



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 12:01 PM UTC

PDB ID : 6YNX / pdb_00006ynx
EMDB ID : EMD-10859
Title : Cryo-EM structure of Tetrahymena thermophila mitochondrial ATP synthase
- Fo-subcomplex
Authors : Kock Flygaard, R.; Muhleip, A.; Amunts, A.
Deposited on : 2020-04-14
Resolution : 2.50 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

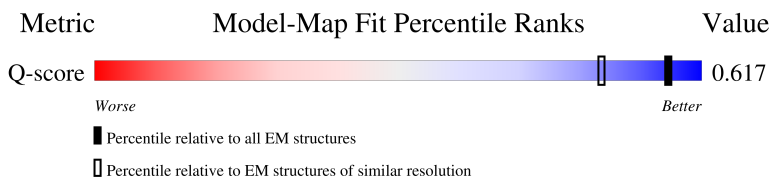
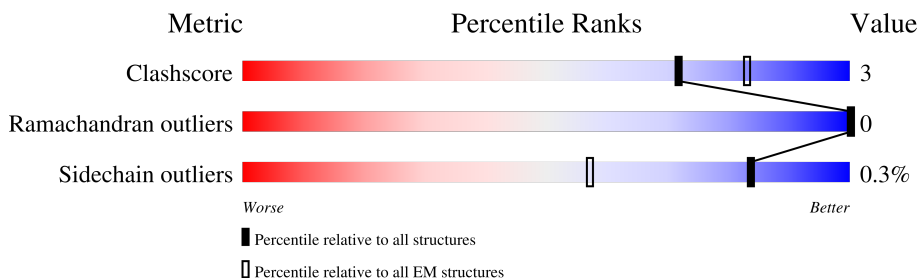
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.50 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.



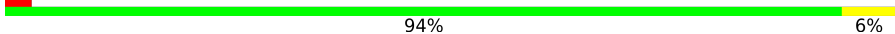
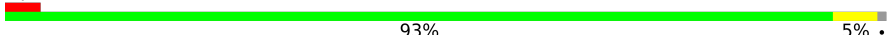
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7115 (2.00 - 3.00)

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	446	
1	a	446	
2	B	381	
2	b	381	

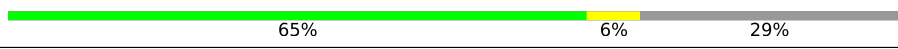
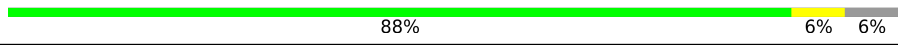
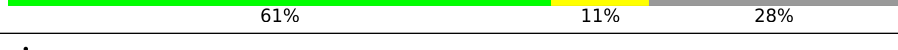
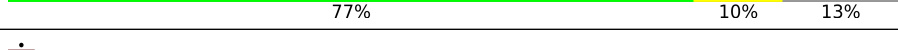
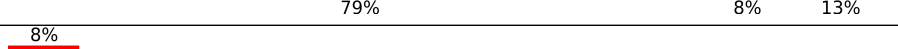
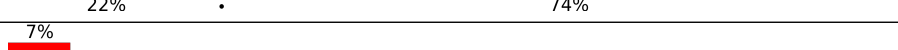
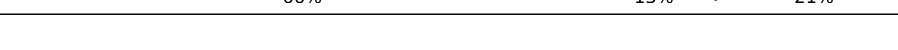
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Mol	Chain	Length	Quality of chain
3	D	234	
3	d	234	
4	F	204	
4	f	204	
5	I	209	
5	i	209	
6	K	179	
6	k	179	
7	C	100	
7	c	100	
8	G	286	
8	g	286	
9	H	268	
9	h	268	
10	J	273	
10	j	273	
11	L	247	
11	l	247	
12	M	221	
12	m	221	
13	N	179	
13	n	179	
14	O	154	
14	o	154	
15	P	152	

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Mol	Chain	Length	Quality of chain
15	p	152	
16	Q	152	
16	q	152	
17	R	149	
17	r	149	
18	S	145	
18	s	145	
19	E	480	
19	e	480	
20	i1	108	
20	i2	108	
21	t	460	

2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 139915 atoms, of which 70075 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called subunit a.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	a	433	Total	C	H	N	O	S	0	0
			7157	2453	3529	526	633	16		
1	A	433	Total	C	H	N	O	S	0	0
			7157	2453	3529	526	633	16		

- Molecule 2 is a protein called subunit b.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	b	161	Total	C	H	N	O	S	0	0
			2678	903	1310	223	232	10		
2	B	161	Total	C	H	N	O	S	0	0
			2675	903	1307	223	232	10		

- Molecule 3 is a protein called subunit d.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	d	110	Total	C	H	N	O	S	0	0
			1764	591	846	147	176	4		
3	D	110	Total	C	H	N	O	S	0	0
			1764	591	846	147	176	4		

- Molecule 4 is a protein called subunit f.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	f	200	Total	C	H	N	O	S	0	0
			3373	1095	1691	299	278	10		
4	F	200	Total	C	H	N	O	S	0	0
			3374	1095	1692	299	278	10		

- Molecule 5 is a protein called subunit i/j.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	i	209	Total	C	H	N	O	S	0	0
			3461	1121	1741	304	285	10		
5	I	209	Total	C	H	N	O	S	0	0
			3461	1121	1741	304	285	10		

- Molecule 6 is a protein called subunit k.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	k	179	Total	C	H	N	O	S	0	0
			2903	939	1430	257	266	11		
6	K	179	Total	C	H	N	O	S	0	0
			2903	939	1430	257	266	11		

- Molecule 7 is a protein called subunit 8.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	c	96	Total	C	H	N	O	S	0	0
			1671	565	830	131	143	2		
7	C	96	Total	C	H	N	O	S	0	0
			1671	565	830	131	143	2		

- Molecule 8 is a protein called ATPTT3.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	g	256	Total	C	H	N	O	S	0	0
			4338	1474	2118	348	388	10		
8	G	256	Total	C	H	N	O	S	0	0
			4338	1474	2118	348	388	10		

- Molecule 9 is a protein called ATPTT4.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	h	231	Total	C	H	N	O	S	0	0
			3836	1236	1883	361	350	6		
9	H	231	Total	C	H	N	O	S	0	0
			3836	1236	1883	361	350	6		

- Molecule 10 is a protein called ATPTT5.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	j	269	Total	C	H	N	O	S	0	0
			4346	1381	2147	406	404	8		

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Mol	Chain	Residues	Atoms						AltConf	Trace
10	J	269	Total	C	H	N	O	S	0	0
			4344	1381	2145	406	404	8		

- Molecule 11 is a protein called ATPTT6.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	I	246	Total	C	H	N	O	S	0	0
			4070	1344	1999	360	361	6		
11	L	246	Total	C	H	N	O	S	0	0
			4070	1344	1999	360	361	6		

- Molecule 12 is a protein called ATPTT7.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	m	221	Total	C	H	N	O	S	0	0
			3696	1205	1835	313	336	7		
12	M	221	Total	C	H	N	O	S	0	0
			3696	1205	1835	313	336	7		

- Molecule 13 is a protein called ATPTT8.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	n	119	Total	C	H	N	O	S	0	0
			1960	655	962	164	173	6		
13	N	119	Total	C	H	N	O	S	0	0
			1960	655	962	164	173	6		

- Molecule 14 is a protein called ATPTT9.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	o	99	Total	C	H	N	O	S	0	0
			1599	507	794	145	147	6		
14	O	99	Total	C	H	N	O	S	0	0
			1599	507	794	145	147	6		

- Molecule 15 is a protein called ATPTT10.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	p	150	Total	C	H	N	O	S	0	0
			2413	788	1196	204	224	1		
15	P	150	Total	C	H	N	O	S	0	0
			2413	788	1196	204	224	1		

- Molecule 16 is a protein called ATPTT11.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	q	108	Total	C	H	N	O	S	0	0
			1749	556	874	149	169	1		
16	Q	108	Total	C	H	N	O	S	0	0
			1749	556	874	149	169	1		

- Molecule 17 is a protein called ATPTT12.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	r	145	Total	C	H	N	O	S	0	0
			2373	776	1180	201	212	4		
17	R	140	Total	C	H	N	O	S	0	0
			2288	750	1134	194	206	4		

- Molecule 18 is a protein called ATPTT13.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	s	105	Total	C	H	N	O	S	0	0
			1714	552	849	148	160	5		
18	S	106	Total	C	H	N	O	S	0	0
			1728	556	856	149	162	5		

- Molecule 19 is a protein called ATPTT1.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	e	417	Total	C	H	N	O	S	0	0
			6681	2171	3286	602	614	8		
19	E	417	Total	C	H	N	O	S	0	0
			6681	2171	3286	602	614	8		

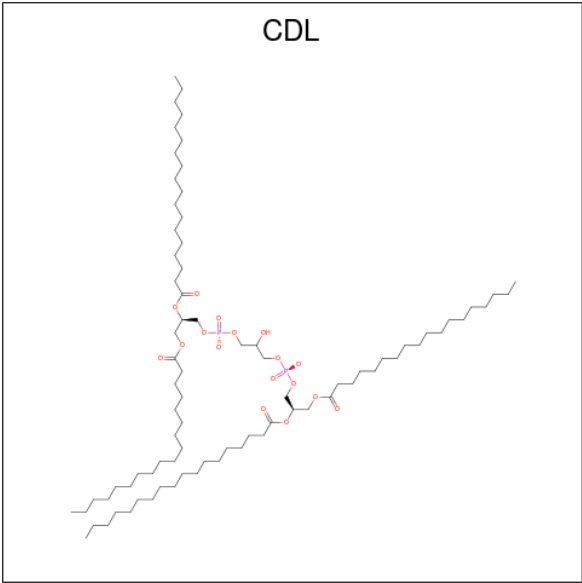
- Molecule 20 is a protein called Inhibitor of F1 (IF1).

Mol	Chain	Residues	Atoms					AltConf	Trace
20	i1	28	Total	C	H	N	O	0	0
			474	154	236	39	45		
20	i2	32	Total	C	H	N	O	0	0
			529	171	262	45	51		

- Molecule 21 is a protein called ATPTT2.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	t	365	Total	C	H	N	O	S	0	0
			5889	1925	2876	533	544	11		

- Molecule 22 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



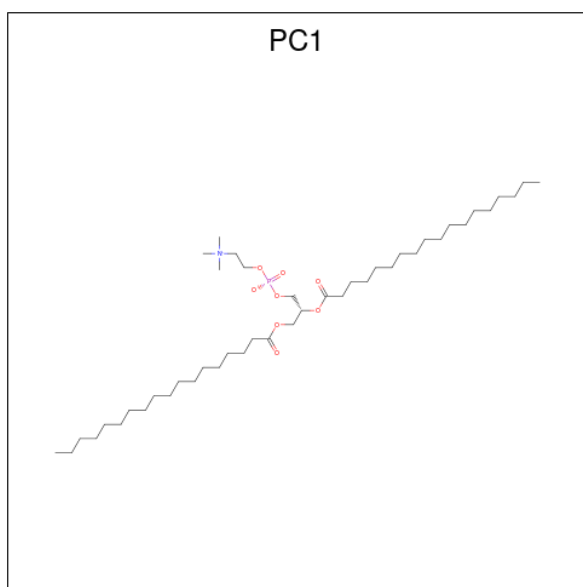
Mol	Chain	Residues	Atoms					AltConf
22	a	1	Total	C	H	O	P	0
			256	81	156	17	2	
22	b	1	Total	C	H	O	P	0
			256	81	156	17	2	
22	b	1	Total	C	H	O	P	0
			256	81	156	17	2	
22	f	1	Total	C	H	O	P	0
			256	81	156	17	2	
22	f	1	Total	C	H	O	P	0
			256	81	156	17	2	
22	f	1	Total	C	H	O	P	0
			256	81	156	17	2	
22	i	1	Total	C	H	O	P	0
			256	81	156	17	2	
22	k	1	Total	C	H	O	P	0
			256	81	156	17	2	
22	k	1	Total	C	H	O	P	0
			256	81	156	17	2	
22	k	1	Total	C	H	O	P	0
			256	81	156	17	2	
22	j	1	Total	C	H	O	P	0
			256	81	156	17	2	

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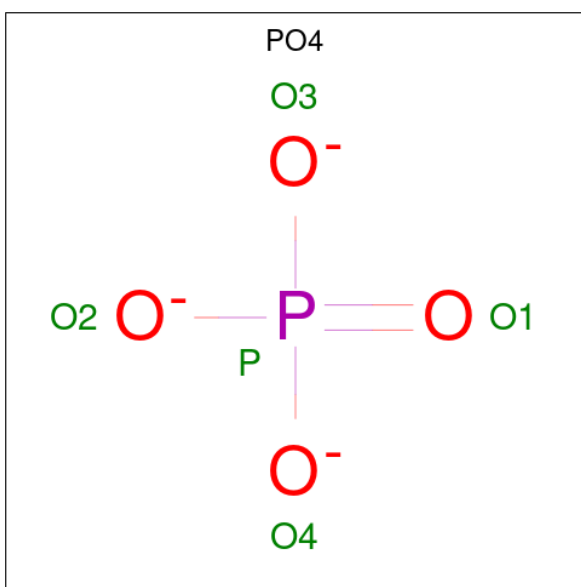
Mol	Chain	Residues	Atoms					AltConf
22	j	1	Total 256	C 81	H 156	O 17	P 2	0
22	l	1	Total 256	C 81	H 156	O 17	P 2	0
22	l	1	Total 256	C 81	H 156	O 17	P 2	0
22	p	1	Total 256	C 81	H 156	O 17	P 2	0
22	r	1	Total 256	C 81	H 156	O 17	P 2	0
22	A	1	Total 256	C 81	H 156	O 17	P 2	0
22	B	1	Total 256	C 81	H 156	O 17	P 2	0
22	B	1	Total 256	C 81	H 156	O 17	P 2	0
22	B	1	Total 256	C 81	H 156	O 17	P 2	0
22	B	1	Total 256	C 81	H 156	O 17	P 2	0
22	B	1	Total 256	C 81	H 156	O 17	P 2	0
22	I	1	Total 256	C 81	H 156	O 17	P 2	0
22	I	1	Total 256	C 81	H 156	O 17	P 2	0
22	K	1	Total 256	C 81	H 156	O 17	P 2	0
22	K	1	Total 256	C 81	H 156	O 17	P 2	0
22	J	1	Total 256	C 81	H 156	O 17	P 2	0
22	J	1	Total 256	C 81	H 156	O 17	P 2	0
22	L	1	Total 256	C 81	H 156	O 17	P 2	0
22	P	1	Total 256	C 81	H 156	O 17	P 2	0

- Molecule 23 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: C₄₄H₈₈NO₈P).



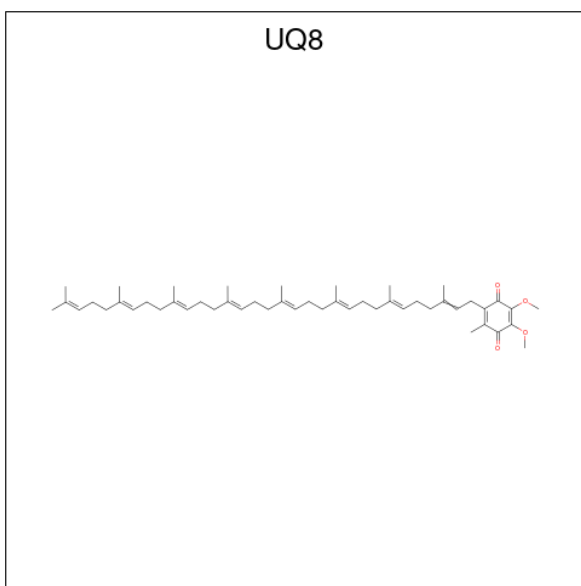
Mol	Chain	Residues	Atoms						AltConf
23	d	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
23	i	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
23	g	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
23	D	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
23	G	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
23	G	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	

- Molecule 24 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



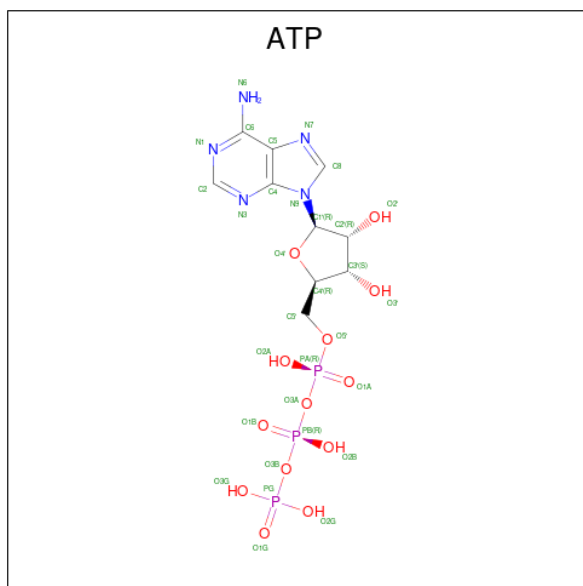
Mol	Chain	Residues	Atoms			AltConf
24	f	1	Total	O	P	0
			5	4	1	
24	F	1	Total	O	P	0
			5	4	1	

- Molecule 25 is Ubiquinone-8 (CCD ID: UQ8) (formula: $C_{49}H_{74}O_4$).



Mol	Chain	Residues	Atoms				AltConf
25	i	1	Total	C	H	O	0
			127	49	74	4	
25	I	1	Total	C	H	O	0
			127	49	74	4	

- Molecule 26 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

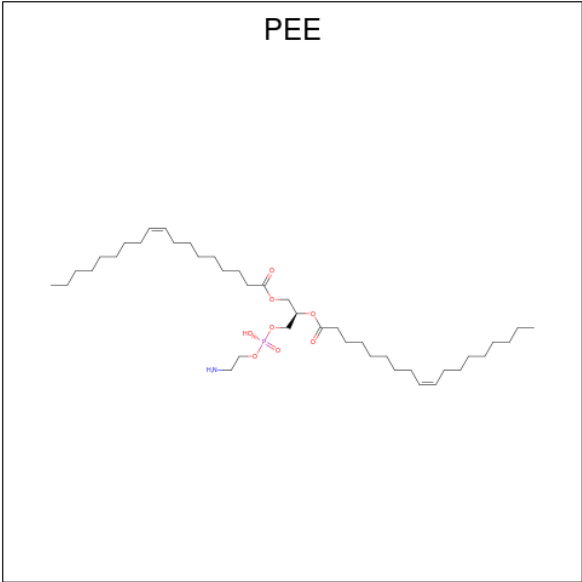


Mol	Chain	Residues	Atoms					AltConf
26	g	1	Total	C	H	N	O	P
			42	10	11	5	13	3
26	G	1	Total	C	H	N	O	P
			42	10	11	5	13	3

- Molecule 27 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

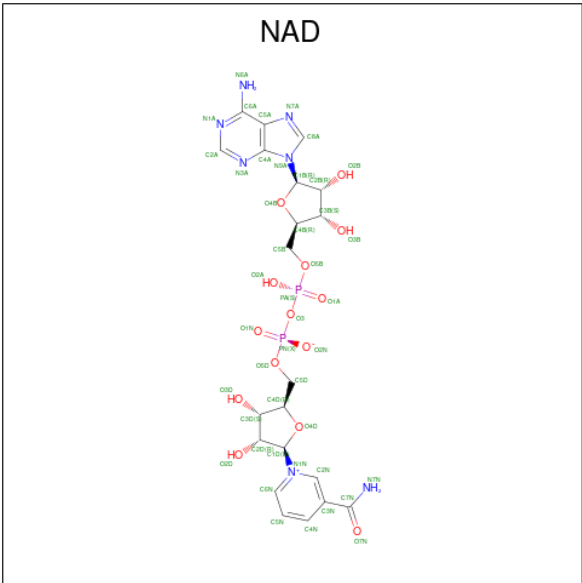
Mol	Chain	Residues	Atoms		AltConf
27	g	1	Total	Mg	0
			1	1	
27	G	1	Total	Mg	0
			1	1	

- Molecule 28 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$).



Mol	Chain	Residues	Atoms						AltConf
28	1	1	Total 123	C 38	H 75	N 1	O 8	P 1	0
28	1	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
28	J	1	Total 123	C 38	H 75	N 1	O 8	P 1	0
28	J	1	Total 133	C 41	H 82	N 1	O 8	P 1	0

- Molecule 29 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms						AltConf
29	e	1	Total	C	H	N	O	P	0
			70	21	26	7	14	2	
29	E	1	Total	C	H	N	O	P	0
			70	21	26	7	14	2	



- Molecule 5: subunit i/j

Chain i: 89% 11%



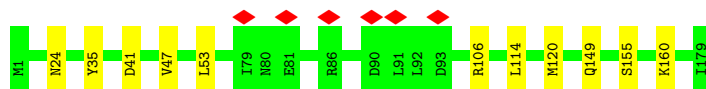
- Molecule 5: subunit i/j

Chain I: 90% 10%



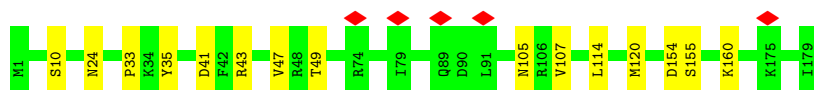
- Molecule 6: subunit k

Chain k: 94% 6%



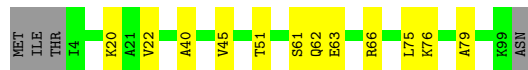
- Molecule 6: subunit k

Chain K: 92% 8%



- Molecule 7: subunit 8

Chain c: 84% 12%



- Molecule 7: subunit 8

Chain C: 85% 11%



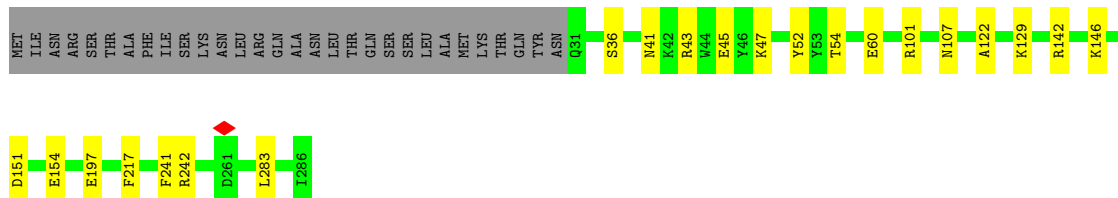
- Molecule 8: ATPPT3

Chain g: 83% 7% 10%



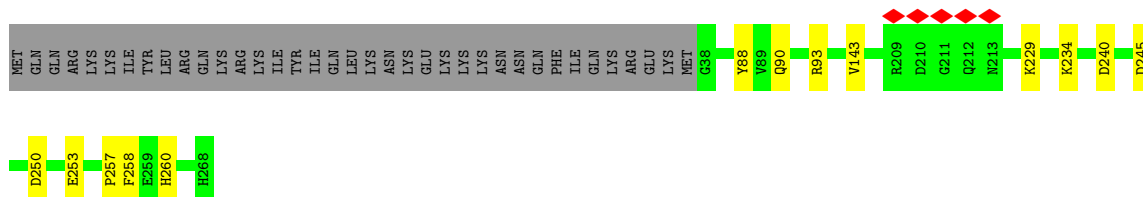
• Molecule 8: ATPTT3

Chain G: 82% 7% 10%



• Molecule 9: ATPTT4

Chain h: 81% 5% 14%



• Molecule 9: ATPTT4

Chain H: 82% 14%



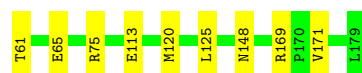
• Molecule 10: ATPTT5

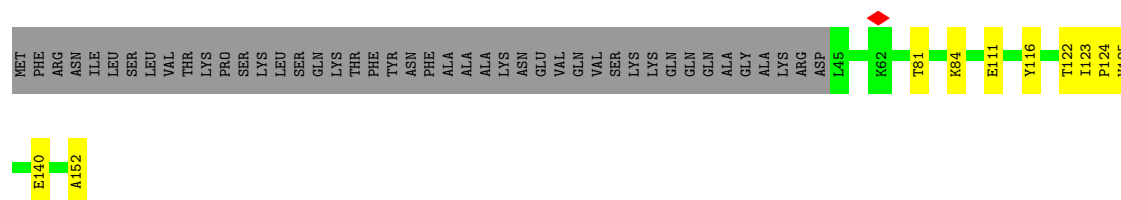
Chain j: 93% 5%



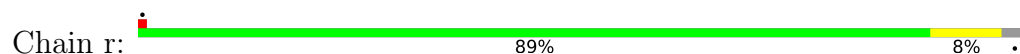
• Molecule 10: ATPTT5

Chain J: 93% 5%





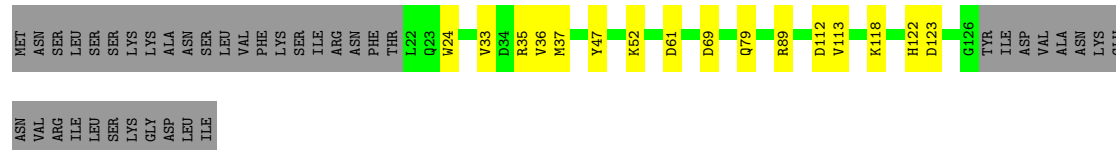
- Molecule 17: ATPTT12



- Molecule 17: ATPTT12



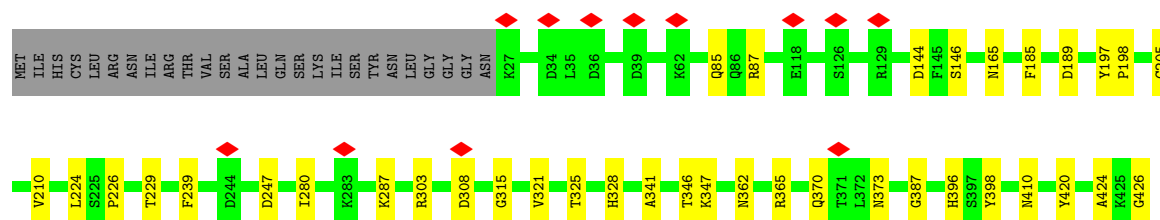
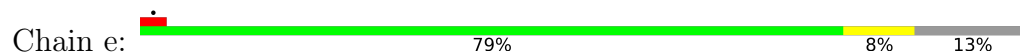
- Molecule 18: ATPTT13

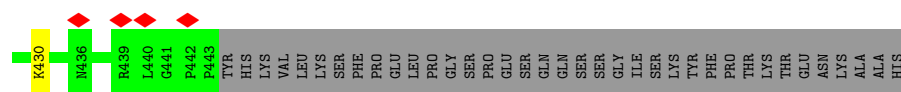


- Molecule 18: ATPTT13

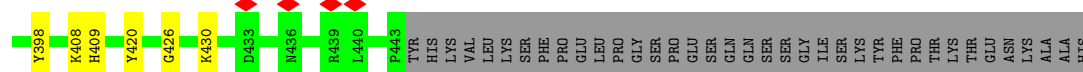
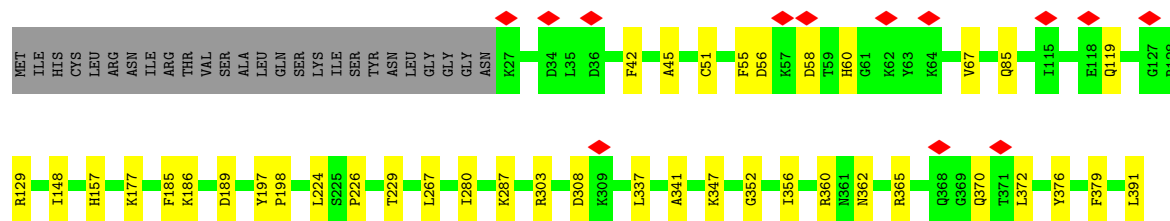
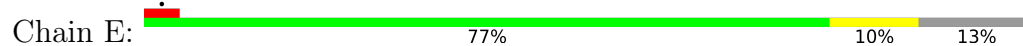


- Molecule 19: ATPTT1

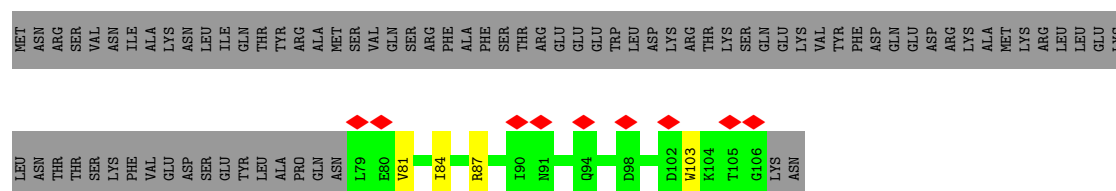




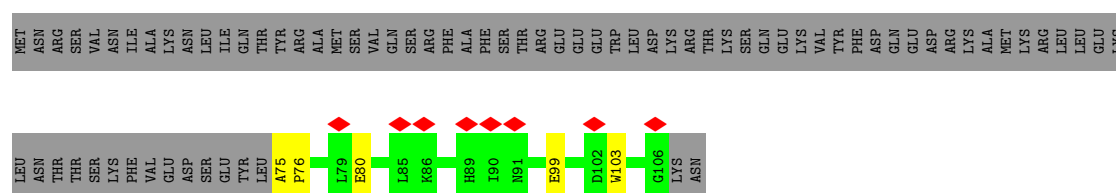
• Molecule 19: ATPTT1



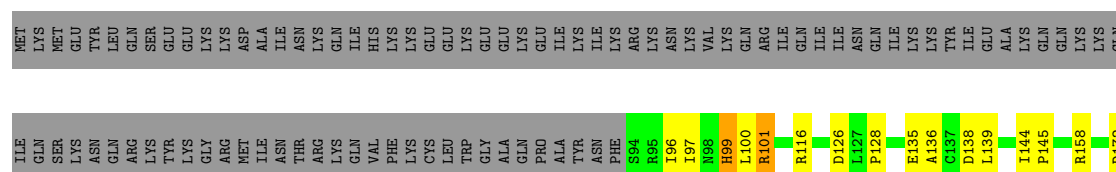
• Molecule 20: Inhibitor of F1 (IF1)

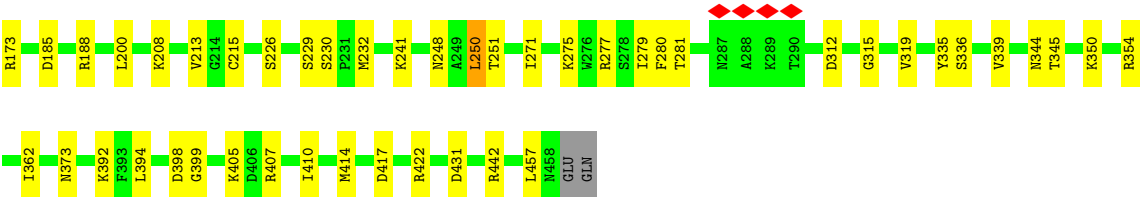


• Molecule 20: Inhibitor of F1 (IF1)



• Molecule 21: ATPTT2





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	61157	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30.9	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	165000	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.159	Depositor
Minimum map value	-0.056	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.018	Depositor
Map size (Å)	498.0, 498.0, 498.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UQ8, PC1, ATP, MG, CDL, NAD, PEE, PO4

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	0.28	0/3752	0.30	0/5109
1	a	0.28	0/3752	0.30	0/5109
2	B	0.30	0/1417	0.34	0/1915
2	b	0.30	0/1417	0.33	0/1915
3	D	0.29	0/944	0.29	0/1278
3	d	0.29	0/944	0.30	0/1278
4	F	0.30	0/1733	0.34	0/2327
4	f	0.30	0/1733	0.32	0/2327
5	I	0.29	0/1771	0.34	0/2394
5	i	0.29	0/1771	0.33	0/2394
6	K	0.23	0/1508	0.30	0/2024
6	k	0.23	0/1508	0.29	0/2024
7	C	0.28	0/866	0.33	0/1176
7	c	0.28	0/866	0.34	0/1176
8	G	0.26	0/2302	0.31	0/3115
8	g	0.26	0/2302	0.31	0/3115
9	H	0.28	0/2006	0.32	0/2704
9	h	0.28	0/2006	0.32	0/2704
10	J	0.27	0/2256	0.31	0/3069
10	j	0.27	0/2256	0.31	0/3069
11	L	0.29	0/2140	0.32	0/2903
11	l	0.28	0/2140	0.32	0/2903
12	M	0.30	0/1912	0.31	0/2598
12	m	0.30	0/1912	0.32	0/2598
13	N	0.30	0/1030	0.32	0/1393
13	n	0.30	0/1030	0.32	0/1393
14	O	0.24	0/821	0.29	0/1104
14	o	0.24	0/821	0.28	0/1104
15	P	0.20	0/1249	0.25	0/1695
15	p	0.20	0/1249	0.25	0/1695
16	Q	0.24	0/888	0.26	0/1200
16	q	0.24	0/888	0.27	0/1200

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	R	0.28	0/1185	0.31	0/1594
17	r	0.27	0/1225	0.32	0/1649
18	S	0.27	0/892	0.34	0/1209
18	s	0.28	0/885	0.33	0/1199
19	E	0.17	0/3492	0.26	0/4720
19	e	0.17	0/3492	0.26	0/4720
20	i1	0.60	0/242	1.02	0/328
20	i2	0.13	0/272	0.26	0/370
21	t	0.27	0/3103	0.34	0/4200
All	All	0.27	0/67978	0.31	0/91997

