y:106:GLN:OE1	2.49	0.45
22:Y:120:LYS:O	22:Y:124:LYS:HB2	2.16	0.45
35:1:41:PHE:HA	51:1:403:PLC:H63	1.98	0.45
37:3:76:TYR:CG	37:3:91:VAL:HG21	2.52	0.45
39:5:428:TYR:O	39:5:431:LYS:HB2	2.17	0.45
1:A:136:CYS:HB3	43:A:801:SF4:S3	2.57	0.45
3:C:257:ARG:HH22	23:Z:35:SER:HB2	1.82	0.45
6:F:99:LEU:HD11	9:I:55:PHE:HE2	1.78	0.45
10:J:119:ILE:HG21	48:J:204:LMN:HAY	1.99	0.45
20:W:56:ARG:NH1	35:1:335:ASP:O	2.45	0.45
1:A:188:ARG:HA	1:A:191:ARG:HE	1.82	0.45
2:B:281:SER:HB3	8:H:173:VAL:HG12	1.98	0.45
52:X:201:CDL:H641	36:2:4:LEU:HG	1.99	0.45
38:4:61:ASN:ND2	38:4:69:SER:OG	2.38	0.45
39:5:92:ILE:HD12	39:5:127:MET:HG3	1.98	0.45
3:C:179:GLU:HG3	3:C:346:ILE:HG21	1.99	0.44
3:C:210:ARG:HH22	11:K:88:VAL:CG1	2.30	0.44
5:E:56:ALA:HA	5:E:124:ILE:O	2.17	0.44
7:G:43:ARG:NH2	23:Z:46:VAL:O	2.50	0.44
9:I:123:TYR:HD2	9:I:127:GLU:HB3	1.81	0.44
10:J:183:ARG:HG2	38:4:405:ARG:CZ	2.48	0.44
21:X:60:LEU:HD23	36:2:438:VAL:HG22	1.99	0.44
1:A:41:ILE:HG12	1:A:107:VAL:HB	2.00	0.44
2:B:414:LEU:HD23	2:B:441:ILE:HD11	1.98	0.44
3:C:260:GLU:OE2	9:I:93:GLN:NE2	2.50	0.44
5:E:140:TYR:HH	5:E:310:SER:HG	1.62	0.44
5:E:150:ARG:CZ	11:K:41:MET:HE3	2.47	0.44
33:j:56:THR:HG23	33:j:60:LEU:HD12	2.00	0.44
35:1:219:TYR:HE2	35:1:227:PHE:HE2	1.64	0.44
38:4:317:VAL:HA	38:4:325:ILE:HD13	2.00	0.44
9:I:145:ILE:HD13	9:I:164:ILE:HG12	1.99	0.44
11:K:81:PHE:CD2	11:K:131:LEU:CG	3.00	0.44
24:a:64:ARG:HE	24:a:70:LEU:HD21	1.83	0.44
35:1:5:ILE:HG12	37:3:6:ILE:HD13	1.99	0.44
35:1:311:PHE:HA	35:1:315:ILE:HD12	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:4:505:T7X:O11	54:4:505:T7X:O2	2.35	0.44
39:5:310:MET:HE3	39:5:310:MET:HB2	1.82	0.44
1:A:157:ARG:HD3	23:Z:69:ILE:O	2.18	0.44
1:A:266:SER:HB2	1:A:289:ASN:HD22	1.81	0.44
5:E:109:LEU:HD11	5:E:129:ILE:HD13	1.99	0.44
9:I:104:PRO:O	31:h:63:TYR:OH	2.33	0.44
34:n:24:TRP:CH2	38:4:459:ILE:HD11	2.53	0.44
1:A:269:ARG:HB3	1:A:281:ILE:CG2	2.47	0.44
1:A:627:ARG:NE	1:A:639:TYR:O	2.41	0.44
3:C:124:GLU:HG2	7:G:210:LEU:HD11	1.99	0.44
50:Q:201:ZMP:H9A	17:R:50:ASN:HD22	1.82	0.44
21:X:155:TRP:CZ3	52:X:201:CDL:H351	2.53	0.44
35:1:340:LEU:HD11	40:6:148:THR:HG21	2.00	0.44
1:A:395:TYR:OH	1:A:533:ASP:OD1	2.27	0.44
9:I:165:ASP:OD2	9:I:168:LYS:NZ	2.37	0.44
17:R:37:ARG:HH21	26:c:9:TRP:HB2	1.83	0.44
29:f:26:VAL:O	29:f:30:ILE:HG12	2.17	0.44
38:4:297:ASP:OD1	38:4:298:LEU:N	2.46	0.44
41:8:16:HIS:CG	41:8:31:VAL:HG21	2.53	0.44
1:A:268:ILE:HG22	1:A:293:ILE:HD11	1.99	0.44
1:A:393:SER:HA	1:A:398:ASN:HD21	1.83	0.44
2:B:40:ILE:HD12	2:B:275:THR:HG21	1.99	0.44
2:B:131:GLU:HG3	2:B:289:THR:HG21	1.99	0.44
2:B:400:ARG:NH2	2:B:410:GLU:OE1	2.51	0.44
3:C:144:TYR:CD1	11:K:85:CYS:HA	2.53	0.44
7:G:164:PRO:HB3	15:P:14:PHE:HE2	1.83	0.44
9:I:123:TYR:CD2	9:I:127:GLU:HB3	2.53	0.44
47:I:501:3PE:H3E2	47:I:501:3PE:H3B2	1.57	0.44
20:W:89:LEU:HD11	20:W:104:ASP:HA	2.00	0.44
21:X:18:ASP:OD1	21:X:18:ASP:N	2.49	0.44
24:a:125:PHE:HB2	24:a:129:GLY:HA2	1.99	0.44
47:a:201:3PE:H271	47:a:201:3PE:H242	1.82	0.44
39:5:499:TYR:HA	39:5:502:THR:HG22	2.00	0.44
2:B:135:LYS:NZ	8:H:217:ASP:OD2	2.45	0.44
3:C:137:PRO:O	3:C:141:ARG:HG2	2.18	0.44
3:C:177:PHE:CZ	3:C:220:VAL:HG21	2.53	0.44
3:C:320:ASP:OD2	3:C:345:ARG:NH1	2.42	0.44
3:C:372:ASN:OD1	3:C:373:LEU:N	2.51	0.44
6:F:63:LYS:HE2	6:F:63:LYS:HB3	1.76	0.44
8:H:40:ASN:HB3	8:H:42:SER:H	1.83	0.44
10:J:128:ALA:HA	47:J:201:3PE:H3D2	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:S:52:ASN:HB3	18:S:55:LYS:HD3	2.00	0.44
38:4:103:ASN:O	38:4:115:TYR:OH	2.34	0.44
4:D:2:ALA:HB2	52:Z:201:CDL:HB21	2.00	0.43
7:G:130:ASP:HB3	7:G:138:PHE:CE1	2.53	0.43
7:G:142:TYR:HB2	7:G:155:LEU:HB3	1.99	0.43
21:X:154:PRO:HB3	52:2:501:CDL:H273	2.00	0.43
21:X:155:TRP:CD2	36:2:55:MET:HE1	2.52	0.43
28:e:34:MET:HE3	28:e:34:MET:HB2	1.82	0.43
1:A:320:PHE:HE2	31:h:133:VAL:O	2.01	0.43
1:A:348:ALA:HA	1:A:551:TRP:HB3	2.00	0.43
2:B:369:ILE:HD12	2:B:440:LEU:HD13	1.99	0.43
3:C:332:ARG:HE	3:C:456:THR:HB	1.82	0.43
3:C:371:ARG:HA	3:C:374:MET:HG3	2.00	0.43
5:E:29:GLN:HG2	15:P:120:LEU:HB3	1.99	0.43
5:E:57:THR:OG1	5:E:122:SER:OG	2.27	0.43
9:I:103:TYR:HH	31:h:70:MET:HG2	1.81	0.43
27:d:20:HIS:HB2	34:n:70:VAL:HG11	1.99	0.43
27:d:87:ARG:HE	38:4:201:VAL:HG22	1.83	0.43
36:2:100:LYS:HG2	36:2:144:TYR:CE1	2.53	0.43
39:5:454:SER:HB2	39:5:458:ILE:HD12	1.99	0.43
16:Q:96:VAL:HG11	16:Q:112:ALA:HB1	1.99	0.43
33:j:83:LYS:HA	33:j:83:LYS:HD3	1.82	0.43
35:1:8:ILE:HD13	37:3:6:ILE:HB	2.01	0.43
36:2:117:ILE:HG22	36:2:247:TYR:HB2	1.99	0.43
38:4:36:LEU:HD23	38:4:93:VAL:HG13	2.01	0.43
41:8:37:ARG:HB3	41:8:42:TYR:CE1	2.53	0.43
2:B:294:MET:HE3	2:B:294:MET:HB3	1.92	0.43
4:D:29:HIS:CD2	35:1:97:ILE:HG23	2.54	0.43
5:E:214:LEU:O	5:E:218:ALA:N	2.52	0.43
39:5:12:PRO:HB2	39:5:125:PHE:HB2	2.00	0.43
39:5:85:THR:O	39:5:89:LEU:HB2	2.18	0.43
2:B:284:VAL:HG21	2:B:306:CYS:HB3	2.01	0.43
3:C:191:CYS:HB3	3:C:203:PHE:HA	2.00	0.43
17:R:28:ASN:HD22	17:R:78:PRO:HA	1.83	0.43
18:S:95:ALA:HB1	18:S:130:TYR:HD1	1.84	0.43
24:a:47:PRO:HG2	24:a:50:LEU:HB2	2.00	0.43
38:4:111:SER:HB2	38:4:115:TYR:HE2	1.84	0.43
38:4:205:ASP:O	38:4:209:ILE:HG12	2.19	0.43
38:4:469:GLN:CD	39:5:69:ASN:H	2.27	0.43
39:5:623:ILE:O	39:5:627:SER:OG	2.28	0.43
2:B:371:ARG:HD2	2:B:371:ARG:HA	1.80	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:136:LEU:HD13	3:C:232:PRO:HD3	1.99	0.43
35:1:121:LEU:HD22	35:1:140:THR:HG21	2.00	0.43
36:2:208:LEU:HD12	36:2:244:ILE:HG23	1.98	0.43
38:4:55:PHE:HB3	47:4:504:3PE:H221	2.01	0.43
3:C:173:ILE:HD13	3:C:173:ILE:HG21	1.80	0.43
3:C:187:LEU:HD21	3:C:209:GLU:HB2	2.01	0.43
3:C:417:ASP:HB2	3:C:423:TYR:HB2	2.00	0.43
9:I:78:PHE:HZ	30:g:25:HIS:HA	1.81	0.43
12:L:20:ARG:HH12	40:6:84:GLU:HG3	1.83	0.43
17:R:82:PRO:HA	17:R:87:GLY:HA3	2.01	0.43
21:X:15:SER:OG	21:X:19:TYR:O	2.30	0.43
48:j:101:LMN:HBE	48:j:101:LMN:HBKA	1.82	0.43
36:2:82:LEU:HD11	36:2:325:MET:HE2	2.00	0.43
52:2:501:CDL:HA32	52:2:501:CDL:HA21	2.01	0.43
39:5:486:ASP:OD1	39:5:486:ASP:N	2.42	0.43
1:A:289:ASN:HA	1:A:423:VAL:HG11	2.01	0.43
1:A:565:ALA:HA	31:h:137:ARG:HD2	2.01	0.43
18:S:191:ILE:HD11	27:d:32:ARG:HG2	2.00	0.43
35:1:48:LEU:HA	35:1:51:PHE:HD2	1.83	0.43
52:5:701:CDL:H312	52:5:701:CDL:HA61	1.89	0.43
1:A:141:GLU:HB2	22:Y:68:THR:CG2	2.34	0.43
2:B:48:TYR:CD2	8:H:232:PRO:HG3	2.54	0.43
5:E:206:PHE:CD1	5:E:235:PRO:HB2	2.54	0.43
18:S:176:LEU:HG	52:4:502:CDL:H561	2.00	0.43
20:W:52:ILE:HG12	20:W:55:ARG:HH22	1.82	0.43
36:2:436:SER:HB3	36:2:439:LEU:HB3	2.01	0.43
42:9:46:GLU:HG3	42:9:52:LYS:H	1.84	0.43
42:9:57:LEU:HA	42:9:60:ILE:HG12	2.01	0.43
1:A:164:LYS:H	13:M:114:PHE:HE2	1.67	0.43
4:D:86:LEU:HD11	40:6:50:ILE:HG13	2.01	0.43
9:I:117:GLU:HB3	9:I:192:TYR:CE1	2.54	0.43
48:J:204:LMN:HBS	48:J:204:LMN:HBP	2.00	0.43
35:1:122:LEU:HD12	40:6:30:MET:HE1	2.01	0.43
37:3:58:LEU:HD21	37:3:110:ALA:HB1	2.01	0.43
38:4:259:LEU:HD23	38:4:263:LEU:HD12	2.00	0.43
39:5:383:SER:O	39:5:392:GLY:HA3	2.19	0.43
42:9:33:SER:O	42:9:33:SER:OG	2.33	0.43
1:A:145:GLN:HG3	3:C:382:ILE:HG23	2.01	0.42
2:B:127:CYS:SG	8:H:172:CYS:N	2.79	0.42
2:B:134:ARG:HG3	2:B:167:GLU:HG3	2.01	0.42
13:M:63:ARG:HH11	13:M:63:ARG:HD2	1.70	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:102:ILE:HG23	14:O:103:LEU:HD22	2.00	0.42
35:1:228:PHE:CZ	53:1:402:UQ9:C12	3.02	0.42
2:B:40:ILE:HG23	2:B:255:THR:HG21	2.00	0.42
5:E:100:GLY:HA2	9:I:198:GLU:OE2	2.19	0.42
13:M:96:VAL:HG13	13:M:114:PHE:CE1	2.54	0.42
15:P:95:GLN:HA	15:P:98:LYS:HG3	2.00	0.42
16:Q:81:LEU:HG	16:Q:87:LEU:HG	2.01	0.42
18:S:202:ARG:NH1	18:S:232:ASP:O	2.52	0.42
21:X:92:ALA:HB2	21:X:150:LEU:HD13	2.01	0.42
36:2:454:PHE:HZ	47:4:503:3PE:H3B1	1.84	0.42
39:5:230:PHE:HB2	39:5:287:THR:HG22	2.01	0.42
3:C:135:ALA:HA	3:C:138:TYR:HD2	1.85	0.42
5:E:134:GLU:HB3	5:E:139:ASN:HA	2.01	0.42
6:F:46:LEU:HD13	6:F:104:VAL:HG22	2.01	0.42
11:K:81:PHE:CE2	11:K:131:LEU:CG	3.03	0.42
11:K:124:THR:HA	11:K:163:VAL:HA	2.00	0.42
47:a:201:3PE:H291	38:4:422:ILE:HD13	2.01	0.42
34:n:111:ILE:HD11	40:6:144:THR:HG21	2.01	0.42
37:3:94:PHE:CD1	40:6:166:ALA:HB2	2.54	0.42
52:5:701:CDL:H552	52:5:701:CDL:H522	1.74	0.42
1:A:168:GLU:N	13:M:116:ASN:HD22	2.16	0.42
1:A:270:ILE:HD13	1:A:593:THR:HG23	2.02	0.42
2:B:39:ARG:CZ	2:B:291:GLU:HB3	2.50	0.42
8:H:189:THR:HG22	8:H:191:GLU:H	1.84	0.42
20:W:88:GLN:OE1	20:W:91:ARG:NH2	2.52	0.42
21:X:130:SER:O	37:3:85:ASN:ND2	2.47	0.42
24:a:66:LEU:HD12	24:a:66:LEU:HA	1.86	0.42
32:i:15:MET:HE2	47:i:101:3PE:H332	2.00	0.42
3:C:342:GLN:O	3:C:346:ILE:HG12	2.19	0.42
12:L:62:LEU:HD11	36:2:128:VAL:HG22	2.02	0.42
14:O:88:GLU:OE1	14:O:101:TYR:OH	2.33	0.42
21:X:151:PHE:HE1	36:2:39:ASP:HB3	1.84	0.42
36:2:299:LEU:HA	36:2:302:LEU:HD23	2.00	0.42
40:6:30:MET:HE2	40:6:30:MET:HB2	1.93	0.42
4:D:10:PRO:HB2	35:1:25:ALA:HB2	2.02	0.42
5:E:267:PHE:HE2	5:E:340:LEU:HB3	1.84	0.42
5:E:363:LEU:HD12	5:E:363:LEU:HA	1.88	0.42
7:G:92:TRP:HA	23:Z:86:THR:HA	2.01	0.42
8:H:103:ARG:HA	8:H:103:ARG:HD3	1.93	0.42
35:1:80:THR:OG1	35:1:119:GLY:HA3	2.20	0.42
42:9:25:CYS:SG	42:9:40:ASN:ND2	2.91	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:ARG:HD3	1:A:81:ARG:HA	1.78	0.42
2:B:137:PRO:O	2:B:141:VAL:HG23	2.20	0.42
3:C:80:ILE:HD12	3:C:80:ILE:HA	1.85	0.42
17:R:34:GLN:OE1	17:R:38:GLN:NE2	2.53	0.42
19:U:117:LEU:HD23	19:U:172:LEU:HD13	2.01	0.42
38:4:223:PRO:HB3	38:4:228:HIS:HA	2.01	0.42
39:5:136:TYR:HD2	39:5:188:ILE:HG21	1.84	0.42
39:5:554:LEU:C	39:5:556:SER:H	2.23	0.42
1:A:286:GLU:HG3	22:Y:138:LYS:H	1.84	0.42
1:A:385:PRO:O	1:A:387:HIS:ND1	2.53	0.42
3:C:202:PRO:HG2	3:C:265:LEU:HD11	2.02	0.42
5:E:32:ASN:O	5:E:40:LEU:HB2	2.20	0.42
5:E:65:LEU:HD12	5:E:205:MET:HE1	2.02	0.42
19:U:42:ILE:HD11	19:U:83:ILE:HD11	2.01	0.42
19:U:136:ARG:HH22	30:g:53:PRO:HG2	1.83	0.42
25:b:53:VAL:HG21	55:2:503:PSC:H082	2.01	0.42
2:B:319:VAL:HG23	2:B:358:VAL:HG12	2.02	0.42
3:C:49:GLN:HG3	3:C:65:TYR:HA	2.02	0.42
11:K:81:PHE:CZ	11:K:127:MET:HG2	2.54	0.42
18:S:193:PHE:HA	18:S:196:LYS:HE3	2.02	0.42
35:1:146:TYR:CZ	35:1:312:CYS:HB2	2.55	0.42
3:C:306:ARG:NH2	3:C:404:GLU:OE1	2.53	0.42
3:C:337:MET:HA	3:C:340:PHE:HD2	1.85	0.42
5:E:131:ARG:NH1	46:E:401:NDP:H2B	2.34	0.42
14:O:94:SER:HB2	14:O:96:ASN:OD1	2.20	0.42
35:1:194:VAL:HG13	35:1:199:ARG:HB2	2.02	0.42
41:8:55:GLU:O	41:8:59:VAL:HG13	2.19	0.42
1:A:76:ILE:HD11	22:Y:142:LYS:HB3	2.02	0.41
1:A:276:GLU:OE2	31:h:126:LYS:CE	2.59	0.41
2:B:317:LEU:HB2	2:B:361:LYS:HA	2.02	0.41
3:C:89:PRO:HB3	11:K:127:MET:HE1	2.02	0.41
3:C:97:VAL:HG21	11:K:83:LEU:HB3	2.02	0.41
4:D:40:PHE:HB2	35:1:167:THR:HG21	2.02	0.41
7:G:176:ASN:HD21	15:P:2:ALA:HB3	1.85	0.41
11:K:82:GLY:HA2	11:K:120:ALA:C	2.45	0.41
17:R:105:ASN:HD22	17:R:108:GLU:HB3	1.84	0.41
52:X:201:CDL:OA7	37:3:85:ASN:HB3	2.20	0.41
52:X:201:CDL:OA7	52:X:201:CDL:CA3	2.68	0.41
27:d:71:LEU:HB2	33:j:84:ARG:HH22	1.85	0.41
27:d:73:MET:HE3	27:d:73:MET:HB2	1.83	0.41
33:j:43:GLN:HG3	39:5:590:VAL:HG21	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:5:215:ILE:HG22	39:5:216:MET:HE2	2.02	0.41
4:D:7:ALA:HB1	35:1:29:THR:HG22	2.01	0.41
8:H:186:GLU:N	8:H:210:PRO:O	2.48	0.41
14:O:84:ILE:HG22	14:O:85:PRO:O	2.19	0.41
50:Q:201:ZMP:H12	17:R:50:ASN:HB3	2.01	0.41
34:n:70:VAL:HG13	38:4:196:ASN:HD21	1.85	0.41
35:1:16:LEU:HA	35:1:19:VAL:HG22	2.02	0.41
36:2:132:LEU:HD13	40:6:168:VAL:HG22	2.00	0.41
38:4:36:LEU:O	38:4:40:VAL:HG23	2.20	0.41
38:4:57:PHE:HB2	38:4:68:LEU:HD11	2.02	0.41
54:4:505:T7X:O2	54:4:505:T7X:P1	2.77	0.41
39:5:103:SER:HB2	39:5:117:PHE:HE1	1.85	0.41
1:A:313:LEU:HD23	1:A:320:PHE:HB3	2.01	0.41
2:B:121:GLU:HG2	2:B:129:ASP:HB2	2.00	0.41
8:H:91:ASN:O	8:H:95:LYS:HG2	2.20	0.41
9:I:70:ALA:HB2	30:g:21:HIS:CE1	2.55	0.41
19:U:35:LEU:HG	20:W:69:LEU:HD22	2.02	0.41
38:4:281:SER:HA	38:4:284:THR:HG22	2.02	0.41
39:5:465:LEU:HD23	39:5:465:LEU:HA	1.91	0.41
39:5:586:ARG:HD3	39:5:586:ARG:HA	1.91	0.41
40:6:158:ASN:HB3	40:6:161:ILE:HD12	2.01	0.41
7:G:120:TYR:HB3	7:G:144:PHE:HB3	2.03	0.41
8:H:119:MET:HE3	8:H:119:MET:HB3	1.87	0.41
16:Q:58:ARG:NH2	16:Q:102:GLU:OE2	2.53	0.41
18:S:113:ASN:ND2	38:4:16:ARG:HH22	2.18	0.41
47:S:501:3PE:H11	38:4:15:ASN:HD21	1.85	0.41
24:a:76:LEU:O	24:a:84:ARG:NH1	2.51	0.41
35:1:11:PHE:CD2	35:1:99:LEU:HD11	2.55	0.41
35:1:16:LEU:HA	35:1:16:LEU:HD23	1.93	0.41
35:1:199:ARG:HD2	35:1:199:ARG:HA	1.80	0.41
54:4:505:T7X:O12	54:4:505:T7X:C8	2.69	0.41
39:5:473:GLY:O	39:5:477:LYS:HB2	2.20	0.41
39:5:595:LEU:HD11	52:5:701:CDL:H161	2.02	0.41
2:B:393:TRP:CD1	2:B:417:LEU:HD13	2.55	0.41
3:C:357:GLY:HA2	7:G:53:VAL:HG21	2.02	0.41
4:D:9:LEU:HD23	4:D:9:LEU:HA	1.92	0.41
8:H:133:GLN:NE2	8:H:138:ASP:OD2	2.47	0.41
11:K:82:GLY:HA3	11:K:120:ALA:O	2.20	0.41
18:S:203:VAL:HG21	18:S:222:ILE:HG23	2.02	0.41
19:U:50:ASN:HB3	20:W:71:PRO:HG2	2.02	0.41
21:X:154:PRO:CG	52:X:201:CDL:H641	2.49	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:a:52:ASN:HB2	24:a:55:LYS:HE2	2.02	0.41
31:h:45:PHE:HZ	31:h:73:VAL:HG13	1.85	0.41
3:C:97:VAL:HB	11:K:83:LEU:HB3	2.02	0.41
3:C:118:LEU:HD23	11:K:126:LYS:HG2	2.01	0.41
5:E:333:LEU:O	15:P:109:ARG:NH2	2.54	0.41
8:H:216:ARG:H	8:H:219:GLU:HG3	1.85	0.41
11:K:138:MET:O	11:K:142:ARG:NH2	2.32	0.41
11:K:196:ARG:CZ	11:K:196:ARG:HB2	2.49	0.41
19:U:14:ASP:OD1	20:W:91:ARG:NH1	2.54	0.41
35:1:86:ILE:HA	37:3:7:PHE:HE2	1.85	0.41
53:1:402:UQ9:H17A	53:1:402:UQ9:H20	1.69	0.41
36:2:334:ILE:HG21	36:2:344:ILE:HD12	2.02	0.41
38:4:157:SER:HB2	38:4:237:GLU:OE2	2.21	0.41
39:5:312:GLN:HB3	39:5:331:HIS:HE1	1.86	0.41
1:A:132:ASP:O	1:A:136:CYS:N	2.53	0.41
1:A:252:LEU:HD13	1:A:271:ASP:HB3	2.03	0.41
2:B:440:LEU:HD12	2:B:444:PHE:HB2	2.03	0.41
3:C:77:ASN:HD21	12:L:80:LEU:HD23	1.85	0.41
7:G:198:ARG:HD2	7:G:203:TYR:HA	2.03	0.41
9:I:190:VAL:HB	11:K:186:ALA:HB2	2.03	0.41
10:J:127:ALA:HB1	47:J:201:3PE:H381	2.01	0.41
16:Q:57:GLU:HA	16:Q:60:VAL:HG22	2.02	0.41
39:5:253:ALA:O	39:5:257:THR:HG23	2.21	0.41
2:B:283:ASN:ND2	8:H:134:LEU:HB3	2.36	0.41
6:F:125:GLU:OE2	23:Z:129:THR:OG1	2.29	0.41
7:G:37:GLU:OE1	7:G:37:GLU:N	2.51	0.41
15:P:6:THR:HG21	15:P:90:TRP:HH2	1.85	0.41
15:P:42:LEU:HD21	15:P:89:ALA:HB2	2.01	0.41
17:R:58:LEU:HA	17:R:61:ARG:HB3	2.03	0.41
36:2:352:GLY:HA3	36:2:424:LYS:HB2	2.02	0.41
40:6:47:LEU:HG	40:6:59:TYR:HE2	1.85	0.41
42:9:61:GLU:OE1	42:9:65:LYS:NZ	2.53	0.41
1:A:405:GLU:HG3	1:A:427:ARG:NH1	2.26	0.41
2:B:68:ILE:HD13	2:B:145:LEU:HD21	2.02	0.41
2:B:158:ILE:HB	2:B:199:ILE:HG12	2.03	0.41
2:B:159:TYR:CG	2:B:214:LEU:HD11	2.55	0.41
3:C:195:MET:HG3	3:C:200:LEU:HG	2.03	0.41
3:C:419:SER:OG	3:C:420:GLU:N	2.54	0.41
7:G:92:TRP:HB2	23:Z:86:THR:HG22	2.02	0.41
8:H:73:PRO:O	8:H:76:ASP:HB3	2.21	0.41
9:I:123:TYR:CE1	9:I:129:ARG:HG2	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:81:PHE:O	11:K:83:LEU:HD21	2.20	0.41
18:S:68:PRO:HD2	18:S:71:LYS:HE2	2.03	0.41
18:S:182:VAL:O	18:S:186:LYS:HB2	2.21	0.41
21:X:147:ILE:HA	21:X:147:ILE:HD12	1.81	0.41
23:Z:14:THR:HG21	23:Z:37:GLY:H	1.86	0.41
35:1:50:ALA:HB1	53:1:402:UQ9:H18	2.02	0.41
35:1:82:ILE:HD11	37:3:12:PRO:HA	2.02	0.41
35:1:86:ILE:HA	35:1:86:ILE:HD13	1.91	0.41
36:2:34:LEU:HD23	36:2:34:LEU:HA	1.91	0.41
37:3:96:LEU:HD23	37:3:96:LEU:HA	1.93	0.41
39:5:33:ARG:O	39:5:37:THR:OG1	2.30	0.41
39:5:123:PHE:HD2	39:5:249:LEU:HD13	1.85	0.41
1:A:131:LEU:HD12	13:M:112:LYS:O	2.21	0.41
3:C:129:TYR:HD2	7:G:216:LEU:HD22	1.86	0.41
7:G:224:TRP:CZ3	11:K:132:ARG:HG2	2.56	0.41
10:J:78:TYR:HB3	39:5:644:PRO:HG3	2.03	0.41
27:d:55:SER:OG	27:d:58:ASN:OD1	2.37	0.41
35:1:226:PHE:CE2	37:3:19:LEU:HB3	2.54	0.41
35:1:235:ILE:HG23	35:1:293:PHE:HD2	1.85	0.41
36:2:302:LEU:HD21	36:2:390:ILE:HD13	2.03	0.41
38:4:124:VAL:HG22	47:4:504:3PE:H2I3	2.02	0.41
1:A:81:ARG:NH2	2:B:426:ILE:HG12	2.33	0.40
3:C:175:THR:OG1	3:C:312:ASP:O	2.36	0.40
5:E:214:LEU:HA	5:E:214:LEU:HD23	1.77	0.40
9:I:209:ALA:HB2	13:M:73:PRO:HB3	2.02	0.40
24:a:31:LYS:HE2	24:a:31:LYS:HB2	1.83	0.40
27:d:14:ASP:OD1	27:d:14:ASP:N	2.54	0.40
47:i:101:3PE:H261	38:4:377:ILE:HD11	2.02	0.40
35:1:67:GLU:HB2	35:1:127:SER:HA	2.03	0.40
38:4:221:LYS:HB3	38:4:221:LYS:HE3	1.90	0.40
52:4:502:CDL:H631	52:4:502:CDL:H602	1.69	0.40
39:5:71:ASP:N	39:5:71:ASP:OD1	2.53	0.40
39:5:294:ILE:HG12	39:5:554:LEU:HD23	2.03	0.40
1:A:355:GLU:HG2	1:A:357:GLU:H	1.86	0.40
1:A:401:ILE:HG12	1:A:424:MET:HE1	2.02	0.40
9:I:129:ARG:HE	9:I:183:ALA:HA	1.86	0.40
10:J:39:ALA:HB2	47:J:203:3PE:H392	2.03	0.40
52:X:201:CDL:OA9	52:X:201:CDL:CA4	2.69	0.40
31:h:69:ASP:HB3	31:h:71:SER:H	1.86	0.40
33:j:38:TRP:O	33:j:45:ARG:NH1	2.54	0.40
35:1:137:ILE:HD13	35:1:137:ILE:HA	1.95	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:3:111:LEU:HA	37:3:111:LEU:HD23	1.91	0.40
38:4:389:THR:HG23	38:4:391:ASN:N	2.36	0.40
1:A:142:CYS:HB3	1:A:145:GLN:HB3	2.02	0.40
1:A:717:PHE:HA	1:A:723:LYS:HD2	2.03	0.40
2:B:145:LEU:HD12	2:B:195:PHE:CD2	2.56	0.40
9:I:88:TYR:CE1	51:W:202:PLC:H6'2	2.57	0.40
13:M:29:ILE:H	13:M:29:ILE:HG12	1.57	0.40
15:P:6:THR:HG21	15:P:90:TRP:CH2	2.56	0.40
16:Q:48:HIS:NE2	39:5:446:ILE:HD11	2.36	0.40
18:S:227:ILE:HG12	27:d:44:VAL:HG22	2.03	0.40
19:U:89:SER:HB2	19:U:126:LEU:HD21	2.03	0.40
24:a:101:LEU:HD23	24:a:101:LEU:HA	1.92	0.40
47:b:201:3PE:H2C1	38:4:147:LEU:HD21	2.04	0.40
27:d:9:LEU:HD23	27:d:9:LEU:HA	1.96	0.40
1:A:161:ILE:HG21	2:B:483:LEU:HD11	2.03	0.40
2:B:80:LYS:HE2	2:B:96:LEU:HD23	2.03	0.40
2:B:130:ARG:NE	2:B:167:GLU:OE2	2.54	0.40
2:B:483:LEU:HA	2:B:484:PRO:HD2	1.93	0.40
9:I:207:LEU:HD23	9:I:207:LEU:HA	1.89	0.40
10:J:46:ALA:HA	40:6:96:LEU:HD22	2.04	0.40
11:K:208:TYR:O	11:K:208:TYR:CG	2.75	0.40
39:5:349:ILE:HG22	39:5:370:LEU:HD22	2.04	0.40
42:9:44:TYR:O	42:9:47:CYS:HB3	2.22	0.40
1:A:577:ASP:H	1:A:580:ALA:HB3	1.86	0.40
3:C:44:VAL:HA	3:C:48:HIS:CD2	2.56	0.40
3:C:107:GLU:HB3	3:C:446:PHE:HD1	1.85	0.40
3:C:204:LEU:HD22	35:1:34:GLN:HB3	2.04	0.40
5:E:140:TYR:HD2	5:E:178:GLU:HG3	1.87	0.40
5:E:145:VAL:HG21	5:E:185:LEU:HB3	2.04	0.40
5:E:213:PHE:HB3	5:E:214:LEU:H	1.67	0.40
12:L:7:ILE:O	12:L:11:SER:CB	2.70	0.40
47:a:201:3PE:H322	39:5:172:LEU:HB3	2.04	0.40
35:1:69:ASN:HB2	35:1:72:ILE:HB	2.03	0.40
39:5:422:ALA:O	39:5:425:THR:HG22	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	690/728 (95%)	641 (93%)	49 (7%)	0	100	100
2	B	454/488 (93%)	424 (93%)	30 (7%)	0	100	100
3	C	429/466 (92%)	402 (94%)	26 (6%)	1 (0%)	43	66
4	D	84/87 (97%)	77 (92%)	7 (8%)	0	100	100
5	E	309/375 (82%)	291 (94%)	18 (6%)	0	100	100
6	F	119/144 (83%)	112 (94%)	7 (6%)	0	100	100
7	G	237/281 (84%)	228 (96%)	8 (3%)	1 (0%)	30	53
8	H	214/243 (88%)	194 (91%)	19 (9%)	1 (0%)	24	49
9	I	188/229 (82%)	179 (95%)	9 (5%)	0	100	100
10	J	177/198 (89%)	169 (96%)	8 (4%)	0	100	100
11	K	173/210 (82%)	161 (93%)	11 (6%)	1 (1%)	21	45
12	L	87/89 (98%)	86 (99%)	1 (1%)	0	100	100
13	M	115/136 (85%)	104 (90%)	11 (10%)	0	100	100
14	O	75/109 (69%)	69 (92%)	6 (8%)	0	100	100
15	P	121/124 (98%)	118 (98%)	3 (2%)	0	100	100
16	Q	83/132 (63%)	82 (99%)	1 (1%)	0	100	100
17	R	104/109 (95%)	96 (92%)	8 (8%)	0	100	100
18	S	168/249 (68%)	160 (95%)	8 (5%)	0	100	100
19	U	169/172 (98%)	161 (95%)	8 (5%)	0	100	100
20	W	119/123 (97%)	114 (96%)	5 (4%)	0	100	100
21	X	165/169 (98%)	160 (97%)	5 (3%)	0	100	100
22	Y	121/161 (75%)	117 (97%)	4 (3%)	0	100	100
23	Z	179/182 (98%)	167 (93%)	12 (7%)	0	100	100
24	a	122/149 (82%)	114 (93%)	8 (7%)	0	100	100
25	b	62/74 (84%)	61 (98%)	1 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	c	42/60 (70%)	37 (88%)	5 (12%)	0	100	100
27	d	88/92 (96%)	86 (98%)	2 (2%)	0	100	100
28	e	50/67 (75%)	49 (98%)	1 (2%)	0	100	100
29	f	78/87 (90%)	73 (94%)	5 (6%)	0	100	100
30	g	74/78 (95%)	70 (95%)	3 (4%)	1 (1%)	9	24
31	h	134/138 (97%)	126 (94%)	7 (5%)	1 (1%)	18	40
32	i	81/90 (90%)	74 (91%)	7 (9%)	0	100	100
33	j	88/93 (95%)	81 (92%)	7 (8%)	0	100	100
34	n	112/120 (93%)	102 (91%)	10 (9%)	0	100	100
35	1	325/341 (95%)	306 (94%)	19 (6%)	0	100	100
36	2	467/469 (100%)	449 (96%)	18 (4%)	0	100	100
37	3	112/128 (88%)	103 (92%)	9 (8%)	0	100	100
38	4	483/486 (99%)	464 (96%)	19 (4%)	0	100	100
39	5	652/655 (100%)	624 (96%)	26 (4%)	2 (0%)	36	59
40	6	178/185 (96%)	169 (95%)	9 (5%)	0	100	100
41	8	75/99 (76%)	71 (95%)	4 (5%)	0	100	100
42	9	84/89 (94%)	76 (90%)	8 (10%)	0	100	100
All	All	7887/8704 (91%)	7447 (94%)	432 (6%)	8 (0%)	49	72

