



Full wwPDB EM Validation Report ⓘ

Aug 6, 2026 – 01:09 AM JST

PDB ID : 6ADQ / pdb_00006adq
EMDB ID : EMD-9610
Title : Respiratory Complex CIII2CIV2SOD2 from Mycobacterium smegmatis
Authors : Gong, H.R.; Xu, A.; Gao, R.G.; Ji, W.X.; Wang, S.H.; Wang, Q.; Li, J.; Rao, Z.H.
Deposited on : 2018-08-01
Resolution : 3.50 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.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

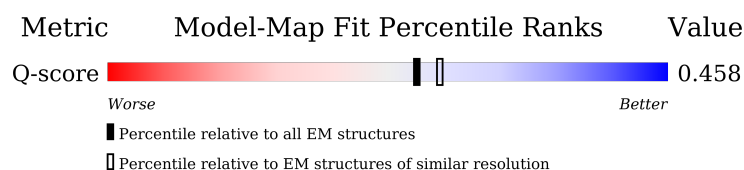
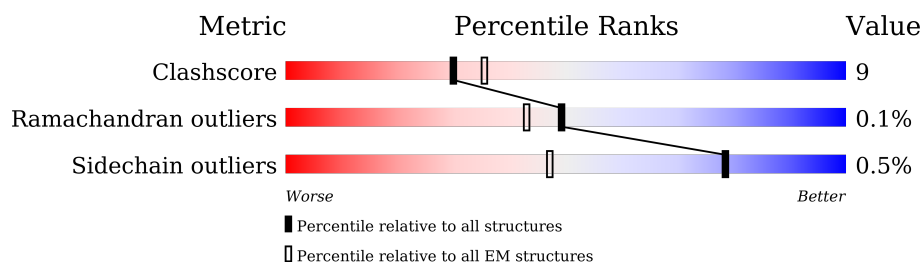
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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	13950 (3.00 - 4.00)

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	E	341	
1	Q	341	
2	F	575	
2	R	575	

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Mol	Chain	Length	Quality of chain
3	G	203	
3	S	203	
4	H	139	
4	T	139	
5	I	79	
5	U	79	
6	J	157	
6	V	157	
7	D	100	
7	P	100	
8	Y	236	
8	Z	236	
9	K	186	
9	W	186	
10	B	546	
10	N	546	
11	C	294	
11	O	294	
12	A	421	
12	M	421	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	HEC	C	302	X	-	-	-
22	HEC	O	302	X	-	-	-
23	FES	M	502	-	-	X	-

2 Entry composition

There are 23 unique types of molecules in this entry. The entry contains 48946 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	E	312	Total	C	N	O	S	0	0
			2465	1592	412	451	10		
1	Q	312	Total	C	N	O	S	0	0
			2465	1592	412	451	10		

- Molecule 2 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	552	Total	C	N	O	S	0	0
			4373	2938	695	714	26		
2	R	552	Total	C	N	O	S	0	0
			4373	2938	695	714	26		

- Molecule 3 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	203	Total	C	N	O	S	0	0
			1560	1039	253	260	8		
3	S	203	Total	C	N	O	S	0	0
			1560	1039	253	260	8		

- Molecule 4 is a protein called Cytochrome c oxidase polypeptide 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	139	Total	C	N	O	S	0	0
			1077	719	167	188	3		
4	T	139	Total	C	N	O	S	0	0
			1077	719	167	188	3		

- Molecule 5 is a protein called Cytochrome c oxidase subunit CtaJ.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	67	Total	C	N	O	S	0	0
			507	334	85	86	2		
5	U	67	Total	C	N	O	S	0	0
			507	334	85	86	2		

- Molecule 6 is a protein called Uncharacterized protein MSMEG_4692/MSMEI_4575.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	145	Total	C	N	O	S	0	0
			1041	658	176	205	2		
6	V	145	Total	C	N	O	S	0	0
			1041	658	176	205	2		

- Molecule 7 is a protein called Prokaryotic respiratory supercomplex associate factor 1 PRSAF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	92	Total	C	N	O	S	0	0
			736	471	136	124	5		
7	P	92	Total	C	N	O	S	0	0
			736	471	136	124	5		

- Molecule 8 is a protein called Superoxide dismutase [Cu-Zn].

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Y	216	Total	C	N	O	S	0	0
			1092	645	217	229	1		
8	Z	216	Total	C	N	O	S	0	0
			1092	645	217	229	1		

- Molecule 9 is a protein called LpqE protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	147	Total	C	N	O	S	0	0
			1072	664	180	227	1		
9	W	147	Total	C	N	O	S	0	0
			1072	664	180	227	1		

- Molecule 10 is a protein called Ubiquinol-cytochrome c reductase cytochrome b subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	B	535	Total	C	N	O	S	0	0
			4181	2751	711	701	18		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	N	535	Total	C	N	O	S	0	0
			4181	2751	711	701	18		

- Molecule 11 is a protein called Cytochrome bc1 complex cytochrome c subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	C	223	Total	C	N	O	S	0	0
			1623	1008	289	314	12		
11	O	223	Total	C	N	O	S	0	0
			1623	1008	289	314	12		

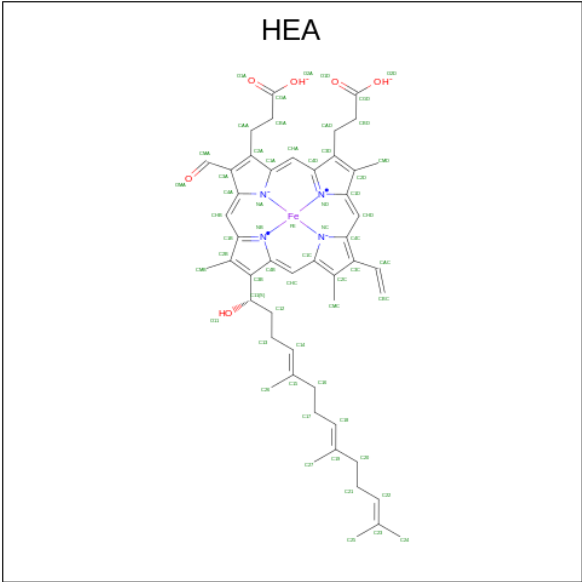
- Molecule 12 is a protein called Rieske iron-sulfur protein QcrA.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	A	382	Total	C	N	O	S	0	0
			2977	1924	504	538	11		
12	M	382	Total	C	N	O	S	0	0
			2977	1924	504	538	11		

- Molecule 13 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

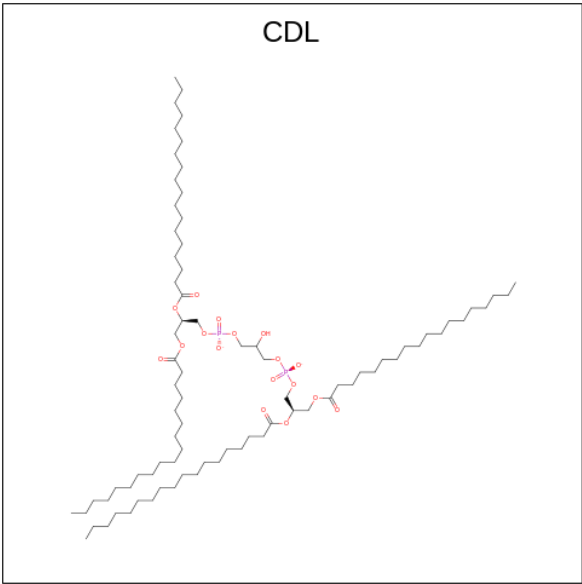
Mol	Chain	Residues	Atoms		AltConf
13	E	2	Total	Cu	0
			2	2	
13	F	2	Total	Cu	0
			2	2	
13	Q	2	Total	Cu	0
			2	2	
13	R	2	Total	Cu	0
			2	2	

- Molecule 14 is HEME-A (CCD ID: HEA) (formula: C₄₉H₅₆FeN₄O₆).



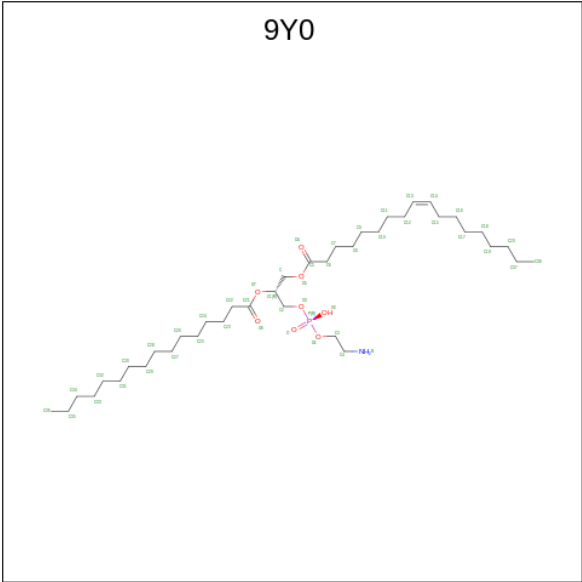
Mol	Chain	Residues	Atoms					AltConf
14	F	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
14	F	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
14	R	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
14	R	1	Total	C	Fe	N	O	0
			60	49	1	4	6	

- Molecule 15 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



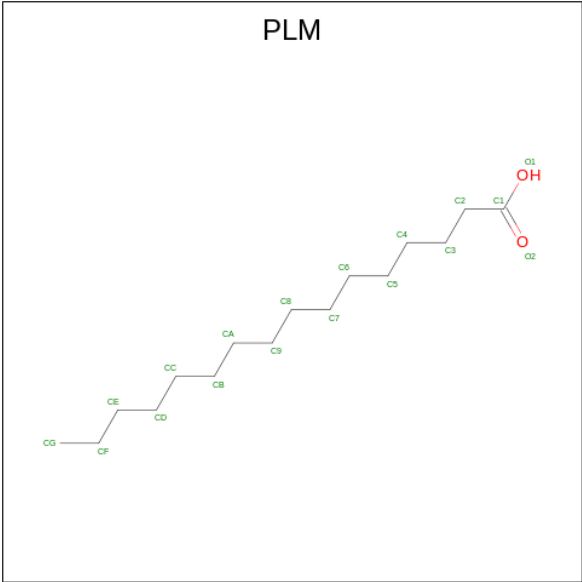
Mol	Chain	Residues	Atoms				AltConf
15	F	1	Total	C	O	P	0
			76	57	17	2	
15	F	1	Total	C	O	P	0
			81	62	17	2	
15	H	1	Total	C	O	P	0
			79	60	17	2	
15	D	1	Total	C	O	P	0
			88	69	17	2	
15	B	1	Total	C	O	P	0
			74	55	17	2	
15	B	1	Total	C	O	P	0
			77	58	17	2	
15	B	1	Total	C	O	P	0
			79	60	17	2	
15	B	1	Total	C	O	P	0
			66	47	17	2	
15	A	1	Total	C	O	P	0
			95	76	17	2	
15	R	1	Total	C	O	P	0
			76	57	17	2	
15	R	1	Total	C	O	P	0
			81	62	17	2	
15	T	1	Total	C	O	P	0
			79	60	17	2	
15	P	1	Total	C	O	P	0
			88	69	17	2	
15	N	1	Total	C	O	P	0
			66	47	17	2	
15	N	1	Total	C	O	P	0
			74	55	17	2	
15	N	1	Total	C	O	P	0
			77	58	17	2	
15	N	1	Total	C	O	P	0
			79	60	17	2	
15	M	1	Total	C	O	P	0
			95	76	17	2	

- Molecule 16 is (2R)-3-(((2-aminoethoxy)(hydroxy)phosphoryl)oxy)-2-(palmitoyloxy)propyl (E)-octadec-9-enoate (CCD ID: 9Y0) (formula: C₃₉H₇₆NO₈P).