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3628	3529	3529	37	0
1	a	3628	3529	3529	35	0
2	B	1368	1307	1307	20	0
2	b	1368	1310	1310	17	0
3	D	918	846	846	4	0
3	d	918	846	846	7	0
4	F	1682	1692	1692	14	0
4	f	1682	1691	1691	16	0
5	I	1720	1741	1740	14	0
5	i	1720	1741	1741	18	0
6	K	1473	1430	1430	10	0
6	k	1473	1430	1430	9	0
7	C	841	830	830	8	0
7	c	841	830	830	9	0
8	G	2220	2118	2118	14	0
8	g	2220	2118	2118	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	H	1953	1883	1882	9	0
9	h	1953	1883	1882	11	0
10	J	2199	2145	2145	13	0
10	j	2199	2147	2147	12	0
11	L	2071	1999	2000	25	0
11	l	2071	1999	2000	20	0
12	M	1861	1835	1835	18	0
12	m	1861	1835	1835	16	0
13	N	998	962	962	10	0
13	n	998	962	962	5	0
14	O	805	794	794	4	0
14	o	805	794	794	4	0
15	P	1217	1196	1196	6	0
15	p	1217	1196	1196	8	0
16	Q	875	874	874	6	0
16	q	875	874	874	5	0
17	R	1154	1134	1134	9	0
17	r	1193	1180	1180	11	0
18	S	872	856	856	4	0
18	s	865	849	849	14	0
19	E	3395	3286	3285	25	0
19	e	3395	3286	3285	22	0
20	i1	238	236	236	12	0
20	i2	267	262	262	13	0
21	t	3013	2876	2876	44	0
22	A	100	156	156	4	0
22	B	500	780	780	28	0
22	I	200	312	312	6	0
22	J	200	312	312	3	0
22	K	200	312	312	2	0
22	L	100	156	156	11	0
22	P	100	156	156	0	0
22	a	100	156	156	4	0
22	b	200	312	312	8	0
22	f	300	468	468	17	0
22	i	100	156	156	1	0
22	j	200	312	312	3	0
22	k	300	468	468	6	0
22	l	200	312	312	14	0
22	p	100	156	156	0	0
22	r	100	156	156	3	0
23	D	54	88	88	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	G	108	176	176	2	0
23	d	54	88	88	1	0
23	g	54	88	88	0	0
23	i	54	88	88	1	0
24	F	5	0	0	0	0
24	f	5	0	0	0	0
25	I	53	74	74	5	0
25	i	53	74	74	8	0
26	G	31	11	12	1	0
26	g	31	11	12	1	0
27	G	1	0	0	0	0
27	g	1	0	0	0	0
28	J	99	157	155	4	0
28	l	99	157	155	3	0
29	E	44	26	25	1	0
29	e	44	26	25	0	0
All	All	69840	70075	70068	481	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 (481) 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)
22:k:203:CDL:O1	11:L:32:LYS:NZ	1.99	0.95
11:l:32:LYS:NZ	22:l:304:CDL:O1	2.03	0.89
17:r:31:GLU:OE1	22:r:201:CDL:O1	1.96	0.84
1:a:374:ILE:O	11:L:128:TYR:OH	1.98	0.82
18:s:36:VAL:O	21:t:407:ARG:NH2	2.13	0.81
4:f:76:ARG:NH1	22:f:303:CDL:OB4	2.16	0.78
2:b:112:ARG:NH2	22:f:303:CDL:OA4	2.18	0.77
10:J:150:ASP:OD1	17:R:142:ARG:NH2	2.18	0.77
1:A:211:ASP:OD2	3:D:198:ARG:NH2	2.18	0.76
21:t:158:ARG:NH1	21:t:398:ASP:OD2	2.19	0.76
20:i:187:ARG:NH1	20:i2:99:GLU:OE1	2.19	0.75
22:I:301:CDL:O1	17:R:31:GLU:OE1	2.03	0.75
20:i1:81:VAL:HG22	20:i2:103:TRP:CH2	2.22	0.75
20:i1:81:VAL:CG2	20:i2:103:TRP:CH2	2.70	0.74
19:E:58:ASP:OD2	19:E:360:ARG:NH1	2.21	0.74
10:j:194:ARG:NH1	12:m:191:ASP:OD1	2.20	0.74
19:E:85:GLN:OE1	19:E:420:TYR:OH	2.06	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:l:124:VAL:HG13	22:l:301:CDL:H312	1.70	0.73
20:i:1:81:VAL:CG2	20:i:2:103:TRP:CZ2	2.71	0.73
1:a:211:ASP:OD2	3:d:198:ARG:NH2	2.21	0.72
21:t:226:SER:OG	21:t:229:SER:OG	2.07	0.71
12:m:49:MET:O	12:m:217:GLN:NE2	2.22	0.71
10:j:54:SER:O	11:l:94:ARG:NH1	2.23	0.71
11:l:128:TYR:OH	1:A:374:ILE:O	2.08	0.70
10:J:54:SER:O	11:L:94:ARG:NH1	2.24	0.69
4:f:39:PRO:O	21:t:350:LYS:NZ	2.26	0.69
1:A:181:LEU:HD22	25:I:303:UQ8:H21A	1.73	0.69
7:c:66:ARG:NH1	18:s:69:ASP:OD1	2.25	0.69
21:t:417:ASP:OD2	21:t:422:ARG:NH1	2.26	0.69
1:A:112:THR:OG1	1:A:146:ASN:OD1	2.06	0.68
9:h:234:LYS:NZ	18:s:61:ASP:OD2	2.27	0.67
21:t:185:ASP:OD1	21:t:188:ARG:NH1	2.26	0.67
9:h:250:ASP:OD2	17:r:20:ARG:NH1	2.27	0.67
1:a:412:LEU:O	1:a:416:THR:OG1	2.13	0.67
1:a:194:LEU:HD13	22:f:302:CDL:H541	1.78	0.66
19:E:303:ARG:NH2	19:E:308:ASP:OD2	2.28	0.66
8:g:107:ASN:OD1	8:g:142:ARG:NH1	2.29	0.66
8:G:107:ASN:OD1	8:G:142:ARG:NH1	2.29	0.66
14:o:55:MET:HE1	13:N:75:ARG:O	1.95	0.65
1:a:184:PHE:HB2	25:i:303:UQ8:H15B	1.79	0.65
9:h:253:GLU:OE2	21:t:422:ARG:NH2	2.29	0.65
22:b:401:CDL:OA4	18:S:23:GLN:NE2	2.30	0.64
3:d:161:ASP:OD2	21:t:405:LYS:NZ	2.29	0.64
1:A:158:GLU:OE1	11:L:176:ARG:NH1	2.29	0.64
2:B:106:GLU:HA	18:S:32:MET:HE1	1.79	0.64
12:M:3:ASN:ND2	12:M:40:GLU:OE2	2.30	0.64
12:M:14:ARG:NH1	13:N:113:GLU:OE2	2.30	0.64
11:l:186:GLU:OE1	13:N:169:ARG:NH1	2.28	0.64
2:B:202:LYS:NZ	9:H:217:GLU:OE1	2.31	0.64
11:L:24:LYS:O	11:L:28:ASN:ND2	2.31	0.63
21:t:116:ARG:NH1	21:t:172:ASP:OD1	2.31	0.63
9:h:258:PHE:O	11:l:118:ARG:NH1	2.33	0.62
5:i:41:PRO:HD3	17:r:7:ILE:HD13	1.82	0.62
9:H:250:ASP:OD2	18:S:49:ARG:NH2	2.33	0.62
5:I:61:MET:HE1	12:M:94:ASN:HB3	1.81	0.61
18:s:35:ARG:NH1	21:t:126:ASP:OD2	2.33	0.61
4:F:87:LYS:NZ	22:L:301:CDL:O1	2.33	0.61
19:E:365:ARG:HE	19:E:370:GLN:HB2	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:205:GLU:OE2	2:b:173:ARG:NE	2.34	0.61
20:i:1:81:VAL:HG22	20:i:2:103:TRP:CZ2	2.36	0.61
21:t:335:TYR:O	21:t:373:ASN:ND2	2.31	0.61
22:B:405:CDL:OB3	4:F:75:LYS:NZ	2.29	0.60
19:e:303:ARG:NH1	19:e:315:GLY:O	2.33	0.60
2:b:113:LYS:NZ	22:f:304:CDL:OB3	2.35	0.60
4:f:13:TRP:O	21:t:442:ARG:NH1	2.34	0.60
5:i:61:MET:HE1	12:m:94:ASN:HB3	1.83	0.60
15:p:126:ASP:OD2	17:r:148:TYR:OH	2.16	0.59
11:L:124:VAL:HG13	22:L:301:CDL:H312	1.84	0.59
11:l:135:LEU:HD12	1:A:374:ILE:HD13	1.84	0.59
1:A:178:ILE:HG23	22:L:301:CDL:H473	1.83	0.59
11:l:24:LYS:O	11:l:28:ASN:ND2	2.36	0.59
6:K:41:ASP:OD2	8:G:242:ARG:NH1	2.36	0.59
1:a:374:ILE:HD13	11:L:135:LEU:HD12	1.83	0.59
10:j:150:ASP:OD1	17:r:142:ARG:NH2	2.35	0.59
12:M:2:ASP:OD1	13:N:61:THR:N	2.36	0.59
12:M:49:MET:O	12:M:217:GLN:NE2	2.35	0.59
19:e:303:ARG:NH2	19:e:308:ASP:OD2	2.35	0.59
22:b:401:CDL:H221	22:l:301:CDL:H671	1.85	0.59
22:k:203:CDL:H1O1	11:L:32:LYS:HZ1	1.45	0.59
8:g:52:TYR:HB3	8:g:54:THR:O	2.03	0.58
21:t:101:ARG:HH21	21:t:101:ARG:HG3	1.68	0.58
10:j:213:ARG:NH1	10:j:220:ASP:OD1	2.35	0.58
22:B:404:CDL:H671	23:D:301:PC1:H3C2	1.84	0.58
17:r:110:ALA:HB2	11:L:180:VAL:HG21	1.86	0.58
11:L:33:SER:OG	11:L:35:ASP:OD1	2.17	0.58
10:J:213:ARG:NH2	10:J:216:THR:O	2.37	0.57
2:b:112:ARG:NH1	4:f:74:ASN:O	2.37	0.57
20:i:1:81:VAL:HG23	20:i:2:103:TRP:CZ2	2.40	0.57
12:m:14:ARG:NH1	13:n:113:GLU:OE2	2.37	0.57
15:p:2:SER:OG	15:p:27:GLN:OE1	2.21	0.57
10:J:194:ARG:NH1	12:M:191:ASP:OD1	2.37	0.57
4:F:43:GLU:N	4:F:43:GLU:OE2	2.37	0.57
14:O:104:LEU:HD12	15:P:143:ARG:HG3	1.86	0.57
1:A:412:LEU:O	1:A:416:THR:OG1	2.22	0.56
11:l:33:SER:OG	11:l:35:ASP:OD1	2.18	0.56
19:E:157:HIS:O	19:E:177:LYS:NZ	2.27	0.56
9:h:93:ARG:NH1	16:q:111:GLU:OE2	2.38	0.56
1:A:205:GLU:OE2	2:B:173:ARG:NE	2.38	0.56
8:G:60:GLU:OE1	9:H:90:GLN:NE2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:l:123:ARG:NE	22:l:301:CDL:OA4	2.27	0.56
11:l:180:VAL:HG21	17:r:110:ALA:HB2	1.88	0.56
7:c:76:LYS:O	18:s:79:GLN:NE2	2.39	0.55
8:G:242:ARG:O	19:E:186:LYS:NZ	2.39	0.55
15:P:126:ASP:OD2	17:r:148:TYR:OH	2.23	0.55
1:a:225:ILE:HG22	1:a:226:THR:HG22	1.89	0.55
10:j:213:ARG:NH2	10:j:216:THR:O	2.40	0.55
1:a:374:ILE:HD12	28:J:303:PEE:H58	1.89	0.55
1:A:229:ASP:OD1	5:I:70:ARG:NH2	2.39	0.55
21:t:407:ARG:HG3	21:t:410:ILE:HD12	1.86	0.55
19:e:426:GLY:O	19:e:430:LYS:NZ	2.31	0.55
1:A:137:GLU:O	12:M:163:TYR:OH	2.21	0.55
18:s:37:MET:HE3	21:t:399:GLY:HA3	1.88	0.55
2:B:196:ASN:OD1	2:B:199:ARG:NH2	2.35	0.55
20:i:184:ILE:CD1	20:i:299:GLU:HB3	2.36	0.55
18:s:118:LYS:O	18:s:122:HIS:ND1	2.39	0.55
11:L:200:ARG:NH2	17:r:88:ASN:OD1	2.39	0.55
10:j:199:VAL:HG13	12:m:191:ASP:HB3	1.89	0.54
10:j:271:LEU:HD12	6:K:160:LYS:HD2	1.88	0.54
12:m:13:LEU:HD21	12:m:18:LEU:HG	1.89	0.54
2:B:112:ARG:NH1	4:F:74:ASN:O	2.41	0.54
11:L:206:ILE:CG2	11:L:207:PRO:HD3	2.38	0.54
20:i:184:ILE:HD11	20:i:299:GLU:CB	2.38	0.54
19:e:365:ARG:NH1	19:e:373:ASN:OD1	2.40	0.54
6:K:105:ASN:OD1	6:K:107:VAL:O	2.25	0.54
8:g:260:CYS:SG	8:g:261:ASP:N	2.79	0.54
1:A:213:LEU:HD21	23:D:301:PC1:H3I2	1.90	0.54
19:E:189:ASP:OD1	19:E:229:THR:OG1	2.23	0.54
2:b:211:HIS:NE2	3:d:129:GLU:OE1	2.34	0.53
10:J:213:ARG:NH1	10:J:220:ASP:OD1	2.37	0.53
13:n:131:ARG:NE	13:n:133:GLU:OE2	2.37	0.53
21:t:100:LEU:HD12	21:t:100:LEU:O	2.09	0.53
22:f:303:CDL:H272	28:l:302:PEE:H74	1.89	0.53
22:A:501:CDL:H791	22:B:402:CDL:H262	1.89	0.53
1:A:44:GLY:H	14:O:58:THR:HB	1.73	0.53
22:B:405:CDL:H391	28:J:303:PEE:H54	1.90	0.53
19:e:365:ARG:HE	19:e:370:GLN:HB2	1.73	0.53
1:a:226:THR:HG21	5:i:88:PHE:HD2	1.74	0.52
3:d:130:ASN:OD1	18:s:89:ARG:NH2	2.42	0.52
5:i:204:ASN:ND2	5:i:206:LEU:O	2.34	0.52
22:l:301:CDL:H741	22:l:301:CDL:H532	1.89	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:LYS:O	1:A:166:ASN:ND2	2.42	0.52
19:E:376:TYR:OH	19:E:379:PHE:O	2.22	0.52
13:n:171:VAL:HG11	17:R:139:VAL:HG21	1.92	0.52
4:f:87:LYS:NZ	22:l:301:CDL:O1	2.42	0.52
1:a:182:ILE:HG12	22:l:301:CDL:H751	1.92	0.52
22:b:401:CDL:H541	22:b:401:CDL:H721	1.92	0.52
2:b:218:ARG:NH1	18:s:123:ASP:OD2	2.42	0.52
10:J:168:ARG:NH2	17:R:120:ASP:OD1	2.39	0.52
5:I:136:ASN:ND2	11:L:191:TYR:O	2.36	0.52
22:L:301:CDL:H562	22:L:301:CDL:H792	1.92	0.52
8:g:60:GLU:OE1	9:h:90:GLN:NE2	2.42	0.52
1:a:44:GLY:H	14:o:58:THR:HB	1.75	0.51
21:t:126:ASP:OD1	21:t:126:ASP:N	2.43	0.51
22:l:304:CDL:H112	22:l:304:CDL:H321	1.91	0.51
1:A:239:ALA:HB1	22:B:403:CDL:H672	1.91	0.51
19:E:119:GLN:OE1	19:E:129:ARG:NH2	2.43	0.51
2:B:169:ARG:NH2	22:B:403:CDL:OB3	2.44	0.51
21:t:336:SER:OG	21:t:339:VAL:O	2.29	0.51
17:r:107:GLU:OE2	13:N:75:ARG:NH2	2.39	0.51
16:Q:122:THR:O	16:Q:125:VAL:HG22	2.10	0.51
1:a:354:SER:HA	2:B:130:ALA:HB1	1.93	0.51
13:n:120:MET:HE2	13:n:125:LEU:HD11	1.92	0.51
6:K:10:SER:O	26:G:301:ATP:N6	2.40	0.51
2:b:172:ARG:NH2	22:f:302:CDL:OB4	2.41	0.51
19:e:144:ASP:OD2	19:e:146:SER:OG	2.28	0.51
11:L:32:LYS:HG3	11:L:47:ARG:HG3	1.93	0.51
5:I:66:VAL:HG21	7:C:45:VAL:HG21	1.93	0.50
1:a:127:GLU:OE1	1:a:127:GLU:N	2.40	0.50
11:L:123:ARG:NE	22:L:301:CDL:OA4	2.30	0.50
21:t:232:MET:HE1	21:t:344:ASN:OD1	2.11	0.50
2:B:188:GLU:HG2	21:t:312:ASP:HB2	1.94	0.50
2:b:135:ASN:ND2	2:B:128:GLY:O	2.44	0.50
16:q:122:THR:O	16:q:125:VAL:HG22	2.12	0.50
6:K:114:LEU:HD22	6:K:120:MET:HE2	1.93	0.50
20:i:184:ILE:HD11	20:i:299:GLU:HB3	1.94	0.50
1:a:330:MET:HG2	1:a:396:VAL:HA	1.94	0.50
8:G:41:ASN:N	16:Q:152:ALA:O	2.42	0.50
1:a:137:GLU:O	12:m:163:TYR:OH	2.23	0.49
9:h:229:LYS:NZ	18:s:24:TRP:O	2.45	0.49
15:P:111:LYS:O	17:R:75:ASN:ND2	2.39	0.49
19:E:426:GLY:O	19:E:430:LYS:NZ	2.36	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:66:ARG:NH1	18:S:69:ASP:OD1	2.41	0.49
6:k:47:VAL:HG21	6:k:53:LEU:HB2	1.94	0.49
19:E:148:ILE:HD13	19:E:267:LEU:HD23	1.94	0.49
6:k:41:ASP:OD2	8:g:242:ARG:NH1	2.46	0.49
3:D:145:ASP:OD2	7:C:76:LYS:NZ	2.40	0.49
11:l:206:ILE:HG22	11:l:207:PRO:HD3	1.94	0.49
11:l:200:ARG:NH2	17:r:88:ASN:OD1	2.46	0.48
21:t:158:ARG:HH11	21:t:394:LEU:HD22	1.78	0.48
21:t:275:LYS:HE3	21:t:279:ILE:HD11	1.94	0.48
4:f:11:TYR:O	4:f:15:LYS:HB2	2.13	0.48
20:i1:103:TRP:NE1	20:i2:80:GLU:OE1	2.43	0.48
1:a:226:THR:OG1	1:a:227:SER:N	2.46	0.48
2:b:130:ALA:HB1	1:A:354:SER:HA	1.94	0.48
12:m:2:ASP:OD1	13:n:61:THR:N	2.46	0.48
21:t:250:LEU:HD11	21:t:271:ILE:HD11	1.95	0.48
1:a:446:ASN:ND2	7:c:62:GLN:O	2.42	0.48
19:e:239:PHE:N	19:e:247:ASP:OD2	2.47	0.48
1:A:275:LEU:HD13	1:A:321:LEU:HD21	1.95	0.48
1:A:330:MET:HG2	1:A:396:VAL:HA	1.94	0.48
2:B:159:LYS:HD2	2:B:166:LEU:HB2	1.95	0.48
12:M:13:LEU:HD21	12:M:18:LEU:HG	1.95	0.48
21:t:271:ILE:HD13	21:t:280:PHE:HD2	1.78	0.48
22:b:401:CDL:H832	22:f:303:CDL:H401	1.96	0.48
6:K:105:ASN:O	6:K:107:VAL:O	2.32	0.48
8:g:101:ARG:NH1	8:g:209:ASP:OD1	2.46	0.48
1:a:177:TRP:CE3	25:i:303:UQ8:H25B	2.48	0.48
22:a:501:CDL:H472	5:i:105:LEU:HD22	1.96	0.48
12:M:205:ASN:ND2	12:M:208:ASP:OD1	2.47	0.47
1:A:251:TRP:CD1	22:B:403:CDL:H582	2.49	0.47
4:f:116:PHE:HB3	22:B:401:CDL:H421	1.95	0.47
19:E:42:PHE:HB2	19:E:67:VAL:HG22	1.96	0.47
5:i:194:LEU:HD23	10:j:196:VAL:HB	1.96	0.47
1:A:46:GLU:HG2	14:O:58:THR:HG22	1.97	0.47
21:t:248:ASN:O	21:t:251:THR:OG1	2.31	0.47
15:P:2:SER:OG	15:P:27:GLN:OE1	2.31	0.47
7:c:61:SER:OG	7:c:63:GLU:OE1	2.18	0.47
9:h:245:ASP:OD2	18:s:33:VAL:HG23	2.15	0.47
10:J:199:VAL:HG13	12:M:191:ASP:HB3	1.96	0.47
21:t:135:GLU:OE1	21:t:136:ALA:N	2.47	0.47
25:I:303:UQ8:H7A	25:I:303:UQ8:H10	1.71	0.47
10:J:184:ALA:HB1	12:M:38:LEU:HD23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:f:107:LEU:N	22:f:302:CDL:OB3	2.46	0.47
11:l:113:ARG:NH2	22:l:301:CDL:OB4	2.47	0.47
19:e:165:ASN:ND2	19:e:205:CYS:SG	2.83	0.47
25:I:303:UQ8:H36A	11:L:107:LEU:HD12	1.97	0.47
9:H:244:PRO:O	21:t:241:LYS:NZ	2.25	0.47
22:B:401:CDL:H671	22:B:401:CDL:H441	1.96	0.46
7:C:75:LEU:HA	7:C:79:ALA:HB3	1.97	0.46
8:G:52:TYR:HB3	8:G:54:THR:O	2.15	0.46
6:k:114:LEU:HD22	6:k:120:MET:HE2	1.97	0.46
6:K:43:ARG:O	6:K:47:VAL:HG22	2.16	0.46
6:k:106:ARG:NH2	6:k:155:SER:O	2.44	0.46
19:E:280:ILE:HA	19:E:287:LYS:HA	1.97	0.46
1:a:209:ASP:OD1	2:b:173:ARG:NH1	2.35	0.46
22:k:203:CDL:H112	22:k:203:CDL:H322	1.98	0.46
22:j:301:CDL:H122	11:l:104:GLY:HA3	1.98	0.46
19:e:87:ARG:HD3	19:e:424:ALA:HB1	1.98	0.46
2:B:193:LYS:O	7:C:62:GLN:NE2	2.49	0.46
11:L:143:PRO:HD3	22:L:301:CDL:H782	1.97	0.46
1:A:77:ASP:O	1:A:81:ASN:ND2	2.47	0.46
2:b:159:LYS:HD2	2:b:166:LEU:HB2	1.98	0.46
22:l:304:CDL:HB32	22:l:304:CDL:H122	1.97	0.46
22:B:401:CDL:H391	22:B:401:CDL:H232	1.98	0.46
8:G:101:ARG:NH2	8:G:146:LYS:O	2.48	0.46
21:t:96:ILE:HG13	21:t:97:ILE:HG13	1.98	0.46
7:c:75:LEU:HA	7:c:79:ALA:HB3	1.98	0.46
19:E:45:ALA:N	29:E:900:NAD:O3B	2.45	0.46
25:i:303:UQ8:H30	25:i:303:UQ8:H27	1.73	0.46
21:t:138:ASP:OD1	21:t:139:LEU:N	2.49	0.46
6:k:47:VAL:HG12	22:k:202:CDL:HA62	1.97	0.45
8:G:47:LYS:NZ	8:G:151:ASP:OD2	2.42	0.45
19:E:341:ALA:O	19:E:347:LYS:NZ	2.49	0.45
2:B:140:SER:OG	4:F:159:TRP:O	2.15	0.45
22:J:301:CDL:H122	11:L:104:GLY:HA3	1.97	0.45
22:r:201:CDL:H752	22:r:201:CDL:H721	1.78	0.45
2:b:95:PHE:HA	5:i:51:ARG:HB3	1.99	0.45
8:g:153:LYS:NZ	26:g:301:ATP:O1A	2.35	0.45
6:k:149:GLN:HB3	11:L:47:ARG:HD3	1.99	0.45
12:m:107:MET:O	12:m:111:PHE:HB2	2.17	0.45
16:q:116:TYR:OH	16:q:140:GLU:OE2	2.33	0.45
5:I:67:ALA:HB1	5:I:95:LEU:HB3	1.99	0.45
25:i:303:UQ8:H22A	25:i:303:UQ8:H25	1.75	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:s:112:ASP:OD1	18:s:113:VAL:N	2.50	0.45
10:j:47:PHE:CD1	22:j:301:CDL:H121	2.51	0.45
25:I:303:UQ8:H30	25:I:303:UQ8:H27A	1.59	0.45
11:L:206:ILE:HG23	11:L:207:PRO:HD3	1.99	0.45
21:t:99:HIS:O	21:t:101:ARG:HD2	2.17	0.45
3:d:157:ASN:HB3	21:t:392:LYS:HE3	1.98	0.45
28:l:302:PEE:H58	1:A:374:ILE:HD12	1.99	0.45
12:m:177:VAL:HG13	12:m:192:SER:HB3	1.99	0.45
15:p:88:VAL:O	15:p:92:SER:OG	2.21	0.45
22:B:402:CDL:H832	22:B:405:CDL:H401	1.99	0.45
19:e:185:PHE:O	19:e:224:LEU:HD13	2.17	0.45
19:e:321:VAL:HA	19:e:328:HIS:HA	1.99	0.45
2:B:187:HIS:NE2	3:D:156:TYR:O	2.49	0.45
5:I:142:THR:N	11:L:164:CYS:O	2.46	0.45
4:f:104:LYS:HD3	4:f:105:PRO:O	2.17	0.44
4:f:70:PRO:HG3	2:B:162:MET:O	2.16	0.44
6:K:24:ASN:HA	8:G:241:PHE:CE1	2.52	0.44
21:t:345:THR:HG23	21:t:362:ILE:HD13	1.99	0.44
22:f:303:CDL:HA61	22:f:303:CDL:H312	1.75	0.44
22:j:302:CDL:OA4	1:A:371:THR:OG1	2.33	0.44
18:s:52:LYS:HA	21:t:405:LYS:HG3	1.99	0.44
22:A:501:CDL:H262	22:B:402:CDL:H392	2.00	0.44
1:a:226:THR:HG21	5:i:88:PHE:CD2	2.51	0.44
5:i:40:GLY:O	11:l:116:PRO:O	2.35	0.44
19:e:346:THR:OG1	19:e:396:HIS:NE2	2.34	0.44
4:F:143:ASN:O	11:L:182:ASN:ND2	2.37	0.44
9:H:93:ARG:NH1	16:Q:111:GLU:OE2	2.51	0.44
22:a:501:CDL:H392	25:i:303:UQ8:H15	2.00	0.44
1:A:416:THR:HB	3:D:223:LYS:HD2	2.00	0.44
2:B:98:PRO:HB2	9:H:252:LEU:HD11	1.99	0.44
1:a:92:VAL:HG22	12:m:175:ALA:HB1	1.99	0.44
22:b:401:CDL:H412	22:l:301:CDL:H672	2.00	0.44
4:f:50:ARG:NH1	21:t:215:CYS:O	2.50	0.44
22:f:304:CDL:H231	22:f:304:CDL:H472	1.98	0.44
2:B:95:PHE:HA	5:I:51:ARG:HB3	2.00	0.44
4:F:85:LEU:HG	22:L:301:CDL:H571	1.98	0.44
22:I:301:CDL:H721	22:I:301:CDL:H752	1.78	0.44
12:M:29:TYR:HE2	13:N:65:GLU:HG3	1.82	0.44
1:a:277:MET:HG3	5:i:87:VAL:HB	2.00	0.44
5:i:66:VAL:HG21	7:c:45:VAL:HG21	2.00	0.44
12:m:148:VAL:O	12:m:152:GLU:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:181:LYS:O	12:M:202:ARG:HD2	2.18	0.44
14:O:77:ILE:O	17:R:95:TYR:OH	2.30	0.44
19:E:352:GLY:O	19:E:356:ILE:HG12	2.17	0.44
6:k:24:ASN:HA	8:g:241:PHE:CE1	2.53	0.44
15:p:111:LYS:O	17:r:75:ASN:ND2	2.50	0.44
13:N:120:MET:HE2	13:N:125:LEU:HD11	1.99	0.44
6:k:160:LYS:HD2	10:J:271:LEU:HD12	2.00	0.44
23:G:303:PC1:H111	23:G:303:PC1:H152	1.75	0.44
1:a:177:TRP:HE3	25:i:303:UQ8:H26	1.83	0.43
19:e:341:ALA:O	19:e:347:LYS:NZ	2.51	0.43
2:B:117:THR:HG21	22:B:401:CDL:H321	1.99	0.43
22:B:403:CDL:H721	7:C:43:THR:HG21	2.01	0.43
10:J:47:PHE:CD1	22:J:301:CDL:H121	2.53	0.43
20:i:184:ILE:HD11	20:i:299:GLU:HB2	2.00	0.43
1:a:226:THR:HG23	1:a:231:TYR:HD2	1.84	0.43
22:a:501:CDL:HB62	4:f:125:ALA:HB2	2.01	0.43
19:e:280:ILE:HA	19:e:287:LYS:HA	2.00	0.43
19:E:185:PHE:O	19:E:224:LEU:HD13	2.17	0.43
22:k:202:CDL:H792	22:k:202:CDL:H761	1.78	0.43
21:t:414:MET:HB3	21:t:431:ASP:HB2	2.01	0.43
1:a:212:TYR:HB2	2:b:172:ARG:HD2	2.01	0.43
1:a:275:LEU:HD13	1:a:321:LEU:HD21	2.00	0.43
8:g:197:GLU:HB3	8:g:283:LEU:HD11	2.00	0.43
10:j:184:ALA:HB1	12:m:38:LEU:HD23	2.00	0.43
22:l:301:CDL:H191	22:l:301:CDL:H162	1.84	0.43
22:l:301:CDL:H361	22:l:301:CDL:H391	1.92	0.43
22:B:401:CDL:H791	22:B:401:CDL:H222	2.00	0.43
7:C:17:LEU:HA	7:C:21:ALA:HB2	1.99	0.43
16:Q:81:THR:O	16:Q:84:LYS:NZ	2.49	0.43
19:e:210:VAL:HG12	19:e:387:GLY:O	2.18	0.43
5:I:204:ASN:ND2	5:I:206:LEU:O	2.36	0.43
19:E:408:LYS:O	19:E:409:HIS:ND1	2.51	0.43
21:t:230:SER:OG	21:t:232:MET:HE2	2.19	0.43
8:g:142:ARG:NE	8:g:286:ILE:O	2.52	0.43
2:B:165:PRO:HB2	2:B:167:LEU:HG	2.01	0.43
4:F:124:LYS:HE3	4:F:128:ILE:HD11	2.00	0.43
25:I:303:UQ8:H22A	25:I:303:UQ8:H25	1.62	0.43
1:a:229:ASP:OD1	5:i:70:ARG:NH2	2.52	0.43
4:f:78:TRP:N	22:f:303:CDL:OA3	2.48	0.43
22:A:501:CDL:H591	22:L:301:CDL:H821	2.00	0.43
22:B:405:CDL:OB4	4:F:76:ARG:NH1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:124:PRO:HA	9:H:131:THR:HG21	2.00	0.43
20:i:1:84:ILE:HD12	20:i:2:99:GLU:HB3	2.00	0.43
22:f:302:CDL:H622	7:c:40:ALA:HB2	2.01	0.43
14:o:134:ASP:HA	14:o:139:GLY:HA2	2.00	0.43
18:s:47:TYR:O	21:t:354:ARG:NH2	2.50	0.43
19:e:85:GLN:OE1	19:e:420:TYR:OH	2.35	0.43
1:a:188:THR:HG21	5:i:52:MET:HG3	2.01	0.43
1:A:115:THR:HB	1:A:124:HIS:CE1	2.54	0.43
22:B:405:CDL:H422	28:J:303:PEE:H57	2.00	0.43
1:a:383:ILE:HG21	22:B:405:CDL:H602	2.01	0.42
1:A:188:THR:HG21	5:I:52:MET:HG3	2.01	0.42
19:E:197:TYR:CG	19:E:198:PRO:HA	2.54	0.42
21:t:200:LEU:HD13	21:t:213:VAL:HB	2.01	0.42
10:J:191:ASN:HA	10:J:194:ARG:HD3	2.02	0.42
5:i:1:MET:HE3	5:i:6:LYS:HG2	2.02	0.42
12:M:107:MET:O	12:M:111:PHE:HB2	2.19	0.42
19:E:56:ASP:O	19:E:60:HIS:N	2.52	0.42
21:t:277:ARG:O	21:t:281:THR:HG23	2.18	0.42
3:d:134:PHE:CE2	3:d:138:ILE:HD11	2.54	0.42
7:c:20:LYS:HB3	7:c:22:VAL:HG23	2.02	0.42
22:B:401:CDL:H541	22:B:401:CDL:H571	1.90	0.42
22:B:403:CDL:H662	22:B:403:CDL:H631	1.89	0.42
15:p:37:VAL:N	15:p:38:PRO:HD2	2.35	0.42
22:b:402:CDL:H801	22:b:402:CDL:H772	1.86	0.42
22:A:501:CDL:H652	22:L:301:CDL:H592	2.01	0.42
22:I:302:CDL:H392	22:I:302:CDL:H421	1.88	0.42
2:b:165:PRO:HB2	2:b:167:LEU:HG	2.00	0.42
5:i:17:TYR:O	5:i:21:GLU:HB2	2.20	0.42
8:G:197:GLU:HG3	19:E:226:PRO:HD2	2.00	0.42
1:A:192:THR:HB	4:F:90:MET:HE2	2.02	0.42
1:A:226:THR:OG1	1:A:227:SER:N	2.53	0.42
22:I:301:CDL:H722	11:L:110:LEU:HD13	2.00	0.42
22:J:302:CDL:H631	22:J:302:CDL:H601	1.91	0.42
4:f:43:GLU:HG3	21:t:319:VAL:HG13	2.01	0.42
4:f:107:LEU:CD1	22:f:302:CDL:H551	2.50	0.42
22:f:302:CDL:H761	22:f:302:CDL:H731	1.76	0.42
11:l:186:GLU:OE2	13:N:169:ARG:NH2	2.52	0.42
10:J:204:TRP:CZ2	12:M:9:THR:HG22	2.54	0.42
20:i:2:75:ALA:N	20:i:2:76:PRO:HD2	2.34	0.42
19:e:189:ASP:OD1	19:e:229:THR:OG1	2.31	0.42
1:A:277:MET:HB3	1:A:278:PRO:HD3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:122:ALA:O	8:G:129:LYS:NZ	2.33	0.42
4:f:86:ILE:HG23	22:l:301:CDL:H511	2.01	0.41
8:g:197:GLU:HG3	19:e:226:PRO:HD2	2.02	0.41
12:m:205:ASN:ND2	12:m:208:ASP:OD1	2.53	0.41
22:r:201:CDL:H432	22:r:201:CDL:H462	1.89	0.41
1:A:62:LEU:HD23	11:L:150:ILE:HB	2.02	0.41
6:K:154:ASP:OD1	6:K:155:SER:N	2.52	0.41
9:H:204:GLU:OE2	9:H:218:ARG:NH1	2.53	0.41
11:L:120:PHE:O	11:L:124:VAL:HG23	2.20	0.41
16:Q:116:TYR:OH	16:Q:140:GLU:OE2	2.21	0.41
21:t:128:PRO:O	21:t:158:ARG:HG2	2.20	0.41
22:f:303:CDL:H401	22:f:303:CDL:H371	1.77	0.41
22:f:303:CDL:H472	22:f:303:CDL:H442	1.82	0.41
22:B:401:CDL:H471	22:B:401:CDL:H262	2.02	0.41
1:a:349:SER:HB2	28:J:303:PEE:H7	2.02	0.41
9:h:257:PRO:HG2	9:h:260:HIS:HB2	2.02	0.41
19:e:410:ASN:OD1	19:e:410:ASN:N	2.47	0.41
22:a:501:CDL:H822	22:b:401:CDL:H261	2.02	0.41
22:K:202:CDL:H812	22:K:202:CDL:H841	1.89	0.41
9:H:88:TYR:HD2	9:H:143:VAL:HG22	1.84	0.41
1:a:115:THR:HB	1:a:124:HIS:CE1	2.55	0.41
25:i:303:UQ8:H35B	25:i:303:UQ8:H37A	1.99	0.41
1:A:145:LEU:HD21	12:M:55:MET:SD	2.60	0.41
22:B:403:CDL:H612	22:B:403:CDL:H642	1.92	0.41
8:G:197:GLU:HB3	8:G:283:LEU:HD11	2.03	0.41
2:b:162:MET:O	4:F:70:PRO:HG3	2.21	0.41
3:d:198:ARG:HG2	7:c:51:THR:HA	2.02	0.41
23:d:301:PC1:H3H1	22:f:302:CDL:H661	2.03	0.41
11:l:87:PRO:HA	11:l:88:PRO:HD3	1.96	0.41
22:B:402:CDL:H571	22:L:301:CDL:H601	2.03	0.41
4:F:82:LEU:O	4:F:86:ILE:HG13	2.21	0.41
22:K:201:CDL:H432	22:K:201:CDL:H402	1.88	0.41
23:G:304:PC1:H261	23:G:304:PC1:H292	1.88	0.41
15:P:126:ASP:OD1	15:P:126:ASP:N	2.51	0.41
16:Q:123:ILE:N	16:Q:124:PRO:HD2	2.36	0.41
19:E:337:LEU:HD11	19:E:356:ILE:HD13	2.02	0.41
2:b:132:VAL:HG22	1:A:355:GLU:OE1	2.21	0.41
5:i:82:PHE:O	5:i:82:PHE:CG	2.74	0.41
1:A:153:TYR:CD1	10:J:126:ILE:HG23	2.56	0.41
12:M:1:MET:HB3	13:N:148:ASN:HB3	2.02	0.41
23:i:301:PC1:H12	8:g:87:ARG:HG2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:p:89:PHE:O	15:p:94:ASN:ND2	2.42	0.41
19:e:325:THR:O	19:e:362:ASN:ND2	2.52	0.41
5:I:156:GLU:O	5:I:160:ARG:NH1	2.50	0.41
12:M:111:PHE:N	12:M:112:PRO:HD2	2.36	0.41
1:a:161:TYR:HB2	11:l:175:ILE:HB	2.01	0.41
5:i:181:LYS:O	12:m:202:ARG:HD2	2.21	0.41
25:i:303:UQ8:H10	25:i:303:UQ8:H7A	1.72	0.41
10:j:212:LEU:HD11	11:l:11:TRP:HB3	2.02	0.41
17:r:139:VAL:HG21	13:N:171:VAL:HG11	2.02	0.41
19:e:197:TYR:CG	19:e:198:PRO:HA	2.55	0.41
1:A:226:THR:HG21	5:I:88:PHE:HD2	1.85	0.41
1:A:247:TYR:O	4:F:111:SER:HB3	2.20	0.41
8:G:36:SER:N	8:G:45:GLU:OE2	2.54	0.41
22:i:302:CDL:H421	22:i:302:CDL:H392	1.92	0.41
10:j:123:ARG:N	10:j:124:PRO:HD2	2.36	0.41
14:o:55:MET:HE2	14:o:59:THR:HG21	2.02	0.41
17:r:10:PRO:HB2	17:r:12:LEU:HG	2.02	0.41
1:A:123:LEU:HB2	1:A:142:ILE:HD11	2.03	0.41
2:B:136:TRP:O	2:B:140:SER:OG	2.39	0.41
22:k:203:CDL:H211	22:k:203:CDL:H182	1.93	0.40
9:h:88:TYR:HD2	9:h:143:VAL:HG22	1.86	0.40
15:p:117:LEU:HD12	15:p:120:LEU:HD12	2.03	0.40
16:q:123:ILE:N	16:q:124:PRO:HD2	2.36	0.40
1:A:48:VAL:HG23	4:F:133:LYS:HG3	2.03	0.40
22:B:401:CDL:H152	22:B:401:CDL:H181	1.88	0.40
8:G:43:ARG:NH2	8:G:154:GLU:OE2	2.54	0.40
1:a:145:LEU:HD21	12:m:55:MET:SD	2.61	0.40
2:b:112:ARG:HD3	2:B:157:GLU:OE2	2.21	0.40
28:l:303:PEE:H79	28:l:303:PEE:H72	1.92	0.40
22:B:402:CDL:H472	22:B:402:CDL:H441	1.81	0.40
5:I:82:PHE:O	5:I:82:PHE:CG	2.75	0.40
15:P:37:VAL:N	15:P:38:PRO:HD2	2.36	0.40
21:t:208:LYS:NZ	21:t:315:GLY:O	2.54	0.40
22:b:401:CDL:H662	22:B:401:CDL:H802	2.03	0.40
5:i:177:ASP:HA	5:i:180:LYS:HG2	2.02	0.40
15:p:126:ASP:N	15:p:126:ASP:OD1	2.55	0.40
22:I:301:CDL:H321	22:I:301:CDL:H352	1.83	0.40
22:L:301:CDL:H432	22:L:301:CDL:H402	1.91	0.40
19:E:51:CYS:O	19:E:55:PHE:N	2.50	0.40
21:t:144:ILE:N	21:t:145:PRO:HD2	2.36	0.40
1:a:379:PRO:O	1:a:383:ILE:HG12	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:k:35:TYR:CD2	19:e:87:ARG:HG2	2.56	0.40
8:g:111:LEU:HB2	8:g:112:PRO:HD3	2.04	0.40
16:q:92:VAL:HG22	16:q:128:LYS:HE2	2.03	0.40
22:B:402:CDL:H762	22:B:402:CDL:H732	1.84	0.40
23:D:301:PC1:H3I3	23:D:301:PC1:H3F1	1.90	0.40
22:I:301:CDL:H752	22:I:301:CDL:H782	1.87	0.40
6:K:33:PRO:HB3	6:K:35:TYR:CE2	2.57	0.40
7:C:69:THR:O	7:C:73:VAL:HG23	2.21	0.40
9:h:240:ASP:OD1	21:t:457:LEU:HD21	2.21	0.40
22:B:403:CDL:H661	23:D:301:PC1:H3H2	2.03	0.40
5:I:79:HIS:NE2	5:I:84:MET:O	2.55	0.40
19:E:362:ASN:HB3	19:E:372:LEU:HD22	2.03	0.40
19:E:391:LEU:C	19:E:391:LEU:HD12	2.46	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	431/446 (97%)	425 (99%)	6 (1%)	0	100	100
1	a	431/446 (97%)	425 (99%)	6 (1%)	0	100	100
2	B	159/381 (42%)	153 (96%)	6 (4%)	0	100	100
2	b	159/381 (42%)	154 (97%)	5 (3%)	0	100	100
3	D	108/234 (46%)	106 (98%)	2 (2%)	0	100	100
3	d	108/234 (46%)	107 (99%)	1 (1%)	0	100	100
4	F	198/204 (97%)	197 (100%)	1 (0%)	0	100	100
4	f	198/204 (97%)	196 (99%)	2 (1%)	0	100	100
5	I	207/209 (99%)	201 (97%)	6 (3%)	0	100	100
5	i	207/209 (99%)	201 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	K	177/179 (99%)	169 (96%)	8 (4%)	0	100	100
6	k	177/179 (99%)	168 (95%)	9 (5%)	0	100	100
7	C	94/100 (94%)	90 (96%)	4 (4%)	0	100	100
7	c	94/100 (94%)	91 (97%)	3 (3%)	0	100	100
8	G	254/286 (89%)	246 (97%)	8 (3%)	0	100	100
8	g	254/286 (89%)	243 (96%)	11 (4%)	0	100	100
9	H	229/268 (85%)	223 (97%)	6 (3%)	0	100	100
9	h	229/268 (85%)	227 (99%)	2 (1%)	0	100	100
10	J	267/273 (98%)	259 (97%)	8 (3%)	0	100	100
10	j	267/273 (98%)	259 (97%)	8 (3%)	0	100	100
11	L	244/247 (99%)	239 (98%)	5 (2%)	0	100	100
11	l	244/247 (99%)	240 (98%)	4 (2%)	0	100	100
12	M	219/221 (99%)	217 (99%)	2 (1%)	0	100	100
12	m	219/221 (99%)	218 (100%)	1 (0%)	0	100	100
13	N	117/179 (65%)	113 (97%)	4 (3%)	0	100	100
13	n	117/179 (65%)	114 (97%)	3 (3%)	0	100	100
14	O	97/154 (63%)	95 (98%)	2 (2%)	0	100	100
14	o	97/154 (63%)	96 (99%)	1 (1%)	0	100	100
15	P	148/152 (97%)	142 (96%)	6 (4%)	0	100	100
15	p	148/152 (97%)	143 (97%)	5 (3%)	0	100	100
16	Q	106/152 (70%)	104 (98%)	2 (2%)	0	100	100
16	q	106/152 (70%)	103 (97%)	3 (3%)	0	100	100
17	R	138/149 (93%)	135 (98%)	3 (2%)	0	100	100
17	r	143/149 (96%)	141 (99%)	2 (1%)	0	100	100
18	S	104/145 (72%)	101 (97%)	3 (3%)	0	100	100
18	s	103/145 (71%)	100 (97%)	3 (3%)	0	100	100
19	E	415/480 (86%)	408 (98%)	7 (2%)	0	100	100
19	e	415/480 (86%)	406 (98%)	9 (2%)	0	100	100
20	i1	26/108 (24%)	26 (100%)	0	0	100	100
20	i2	30/108 (28%)	30 (100%)	0	0	100	100
21	t	363/460 (79%)	356 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	7847/9594 (82%)	7667 (98%)	180 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	397/409 (97%)	397 (100%)	0	100	100
1	a	397/409 (97%)	396 (100%)	1 (0%)	86	94
2	B	143/331 (43%)	142 (99%)	1 (1%)	76	89
2	b	143/331 (43%)	143 (100%)	0	100	100
3	D	95/206 (46%)	95 (100%)	0	100	100
3	d	95/206 (46%)	95 (100%)	0	100	100
4	F	175/178 (98%)	175 (100%)	0	100	100
4	f	175/178 (98%)	173 (99%)	2 (1%)	65	84
5	I	182/182 (100%)	180 (99%)	2 (1%)	65	84
5	i	182/182 (100%)	181 (100%)	1 (0%)	81	92
6	K	152/152 (100%)	151 (99%)	1 (1%)	76	89
6	k	152/152 (100%)	152 (100%)	0	100	100
7	C	93/97 (96%)	93 (100%)	0	100	100
7	c	93/97 (96%)	93 (100%)	0	100	100
8	G	235/262 (90%)	234 (100%)	1 (0%)	84	93
8	g	235/262 (90%)	234 (100%)	1 (0%)	84	93
9	H	208/245 (85%)	208 (100%)	0	100	100
9	h	208/245 (85%)	208 (100%)	0	100	100
10	J	235/239 (98%)	235 (100%)	0	100	100
10	j	235/239 (98%)	235 (100%)	0	100	100
11	L	219/220 (100%)	218 (100%)	1 (0%)	81	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	l	219/220 (100%)	218 (100%)	1 (0%)	81	92
12	M	202/202 (100%)	202 (100%)	0	100	100
12	m	202/202 (100%)	202 (100%)	0	100	100
13	N	104/162 (64%)	104 (100%)	0	100	100
13	n	104/162 (64%)	104 (100%)	0	100	100
14	O	89/142 (63%)	89 (100%)	0	100	100
14	o	89/142 (63%)	89 (100%)	0	100	100
15	P	131/133 (98%)	130 (99%)	1 (1%)	73	88
15	p	131/133 (98%)	131 (100%)	0	100	100
16	Q	97/135 (72%)	97 (100%)	0	100	100
16	q	97/135 (72%)	97 (100%)	0	100	100
17	R	120/129 (93%)	120 (100%)	0	100	100
17	r	125/129 (97%)	125 (100%)	0	100	100
18	S	95/131 (72%)	94 (99%)	1 (1%)	65	84
18	s	94/131 (72%)	94 (100%)	0	100	100
19	E	359/414 (87%)	358 (100%)	1 (0%)	86	94
19	e	359/414 (87%)	358 (100%)	1 (0%)	86	94
20	i1	26/101 (26%)	26 (100%)	0	100	100
20	i2	29/101 (29%)	29 (100%)	0	100	100
21	t	325/414 (78%)	321 (99%)	4 (1%)	63	83
All	All	7046/8554 (82%)	7026 (100%)	20 (0%)	84	94

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	364	LEU
4	f	19	GLN
4	f	43	GLU
5	i	124	LEU
8	g	217	PHE
11	l	205	TRP
19	e	398	TYR
2	B	188	GLU
5	I	90	HIS
5	I	124	LEU

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Mol	Chain	Res	Type
6	K	49	THR
8	G	217	PHE
11	L	205	TRP
15	P	126	ASP
18	S	62	LYS
19	E	398	TYR
21	t	99	HIS
21	t	101	ARG
21	t	173	ARG
21	t	250	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	a	443	ASN
2	b	168	GLN
7	c	52	HIS
8	g	61	HIS
8	g	93	ASN
9	h	58	HIS
9	h	178	GLN
10	j	30	GLN
10	j	186	GLN
10	j	211	HIS
10	j	232	ASN
11	l	50	GLN
11	l	78	GLN
11	l	217	HIS
11	l	221	HIS
12	m	16	GLN
12	m	74	HIS
12	m	97	ASN
13	n	76	ASN
14	o	108	GLN
16	q	137	ASN
16	q	146	ASN
18	s	48	GLN
19	e	54	HIS
19	e	165	ASN
19	e	219	GLN
19	e	221	HIS
19	e	293	ASN

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Mol	Chain	Res	Type
19	e	361	ASN
1	A	202	ASN
2	B	104	HIS
2	B	168	GLN
2	B	177	ASN
4	F	81	ASN
4	F	134	GLN
5	I	57	ASN
5	I	83	HIS
5	I	139	ASN
5	I	201	ASN
6	K	32	GLN
7	C	52	HIS
8	G	61	HIS
8	G	93	ASN
9	H	101	GLN
9	H	136	HIS
11	L	40	ASN
11	L	50	GLN
11	L	90	HIS
11	L	183	ASN
11	L	217	HIS
12	M	74	HIS
12	M	94	ASN
14	O	108	GLN
16	Q	69	GLN
16	Q	146	ASN
18	S	100	ASN
19	E	220	HIS
19	E	221	HIS
19	E	275	GLN
19	E	370	GLN
21	t	254	ASN
21	t	270	ASN
21	t	304	HIS
21	t	316	ASN
21	t	360	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 50 ligands modelled in this entry, 2 are monoatomic - leaving 48 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$
22	CDL	b	402	-	99,99,99	0.90	7 (7%)	105,111,111	0.94	4 (3%)
22	CDL	i	302	-	99,99,99	0.91	8 (8%)	105,111,111	0.95	4 (3%)
22	CDL	I	302	-	99,99,99	0.90	8 (8%)	105,111,111	0.99	4 (3%)
26	ATP	G	301	27	32,33,33	3.48	12 (37%)	48,52,52	2.18	12 (25%)
22	CDL	f	303	-	99,99,99	0.91	8 (8%)	105,111,111	1.13	6 (5%)
22	CDL	P	201	-	99,99,99	0.89	8 (8%)	105,111,111	1.04	5 (4%)
24	PO4	F	900	-	4,4,4	1.11	0	6,6,6	0.49	0
23	PC1	G	304	-	53,53,53	0.98	3 (5%)	59,61,61	1.05	2 (3%)
22	CDL	B	404	-	99,99,99	0.90	8 (8%)	105,111,111	0.96	4 (3%)
29	NAD	e	900	-	46,48,48	4.04	22 (47%)	64,73,73	2.08	13 (20%)
29	NAD	E	900	-	46,48,48	4.03	22 (47%)	64,73,73	2.07	14 (21%)
24	PO4	f	301	-	4,4,4	1.11	0	6,6,6	0.45	0
22	CDL	p	201	-	99,99,99	0.90	8 (8%)	105,111,111	1.01	4 (3%)
22	CDL	I	301	-	99,99,99	0.89	6 (6%)	105,111,111	0.96	4 (3%)
28	PEE	J	304	-	50,50,50	1.18	6 (12%)	53,55,55	1.14	4 (7%)
22	CDL	L	301	-	99,99,99	0.90	8 (8%)	105,111,111	0.99	4 (3%)
22	CDL	K	201	-	99,99,99	0.90	8 (8%)	105,111,111	1.02	4 (3%)
22	CDL	B	405	-	99,99,99	0.89	8 (8%)	105,111,111	1.11	5 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CDL	j	301	-	99,99,99	0.90	8 (8%)	105,111,111	1.08	5 (4%)
22	CDL	b	401	-	99,99,99	0.89	8 (8%)	105,111,111	0.99	4 (3%)
25	UQ8	i	303	-	53,53,53	1.86	7 (13%)	66,67,67	1.57	15 (22%)
22	CDL	k	203	-	99,99,99	0.90	8 (8%)	105,111,111	1.00	4 (3%)
22	CDL	l	301	-	99,99,99	0.90	7 (7%)	105,111,111	1.02	4 (3%)
23	PC1	i	301	-	53,53,53	0.98	4 (7%)	59,61,61	0.97	2 (3%)
28	PEE	J	303	-	47,47,50	1.20	6 (12%)	50,52,55	1.14	4 (8%)
22	CDL	B	403	-	99,99,99	0.88	7 (7%)	105,111,111	1.10	4 (3%)
22	CDL	B	402	-	99,99,99	0.89	8 (8%)	105,111,111	1.07	4 (3%)
22	CDL	K	202	-	99,99,99	0.90	7 (7%)	105,111,111	1.07	5 (4%)
28	PEE	l	302	-	47,47,50	1.21	6 (12%)	50,52,55	1.10	4 (8%)
22	CDL	J	301	-	99,99,99	0.90	7 (7%)	105,111,111	1.08	4 (3%)
22	CDL	l	304	-	99,99,99	0.90	8 (8%)	105,111,111	1.05	4 (3%)
23	PC1	G	303	-	53,53,53	0.99	4 (7%)	59,61,61	0.95	2 (3%)
28	PEE	l	303	-	50,50,50	1.17	6 (12%)	53,55,55	1.14	4 (7%)
22	CDL	r	201	-	99,99,99	0.88	6 (6%)	105,111,111	0.98	4 (3%)
23	PC1	D	301	-	53,53,53	0.96	4 (7%)	59,61,61	1.10	3 (5%)
22	CDL	A	501	-	99,99,99	0.89	7 (7%)	105,111,111	1.02	6 (5%)
22	CDL	J	302	-	99,99,99	0.89	7 (7%)	105,111,111	1.00	4 (3%)
23	PC1	g	303	-	53,53,53	0.98	4 (7%)	59,61,61	1.05	3 (5%)
22	CDL	k	201	-	99,99,99	0.90	8 (8%)	105,111,111	1.08	5 (4%)
22	CDL	B	401	-	99,99,99	0.90	8 (8%)	105,111,111	1.00	5 (4%)
25	UQ8	I	303	-	53,53,53	1.86	7 (13%)	66,67,67	1.55	13 (19%)
23	PC1	d	301	-	53,53,53	0.95	4 (7%)	59,61,61	1.09	3 (5%)
26	ATP	g	301	27	32,33,33	3.47	13 (40%)	48,52,52	2.16	12 (25%)
22	CDL	f	302	-	99,99,99	0.90	8 (8%)	105,111,111	1.07	5 (4%)
22	CDL	k	202	-	99,99,99	0.90	7 (7%)	105,111,111	1.04	5 (4%)
22	CDL	f	304	-	99,99,99	0.89	8 (8%)	105,111,111	1.06	5 (4%)
22	CDL	a	501	-	99,99,99	0.90	7 (7%)	105,111,111	1.02	3 (2%)
22	CDL	j	302	-	99,99,99	0.88	7 (7%)	105,111,111	1.03	4 (3%)

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
22	CDL	b	402	-	-	42/110/110/110	-
22	CDL	i	302	-	-	40/110/110/110	-
22	CDL	I	302	-	-	38/110/110/110	-
26	ATP	G	301	27	-	0/22/38/38	0/3/3/3
22	CDL	f	303	-	-	42/110/110/110	-
22	CDL	P	201	-	-	39/110/110/110	-
23	PC1	G	304	-	-	19/57/57/57	-
22	CDL	B	404	-	-	38/110/110/110	-
29	NAD	e	900	-	-	7/30/62/62	0/5/5/5
29	NAD	E	900	-	-	7/30/62/62	0/5/5/5
22	CDL	p	201	-	-	33/110/110/110	-
22	CDL	I	301	-	-	50/110/110/110	-
28	PEE	J	304	-	-	24/54/54/54	-
22	CDL	L	301	-	-	44/110/110/110	-
22	CDL	K	201	-	-	33/110/110/110	-
22	CDL	B	405	-	-	40/110/110/110	-
22	CDL	j	301	-	-	40/110/110/110	-
22	CDL	b	401	-	-	55/110/110/110	-
25	UQ8	i	303	-	-	8/51/75/75	0/1/1/1
22	CDL	k	203	-	-	45/110/110/110	-
22	CDL	l	301	-	-	36/110/110/110	-
23	PC1	i	301	-	-	16/57/57/57	-
28	PEE	J	303	-	-	23/51/51/54	-
22	CDL	B	403	-	-	42/110/110/110	-
22	CDL	B	402	-	-	53/110/110/110	-
22	CDL	K	202	-	-	39/110/110/110	-
28	PEE	l	302	-	-	26/51/51/54	-
22	CDL	J	301	-	-	33/110/110/110	-
22	CDL	l	304	-	-	40/110/110/110	-
23	PC1	G	303	-	-	17/57/57/57	-
28	PEE	l	303	-	-	24/54/54/54	-
22	CDL	r	201	-	-	45/110/110/110	-
23	PC1	D	301	-	-	14/57/57/57	-
22	CDL	A	501	-	-	49/110/110/110	-
22	CDL	J	302	-	-	36/110/110/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	PC1	g	303	-	-	16/57/57/57	-
22	CDL	k	201	-	-	35/110/110/110	-
22	CDL	B	401	-	-	51/110/110/110	-
25	UQ8	I	303	-	-	11/51/75/75	0/1/1/1
23	PC1	d	301	-	-	17/57/57/57	-
26	ATP	g	301	27	-	0/22/38/38	0/3/3/3
22	CDL	f	302	-	-	43/110/110/110	-
22	CDL	k	202	-	-	42/110/110/110	-
22	CDL	f	304	-	-	58/110/110/110	-
22	CDL	a	501	-	-	47/110/110/110	-
22	CDL	j	302	-	-	37/110/110/110	-

