



Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 12:30 PM UTC

PDB ID : 9F5Y / pdb_00009f5y
EMDB ID : EMD-50203
Title : Structure of the Chlamydomonas reinhardtii respiratory complex I from respiratory supercomplex
Authors : Waltz, F.; Righetto, R.; Kotecha, A.; Engel, B.D.
Deposited on : 2024-04-30
Resolution : 2.51 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

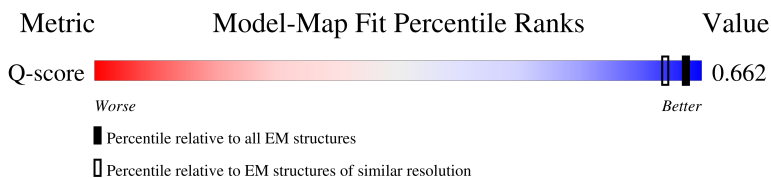
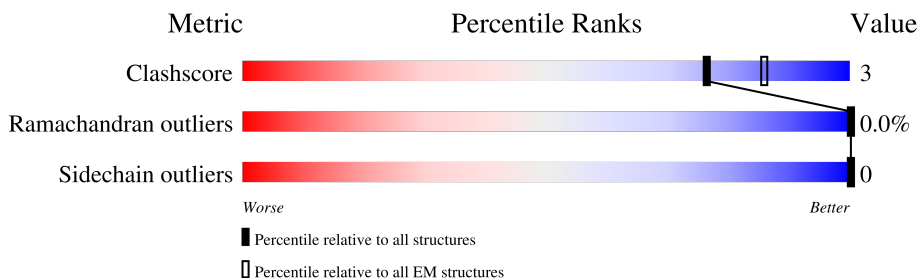
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.51 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.



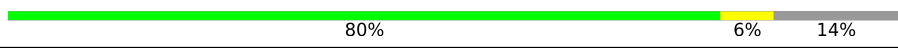
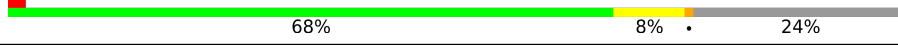
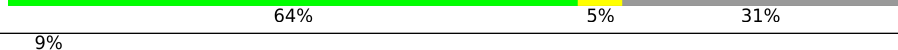
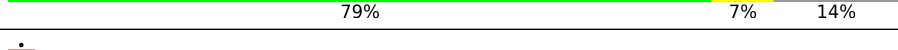
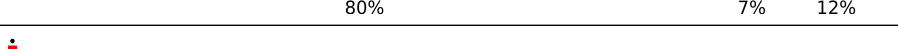
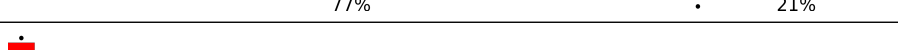
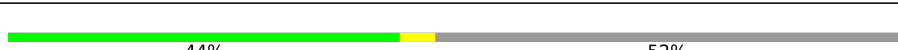
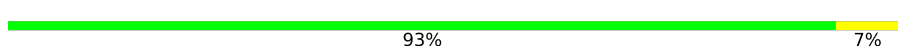
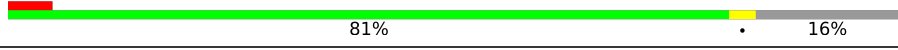
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7159 (2.01 - 3.01)

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	282	
2	B	484	
3	C	733	
4	D	282	

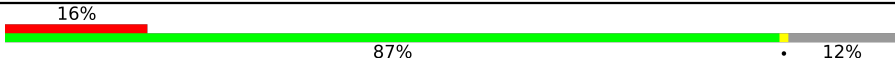
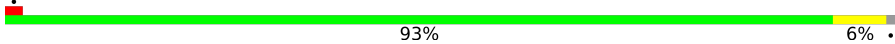
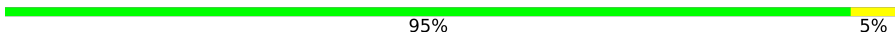
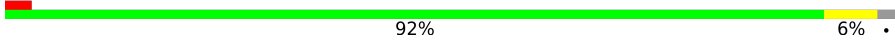
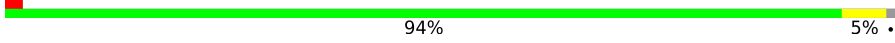
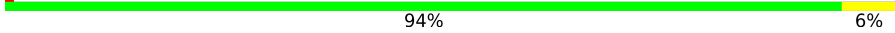
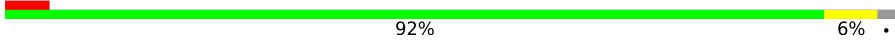
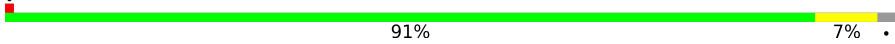
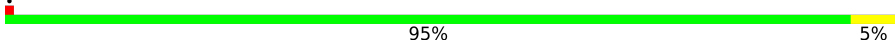
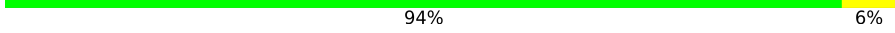
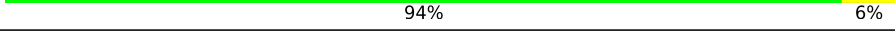
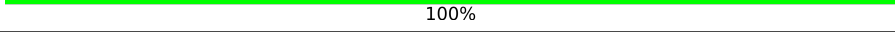
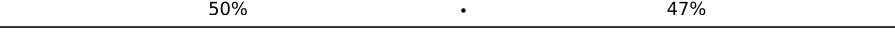
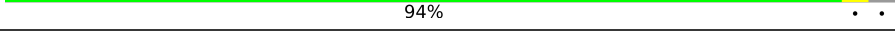
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Mol	Chain	Length	Quality of chain
5	E	467	
6	F	164	
7	G	231	
8	H	118	
9	I	165	
10	J	128	
10	r	128	
11	K	138	
12	L	187	
13	M	154	
14	N	156	
15	O	101	
16	P	397	
17	Q	292	
18	R	387	
19	S	279	
20	T	443	
21	U	227	
22	V	546	
23	W	162	
24	X	149	
25	Y	64	
26	Z	124	
27	a	129	
28	b	172	

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Mol	Chain	Length	Quality of chain
29	c	67	
30	d	86	
31	e	219	
32	f	65	
33	g	55	
34	h	142	
35	i	81	
36	j	86	
37	k	117	
38	l	121	
39	m	142	
40	n	106	
41	o	155	
42	p	130	
43	q	197	
44	s	312	
45	t	279	
46	u	229	
47	v	45	
48	w	109	
49	x	157	
50	y	118	

2 Entry composition

There are 64 unique types of molecules in this entry. The entry contains 75117 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called NADH:ubiquinone oxidoreductase 24 kD subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	239	Total	C	N	O	S	0	0
			1839	1165	311	352	11		

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	435	Total	C	N	O	S	0	0
			3331	2099	592	614	26		

- Molecule 3 is a protein called NADH:ubiquinone oxidoreductase 78 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	688	Total	C	N	O	S	0	0
			5175	3235	936	972	32		

- Molecule 4 is a protein called NADH:ubiquinone oxidoreductase 30kDa subunit domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	216	Total	C	N	O	S	0	0
			1790	1156	301	325	8		

- Molecule 5 is a protein called NADH:ubiquinone oxidoreductase 49 kD subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	383	Total	C	N	O	S	0	0
			3085	1971	537	554	23		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	157	Total	C	N	O	S	0	0
			1225	787	211	215	12		

- Molecule 7 is a protein called NADH:ubiquinone oxidoreductase subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	199	Total	C	N	O	S	0	0
			1615	1007	281	315	12		

- Molecule 8 is a protein called B14.5a.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	90	Total	C	N	O	S	0	0
			750	486	129	132	3		

- Molecule 9 is a protein called Mitochondrial NADH:ubiquinone oxidoreductase 18 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	135	Total	C	N	O	S	0	0
			1044	661	173	208	2		

- Molecule 10 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	84	Total	C	N	O	S	0	0
			640	404	100	133	3		
10	r	88	Total	C	N	O	S	0	0
			663	419	104	137	3		

- Molecule 11 is a protein called NADH:ubiquinone oxidoreductase B14 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	119	Total	C	N	O	S	0	0
			986	640	173	168	5		

- Molecule 12 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	164	Total	C	N	O	S	0	0
			1275	803	221	245	6		

- Molecule 13 is a protein called NADH:ubiquinone oxidoreductase 13 kD-like subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	121	Total	C	N	O	S	0	0
			913	582	150	178	3		

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	150	Total	C	N	O	S	0	0
			1235	791	214	227	3		

- Molecule 15 is a protein called NADH:ubiquinone oxidoreductase B8 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	100	Total	C	N	O	S	0	0
			761	471	138	147	5		

- Molecule 16 is a protein called Putative NADH:ubiquinone oxidoreductase 39 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	363	Total	C	N	O	S	0	0
			2823	1793	489	527	14		

- Molecule 17 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	286	Total	C	N	O	S	0	0
			2179	1448	338	374	19		

- Molecule 18 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	387	Total	C	N	O	S	0	0
			3014	2026	467	496	25		

- Molecule 19 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	134	Total	C	N	O	S	0	0
			1071	715	159	192	5		

- Molecule 20 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	443	Total	C	N	O	S	0	0
			3434	2321	526	557	30		

- Molecule 21 is a protein called NADH dehydrogenase subunit 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	105	Total	C	N	O	S	0	0
			805	524	124	146	11		

- Molecule 22 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	546	Total	C	N	O	S	0	0
			4152	2731	668	716	37		

- Molecule 23 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	157	Total	C	N	O	S	0	0
			1210	820	180	201	9		

- Molecule 24 is a protein called ASH1.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	125	Total	C	N	O	S	0	0
			1037	685	168	178	6		

- Molecule 25 is a protein called P9.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	54	Total	C	N	O	S	0	0
			405	256	74	74	1		

- Molecule 26 is a protein called KFYI.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	107	Total	C	N	O	S	0	0
			861	555	149	152	5		

- Molecule 27 is a protein called AGGG.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	a	82	Total	C	N	O	S	0	0
			674	440	109	123	2		

- Molecule 28 is a protein called ESSS.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	b	144	Total	C	N	O	S	0	0
			1169	756	192	214	7		

- Molecule 29 is a protein called B9.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	c	59	Total	C	N	O	S	0	0
			453	298	71	79	5		

- Molecule 30 is a protein called Mitochondrial NADH:ubiquinone oxidoreductase 10 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	d	85	Total	C	N	O	S	0	0
			699	456	120	120	3		

- Molecule 31 is a protein called Mitochondrial NADH:ubiquinone oxidoreductase 23 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	e	218	Total	C	N	O	S	0	0
			1639	1055	279	297	8		

- Molecule 32 is a protein called Mitochondrial NADH:ubiquinone oxidoreductase 7.5 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	f	64	Total	C	N	O	S	0	0
			532	345	93	92	2		

- Molecule 33 is a protein called Mitochondrial putative NADH:ubiquinone oxidoreductase 6.5 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	g	50	Total	C	N	O	S	0	0
			416	277	73	65	1		

- Molecule 34 is a protein called Mitochondrial NADH:ubiquinone oxidoreductase 13 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	h	108	Total	C	N	O	S	0	0
			915	597	157	159	2		

- Molecule 35 is a protein called NADH:ubiquinone oxidoreductase 15 kDa subunit-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	i	76	Total	C	N	O	S	0	0
			633	387	122	116	8		

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	j	85	Total	C	N	O	S	0	0
			712	449	131	125	7		

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	k	117	Total	C	N	O	S	0	0
			984	631	176	173	4		

- Molecule 38 is a protein called NADH:ubiquinone oxidoreductase 20,9 kD-like subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	l	116	Total	C	N	O	S	0	0
			904	589	150	161	4		

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	m	138	Total	C	N	O	S	0	0
			1126	724	205	193	4		

- Molecule 40 is a protein called Putative NADH:ubiquinone oxidoreductase 12.5 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	n	104	Total	C	N	O	S	0	0
			864	547	152	159	6		

- Molecule 41 is a protein called Putative NADH:ubiquinone oxidoreductase 17.8 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	o	152	Total	C	N	O	S	0	0
			1240	771	238	228	3		

- Molecule 42 is a protein called Mitochondrial NADH:ubiquinone oxidoreductase 16 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	p	129	Total	C	N	O	S	0	0
			1069	670	192	204	3		

- Molecule 43 is a protein called Mitochondrial NADH:ubiquinone oxidoreductase 19 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	q	157	Total	C	N	O	S	0	0
			1268	818	217	229	4		

- Molecule 44 is a protein called Mitochondrial NADH:ubiquinone oxidoreductase 32 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	s	312	Total	C	N	O	S	0	0
			2302	1451	407	435	9		

- Molecule 45 is a protein called CAG2 - CA-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	t	253	Total	C	N	O	S	0	0
			1997	1268	357	367	5		

- Molecule 46 is a protein called CAG1.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	u	228	Total	C	N	O	S	0	0
			1698	1063	300	327	8		

- Molecule 47 is a protein called P10.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	v	45	Total	C	N	O	S	0	0
			361	233	61	66	1		

- Molecule 48 is a protein called Mitochondrial NADH:ubiquinone oxidoreductase 9 kDa sub-unit.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	w	64	Total	C	N	O	S	0	0
			508	334	78	91	5		

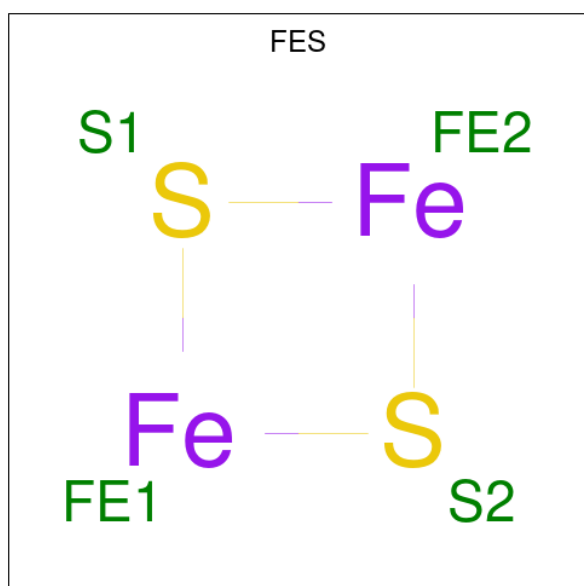
- Molecule 49 is a protein called NUOP8.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	x	83	Total	C	N	O	S	0	0
			699	467	110	121	1		

- Molecule 50 is a protein called NUOP7.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	y	114	Total	C	N	O	S	0	0
			932	615	154	161	2		

- Molecule 51 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



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

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Mol	Chain	Residues	Atoms			AltConf
51	C	1	Total	Fe	S	0
			4	2	2	

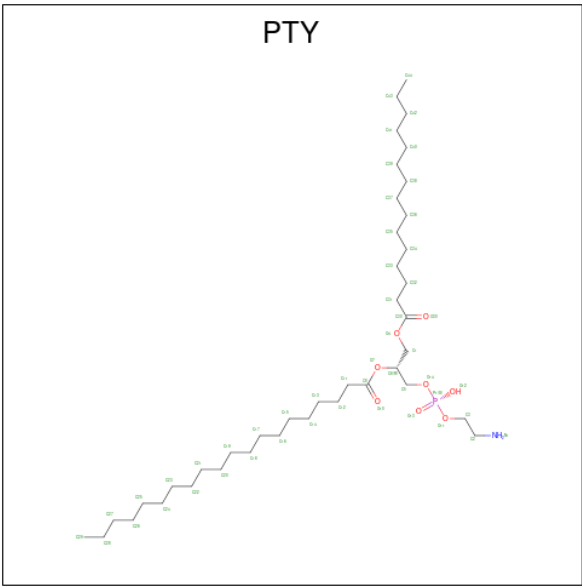
-
- The image displays the chemical structure of Flavin Mononucleotide (FMN). It features an isoalloxazine ring system, which is a tricyclic aromatic heterocycle consisting of a benzene ring fused to two pyrimidine rings. The atoms in the ring are labeled: N1, N5, N10 for the nitrogen atoms, and C2, C4, C6, C7, C8, C9, C10, C4A, C5A for the carbon atoms. Substituents on the ring include a dimethylamino group at C8 (C8M, C7M), a carbonyl group at C2 (C2=O, O2), and a ribityl side chain at C10 (C10A). The ribityl side chain consists of a ribitol chain (C1', C2', C3', C4') with a phosphate group (O1P, O2P, O3P) attached to the terminal carbon (C4'). Stereochemistry is indicated with wedges and dashes at C2' and C3'.

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

-
- A chemical structure diagram of a cubane-like molecule, [Fe₄S₄]²⁺. The structure consists of four iron (Fe) atoms at the corners of a cube and four sulfur (S) atoms at the centers of the edges. The atoms are color-coded: Fe atoms are purple and S atoms are yellow. The diagram is labeled with SF₄ at the top, S₃, FE₁, FE₄, FE₂, S₂, S₄, S₁, and FE₃ at the bottom.

Mol	Chain	Residues	Atoms			AltConf
53	B	1	Total	Fe	S	0
			8	4	4	
53	C	1	Total	Fe	S	0
			8	4	4	
53	C	1	Total	Fe	S	0
			8	4	4	
53	F	1	Total	Fe	S	0
			8	4	4	
53	G	1	Total	Fe	S	0
			8	4	4	
53	G	1	Total	Fe	S	0
			8	4	4	

- Molecule 54 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: C₄₀H₈₀NO₈P).



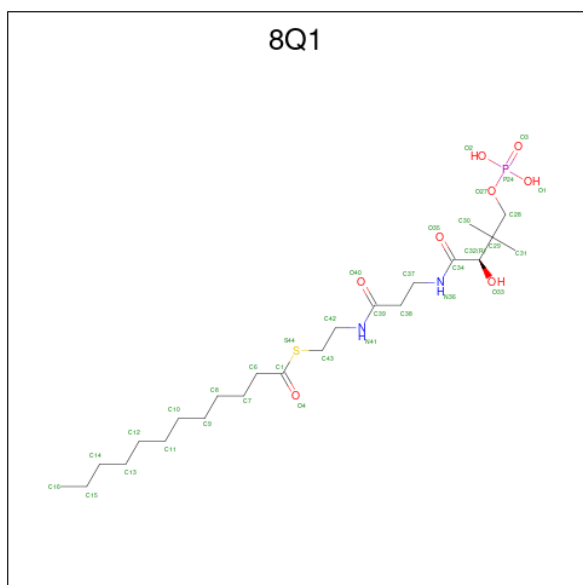
Mol	Chain	Residues	Atoms					AltConf
54	G	1	Total	C	N	O	P	0
			43	33	1	8	1	
54	R	1	Total	C	N	O	P	0
			34	24	1	8	1	
54	R	1	Total	C	N	O	P	0
			44	34	1	8	1	
54	R	1	Total	C	N	O	P	0
			40	30	1	8	1	
54	S	1	Total	C	N	O	P	0
			46	36	1	8	1	
54	T	1	Total	C	N	O	P	0
			50	40	1	8	1	

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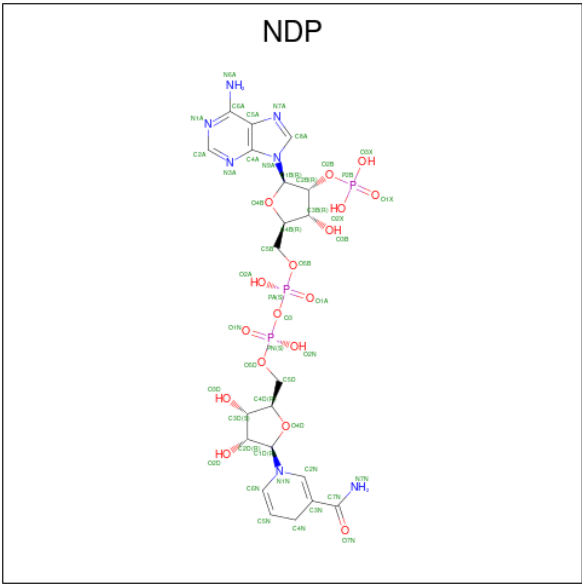
Mol	Chain	Residues	Atoms					AltConf
54	T	1	Total	C	N	O	P	0
			28	18	1	8	1	
54	T	1	Total	C	N	O	P	0
			26	16	1	8	1	
54	V	1	Total	C	N	O	P	0
			40	30	1	8	1	
54	V	1	Total	C	N	O	P	0
			50	40	1	8	1	
54	V	1	Total	C	N	O	P	0
			35	25	1	8	1	
54	e	1	Total	C	N	O	P	0
			25	15	1	8	1	
54	e	1	Total	C	N	O	P	0
			43	33	1	8	1	
54	h	1	Total	C	N	O	P	0
			46	36	1	8	1	
54	x	1	Total	C	N	O	P	0
			50	40	1	8	1	

- Molecule 55 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (CCD ID: 8Q1) (formula: C₂₃H₄₅N₂O₈PS).



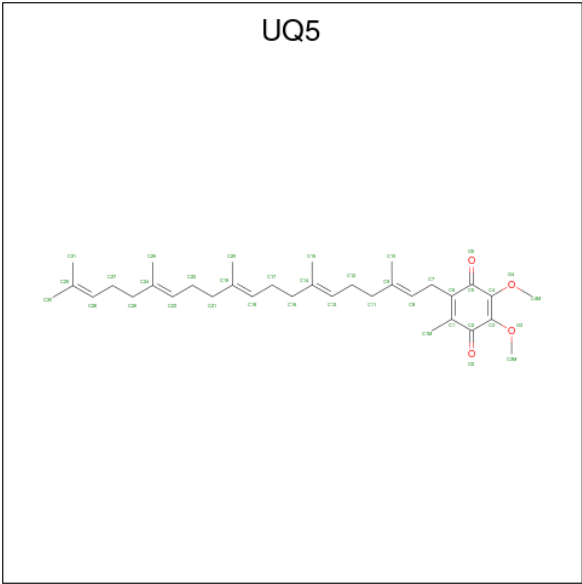
Mol	Chain	Residues	Atoms						AltConf
55	J	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	
55	r	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	

- Molecule 56 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



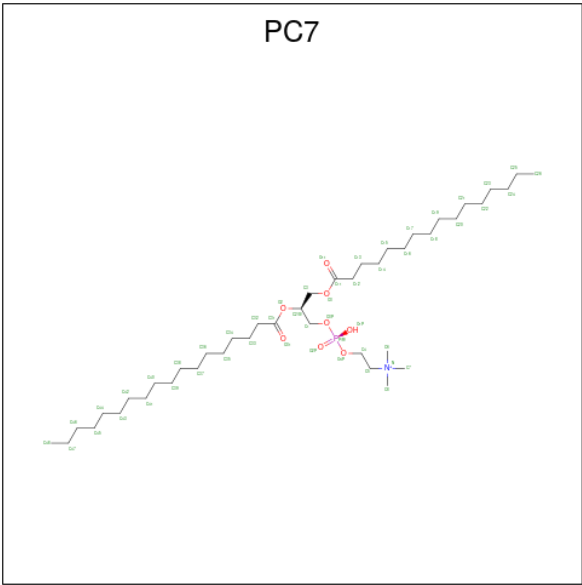
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
56	P	1	48	21	7	17	3	0

- Molecule 57 is 2,3-DIMETHOXY-5-METHYL-6-(3,11,15,19-TETRAMETHYL-EICOSA-2,6,10,14,18-PENTAENYL)-[1,4]BENZOQUINONE (CCD ID: UQ5) (formula: C₃₄H₅₀O₄).



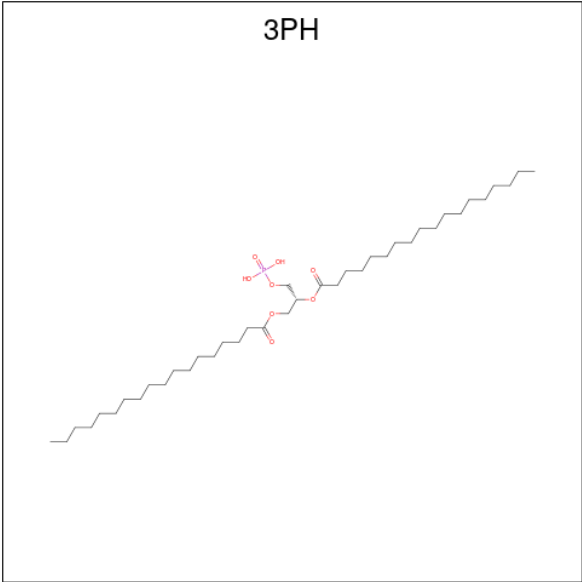
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
57	Q	1	38	34	4	0

- Molecule 58 is (7S)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY) METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSAN-1-AMINIUM 4-OXIDE (CCD ID: PC7) (formula: C₄₂H₈₅NO₈P).



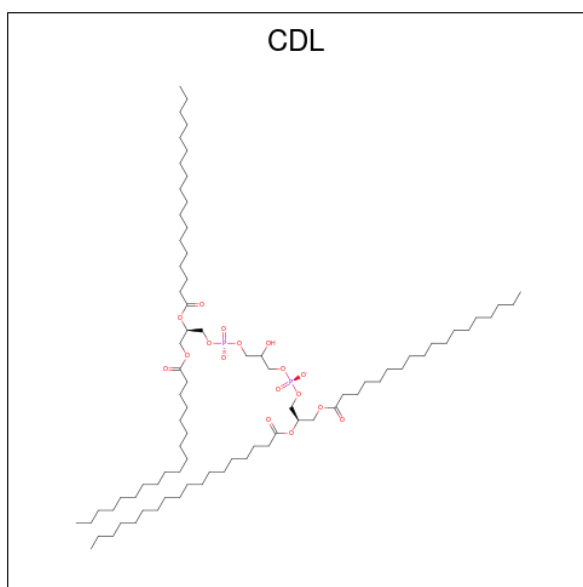
Mol	Chain	Residues	Atoms					AltConf
58	Q	1	Total	C	N	O	P	0
			33	23	1	8	1	
58	R	1	Total	C	N	O	P	0
			44	34	1	8	1	
58	T	1	Total	C	N	O	P	0
			52	42	1	8	1	
58	u	1	Total	C	N	O	P	0
			42	32	1	8	1	

- Molecule 59 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (CCD ID: 3PH) (formula: C₃₉H₇₇O₈P).



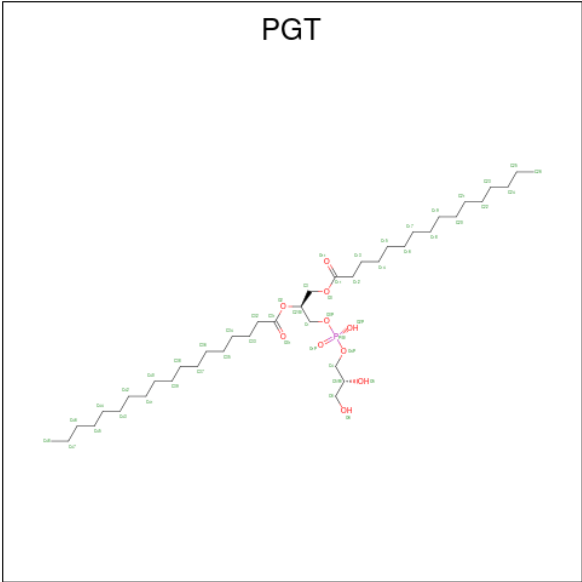
Mol	Chain	Residues	Atoms				AltConf
59	R	1	Total	C	O	P	0
			32	23	8	1	
59	S	1	Total	C	O	P	0
			37	28	8	1	
59	V	1	Total	C	O	P	0
			42	33	8	1	
59	V	1	Total	C	O	P	0
			41	32	8	1	
59	c	1	Total	C	O	P	0
			48	39	8	1	
59	g	1	Total	C	O	P	0
			37	28	8	1	
59	h	1	Total	C	O	P	0
			45	36	8	1	
59	w	1	Total	C	O	P	0
			45	36	8	1	

- Molecule 60 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



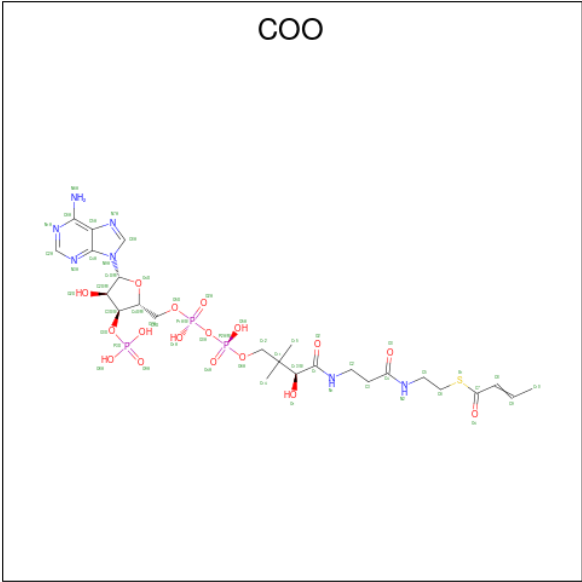
Mol	Chain	Residues	Atoms				AltConf
60	R	1	Total	C	O	P	0
			63	44	17	2	
60	V	1	Total	C	O	P	0
			64	45	17	2	
60	W	1	Total	C	O	P	0
			95	76	17	2	
60	h	1	Total	C	O	P	0
			77	58	17	2	
60	u	1	Total	C	O	P	0
			83	64	17	2	
60	u	1	Total	C	O	P	0
			71	52	17	2	
60	x	1	Total	C	O	P	0
			92	73	17	2	
60	y	1	Total	C	O	P	0
			55	36	17	2	

- Molecule 61 is (1S)-2-[[[(2R)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (CCD ID: PGT) (formula: C₄₀H₇₉O₁₀P).



Mol	Chain	Residues	Atoms				AltConf
61	T	1	Total	C	O	P	0
			48	37	10	1	
61	T	1	Total	C	O	P	0
			40	29	10	1	
61	b	1	Total	C	O	P	0
			44	33	10	1	
61	l	1	Total	C	O	P	0
			51	40	10	1	

- Molecule 62 is CROTONYL COENZYME A (CCD ID: COO) (formula: C₂₅H₄₀N₇O₁₇P₃S).



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

- Molecule 63 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
63	s	1	Total	Zn	0
			1	1	

- Molecule 64 is water.

Mol	Chain	Residues	Atoms		AltConf
64	A	24	Total	O	0
			24	24	
64	B	66	Total	O	0
			66	66	
64	C	168	Total	O	0
			168	168	
64	D	66	Total	O	0
			66	66	
64	E	87	Total	O	0
			87	87	
64	F	39	Total	O	0
			39	39	
64	G	62	Total	O	0
			62	62	
64	H	16	Total	O	0
			16	16	
64	I	19	Total	O	0
			19	19	
64	K	16	Total	O	0
			16	16	
64	L	68	Total	O	0
			68	68	
64	M	30	Total	O	0
			30	30	
64	N	53	Total	O	0
			53	53	
64	O	6	Total	O	0
			6	6	
64	P	69	Total	O	0
			69	69	
64	Q	24	Total	O	0
			24	24	

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Mol	Chain	Residues	Atoms		AltConf
64	R	64	Total 64	O 64	0
64	S	22	Total 22	O 22	0
64	T	85	Total 85	O 85	0
64	U	14	Total 14	O 14	0
64	V	99	Total 99	O 99	0
64	W	25	Total 25	O 25	0
64	X	50	Total 50	O 50	0
64	Y	4	Total 4	O 4	0
64	Z	20	Total 20	O 20	0
64	a	6	Total 6	O 6	0
64	b	24	Total 24	O 24	0
64	c	1	Total 1	O 1	0
64	d	12	Total 12	O 12	0
64	e	55	Total 55	O 55	0
64	f	10	Total 10	O 10	0
64	g	7	Total 7	O 7	0
64	h	38	Total 38	O 38	0
64	i	30	Total 30	O 30	0
64	j	29	Total 29	O 29	0
64	k	51	Total 51	O 51	0
64	l	17	Total 17	O 17	0

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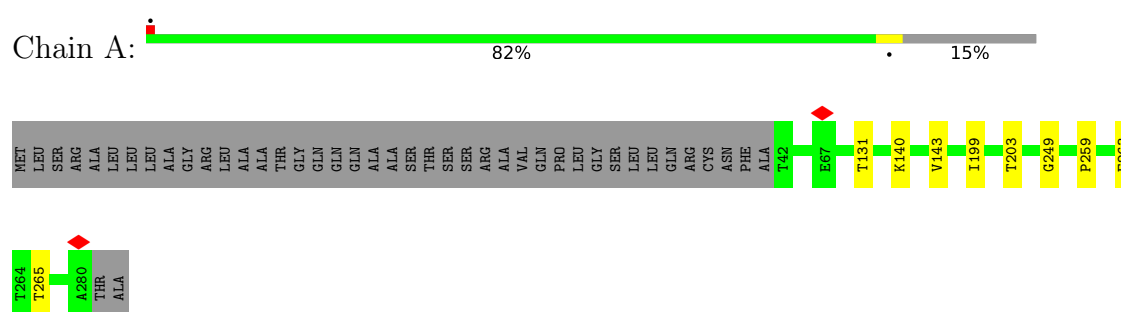
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Mol	Chain	Residues	Atoms		AltConf
64	m	32	Total 32	O 32	0
64	n	7	Total 7	O 7	0
64	o	51	Total 51	O 51	0
64	p	21	Total 21	O 21	0
64	q	24	Total 24	O 24	0
64	r	12	Total 12	O 12	0
64	s	39	Total 39	O 39	0
64	t	55	Total 55	O 55	0
64	u	41	Total 41	O 41	0
64	v	2	Total 2	O 2	0
64	w	16	Total 16	O 16	0
64	x	22	Total 22	O 22	0
64	y	29	Total 29	O 29	0

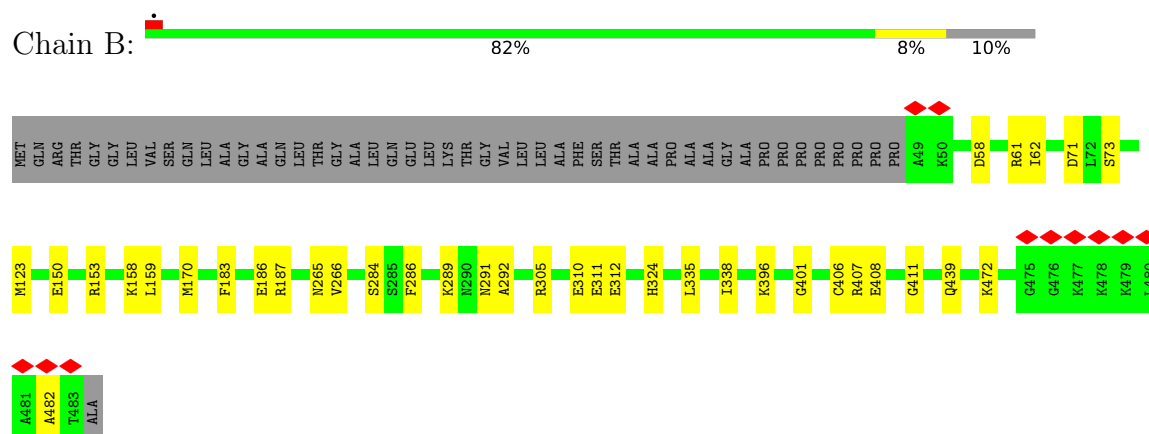
3 Residue-property plots

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

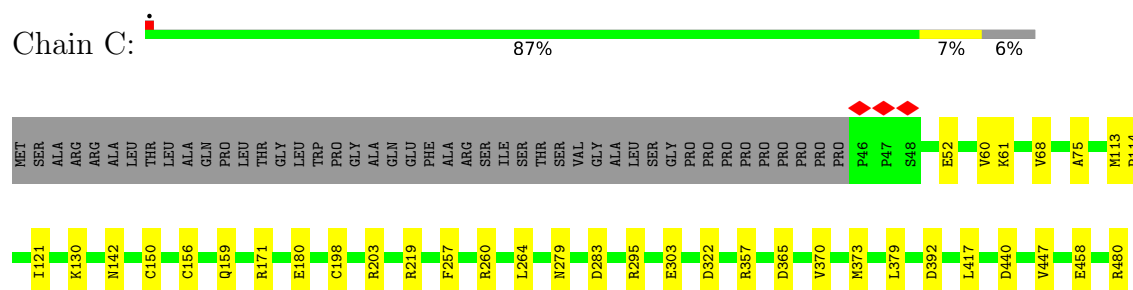
- Molecule 1: NADH:ubiquinone oxidoreductase 24 kD subunit

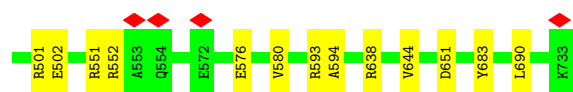


- Molecule 2: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



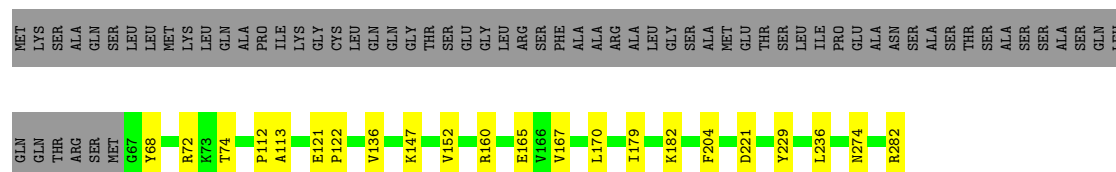
- Molecule 3: NADH:ubiquinone oxidoreductase 78 kDa subunit





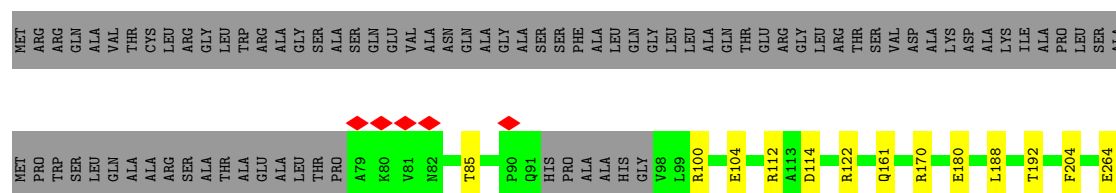
- Molecule 4: NADH:ubiquinone oxidoreductase 30kDa subunit domain-containing protein

Chain D: 69% 8% 23%



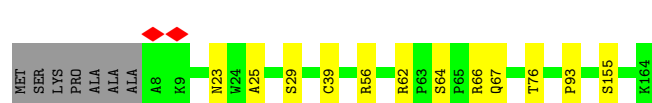
- Molecule 5: NADH:ubiquinone oxidoreductase 49 kD subunit