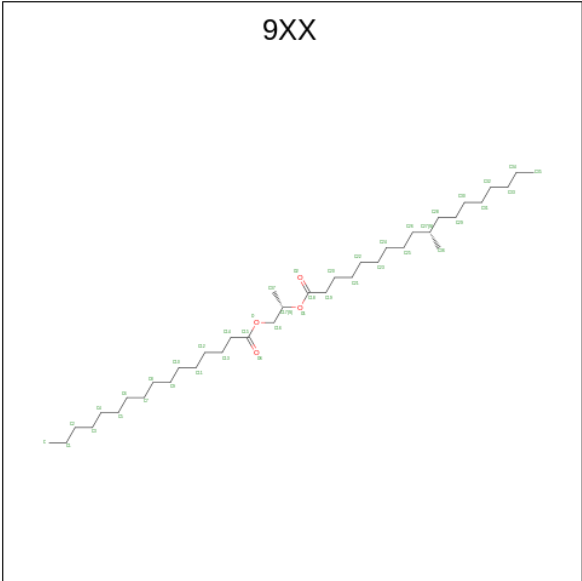
Mol	Chain	Residues	Atoms					AltConf
16	G	1	Total	C	N	O	P	0
			43	33	1	8	1	
16	D	1	Total	C	N	O	P	0
			41	31	1	8	1	
16	K	1	Total	C	N	O	P	0
			38	28	1	8	1	
16	B	1	Total	C	N	O	P	0
			49	39	1	8	1	
16	B	1	Total	C	N	O	P	0
			49	39	1	8	1	
16	S	1	Total	C	N	O	P	0
			43	33	1	8	1	
16	P	1	Total	C	N	O	P	0
			41	31	1	8	1	
16	W	1	Total	C	N	O	P	0
			38	28	1	8	1	

- Molecule 17 is PALMITIC ACID (CCD ID: PLM) (formula: C₁₆H₃₂O₂).



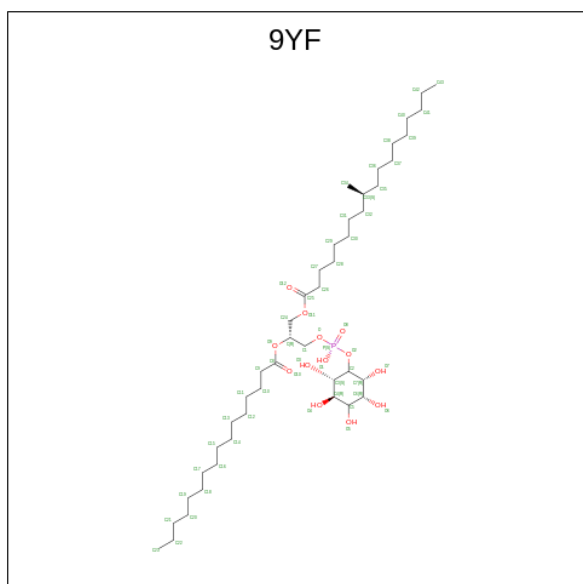
Mol	Chain	Residues	Atoms			AltConf
17	Y	1	Total	C	O	0
			11	10	1	
17	K	1	Total	C	O	0
			17	16	1	
17	Z	1	Total	C	O	0
			11	10	1	
17	W	1	Total	C	O	0
			17	16	1	

- Molecule 18 is (2S)-1-(hexadecanoyloxy)propan-2-yl (10S)-10-methyloctadecanoate (CCD ID: 9XX) (formula: C₃₈H₇₄O₄).



Mol	Chain	Residues	Atoms			AltConf
18	Y	1	Total	C	O	0
			32	28	4	
18	K	1	Total	C	O	0
			42	38	4	
18	Z	1	Total	C	O	0
			32	28	4	
18	W	1	Total	C	O	0
			42	38	4	

- Molecule 19 is (2R)-2-(hexadecanoyloxy)-3-{[(S)-hydroxy{[(1R,2R,3R,4R,5R,6S)-2,3,4,5,6-pentahydroxycyclohexyl]oxy}phosphoryl]oxy}propyl (9S)-9-methyloctadecanoate (CCD ID: 9YF) (formula: C₄₄H₈₅O₁₃P).



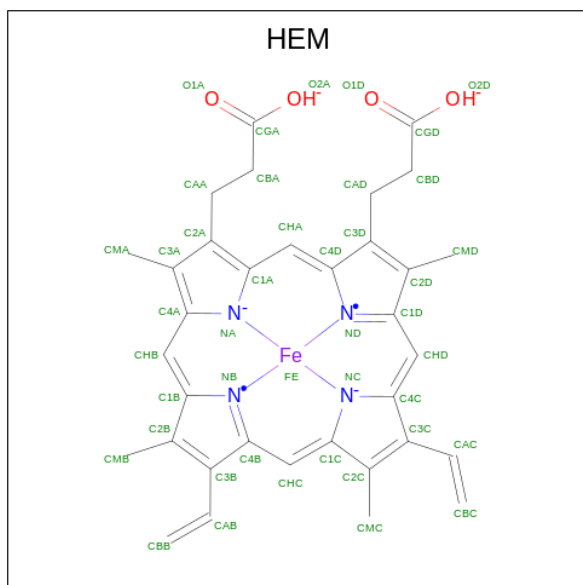
Mol	Chain	Residues	Atoms				AltConf
19	K	1	Total	C	O	P	0
			58	44	13	1	
19	C	1	Total	C	O	P	0
			58	44	13	1	
19	A	1	Total	C	O	P	0
			58	44	13	1	
19	A	1	Total	C	O	P	0
			58	44	13	1	
19	W	1	Total	C	O	P	0
			58	44	13	1	
19	O	1	Total	C	O	P	0
			58	44	13	1	
19	M	1	Total	C	O	P	0
			58	44	13	1	

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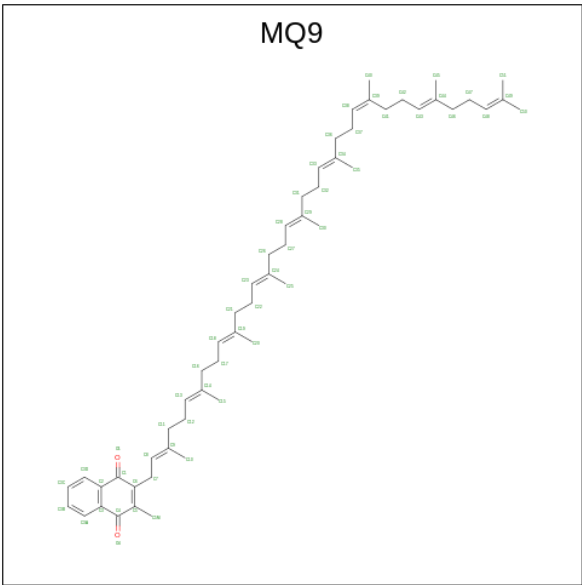
Mol	Chain	Residues	Atoms				AltConf
19	M	1	Total	C	O	P	0
			58	44	13	1	

- Molecule 20 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



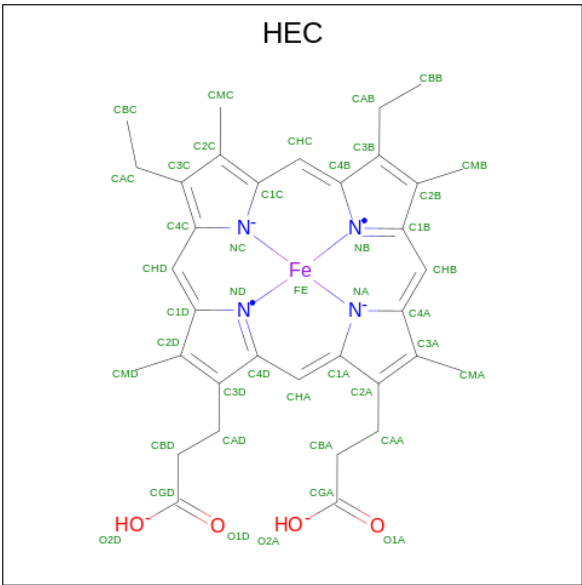
Mol	Chain	Residues	Atoms					AltConf
20	B	1	Total	C	Fe	N	O	0
			42	33	1	4	4	
20	B	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
20	N	1	Total	C	Fe	N	O	0
			42	33	1	4	4	
20	N	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 21 is MENAQUINONE-9 (CCD ID: MQ9) (formula: $C_{56}H_{80}O_2$).



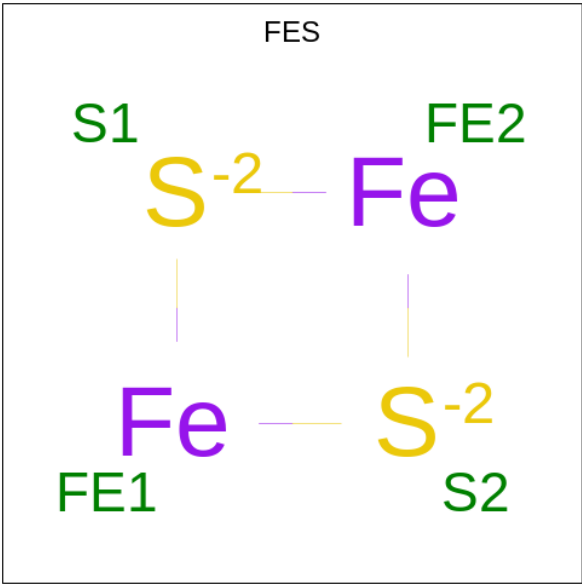
Mol	Chain	Residues	Atoms			AltConf
21	B	1	Total	C	O	0
			43	41	2	
21	B	1	Total	C	O	0
			48	46	2	
21	B	1	Total	C	O	0
			58	56	2	
21	B	1	Total	C	O	0
			43	41	2	
21	C	1	Total	C	O	0
			58	56	2	
21	N	1	Total	C	O	0
			43	41	2	
21	N	1	Total	C	O	0
			48	46	2	
21	N	1	Total	C	O	0
			58	56	2	
21	N	1	Total	C	O	0
			43	41	2	
21	O	1	Total	C	O	0
			58	56	2	

- Molecule 22 is HEME C (CCD ID: HEC) (formula: C₃₄H₃₆FeN₄O₄).



Mol	Chain	Residues	Atoms					AltConf
22	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
22	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
22	O	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
22	O	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 23 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).