All (356) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	e	900	NAD	O4D-C1D	-10.29	1.27	1.40
29	E	900	NAD	O4D-C1D	-10.21	1.27	1.40
25	i	303	UQ8	C6-C1	9.99	1.53	1.35
25	I	303	UQ8	C6-C1	9.94	1.53	1.35
29	e	900	NAD	PN-O3	9.64	1.69	1.59
26	G	301	ATP	C3'-C4'	-9.61	1.28	1.53
26	g	301	ATP	C3'-C4'	-9.58	1.28	1.53
29	E	900	NAD	PN-O3	9.47	1.69	1.59
29	E	900	NAD	C3B-C4B	-9.35	1.29	1.53
29	e	900	NAD	C3B-C4B	-9.32	1.29	1.53
29	E	900	NAD	C7N-N7N	8.72	1.49	1.33
29	e	900	NAD	C7N-N7N	8.71	1.49	1.33
29	E	900	NAD	C3D-C4D	-8.57	1.31	1.53
29	e	900	NAD	C3D-C4D	-8.55	1.31	1.53
26	g	301	ATP	C2'-C1'	-8.22	1.27	1.53
26	G	301	ATP	C2'-C1'	-8.14	1.27	1.53
29	e	900	NAD	O4D-C4D	7.58	1.61	1.45
29	E	900	NAD	O4D-C4D	7.56	1.61	1.45
29	e	900	NAD	O4B-C4B	7.55	1.61	1.45
29	E	900	NAD	O4B-C4B	7.54	1.61	1.45
26	G	301	ATP	O4'-C1'	6.28	1.56	1.42
26	g	301	ATP	O4'-C1'	6.20	1.56	1.42
29	e	900	NAD	C6A-N6A	5.97	1.49	1.34
29	E	900	NAD	C6A-N6A	5.96	1.49	1.34
26	G	301	ATP	PA-O3A	5.67	1.65	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	g	301	ATP	PA-O3A	5.59	1.65	1.59
26	G	301	ATP	PB-O3A	5.32	1.65	1.59
26	g	301	ATP	PB-O3A	5.26	1.65	1.59
29	E	900	NAD	C3N-C7N	4.75	1.57	1.50
26	G	301	ATP	PB-O3B	4.73	1.64	1.59
26	G	301	ATP	C2'-C3'	4.73	1.66	1.53
26	g	301	ATP	PB-O3B	4.70	1.64	1.59
26	g	301	ATP	C2'-C3'	4.65	1.66	1.53
29	e	900	NAD	C3N-C7N	4.63	1.57	1.50
25	I	303	UQ8	C4-C3	4.62	1.53	1.36
29	e	900	NAD	PA-O3	4.60	1.64	1.59
29	E	900	NAD	PA-O3	4.58	1.64	1.59
25	i	303	UQ8	C4-C3	4.58	1.52	1.36
26	g	301	ATP	O4'-C4'	4.45	1.54	1.45
26	G	301	ATP	O4'-C4'	4.45	1.54	1.45
26	G	301	ATP	C6-N6	4.41	1.45	1.34
29	e	900	NAD	O4B-C1B	-4.40	1.31	1.42
29	E	900	NAD	O3D-C3D	4.32	1.53	1.43
29	e	900	NAD	O3D-C3D	4.32	1.53	1.43
26	g	301	ATP	C6-N6	4.29	1.45	1.34
29	E	900	NAD	O4B-C1B	-4.19	1.32	1.42
28	J	303	PEE	C39-C38	3.86	1.53	1.31
28	l	303	PEE	C18-C19	3.85	1.53	1.31
28	J	304	PEE	C39-C38	3.83	1.53	1.31
28	l	303	PEE	C39-C38	3.82	1.53	1.31
28	J	304	PEE	C18-C19	3.80	1.53	1.31
28	l	302	PEE	C39-C38	3.76	1.53	1.31
28	l	302	PEE	C18-C19	3.70	1.52	1.31
28	J	303	PEE	C18-C19	3.68	1.52	1.31
22	A	501	CDL	OA6-CA4	-3.14	1.39	1.46
22	l	301	CDL	OA6-CA4	-3.12	1.39	1.46
22	K	202	CDL	OA6-CA4	-3.09	1.39	1.46
26	g	301	ATP	C5-C4	-3.09	1.33	1.39
22	k	202	CDL	OA6-CA4	-3.07	1.39	1.46
22	a	501	CDL	OA6-CA4	-3.03	1.39	1.46
26	G	301	ATP	C5-C4	-3.02	1.33	1.39
22	L	301	CDL	OA6-CA4	-3.02	1.39	1.46
22	B	403	CDL	OA6-CA4	-3.01	1.39	1.46
29	e	900	NAD	O3B-C3B	3.00	1.50	1.43
29	E	900	NAD	O3B-C3B	2.98	1.50	1.43
22	B	404	CDL	OB6-CB4	-2.95	1.39	1.46
22	f	302	CDL	OB6-CB4	-2.95	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	E	900	NAD	C2N-N1N	2.94	1.38	1.35
22	J	301	CDL	OA6-CA4	-2.92	1.39	1.46
22	f	302	CDL	OA6-CA4	-2.91	1.39	1.46
22	b	402	CDL	OB6-CB4	-2.91	1.39	1.46
22	I	301	CDL	OB6-CB4	-2.90	1.39	1.46
22	a	501	CDL	OB6-CB4	-2.90	1.39	1.46
22	L	301	CDL	OB6-CB4	-2.89	1.39	1.46
22	r	201	CDL	OB6-CB4	-2.89	1.39	1.46
23	G	303	PC1	O21-C2	-2.87	1.39	1.46
23	i	301	PC1	O21-C2	-2.85	1.39	1.46
29	e	900	NAD	C2N-N1N	2.84	1.38	1.35
22	j	301	CDL	OA6-CA4	-2.83	1.39	1.46
22	B	401	CDL	OB6-CB4	-2.83	1.39	1.46
22	K	202	CDL	OB6-CB4	-2.80	1.40	1.46
22	A	501	CDL	OB6-CB4	-2.79	1.40	1.46
22	I	302	CDL	OA6-CA4	-2.79	1.40	1.46
22	p	201	CDL	OA6-CA4	-2.78	1.40	1.46
28	J	303	PEE	O2-C2	-2.78	1.40	1.46
22	p	201	CDL	OB6-CB4	-2.78	1.40	1.46
22	B	401	CDL	OA6-CA4	-2.77	1.40	1.46
22	P	201	CDL	OA6-CA4	-2.76	1.40	1.46
22	J	302	CDL	OB6-CB4	-2.76	1.40	1.46
22	b	401	CDL	OB6-CB4	-2.76	1.40	1.46
22	j	301	CDL	OB6-CB4	-2.76	1.40	1.46
29	E	900	NAD	C8A-N9A	-2.75	1.32	1.37
22	i	302	CDL	OA6-CA4	-2.74	1.40	1.46
22	l	304	CDL	OB6-CB4	-2.74	1.40	1.46
22	j	302	CDL	OB6-CB4	-2.72	1.40	1.46
22	B	402	CDL	OB6-CB4	-2.71	1.40	1.46
29	e	900	NAD	C8A-N9A	-2.71	1.32	1.37
29	E	900	NAD	C5A-C4A	-2.71	1.34	1.39
28	l	302	PEE	O2-C2	-2.70	1.40	1.46
22	J	301	CDL	OB6-CB4	-2.69	1.40	1.46
22	l	304	CDL	OA8-CA7	2.69	1.41	1.33
23	G	304	PC1	O21-C2	-2.69	1.40	1.46
22	f	304	CDL	OA6-CA4	-2.69	1.40	1.46
22	I	301	CDL	OA6-CA4	-2.69	1.40	1.46
22	l	301	CDL	OB6-CB4	-2.68	1.40	1.46
29	e	900	NAD	C5A-C4A	-2.68	1.34	1.39
28	J	304	PEE	O2-C2	-2.68	1.40	1.46
28	l	303	PEE	O2-C2	-2.68	1.40	1.46
22	B	405	CDL	OB6-CB4	-2.67	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	K	201	CDL	OB6-CB4	-2.66	1.40	1.46
22	k	202	CDL	OB6-CB4	-2.66	1.40	1.46
22	k	203	CDL	OB6-CB4	-2.66	1.40	1.46
22	P	201	CDL	OB6-CB4	-2.65	1.40	1.46
22	b	402	CDL	OA8-CA7	2.65	1.41	1.33
29	E	900	NAD	O2B-C2B	-2.65	1.36	1.43
22	f	303	CDL	OB6-CB4	-2.65	1.40	1.46
22	J	302	CDL	OA6-CA4	-2.65	1.40	1.46
22	r	201	CDL	OA6-CA4	-2.63	1.40	1.46
22	B	403	CDL	OB6-CB4	-2.62	1.40	1.46
22	b	401	CDL	OA6-CA4	-2.62	1.40	1.46
23	g	303	PC1	O21-C2	-2.61	1.40	1.46
22	I	302	CDL	OB6-CB4	-2.60	1.40	1.46
22	f	304	CDL	OB6-CB4	-2.60	1.40	1.46
22	B	404	CDL	OA6-CA4	-2.59	1.40	1.46
22	J	301	CDL	OA8-CA7	2.59	1.40	1.33
22	i	302	CDL	OB6-CB4	-2.58	1.40	1.46
29	e	900	NAD	O2B-C2B	-2.58	1.36	1.43
22	k	201	CDL	OB6-CB4	-2.58	1.40	1.46
22	f	302	CDL	OA8-CA7	2.57	1.40	1.33
22	k	203	CDL	OA8-CA7	2.57	1.40	1.33
22	f	303	CDL	OA6-CA4	-2.57	1.40	1.46
29	e	900	NAD	C2A-N1A	2.57	1.38	1.33
23	D	301	PC1	O21-C2	-2.56	1.40	1.46
22	k	203	CDL	OA6-CA4	-2.56	1.40	1.46
29	E	900	NAD	C2A-N1A	2.56	1.38	1.33
22	j	302	CDL	OA6-CA4	-2.56	1.40	1.46
25	i	303	UQ8	O4-C4M	-2.56	1.39	1.45
22	b	401	CDL	OB8-CB6	-2.56	1.39	1.45
22	f	303	CDL	OA8-CA7	2.55	1.40	1.33
22	k	202	CDL	OA8-CA7	2.55	1.40	1.33
22	b	402	CDL	OA6-CA4	-2.55	1.40	1.46
22	I	301	CDL	OA8-CA7	2.55	1.40	1.33
22	K	202	CDL	OA8-CA7	2.54	1.40	1.33
22	l	301	CDL	OB8-CB6	-2.54	1.39	1.45
22	j	301	CDL	OA8-CA7	2.54	1.40	1.33
22	K	201	CDL	OB8-CB7	2.53	1.40	1.33
22	l	304	CDL	OA6-CA4	-2.53	1.40	1.46
23	g	303	PC1	O31-C31	2.53	1.40	1.33
22	r	201	CDL	OA8-CA7	2.53	1.40	1.33
22	J	302	CDL	OB8-CB7	2.52	1.40	1.33
22	j	302	CDL	OB8-CB7	2.52	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	404	CDL	OA8-CA7	2.52	1.40	1.33
22	K	201	CDL	OA6-CA4	-2.52	1.40	1.46
22	B	405	CDL	OA6-CA4	-2.52	1.40	1.46
23	G	304	PC1	O31-C31	2.52	1.40	1.33
22	k	201	CDL	OB8-CB7	2.51	1.40	1.33
22	B	405	CDL	OA8-CA7	2.51	1.40	1.33
22	j	302	CDL	OA8-CA7	2.51	1.40	1.33
22	B	405	CDL	OB8-CB7	2.50	1.40	1.33
26	g	301	ATP	C5-N7	-2.49	1.34	1.39
22	P	201	CDL	OB8-CB7	2.49	1.40	1.33
25	i	303	UQ8	O3-C3M	-2.49	1.39	1.45
22	p	201	CDL	OB8-CB7	2.49	1.40	1.33
22	B	402	CDL	OA6-CA4	-2.49	1.40	1.46
22	r	201	CDL	OB8-CB6	-2.49	1.39	1.45
23	i	301	PC1	O31-C31	2.48	1.40	1.33
26	G	301	ATP	C8-N9	-2.48	1.33	1.37
22	k	201	CDL	OA6-CA5	2.47	1.41	1.34
22	a	501	CDL	OA8-CA7	2.47	1.40	1.33
22	B	402	CDL	OB8-CB6	-2.47	1.39	1.45
22	f	303	CDL	OA6-CA5	2.47	1.41	1.34
22	j	301	CDL	OB8-CB7	2.46	1.40	1.33
22	B	402	CDL	OA8-CA6	-2.46	1.39	1.45
29	E	900	NAD	O7N-C7N	-2.46	1.19	1.24
22	f	303	CDL	OB8-CB7	2.46	1.40	1.33
25	I	303	UQ8	O3-C3M	-2.46	1.39	1.45
22	L	301	CDL	OB8-CB7	2.46	1.40	1.33
22	k	201	CDL	OA8-CA7	2.46	1.40	1.33
22	a	501	CDL	OB8-CB7	2.45	1.40	1.33
22	P	201	CDL	OA8-CA7	2.45	1.40	1.33
26	g	301	ATP	C8-N9	-2.44	1.33	1.37
25	I	303	UQ8	O4-C4M	-2.44	1.39	1.45
22	L	301	CDL	OA8-CA7	2.44	1.40	1.33
22	b	401	CDL	OA8-CA7	2.44	1.40	1.33
22	l	304	CDL	OB8-CB7	2.43	1.40	1.33
22	B	403	CDL	OA8-CA7	2.43	1.40	1.33
22	k	203	CDL	OB8-CB7	2.43	1.40	1.33
22	i	302	CDL	OA8-CA7	2.43	1.40	1.33
28	l	302	PEE	O3-C3	-2.43	1.39	1.45
26	G	301	ATP	C5-N7	-2.43	1.34	1.39
22	B	401	CDL	OB8-CB7	2.43	1.40	1.33
22	I	302	CDL	OA8-CA7	2.42	1.40	1.33
22	J	301	CDL	OB8-CB7	2.42	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	D	301	PC1	O31-C3	-2.42	1.39	1.45
22	k	201	CDL	OA6-CA4	-2.42	1.40	1.46
22	A	501	CDL	OB8-CB7	2.41	1.40	1.33
22	f	304	CDL	OA8-CA7	2.41	1.40	1.33
22	K	201	CDL	OA8-CA7	2.41	1.40	1.33
22	K	202	CDL	OB8-CB7	2.41	1.40	1.33
28	J	303	PEE	O3-C3	-2.40	1.39	1.45
22	I	301	CDL	OB8-CB6	-2.40	1.39	1.45
22	f	302	CDL	OB8-CB6	-2.39	1.39	1.45
29	e	900	NAD	O7N-C7N	-2.39	1.19	1.24
23	d	301	PC1	O21-C2	-2.39	1.41	1.46
22	J	302	CDL	OA8-CA7	2.38	1.40	1.33
22	p	201	CDL	OA8-CA7	2.38	1.40	1.33
22	B	402	CDL	OB8-CB7	2.38	1.40	1.33
22	I	301	CDL	OB8-CB7	2.38	1.40	1.33
22	I	302	CDL	OB8-CB6	-2.37	1.39	1.45
28	J	304	PEE	O3-C30	2.37	1.40	1.33
22	l	301	CDL	OA8-CA7	2.37	1.40	1.33
22	i	302	CDL	OB8-CB7	2.37	1.40	1.33
22	B	403	CDL	OB8-CB6	-2.37	1.39	1.45
23	G	303	PC1	O31-C31	2.36	1.40	1.33
22	k	202	CDL	OB8-CB7	2.36	1.40	1.33
28	l	303	PEE	O3-C30	2.35	1.40	1.33
23	g	303	PC1	O21-C21	2.35	1.40	1.34
22	b	402	CDL	OB8-CB7	2.35	1.40	1.33
22	f	304	CDL	OB8-CB7	2.34	1.40	1.33
23	G	303	PC1	O31-C3	-2.34	1.39	1.45
23	d	301	PC1	O21-C21	2.34	1.40	1.34
23	D	301	PC1	O21-C21	2.33	1.40	1.34
22	A	501	CDL	OA8-CA6	-2.33	1.40	1.45
22	B	401	CDL	OA8-CA7	2.33	1.40	1.33
22	f	304	CDL	OB8-CB6	-2.33	1.40	1.45
22	b	401	CDL	OB8-CB7	2.33	1.40	1.33
28	J	304	PEE	O3-C3	-2.32	1.40	1.45
22	B	404	CDL	OB8-CB7	2.32	1.40	1.33
22	i	302	CDL	OB8-CB6	-2.32	1.40	1.45
22	B	404	CDL	OB8-CB6	-2.32	1.40	1.45
22	f	302	CDL	OB8-CB7	2.31	1.40	1.33
22	I	302	CDL	OB8-CB7	2.31	1.40	1.33
22	K	201	CDL	OA6-CA5	2.31	1.40	1.34
23	d	301	PC1	O31-C31	2.31	1.40	1.33
22	f	303	CDL	OB6-CB5	2.30	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	i	302	CDL	OB6-CB5	2.30	1.40	1.34
22	A	501	CDL	OB8-CB6	-2.30	1.40	1.45
22	a	501	CDL	OA8-CA6	-2.30	1.40	1.45
22	A	501	CDL	OA8-CA7	2.29	1.40	1.33
22	B	402	CDL	OA8-CA7	2.29	1.40	1.33
23	d	301	PC1	O31-C3	-2.29	1.40	1.45
22	k	202	CDL	OB8-CB6	-2.29	1.40	1.45
22	b	402	CDL	OB8-CB6	-2.28	1.40	1.45
28	l	302	PEE	O3-C30	2.28	1.40	1.33
22	B	403	CDL	OB8-CB7	2.27	1.40	1.33
22	l	301	CDL	OB8-CB7	2.27	1.40	1.33
22	B	405	CDL	OA6-CA5	2.27	1.40	1.34
22	L	301	CDL	OB8-CB6	-2.26	1.40	1.45
22	k	201	CDL	OB6-CB5	2.26	1.40	1.34
22	a	501	CDL	OB8-CB6	-2.26	1.40	1.45
28	J	303	PEE	O3-C30	2.26	1.39	1.33
22	k	203	CDL	OB8-CB6	-2.26	1.40	1.45
22	I	302	CDL	OB6-CB5	2.26	1.40	1.34
22	B	402	CDL	OB6-CB5	2.25	1.40	1.34
22	r	201	CDL	OB8-CB7	2.25	1.39	1.33
22	l	301	CDL	OA8-CA6	-2.25	1.40	1.45
22	B	401	CDL	OA6-CA5	2.25	1.40	1.34
22	B	401	CDL	OA8-CA6	-2.25	1.40	1.45
22	l	304	CDL	OB6-CB5	2.25	1.40	1.34
22	k	203	CDL	OB6-CB5	2.24	1.40	1.34
23	G	304	PC1	O21-C21	2.24	1.40	1.34
28	l	302	PEE	O2-C10	2.24	1.40	1.34
22	J	302	CDL	OA8-CA6	-2.24	1.40	1.45
25	I	303	UQ8	C6-C5	2.23	1.52	1.46
22	K	201	CDL	OB6-CB5	2.23	1.40	1.34
22	k	202	CDL	OB6-CB5	2.23	1.40	1.34
22	f	304	CDL	OB6-CB5	2.22	1.40	1.34
22	l	304	CDL	OB8-CB6	-2.22	1.40	1.45
28	J	304	PEE	O2-C10	2.21	1.40	1.34
22	j	302	CDL	OA8-CA6	-2.21	1.40	1.45
22	L	301	CDL	OA8-CA6	-2.21	1.40	1.45
23	D	301	PC1	O31-C31	2.21	1.39	1.33
22	B	405	CDL	OB6-CB5	2.21	1.40	1.34
22	k	203	CDL	OA6-CA5	2.20	1.40	1.34
22	i	302	CDL	OA6-CA5	2.20	1.40	1.34
22	f	304	CDL	OA8-CA6	-2.19	1.40	1.45
22	J	301	CDL	OB6-CB5	2.19	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	P	201	CDL	OB6-CB5	2.19	1.40	1.34
22	j	301	CDL	OB6-CB5	2.19	1.40	1.34
28	l	303	PEE	O2-C10	2.18	1.40	1.34
22	f	303	CDL	OB8-CB6	-2.17	1.40	1.45
22	B	404	CDL	OA6-CA5	2.17	1.40	1.34
22	K	202	CDL	OB6-CB5	2.17	1.40	1.34
22	K	201	CDL	OA8-CA6	-2.17	1.40	1.45
22	B	402	CDL	OA6-CA5	2.16	1.40	1.34
22	b	401	CDL	OA6-CA5	2.16	1.40	1.34
25	i	303	UQ8	O2-C2	-2.16	1.18	1.23
22	b	402	CDL	OA6-CA5	2.16	1.40	1.34
22	i	302	CDL	OA8-CA6	-2.16	1.40	1.45
22	I	302	CDL	OA6-CA5	2.16	1.40	1.34
28	l	303	PEE	O3-C3	-2.16	1.40	1.45
22	j	301	CDL	OB8-CB6	-2.16	1.40	1.45
22	B	401	CDL	OB8-CB6	-2.16	1.40	1.45
25	I	303	UQ8	O5-C5	-2.16	1.18	1.23
22	J	301	CDL	OB8-CB6	-2.16	1.40	1.45
22	K	202	CDL	OA8-CA6	-2.15	1.40	1.45
22	K	202	CDL	OB8-CB6	-2.15	1.40	1.45
28	J	303	PEE	O2-C10	2.15	1.40	1.34
22	J	302	CDL	OB8-CB6	-2.15	1.40	1.45
25	i	303	UQ8	C6-C5	2.15	1.52	1.46
25	i	303	UQ8	O5-C5	-2.15	1.18	1.23
22	f	304	CDL	OA6-CA5	2.14	1.40	1.34
22	b	401	CDL	OA8-CA6	-2.14	1.40	1.45
22	J	302	CDL	OB6-CB5	2.14	1.40	1.34
22	k	202	CDL	OA8-CA6	-2.13	1.40	1.45
22	j	302	CDL	OB6-CB5	2.13	1.40	1.34
22	p	201	CDL	OA6-CA5	2.13	1.40	1.34
22	B	403	CDL	OA8-CA6	-2.13	1.40	1.45
22	P	201	CDL	OA8-CA6	-2.13	1.40	1.45
22	B	404	CDL	OA8-CA6	-2.12	1.40	1.45
22	p	201	CDL	OB6-CB5	2.12	1.40	1.34
22	I	302	CDL	OA8-CA6	-2.12	1.40	1.45
23	i	301	PC1	O31-C3	-2.12	1.40	1.45
22	L	301	CDL	OB6-CB5	2.11	1.40	1.34
29	e	900	NAD	C8A-N7A	2.11	1.35	1.31
25	I	303	UQ8	O2-C2	-2.11	1.18	1.23
22	A	501	CDL	OB6-CB5	2.10	1.40	1.34
22	k	201	CDL	OB8-CB6	-2.10	1.40	1.45
22	b	402	CDL	OB6-CB5	2.10	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	p	201	CDL	OA8-CA6	-2.10	1.40	1.45
22	l	304	CDL	OA6-CA5	2.10	1.40	1.34
22	K	201	CDL	OB8-CB6	-2.09	1.40	1.45
23	G	303	PC1	O21-C21	2.09	1.40	1.34
29	e	900	NAD	PA-O5B	2.09	1.67	1.59
22	k	201	CDL	OA8-CA6	-2.08	1.40	1.45
22	f	302	CDL	OB6-CB5	2.08	1.40	1.34
22	f	302	CDL	OA8-CA6	-2.08	1.40	1.45
22	j	302	CDL	OB8-CB6	-2.07	1.40	1.45
22	P	201	CDL	OA6-CA5	2.07	1.40	1.34
22	P	201	CDL	OB8-CB6	-2.07	1.40	1.45
22	j	301	CDL	OA6-CA5	2.07	1.40	1.34
22	B	405	CDL	OA8-CA6	-2.07	1.40	1.45
22	f	302	CDL	OA6-CA5	2.07	1.40	1.34
22	B	405	CDL	OB8-CB6	-2.06	1.40	1.45
22	B	403	CDL	OB6-CB5	2.06	1.40	1.34
22	f	303	CDL	OA8-CA6	-2.06	1.40	1.45
29	E	900	NAD	PA-O5B	2.06	1.67	1.59
22	a	501	CDL	OA6-CA5	2.05	1.40	1.34
22	I	301	CDL	OA8-CA6	-2.05	1.40	1.45
22	B	401	CDL	OB6-CB5	2.05	1.40	1.34
22	p	201	CDL	OB8-CB6	-2.05	1.40	1.45
23	i	301	PC1	O21-C21	2.05	1.40	1.34
23	g	303	PC1	O31-C3	-2.04	1.40	1.45
22	k	203	CDL	OA8-CA6	-2.04	1.40	1.45
22	J	301	CDL	OA8-CA6	-2.04	1.40	1.45
22	b	401	CDL	OB6-CB5	2.03	1.40	1.34
22	B	404	CDL	OB6-CB5	2.03	1.40	1.34
22	l	301	CDL	OB6-CB5	2.02	1.40	1.34
26	g	301	ATP	C5'-C4'	2.02	1.57	1.51
22	L	301	CDL	OA6-CA5	2.02	1.40	1.34
29	E	900	NAD	C8A-N7A	2.02	1.35	1.31
22	l	304	CDL	OA8-CA6	-2.01	1.40	1.45
22	j	301	CDL	OA8-CA6	-2.01	1.40	1.45
22	r	201	CDL	OB6-CB5	2.01	1.39	1.34
29	e	900	NAD	C5A-N7A	-2.01	1.35	1.39
29	E	900	NAD	C5A-N7A	-2.01	1.35	1.39

All (242) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	e	900	NAD	C4A-N9A-C1B	-6.28	111.94	126.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	E	900	NAD	C4A-N9A-C1B	-6.09	112.38	126.63
26	G	301	ATP	C1'-N9-C8	-5.67	114.51	127.09
29	e	900	NAD	N3A-C2A-N1A	-5.56	120.17	128.58
26	g	301	ATP	C1'-N9-C8	-5.52	114.85	127.09
26	G	301	ATP	N3-C2-N1	-5.50	120.26	128.58
29	E	900	NAD	N3A-C2A-N1A	-5.49	120.27	128.58
26	g	301	ATP	N3-C2-N1	-5.42	120.37	128.58
29	E	900	NAD	N9A-C8A-N7A	-5.02	106.81	113.94
22	k	201	CDL	OA6-CA5-C11	4.99	122.28	111.48
29	E	900	NAD	C5A-C4A-N3A	-4.98	119.86	126.72
29	e	900	NAD	N9A-C8A-N7A	-4.97	106.89	113.94
29	e	900	NAD	C1B-N9A-C8A	4.97	138.12	127.09
29	e	900	NAD	N6A-C6A-N1A	-4.95	107.34	118.38
23	D	301	PC1	O21-C21-C22	4.93	122.14	111.48
23	d	301	PC1	O21-C21-C22	4.90	122.08	111.48
29	E	900	NAD	N6A-C6A-N1A	-4.88	107.51	118.38
22	f	304	CDL	OB6-CB5-C51	4.82	121.90	111.48
23	g	303	PC1	O21-C21-C22	4.81	121.89	111.48
29	e	900	NAD	C5A-C4A-N3A	-4.74	120.18	126.72
29	E	900	NAD	C1B-N9A-C8A	4.73	137.60	127.09
22	f	302	CDL	OB6-CB5-C51	4.73	121.71	111.48
22	f	303	CDL	OA6-CA5-C11	4.73	121.70	111.48
22	B	403	CDL	OB6-CB5-C51	4.68	121.62	111.48
23	G	304	PC1	O21-C21-C22	4.64	121.52	111.48
26	g	301	ATP	N6-C6-N1	-4.61	108.10	118.38
26	G	301	ATP	N6-C6-N1	-4.53	108.30	118.38
26	G	301	ATP	N9-C8-N7	-4.52	107.52	113.94
26	G	301	ATP	C5-C4-N3	-4.51	120.51	126.72
26	g	301	ATP	C5-C4-N3	-4.48	120.54	126.72
26	g	301	ATP	N9-C8-N7	-4.46	107.61	113.94
22	l	301	CDL	OB6-CB5-C51	4.45	121.10	111.48
22	B	405	CDL	OA6-CA5-C11	4.41	121.03	111.48
22	K	201	CDL	OA6-CA5-C11	4.36	120.91	111.48
22	B	402	CDL	OA6-CA5-C11	4.32	120.83	111.48
25	I	303	UQ8	C40-C39-C41	4.21	122.53	115.23
26	G	301	ATP	C4-N9-C1'	4.20	136.46	126.63
22	P	201	CDL	OB6-CB5-C51	4.17	120.51	111.48
22	j	301	CDL	OA6-CA5-C11	4.17	120.50	111.48
22	J	301	CDL	OA6-CA5-C11	4.12	120.39	111.48
28	l	303	PEE	O2-C10-C11	4.12	120.39	111.48
22	J	301	CDL	OB6-CB5-C51	4.11	120.38	111.48
22	j	301	CDL	OB6-CB5-C51	4.11	120.37	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	g	301	ATP	C4-N9-C1'	4.10	136.23	126.63
29	E	900	NAD	C4A-N9A-C8A	4.08	110.02	105.74
22	k	203	CDL	OB6-CB5-C51	4.05	120.24	111.48
22	j	302	CDL	OB6-CB5-C51	4.04	120.21	111.48
29	e	900	NAD	C4A-N9A-C8A	4.01	109.94	105.74
22	k	202	CDL	OB6-CB5-C51	3.99	120.11	111.48
22	I	302	CDL	OB6-CB5-C51	3.97	120.08	111.48
22	J	302	CDL	OB6-CB5-C51	3.97	120.06	111.48
22	k	201	CDL	OB6-CB5-C51	3.97	120.06	111.48
22	K	202	CDL	OB6-CB5-C51	3.94	120.01	111.48
22	b	401	CDL	OB6-CB5-C51	3.94	120.00	111.48
22	i	302	CDL	OB6-CB5-C51	3.91	119.93	111.48
22	B	401	CDL	OA6-CA5-C11	3.89	119.90	111.48
22	f	303	CDL	OB6-CB5-C51	3.88	119.88	111.48
29	E	900	NAD	N3A-C4A-N9A	3.86	133.74	127.17
22	l	304	CDL	OB6-CB5-C51	3.85	119.80	111.48
22	p	201	CDL	OA6-CA5-C11	3.84	119.79	111.48
22	a	501	CDL	OB6-CB5-C51	3.81	119.72	111.48
22	B	404	CDL	OA6-CA5-C11	3.81	119.72	111.48
22	b	401	CDL	OA6-CA5-C11	3.80	119.71	111.48
22	I	302	CDL	OA6-CA5-C11	3.79	119.69	111.48
29	e	900	NAD	C5A-C6A-N6A	3.79	132.67	123.29
23	i	301	PC1	O21-C21-C22	3.78	119.66	111.48
22	p	201	CDL	OB6-CB5-C51	3.77	119.64	111.48
22	B	405	CDL	OB6-CB5-C51	3.77	119.64	111.48
22	f	304	CDL	OA6-CA5-C11	3.76	119.61	111.48
22	A	501	CDL	OB6-CB5-C51	3.70	119.49	111.48
22	P	201	CDL	OA6-CA5-C11	3.70	119.48	111.48
29	E	900	NAD	C5A-C6A-N6A	3.68	132.39	123.29
22	L	301	CDL	OA6-CA5-C11	3.67	119.42	111.48
23	G	303	PC1	O21-C21-C22	3.65	119.38	111.48
22	B	401	CDL	OB6-CB5-C51	3.64	119.36	111.48
29	e	900	NAD	N3A-C4A-N9A	3.62	133.32	127.17
28	J	304	PEE	O2-C10-C11	3.61	119.30	111.48
22	A	501	CDL	OA6-CA5-C11	3.61	119.28	111.48
22	f	302	CDL	OA6-CA5-C11	3.59	119.25	111.48
22	l	304	CDL	OA6-CA5-C11	3.58	119.23	111.48
22	a	501	CDL	OA6-CA5-C11	3.57	119.21	111.48
28	l	302	PEE	O2-C10-C11	3.57	119.20	111.48
22	B	402	CDL	OB6-CB5-C51	3.56	119.18	111.48
25	I	303	UQ8	C27-C28-C29	-3.56	119.48	127.62
22	L	301	CDL	OB6-CB5-C51	3.49	119.03	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	f	303	CDL	OA8-CA7-C31	3.48	122.44	111.83
22	b	402	CDL	OA6-CA5-C11	3.48	119.00	111.48
25	i	303	UQ8	C25-C24-C26	3.48	121.26	115.23
22	k	202	CDL	OA6-CA5-C11	3.46	118.97	111.48
22	K	201	CDL	OB6-CB5-C51	3.44	118.93	111.48
25	I	303	UQ8	C17-C18-C19	-3.41	119.82	127.62
28	J	303	PEE	O2-C10-C11	3.40	118.84	111.48
26	G	301	ATP	C5-C6-N6	3.39	131.68	123.29
26	g	301	ATP	C5-C6-N6	3.38	131.66	123.29
22	l	301	CDL	OA6-CA5-C11	3.34	118.72	111.48
22	k	203	CDL	OA6-CA5-C11	3.33	118.68	111.48
22	B	403	CDL	OA6-CA5-C11	3.31	118.63	111.48
29	E	900	NAD	C2A-N3A-C4A	3.30	119.90	111.83
25	i	303	UQ8	C17-C18-C19	-3.27	120.15	127.62
22	K	202	CDL	OA6-CA5-C11	3.26	118.52	111.48
25	i	303	UQ8	C7-C8-C9	-3.25	121.23	126.83
22	I	301	CDL	OA6-CA5-C11	3.25	118.51	111.48
29	e	900	NAD	C2A-N3A-C4A	3.24	119.75	111.83
22	r	201	CDL	OA6-CA5-C11	3.21	118.42	111.48
25	I	303	UQ8	C20-C19-C21	3.21	120.79	115.23
22	i	302	CDL	OA6-CA5-C11	3.20	118.41	111.48
26	g	301	ATP	C2-N3-C4	3.19	119.61	111.83
26	G	301	ATP	C2-N3-C4	3.17	119.58	111.83
25	i	303	UQ8	C35-C34-C36	3.17	120.74	115.23
22	l	304	CDL	OA8-CA7-C31	3.16	121.46	111.83
25	I	303	UQ8	C7-C8-C9	-3.15	121.41	126.83
29	E	900	NAD	C5A-N7A-C8A	3.14	108.38	103.45
26	G	301	ATP	C4-N9-C8	3.14	109.03	105.74
22	r	201	CDL	OB6-CB5-C51	3.13	118.26	111.48
26	G	301	ATP	C3'-C2'-C1'	3.11	107.36	101.46
26	g	301	ATP	C3'-C2'-C1'	3.11	107.35	101.46
22	I	301	CDL	OB6-CB5-C51	3.07	118.13	111.48
25	i	303	UQ8	C30-C29-C31	3.06	120.54	115.23
29	e	900	NAD	C5A-N7A-C8A	3.04	108.23	103.45
22	j	302	CDL	OA8-CA7-C31	3.04	121.10	111.83
26	g	301	ATP	C4-N9-C8	3.03	108.92	105.74
22	b	402	CDL	OB6-CB5-C51	3.02	118.01	111.48
22	K	201	CDL	OB8-CB7-C71	3.02	121.04	111.83
25	I	303	UQ8	C25-C24-C26	3.01	120.45	115.23
22	f	302	CDL	OA8-CA7-C31	3.00	120.99	111.83
26	G	301	ATP	N3-C4-N9	3.00	132.27	127.17
23	G	304	PC1	O31-C31-C32	2.99	120.96	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	E	900	NAD	C4D-O4D-C1D	-2.98	107.20	109.92
25	i	303	UQ8	C27-C28-C29	-2.95	120.87	127.62
22	J	301	CDL	OB8-CB7-C71	2.94	120.80	111.83
22	B	403	CDL	OA8-CA7-C31	2.93	120.78	111.83
22	K	202	CDL	OA8-CA7-C31	2.93	120.76	111.83
26	g	301	ATP	N3-C4-N9	2.91	132.12	127.17
22	I	301	CDL	OA8-CA7-C31	2.90	120.67	111.83
22	B	404	CDL	OB6-CB5-C51	2.89	117.73	111.48
28	J	304	PEE	O3-C30-C31	2.88	120.63	111.83
22	B	405	CDL	OA8-CA7-C31	2.88	120.63	111.83
22	p	201	CDL	OB8-CB7-C71	2.88	120.61	111.83
22	k	201	CDL	OB8-CB7-C71	2.86	120.55	111.83
28	l	303	PEE	O3-C30-C31	2.84	120.49	111.83
26	G	301	ATP	C5-N7-C8	2.83	107.90	103.45
22	J	302	CDL	OA6-CA5-C11	2.83	117.61	111.48
22	p	201	CDL	OA8-CA7-C31	2.83	120.46	111.83
22	J	301	CDL	OA8-CA7-C31	2.83	120.45	111.83
25	i	303	UQ8	C22-C23-C24	-2.83	121.16	127.62
25	i	303	UQ8	C40-C39-C41	2.82	120.13	115.23
22	P	201	CDL	OA8-CA7-C31	2.82	120.44	111.83
22	B	405	CDL	OB8-CB7-C71	2.81	120.41	111.83
22	j	301	CDL	OA8-CA7-C31	2.81	120.41	111.83
22	k	202	CDL	OA8-CA7-C31	2.79	120.33	111.83
22	f	303	CDL	OB8-CB7-C71	2.79	120.33	111.83
28	J	303	PEE	O3-C30-C31	2.77	120.27	111.83
25	I	303	UQ8	C22-C23-C24	-2.76	121.31	127.62
22	j	302	CDL	OA6-CA5-C11	2.75	117.42	111.48
22	r	201	CDL	OA8-CA7-C31	2.72	120.12	111.83
23	G	303	PC1	O31-C31-C32	2.71	120.10	111.83
22	j	302	CDL	OB8-CB7-C71	2.70	120.07	111.83
26	g	301	ATP	C5-N7-C8	2.69	107.67	103.45
22	B	401	CDL	OA8-CA7-C31	2.68	120.01	111.83
22	K	202	CDL	CA4-OA6-CA5	-2.68	111.39	117.80
22	k	201	CDL	OA8-CA7-C31	2.67	119.97	111.83
23	i	301	PC1	O31-C31-C32	2.65	119.92	111.83
29	e	900	NAD	C4D-O4D-C1D	-2.65	107.50	109.92
25	i	303	UQ8	C12-C13-C14	-2.64	121.59	127.62
22	b	401	CDL	OA8-CA7-C31	2.63	119.86	111.83
22	P	201	CDL	OB8-CB7-C71	2.63	119.86	111.83
22	K	202	CDL	OB8-CB7-C71	2.62	119.83	111.83
22	i	302	CDL	OB8-CB7-C71	2.61	119.79	111.83
22	k	202	CDL	CA4-OA6-CA5	-2.61	111.56	117.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	501	CDL	OB8-CB7-C71	2.60	119.77	111.83
22	K	201	CDL	OA8-CA7-C31	2.60	119.75	111.83
22	j	301	CDL	OB8-CB7-C71	2.59	119.74	111.83
22	b	402	CDL	OB8-CB7-C71	2.56	119.65	111.83
22	L	301	CDL	OA8-CA7-C31	2.56	119.65	111.83
22	f	304	CDL	OA8-CA7-C31	2.55	119.62	111.83
25	i	303	UQ8	C20-C19-C21	2.55	119.65	115.23
22	J	302	CDL	OB8-CB7-C71	2.53	119.55	111.83
22	l	301	CDL	OA8-CA7-C31	2.52	119.52	111.83
22	B	404	CDL	OA8-CA7-C31	2.50	119.47	111.83
22	r	201	CDL	OB8-CB7-C71	2.49	119.43	111.83
22	A	501	CDL	OA8-CA7-C31	2.49	119.42	111.83
22	I	302	CDL	OA8-CA7-C31	2.48	119.40	111.83
23	g	303	PC1	O31-C31-C32	2.48	119.39	111.83
22	k	203	CDL	OA8-CA7-C31	2.48	119.38	111.83
23	D	301	PC1	O31-C31-C32	2.47	119.37	111.83
22	I	302	CDL	OB8-CB7-C71	2.47	119.36	111.83
22	B	403	CDL	OB8-CB7-C71	2.46	119.35	111.83
28	l	302	PEE	O3-C30-C31	2.46	119.33	111.83
22	f	304	CDL	OB8-CB7-C71	2.44	119.28	111.83
22	i	302	CDL	OA8-CA7-C31	2.44	119.26	111.83
22	b	402	CDL	OA8-CA7-C31	2.43	119.25	111.83
22	L	301	CDL	OB8-CB7-C71	2.43	119.25	111.83
22	B	401	CDL	OB8-CB7-C71	2.41	119.19	111.83
22	A	501	CDL	CB4-OB6-CB5	-2.40	112.05	117.80
25	I	303	UQ8	C12-C13-C14	-2.40	122.14	127.62
25	I	303	UQ8	C1M-C1-C6	-2.39	120.52	124.45
22	k	202	CDL	OB8-CB7-C71	2.39	119.11	111.83
23	d	301	PC1	O31-C31-C32	2.38	119.10	111.83
22	b	401	CDL	OB8-CB7-C71	2.36	119.02	111.83
22	J	302	CDL	OA8-CA7-C31	2.34	118.97	111.83
22	l	304	CDL	OB8-CB7-C71	2.34	118.97	111.83
25	i	303	UQ8	C1M-C1-C6	-2.30	120.67	124.45
25	I	303	UQ8	C7-C6-C1	-2.29	120.97	124.89
22	B	402	CDL	OA8-CA7-C31	2.28	118.78	111.83
22	f	303	CDL	OA6-CA5-OA7	-2.27	118.40	123.70
28	J	304	PEE	C17-C18-C19	-2.25	107.94	124.83
22	B	404	CDL	OB8-CB7-C71	2.25	118.69	111.83
22	k	203	CDL	OB8-CB7-C71	2.24	118.66	111.83
29	e	900	NAD	C6N-N1N-C2N	-2.23	119.98	121.88
22	k	201	CDL	OA6-CA5-OA7	-2.23	118.50	123.70
22	B	402	CDL	OB8-CB7-C71	2.22	118.61	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	i	303	UQ8	C46-C44-C45	2.22	119.70	114.59
22	l	301	CDL	OB8-CB7-C71	2.21	118.57	111.83
25	i	303	UQ8	C40-C39-C38	-2.20	117.97	123.63
25	I	303	UQ8	C35-C34-C33	-2.20	117.98	123.63
22	A	501	CDL	OB8-CB7-C71	2.20	118.53	111.83
22	B	405	CDL	OA6-CA5-OA7	-2.18	118.60	123.70
28	J	303	PEE	C17-C18-C19	-2.18	108.48	124.83
29	E	900	NAD	C6N-N1N-C2N	-2.18	120.02	121.88
25	i	303	UQ8	C37-C38-C39	-2.17	122.65	127.62
28	l	302	PEE	C37-C38-C39	-2.14	108.78	124.83
25	I	303	UQ8	C42-C43-C44	-2.14	120.50	127.64
25	i	303	UQ8	C32-C33-C34	-2.13	122.74	127.62
22	f	302	CDL	OB8-CB7-C71	2.11	118.26	111.83
28	J	303	PEE	C40-C39-C38	-2.10	109.12	124.83
22	B	401	CDL	CB4-OB6-CB5	-2.08	112.81	117.80
28	l	303	PEE	C17-C18-C19	-2.08	109.27	124.83
22	I	301	CDL	OB8-CB7-C71	2.08	118.16	111.83
23	d	301	PC1	O21-C21-O22	-2.07	118.85	123.70
22	P	201	CDL	CA4-OA6-CA5	-2.07	112.84	117.80
29	E	900	NAD	C6A-C5A-C4A	2.06	119.98	117.18
25	I	303	UQ8	C41-C39-C38	-2.06	116.55	121.17
22	j	301	CDL	CB4-OB6-CB5	-2.06	112.88	117.80
22	A	501	CDL	CA4-OA6-CA5	-2.05	112.89	117.80
23	D	301	PC1	O21-C21-O22	-2.05	118.91	123.70
28	l	303	PEE	C37-C38-C39	-2.05	109.47	124.83
23	g	303	PC1	O21-C21-O22	-2.04	118.94	123.70
28	l	302	PEE	C40-C39-C38	-2.03	109.59	124.83
22	f	302	CDL	OB6-CB5-OB7	-2.03	118.96	123.70
22	f	304	CDL	OB6-CB5-OB7	-2.02	118.99	123.70
22	f	303	CDL	OA8-CA7-OA9	-2.01	118.60	123.63
28	J	304	PEE	C40-C39-C38	-2.00	109.82	124.83

There are no chirality outliers.