Chain E: 75% 7% 18%



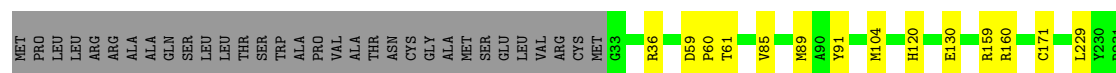
- Molecule 6: NADH:ubiquinone oxidoreductase subunit 10

Chain F: 88% 7% 5%



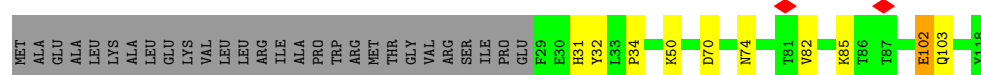
- Molecule 7: NADH:ubiquinone oxidoreductase subunit 8

Chain G: 80% 6% 14%



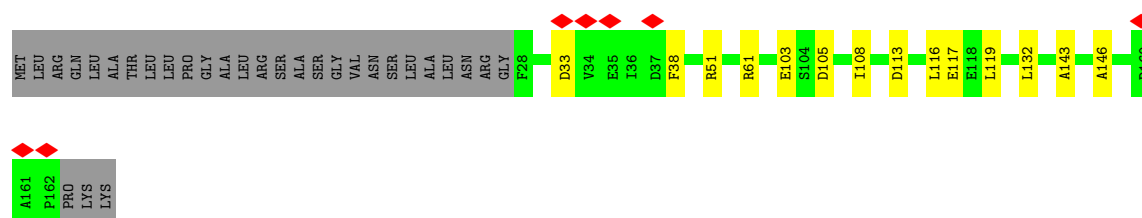
- Molecule 8: B14.5a

Chain H: 68% 8% 24%



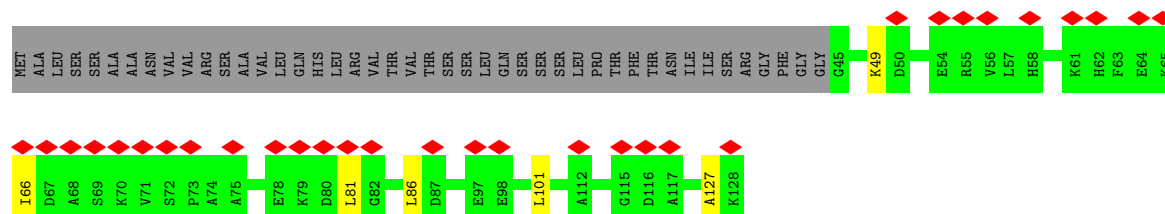
- Molecule 9: Mitochondrial NADH:ubiquinone oxidoreductase 18 kDa subunit

Chain I: 



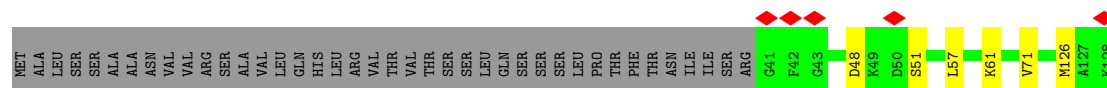
- Molecule 10: Acyl carrier protein

Chain J: 



- Molecule 10: Acyl carrier protein

Chain r: 



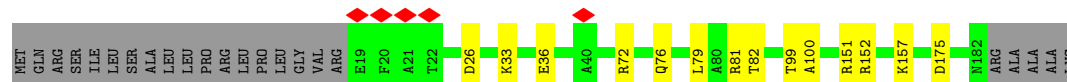
- Molecule 11: NADH:ubiquinone oxidoreductase B14 subunit

Chain K: 



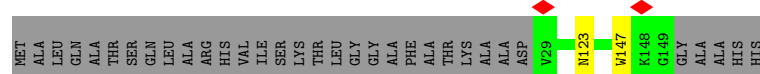
- Molecule 12: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain L: 



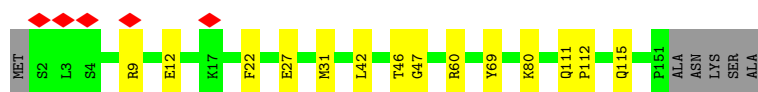
- Molecule 13: NADH:ubiquinone oxidoreductase 13 kD-like subunit

Chain M: 



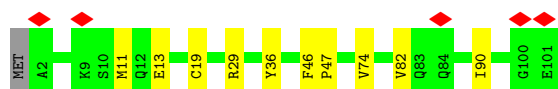
- Molecule 14: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain N:  87% 9%



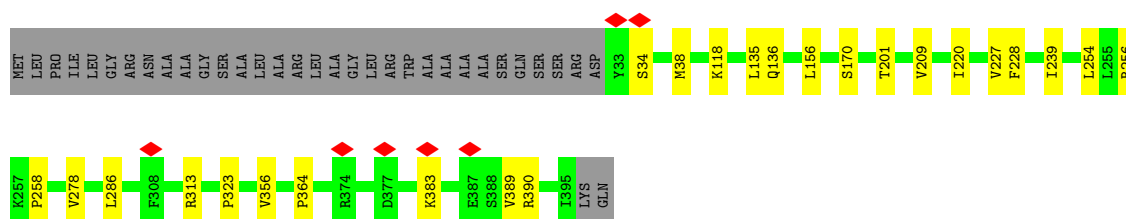
- Molecule 15: NADH:ubiquinone oxidoreductase B8 subunit

Chain O:  5% 89% 10%



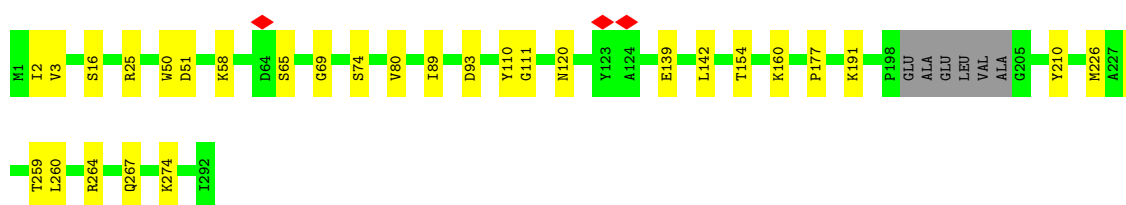
- Molecule 16: Putative NADH:ubiquinone oxidoreductase 39 kDa subunit

Chain P:  85% 6% 9%



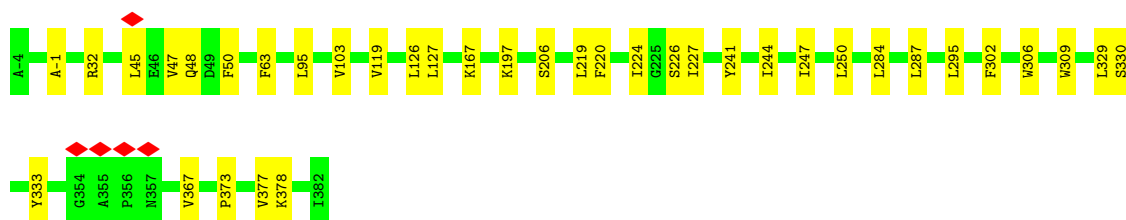
- Molecule 17: NADH-ubiquinone oxidoreductase chain 1

Chain Q:  88% 10%



- Molecule 18: NADH-ubiquinone oxidoreductase chain 2

Chain R:  90% 10%



- Molecule 19: NADH-ubiquinone oxidoreductase chain 3

- Molecule 20: NADH-ubiquinone oxidoreductase chain 4

R238	F252	S256	L260	D275	K278	Y292	M288	S299	S307	P318	A362	E372	V389	G397	Y400	F405	N406	R407	V408	V409	M442	A443									
M1	L7	P36	W44	L54	L57	L60	R62	D70	L76	V82	G96	L108	L127	F131	V149	F164	S168	W190	V195	L196	T200	P201	L202	M203	H206	P210	V222	L224	L228	L229	L234

- Molecule 21: NADH dehydrogenase subunit 4L

[illegible]

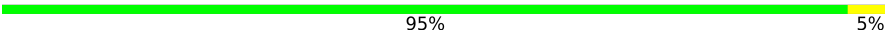
- Molecule 22: NADH-ubiquinone oxidoreductase chain 5

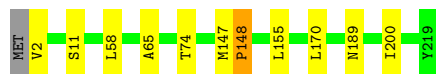
L378	M1
S379	F2
K394	F8
I398	L11
R438	C36
T461	S43
F515	I47
P519	M126
G542	W156
A546	K164
	K168
	S176
	S205
	G215
	T223
	D231
	T237
	T243
	T247
	L248
	F266
	V270
	S295
	Y302
	G310
	G314
	G319
	T323
	K328
	G336
	R350

- Molecule 23: NADH-ubiquinone oxidoreductase chain 6

M1		E4	M43	V59	L73	A77	T78	E79	L80	R81	A82	Y83	S84	R85	G86	W87	F101	T123	G126	D135	V143	R151	I154	V157	ARG THR	THR GLY	ARG
----	--	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	---------	---------	-----

- Molecule 31: Mitochondrial NADH:ubiquinone oxidoreductase 23 kDa subunit

Chain e:  95% 5%



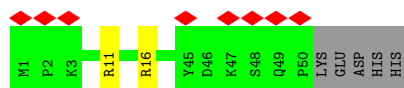
- Molecule 32: Mitochondrial NADH:ubiquinone oxidoreductase 7.5 kDa subunit

Chain f:  92% 6%



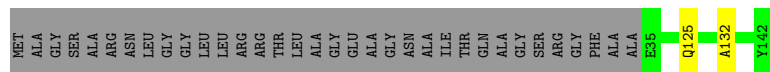
- Molecule 33: Mitochondrial putative NADH:ubiquinone oxidoreductase 6.5 kDa subunit

Chain g:  15% 87% 9%



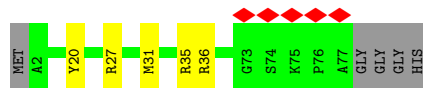
- Molecule 34: Mitochondrial NADH:ubiquinone oxidoreductase 13 kDa subunit

Chain h:  75% 24%

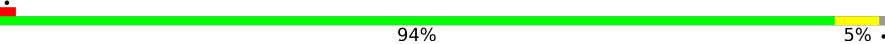


- Molecule 35: NADH:ubiquinone oxidoreductase 15 kDa subunit-like

Chain i:  6% 88% 6% 6%

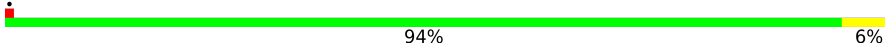


- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain j:  94% 5%

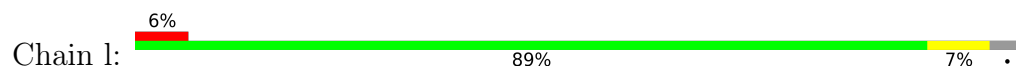


- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

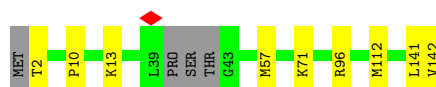
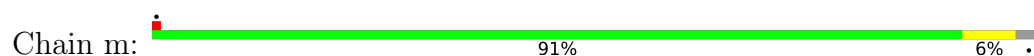
Chain k:  94% 6%



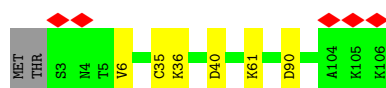
- Molecule 38: NADH:ubiquinone oxidoreductase 20,9 kD-like subunit



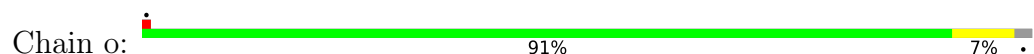
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



- Molecule 40: Putative NADH:ubiquinone oxidoreductase 12.5 kDa subunit



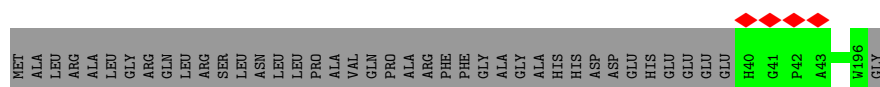
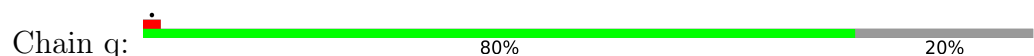
- Molecule 41: Putative NADH:ubiquinone oxidoreductase 17.8 kDa subunit



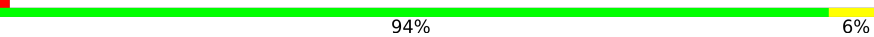
- Molecule 42: Mitochondrial NADH:ubiquinone oxidoreductase 16 kDa subunit



- Molecule 43: Mitochondrial NADH:ubiquinone oxidoreductase 19 kDa subunit



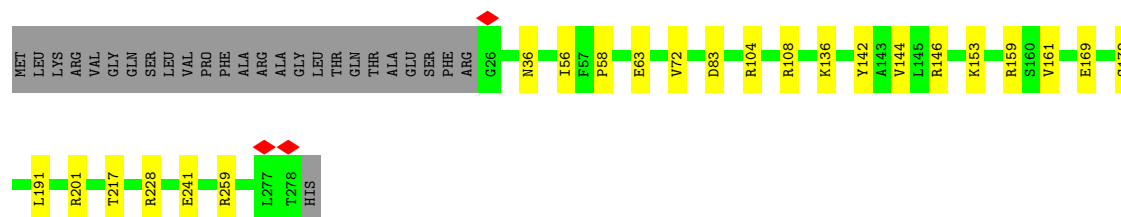
- Molecule 44: Mitochondrial NADH:ubiquinone oxidoreductase 32 kDa subunit

Chain s:  94% 6%

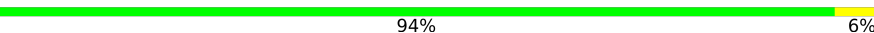


- Molecule 45: CAG2 - CA-like

Chain t:  82% 8% 9%

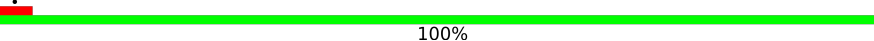


- Molecule 46: CAG1

Chain u:  94% 6%



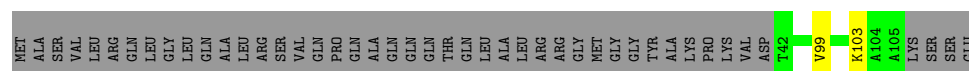
- Molecule 47: P10

Chain v:  100%



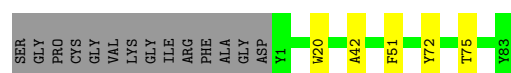
- Molecule 48: Mitochondrial NADH:ubiquinone oxidoreductase 9 kDa subunit

Chain w:  57% 41%

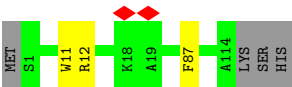
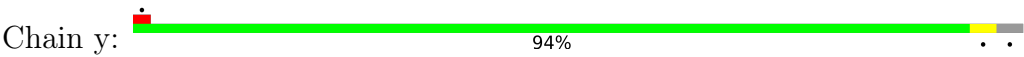


- Molecule 49: NUOP8

Chain x:  50% 47%



- Molecule 50: NUOP7



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	83443	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	1.068	Depositor
Minimum map value	0.000	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.141	Depositor
Map size (Å)	589.6, 589.6, 589.6	wwPDB
Map dimensions	588, 588, 588	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0027211, 1.0027211, 1.0027211	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.22	0/1878	0.47	0/2549
2	B	0.24	0/3400	0.45	0/4573
3	C	0.23	0/5272	0.42	0/7143
4	D	0.27	0/1843	0.49	0/2506
5	E	0.29	0/3158	0.49	0/4270
6	F	0.30	0/1258	0.48	0/1706
7	G	0.25	0/1648	0.50	0/2222
8	H	0.24	0/773	0.58	2/1046 (0.2%)
9	I	0.21	0/1061	0.38	0/1441
10	J	0.20	0/649	0.47	0/875
10	r	0.22	0/673	0.40	0/906
11	K	0.24	0/1007	0.54	1/1348 (0.1%)
12	L	0.23	0/1306	0.47	0/1769
13	M	0.23	0/936	0.43	0/1276
14	N	0.21	0/1277	0.37	0/1735
15	O	0.18	0/772	0.45	0/1037
16	P	0.22	0/2879	0.44	0/3905
17	Q	0.29	0/2234	0.52	0/3034
18	R	0.30	0/3100	0.54	0/4226
19	S	0.28	0/1106	0.49	0/1512
20	T	0.31	0/3533	0.55	0/4825
21	U	0.28	0/819	0.48	0/1112
22	V	0.29	0/4258	0.52	0/5792
23	W	0.26	0/1239	0.52	0/1686
24	X	0.27	0/1081	0.51	0/1479
25	Y	0.24	0/411	0.41	0/557
26	Z	0.23	0/894	0.42	0/1218
27	a	0.21	0/698	0.43	0/949
28	b	0.26	0/1201	0.49	0/1623
29	c	0.22	0/463	0.50	0/623
30	d	0.27	0/721	0.41	0/968
31	e	0.27	0/1688	0.46	0/2301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	f	0.25	0/547	0.42	0/740
33	g	0.20	0/433	0.46	0/587
34	h	0.24	0/948	0.49	0/1285
35	i	0.22	0/644	0.40	0/860
36	j	0.23	0/732	0.38	0/983
37	k	0.25	0/1011	0.43	0/1361
38	l	0.25	0/936	0.43	0/1278
39	m	0.27	0/1155	0.41	0/1558
40	n	0.23	0/886	0.39	0/1188
41	o	0.27	0/1265	0.50	0/1705
42	p	0.22	0/1095	0.39	0/1480
43	q	0.23	0/1308	0.38	0/1779
44	s	0.22	0/2353	0.42	0/3202
45	t	0.25	0/2043	0.48	0/2778
46	u	0.25	0/1730	0.47	0/2341
47	v	0.22	0/369	0.37	0/498
48	w	0.24	0/521	0.41	0/702
49	x	0.23	0/727	0.39	0/994
50	y	0.25	0/963	0.48	0/1313
All	All	0.25	0/72902	0.47	3/98844 (0.0%)

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
31	e	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	102	GLU	CA-C-N	7.46	135.79	121.54
8	H	102	GLU	C-N-CA	7.46	135.79	121.54
11	K	85	GLU	N-CA-CB	5.25	118.96	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
31	e	147	MET	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	1839	0	1827	6	0
2	B	3331	0	3328	23	0
3	C	5175	0	5182	32	0
4	D	1790	0	1740	16	0
5	E	3085	0	3058	20	0
6	F	1225	0	1224	11	0
7	G	1615	0	1551	11	0
8	H	750	0	751	8	0
9	I	1044	0	1046	10	0
10	J	640	0	629	5	0
10	r	663	0	647	5	0
11	K	986	0	1017	7	0
12	L	1275	0	1243	12	0
13	M	913	0	909	2	0
14	N	1235	0	1161	9	0
15	O	761	0	759	6	0
16	P	2823	0	2854	14	0
17	Q	2179	0	2241	26	0
18	R	3014	0	3102	31	0
19	S	1071	0	1035	12	0
20	T	3434	0	3590	36	0
21	U	805	0	812	9	0
22	V	4152	0	4212	27	0
23	W	1210	0	1275	19	0
24	X	1037	0	981	5	0
25	Y	405	0	404	2	0
26	Z	861	0	826	3	0
27	a	674	0	620	2	0
28	b	1169	0	1144	6	0
29	c	453	0	475	1	0
30	d	699	0	670	4	0
31	e	1639	0	1618	12	0
32	f	532	0	524	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	g	416	0	402	2	0
34	h	915	0	866	1	0
35	i	633	0	612	3	0
36	j	712	0	684	3	0
37	k	984	0	980	5	0
38	l	904	0	875	4	0
39	m	1126	0	1148	11	0
40	n	864	0	839	6	0
41	o	1240	0	1222	9	0
42	p	1069	0	1014	5	0
43	q	1268	0	1209	0	0
44	s	2302	0	2299	15	0
45	t	1997	0	1985	17	0
46	u	1698	0	1686	9	0
47	v	361	0	359	0	0
48	w	508	0	494	2	0
49	x	699	0	662	4	0
50	y	932	0	950	3	0
51	A	4	0	0	0	0
51	C	4	0	0	0	0
52	B	31	0	19	1	0
53	B	8	0	0	1	0
53	C	16	0	0	0	0
53	F	8	0	0	1	0
53	G	16	0	0	0	0
54	G	43	0	62	2	0
54	R	118	0	161	2	0
54	S	46	0	68	3	0
54	T	104	0	133	1	0
54	V	125	0	175	3	0
54	e	68	0	85	3	0
54	h	46	0	68	1	0
54	x	50	0	79	0	0
55	J	35	0	0	0	0
55	r	35	0	0	0	0
56	P	48	0	26	1	0
57	Q	38	0	50	2	0
58	Q	33	0	40	1	0
58	R	44	0	62	0	0
58	T	52	0	84	3	0
58	u	42	0	58	2	0
59	R	32	0	37	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	S	37	0	47	0	0
59	V	83	0	115	3	0
59	c	48	0	75	2	0
59	g	37	0	50	0	0
59	h	45	0	63	2	0
59	w	45	0	66	3	0
60	R	63	0	70	1	0
60	V	64	0	72	1	0
60	W	95	0	143	8	0
60	h	77	0	98	3	0
60	u	154	0	205	5	0
60	x	92	0	137	9	0
60	y	55	0	54	4	0
61	T	88	0	122	3	0
61	b	44	0	58	1	0
61	l	51	0	78	1	0
62	s	53	0	37	5	0
63	s	1	0	0	0	0
64	A	24	0	0	0	0
64	B	66	0	0	1	0
64	C	168	0	0	1	0
64	D	66	0	0	0	0
64	E	87	0	0	1	0
64	F	39	0	0	0	0
64	G	62	0	0	0	0
64	H	16	0	0	0	0
64	I	19	0	0	0	0
64	K	16	0	0	0	0
64	L	68	0	0	1	0
64	M	30	0	0	0	0
64	N	53	0	0	0	0
64	O	6	0	0	0	0
64	P	69	0	0	0	0
64	Q	24	0	0	0	0
64	R	64	0	0	0	0
64	S	22	0	0	1	0
64	T	85	0	0	1	0
64	U	14	0	0	1	0
64	V	99	0	0	1	0
64	W	25	0	0	0	0
64	X	50	0	0	0	0
64	Y	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
64	Z	20	0	0	0	0
64	a	6	0	0	0	0
64	b	24	0	0	0	0
64	c	1	0	0	0	0
64	d	12	0	0	0	0
64	e	55	0	0	1	0
64	f	10	0	0	0	0
64	g	7	0	0	1	0
64	h	38	0	0	0	0
64	i	30	0	0	0	0
64	j	29	0	0	0	0
64	k	51	0	0	0	0
64	l	17	0	0	0	0
64	m	32	0	0	1	0
64	n	7	0	0	0	0
64	o	51	0	0	0	0
64	p	21	0	0	0	0
64	q	24	0	0	0	0
64	r	12	0	0	0	0
64	s	39	0	0	0	0
64	t	55	0	0	0	0
64	u	41	0	0	0	0
64	v	2	0	0	0	0
64	w	16	0	0	0	0
64	x	22	0	0	0	0
64	y	29	0	0	0	0
All	All	75117	0	73438	433	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 3.