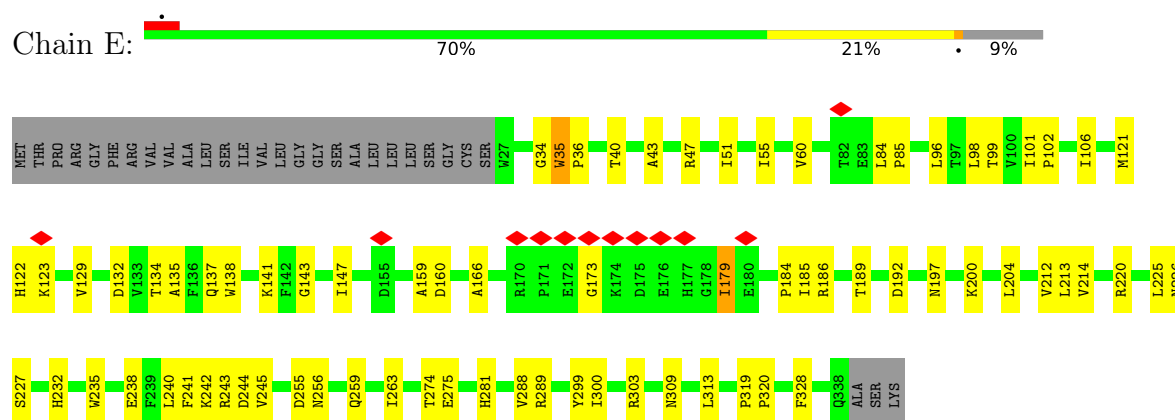


Mol	Chain	Residues	Atoms			AltConf
23	A	1	Total 4	Fe 2	S 2	0
23	M	1	Total 4	Fe 2	S 2	0

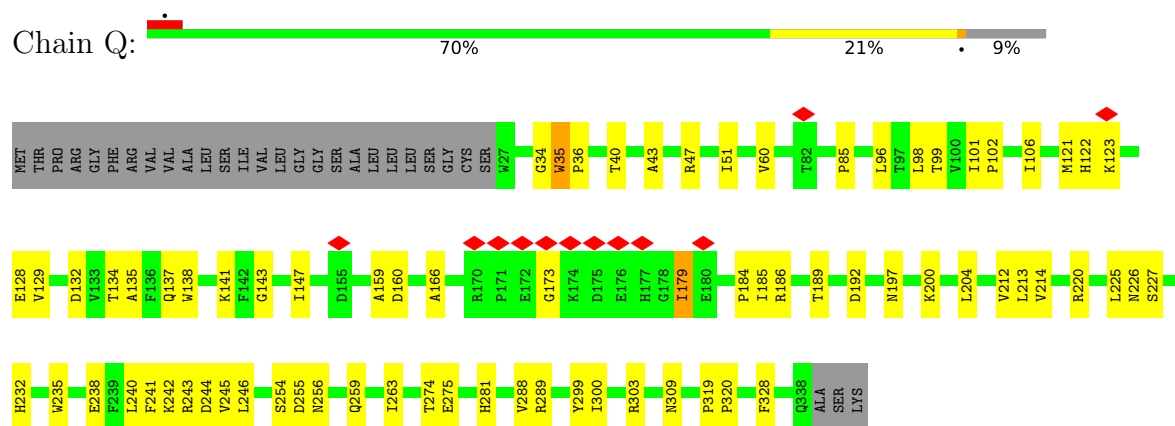
3 Residue-property plots

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

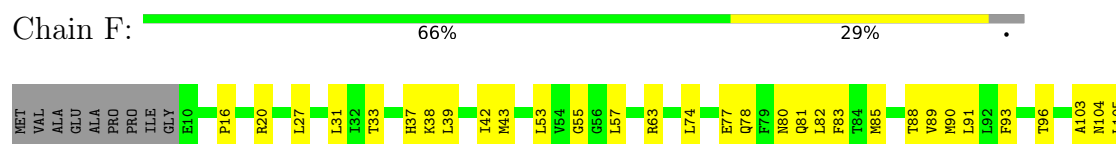
• Molecule 1: Cytochrome c oxidase subunit 2

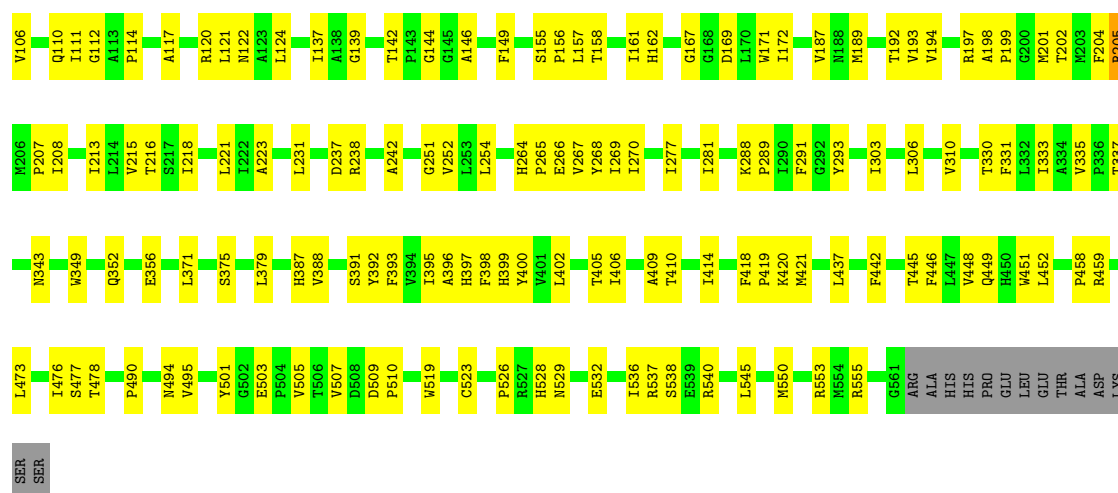


• Molecule 1: Cytochrome c oxidase subunit 2



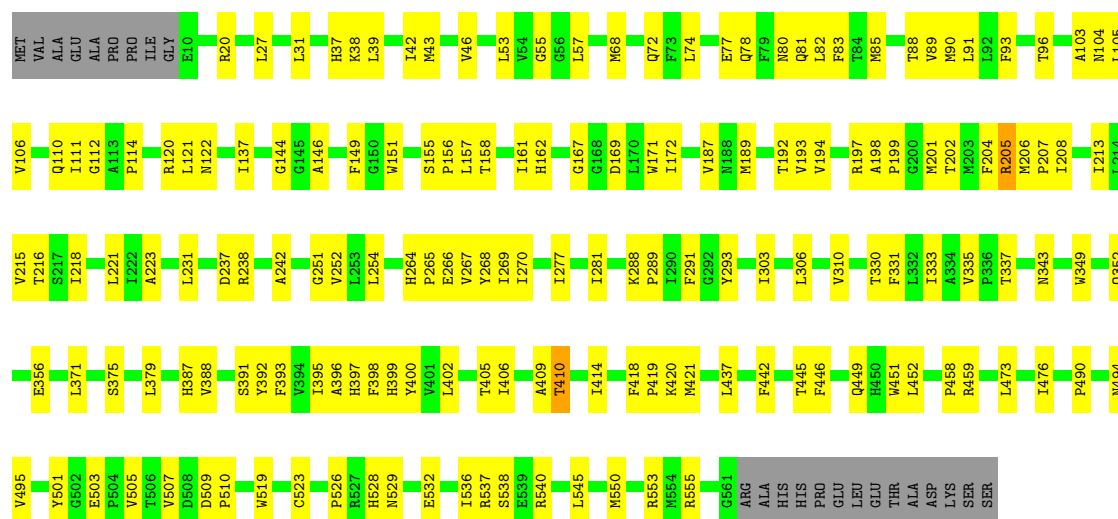
• Molecule 2: Cytochrome c oxidase subunit 1





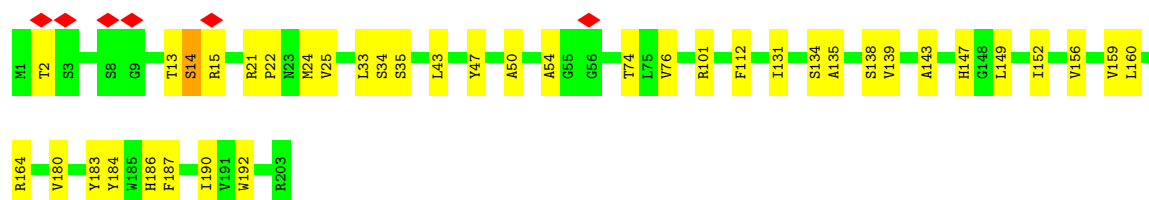
• Molecule 2: Cytochrome c oxidase subunit 1

Chain R: 67% 28%



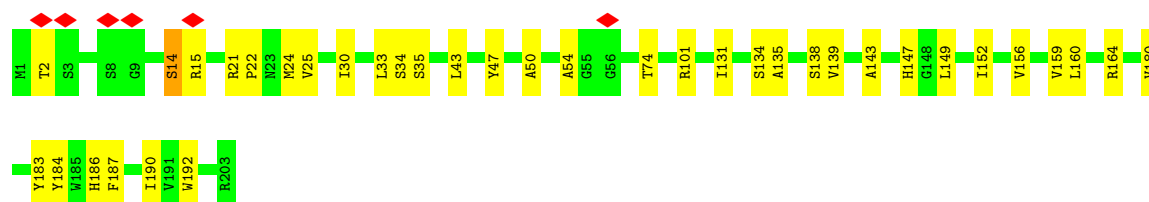
• Molecule 3: Cytochrome c oxidase subunit 3

Chain G: 81% 19%



• Molecule 3: Cytochrome c oxidase subunit 3

Chain S: 82% 18%



- Molecule 4: Cytochrome c oxidase polypeptide 4

Chain H: 87% 13%



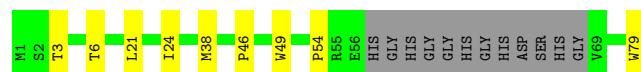
- Molecule 4: Cytochrome c oxidase polypeptide 4

Chain T: 88% 12%



- Molecule 5: Cytochrome c oxidase subunit CtaJ

Chain I: 73% 11% 15%



- Molecule 5: Cytochrome c oxidase subunit CtaJ

Chain U: 73% 11% 15%



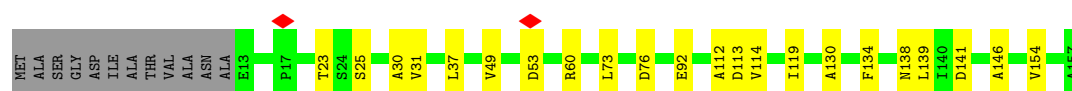
- Molecule 6: Uncharacterized protein MSMEG_4692/MSMEI_4575

Chain J: 77% 15% 8%

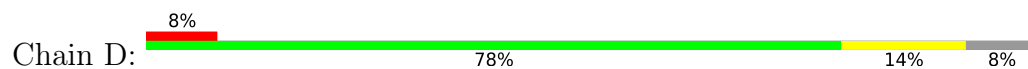


- Molecule 6: Uncharacterized protein MSMEG_4692/MSMEI_4575

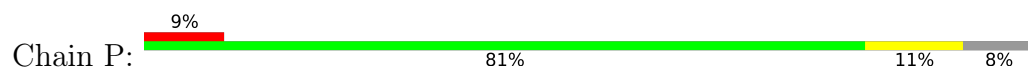
Chain V: 78% 14% 8%



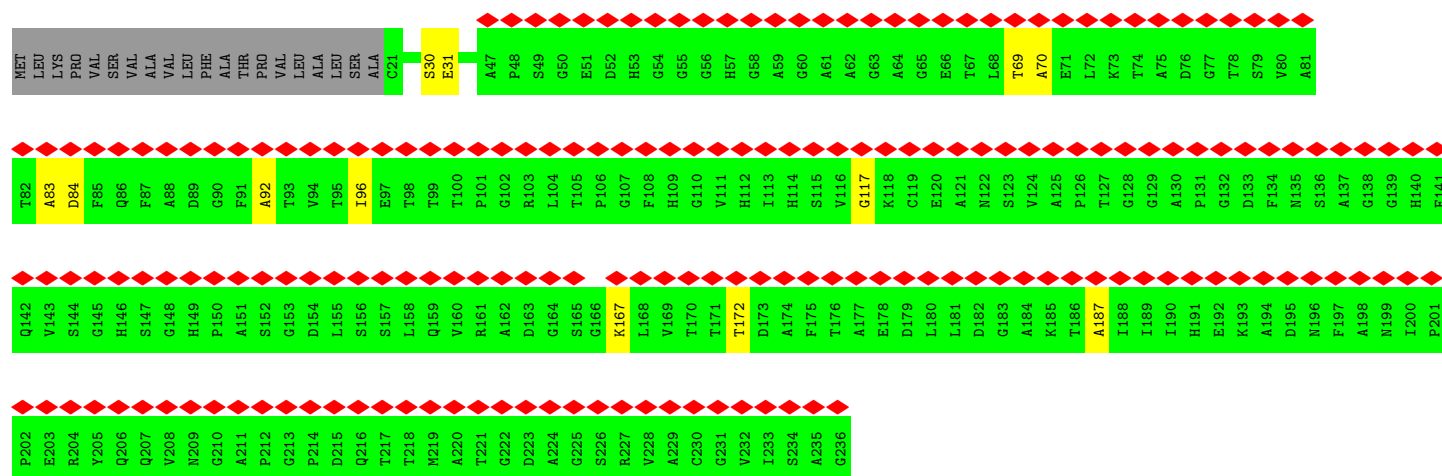
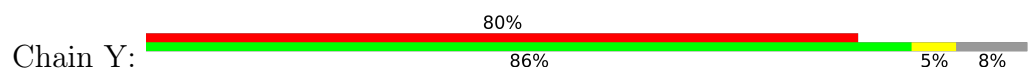
- Molecule 7: Prokaryotic respiratory supercomplex associate factor 1 PRSAF1