All (1494) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	a	501	CDL	CB3-OB5-PB2-OB2
22	a	501	CDL	CB3-OB5-PB2-OB3
22	a	501	CDL	CB3-OB5-PB2-OB4
22	a	501	CDL	OB7-CB5-OB6-CB4
22	a	501	CDL	C51-CB5-OB6-CB4
22	b	401	CDL	C1-CA2-OA2-PA1

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Mol	Chain	Res	Type	Atoms
22	b	401	CDL	CA2-OA2-PA1-OA4
22	b	401	CDL	CA2-OA2-PA1-OA5
22	b	401	CDL	CA4-CA3-OA5-PA1
22	b	401	CDL	C11-CA5-OA6-CA4
22	b	401	CDL	CB2-OB2-PB2-OB5
22	f	302	CDL	CA3-OA5-PA1-OA2
22	f	302	CDL	CA3-OA5-PA1-OA3
22	f	302	CDL	CA3-OA5-PA1-OA4
22	f	302	CDL	C11-CA5-OA6-CA4
22	f	302	CDL	CB3-OB5-PB2-OB2
22	f	302	CDL	CB3-OB5-PB2-OB3
22	f	302	CDL	CB3-OB5-PB2-OB4
22	f	302	CDL	OB7-CB5-OB6-CB4
22	f	302	CDL	C51-CB5-OB6-CB4
22	f	303	CDL	CA2-C1-CB2-OB2
22	f	303	CDL	OA7-CA5-OA6-CA4
22	f	303	CDL	C11-CA5-OA6-CA4
22	f	303	CDL	OA9-CA7-OA8-CA6
22	f	303	CDL	C31-CA7-OA8-CA6
22	f	303	CDL	CB2-OB2-PB2-OB3
22	f	303	CDL	CB2-OB2-PB2-OB5
22	f	303	CDL	CB3-OB5-PB2-OB2
22	f	303	CDL	CB3-OB5-PB2-OB3
22	f	303	CDL	CB3-OB5-PB2-OB4
22	f	303	CDL	OB6-CB4-CB6-OB8
22	f	304	CDL	CB2-C1-CA2-OA2
22	f	304	CDL	CA2-C1-CB2-OB2
22	f	304	CDL	CA2-OA2-PA1-OA3
22	f	304	CDL	CA3-OA5-PA1-OA3
22	f	304	CDL	CB2-OB2-PB2-OB3
22	f	304	CDL	CB3-OB5-PB2-OB2
22	f	304	CDL	CB3-OB5-PB2-OB3
22	f	304	CDL	CB3-OB5-PB2-OB4
22	f	304	CDL	OB7-CB5-OB6-CB4
22	i	302	CDL	CB3-OB5-PB2-OB2
22	i	302	CDL	CB3-OB5-PB2-OB3
22	i	302	CDL	CB3-OB5-PB2-OB4
22	i	302	CDL	OB7-CB5-OB6-CB4
22	i	302	CDL	C51-CB5-OB6-CB4
22	k	201	CDL	OA7-CA5-OA6-CA4
22	k	201	CDL	C11-CA5-OA6-CA4
22	k	201	CDL	CB2-OB2-PB2-OB3

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Mol	Chain	Res	Type	Atoms
22	k	201	CDL	CB2-OB2-PB2-OB5
22	k	201	CDL	CB3-OB5-PB2-OB2
22	k	201	CDL	CB3-OB5-PB2-OB3
22	k	202	CDL	C11-CA5-OA6-CA4
22	k	202	CDL	CB2-OB2-PB2-OB4
22	k	202	CDL	CB2-OB2-PB2-OB5
22	k	202	CDL	CB3-OB5-PB2-OB2
22	k	202	CDL	CB3-OB5-PB2-OB3
22	k	202	CDL	CB3-OB5-PB2-OB4
22	k	203	CDL	CB3-OB5-PB2-OB2
22	k	203	CDL	CB3-OB5-PB2-OB3
22	j	301	CDL	C51-CB5-OB6-CB4
22	j	302	CDL	CA3-OA5-PA1-OA2
22	j	302	CDL	CA3-OA5-PA1-OA3
22	j	302	CDL	CA3-OA5-PA1-OA4
22	j	302	CDL	CB3-OB5-PB2-OB2
22	j	302	CDL	CB3-OB5-PB2-OB3
22	j	302	CDL	CB3-OB5-PB2-OB4
22	l	301	CDL	CA3-OA5-PA1-OA2
22	l	301	CDL	CA3-OA5-PA1-OA4
22	l	304	CDL	CB3-OB5-PB2-OB3
22	p	201	CDL	CB2-OB2-PB2-OB3
22	p	201	CDL	CB3-OB5-PB2-OB3
22	p	201	CDL	CB3-OB5-PB2-OB4
22	r	201	CDL	CA3-OA5-PA1-OA2
22	r	201	CDL	CA3-OA5-PA1-OA4
22	r	201	CDL	CB2-OB2-PB2-OB3
22	r	201	CDL	CB2-OB2-PB2-OB5
22	A	501	CDL	CB2-C1-CA2-OA2
22	A	501	CDL	C1-CA2-OA2-PA1
22	A	501	CDL	CA2-OA2-PA1-OA3
22	A	501	CDL	CB3-OB5-PB2-OB2
22	A	501	CDL	CB3-OB5-PB2-OB3
22	A	501	CDL	CB3-OB5-PB2-OB4
22	A	501	CDL	C51-CB5-OB6-CB4
22	B	401	CDL	CB2-C1-CA2-OA2
22	B	401	CDL	O1-C1-CB2-OB2
22	B	401	CDL	CB3-OB5-PB2-OB2
22	B	401	CDL	CB3-OB5-PB2-OB3
22	B	401	CDL	C51-CB5-OB6-CB4
22	B	402	CDL	CA4-CA3-OA5-PA1
22	B	402	CDL	C11-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
22	B	402	CDL	CB3-OB5-PB2-OB3
22	B	403	CDL	OA7-CA5-OA6-CA4
22	B	403	CDL	CB3-OB5-PB2-OB2
22	B	403	CDL	CB3-OB5-PB2-OB3
22	B	403	CDL	CB3-OB5-PB2-OB4
22	B	403	CDL	OB7-CB5-OB6-CB4
22	B	404	CDL	CA3-OA5-PA1-OA2
22	B	405	CDL	CA2-C1-CB2-OB2
22	B	405	CDL	OA7-CA5-OA6-CA4
22	B	405	CDL	OA9-CA7-OA8-CA6
22	B	405	CDL	C31-CA7-OA8-CA6
22	B	405	CDL	CB2-OB2-PB2-OB3
22	B	405	CDL	CB3-OB5-PB2-OB2
22	B	405	CDL	CB3-OB5-PB2-OB3
22	B	405	CDL	CB3-OB5-PB2-OB4
22	I	301	CDL	CA3-OA5-PA1-OA2
22	I	301	CDL	CA3-OA5-PA1-OA4
22	I	301	CDL	CB3-OB5-PB2-OB2
22	I	301	CDL	CB3-OB5-PB2-OB3
22	I	301	CDL	CB3-OB5-PB2-OB4
22	I	302	CDL	CB2-C1-CA2-OA2
22	I	302	CDL	O1-C1-CB2-OB2
22	I	302	CDL	CB3-OB5-PB2-OB2
22	I	302	CDL	CB3-OB5-PB2-OB3
22	I	302	CDL	CB3-OB5-PB2-OB4
22	I	302	CDL	OB7-CB5-OB6-CB4
22	I	302	CDL	C51-CB5-OB6-CB4
22	K	201	CDL	CB2-C1-CA2-OA2
22	K	201	CDL	CA3-OA5-PA1-OA3
22	K	201	CDL	OA7-CA5-OA6-CA4
22	K	201	CDL	C11-CA5-OA6-CA4
22	K	201	CDL	CB2-OB2-PB2-OB3
22	K	201	CDL	CB2-OB2-PB2-OB5
22	K	201	CDL	CB3-OB5-PB2-OB2
22	K	201	CDL	CB3-OB5-PB2-OB3
22	K	202	CDL	OA5-CA3-CA4-OA6
22	K	202	CDL	OA7-CA5-OA6-CA4
22	K	202	CDL	C11-CA5-OA6-CA4
22	K	202	CDL	CB2-OB2-PB2-OB5
22	K	202	CDL	CB3-OB5-PB2-OB2
22	K	202	CDL	CB3-OB5-PB2-OB3
22	K	202	CDL	CB3-OB5-PB2-OB4

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Mol	Chain	Res	Type	Atoms
22	J	301	CDL	OB7-CB5-OB6-CB4
22	J	302	CDL	CA3-OA5-PA1-OA2
22	J	302	CDL	CA3-OA5-PA1-OA4
22	J	302	CDL	CB3-OB5-PB2-OB2
22	J	302	CDL	CB3-OB5-PB2-OB3
22	J	302	CDL	CB3-OB5-PB2-OB4
22	L	301	CDL	O1-C1-CA2-OA2
22	L	301	CDL	CA3-OA5-PA1-OA2
22	L	301	CDL	CA3-OA5-PA1-OA4
22	P	201	CDL	CB2-OB2-PB2-OB3
22	P	201	CDL	CB2-OB2-PB2-OB5
22	P	201	CDL	CB3-OB5-PB2-OB2
22	P	201	CDL	CB3-OB5-PB2-OB3
22	P	201	CDL	CB3-OB5-PB2-OB4
23	d	301	PC1	O22-C21-O21-C2
23	d	301	PC1	C22-C21-O21-C2
23	g	303	PC1	O22-C21-O21-C2
23	g	303	PC1	C22-C21-O21-C2
23	D	301	PC1	O13-C11-C12-N
23	D	301	PC1	O22-C21-O21-C2
23	D	301	PC1	C22-C21-O21-C2
23	G	303	PC1	C1-O11-P-O12
23	G	303	PC1	C1-O11-P-O14
23	G	303	PC1	C1-O11-P-O13
23	G	304	PC1	O22-C21-O21-C2
25	i	303	UQ8	C29-C31-C32-C33
28	l	302	PEE	C1-O3P-P-O1P
28	l	302	PEE	C1-O3P-P-O4P
28	l	302	PEE	C4-O4P-P-O3P
28	l	302	PEE	C4-O4P-P-O2P
28	l	302	PEE	C4-O4P-P-O1P
28	l	303	PEE	C1-O3P-P-O2P
28	l	303	PEE	C1-O3P-P-O4P
28	l	303	PEE	C4-O4P-P-O3P
28	l	303	PEE	C4-O4P-P-O2P
28	l	303	PEE	C4-O4P-P-O1P
28	J	303	PEE	C1-O3P-P-O2P
28	J	303	PEE	C1-O3P-P-O1P
28	J	303	PEE	C1-O3P-P-O4P
28	J	304	PEE	C17-C18-C19-C20
28	J	304	PEE	C1-O3P-P-O2P
28	J	304	PEE	C1-O3P-P-O4P

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Mol	Chain	Res	Type	Atoms
28	J	304	PEE	C4-O4P-P-O3P
28	J	304	PEE	C4-O4P-P-O2P
28	J	304	PEE	C4-O4P-P-O1P
29	e	900	NAD	C5B-O5B-PA-O2A
29	E	900	NAD	C5D-O5D-PN-O3
29	E	900	NAD	C5D-O5D-PN-O2N
28	J	303	PEE	O5-C30-O3-C3
22	f	303	CDL	OB9-CB7-OB8-CB6
22	k	201	CDL	OB9-CB7-OB8-CB6
22	k	202	CDL	OA9-CA7-OA8-CA6
22	l	304	CDL	OB9-CB7-OB8-CB6
22	r	201	CDL	OA9-CA7-OA8-CA6
22	r	201	CDL	OB9-CB7-OB8-CB6
22	B	404	CDL	OB9-CB7-OB8-CB6
22	B	405	CDL	OB9-CB7-OB8-CB6
22	I	301	CDL	OA9-CA7-OA8-CA6
22	I	301	CDL	OB9-CB7-OB8-CB6
22	J	302	CDL	OA9-CA7-OA8-CA6
28	l	302	PEE	O5-C30-O3-C3
28	l	303	PEE	O5-C30-O3-C3
22	j	302	CDL	OA9-CA7-OA8-CA6
22	b	401	CDL	OA7-CA5-OA6-CA4
22	f	302	CDL	OA7-CA5-OA6-CA4
22	k	202	CDL	OA7-CA5-OA6-CA4
22	j	301	CDL	OB7-CB5-OB6-CB4
22	p	201	CDL	OA7-CA5-OA6-CA4
22	A	501	CDL	OB7-CB5-OB6-CB4
22	B	401	CDL	OB7-CB5-OB6-CB4
22	B	404	CDL	OA7-CA5-OA6-CA4
22	P	201	CDL	OA7-CA5-OA6-CA4
22	k	201	CDL	C71-CB7-OB8-CB6
22	k	203	CDL	C71-CB7-OB8-CB6
22	r	201	CDL	C31-CA7-OA8-CA6
22	B	405	CDL	C71-CB7-OB8-CB6
22	I	301	CDL	C31-CA7-OA8-CA6
28	l	303	PEE	C31-C30-O3-C3
28	J	303	PEE	C31-C30-O3-C3
22	f	304	CDL	C51-CB5-OB6-CB4
22	p	201	CDL	C11-CA5-OA6-CA4
22	B	403	CDL	C11-CA5-OA6-CA4
22	B	403	CDL	C51-CB5-OB6-CB4
22	B	405	CDL	C11-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
22	J	301	CDL	C51-CB5-OB6-CB4
22	P	201	CDL	C11-CA5-OA6-CA4
23	G	304	PC1	C22-C21-O21-C2
25	I	303	UQ8	C40-C39-C41-C42
25	I	303	UQ8	C38-C39-C41-C42
22	f	303	CDL	C71-CB7-OB8-CB6
22	k	202	CDL	C31-CA7-OA8-CA6
22	j	302	CDL	C31-CA7-OA8-CA6
22	l	304	CDL	C71-CB7-OB8-CB6
22	r	201	CDL	C71-CB7-OB8-CB6
22	B	401	CDL	C31-CA7-OA8-CA6
22	B	404	CDL	C71-CB7-OB8-CB6
22	I	301	CDL	C71-CB7-OB8-CB6
22	K	202	CDL	C31-CA7-OA8-CA6
22	J	302	CDL	C31-CA7-OA8-CA6
28	l	302	PEE	C31-C30-O3-C3
22	b	402	CDL	OB9-CB7-OB8-CB6
22	k	203	CDL	OB9-CB7-OB8-CB6
22	K	201	CDL	OB9-CB7-OB8-CB6
22	K	202	CDL	OA9-CA7-OA8-CA6
22	B	402	CDL	OA7-CA5-OA6-CA4
22	f	303	CDL	O1-C1-CB2-OB2
22	f	304	CDL	O1-C1-CB2-OB2
22	k	201	CDL	O1-C1-CA2-OA2
22	k	202	CDL	O1-C1-CA2-OA2
22	B	405	CDL	O1-C1-CB2-OB2
22	I	301	CDL	O1-C1-CA2-OA2
22	K	201	CDL	O1-C1-CA2-OA2
23	d	301	PC1	C32-C31-O31-C3
22	B	401	CDL	OA9-CA7-OA8-CA6
22	a	501	CDL	C11-CA5-OA6-CA4
22	b	402	CDL	C11-CA5-OA6-CA4
22	j	302	CDL	C11-CA5-OA6-CA4
22	l	304	CDL	C11-CA5-OA6-CA4
22	r	201	CDL	C11-CA5-OA6-CA4
22	B	404	CDL	C11-CA5-OA6-CA4
22	I	301	CDL	C11-CA5-OA6-CA4
22	J	302	CDL	C11-CA5-OA6-CA4
29	E	900	NAD	O4D-C4D-C5D-O5D
22	b	402	CDL	C71-CB7-OB8-CB6
22	K	201	CDL	C71-CB7-OB8-CB6
23	D	301	PC1	C32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
23	d	301	PC1	O32-C31-O31-C3
22	a	501	CDL	OA7-CA5-OA6-CA4
22	b	402	CDL	OA7-CA5-OA6-CA4
22	r	201	CDL	OA7-CA5-OA6-CA4
22	I	301	CDL	OA7-CA5-OA6-CA4
25	i	303	UQ8	C34-C36-C37-C38
25	I	303	UQ8	C39-C41-C42-C43
25	I	303	UQ8	C34-C36-C37-C38
25	I	303	UQ8	C29-C31-C32-C33
23	D	301	PC1	O32-C31-O31-C3
22	k	203	CDL	C11-CA5-OA6-CA4
28	l	302	PEE	C34-C35-C36-C37
22	j	302	CDL	OA7-CA5-OA6-CA4
22	l	304	CDL	OA7-CA5-OA6-CA4
22	J	302	CDL	OA7-CA5-OA6-CA4
22	b	402	CDL	CB2-C1-CA2-OA2
22	i	302	CDL	CB2-C1-CA2-OA2
22	k	201	CDL	CB2-C1-CA2-OA2
22	B	401	CDL	CA2-C1-CB2-OB2
22	B	402	CDL	CA2-C1-CB2-OB2
22	B	404	CDL	CB2-C1-CA2-OA2
22	I	301	CDL	CB2-C1-CA2-OA2
22	I	302	CDL	CA2-C1-CB2-OB2
22	L	301	CDL	CB2-C1-CA2-OA2
22	B	401	CDL	C71-CB7-OB8-CB6
28	J	303	PEE	C34-C35-C36-C37
22	L	301	CDL	CA7-C31-C32-C33
22	b	402	CDL	O1-C1-CA2-OA2
22	f	302	CDL	O1-C1-CB2-OB2
22	A	501	CDL	O1-C1-CA2-OA2
22	B	401	CDL	O1-C1-CA2-OA2
22	B	402	CDL	O1-C1-CB2-OB2
22	B	403	CDL	O1-C1-CB2-OB2
22	B	404	CDL	O1-C1-CA2-OA2
22	b	402	CDL	CA5-C11-C12-C13
22	B	401	CDL	OA5-CA3-CA4-OA6
22	f	304	CDL	C11-CA5-OA6-CA4
22	A	501	CDL	C11-CA5-OA6-CA4
22	B	405	CDL	OB6-CB4-CB6-OB8
28	J	304	PEE	O2-C2-C3-O3
22	B	401	CDL	OB9-CB7-OB8-CB6
22	l	301	CDL	C71-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
22	B	401	CDL	CB5-C51-C52-C53
22	B	405	CDL	CB5-C51-C52-C53
22	k	203	CDL	OA7-CA5-OA6-CA4
22	f	303	CDL	CA5-C11-C12-C13
22	f	303	CDL	CB7-C71-C72-C73
22	f	304	CDL	CB5-C51-C52-C53
22	i	302	CDL	CB5-C51-C52-C53
22	k	201	CDL	CA5-C11-C12-C13
22	l	301	CDL	CB5-C51-C52-C53
22	B	403	CDL	CA5-C11-C12-C13
22	B	404	CDL	CA5-C11-C12-C13
22	J	302	CDL	CA5-C11-C12-C13
22	k	203	CDL	CA5-C11-C12-C13
22	B	404	CDL	CB7-C71-C72-C73
22	i	302	CDL	O1-C1-CA2-OA2
22	I	302	CDL	O1-C1-CA2-OA2
22	A	501	CDL	OA7-CA5-OA6-CA4
22	B	405	CDL	CA5-C11-C12-C13
22	j	301	CDL	C11-CA5-OA6-CA4
22	B	401	CDL	C11-CA5-OA6-CA4
22	b	402	CDL	CA7-C31-C32-C33
22	f	304	CDL	OA7-CA5-OA6-CA4
22	j	301	CDL	OA7-CA5-OA6-CA4
22	B	401	CDL	OA7-CA5-OA6-CA4
22	k	202	CDL	CB2-C1-CA2-OA2
22	r	201	CDL	CA5-C11-C12-C13
22	b	401	CDL	CB5-C51-C52-C53
22	i	302	CDL	CB7-C71-C72-C73
22	l	301	CDL	OB9-CB7-OB8-CB6
22	f	304	CDL	O1-C1-CA2-OA2
22	i	302	CDL	O1-C1-CB2-OB2
22	K	202	CDL	O1-C1-CA2-OA2
22	j	302	CDL	CA5-C11-C12-C13
22	A	501	CDL	CA7-C31-C32-C33
22	B	402	CDL	CA3-CA4-OA6-CA5
23	G	304	PC1	C32-C31-O31-C3
22	a	501	CDL	C33-C34-C35-C36
22	f	304	CDL	C79-C80-C81-C82
22	k	202	CDL	C74-C75-C76-C77
22	j	301	CDL	C14-C15-C16-C17
22	j	302	CDL	C72-C73-C74-C75
22	l	304	CDL	C78-C79-C80-C81

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Mol	Chain	Res	Type	Atoms
22	A	501	CDL	C36-C37-C38-C39
22	B	403	CDL	C51-C52-C53-C54
22	B	403	CDL	C81-C82-C83-C84
22	B	404	CDL	C51-C52-C53-C54
22	I	302	CDL	C19-C20-C21-C22
22	K	201	CDL	C72-C73-C74-C75
22	J	301	CDL	C33-C34-C35-C36
23	d	301	PC1	C28-C29-C2A-C2B
28	l	302	PEE	C42-C43-C44-C45
22	k	203	CDL	C78-C79-C80-C81
22	r	201	CDL	C20-C21-C22-C23
22	r	201	CDL	C53-C54-C55-C56
22	A	501	CDL	C16-C17-C18-C19
22	B	402	CDL	C38-C39-C40-C41
22	B	404	CDL	C82-C83-C84-C85
22	I	302	CDL	C12-C13-C14-C15
22	i	302	CDL	C31-CA7-OA8-CA6
22	a	501	CDL	C74-C75-C76-C77
22	b	401	CDL	C77-C78-C79-C80
22	k	203	CDL	C15-C16-C17-C18
22	A	501	CDL	C74-C75-C76-C77
22	B	403	CDL	C72-C73-C74-C75
22	B	404	CDL	C74-C75-C76-C77
22	B	405	CDL	C16-C17-C18-C19
22	I	301	CDL	C43-C44-C45-C46
22	k	203	CDL	C79-C80-C81-C82
22	A	501	CDL	C55-C56-C57-C58
22	J	302	CDL	C21-C22-C23-C24
22	J	302	CDL	C72-C73-C74-C75
22	B	404	CDL	CA7-C31-C32-C33
22	K	201	CDL	CA5-C11-C12-C13
22	b	401	CDL	C35-C36-C37-C38
22	f	304	CDL	C40-C41-C42-C43
22	A	501	CDL	C13-C14-C15-C16
22	L	301	CDL	C61-C62-C63-C64
22	f	303	CDL	C35-C36-C37-C38
22	A	501	CDL	C14-C15-C16-C17
22	B	405	CDL	C51-C52-C53-C54
22	l	301	CDL	O1-C1-CA2-OA2
22	B	402	CDL	CB5-C51-C52-C53
29	E	900	NAD	C3B-C4B-C5B-O5B
22	a	501	CDL	C55-C56-C57-C58

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Mol	Chain	Res	Type	Atoms
22	j	301	CDL	C20-C21-C22-C23
22	l	301	CDL	C72-C73-C74-C75
22	B	401	CDL	C74-C75-C76-C77
22	B	402	CDL	C18-C19-C20-C21
22	B	401	CDL	C39-C40-C41-C42
22	f	304	CDL	C22-C23-C24-C25
22	k	203	CDL	C71-C72-C73-C74
22	I	301	CDL	C18-C19-C20-C21
22	J	301	CDL	C20-C21-C22-C23
22	j	301	CDL	C31-C32-C33-C34
22	r	201	CDL	CB2-C1-CA2-OA2
22	k	202	CDL	C71-CB7-OB8-CB6
22	b	402	CDL	C73-C74-C75-C76
22	f	304	CDL	C38-C39-C40-C41
22	j	301	CDL	C13-C14-C15-C16
22	p	201	CDL	C57-C58-C59-C60
22	p	201	CDL	C74-C75-C76-C77
22	B	401	CDL	C18-C19-C20-C21
22	K	202	CDL	C78-C79-C80-C81
22	J	302	CDL	C31-C32-C33-C34
22	L	301	CDL	C57-C58-C59-C60
22	P	201	CDL	C23-C24-C25-C26
23	d	301	PC1	C2D-C2E-C2F-C2G
22	I	301	CDL	CA5-C11-C12-C13
23	G	303	PC1	C31-C32-C33-C34
22	a	501	CDL	C42-C43-C44-C45
22	f	303	CDL	C12-C13-C14-C15
22	f	303	CDL	C43-C44-C45-C46
22	f	304	CDL	C63-C64-C65-C66
22	k	203	CDL	C52-C53-C54-C55
22	j	301	CDL	C33-C34-C35-C36
22	B	405	CDL	C35-C36-C37-C38
22	J	301	CDL	C31-C32-C33-C34
22	k	201	CDL	C39-C40-C41-C42
22	r	201	CDL	C82-C83-C84-C85
22	B	403	CDL	C19-C20-C21-C22
22	B	404	CDL	C75-C76-C77-C78
22	I	301	CDL	C81-C82-C83-C84
28	l	302	PEE	C43-C44-C45-C46
22	j	302	CDL	C31-C32-C33-C34
22	f	304	CDL	C82-C83-C84-C85
22	j	302	CDL	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
22	B	401	CDL	C63-C64-C65-C66
23	i	301	PC1	C35-C36-C37-C38
28	l	302	PEE	C40-C41-C42-C43
22	f	304	CDL	CA5-C11-C12-C13
22	f	304	CDL	CB7-C71-C72-C73
22	l	304	CDL	CA5-C11-C12-C13
22	L	301	CDL	CA5-C11-C12-C13
28	J	303	PEE	C10-C11-C12-C13
22	j	302	CDL	C51-CB5-OB6-CB4
22	J	301	CDL	C11-CA5-OA6-CA4
22	B	402	CDL	C31-CA7-OA8-CA6
28	l	303	PEE	C17-C18-C19-C20
22	l	304	CDL	C76-C77-C78-C79
22	k	203	CDL	C16-C17-C18-C19
22	a	501	CDL	C36-C37-C38-C39
22	k	203	CDL	C31-C32-C33-C34
22	j	301	CDL	C78-C79-C80-C81
22	i	302	CDL	OA9-CA7-OA8-CA6
23	G	304	PC1	O32-C31-O31-C3
22	b	402	CDL	C51-C52-C53-C54
22	r	201	CDL	C18-C19-C20-C21
25	i	303	UQ8	C30-C29-C31-C32
22	f	303	CDL	C79-C80-C81-C82
22	P	201	CDL	C52-C53-C54-C55
22	P	201	CDL	C76-C77-C78-C79
22	b	401	CDL	C32-C33-C34-C35
22	k	202	CDL	C53-C54-C55-C56
22	k	203	CDL	C14-C15-C16-C17
22	k	203	CDL	C74-C75-C76-C77
22	j	301	CDL	C60-C61-C62-C63
22	K	202	CDL	C56-C57-C58-C59
22	l	301	CDL	C31-CA7-OA8-CA6
22	B	403	CDL	C71-CB7-OB8-CB6
22	I	302	CDL	C31-CA7-OA8-CA6
22	k	203	CDL	C75-C76-C77-C78
22	B	401	CDL	C21-C22-C23-C24
22	B	405	CDL	C12-C13-C14-C15
28	J	303	PEE	C42-C43-C44-C45
22	p	201	CDL	C54-C55-C56-C57
22	I	301	CDL	C20-C21-C22-C23
22	P	201	CDL	C80-C81-C82-C83
22	a	501	CDL	C51-C52-C53-C54

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Mol	Chain	Res	Type	Atoms
22	b	401	CDL	C74-C75-C76-C77
22	p	201	CDL	C23-C24-C25-C26
22	b	402	CDL	C75-C76-C77-C78
22	f	302	CDL	C53-C54-C55-C56
22	B	401	CDL	C11-C12-C13-C14
22	I	302	CDL	C74-C75-C76-C77
28	l	302	PEE	C32-C33-C34-C35
22	b	401	CDL	C31-C32-C33-C34
22	B	402	CDL	C78-C79-C80-C81
22	B	405	CDL	C43-C44-C45-C46
22	J	302	CDL	C74-C75-C76-C77
22	f	303	CDL	C51-CB5-OB6-CB4
22	I	302	CDL	C11-CA5-OA6-CA4
22	K	202	CDL	CA5-C11-C12-C13
28	l	303	PEE	C30-C31-C32-C33
22	k	203	CDL	C53-C54-C55-C56
22	B	402	CDL	C41-C42-C43-C44
22	f	303	CDL	OB7-CB5-OB6-CB4
22	K	201	CDL	C60-C61-C62-C63
28	J	304	PEE	C19-C20-C21-C22
22	b	402	CDL	C58-C59-C60-C61
22	k	203	CDL	C54-C55-C56-C57
29	e	900	NAD	O4D-C4D-C5D-O5D
22	k	202	CDL	C78-C79-C80-C81
22	p	201	CDL	C58-C59-C60-C61
22	A	501	CDL	C75-C76-C77-C78
22	f	304	CDL	C81-C82-C83-C84
22	j	302	CDL	C12-C13-C14-C15
22	K	202	CDL	C40-C41-C42-C43
22	L	301	CDL	C52-C53-C54-C55
28	J	303	PEE	C40-C41-C42-C43
22	b	402	CDL	C82-C83-C84-C85
22	J	301	CDL	C72-C73-C74-C75
22	i	302	CDL	C12-C13-C14-C15
28	l	303	PEE	C20-C21-C22-C23
22	p	201	CDL	C80-C81-C82-C83
22	K	202	CDL	C74-C75-C76-C77
22	P	201	CDL	C37-C38-C39-C40
22	k	202	CDL	OB9-CB7-OB8-CB6
22	b	401	CDL	C53-C54-C55-C56
28	J	304	PEE	C23-C24-C25-C26
22	b	402	CDL	CB7-C71-C72-C73

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Mol	Chain	Res	Type	Atoms
22	k	201	CDL	C72-C73-C74-C75
22	k	202	CDL	C11-C12-C13-C14
22	I	301	CDL	C17-C18-C19-C20
22	J	301	CDL	OA7-CA5-OA6-CA4
22	a	501	CDL	OA5-CA3-CA4-OA6
22	i	302	CDL	OB5-CB3-CB4-OB6
22	k	202	CDL	OA5-CA3-CA4-OA6
22	b	402	CDL	C12-C13-C14-C15
22	A	501	CDL	C56-C57-C58-C59
22	B	405	CDL	C79-C80-C81-C82
22	j	301	CDL	C37-C38-C39-C40
22	J	301	CDL	C21-C22-C23-C24
22	k	201	CDL	CA7-C31-C32-C33
22	k	203	CDL	C33-C34-C35-C36
22	B	403	CDL	C76-C77-C78-C79
23	d	301	PC1	C37-C38-C39-C3A
22	r	201	CDL	C16-C17-C18-C19
22	b	401	CDL	C71-CB7-OB8-CB6
22	a	501	CDL	C21-C22-C23-C24
22	B	402	CDL	C22-C23-C24-C25
28	l	302	PEE	C41-C42-C43-C44
22	i	302	CDL	C74-C75-C76-C77
22	B	401	CDL	C72-C73-C74-C75
22	J	302	CDL	C14-C15-C16-C17
23	d	301	PC1	C22-C23-C24-C25
22	l	304	CDL	C61-C62-C63-C64
22	B	401	CDL	C13-C14-C15-C16
22	B	404	CDL	C11-C12-C13-C14
28	l	302	PEE	C12-C13-C14-C15
22	a	501	CDL	C61-C62-C63-C64
22	f	304	CDL	C17-C18-C19-C20
22	f	304	CDL	C62-C63-C64-C65
22	f	304	CDL	C83-C84-C85-C86
22	k	201	CDL	C56-C57-C58-C59
22	l	301	CDL	C11-C12-C13-C14
22	B	405	CDL	C56-C57-C58-C59
22	K	202	CDL	C77-C78-C79-C80
22	a	501	CDL	C22-C23-C24-C25
22	p	201	CDL	C11-C12-C13-C14
22	K	202	CDL	C13-C14-C15-C16
23	D	301	PC1	C28-C29-C2A-C2B
22	j	301	CDL	C52-C53-C54-C55

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Mol	Chain	Res	Type	Atoms
22	l	301	CDL	C21-C22-C23-C24
22	b	401	CDL	C22-C23-C24-C25
22	f	304	CDL	C76-C77-C78-C79
22	j	301	CDL	C72-C73-C74-C75
22	K	201	CDL	C71-C72-C73-C74
23	G	304	PC1	C27-C28-C29-C2A
22	B	402	CDL	OA9-CA7-OA8-CA6
28	J	304	PEE	C40-C41-C42-C43
22	f	303	CDL	C19-C20-C21-C22
22	B	401	CDL	C35-C36-C37-C38
22	B	403	CDL	C22-C23-C24-C25
28	J	304	PEE	C41-C42-C43-C44
22	k	203	CDL	C77-C78-C79-C80
22	L	301	CDL	C81-C82-C83-C84
22	b	401	CDL	C33-C34-C35-C36
28	l	303	PEE	C35-C36-C37-C38
22	I	302	CDL	OA9-CA7-OA8-CA6
22	f	302	CDL	OA5-CA3-CA4-CA6
22	f	304	CDL	OB5-CB3-CB4-CB6
22	k	202	CDL	OA5-CA3-CA4-CA6
22	B	402	CDL	OA5-CA3-CA4-CA6
22	K	202	CDL	OA5-CA3-CA4-CA6
23	G	304	PC1	O11-C1-C2-C3
22	j	302	CDL	OB7-CB5-OB6-CB4
22	a	501	CDL	C12-C13-C14-C15
22	B	404	CDL	C79-C80-C81-C82
28	J	303	PEE	C32-C33-C34-C35
22	I	302	CDL	C15-C16-C17-C18
22	B	403	CDL	OB9-CB7-OB8-CB6
22	L	301	CDL	C11-C12-C13-C14
22	f	302	CDL	CB5-C51-C52-C53
22	l	301	CDL	CA5-C11-C12-C13
28	J	304	PEE	C10-C11-C12-C13
22	b	402	CDL	C52-C53-C54-C55
25	I	303	UQ8	C15-C14-C16-C17
25	i	303	UQ8	C13-C14-C16-C17
22	f	302	CDL	C71-C72-C73-C74
22	l	301	CDL	OA9-CA7-OA8-CA6
22	i	302	CDL	C76-C77-C78-C79
22	J	301	CDL	C12-C13-C14-C15
22	L	301	CDL	C19-C20-C21-C22
22	B	402	CDL	C39-C40-C41-C42

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Mol	Chain	Res	Type	Atoms
22	I	301	CDL	C79-C80-C81-C82
22	I	302	CDL	C14-C15-C16-C17
22	k	202	CDL	C15-C16-C17-C18
22	k	203	CDL	C32-C33-C34-C35
22	f	303	CDL	CB3-CB4-CB6-OB8
22	j	301	CDL	CB3-CB4-CB6-OB8
22	r	201	CDL	CB3-CB4-CB6-OB8
22	B	401	CDL	CA3-CA4-CA6-OA8
22	B	405	CDL	CB3-CB4-CB6-OB8
22	I	301	CDL	CB3-CB4-CB6-OB8
22	I	302	CDL	CB3-CB4-CB6-OB8
22	J	302	CDL	CA3-CA4-CA6-OA8
23	d	301	PC1	C1-C2-C3-O31
28	l	303	PEE	C1-C2-C3-O3
22	j	302	CDL	C22-C23-C24-C25
22	B	404	CDL	C12-C13-C14-C15
22	B	405	CDL	C74-C75-C76-C77
28	J	304	PEE	C35-C36-C37-C38
22	r	201	CDL	C62-C63-C64-C65
22	J	301	CDL	C39-C40-C41-C42
22	K	202	CDL	C71-CB7-OB8-CB6
22	b	402	CDL	C43-C44-C45-C46
22	A	501	CDL	C78-C79-C80-C81
22	J	302	CDL	C12-C13-C14-C15
22	f	304	CDL	C60-C61-C62-C63
22	l	301	CDL	C62-C63-C64-C65
22	A	501	CDL	C15-C16-C17-C18
22	J	301	CDL	C78-C79-C80-C81
22	B	403	CDL	C53-C54-C55-C56
22	f	304	CDL	C36-C37-C38-C39
22	i	302	CDL	C57-C58-C59-C60
22	b	401	CDL	OB9-CB7-OB8-CB6
22	B	404	CDL	C76-C77-C78-C79
22	L	301	CDL	C53-C54-C55-C56
22	J	301	CDL	C35-C36-C37-C38
22	f	303	CDL	C13-C14-C15-C16
22	j	301	CDL	CB5-C51-C52-C53
22	l	304	CDL	CB7-C71-C72-C73
22	a	501	CDL	C56-C57-C58-C59
22	B	405	CDL	C13-C14-C15-C16
22	J	301	CDL	C57-C58-C59-C60
22	f	302	CDL	C71-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
22	b	402	CDL	CA6-CA4-OA6-CA5
22	B	404	CDL	CA6-CA4-OA6-CA5
22	I	301	CDL	CA6-CA4-OA6-CA5
22	P	201	CDL	C72-C73-C74-C75
28	l	302	PEE	C33-C34-C35-C36
28	l	303	PEE	C11-C12-C13-C14
28	l	302	PEE	C35-C36-C37-C38
28	l	303	PEE	C19-C20-C21-C22
28	J	303	PEE	C19-C20-C21-C22
28	J	303	PEE	C35-C36-C37-C38
22	k	201	CDL	C76-C77-C78-C79
22	B	403	CDL	C71-C72-C73-C74
22	B	405	CDL	C59-C60-C61-C62
23	G	304	PC1	C3B-C3C-C3D-C3E
22	l	301	CDL	C80-C81-C82-C83
22	l	301	CDL	CA7-C31-C32-C33
28	J	304	PEE	C37-C38-C39-C40
22	l	304	CDL	C32-C33-C34-C35
22	B	404	CDL	C43-C44-C45-C46
22	K	202	CDL	C53-C54-C55-C56
28	J	303	PEE	C14-C15-C16-C17
22	b	401	CDL	C24-C25-C26-C27
22	a	501	CDL	OB5-CB3-CB4-OB6
22	B	401	CDL	OB5-CB3-CB4-OB6
22	I	302	CDL	OB5-CB3-CB4-OB6
22	b	401	CDL	C14-C15-C16-C17
22	b	401	CDL	C23-C24-C25-C26
22	j	301	CDL	C74-C75-C76-C77
22	J	302	CDL	C23-C24-C25-C26
22	f	303	CDL	C38-C39-C40-C41
22	j	302	CDL	C74-C75-C76-C77
22	B	405	CDL	C78-C79-C80-C81
22	L	301	CDL	C21-C22-C23-C24
23	D	301	PC1	C37-C38-C39-C3A
25	I	303	UQ8	C13-C14-C16-C17
22	B	404	CDL	C78-C79-C80-C81
22	J	302	CDL	C13-C14-C15-C16
22	f	304	CDL	C77-C78-C79-C80
22	k	201	CDL	C80-C81-C82-C83
22	k	202	CDL	C52-C53-C54-C55
22	j	301	CDL	C34-C35-C36-C37
22	l	304	CDL	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
22	l	304	CDL	C17-C18-C19-C20
22	B	401	CDL	C41-C42-C43-C44
22	J	301	CDL	C22-C23-C24-C25
22	L	301	CDL	C80-C81-C82-C83
22	k	201	CDL	OB6-CB4-CB6-OB8
22	A	501	CDL	OB6-CB4-CB6-OB8
22	k	203	CDL	C41-C42-C43-C44
22	K	202	CDL	C79-C80-C81-C82
22	k	203	CDL	C31-CA7-OA8-CA6
22	f	303	CDL	C56-C57-C58-C59
22	B	402	CDL	C13-C14-C15-C16
22	B	402	CDL	C15-C16-C17-C18
22	l	304	CDL	C32-C31-CA7-OA8
22	r	201	CDL	C14-C15-C16-C17
22	B	402	CDL	C76-C77-C78-C79
22	B	403	CDL	C54-C55-C56-C57
22	K	202	CDL	C22-C23-C24-C25
22	K	202	CDL	C43-C44-C45-C46
22	I	302	CDL	OA7-CA5-OA6-CA4
22	K	201	CDL	C74-C75-C76-C77
22	J	301	CDL	C71-C72-C73-C74
22	b	401	CDL	CA5-C11-C12-C13
23	i	301	PC1	C31-C32-C33-C34
22	p	201	CDL	C31-CA7-OA8-CA6
23	g	303	PC1	C32-C31-O31-C3
22	b	401	CDL	C81-C82-C83-C84
22	l	304	CDL	C74-C75-C76-C77
22	K	202	CDL	C80-C81-C82-C83
23	g	303	PC1	C38-C39-C3A-C3B
22	K	201	CDL	C22-C23-C24-C25
22	k	202	CDL	CA5-C11-C12-C13
22	P	201	CDL	CA7-C31-C32-C33
22	i	302	CDL	C17-C18-C19-C20
22	k	201	CDL	C54-C55-C56-C57
22	j	302	CDL	C14-C15-C16-C17
22	B	402	CDL	C57-C58-C59-C60
22	B	403	CDL	C56-C57-C58-C59
22	J	302	CDL	C54-C55-C56-C57
23	g	303	PC1	C29-C2A-C2B-C2C
22	f	303	CDL	C76-C77-C78-C79
22	P	201	CDL	C11-C12-C13-C14
22	P	201	CDL	C58-C59-C60-C61

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Mol	Chain	Res	Type	Atoms
22	a	501	CDL	C1-CB2-OB2-PB2
22	f	302	CDL	C16-C17-C18-C19
22	k	202	CDL	C76-C77-C78-C79
22	I	302	CDL	C52-C53-C54-C55
22	B	404	CDL	C24-C25-C26-C27
22	B	403	CDL	C43-C44-C45-C46
22	f	303	CDL	C16-C17-C18-C19
22	i	302	CDL	C56-C57-C58-C59
22	j	301	CDL	C54-C55-C56-C57
22	K	202	CDL	C52-C53-C54-C55
22	a	501	CDL	OA5-CA3-CA4-CA6
22	a	501	CDL	OB5-CB3-CB4-CB6
22	b	401	CDL	OA5-CA3-CA4-CA6
22	i	302	CDL	OB5-CB3-CB4-CB6
22	j	301	CDL	OA5-CA3-CA4-CA6
22	p	201	CDL	OB5-CB3-CB4-CB6
22	B	401	CDL	OA5-CA3-CA4-CA6
22	I	301	CDL	OA5-CA3-CA4-CA6
22	I	301	CDL	OB5-CB3-CB4-CB6
22	I	302	CDL	OB5-CB3-CB4-CB6
23	g	303	PC1	O11-C1-C2-C3
28	J	304	PEE	O3P-C1-C2-C3
29	E	900	NAD	O4B-C4B-C5B-O5B
29	E	900	NAD	C3D-C4D-C5D-O5D
22	b	401	CDL	C16-C17-C18-C19
22	B	404	CDL	C52-C53-C54-C55
22	I	301	CDL	C77-C78-C79-C80
23	D	301	PC1	C23-C24-C25-C26
22	r	201	CDL	C83-C84-C85-C86
22	A	501	CDL	C44-C45-C46-C47
25	i	303	UQ8	C15-C14-C16-C17
28	J	303	PEE	C12-C13-C14-C15
22	K	202	CDL	OB9-CB7-OB8-CB6
22	K	201	CDL	C31-CA7-OA8-CA6
22	r	201	CDL	C76-C77-C78-C79
22	K	201	CDL	C58-C59-C60-C61
22	j	302	CDL	C13-C14-C15-C16
22	l	301	CDL	C37-C38-C39-C40
22	B	401	CDL	C38-C39-C40-C41
22	B	405	CDL	C38-C39-C40-C41
28	J	303	PEE	C41-C42-C43-C44
22	p	201	CDL	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
22	f	302	CDL	C76-C77-C78-C79
22	K	202	CDL	CB2-C1-CA2-OA2
22	f	302	CDL	C79-C80-C81-C82
23	i	301	PC1	C3E-C3F-C3G-C3H
22	b	401	CDL	CB3-CB4-CB6-OB8
22	f	302	CDL	CB3-CB4-CB6-OB8
22	f	304	CDL	CA3-CA4-CA6-OA8
22	i	302	CDL	CB3-CB4-CB6-OB8
22	A	501	CDL	CB3-CB4-CB6-OB8
22	J	301	CDL	CA3-CA4-CA6-OA8
22	J	302	CDL	CB3-CB4-CB6-OB8
28	J	304	PEE	C1-C2-C3-O3
22	r	201	CDL	C35-C36-C37-C38
22	I	301	CDL	C44-C45-C46-C47
22	k	203	CDL	CB5-C51-C52-C53
22	A	501	CDL	C61-C62-C63-C64
22	f	304	CDL	C19-C20-C21-C22
22	B	401	CDL	C20-C21-C22-C23
25	i	303	UQ8	C40-C39-C41-C42
22	J	302	CDL	CA7-C31-C32-C33
22	B	404	CDL	C73-C74-C75-C76
28	l	302	PEE	C13-C14-C15-C16
22	B	402	CDL	C80-C81-C82-C83
23	i	301	PC1	C24-C25-C26-C27
22	p	201	CDL	C76-C77-C78-C79
22	b	401	CDL	OB5-CB3-CB4-OB6
22	f	302	CDL	OA5-CA3-CA4-OA6
22	p	201	CDL	OB5-CB3-CB4-OB6
22	r	201	CDL	OA5-CA3-CA4-OA6
22	A	501	CDL	OB5-CB3-CB4-OB6
23	d	301	PC1	O11-C1-C2-O21
28	J	304	PEE	O3P-C1-C2-O2
22	f	302	CDL	C83-C84-C85-C86
22	k	202	CDL	C31-C32-C33-C34
28	J	303	PEE	C37-C38-C39-C40
22	i	302	CDL	C31-C32-C33-C34
22	k	203	CDL	C37-C38-C39-C40
22	A	501	CDL	C32-C33-C34-C35
22	b	402	CDL	C77-C78-C79-C80
22	I	302	CDL	C41-C42-C43-C44
22	J	301	CDL	C34-C35-C36-C37
22	b	402	CDL	C76-C77-C78-C79

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Mol	Chain	Res	Type	Atoms
22	b	402	CDL	C79-C80-C81-C82
22	f	304	CDL	C35-C36-C37-C38
22	k	202	CDL	C13-C14-C15-C16
22	j	301	CDL	C11-C12-C13-C14
22	I	301	CDL	C36-C37-C38-C39
22	B	402	CDL	C32-C31-CA7-OA8
22	L	301	CDL	C72-C71-CB7-OB8
22	a	501	CDL	CB7-C71-C72-C73
22	b	401	CDL	OB6-CB4-CB6-OB8
22	i	302	CDL	OB6-CB4-CB6-OB8
22	j	302	CDL	OB6-CB4-CB6-OB8
22	B	402	CDL	OB6-CB4-CB6-OB8
22	B	405	CDL	OA6-CA4-CA6-OA8
22	J	302	CDL	OA6-CA4-CA6-OA8
22	J	302	CDL	OB6-CB4-CB6-OB8
23	d	301	PC1	O21-C2-C3-O31
22	f	303	CDL	C44-C45-C46-C47
22	B	402	CDL	CA5-C11-C12-C13
22	f	302	CDL	OB9-CB7-OB8-CB6
22	k	202	CDL	C72-C73-C74-C75
22	a	501	CDL	C38-C39-C40-C41
22	k	201	CDL	C22-C23-C24-C25
22	k	203	CDL	C76-C77-C78-C79
22	l	301	CDL	C23-C24-C25-C26
22	j	302	CDL	CA7-C31-C32-C33
22	B	402	CDL	CB7-C71-C72-C73
22	J	302	CDL	C51-CB5-OB6-CB4
22	f	302	CDL	C84-C85-C86-C87
22	B	402	CDL	C77-C78-C79-C80
22	j	302	CDL	C11-C12-C13-C14
22	K	201	CDL	C39-C40-C41-C42
25	I	303	UQ8	C14-C16-C17-C18
22	B	402	CDL	C63-C64-C65-C66
22	b	401	CDL	C42-C43-C44-C45
22	B	402	CDL	C73-C74-C75-C76
22	I	302	CDL	C71-CB7-OB8-CB6
22	B	403	CDL	C32-C31-CA7-OA8
22	b	401	CDL	C11-C12-C13-C14
22	P	201	CDL	C22-C23-C24-C25
22	r	201	CDL	C37-C38-C39-C40
22	A	501	CDL	C33-C34-C35-C36
22	B	404	CDL	C39-C40-C41-C42

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Mol	Chain	Res	Type	Atoms
22	l	304	CDL	C31-CA7-OA8-CA6
22	k	202	CDL	C80-C81-C82-C83
22	r	201	CDL	C58-C59-C60-C61
22	b	401	CDL	OB5-CB3-CB4-CB6
22	r	201	CDL	OA5-CA3-CA4-CA6
22	B	401	CDL	OB5-CB3-CB4-CB6
22	J	301	CDL	OA5-CA3-CA4-CA6
22	p	201	CDL	C71-C72-C73-C74
22	K	201	CDL	OA9-CA7-OA8-CA6
22	k	201	CDL	C36-C37-C38-C39
22	k	203	CDL	OA9-CA7-OA8-CA6
22	k	203	CDL	C12-C13-C14-C15
23	g	303	PC1	C27-C28-C29-C2A
25	I	303	UQ8	C30-C29-C31-C32
22	p	201	CDL	OA9-CA7-OA8-CA6
22	a	501	CDL	C14-C15-C16-C17
22	j	302	CDL	CA6-CA4-OA6-CA5
22	l	304	CDL	CA6-CA4-OA6-CA5
22	r	201	CDL	CA6-CA4-OA6-CA5
22	B	403	CDL	CB6-CB4-OB6-CB5
22	J	302	CDL	CA6-CA4-OA6-CA5
23	g	303	PC1	O32-C31-O31-C3
22	f	303	CDL	C58-C59-C60-C61
22	A	501	CDL	C72-C73-C74-C75
22	b	402	CDL	C34-C35-C36-C37
22	J	302	CDL	C16-C17-C18-C19
22	j	301	CDL	OA5-CA3-CA4-OA6
22	j	302	CDL	OB5-CB3-CB4-OB6
22	l	304	CDL	OB5-CB3-CB4-OB6
22	B	402	CDL	OA5-CA3-CA4-OA6
22	B	403	CDL	OB5-CB3-CB4-OB6
22	I	301	CDL	OB5-CB3-CB4-OB6
23	g	303	PC1	O11-C1-C2-O21
28	l	302	PEE	O3P-C1-C2-O2
22	f	304	CDL	CB3-CB4-CB6-OB8
22	j	302	CDL	CA3-CA4-CA6-OA8
22	j	302	CDL	CB3-CB4-CB6-OB8
22	B	405	CDL	CA3-CA4-CA6-OA8
22	I	301	CDL	CA3-CA4-CA6-OA8
23	D	301	PC1	C1-C2-C3-O31
22	f	303	CDL	C59-C60-C61-C62
22	l	304	CDL	C41-C42-C43-C44