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	97	VAL
7	G	94	ASP
11	K	85	CYS
39	5	555	VAL
31	h	108	PRO
8	H	30	VAL
39	5	556	SER
30	g	12	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	565/595 (95%)	565 (100%)	0	100	100
2	B	364/389 (94%)	360 (99%)	4 (1%)	65	80
3	C	368/394 (93%)	367 (100%)	1 (0%)	86	92
4	D	68/69 (99%)	68 (100%)	0	100	100
5	E	274/329 (83%)	272 (99%)	2 (1%)	76	87
6	F	109/129 (84%)	108 (99%)	1 (1%)	70	83
7	G	216/245 (88%)	216 (100%)	0	100	100
8	H	191/212 (90%)	189 (99%)	2 (1%)	68	82
9	I	156/187 (83%)	156 (100%)	0	100	100
10	J	130/147 (88%)	130 (100%)	0	100	100
11	K	152/180 (84%)	151 (99%)	1 (1%)	76	87
12	L	77/77 (100%)	76 (99%)	1 (1%)	61	78
13	M	97/115 (84%)	96 (99%)	1 (1%)	68	82
14	O	65/91 (71%)	65 (100%)	0	100	100
15	P	108/109 (99%)	108 (100%)	0	100	100
16	Q	72/111 (65%)	72 (100%)	0	100	100
17	R	97/100 (97%)	97 (100%)	0	100	100
18	S	149/211 (71%)	149 (100%)	0	100	100
19	U	147/148 (99%)	146 (99%)	1 (1%)	76	87
20	W	100/102 (98%)	100 (100%)	0	100	100
21	X	131/133 (98%)	131 (100%)	0	100	100
22	Y	105/140 (75%)	105 (100%)	0	100	100
23	Z	147/148 (99%)	147 (100%)	0	100	100
24	a	108/129 (84%)	107 (99%)	1 (1%)	70	83
25	b	50/59 (85%)	50 (100%)	0	100	100
26	c	30/45 (67%)	30 (100%)	0	100	100
27	d	83/85 (98%)	83 (100%)	0	100	100
28	e	44/55 (80%)	44 (100%)	0	100	100
29	f	69/73 (94%)	69 (100%)	0	100	100
30	g	62/64 (97%)	62 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	h	121/123 (98%)	121 (100%)	0	100	100
32	i	64/68 (94%)	64 (100%)	0	100	100
33	j	71/73 (97%)	71 (100%)	0	100	100
34	n	98/102 (96%)	98 (100%)	0	100	100
35	1	292/302 (97%)	289 (99%)	3 (1%)	68	82
36	2	433/433 (100%)	432 (100%)	1 (0%)	87	94
37	3	104/114 (91%)	104 (100%)	0	100	100
38	4	433/434 (100%)	432 (100%)	1 (0%)	87	94
39	5	579/580 (100%)	578 (100%)	1 (0%)	87	94
40	6	162/167 (97%)	160 (99%)	2 (1%)	63	79
41	8	68/76 (90%)	67 (98%)	1 (2%)	57	76
42	9	73/76 (96%)	72 (99%)	1 (1%)	59	77
All	All	6832/7419 (92%)	6807 (100%)	25 (0%)	81	92

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	34	LEU
2	B	68	ILE
2	B	431	ASP
2	B	459	VAL
3	C	78	THR
5	E	135	THR
5	E	278	GLU
6	F	44	PRO
8	H	30	VAL
8	H	36	THR
11	K	85	CYS
12	L	51	SER
13	M	29	ILE
19	U	138	ASP
24	a	82	PRO
35	1	5	ILE
35	1	82	ILE
35	1	86	ILE
36	2	378	LEU
38	4	8	LEU
39	5	525	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
40	6	91	ILE
40	6	111	ILE
41	8	63	GLN
42	9	25	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (117) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	194	ASN
1	A	285	HIS
1	A	398	ASN
1	A	499	ASN
1	A	696	ASN
2	B	30	GLN
2	B	42	GLN
2	B	285	ASN
2	B	315	ASN
3	C	57	HIS
3	C	77	ASN
3	C	120	HIS
3	C	445	HIS
4	D	33	ASN
4	D	60	GLN
5	E	62	ASN
5	E	170	ASN
5	E	234	ASN
5	E	237	HIS
5	E	269	GLN
6	F	73	ASN
6	F	77	HIS
6	F	93	ASN
6	F	106	GLN
6	F	108	HIS
7	G	38	ASN
7	G	208	HIS
8	H	91	ASN
8	H	146	ASN
8	H	174	ASN
9	I	210	ASN
10	J	96	ASN
10	J	186	ASN
11	K	100	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	K	158	HIS
12	L	43	ASN
13	M	72	GLN
13	M	116	ASN
13	M	123	HIS
14	O	97	GLN
15	P	80	HIS
15	P	107	GLN
15	P	122	ASN
17	R	28	ASN
17	R	38	GLN
17	R	45	HIS
17	R	50	ASN
17	R	93	ASN
18	S	113	ASN
18	S	166	ASN
18	S	201	GLN
18	S	211	ASN
19	U	17	ASN
19	U	50	ASN
19	U	127	ASN
20	W	22	ASN
21	X	142	ASN
21	X	157	ASN
22	Y	63	GLN
22	Y	109	GLN
22	Y	157	HIS
23	Z	79	HIS
24	a	52	ASN
26	c	25	ASN
27	d	4	HIS
27	d	69	GLN
29	f	11	HIS
31	h	25	ASN
31	h	51	GLN
31	h	55	HIS
32	i	78	HIS
33	j	73	GLN
34	n	45	ASN
34	n	64	ASN
34	n	95	HIS
35	1	310	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	2	50	GLN
36	2	86	ASN
36	2	90	ASN
36	2	173	ASN
36	2	185	HIS
36	2	227	ASN
36	2	339	ASN
36	2	385	ASN
36	2	422	GLN
36	2	469	ASN
37	3	22	ASN
38	4	15	ASN
38	4	56	ASN
38	4	103	ASN
38	4	128	ASN
38	4	153	HIS
38	4	193	ASN
38	4	196	ASN
38	4	270	GLN
38	4	355	HIS
38	4	371	GLN
38	4	424	GLN
38	4	429	ASN
38	4	480	ASN
39	5	25	GLN
39	5	66	ASN
39	5	78	ASN
39	5	112	HIS
39	5	229	GLN
39	5	299	ASN
39	5	335	HIS
39	5	450	ASN
39	5	491	HIS
39	5	552	GLN
39	5	562	HIS
39	5	578	HIS
39	5	602	ASN
39	5	638	ASN
40	6	81	ASN
40	6	143	ASN
40	6	152	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 44 ligands modelled in this entry, 1 is monoatomic - leaving 43 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	$\# Z > 2$
44	FES	A	803	1	0,4,4	-	-	-		
50	ZMP	O	201	14	27,32,36	1.69	5 (18%)	31,39,45	1.88	7 (22%)
51	PLC	W	201	-	40,40,41	1.35	5 (12%)	46,48,49	1.13	2 (4%)
47	3PE	4	503	-	41,41,50	1.05	4 (9%)	44,46,55	1.28	3 (6%)
53	UQ9	1	402	-	35,35,58	2.53	14 (40%)	43,45,73	2.13	13 (30%)
47	3PE	J	201	-	40,40,50	0.96	3 (7%)	43,45,55	1.08	2 (4%)
48	LMN	J	202	-	72,72,72	1.63	12 (16%)	92,98,98	1.97	29 (31%)
52	CDL	X	201	-	85,85,99	0.67	1 (1%)	91,97,111	0.87	4 (4%)
54	T7X	2	504	-	52,52,61	0.53	0	61,64,73	0.98	4 (6%)
45	FMN	B	502	-	33,33,33	2.94	13 (39%)	48,50,50	1.65	10 (20%)
47	3PE	i	101	-	41,41,50	0.96	4 (9%)	44,46,55	1.22	2 (4%)
47	3PE	b	201	-	41,41,50	0.95	3 (7%)	44,46,55	1.19	2 (4%)
47	3PE	S	501	-	41,41,50	0.95	4 (9%)	44,46,55	1.09	1 (2%)
51	PLC	1	403	-	34,34,41	1.50	7 (20%)	40,42,49	1.25	3 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
50	ZMP	Q	201	16	27,32,36	1.63	6 (22%)	31,39,45	2.27	8 (25%)
46	NDP	E	401	-	51,52,52	3.63	24 (47%)	71,80,80	2.05	13 (18%)
51	PLC	5	702	-	41,41,41	1.33	5 (12%)	47,49,49	1.14	2 (4%)
47	3PE	3	201	-	42,42,50	0.30	0	45,47,55	0.36	0
52	CDL	2	501	-	82,82,99	0.50	0	88,94,111	0.68	3 (3%)
47	3PE	I	501	-	50,50,50	0.90	3 (6%)	53,55,55	1.05	3 (5%)
55	PSC	2	503	-	51,51,51	1.03	5 (9%)	57,59,59	1.08	3 (5%)
52	CDL	4	502	-	91,91,99	0.93	6 (6%)	97,103,111	1.15	6 (6%)
52	CDL	Z	201	-	75,75,99	1.01	8 (10%)	81,87,111	1.17	6 (7%)
43	SF4	A	801	1	0,12,12	-	-	-	-	-
47	3PE	4	501	-	42,42,50	0.94	4 (9%)	45,47,55	1.12	2 (4%)
47	3PE	4	504	-	50,50,50	0.86	4 (8%)	53,55,55	1.20	3 (5%)
54	T7X	3	202	-	49,49,61	0.97	5 (10%)	58,61,73	1.45	7 (12%)
52	CDL	5	701	-	77,77,99	1.03	8 (10%)	83,89,111	1.26	5 (6%)
54	T7X	4	505	-	43,43,61	0.67	1 (2%)	52,55,73	1.39	8 (15%)
54	T7X	2	502	-	48,48,61	1.00	4 (8%)	57,60,73	1.37	8 (14%)
48	LMN	j	101	-	72,72,72	1.63	11 (15%)	92,98,98	1.84	20 (21%)
43	SF4	I	503	9	0,12,12	-	-	-	-	-
44	FES	H	301	8	0,4,4	-	-	-	-	-
48	LMN	J	204	-	68,68,72	1.62	13 (19%)	88,94,98	1.50	15 (17%)
43	SF4	B	501	2	0,12,12	-	-	-	-	-
43	SF4	A	802	1	0,12,12	-	-	-	-	-
51	PLC	1	401	-	41,41,41	1.35	5 (12%)	47,49,49	1.20	3 (6%)
51	PLC	5	703	-	30,30,41	1.51	5 (16%)	36,38,49	1.10	3 (8%)
43	SF4	I	502	9	0,12,12	-	-	-	-	-
51	PLC	W	202	-	41,41,41	1.33	5 (12%)	47,49,49	1.01	3 (6%)
43	SF4	K	301	11	0,12,12	-	-	-	-	-
47	3PE	a	201	-	50,50,50	0.88	4 (8%)	53,55,55	1.12	3 (5%)
47	3PE	J	203	-	43,43,50	0.96	4 (9%)	46,48,55	1.32	3 (6%)

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
44	FES	A	803	1	-	-	0/1/1/1
50	ZMP	O	201	14	-	5/37/39/43	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
51	PLC	W	201	-	-	15/44/44/45	-
47	3PE	4	503	-	-	14/45/45/54	-
53	UQ9	1	402	-	-	6/30/54/81	0/1/1/1
47	3PE	J	201	-	-	9/44/44/54	-
48	LMN	J	202	-	-	26/50/130/130	0/4/4/4
52	CDL	X	201	-	-	41/96/96/110	-
54	T7X	2	504	-	-	13/47/71/80	0/1/1/1
45	FMN	B	502	-	-	13/18/18/18	0/3/3/3
47	3PE	i	101	-	-	20/45/45/54	-
47	3PE	b	201	-	-	11/45/45/54	-
47	3PE	S	501	-	-	18/45/45/54	-
51	PLC	1	403	-	-	6/38/38/45	-
50	ZMP	Q	201	16	-	12/37/39/43	-
46	NDP	E	401	-	-	10/34/77/77	0/5/5/5
51	PLC	5	702	-	-	20/45/45/45	-
47	3PE	3	201	-	-	4/46/46/54	-
52	CDL	2	501	-	-	24/93/93/110	-
47	3PE	I	501	-	-	23/54/54/54	-
55	PSC	2	503	-	-	24/55/55/55	-
52	CDL	4	502	-	-	44/102/102/110	-
52	CDL	Z	201	-	-	32/86/86/110	-
47	3PE	4	501	-	-	7/46/46/54	-
47	3PE	4	504	-	-	25/54/54/54	-
54	T7X	3	202	-	-	13/44/68/80	0/1/1/1
43	SF4	A	801	1	-	-	0/6/5/5
52	CDL	5	701	-	-	32/88/88/110	-
54	T7X	4	505	-	-	23/38/62/80	0/1/1/1
54	T7X	2	502	-	-	12/43/67/80	0/1/1/1
48	LMN	j	101	-	-	31/50/130/130	0/4/4/4
43	SF4	I	503	9	-	-	0/6/5/5
44	FES	H	301	8	-	-	0/1/1/1
48	LMN	J	204	-	-	17/46/126/130	0/4/4/4
43	SF4	B	501	2	-	-	0/6/5/5
51	PLC	1	401	-	-	14/45/45/45	-
51	PLC	5	703	-	-	11/34/34/45	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
43	SF4	A	802	1	-	-	0/6/5/5
43	SF4	I	502	9	-	-	0/6/5/5
51	PLC	W	202	-	-	16/45/45/45	-
43	SF4	K	301	11	-	-	0/6/5/5
47	3PE	a	201	-	-	10/54/54/54	-
47	3PE	J	203	-	-	20/47/47/54	-

All (205) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	1	402	UQ9	C6-C1	9.63	1.52	1.35
46	E	401	NDP	PN-O3	8.24	1.68	1.59
46	E	401	NDP	O4B-C1B	8.11	1.60	1.42
46	E	401	NDP	O4D-C1D	8.06	1.60	1.42
46	E	401	NDP	C2B-C1B	-7.53	1.34	1.53
46	E	401	NDP	C6N-C5N	7.21	1.55	1.33
46	E	401	NDP	C2D-C1D	-7.12	1.31	1.53
45	B	502	FMN	C4A-N5	7.06	1.46	1.30
45	B	502	FMN	C10-N1	7.01	1.47	1.33
46	E	401	NDP	O4D-C4D	-6.83	1.29	1.45
46	E	401	NDP	O4B-C4B	-6.30	1.31	1.45
48	J	202	LMN	O1-C1	-5.98	1.30	1.40
48	j	101	LMN	O1-C1	-5.87	1.30	1.40
45	B	502	FMN	C5A-N5	5.67	1.49	1.39
48	J	204	LMN	O1-C1	-5.35	1.31	1.40
46	E	401	NDP	C2N-C3N	5.25	1.49	1.35
46	E	401	NDP	PA-O3	5.23	1.65	1.59
45	B	502	FMN	C2-N1	5.17	1.48	1.36
48	J	204	LMN	O5-C1	5.15	1.55	1.41
50	O	201	ZMP	C16-N2	5.08	1.45	1.33
50	O	201	ZMP	C13-N1	5.03	1.45	1.33
48	j	101	LMN	O5-C1	4.90	1.54	1.41
48	J	202	LMN	O5-C1	4.88	1.54	1.41
50	Q	201	ZMP	C13-N1	4.85	1.44	1.33
45	B	502	FMN	C9A-N10	4.76	1.49	1.41
46	E	401	NDP	P2B-O2B	4.73	1.67	1.59
46	E	401	NDP	C6A-N6A	4.61	1.46	1.34
50	Q	201	ZMP	C16-N2	4.51	1.44	1.33
45	B	502	FMN	C2-N3	4.47	1.48	1.39
53	1	402	UQ9	C4-C3	4.40	1.52	1.36
45	B	502	FMN	C10-N10	4.31	1.46	1.37
46	E	401	NDP	C4N-C3N	4.19	1.57	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	E	401	NDP	O2D-C2D	4.18	1.53	1.43
45	B	502	FMN	C4-N3	3.95	1.46	1.38
51	W	202	PLC	O2-C'	3.80	1.45	1.34
48	J	202	LMN	O4-C4	3.70	1.53	1.43
53	1	402	UQ9	C7-C8	3.67	1.56	1.50
48	J	202	LMN	CCV-CCT	-3.54	1.43	1.52
48	j	101	LMN	CBS-CCM	3.48	1.61	1.53
51	5	702	PLC	O2-C'	3.48	1.44	1.34
47	I	501	3PE	O21-C2	-3.47	1.38	1.46
53	1	402	UQ9	C11-C9	3.45	1.58	1.51
51	1	403	PLC	O2-C'	3.45	1.44	1.34
48	J	202	LMN	CCT-CCN	3.45	1.61	1.52
51	W	201	PLC	O2-C'	3.44	1.44	1.34
51	1	403	PLC	O3-CB	3.38	1.43	1.33
51	W	201	PLC	O3-CB	3.37	1.43	1.33
51	1	401	PLC	O3-CB	3.33	1.43	1.33
51	1	401	PLC	O2-C'	3.32	1.43	1.34
51	5	702	PLC	O3-CB	3.31	1.43	1.33
46	E	401	NDP	C6N-N1N	3.20	1.45	1.37
48	j	101	LMN	CBR-CCM	3.17	1.59	1.54
51	5	703	PLC	O3-CB	3.17	1.42	1.33
48	j	101	LMN	OBY-CCR	3.15	1.50	1.41
51	W	202	PLC	O3-CB	3.13	1.42	1.33
48	j	101	LMN	CBT-CCM	3.11	1.60	1.53
46	E	401	NDP	C7N-N7N	3.10	1.42	1.33
47	J	201	3PE	O21-C2	-3.08	1.39	1.46
48	J	204	LMN	CBS-CCM	3.06	1.60	1.53
51	5	703	PLC	O2-C2	-3.05	1.39	1.46
47	a	201	3PE	O21-C2	-3.05	1.39	1.46
48	J	204	LMN	CBT-CCM	3.04	1.60	1.53
48	j	101	LMN	O4-C4	3.03	1.51	1.43
48	j	101	LMN	CBQ-CCM	3.01	1.59	1.54
48	J	202	LMN	OBZ-CCS	2.99	1.49	1.41
52	4	502	CDL	OA6-CA4	-2.95	1.39	1.46
52	5	701	CDL	OB6-CB4	-2.95	1.39	1.46
52	4	502	CDL	OB6-CB4	-2.92	1.39	1.46
47	b	201	3PE	O21-C2	-2.91	1.39	1.46
51	5	703	PLC	O2-C'	2.87	1.42	1.34
47	i	101	3PE	O21-C2	-2.86	1.39	1.46
46	E	401	NDP	C5D-C4D	2.85	1.60	1.51
53	1	402	UQ9	O4-C4M	-2.85	1.38	1.45
53	1	402	UQ9	C21-C19	2.85	1.57	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	j	101	LMN	OBZ-CCS	2.85	1.49	1.41
47	4	503	3PE	O31-C31	2.84	1.41	1.33
47	4	503	3PE	O21-C21	2.84	1.42	1.34
45	B	502	FMN	O4-C4	-2.83	1.18	1.23
47	4	504	3PE	O21-C2	-2.82	1.40	1.46
53	1	402	UQ9	C16-C14	2.82	1.57	1.51
47	J	203	3PE	O21-C2	-2.81	1.40	1.46
47	4	501	3PE	O21-C2	-2.79	1.40	1.46
48	J	204	LMN	OBZ-CCS	2.79	1.49	1.41
55	2	503	PSC	O03-C01	-2.76	1.39	1.45
46	E	401	NDP	C5A-C4A	-2.75	1.34	1.39
52	Z	201	CDL	OB8-CB7	2.73	1.41	1.33
46	E	401	NDP	C4N-C5N	2.69	1.56	1.49
51	1	401	PLC	O2-C2	-2.67	1.40	1.46
54	2	502	T7X	P1-O1	2.67	1.67	1.59
54	3	202	T7X	O16-C8	-2.63	1.40	1.46
51	W	201	PLC	O2-C2	-2.63	1.40	1.46
48	J	204	LMN	OBX-CCR	2.62	1.48	1.41
45	B	502	FMN	O2-C2	-2.62	1.19	1.24
55	2	503	PSC	O01-C1	2.61	1.41	1.34
54	3	202	T7X	O16-C10	2.61	1.41	1.34
48	J	204	LMN	OBX-CCJ	2.60	1.48	1.41
47	b	201	3PE	O31-C3	-2.60	1.39	1.45
47	a	201	3PE	O31-C3	-2.59	1.39	1.45
52	4	502	CDL	OA8-CA7	2.58	1.40	1.33
47	4	504	3PE	O31-C3	-2.57	1.39	1.45
53	1	402	UQ9	C6-C5	2.55	1.53	1.46
52	5	701	CDL	OA6-CA4	-2.55	1.40	1.46
52	5	701	CDL	OA8-CA7	2.55	1.40	1.33
52	Z	201	CDL	OA8-CA7	2.54	1.40	1.33
52	Z	201	CDL	OB6-CB5	2.54	1.41	1.34
53	1	402	UQ9	C26-C24	2.53	1.56	1.51
51	1	403	PLC	O2-C2	-2.52	1.40	1.46
52	5	701	CDL	OA6-CA5	2.51	1.41	1.34
53	1	402	UQ9	O2-C2	-2.51	1.17	1.23
47	S	501	3PE	O21-C2	-2.51	1.40	1.46
48	J	204	LMN	O4-C4	2.50	1.50	1.43
48	J	202	LMN	OBX-CCR	2.50	1.48	1.41
47	i	101	3PE	O31-C3	-2.49	1.39	1.45
52	Z	201	CDL	OB6-CB4	-2.48	1.40	1.46
50	Q	201	ZMP	O2-C13	-2.48	1.18	1.23
52	4	502	CDL	OB8-CB7	2.47	1.40	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	5	701	CDL	OB8-CB7	2.46	1.40	1.33
52	5	701	CDL	OB6-CB5	2.45	1.41	1.34
46	E	401	NDP	C5A-N7A	-2.45	1.34	1.39
45	B	502	FMN	C5'-C4'	-2.45	1.48	1.51
52	Z	201	CDL	OA6-CA5	2.41	1.41	1.34
48	J	202	LMN	OBZ-CCD	2.41	1.50	1.44
47	J	203	3PE	O31-C31	2.40	1.40	1.33
47	4	503	3PE	O21-C2	-2.40	1.41	1.46
51	5	703	PLC	P-O4P	2.39	1.68	1.59
47	4	501	3PE	O31-C3	-2.39	1.39	1.45
54	3	202	T7X	O18-C11	2.39	1.40	1.33
54	2	502	T7X	O16-C10	2.39	1.41	1.34
48	J	202	LMN	CBS-CCM	2.38	1.58	1.53
48	J	204	LMN	OBX-CCF	2.38	1.50	1.44
50	O	201	ZMP	C10-S1	2.38	1.81	1.76
54	2	502	T7X	O18-C11	2.36	1.40	1.33
51	5	702	PLC	O2-C2	-2.36	1.41	1.46
47	i	101	3PE	O31-C31	2.35	1.40	1.33
55	2	503	PSC	O01-C02	-2.35	1.41	1.46
48	J	202	LMN	CBT-CCM	2.35	1.58	1.53
50	O	201	ZMP	O3-C16	-2.35	1.18	1.23
48	J	202	LMN	OAQ-CCN	2.35	1.48	1.43
51	5	703	PLC	P-O3P	2.34	1.68	1.59
47	S	501	3PE	O31-C3	-2.34	1.39	1.45
48	J	204	LMN	CBR-CCM	2.33	1.58	1.54
51	1	403	PLC	C8-N	-2.32	1.43	1.50
50	O	201	ZMP	O2-C13	-2.31	1.18	1.23
51	5	702	PLC	P-O4P	2.29	1.68	1.59
54	3	202	T7X	P1-O1	2.29	1.66	1.59
53	1	402	UQ9	O3-C3M	-2.28	1.40	1.45
52	5	701	CDL	OA8-CA6	-2.28	1.40	1.45
53	1	402	UQ9	O5-C5	-2.28	1.18	1.23
53	1	402	UQ9	C22-C23	2.27	1.57	1.50
47	S	501	3PE	O21-C21	2.26	1.40	1.34
51	W	201	PLC	P-O3P	2.26	1.68	1.59
48	j	101	LMN	OBZ-CCD	2.26	1.49	1.44
51	5	702	PLC	P-O3P	2.24	1.68	1.59
51	1	403	PLC	P-O3P	2.24	1.68	1.59
47	J	203	3PE	O21-C21	2.24	1.40	1.34
51	W	202	PLC	P-O4P	2.23	1.68	1.59
47	a	201	3PE	O21-C21	2.23	1.40	1.34
48	J	204	LMN	OCB-CCQ	2.23	1.49	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	4	501	3PE	O31-C31	2.22	1.39	1.33
47	I	501	3PE	O31-C3	-2.22	1.40	1.45
47	4	504	3PE	O21-C21	2.21	1.40	1.34
47	a	201	3PE	O31-C31	2.21	1.39	1.33
51	1	403	PLC	P-O4P	2.20	1.68	1.59
52	4	502	CDL	OA8-CA6	-2.20	1.40	1.45
50	Q	201	ZMP	C10-S1	2.19	1.81	1.76
54	2	502	T7X	O18-C9	-2.18	1.40	1.45
47	4	504	3PE	O31-C31	2.18	1.39	1.33
51	W	202	PLC	P-O3P	2.17	1.67	1.59
47	J	201	3PE	O31-C31	2.16	1.39	1.33
46	E	401	NDP	PA-O5B	2.16	1.67	1.59
48	J	204	LMN	CBQ-CCM	2.16	1.58	1.54
48	j	101	LMN	OBY-CCC	2.16	1.49	1.44
45	B	502	FMN	O2'-C2'	-2.16	1.38	1.43
47	J	203	3PE	O31-C3	-2.16	1.40	1.45
47	S	501	3PE	O31-C31	2.15	1.39	1.33
46	E	401	NDP	PA-O2A	-2.15	1.45	1.55
51	1	401	PLC	P-O4P	2.15	1.67	1.59
47	4	501	3PE	O21-C21	2.15	1.40	1.34
54	3	202	T7X	O18-C9	-2.15	1.40	1.45
52	Z	201	CDL	OA6-CA4	-2.14	1.41	1.46
52	Z	201	CDL	OB8-CB6	-2.14	1.40	1.45
50	Q	201	ZMP	C9-C10	2.13	1.53	1.50
47	J	201	3PE	O31-C3	-2.13	1.40	1.45
52	Z	201	CDL	OA8-CA6	-2.13	1.40	1.45
54	4	505	T7X	C31-C11	-2.11	1.44	1.50
50	Q	201	ZMP	O3-C16	-2.10	1.19	1.23
51	W	201	PLC	P-O4P	2.09	1.67	1.59
47	I	501	3PE	O31-C31	2.09	1.39	1.33
53	1	402	UQ9	C17-C18	2.08	1.56	1.50
47	i	101	3PE	O21-C21	2.07	1.40	1.34
48	J	202	LMN	O5-C5	2.07	1.49	1.44
55	2	503	PSC	C05-N	-2.05	1.45	1.51
46	E	401	NDP	C8A-N9A	-2.05	1.34	1.37
52	X	201	CDL	OA9-CA7	-2.05	1.16	1.22
47	b	201	3PE	O21-C21	2.04	1.40	1.34
47	4	503	3PE	O31-C3	-2.04	1.40	1.45
48	J	204	LMN	OBY-CCC	2.03	1.49	1.44
52	4	502	CDL	OB8-CB6	-2.03	1.40	1.45
51	1	401	PLC	P-O3P	2.03	1.67	1.59
55	2	503	PSC	O03-C19	2.03	1.39	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	W	202	PLC	O2-C2	-2.03	1.41	1.46
46	E	401	NDP	O2B-C2B	2.03	1.51	1.44
52	5	701	CDL	OB8-CB6	-2.02	1.40	1.45
51	1	403	PLC	C1'-C'	2.02	1.56	1.50
45	B	502	FMN	C7M-C7	2.00	1.54	1.51