All (433) 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)
19:S:224:LEU:HD12	23:W:151:ARG:HH22	1.57	0.70
33:g:16:ARG:HH12	37:k:33:ARG:HD3	1.58	0.68
40:n:35:CYS:SG	42:p:102:ARG:NH2	2.67	0.67
5:E:122:ARG:HD3	6:F:76:THR:HG21	1.76	0.67
17:Q:69:GLY:HA3	60:W:701:CDL:HB4	1.76	0.65
23:W:81:ARG:HA	23:W:84:SER:HB3	1.79	0.64
60:u:603:CDL:HB62	60:u:603:CDL:HB22	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:302:PHE:HB3	18:R:306:TRP:HZ3	1.63	0.62
31:e:58:LEU:HD22	49:x:51:PHE:HD2	1.65	0.62
22:V:319:GLY:HA2	22:V:461:THR:HG21	1.81	0.61
16:P:136:GLN:OE1	16:P:313:ARG:NH1	2.33	0.61
2:B:286:PHE:HB3	2:B:312:GLU:HG3	1.82	0.61
10:J:101:LEU:HD21	10:J:127:ALA:HA	1.83	0.61
5:E:298:ARG:NH1	5:E:340:GLU:OE2	2.34	0.60
36:j:78:LYS:HG2	36:j:83:LEU:HD12	1.83	0.60
5:E:85:THR:HG22	5:E:104:GLU:HG2	1.83	0.60
10:J:49:LYS:O	10:J:49:LYS:HG2	2.00	0.60
44:s:29:LEU:HD21	58:u:601:PC7:H151	1.83	0.60
5:E:306:LEU:HB2	5:E:405:GLU:HB2	1.83	0.59
16:P:135:LEU:HD21	16:P:323:PRO:HA	1.83	0.59
17:Q:154:THR:HG22	17:Q:160:LYS:HG2	1.84	0.59
44:s:214:ALA:HB2	62:s:401:COO:H22	1.84	0.59
6:F:93:PRO:HG2	17:Q:58:LYS:HE3	1.84	0.59
44:s:280:ILE:HD11	45:t:259:ARG:HG2	1.85	0.59
14:N:12:GLU:OE1	14:N:60:ARG:NH2	2.35	0.59
4:D:274:ASN:O	12:L:81:ARG:NH2	2.35	0.59
20:T:54:LEU:HB3	20:T:57:LEU:HD21	1.83	0.58
3:C:180:GLU:HG2	13:M:123:ASN:HD22	1.68	0.58
19:S:245:THR:HG22	23:W:123:THR:HA	1.86	0.58
22:V:295:SER:OG	22:V:328:LYS:NZ	2.36	0.58
29:c:26:VAL:HG11	59:c:101:3PH:H3G2	1.86	0.58
7:G:89:MET:HG2	17:Q:259:THR:HG21	1.85	0.58
3:C:501:ARG:NH1	3:C:502:GLU:OE2	2.37	0.57
45:t:159:ARG:HB2	46:u:149:ILE:HD11	1.87	0.57
2:B:61:ARG:NH1	2:B:310:GLU:O	2.37	0.57
38:l:112:LEU:HB3	38:l:115:VAL:HB	1.85	0.57
18:R:95:LEU:HD13	18:R:167:LYS:HE3	1.87	0.57
7:G:120:HIS:CE1	7:G:171:CYS:SG	2.97	0.56
18:R:309:TRP:NE1	20:T:168:SER:OG	2.34	0.56
22:V:205:SER:O	22:V:205:SER:OG	2.23	0.56
46:u:24:ALA:HB1	60:u:602:CDL:HA62	1.87	0.56
22:V:2:PHE:HA	22:V:47:ILE:HD11	1.88	0.56
16:P:220:ILE:HD12	16:P:286:LEU:HD11	1.88	0.56
18:R:241:TYR:HA	18:R:244:ILE:HD12	1.87	0.56
21:U:223:LEU:HD11	23:W:73:LEU:HD23	1.86	0.56
27:a:56:ASP:OD2	27:a:66:LYS:NZ	2.34	0.56
3:C:303:GLU:OE2	12:L:72:ARG:NH2	2.39	0.56
54:h:202:PTY:H381	54:h:202:PTY:H202	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:l:2:THR:OG1	38:l:3:TRP:N	2.34	0.55
5:E:188:LEU:HG	5:E:341:MET:HE1	1.89	0.55
8:H:31:HIS:ND1	8:H:32:TYR:O	2.29	0.55
18:R:47:VAL:HA	59:R:401:3PH:H221	1.89	0.55
20:T:62:ARG:NH2	30:d:84:GLN:OE1	2.39	0.55
28:b:164:LYS:NZ	28:b:168:GLU:OE2	2.39	0.55
17:Q:65:SER:O	17:Q:120:ASN:ND2	2.39	0.55
18:R:378:LYS:HD2	20:T:62:ARG:HG3	1.88	0.55
22:V:323:THR:HG1	22:V:379:SER:HG	1.51	0.55
31:e:74:THR:HG23	49:x:75:THR:HG21	1.88	0.55
12:L:79:LEU:HD11	12:L:151:ARG:HH12	1.70	0.55
17:Q:274:LYS:NZ	19:S:276:GLU:OE2	2.39	0.55
2:B:406:CYS:HB3	53:B:502:SF4:S4	2.47	0.55
6:F:66:ARG:NH2	19:S:202:SER:O	2.40	0.55
31:e:2:VAL:N	64:e:406:HOH:O	2.39	0.55
48:w:99:VAL:O	48:w:103:LYS:HB2	2.06	0.55
23:W:101:PHE:O	25:Y:28:ARG:NH2	2.40	0.55
20:T:195:VAL:HG23	20:T:196:LEU:HG	1.88	0.54
3:C:52:GLU:OE2	3:C:61:LYS:NZ	2.40	0.54
41:o:127:ARG:NH1	41:o:130:GLU:OE1	2.40	0.54
9:I:116:LEU:HA	9:I:119:LEU:HD12	1.88	0.54
59:h:201:3PH:H32	59:w:201:3PH:H371	1.89	0.54
44:s:184:HIS:ND1	44:s:202:ASP:OD1	2.37	0.54
60:y:201:CDL:H1	60:y:201:CDL:H111	1.88	0.54
18:R:48:GLN:HG3	54:R:404:PTY:H112	1.89	0.54
15:O:13:GLU:HG3	15:O:47:PRO:HB2	1.88	0.54
44:s:284:ARG:NH2	45:t:36:ASN:OD1	2.39	0.54
2:B:482:ALA:HB2	39:m:10:PRO:HB2	1.90	0.53
11:K:52:GLU:OE1	11:K:106:TYR:OH	2.27	0.53
54:G:303:PTY:H362	17:Q:177:PRO:HB3	1.90	0.53
2:B:265:ASN:ND2	52:B:501:FMN:O2	2.40	0.53
6:F:62:ARG:NH2	57:Q:301:UQ5:O5	2.42	0.53
20:T:362:ALA:HB1	20:T:372:GLU:HG2	1.89	0.53
35:i:20:TYR:OH	35:i:36:ARG:NH1	2.38	0.53
2:B:401:GLY:HA2	2:B:407:ARG:HB2	1.91	0.53
4:D:113:ALA:HA	4:D:121:GLU:HB2	1.91	0.53
18:R:119:VAL:HG21	21:U:214:MET:HE1	1.91	0.53
20:T:131:PHE:HB2	20:T:149:VAL:HG21	1.90	0.53
4:D:122:PRO:HG2	4:D:179:ILE:HG13	1.91	0.53
44:s:17:ARG:NH2	45:t:241:GLU:OE1	2.41	0.53
35:i:27:ARG:HB2	35:i:35:ARG:HD3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:s:68:ALA:HB3	44:s:117:LEU:HG	1.92	0.52
31:e:200:ILE:H	42:p:46:GLU:HG2	1.75	0.52
58:u:601:PC7:H352	58:u:601:PC7:H31	1.91	0.52
20:T:299:SER:HB2	41:o:114:ALA:HB2	1.90	0.52
45:t:56:ILE:HD11	45:t:72:VAL:HG21	1.92	0.52
18:R:219:LEU:HB3	60:x:101:CDL:H592	1.92	0.52
41:o:107:ASN:HA	41:o:110:ARG:HD3	1.92	0.52
18:R:220:PHE:O	18:R:224:ILE:HB	2.10	0.51
5:E:293:SER:HA	5:E:297:LEU:HD22	1.91	0.51
1:A:265:THR:OG1	2:B:58:ASP:OD1	2.28	0.51
45:t:108:ARG:HH12	45:t:217:THR:HG23	1.75	0.51
3:C:365:ASP:OD1	3:C:365:ASP:N	2.43	0.51
5:E:170:ARG:NH1	5:E:356:PRO:O	2.40	0.51
59:h:201:3PH:H371	59:w:201:3PH:H2B1	1.93	0.51
46:u:111:ALA:HB2	46:u:119:VAL:HG23	1.92	0.51
3:C:156:CYS:HB3	3:C:159:GLN:HB2	1.92	0.51
16:P:209:VAL:HG21	16:P:356:VAL:HG13	1.92	0.51
18:R:287:LEU:HD22	18:R:367:VAL:HG13	1.91	0.51
20:T:82:VAL:HG21	58:T:503:PC7:H201	1.92	0.51
60:W:701:CDL:HA62	25:Y:6:ASN:HB3	1.93	0.51
45:t:191:LEU:HD23	45:t:201:ARG:HG2	1.91	0.51
60:x:101:CDL:H792	60:y:201:CDL:H122	1.92	0.51
54:e:302:PTY:H381	54:e:302:PTY:H212	1.93	0.51
38:l:87:LEU:HG	38:l:91:MET:HE2	1.92	0.51
18:R:206:SER:OG	42:p:72:ARG:NH2	2.44	0.51
22:V:126:MET:HB2	22:V:247:THR:HG23	1.93	0.51
28:b:104:LEU:HD21	41:o:72:LEU:HG	1.93	0.51
2:B:187:ARG:NH1	64:B:604:HOH:O	2.45	0.50
59:w:201:3PH:H261	59:w:201:3PH:H352	1.94	0.50
17:Q:2:ILE:HB	58:Q:302:PC7:H71	1.94	0.50
8:H:70:ASP:O	8:H:74:ASN:ND2	2.35	0.50
2:B:62:ILE:O	2:B:158:LYS:NZ	2.41	0.50
20:T:275:ASP:HB3	20:T:278:LYS:HB2	1.92	0.50
40:n:90:ASP:OD1	40:n:90:ASP:N	2.44	0.50
6:F:67:GLN:NE2	17:Q:210:TYR:O	2.41	0.50
45:t:58:PRO:HB3	45:t:63:GLU:HG3	1.94	0.50
3:C:638:ARG:NH2	3:C:651:ASP:OD1	2.44	0.49
6:F:56:ARG:HH12	7:G:104:MET:HA	1.77	0.49
31:e:189:ASN:HB3	41:o:8:ARG:HB3	1.92	0.49
5:E:449:ALA:HB3	17:Q:264:ARG:HD2	1.94	0.49
11:K:106:TYR:O	11:K:110:ARG:CB	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:s:120:VAL:HG22	44:s:141:ILE:HB	1.94	0.49
5:E:414:TYR:HB3	5:E:427:LYS:HB3	1.94	0.49
12:L:72:ARG:NH1	12:L:76:GLN:O	2.45	0.49
31:e:148:PRO:HG2	50:y:11:TRP:HB3	1.94	0.49
17:Q:80:VAL:HG11	60:W:701:CDL:H792	1.94	0.49
21:U:196:ILE:HD13	23:W:143:VAL:HG11	1.94	0.49
59:V:602:3PH:H3B1	24:X:87:ALA:HB2	1.95	0.49
44:s:93:THR:HG21	46:u:222:MET:HE1	1.95	0.49
20:T:44:TRP:HE1	58:T:503:PC7:H321	1.78	0.49
22:V:205:SER:OG	24:X:145:TRP:O	2.31	0.49
46:u:127:VAL:HA	46:u:144:ILE:HB	1.95	0.49
2:B:150:GLU:OE2	2:B:153:ARG:NH2	2.46	0.48
7:G:130:GLU:O	7:G:160:ARG:NH1	2.44	0.48
19:S:174:THR:HG21	54:S:302:PTY:H372	1.94	0.48
37:k:2:ALA:HB1	37:k:6:VAL:HB	1.94	0.48
2:B:183:PHE:HB3	2:B:186:GLU:HB2	1.94	0.48
20:T:252:PHE:O	20:T:256:SER:HB2	2.12	0.48
21:U:129:ILE:O	21:U:133:THR:OG1	2.27	0.48
7:G:229:LEU:HD22	8:H:50:LYS:HE2	1.95	0.48
18:R:119:VAL:HG13	21:U:207:LEU:HD22	1.95	0.48
38:l:41:ASN:ND2	38:l:111:ASN:OD1	2.46	0.48
54:V:605:PTY:H332	54:V:605:PTY:H362	1.67	0.48
54:V:606:PTY:H151	50:y:87:PHE:HE2	1.79	0.48
44:s:214:ALA:CB	62:s:401:COO:H22	2.43	0.48
4:D:112:PRO:O	5:E:161:GLN:NE2	2.46	0.48
6:F:23:ASN:ND2	6:F:155:SER:O	2.42	0.48
22:V:438:ARG:NH1	64:V:709:HOH:O	2.41	0.48
54:R:406:PTY:H442	60:x:101:CDL:H582	1.94	0.48
22:V:176:SER:HB2	22:V:215:GLY:HA2	1.95	0.48
20:T:96:GLY:HA2	37:k:117:LEU:HD23	1.95	0.48
2:B:284:SER:HA	2:B:292:ALA:HB1	1.94	0.48
5:E:180:GLU:OE2	5:E:315:TYR:OH	2.28	0.48
19:S:224:LEU:HG	23:W:151:ARG:HH12	1.78	0.48
3:C:502:GLU:HG3	3:C:690:LEU:HB3	1.96	0.48
8:H:34:PRO:HD2	14:N:69:TYR:CE1	2.49	0.48
61:l:701:PGT:H32	61:l:701:PGT:H332	1.96	0.48
18:R:247:ILE:HD12	18:R:250:LEU:HD12	1.96	0.47
31:e:11:SER:HB3	41:o:112:PRO:HG3	1.95	0.47
41:o:118:ASP:HB3	41:o:123:TYR:CD2	2.48	0.47
5:E:377:GLN:NE2	64:E:506:HOH:O	2.46	0.47
45:t:169:GLU:O	45:t:172:SER:OG	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:227:ILE:HD13	60:x:101:CDL:H512	1.96	0.47
62:s:401:COO:H103	45:t:146:ARG:NE	2.29	0.47
62:s:401:COO:H121	62:s:401:COO:C8A	2.44	0.47
2:B:289:LYS:O	2:B:291:ASN:ND2	2.45	0.47
11:K:99:THR:HG23	11:K:100:GLU:HG3	1.97	0.47
44:s:213:ALA:HB2	62:s:401:COO:H142	1.96	0.47
3:C:322:ASP:OD1	3:C:322:ASP:N	2.46	0.47
9:I:51:ARG:NH2	9:I:117:GLU:OE2	2.43	0.47
16:P:170:SER:O	56:P:401:NDP:H6N	2.14	0.47
22:V:266:PHE:HD1	59:V:602:3PH:H272	1.78	0.47
4:D:160:ARG:NH1	4:D:165:GLU:OE2	2.41	0.47
12:L:99:THR:HG22	12:L:100:ALA:H	1.79	0.47
19:S:195:ARG:NH1	64:S:403:HOH:O	2.39	0.47
22:V:11:LEU:HB2	54:V:605:PTY:H411	1.97	0.47
23:W:1:MET:HG2	23:W:4:GLU:HB2	1.97	0.47
4:D:68:TYR:HE2	4:D:147:LYS:HE3	1.80	0.47
15:O:74:VAL:HB	15:O:82:VAL:HG12	1.97	0.47
4:D:167:VAL:HG22	4:D:182:LYS:HG2	1.97	0.47
20:T:222:VAL:HG13	20:T:318:PRO:HB3	1.96	0.47
21:U:164:GLU:OE2	21:U:201:THR:OG1	2.32	0.47
22:V:1:MET:HE3	22:V:43:SER:HA	1.96	0.47
30:d:22:ASN:ND2	30:d:31:ARG:O	2.43	0.47
3:C:357:ARG:HH12	3:C:552:ARG:HD2	1.78	0.46
16:P:227:VAL:HG23	16:P:228:PHE:HD1	1.80	0.46
54:T:501:PTY:H331	54:T:501:PTY:H361	1.73	0.46
4:D:229:TYR:OH	5:E:100:ARG:NH1	2.47	0.46
9:I:105:ASP:HA	9:I:108:ILE:HD12	1.98	0.46
17:Q:16:SER:OG	32:f:16:TRP:NE1	2.49	0.46
17:Q:139:GLU:HA	17:Q:142:LEU:HD12	1.97	0.46
22:V:542:GLY:N	60:y:201:CDL:OA7	2.41	0.46
46:u:6:GLY:HA2	60:u:603:CDL:HB61	1.96	0.46
12:L:175:ASP:OD1	12:L:175:ASP:N	2.41	0.46
18:R:306:TRP:HH2	18:R:377:VAL:HA	1.79	0.46
20:T:201:PRO:HD3	20:T:229:LEU:HD22	1.96	0.46
44:s:1:MET:HA	44:s:5:LYS:HD2	1.98	0.46
20:T:397:GLY:HA2	20:T:400:TYR:CE2	2.51	0.46
39:m:71:LYS:NZ	64:m:202:HOH:O	2.48	0.46
3:C:257:PHE:HB3	7:G:159:ARG:HG3	1.98	0.46
5:E:264:GLU:HG3	7:G:91:TYR:CZ	2.51	0.46
60:h:203:CDL:H132	60:h:203:CDL:H531	1.98	0.46
40:n:36:LYS:HD2	40:n:36:LYS:HA	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:w:99:VAL:HG13	48:w:103:LYS:HE2	1.98	0.46
1:A:249:GLY:HA3	1:A:259:PRO:HA	1.98	0.46
3:C:580:VAL:HB	3:C:594:ALA:HA	1.97	0.46
5:E:374:THR:HG23	39:m:2:THR:HG21	1.97	0.46
18:R:45:LEU:HD23	18:R:50:PHE:HE2	1.80	0.46
6:F:64:SER:OG	6:F:67:GLN:OE1	2.34	0.46
9:I:33:ASP:N	9:I:33:ASP:OD1	2.45	0.46
13:M:147:TRP:H	13:M:147:TRP:CD1	2.33	0.46
61:T:502:PGT:H152	61:T:502:PGT:H202	1.98	0.46
5:E:329:ASP:OD2	7:G:36:ARG:NH1	2.49	0.45
9:I:61:ARG:HH12	9:I:103:GLU:HA	1.82	0.45
18:R:284:LEU:HD21	30:d:20:LEU:HD11	1.98	0.45
20:T:203:MET:HG2	20:T:206:HIS:CE1	2.51	0.45
4:D:74:THR:HG21	9:I:38:PHE:HB3	1.99	0.45
28:b:95:TRP:O	28:b:99:ARG:NH1	2.42	0.45
2:B:408:GLU:OE1	3:C:142:ASN:ND2	2.40	0.45
3:C:551:ARG:NH2	64:C:920:HOH:O	2.40	0.45
14:N:27:GLU:HG2	14:N:80:LYS:HG3	1.99	0.45
19:S:148:VAL:HG12	32:f:56:ARG:HB3	1.98	0.45
49:x:20:TRP:HH2	49:x:72:TYR:HA	1.81	0.45
23:W:135:ASP:OD1	23:W:135:ASP:N	2.48	0.45
32:f:57:GLU:OE1	39:m:96:ARG:NH2	2.44	0.45
45:t:228:ARG:NH1	60:u:603:CDL:OA4	2.43	0.45
5:E:334:TYR:CZ	5:E:338:LEU:HD11	2.51	0.45
20:T:8:ILE:HG13	61:T:502:PGT:H222	1.99	0.45
60:V:603:CDL:H341	60:V:603:CDL:H371	1.69	0.45
16:P:201:THR:HG21	16:P:254:LEU:HD22	1.98	0.45
18:R:309:TRP:CD1	20:T:164:PHE:HB3	2.51	0.45
20:T:442:MET:HE2	20:T:442:MET:HB3	1.82	0.45
34:h:125:GLN:HB2	34:h:132:ALA:HB3	1.97	0.45
4:D:221:ASP:N	4:D:221:ASP:OD1	2.48	0.45
21:U:178:ALA:HB2	21:U:186:GLY:HA3	1.98	0.45
22:V:164:LYS:NZ	24:X:57:PRO:O	2.50	0.45
60:h:203:CDL:H751	60:h:203:CDL:H782	1.56	0.45
40:n:40:ASP:OD1	40:n:40:ASP:N	2.50	0.45
41:o:118:ASP:OD1	41:o:118:ASP:N	2.49	0.45
11:K:88:LEU:HD13	16:P:389:VAL:HG21	1.98	0.45
8:H:82:VAL:HG11	9:I:146:ALA:HB1	1.98	0.44
60:W:701:CDL:H742	60:W:701:CDL:H771	1.66	0.44
15:O:19:CYS:O	15:O:29:ARG:NH1	2.50	0.44
22:V:1:MET:O	22:V:43:SER:OG	2.25	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:156:TRP:CG	37:k:92:ILE:HG23	2.52	0.44
39:m:112:MET:HE3	39:m:112:MET:HB3	1.94	0.44
44:s:73:LYS:HB2	44:s:76:VAL:HB	1.99	0.44
60:x:101:CDL:H131	60:x:101:CDL:H161	1.59	0.44
6:F:39:CYS:HB3	53:F:201:SF4:S3	2.58	0.44
17:Q:110:TYR:OH	23:W:59:VAL:O	2.32	0.44
28:b:59:LYS:HE3	28:b:59:LYS:HB2	1.77	0.44
3:C:198:CYS:O	3:C:203:ARG:NH2	2.49	0.44
3:C:264:LEU:HB3	3:C:283:ASP:HB3	1.99	0.44
12:L:33:LYS:HA	12:L:36:GLU:HG2	2.00	0.44
20:T:408:VAL:HG23	20:T:409:VAL:HG23	2.00	0.44
37:k:18:MET:HE3	37:k:66:GLY:HA3	2.00	0.44
10:r:48:ASP:OD1	10:r:51:SER:OG	2.29	0.44
10:J:66:ILE:HD11	10:J:81:LEU:HB3	1.99	0.44
18:R:330:SER:HA	18:R:333:TYR:CE2	2.53	0.44
19:S:227:ILE:HD13	23:W:151:ARG:HG3	2.00	0.44
18:R:309:TRP:HD1	20:T:164:PHE:HB3	1.83	0.44
20:T:200:ILE:HG23	20:T:288:MET:HB3	2.00	0.44
17:Q:89:ILE:HD11	17:Q:228:VAL:HG13	1.98	0.44
22:V:168:LYS:NZ	22:V:231:ASP:OD2	2.36	0.44
3:C:576:GLU:HA	3:C:593:ARG:HH21	1.83	0.44
6:F:29:SER:OG	17:Q:51:ASP:OD1	2.32	0.44
26:Z:16:TRP:HB3	28:b:51:VAL:HG11	2.00	0.44
45:t:144:VAL:HB	45:t:161:VAL:HG12	2.00	0.44
49:x:42:ALA:HA	60:x:101:CDL:H262	1.99	0.44
2:B:335:LEU:HD11	2:B:338:ILE:HG13	2.00	0.44
7:G:59:ASP:OD2	7:G:61:THR:OG1	2.32	0.44
14:N:112:PRO:HG2	14:N:115:GLN:HB2	2.00	0.44
2:B:439:GLN:OE1	3:C:171:ARG:NH2	2.51	0.43
20:T:70:ASP:OD1	20:T:238:ARG:NH2	2.46	0.43
59:V:602:3PH:H342	59:V:602:3PH:H242	2.00	0.43
60:W:701:CDL:H312	60:W:701:CDL:HB61	2.00	0.43
40:n:61:LYS:HB3	40:n:61:LYS:HE3	1.78	0.43
44:s:306:LEU:HD11	45:t:259:ARG:HB3	1.98	0.43
1:A:140:LYS:HB3	1:A:203:THR:HG22	2.00	0.43
2:B:71:ASP:OD2	2:B:73:SER:OG	2.35	0.43
3:C:68:VAL:HG13	3:C:121:ILE:HG12	1.99	0.43
3:C:113:MET:HE3	3:C:114:PRO:HD2	1.99	0.43
18:R:302:PHE:O	18:R:306:TRP:HE3	2.01	0.43
60:h:203:CDL:H712	60:h:203:CDL:H741	1.44	0.43
54:G:303:PTY:H441	39:m:57:MET:HE1	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:264:ARG:HB2	17:Q:267:GLN:HG3	1.98	0.43
18:R:226:SER:HB3	18:R:329:LEU:HD23	2.01	0.43
20:T:190:TRP:HE1	54:e:302:PTY:H121	1.83	0.43
26:Z:103:ARG:NH2	36:j:36:ASP:OD1	2.47	0.43
36:j:3:ASP:OD1	36:j:3:ASP:N	2.48	0.43
60:x:101:CDL:H751	60:x:101:CDL:H722	1.75	0.43
10:J:49:LYS:O	10:J:49:LYS:CG	2.67	0.43
20:T:7:LEU:HD23	20:T:36:PRO:HG3	1.99	0.43
61:b:601:PGT:H401	61:b:601:PGT:H432	1.80	0.43
45:t:142:TYR:HB3	45:t:159:ARG:HD2	2.00	0.43
3:C:150:CYS:O	3:C:260:ARG:NH1	2.49	0.43
3:C:279:ASN:HD22	3:C:295:ARG:NH2	2.17	0.43
12:L:79:LEU:O	12:L:82:THR:OG1	2.33	0.43
23:W:78:THR:HA	23:W:82:ALA:HB3	2.00	0.43
10:r:48:ASP:OD1	10:r:48:ASP:N	2.51	0.43
16:P:383:LYS:O	16:P:390:ARG:NH2	2.52	0.43
26:Z:99:PRO:HB2	26:Z:107:LEU:HD12	2.00	0.43
39:m:96:ARG:NE	40:n:6:VAL:O	2.52	0.43
3:C:417:LEU:HD11	3:C:447:VAL:HG23	2.00	0.43
17:Q:74:SER:OG	17:Q:111:GLY:O	2.32	0.43
5:E:283:THR:H	5:E:286:MET:HE2	1.83	0.43
10:J:86:LEU:HD12	11:K:62:LYS:HZ3	1.83	0.43
59:c:101:3PH:H2C1	59:c:101:3PH:H292	1.87	0.43
3:C:392:ASP:OD1	3:C:392:ASP:N	2.49	0.43
22:V:302:TYR:HE2	22:V:384:LYS:HD2	1.84	0.43
22:V:398:ILE:HD11	24:X:94:ALA:HB2	2.00	0.43
2:B:396:LYS:HD2	2:B:411:GLY:HA2	2.01	0.42
3:C:60:VAL:HG21	3:C:75:ALA:HB2	2.00	0.42
14:N:22:PHE:HZ	14:N:31:MET:HE1	1.84	0.42
17:Q:226:MET:HE3	17:Q:226:MET:HB3	1.84	0.42
54:S:302:PTY:H321	54:S:302:PTY:H171	2.01	0.42
28:b:99:ARG:HA	28:b:102:LYS:HE2	2.01	0.42
15:O:11:MET:HG3	15:O:46:PHE:HZ	1.84	0.42
7:G:59:ASP:HA	7:G:60:PRO:HD3	1.91	0.42
20:T:127:LEU:HD11	20:T:149:VAL:HA	2.01	0.42
7:G:85:VAL:HG13	17:Q:260:LEU:HD21	2.01	0.42
60:W:701:CDL:H411	60:W:701:CDL:H442	1.83	0.42
6:F:25:ALA:HA	17:Q:50:TRP:HB3	2.02	0.42
61:T:502:PGT:H331	61:T:502:PGT:H122	2.01	0.42
64:U:304:HOH:O	23:W:85:ARG:NH1	2.51	0.42
2:B:311:GLU:OE1	2:B:324:HIS:NE2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:136:VAL:HG11	9:I:132:LEU:HD23	2.01	0.42
16:P:38:MET:HG3	16:P:256:ARG:HA	2.02	0.42
18:R:32:ARG:NH1	18:R:63:PHE:O	2.53	0.42
18:R:302:PHE:CE2	18:R:373:PRO:HB3	2.55	0.42
60:W:701:CDL:H661	60:W:701:CDL:H631	1.64	0.42
46:u:205:ARG:O	46:u:208:GLU:HG2	2.19	0.42
11:K:106:TYR:O	11:K:110:ARG:HB3	2.19	0.42
24:X:133:ASP:OD1	24:X:133:ASP:N	2.51	0.42
60:x:101:CDL:H561	60:x:101:CDL:H591	1.81	0.42
2:B:123:MET:HG3	2:B:170:MET:HB3	2.00	0.42
3:C:130:LYS:HA	3:C:130:LYS:HD2	1.78	0.42
4:D:170:LEU:HB2	4:D:179:ILE:HG22	2.01	0.42
23:W:151:ARG:HA	23:W:154:ILE:HG22	2.01	0.42
46:u:83:TRP:CZ2	46:u:206:TYR:HD1	2.38	0.42
8:H:34:PRO:HD2	14:N:69:TYR:HE1	1.85	0.42
8:H:102:GLU:O	8:H:103:GLN:HG2	2.20	0.42
17:Q:3:VAL:HG13	19:S:176:ILE:HD11	2.02	0.42
10:r:61:LYS:HG2	10:r:71:VAL:HG21	2.01	0.42
1:A:263:GLU:O	2:B:305:ARG:NH2	2.53	0.42
16:P:239:ILE:HD11	16:P:278:VAL:HG21	2.02	0.42
17:Q:191:LYS:HE2	17:Q:191:LYS:HB2	1.89	0.42
20:T:405:PHE:CE1	20:T:409:VAL:HG21	2.55	0.42
22:V:223:ILE:HG22	22:V:270:VAL:HG13	2.00	0.42
31:e:65:ALA:HA	60:x:101:CDL:H202	2.02	0.42
2:B:472:LYS:HA	39:m:13:LYS:HD2	2.01	0.41
18:R:-1:ALA:HB1	42:p:64:LYS:HE3	2.01	0.41
18:R:302:PHE:HB3	18:R:306:TRP:CZ3	2.50	0.41
22:V:378:LEU:HD23	22:V:378:LEU:HA	1.91	0.41
11:K:48:VAL:HG11	11:K:102:VAL:HG21	2.03	0.41
14:N:111:GLN:OE1	14:N:115:GLN:NE2	2.49	0.41
16:P:34:SER:O	16:P:258:PRO:HB3	2.20	0.41
20:T:1:MET:HE3	20:T:60:LEU:HD11	2.01	0.41
20:T:76:LEU:HD12	20:T:234:ILE:HD12	2.01	0.41
22:V:8:PHE:CE2	22:V:36:CYS:HA	2.56	0.41
22:V:310:GLY:O	22:V:314:GLY:N	2.51	0.41
4:D:152:VAL:HB	4:D:204:PHE:HB3	2.03	0.41
20:T:260:LEU:HD22	20:T:389:VAL:HG11	2.01	0.41
3:C:379:LEU:HD11	3:C:644:VAL:HG11	2.01	0.41
14:N:42:LEU:O	14:N:46:THR:OG1	2.36	0.41
19:S:245:THR:HG21	23:W:126:GLY:HA3	2.02	0.41
20:T:224:LEU:HD23	20:T:228:LEU:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:458:GLU:OE1	3:C:480:ARG:NH1	2.53	0.41
18:R:127:LEU:HD11	21:U:156:LEU:HD22	2.02	0.41
18:R:197:LYS:HD3	18:R:247:ILE:HD13	2.02	0.41
31:e:200:ILE:HG23	35:i:31:MET:HE3	2.02	0.41
2:B:159:LEU:HD13	2:B:266:VAL:HG13	2.01	0.41
22:V:243:ILE:HG23	22:V:248:LEU:HD23	2.02	0.41
31:e:189:ASN:HA	41:o:9:GLN:HG3	2.03	0.41
45:t:83:ASP:HB2	45:t:104:ARG:HG2	2.03	0.41
17:Q:25:ARG:HD2	57:Q:301:UQ5:H1M1	2.03	0.41
22:V:515:PHE:O	22:V:519:PRO:HD2	2.21	0.41
31:e:155:LEU:HD23	31:e:155:LEU:HA	1.91	0.41
4:D:72:ARG:NH2	9:I:113:ASP:OD1	2.53	0.41
12:L:26:ASP:N	12:L:26:ASP:OD1	2.54	0.41
12:L:152:ARG:NH1	64:L:210:HOH:O	2.54	0.41
44:s:135:ARG:NH2	46:u:105:ASP:OD1	2.49	0.41
3:C:440:ASP:HB2	12:L:157:LYS:HB2	2.03	0.41
4:D:236:LEU:HD23	4:D:236:LEU:HA	1.91	0.41
5:E:112:ARG:NH1	5:E:114:ASP:OD2	2.54	0.41
8:H:85:LYS:NZ	9:I:143:ALA:O	2.38	0.41
14:N:9:ARG:NH1	14:N:47:GLY:O	2.54	0.41
60:R:405:CDL:H532	60:R:405:CDL:H111	2.03	0.41
54:S:302:PTY:H122	54:S:302:PTY:H152	1.78	0.41
20:T:407:ARG:NH2	64:T:615:HOH:O	2.53	0.41
22:V:237:THR:HG21	22:V:336:GLY:HA3	2.02	0.41
23:W:77:ALA:HB1	23:W:80:LEU:HB3	2.02	0.41
60:W:701:CDL:H552	60:W:701:CDL:H581	1.85	0.41
27:a:65:MET:HE2	27:a:65:MET:HB3	1.93	0.41
42:p:66:THR:HG23	42:p:71:TRP:HZ3	1.86	0.41
10:r:57:LEU:HD22	10:r:71:VAL:HG12	2.03	0.41
1:A:131:THR:HG23	3:C:219:ARG:HH12	1.86	0.41
15:O:11:MET:HE3	15:O:90:ILE:HD13	2.03	0.41
22:V:350:ARG:HE	22:V:350:ARG:HB3	1.72	0.41
10:r:126:MET:HE3	10:r:126:MET:HB3	1.89	0.41
60:u:602:CDL:H552	60:u:602:CDL:H521	1.92	0.41
20:T:108:LEU:HD23	20:T:108:LEU:HA	1.94	0.40
20:T:307:SER:HB2	58:T:503:PC7:H442	2.02	0.40
1:A:143:VAL:HG22	1:A:199:ILE:HG12	2.04	0.40
3:C:683:TYR:HA	15:O:36:TYR:HE2	1.85	0.40
17:Q:2:ILE:HD13	17:Q:2:ILE:HA	1.92	0.40
18:R:295:LEU:HD23	18:R:295:LEU:HA	1.85	0.40
32:f:57:GLU:CD	39:m:96:ARG:HH22	2.28	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:t:136:LYS:HE2	45:t:153:LYS:HG2	2.03	0.40
4:D:282:ARG:NE	12:L:26:ASP:OD2	2.46	0.40
16:P:364:PRO:HB3	19:S:198:LEU:HD11	2.03	0.40
18:R:103:VAL:HG21	18:R:126:LEU:HD13	2.03	0.40
20:T:210:PRO:HB3	20:T:282:TYR:HE1	1.86	0.40
30:d:28:ALA:HB2	45:t:228:ARG:HG2	2.03	0.40
33:g:11:ARG:NH1	64:g:202:HOH:O	2.54	0.40
5:E:192:THR:HB	5:E:204:PHE:HA	2.04	0.40
16:P:118:LYS:HG3	16:P:156:LEU:HD22	2.04	0.40
17:Q:93:ASP:OD2	32:f:40:LYS:NZ	2.42	0.40
21:U:152:PHE:HA	23:W:87:TRP:HB3	2.04	0.40
23:W:43:MET:HG2	39:m:141:LEU:HB2	2.02	0.40
3:C:370:VAL:HG23	3:C:373:MET:HE2	2.04	0.40
23:W:43:MET:HE3	39:m:142:VAL:HB	2.03	0.40
31:e:170:LEU:HD13	54:e:302:PTY:HC51	2.02	0.40
50:y:12:ARG:NH2	60:y:201:CDL:OB7	2.48	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	237/282 (84%)	228 (96%)	9 (4%)	0	100	100
2	B	433/484 (90%)	417 (96%)	16 (4%)	0	100	100
3	C	686/733 (94%)	667 (97%)	19 (3%)	0	100	100
4	D	214/282 (76%)	204 (95%)	10 (5%)	0	100	100
5	E	379/467 (81%)	368 (97%)	11 (3%)	0	100	100
6	F	155/164 (94%)	149 (96%)	6 (4%)	0	100	100
7	G	197/231 (85%)	189 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	H	88/118 (75%)	81 (92%)	7 (8%)	0	100	100
9	I	133/165 (81%)	130 (98%)	3 (2%)	0	100	100
10	J	82/128 (64%)	76 (93%)	6 (7%)	0	100	100
10	r	86/128 (67%)	84 (98%)	2 (2%)	0	100	100
11	K	117/138 (85%)	115 (98%)	2 (2%)	0	100	100
12	L	162/187 (87%)	155 (96%)	7 (4%)	0	100	100
13	M	119/154 (77%)	111 (93%)	8 (7%)	0	100	100
14	N	148/156 (95%)	145 (98%)	3 (2%)	0	100	100
15	O	98/101 (97%)	94 (96%)	4 (4%)	0	100	100
16	P	361/397 (91%)	350 (97%)	11 (3%)	0	100	100
17	Q	282/292 (97%)	274 (97%)	8 (3%)	0	100	100
18	R	385/387 (100%)	369 (96%)	16 (4%)	0	100	100
19	S	130/279 (47%)	128 (98%)	2 (2%)	0	100	100
20	T	441/443 (100%)	431 (98%)	10 (2%)	0	100	100
21	U	103/227 (45%)	102 (99%)	1 (1%)	0	100	100
22	V	544/546 (100%)	525 (96%)	18 (3%)	1 (0%)	43	63
23	W	155/162 (96%)	151 (97%)	4 (3%)	0	100	100
24	X	123/149 (83%)	117 (95%)	6 (5%)	0	100	100
25	Y	52/64 (81%)	52 (100%)	0	0	100	100
26	Z	105/124 (85%)	100 (95%)	5 (5%)	0	100	100
27	a	80/129 (62%)	78 (98%)	1 (1%)	1 (1%)	9	18
28	b	142/172 (83%)	139 (98%)	3 (2%)	0	100	100
29	c	55/67 (82%)	52 (94%)	3 (6%)	0	100	100
30	d	83/86 (96%)	82 (99%)	1 (1%)	0	100	100
31	e	216/219 (99%)	214 (99%)	1 (0%)	1 (0%)	24	43
32	f	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
33	g	48/55 (87%)	42 (88%)	6 (12%)	0	100	100
34	h	106/142 (75%)	97 (92%)	9 (8%)	0	100	100
35	i	74/81 (91%)	73 (99%)	1 (1%)	0	100	100
36	j	83/86 (96%)	80 (96%)	3 (4%)	0	100	100
37	k	115/117 (98%)	110 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	l	114/121 (94%)	110 (96%)	4 (4%)	0	100	100
39	m	134/142 (94%)	133 (99%)	1 (1%)	0	100	100
40	n	102/106 (96%)	100 (98%)	2 (2%)	0	100	100
41	o	150/155 (97%)	145 (97%)	5 (3%)	0	100	100
42	p	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
43	q	155/197 (79%)	149 (96%)	6 (4%)	0	100	100
44	s	310/312 (99%)	303 (98%)	7 (2%)	0	100	100
45	t	251/279 (90%)	243 (97%)	8 (3%)	0	100	100
46	u	226/229 (99%)	220 (97%)	6 (3%)	0	100	100
47	v	43/45 (96%)	43 (100%)	0	0	100	100
48	w	62/109 (57%)	61 (98%)	1 (2%)	0	100	100
49	x	81/157 (52%)	81 (100%)	0	0	100	100
50	y	112/118 (95%)	111 (99%)	1 (1%)	0	100	100
All	All	8946/10307 (87%)	8662 (97%)	281 (3%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
27	a	43	TYR
22	V	519	PRO
31	e	148	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	197/228 (86%)	197 (100%)	0	100	100
2	B	344/377 (91%)	344 (100%)	0	100	100
3	C	537/572 (94%)	537 (100%)	0	100	100
4	D	196/248 (79%)	196 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	329/388 (85%)	329 (100%)	0	100	100
6	F	129/133 (97%)	129 (100%)	0	100	100
7	G	172/198 (87%)	172 (100%)	0	100	100
8	H	82/105 (78%)	82 (100%)	0	100	100
9	I	111/134 (83%)	111 (100%)	0	100	100
10	J	71/108 (66%)	71 (100%)	0	100	100
10	r	72/108 (67%)	72 (100%)	0	100	100
11	K	106/122 (87%)	106 (100%)	0	100	100
12	L	130/148 (88%)	130 (100%)	0	100	100
13	M	100/121 (83%)	100 (100%)	0	100	100
14	N	128/132 (97%)	128 (100%)	0	100	100
15	O	80/81 (99%)	80 (100%)	0	100	100
16	P	305/327 (93%)	305 (100%)	0	100	100
17	Q	230/234 (98%)	230 (100%)	0	100	100
18	R	321/321 (100%)	321 (100%)	0	100	100
19	S	111/217 (51%)	111 (100%)	0	100	100
20	T	374/374 (100%)	374 (100%)	0	100	100
21	U	84/180 (47%)	84 (100%)	0	100	100
22	V	439/439 (100%)	439 (100%)	0	100	100
23	W	131/135 (97%)	131 (100%)	0	100	100
24	X	105/122 (86%)	105 (100%)	0	100	100
25	Y	38/46 (83%)	38 (100%)	0	100	100
26	Z	93/102 (91%)	93 (100%)	0	100	100
27	a	68/98 (69%)	68 (100%)	0	100	100
28	b	119/138 (86%)	119 (100%)	0	100	100
29	c	49/56 (88%)	49 (100%)	0	100	100
30	d	63/64 (98%)	63 (100%)	0	100	100
31	e	163/164 (99%)	163 (100%)	0	100	100
32	f	52/53 (98%)	52 (100%)	0	100	100
33	g	40/45 (89%)	40 (100%)	0	100	100
34	h	91/110 (83%)	91 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	i	65/67 (97%)	65 (100%)	0	100	100
36	j	72/73 (99%)	72 (100%)	0	100	100
37	k	102/102 (100%)	102 (100%)	0	100	100
38	l	94/99 (95%)	94 (100%)	0	100	100
39	m	118/122 (97%)	118 (100%)	0	100	100
40	n	92/94 (98%)	92 (100%)	0	100	100
41	o	130/132 (98%)	130 (100%)	0	100	100
42	p	109/110 (99%)	109 (100%)	0	100	100
43	q	135/165 (82%)	135 (100%)	0	100	100
44	s	243/243 (100%)	243 (100%)	0	100	100
45	t	212/233 (91%)	212 (100%)	0	100	100
46	u	180/181 (99%)	180 (100%)	0	100	100
47	v	38/38 (100%)	38 (100%)	0	100	100
48	w	55/91 (60%)	55 (100%)	0	100	100
49	x	70/130 (54%)	70 (100%)	0	100	100
50	y	102/106 (96%)	102 (100%)	0	100	100
All	All	7477/8414 (89%)	7477 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	ASN
1	A	110	ASN
1	A	142	HIS
2	B	100	GLN
2	B	241	GLN
2	B	402	GLN
2	B	462	HIS
3	C	279	ASN
3	C	297	ASN
3	C	708	ASN
4	D	92	GLN
4	D	274	ASN
5	E	153	HIS

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Mol	Chain	Res	Type
5	E	339	GLN
6	F	147	GLN
6	F	159	GLN
7	G	58	ASN
11	K	93	GLN
11	K	95	HIS
12	L	103	GLN
12	L	149	ASN
14	N	40	ASN
14	N	142	ASN
15	O	35	ASN
17	Q	47	GLN
17	Q	83	GLN
18	R	23	ASN
18	R	98	GLN
18	R	145	GLN
19	S	147	HIS
19	S	246	HIS
20	T	332	HIS
22	V	79	ASN
22	V	173	ASN
23	W	127	HIS
24	X	119	GLN
24	X	127	HIS
26	Z	54	ASN
31	e	89	GLN
34	h	66	ASN
37	k	34	HIS
38	l	41	ASN
39	m	65	HIS
39	m	90	GLN
39	m	100	HIS
40	n	12	HIS
40	n	29	HIS
40	n	76	GLN
41	o	21	ASN
41	o	150	GLN
43	q	92	ASN
44	s	221	ASN
45	t	257	ASN
46	u	45	HIS
46	u	102	ASN

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Mol	Chain	Res	Type
46	u	104	GLN
46	u	147	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 54 ligands modelled in this entry, 1 is monoatomic - leaving 53 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	$\# Z > 2$
54	PTY	T	506	-	25,25,49	0.65	0	28,30,54	0.48	0
59	3PH	V	602	-	40,40,47	0.67	1 (2%)	43,45,52	0.83	1 (2%)
59	3PH	c	101	-	47,47,47	0.63	1 (2%)	50,52,52	0.63	1 (2%)
54	PTY	T	501	-	49,49,49	0.46	0	52,54,54	0.63	1 (1%)
54	PTY	R	406	-	39,39,49	0.54	0	42,44,54	0.51	0
54	PTY	h	202	-	45,45,49	0.47	0	48,50,54	0.46	0
59	3PH	S	301	-	36,36,47	0.71	1 (2%)	39,41,52	0.71	1 (2%)
53	SF4	F	201	6	0,12,12	-	-	-	-	-
60	CDL	y	201	-	54,54,99	0.54	2 (3%)	60,66,111	0.32	0
53	SF4	G	302	7	0,12,12	-	-	-	-	-
54	PTY	V	605	-	49,49,49	0.46	0	52,54,54	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
53	SF4	C	803	3	0,12,12	-	-	-		
55	8Q1	J	200	-	32,34,34	1.61	6 (18%)	39,43,43	1.73	5 (12%)
54	PTY	V	606	-	34,34,49	0.57	0	37,39,54	0.44	0
60	CDL	x	101	-	91,91,99	0.40	1 (1%)	97,103,111	0.24	0
59	3PH	R	401	-	31,31,47	0.76	1 (3%)	34,36,52	0.73	2 (5%)
54	PTY	x	102	-	49,49,49	0.46	0	52,54,54	0.40	0
55	8Q1	r	200	-	32,34,34	1.68	5 (15%)	39,43,43	1.93	10 (25%)
58	PC7	T	503	-	51,51,51	0.50	0	57,59,59	0.59	0
54	PTY	R	402	-	33,33,49	0.54	0	36,38,54	0.44	0
60	CDL	V	603	-	63,63,99	0.41	1 (1%)	69,75,111	0.26	0
61	PGT	l	701	-	50,50,50	0.48	0	53,56,56	0.60	1 (1%)
58	PC7	Q	302	-	32,32,51	0.60	0	38,40,59	0.70	0
52	FMN	B	501	-	33,33,33	1.08	2 (6%)	48,50,50	1.26	8 (16%)
51	FES	C	801	3	0,4,4	-	-	-		
59	3PH	h	201	-	44,44,47	0.66	1 (2%)	47,49,52	3.86	5 (10%)
53	SF4	G	301	7	0,12,12	-	-	-		
54	PTY	R	404	-	43,43,49	0.51	0	46,48,54	0.47	0
62	COO	s	401	-	51,55,55	1.17	4 (7%)	73,81,81	3.87	16 (21%)
54	PTY	S	302	-	45,45,49	0.50	0	48,50,54	0.42	0
54	PTY	G	303	-	42,42,49	0.49	0	45,47,54	0.45	0
51	FES	A	301	1	0,4,4	-	-	-		
56	NDP	P	401	-	51,52,52	1.17	5 (9%)	71,80,80	1.53	8 (11%)
58	PC7	R	403	-	43,43,51	0.53	0	49,51,59	0.62	0
60	CDL	u	603	-	70,70,99	0.44	0	76,82,111	0.28	0
60	CDL	u	602	-	82,82,99	0.39	0	88,94,111	0.30	0
53	SF4	C	802	3	0,12,12	-	-	-		
54	PTY	e	302	-	42,42,49	0.53	0	45,47,54	0.43	0
59	3PH	g	101	-	36,36,47	0.72	1 (2%)	39,41,52	0.70	1 (2%)
61	PGT	b	601	-	43,43,50	0.53	0	46,49,56	0.52	0
54	PTY	e	301	-	24,24,49	0.65	0	27,29,54	0.53	0
60	CDL	h	203	-	76,76,99	0.37	0	82,88,111	0.26	0
61	PGT	T	505	-	39,39,50	0.54	0	42,45,56	0.51	0
53	SF4	B	502	2	0,12,12	-	-	-		
57	UQ5	Q	301	-	38,38,38	0.51	0	48,49,49	0.87	3 (6%)
61	PGT	T	502	-	47,47,50	0.53	0	50,53,56	0.57	1 (2%)
59	3PH	w	201	-	44,44,47	0.64	1 (2%)	47,49,52	0.76	3 (6%)
60	CDL	R	405	-	62,62,99	0.40	0	68,74,111	0.28	0
58	PC7	u	601	-	41,41,51	0.56	0	47,49,59	0.69	2 (4%)
60	CDL	W	701	-	94,94,99	0.36	0	100,106,111	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
54	PTY	V	604	-	39,39,49	0.54	0	42,44,54	0.50	0
59	3PH	V	601	-	41,41,47	0.67	1 (2%)	44,46,52	0.64	1 (2%)
54	PTY	T	504	-	27,27,49	0.66	0	30,32,54	0.48	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	PTY	T	506	-	-	15/29/29/53	-
59	3PH	V	602	-	-	17/42/42/49	-
59	3PH	c	101	-	-	13/49/49/49	-
54	PTY	T	501	-	-	19/53/53/53	-
54	PTY	R	406	-	-	14/43/43/53	-
54	PTY	h	202	-	-	19/49/49/53	-
59	3PH	S	301	-	-	13/38/38/49	-
60	CDL	y	201	-	-	29/65/65/110	-
53	SF4	F	201	6	-	-	0/6/5/5
53	SF4	G	302	7	-	-	0/6/5/5
54	PTY	V	605	-	-	25/53/53/53	-
53	SF4	C	803	3	-	-	0/6/5/5
55	8Q1	J	200	-	-	11/41/41/41	-
54	PTY	V	606	-	-	16/38/38/53	-
60	CDL	x	101	-	-	62/102/102/110	-
59	3PH	R	401	-	-	13/33/33/49	-
54	PTY	x	102	-	-	17/53/53/53	-
55	8Q1	r	200	-	-	19/41/41/41	-
58	PC7	T	503	-	-	21/55/55/55	-
54	PTY	R	402	-	-	11/37/37/53	-
60	CDL	V	603	-	-	40/74/74/110	-
61	PGT	l	701	-	-	26/55/55/55	-
58	PC7	Q	302	-	-	13/36/36/55	-
52	FMN	B	501	-	-	4/18/18/18	0/3/3/3
51	FES	C	801	3	-	-	0/1/1/1
59	3PH	h	201	-	-	19/46/46/49	-
53	SF4	G	301	7	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	PTY	R	404	-	-	21/47/47/53	-
62	COO	s	401	-	-	21/54/70/70	0/3/3/3
54	PTY	S	302	-	-	20/49/49/53	-
54	PTY	G	303	-	-	5/46/46/53	-
58	PC7	R	403	-	-	14/47/47/55	-
56	NDP	P	401	-	-	7/34/77/77	0/5/5/5
60	CDL	u	603	-	-	57/81/81/110	-
51	FES	A	301	1	-	-	0/1/1/1
60	CDL	u	602	-	-	50/93/93/110	-
54	PTY	e	302	-	-	21/46/46/53	-
53	SF4	C	802	3	-	-	0/6/5/5
59	3PH	g	101	-	-	10/38/38/49	-
61	PGT	b	601	-	-	26/48/48/55	-
54	PTY	e	301	-	-	8/28/28/53	-
60	CDL	h	203	-	-	57/87/87/110	-
61	PGT	T	505	-	-	18/44/44/55	-
53	SF4	B	502	2	-	-	0/6/5/5
57	UQ5	Q	301	-	-	5/33/57/57	0/1/1/1
61	PGT	T	502	-	-	20/52/52/55	-
59	3PH	w	201	-	-	21/46/46/49	-
60	CDL	R	405	-	-	41/73/73/110	-
58	PC7	u	601	-	-	15/45/45/55	-
60	CDL	W	701	-	-	62/105/105/110	-
54	PTY	V	604	-	-	15/43/43/53	-
59	3PH	V	601	-	-	18/43/43/49	-
54	PTY	T	504	-	-	10/31/31/53	-