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Mol	Chain	Res	Type	Atoms
22	f	304	CDL	C71-CB7-OB8-CB6
22	f	302	CDL	C41-C42-C43-C44
22	i	302	CDL	C78-C79-C80-C81
22	B	404	CDL	C81-C82-C83-C84
25	i	303	UQ8	C28-C29-C31-C32
22	B	404	CDL	C55-C56-C57-C58
22	f	302	CDL	OB6-CB4-CB6-OB8
22	f	304	CDL	OA6-CA4-CA6-OA8
22	j	301	CDL	OB6-CB4-CB6-OB8
22	r	201	CDL	OB6-CB4-CB6-OB8
22	I	301	CDL	OA6-CA4-CA6-OA8
22	I	302	CDL	OB6-CB4-CB6-OB8
22	J	301	CDL	OA6-CA4-CA6-OA8
23	D	301	PC1	O21-C2-C3-O31
22	k	202	CDL	C56-C57-C58-C59
22	l	301	CDL	C34-C35-C36-C37
22	B	404	CDL	C35-C36-C37-C38
22	b	401	CDL	C76-C77-C78-C79
22	B	402	CDL	C81-C82-C83-C84
22	k	203	CDL	C42-C43-C44-C45
22	p	201	CDL	C37-C38-C39-C40
22	B	401	CDL	C32-C33-C34-C35
22	I	302	CDL	OB9-CB7-OB8-CB6
22	A	501	CDL	C63-C64-C65-C66
22	B	403	CDL	C75-C76-C77-C78
28	J	304	PEE	C31-C32-C33-C34
29	e	900	NAD	O4B-C4B-C5B-O5B
22	B	403	CDL	C33-C34-C35-C36
22	B	402	CDL	C71-C72-C73-C74
23	d	301	PC1	O13-C11-C12-N
23	g	303	PC1	O13-C11-C12-N
23	G	304	PC1	O13-C11-C12-N
22	B	404	CDL	C15-C16-C17-C18
22	r	201	CDL	C72-C73-C74-C75
22	B	403	CDL	CA2-C1-CB2-OB2
22	r	201	CDL	O1-C1-CA2-OA2
22	j	301	CDL	C55-C56-C57-C58
22	J	301	CDL	C74-C75-C76-C77
23	G	304	PC1	C21-C22-C23-C24
22	I	302	CDL	C60-C61-C62-C63
22	l	304	CDL	OA9-CA7-OA8-CA6
22	f	302	CDL	C77-C78-C79-C80

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Mol	Chain	Res	Type	Atoms
22	k	202	CDL	C40-C41-C42-C43
22	l	304	CDL	C51-C52-C53-C54
23	G	304	PC1	C24-C25-C26-C27
28	J	304	PEE	C21-C22-C23-C24
22	B	405	CDL	C17-C18-C19-C20
22	B	401	CDL	C76-C77-C78-C79
22	f	304	CDL	OB9-CB7-OB8-CB6
28	l	303	PEE	C12-C13-C14-C15
22	b	402	CDL	OB5-CB3-CB4-CB6
22	B	404	CDL	OB5-CB3-CB4-CB6
22	P	201	CDL	OB5-CB3-CB4-CB6
23	d	301	PC1	O11-C1-C2-C3
28	l	302	PEE	O3P-C1-C2-C3
22	I	301	CDL	C74-C75-C76-C77
22	J	302	CDL	OB7-CB5-OB6-CB4
22	f	304	CDL	C14-C15-C16-C17
23	g	303	PC1	C21-C22-C23-C24
22	f	303	CDL	C64-C65-C66-C67
22	k	203	CDL	C17-C18-C19-C20
22	r	201	CDL	C21-C22-C23-C24
23	G	304	PC1	C38-C39-C3A-C3B
22	K	202	CDL	C44-C45-C46-C47
22	B	402	CDL	C43-C44-C45-C46
22	a	501	CDL	C31-C32-C33-C34
22	L	301	CDL	CB7-C71-C72-C73
22	b	402	CDL	C1-CB2-OB2-PB2
22	k	201	CDL	C1-CB2-OB2-PB2
22	j	301	CDL	C1-CB2-OB2-PB2
22	B	404	CDL	C1-CB2-OB2-PB2
22	J	301	CDL	C1-CB2-OB2-PB2
22	k	201	CDL	C44-C45-C46-C47
22	l	301	CDL	C17-C18-C19-C20
22	r	201	CDL	C11-C12-C13-C14
22	B	402	CDL	C84-C85-C86-C87
22	i	302	CDL	C80-C81-C82-C83
22	k	201	CDL	C12-C13-C14-C15
22	b	401	CDL	OA5-CA3-CA4-OA6
22	I	301	CDL	OA5-CA3-CA4-OA6
22	J	301	CDL	OA5-CA3-CA4-OA6
22	P	201	CDL	OB5-CB3-CB4-OB6
23	G	304	PC1	O11-C1-C2-O21
22	b	401	CDL	CA7-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
22	b	402	CDL	C61-C62-C63-C64
22	i	302	CDL	C11-CA5-OA6-CA4
22	L	301	CDL	C11-CA5-OA6-CA4
22	L	301	CDL	C76-C77-C78-C79
22	K	201	CDL	CB5-C51-C52-C53
22	l	304	CDL	C82-C83-C84-C85
23	G	304	PC1	C2B-C2C-C2D-C2E
22	f	304	CDL	OB6-CB4-CB6-OB8
22	k	201	CDL	OA6-CA4-CA6-OA8
22	j	302	CDL	OA6-CA4-CA6-OA8
22	r	201	CDL	OA6-CA4-CA6-OA8
22	B	401	CDL	OA6-CA4-CA6-OA8
22	B	403	CDL	OB6-CB4-CB6-OB8
22	J	301	CDL	OB6-CB4-CB6-OB8
23	i	301	PC1	O21-C2-C3-O31
28	l	303	PEE	O2-C2-C3-O3
22	b	402	CDL	C22-C23-C24-C25
22	f	302	CDL	CA2-C1-CB2-OB2
22	k	201	CDL	CB3-CB4-CB6-OB8
22	p	201	CDL	CA3-CA4-CA6-OA8
22	r	201	CDL	CA3-CA4-CA6-OA8
22	B	402	CDL	CB3-CB4-CB6-OB8
22	P	201	CDL	CA3-CA4-CA6-OA8
22	B	402	CDL	C54-C55-C56-C57
22	B	405	CDL	C39-C40-C41-C42
22	I	302	CDL	C34-C35-C36-C37
22	B	403	CDL	C79-C80-C81-C82
22	P	201	CDL	C74-C75-C76-C77
22	a	501	CDL	C75-C76-C77-C78
22	k	202	CDL	C23-C24-C25-C26
22	B	405	CDL	C19-C20-C21-C22
22	b	401	CDL	C31-CA7-OA8-CA6
22	l	301	CDL	C74-C75-C76-C77
22	a	501	CDL	CA2-OA2-PA1-OA4
22	b	401	CDL	CB2-OB2-PB2-OB4
22	b	401	CDL	CB3-OB5-PB2-OB2
22	b	401	CDL	CB3-OB5-PB2-OB3
22	b	401	CDL	CB3-OB5-PB2-OB4
22	b	402	CDL	CA3-OA5-PA1-OA2
22	f	304	CDL	CA2-OA2-PA1-OA4
22	f	304	CDL	CA2-OA2-PA1-OA5
22	k	201	CDL	CB3-OB5-PB2-OB4

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Mol	Chain	Res	Type	Atoms
22	k	203	CDL	CA3-OA5-PA1-OA4
22	k	203	CDL	CB2-OB2-PB2-OB3
22	k	203	CDL	CB3-OB5-PB2-OB4
22	j	301	CDL	CA2-OA2-PA1-OA3
22	j	301	CDL	CB3-OB5-PB2-OB2
22	j	301	CDL	CB3-OB5-PB2-OB3
22	j	301	CDL	CB3-OB5-PB2-OB4
22	l	301	CDL	CB3-OB5-PB2-OB2
22	l	301	CDL	CB3-OB5-PB2-OB3
22	l	301	CDL	CB3-OB5-PB2-OB4
22	l	304	CDL	CA3-OA5-PA1-OA4
22	l	304	CDL	CB2-OB2-PB2-OB3
22	l	304	CDL	CB3-OB5-PB2-OB2
22	l	304	CDL	CB3-OB5-PB2-OB4
22	p	201	CDL	CB3-OB5-PB2-OB2
22	r	201	CDL	CB3-OB5-PB2-OB3
22	A	501	CDL	CB2-OB2-PB2-OB3
22	B	401	CDL	CA2-OA2-PA1-OA3
22	B	401	CDL	CA3-OA5-PA1-OA3
22	B	401	CDL	CB3-OB5-PB2-OB4
22	B	402	CDL	CB3-OB5-PB2-OB2
22	B	405	CDL	CB2-OB2-PB2-OB5
22	I	301	CDL	CB2-OB2-PB2-OB3
22	I	301	CDL	CB2-OB2-PB2-OB4
22	I	301	CDL	CB2-OB2-PB2-OB5
22	K	201	CDL	CB3-OB5-PB2-OB4
22	K	202	CDL	CA2-OA2-PA1-OA3
22	K	202	CDL	CB2-OB2-PB2-OB4
22	J	301	CDL	CB2-OB2-PB2-OB3
22	J	301	CDL	CB3-OB5-PB2-OB2
22	J	301	CDL	CB3-OB5-PB2-OB3
22	J	301	CDL	CB3-OB5-PB2-OB4
22	L	301	CDL	CB3-OB5-PB2-OB2
22	L	301	CDL	CB3-OB5-PB2-OB3
22	L	301	CDL	CB3-OB5-PB2-OB4
23	i	301	PC1	C11-O13-P-O12
23	i	301	PC1	C11-O13-P-O14
23	i	301	PC1	C11-O13-P-O11
23	i	301	PC1	C1-O11-P-O14
23	D	301	PC1	C1-O11-P-O14
23	G	303	PC1	C11-O13-P-O12
23	G	303	PC1	C11-O13-P-O14

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Mol	Chain	Res	Type	Atoms
23	G	303	PC1	C11-O13-P-O11
28	J	303	PEE	C4-O4P-P-O3P
28	J	303	PEE	C4-O4P-P-O2P
29	e	900	NAD	C5B-O5B-PA-O1A
29	e	900	NAD	C5B-O5B-PA-O3
29	E	900	NAD	C5B-O5B-PA-O1A
22	l	304	CDL	C44-C45-C46-C47
22	B	401	CDL	C75-C76-C77-C78
22	B	404	CDL	C22-C23-C24-C25
22	b	401	CDL	C17-C18-C19-C20
22	f	304	CDL	C71-C72-C73-C74
22	B	403	CDL	C32-C33-C34-C35
25	I	303	UQ8	C28-C29-C31-C32
22	b	402	CDL	C37-C38-C39-C40
22	I	301	CDL	CB5-C51-C52-C53
22	a	501	CDL	C1-CA2-OA2-PA1
22	k	203	CDL	C1-CA2-OA2-PA1
22	l	301	CDL	CA4-CA3-OA5-PA1
22	l	304	CDL	C1-CA2-OA2-PA1
22	L	301	CDL	C1-CA2-OA2-PA1
22	L	301	CDL	CA4-CA3-OA5-PA1
22	L	301	CDL	C1-CB2-OB2-PB2
23	G	303	PC1	C2-C1-O11-P
22	L	301	CDL	OA7-CA5-OA6-CA4
22	I	302	CDL	C76-C77-C78-C79
22	f	304	CDL	C11-C12-C13-C14
22	B	404	CDL	C34-C35-C36-C37
22	r	201	CDL	CB7-C71-C72-C73
22	b	401	CDL	OA9-CA7-OA8-CA6
22	B	403	CDL	C80-C81-C82-C83
22	i	302	CDL	C58-C59-C60-C61
22	b	401	CDL	CA6-CA4-OA6-CA5
22	k	203	CDL	CA6-CA4-OA6-CA5
22	l	301	CDL	C72-C71-CB7-OB8
22	a	501	CDL	C34-C35-C36-C37
22	f	304	CDL	C12-C13-C14-C15
22	K	201	CDL	C59-C60-C61-C62
22	b	402	CDL	C39-C40-C41-C42
22	K	202	CDL	C54-C55-C56-C57
28	l	303	PEE	O3P-C1-C2-C3
22	b	402	CDL	C31-C32-C33-C34
22	I	301	CDL	C82-C83-C84-C85

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Mol	Chain	Res	Type	Atoms
22	k	202	CDL	C16-C17-C18-C19
23	G	304	PC1	C3C-C3D-C3E-C3F
22	J	301	CDL	C72-C71-CB7-OB8
23	i	301	PC1	C23-C24-C25-C26
22	k	203	CDL	C44-C45-C46-C47
22	b	402	CDL	OB5-CB3-CB4-OB6
22	f	304	CDL	OB5-CB3-CB4-OB6
22	B	404	CDL	OB5-CB3-CB4-OB6
22	J	302	CDL	C33-C34-C35-C36
22	J	302	CDL	C77-C78-C79-C80
22	P	201	CDL	C54-C55-C56-C57
29	e	900	NAD	C3B-C4B-C5B-O5B
22	j	301	CDL	C31-CA7-OA8-CA6
28	l	303	PEE	C14-C15-C16-C17
22	j	301	CDL	OA9-CA7-OA8-CA6
22	i	302	CDL	OA7-CA5-OA6-CA4
22	k	203	CDL	C13-C14-C15-C16
22	B	404	CDL	CB4-CB3-OB5-PB2
23	i	301	PC1	C2-C1-O11-P
22	f	304	CDL	C78-C79-C80-C81
22	j	301	CDL	C15-C16-C17-C18
22	B	401	CDL	C71-C72-C73-C74
22	P	201	CDL	C81-C82-C83-C84
22	f	303	CDL	OA6-CA4-CA6-OA8
22	I	301	CDL	OB6-CB4-CB6-OB8
22	P	201	CDL	C31-CA7-OA8-CA6
22	f	302	CDL	C32-C33-C34-C35
22	l	301	CDL	C19-C20-C21-C22
22	P	201	CDL	C13-C14-C15-C16
22	L	301	CDL	C51-CB5-OB6-CB4
22	p	201	CDL	C72-C71-CB7-OB8
22	I	302	CDL	C72-C71-CB7-OB8
22	k	201	CDL	CB5-C51-C52-C53
22	L	301	CDL	C71-CB7-OB8-CB6
22	P	201	CDL	OA9-CA7-OA8-CA6
22	i	302	CDL	C22-C23-C24-C25
22	i	302	CDL	C71-C72-C73-C74
22	l	304	CDL	C12-C13-C14-C15
22	B	403	CDL	C18-C19-C20-C21
22	B	403	CDL	CB3-CB4-CB6-OB8
23	i	301	PC1	C1-C2-C3-O31
22	f	302	CDL	C32-C31-CA7-OA8

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Mol	Chain	Res	Type	Atoms
22	i	302	CDL	C72-C71-CB7-OB8
22	k	202	CDL	C12-C13-C14-C15
22	l	304	CDL	C39-C40-C41-C42
22	j	301	CDL	C72-C71-CB7-OB8
22	I	301	CDL	C32-C33-C34-C35
22	J	302	CDL	C11-C12-C13-C14
22	I	302	CDL	CB7-C71-C72-C73
22	a	501	CDL	CA5-C11-C12-C13
22	b	402	CDL	CB4-CB3-OB5-PB2
22	a	501	CDL	C71-CB7-OB8-CB6
22	a	501	CDL	CA7-C31-C32-C33
22	L	301	CDL	OB9-CB7-OB8-CB6
22	I	302	CDL	C31-C32-C33-C34
25	I	303	UQ8	C19-C21-C22-C23
22	p	201	CDL	C52-C53-C54-C55
22	f	304	CDL	C75-C76-C77-C78
22	L	301	CDL	C74-C75-C76-C77
23	D	301	PC1	C39-C3A-C3B-C3C
22	b	401	CDL	C80-C81-C82-C83
22	f	302	CDL	C62-C63-C64-C65
22	i	302	CDL	C14-C15-C16-C17
22	b	402	CDL	C11-C12-C13-C14
22	b	402	CDL	C55-C56-C57-C58
22	L	301	CDL	OB7-CB5-OB6-CB4
22	b	401	CDL	C72-C71-CB7-OB8
22	P	201	CDL	C36-C37-C38-C39
28	J	304	PEE	C36-C37-C38-C39
22	a	501	CDL	OB9-CB7-OB8-CB6
22	a	501	CDL	OA6-CA4-CA6-OA8
22	K	201	CDL	OA6-CA4-CA6-OA8
22	k	202	CDL	C38-C39-C40-C41
22	f	304	CDL	C74-C75-C76-C77
23	g	303	PC1	C36-C37-C38-C39
22	K	201	CDL	C16-C17-C18-C19
22	j	302	CDL	C16-C17-C18-C19
22	B	401	CDL	C78-C79-C80-C81
22	I	301	CDL	C34-C35-C36-C37
23	d	301	PC1	C35-C36-C37-C38
22	p	201	CDL	CA7-C31-C32-C33
22	A	501	CDL	C11-C12-C13-C14
22	b	401	CDL	C78-C79-C80-C81
22	K	201	CDL	C1-CB2-OB2-PB2

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Mol	Chain	Res	Type	Atoms
22	f	302	CDL	C19-C20-C21-C22
22	f	302	CDL	C23-C24-C25-C26
22	p	201	CDL	C13-C14-C15-C16
22	a	501	CDL	C16-C17-C18-C19
22	f	304	CDL	C37-C38-C39-C40
22	k	203	CDL	C21-C22-C23-C24
22	I	302	CDL	C22-C23-C24-C25
22	B	403	CDL	C41-C42-C43-C44
22	i	302	CDL	C24-C25-C26-C27
22	l	304	CDL	C32-C31-CA7-OA9
22	k	202	CDL	C79-C80-C81-C82
22	A	501	CDL	C73-C74-C75-C76
22	f	303	CDL	CB5-C51-C52-C53
22	L	301	CDL	C79-C80-C81-C82
22	b	402	CDL	C31-CA7-OA8-CA6
22	f	302	CDL	C33-C34-C35-C36
22	f	304	CDL	CA6-CA4-OA6-CA5
22	f	304	CDL	C52-C53-C54-C55
22	l	304	CDL	C75-C76-C77-C78
22	P	201	CDL	C43-C44-C45-C46
22	A	501	CDL	C32-C31-CA7-OA8
22	I	301	CDL	C71-C72-C73-C74
22	B	403	CDL	C64-C65-C66-C67
23	D	301	PC1	O11-C1-C2-O21
22	l	301	CDL	C63-C64-C65-C66
22	B	402	CDL	C74-C75-C76-C77
22	L	301	CDL	C44-C45-C46-C47
22	B	405	CDL	C77-C78-C79-C80
22	P	201	CDL	C71-CB7-OB8-CB6
22	B	401	CDL	C1-CB2-OB2-PB2
22	K	202	CDL	CB4-CB3-OB5-PB2
22	L	301	CDL	CB4-CB3-OB5-PB2
22	k	201	CDL	C58-C59-C60-C61
23	d	301	PC1	C36-C37-C38-C39
22	B	401	CDL	C40-C41-C42-C43
22	B	402	CDL	C32-C33-C34-C35
22	B	402	CDL	C37-C38-C39-C40
22	I	301	CDL	C22-C23-C24-C25
28	l	302	PEE	C14-C15-C16-C17
22	a	501	CDL	C77-C78-C79-C80
22	B	402	CDL	C52-C53-C54-C55
22	B	403	CDL	C74-C75-C76-C77

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Mol	Chain	Res	Type	Atoms
28	l	303	PEE	C23-C24-C25-C26
22	a	501	CDL	C17-C18-C19-C20
22	l	301	CDL	C59-C60-C61-C62
23	d	301	PC1	C34-C35-C36-C37
22	J	302	CDL	C72-C71-CB7-OB8
22	l	301	CDL	C54-C55-C56-C57
22	f	302	CDL	C73-C74-C75-C76
22	j	302	CDL	C18-C19-C20-C21
22	I	301	CDL	C72-C73-C74-C75
22	B	402	CDL	C72-C71-CB7-OB8
23	i	301	PC1	C3D-C3E-C3F-C3G
22	l	301	CDL	C22-C23-C24-C25
22	B	403	CDL	C77-C78-C79-C80
22	k	203	CDL	O1-C1-CA2-OA2
22	k	201	CDL	C31-CA7-OA8-CA6
22	b	402	CDL	OA9-CA7-OA8-CA6
22	I	302	CDL	C64-C65-C66-C67
22	B	404	CDL	C71-C72-C73-C74
22	l	301	CDL	C44-C45-C46-C47
22	b	401	CDL	CB7-C71-C72-C73
22	j	301	CDL	C53-C54-C55-C56
22	k	202	CDL	CB4-CB3-OB5-PB2
22	B	405	CDL	CA4-CA3-OA5-PA1
22	I	302	CDL	CB4-CB3-OB5-PB2
22	j	302	CDL	C24-C25-C26-C27
25	i	303	UQ8	C38-C39-C41-C42
22	P	201	CDL	OB9-CB7-OB8-CB6
22	A	501	CDL	C80-C81-C82-C83
22	A	501	CDL	C31-CA7-OA8-CA6
22	B	402	CDL	C71-CB7-OB8-CB6
22	A	501	CDL	C60-C61-C62-C63
22	B	402	CDL	OB9-CB7-OB8-CB6
22	k	202	CDL	CB3-CB4-CB6-OB8
22	k	201	CDL	OA9-CA7-OA8-CA6
22	l	304	CDL	C77-C78-C79-C80
22	I	301	CDL	C60-C61-C62-C63
22	K	202	CDL	C24-C25-C26-C27
22	r	201	CDL	C44-C45-C46-C47
23	G	303	PC1	O22-C21-O21-C2
22	K	201	CDL	OB5-CB3-CB4-OB6
22	P	201	CDL	C72-C71-CB7-OB8
22	a	501	CDL	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
22	f	302	CDL	C54-C55-C56-C57
22	f	302	CDL	C72-C73-C74-C75
22	k	202	CDL	C77-C78-C79-C80
22	b	401	CDL	C73-C74-C75-C76
22	B	402	CDL	C56-C57-C58-C59
22	A	501	CDL	OA9-CA7-OA8-CA6
22	b	402	CDL	C41-C42-C43-C44
22	j	302	CDL	C72-C71-CB7-OB8
23	G	304	PC1	O31-C31-C32-C33
22	l	304	CDL	C83-C84-C85-C86
23	G	303	PC1	C23-C24-C25-C26
22	i	302	CDL	CA2-C1-CB2-OB2
22	l	301	CDL	CB2-C1-CA2-OA2
22	B	401	CDL	C19-C20-C21-C22
22	b	401	CDL	C44-C45-C46-C47
22	b	402	CDL	C38-C39-C40-C41
22	K	201	CDL	C20-C21-C22-C23
22	j	302	CDL	OB5-CB3-CB4-CB6
22	l	304	CDL	OB5-CB3-CB4-CB6
22	A	501	CDL	OB5-CB3-CB4-CB6
22	B	403	CDL	OB5-CB3-CB4-CB6
22	r	201	CDL	C12-C13-C14-C15
22	f	304	CDL	C16-C17-C18-C19
22	a	501	CDL	CB4-CB3-OB5-PB2
22	j	302	CDL	CB4-CB3-OB5-PB2
22	l	301	CDL	C1-CA2-OA2-PA1
22	B	401	CDL	C1-CA2-OA2-PA1
22	f	302	CDL	C14-C15-C16-C17
22	B	402	CDL	C35-C36-C37-C38
22	f	304	CDL	C18-C19-C20-C21
22	r	201	CDL	C43-C44-C45-C46
23	G	304	PC1	C33-C34-C35-C36
28	l	302	PEE	C44-C45-C46-C47
22	A	501	CDL	OB9-CB7-OB8-CB6
28	J	304	PEE	C16-C17-C18-C19
22	I	302	CDL	C78-C79-C80-C81
22	B	404	CDL	C41-C42-C43-C44
23	d	301	PC1	C25-C26-C27-C28
22	B	402	CDL	C32-C31-CA7-OA9
22	B	402	CDL	C16-C17-C18-C19
22	A	501	CDL	C71-CB7-OB8-CB6
23	g	303	PC1	C39-C3A-C3B-C3C

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Mol	Chain	Res	Type	Atoms
22	b	401	CDL	C12-C11-CA5-OA6
23	g	303	PC1	O31-C31-C32-C33
22	l	304	CDL	C59-C60-C61-C62
28	l	302	PEE	C36-C37-C38-C39
22	B	405	CDL	C41-C42-C43-C44
22	j	301	CDL	C83-C84-C85-C86
22	J	302	CDL	C41-C42-C43-C44
22	L	301	CDL	C42-C43-C44-C45
22	f	303	CDL	CA4-CA3-OA5-PA1
22	i	302	CDL	CB4-CB3-OB5-PB2
22	J	301	CDL	CA4-CA3-OA5-PA1
22	B	403	CDL	C62-C63-C64-C65
22	J	302	CDL	OB5-CB3-CB4-OB6
22	P	201	CDL	OA5-CA3-CA4-OA6
22	k	201	CDL	CA3-CA4-CA6-OA8
22	K	201	CDL	CA3-CA4-CA6-OA8
22	J	301	CDL	CB3-CB4-CB6-OB8
23	G	303	PC1	C1-C2-C3-O31
22	k	201	CDL	C11-C12-C13-C14
22	p	201	CDL	C43-C44-C45-C46
22	r	201	CDL	C32-C33-C34-C35
22	J	301	CDL	C54-C55-C56-C57
28	l	303	PEE	C36-C37-C38-C39
22	k	201	CDL	C78-C79-C80-C81
22	p	201	CDL	C15-C16-C17-C18
22	L	301	CDL	C75-C76-C77-C78
22	L	301	CDL	C72-C71-CB7-OB9
22	K	202	CDL	C31-C32-C33-C34
22	K	201	CDL	C12-C13-C14-C15
22	b	401	CDL	C72-C73-C74-C75
22	l	301	CDL	C56-C57-C58-C59
22	P	201	CDL	OA5-CA3-CA4-CA6
22	k	203	CDL	C59-C60-C61-C62
22	i	302	CDL	C51-C52-C53-C54
22	k	202	CDL	C19-C20-C21-C22
22	k	203	CDL	C39-C40-C41-C42
22	k	201	CDL	C24-C25-C26-C27
22	B	402	CDL	C42-C43-C44-C45
28	J	303	PEE	C36-C37-C38-C39
23	g	303	PC1	C2D-C2E-C2F-C2G
22	j	302	CDL	C1-CB2-OB2-PB2
22	a	501	CDL	C72-C73-C74-C75

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Mol	Chain	Res	Type	Atoms
22	L	301	CDL	C71-C72-C73-C74
23	G	304	PC1	C36-C37-C38-C39
22	B	401	CDL	C72-C71-CB7-OB8
23	G	303	PC1	O31-C31-C32-C33
22	B	403	CDL	C32-C31-CA7-OA9
28	l	302	PEE	C31-C32-C33-C34
22	a	501	CDL	CB5-C51-C52-C53
22	a	501	CDL	C32-C31-CA7-OA8
22	f	303	CDL	C32-C31-CA7-OA8
22	j	301	CDL	C16-C17-C18-C19
22	j	301	CDL	OB9-CB7-OB8-CB6
23	G	303	PC1	C22-C21-O21-C2
22	f	302	CDL	C64-C65-C66-C67
22	a	501	CDL	C79-C80-C81-C82
22	B	404	CDL	C20-C21-C22-C23
22	B	401	CDL	C36-C37-C38-C39
22	K	202	CDL	C12-C11-CA5-OA6
28	J	304	PEE	O2-C10-C11-C12
28	l	302	PEE	C37-C38-C39-C40
22	J	301	CDL	C17-C18-C19-C20
22	B	401	CDL	C54-C55-C56-C57
22	b	401	CDL	C13-C14-C15-C16
22	l	301	CDL	C81-C82-C83-C84
22	f	302	CDL	C52-C51-CB5-OB6
22	l	304	CDL	C52-C51-CB5-OB6
28	l	303	PEE	O2-C10-C11-C12
22	I	302	CDL	C39-C40-C41-C42
22	b	401	CDL	C12-C13-C14-C15
22	K	202	CDL	C72-C71-CB7-OB8
22	j	302	CDL	C59-C60-C61-C62
22	A	501	CDL	C51-C52-C53-C54
22	A	501	CDL	C18-C19-C20-C21
22	k	203	CDL	C32-C31-CA7-OA8
22	I	301	CDL	C72-C71-CB7-OB8
22	j	301	CDL	C22-C23-C24-C25
22	j	301	CDL	C32-C33-C34-C35
22	r	201	CDL	C56-C57-C58-C59
22	B	403	CDL	C16-C17-C18-C19
22	i	302	CDL	C64-C65-C66-C67
22	r	201	CDL	C34-C35-C36-C37
22	f	303	CDL	C72-C71-CB7-OB8
22	k	202	CDL	C72-C71-CB7-OB8

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Mol	Chain	Res	Type	Atoms
22	L	301	CDL	C32-C31-CA7-OA8
22	P	201	CDL	C12-C11-CA5-OA6
23	i	301	PC1	O31-C31-C32-C33
28	J	303	PEE	C31-C32-C33-C34
22	p	201	CDL	C12-C11-CA5-OA6
22	A	501	CDL	C52-C51-CB5-OB6
22	B	405	CDL	C72-C71-CB7-OB8
28	J	303	PEE	O2-C10-C11-C12
22	f	303	CDL	C36-C37-C38-C39
22	l	304	CDL	CA7-C31-C32-C33
22	l	304	CDL	CB5-C51-C52-C53
22	k	202	CDL	C12-C11-CA5-OA6
28	l	302	PEE	O2-C10-C11-C12
22	A	501	CDL	C76-C77-C78-C79
22	i	302	CDL	C44-C45-C46-C47
22	f	302	CDL	C55-C56-C57-C58
22	I	301	CDL	C52-C53-C54-C55
22	f	304	CDL	C52-C51-CB5-OB6
22	p	201	CDL	C32-C31-CA7-OA8
22	j	301	CDL	C71-CB7-OB8-CB6
22	P	201	CDL	C75-C76-C77-C78
28	J	303	PEE	C20-C21-C22-C23
22	A	501	CDL	O1-C1-CB2-OB2
22	J	302	CDL	C60-C61-C62-C63
22	r	201	CDL	C79-C80-C81-C82
28	l	303	PEE	C43-C44-C45-C46
22	L	301	CDL	C52-C51-CB5-OB6
22	B	405	CDL	C15-C16-C17-C18
22	B	401	CDL	CA4-CA3-OA5-PA1
22	K	202	CDL	C12-C11-CA5-OA7
22	I	301	CDL	CB7-C71-C72-C73
22	r	201	CDL	C36-C37-C38-C39
22	L	301	CDL	C78-C79-C80-C81
22	f	303	CDL	C37-C38-C39-C40
23	G	304	PC1	C26-C27-C28-C29
22	p	201	CDL	C12-C13-C14-C15
22	I	302	CDL	C36-C37-C38-C39
23	g	303	PC1	C26-C27-C28-C29
22	B	402	CDL	OB5-CB3-CB4-OB6
23	G	303	PC1	O21-C21-C22-C23
28	l	303	PEE	C16-C17-C18-C19
22	a	501	CDL	C32-C31-CA7-OA9

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Mol	Chain	Res	Type	Atoms
23	G	303	PC1	O32-C31-C32-C33
22	b	401	CDL	C62-C63-C64-C65
22	B	402	CDL	C60-C61-C62-C63
22	f	304	CDL	C52-C51-CB5-OB7
22	B	401	CDL	C72-C71-CB7-OB9
22	i	302	CDL	C79-C80-C81-C82
22	i	302	CDL	C32-C33-C34-C35
22	P	201	CDL	C12-C11-CA5-OA7
28	l	303	PEE	O4-C10-C11-C12
22	a	501	CDL	C32-C33-C34-C35
22	b	401	CDL	C56-C57-C58-C59
22	B	402	CDL	C83-C84-C85-C86
22	P	201	CDL	C42-C43-C44-C45
29	e	900	NAD	C3D-C4D-C5D-O5D
22	f	303	CDL	C72-C71-CB7-OB9
22	k	202	CDL	C12-C11-CA5-OA7
22	B	405	CDL	C72-C71-CB7-OB9
22	K	202	CDL	C72-C71-CB7-OB9
28	J	303	PEE	O4-C10-C11-C12
28	J	304	PEE	O4-C10-C11-C12
22	I	301	CDL	C39-C40-C41-C42
23	G	303	PC1	O21-C2-C3-O31
23	i	301	PC1	O32-C31-C32-C33
22	k	203	CDL	C61-C62-C63-C64
22	A	501	CDL	C34-C35-C36-C37
22	P	201	CDL	C15-C16-C17-C18
28	J	304	PEE	C12-C13-C14-C15
22	p	201	CDL	C12-C11-CA5-OA7
22	b	402	CDL	C1-CA2-OA2-PA1
22	f	302	CDL	C72-C71-CB7-OB8
22	l	301	CDL	C12-C11-CA5-OA6
22	B	401	CDL	C12-C11-CA5-OA6
22	P	201	CDL	C32-C31-CA7-OA8
22	I	301	CDL	C55-C56-C57-C58
22	k	203	CDL	C32-C31-CA7-OA9
22	I	301	CDL	C72-C71-CB7-OB9
22	b	402	CDL	C32-C33-C34-C35
22	J	302	CDL	C32-C33-C34-C35
22	L	301	CDL	C24-C25-C26-C27
22	K	201	CDL	C75-C76-C77-C78
28	l	302	PEE	O4-C10-C11-C12
22	K	202	CDL	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
22	b	402	CDL	C33-C34-C35-C36
22	f	302	CDL	C52-C51-CB5-OB7
22	f	303	CDL	C32-C31-CA7-OA9
22	l	304	CDL	C52-C51-CB5-OB7
22	f	304	CDL	CA7-C31-C32-C33
22	K	201	CDL	C56-C57-C58-C59
22	p	201	CDL	C32-C31-CA7-OA9
22	A	501	CDL	C52-C51-CB5-OB7
22	B	402	CDL	C12-C11-CA5-OA6
22	k	202	CDL	C72-C71-CB7-OB9
22	b	402	CDL	C74-C75-C76-C77
22	b	401	CDL	C84-C85-C86-C87
22	L	301	CDL	C12-C11-CA5-OA6
23	i	301	PC1	O21-C21-C22-C23
22	L	301	CDL	C32-C31-CA7-OA9
23	G	303	PC1	O22-C21-C22-C23
23	G	304	PC1	C3A-C3B-C3C-C3D
23	D	301	PC1	C36-C37-C38-C39

There are no ring outliers.

40 monomers are involved in 124 short contacts:

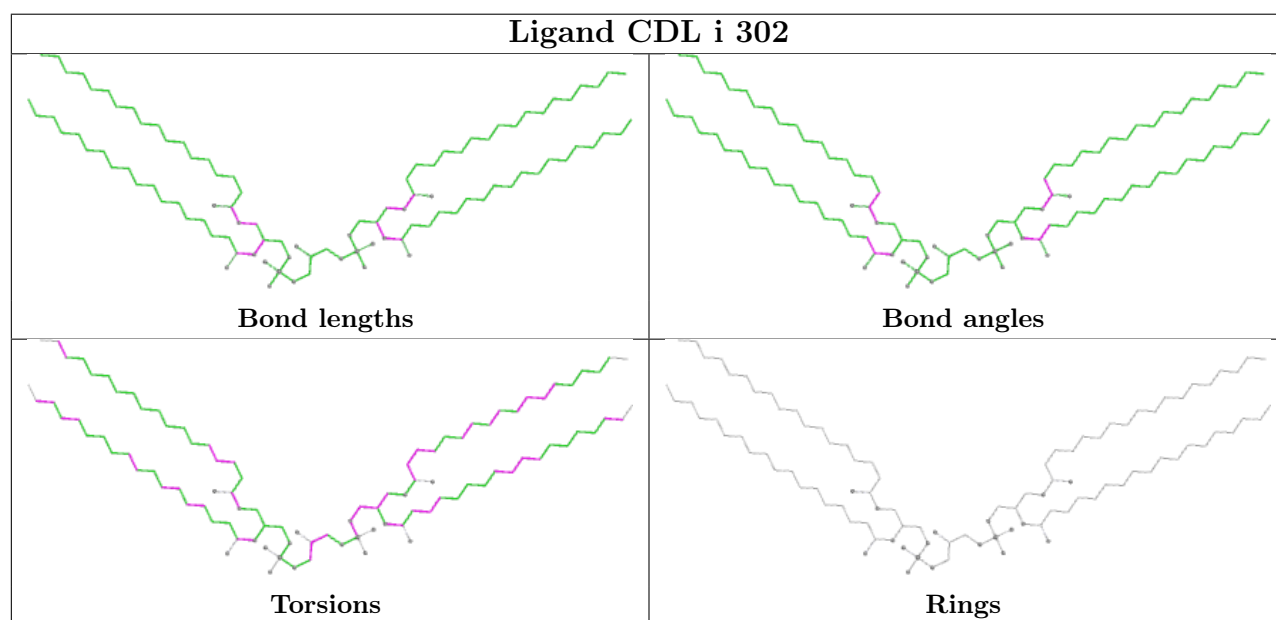
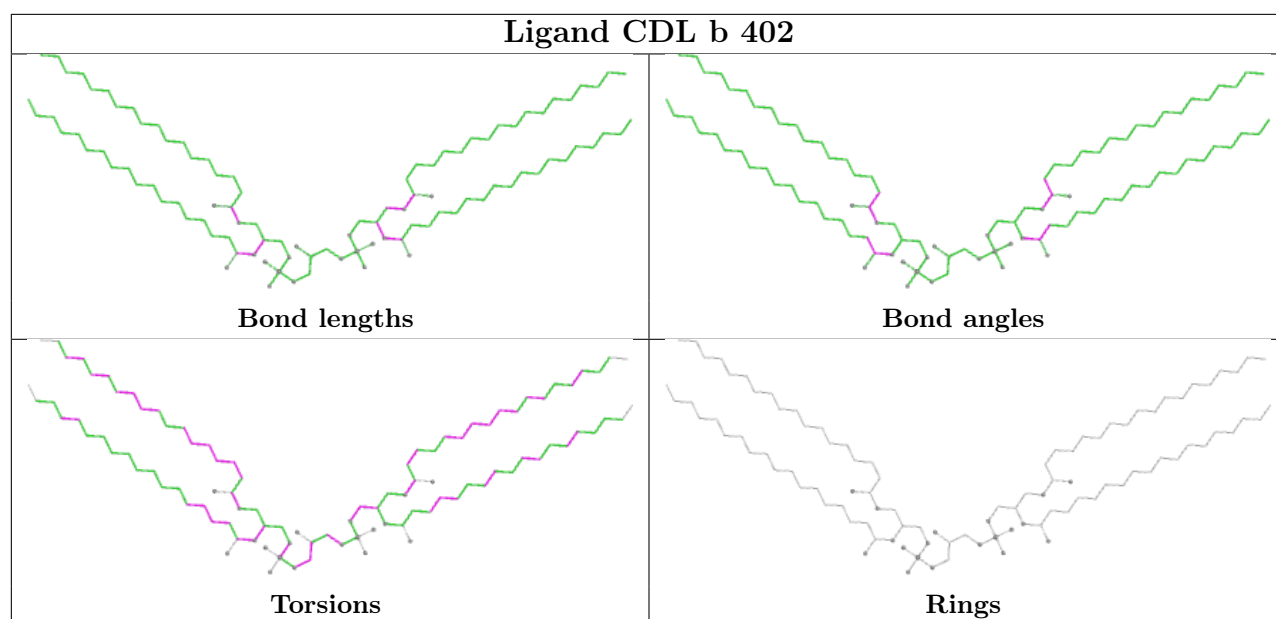
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	b	402	CDL	1	0
22	i	302	CDL	1	0
22	I	302	CDL	1	0
26	G	301	ATP	1	0
22	f	303	CDL	8	0
23	G	304	PC1	1	0
22	B	404	CDL	1	0
29	E	900	NAD	1	0
22	I	301	CDL	5	0
22	L	301	CDL	11	0
22	K	201	CDL	1	0
22	B	405	CDL	6	0
22	j	301	CDL	2	0
22	b	401	CDL	7	0
25	i	303	UQ8	8	0
22	k	203	CDL	4	0
22	l	301	CDL	11	0
23	i	301	PC1	1	0
28	J	303	PEE	4	0