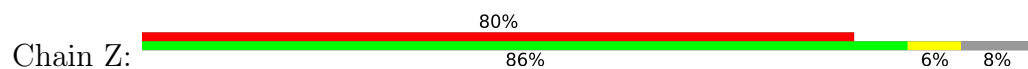
- Molecule 7: Prokaryotic respiratory supercomplex associate factor 1 PRSAF1

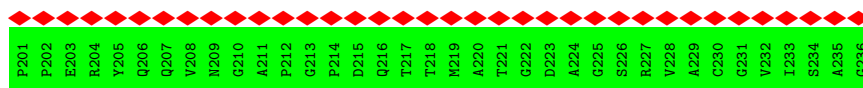


- Molecule 8: Superoxide dismutase [Cu-Zn]

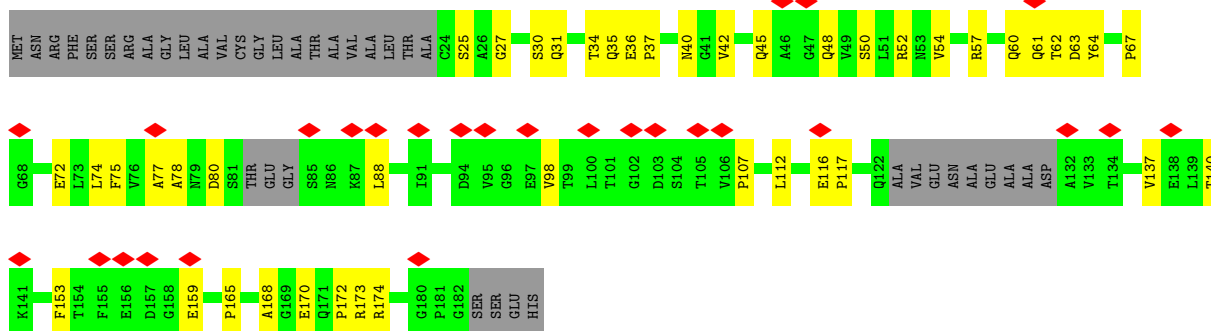


- Molecule 8: Superoxide dismutase [Cu-Zn]

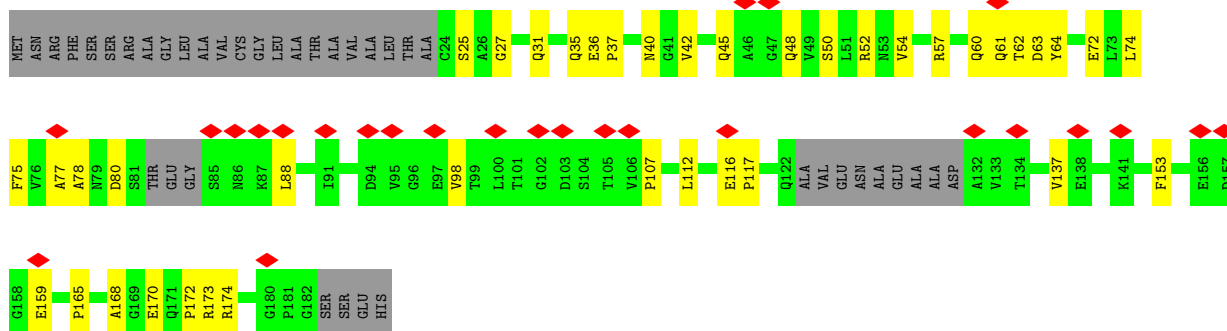




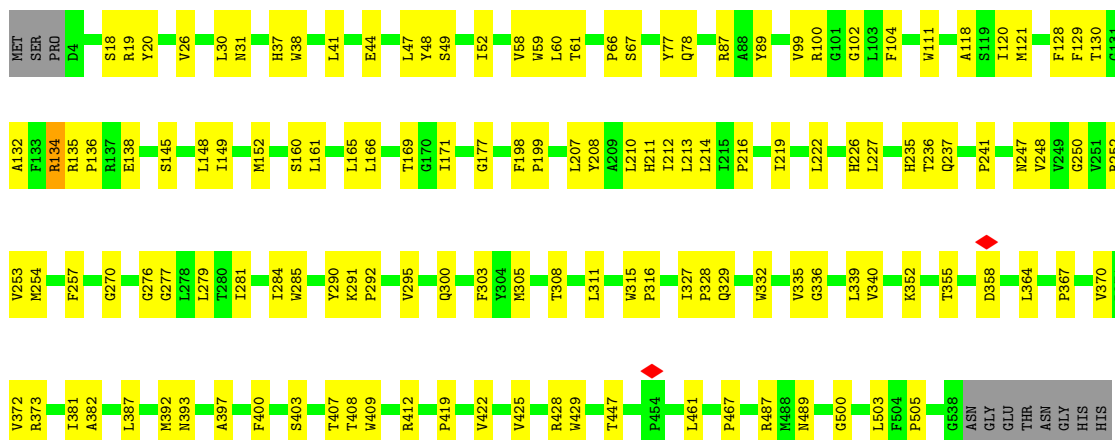
• Molecule 9: LpqE protein



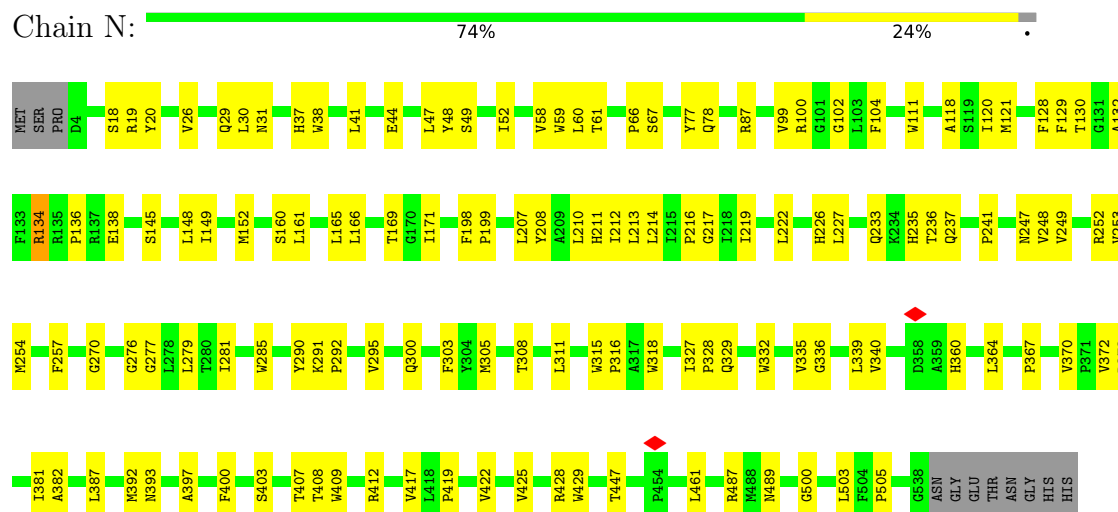
• Molecule 9: LpqE protein

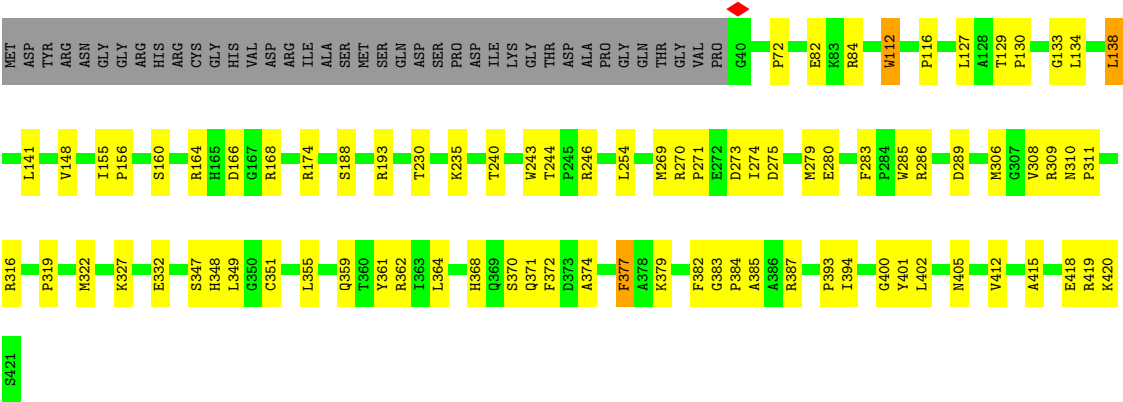


• Molecule 10: Ubiquinol-cytochrome c reductase cytochrome b subunit

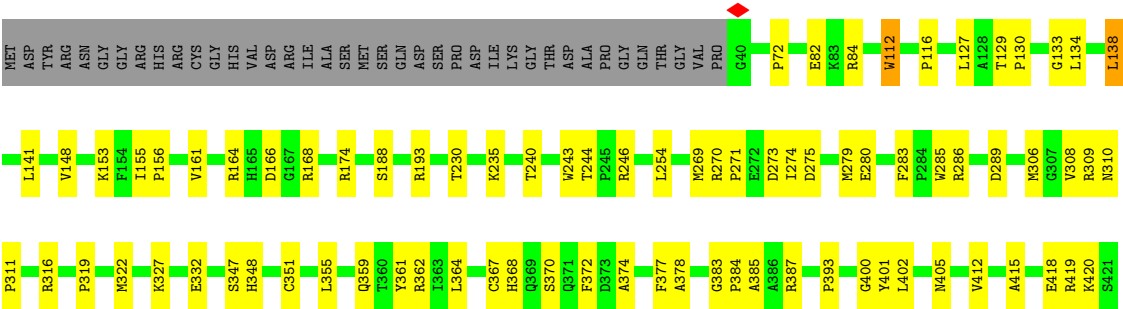


- Molecule 10: Ubiquinol-cytochrome c reductase cytochrome b subunit





• Molecule 12: Rieske iron-sulfur protein QcrA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	202215	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.563	Depositor
Minimum map value	-0.271	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.0452	Depositor
Map size ($\text{\AA}$)	379.59998, 379.59998, 379.59998	wwPDB
Map dimensions	292, 292, 292	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.3, 1.3, 1.3	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CU, HEC, HEM, CDL, HEA, FES, MQ9, 9XX, PLM, 9Y0, 9YF