All (209) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	Q	201	ZMP	C14-C15-N2	-8.24	94.46	112.00
48	j	101	LMN	CBR-CBL-CBJ	7.32	134.98	113.19
48	J	202	LMN	CBM-CCC-CCN	-6.40	97.30	113.02
48	J	204	LMN	CBR-CBL-CBJ	6.28	131.88	113.19
46	E	401	NDP	N6A-C6A-N1A	-6.14	104.71	118.38
50	O	201	ZMP	C9-C10-S1	5.77	120.28	113.40
54	4	505	T7X	O16-C10-C12	5.58	123.55	111.48
46	E	401	NDP	N3A-C2A-N1A	-5.57	120.14	128.58
47	J	203	3PE	O21-C21-C22	5.45	123.28	111.48
46	E	401	NDP	C5A-C4A-N3A	-5.44	119.22	126.72
46	E	401	NDP	C4A-N9A-C1B	-5.39	114.02	126.63
50	Q	201	ZMP	C9-C10-S1	5.33	119.75	113.40
51	1	401	PLC	O2-C'-C1'	5.30	122.94	111.48
52	5	701	CDL	OA6-CA5-C11	5.21	122.75	111.48
48	J	202	LMN	CBR-CBL-CBJ	5.16	128.57	113.19
46	E	401	NDP	C1B-N9A-C8A	5.14	138.51	127.09
51	1	403	PLC	O2-C'-C1'	5.08	122.47	111.48
48	j	101	LMN	C2-C3-C4	5.03	121.09	109.68
48	j	101	LMN	OBX-CCF-CBP	-4.94	94.21	106.44
48	j	101	LMN	OBX-CCJ-OBV	-4.73	98.87	110.04
46	E	401	NDP	C5A-C6A-N6A	4.72	134.97	123.29
53	1	402	UQ9	C8-C7-C6	-4.67	100.57	112.08
45	B	502	FMN	C7M-C7-C6	-4.65	111.38	119.57
48	j	101	LMN	OCB-CCS-CCW	4.50	119.15	108.09
50	O	201	ZMP	C11-C12-N1	-4.32	103.38	112.41
47	i	101	3PE	O21-C21-C22	4.28	120.74	111.48
53	1	402	UQ9	C12-C13-C14	-4.26	117.88	127.62
54	3	202	T7X	C6-C1-C2	4.25	116.75	110.86
53	1	402	UQ9	C15-C14-C13	-4.23	112.77	123.63
51	5	702	PLC	O2-C'-C1'	4.18	120.52	111.48
48	J	202	LMN	CCR-CCV-CCT	4.15	118.73	110.01
47	S	501	3PE	O21-C21-C22	4.14	120.43	111.48
53	1	402	UQ9	C17-C18-C19	-4.03	118.41	127.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	4	503	3PE	O31-C31-C32	3.99	123.99	111.83
55	2	503	PSC	O01-C1-C2	3.97	120.07	111.48
48	J	202	LMN	O3-C3-C2	-3.97	101.03	110.38
48	J	202	LMN	OCB-CCQ-CCF	-3.96	99.10	109.48
53	1	402	UQ9	C12-C11-C9	-3.95	100.09	113.19
45	B	502	FMN	C4-N3-C2	-3.95	118.63	125.64
47	b	201	3PE	O21-C21-C22	3.92	119.97	111.48
52	4	502	CDL	OB6-CB5-C51	3.90	119.92	111.48
53	1	402	UQ9	C7-C8-C9	-3.90	120.11	126.83
50	Q	201	ZMP	C20-C18-C17	3.88	115.38	108.77
54	3	202	T7X	C5-C6-C1	3.82	118.35	109.68
48	J	202	LMN	OBZ-CCD-CCO	3.80	116.56	109.70
54	3	202	T7X	C12-C13-C14	-3.74	105.18	113.35
47	4	503	3PE	O21-C21-C22	3.73	119.54	111.48
53	1	402	UQ9	C7-C6-C1	-3.63	118.66	124.89
52	X	201	CDL	OB6-CB5-C51	3.62	119.32	111.48
52	Z	201	CDL	OA6-CA5-C11	3.60	119.28	111.48
48	J	202	LMN	O4-CCR-CCV	3.58	116.89	108.09
53	1	402	UQ9	C15-C14-C16	3.57	121.43	115.23
54	2	502	T7X	C12-C13-C14	-3.57	105.56	113.35
46	E	401	NDP	N9A-C8A-N7A	-3.55	108.90	113.94
50	O	201	ZMP	O1-C10-C9	-3.54	119.89	123.98
46	E	401	NDP	C2A-N3A-C4A	3.54	120.48	111.83
52	4	502	CDL	OB8-CB7-C71	3.52	122.57	111.83
54	2	502	T7X	C3-C2-C1	3.50	117.63	109.68
48	j	101	LMN	OCB-CCQ-CCF	3.50	118.65	109.48
46	E	401	NDP	N3A-C4A-N9A	3.48	133.08	127.17
45	B	502	FMN	C7M-C7-C8	3.44	127.78	120.76
54	2	504	T7X	C5-C4-C3	3.43	116.86	110.83
48	j	101	LMN	CBP-CCF-CCQ	3.43	123.03	113.38
47	4	501	3PE	O21-C21-C22	3.43	118.90	111.48
51	5	703	PLC	O2-C'-C1'	3.42	118.88	111.48
48	J	202	LMN	CCL-CCH-CCQ	3.38	117.36	109.68
54	3	202	T7X	O16-C10-C12	3.36	118.75	111.48
48	J	202	LMN	CCJ-CCL-CCH	3.36	117.07	110.01
47	4	504	3PE	O21-C21-C22	3.34	118.71	111.48
47	J	203	3PE	O31-C31-C32	3.33	121.99	111.83
48	J	202	LMN	CCS-OBZ-CCD	3.32	120.21	113.72
52	Z	201	CDL	OB6-CB5-C51	3.25	118.51	111.48
47	I	501	3PE	O31-C31-C32	3.23	121.69	111.83
51	W	201	PLC	O2-C'-C1'	3.23	118.47	111.48
53	1	402	UQ9	C22-C23-C24	-3.19	120.31	127.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	B	502	FMN	O4-C4-C4A	-3.19	118.12	126.53
48	J	202	LMN	CBQ-CBK-CBI	-3.18	103.74	113.19
52	4	502	CDL	OA8-CA7-C31	3.17	121.49	111.83
54	3	202	T7X	O18-C11-C31	3.16	121.47	111.83
51	5	702	PLC	O3-CB-C1B	3.15	121.43	111.83
48	J	204	LMN	CCJ-OBX-CCF	3.15	119.86	113.72
47	a	201	3PE	C3-C2-C1	-3.13	104.49	111.78
48	J	202	LMN	OCB-CCS-CCW	-3.11	100.44	108.09
54	4	505	T7X	O1-P1-O11	-3.10	99.89	109.81
47	a	201	3PE	O21-C21-C22	3.09	118.17	111.48
45	B	502	FMN	C4A-C4-N3	3.09	121.11	113.25
48	j	101	LMN	O4-CCR-CCV	3.08	115.66	108.09
52	4	502	CDL	OA6-CA5-C11	3.07	118.13	111.48
47	4	504	3PE	C3-C2-C1	-3.05	104.66	111.78
51	W	201	PLC	O3-CB-C1B	3.03	121.07	111.83
54	4	505	T7X	O16-C8-C7	3.03	119.20	108.34
54	2	502	T7X	O16-C10-C12	3.00	117.97	111.48
52	5	701	CDL	OB8-CB7-C71	3.00	120.97	111.83
47	i	101	3PE	O31-C31-C32	2.99	120.96	111.83
51	1	403	PLC	O3-CB-C1B	2.98	120.93	111.83
47	4	501	3PE	O31-C31-C32	2.95	120.84	111.83
48	J	204	LMN	CCW-CCU-CCO	2.94	115.99	110.83
54	2	502	T7X	C8-O16-C10	2.92	124.77	117.80
53	1	402	UQ9	C25-C24-C26	2.91	120.28	115.23
48	j	101	LMN	C1-O5-C5	-2.91	108.04	113.72
46	E	401	NDP	C2B-C1B-N9A	-2.90	108.98	113.75
48	J	202	LMN	C2-C3-C4	2.87	116.19	109.68
48	J	202	LMN	O5-C5-C4	2.87	115.65	109.72
48	J	202	LMN	OAS-CCT-CCV	-2.86	103.63	110.38
48	J	204	LMN	C2-C3-C4	2.84	116.12	109.68
48	j	101	LMN	OBY-CCC-CCN	2.83	114.80	109.70
48	J	202	LMN	OCB-CCQ-CCH	2.81	114.37	107.23
47	J	201	3PE	O31-C31-C32	2.81	120.39	111.83
50	Q	201	ZMP	O1-C10-C9	-2.80	120.75	123.98
52	5	701	CDL	CA6-CA4-CA3	-2.79	105.28	111.78
47	J	201	3PE	O21-C21-C22	2.79	117.52	111.48
48	J	202	LMN	O4-C4-C3	2.78	114.29	107.23
52	Z	201	CDL	OA8-CA7-C31	2.77	120.27	111.83
54	2	502	T7X	O18-C11-C31	2.74	120.19	111.83
54	2	502	T7X	C4-C3-C2	2.71	115.59	110.83
52	2	501	CDL	OB6-CB4-CB6	2.71	118.08	108.34
48	J	204	LMN	CCJ-CCL-CCH	2.70	115.69	110.01

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	J	202	LMN	OAQ-CCN-CCT	2.70	116.74	110.38
52	5	701	CDL	OA8-CA7-C31	2.69	120.05	111.83
51	W	202	PLC	O2-C'-C1'	2.69	117.31	111.48
48	J	204	LMN	CCL-CCH-CCQ	2.68	115.75	109.68
54	3	202	T7X	C4-C3-C2	2.65	115.49	110.83
48	J	204	LMN	OBY-CCC-CCN	2.65	114.47	109.70
48	J	202	LMN	OBY-CCC-CCN	2.64	114.46	109.70
54	2	504	T7X	O16-C10-C12	2.64	117.20	111.48
52	X	201	CDL	OB6-CB4-CB6	2.62	117.75	108.34
54	2	504	T7X	C6-C1-C2	-2.61	107.23	110.86
47	J	203	3PE	O21-C21-O22	-2.60	117.64	123.70
45	B	502	FMN	C10-N1-C2	2.58	122.44	116.85
50	Q	201	ZMP	C11-C12-N1	-2.57	107.04	112.41
51	W	202	PLC	C2-O2-C'	2.57	123.95	117.80
48	j	101	LMN	CCW-CCU-CCO	2.56	115.33	110.83
47	b	201	3PE	C33-C32-C31	-2.56	104.33	113.69
54	3	202	T7X	C3-C2-C1	2.55	115.48	109.68
46	E	401	NDP	C5A-N7A-C8A	2.55	107.46	103.45
48	J	204	LMN	O3-C3-C2	-2.54	104.39	110.38
54	2	502	T7X	O6-C6-C5	-2.52	104.42	110.38
48	J	202	LMN	CBN-CCD-CCO	-2.52	106.83	113.02
50	Q	201	ZMP	O1-C10-S1	-2.51	119.49	122.68
54	2	502	T7X	C5-C4-C3	2.50	115.21	110.83
52	2	501	CDL	OB6-CB4-CB3	-2.48	99.44	108.34
54	4	505	T7X	C6-C1-C2	2.48	114.30	110.86
50	O	201	ZMP	C17-C16-N2	2.48	121.19	116.48
48	J	202	LMN	OBY-CCC-CBM	2.47	112.56	106.44
51	5	703	PLC	O3-CB-C1B	2.47	119.35	111.83
48	J	204	LMN	OCB-CCQ-CCF	2.46	115.92	109.48
45	B	502	FMN	C4A-C10-N1	-2.45	118.58	124.59
51	1	401	PLC	O3-CB-C1B	2.45	119.30	111.83
51	W	202	PLC	O3-CB-C1B	2.44	119.28	111.83
48	J	202	LMN	CCS-CCW-CCU	-2.44	104.88	110.01
47	4	504	3PE	O31-C31-C32	2.43	119.24	111.83
52	4	502	CDL	CB4-OB6-CB5	-2.43	111.98	117.80
48	J	204	LMN	CBL-CBR-CCM	-2.42	109.84	117.19
48	J	202	LMN	O5-C1-C2	-2.40	105.43	110.37
50	Q	201	ZMP	C15-C14-C13	2.40	116.39	112.39
53	1	402	UQ9	C17-C16-C14	-2.40	105.23	113.19
48	j	101	LMN	CCJ-OBX-CCF	2.40	118.40	113.72
50	O	201	ZMP	C15-N2-C16	-2.40	118.24	122.55
48	j	101	LMN	CBS-O1-C1	2.36	119.31	113.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	5	701	CDL	OB6-CB5-C51	2.36	116.58	111.48
52	Z	201	CDL	OB8-CB7-C71	2.34	118.98	111.83
46	E	401	NDP	C3N-C2N-N1N	-2.34	119.78	123.20
48	j	101	LMN	OBZ-CCD-CCO	2.32	113.88	109.70
51	1	401	PLC	O2-C'-O'	-2.31	118.30	123.70
48	J	202	LMN	OBY-CCR-CCV	-2.31	105.63	110.37
48	J	204	LMN	CBQ-CBK-CBI	-2.30	106.33	113.19
47	I	501	3PE	O21-C21-C22	2.30	116.45	111.48
48	J	202	LMN	OAN-CCH-CCL	-2.28	105.00	110.38
48	j	101	LMN	CCR-OBY-CCC	2.27	118.16	113.72
48	J	202	LMN	OBX-CCJ-CCL	2.27	115.04	110.37
48	J	202	LMN	CCU-CCO-CCD	2.25	114.31	110.23
50	O	201	ZMP	O1-C10-S1	-2.25	119.83	122.68
48	j	101	LMN	CCL-CCH-CCQ	2.24	114.77	109.68
48	J	204	LMN	CCR-CCV-CCT	2.24	114.73	110.01
48	J	204	LMN	CCV-CCT-CCN	2.24	114.76	110.83
55	2	503	PSC	C03-C02-C01	-2.24	106.57	111.78
46	E	401	NDP	C6A-C5A-C4A	2.23	120.22	117.18
48	J	202	LMN	CBL-CBR-CCM	-2.23	110.43	117.19
52	X	201	CDL	OB2-PB2-OB3	-2.21	100.18	108.94
48	j	101	LMN	OBV-CCJ-CCL	2.20	111.62	108.27
48	J	204	LMN	O5-C1-C2	-2.19	105.86	110.37
45	B	502	FMN	O3P-P-O5'	2.19	112.38	106.67
51	5	703	PLC	C2-O2-C'	-2.18	112.58	117.80
53	1	402	UQ9	C20-C19-C21	2.17	119.00	115.23
55	2	503	PSC	O03-C19-C20	2.17	118.44	111.83
50	Q	201	ZMP	C20-C18-C19	-2.15	104.92	109.20
52	X	201	CDL	OB4-PB2-OB3	2.14	122.40	112.44
51	1	403	PLC	O2-C'-O'	-2.14	118.71	123.70
48	J	202	LMN	CBK-CBQ-CCM	-2.12	110.76	117.19
52	4	502	CDL	OB6-CB5-OB7	-2.12	118.76	123.70
48	j	101	LMN	C3-C4-C5	2.11	115.62	110.93
54	4	505	T7X	O17-C10-C12	-2.11	115.54	123.78
54	4	505	T7X	O12-P1-O11	2.10	122.22	112.44
45	B	502	FMN	C10-C4A-N5	-2.10	120.53	124.81
54	2	504	T7X	O13-P1-O11	-2.09	100.67	108.94
52	Z	201	CDL	OA6-CA4-CA3	2.08	115.79	108.34
47	4	503	3PE	O31-C31-O32	-2.07	118.44	123.63
45	B	502	FMN	C9A-C5A-N5	-2.07	120.25	122.45
54	4	505	T7X	O4-C4-C5	-2.06	105.51	110.38
53	1	402	UQ9	C16-C14-C13	2.06	125.80	121.17
48	J	204	LMN	OCB-CCQ-CCH	2.05	112.44	107.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	O	201	ZMP	C19-C18-C17	2.05	112.26	108.77
47	a	201	3PE	O31-C31-C32	2.04	118.05	111.83
48	j	101	LMN	C1-C2-C3	2.04	114.30	110.01
52	2	501	CDL	OB2-PB2-OB3	-2.03	100.88	108.94
52	Z	201	CDL	CB6-CB4-CB3	-2.03	107.06	111.78
54	4	505	T7X	C5-C4-C3	-2.02	107.28	110.83
47	I	501	3PE	C24-C23-C22	-2.01	105.75	113.13
48	j	101	LMN	CCH-CCQ-CCF	-2.01	106.48	110.93

There are no chirality outliers.