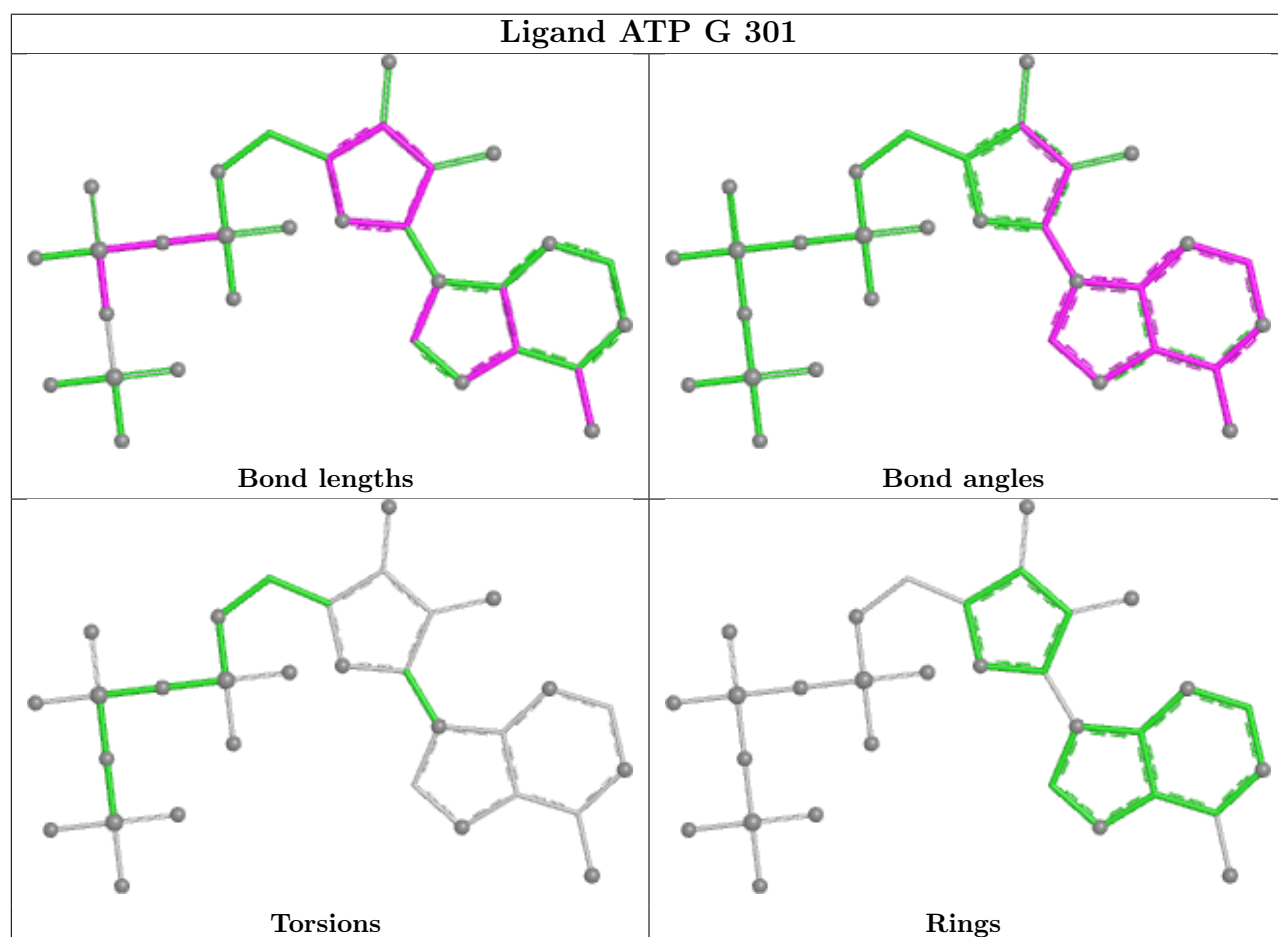
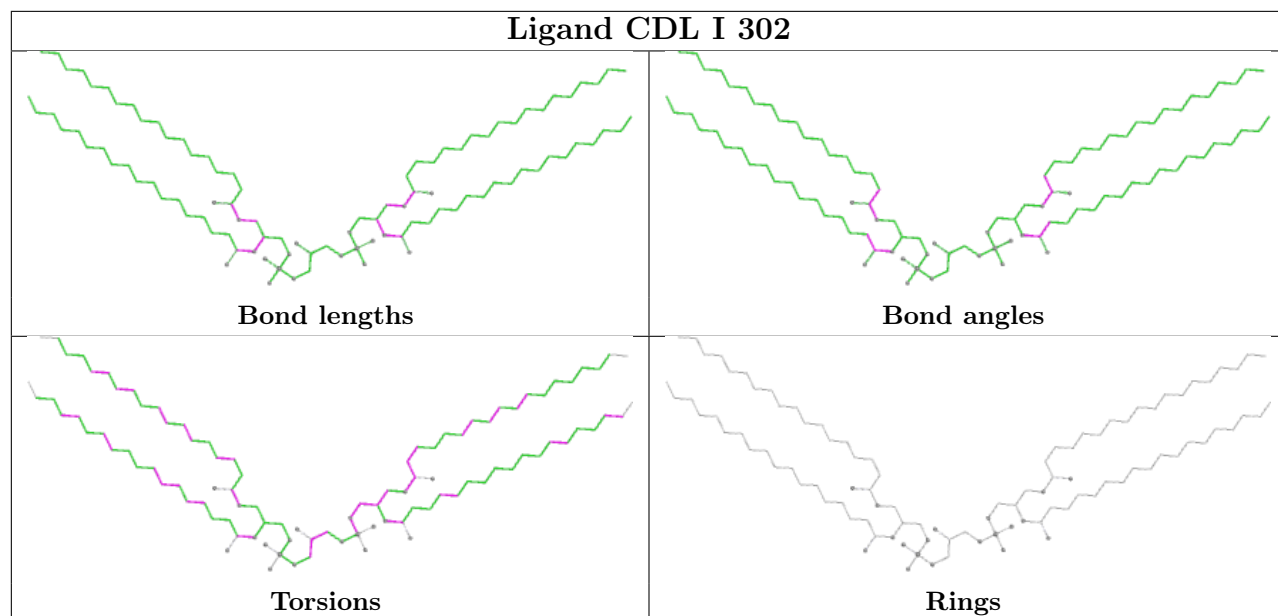
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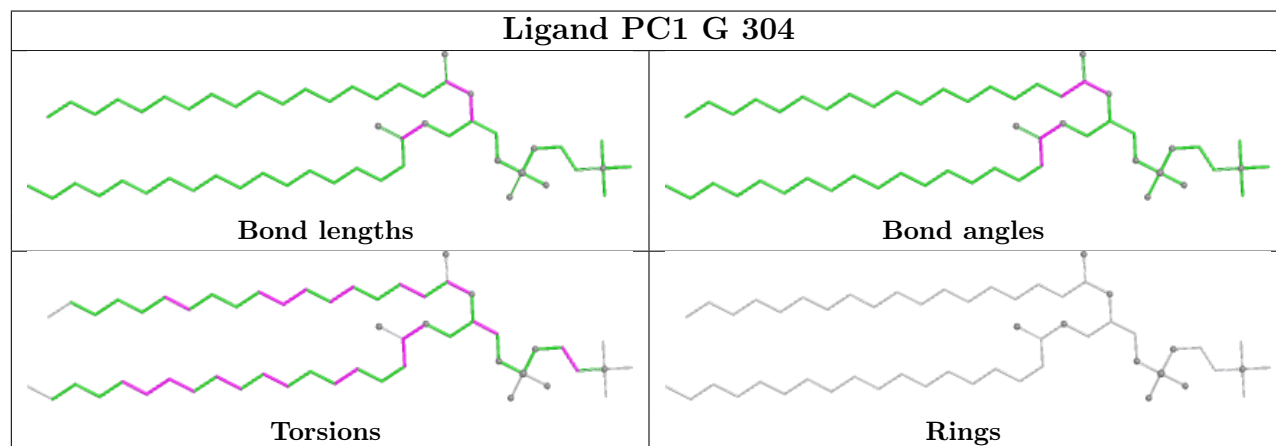
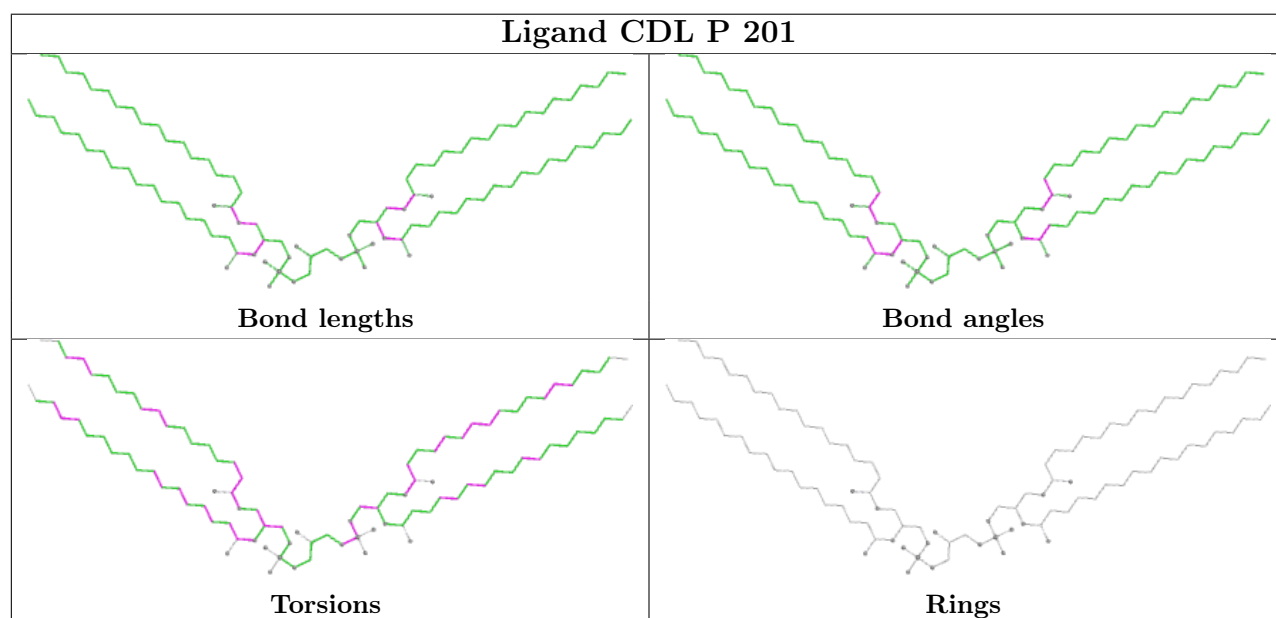
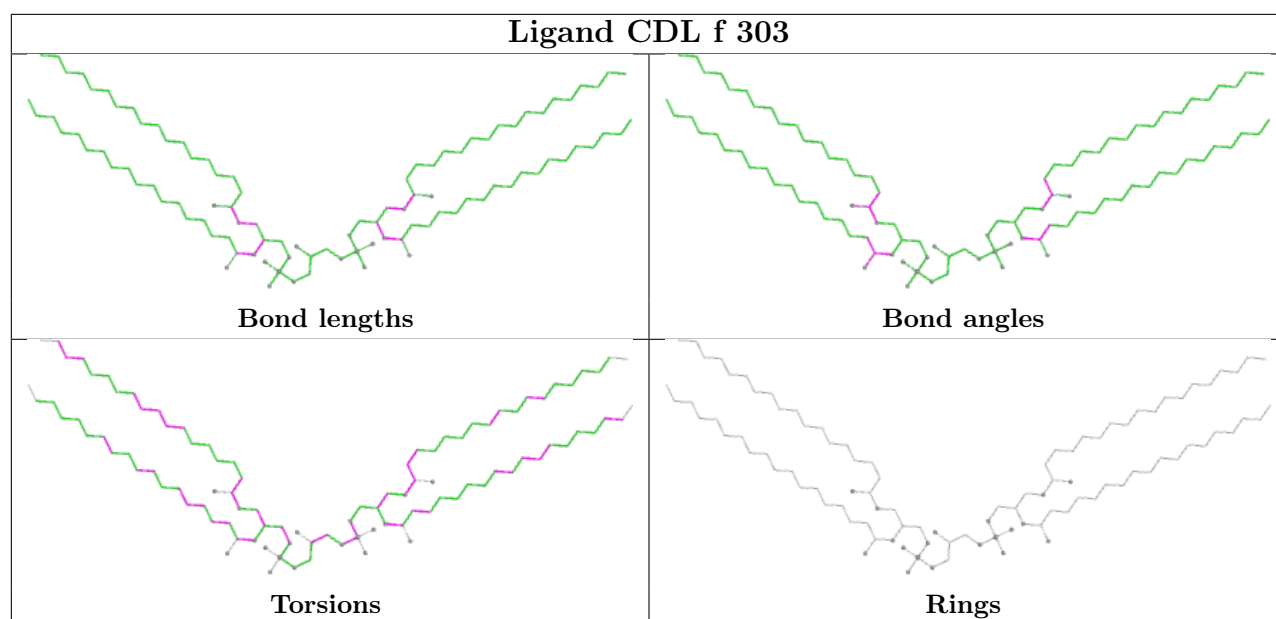
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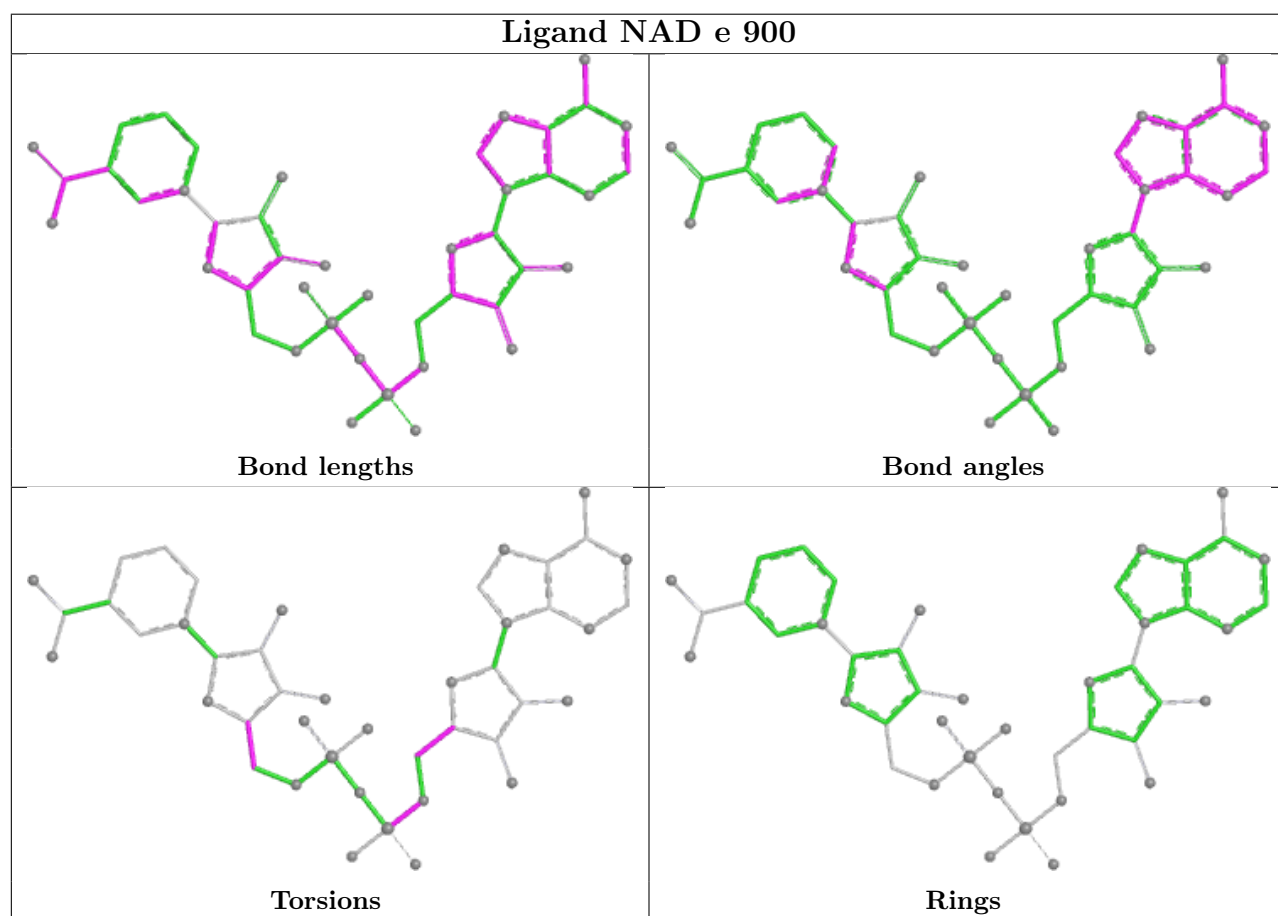
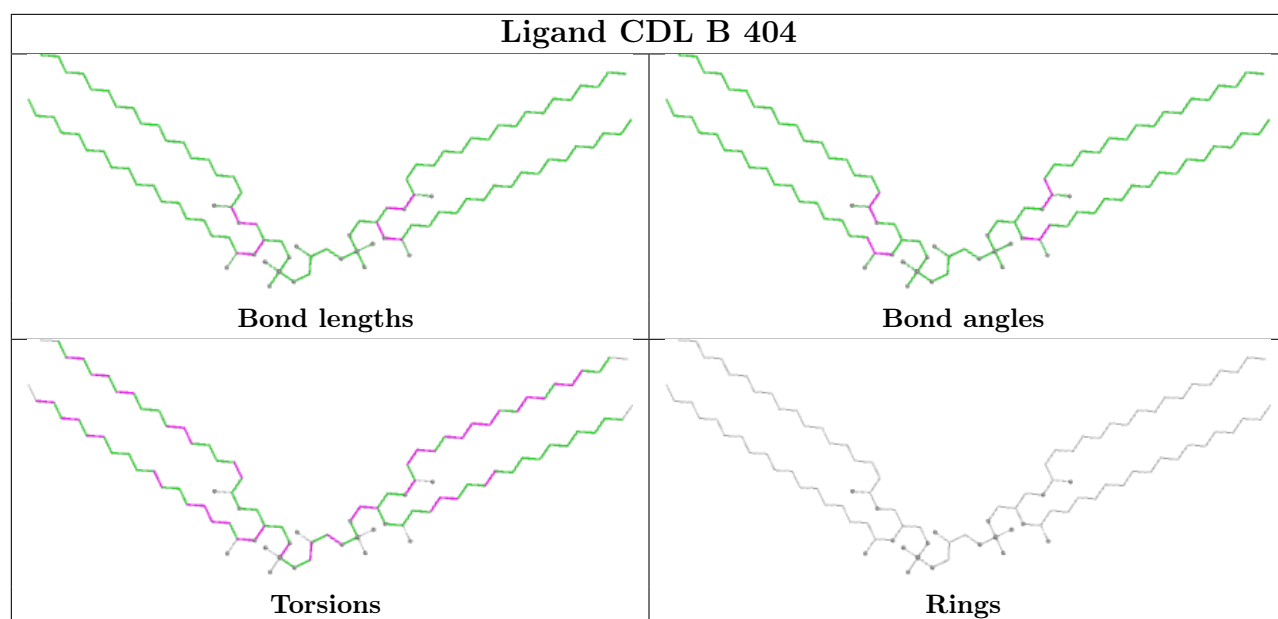
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	B	403	CDL	7	0
22	B	402	CDL	6	0
22	K	202	CDL	1	0
28	l	302	PEE	2	0
22	J	301	CDL	2	0
22	l	304	CDL	3	0
23	G	303	PC1	1	0
28	l	303	PEE	1	0
22	r	201	CDL	3	0
23	D	301	PC1	4	0
22	A	501	CDL	4	0
22	J	302	CDL	1	0
22	B	401	CDL	9	0
25	I	303	UQ8	5	0
23	d	301	PC1	1	0
26	g	301	ATP	1	0
22	f	302	CDL	7	0
22	k	202	CDL	2	0
22	f	304	CDL	2	0
22	a	501	CDL	4	0
22	j	302	CDL	1	0

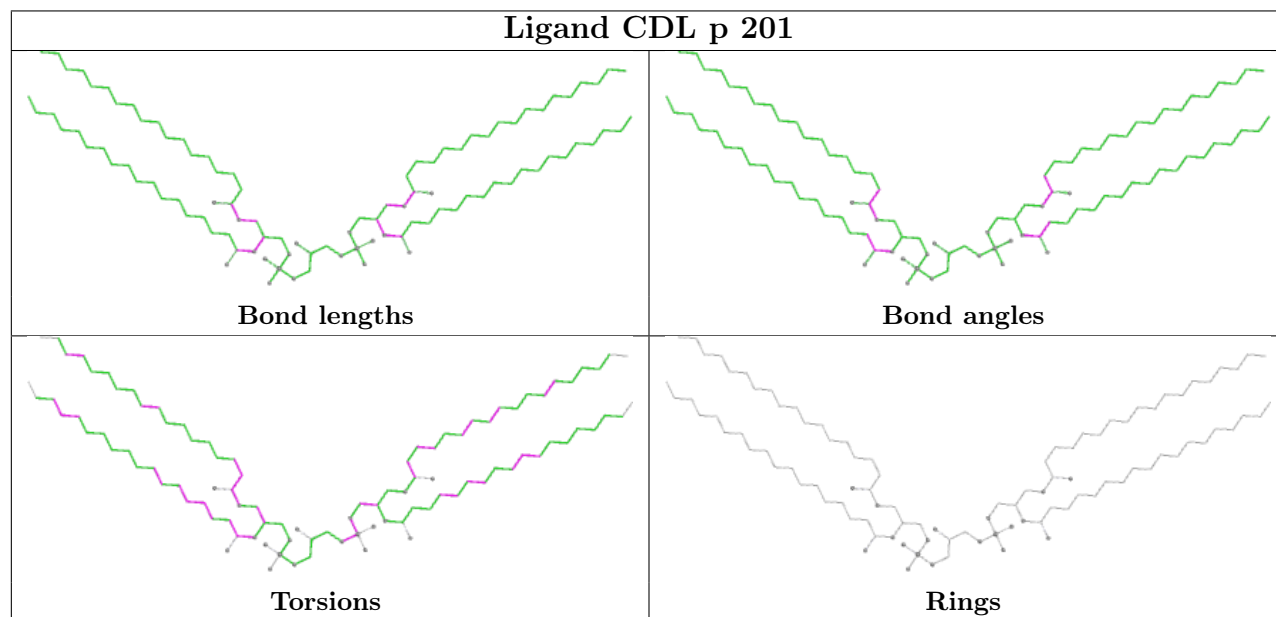
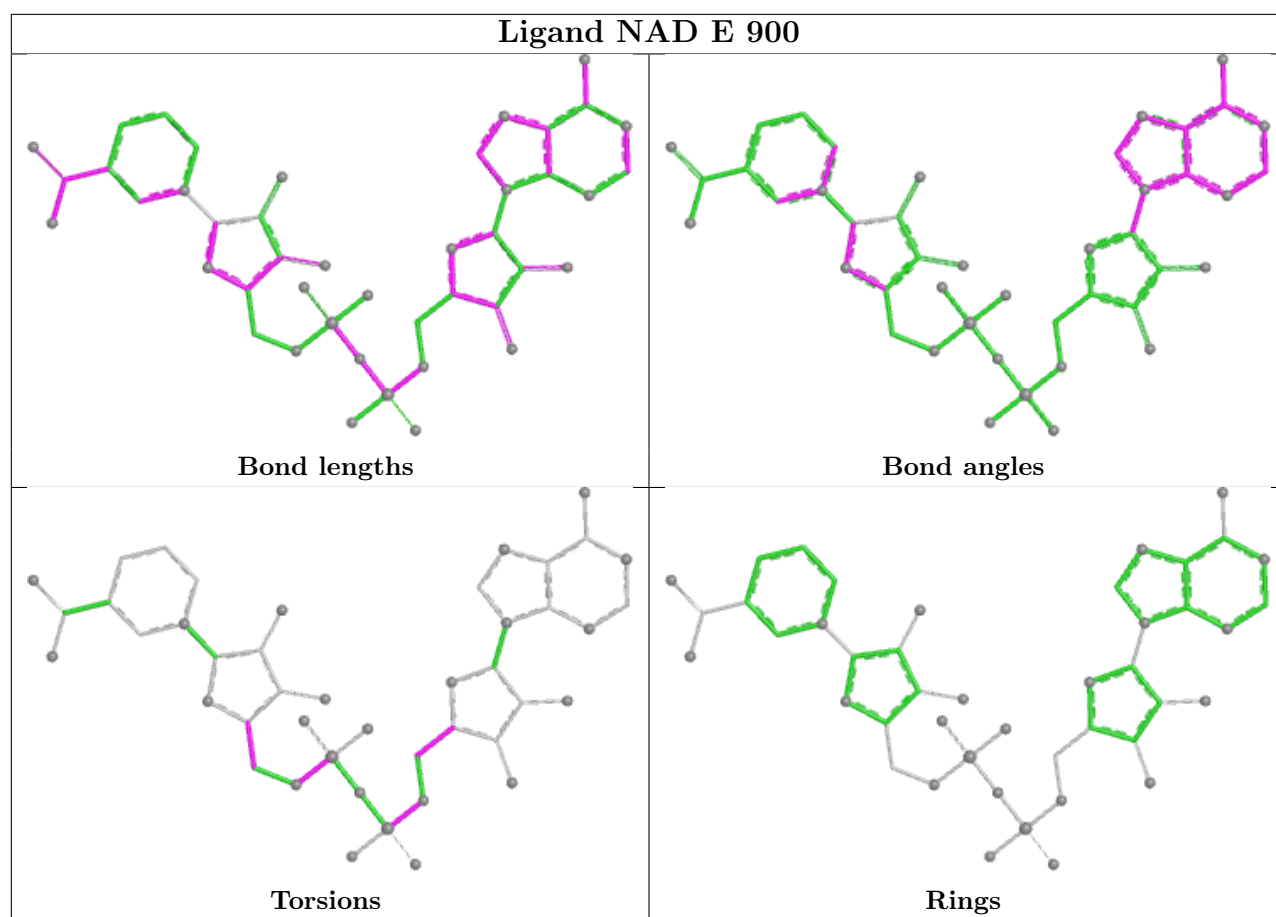
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

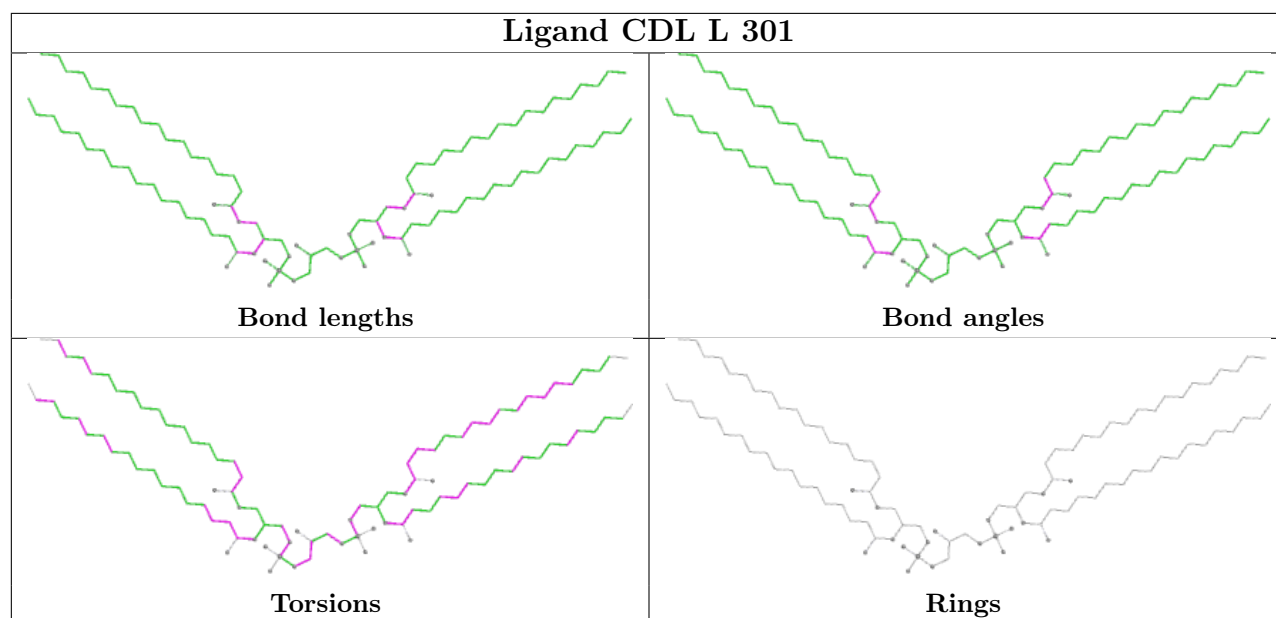
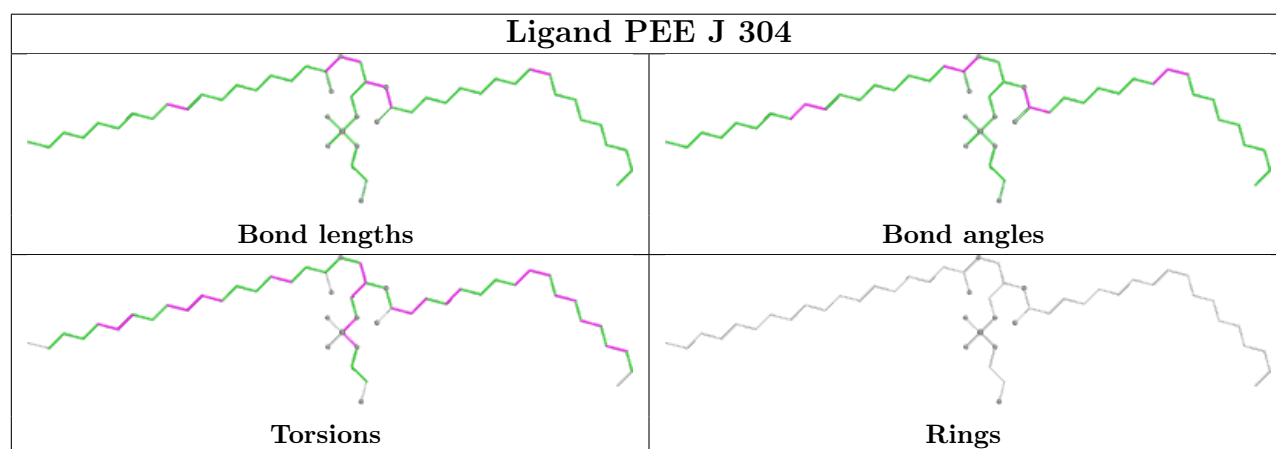
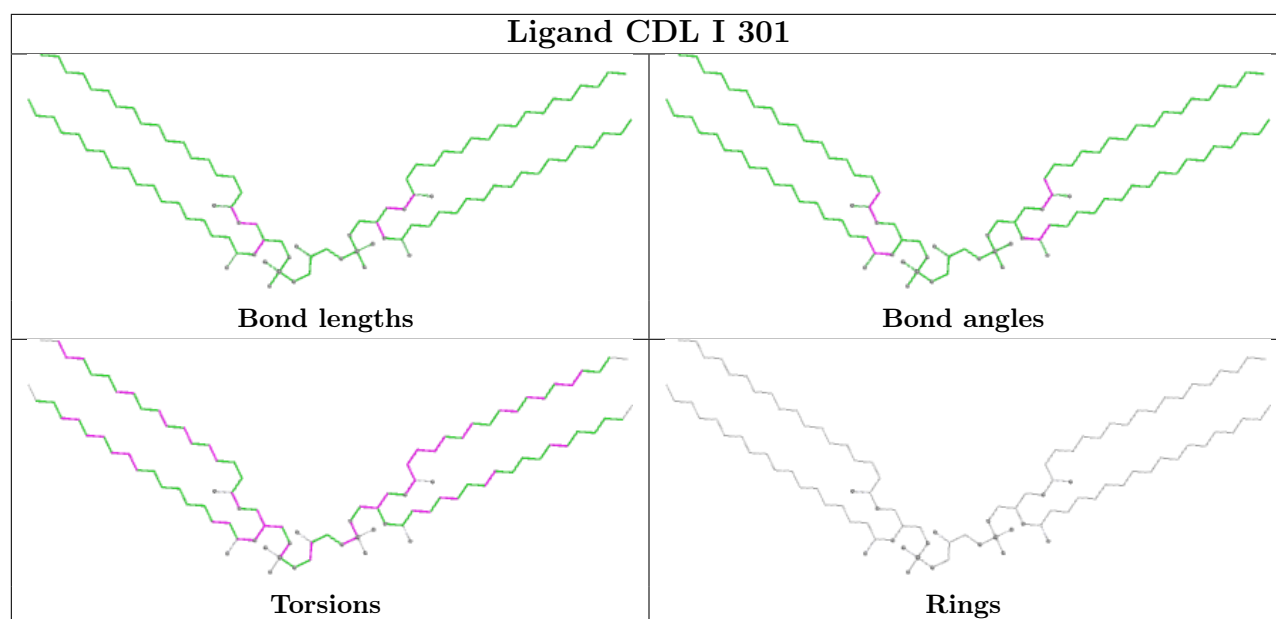


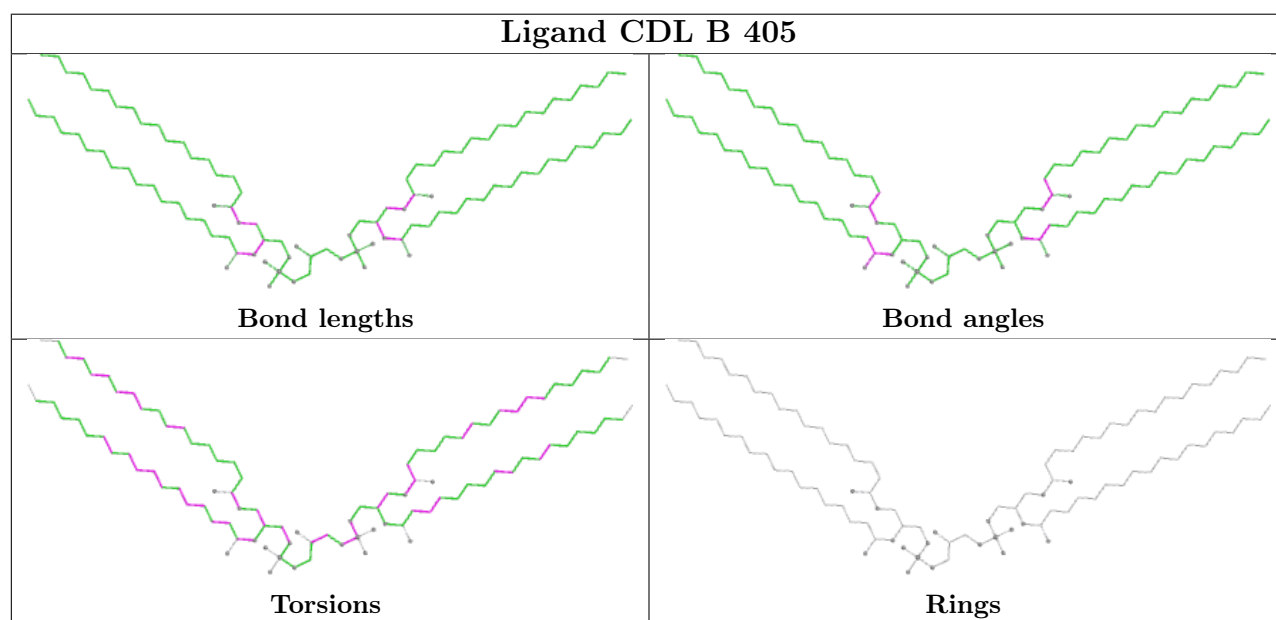
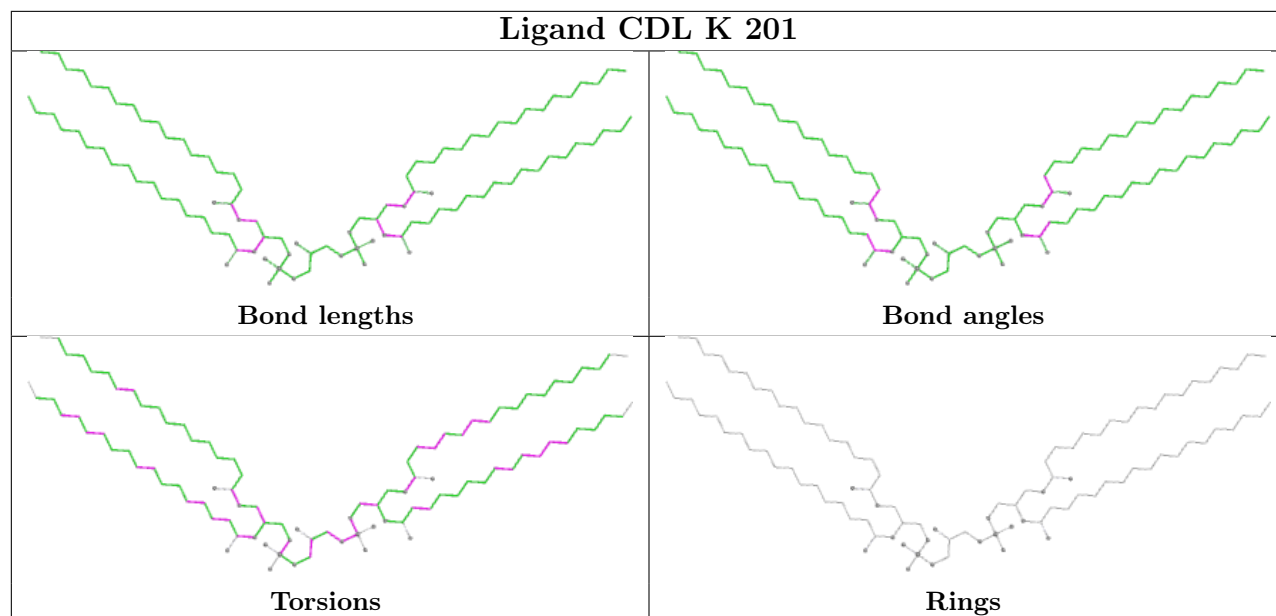


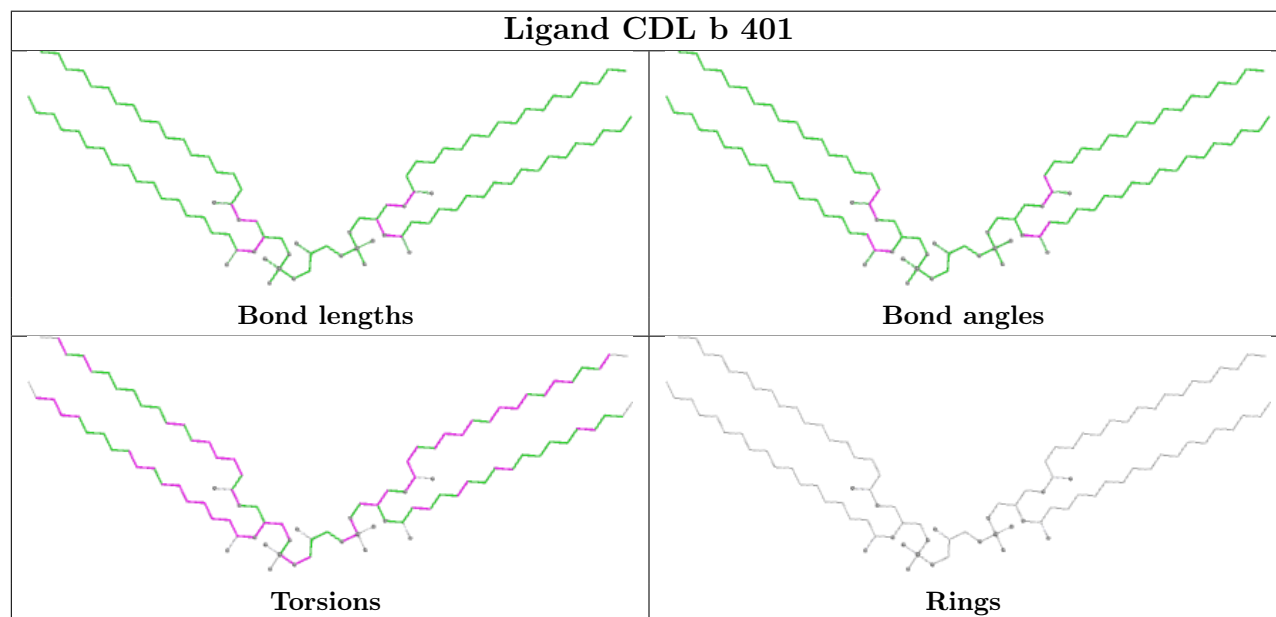
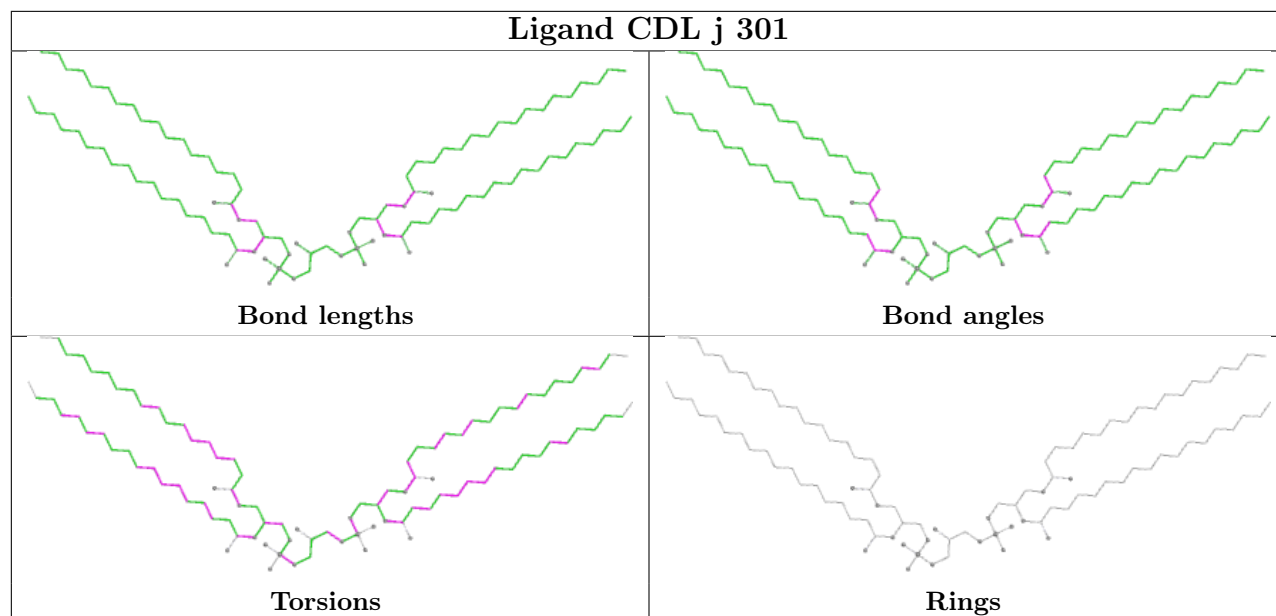


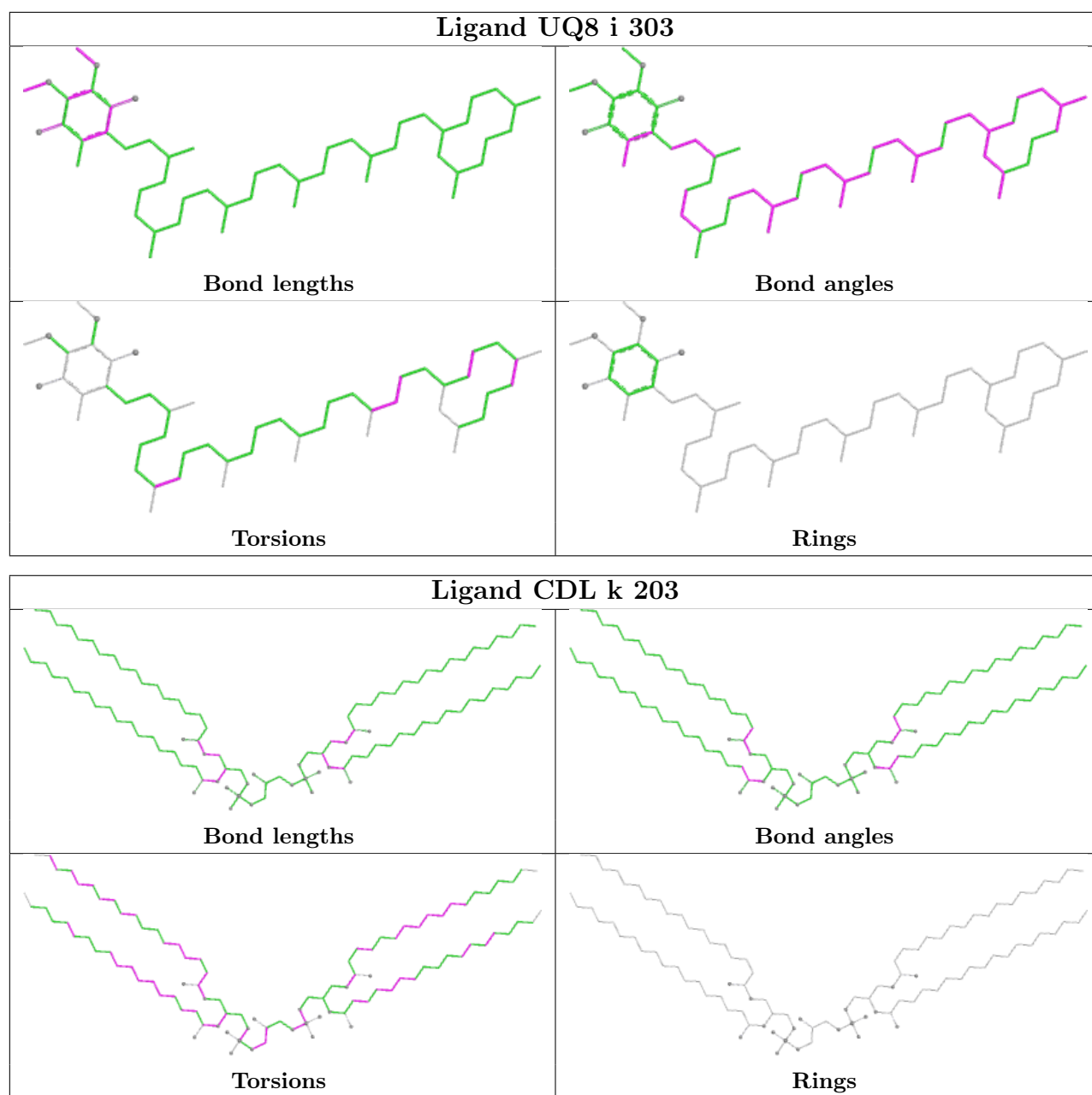


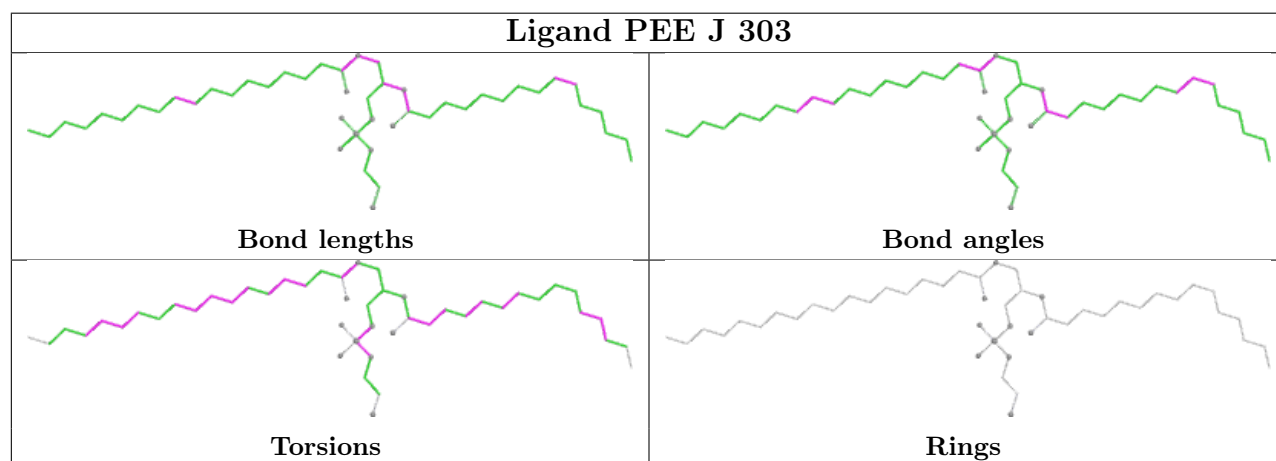
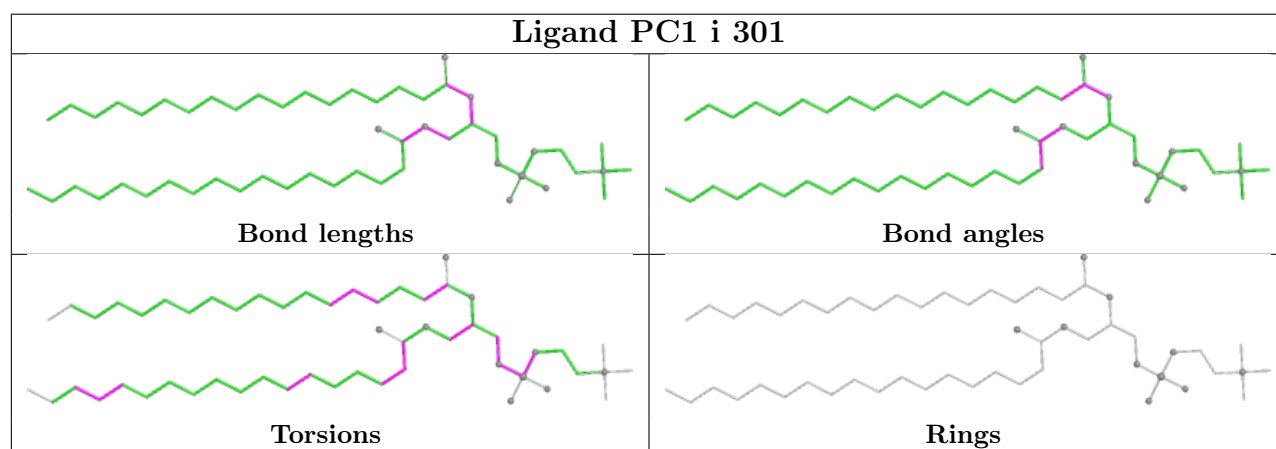
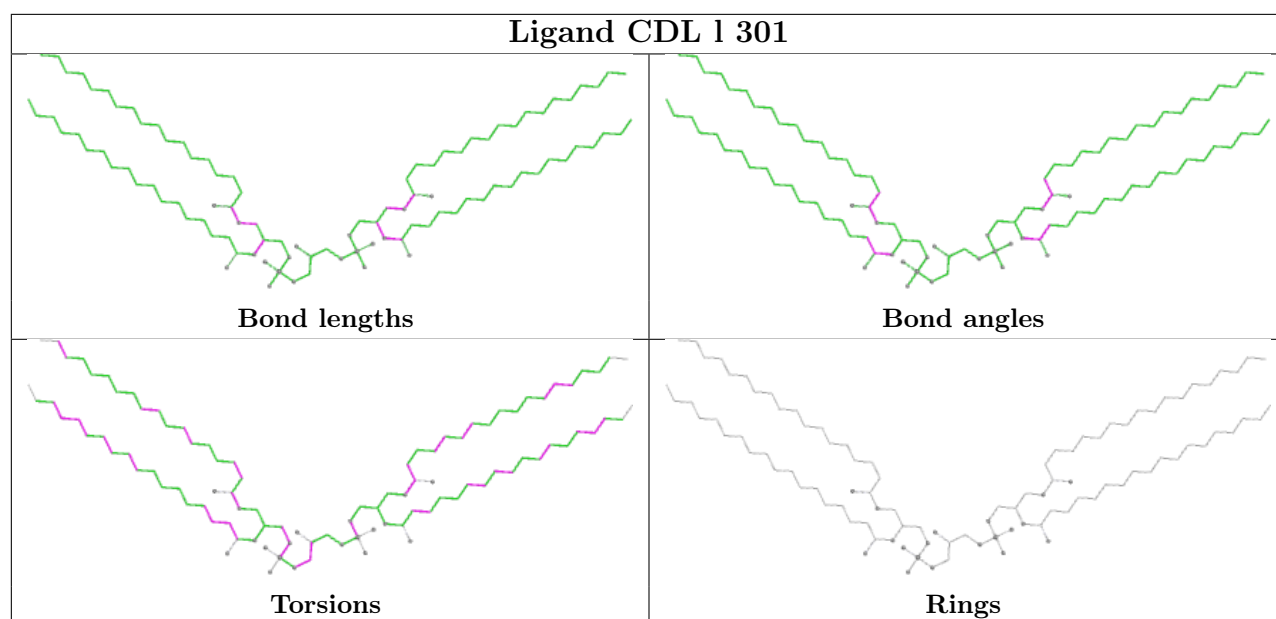