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	r	200	8Q1	C34-N36	5.57	1.46	1.33
55	J	200	8Q1	C34-N36	5.10	1.45	1.33
55	r	200	8Q1	C39-N41	5.02	1.45	1.33
55	J	200	8Q1	C39-N41	4.92	1.45	1.33
62	s	401	COO	C5A-C4A	4.64	1.47	1.39
56	P	401	NDP	C5A-C4A	4.43	1.47	1.39
59	V	602	3PH	P-O11	3.42	1.71	1.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	h	201	3PH	P-O11	3.33	1.70	1.60
59	c	101	3PH	P-O11	3.32	1.70	1.60
59	V	601	3PH	P-O11	3.30	1.70	1.60
59	w	201	3PH	P-O11	3.29	1.70	1.60
59	R	401	3PH	P-O11	3.29	1.70	1.60
59	S	301	3PH	P-O11	3.27	1.70	1.60
52	B	501	FMN	C4A-N5	3.23	1.37	1.30
59	g	101	3PH	P-O11	3.22	1.70	1.60
62	s	401	COO	C5A-C6A	2.75	1.48	1.41
56	P	401	NDP	C5A-C6A	2.57	1.48	1.41
55	r	200	8Q1	C1-S44	2.57	1.82	1.76
56	P	401	NDP	C5A-N7A	-2.48	1.34	1.39
55	r	200	8Q1	C6-C1	2.44	1.53	1.50
55	r	200	8Q1	O40-C39	-2.44	1.18	1.23
55	J	200	8Q1	O40-C39	-2.41	1.18	1.23
62	s	401	COO	C8A-N7A	2.39	1.36	1.31
55	J	200	8Q1	C1-S44	2.32	1.81	1.76
55	J	200	8Q1	C6-C1	2.27	1.53	1.50
62	s	401	COO	C5A-N7A	-2.26	1.35	1.39
60	x	101	CDL	PB2-OB4	-2.22	1.45	1.55
56	P	401	NDP	C8A-N7A	2.17	1.35	1.31
52	B	501	FMN	C10-N1	2.15	1.37	1.33
56	P	401	NDP	C4A-N9A	-2.05	1.33	1.37
60	y	201	CDL	PB2-OB4	-2.04	1.45	1.55
55	J	200	8Q1	O35-C34	-2.04	1.19	1.23
60	y	201	CDL	PA1-OA4	-2.02	1.46	1.55
60	V	603	CDL	PA1-OA4	-2.01	1.46	1.55

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
62	s	401	COO	C15-C11-C12	-18.90	77.03	108.22
59	h	201	3PH	O31-C31-O32	-18.11	78.33	123.63
62	s	401	COO	C15-C11-C13	-16.99	79.80	108.77
62	s	401	COO	C15-C11-C14	-15.54	78.23	109.20
59	h	201	3PH	O31-C31-C32	14.79	156.94	111.83
59	h	201	3PH	O32-C31-C32	-11.55	78.63	123.78
55	J	200	8Q1	C6-C1-S44	6.54	121.19	113.40
56	P	401	NDP	C5A-C4A-N3A	-5.82	118.70	126.72
62	s	401	COO	C5A-C4A-N3A	-5.70	118.88	126.72
55	r	200	8Q1	C6-C1-S44	5.42	119.86	113.40
55	r	200	8Q1	C32-C34-N36	5.29	126.53	116.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
62	s	401	COO	C14-C11-C12	4.91	116.33	108.22
56	P	401	NDP	N3A-C4A-N9A	4.57	134.94	127.17
62	s	401	COO	N3A-C4A-N9A	4.41	134.67	127.17
62	s	401	COO	C14-C11-C13	4.15	115.84	108.77
55	J	200	8Q1	O4-C1-C6	-3.94	119.43	123.98
62	s	401	COO	C4A-C5A-N7A	-3.72	106.33	110.58
56	P	401	NDP	C2A-N3A-C4A	3.67	120.80	111.83
62	s	401	COO	C2A-N3A-C4A	3.64	120.72	111.83
56	P	401	NDP	C4A-C5A-N7A	-3.45	106.64	110.58
59	V	602	3PH	C2-O21-C21	3.44	126.03	117.80
55	r	200	8Q1	C37-C38-C39	-3.34	106.83	112.39
55	r	200	8Q1	O4-C1-C6	-3.31	120.16	123.98
52	B	501	FMN	C4-N3-C2	-3.24	119.88	125.64
56	P	401	NDP	N3A-C2A-N1A	-3.22	123.71	128.58
62	s	401	COO	N1A-C2A-N3A	-3.21	123.72	128.58
54	T	501	PTY	C6-O7-C8	3.14	125.32	117.80
55	r	200	8Q1	O35-C34-N36	-3.10	116.42	122.98
62	s	401	COO	C3X-C2X-C1X	2.95	106.37	99.89
52	B	501	FMN	C4A-C10-N10	2.81	120.51	116.48
62	s	401	COO	C4A-N9A-C8A	2.80	108.68	105.74
62	s	401	COO	C10-C9-C8	-2.80	119.65	125.28
55	r	200	8Q1	C43-S44-C1	2.79	110.08	101.84
62	s	401	COO	C5A-N7A-C8A	2.69	107.67	103.45
52	B	501	FMN	C4A-C4-N3	2.67	120.06	113.25
56	P	401	NDP	C4A-N9A-C8A	2.61	108.47	105.74
55	J	200	8Q1	O4-C1-S44	-2.60	119.38	122.68
57	Q	301	UQ5	C8-C7-C6	2.56	118.39	112.08
57	Q	301	UQ5	C12-C13-C14	2.56	133.47	127.62
56	P	401	NDP	C5A-N7A-C8A	2.51	107.39	103.45
55	r	200	8Q1	C38-C39-N41	2.49	120.87	116.34
59	w	201	3PH	C2-O21-C21	2.48	123.74	117.80
55	J	200	8Q1	C43-S44-C1	2.47	109.15	101.84
52	B	501	FMN	O4-C4-C4A	-2.45	120.07	126.53
59	w	201	3PH	O13-P-O11	-2.42	100.35	106.67
58	u	601	PC7	O3-C3-C2	2.39	115.29	108.40
55	J	200	8Q1	C38-C39-N41	2.30	120.53	116.34
52	B	501	FMN	C5A-C9A-N10	2.30	120.04	117.97
61	T	502	PGT	C3-C2-C1	2.29	117.11	111.78
52	B	501	FMN	C10-C4A-N5	-2.28	120.14	124.81
55	r	200	8Q1	C37-N36-C34	2.28	126.64	122.55
62	s	401	COO	C6A-C5A-N7A	2.25	136.43	132.09
61	l	701	PGT	C2-O2-C31	2.23	123.14	117.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	r	200	8Q1	C31-C29-C32	2.22	112.55	108.77
57	Q	301	UQ5	C12-C11-C9	2.21	120.50	113.19
62	s	401	COO	N9A-C8A-N7A	-2.17	110.85	113.94
59	c	101	3PH	O13-P-O11	-2.16	101.03	106.67
52	B	501	FMN	C9A-C5A-N5	-2.14	120.19	122.45
55	r	200	8Q1	O4-C1-S44	-2.13	119.98	122.68
59	h	201	3PH	O14-P-O13	2.13	115.77	107.80
59	g	101	3PH	O13-P-O11	-2.12	101.14	106.67
59	R	401	3PH	O13-P-O11	-2.11	101.17	106.67
59	S	301	3PH	O13-P-O11	-2.11	101.17	106.67
52	B	501	FMN	C4A-C10-N1	-2.09	119.47	124.59
59	h	201	3PH	O13-P-O11	-2.08	101.24	106.67
58	u	601	PC7	C3-C2-C1	2.06	116.59	111.78
56	P	401	NDP	C6N-N1N-C2N	2.06	121.52	119.32
59	V	601	3PH	O13-P-O11	-2.05	101.31	106.67
59	R	401	3PH	O14-P-O13	2.01	115.35	107.80
59	w	201	3PH	O14-P-O13	2.01	115.35	107.80

There are no chirality outliers.

All (978) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
52	B	501	FMN	C5'-O5'-P-O1P
52	B	501	FMN	C5'-O5'-P-O2P
52	B	501	FMN	C5'-O5'-P-O3P
54	G	303	PTY	C3-O11-P1-O13
54	R	402	PTY	C2-C3-O11-P1
54	R	402	PTY	C6-C5-O14-P1
54	R	402	PTY	C3-O11-P1-O12
54	R	402	PTY	C3-O11-P1-O14
54	R	402	PTY	C5-O14-P1-O11
54	R	404	PTY	C11-C8-O7-C6
54	R	404	PTY	C5-O14-P1-O11
54	R	404	PTY	C5-O14-P1-O12
54	R	406	PTY	O14-C5-C6-O7
54	R	406	PTY	C11-C8-O7-C6
54	R	406	PTY	C5-O14-P1-O11
54	R	406	PTY	C5-O14-P1-O12
54	S	302	PTY	C3-O11-P1-O12
54	S	302	PTY	C3-O11-P1-O14
54	S	302	PTY	C5-O14-P1-O13
54	T	501	PTY	N1-C2-C3-O11

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Mol	Chain	Res	Type	Atoms
54	T	501	PTY	C3-O11-P1-O12
54	T	501	PTY	C3-O11-P1-O14
54	T	501	PTY	C5-O14-P1-O11
54	T	501	PTY	C5-O14-P1-O12
54	T	504	PTY	N1-C2-C3-O11
54	T	504	PTY	C5-O14-P1-O11
54	T	504	PTY	C5-O14-P1-O12
54	T	506	PTY	C3-O11-P1-O14
54	T	506	PTY	C5-O14-P1-O12
54	V	604	PTY	N1-C2-C3-O11
54	V	604	PTY	C3-O11-P1-O12
54	V	604	PTY	C3-O11-P1-O13
54	V	604	PTY	C3-O11-P1-O14
54	V	604	PTY	C5-O14-P1-O11
54	V	605	PTY	N1-C2-C3-O11
54	V	605	PTY	C3-O11-P1-O13
54	V	605	PTY	C3-O11-P1-O14
54	V	605	PTY	C5-O14-P1-O11
54	V	605	PTY	C5-O14-P1-O12
54	e	301	PTY	N1-C2-C3-O11
54	e	301	PTY	C3-O11-P1-O13
54	e	301	PTY	C3-O11-P1-O14
54	e	302	PTY	O14-C5-C6-O7
54	e	302	PTY	O10-C8-O7-C6
54	e	302	PTY	C11-C8-O7-C6
54	e	302	PTY	C5-O14-P1-O11
54	e	302	PTY	C5-O14-P1-O12
54	h	202	PTY	O10-C8-O7-C6
54	h	202	PTY	C3-O11-P1-O12
54	h	202	PTY	C3-O11-P1-O14
54	h	202	PTY	C5-O14-P1-O11
54	h	202	PTY	C5-O14-P1-O12
54	x	102	PTY	O10-C8-O7-C6
54	x	102	PTY	C3-O11-P1-O13
55	J	200	8Q1	C1-C6-C7-C8
55	J	200	8Q1	O27-C28-C29-C30
55	J	200	8Q1	O27-C28-C29-C31
55	J	200	8Q1	O27-C28-C29-C32
55	r	200	8Q1	C1-C6-C7-C8
55	r	200	8Q1	O4-C1-S44-C43
55	r	200	8Q1	C6-C1-S44-C43
55	r	200	8Q1	C28-C29-C32-C34

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Mol	Chain	Res	Type	Atoms
55	r	200	8Q1	C28-C29-C32-O33
55	r	200	8Q1	C30-C29-C32-C34
55	r	200	8Q1	C30-C29-C32-O33
55	r	200	8Q1	C31-C29-C32-C34
55	r	200	8Q1	C31-C29-C32-O33
55	r	200	8Q1	O33-C32-C34-N36
55	r	200	8Q1	C32-C34-N36-C37
55	r	200	8Q1	C28-O27-P24-O1
56	P	401	NDP	C5B-O5B-PA-O1A
56	P	401	NDP	C5D-O5D-PN-O3
56	P	401	NDP	C5D-O5D-PN-O1N
56	P	401	NDP	C5D-O5D-PN-O2N
58	Q	302	PC7	C4-O4P-P-O3P
58	Q	302	PC7	C4-O4P-P-O1P
58	Q	302	PC7	C4-O4P-P-O2P
58	R	403	PC7	C1-O3P-P-O1P
58	R	403	PC7	C1-O3P-P-O2P
58	R	403	PC7	C1-O3P-P-O4P
58	R	403	PC7	O4P-C4-C5-N
58	T	503	PC7	C32-C31-O2-C2
58	T	503	PC7	C4-O4P-P-O2P
58	T	503	PC7	O4P-C4-C5-N
58	u	601	PC7	C32-C31-O2-C2
58	u	601	PC7	C4-O4P-P-O3P
58	u	601	PC7	C4-O4P-P-O1P
59	R	401	3PH	C1-O11-P-O13
59	R	401	3PH	C1-O11-P-O14
59	S	301	3PH	C1-O11-P-O13
59	S	301	3PH	C1-O11-P-O14
59	S	301	3PH	C1-O11-P-O12
59	V	601	3PH	C1-O11-P-O13
59	V	601	3PH	C1-O11-P-O14
59	V	601	3PH	O22-C21-O21-C2
59	V	601	3PH	C22-C21-O21-C2
59	V	602	3PH	C1-O11-P-O13
59	V	602	3PH	C1-O11-P-O14
59	V	602	3PH	C1-O11-P-O12
59	V	602	3PH	C22-C21-O21-C2
59	c	101	3PH	C1-O11-P-O13
59	c	101	3PH	C1-O11-P-O14
59	c	101	3PH	C1-O11-P-O12
59	h	201	3PH	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
59	h	201	3PH	C1-O11-P-O14
59	h	201	3PH	O11-C1-C2-O21
59	h	201	3PH	C22-C21-O21-C2
60	R	405	CDL	CA2-OA2-PA1-OA3
60	R	405	CDL	CA2-OA2-PA1-OA4
60	R	405	CDL	CA2-OA2-PA1-OA5
60	R	405	CDL	CA3-OA5-PA1-OA2
60	R	405	CDL	CA3-OA5-PA1-OA3
60	R	405	CDL	CA3-OA5-PA1-OA4
60	R	405	CDL	CB2-OB2-PB2-OB3
60	R	405	CDL	CB2-OB2-PB2-OB4
60	R	405	CDL	CB2-OB2-PB2-OB5
60	R	405	CDL	CB3-OB5-PB2-OB3
60	R	405	CDL	OB5-CB3-CB4-OB6
60	R	405	CDL	C51-CB5-OB6-CB4
60	V	603	CDL	CA2-OA2-PA1-OA3
60	V	603	CDL	CA3-OA5-PA1-OA3
60	V	603	CDL	C11-CA5-OA6-CA4
60	V	603	CDL	CB2-OB2-PB2-OB4
60	V	603	CDL	CB2-OB2-PB2-OB5
60	V	603	CDL	CB3-OB5-PB2-OB3
60	V	603	CDL	CB3-OB5-PB2-OB4
60	W	701	CDL	CA2-OA2-PA1-OA3
60	W	701	CDL	CA2-OA2-PA1-OA5
60	W	701	CDL	CA3-OA5-PA1-OA2
60	W	701	CDL	CA3-OA5-PA1-OA3
60	W	701	CDL	CA3-OA5-PA1-OA4
60	W	701	CDL	OA7-CA5-OA6-CA4
60	W	701	CDL	C11-CA5-OA6-CA4
60	W	701	CDL	CB3-OB5-PB2-OB2
60	h	203	CDL	CA2-C1-CB2-OB2
60	h	203	CDL	CA2-OA2-PA1-OA3
60	h	203	CDL	CA2-OA2-PA1-OA4
60	h	203	CDL	CA2-OA2-PA1-OA5
60	h	203	CDL	CA3-OA5-PA1-OA2
60	h	203	CDL	CA3-OA5-PA1-OA3
60	h	203	CDL	CA3-OA5-PA1-OA4
60	h	203	CDL	CB2-OB2-PB2-OB3
60	h	203	CDL	CB2-OB2-PB2-OB5
60	h	203	CDL	CB3-OB5-PB2-OB3
60	u	602	CDL	CA2-C1-CB2-OB2
60	u	602	CDL	CA2-OA2-PA1-OA3

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Mol	Chain	Res	Type	Atoms
60	u	602	CDL	CA2-OA2-PA1-OA4
60	u	602	CDL	CA2-OA2-PA1-OA5
60	u	602	CDL	CA3-OA5-PA1-OA2
60	u	602	CDL	CA3-OA5-PA1-OA3
60	u	602	CDL	CA3-OA5-PA1-OA4
60	u	602	CDL	C51-CB5-OB6-CB4
60	u	603	CDL	O1-C1-CB2-OB2
60	u	603	CDL	CA2-OA2-PA1-OA4
60	u	603	CDL	CA2-OA2-PA1-OA5
60	u	603	CDL	CA3-OA5-PA1-OA3
60	u	603	CDL	CB2-OB2-PB2-OB4
60	u	603	CDL	CB3-OB5-PB2-OB2
60	u	603	CDL	CB3-OB5-PB2-OB3
60	x	101	CDL	CA3-OA5-PA1-OA2
60	x	101	CDL	CA3-OA5-PA1-OA4
60	x	101	CDL	CB2-OB2-PB2-OB3
60	y	201	CDL	O1-C1-CB2-OB2
60	y	201	CDL	CA2-C1-CB2-OB2
60	y	201	CDL	CA3-OA5-PA1-OA2
60	y	201	CDL	CA3-OA5-PA1-OA3
60	y	201	CDL	CA3-OA5-PA1-OA4
61	T	502	PGT	C4-O4P-P-O3P
61	T	502	PGT	C4-O4P-P-O1P
61	T	505	PGT	C1-O3P-P-O2P
61	b	601	PGT	C2-C1-O3P-P
61	b	601	PGT	C1-O3P-P-O2P
61	b	601	PGT	C1-O3P-P-O4P
61	b	601	PGT	C4-O4P-P-O1P
61	l	701	PGT	O3P-C1-C2-O2
61	l	701	PGT	C4-O4P-P-O3P
61	l	701	PGT	C4-O4P-P-O1P
62	s	401	COO	C14-C11-C13-O1
62	s	401	COO	C12-C11-C13-O1
62	s	401	COO	C14-C11-C13-C1
62	s	401	COO	C12-C11-C13-C1
62	s	401	COO	C13-C11-C12-O6A
62	s	401	COO	C15-C11-C12-O6A
62	s	401	COO	C13-C1-N1-C2
62	s	401	COO	O2-C1-N1-C2
62	s	401	COO	C3-C4-N2-C5
62	s	401	COO	O3-C4-N2-C5
62	s	401	COO	O4-C7-S1-C6

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Mol	Chain	Res	Type	Atoms
62	s	401	COO	C8-C7-S1-C6
62	s	401	COO	S1-C7-C8-C9
54	R	404	PTY	O30-C30-O4-C1
54	V	606	PTY	O30-C30-O4-C1
59	g	101	3PH	O32-C31-O31-C3
60	V	603	CDL	OB9-CB7-OB8-CB6
60	W	701	CDL	OB9-CB7-OB8-CB6
60	u	602	CDL	OA9-CA7-OA8-CA6
61	l	701	PGT	O11-C11-O3-C3
54	R	404	PTY	C31-C30-O4-C1
54	V	606	PTY	C31-C30-O4-C1
60	V	603	CDL	C71-CB7-OB8-CB6
60	u	602	CDL	C31-CA7-OA8-CA6
61	b	601	PGT	C12-C11-O3-C3
54	h	202	PTY	O30-C30-O4-C1
59	h	201	3PH	O32-C31-O31-C3
61	b	601	PGT	O11-C11-O3-C3
54	R	404	PTY	O10-C8-O7-C6
54	R	406	PTY	O10-C8-O7-C6
58	T	503	PC7	O31-C31-O2-C2
58	u	601	PC7	O31-C31-O2-C2
59	V	602	3PH	O22-C21-O21-C2
60	R	405	CDL	OB7-CB5-OB6-CB4
60	V	603	CDL	OA7-CA5-OA6-CA4
60	W	701	CDL	OB7-CB5-OB6-CB4
60	u	602	CDL	OB7-CB5-OB6-CB4
59	g	101	3PH	C32-C31-O31-C3
60	W	701	CDL	C71-CB7-OB8-CB6
61	T	505	PGT	C12-C11-O3-C3
61	l	701	PGT	C12-C11-O3-C3
54	h	202	PTY	C11-C8-O7-C6
54	x	102	PTY	C11-C8-O7-C6
54	h	202	PTY	C31-C30-O4-C1
59	h	201	3PH	C32-C31-O31-C3
54	e	302	PTY	O30-C30-O4-C1
58	R	403	PC7	O11-C11-O3-C3
61	T	505	PGT	O11-C11-O3-C3
59	h	201	3PH	O22-C21-O21-C2
60	R	405	CDL	O1-C1-CA2-OA2
60	h	203	CDL	O1-C1-CB2-OB2
60	u	602	CDL	O1-C1-CB2-OB2
60	x	101	CDL	O1-C1-CB2-OB2

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Mol	Chain	Res	Type	Atoms
60	y	201	CDL	O1-C1-CA2-OA2
61	b	601	PGT	O4P-C4-C5-O5
54	e	301	PTY	C31-C30-O4-C1
54	e	302	PTY	C31-C30-O4-C1
60	u	603	CDL	C31-CA7-OA8-CA6
61	T	502	PGT	C12-C11-O3-C3
55	r	200	8Q1	O35-C34-N36-C37
54	T	501	PTY	C11-C8-O7-C6
60	W	701	CDL	C51-CB5-OB6-CB4
61	T	502	PGT	O11-C11-O3-C3
58	R	403	PC7	C12-C11-O3-C3
60	u	603	CDL	OA9-CA7-OA8-CA6
54	T	501	PTY	O10-C8-O7-C6
57	Q	301	UQ5	C19-C21-C22-C23
60	h	203	CDL	C71-C72-C73-C74
54	e	301	PTY	O30-C30-O4-C1
60	R	405	CDL	C71-CB7-OB8-CB6
59	S	301	3PH	C22-C21-O21-C2
60	R	405	CDL	OB9-CB7-OB8-CB6
60	W	701	CDL	CA2-C1-CB2-OB2
60	u	603	CDL	CA2-C1-CB2-OB2
60	y	201	CDL	CB2-C1-CA2-OA2
59	R	401	3PH	C32-C31-O31-C3
60	x	101	CDL	C31-CA7-OA8-CA6
60	h	203	CDL	C75-C76-C77-C78
60	x	101	CDL	C72-C73-C74-C75
58	Q	302	PC7	C4-C5-N-C7
60	u	603	CDL	C13-C14-C15-C16
60	h	203	CDL	CB7-C71-C72-C73
59	h	201	3PH	C3B-C3C-C3D-C3E
61	T	502	PGT	C17-C18-C19-C20
59	R	401	3PH	O32-C31-O31-C3
60	W	701	CDL	C63-C64-C65-C66
58	T	503	PC7	O2-C2-C3-O3
60	u	603	CDL	OB6-CB4-CB6-OB8
60	y	201	CDL	OA6-CA4-CA6-OA8
61	b	601	PGT	O5-C5-C6-O6
59	S	301	3PH	C21-C22-C23-C24
54	S	302	PTY	C30-C31-C32-C33
60	h	203	CDL	CA7-C31-C32-C33
61	l	701	PGT	C31-C32-C33-C34
58	Q	302	PC7	C4-C5-N-C8

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Mol	Chain	Res	Type	Atoms
60	h	203	CDL	C12-C13-C14-C15
54	R	404	PTY	C30-C31-C32-C33
54	x	102	PTY	C8-C11-C12-C13
60	V	603	CDL	CB7-C71-C72-C73
60	u	602	CDL	CB7-C71-C72-C73
60	y	201	CDL	CB7-C71-C72-C73
59	R	401	3PH	C22-C21-O21-C2
58	T	503	PC7	C11-C12-C13-C14
58	u	601	PC7	C31-C32-C33-C34
60	R	405	CDL	CA7-C31-C32-C33
60	R	405	CDL	CB7-C71-C72-C73
60	x	101	CDL	CB5-C51-C52-C53
60	x	101	CDL	OA9-CA7-OA8-CA6
60	u	603	CDL	C39-C40-C41-C42
60	h	203	CDL	C15-C16-C17-C18
60	W	701	CDL	O1-C1-CB2-OB2
61	T	505	PGT	O4P-C4-C5-O5
54	V	605	PTY	C30-C31-C32-C33
59	c	101	3PH	C31-C32-C33-C34
60	u	603	CDL	CB7-C71-C72-C73
59	S	301	3PH	O22-C21-O21-C2
60	V	603	CDL	CA7-C31-C32-C33
60	W	701	CDL	CB5-C51-C52-C53
54	V	605	PTY	C13-C14-C15-C16
60	u	603	CDL	C11-CA5-OA6-CA4
60	u	603	CDL	CA7-C31-C32-C33
59	R	401	3PH	O22-C21-O21-C2
60	u	603	CDL	OA7-CA5-OA6-CA4
60	x	101	CDL	CA2-C1-CB2-OB2
61	T	505	PGT	O4P-C4-C5-C6
59	w	201	3PH	C32-C31-O31-C3
60	W	701	CDL	C74-C75-C76-C77
60	x	101	CDL	C13-C14-C15-C16
59	w	201	3PH	C21-C22-C23-C24
54	V	605	PTY	C11-C8-O7-C6
61	T	505	PGT	C32-C31-O2-C2
54	V	605	PTY	C19-C20-C21-C22
61	T	502	PGT	C4-C5-C6-O6
61	b	601	PGT	C4-C5-C6-O6
60	W	701	CDL	C18-C19-C20-C21
61	l	701	PGT	C32-C31-O2-C2
59	w	201	3PH	O32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
54	S	302	PTY	C11-C12-C13-C14
59	V	602	3PH	C26-C27-C28-C29
61	T	502	PGT	C14-C15-C16-C17
60	h	203	CDL	C19-C20-C21-C22
60	u	602	CDL	C36-C37-C38-C39
60	u	603	CDL	C14-C15-C16-C17
60	u	603	CDL	C20-C21-C22-C23
60	u	603	CDL	C33-C34-C35-C36
60	x	101	CDL	C77-C78-C79-C80
54	e	302	PTY	C34-C35-C36-C37
60	W	701	CDL	C83-C84-C85-C86
60	h	203	CDL	C11-C12-C13-C14
60	u	603	CDL	C36-C37-C38-C39
61	b	601	PGT	C37-C38-C39-C40
54	V	605	PTY	C32-C33-C34-C35
54	V	606	PTY	C13-C14-C15-C16
58	T	503	PC7	C32-C33-C34-C35
60	W	701	CDL	C61-C62-C63-C64
60	u	603	CDL	C31-C32-C33-C34
61	l	701	PGT	C39-C40-C41-C42
54	V	605	PTY	O10-C8-O7-C6
61	T	505	PGT	O31-C31-O2-C2
61	l	701	PGT	O31-C31-O2-C2
54	T	501	PTY	C37-C38-C39-C40
59	g	101	3PH	C3E-C3F-C3G-C3H
60	R	405	CDL	C72-C73-C74-C75
60	W	701	CDL	C77-C78-C79-C80
60	x	101	CDL	C23-C24-C25-C26
62	s	401	COO	N2-C5-C6-S1
61	b	601	PGT	C36-C37-C38-C39
59	V	601	3PH	C2C-C2D-C2E-C2F
60	h	203	CDL	C11-CA5-OA6-CA4
60	h	203	CDL	C51-CB5-OB6-CB4
60	W	701	CDL	C72-C73-C74-C75
60	u	603	CDL	C12-C13-C14-C15
54	R	402	PTY	C8-C11-C12-C13
54	e	302	PTY	C30-C31-C32-C33
60	u	603	CDL	CA5-C11-C12-C13
60	W	701	CDL	C59-C60-C61-C62
60	h	203	CDL	C72-C73-C74-C75
60	y	201	CDL	C72-C73-C74-C75
60	W	701	CDL	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
60	W	701	CDL	C51-C52-C53-C54
60	u	602	CDL	C63-C64-C65-C66
55	r	200	8Q1	C12-C13-C14-C15
59	h	201	3PH	C2A-C2B-C2C-C2D
54	S	302	PTY	C33-C34-C35-C36
58	T	503	PC7	C13-C14-C15-C16
60	R	405	CDL	C11-C12-C13-C14
60	u	603	CDL	C40-C41-C42-C43
59	g	101	3PH	C21-C22-C23-C24
54	x	102	PTY	C16-C17-C18-C19
58	T	503	PC7	C33-C34-C35-C36
59	S	301	3PH	C37-C38-C39-C3A
60	u	602	CDL	C57-C58-C59-C60
60	x	101	CDL	C62-C63-C64-C65
60	x	101	CDL	C63-C64-C65-C66
54	e	302	PTY	C13-C14-C15-C16
59	c	101	3PH	C35-C36-C37-C38
60	W	701	CDL	C35-C36-C37-C38
60	u	603	CDL	C16-C17-C18-C19
54	R	404	PTY	C25-C26-C27-C28
60	h	203	CDL	C31-C32-C33-C34
60	u	602	CDL	C62-C63-C64-C65
60	x	101	CDL	C11-C12-C13-C14
54	V	605	PTY	C33-C34-C35-C36
54	T	504	PTY	C11-C8-O7-C6
60	u	603	CDL	C71-CB7-OB8-CB6
60	R	405	CDL	C75-C76-C77-C78
60	u	603	CDL	C71-C72-C73-C74
60	u	602	CDL	C16-C17-C18-C19
58	Q	302	PC7	C11-C12-C13-C14
58	T	503	PC7	C39-C40-C41-C42
59	g	101	3PH	C37-C38-C39-C3A
60	x	101	CDL	C57-C58-C59-C60
61	b	601	PGT	C17-C18-C19-C20
54	T	504	PTY	C32-C33-C34-C35
60	x	101	CDL	C79-C80-C81-C82
59	w	201	3PH	O22-C21-O21-C2
60	h	203	CDL	OA7-CA5-OA6-CA4
60	h	203	CDL	OB7-CB5-OB6-CB4
59	V	602	3PH	C2B-C2C-C2D-C2E
60	u	603	CDL	C38-C39-C40-C41
60	x	101	CDL	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
60	W	701	CDL	C32-C33-C34-C35
60	h	203	CDL	C20-C21-C22-C23
60	h	203	CDL	C73-C74-C75-C76
60	u	603	CDL	C42-C43-C44-C45
54	x	102	PTY	C22-C23-C24-C25
58	Q	302	PC7	C12-C13-C14-C15
58	T	503	PC7	C17-C18-C19-C20
60	V	603	CDL	C34-C35-C36-C37
60	x	101	CDL	C21-C22-C23-C24
61	T	505	PGT	C19-C20-C21-C22
60	h	203	CDL	C57-C58-C59-C60
61	T	505	PGT	C32-C33-C34-C35
59	c	101	3PH	C33-C34-C35-C36
60	x	101	CDL	C15-C16-C17-C18
55	r	200	8Q1	C11-C10-C9-C8
58	T	503	PC7	C40-C41-C42-C43
60	V	603	CDL	C71-C72-C73-C74
61	b	601	PGT	C16-C17-C18-C19
54	R	406	PTY	C14-C15-C16-C17
58	Q	302	PC7	C32-C31-O2-C2
59	w	201	3PH	C22-C21-O21-C2
60	R	405	CDL	C11-CA5-OA6-CA4
60	u	602	CDL	C11-CA5-OA6-CA4
60	y	201	CDL	C51-CB5-OB6-CB4
54	T	501	PTY	C6-C1-O4-C30
60	y	201	CDL	OB7-CB5-OB6-CB4
60	x	101	CDL	C80-C81-C82-C83
61	l	701	PGT	C11-C12-C13-C14
54	S	302	PTY	C37-C38-C39-C40
61	T	502	PGT	C16-C17-C18-C19
60	W	701	CDL	C11-C12-C13-C14
59	w	201	3PH	C38-C39-C3A-C3B
61	b	601	PGT	C32-C33-C34-C35
58	Q	302	PC7	C4-C5-N-C6
60	W	701	CDL	C76-C77-C78-C79
60	h	203	CDL	C32-C33-C34-C35
61	T	505	PGT	C15-C16-C17-C18
54	R	404	PTY	C24-C25-C26-C27
60	h	203	CDL	C80-C81-C82-C83
60	W	701	CDL	C14-C15-C16-C17
58	Q	302	PC7	O31-C31-O2-C2
60	V	603	CDL	C51-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
54	T	506	PTY	C12-C13-C14-C15
60	V	603	CDL	C11-C12-C13-C14
54	T	501	PTY	C19-C20-C21-C22
60	V	603	CDL	C13-C14-C15-C16
58	T	503	PC7	C38-C39-C40-C41
58	T	503	PC7	C15-C16-C17-C18
54	R	402	PTY	O4-C1-C6-O7
54	T	506	PTY	O4-C1-C6-O7
60	u	602	CDL	C13-C14-C15-C16
60	x	101	CDL	C54-C55-C56-C57
60	x	101	CDL	C71-CB7-OB8-CB6
55	J	200	8Q1	C10-C11-C12-C13
60	W	701	CDL	C17-C18-C19-C20
60	W	701	CDL	C80-C81-C82-C83
60	u	602	CDL	C33-C34-C35-C36
61	T	505	PGT	C18-C19-C20-C21
61	l	701	PGT	C40-C41-C42-C43
54	V	605	PTY	C6-C5-O14-P1
60	h	203	CDL	CB4-CB3-OB5-PB2
60	W	701	CDL	CB2-C1-CA2-OA2
54	V	604	PTY	C34-C35-C36-C37
60	u	603	CDL	C34-C35-C36-C37
59	V	602	3PH	C2A-C2B-C2C-C2D
62	s	401	COO	O4-C7-C8-C9
59	R	401	3PH	C36-C37-C38-C39
60	R	405	CDL	C32-C33-C34-C35
60	u	603	CDL	OB9-CB7-OB8-CB6
60	W	701	CDL	C62-C63-C64-C65
60	u	602	CDL	C54-C55-C56-C57
55	r	200	8Q1	O33-C32-C34-O35
60	V	603	CDL	C33-C34-C35-C36
59	h	201	3PH	C33-C34-C35-C36
60	W	701	CDL	C81-C82-C83-C84
58	T	503	PC7	C44-C45-C46-C47
59	V	601	3PH	O11-C1-C2-C3
59	c	101	3PH	O11-C1-C2-C3
59	h	201	3PH	O11-C1-C2-C3
61	l	701	PGT	O3P-C1-C2-C3
54	T	504	PTY	O10-C8-O7-C6
54	x	102	PTY	C20-C21-C22-C23
54	T	504	PTY	C30-C31-C32-C33
60	h	203	CDL	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
61	T	502	PGT	C36-C37-C38-C39
54	T	506	PTY	C31-C30-O4-C1
54	T	501	PTY	C21-C22-C23-C24
60	x	101	CDL	C12-C13-C14-C15
59	V	602	3PH	C34-C35-C36-C37
54	R	404	PTY	O4-C1-C6-C5
60	h	203	CDL	CB3-CB4-CB6-OB8
60	u	603	CDL	CB3-CB4-CB6-OB8
60	x	101	CDL	CA3-CA4-CA6-OA8
60	y	201	CDL	CA3-CA4-CA6-OA8
58	T	503	PC7	C42-C43-C44-C45
59	w	201	3PH	C2A-C2B-C2C-C2D
60	x	101	CDL	C74-C75-C76-C77
54	R	404	PTY	C33-C34-C35-C36
60	V	603	CDL	C21-C22-C23-C24
60	x	101	CDL	C83-C84-C85-C86
54	T	501	PTY	C31-C30-O4-C1
58	u	601	PC7	C39-C40-C41-C42
61	l	701	PGT	C41-C42-C43-C44
59	h	201	3PH	C36-C37-C38-C39
60	x	101	CDL	C55-C56-C57-C58
60	u	602	CDL	C11-C12-C13-C14
60	x	101	CDL	C19-C20-C21-C22
58	R	403	PC7	C2-C1-O3P-P
60	u	602	CDL	OA7-CA5-OA6-CA4
59	h	201	3PH	C1-O11-P-O12
54	R	404	PTY	C16-C17-C18-C19
61	l	701	PGT	C4-C5-C6-O6
60	x	101	CDL	OB9-CB7-OB8-CB6
60	x	101	CDL	C51-C52-C53-C54
60	W	701	CDL	CB6-CB4-OB6-CB5
54	V	605	PTY	C35-C36-C37-C38
60	x	101	CDL	C60-C61-C62-C63
60	u	603	CDL	C15-C16-C17-C18
60	x	101	CDL	CB7-C71-C72-C73
58	T	503	PC7	C45-C46-C47-C48
54	S	302	PTY	O14-C5-C6-O7
60	W	701	CDL	C31-CA7-OA8-CA6
60	u	602	CDL	C18-C19-C20-C21
54	e	302	PTY	C31-C32-C33-C34
54	S	302	PTY	O4-C1-C6-O7
54	R	402	PTY	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
60	u	602	CDL	C71-CB7-OB8-CB6
60	R	405	CDL	C12-C13-C14-C15
60	R	405	CDL	C77-C78-C79-C80
60	V	603	CDL	C32-C33-C34-C35
60	h	203	CDL	C76-C77-C78-C79
61	b	601	PGT	C18-C19-C20-C21
60	u	603	CDL	C37-C38-C39-C40
60	u	603	CDL	C44-C45-C46-C47
60	R	405	CDL	OA7-CA5-OA6-CA4
59	g	101	3PH	C38-C39-C3A-C3B
58	T	503	PC7	C23-C24-C25-C26
59	V	601	3PH	C37-C38-C39-C3A
60	u	602	CDL	C61-C62-C63-C64
61	T	502	PGT	C20-C21-C22-C23
62	s	401	COO	P1A-O3A-P2A-O4A
60	u	602	CDL	C37-C38-C39-C40
54	e	302	PTY	C17-C18-C19-C20
60	V	603	CDL	C23-C24-C25-C26
54	T	501	PTY	C32-C33-C34-C35
54	G	303	PTY	C8-C11-C12-C13
54	e	302	PTY	C8-C11-C12-C13
60	x	101	CDL	C36-C37-C38-C39
60	W	701	CDL	C19-C20-C21-C22
60	u	603	CDL	C51-C52-C53-C54
59	h	201	3PH	C3D-C3E-C3F-C3G
60	x	101	CDL	C61-C62-C63-C64
60	u	603	CDL	CA4-CA3-OA5-PA1
60	u	602	CDL	C74-C75-C76-C77
54	T	501	PTY	O30-C30-O4-C1
54	T	506	PTY	O30-C30-O4-C1
54	V	605	PTY	C39-C40-C41-C42
60	W	701	CDL	C54-C55-C56-C57
54	V	605	PTY	C12-C11-C8-O7
60	h	203	CDL	C33-C34-C35-C36
60	W	701	CDL	C75-C76-C77-C78
60	y	201	CDL	C73-C74-C75-C76
54	R	404	PTY	O14-C5-C6-C1
54	R	406	PTY	O14-C5-C6-C1
54	e	302	PTY	O14-C5-C6-C1
60	R	405	CDL	OB5-CB3-CB4-CB6
60	V	603	CDL	OA5-CA3-CA4-CA6
60	y	201	CDL	OB5-CB3-CB4-CB6