All (621) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	B	502	FMN	N10-C1'-C2'-O2'
45	B	502	FMN	N10-C1'-C2'-C3'
45	B	502	FMN	C1'-C2'-C3'-O3'
45	B	502	FMN	C1'-C2'-C3'-C4'
45	B	502	FMN	O3'-C3'-C4'-O4'
45	B	502	FMN	O3'-C3'-C4'-C5'
45	B	502	FMN	C5'-O5'-P-O2P
45	B	502	FMN	C5'-O5'-P-O3P
46	E	401	NDP	C4B-C5B-O5B-PA
46	E	401	NDP	O4B-C4B-C5B-O5B
46	E	401	NDP	C3B-C4B-C5B-O5B
47	I	501	3PE	O13-C11-C12-N
47	J	201	3PE	C1-O11-P-O12
47	J	201	3PE	C1-O11-P-O13
47	J	201	3PE	C1-O11-P-O14
47	J	203	3PE	C1-O11-P-O13
47	J	203	3PE	C11-O13-P-O11
47	J	203	3PE	C11-O13-P-O12
47	J	203	3PE	O22-C21-O21-C2
47	S	501	3PE	C1-O11-P-O12
47	S	501	3PE	C1-O11-P-O13
47	S	501	3PE	C1-O11-P-O14
47	S	501	3PE	C11-O13-P-O11
47	S	501	3PE	C11-O13-P-O12
47	S	501	3PE	C11-O13-P-O14
47	S	501	3PE	O13-C11-C12-N
47	a	201	3PE	C1-O11-P-O14
47	a	201	3PE	O13-C11-C12-N
47	i	101	3PE	C11-O13-P-O11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
47	i	101	3PE	C11-O13-P-O12
47	i	101	3PE	C11-O13-P-O14
47	i	101	3PE	O13-C11-C12-N
47	4	503	3PE	C11-O13-P-O11
47	4	503	3PE	C11-O13-P-O14
47	4	503	3PE	O32-C31-O31-C3
47	4	503	3PE	C32-C31-O31-C3
47	4	504	3PE	C1-O11-P-O12
47	4	504	3PE	C1-O11-P-O13
47	4	504	3PE	C1-O11-P-O14
47	4	504	3PE	C11-O13-P-O12
48	J	202	LMN	O1-CBS-CCM-CBQ
48	j	101	LMN	O5-C1-O1-CBS
48	j	101	LMN	CBL-CBR-CCM-CBQ
48	j	101	LMN	CBL-CBR-CCM-CBS
48	j	101	LMN	CBL-CBR-CCM-CBT
48	j	101	LMN	OBV-CBT-CCM-CBQ
48	j	101	LMN	OBV-CBT-CCM-CBR
50	O	201	ZMP	S1-C11-C12-N1
50	Q	201	ZMP	C20-C18-C21-O5
50	Q	201	ZMP	O4-C17-C18-C21
50	Q	201	ZMP	C16-C17-C18-C21
50	Q	201	ZMP	O4-C17-C18-C19
50	Q	201	ZMP	C16-C17-C18-C19
50	Q	201	ZMP	O4-C17-C18-C20
50	Q	201	ZMP	C16-C17-C18-C20
50	Q	201	ZMP	O1-C10-S1-C11
50	Q	201	ZMP	C9-C10-S1-C11
51	W	202	PLC	O4P-C4-C5-N
51	1	401	PLC	C1'-C'-O2-C2
51	1	401	PLC	O'-C'-O2-C2
51	1	401	PLC	C1-O3P-P-O1P
51	1	401	PLC	C4-O4P-P-O3P
51	1	403	PLC	C1'-C'-O2-C2
51	1	403	PLC	O'-C'-O2-C2
51	5	702	PLC	O2-C2-C3-O3
51	5	702	PLC	C1'-C'-O2-C2
51	5	702	PLC	C1-O3P-P-O2P
51	5	703	PLC	C1'-C'-O2-C2
51	5	703	PLC	C4-O4P-P-O1P
52	X	201	CDL	CA3-OA5-PA1-OA2
52	Z	201	CDL	CA2-OA2-PA1-OA4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
52	Z	201	CDL	CA2-OA2-PA1-OA5
52	Z	201	CDL	C11-CA5-OA6-CA4
52	Z	201	CDL	CB3-OB5-PB2-OB2
52	Z	201	CDL	CB3-OB5-PB2-OB3
52	Z	201	CDL	CB3-OB5-PB2-OB4
52	2	501	CDL	CA2-OA2-PA1-OA3
52	2	501	CDL	CA2-OA2-PA1-OA5
52	2	501	CDL	CB2-OB2-PB2-OB3
52	2	501	CDL	CB3-OB5-PB2-OB3
52	4	502	CDL	CA2-OA2-PA1-OA4
52	4	502	CDL	CA3-OA5-PA1-OA2
52	4	502	CDL	CA3-OA5-PA1-OA3
52	4	502	CDL	CA3-OA5-PA1-OA4
52	4	502	CDL	CB2-OB2-PB2-OB3
52	4	502	CDL	CB2-OB2-PB2-OB4
52	4	502	CDL	CB2-OB2-PB2-OB5
52	4	502	CDL	CB3-OB5-PB2-OB2
52	4	502	CDL	CB3-OB5-PB2-OB3
52	4	502	CDL	OB7-CB5-OB6-CB4
52	5	701	CDL	C11-CA5-OA6-CA4
52	5	701	CDL	CB2-OB2-PB2-OB4
54	2	502	T7X	C7-O13-P1-O1
54	2	502	T7X	C7-O13-P1-O12
54	2	502	T7X	C18-C19-C20-C21
54	3	202	T7X	C2-C1-O1-P1
54	3	202	T7X	C6-C1-O1-P1
54	3	202	T7X	C7-O13-P1-O11
54	4	505	T7X	C2-C1-O1-P1
54	4	505	T7X	C6-C1-O1-P1
54	4	505	T7X	C7-O13-P1-O1
54	4	505	T7X	C8-C7-O13-P1
55	2	503	PSC	C03-O11-P-O12
55	2	503	PSC	C03-O11-P-O13
55	2	503	PSC	C03-O11-P-O14
55	2	503	PSC	C02-C03-O11-P
55	2	503	PSC	O12-C04-C05-N
52	4	502	CDL	OA9-CA7-OA8-CA6
52	5	701	CDL	OA9-CA7-OA8-CA6
54	2	504	T7X	O19-C11-O18-C9
54	4	505	T7X	O19-C11-O18-C9
48	j	101	LMN	C4-C5-C6-O6
52	4	502	CDL	C31-CA7-OA8-CA6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
52	5	701	CDL	C31-CA7-OA8-CA6
54	2	504	T7X	C31-C11-O18-C9
54	4	505	T7X	C31-C11-O18-C9
54	3	202	T7X	O19-C11-O18-C9
48	j	101	LMN	CCV-CCR-O4-C4
51	5	703	PLC	O'-C'-O2-C2
52	Z	201	CDL	OA7-CA5-OA6-CA4
52	4	502	CDL	OA7-CA5-OA6-CA4
52	5	701	CDL	OA7-CA5-OA6-CA4
52	4	502	CDL	C71-CB7-OB8-CB6
54	3	202	T7X	C31-C11-O18-C9
47	J	203	3PE	C22-C21-O21-C2
52	4	502	CDL	C11-CA5-OA6-CA4
52	4	502	CDL	C51-CB5-OB6-CB4
53	1	402	UQ9	C20-C19-C21-C22
53	1	402	UQ9	C15-C14-C16-C17
53	1	402	UQ9	C18-C19-C21-C22
52	Z	201	CDL	C31-CA7-OA8-CA6
48	J	204	LMN	CCF-CCQ-OCB-CCS
48	J	202	LMN	OAJ-CBN-CCD-OBZ
47	J	203	3PE	O32-C31-O31-C3
52	4	502	CDL	OB9-CB7-OB8-CB6
51	5	702	PLC	O'-C'-O2-C2
48	j	101	LMN	O5-C5-C6-O6
52	X	201	CDL	O1-C1-CA2-OA2
52	4	502	CDL	O1-C1-CB2-OB2
47	J	203	3PE	C32-C31-O31-C3
48	j	101	LMN	OAJ-CBN-CCD-OBZ
48	j	101	LMN	OAJ-CBN-CCD-CCO
47	i	101	3PE	C22-C21-O21-C2
45	B	502	FMN	O2'-C2'-C3'-C4'
45	B	502	FMN	C2'-C3'-C4'-O4'
52	2	501	CDL	C1-CB2-OB2-PB2
48	J	202	LMN	OAJ-CBN-CCD-CCO
52	Z	201	CDL	OA9-CA7-OA8-CA6
48	J	202	LMN	O5-C1-O1-CBS
48	J	202	LMN	OBX-CCJ-OBV-CBT
48	j	101	LMN	OBV-CBT-CCM-CBS
48	j	101	LMN	OBX-CCJ-OBV-CBT
48	J	202	LMN	O5-C5-C6-O6
48	J	202	LMN	CBC-CBE-CBG-CBI
48	J	202	LMN	OAI-CBM-CCC-OBY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
46	E	401	NDP	C3B-C2B-O2B-P2B
47	i	101	3PE	O22-C21-O21-C2
52	X	201	CDL	CB2-C1-CA2-OA2
52	4	502	CDL	CA2-C1-CB2-OB2
52	X	201	CDL	C71-CB7-OB8-CB6
48	J	202	LMN	OAI-CBM-CCC-CCN
47	4	501	3PE	C2E-C2F-C2G-C2H
53	1	402	UQ9	C13-C14-C16-C17
48	j	101	LMN	CCL-CCJ-OBV-CBT
52	X	201	CDL	O1-C1-CB2-OB2
48	J	204	LMN	CCV-CCR-O4-C4
47	I	501	3PE	C3B-C3C-C3D-C3E
54	4	505	T7X	C12-C10-O16-C8
48	J	202	LMN	CCH-CCQ-OCB-CCS
48	j	101	LMN	OAL-CBP-CCF-OBX
52	X	201	CDL	C54-C55-C56-C57
52	X	201	CDL	C58-C59-C60-C61
48	j	101	LMN	OAL-CBP-CCF-CCQ
47	I	501	3PE	C26-C27-C28-C29
47	J	203	3PE	C21-C22-C23-C24
48	J	204	LMN	OBY-CCR-O4-C4
53	1	402	UQ9	C9-C11-C12-C13
45	B	502	FMN	C2'-C3'-C4'-C5'
47	4	504	3PE	C21-C22-C23-C24
47	i	101	3PE	C31-C32-C33-C34
51	W	201	PLC	CB-C1B-C2B-C3B
48	J	204	LMN	CBJ-CBL-CBR-CCM
48	j	101	LMN	CBJ-CBL-CBR-CCM
52	X	201	CDL	OB9-CB7-OB8-CB6
48	J	204	LMN	O5-C1-O1-CBS
51	5	703	PLC	C'-C1'-C2'-C3'
54	2	504	T7X	C17-C18-C19-C20
45	B	502	FMN	O2'-C2'-C3'-O3'
48	J	204	LMN	C4-C5-C6-O6
55	2	503	PSC	C2-C1-O01-C02
52	2	501	CDL	CB7-C71-C72-C73
54	4	505	T7X	C11-C31-C32-C33
47	4	504	3PE	O22-C21-O21-C2
54	4	505	T7X	O17-C10-O16-C8
55	2	503	PSC	O02-C1-O01-C02
55	2	503	PSC	C20-C19-O03-C01
48	J	202	LMN	CCF-CCQ-OCB-CCS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
47	4	503	3PE	C22-C21-O21-C2
47	4	504	3PE	C22-C21-O21-C2
47	4	503	3PE	O22-C21-O21-C2
48	J	202	LMN	C2-C1-O1-CBS
48	J	204	LMN	C2-C1-O1-CBS
48	j	101	LMN	C2-C1-O1-CBS
52	Z	201	CDL	CA3-CA4-OA6-CA5
48	J	204	LMN	CAW-CAY-CBA-CBC
48	J	204	LMN	OBX-CCJ-OBV-CBT
54	4	505	T7X	C10-C12-C13-C14
47	I	501	3PE	C32-C31-O31-C3
52	2	501	CDL	C38-C39-C40-C41
51	W	202	PLC	C4'-C5'-C6'-C7'
47	I	501	3PE	C21-C22-C23-C24
52	5	701	CDL	C76-C77-C78-C79
52	X	201	CDL	C38-C39-C40-C41
47	i	101	3PE	C34-C35-C36-C37
52	X	201	CDL	C31-C32-C33-C34
46	E	401	NDP	C1B-C2B-O2B-P2B
51	5	702	PLC	C'-C1'-C2'-C3'
48	j	101	LMN	OAI-CBM-CCC-OBY
55	2	503	PSC	O04-C19-O03-C01
47	4	501	3PE	C2D-C2E-C2F-C2G
52	5	701	CDL	C11-C12-C13-C14
52	2	501	CDL	CA2-C1-CB2-OB2
51	W	202	PLC	C3'-C4'-C5'-C6'
51	1	403	PLC	CB-C1B-C2B-C3B
52	4	502	CDL	CA7-C31-C32-C33
52	4	502	CDL	C33-C34-C35-C36
52	2	501	CDL	C43-C44-C45-C46
52	5	701	CDL	C32-C33-C34-C35
47	4	501	3PE	C32-C31-O31-C3
52	5	701	CDL	C62-C63-C64-C65
47	I	501	3PE	C3C-C3D-C3E-C3F
47	I	501	3PE	C3D-C3E-C3F-C3G
47	I	501	3PE	O32-C31-O31-C3
47	4	504	3PE	C3B-C3C-C3D-C3E
47	4	504	3PE	C3C-C3D-C3E-C3F
47	4	504	3PE	C23-C24-C25-C26
55	2	503	PSC	C5-C6-C7-C8
48	j	101	LMN	CAW-CAY-CBA-CBC
47	S	501	3PE	C3D-C3E-C3F-C3G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
47	J	203	3PE	C31-C32-C33-C34
51	W	202	PLC	C1B-CB-O3-C3
51	W	201	PLC	C1'-C'-O2-C2
47	J	203	3PE	C39-C3A-C3B-C3C
47	S	501	3PE	C3C-C3D-C3E-C3F
48	J	202	LMN	C3-C4-O4-CCR
48	j	101	LMN	CCH-CCQ-OCB-CCS
52	Z	201	CDL	C73-C74-C75-C76
52	5	701	CDL	C73-C74-C75-C76
47	S	501	3PE	C22-C23-C24-C25
51	W	201	PLC	O'-C'-O2-C2
47	b	201	3PE	O11-C1-C2-O21
48	j	101	LMN	CBF-CBH-CBJ-CBL
52	4	502	CDL	C59-C60-C61-C62
51	5	702	PLC	C3B-C4B-C5B-C6B
55	2	503	PSC	C1-C2-C3-C4
47	I	501	3PE	C37-C38-C39-C3A
47	J	203	3PE	C2A-C2B-C2C-C2D
55	2	503	PSC	C7-C8-C9-C10
52	Z	201	CDL	C15-C16-C17-C18
52	4	502	CDL	C1-CA2-OA2-PA1
52	Z	201	CDL	C38-C39-C40-C41
52	Z	201	CDL	C18-C19-C20-C21
52	4	502	CDL	C41-C42-C43-C44
48	J	202	LMN	C4-C5-C6-O6
47	4	501	3PE	O32-C31-O31-C3
52	5	701	CDL	OB5-CB3-CB4-CB6
55	2	503	PSC	C23-C24-C25-C26
48	J	202	LMN	CBI-CBK-CBQ-CCM
47	i	101	3PE	C21-C22-C23-C24
51	5	703	PLC	CB-C1B-C2B-C3B
52	Z	201	CDL	CB5-C51-C52-C53
51	W	202	PLC	OB-CB-O3-C3
51	W	201	PLC	C1-C2-C3-O3
52	2	501	CDL	C22-C23-C24-C25
48	J	202	LMN	C5-C4-O4-CCR
47	I	501	3PE	C3F-C3G-C3H-C3I
52	X	201	CDL	C73-C74-C75-C76
52	5	701	CDL	C74-C75-C76-C77
52	X	201	CDL	CA4-CA6-OA8-CA7
47	i	101	3PE	C33-C34-C35-C36
51	W	201	PLC	C5B-C6B-C7B-C8B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
52	2	501	CDL	C73-C74-C75-C76
48	J	202	LMN	CAY-CBA-CBC-CBE
54	3	202	T7X	C12-C13-C14-C15
54	4	505	T7X	C12-C13-C14-C15
48	j	101	LMN	CAZ-CBB-CBD-CBF
54	4	505	T7X	C32-C33-C34-C35
47	I	501	3PE	O11-C1-C2-O21
52	5	701	CDL	OA5-CA3-CA4-OA6
48	j	101	LMN	CCF-CCQ-OCB-CCS
47	I	501	3PE	C33-C34-C35-C36
47	J	203	3PE	C35-C36-C37-C38
52	4	502	CDL	C19-C20-C21-C22
47	J	203	3PE	C38-C39-C3A-C3B
51	1	401	PLC	C4B-C5B-C6B-C7B
52	4	502	CDL	C44-C45-C46-C47
52	X	201	CDL	OA6-CA4-CA6-OA8
54	2	504	T7X	O16-C8-C9-O18
52	2	501	CDL	O1-C1-CB2-OB2
52	2	501	CDL	C20-C21-C22-C23
47	I	501	3PE	C2C-C2D-C2E-C2F
47	J	201	3PE	C37-C38-C39-C3A
52	Z	201	CDL	C55-C56-C57-C58
47	4	504	3PE	C3F-C3G-C3H-C3I
52	4	502	CDL	C42-C43-C44-C45
47	i	101	3PE	C32-C33-C34-C35
52	5	701	CDL	C60-C61-C62-C63
46	E	401	NDP	PN-O3-PA-O1A
51	W	202	PLC	C8'-C9'-CA'-CB'
51	W	202	PLC	C6B-C7B-C8B-C9B
54	2	502	T7X	C6-C1-O1-P1
51	5	702	PLC	C1B-CB-O3-C3
47	J	203	3PE	C34-C35-C36-C37
52	X	201	CDL	C13-C14-C15-C16
52	5	701	CDL	C16-C17-C18-C19
52	Z	201	CDL	C74-C75-C76-C77
47	4	504	3PE	C2D-C2E-C2F-C2G
48	J	204	LMN	O5-C5-C6-O6
47	b	201	3PE	O11-C1-C2-C3
47	i	101	3PE	O11-C1-C2-C3
47	S	501	3PE	C35-C36-C37-C38
48	J	204	LMN	CAA-CAW-CAY-CBA
50	O	201	ZMP	C22-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
51	W	202	PLC	C3B-C4B-C5B-C6B
48	j	101	LMN	CBB-CBD-CBF-CBH
51	5	702	PLC	C1B-C2B-C3B-C4B
52	X	201	CDL	C71-C72-C73-C74
52	Z	201	CDL	C72-C73-C74-C75
47	i	101	3PE	C1-C2-C3-O31
51	5	702	PLC	C1-C2-C3-O3
52	Z	201	CDL	CB3-CB4-CB6-OB8
47	4	504	3PE	C31-C32-C33-C34
52	Z	201	CDL	C20-C21-C22-C23
47	J	203	3PE	C28-C29-C2A-C2B
51	5	703	PLC	C1B-C2B-C3B-C4B
51	5	702	PLC	OB-CB-O3-C3
52	Z	201	CDL	CA5-C11-C12-C13
52	5	701	CDL	C56-C57-C58-C59
52	5	701	CDL	C12-C11-CA5-OA6
47	i	101	3PE	O21-C2-C3-O31
51	W	201	PLC	O2-C2-C3-O3
52	Z	201	CDL	OB6-CB4-CB6-OB8
54	4	505	T7X	O16-C8-C9-O18
54	2	502	T7X	C22-C23-C24-C25
54	2	504	T7X	C16-C17-C18-C19
54	2	504	T7X	C21-C22-C23-C24
54	3	202	T7X	C15-C16-C17-C18
54	3	202	T7X	C18-C19-C20-C21
55	2	503	PSC	C9-C10-C11-C12
52	Z	201	CDL	C53-C54-C55-C56
52	Z	201	CDL	C14-C15-C16-C17
52	4	502	CDL	C74-C75-C76-C77
52	X	201	CDL	C17-C18-C19-C20
54	3	202	T7X	C10-C12-C13-C14
52	X	201	CDL	C31-CA7-OA8-CA6
48	J	202	LMN	CBD-CBF-CBH-CBJ
47	4	503	3PE	C37-C38-C39-C3A
47	a	201	3PE	C34-C35-C36-C37
52	5	701	CDL	C51-C52-C53-C54
47	S	501	3PE	C39-C3A-C3B-C3C
48	J	204	LMN	CBF-CBH-CBJ-CBL
52	5	701	CDL	C12-C13-C14-C15
55	2	503	PSC	C25-C26-C27-C28
52	4	502	CDL	CB2-C1-CA2-OA2
47	4	501	3PE	C31-C32-C33-C34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
52	X	201	CDL	C18-C19-C20-C21
52	Z	201	CDL	OB5-CB3-CB4-CB6
52	4	502	CDL	C37-C38-C39-C40
55	2	503	PSC	O03-C19-C20-C21
52	X	201	CDL	OA9-CA7-OA8-CA6
48	J	202	LMN	CBF-CBH-CBJ-CBL
51	W	201	PLC	C1'-C2'-C3'-C4'
54	2	502	T7X	C2-C1-O1-P1
54	2	504	T7X	C2-C1-O1-P1
48	J	202	LMN	CBH-CBJ-CBL-CBR
47	4	504	3PE	C38-C39-C3A-C3B
47	J	203	3PE	C23-C24-C25-C26
47	a	201	3PE	C29-C2A-C2B-C2C
47	i	101	3PE	O11-C1-C2-O21
52	Z	201	CDL	OB5-CB3-CB4-OB6
52	5	701	CDL	OB5-CB3-CB4-OB6
52	X	201	CDL	CB3-CB4-CB6-OB8
51	1	403	PLC	C1'-C2'-C3'-C4'
52	2	501	CDL	C51-C52-C53-C54
51	W	201	PLC	O2-C'-C1'-C2'
47	S	501	3PE	C12-C11-O13-P
47	4	503	3PE	C12-C11-O13-P
51	5	703	PLC	C5-C4-O4P-P
47	4	503	3PE	C3D-C3E-C3F-C3G
47	4	503	3PE	O21-C2-C3-O31
52	5	701	CDL	C31-C32-C33-C34
52	X	201	CDL	C34-C35-C36-C37
47	S	501	3PE	C34-C35-C36-C37
51	W	201	PLC	C4B-C5B-C6B-C7B
51	5	703	PLC	C2'-C3'-C4'-C5'
51	1	401	PLC	O4P-C4-C5-N
51	1	403	PLC	O4P-C4-C5-N
51	5	702	PLC	O4P-C4-C5-N
51	5	703	PLC	O4P-C4-C5-N
54	3	202	T7X	C1-O1-P1-O11
47	S	501	3PE	C25-C26-C27-C28
47	4	504	3PE	C2A-C2B-C2C-C2D
48	J	202	LMN	O1-CBS-CCM-CBR
47	i	101	3PE	C23-C24-C25-C26
52	4	502	CDL	C12-C13-C14-C15
47	b	201	3PE	C31-C32-C33-C34
52	4	502	CDL	CB5-C51-C52-C53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
52	Z	201	CDL	C71-C72-C73-C74
47	I	501	3PE	O11-C1-C2-C3
52	5	701	CDL	OA5-CA3-CA4-CA6
51	W	202	PLC	C7'-C8'-C9'-CA'
50	Q	201	ZMP	C19-C18-C21-O5
52	X	201	CDL	C60-C61-C62-C63
47	I	501	3PE	C3E-C3F-C3G-C3H
47	i	101	3PE	C39-C3A-C3B-C3C
47	a	201	3PE	C33-C34-C35-C36
52	4	502	CDL	C51-C52-C53-C54
52	5	701	CDL	OB7-CB5-OB6-CB4
54	3	202	T7X	O13-C7-C8-O16
47	4	501	3PE	C29-C2A-C2B-C2C
52	4	502	CDL	C58-C59-C60-C61
48	J	202	LMN	CBG-CBI-CBK-CBQ
48	J	204	LMN	CBH-CBJ-CBL-CBR
52	X	201	CDL	OB6-CB4-CB6-OB8
52	4	502	CDL	OA6-CA4-CA6-OA8
52	X	201	CDL	CA2-C1-CB2-OB2
54	2	504	T7X	C11-C31-C32-C33
47	4	503	3PE	C1-C2-C3-O31
52	4	502	CDL	CA3-CA4-CA6-OA8
52	Z	201	CDL	CB7-C71-C72-C73
51	1	401	PLC	C1B-C2B-C3B-C4B
47	S	501	3PE	C36-C37-C38-C39
46	E	401	NDP	O4D-C4D-C5D-O5D
47	J	203	3PE	C1-O11-P-O14
47	a	201	3PE	C1-O11-P-O12
47	a	201	3PE	C1-O11-P-O13
47	a	201	3PE	C11-O13-P-O12
47	4	501	3PE	O13-C11-C12-N
47	4	504	3PE	C11-O13-P-O11
47	4	504	3PE	C11-O13-P-O14
47	4	504	3PE	O13-C11-C12-N
51	W	201	PLC	C1-O3P-P-O1P
51	W	201	PLC	C4-O4P-P-O1P
51	1	403	PLC	C1-O3P-P-O1P
51	5	702	PLC	C1-O3P-P-O1P
51	5	702	PLC	C1-O3P-P-O4P
51	5	702	PLC	C4-O4P-P-O2P
52	X	201	CDL	CA3-OA5-PA1-OA3
52	2	501	CDL	CA2-OA2-PA1-OA4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
52	2	501	CDL	CB2-OB2-PB2-OB5
52	4	502	CDL	CA2-OA2-PA1-OA5
52	4	502	CDL	CB3-OB5-PB2-OB4
52	5	701	CDL	CA3-OA5-PA1-OA3
54	2	502	T7X	C7-O13-P1-O11
54	4	505	T7X	C7-O13-P1-O11
52	4	502	CDL	C54-C55-C56-C57
52	X	201	CDL	C1-CB2-OB2-PB2
51	W	202	PLC	C8B-C9B-CAA-CBA
47	b	201	3PE	C2A-C2B-C2C-C2D
48	J	204	LMN	CCH-CCQ-OCB-CCS
52	2	501	CDL	CB5-C51-C52-C53
50	Q	201	ZMP	C2-C3-C4-C5
51	5	702	PLC	C1'-C2'-C3'-C4'
50	O	201	ZMP	C1-C2-C3-C4
52	X	201	CDL	CA3-CA4-OA6-CA5
52	2	501	CDL	CB6-CB4-OB6-CB5
55	2	503	PSC	C29-C30-C31-C32
51	W	201	PLC	C4-C5-N-C8
47	3	201	3PE	O11-C1-C2-C3
52	X	201	CDL	OB5-CB3-CB4-CB6
54	2	502	T7X	O13-C7-C8-C9
54	3	202	T7X	O13-C7-C8-C9
48	J	204	LMN	CAY-CBA-CBC-CBE
47	4	504	3PE	C2F-C2G-C2H-C2I
47	b	201	3PE	C2C-C2D-C2E-C2F
47	4	503	3PE	C31-C32-C33-C34
54	4	505	T7X	C34-C35-C36-C37
47	I	501	3PE	O22-C21-O21-C2
52	X	201	CDL	C56-C57-C58-C59
52	X	201	CDL	CA5-C11-C12-C13
47	3	201	3PE	C22-C21-O21-C2
51	W	201	PLC	C4-C5-N-C6
52	2	501	CDL	C13-C14-C15-C16
47	I	501	3PE	C27-C28-C29-C2A
47	I	501	3PE	C22-C21-O21-C2
54	2	504	T7X	C6-C1-O1-P1
51	W	202	PLC	C6'-C7'-C8'-C9'
47	a	201	3PE	C32-C33-C34-C35
52	5	701	CDL	C12-C11-CA5-OA7
52	X	201	CDL	C63-C64-C65-C66
52	5	701	CDL	CB5-C51-C52-C53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
47	4	504	3PE	O11-C1-C2-O21
54	2	504	T7X	C24-C25-C26-C27
52	4	502	CDL	C34-C35-C36-C37
52	5	701	CDL	C17-C18-C19-C20
51	5	702	PLC	C8B-C9B-CAA-CBA
52	4	502	CDL	O1-C1-CA2-OA2
47	J	203	3PE	C29-C2A-C2B-C2C
47	4	503	3PE	C3A-C3B-C3C-C3D
47	J	201	3PE	O22-C21-O21-C2
47	4	503	3PE	C34-C35-C36-C37
48	j	101	LMN	CBD-CBF-CBH-CBJ
47	I	501	3PE	C34-C35-C36-C37
46	E	401	NDP	O4D-C1D-N1N-C6N
48	J	202	LMN	OBY-CCR-O4-C4
52	4	502	CDL	C1-CB2-OB2-PB2
51	W	201	PLC	C4-C5-N-C7
51	W	202	PLC	C1B-C2B-C3B-C4B
54	4	505	T7X	C35-C36-C37-C38
52	X	201	CDL	C72-C73-C74-C75
54	2	502	T7X	C9-C8-O16-C10
51	1	401	PLC	C1'-C2'-C3'-C4'
52	X	201	CDL	C51-C52-C53-C54
48	j	101	LMN	OBY-CCR-O4-C4
47	I	501	3PE	C3A-C3B-C3C-C3D
52	5	701	CDL	C51-CB5-OB6-CB4
48	J	202	LMN	O1-CBS-CCM-CBT
47	4	504	3PE	C32-C31-O31-C3
51	W	202	PLC	C2B-C3B-C4B-C5B
51	1	401	PLC	C3B-C4B-C5B-C6B
51	1	401	PLC	C8'-C9'-CA'-CB'
51	1	401	PLC	C2'-C3'-C4'-C5'
52	5	701	CDL	CB2-C1-CA2-OA2
48	J	202	LMN	CAW-CAY-CBA-CBC
47	4	504	3PE	C33-C34-C35-C36
51	1	401	PLC	CB-C1B-C2B-C3B
52	Z	201	CDL	C31-C32-C33-C34
48	j	101	LMN	CAB-CAX-CAZ-CBB
48	j	101	LMN	C3-C4-O4-CCR
47	a	201	3PE	C26-C27-C28-C29
47	b	201	3PE	C2-C1-O11-P
51	5	702	PLC	C2'-C3'-C4'-C5'
52	X	201	CDL	C74-C75-C76-C77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
52	4	502	CDL	C56-C57-C58-C59
47	J	201	3PE	C22-C21-O21-C2
47	4	504	3PE	O32-C31-O31-C3
51	5	703	PLC	C1-C2-C3-O3
53	1	402	UQ9	C12-C11-C9-C10
54	2	502	T7X	C32-C33-C34-C35
54	4	505	T7X	C16-C17-C18-C19
48	J	204	LMN	CBD-CBF-CBH-CBJ
51	5	703	PLC	O2-C2-C3-O3
47	J	201	3PE	C39-C3A-C3B-C3C
52	2	501	CDL	C18-C19-C20-C21
46	E	401	NDP	C2D-C1D-N1N-C6N
47	i	101	3PE	C29-C2A-C2B-C2C
45	B	502	FMN	C5'-O5'-P-O1P
47	4	504	3PE	C3E-C3F-C3G-C3H
55	2	503	PSC	C20-C21-C22-C23
50	Q	201	ZMP	C5-C6-C7-C8
47	S	501	3PE	C37-C38-C39-C3A
55	2	503	PSC	C4-C5-C6-C7
47	b	201	3PE	C32-C33-C34-C35
54	4	505	T7X	C33-C34-C35-C36
54	4	505	T7X	C13-C14-C15-C16
47	S	501	3PE	C38-C39-C3A-C3B
47	J	203	3PE	O11-C1-C2-O21
54	4	505	T7X	O13-C7-C8-O16
54	4	505	T7X	C7-C8-C9-O18
48	J	202	LMN	CCV-CCR-O4-C4
48	J	204	LMN	CBC-CBE-CBG-CBI
51	5	702	PLC	C3'-C4'-C5'-C6'
54	2	502	T7X	O17-C10-O16-C8
47	J	201	3PE	O21-C21-C22-C23
52	2	501	CDL	C76-C77-C78-C79
47	I	501	3PE	O31-C31-C32-C33
52	5	701	CDL	C72-C71-CB7-OB8
52	5	701	CDL	C34-C35-C36-C37
52	X	201	CDL	C51-CB5-OB6-CB4
47	b	201	3PE	O31-C31-C32-C33
47	4	504	3PE	C26-C27-C28-C29
52	X	201	CDL	C52-C53-C54-C55
51	5	702	PLC	O2-C'-C1'-C2'
51	W	201	PLC	O'-C'-C1'-C2'
55	2	503	PSC	O04-C19-C20-C21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
47	b	201	3PE	C38-C39-C3A-C3B
48	j	101	LMN	CBH-CBJ-CBL-CBR
47	3	201	3PE	O22-C21-O21-C2
47	b	201	3PE	O21-C21-C22-C23
47	J	203	3PE	C1-C2-C3-O31
51	W	202	PLC	C2B-C1B-CB-O3
54	2	504	T7X	O18-C11-C31-C32
50	O	201	ZMP	C2-C3-C4-C5
55	2	503	PSC	O03-C01-C02-O01
47	i	101	3PE	O21-C21-C22-C23
52	X	201	CDL	C12-C11-CA5-OA6
55	2	503	PSC	O01-C1-C2-C3
51	1	401	PLC	O2-C'-C1'-C2'
52	2	501	CDL	C12-C11-CA5-OA6
54	4	505	T7X	O18-C11-C31-C32
52	X	201	CDL	C32-C31-CA7-OA8
51	W	202	PLC	C1-C2-O2-C'
54	4	505	T7X	C7-C8-O16-C10
54	2	502	T7X	C24-C25-C26-C27
55	2	503	PSC	C6-C7-C8-C9
52	2	501	CDL	C41-C42-C43-C44
47	J	201	3PE	O22-C21-C22-C23
52	4	502	CDL	C52-C53-C54-C55
51	W	202	PLC	C2B-C1B-CB-OB
47	3	201	3PE	O11-C1-C2-O21
55	2	503	PSC	O02-C1-C2-C3
52	Z	201	CDL	CB4-CB6-OB8-CB7
52	X	201	CDL	C32-C31-CA7-OA9
54	2	504	T7X	O19-C11-C31-C32
47	b	201	3PE	O32-C31-C32-C33
52	Z	201	CDL	C32-C31-CA7-OA8
48	j	101	LMN	CCM-CBS-O1-C1
47	I	501	3PE	O32-C31-C32-C33
51	5	702	PLC	O'-C'-C1'-C2'
50	O	201	ZMP	N2-C16-C17-O4
47	i	101	3PE	O22-C21-C22-C23
52	5	701	CDL	C72-C71-CB7-OB9
52	2	501	CDL	C12-C11-CA5-OA7
51	1	401	PLC	O'-C'-C1'-C2'
52	X	201	CDL	C12-C11-CA5-OA7
54	2	504	T7X	O13-C7-C8-C9
52	X	201	CDL	C61-C62-C63-C64

Continued on next page...

Continued from previous page...

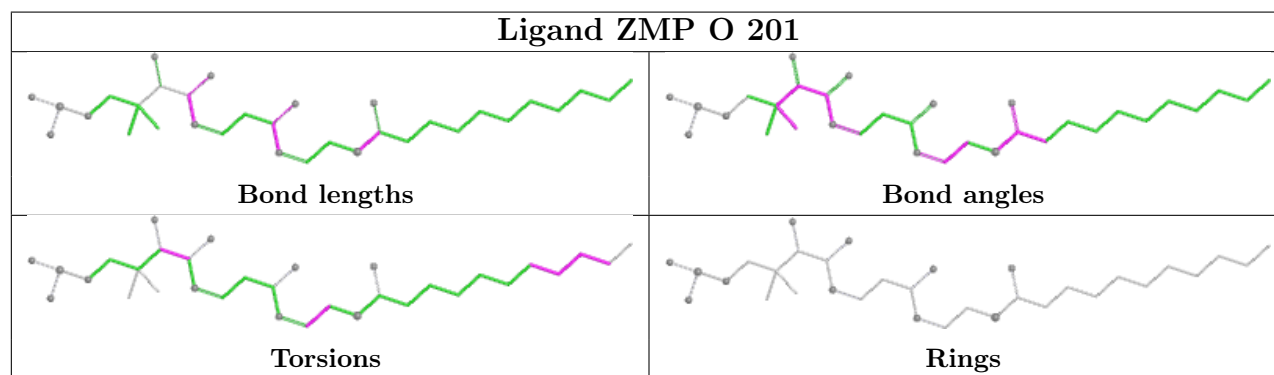
Mol	Chain	Res	Type	Atoms
52	Z	201	CDL	C32-C31-CA7-OA9
47	I	501	3PE	O21-C21-C22-C23
46	E	401	NDP	PN-O3-PA-O2A
54	3	202	T7X	O16-C10-C12-C13

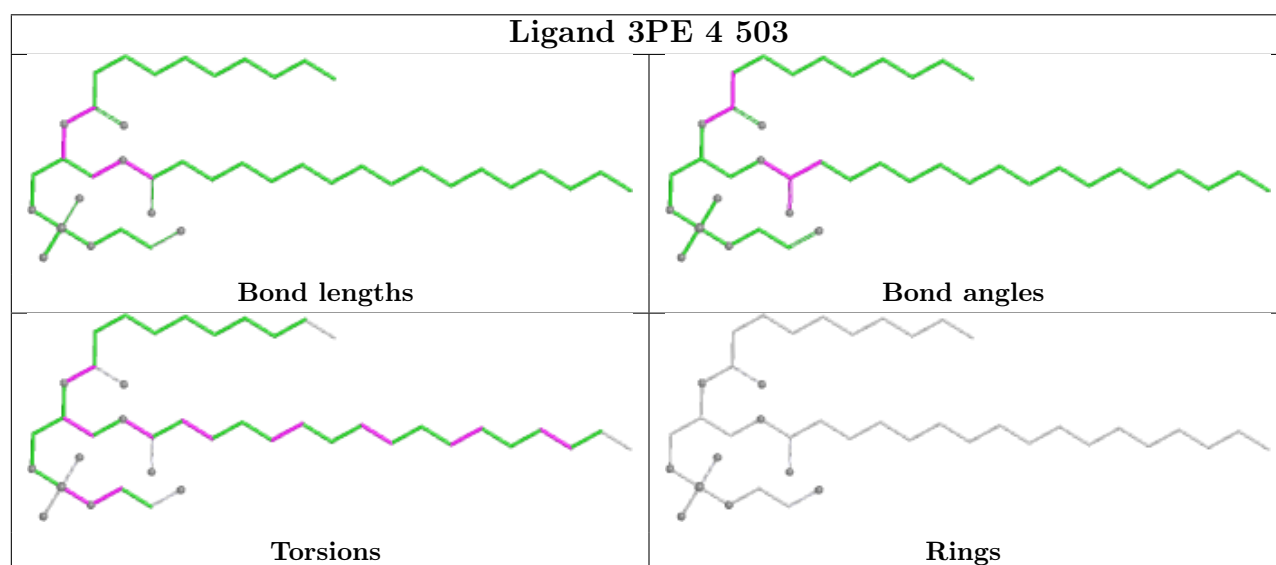
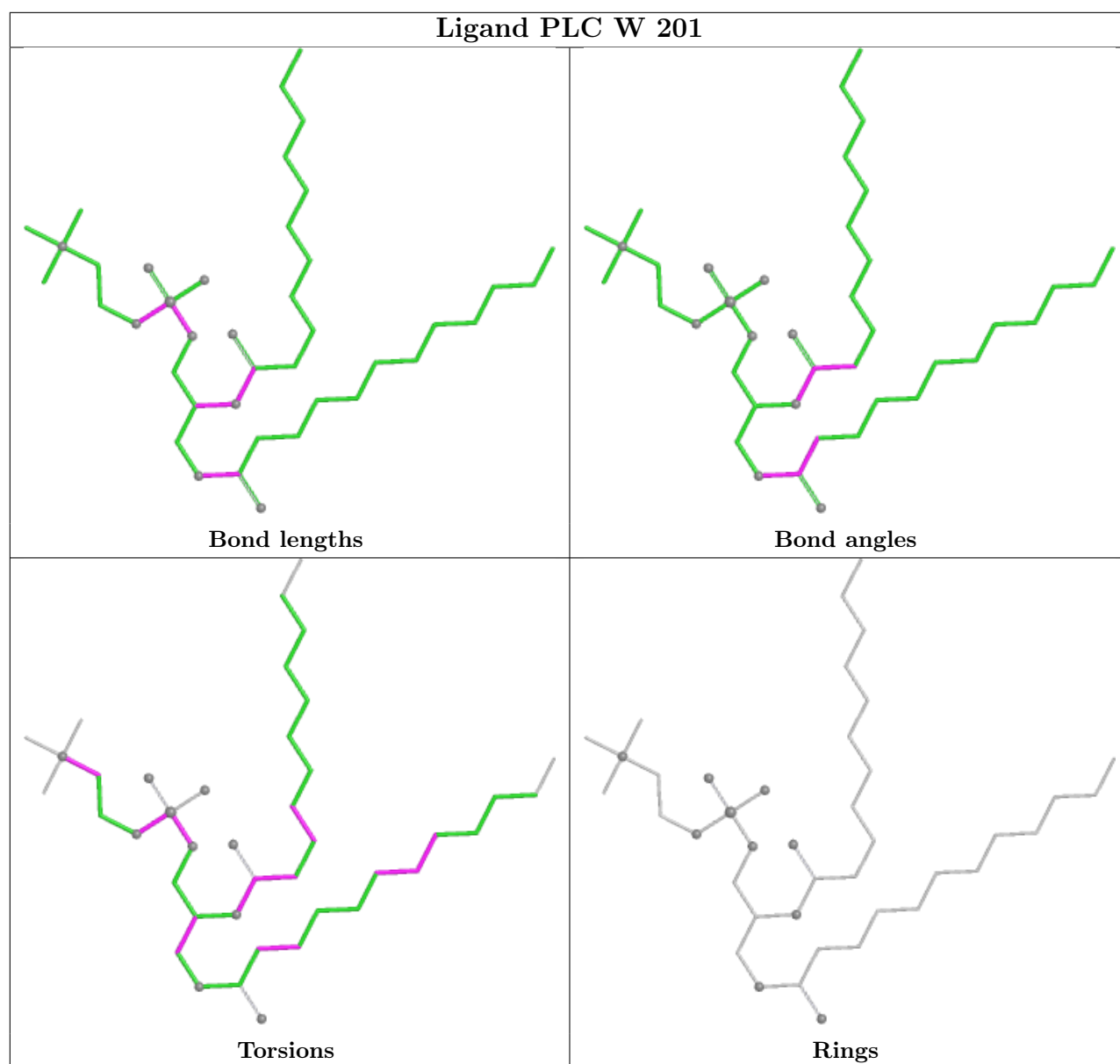
There are no ring outliers.