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	E	0.36	0/2534	0.67	0/3451
1	Q	0.36	0/2534	0.67	0/3451
2	F	0.48	0/4533	0.78	1/6192 (0.0%)
2	R	0.48	0/4533	0.78	1/6192 (0.0%)
3	G	0.37	0/1608	0.73	0/2195
3	S	0.37	0/1608	0.72	0/2195
4	H	0.34	0/1112	0.62	0/1524
4	T	0.35	0/1112	0.62	0/1524
5	I	0.30	0/523	0.60	0/714
5	U	0.30	0/523	0.60	0/714
6	J	0.28	0/1059	0.58	0/1446
6	V	0.28	0/1059	0.58	0/1446
7	D	0.30	0/757	0.56	0/1027
7	P	0.30	0/757	0.56	0/1027
8	Y	0.18	0/1099	0.44	0/1519
8	Z	0.18	0/1099	0.45	0/1519
9	K	0.30	0/1088	0.65	0/1490
9	W	0.28	0/1088	0.66	0/1490
10	B	0.40	0/4314	0.64	2/5882 (0.0%)
10	N	0.40	0/4314	0.65	2/5882 (0.0%)
11	C	0.39	0/1660	0.67	0/2250
11	O	0.39	0/1660	0.67	0/2250
12	A	0.36	0/3056	0.69	3/4142 (0.1%)
12	M	0.36	0/3056	0.71	5/4142 (0.1%)
All	All	0.38	0/46686	0.68	14/63664 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	3
1	Q	0	3
2	F	0	4
2	R	0	4
3	G	0	3
3	S	0	3
9	K	0	1
9	W	0	1
10	B	0	1
10	N	0	1
All	All	0	24

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	M	378	ALA	CA-C-N	7.35	130.93	120.49
12	M	378	ALA	C-N-CA	7.35	130.93	120.49
12	M	377	PHE	N-CA-C	-6.50	98.65	108.52
12	A	377	PHE	N-CA-C	-6.49	97.75	108.07
2	R	155	SER	N-CA-C	6.47	122.50	113.57
2	F	155	SER	N-CA-C	6.46	122.49	113.57
12	M	112	TRP	CA-C-N	5.36	134.51	122.19
12	M	112	TRP	C-N-CA	5.36	134.51	122.19
12	A	112	TRP	CA-C-N	5.35	134.50	122.19
12	A	112	TRP	C-N-CA	5.35	134.50	122.19
10	N	392	MET	CA-C-N	5.27	131.60	121.54
10	N	392	MET	C-N-CA	5.27	131.60	121.54
10	B	392	MET	CA-C-N	5.23	131.53	121.54
10	B	392	MET	C-N-CA	5.23	131.53	121.54

There are no chirality outliers.

All (24) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	B	134	ARG	Peptide
1	E	160	ASP	Peptide
1	E	328	PHE	Peptide
1	E	35	TRP	Peptide
2	F	356	GLU	Peptide
2	F	437	LEU	Peptide
2	F	523	CYS	Peptide

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Mol	Chain	Res	Type	Group
2	F	528	HIS	Peptide
3	G	14	SER	Peptide
3	G	2	THR	Peptide
3	G	50	ALA	Peptide
9	K	27	GLY	Peptide
10	N	134	ARG	Peptide
1	Q	160	ASP	Peptide
1	Q	328	PHE	Peptide
1	Q	35	TRP	Peptide
2	R	356	GLU	Peptide
2	R	437	LEU	Peptide
2	R	523	CYS	Peptide
2	R	528	HIS	Peptide
3	S	14	SER	Peptide
3	S	2	THR	Peptide
3	S	50	ALA	Peptide
9	W	27	GLY	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2465	0	2392	52	0
1	Q	2465	0	2392	51	0
2	F	4373	0	4347	118	0
2	R	4373	0	4347	114	0
3	G	1560	0	1547	27	0
3	S	1560	0	1547	25	0
4	H	1077	0	1058	18	0
4	T	1077	0	1058	16	0
5	I	507	0	516	8	0
5	U	507	0	516	6	0
6	J	1041	0	1052	20	0
6	V	1041	0	1052	18	0
7	D	736	0	717	13	0
7	P	736	0	717	11	0
8	Y	1092	0	640	7	0
8	Z	1092	0	640	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	K	1072	0	1045	29	0
9	W	1072	0	1045	26	0
10	B	4181	0	4201	103	0
10	N	4181	0	4201	102	0
11	C	1623	0	1564	43	0
11	O	1623	0	1564	41	0
12	A	2977	0	2986	76	0
12	M	2977	0	2986	63	0
13	E	2	0	0	0	0
13	F	2	0	0	0	0
13	Q	2	0	0	0	0
13	R	2	0	0	0	0
14	F	120	0	107	11	0
14	R	120	0	107	11	0
15	A	95	0	143	3	0
15	B	296	0	371	14	0
15	D	88	0	126	6	0
15	F	157	0	208	6	0
15	H	79	0	105	2	0
15	M	95	0	143	3	0
15	N	296	0	371	16	0
15	P	88	0	126	5	0
15	R	157	0	208	8	0
15	T	79	0	105	2	0
16	B	98	0	0	0	0
16	D	41	0	0	0	0
16	G	43	0	0	0	0
16	K	38	0	0	0	0
16	P	41	0	0	0	0
16	S	43	0	0	0	0
16	W	38	0	0	0	0
17	K	17	0	31	1	0
17	W	17	0	31	0	0
17	Y	11	0	16	0	0
17	Z	11	0	16	0	0
18	K	42	0	0	0	0
18	W	42	0	0	0	0
18	Y	32	0	0	0	0
18	Z	32	0	0	0	0
19	A	116	0	0	17	0
19	C	58	0	0	1	0
19	K	58	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	M	116	0	0	6	0
19	O	58	0	0	1	0
19	W	58	0	0	1	0
20	B	85	0	57	3	0
20	N	85	0	57	3	0
21	B	192	0	247	7	0
21	C	58	0	80	7	0
21	N	192	0	247	6	0
21	O	58	0	80	7	0
22	C	86	0	64	5	0
22	O	86	0	64	5	0
23	A	4	0	0	1	0
23	M	4	0	0	2	0
All	All	48946	0	47240	879	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 9.