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Mol	Chain	Res	Type	Atoms
59	S	301	3PH	C32-C33-C34-C35
60	h	203	CDL	C56-C57-C58-C59
60	x	101	CDL	C32-C33-C34-C35
60	y	201	CDL	C12-C13-C14-C15
59	S	301	3PH	C38-C39-C3A-C3B
59	S	301	3PH	C39-C3A-C3B-C3C
59	h	201	3PH	C26-C27-C28-C29
60	W	701	CDL	C82-C83-C84-C85
61	b	601	PGT	C11-C12-C13-C14
60	V	603	CDL	C19-C20-C21-C22
58	Q	302	PC7	C14-C15-C16-C17
54	R	402	PTY	O4-C1-C6-C5
54	S	302	PTY	O4-C1-C6-C5
54	T	506	PTY	O4-C1-C6-C5
54	V	604	PTY	O4-C1-C6-C5
58	T	503	PC7	C1-C2-C3-O3
60	V	603	CDL	CA3-CA4-CA6-OA8
60	y	201	CDL	CB3-CB4-CB6-OB8
61	T	505	PGT	C1-C2-C3-O3
54	e	302	PTY	C39-C40-C41-C42
60	x	101	CDL	C56-C57-C58-C59
54	h	202	PTY	C31-C32-C33-C34
59	w	201	3PH	C3C-C3D-C3E-C3F
60	W	701	CDL	C40-C41-C42-C43
60	W	701	CDL	C52-C53-C54-C55
60	x	101	CDL	C18-C19-C20-C21
61	T	502	PGT	C18-C19-C20-C21
59	V	601	3PH	C2B-C2C-C2D-C2E
61	l	701	PGT	C34-C35-C36-C37
60	h	203	CDL	C77-C78-C79-C80
60	V	603	CDL	OB7-CB5-OB6-CB4
54	S	302	PTY	C8-C11-C12-C13
54	T	504	PTY	O14-C5-C6-O7
54	V	604	PTY	C6-C5-O14-P1
59	R	401	3PH	C2-C1-O11-P
54	V	606	PTY	C14-C15-C16-C17
54	V	604	PTY	O4-C1-C6-O7
58	R	403	PC7	O2-C2-C3-O3
58	u	601	PC7	O2-C2-C3-O3
59	h	201	3PH	O21-C2-C3-O31
60	y	201	CDL	OB6-CB4-CB6-OB8
61	T	505	PGT	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
61	b	601	PGT	O2-C2-C3-O3
54	V	604	PTY	C37-C38-C39-C40
54	S	302	PTY	C12-C13-C14-C15
58	T	503	PC7	C16-C17-C18-C19
60	V	603	CDL	C14-C15-C16-C17
60	u	602	CDL	C24-C25-C26-C27
60	W	701	CDL	C60-C61-C62-C63
61	T	505	PGT	C14-C15-C16-C17
58	Q	302	PC7	C12-C11-O3-C3
54	V	606	PTY	C11-C8-O7-C6
58	u	601	PC7	C16-C17-C18-C19
54	S	302	PTY	C38-C39-C40-C41
59	c	101	3PH	C22-C23-C24-C25
60	u	602	CDL	C22-C23-C24-C25
54	R	404	PTY	C23-C24-C25-C26
54	S	302	PTY	C13-C14-C15-C16
58	u	601	PC7	C32-C33-C34-C35
61	T	502	PGT	O5-C5-C6-O6
60	R	405	CDL	CB2-C1-CA2-OA2
60	u	603	CDL	CB2-C1-CA2-OA2
61	l	701	PGT	C20-C21-C22-C23
61	T	502	PGT	O2-C31-C32-C33
54	x	102	PTY	C31-C30-O4-C1
54	V	606	PTY	C11-C12-C13-C14
54	T	501	PTY	C11-C12-C13-C14
54	S	302	PTY	O14-C5-C6-C1
54	T	506	PTY	O14-C5-C6-C1
58	u	601	PC7	O3P-C1-C2-C3
60	u	602	CDL	OB5-CB3-CB4-CB6
61	T	502	PGT	O3P-C1-C2-C3
61	T	505	PGT	O3P-C1-C2-C3
60	h	203	CDL	C55-C56-C57-C58
60	u	602	CDL	C51-C52-C53-C54
54	G	303	PTY	C37-C38-C39-C40
54	R	406	PTY	C39-C40-C41-C42
60	R	405	CDL	C74-C75-C76-C77
54	x	102	PTY	C26-C27-C28-C29
60	W	701	CDL	OA9-CA7-OA8-CA6
60	V	603	CDL	C72-C73-C74-C75
55	r	200	8Q1	C28-O27-P24-O2
60	u	603	CDL	C21-C22-C23-C24
60	y	201	CDL	C51-C52-C53-C54

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Mol	Chain	Res	Type	Atoms
59	R	401	3PH	C3-C2-O21-C21
59	w	201	3PH	C3-C2-O21-C21
61	l	701	PGT	C3-C2-O2-C31
60	u	602	CDL	OB9-CB7-OB8-CB6
59	R	401	3PH	C26-C27-C28-C29
60	h	203	CDL	CA5-C11-C12-C13
60	u	602	CDL	C15-C16-C17-C18
60	W	701	CDL	C64-C65-C66-C67
54	T	501	PTY	C33-C34-C35-C36
60	x	101	CDL	C75-C76-C77-C78
54	R	404	PTY	O14-C5-C6-O7
54	T	506	PTY	O14-C5-C6-O7
58	u	601	PC7	O3P-C1-C2-O2
59	c	101	3PH	O11-C1-C2-O21
59	w	201	3PH	O11-C1-C2-O21
60	V	603	CDL	OA5-CA3-CA4-OA6
60	h	203	CDL	OB5-CB3-CB4-OB6
60	u	602	CDL	C20-C21-C22-C23
54	T	501	PTY	C40-C41-C42-C43
58	u	601	PC7	C1-C2-C3-O3
59	h	201	3PH	C1-C2-C3-O31
60	R	405	CDL	CB3-CB4-CB6-OB8
60	h	203	CDL	CA3-CA4-CA6-OA8
61	b	601	PGT	C1-C2-C3-O3
54	e	301	PTY	C30-C31-C32-C33
60	u	602	CDL	CA5-C11-C12-C13
55	J	200	8Q1	C7-C8-C9-C10
60	u	602	CDL	C59-C60-C61-C62
54	S	302	PTY	C2-C3-O11-P1
54	V	606	PTY	C2-C3-O11-P1
54	R	404	PTY	O4-C1-C6-O7
54	R	406	PTY	O4-C1-C6-O7
54	V	605	PTY	O4-C1-C6-O7
54	V	606	PTY	O4-C1-C6-O7
59	w	201	3PH	O21-C2-C3-O31
60	R	405	CDL	OB6-CB4-CB6-OB8
60	V	603	CDL	OA6-CA4-CA6-OA8
60	W	701	CDL	OB6-CB4-CB6-OB8
60	h	203	CDL	OA6-CA4-CA6-OA8
61	l	701	PGT	O2-C2-C3-O3
60	u	602	CDL	C58-C59-C60-C61
60	R	405	CDL	C31-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
59	g	101	3PH	C32-C33-C34-C35
54	G	303	PTY	C32-C33-C34-C35
59	c	101	3PH	C29-C2A-C2B-C2C
60	h	203	CDL	C17-C18-C19-C20
54	x	102	PTY	O30-C30-O4-C1
58	Q	302	PC7	O11-C11-O3-C3
60	y	201	CDL	C11-C12-C13-C14
54	V	604	PTY	C11-C8-O7-C6
59	w	201	3PH	C29-C2A-C2B-C2C
60	V	603	CDL	C12-C13-C14-C15
60	V	603	CDL	O1-C1-CA2-OA2
60	h	203	CDL	C51-C52-C53-C54
60	h	203	CDL	C78-C79-C80-C81
54	x	102	PTY	C32-C33-C34-C35
60	W	701	CDL	C71-C72-C73-C74
60	W	701	CDL	C44-C45-C46-C47
56	P	401	NDP	O4D-C1D-N1N-C6N
60	h	203	CDL	C74-C75-C76-C77
60	V	603	CDL	OB5-CB3-CB4-CB6
60	h	203	CDL	OB5-CB3-CB4-CB6
54	V	604	PTY	O10-C8-O7-C6
54	V	606	PTY	O10-C8-O7-C6
59	R	401	3PH	C25-C26-C27-C28
52	B	501	FMN	N10-C1'-C2'-O2'
54	R	404	PTY	C13-C14-C15-C16
60	W	701	CDL	O1-C1-CA2-OA2
60	V	603	CDL	C32-C31-CA7-OA8
60	W	701	CDL	C43-C44-C45-C46
56	P	401	NDP	C2B-O2B-P2B-O1X
60	x	101	CDL	C84-C85-C86-C87
59	V	601	3PH	O11-C1-C2-O21
60	V	603	CDL	OB5-CB3-CB4-OB6
60	u	602	CDL	OB5-CB3-CB4-OB6
60	u	603	CDL	OB5-CB3-CB4-OB6
60	y	201	CDL	OB5-CB3-CB4-OB6
61	T	502	PGT	O3P-C1-C2-O2
61	T	502	PGT	C35-C36-C37-C38
60	R	405	CDL	OA9-CA7-OA8-CA6
54	e	302	PTY	C18-C19-C20-C21
59	w	201	3PH	C3A-C3B-C3C-C3D
61	T	502	PGT	C41-C42-C43-C44
61	l	701	PGT	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
60	W	701	CDL	C36-C37-C38-C39
60	W	701	CDL	C31-C32-C33-C34
60	V	603	CDL	C35-C36-C37-C38
60	x	101	CDL	C58-C59-C60-C61
60	h	203	CDL	OB6-CB4-CB6-OB8
60	u	603	CDL	OA6-CA4-CA6-OA8
54	R	406	PTY	O4-C1-C6-C5
54	V	605	PTY	O4-C1-C6-C5
59	S	301	3PH	C22-C23-C24-C25
58	R	403	PC7	C12-C13-C14-C15
61	b	601	PGT	C40-C41-C42-C43
60	x	101	CDL	C78-C79-C80-C81
54	S	302	PTY	C15-C16-C17-C18
54	V	606	PTY	C32-C33-C34-C35
54	R	402	PTY	C5-O14-P1-O13
54	R	406	PTY	C3-O11-P1-O13
54	T	501	PTY	C3-O11-P1-O13
54	T	506	PTY	C3-O11-P1-O13
54	T	506	PTY	C5-O14-P1-O11
54	T	506	PTY	C5-O14-P1-O13
54	V	604	PTY	C5-O14-P1-O13
54	V	605	PTY	C3-O11-P1-O12
60	R	405	CDL	CB3-OB5-PB2-OB4
60	V	603	CDL	CA2-OA2-PA1-OA4
60	V	603	CDL	CB3-OB5-PB2-OB2
60	W	701	CDL	CA2-OA2-PA1-OA4
60	W	701	CDL	CB3-OB5-PB2-OB3
60	h	203	CDL	CB3-OB5-PB2-OB2
60	h	203	CDL	CB3-OB5-PB2-OB4
60	u	602	CDL	CB2-OB2-PB2-OB3
60	u	602	CDL	CB2-OB2-PB2-OB4
60	u	602	CDL	CB2-OB2-PB2-OB5
60	u	602	CDL	CB3-OB5-PB2-OB3
60	u	603	CDL	CA3-OA5-PA1-OA2
60	u	603	CDL	CA3-OA5-PA1-OA4
60	u	603	CDL	CB2-OB2-PB2-OB3
60	u	603	CDL	CB2-OB2-PB2-OB5
60	u	603	CDL	CB3-OB5-PB2-OB4
60	x	101	CDL	CA3-OA5-PA1-OA3
60	x	101	CDL	CB3-OB5-PB2-OB2
60	y	201	CDL	CB2-OB2-PB2-OB3
60	y	201	CDL	CB2-OB2-PB2-OB4

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Mol	Chain	Res	Type	Atoms
60	y	201	CDL	CB2-OB2-PB2-OB5
60	y	201	CDL	CB3-OB5-PB2-OB3
61	T	502	PGT	C4-O4P-P-O2P
61	T	505	PGT	C1-O3P-P-O4P
61	T	505	PGT	C4-O4P-P-O1P
61	b	601	PGT	C4-O4P-P-O3P
60	u	602	CDL	C17-C18-C19-C20
60	x	101	CDL	C82-C83-C84-C85
61	b	601	PGT	C32-C31-O2-C2
54	h	202	PTY	C36-C37-C38-C39
60	V	603	CDL	C1-CA2-OA2-PA1
60	W	701	CDL	CB4-CB3-OB5-PB2
54	V	604	PTY	C11-C12-C13-C14
54	h	202	PTY	C33-C34-C35-C36
61	b	601	PGT	C38-C39-C40-C41
59	g	101	3PH	C39-C3A-C3B-C3C
55	r	200	8Q1	C28-O27-P24-O3
54	e	302	PTY	C40-C41-C42-C43
60	x	101	CDL	C52-C53-C54-C55
60	x	101	CDL	CA7-C31-C32-C33
54	V	605	PTY	C34-C35-C36-C37
54	R	404	PTY	C1-C6-O7-C8
54	T	501	PTY	C1-C6-O7-C8
59	V	602	3PH	C1-C2-O21-C21
60	R	405	CDL	CB6-CB4-OB6-CB5
60	u	602	CDL	CB6-CB4-OB6-CB5
54	e	302	PTY	C33-C34-C35-C36
60	y	201	CDL	C15-C16-C17-C18
59	V	601	3PH	C29-C2A-C2B-C2C
62	s	401	COO	C2X-C3X-O3X-P3X
54	V	605	PTY	O14-C5-C6-C1
60	h	203	CDL	OA5-CA3-CA4-CA6
60	y	201	CDL	OA5-CA3-CA4-CA6
61	b	601	PGT	O4P-C4-C5-C6
61	T	505	PGT	O3P-C1-C2-O2
54	S	302	PTY	C17-C18-C19-C20
54	V	606	PTY	C15-C16-C17-C18
60	u	603	CDL	C32-C33-C34-C35
61	l	701	PGT	C21-C22-C23-C24
54	V	606	PTY	C36-C37-C38-C39
60	x	101	CDL	OA6-CA4-CA6-OA8
58	u	601	PC7	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
60	x	101	CDL	C17-C18-C19-C20
60	W	701	CDL	CB3-CB4-CB6-OB8
60	W	701	CDL	C84-C85-C86-C87
62	s	401	COO	P1A-O3A-P2A-O5A
60	R	405	CDL	C52-C53-C54-C55
62	s	401	COO	O2-C1-C13-C11
59	h	201	3PH	C3A-C3B-C3C-C3D
61	b	601	PGT	O31-C31-O2-C2
61	l	701	PGT	O5-C5-C6-O6
54	R	406	PTY	C35-C36-C37-C38
54	V	604	PTY	C32-C33-C34-C35
59	V	601	3PH	C2D-C2E-C2F-C2G
59	V	601	3PH	C23-C24-C25-C26
61	l	701	PGT	C37-C38-C39-C40
59	V	601	3PH	C33-C34-C35-C36
59	V	602	3PH	C33-C34-C35-C36
62	s	401	COO	N1-C1-C13-C11
54	G	303	PTY	C33-C34-C35-C36
54	e	301	PTY	O4-C1-C6-O7
55	J	200	8Q1	C11-C12-C13-C14
60	u	603	CDL	C17-C18-C19-C20
60	x	101	CDL	C14-C15-C16-C17
54	x	102	PTY	C31-C32-C33-C34
54	h	202	PTY	C8-C11-C12-C13
60	x	101	CDL	CA5-C11-C12-C13
54	R	404	PTY	C22-C23-C24-C25
54	x	102	PTY	C38-C39-C40-C41
54	x	102	PTY	C40-C41-C42-C43
58	R	403	PC7	C1-C2-C3-O3
59	w	201	3PH	C1-C2-C3-O31
54	V	605	PTY	C12-C11-C8-O10
60	W	701	CDL	C42-C43-C44-C45
54	e	302	PTY	C14-C15-C16-C17
59	V	601	3PH	C34-C35-C36-C37
54	V	605	PTY	C17-C18-C19-C20
59	R	401	3PH	C37-C38-C39-C3A
60	y	201	CDL	C32-C33-C34-C35
54	h	202	PTY	C41-C42-C43-C44
58	u	601	PC7	C35-C36-C37-C38
60	u	602	CDL	CA7-C31-C32-C33
60	x	101	CDL	C71-C72-C73-C74
54	V	606	PTY	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
54	R	402	PTY	C11-C12-C13-C14
54	R	406	PTY	C32-C33-C34-C35
60	V	603	CDL	C17-C18-C19-C20
54	h	202	PTY	C38-C39-C40-C41
61	b	601	PGT	C34-C35-C36-C37
60	h	203	CDL	C72-C71-CB7-OB8
58	u	601	PC7	C37-C38-C39-C40
55	J	200	8Q1	C13-C14-C15-C16
60	h	203	CDL	C13-C14-C15-C16
59	c	101	3PH	C34-C35-C36-C37
59	w	201	3PH	C22-C23-C24-C25
59	S	301	3PH	C2-C1-O11-P
60	u	602	CDL	CA4-CA3-OA5-PA1
58	R	403	PC7	C36-C37-C38-C39
60	u	602	CDL	C72-C71-CB7-OB8
54	V	606	PTY	O4-C1-C6-C5
54	x	102	PTY	O4-C1-C6-C5
57	Q	301	UQ5	C14-C16-C17-C18
59	V	602	3PH	C1-C2-C3-O31
54	V	606	PTY	C31-C32-C33-C34
60	W	701	CDL	C55-C56-C57-C58
55	r	200	8Q1	C6-C7-C8-C9
60	W	701	CDL	CA7-C31-C32-C33
54	V	605	PTY	O14-C5-C6-O7
60	h	203	CDL	OA5-CA3-CA4-OA6
60	h	203	CDL	C54-C55-C56-C57
54	T	506	PTY	C14-C15-C16-C17
59	g	101	3PH	C24-C25-C26-C27
59	V	602	3PH	C3A-C3B-C3C-C3D
54	T	504	PTY	O14-C5-C6-C1
54	h	202	PTY	O4-C1-C6-O7
60	y	201	CDL	CA5-C11-C12-C13
60	u	603	CDL	C43-C44-C45-C46
60	R	405	CDL	C1-CB2-OB2-PB2
60	R	405	CDL	C33-C34-C35-C36
54	T	504	PTY	C33-C34-C35-C36
59	w	201	3PH	C35-C36-C37-C38
59	R	401	3PH	C1-O11-P-O12
59	V	601	3PH	C1-O11-P-O12
57	Q	301	UQ5	C11-C12-C13-C14
59	V	602	3PH	C23-C24-C25-C26
59	w	201	3PH	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
60	u	603	CDL	C12-C11-CA5-OA6
60	x	101	CDL	C35-C36-C37-C38
59	h	201	3PH	C24-C25-C26-C27
61	l	701	PGT	C33-C34-C35-C36
61	l	701	PGT	C1-C2-C3-O3
59	w	201	3PH	C2B-C2C-C2D-C2E
60	x	101	CDL	C33-C34-C35-C36
55	J	200	8Q1	C9-C10-C11-C12
58	T	503	PC7	C37-C38-C39-C40
59	w	201	3PH	C32-C33-C34-C35
58	R	403	PC7	C44-C45-C46-C47
54	e	302	PTY	C12-C11-C8-O7
60	u	603	CDL	OB5-CB3-CB4-CB6
59	V	601	3PH	C2A-C2B-C2C-C2D
59	S	301	3PH	C27-C28-C29-C2A
61	l	701	PGT	C35-C36-C37-C38
60	x	101	CDL	C72-C71-CB7-OB8
60	x	101	CDL	C76-C77-C78-C79
56	P	401	NDP	PA-O3-PN-O2N
59	w	201	3PH	C39-C3A-C3B-C3C
54	S	302	PTY	C12-C11-C8-O7
54	T	506	PTY	O10-C8-O7-C6
54	T	506	PTY	C11-C8-O7-C6
54	h	202	PTY	C14-C15-C16-C17
54	R	406	PTY	C16-C17-C18-C19
54	R	404	PTY	C17-C18-C19-C20
60	x	101	CDL	C52-C51-CB5-OB6
54	x	102	PTY	C21-C22-C23-C24
59	g	101	3PH	C23-C24-C25-C26
60	x	101	CDL	C81-C82-C83-C84
60	u	602	CDL	C32-C33-C34-C35
61	T	502	PGT	O31-C31-C32-C33
59	V	601	3PH	C27-C28-C29-C2A
54	h	202	PTY	O4-C30-C31-C32
61	l	701	PGT	O4P-C4-C5-O5
54	e	301	PTY	O4-C1-C6-C5
60	u	603	CDL	CA3-CA4-CA6-OA8
57	Q	301	UQ5	C5-C4-O4-C4M
59	V	602	3PH	C35-C36-C37-C38
60	R	405	CDL	C72-C71-CB7-OB8
55	J	200	8Q1	C6-C7-C8-C9
60	W	701	CDL	C41-C42-C43-C44

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Mol	Chain	Res	Type	Atoms
60	u	603	CDL	C52-C51-CB5-OB6
60	V	603	CDL	CA2-C1-CB2-OB2
59	c	101	3PH	C2D-C2E-C2F-C2G
58	R	403	PC7	C13-C14-C15-C16
59	V	602	3PH	C32-C33-C34-C35
60	R	405	CDL	C34-C35-C36-C37
54	e	302	PTY	C12-C11-C8-O10
60	u	603	CDL	C35-C36-C37-C38
61	T	502	PGT	C31-C32-C33-C34
57	Q	301	UQ5	C20-C19-C21-C22
62	s	401	COO	C5-C6-S1-C7
54	S	302	PTY	C12-C11-C8-O10
59	V	602	3PH	C25-C26-C27-C28
59	w	201	3PH	C36-C37-C38-C39
59	c	101	3PH	C37-C38-C39-C3A
60	R	405	CDL	C35-C36-C37-C38
54	h	202	PTY	O30-C30-C31-C32
60	u	603	CDL	O1-C1-CA2-OA2
58	R	403	PC7	C16-C17-C18-C19
60	u	603	CDL	C52-C51-CB5-OB7
60	x	101	CDL	C52-C51-CB5-OB7
54	V	606	PTY	C33-C34-C35-C36
54	h	202	PTY	C37-C38-C39-C40
60	x	101	CDL	C72-C71-CB7-OB9
55	J	200	8Q1	O33-C32-C34-N36
60	h	203	CDL	C12-C11-CA5-OA6
54	V	605	PTY	O4-C30-C31-C32
54	x	102	PTY	C23-C24-C25-C26
59	V	601	3PH	C2F-C2G-C2H-C2I
61	b	601	PGT	C31-C32-C33-C34
54	R	404	PTY	C20-C21-C22-C23
60	x	101	CDL	C12-C11-CA5-OA6
60	h	203	CDL	C52-C51-CB5-OB6
60	x	101	CDL	C12-C11-CA5-OA7

There are no ring outliers.

34 monomers are involved in 75 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	V	602	3PH	3	0
59	c	101	3PH	2	0
54	T	501	PTY	1	0

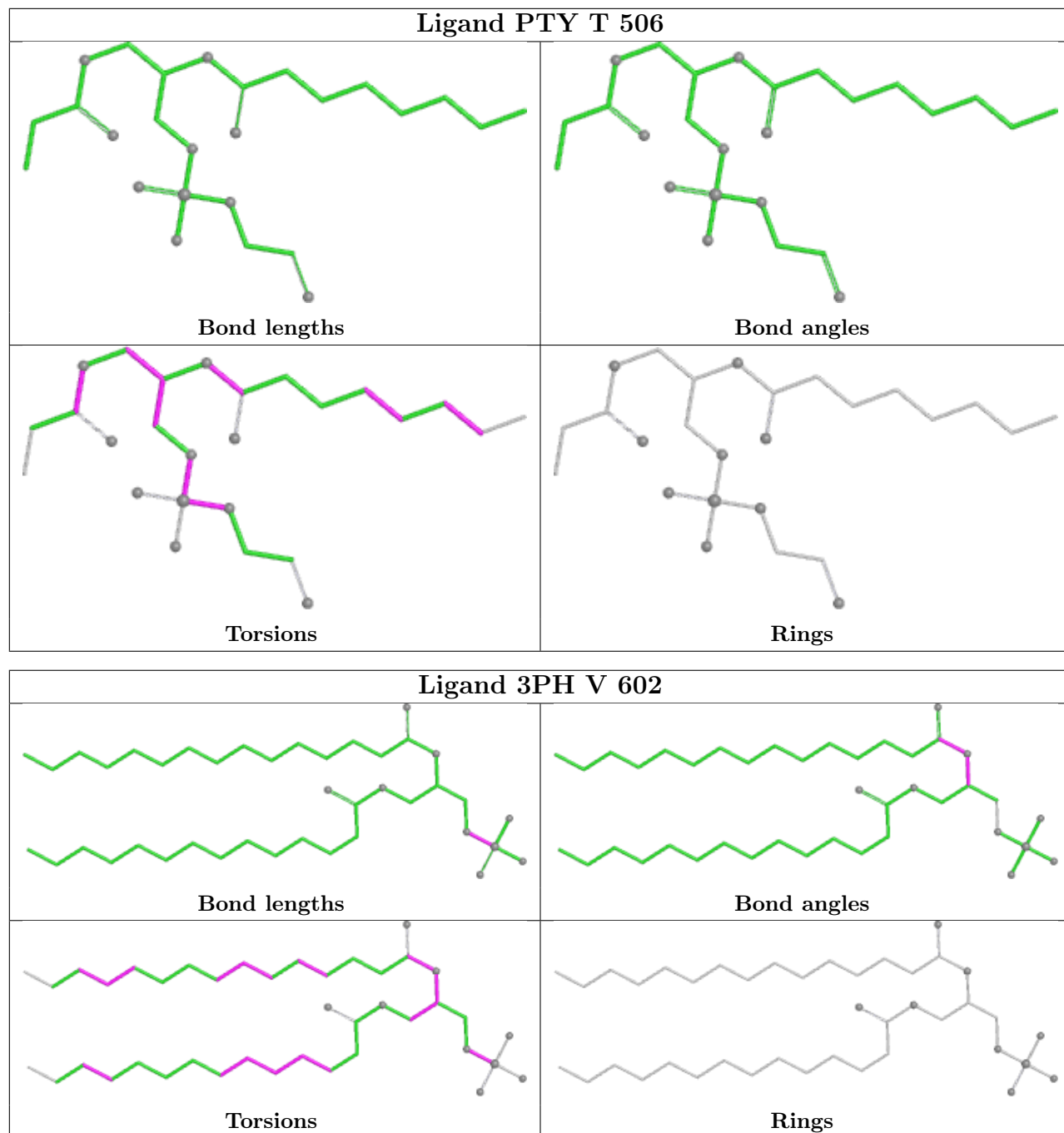
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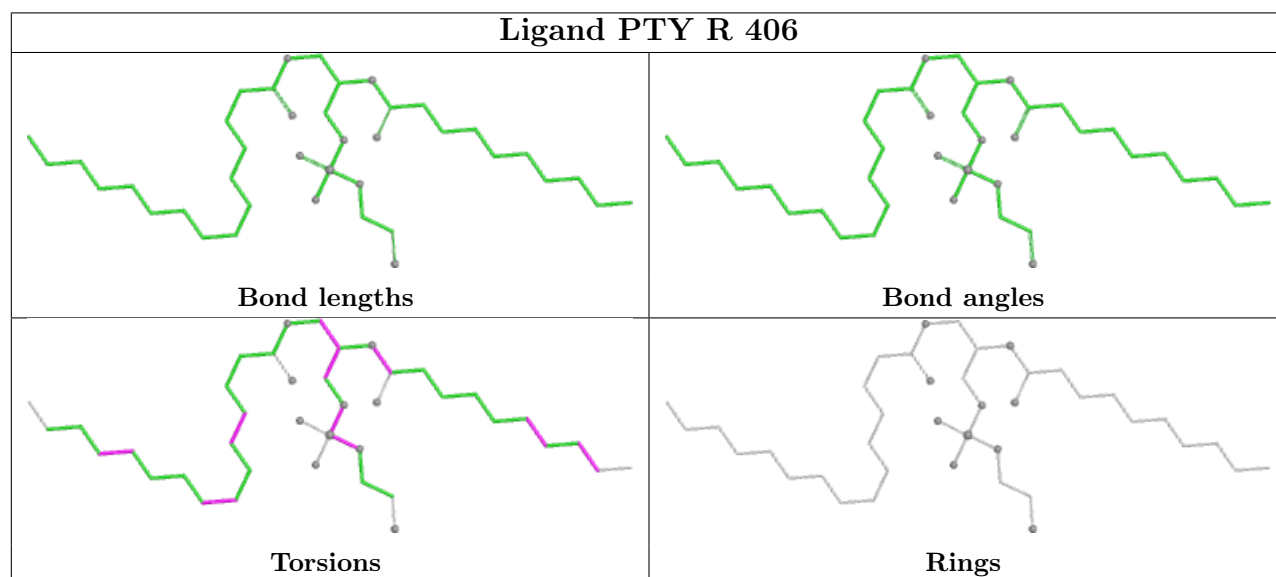
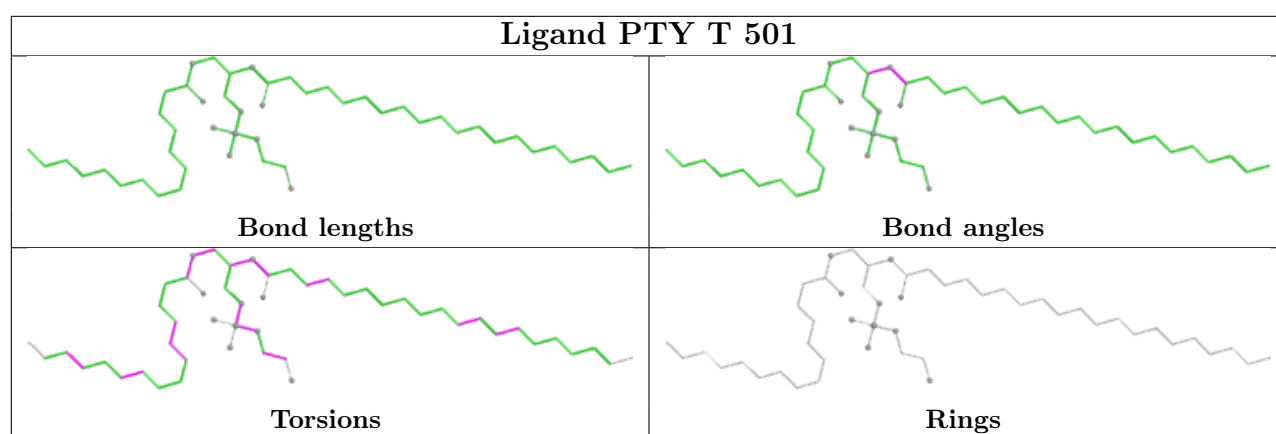
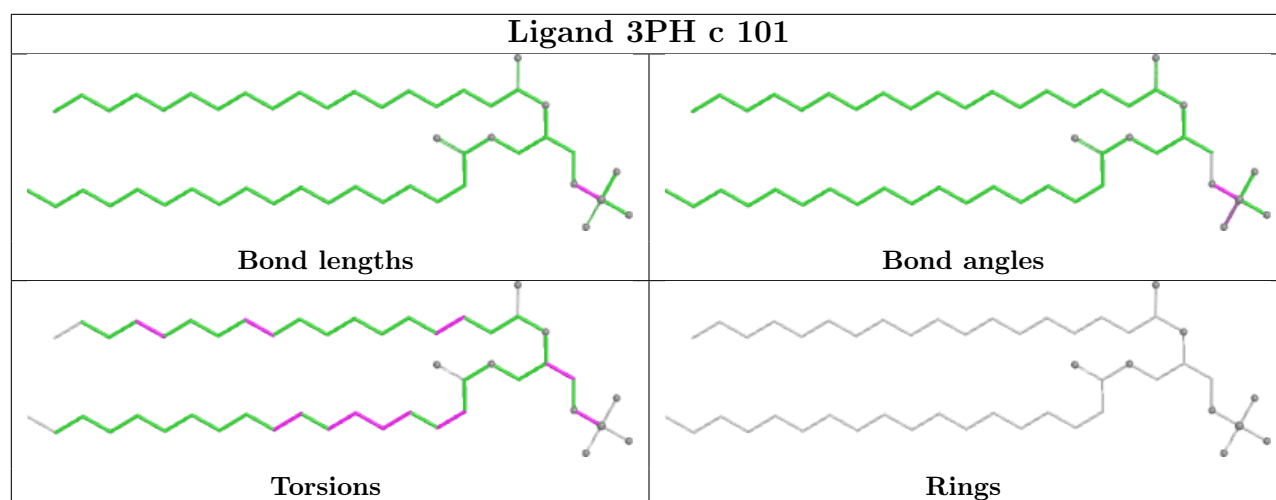
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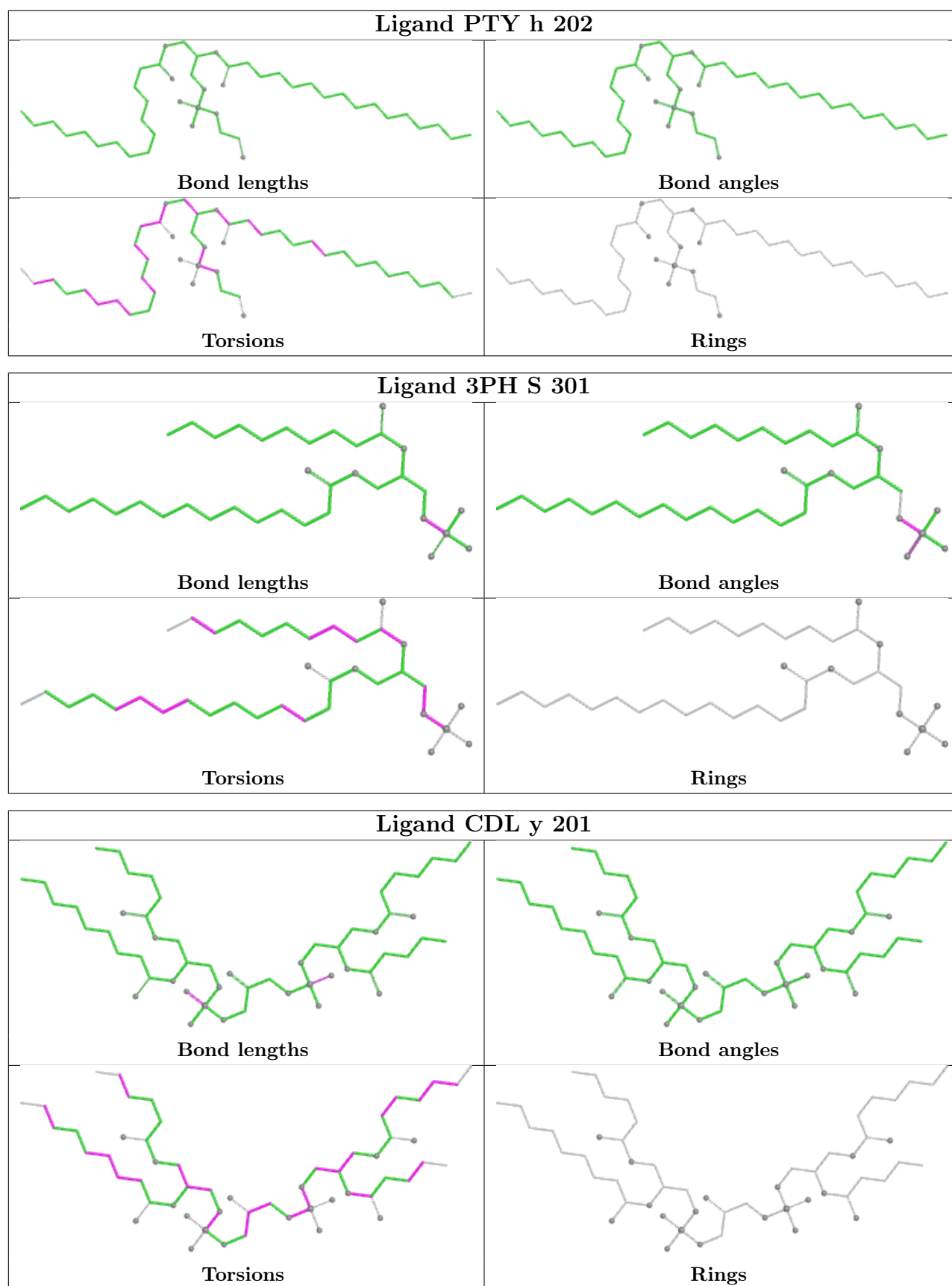
Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	R	406	PTY	1	0
54	h	202	PTY	1	0
53	F	201	SF4	1	0
60	y	201	CDL	4	0
54	V	605	PTY	2	0
54	V	606	PTY	1	0
60	x	101	CDL	9	0
59	R	401	3PH	1	0
58	T	503	PC7	3	0
60	V	603	CDL	1	0
61	l	701	PGT	1	0
58	Q	302	PC7	1	0
52	B	501	FMN	1	0
59	h	201	3PH	2	0
54	R	404	PTY	1	0
62	s	401	COO	5	0
54	S	302	PTY	3	0
54	G	303	PTY	2	0
56	P	401	NDP	1	0
60	u	603	CDL	3	0
60	u	602	CDL	2	0
54	e	302	PTY	3	0
61	b	601	PGT	1	0
60	h	203	CDL	3	0
53	B	502	SF4	1	0
57	Q	301	UQ5	2	0
61	T	502	PGT	3	0
59	w	201	3PH	3	0
60	R	405	CDL	1	0
58	u	601	PC7	2	0
60	W	701	CDL	8	0