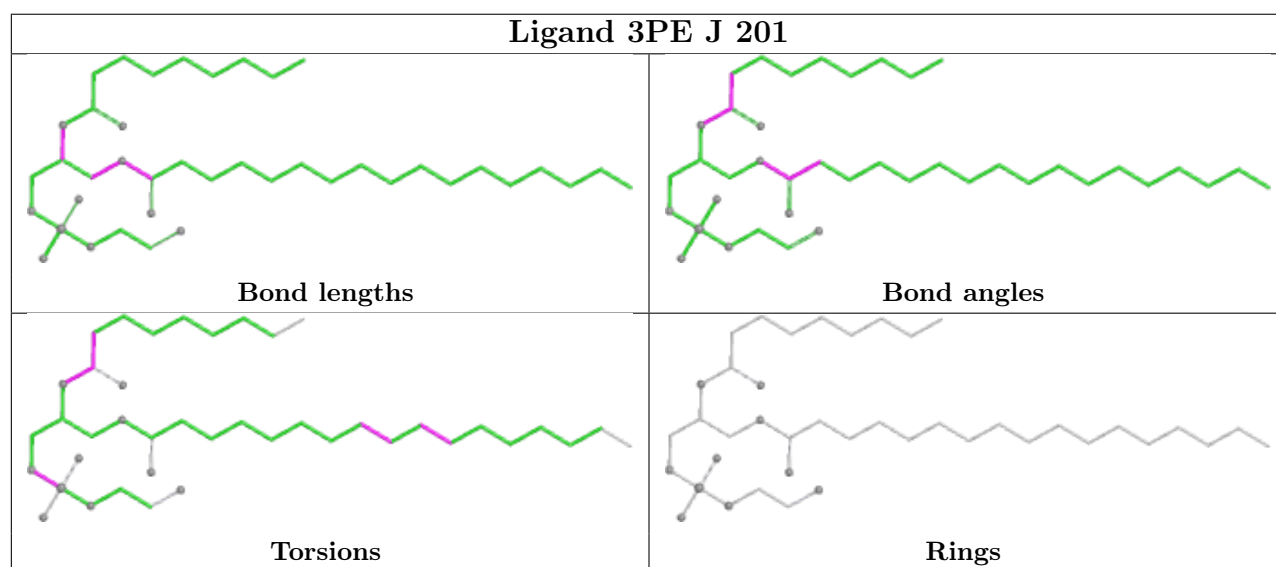
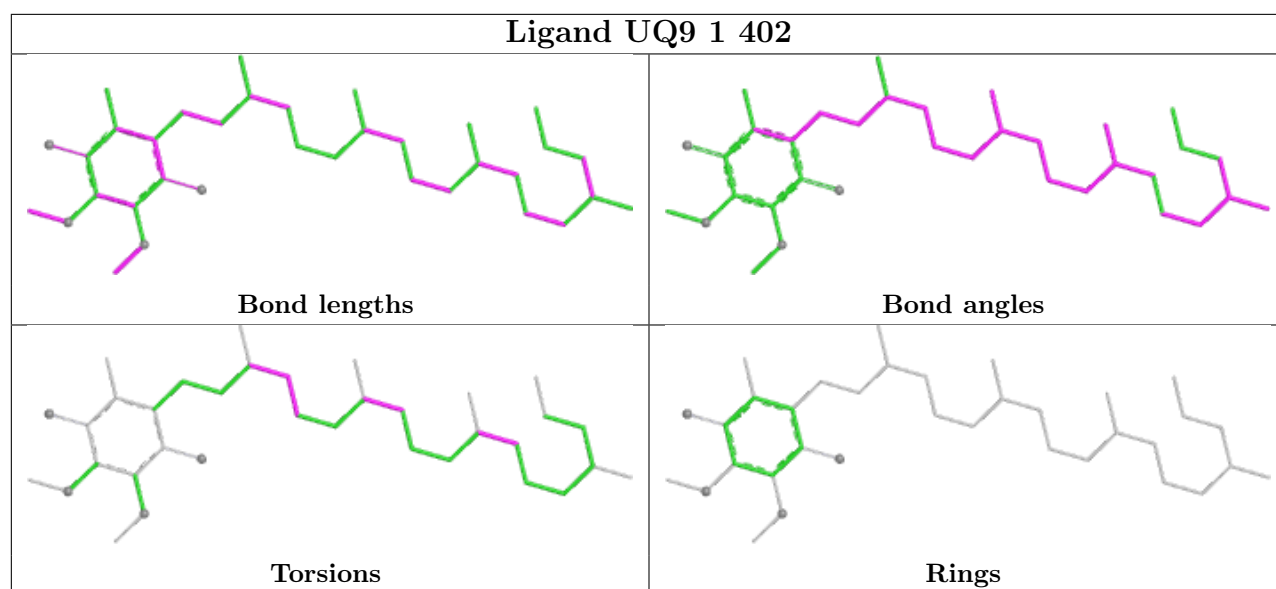
32 monomers are involved in 122 short contacts:

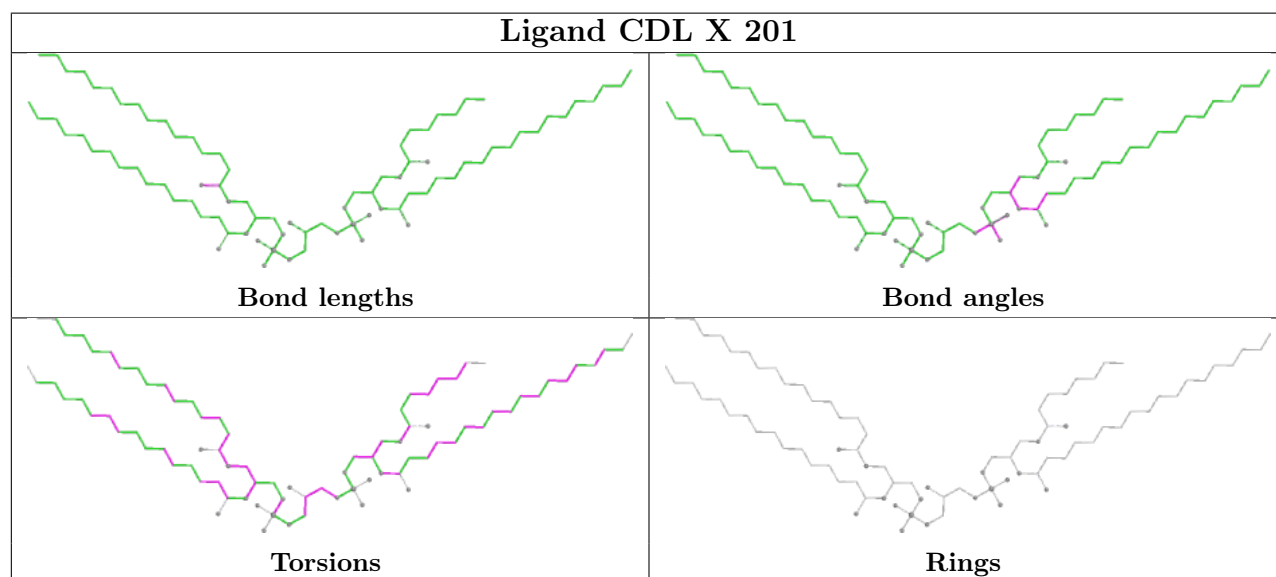
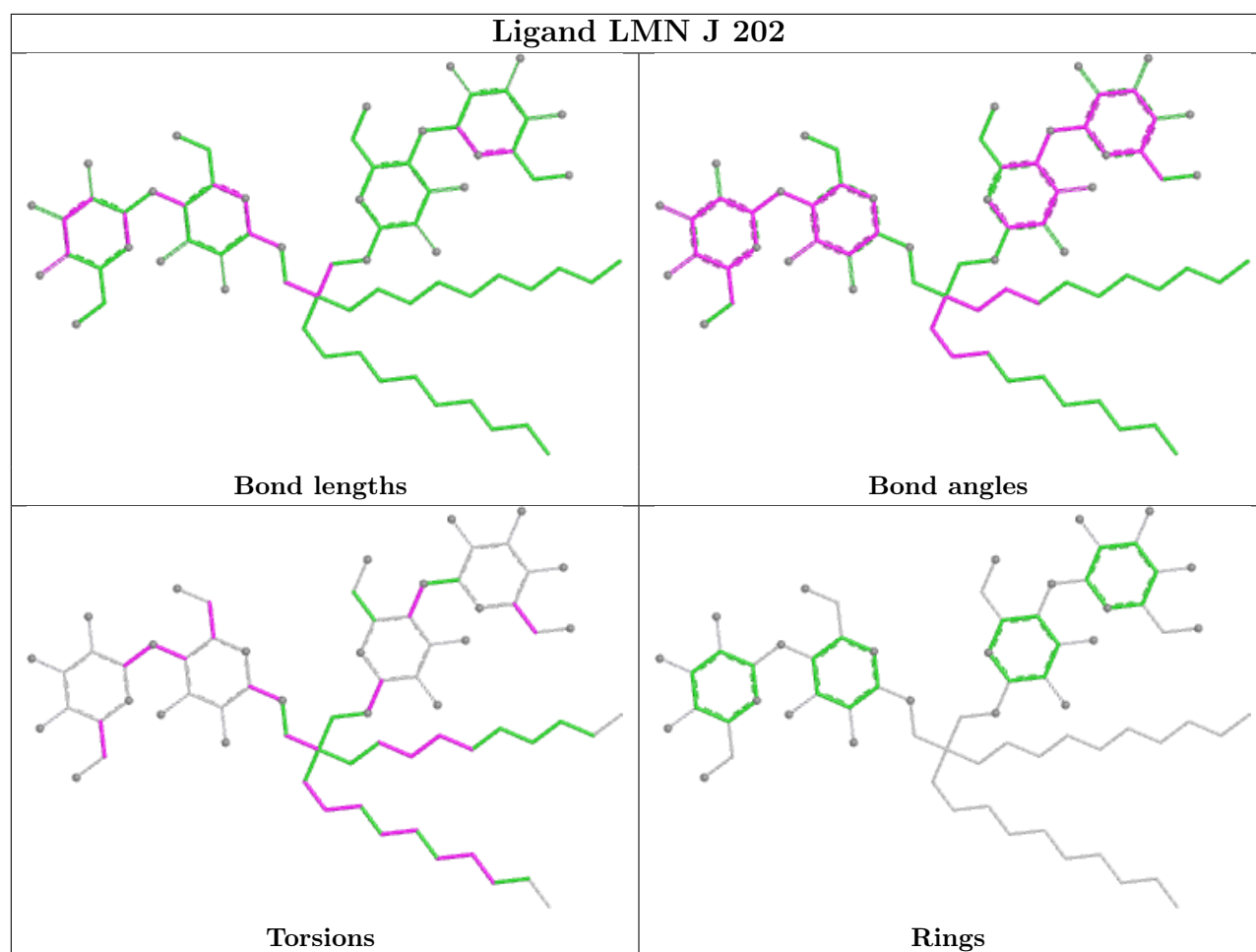
Mol	Chain	Res	Type	Clashes	Symm-Clashes
50	O	201	ZMP	1	0
51	W	201	PLC	5	0
47	4	503	3PE	3	0
53	1	402	UQ9	11	0
47	J	201	3PE	2	0
48	J	202	LMN	3	0
52	X	201	CDL	14	0
45	B	502	FMN	1	0
47	i	101	3PE	2	0
47	b	201	3PE	2	0
47	S	501	3PE	2	0
51	1	403	PLC	1	0
50	Q	201	ZMP	2	0
46	E	401	NDP	1	0
51	5	702	PLC	1	0
47	3	201	3PE	10	0
52	2	501	CDL	19	0
47	I	501	3PE	3	0
55	2	503	PSC	1	0
52	4	502	CDL	4	0
52	Z	201	CDL	2	0
43	A	801	SF4	1	0
47	4	501	3PE	3	0
47	4	504	3PE	9	0
52	5	701	CDL	4	0
54	4	505	T7X	3	0
48	j	101	LMN	3	0
48	J	204	LMN	4	0
51	1	401	PLC	3	0
51	W	202	PLC	4	0
47	a	201	3PE	3	0
47	J	203	3PE	2	0

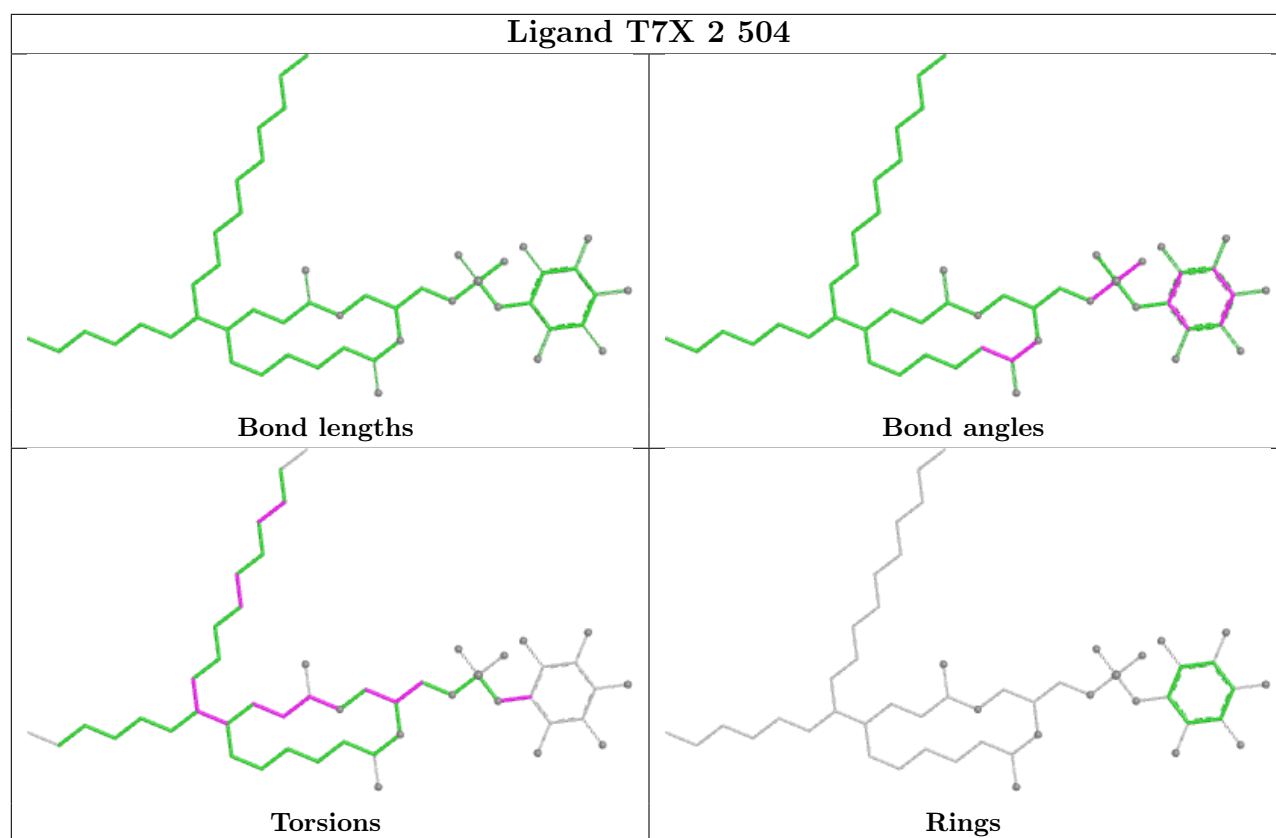
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

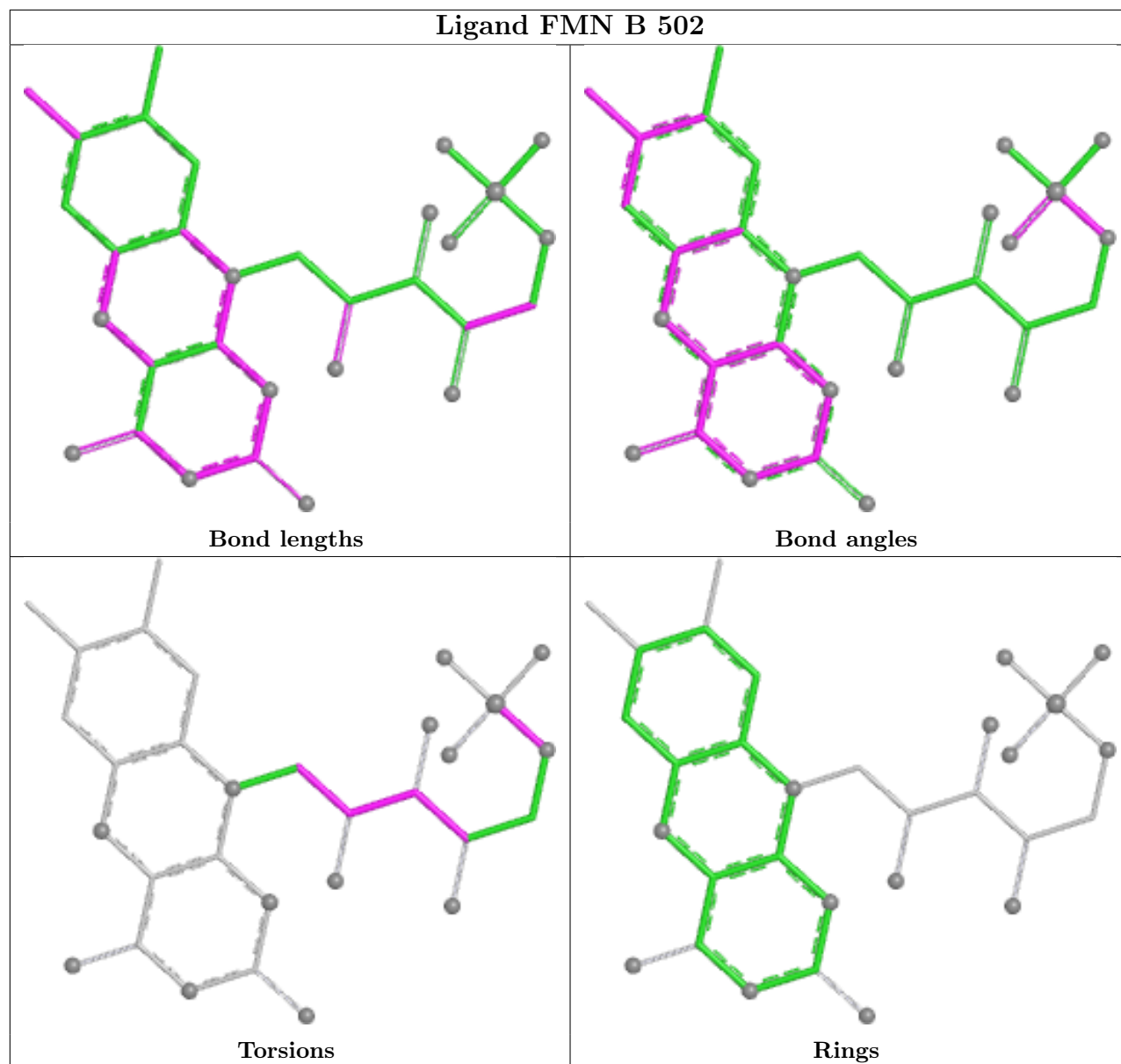


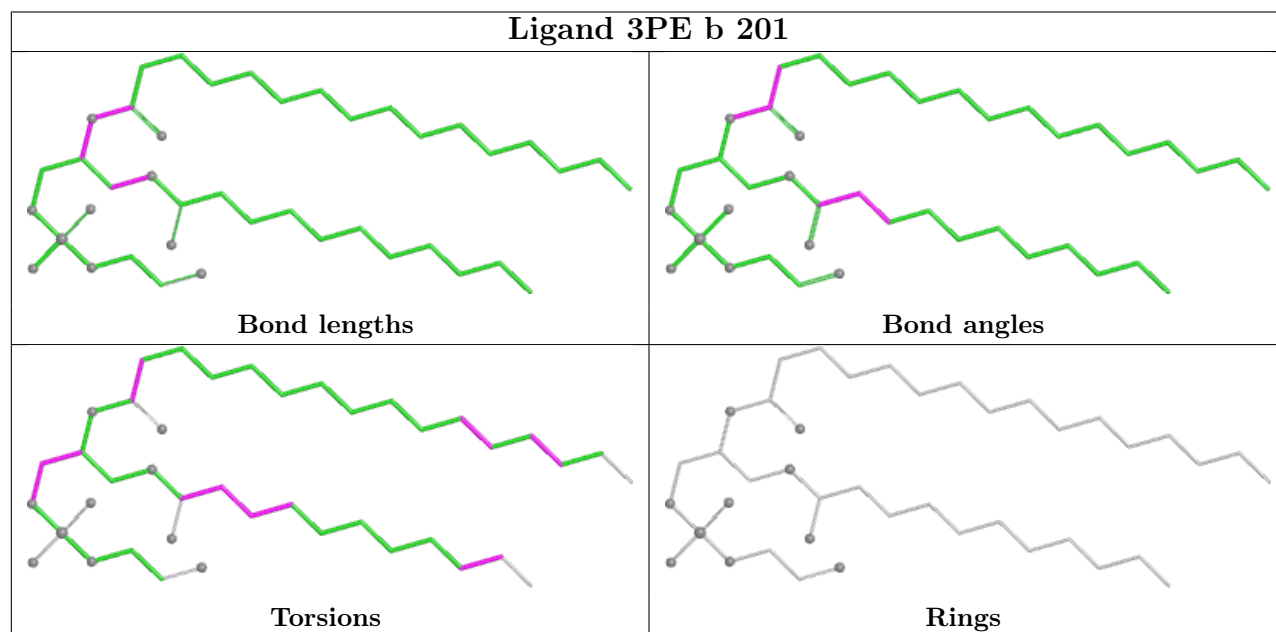
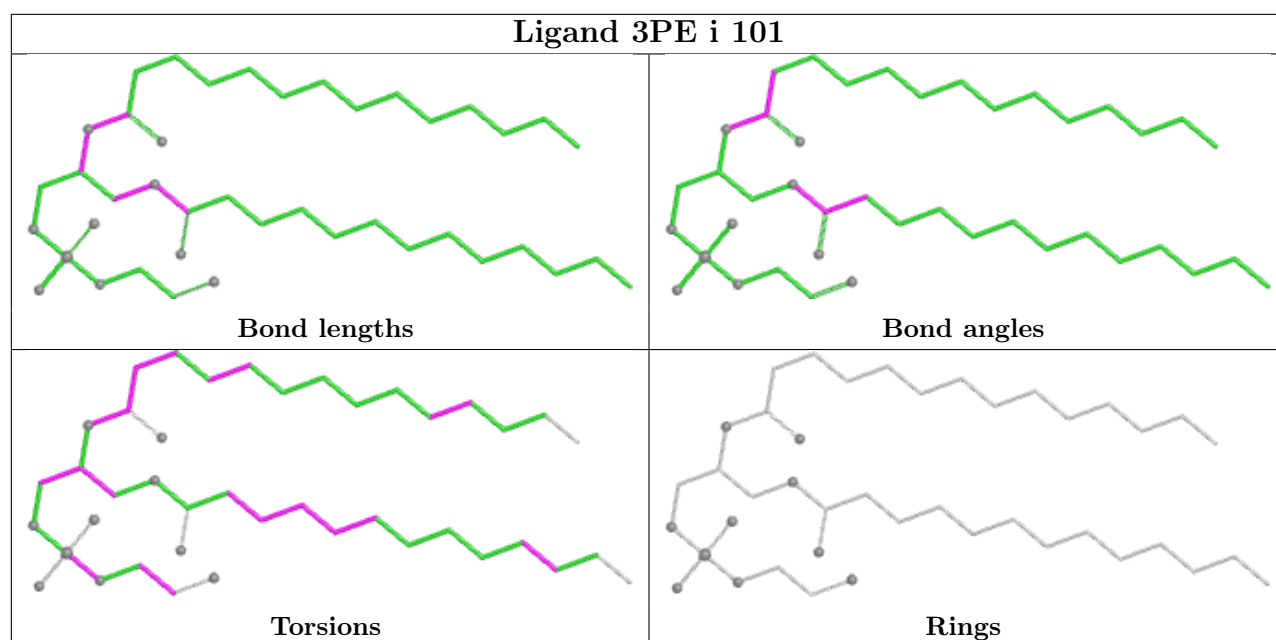


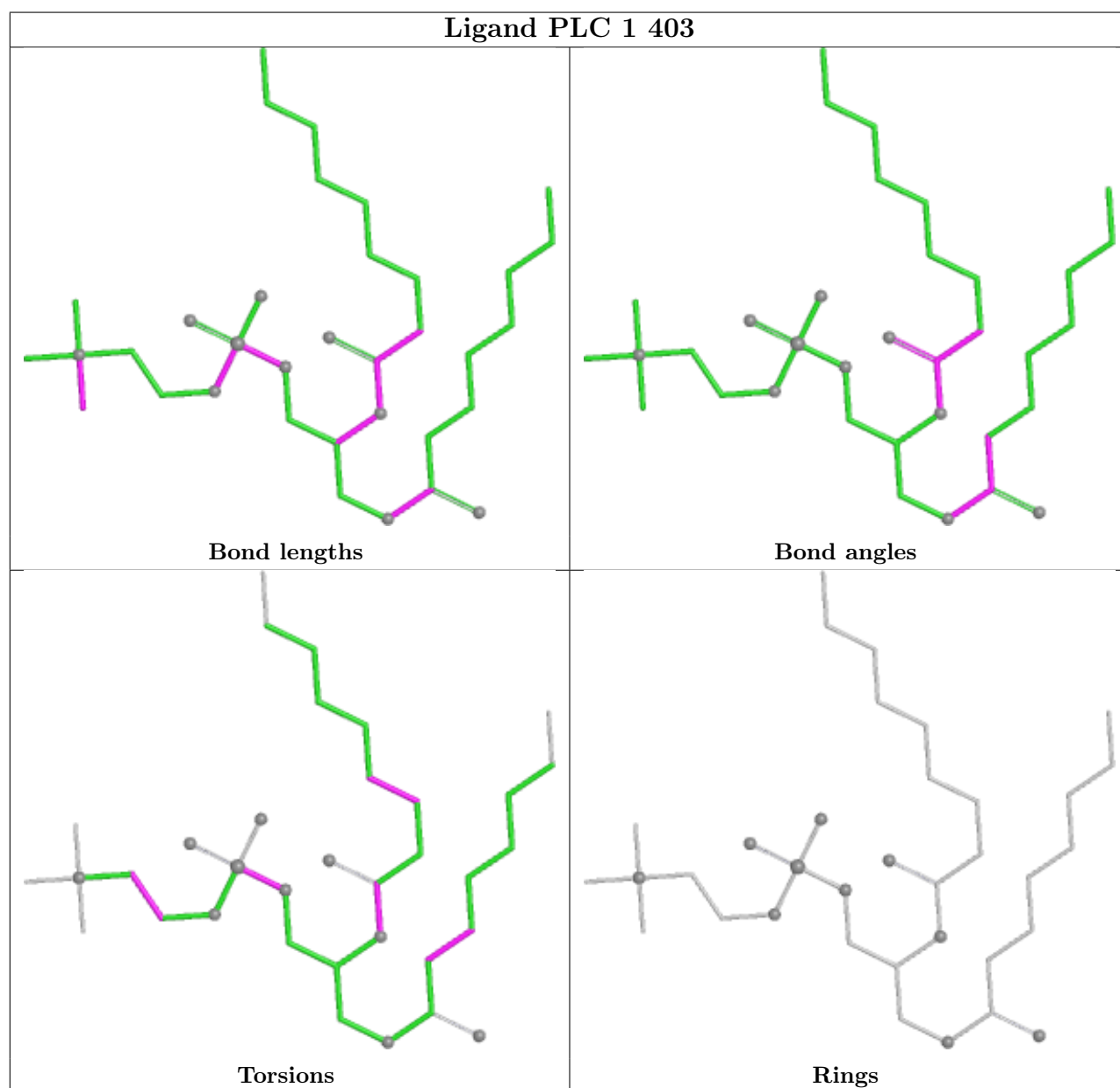
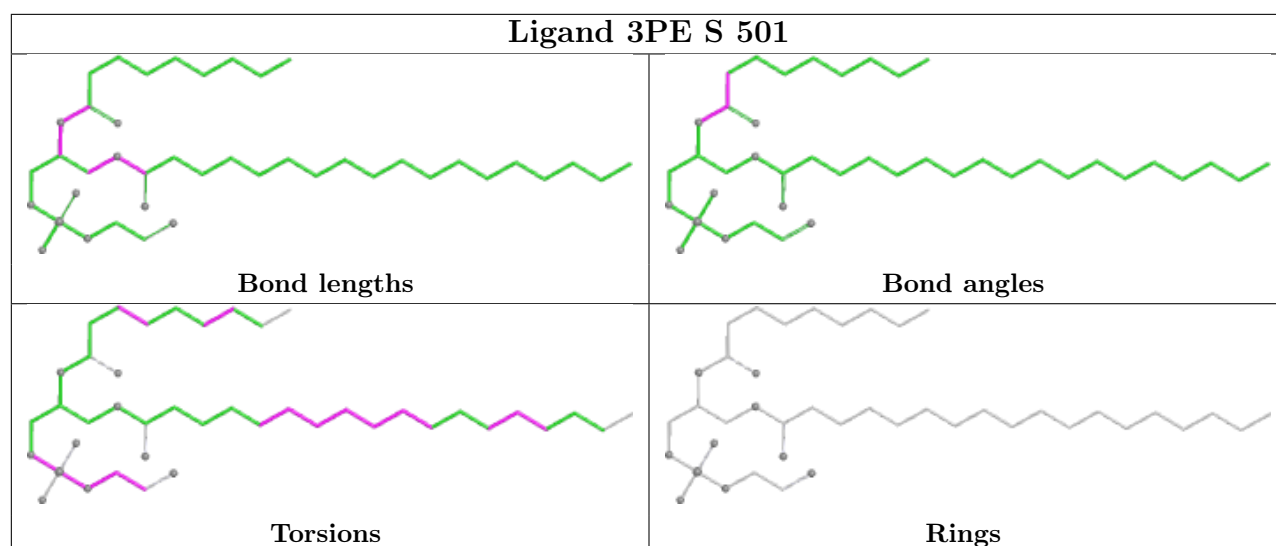