All (879) 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)
2:F:398:PHE:O	2:F:402:LEU:HB3	1.65	0.96
2:R:398:PHE:O	2:R:402:LEU:HB3	1.66	0.95
12:A:355:LEU:HB2	12:A:364:LEU:O	1.70	0.91
12:M:355:LEU:HB2	12:M:364:LEU:O	1.69	0.90
2:F:88:THR:HG21	2:F:171:TRP:HE1	1.44	0.83
2:R:414:ILE:O	2:R:418:PHE:HB2	1.79	0.82
2:R:88:THR:HG21	2:R:171:TRP:HE1	1.44	0.82
2:F:414:ILE:O	2:F:418:PHE:HB2	1.79	0.81
12:A:418:GLU:OE1	19:A:503:9YF:O1	1.99	0.80
12:A:418:GLU:OE1	19:A:503:9YF:P	2.44	0.76
12:A:418:GLU:HB3	19:A:503:9YF:O8	1.87	0.74
2:F:406:ILE:O	2:F:410:THR:HB	1.89	0.73
2:R:406:ILE:O	2:R:410:THR:HB	1.88	0.73
2:R:550:MET:HE1	2:R:553:ARG:HH11	1.56	0.70
10:N:30:LEU:HB2	10:N:254:MET:HB2	1.73	0.70
2:F:550:MET:HE1	2:F:553:ARG:HH11	1.56	0.70
11:C:114:TYR:O	11:C:118:SER:HB3	1.92	0.70
11:O:114:TYR:O	11:O:118:SER:HB3	1.92	0.70
1:Q:232:HIS:HA	1:Q:275:GLU:HB2	1.73	0.70
2:R:162:HIS:HA	11:O:125:MET:HG3	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:90:MET:HB3	14:F:602:HEA:HBC1	1.74	0.70
2:R:90:MET:HB3	14:R:602:HEA:HBC1	1.74	0.70
12:A:418:GLU:CD	19:A:503:9YF:P	2.75	0.69
1:E:232:HIS:HA	1:E:275:GLU:HB2	1.73	0.69
1:Q:303:ARG:HH12	1:Q:309:ASN:HA	1.57	0.69
11:C:193:ASN:HD22	11:C:197:LYS:HB2	1.57	0.69
10:B:30:LEU:HB2	10:B:254:MET:HB2	1.73	0.69
11:O:193:ASN:HD22	11:O:197:LYS:HB2	1.57	0.68
1:E:303:ARG:HH12	1:E:309:ASN:HA	1.58	0.68
2:F:162:HIS:HA	11:C:125:MET:HG3	1.74	0.68
9:K:54:VAL:HA	9:K:74:LEU:O	1.94	0.67
9:W:54:VAL:HA	9:W:74:LEU:O	1.95	0.67
10:B:128:PHE:O	10:B:373:ARG:NH1	2.24	0.67
12:A:347:SER:O	12:A:387:ARG:NH2	2.29	0.66
11:O:192:HIS:NE2	22:O:302:HEC:NB	2.44	0.66
11:C:192:HIS:NE2	22:C:302:HEC:NB	2.44	0.66
2:R:172:ILE:HG23	2:R:231:LEU:HG	1.76	0.66
2:F:538:SER:HB3	2:F:555:ARG:HH21	1.61	0.66
12:A:348:HIS:HD2	12:A:349:LEU:HD13	1.61	0.65
3:S:74:THR:HG22	3:S:192:TRP:HE1	1.62	0.65
12:M:418:GLU:CD	19:M:504:9YF:O8	2.39	0.65
10:N:128:PHE:O	10:N:373:ARG:NH1	2.23	0.65
2:F:172:ILE:HG23	2:F:231:LEU:HG	1.76	0.65
3:G:74:THR:HG22	3:G:192:TRP:HE1	1.62	0.65
2:R:538:SER:HB3	2:R:555:ARG:HH21	1.62	0.65
8:Z:92:ALA:HB3	8:Z:172:THR:O	1.97	0.65
12:M:347:SER:O	12:M:387:ARG:NH2	2.30	0.65
10:B:210:LEU:HA	10:B:214:LEU:HB3	1.79	0.64
8:Y:92:ALA:HB3	8:Y:172:THR:O	1.96	0.64
1:Q:243:ARG:NH1	1:Q:255:ASP:O	2.31	0.64
11:C:115:PHE:HE2	11:C:226:PRO:HG3	1.63	0.64
2:R:105:LEU:HB3	2:R:106:VAL:HG13	1.80	0.64
12:M:368:HIS:ND1	23:M:502:FES:S2	2.69	0.64
2:F:105:LEU:HB3	2:F:106:VAL:HG13	1.79	0.64
10:N:210:LEU:HA	10:N:214:LEU:HB3	1.79	0.64
10:N:277:GLY:HA3	12:M:133:GLY:HA3	1.80	0.63
11:O:115:PHE:HE2	11:O:226:PRO:HG3	1.63	0.63
2:F:112:GLY:HA3	2:F:198:ALA:HB2	1.80	0.63
12:M:418:GLU:CG	19:M:504:9YF:O8	2.46	0.63
9:K:31:GLN:O	9:K:35:GLN:NE2	2.32	0.63
1:E:243:ARG:NH1	1:E:255:ASP:O	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:31:LEU:HA	2:F:43:MET:HE1	1.80	0.63
2:R:112:GLY:HA3	2:R:198:ALA:HB2	1.82	0.62
15:B:603:CDL:H321	15:N:604:CDL:H522	1.81	0.62
2:F:27:LEU:HD21	15:F:606:CDL:H521	1.82	0.62
2:R:31:LEU:HA	2:R:43:MET:HE1	1.80	0.62
9:W:31:GLN:O	9:W:35:GLN:NE2	2.32	0.62
2:R:27:LEU:HD21	15:R:606:CDL:H521	1.82	0.61
5:I:54:PRO:O	6:J:65:ARG:NH2	2.32	0.61
2:F:251:GLY:HA2	2:F:254:LEU:HB3	1.82	0.61
9:K:60:GLN:NE2	9:K:62:THR:O	2.33	0.61
10:N:315:TRP:HB3	10:N:329:GLN:HE21	1.64	0.61
3:G:33:LEU:HD11	3:G:184:TYR:HA	1.83	0.61
10:B:277:GLY:HA3	12:A:133:GLY:HA3	1.80	0.61
12:M:254:LEU:HD12	12:M:402:LEU:HB3	1.83	0.61
2:F:503:GLU:HG2	6:J:37:LEU:HD22	1.83	0.61
3:G:159:VAL:HG23	15:A:502:CDL:H192	1.83	0.61
11:O:230:PRO:HB3	12:M:279:MET:H	1.66	0.61
10:B:315:TRP:HB3	10:B:329:GLN:HE21	1.65	0.60
12:A:418:GLU:CD	19:A:503:9YF:O	2.44	0.60
9:W:60:GLN:NE2	9:W:62:THR:O	2.33	0.60
10:B:161:LEU:HD21	10:B:208:TYR:HD1	1.66	0.60
3:S:33:LEU:HD11	3:S:184:TYR:HA	1.83	0.60
12:A:254:LEU:HD12	12:A:402:LEU:HB3	1.82	0.60
2:R:251:GLY:HA2	2:R:254:LEU:HB3	1.82	0.60
10:N:161:LEU:HD21	10:N:208:TYR:HD1	1.66	0.60
11:C:121:ARG:HH22	22:C:302:HEC:HHA	1.67	0.60
11:C:215:PRO:HG3	11:C:250:ARG:HG3	1.84	0.60
11:O:121:ARG:HH22	22:O:302:HEC:HHA	1.67	0.60
11:C:230:PRO:HB3	12:A:279:MET:H	1.66	0.59
11:O:215:PRO:HG3	11:O:250:ARG:HG3	1.84	0.59
1:E:184:PRO:HA	3:G:134:SER:HA	1.84	0.59
1:E:299:TYR:OH	1:E:303:ARG:NH1	2.34	0.59
1:E:242:LYS:NZ	1:E:244:ASP:OD1	2.36	0.59
1:E:242:LYS:HE3	1:E:274:THR:HB	1.85	0.59
10:B:67:SER:HB3	10:B:87:ARG:HB3	1.83	0.59
10:B:26:VAL:HG22	15:B:603:CDL:H531	1.85	0.59
2:R:237:ASP:HA	2:R:242:ALA:H	1.67	0.59
2:F:89:VAL:HA	2:F:93:PHE:HB2	1.84	0.59
1:Q:299:TYR:OH	1:Q:303:ARG:NH1	2.34	0.59
6:J:130:ALA:HB2	6:J:146:ALA:HB2	1.85	0.59
2:R:20:ARG:NH2	6:V:53:ASP:OD1	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:N:222:LEU:O	10:N:226:HIS:HB2	2.02	0.59
2:R:501:TYR:HE1	6:V:49:VAL:HG11	1.67	0.58
2:F:237:ASP:HA	2:F:242:ALA:H	1.67	0.58
12:A:155:ILE:HG12	12:M:188:SER:HB2	1.86	0.58
3:S:159:VAL:HG23	15:M:503:CDL:H192	1.83	0.58
2:F:501:TYR:HE1	6:J:49:VAL:HG11	1.69	0.58
10:B:222:LEU:O	10:B:226:HIS:HB2	2.03	0.58
1:Q:242:LYS:HE3	1:Q:274:THR:HB	1.85	0.58
2:R:120:ARG:NH1	4:T:128:LEU:O	2.33	0.58
15:B:603:CDL:H772	21:B:607:MQ9:H3D	1.86	0.58
2:R:89:VAL:HA	2:R:93:PHE:HB2	1.84	0.58
10:N:67:SER:HB3	10:N:87:ARG:HB3	1.83	0.58
10:B:425:VAL:O	10:B:429:TRP:HB2	2.04	0.58
15:B:603:CDL:H522	15:N:604:CDL:H321	1.85	0.58
3:S:15:ARG:NH2	4:T:84:PHE:O	2.36	0.58
6:V:130:ALA:HB2	6:V:146:ALA:HB2	1.85	0.58
10:N:26:VAL:HG22	15:N:604:CDL:H531	1.85	0.58
10:N:279:LEU:HD23	11:O:263:LEU:HD11	1.86	0.58
1:E:275:GLU:O	1:E:281:HIS:NE2	2.37	0.58
2:F:303:ILE:HD12	2:F:337:THR:HB	1.86	0.58
2:F:532:GLU:HG2	6:J:25:SER:H	1.69	0.58
2:F:267:VAL:HB	14:F:601:HEA:HAC	1.86	0.57
2:R:111:ILE:HB	2:R:197:ARG:HG3	1.86	0.57
10:N:425:VAL:O	10:N:429:TRP:HB2	2.03	0.57
12:M:285:TRP:NE1	12:M:289:ASP:O	2.37	0.57
1:Q:184:PRO:HA	3:S:134:SER:HA	1.84	0.57
2:R:371:LEU:HB3	2:R:400:TYR:HE2	1.68	0.57
2:R:391:SER:HA	2:R:458:PRO:HA	1.87	0.57
12:A:82:GLU:OE2	12:M:193:ARG:NH2	2.36	0.57
12:A:188:SER:HB2	12:M:155:ILE:HG12	1.85	0.57
1:Q:242:LYS:NZ	1:Q:244:ASP:OD1	2.36	0.57
3:G:15:ARG:NH2	4:H:84:PHE:O	2.36	0.57
7:D:66:ASN:ND2	12:A:385:ALA:O	2.37	0.57
1:Q:275:GLU:O	1:Q:281:HIS:NE2	2.37	0.57
9:W:98:VAL:HG22	9:W:137:VAL:HG12	1.87	0.57
2:F:27:LEU:O	2:F:31:LEU:N	2.38	0.57
10:B:138:GLU:OE1	10:B:352:LYS:NZ	2.38	0.57
2:R:388:VAL:HG13	2:R:393:PHE:HB3	1.86	0.57
15:N:604:CDL:H772	21:N:607:MQ9:H3D	1.86	0.57
2:F:111:ILE:HB	2:F:197:ARG:HG3	1.86	0.57
2:F:371:LEU:HB3	2:F:400:TYR:HE2	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:303:ILE:HD12	2:R:337:THR:HB	1.86	0.57
2:R:545:LEU:HD11	6:V:23:THR:HG22	1.87	0.57
9:W:57:ARG:NH2	9:W:72:GLU:OE1	2.38	0.57
2:F:391:SER:HA	2:F:458:PRO:HA	1.87	0.57
9:K:57:ARG:NH2	9:K:72:GLU:OE1	2.38	0.57
1:E:235:TRP:HD1	1:E:242:LYS:HB3	1.71	0.56
12:A:418:GLU:OE2	19:A:503:9YF:C1	2.53	0.56
2:R:267:VAL:HB	14:R:601:HEA:HAC	1.86	0.56
7:P:90:ASN:OD1	7:P:94:ARG:NH1	2.38	0.56
2:F:20:ARG:NH2	6:J:53:ASP:OD1	2.38	0.56
10:B:248:VAL:HG23	12:A:164:ARG:HD2	1.86	0.56
12:A:285:TRP:NE1	12:A:289:ASP:O	2.37	0.56
2:R:532:GLU:HG2	6:V:25:SER:H	1.69	0.56
7:D:90:ASN:OD1	7:D:94:ARG:NH1	2.38	0.56
9:K:98:VAL:HG22	9:K:137:VAL:HG12	1.86	0.56
7:P:66:ASN:ND2	12:M:385:ALA:O	2.38	0.56