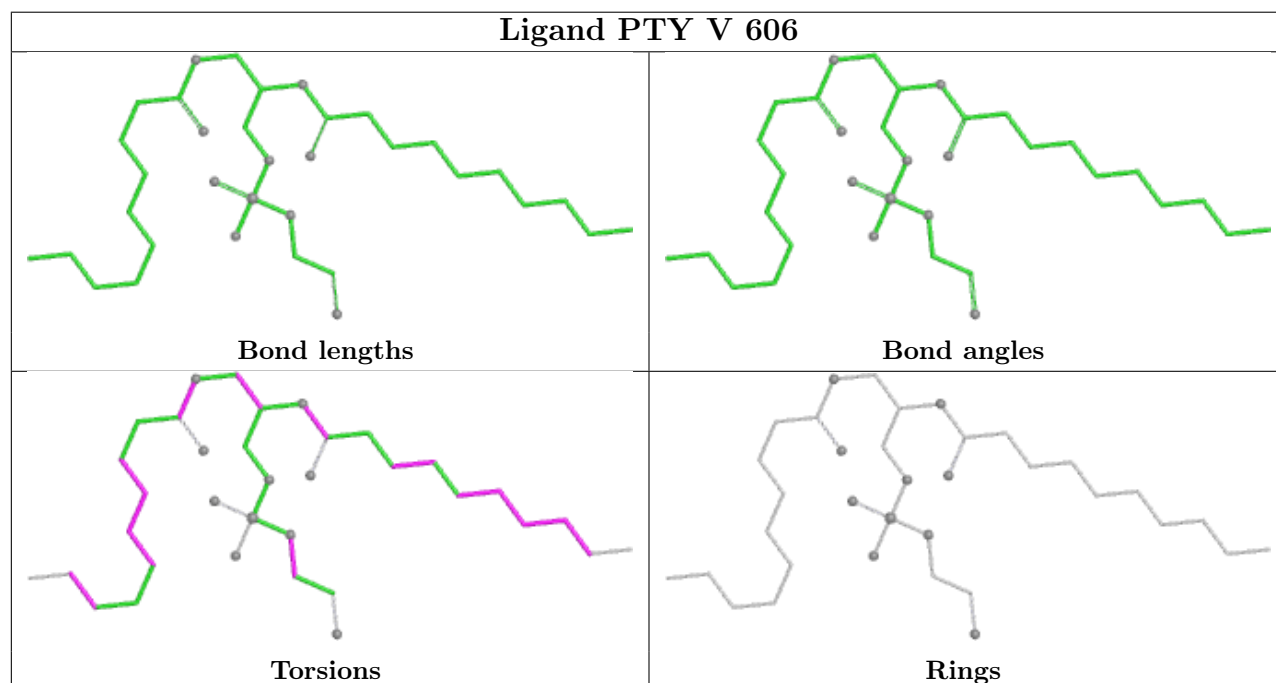
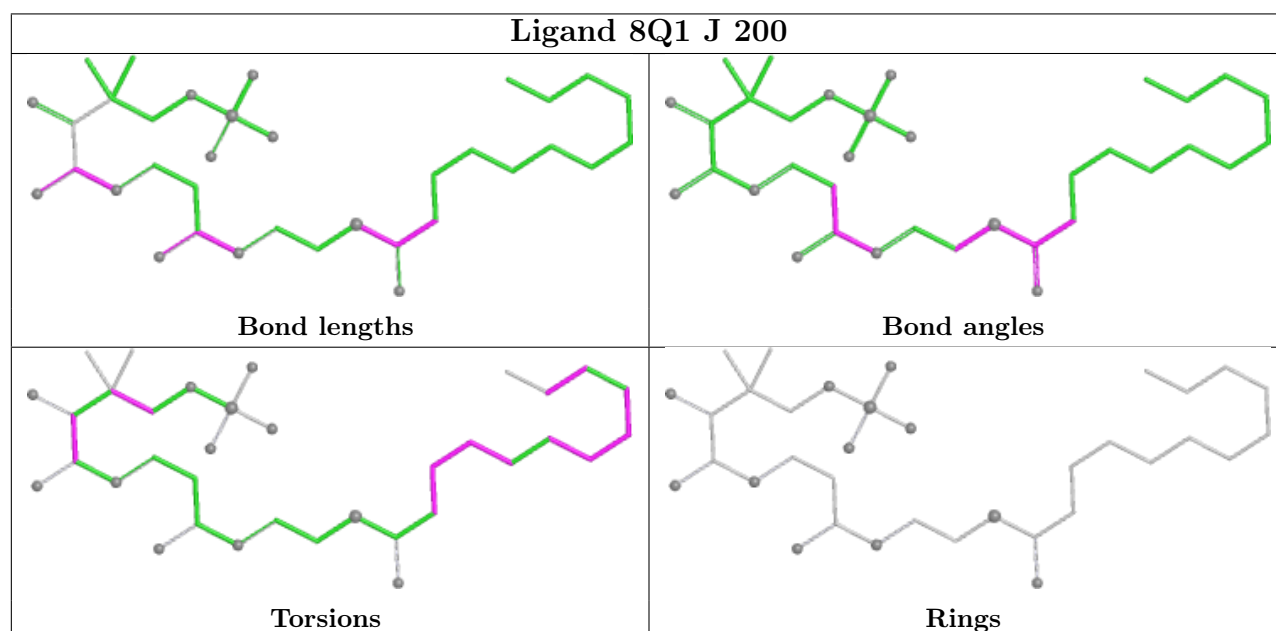
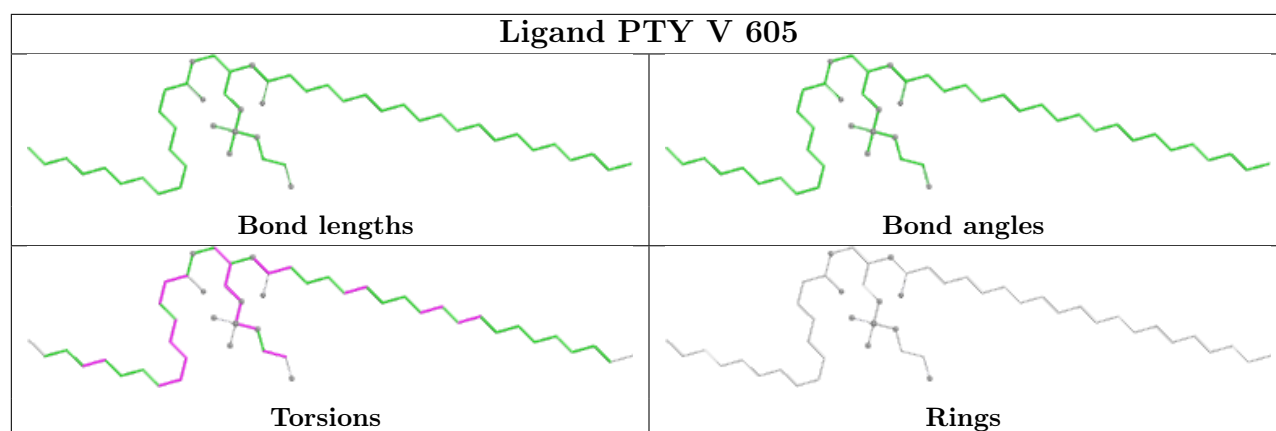
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

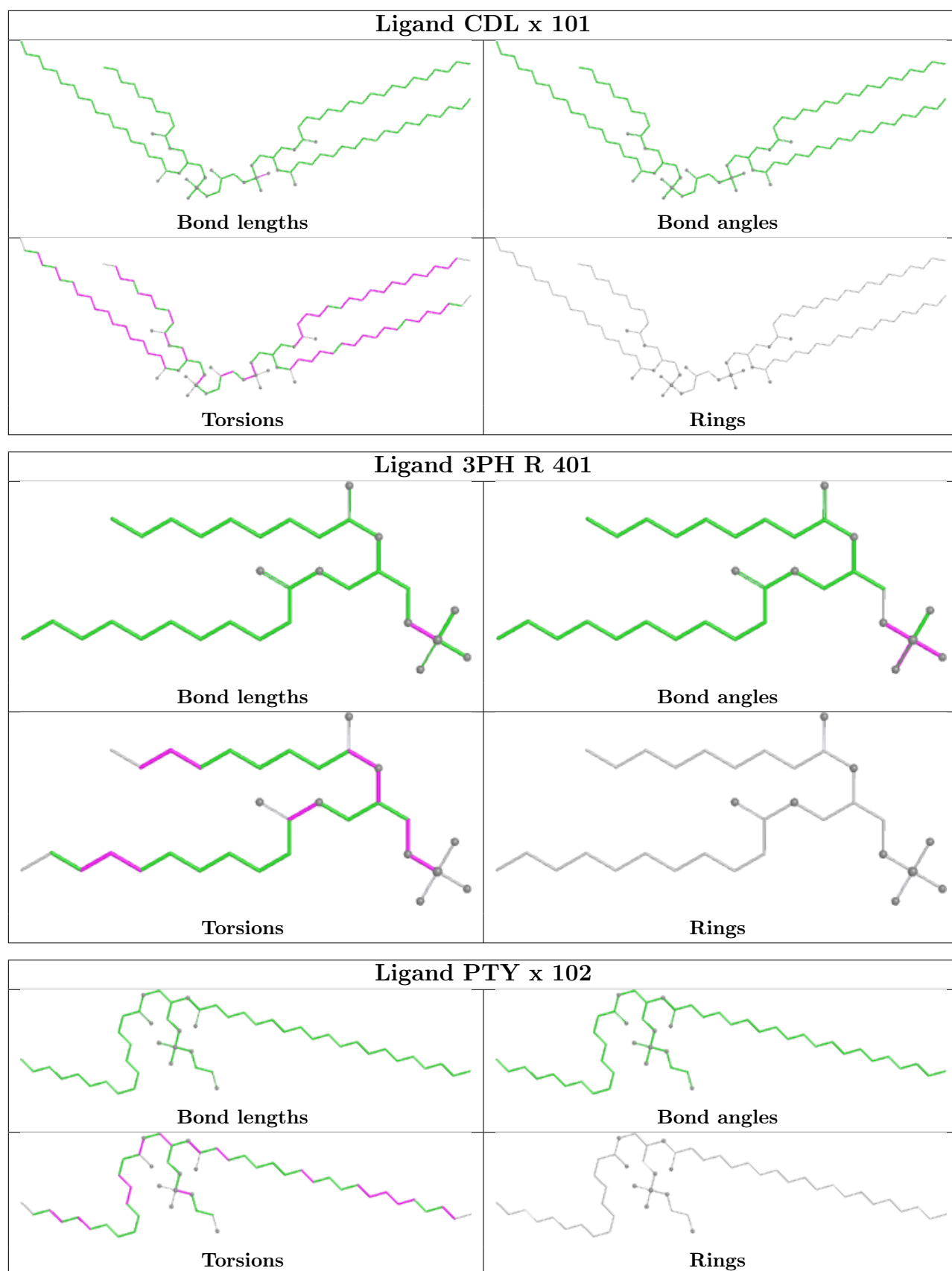
equivalents in the CSD to analyse the geometry.

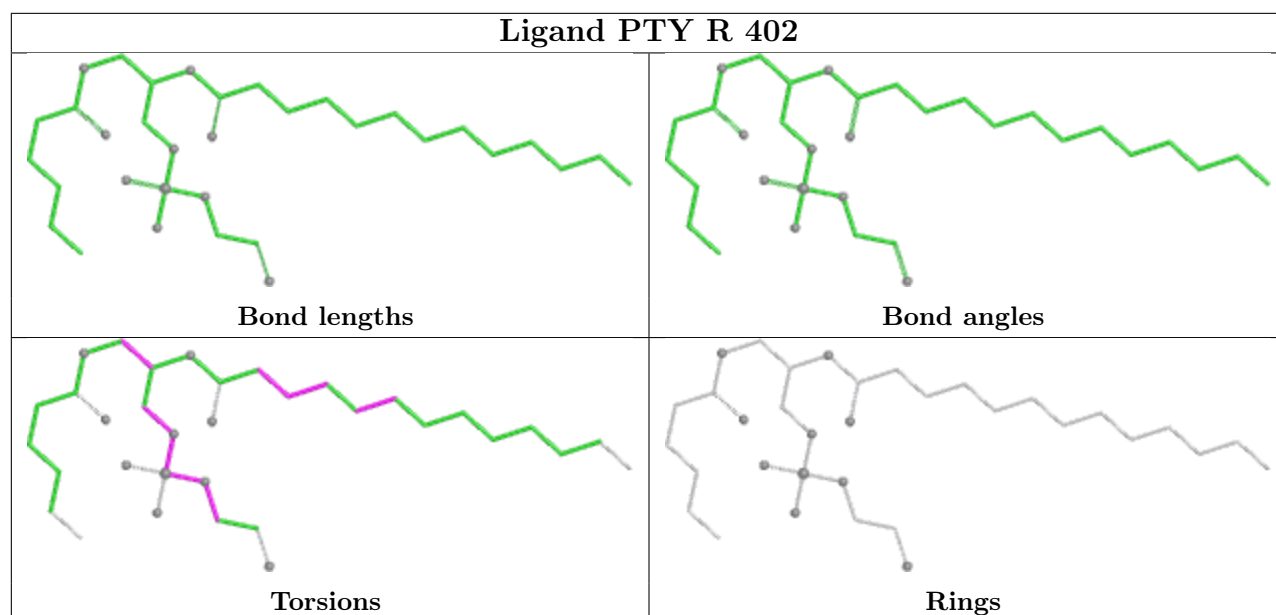
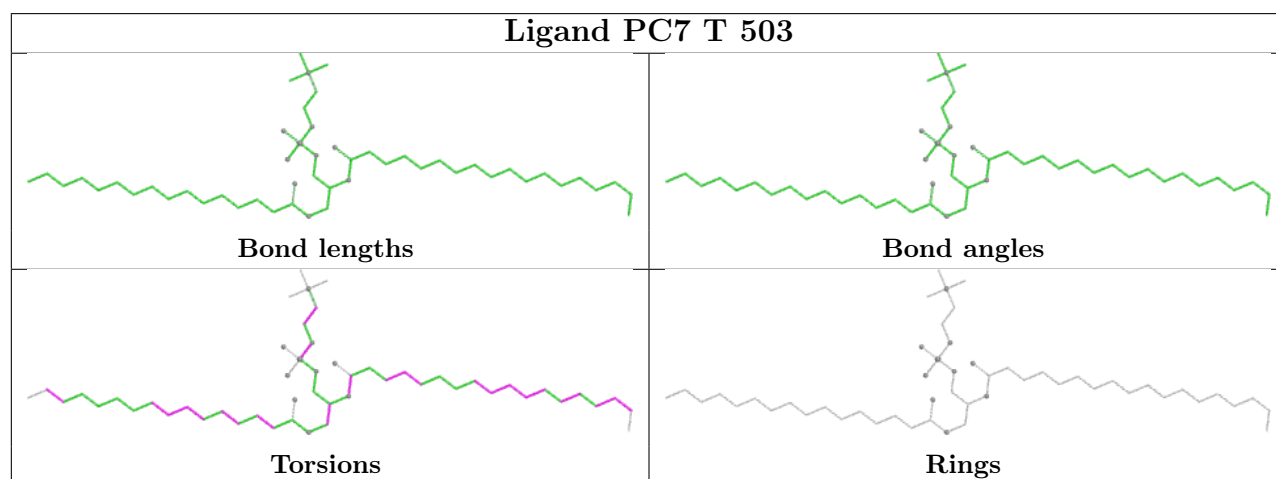
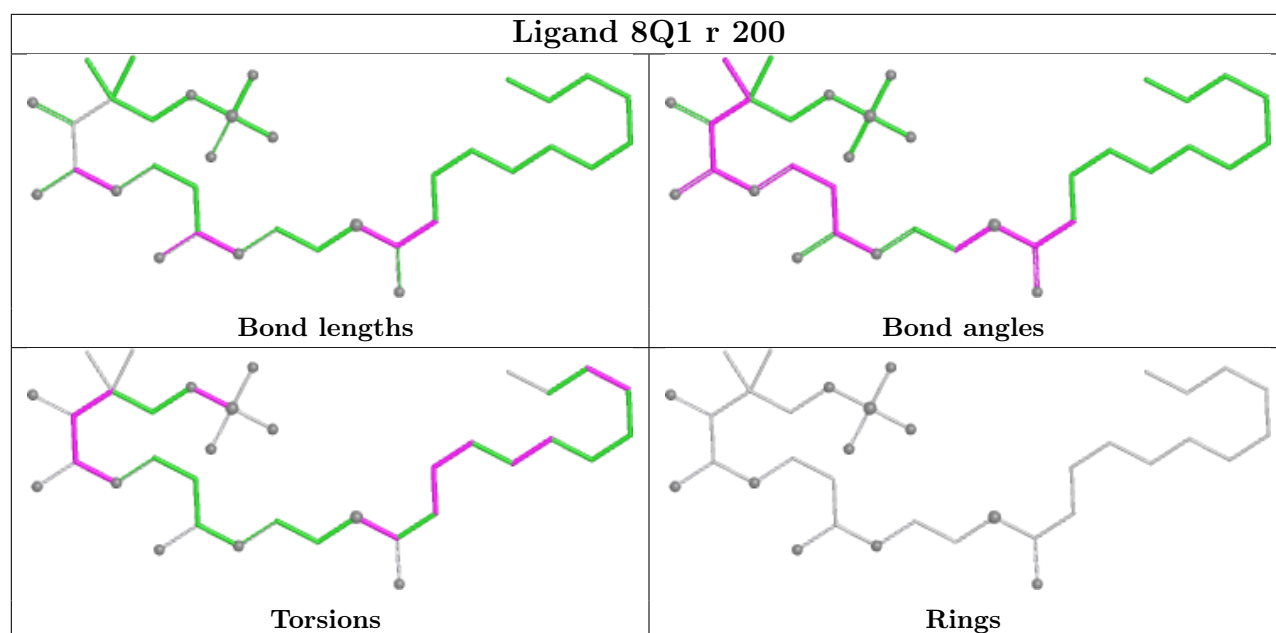


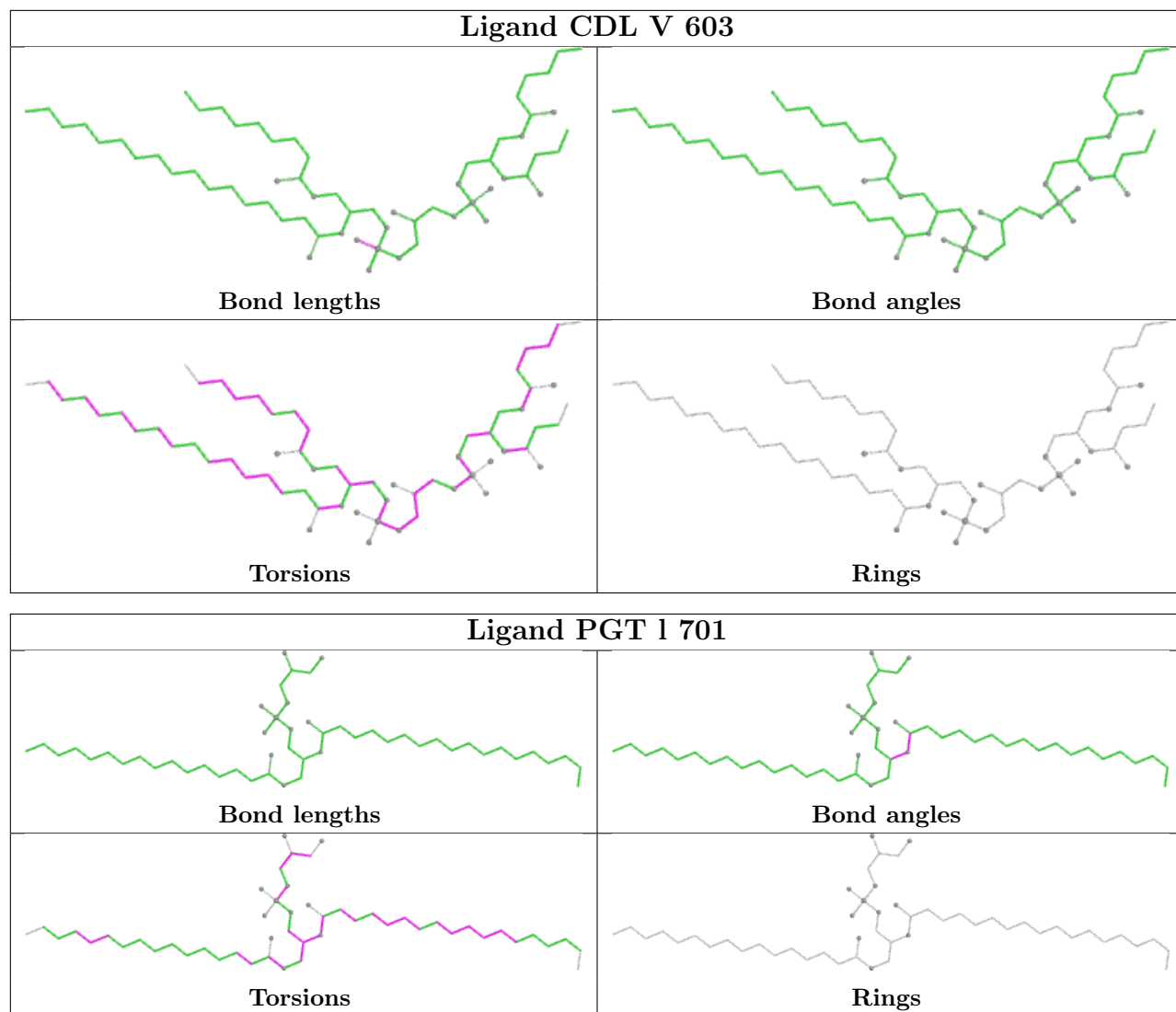


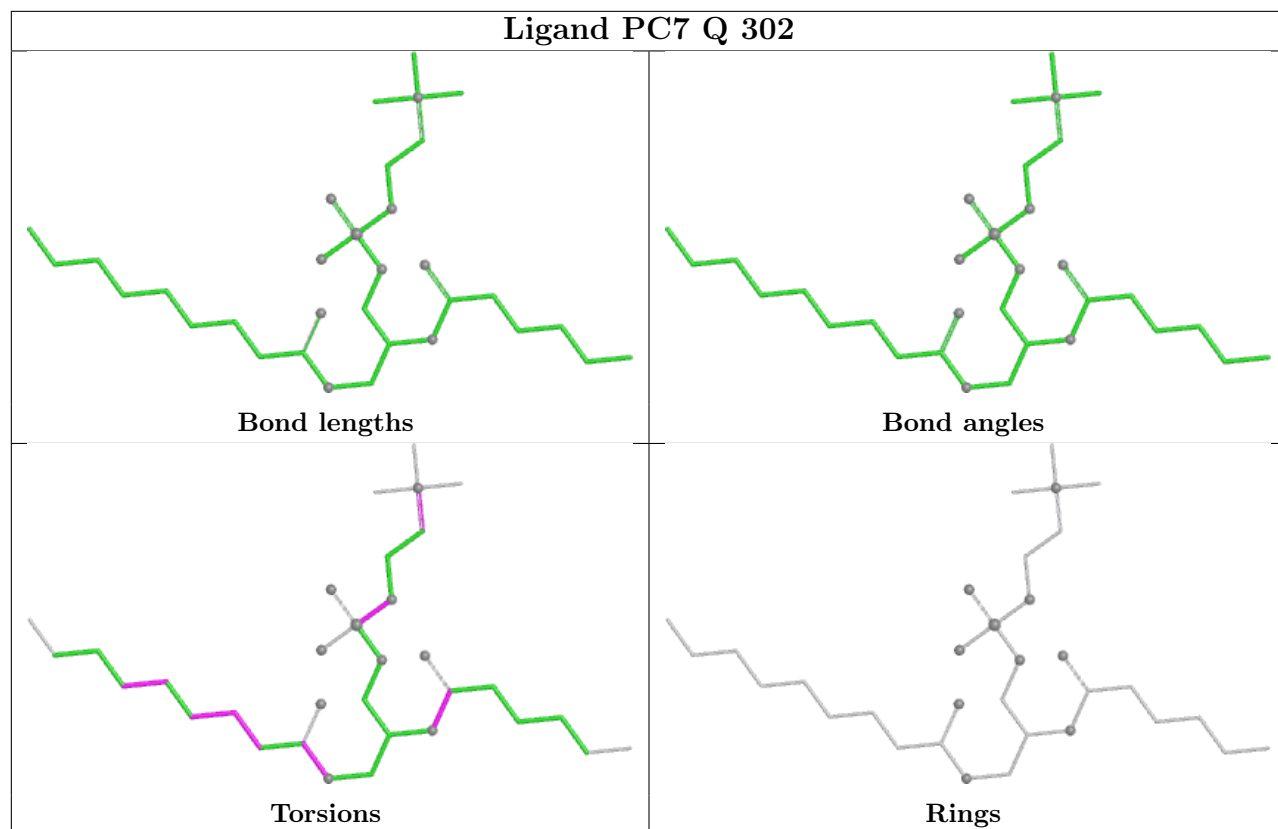


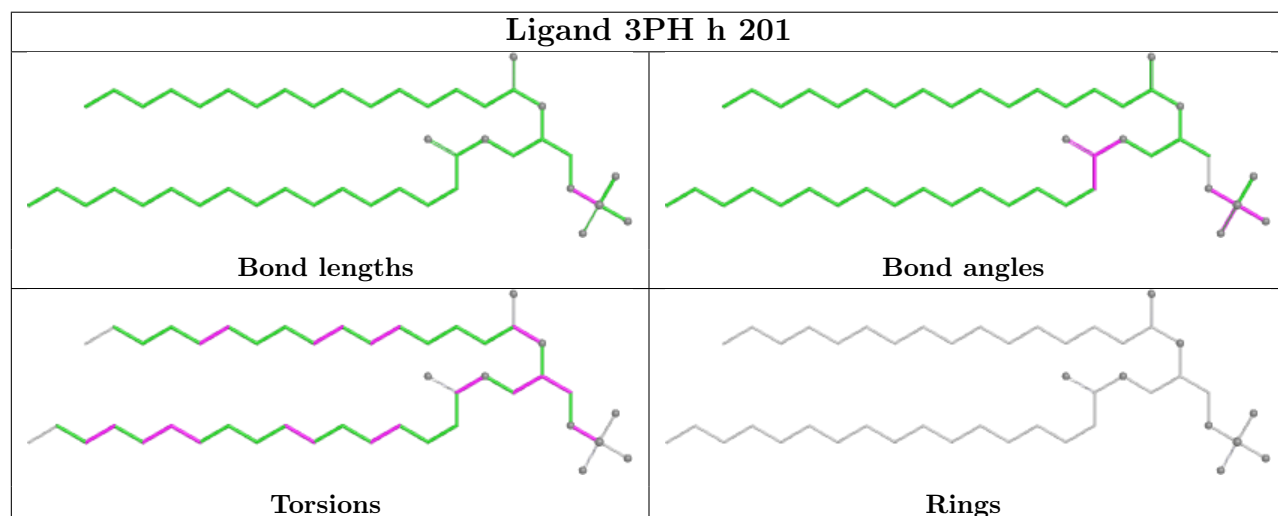
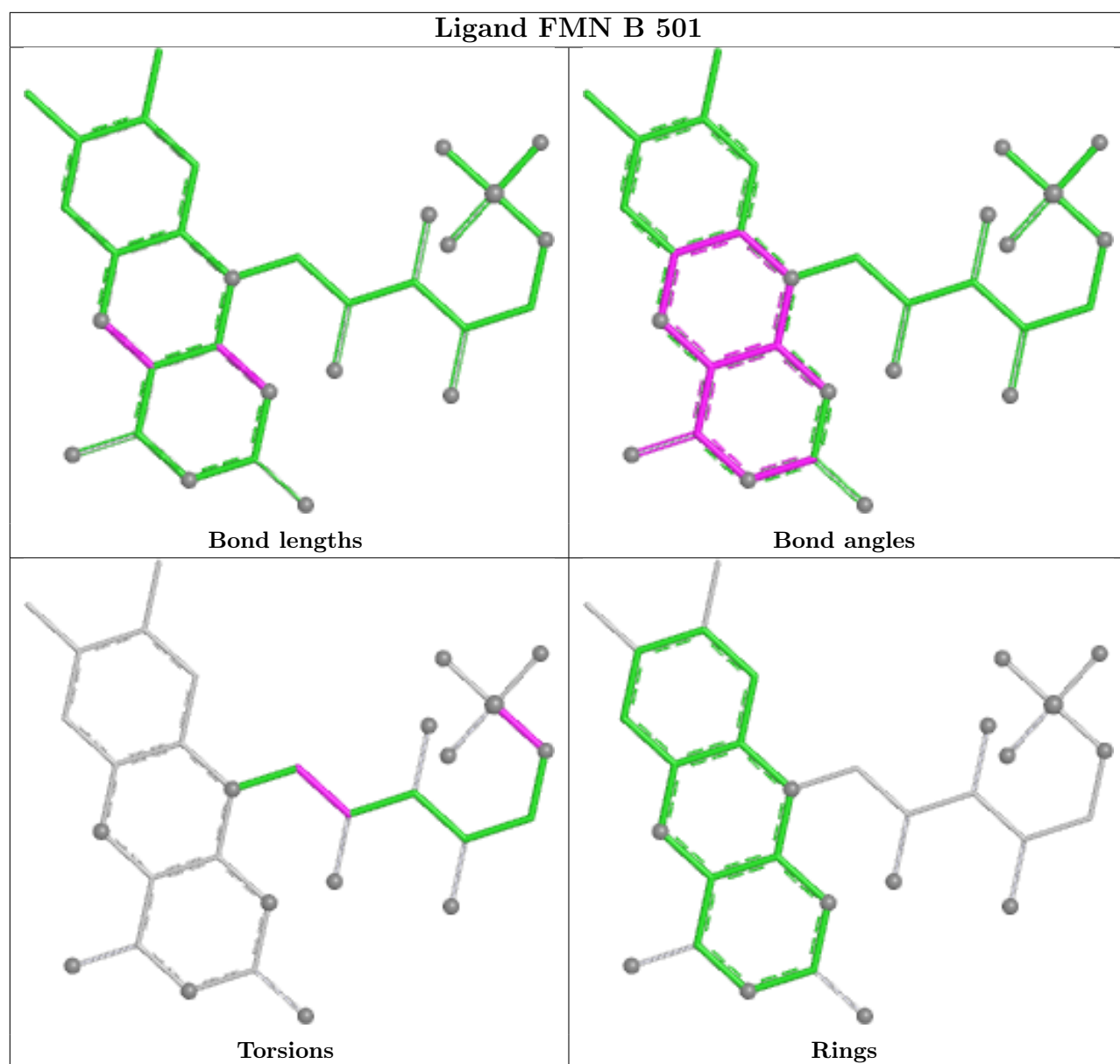


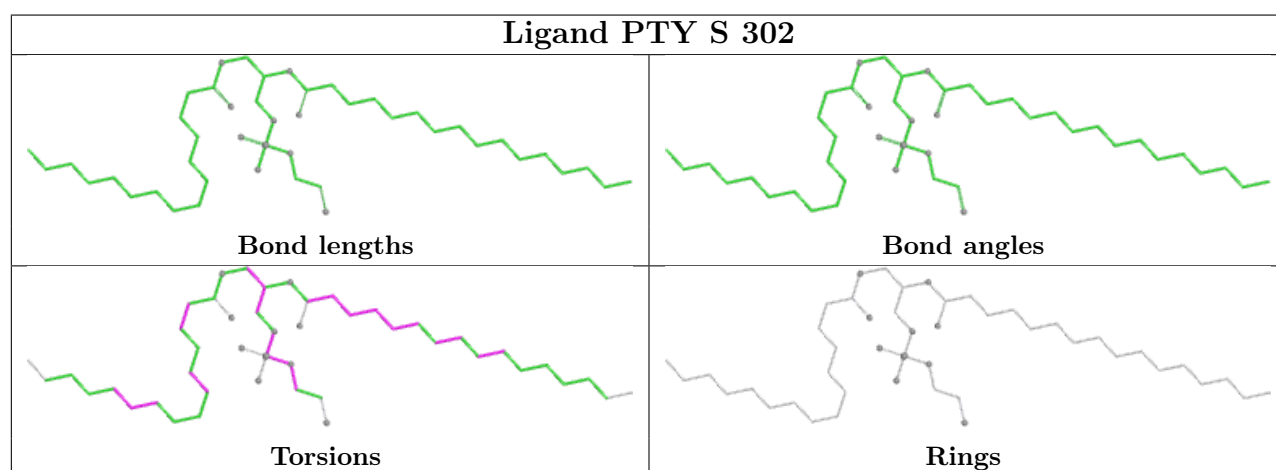
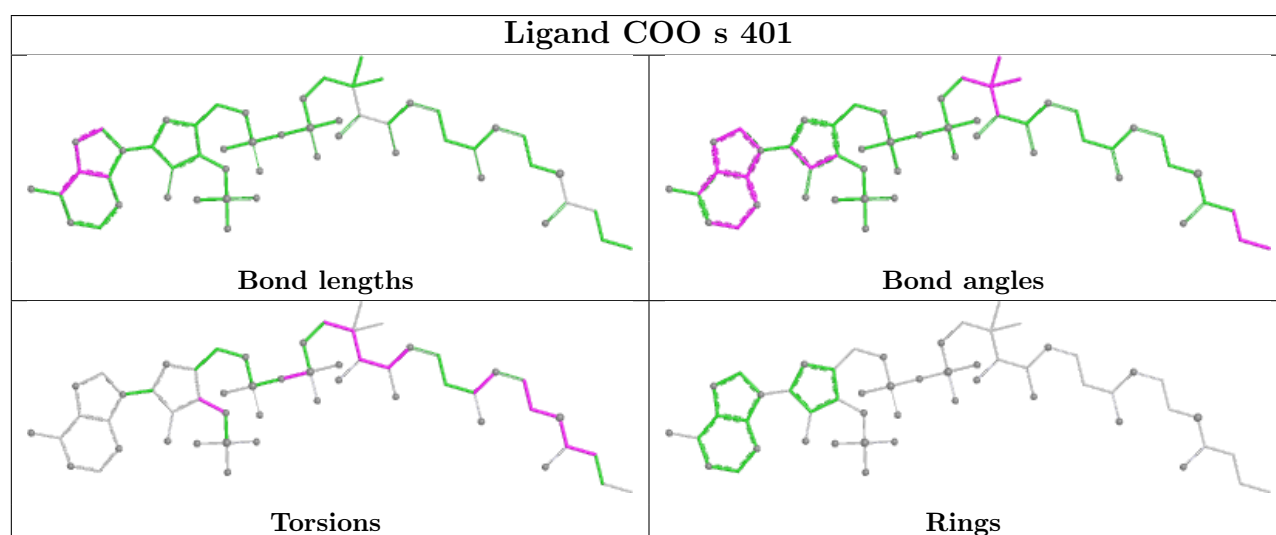
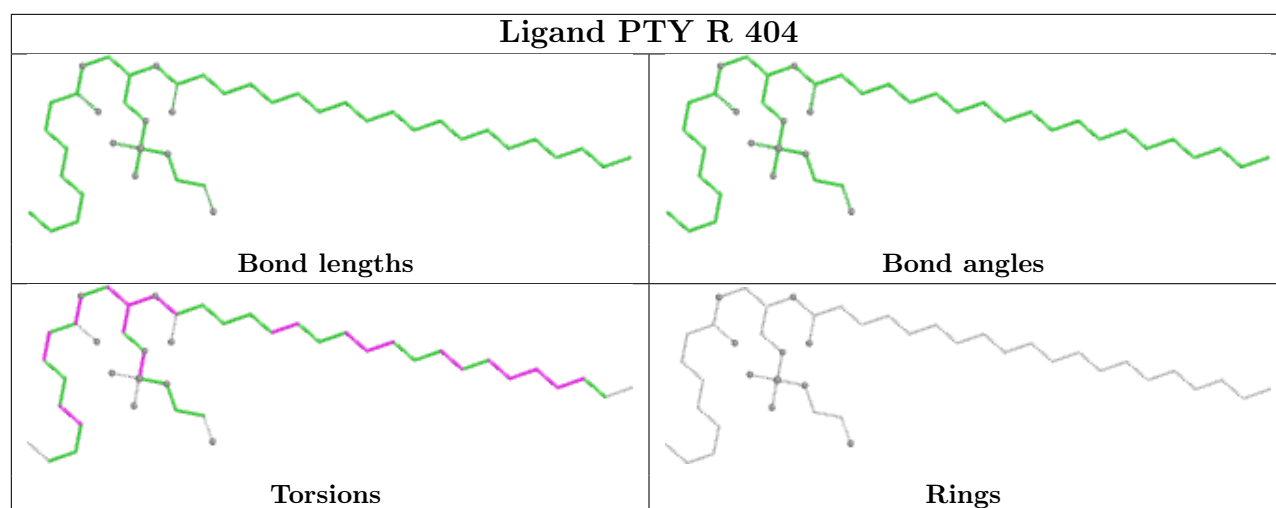


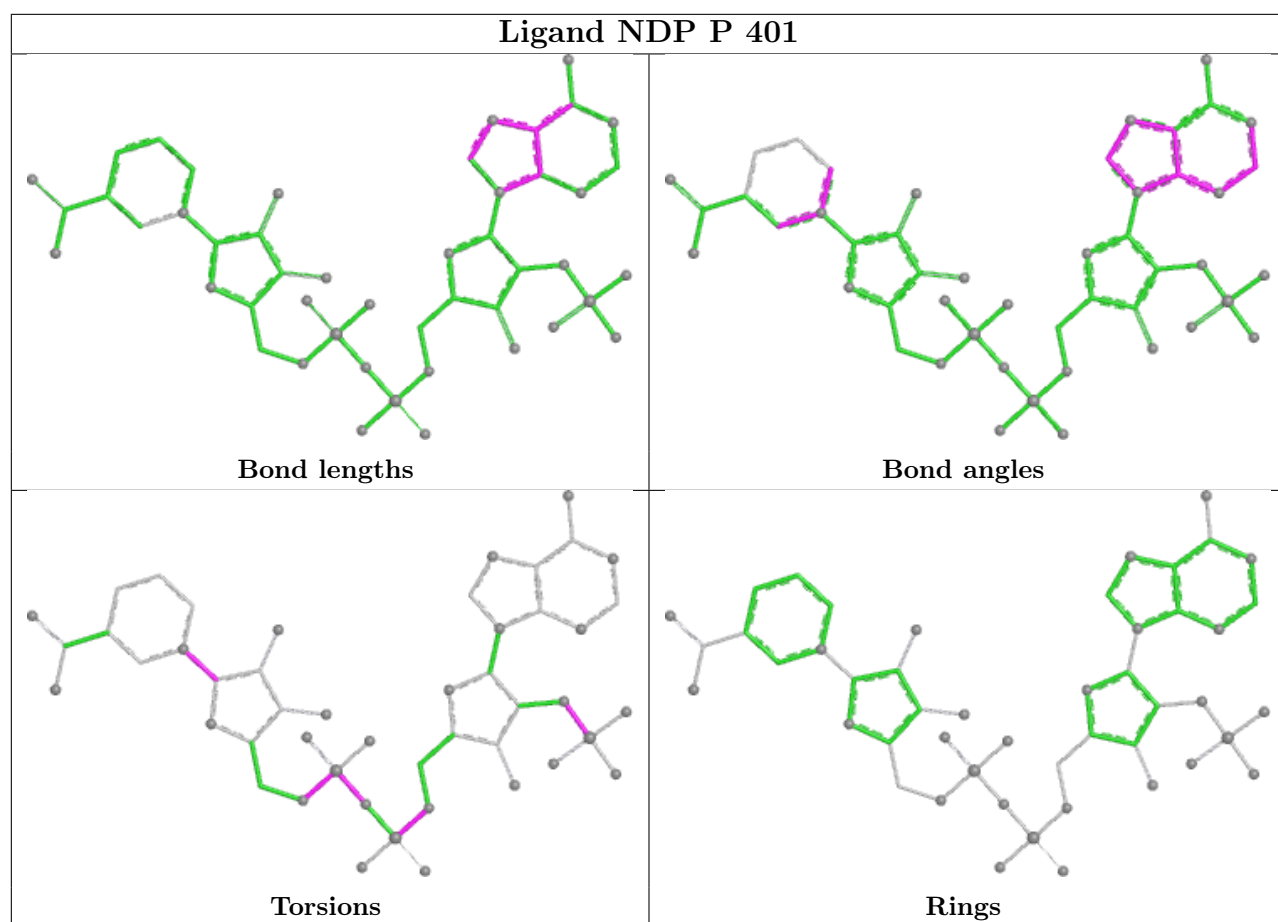
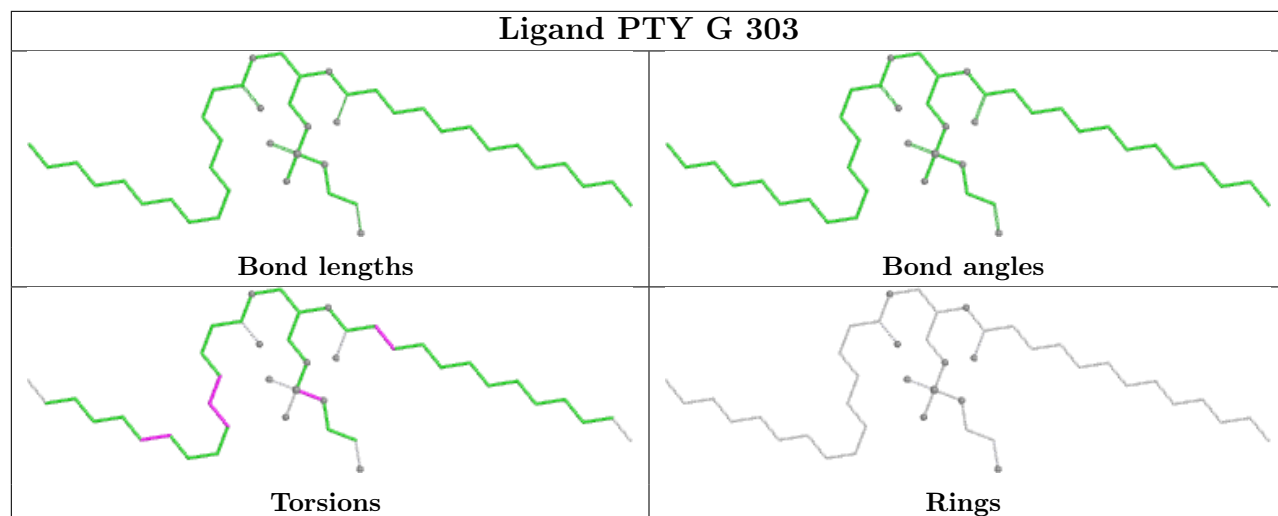