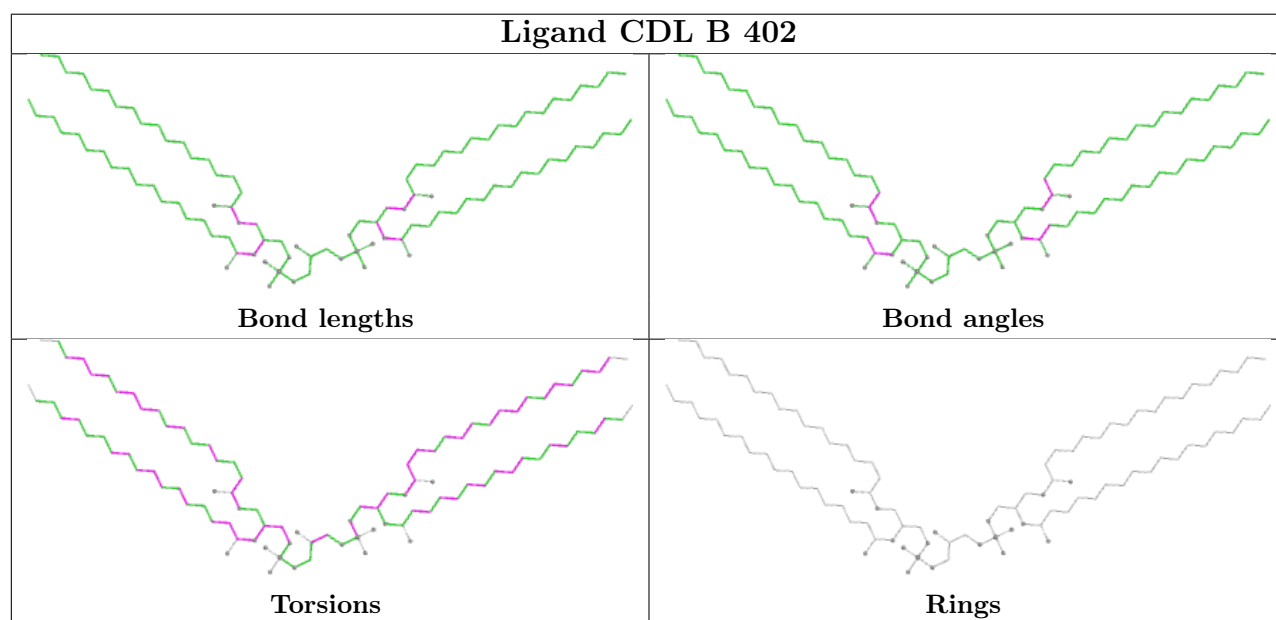
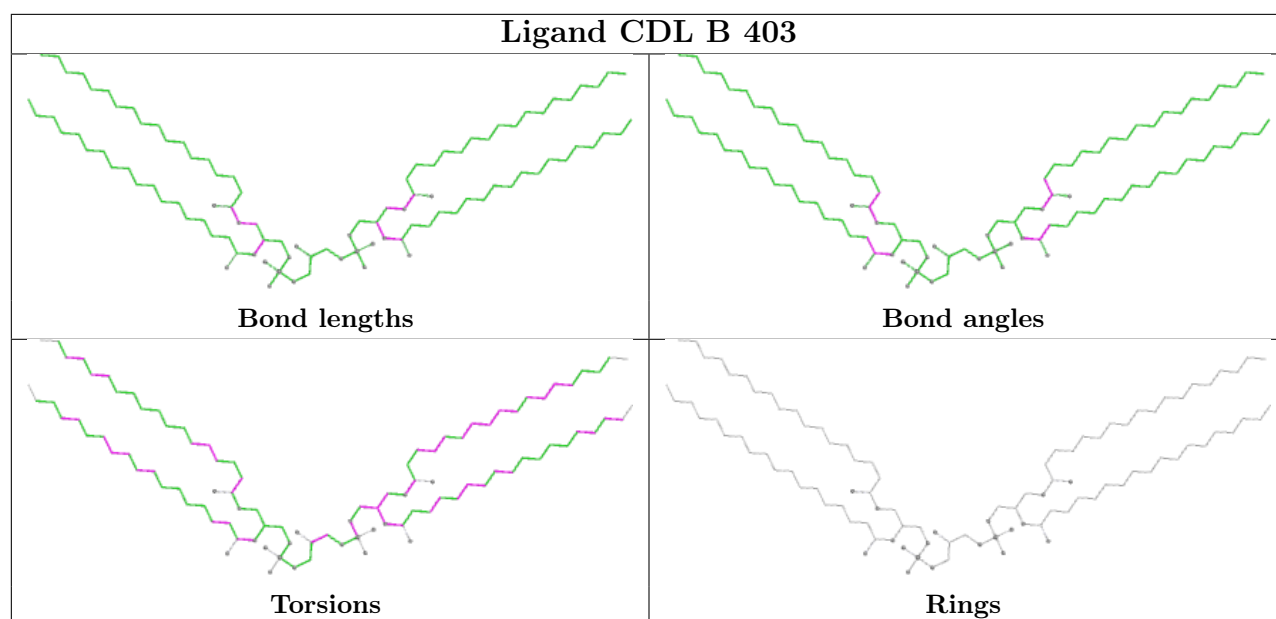


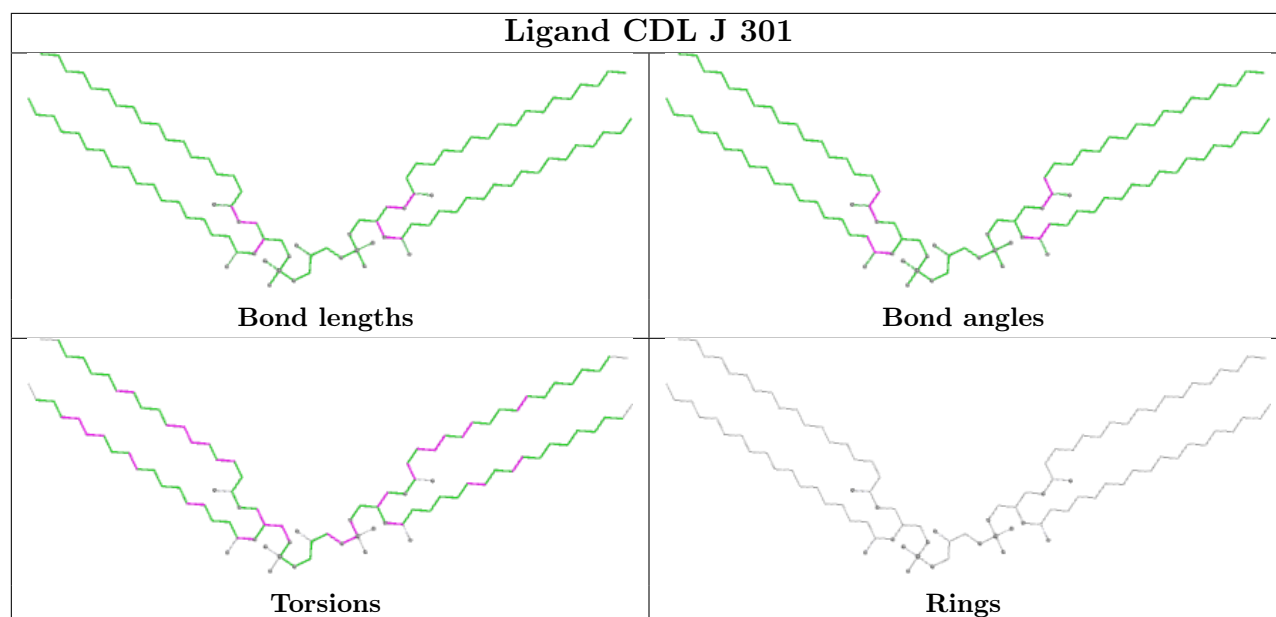
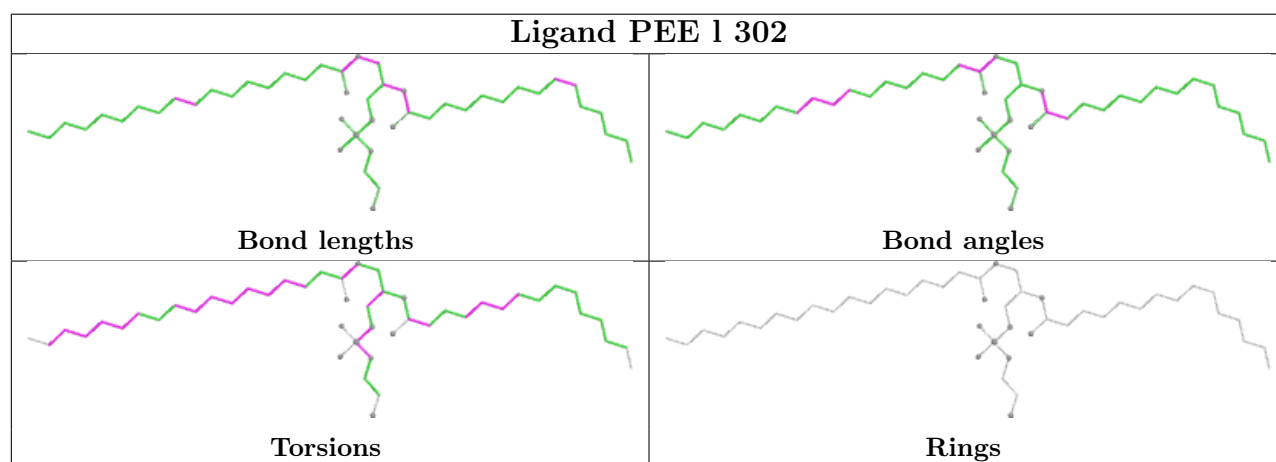
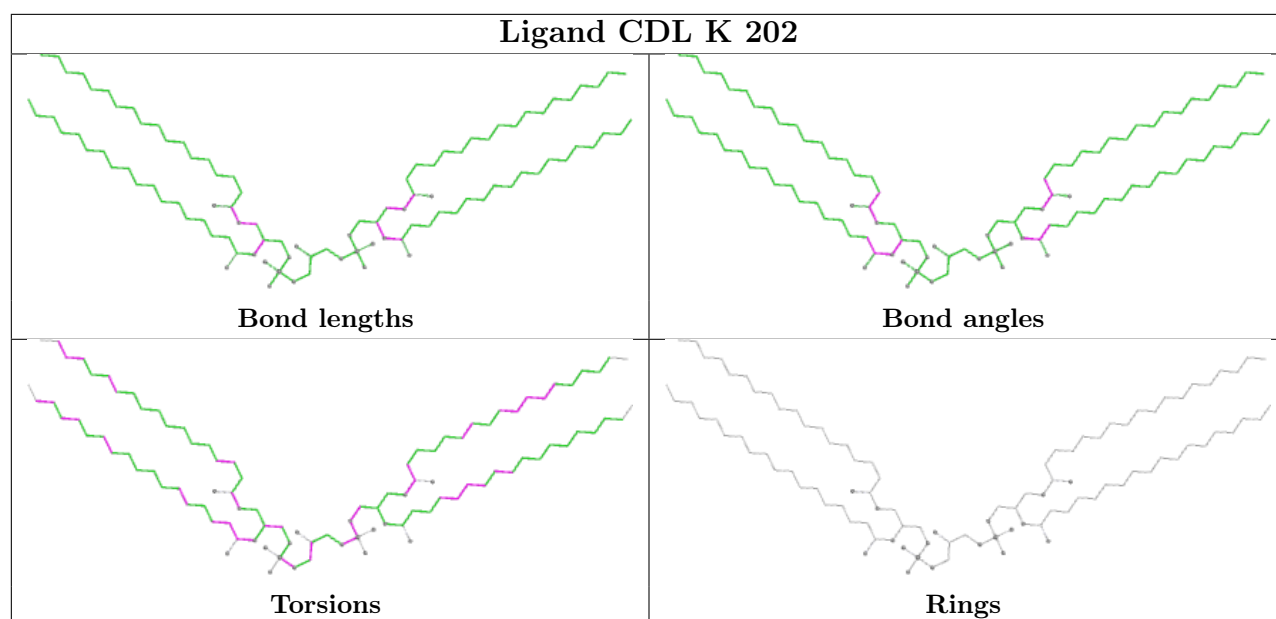


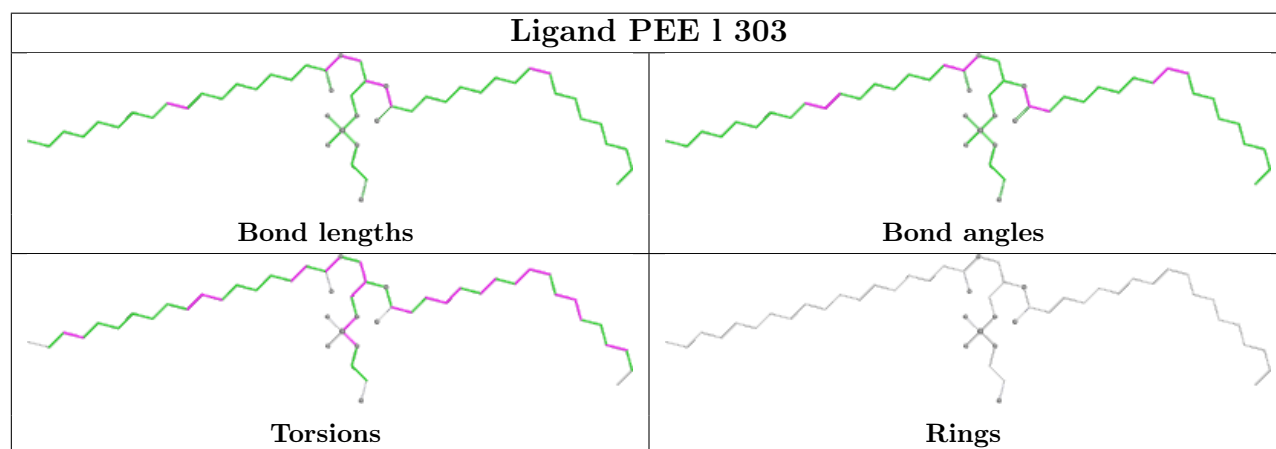
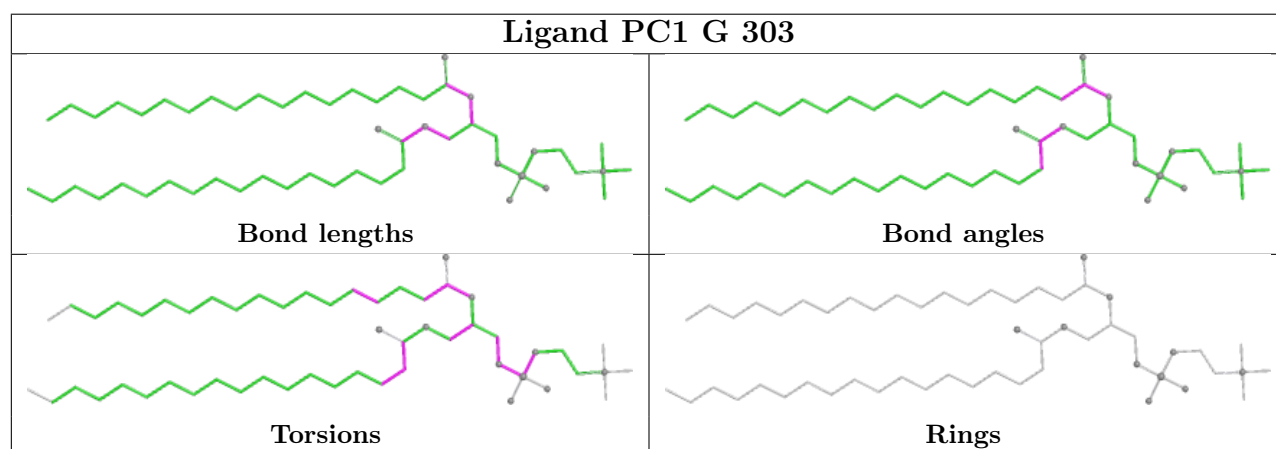
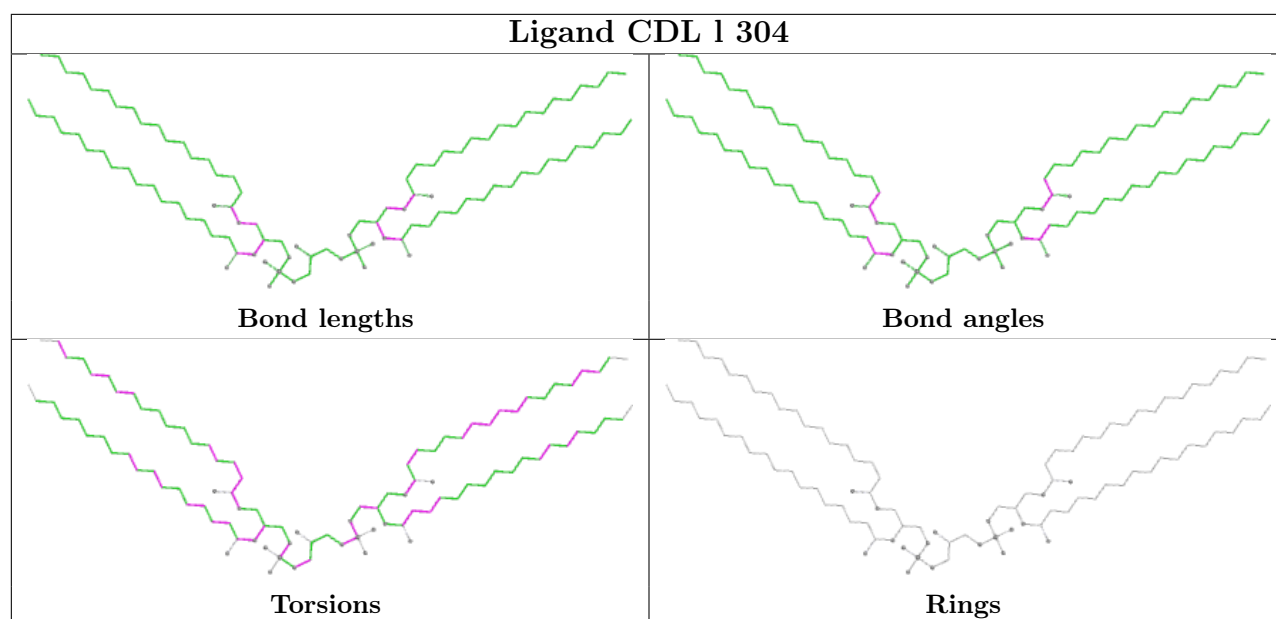


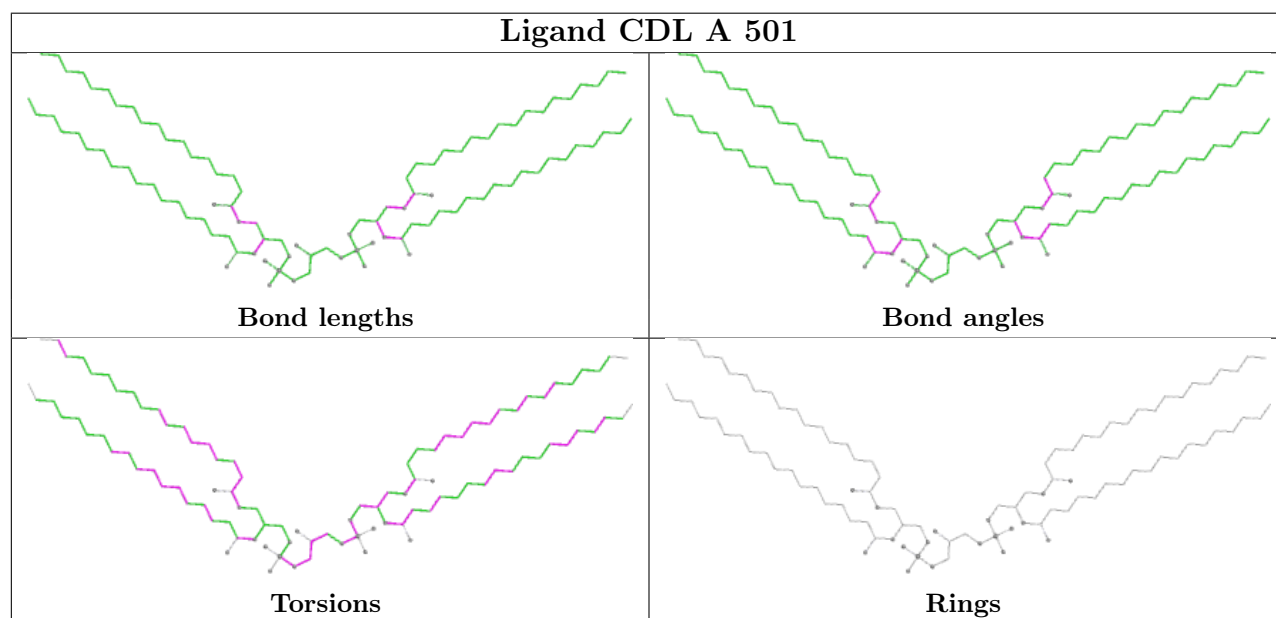
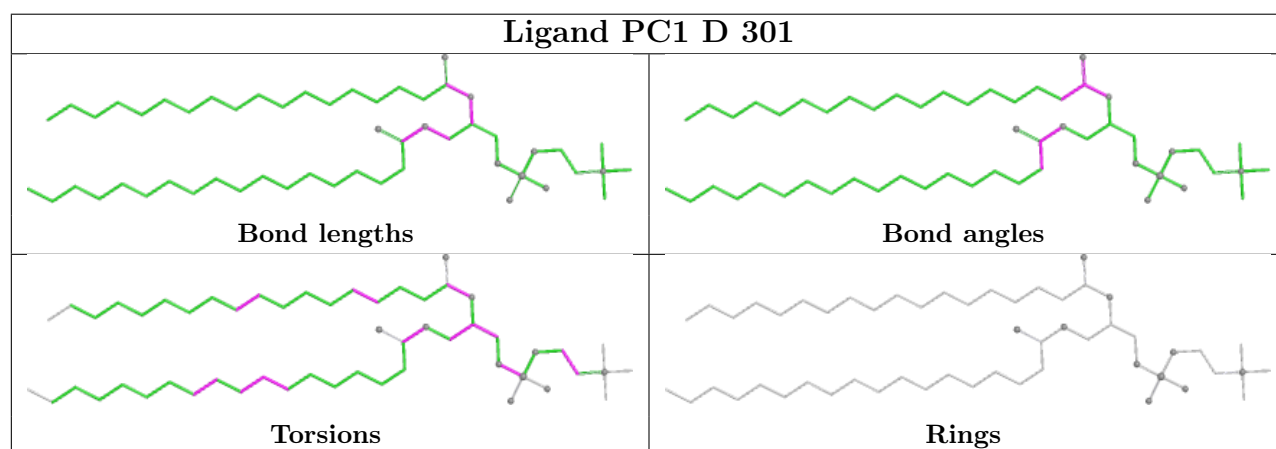
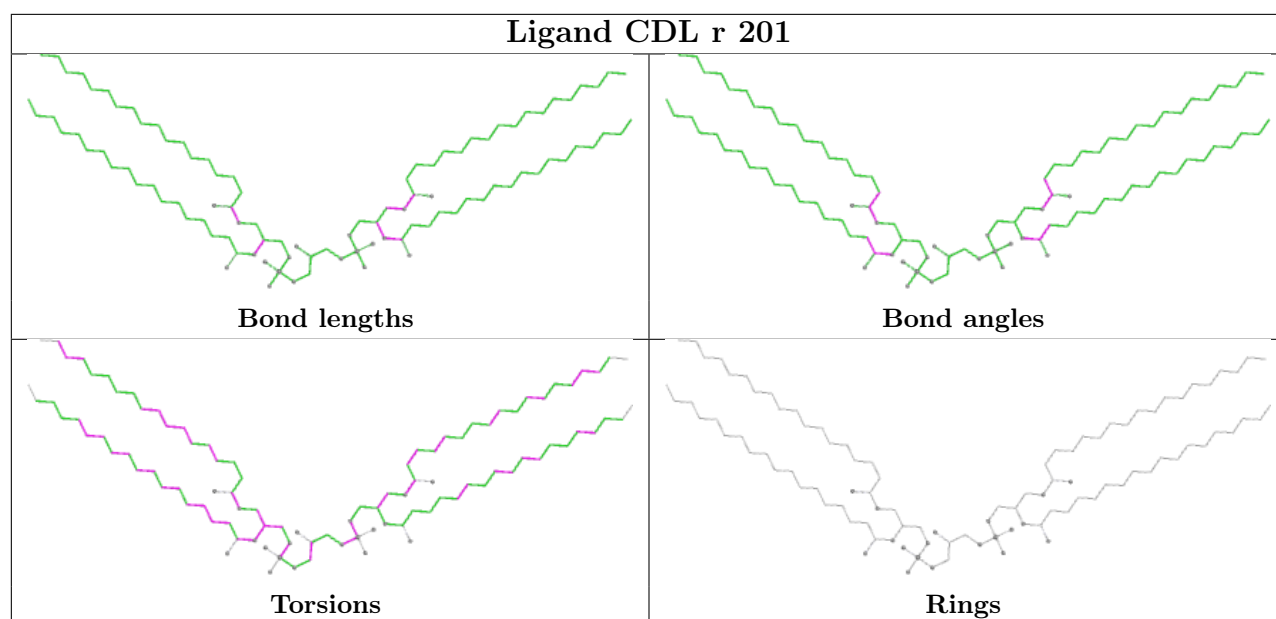


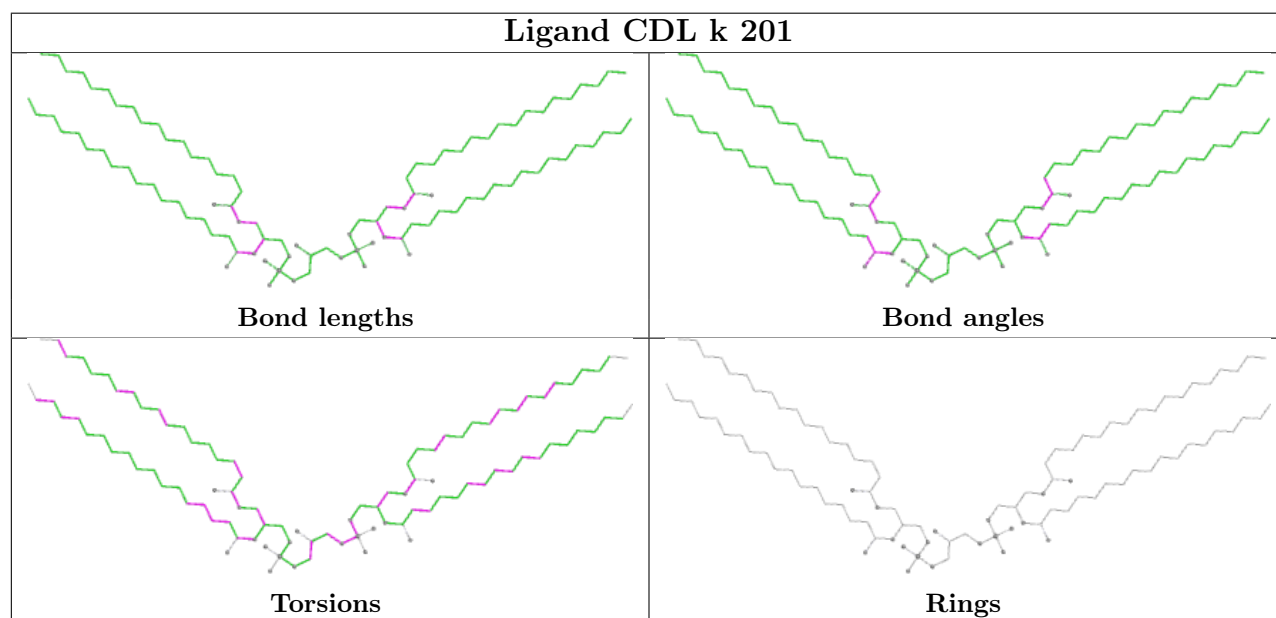
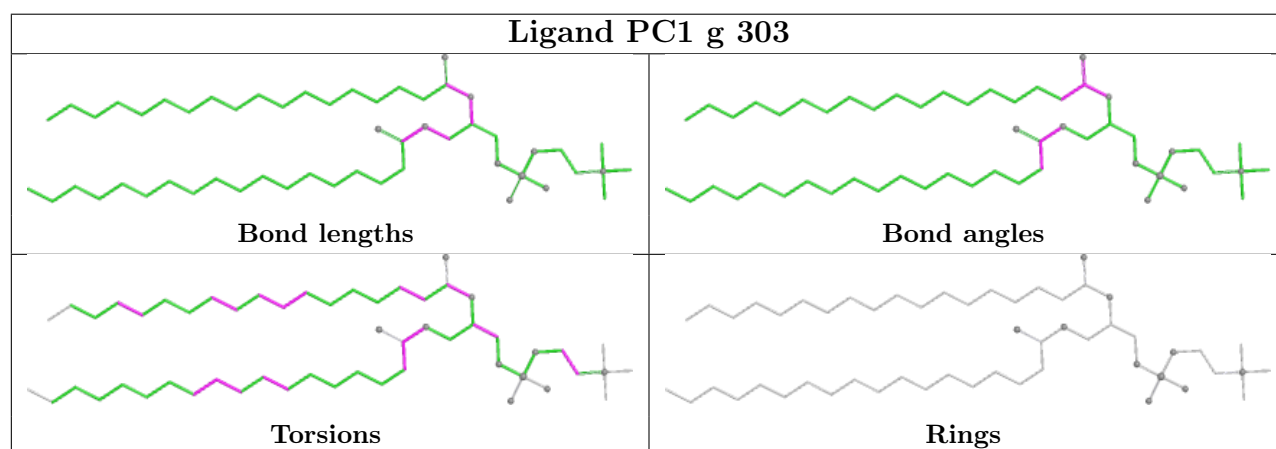
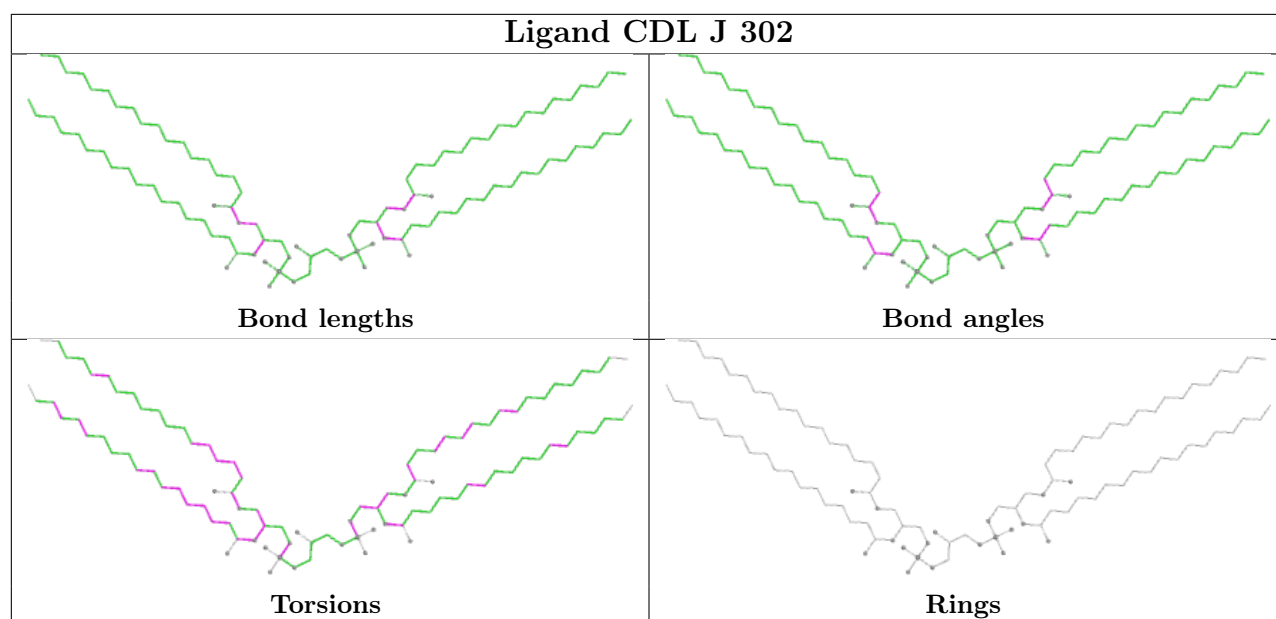


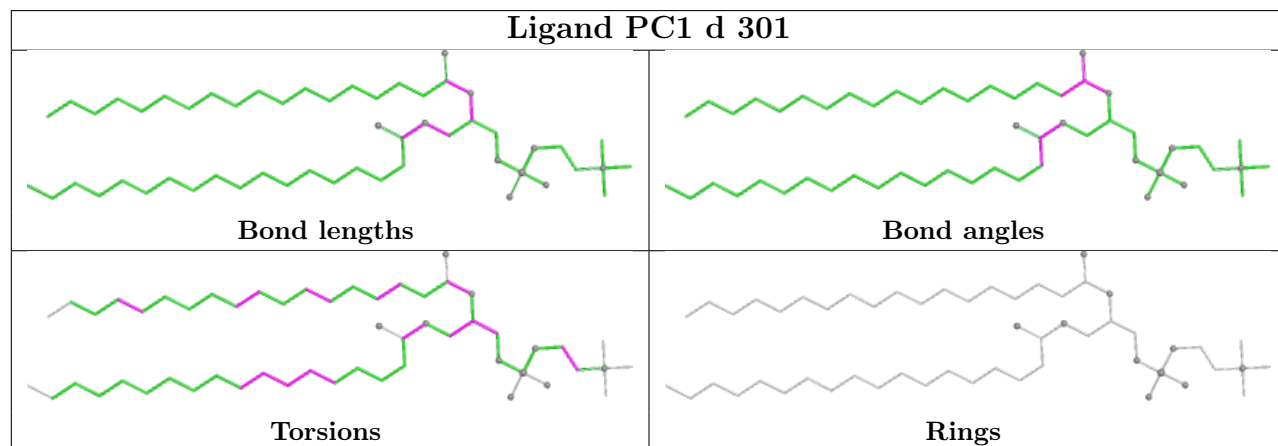
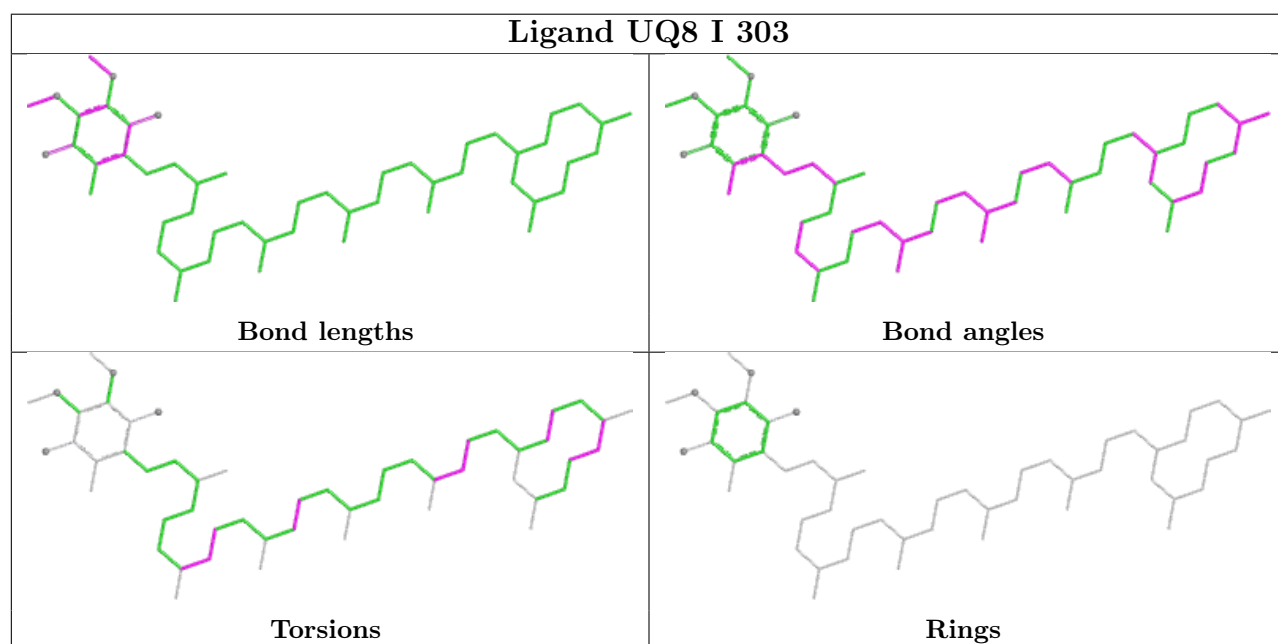
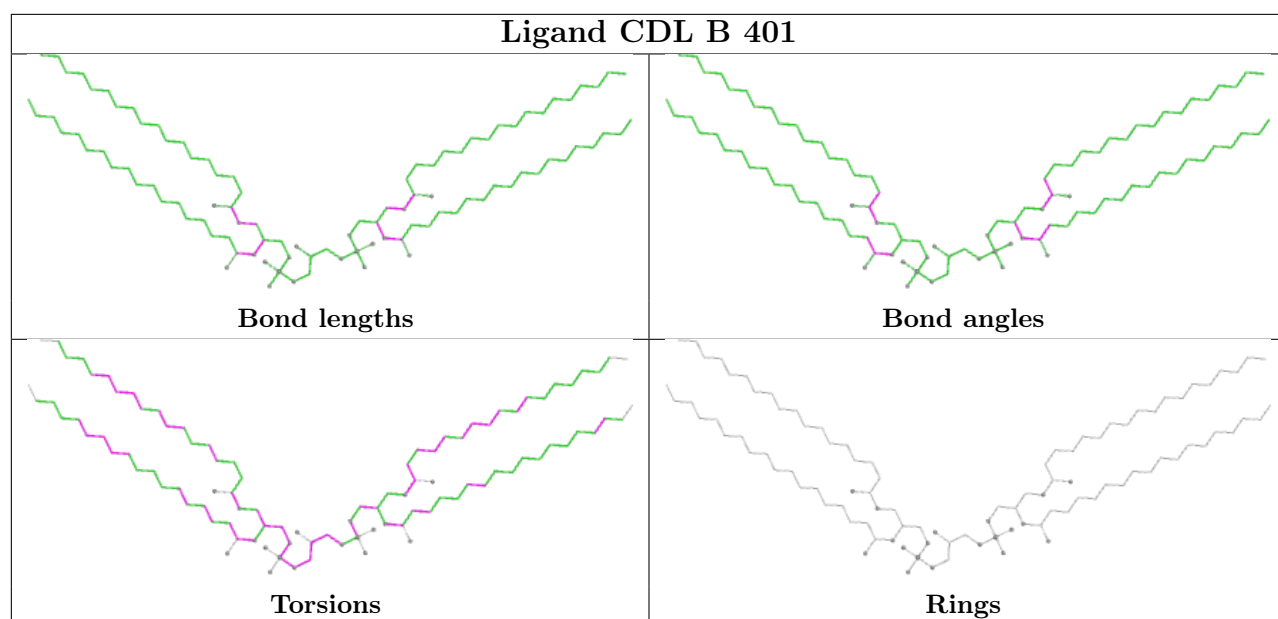


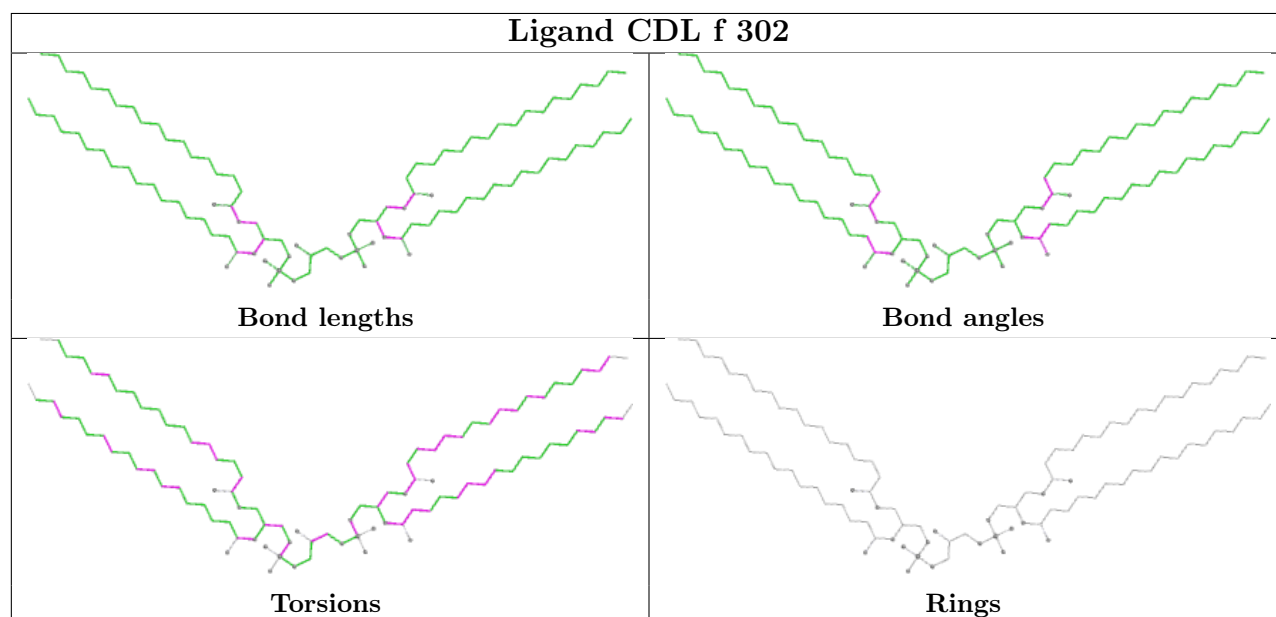
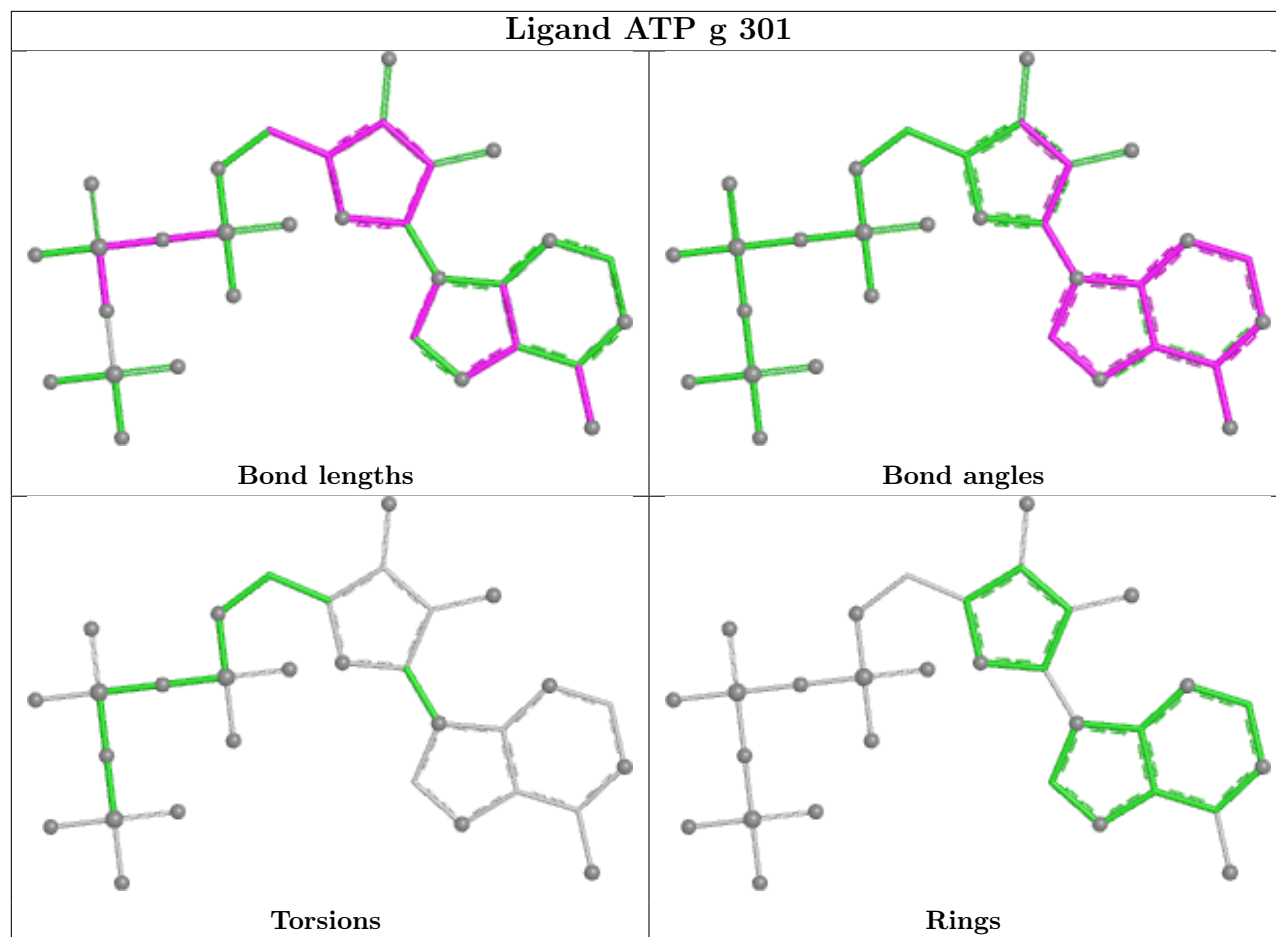


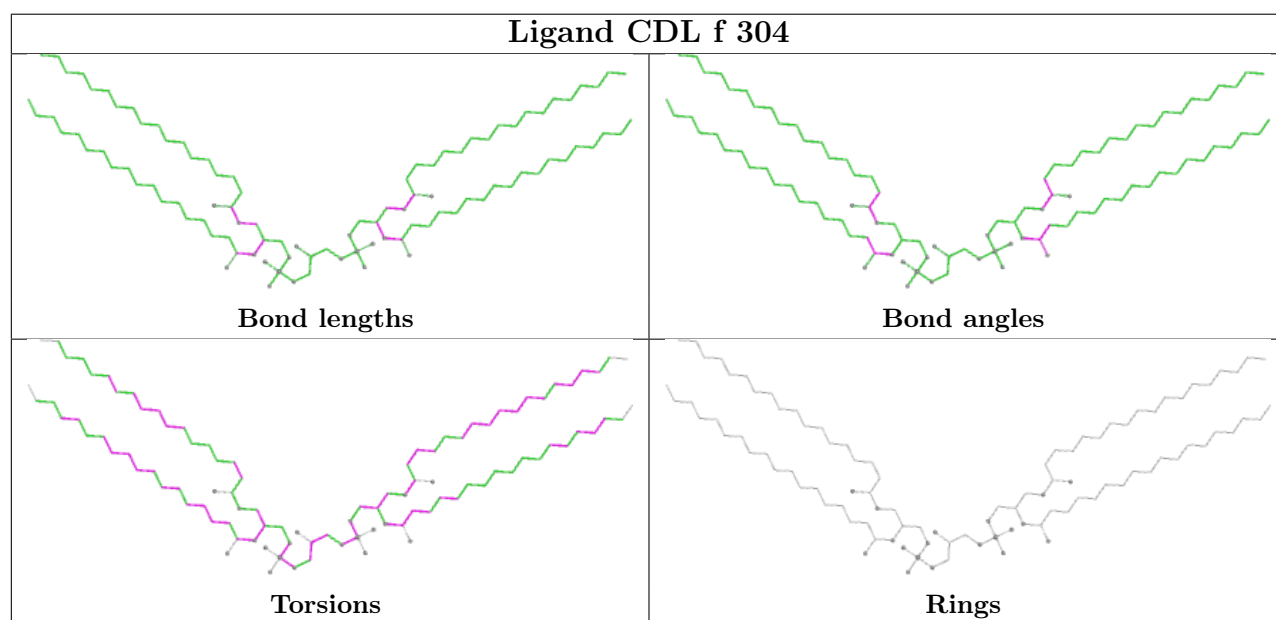
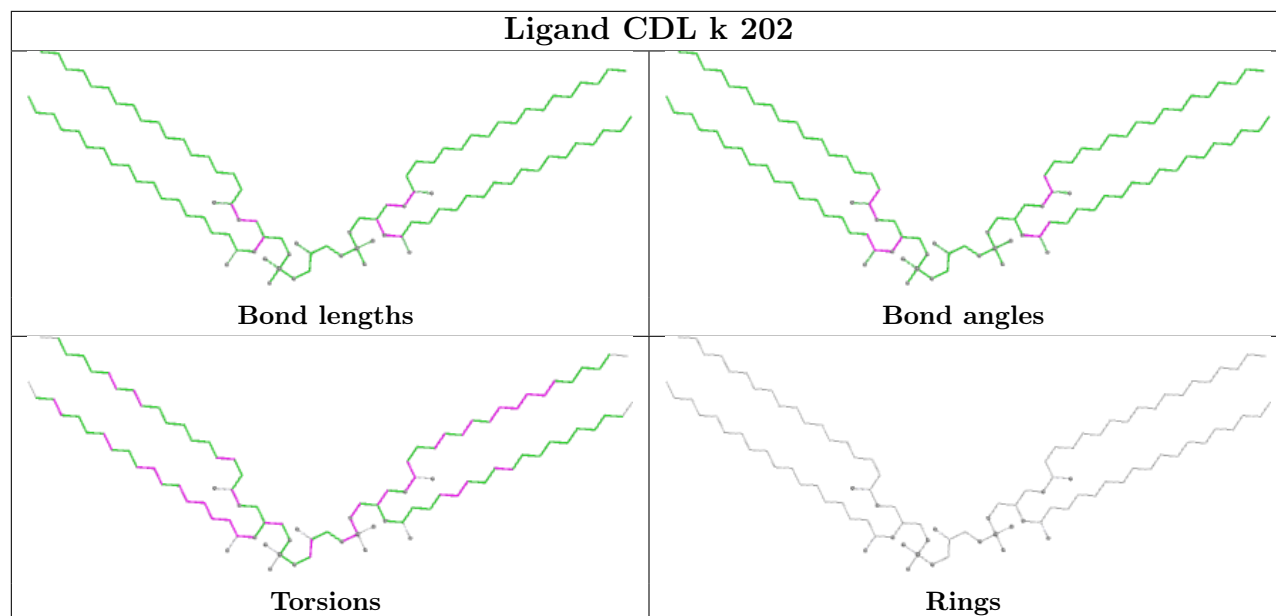


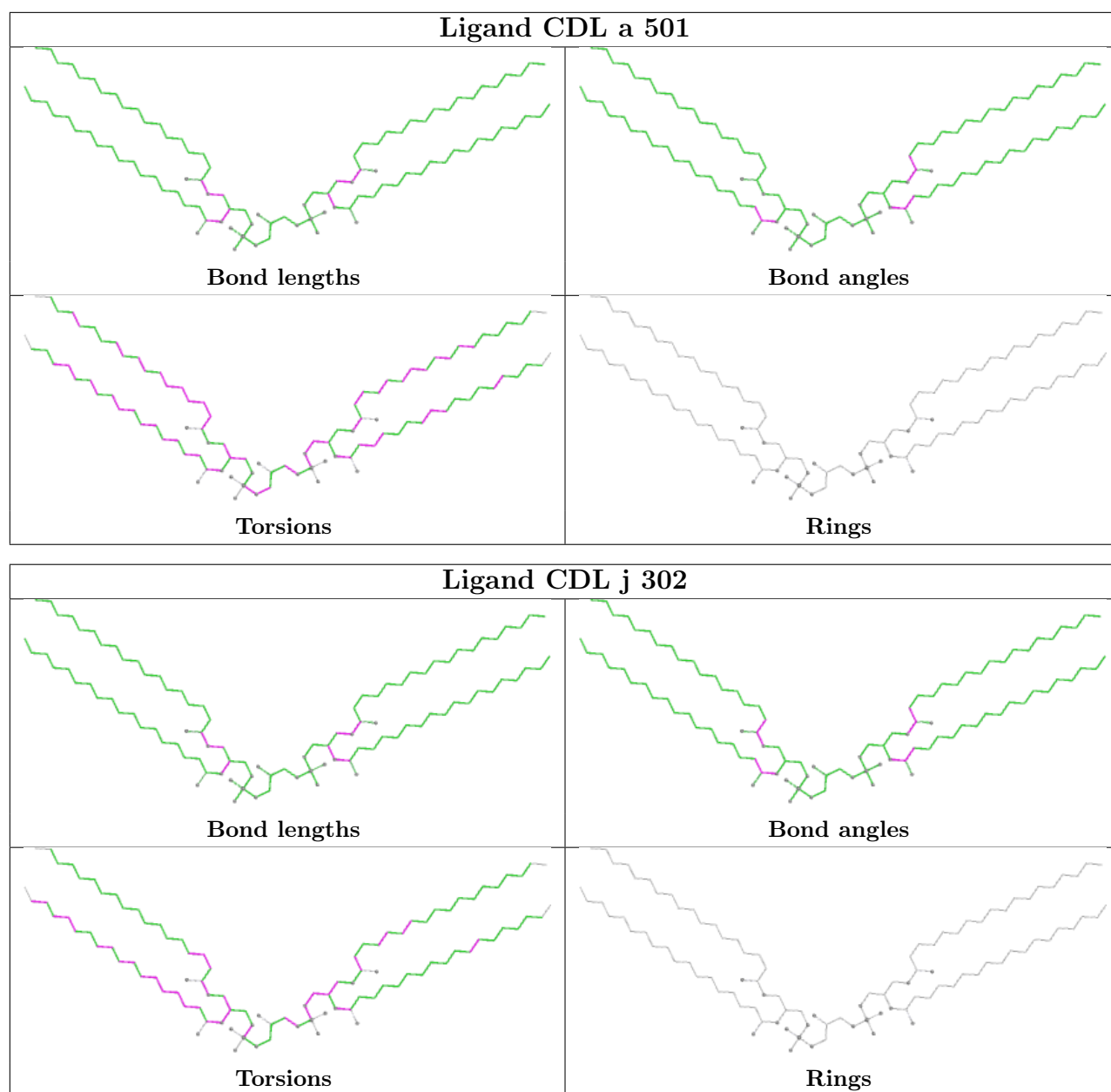












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

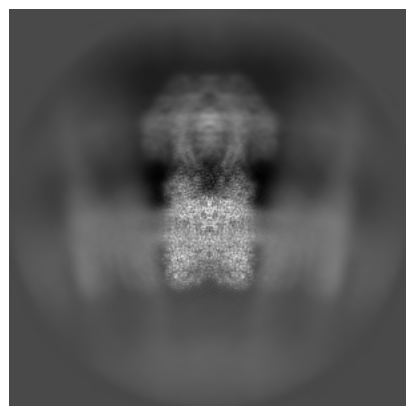
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10859. These allow visual inspection of the internal detail of the map and identification of artifacts.