2:F:201:MET:HB3	2:F:536:ILE:HG21	1.86	0.56
10:B:279:LEU:HD23	11:C:263:LEU:HD11	1.86	0.56
12:A:274:ILE:HD13	12:A:280:GLU:HB2	1.88	0.56
1:Q:235:TRP:HD1	1:Q:242:LYS:HB3	1.70	0.56
2:R:268:TYR:HH	14:R:601:HEA:HO1	1.45	0.56
7:P:94:ARG:NH2	15:P:201:CDL:OA4	2.39	0.56
10:B:332:TRP:O	10:B:336:GLY:N	2.39	0.56
1:E:134:THR:HA	1:E:226:ASN:O	2.06	0.56
2:F:288:LYS:NZ	2:F:349:TRP:O	2.37	0.56
2:F:505:VAL:HG11	2:F:510:PRO:HB3	1.88	0.56
2:R:110:GLN:HB3	2:R:207:PRO:HG2	1.88	0.56
2:R:288:LYS:NZ	2:R:349:TRP:O	2.38	0.56
12:M:274:ILE:HD13	12:M:280:GLU:HB2	1.88	0.56
2:F:114:PRO:O	2:F:529:ASN:ND2	2.39	0.56
2:F:388:VAL:HG13	2:F:393:PHE:HB3	1.86	0.56
4:H:108:LEU:HD13	10:B:400:PHE:HA	1.88	0.56
2:R:201:MET:HB3	2:R:536:ILE:HG21	1.87	0.56
10:N:300:GLN:HG3	11:O:268:PRO:HG2	1.88	0.56
1:Q:134:THR:HA	1:Q:226:ASN:O	2.06	0.56
2:R:505:VAL:HG11	2:R:510:PRO:HB3	1.88	0.56
1:E:102:PRO:HB2	2:F:335:VAL:HG23	1.88	0.56
8:Z:117:GLY:HA2	8:Z:187:ALA:HB2	1.88	0.56
2:R:503:GLU:HG2	6:V:37:LEU:HD22	1.88	0.55
1:Q:102:PRO:HB2	2:R:335:VAL:HG23	1.88	0.55
2:R:39:LEU:HG	2:R:43:MET:HE3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:223:ALA:HB2	2:R:265:PRO:HB2	1.87	0.55
10:N:248:VAL:HG23	12:M:164:ARG:HD2	1.87	0.55
12:M:418:GLU:OE1	19:M:504:9YF:O8	2.24	0.55
1:E:214:VAL:HG12	1:E:289:ARG:HB2	1.88	0.55
2:F:39:LEU:HG	2:F:43:MET:HE3	1.88	0.55
9:K:45:GLN:HG2	9:K:52:ARG:HH22	1.71	0.55
8:Y:117:GLY:HA2	8:Y:187:ALA:HB2	1.88	0.55
1:Q:214:VAL:HG12	1:Q:289:ARG:HB2	1.88	0.55
10:N:332:TRP:O	10:N:336:GLY:N	2.39	0.55
10:N:500:GLY:HA3	10:N:505:PRO:HA	1.89	0.55
12:M:72:PRO:HA	12:M:156:PRO:HB3	1.88	0.55
1:E:186:ARG:HG2	3:G:54:ALA:HA	1.88	0.55
4:T:108:LEU:HD13	10:N:400:PHE:HA	1.88	0.55
10:N:308:THR:O	10:N:311:LEU:HB3	2.07	0.55
9:K:25:SER:OG	19:K:202:9YF:O3	2.24	0.55
1:E:185:ILE:HG22	3:G:135:ALA:HB2	1.89	0.55
2:F:223:ALA:HB2	2:F:265:PRO:HB2	1.87	0.55
2:R:114:PRO:O	2:R:529:ASN:ND2	2.39	0.55
12:A:72:PRO:HA	12:A:156:PRO:HB3	1.88	0.54
1:Q:106:ILE:HB	2:R:331:PHE:HB3	1.89	0.54
1:Q:166:ALA:HB3	1:Q:192:ASP:HA	1.89	0.54
2:F:110:GLN:HB3	2:F:207:PRO:HG2	1.89	0.54
10:B:300:GLN:HG3	11:C:268:PRO:HG2	1.88	0.54
1:Q:225:LEU:O	1:Q:256:ASN:ND2	2.38	0.54
2:F:74:LEU:HD11	2:F:82:LEU:HD22	1.88	0.54
10:B:308:THR:O	10:B:311:LEU:HB3	2.07	0.54
19:A:503:9YF:C31	19:A:503:9YF:C27	2.85	0.54
1:Q:186:ARG:HG2	3:S:54:ALA:HA	1.89	0.54
2:R:27:LEU:O	2:R:31:LEU:N	2.38	0.54
2:R:375:SER:O	2:R:379:LEU:HB2	2.07	0.54
21:B:608:MQ9:H203	21:B:608:MQ9:H301	1.88	0.54
2:R:205:ARG:NH2	2:R:537:ARG:O	2.41	0.54
21:N:608:MQ9:H203	21:N:608:MQ9:H301	1.88	0.54
2:F:375:SER:O	2:F:379:LEU:HB2	2.07	0.54
6:V:119:ILE:HG22	6:V:154:VAL:HG22	1.90	0.54
10:N:291:LYS:HG2	12:M:306:MET:HE1	1.90	0.54
5:I:46:PRO:HG3	6:J:72:PRO:HD2	1.90	0.54
7:D:94:ARG:NH2	15:D:201:CDL:OA4	2.39	0.54
19:M:504:9YF:C31	19:M:504:9YF:C27	2.85	0.54
2:F:221:LEU:HD22	3:G:35:SER:HB3	1.90	0.54
2:R:158:THR:O	2:R:238:ARG:NH1	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:N:235:HIS:ND1	10:N:236:THR:O	2.41	0.54
1:E:204:LEU:HD11	11:C:88:VAL:HG21	1.89	0.54
10:B:208:TYR:CZ	10:B:212:ILE:HD11	2.43	0.54
10:B:291:LYS:HG2	12:A:306:MET:HE1	1.90	0.54
10:B:500:GLY:HA3	10:B:505:PRO:HA	1.89	0.54
7:P:62:MET:HE3	10:N:412:ARG:HG2	1.90	0.54
10:B:37:HIS:HD2	11:C:294:ALA:H	1.56	0.54
1:E:106:ILE:HB	2:F:331:PHE:HB3	1.89	0.54
6:J:119:ILE:HG22	6:J:154:VAL:HG22	1.90	0.54
10:B:235:HIS:ND1	10:B:236:THR:O	2.41	0.54
12:A:418:GLU:OE1	19:A:503:9YF:O8	2.26	0.54
19:A:503:9YF:C30	19:A:503:9YF:C34	2.85	0.54
10:N:37:HIS:HD2	11:O:294:ALA:H	1.56	0.54
12:M:168:ARG:HB3	12:M:174:ARG:HH21	1.73	0.54
12:A:168:ARG:HB3	12:A:174:ARG:HH21	1.72	0.53
1:Q:185:ILE:HG22	3:S:135:ALA:HB2	1.89	0.53
9:W:40:ASN:HD21	12:M:275:ASP:HB2	1.73	0.53
9:W:45:GLN:HG2	9:W:52:ARG:HH22	1.73	0.53
10:N:253:VAL:HA	10:N:257:PHE:HB3	1.90	0.53
5:I:54:PRO:HD2	6:J:65:ARG:HG3	1.89	0.53
2:R:495:VAL:HG21	15:R:606:CDL:H801	1.90	0.53
2:F:120:ARG:NH1	4:H:128:LEU:O	2.33	0.53
9:K:173:ARG:NH2	11:C:235:ARG:O	2.41	0.53
10:B:253:VAL:HA	10:B:257:PHE:HB3	1.89	0.53
19:A:503:9YF:C39	19:A:503:9YF:C43	2.85	0.53
19:M:504:9YF:C34	19:M:504:9YF:C30	2.85	0.53
2:F:91:LEU:HD21	2:F:402:LEU:HD21	1.91	0.53
2:F:199:PRO:HA	4:H:68:GLU:HA	1.90	0.53
12:A:168:ARG:NE	10:N:18:SER:OG	2.39	0.53
2:R:199:PRO:HA	4:T:68:GLU:HA	1.90	0.53
11:O:290:ILE:HG12	12:M:148:VAL:HG21	1.90	0.53
1:E:166:ALA:HB3	1:E:192:ASP:HA	1.89	0.53
2:F:268:TYR:OH	14:F:601:HEA:O11	2.22	0.53
10:N:208:TYR:CZ	10:N:212:ILE:HD11	2.43	0.53
2:F:96:THR:OG1	2:F:266:GLU:OE2	2.27	0.53
2:F:205:ARG:NH2	2:F:537:ARG:O	2.41	0.53
2:F:495:VAL:HG21	15:F:606:CDL:H801	1.91	0.53
6:J:134:PHE:HE1	6:J:139:LEU:HD22	1.73	0.53
10:B:212:ILE:HG22	10:N:213:LEU:HD13	1.91	0.53
1:Q:204:LEU:HD11	11:O:88:VAL:HG21	1.89	0.53
2:R:89:VAL:HG11	2:R:137:ILE:HD11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:N:20:TYR:HE2	15:N:604:CDL:H612	1.73	0.53
2:F:55:GLY:HA3	2:F:90:MET:HE2	1.90	0.53
15:F:606:CDL:HA32	10:B:428:ARG:HH11	1.74	0.53
9:W:173:ARG:NH2	11:O:235:ARG:O	2.41	0.53
2:R:81:GLN:NE2	2:R:144:GLY:O	2.42	0.53
9:W:25:SER:OG	19:W:202:9YF:O3	2.23	0.53
10:B:138:GLU:OE2	10:N:19:ARG:NH2	2.38	0.53
10:B:500:GLY:O	12:A:84:ARG:NH1	2.42	0.53
1:Q:85:PRO:HG3	2:R:352:GLN:HG3	1.91	0.53
2:R:74:LEU:HD11	2:R:82:LEU:HD22	1.90	0.53
9:W:48:GLN:NE2	9:W:80:ASP:O	2.42	0.53
11:O:199:GLY:H	11:O:207:ALA:HB3	1.74	0.53
1:E:225:LEU:O	1:E:256:ASN:ND2	2.38	0.52
10:B:316:PRO:HB3	10:B:412:ARG:HD3	1.92	0.52
2:R:221:LEU:HD22	3:S:35:SER:HB3	1.90	0.52
1:E:85:PRO:HG3	2:F:352:GLN:HG3	1.91	0.52
9:K:40:ASN:HD21	12:A:275:ASP:HB2	1.73	0.52
11:C:290:ILE:HG12	12:A:148:VAL:HG21	1.90	0.52
2:R:55:GLY:HA3	2:R:90:MET:HE2	1.90	0.52
7:D:62:MET:HE3	10:B:412:ARG:HG2	1.91	0.52
2:R:91:LEU:HD21	2:R:402:LEU:HD21	1.91	0.52
2:R:96:THR:OG1	2:R:266:GLU:OE2	2.26	0.52
2:F:392:TYR:HE1	2:F:459:ARG:HA	1.73	0.52
3:G:34:SER:HB3	4:H:48:LEU:HG	1.91	0.52
3:G:43:LEU:HD23	3:G:143:ALA:HA	1.91	0.52
2:R:392:TYR:HE1	2:R:459:ARG:HA	1.73	0.52
8:Z:69:THR:HA	8:Z:84:ASP:HA	1.92	0.52
2:F:81:GLN:NE2	2:F:144:GLY:O	2.43	0.52
10:N:447:THR:OG1	10:N:461:LEU:O	2.28	0.52
3:S:34:SER:HB3	4:T:48:LEU:HG	1.91	0.52
6:V:134:PHE:HE1	6:V:139:LEU:HD22	1.73	0.52
10:B:213:LEU:HD13	10:N:212:ILE:HG22	1.90	0.52
10:B:447:THR:OG1	10:B:461:LEU:O	2.28	0.52
19:C:303:9YF:O3	19:C:303:9YF:O11	2.28	0.52
6:J:114:VAL:HG12	6:J:119:ILE:HD13	1.92	0.52
11:C:114:TYR:O	11:C:118:SER:CB	2.58	0.52
11:C:273:MET:SD	21:C:304:MQ9:O1	2.68	0.52
3:S:43:LEU:HD23	3:S:143:ALA:HA	1.91	0.52
2:R:78:GLN:O	2:R:82:LEU:HB2	2.09	0.51
1:E:40:THR:HG23	1:E:43:ALA:H	1.75	0.51
11:O:114:TYR:O	11:O:118:SER:CB	2.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:48:GLN:NE2	9:K:80:ASP:O	2.42	0.51
2:F:89:VAL:HG11	2:F:137:ILE:HD11	1.92	0.51
11:C:199:GLY:H	11:C:207:ALA:HB3	1.74	0.51
12:A:193:ARG:NH2	12:M:82:GLU:OE2	2.36	0.51
10:N:500:GLY:O	12:M:84:ARG:NH1	2.42	0.51
11:O:273:MET:SD	21:O:304:MQ9:O1	2.68	0.51
1:Q:40:THR:HG23	1:Q:43:ALA:H	1.75	0.51
6:V:114:VAL:HG12	6:V:119:ILE:HD13	1.92	0.51
2:F:78:GLN:O	2:F:82:LEU:HB2	2.11	0.51
12:A:361:TYR:HB3	12:A:374:ALA:HB3	1.92	0.51
10:N:169:THR:OG1	12:M:351:CYS:SG	2.68	0.51
1:E:159:ALA:HB2	1:E:200:LYS:HG3	1.92	0.51