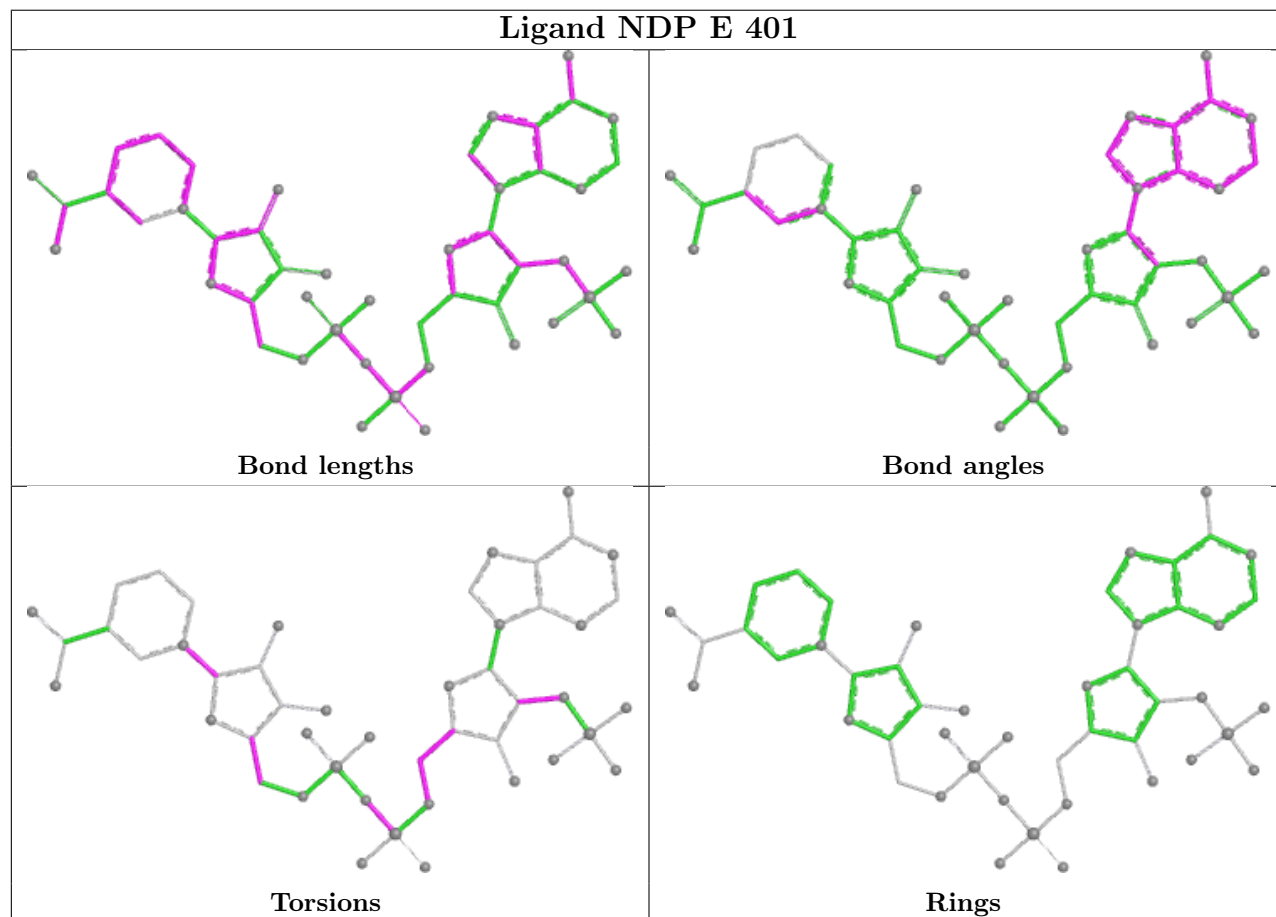
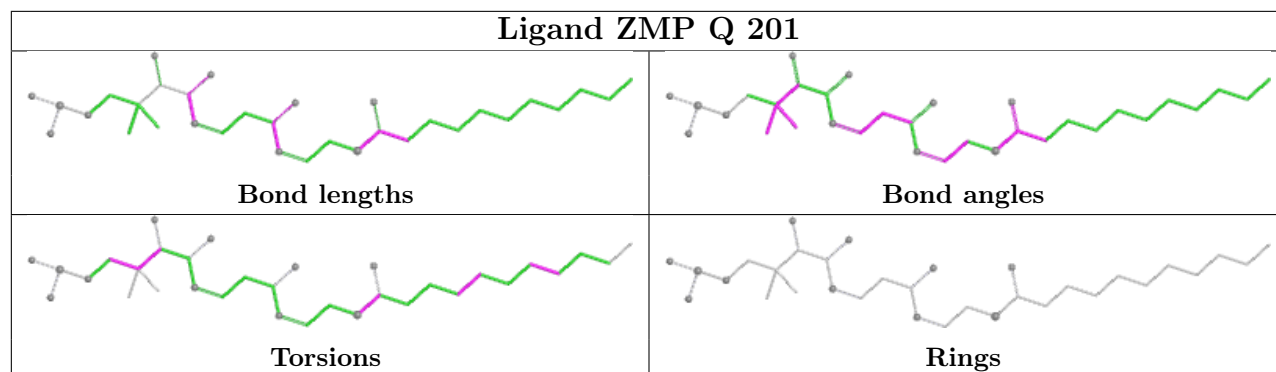


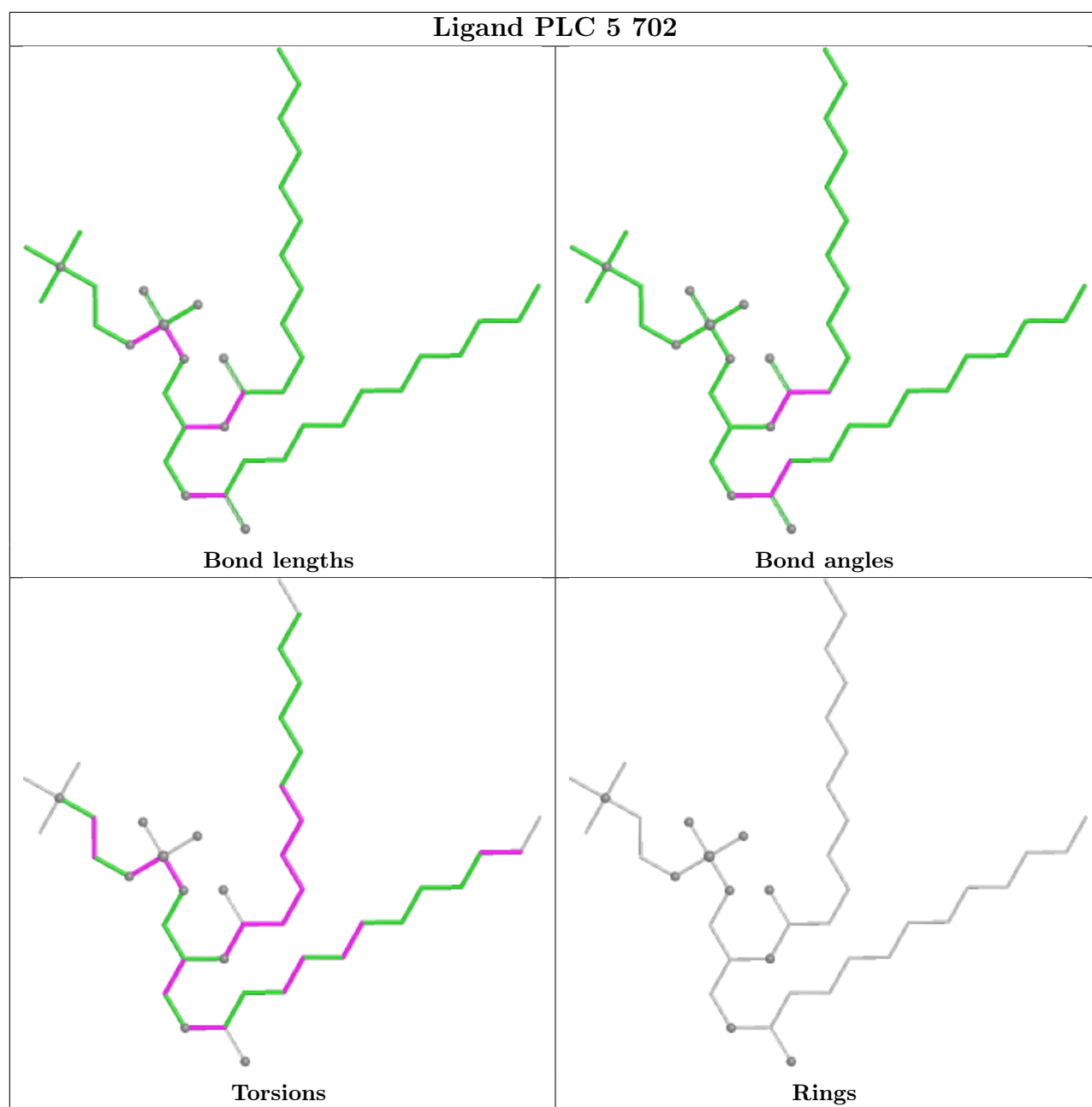


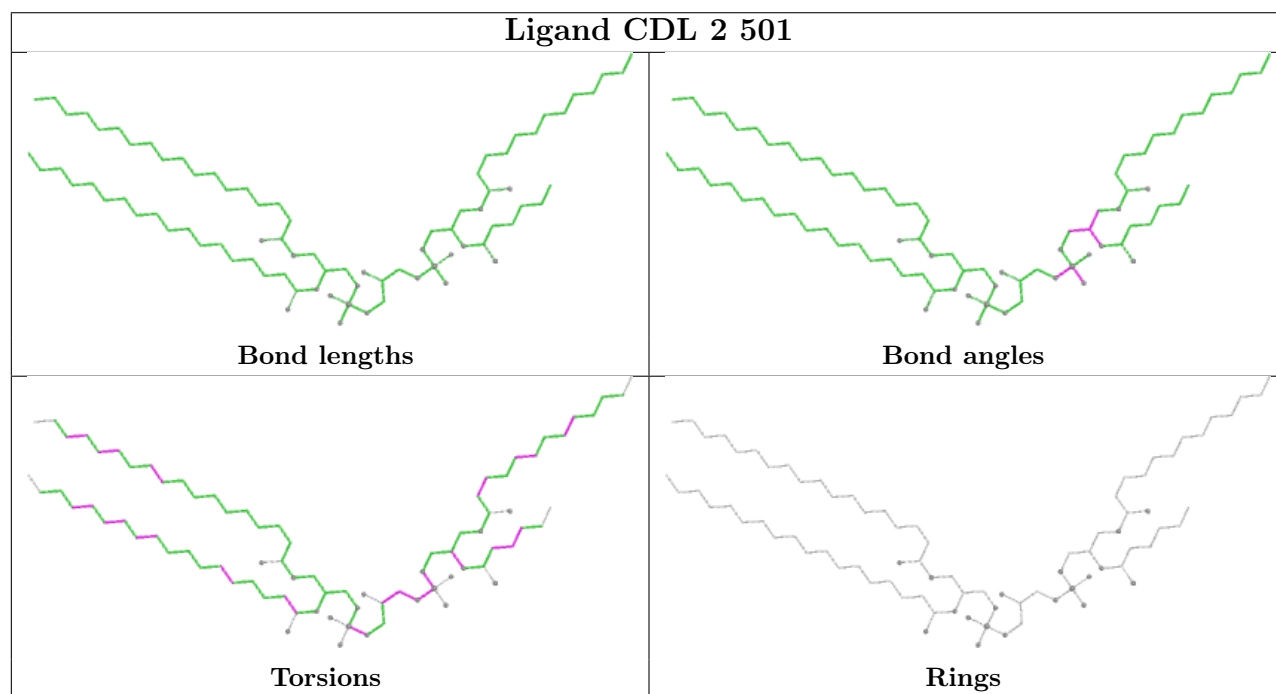
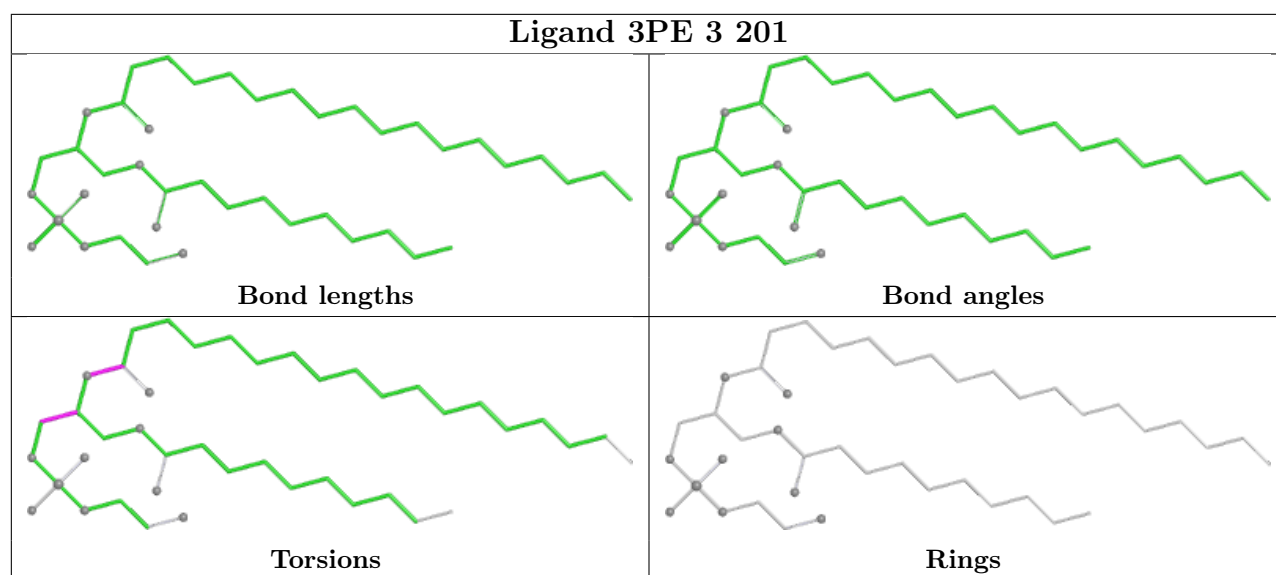


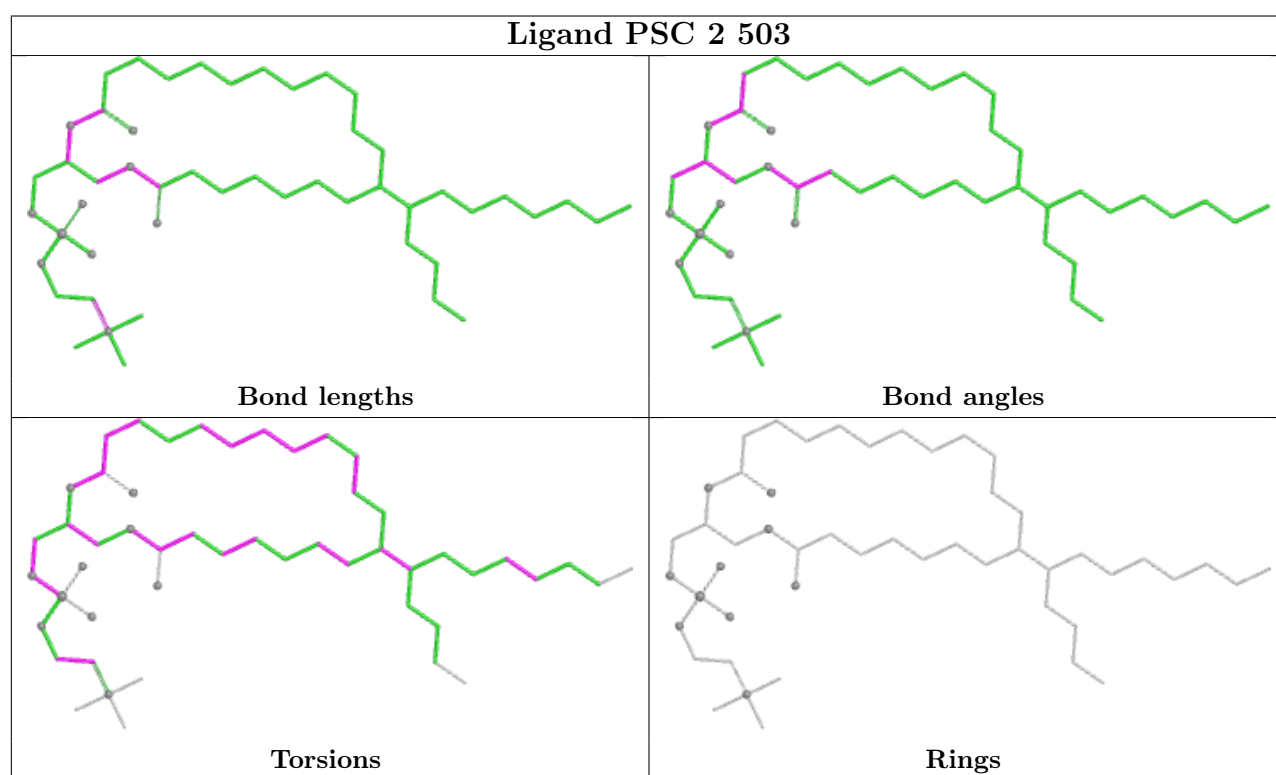
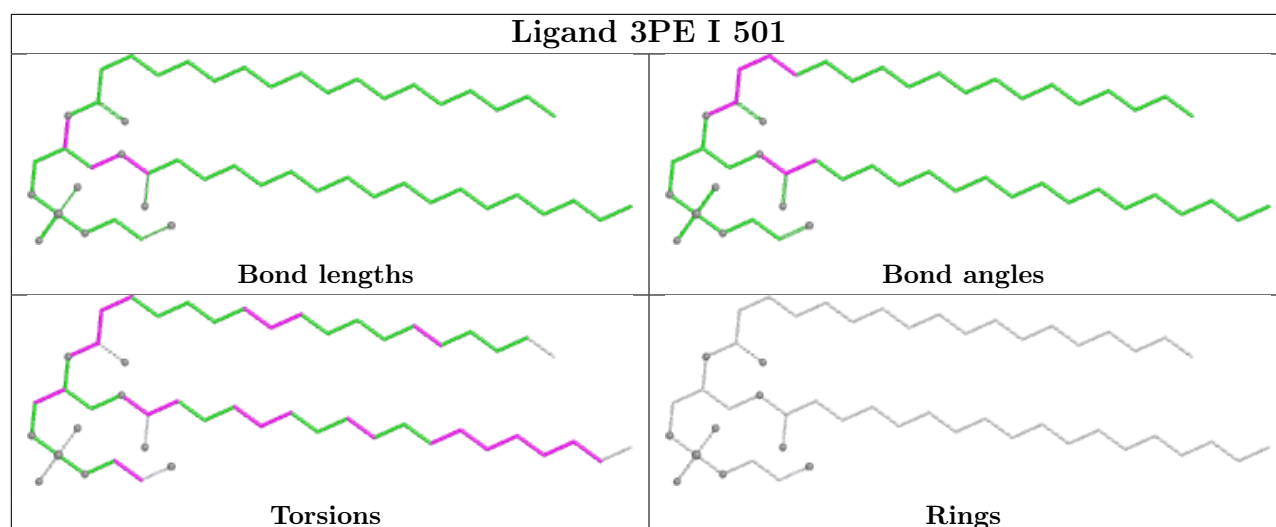


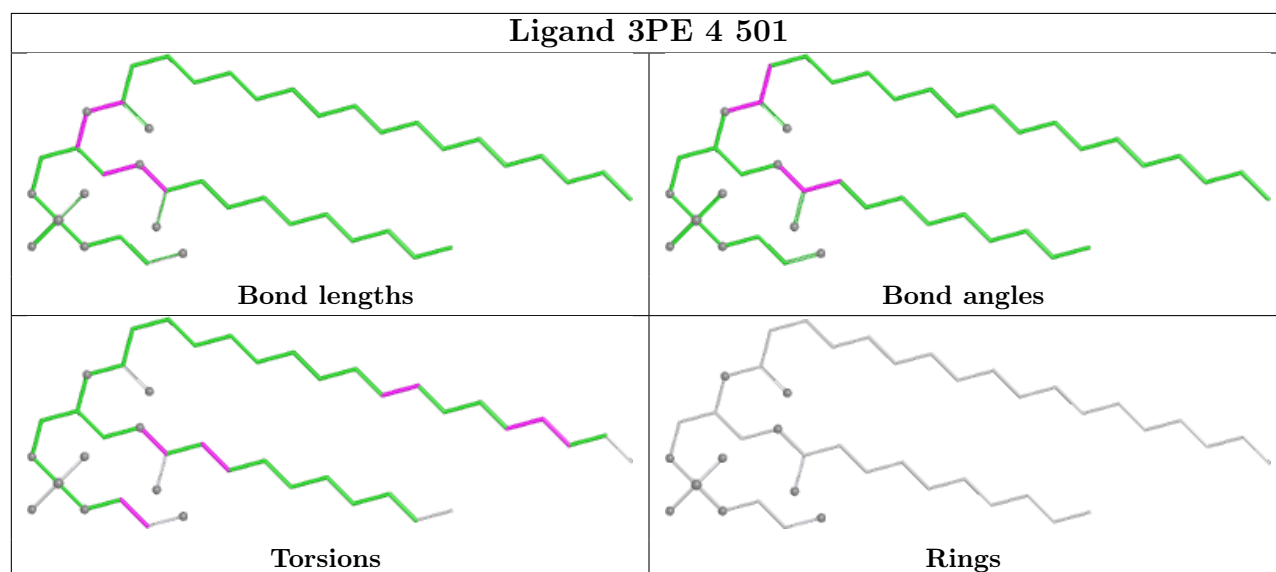
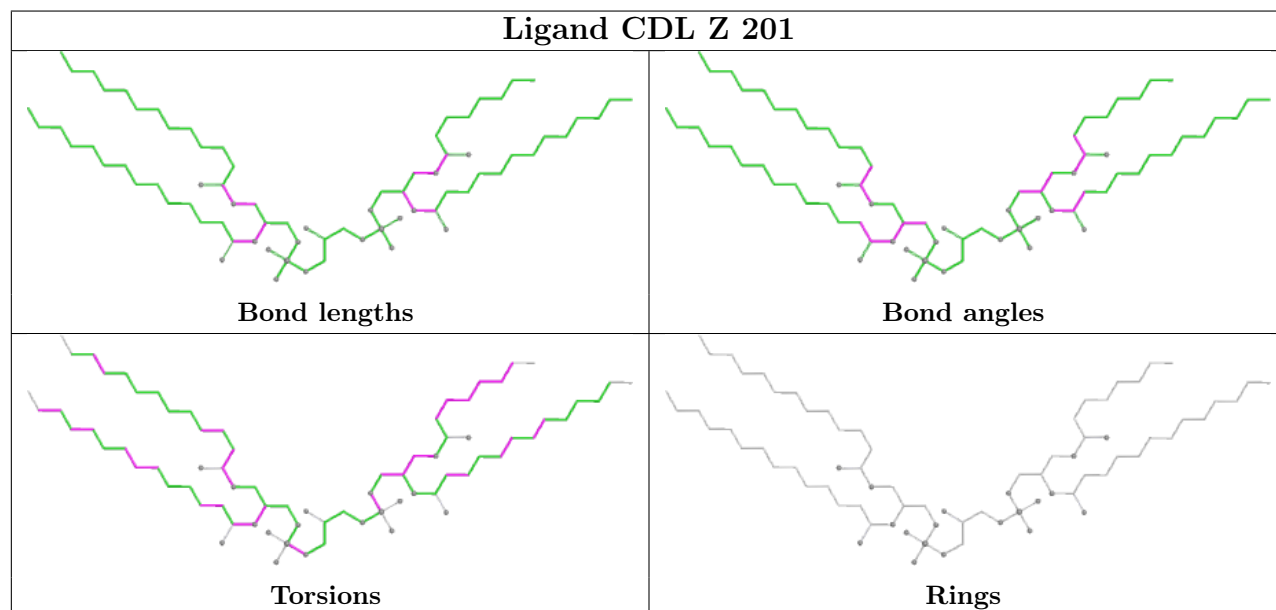
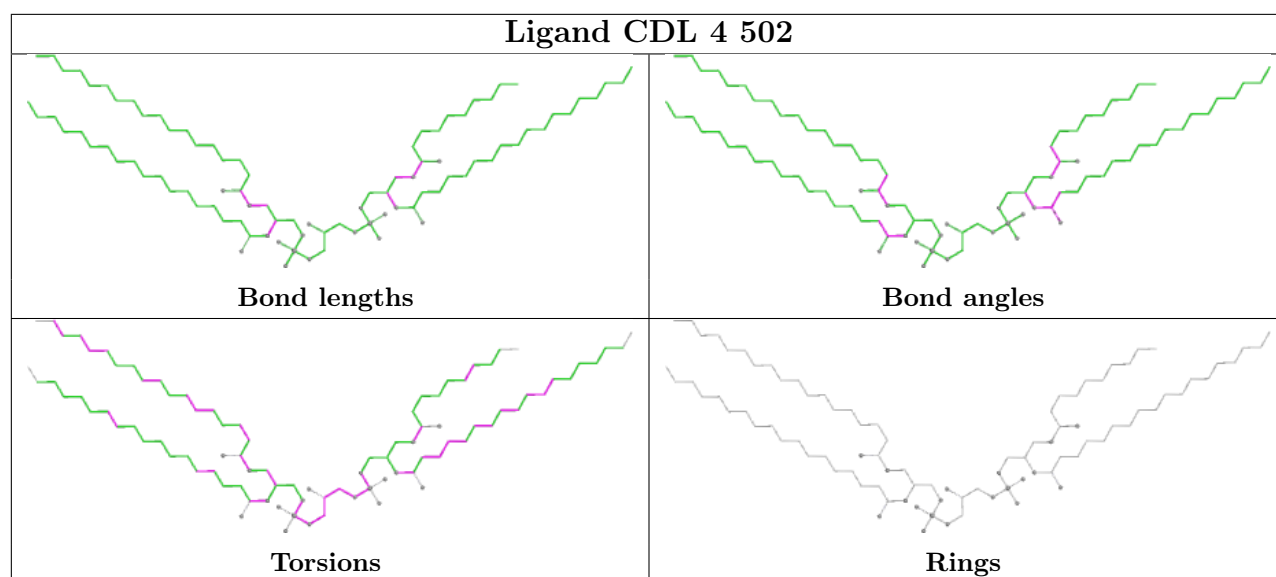


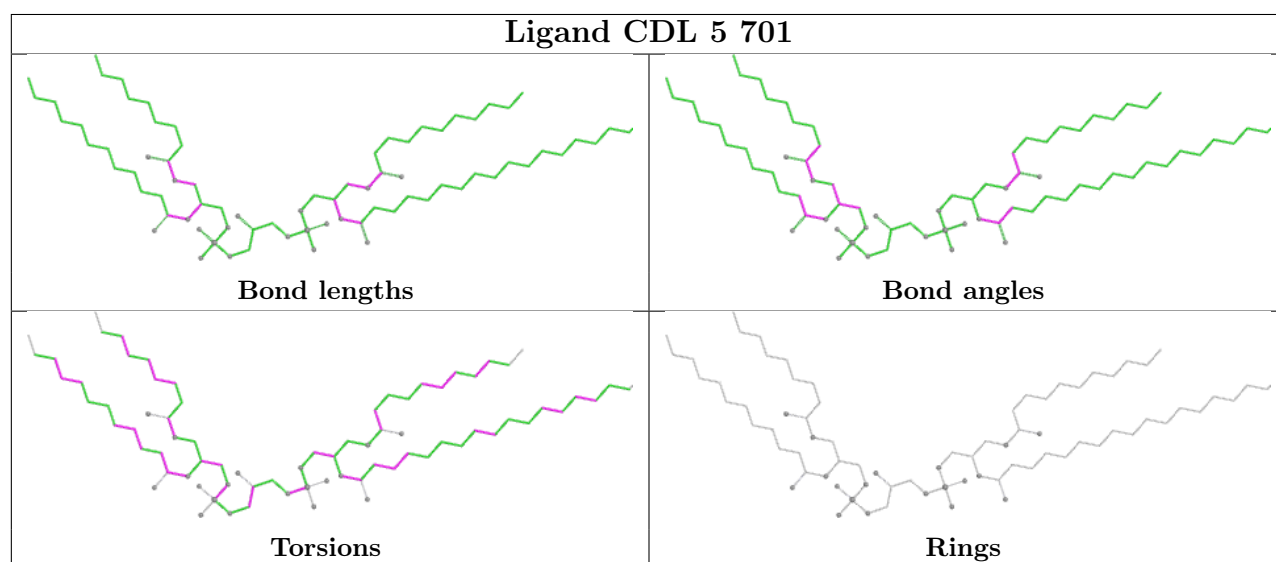
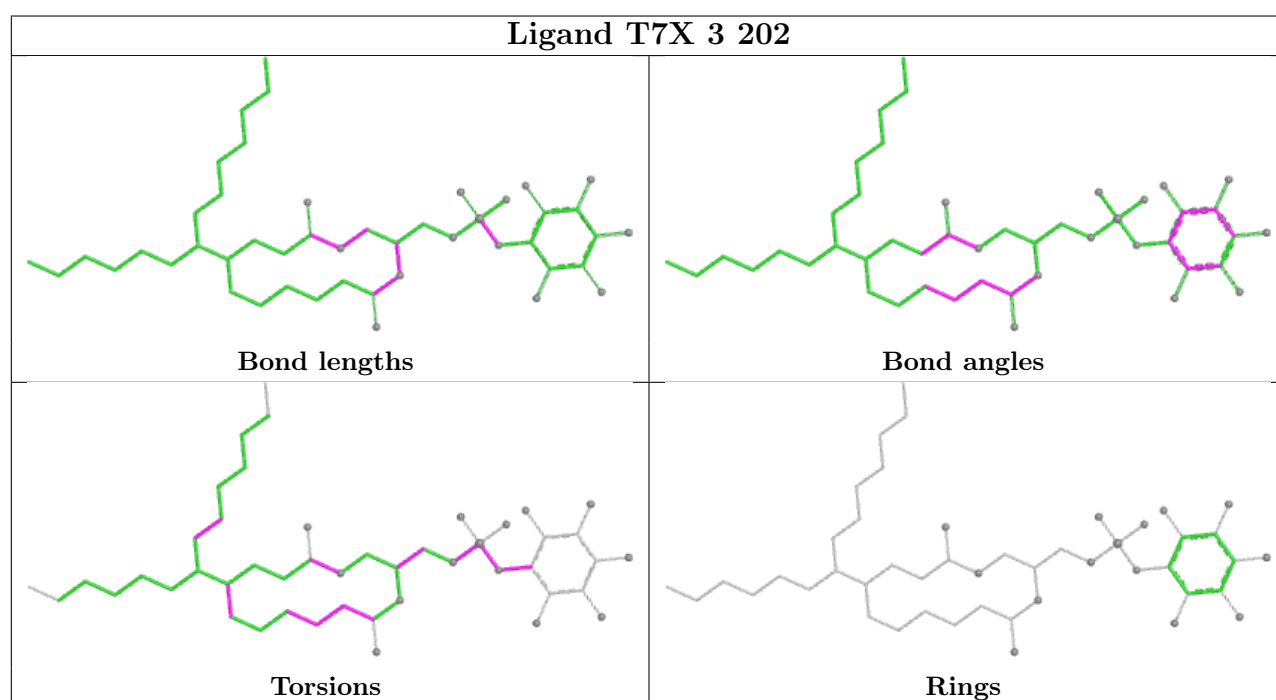
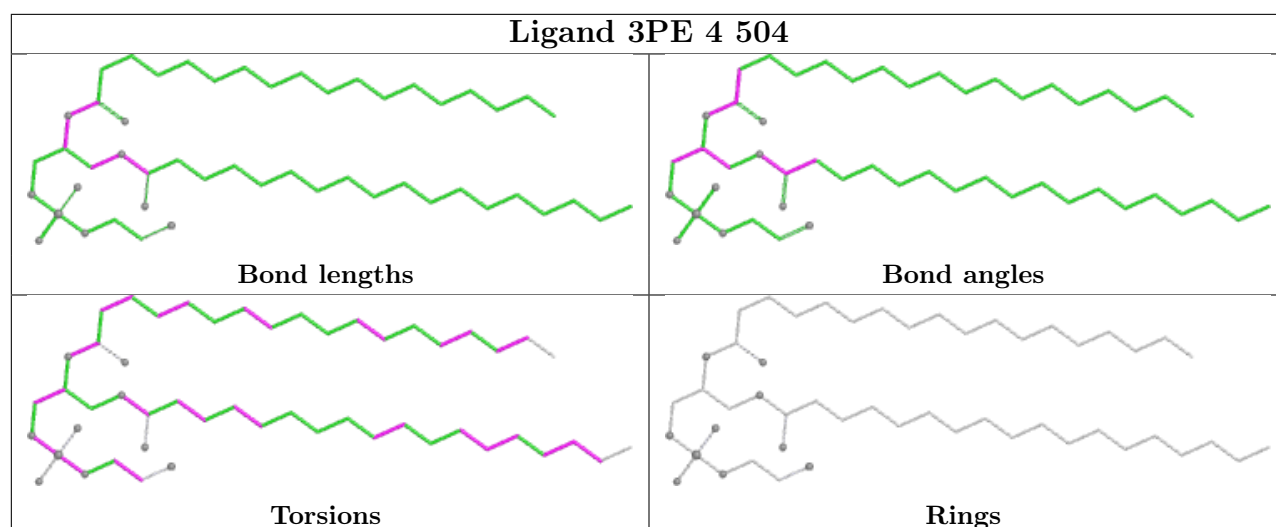