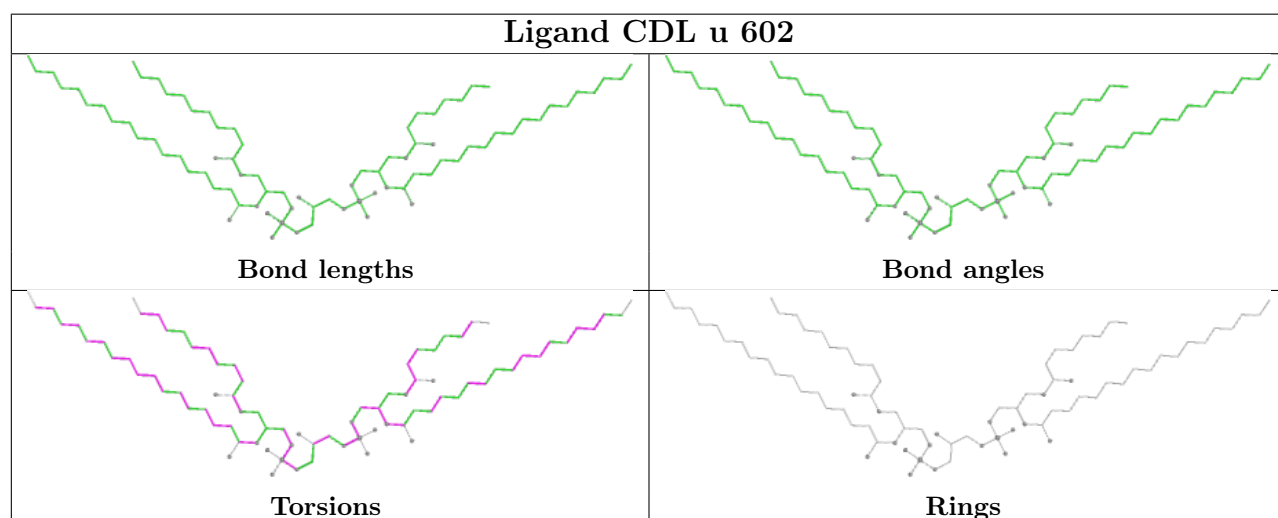
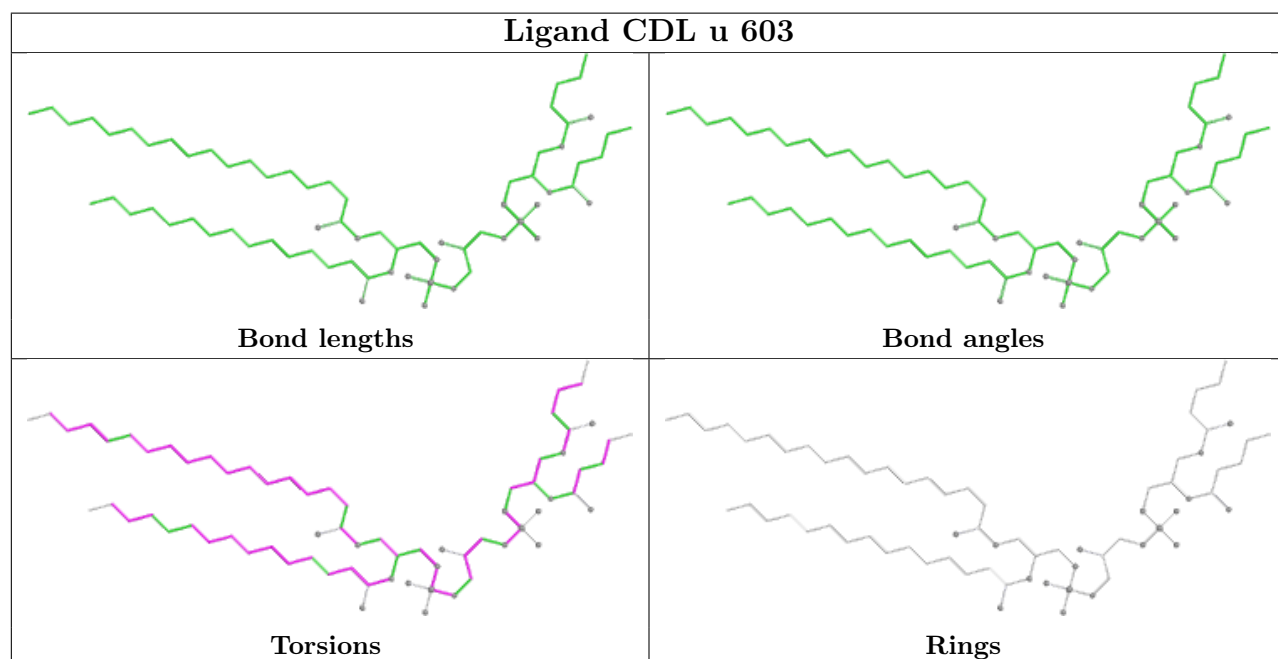
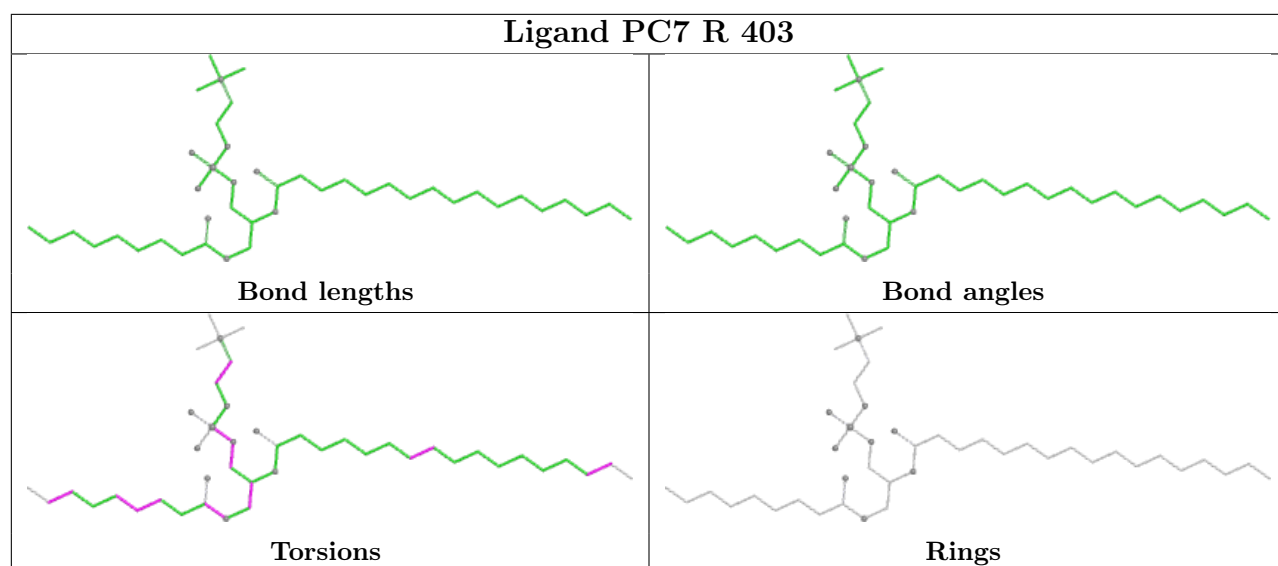


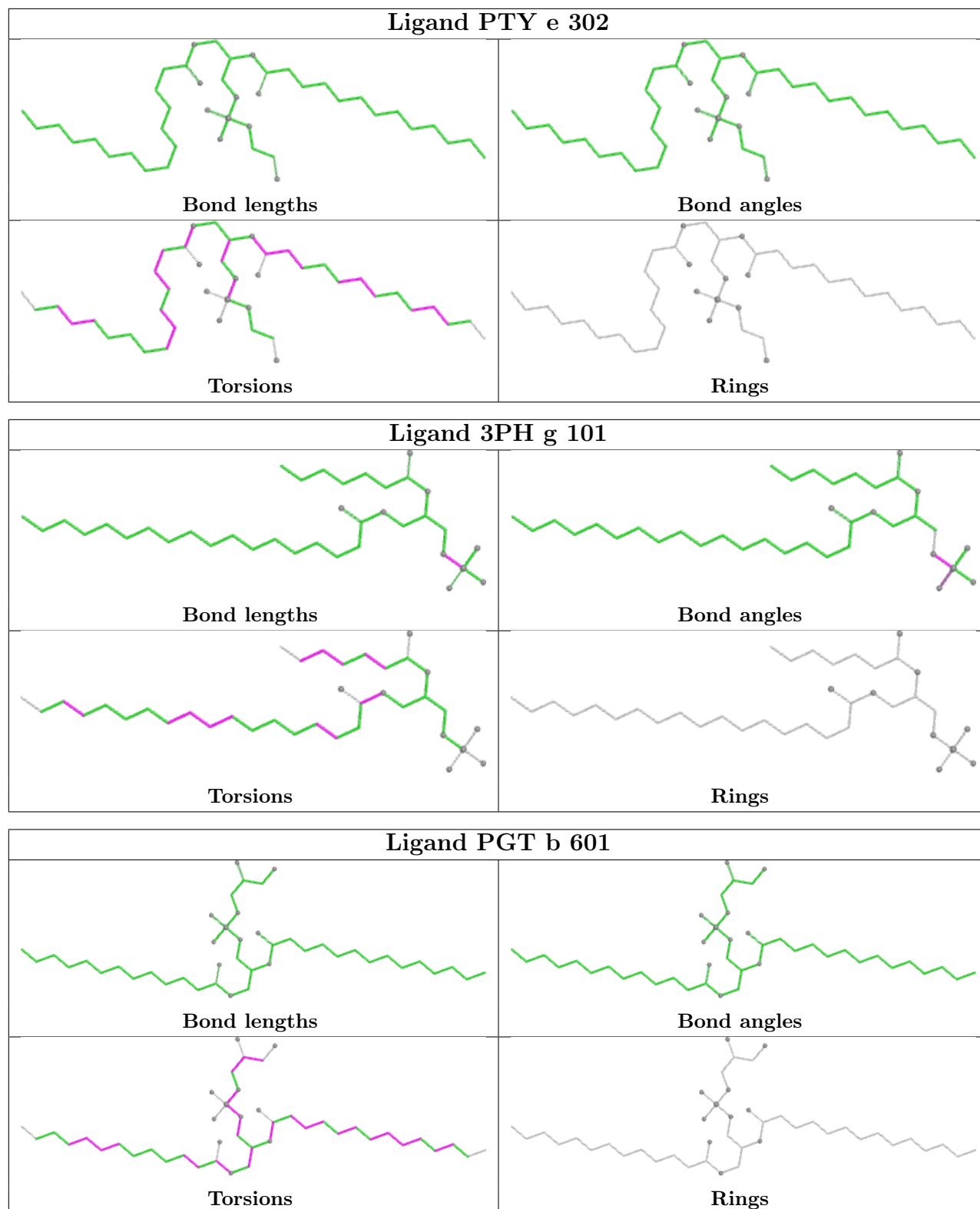


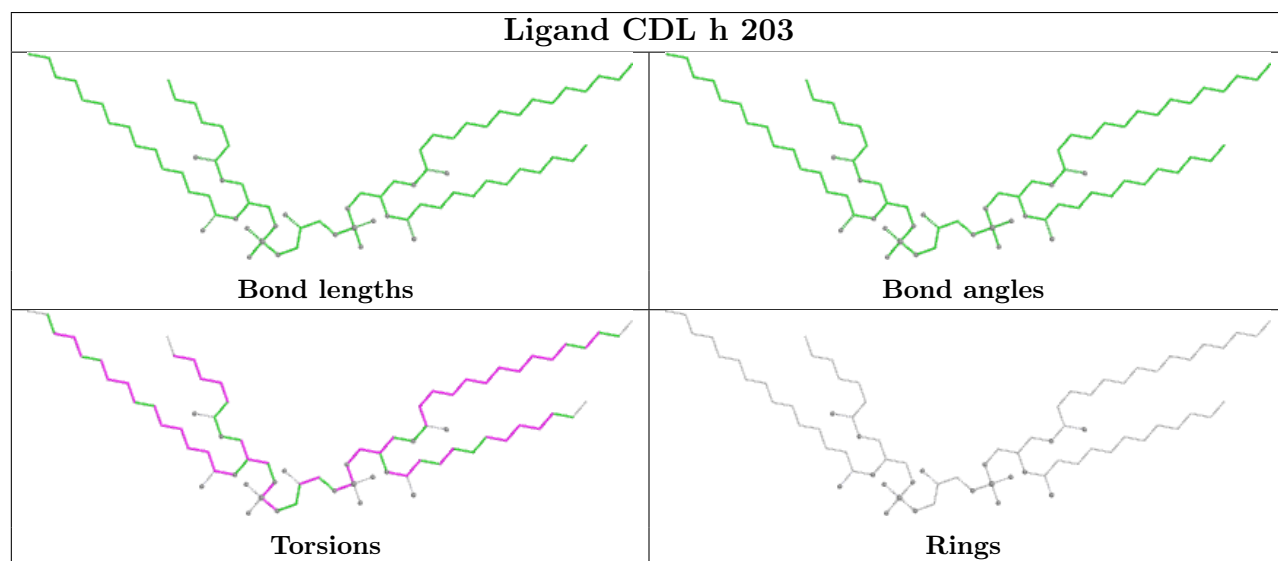
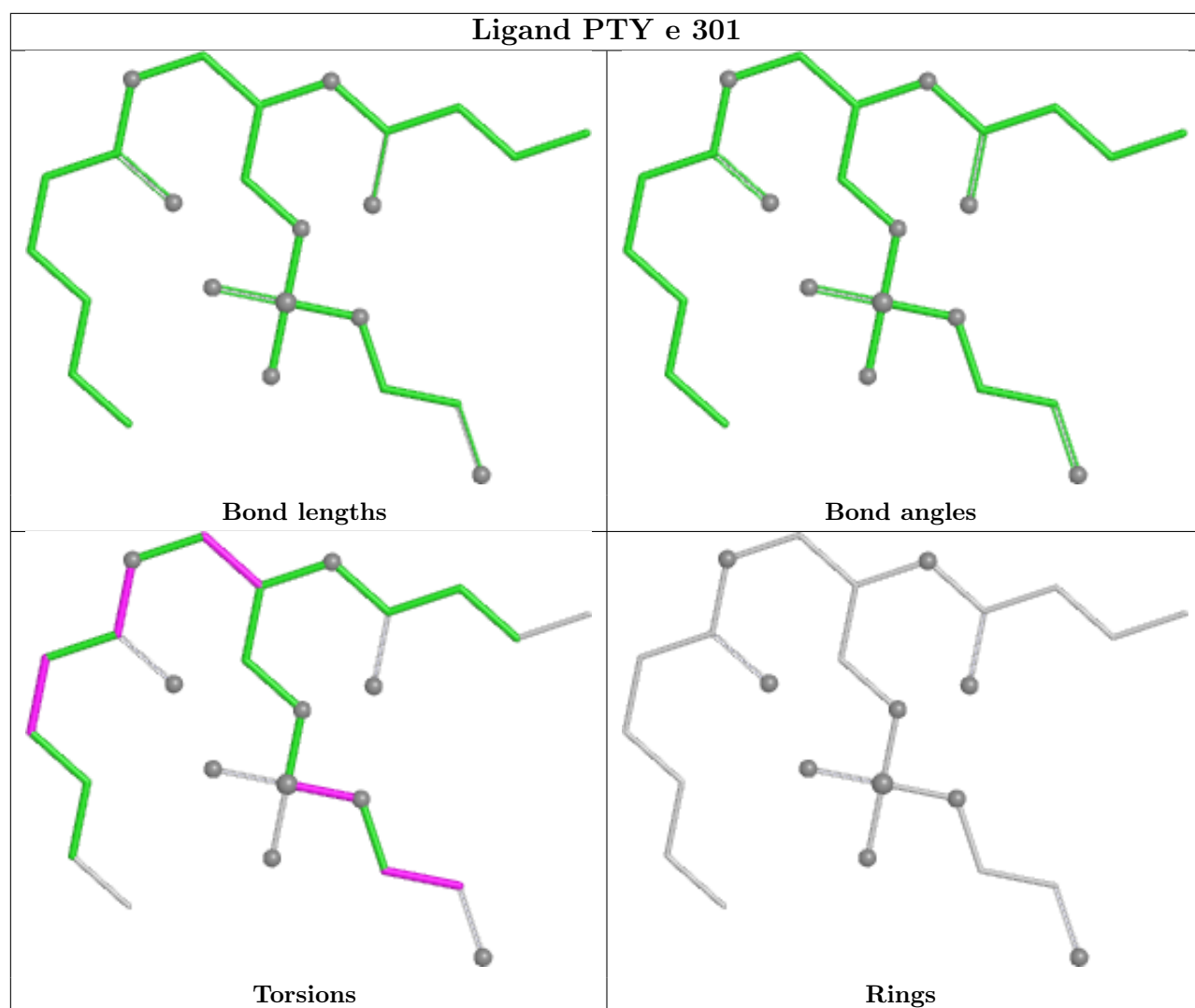


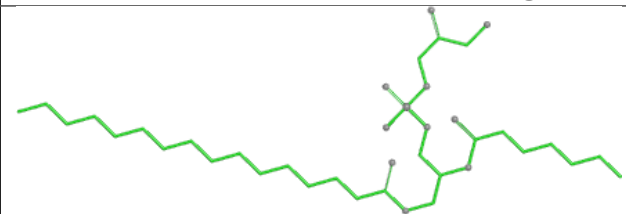
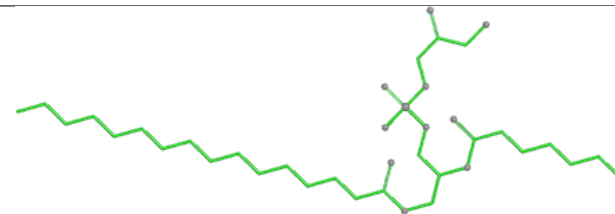
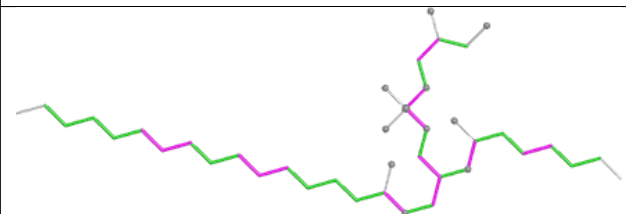
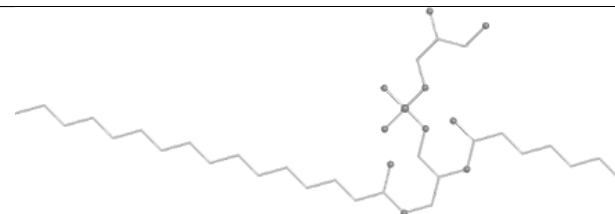


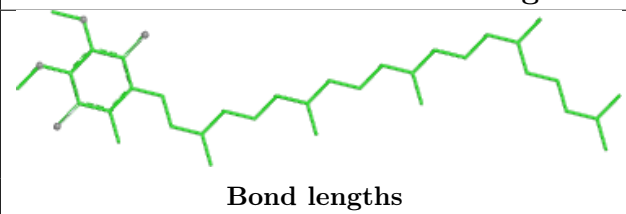
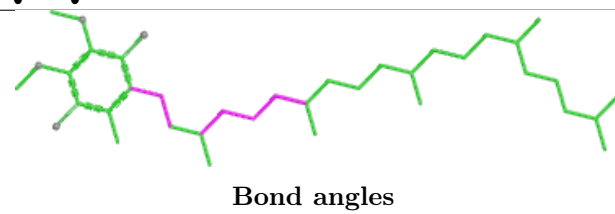
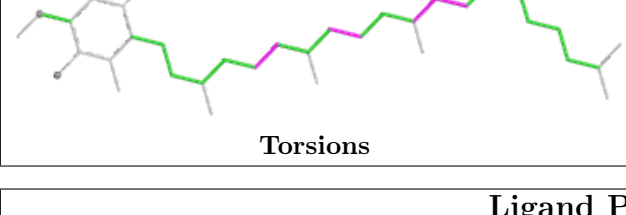
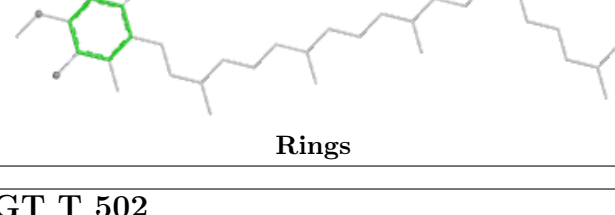


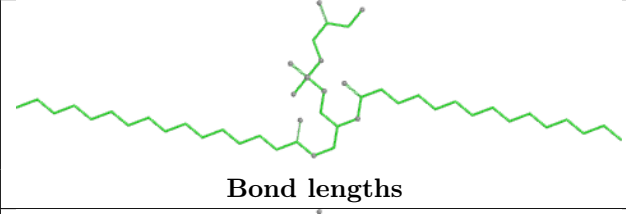
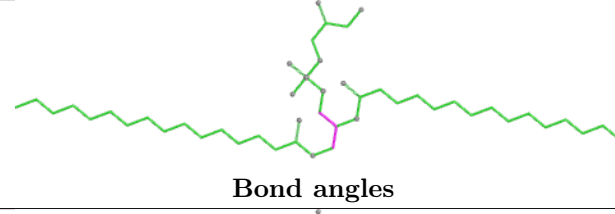
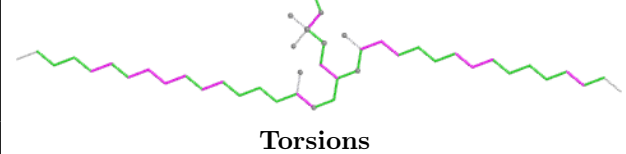
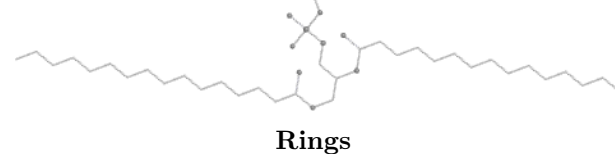


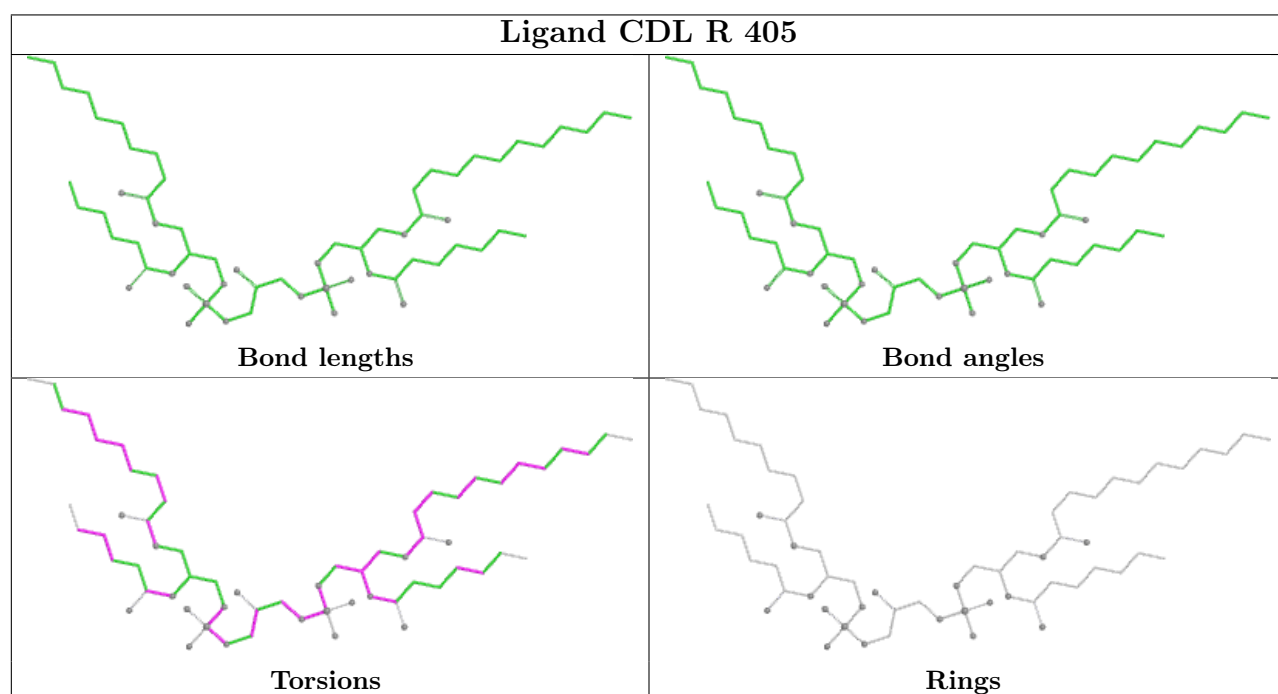
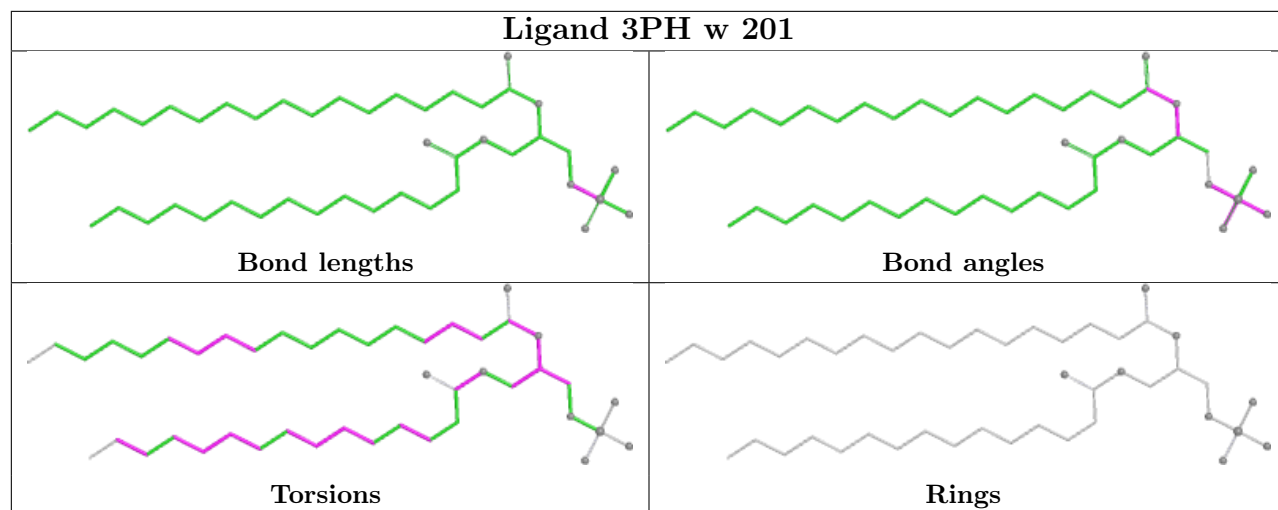


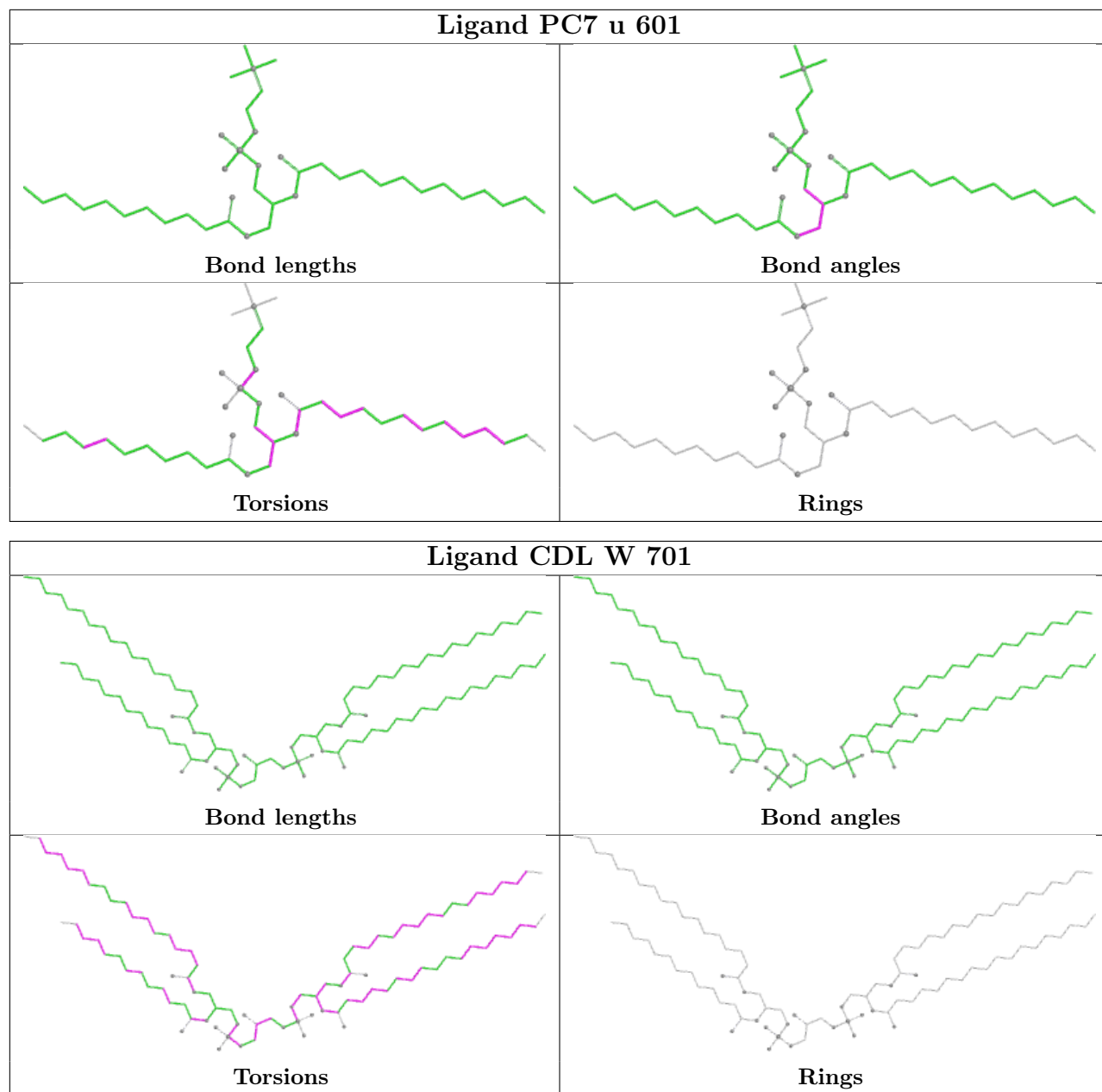


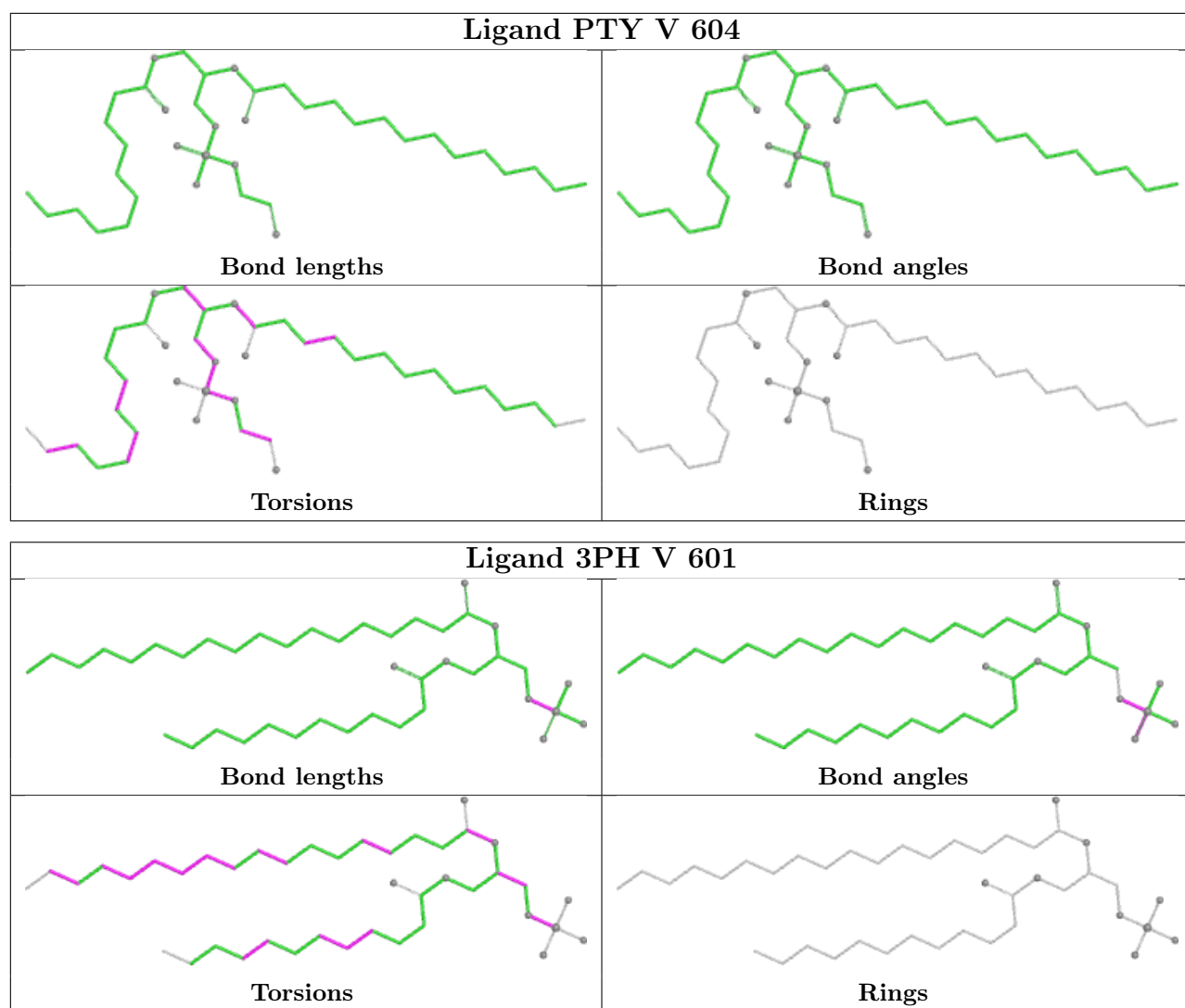
Ligand PGT T 505	
	
Bond lengths	Bond angles
	
Torsions	Rings

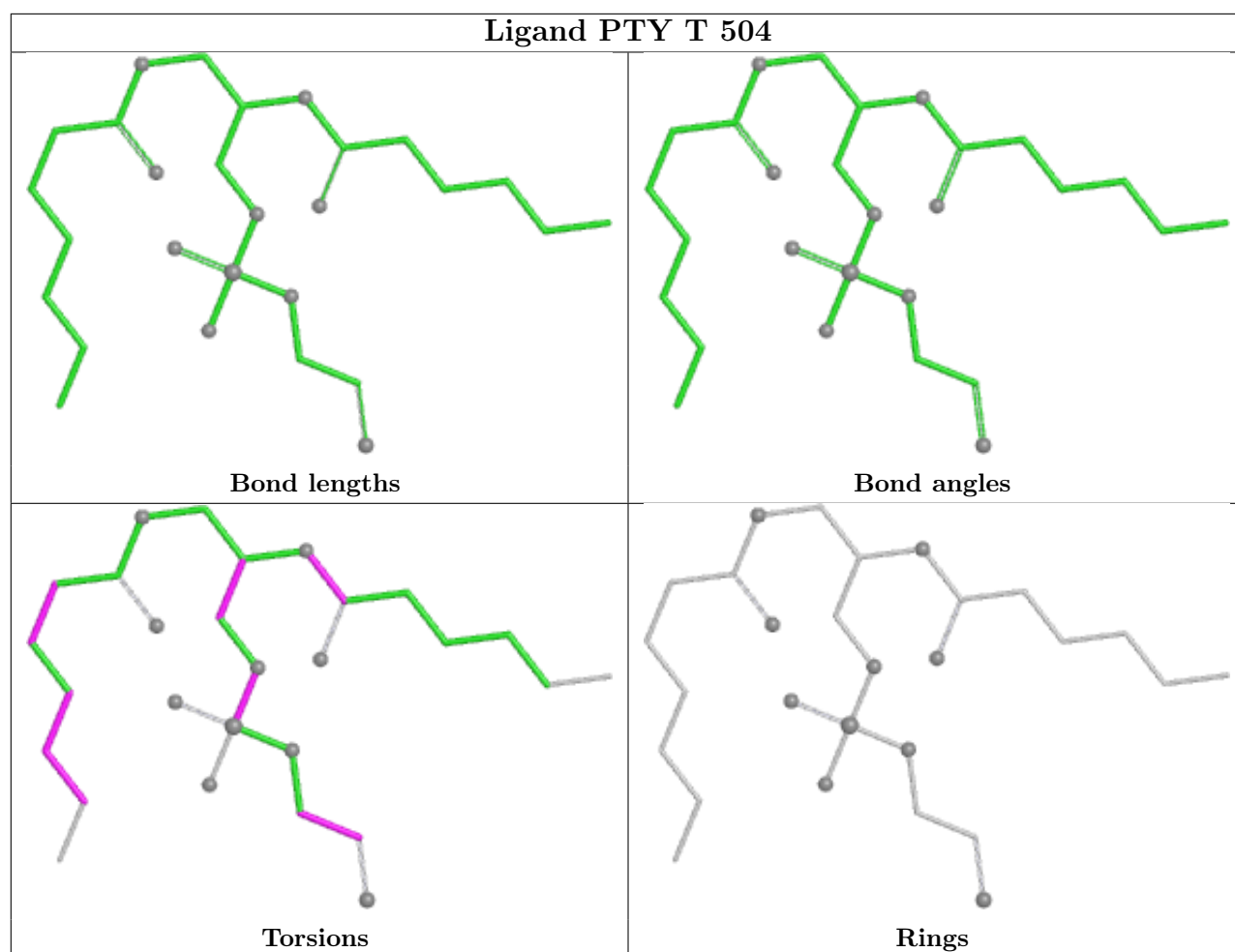
Ligand UQ5 Q 301	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PGT T 502	
	
Bond lengths	Bond angles
	
Torsions	Rings









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.