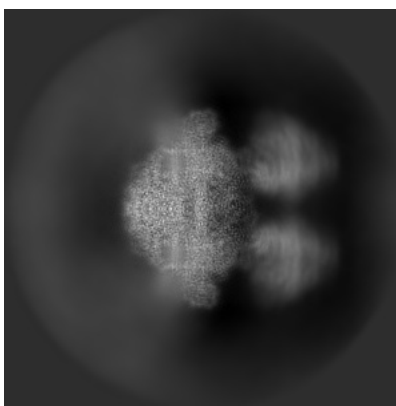
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

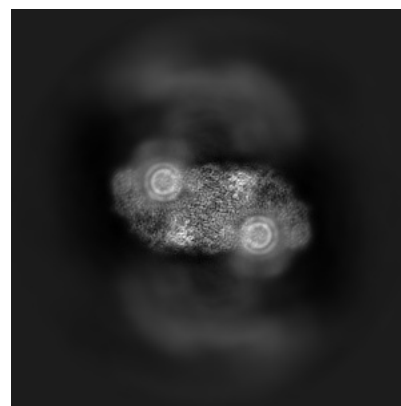
6.1.1 Primary map



X

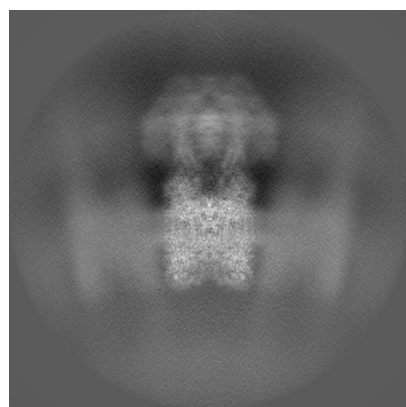


Y

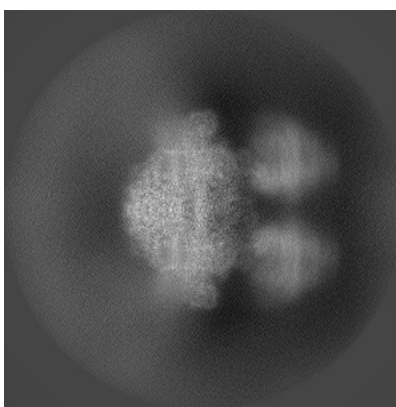


Z

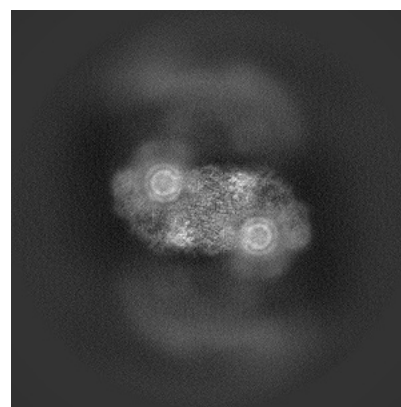
6.1.2 Raw map



X



Y

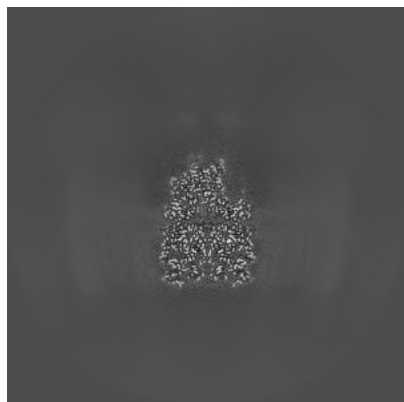


Z

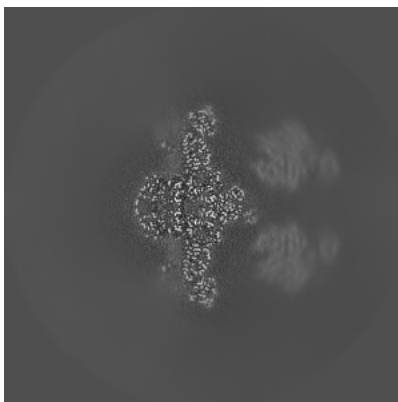
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 300

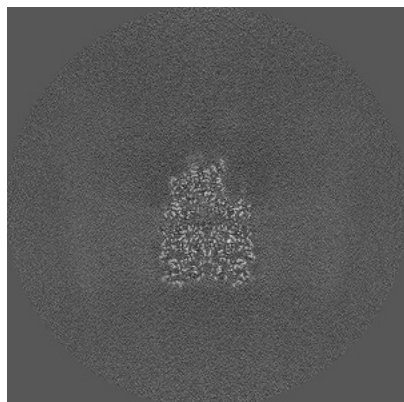


Y Index: 300

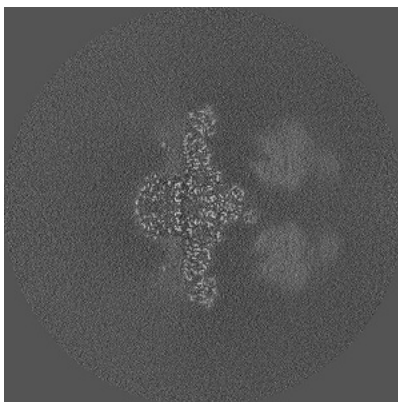


Z Index: 300

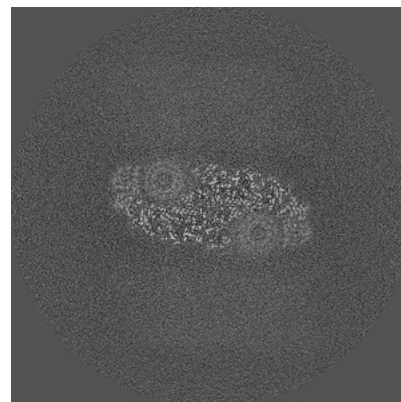
6.2.2 Raw map



X Index: 300



Y Index: 300

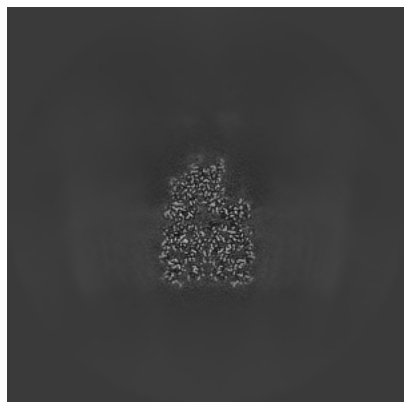


Z Index: 300

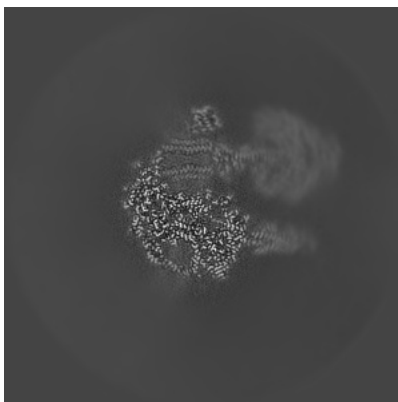
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 299

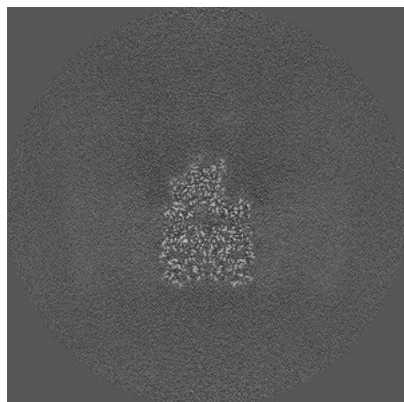


Y Index: 259

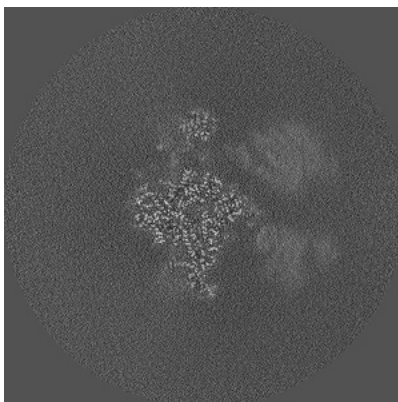


Z Index: 292

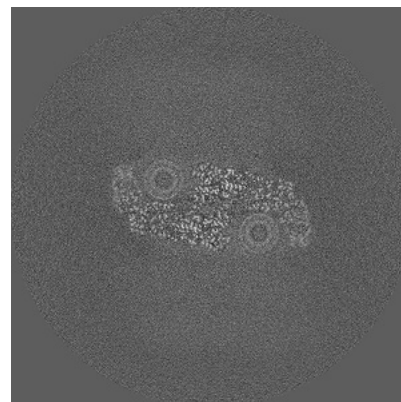
6.3.2 Raw map



X Index: 299



Y Index: 290

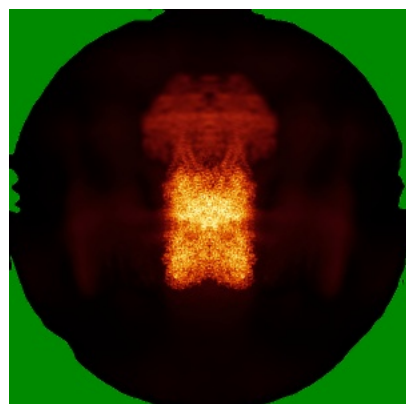


Z Index: 292

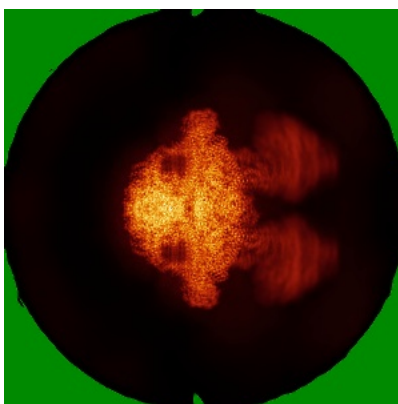
The images above show the largest variance slices of the map in three orthogonal directions.

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

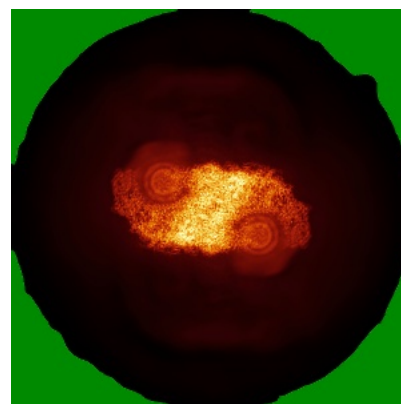
6.4.1 Primary map



X

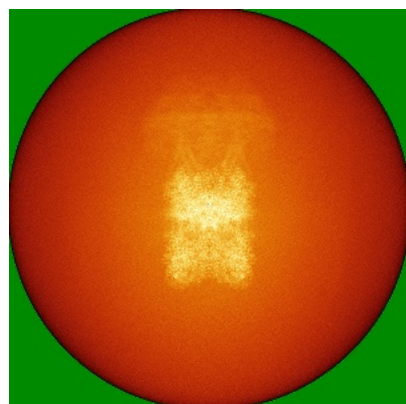


Y

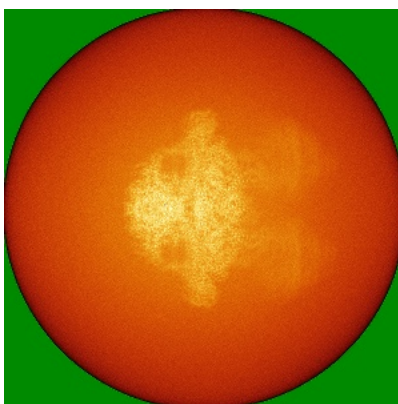


Z

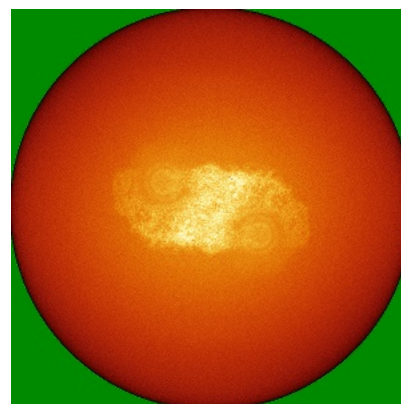
6.4.2 Raw map



X



Y



Z

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

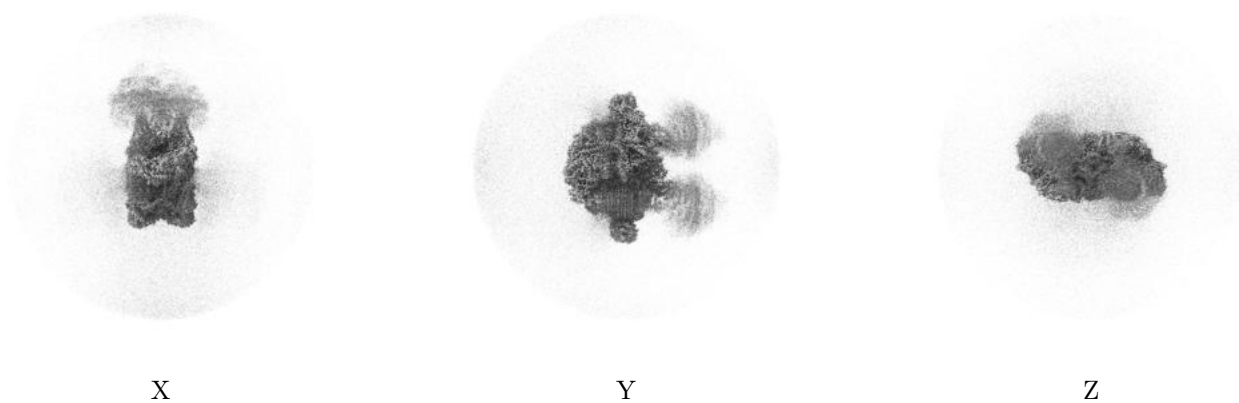
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.018. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

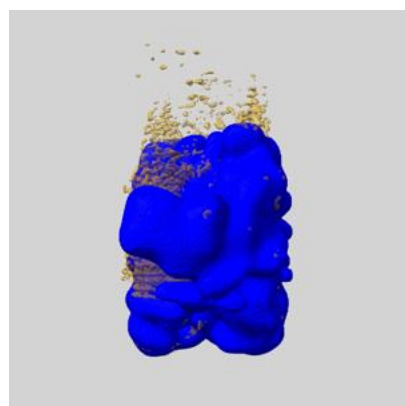
6.6 Mask visualisation [i](#)

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

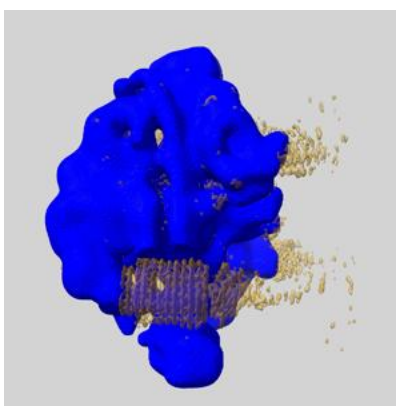
A mask typically either:

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

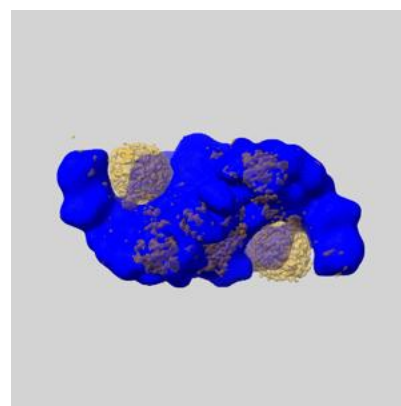
6.6.1 emd_10859_msk_1.map [i](#)



X



Y

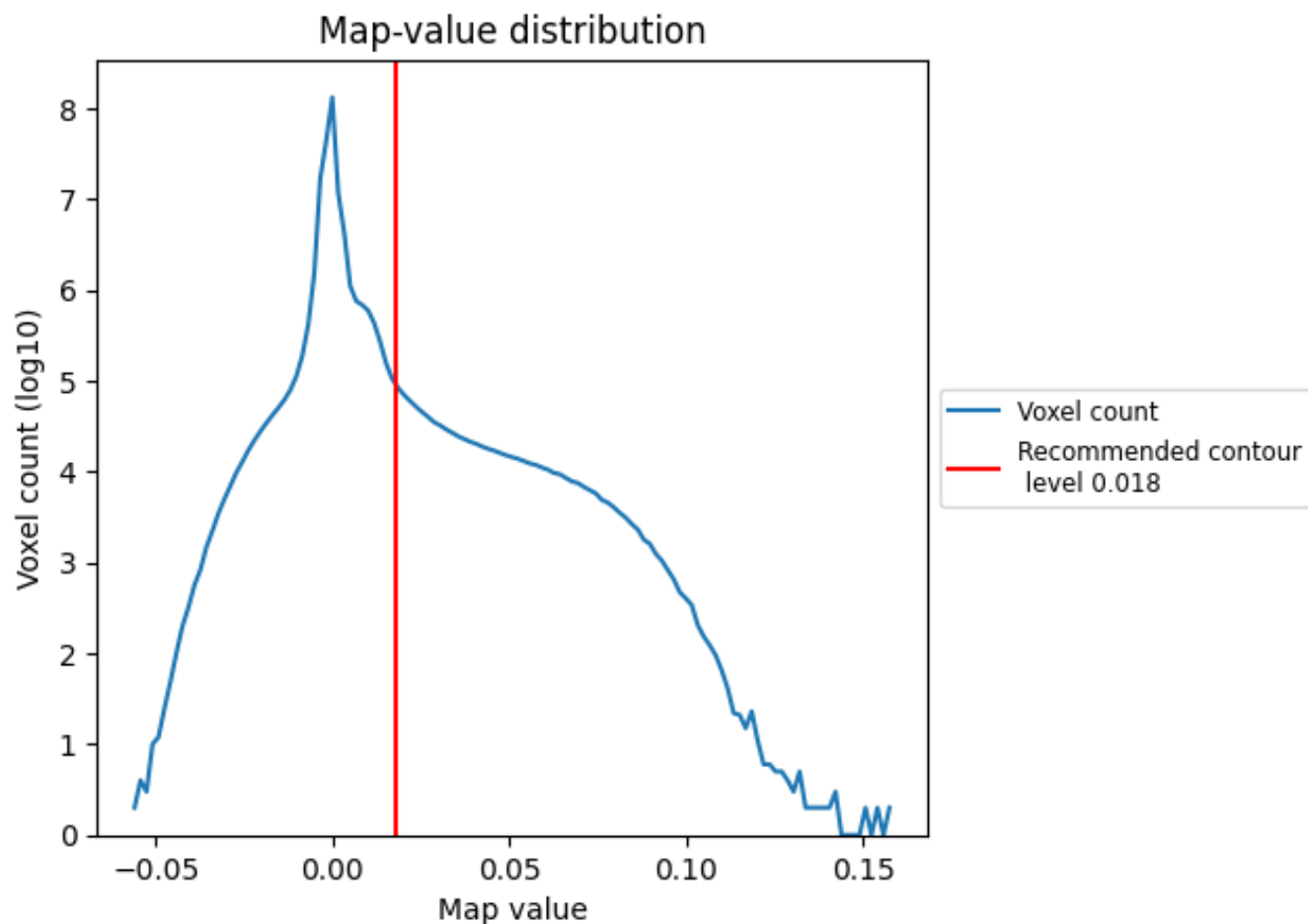


Z

7 Map analysis [i](#)

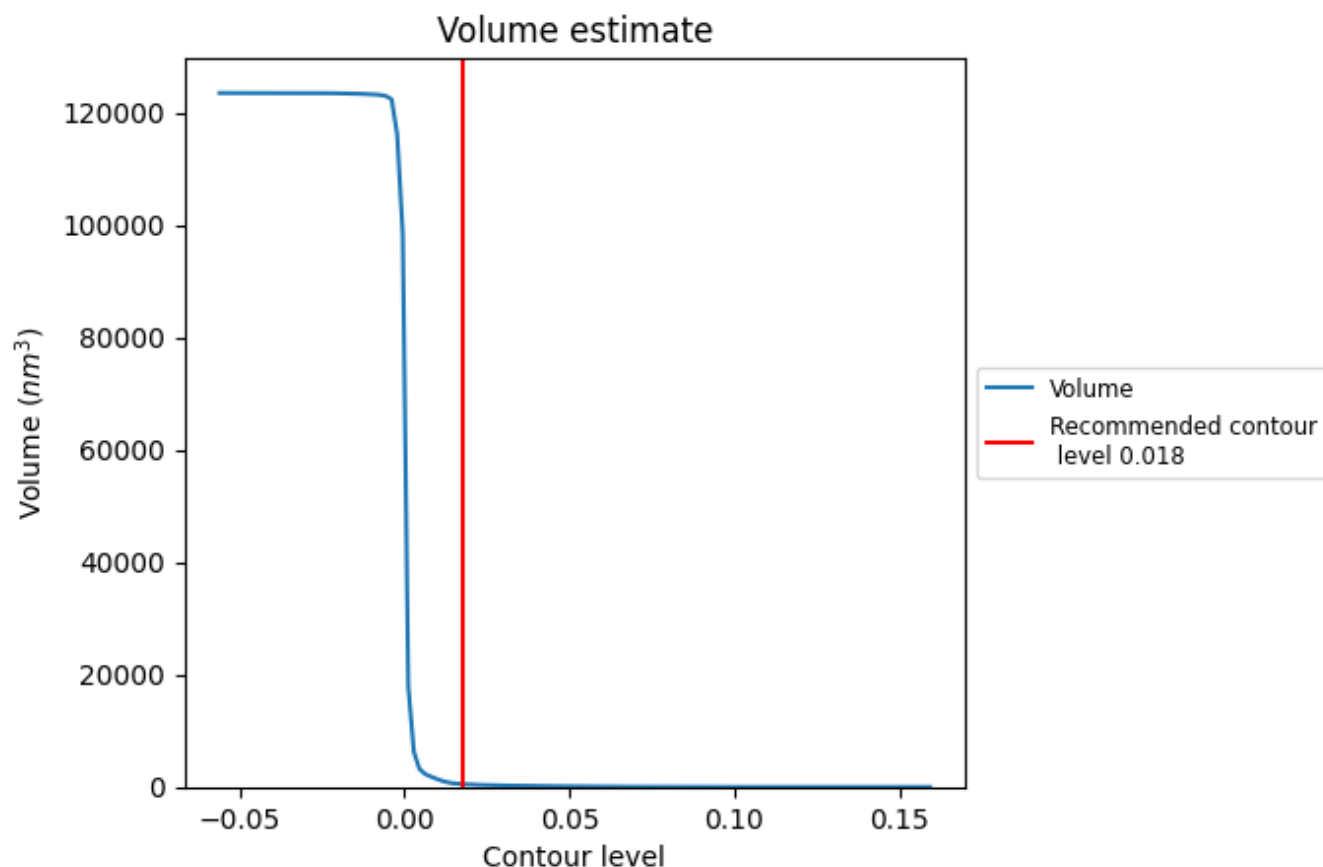
This section contains the results of statistical analysis of the map.

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.

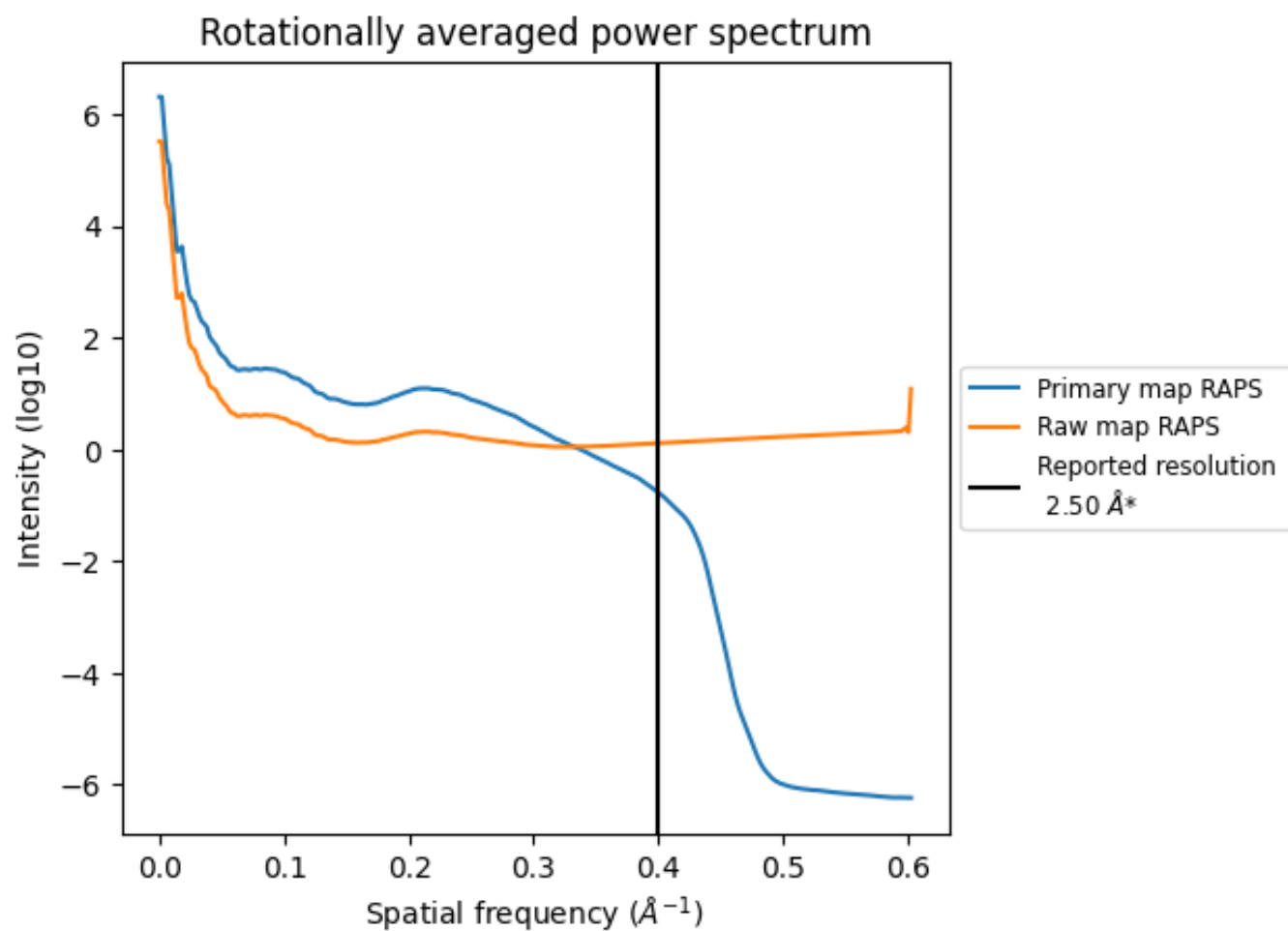
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 494 nm^3 ; this corresponds to an approximate mass of 446 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 ⓘ

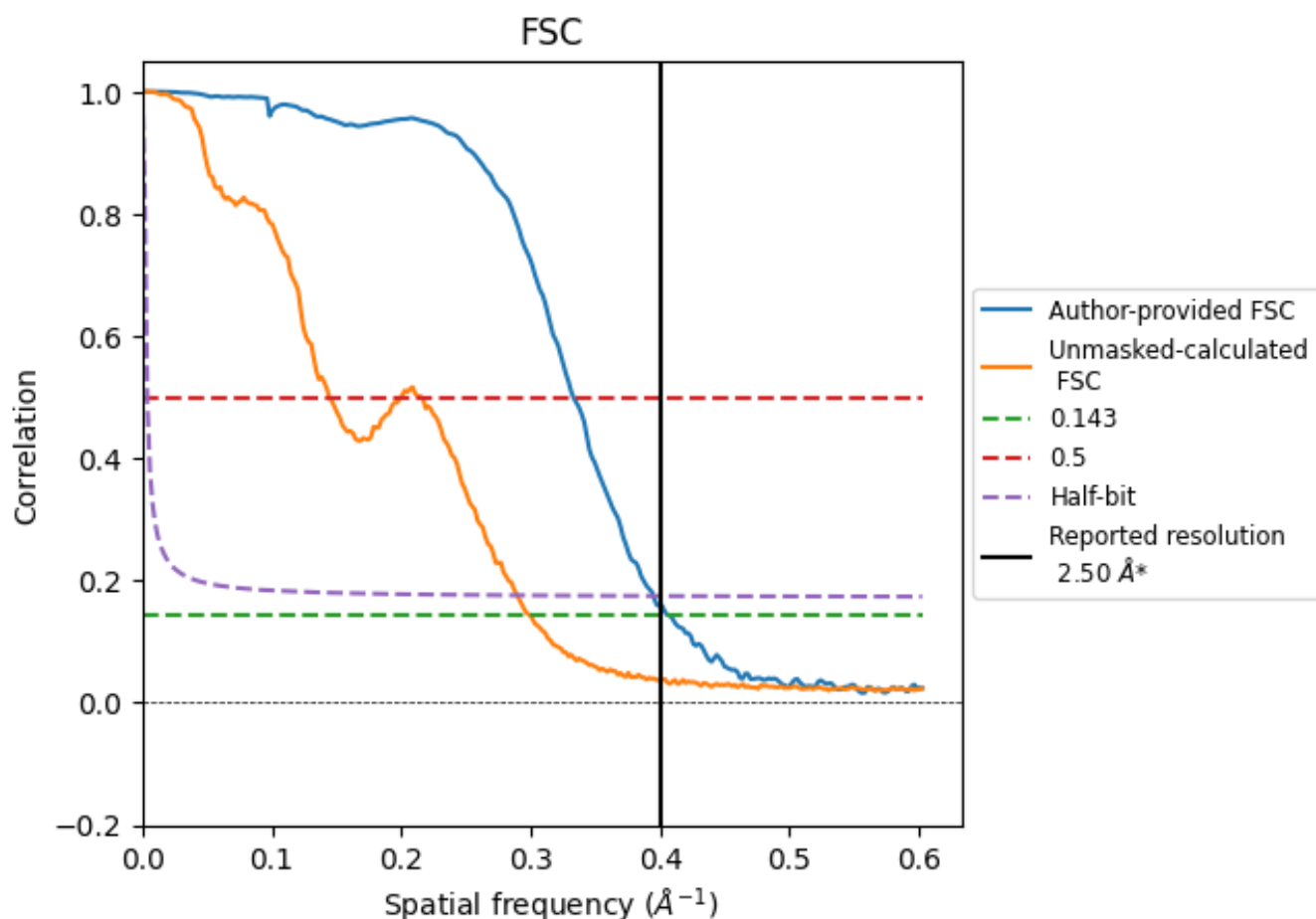


*Reported resolution corresponds to spatial frequency of 0.400 Å⁻¹

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 0.400 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

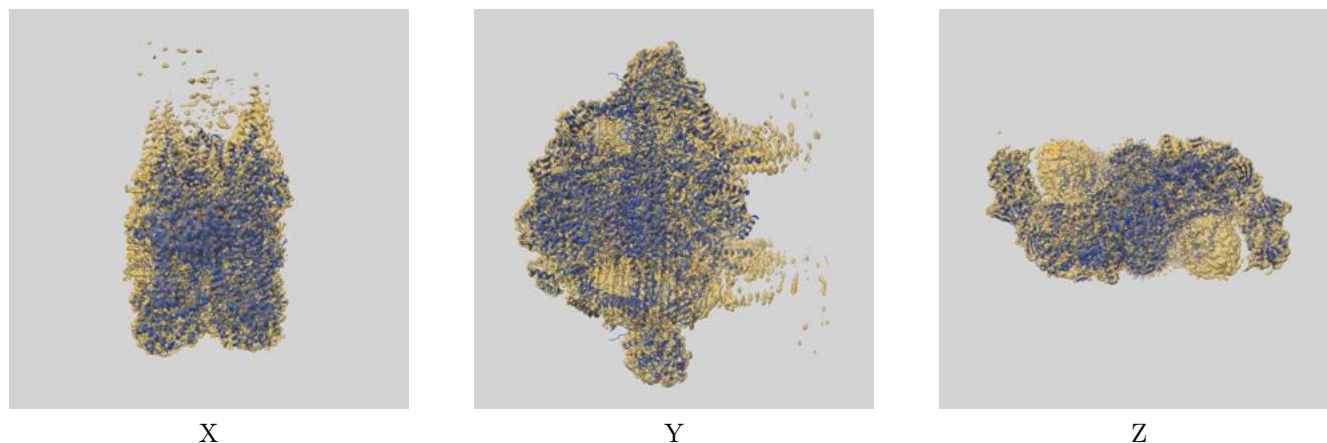
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	2.46	3.00	2.53
Unmasked-calculated*	3.34	6.92	3.45

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.34 differs from the reported value 2.5 by more than 10 %

9 Map-model fit [i](#)

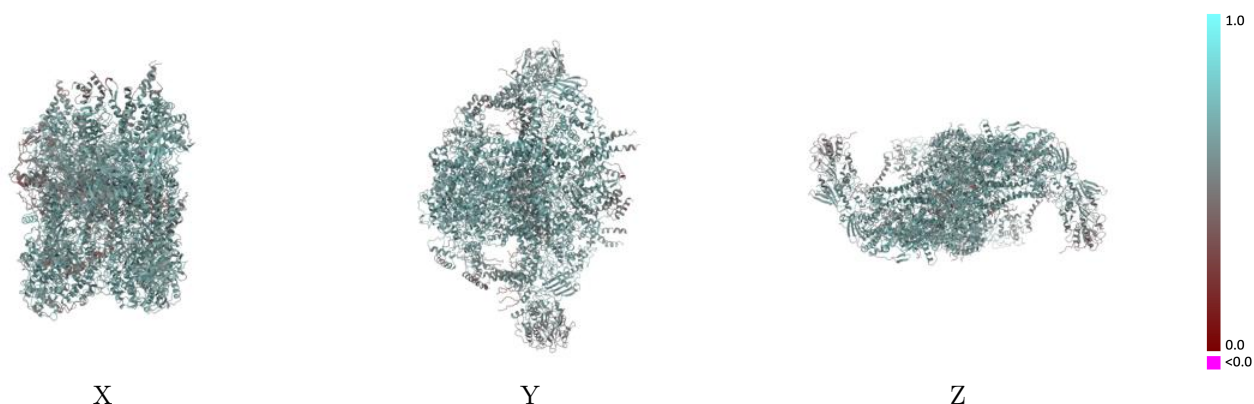
This section contains information regarding the fit between EMDB map EMD-10859 and PDB model 6YNX. Per-residue inclusion information can be found in section [3](#) on page [16](#).

9.1 Map-model overlay [i](#)



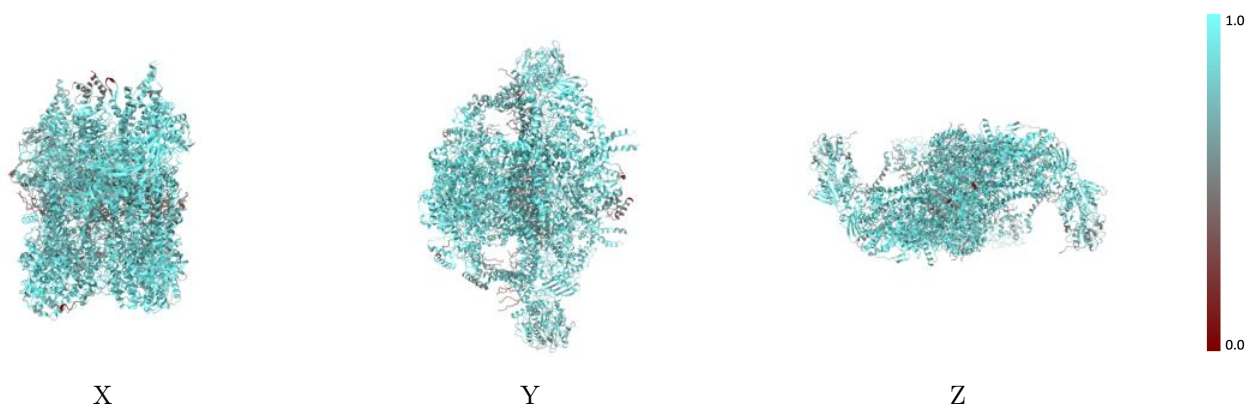
The images above show the 3D surface view of the map at the recommended contour level 0.018 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



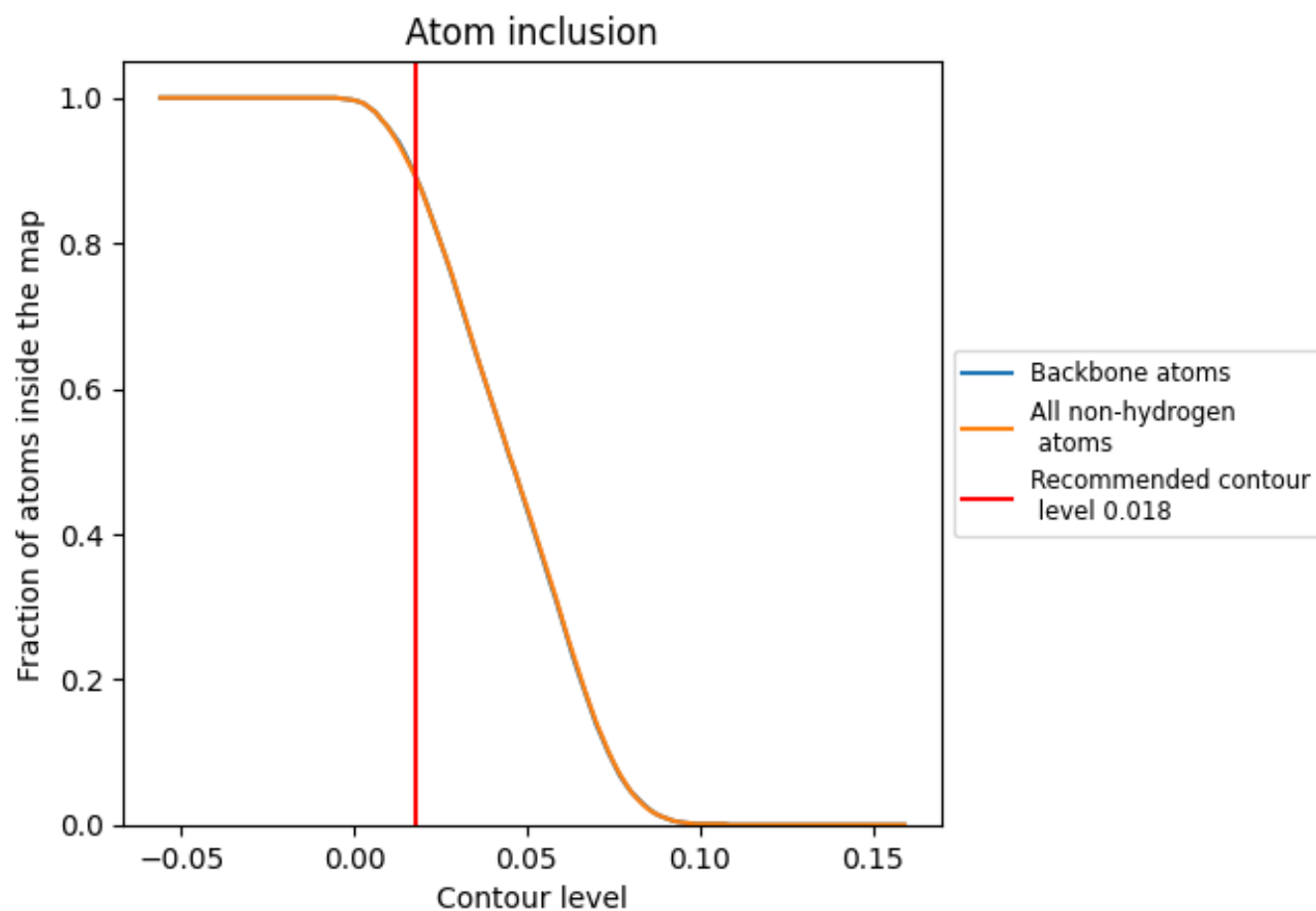
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.018).

9.4 Atom inclusion ⓘ



At the recommended contour level, 89% of all backbone atoms, 89% 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 (0.018) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8900	 0.6170
A	 0.9410	 0.6470
B	 0.8590	 0.6150
C	 0.9720	 0.6630
D	 0.9470	 0.6500
E	 0.7790	 0.5230
F	 0.9700	 0.6710
G	 0.9030	 0.6150
H	 0.9170	 0.6300
I	 0.8920	 0.6220
J	 0.8580	 0.6070
K	 0.8170	 0.5610
L	 0.9280	 0.6450
M	 0.9640	 0.6530
N	 0.9630	 0.6550
O	 0.9300	 0.6230
P	 0.7830	 0.5660
Q	 0.9060	 0.6210
R	 0.9350	 0.6420
S	 0.9270	 0.6240
a	 0.9430	 0.6470
b	 0.8970	 0.6280
c	 0.9710	 0.6650
d	 0.9510	 0.6560
e	 0.7880	 0.5250
f	 0.9220	 0.6510
g	 0.9170	 0.6200
h	 0.9230	 0.6370
i	 0.8890	 0.6240
i1	 0.5450	 0.4790
i2	 0.5300	 0.4990
j	 0.8640	 0.6130
k	 0.7810	 0.5550
l	 0.9020	 0.6320
m	 0.9680	 0.6550



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
n	 0.9550	 0.6560
o	 0.9220	 0.6200
p	 0.7930	 0.5660
q	 0.9180	 0.6240
r	 0.9270	 0.6350
s	 0.9130	 0.6170
t	 0.9230	 0.6310