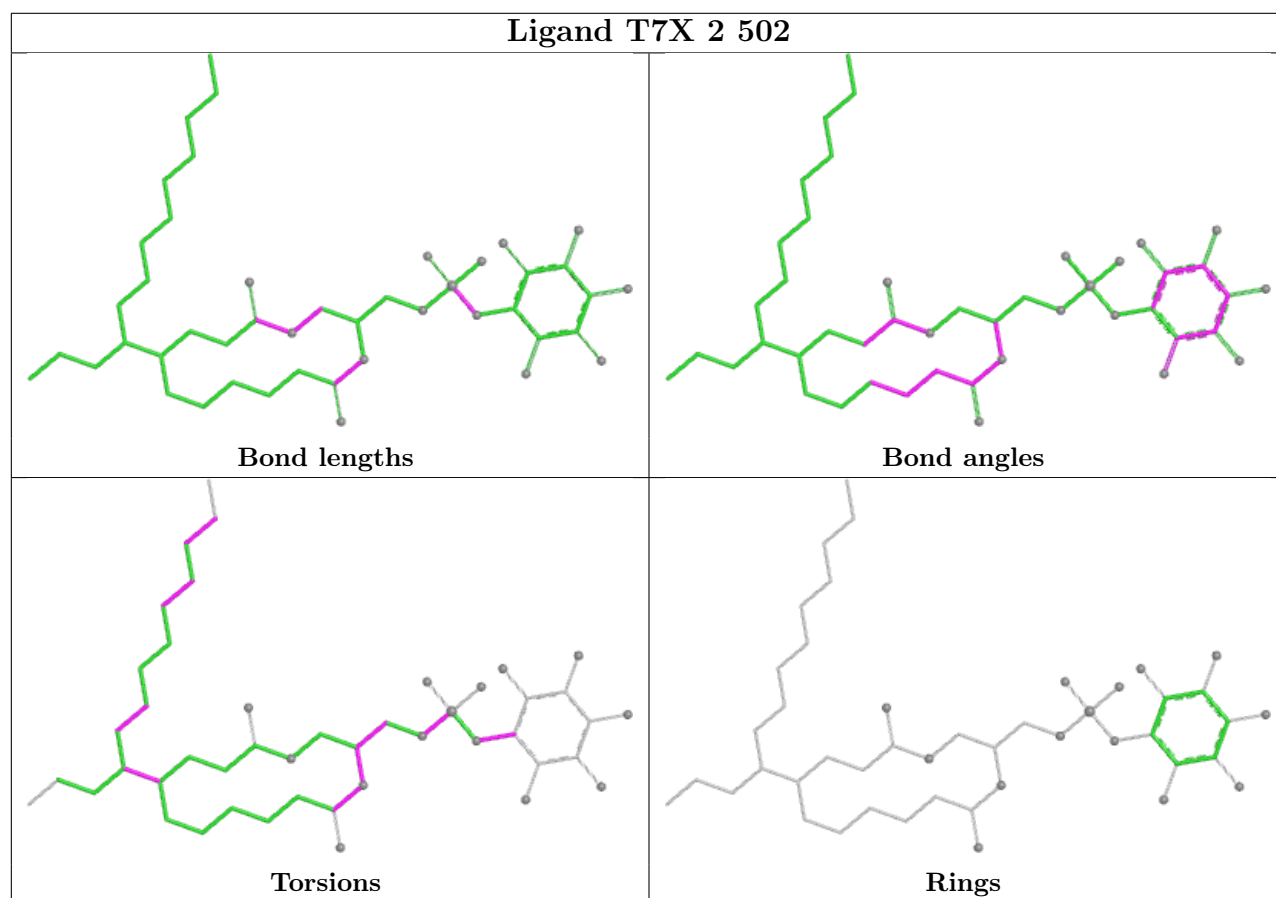
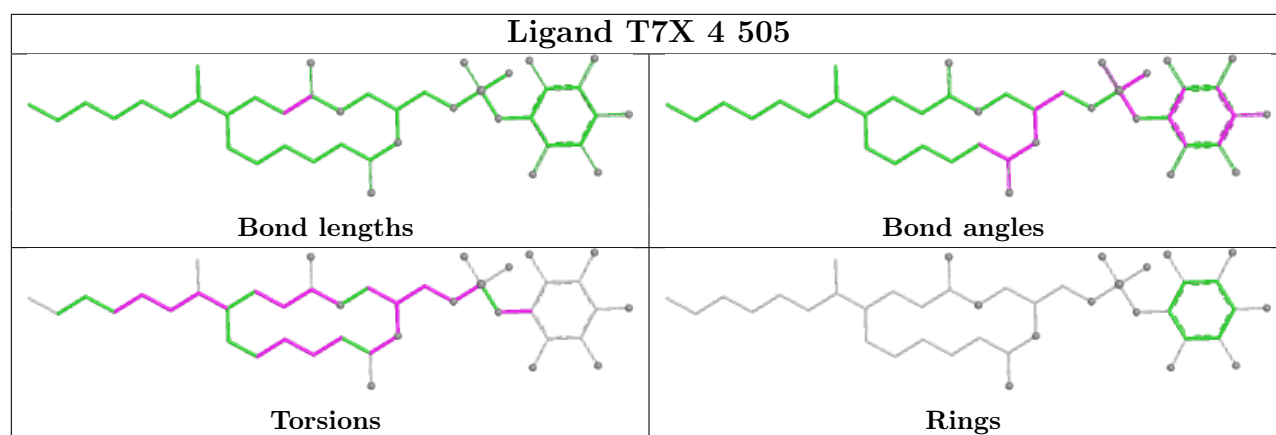


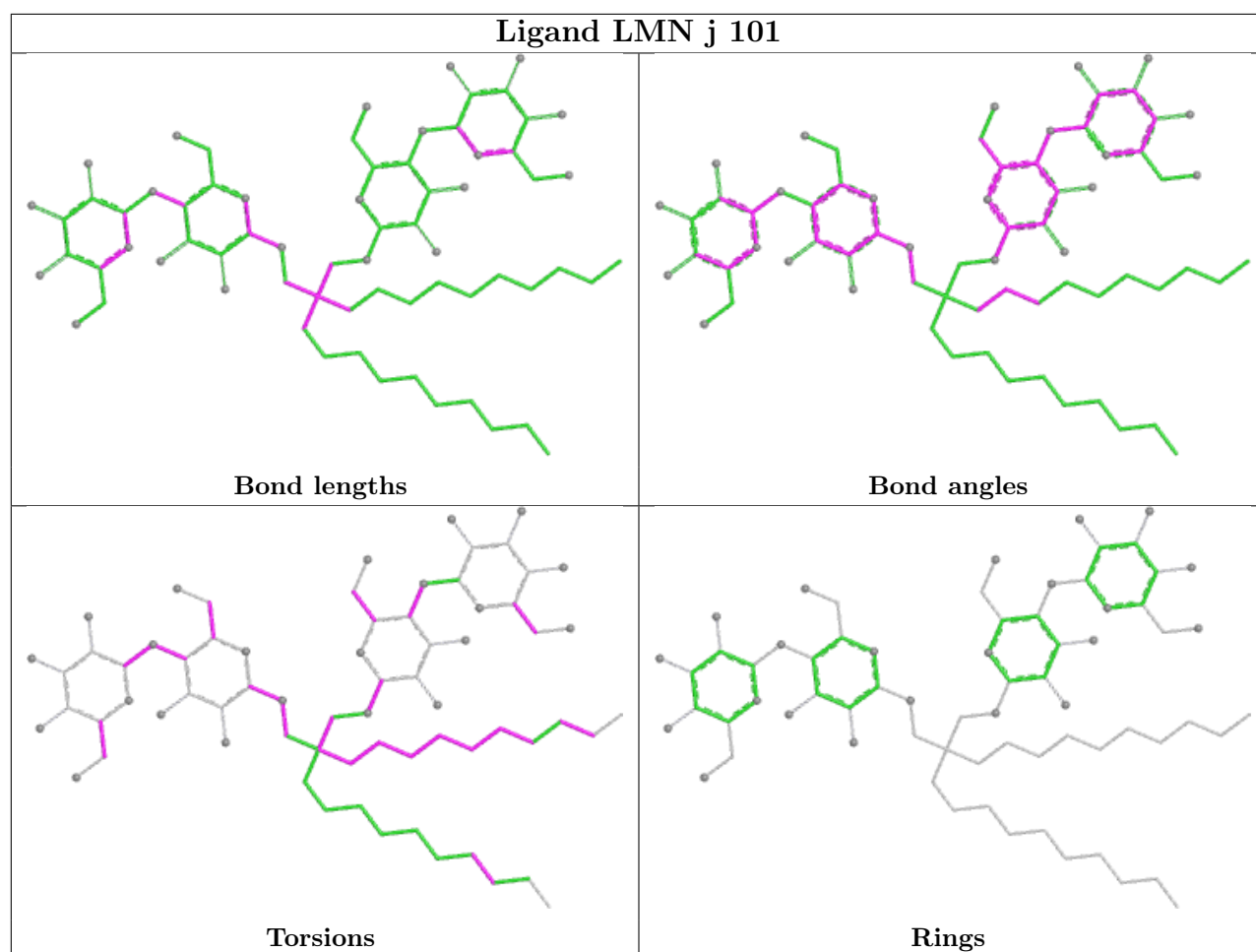


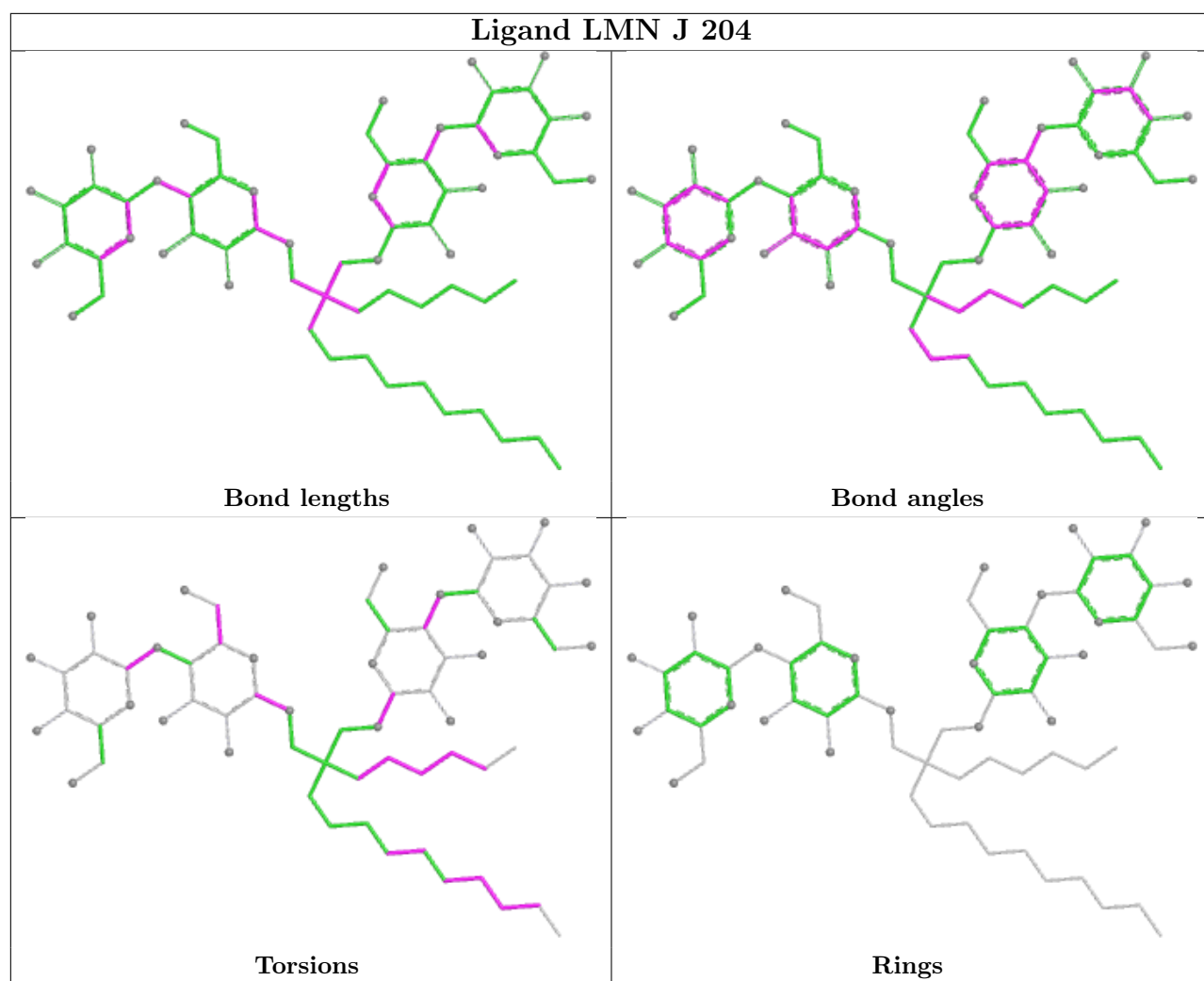


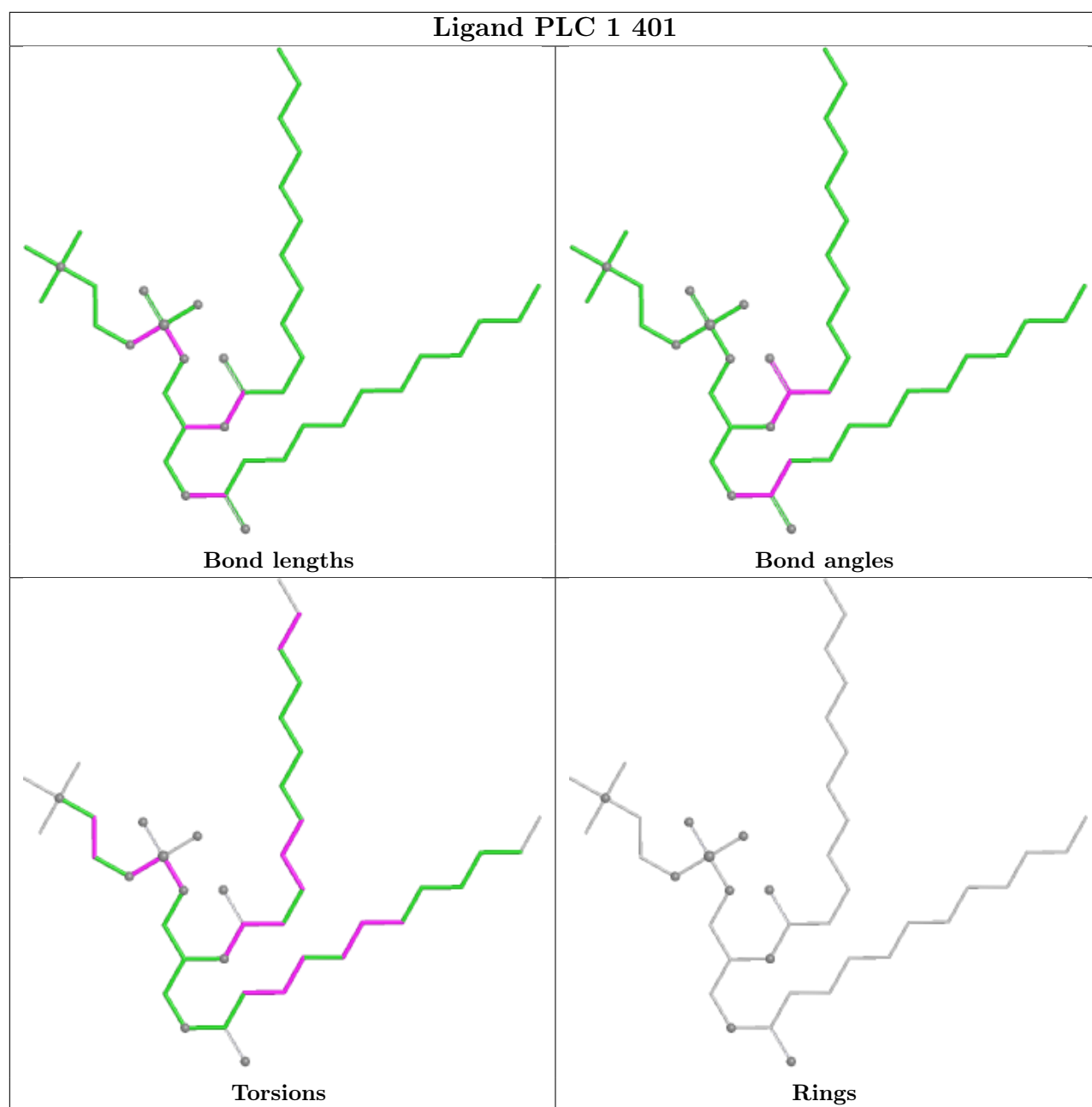


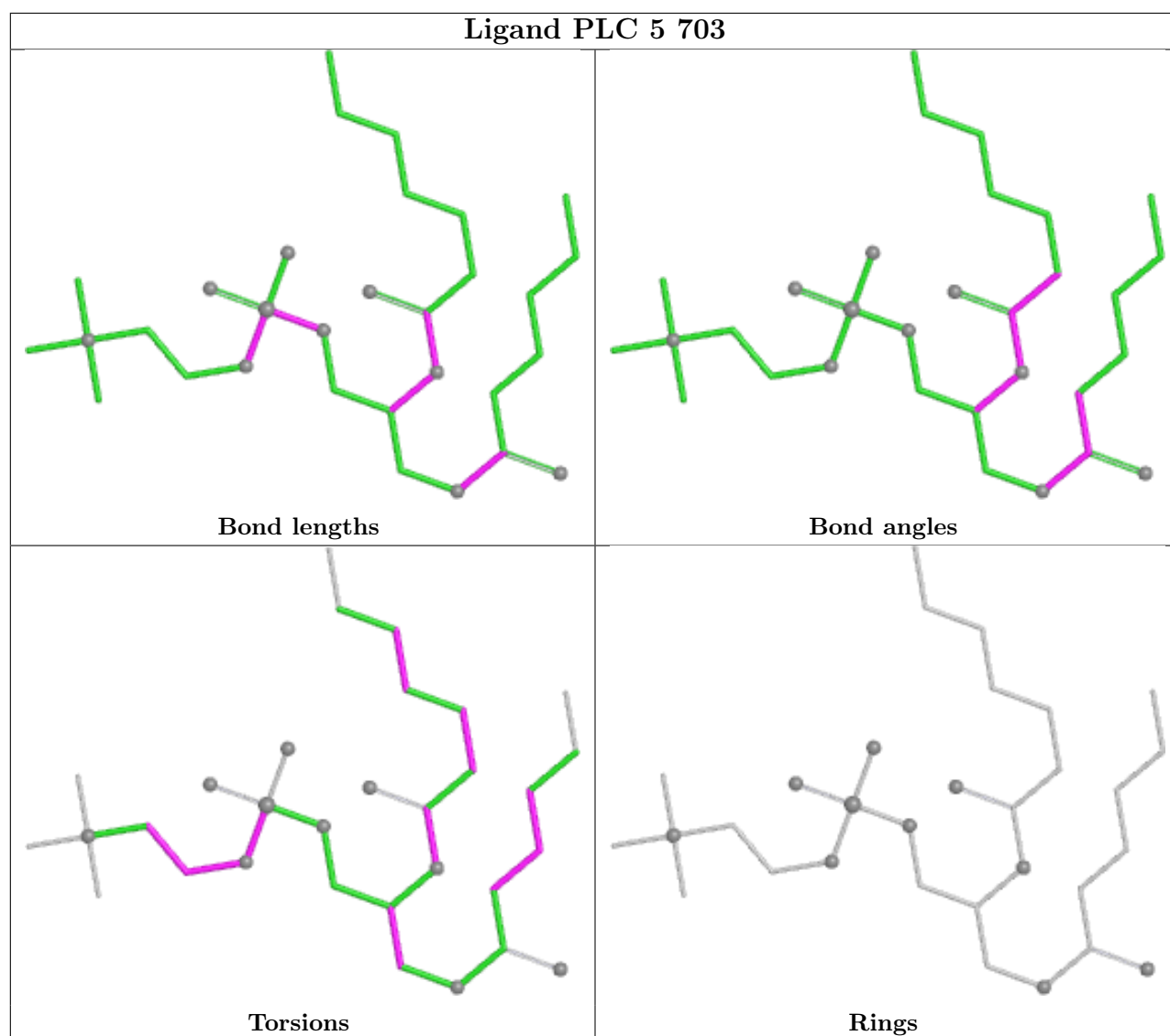


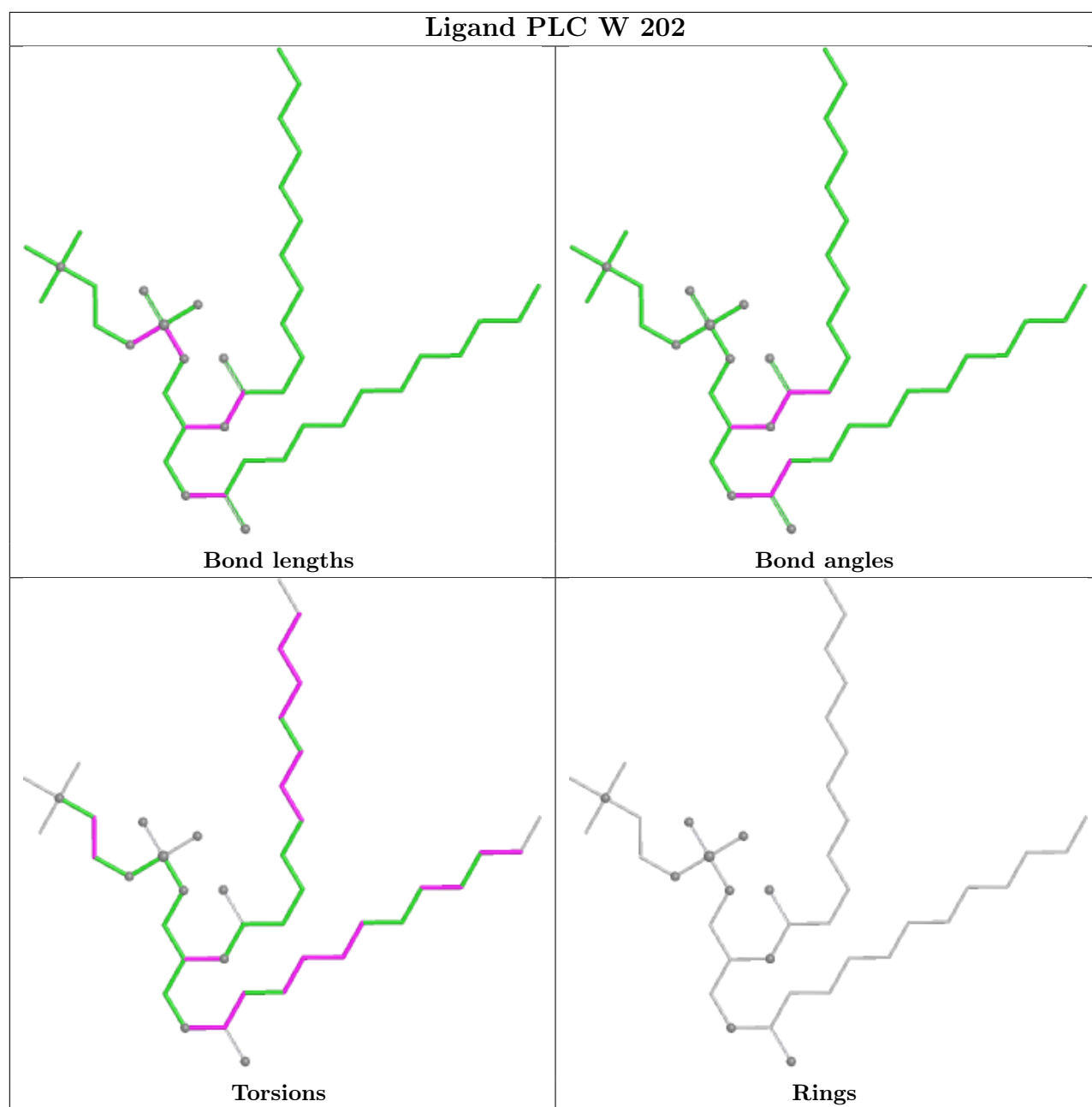


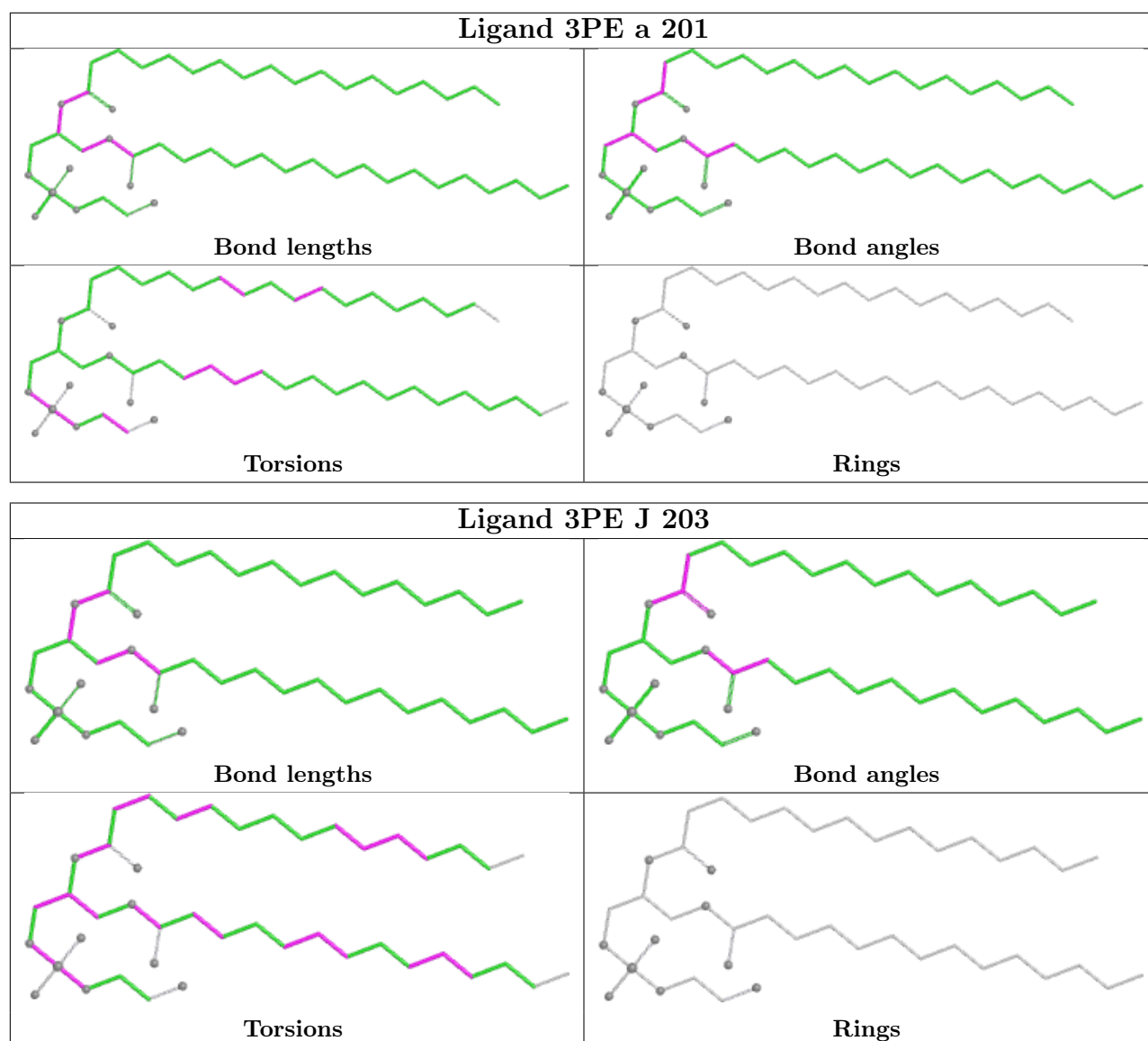












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

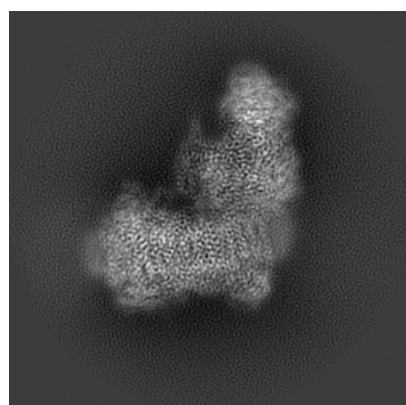
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10711. These allow visual inspection of the internal detail of the map and identification of artifacts.