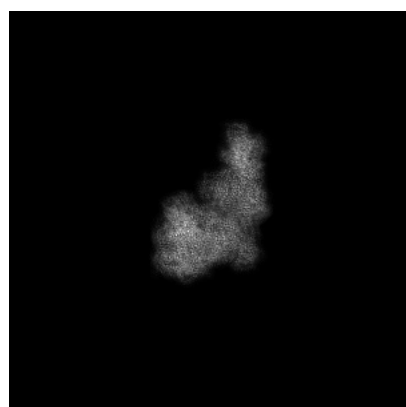
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50203. These allow visual inspection of the internal detail of the map and identification of artifacts.

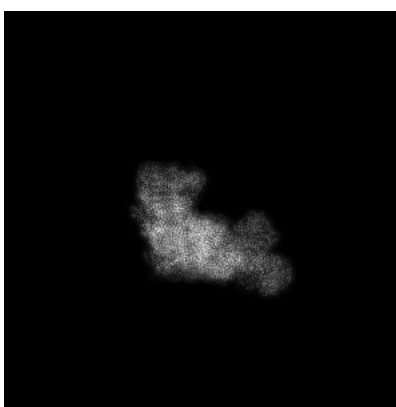
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

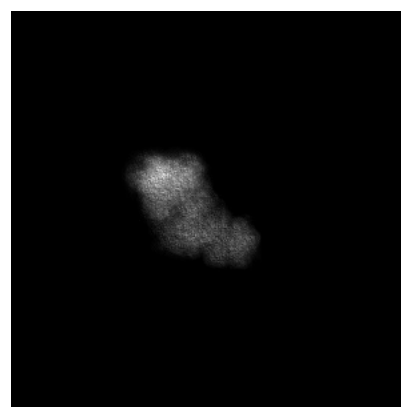
6.1.1 Primary map



X



Y

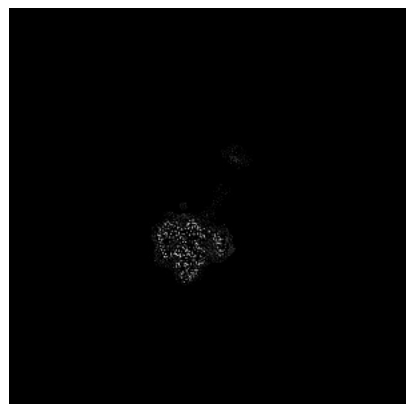


Z

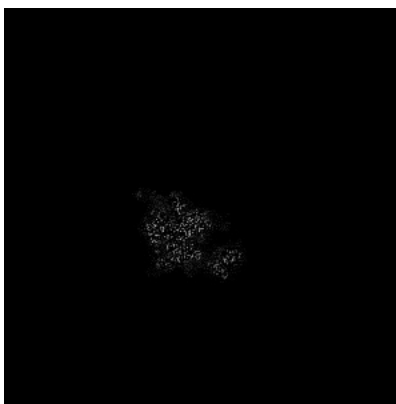
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

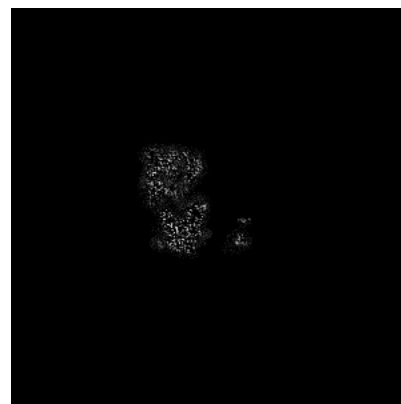
6.2.1 Primary map



X Index: 294



Y Index: 294

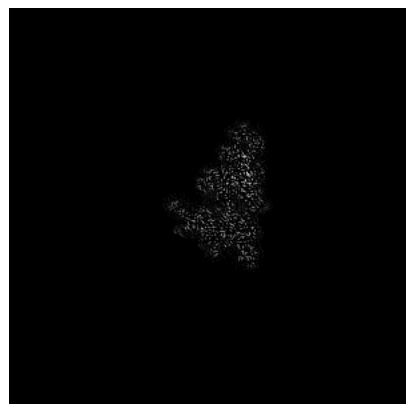


Z Index: 294

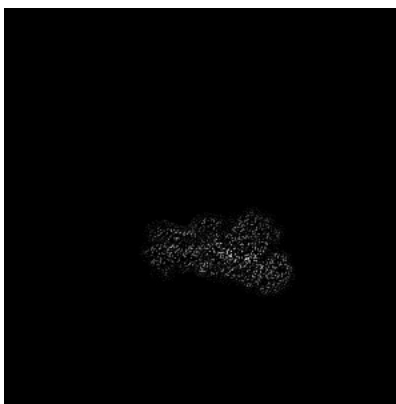
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

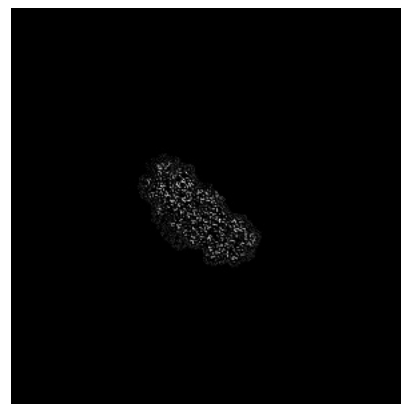
6.3.1 Primary map



X Index: 221



Y Index: 345

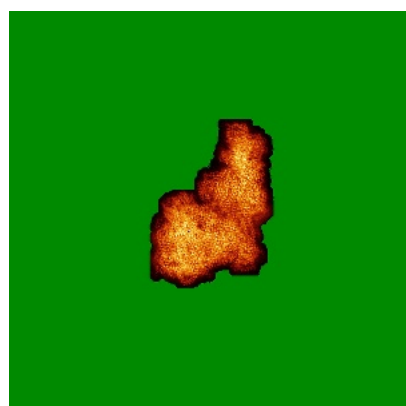


Z Index: 252

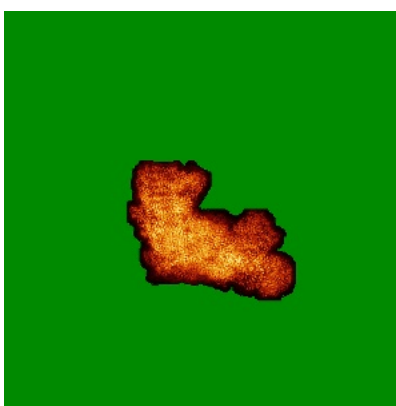
The images above show the largest variance slices of the map in three orthogonal directions.

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

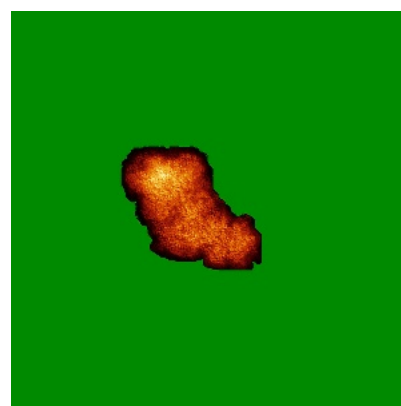
6.4.1 Primary map



X



Y

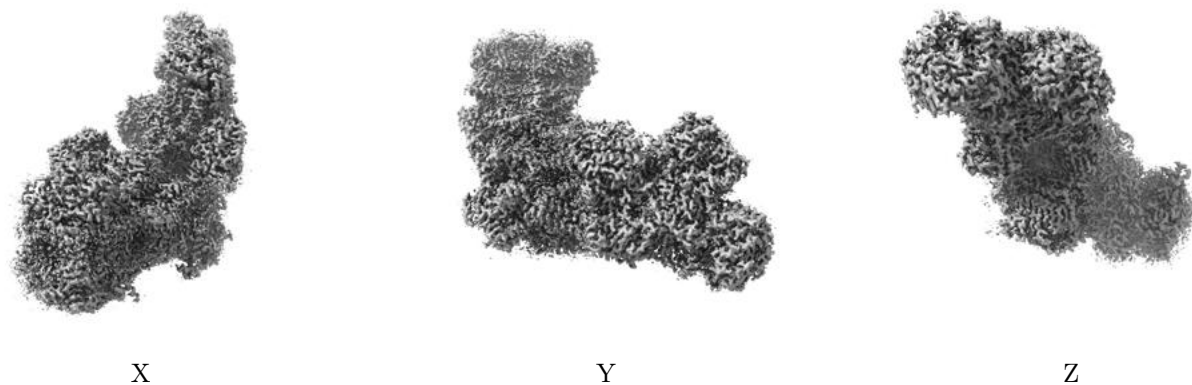


Z

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 [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.141. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

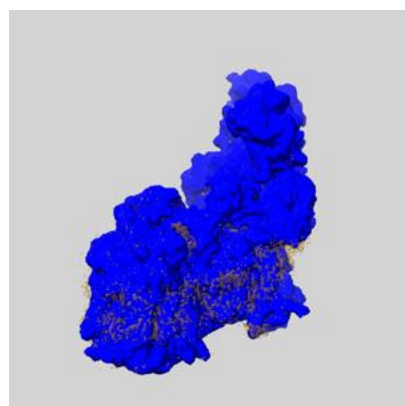
6.6 Mask visualisation [i](#)

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

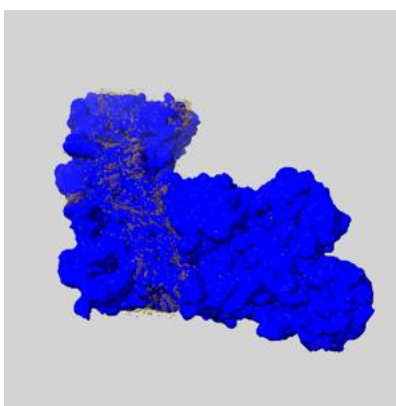
A mask typically either:

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

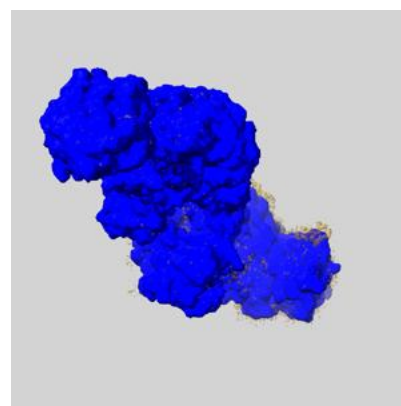
6.6.1 emd_50203_msk_1.map [i](#)



X



Y

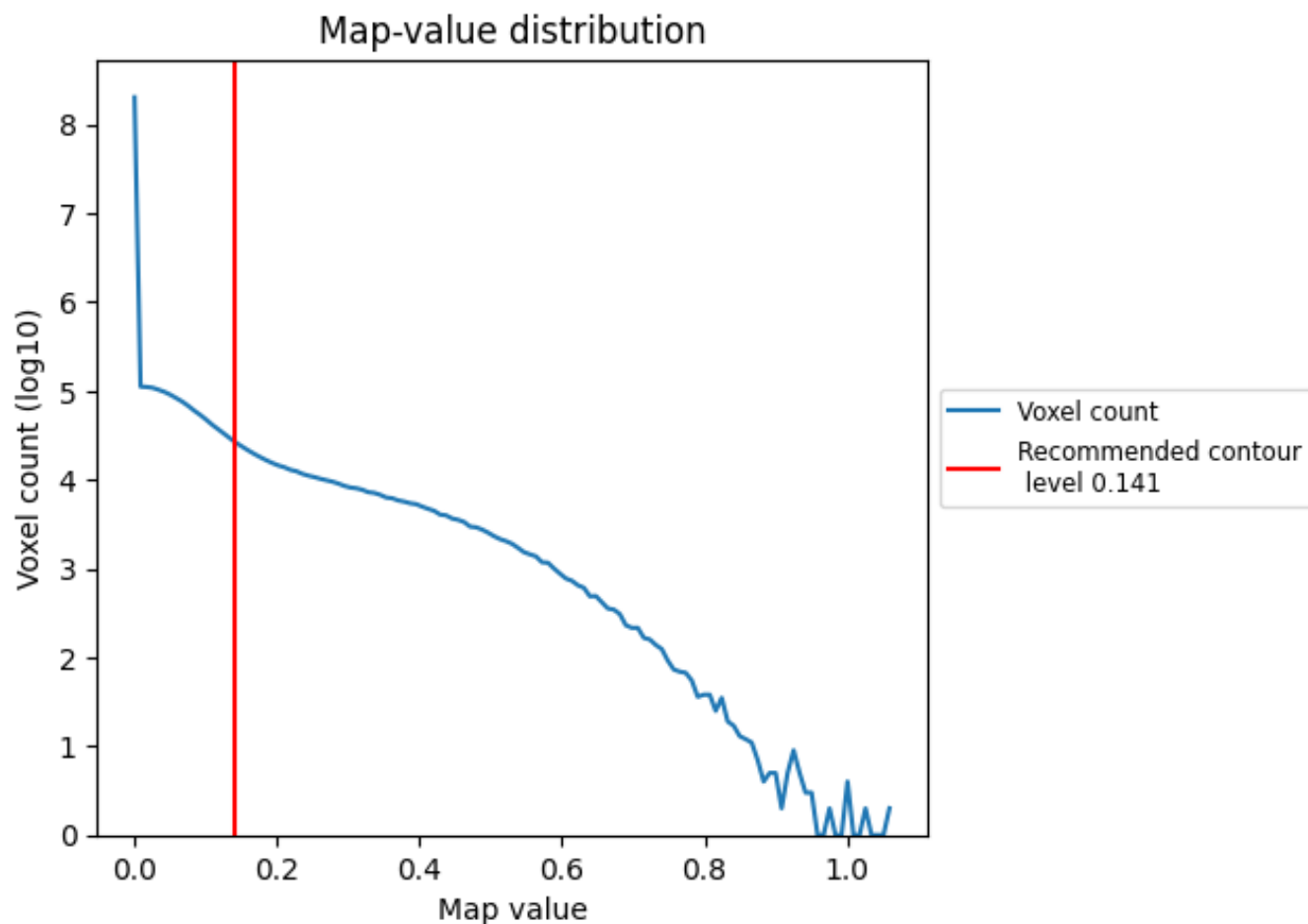


Z

7 Map analysis [i](#)

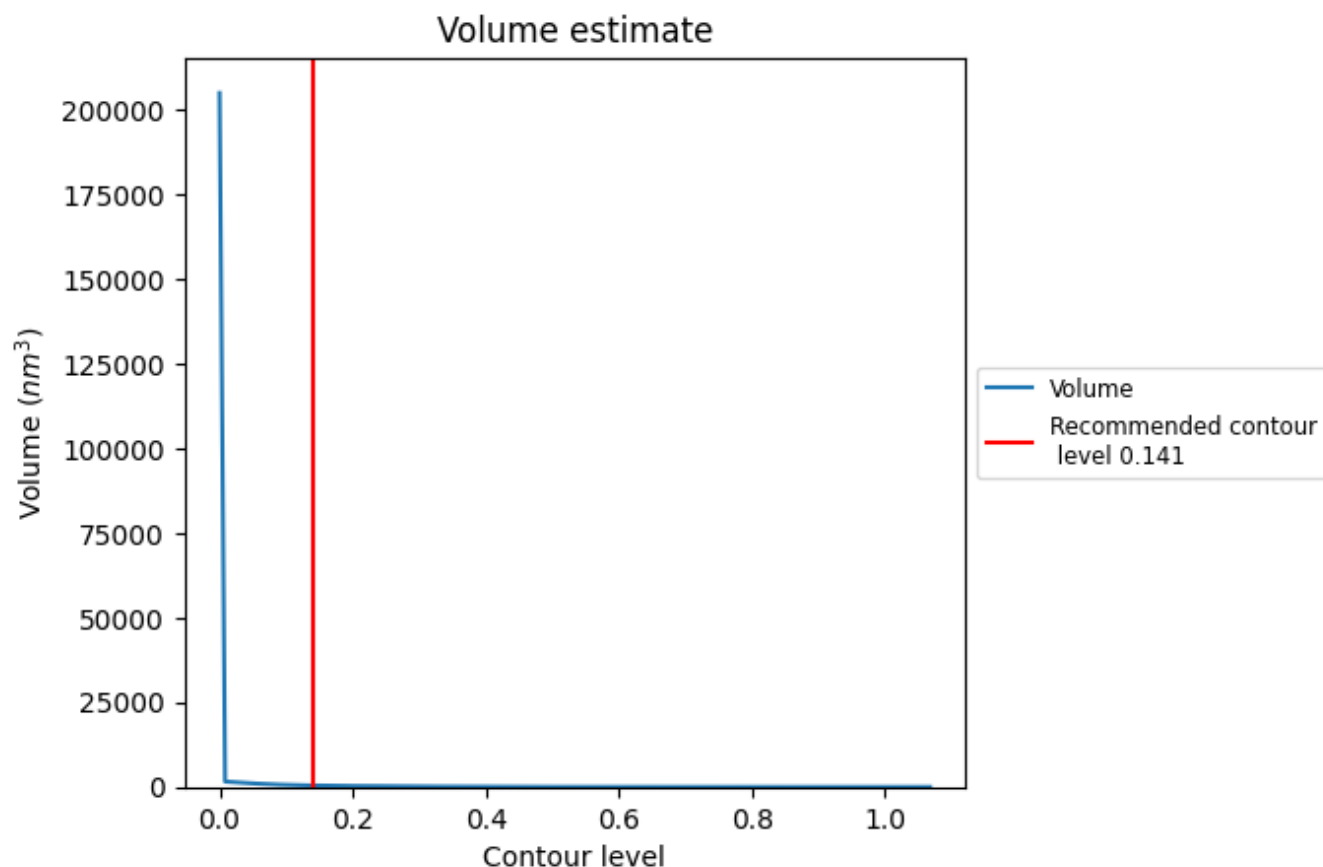
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

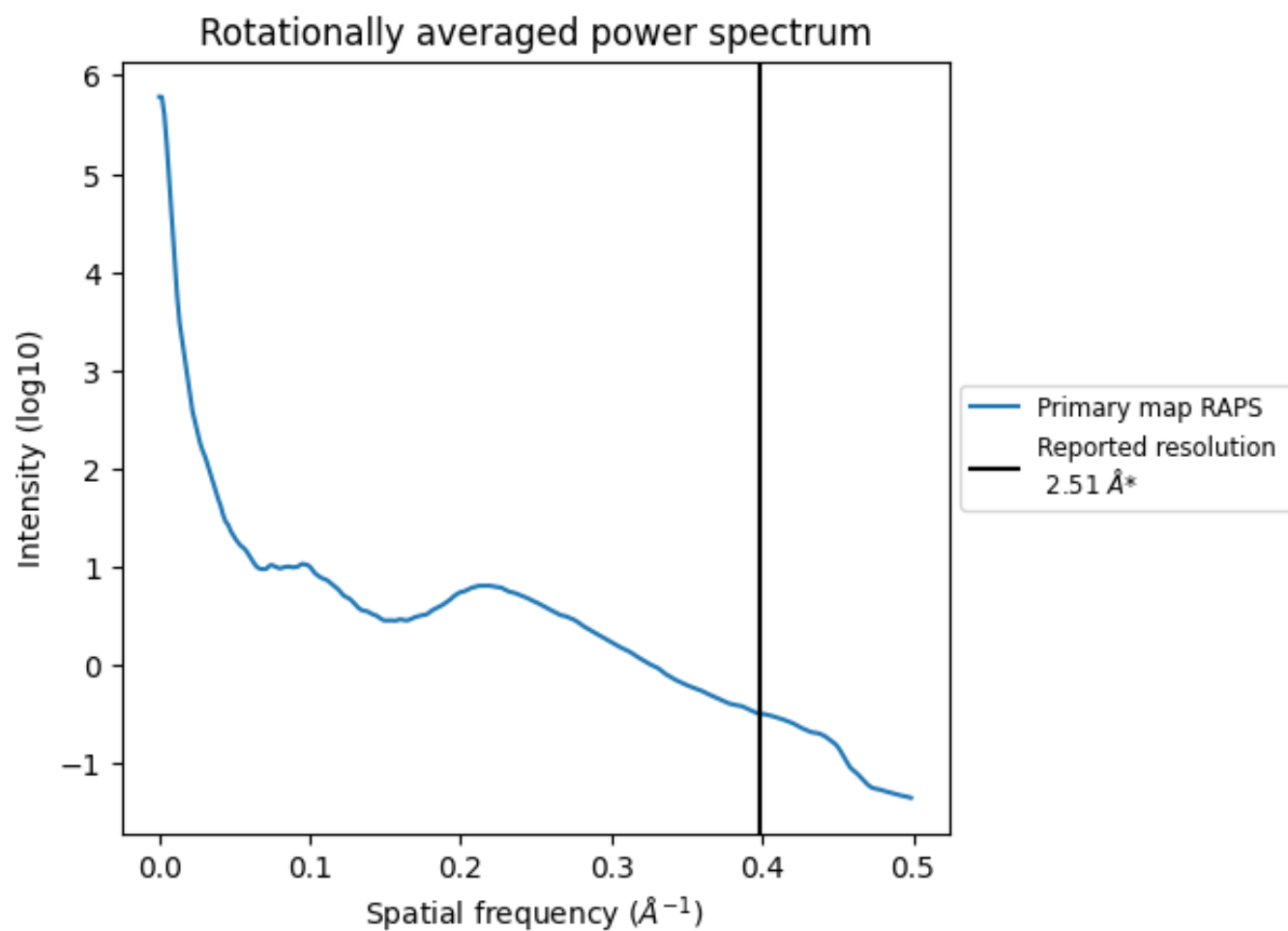
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 434 nm^3 ; this corresponds to an approximate mass of 392 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 ⓘ

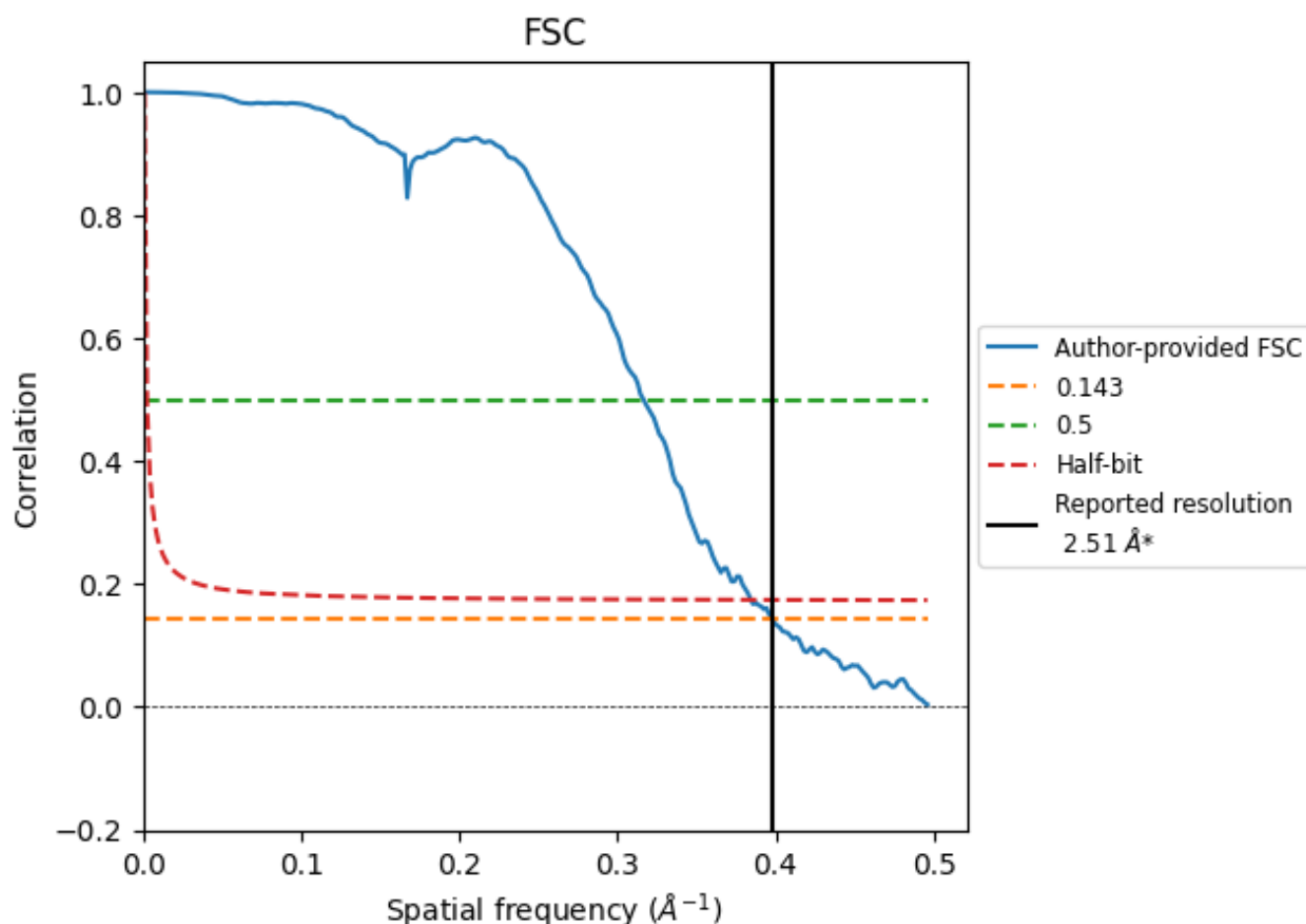


*Reported resolution corresponds to spatial frequency of 0.398 Å⁻¹

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 0.398 Å⁻¹

8.2 Resolution estimates [i](#)

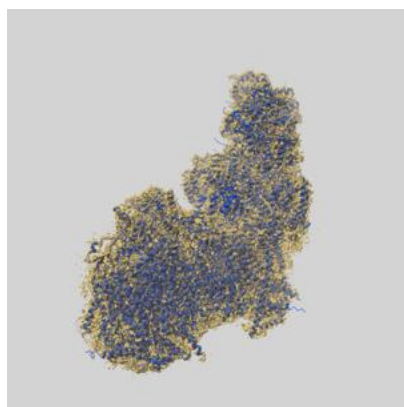
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.51	-	-
Author-provided FSC curve	2.51	3.16	2.60
Unmasked-calculated*	-	-	-

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

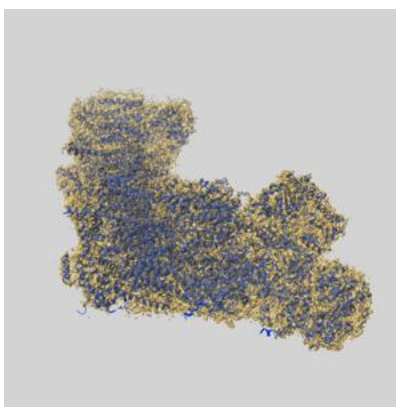
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-50203 and PDB model 9F5Y. Per-residue inclusion information can be found in section [3](#) on page [24](#).

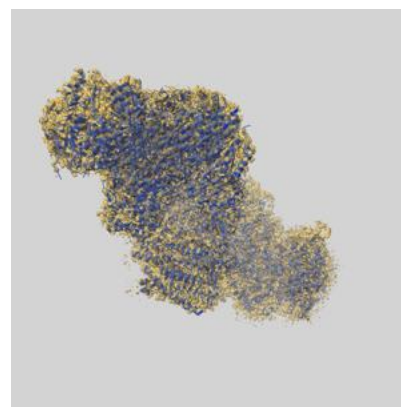
9.1 Map-model overlay [i](#)



X



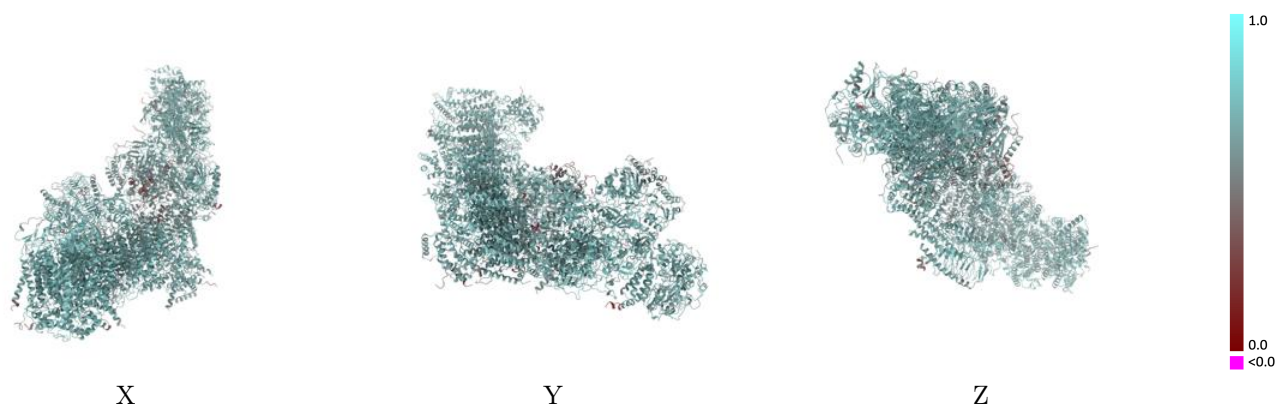
Y



Z

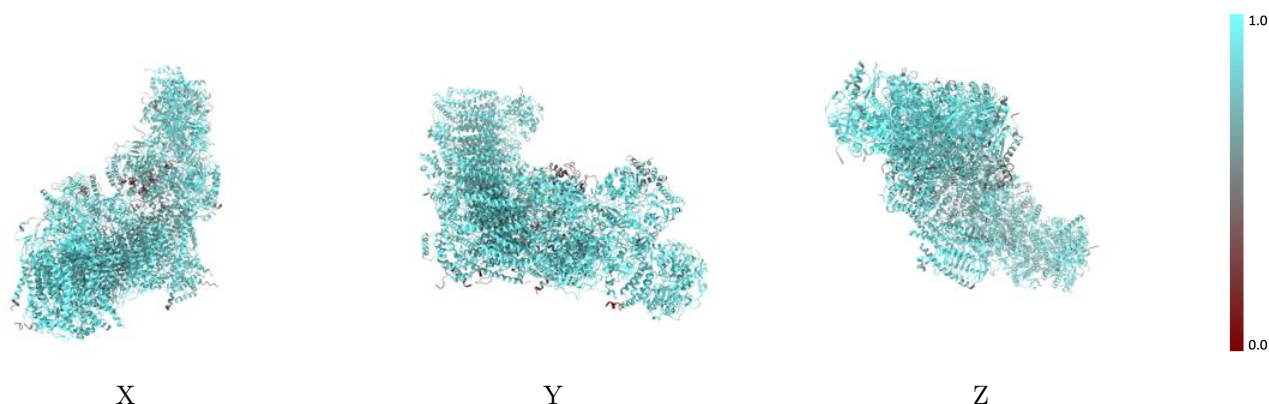
The images above show the 3D surface view of the map at the recommended contour level 0.141 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



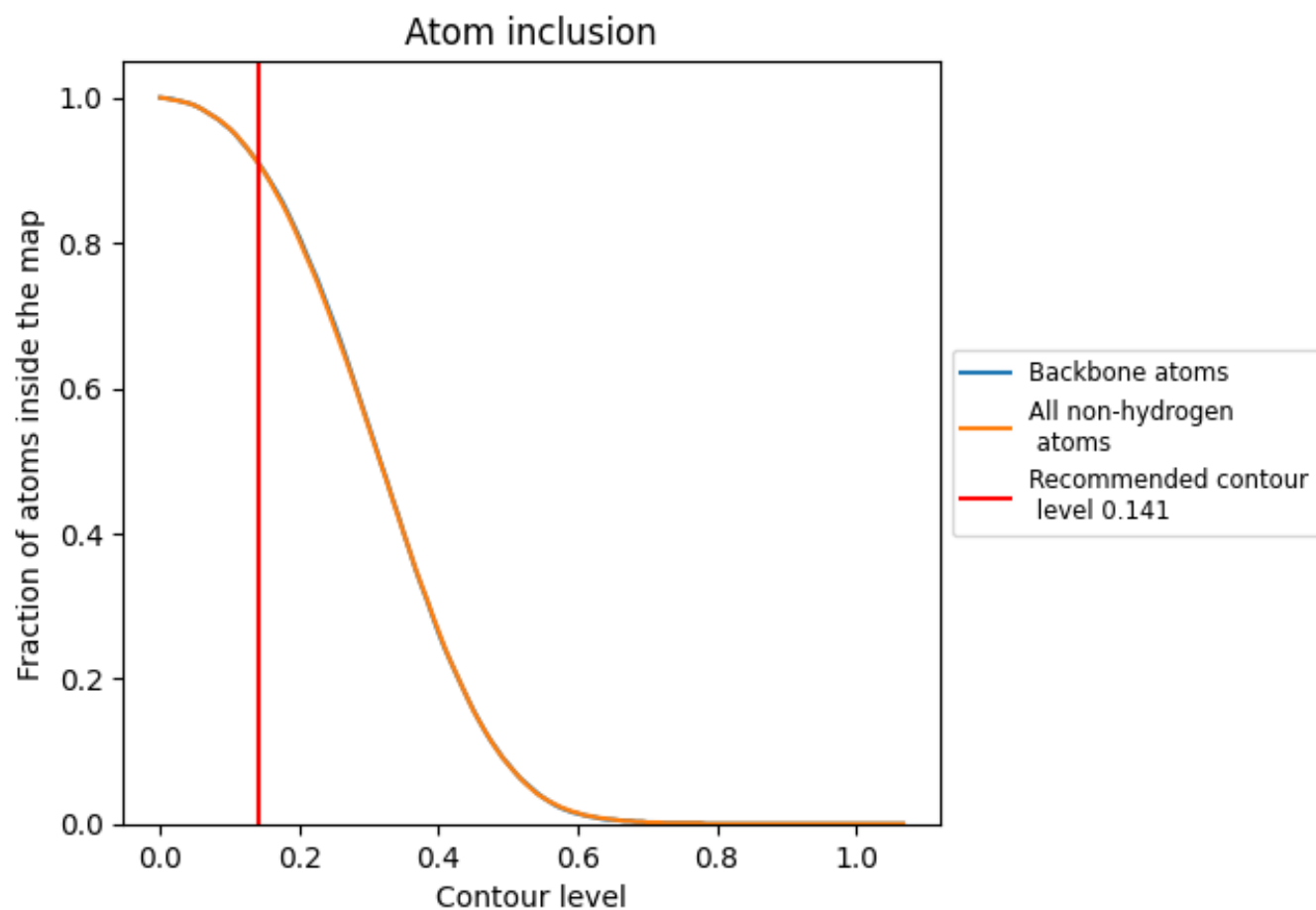
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.141).

9.4 Atom inclusion ⓘ



At the recommended contour level, 91% of all backbone atoms, 91% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.141) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9090	 0.6620
A	 0.8780	 0.6380
B	 0.9170	 0.6520
C	 0.9200	 0.6640
D	 0.9500	 0.6840
E	 0.9470	 0.6730
F	 0.9480	 0.6620
G	 0.9390	 0.6720
H	 0.8900	 0.6480
I	 0.8450	 0.6330
J	 0.5040	 0.4580
K	 0.7710	 0.5790
L	 0.8820	 0.6440
M	 0.8960	 0.6650
N	 0.8970	 0.6540
O	 0.7580	 0.5770
P	 0.8800	 0.6270
Q	 0.9240	 0.6520
R	 0.9450	 0.6840
S	 0.9150	 0.6560
T	 0.9710	 0.7050
U	 0.9550	 0.6910
V	 0.9620	 0.6990
W	 0.9190	 0.6630
X	 0.9600	 0.6950
Y	 0.8980	 0.6440
Z	 0.9250	 0.6820
a	 0.8750	 0.6360
b	 0.9210	 0.6870
c	 0.6900	 0.5460
d	 0.9350	 0.6700
e	 0.9500	 0.6790
f	 0.8990	 0.6490
g	 0.7460	 0.5720
h	 0.9030	 0.6750



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Chain	Atom inclusion	Q-score
i	 0.8940	 0.6610
j	 0.9370	 0.6780
k	 0.9370	 0.6800
l	 0.8550	 0.6300
m	 0.8840	 0.6450
n	 0.8340	 0.6300
o	 0.9440	 0.6840
p	 0.9140	 0.6620
q	 0.9200	 0.6730
r	 0.8600	 0.6350
s	 0.8950	 0.6520
t	 0.9480	 0.6940
u	 0.9060	 0.6670
v	 0.8770	 0.6370
w	 0.9070	 0.6680
x	 0.9110	 0.6670
y	 0.9240	 0.6780