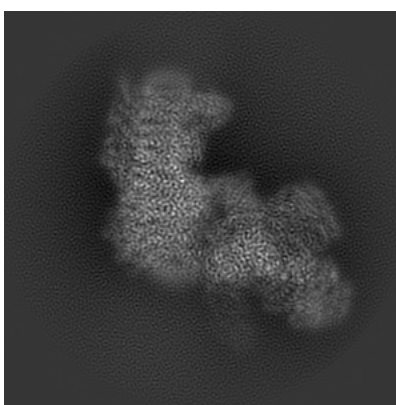
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

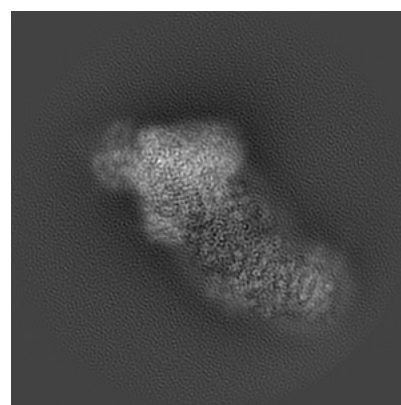
6.1.1 Primary map



X



Y

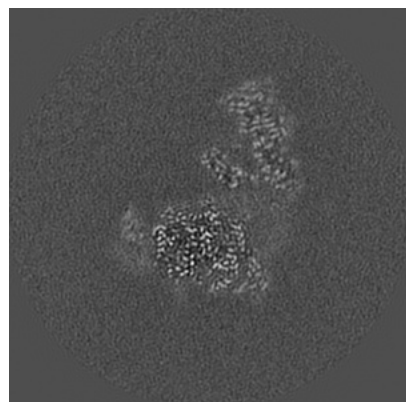


Z

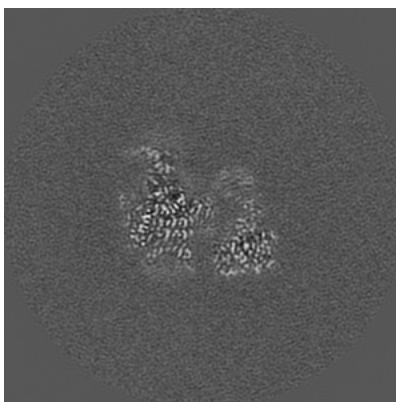
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

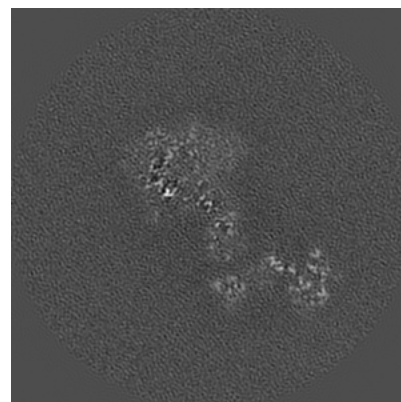
6.2.1 Primary map



X Index: 200



Y Index: 200

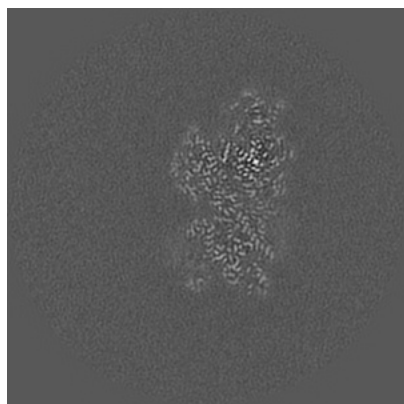


Z Index: 200

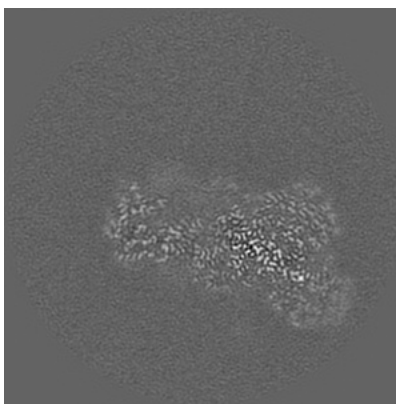
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

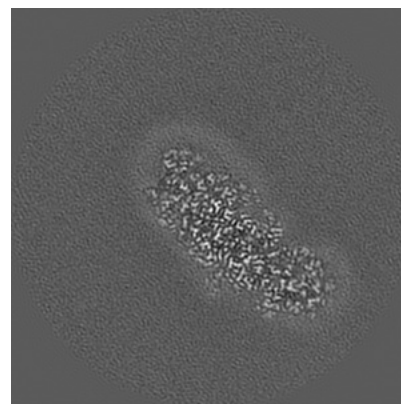
6.3.1 Primary map



X Index: 159



Y Index: 244

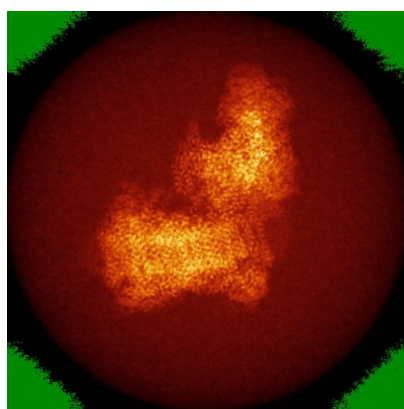


Z Index: 174

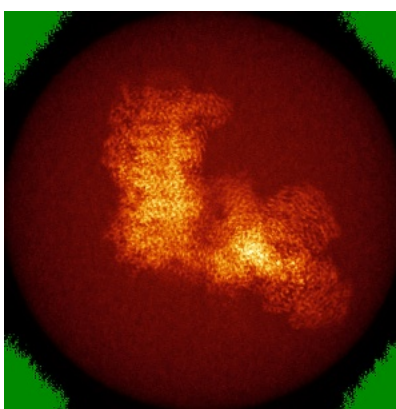
The images above show the largest variance slices of the map in three orthogonal directions.

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

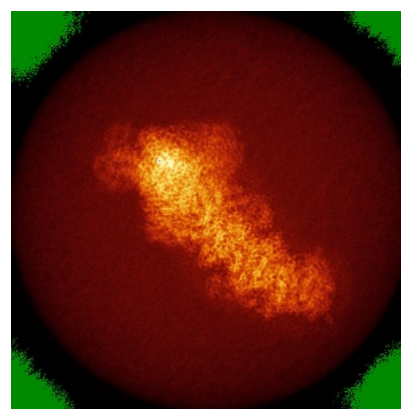
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views

This section was not generated.

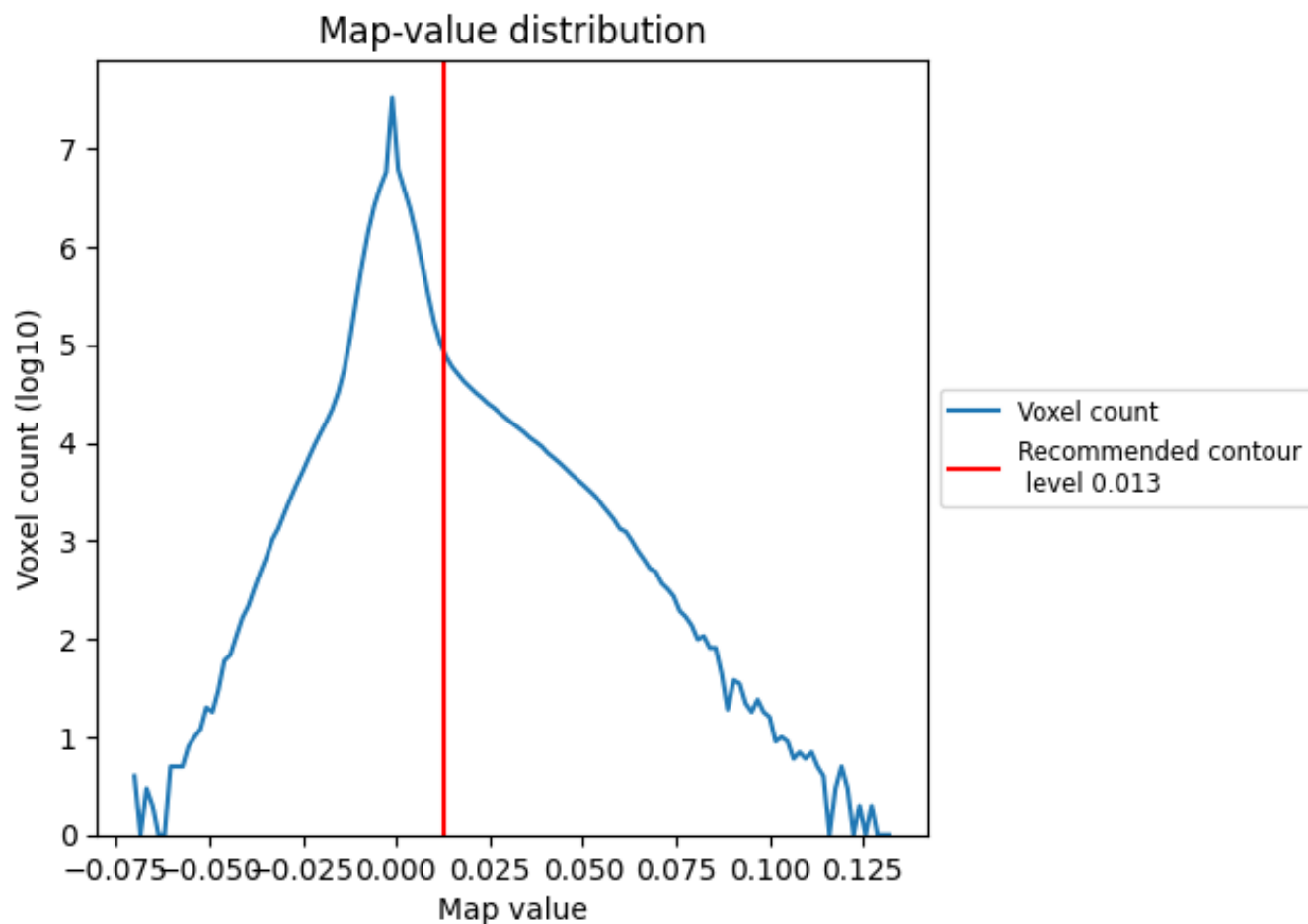
6.6 Mask visualisation

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

7 Map analysis [i](#)

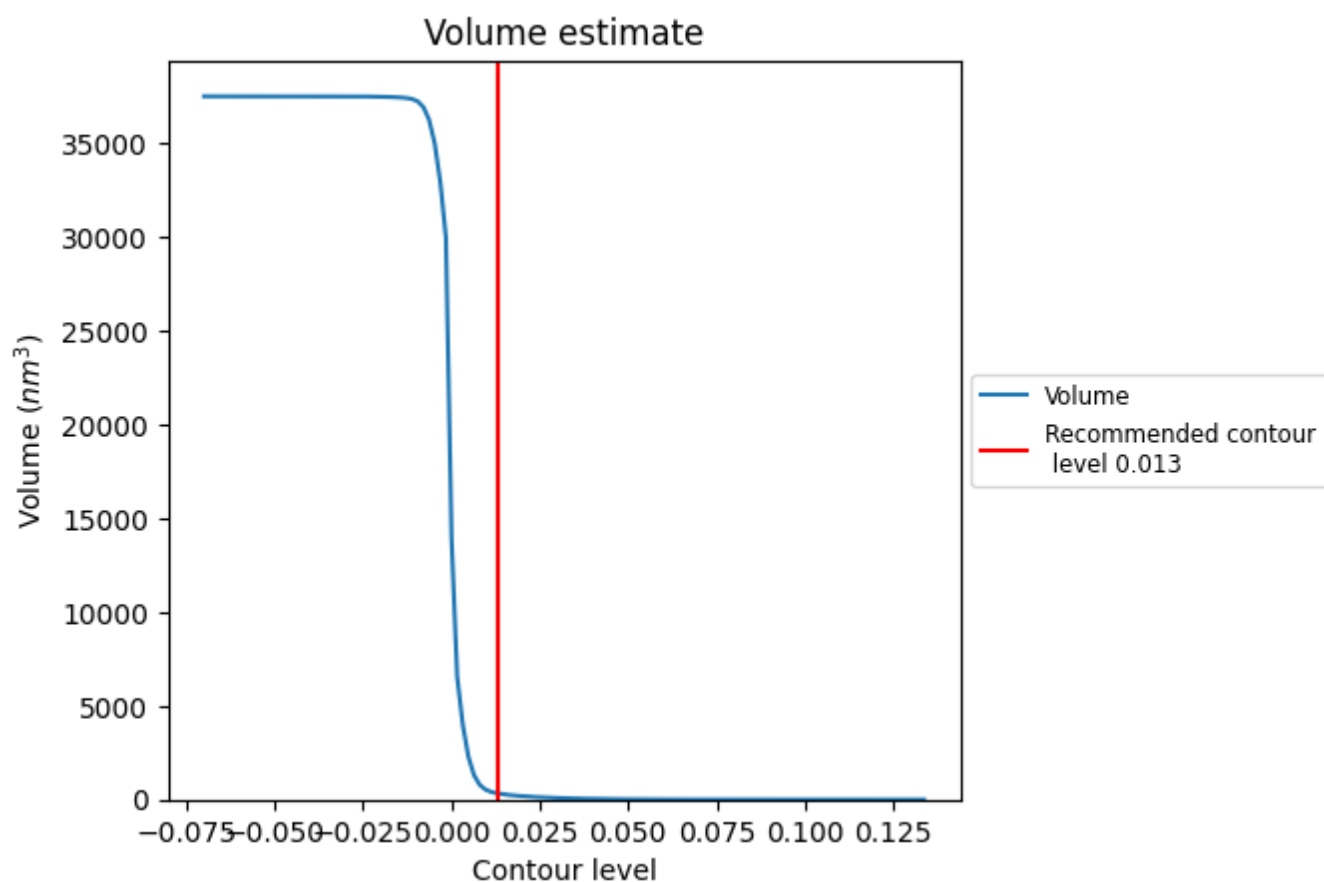
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

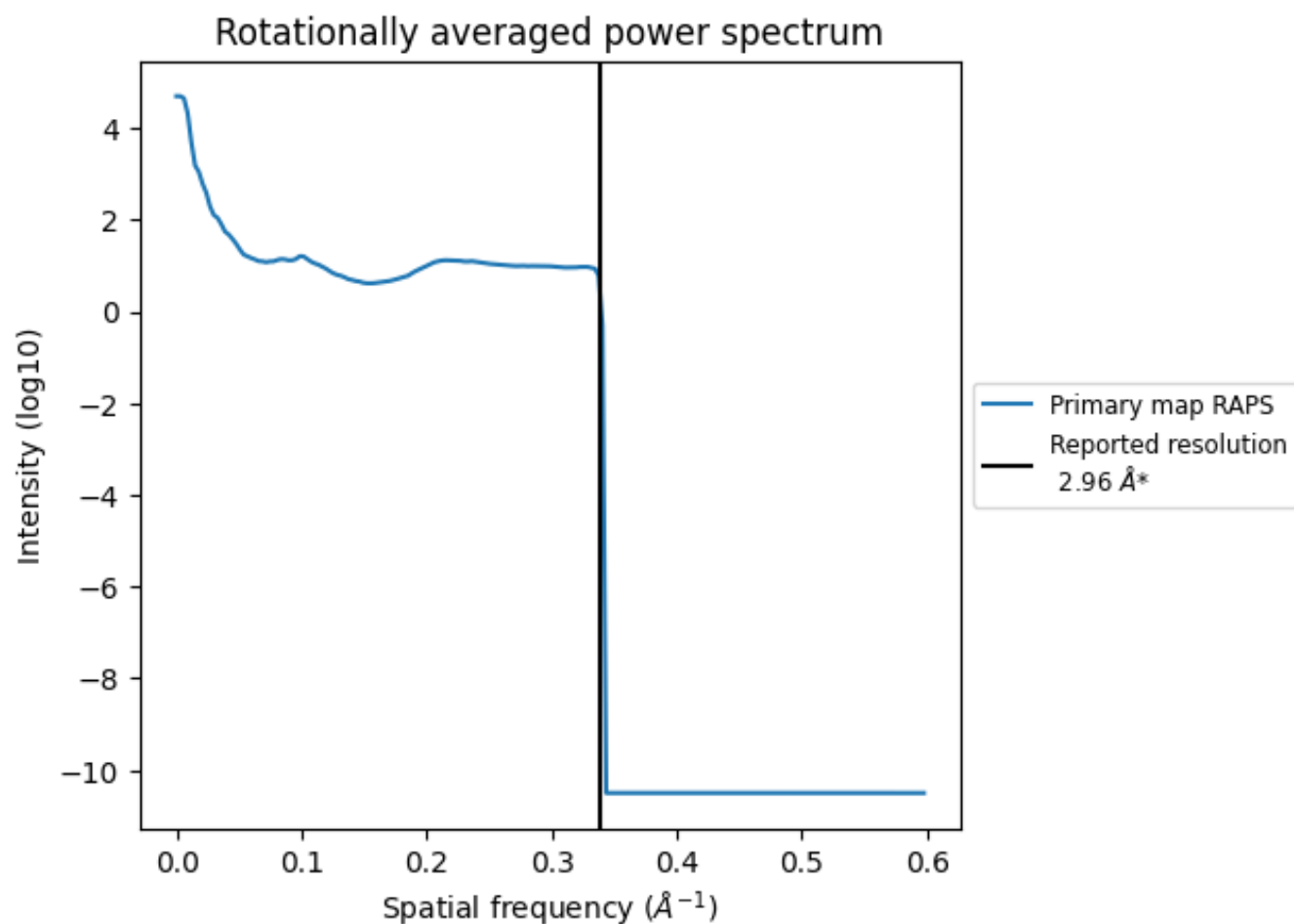
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 333 nm^3 ; this corresponds to an approximate mass of 301 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 ⓘ

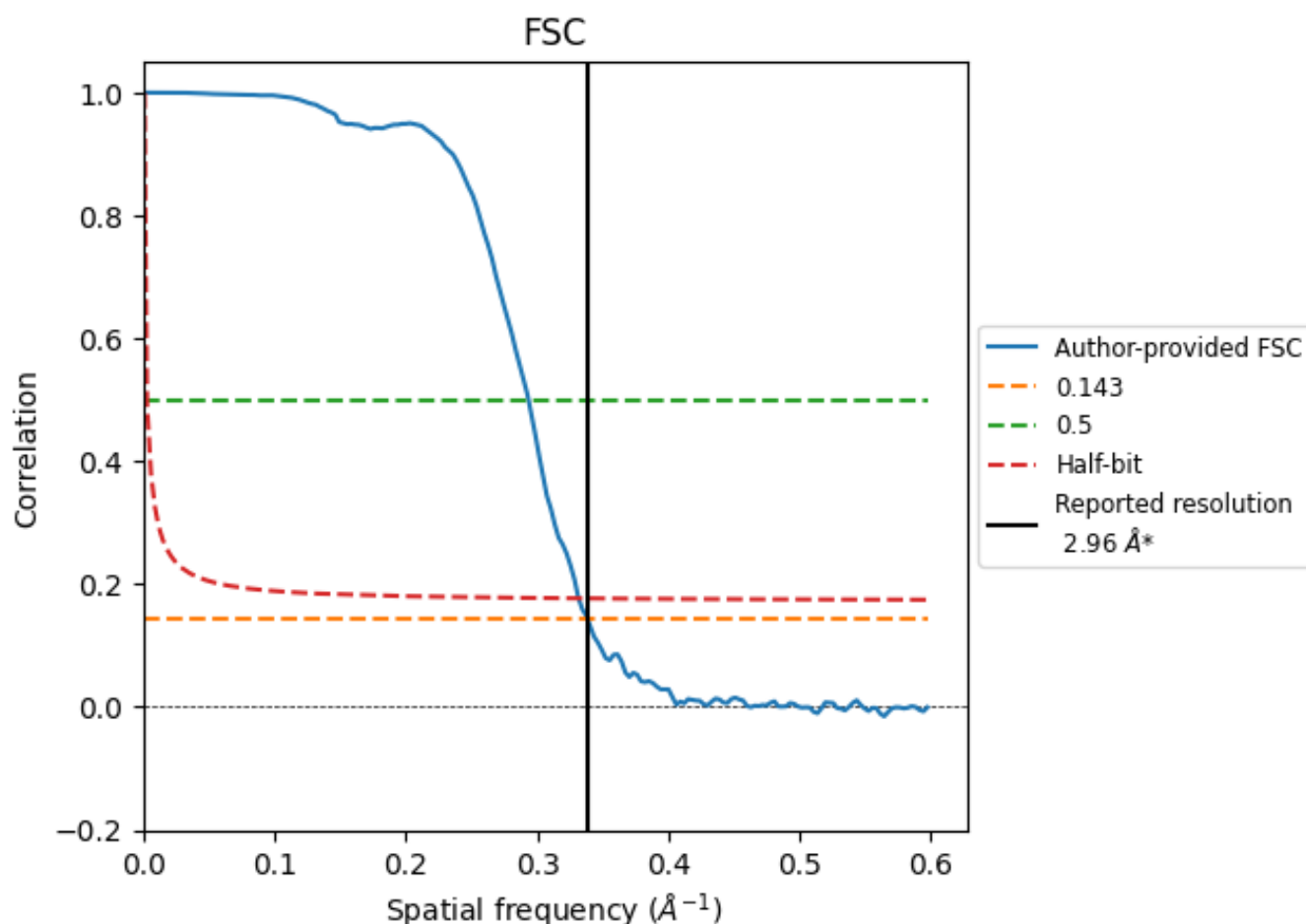


*Reported resolution corresponds to spatial frequency of 0.338 Å⁻¹

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 0.338 Å⁻¹

8.2 Resolution estimates [i](#)

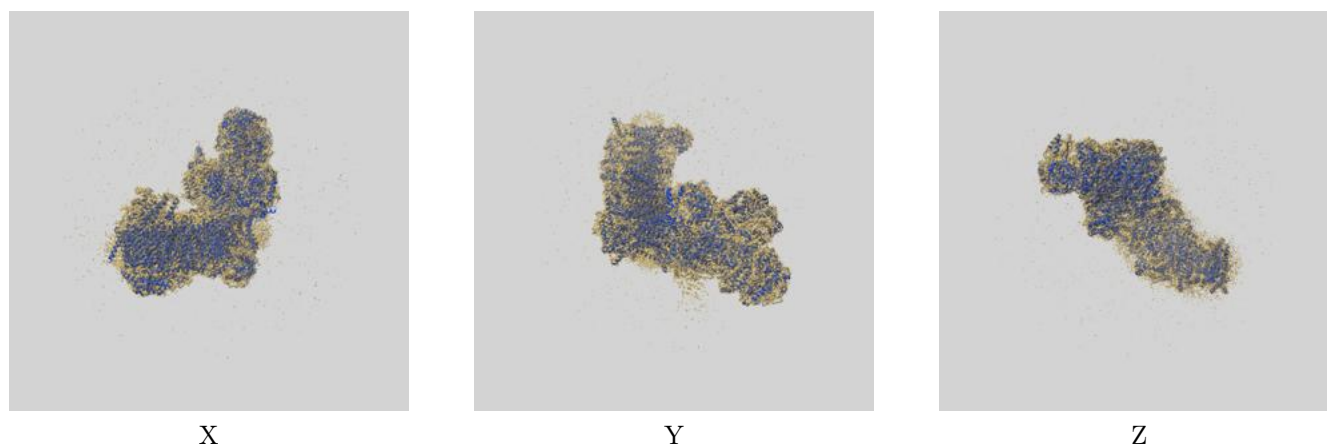
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.96	-	-
Author-provided FSC curve	2.95	3.41	3.01
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

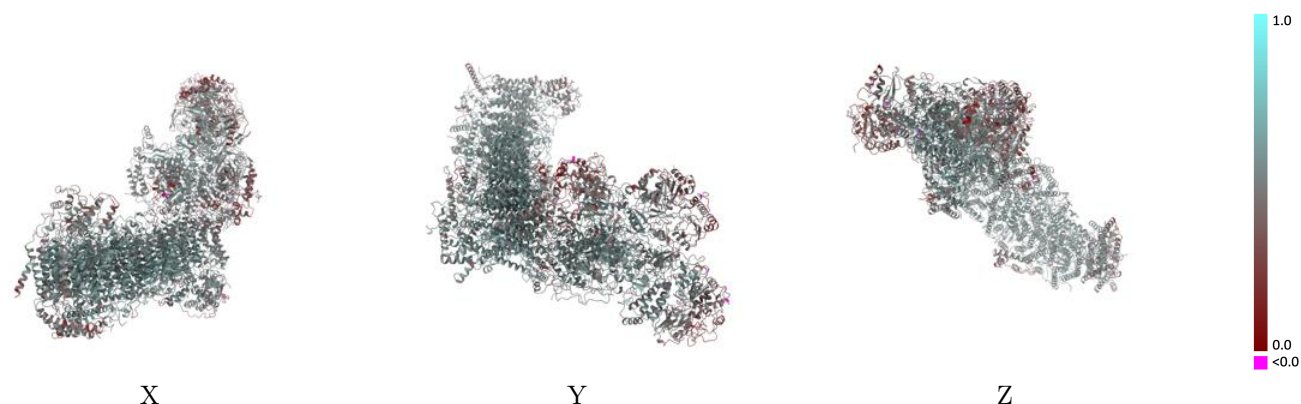
This section contains information regarding the fit between EMDB map EMD-10711 and PDB model 6Y79. Per-residue inclusion information can be found in section [3](#) on page [21](#).

9.1 Map-model overlay [i](#)



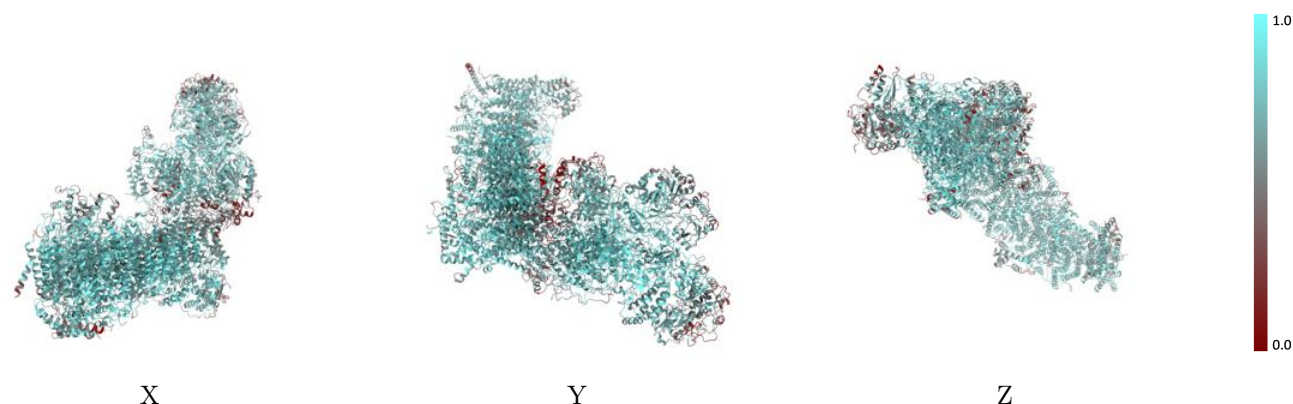
The images above show the 3D surface view of the map at the recommended contour level 0.013 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



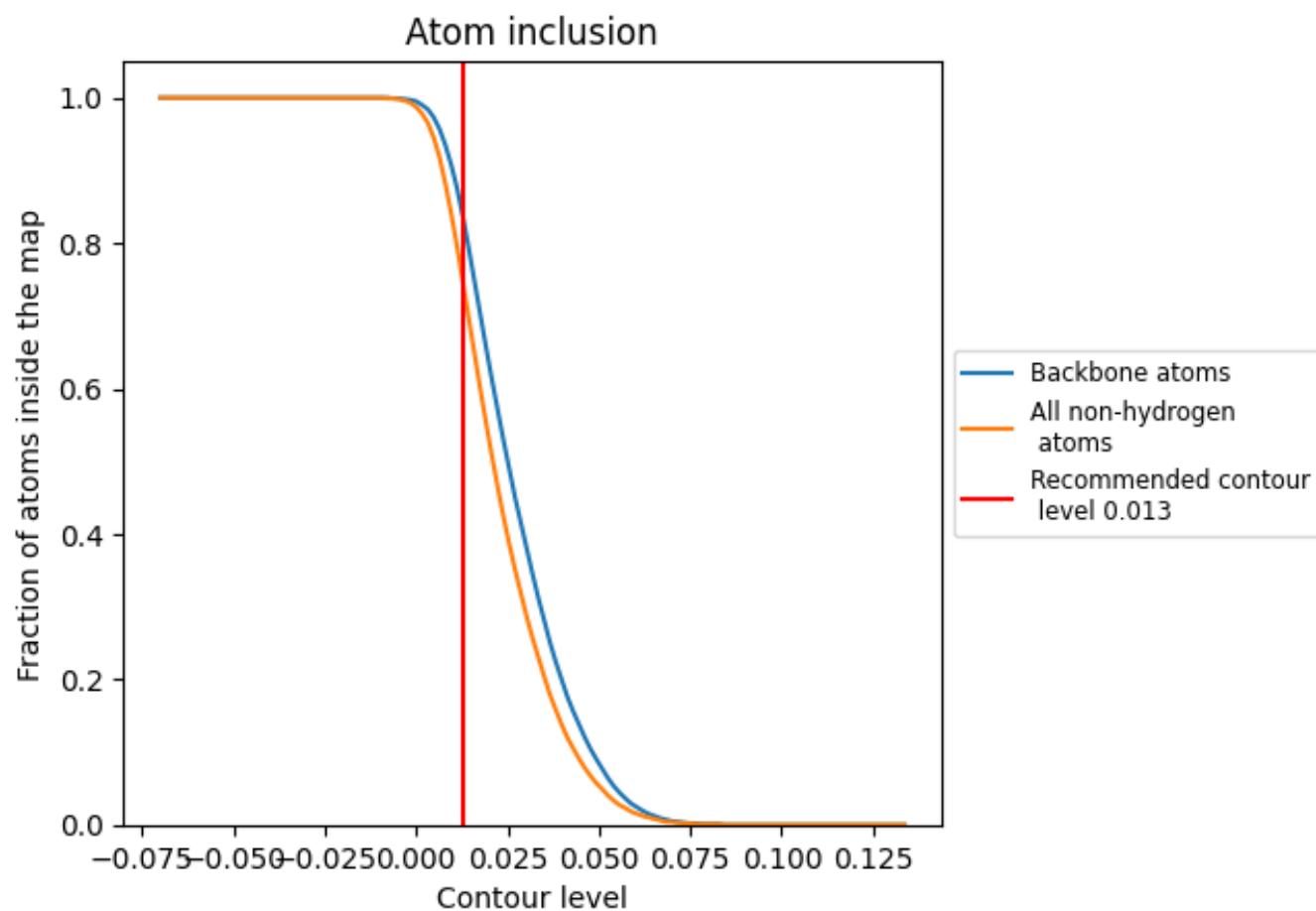
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.013).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 74% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.013) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7390	 0.5050
1	 0.7210	 0.5160
2	 0.8890	 0.5870
3	 0.6210	 0.4840
4	 0.8670	 0.5810
5	 0.8030	 0.5500
6	 0.7540	 0.5340
8	 0.6170	 0.4360
9	 0.6450	 0.4770
A	 0.7030	 0.4450
B	 0.6200	 0.4310
C	 0.8330	 0.5500
D	 0.7470	 0.5110
E	 0.5740	 0.4060
F	 0.7460	 0.5090
G	 0.8300	 0.5570
H	 0.5820	 0.4270
I	 0.8120	 0.5120
J	 0.7430	 0.5310
K	 0.6780	 0.4590
L	 0.8270	 0.5580
M	 0.7830	 0.5100
O	 0.4220	 0.3240
P	 0.7230	 0.4990
Q	 0.5620	 0.4290
R	 0.6780	 0.4640
S	 0.6360	 0.4490
U	 0.7360	 0.5100
W	 0.7480	 0.5200
X	 0.8200	 0.5570
Y	 0.8030	 0.5380
Z	 0.6960	 0.5090
a	 0.7230	 0.5080
b	 0.8610	 0.5740
c	 0.6370	 0.4420



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
d	 0.8080	 0.5300
e	 0.5860	 0.4580
f	 0.5880	 0.4050
g	 0.7940	 0.5220
h	 0.6840	 0.5010
i	 0.7750	 0.5190
j	 0.7590	 0.5210
n	 0.7520	 0.5140