1:Q:159:ALA:HB2	1:Q:200:LYS:HG3	1.92	0.51
10:B:18:SER:OG	12:M:168:ARG:NE	2.39	0.51
2:F:545:LEU:HD11	6:J:23:THR:HG22	1.92	0.51
2:R:202:THR:HG22	2:R:205:ARG:HD3	1.93	0.51
19:O:303:9YF:O11	19:O:303:9YF:O3	2.28	0.51
12:M:269:MET:HG3	12:M:402:LEU:HD12	1.93	0.51
1:E:212:VAL:HB	1:E:309:ASN:HD21	1.76	0.50
2:F:169:ASP:OD1	2:F:238:ARG:NE	2.42	0.50
4:H:131:GLU:O	10:B:487:ARG:NH1	2.44	0.50
4:T:131:GLU:O	10:N:487:ARG:NH1	2.45	0.50
12:M:361:TYR:HB3	12:M:374:ALA:HB3	1.93	0.50
10:N:370:VAL:HG11	10:N:373:ARG:HH21	1.75	0.50
1:E:225:LEU:HB3	1:E:245:VAL:HG12	1.93	0.50
2:F:53:LEU:HB3	14:F:602:HEA:H22	1.93	0.50
9:K:168:ALA:HB1	9:K:170:GLU:HB2	1.93	0.50
10:B:89:TYR:OH	10:B:284:ILE:O	2.24	0.50
11:C:259:GLY:HA2	12:A:129:THR:HB	1.94	0.50
2:R:90:MET:HE3	14:R:602:HEA:HHC	1.93	0.50
11:O:87:CYS:HB3	22:O:301:HEC:HBB3	1.93	0.50
2:F:90:MET:HE3	14:F:602:HEA:HHC	1.94	0.50
8:Y:69:THR:HA	8:Y:84:ASP:HA	1.93	0.50
10:B:382:ALA:HB2	15:B:604:CDL:H182	1.93	0.50
11:C:87:CYS:HB3	22:C:301:HEC:HBB3	1.93	0.50
3:G:21:ARG:HD3	3:G:22:PRO:HD2	1.94	0.50
1:Q:212:VAL:HB	1:Q:309:ASN:HD21	1.76	0.50
5:I:79:TRP:HA	6:J:131:ALA:HB1	1.94	0.50
11:C:227:GLN:HB2	22:C:302:HEC:HBD2	1.94	0.50
12:A:418:GLU:CB	19:A:503:9YF:O8	2.57	0.50
4:T:1:MET:HB3	4:T:66:ARG:HH12	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:490:PRO:O	2:F:494:ASN:HB2	2.12	0.50
10:N:165:LEU:HB3	10:N:290:TYR:HA	1.93	0.50
2:F:202:THR:HG22	2:F:205:ARG:HD3	1.94	0.49
10:B:165:LEU:HB3	10:B:290:TYR:HA	1.92	0.49
12:A:419:ARG:HG2	12:A:420:LYS:HG2	1.93	0.49
4:H:1:MET:HB3	4:H:66:ARG:HH12	1.77	0.49
10:B:235:HIS:NE2	20:B:601:HEM:O2A	2.37	0.49
10:B:370:VAL:HG11	10:B:373:ARG:HH21	1.77	0.49
12:A:269:MET:HG3	12:A:402:LEU:HD12	1.93	0.49
1:Q:173:GLY:H	1:Q:179:ILE:HD11	1.76	0.49
2:R:53:LEU:HB3	14:R:602:HEA:H22	1.93	0.49
2:R:193:VAL:O	2:R:197:ARG:NH1	2.45	0.49
1:E:173:GLY:H	1:E:179:ILE:HD11	1.77	0.49
10:B:169:THR:OG1	12:A:351:CYS:SG	2.70	0.49
2:R:169:ASP:OD1	2:R:238:ARG:NE	2.42	0.49
12:M:362:ARG:HA	12:M:372:PHE:O	2.13	0.49
2:F:402:LEU:HG	14:F:602:HEA:HAC	1.95	0.49
10:B:198:PHE:HB3	12:A:308:VAL:HG21	1.94	0.49
6:V:92:GLU:O	6:V:113:ASP:N	2.45	0.49
11:O:259:GLY:HA2	12:M:129:THR:HB	1.94	0.49
12:M:419:ARG:HG2	12:M:420:LYS:HG2	1.93	0.49
1:Q:225:LEU:HB3	1:Q:245:VAL:HG12	1.93	0.49
2:R:375:SER:OG	2:R:397:HIS:ND1	2.40	0.49
3:G:15:ARG:HG3	3:G:24:MET:HE2	1.95	0.49
3:S:15:ARG:HG3	3:S:24:MET:HE2	1.95	0.49
3:S:21:ARG:HD3	3:S:22:PRO:HD2	1.94	0.49
9:W:42:VAL:HG13	9:W:165:PRO:HD3	1.94	0.49
9:W:107:PRO:HG3	9:W:112:LEU:HB2	1.94	0.49
10:N:47:LEU:HD21	21:N:609:MQ9:H8	1.94	0.49
9:K:42:VAL:HG13	9:K:165:PRO:HD3	1.95	0.49
12:A:418:GLU:CG	19:A:503:9YF:O8	2.60	0.49
2:R:405:THR:O	2:R:409:ALA:HB3	2.13	0.49
10:N:316:PRO:HB3	10:N:412:ARG:HD3	1.95	0.49
10:N:340:VAL:HG21	21:O:304:MQ9:H361	1.95	0.49
12:M:327:LYS:HG2	12:M:332:GLU:HA	1.94	0.49
2:F:202:THR:HG23	2:F:204:PHE:H	1.77	0.49
8:Y:96:ILE:O	8:Y:167:LYS:HA	2.13	0.49
9:K:50:SER:HB3	9:K:78:ALA:HB3	1.95	0.49
9:K:107:PRO:HG3	9:K:112:LEU:HB2	1.95	0.49
10:B:47:LEU:HD21	21:B:609:MQ9:H8	1.94	0.49
12:A:327:LYS:HG2	12:A:332:GLU:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:N:120:ILE:HG22	10:N:148:LEU:HD12	1.95	0.49
10:N:198:PHE:HB3	12:M:308:VAL:HG21	1.94	0.49
10:N:419:PRO:HA	10:N:422:VAL:HG12	1.94	0.49
2:F:193:VAL:O	2:F:197:ARG:NH1	2.45	0.49
2:R:402:LEU:HG	14:R:602:HEA:HAC	1.95	0.49
2:R:490:PRO:O	2:R:494:ASN:HB2	2.13	0.49
12:M:367:CYS:HB2	23:M:502:FES:S2	2.53	0.49
3:G:131:ILE:HG13	3:G:138:SER:HA	1.95	0.49
10:B:160:SER:HB2	10:B:171:ILE:HD11	1.94	0.49
10:B:166:LEU:HD12	11:C:194:PHE:HE2	1.78	0.49
2:R:77:GLU:OE2	11:O:127:GLY:N	2.44	0.49
2:F:42:ILE:HD11	2:F:421:MET:HB3	1.95	0.48
6:J:92:GLU:O	6:J:113:ASP:N	2.45	0.48
10:B:340:VAL:HG21	21:C:304:MQ9:H361	1.95	0.48
10:B:419:PRO:HA	10:B:422:VAL:HG12	1.94	0.48
12:A:348:HIS:CE1	12:A:384:PRO:HB2	2.48	0.48
15:N:605:CDL:H152	15:N:605:CDL:H571	1.95	0.48
11:O:80:LYS:NZ	11:O:84:GLU:OE2	2.45	0.48
11:O:227:GLN:HB2	22:O:302:HEC:HBD2	1.94	0.48
11:O:235:ARG:HB3	12:M:273:ASP:HA	1.95	0.48
15:F:606:CDL:H321	15:D:201:CDL:H542	1.95	0.48
15:A:502:CDL:H722	15:A:502:CDL:H551	1.95	0.48
2:R:396:ALA:HB2	2:R:449:GLN:HB2	1.95	0.48
8:Z:70:ALA:HB3	8:Z:83:ALA:HB3	1.95	0.48
10:N:382:ALA:HB2	15:N:605:CDL:H182	1.94	0.48
3:S:160:LEU:HD21	4:T:129:VAL:HG11	1.95	0.48
10:N:199:PRO:HD3	12:M:308:VAL:HG23	1.96	0.48
3:G:160:LEU:HD21	4:H:129:VAL:HG11	1.95	0.48
10:N:129:PHE:HB3	10:N:367:PRO:HB3	1.95	0.48
10:N:160:SER:HB2	10:N:171:ILE:HD11	1.94	0.48
2:R:189:MET:O	2:R:192:THR:OG1	2.31	0.48
1:E:36:PRO:HB2	1:E:238:GLU:HG2	1.95	0.48
2:F:405:THR:O	2:F:409:ALA:HB3	2.13	0.48
10:B:129:PHE:HB3	10:B:367:PRO:HB3	1.95	0.48
9:W:50:SER:HB3	9:W:78:ALA:HB3	1.95	0.48
1:E:235:TRP:CD1	1:E:242:LYS:HB3	2.49	0.48
3:G:149:LEU:HA	3:G:152:ILE:HG22	1.96	0.48
10:B:199:PRO:HD3	12:A:308:VAL:HG23	1.95	0.48
9:W:168:ALA:HB1	9:W:170:GLU:HB2	1.96	0.48
2:F:158:THR:O	2:F:238:ARG:NH1	2.40	0.48
12:A:240:THR:HG23	12:A:244:THR:HG21	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:289:ASP:OD1	12:A:289:ASP:N	2.45	0.48
2:R:202:THR:HG23	2:R:204:PHE:H	1.79	0.48
3:S:131:ILE:HG13	3:S:138:SER:HA	1.95	0.48
9:W:60:GLN:NE2	9:W:63:ASP:O	2.47	0.48
11:C:80:LYS:NZ	11:C:84:GLU:OE2	2.45	0.48
11:C:235:ARG:HB3	12:A:273:ASP:HA	1.95	0.48
2:F:419:PRO:HB2	2:F:510:PRO:HG3	1.95	0.48
8:Z:96:ILE:O	8:Z:167:LYS:HA	2.14	0.48
10:N:66:PRO:HG3	10:N:208:TYR:CD2	2.49	0.48
2:F:63:ARG:HG3	2:F:478:THR:HG23	1.95	0.47
9:K:60:GLN:NE2	9:K:63:ASP:O	2.47	0.47
4:T:42:LEU:HA	4:T:45:THR:HG22	1.96	0.47
10:B:120:ILE:HG22	10:B:148:LEU:HD12	1.95	0.47
10:B:222:LEU:O	10:B:226:HIS:CB	2.62	0.47
11:C:225:GLY:H	11:C:231:LYS:HB3	1.79	0.47
12:A:362:ARG:HA	12:A:372:PHE:O	2.14	0.47
1:Q:36:PRO:HB2	1:Q:238:GLU:HG2	1.95	0.47
2:R:37:HIS:HE1	2:R:529:ASN:HD21	1.62	0.47
2:R:242:ALA:O	3:S:138:SER:OG	2.29	0.47
15:P:201:CDL:OA2	10:N:428:ARG:NH2	2.47	0.47
12:M:418:GLU:HG3	19:M:504:9YF:O8	2.13	0.47
2:F:38:LYS:NZ	2:F:526:PRO:O	2.43	0.47
2:F:291:PHE:HD2	2:F:343:ASN:HA	1.79	0.47
2:F:37:HIS:HE1	2:F:529:ASN:HD21	1.63	0.47
3:S:149:LEU:HA	3:S:152:ILE:HG22	1.96	0.47
2:F:396:ALA:HB2	2:F:449:GLN:HB2	1.95	0.47
2:R:42:ILE:HD11	2:R:421:MET:HB3	1.96	0.47
10:B:66:PRO:HG3	10:B:208:TYR:CD2	2.49	0.47
10:B:132:ALA:HB1	20:B:601:HEM:HBD2	1.97	0.47
2:R:291:PHE:HD2	2:R:343:ASN:HA	1.79	0.47
2:R:419:PRO:HB2	2:R:510:PRO:HG3	1.96	0.47
9:W:36:GLU:O	12:M:359:GLN:NE2	2.47	0.47
10:N:166:LEU:HD12	11:O:194:PHE:HE2	1.78	0.47
15:D:201:CDL:OA2	10:B:428:ARG:NH2	2.47	0.47
9:K:36:GLU:O	12:A:359:GLN:NE2	2.47	0.47
5:U:3:THR:HA	5:U:6:THR:HG22	1.97	0.47
10:N:121:MET:HB3	21:O:304:MQ9:H262	1.97	0.47
2:F:395:ILE:O	2:F:399:HIS:ND1	2.39	0.47
15:B:611:CDL:H552	15:B:611:CDL:H581	1.84	0.47
15:N:601:CDL:H531	15:N:604:CDL:H602	1.97	0.47
11:O:273:MET:SD	21:O:304:MQ9:H3D	2.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:37:HIS:CE1	2:F:529:ASN:HD21	2.33	0.46
15:F:605:CDL:OB4	3:G:164:ARG:NH1	2.36	0.46
4:H:42:LEU:HA	4:H:45:THR:HG22	1.96	0.46
1:Q:220:ARG:HE	1:Q:259:GLN:HB3	1.80	0.46
2:R:37:HIS:CE1	2:R:529:ASN:HD21	2.33	0.46
15:R:605:CDL:OB4	3:S:164:ARG:NH1	2.37	0.46
10:N:104:PHE:HB2	12:M:129:THR:HG23	1.97	0.46
11:O:130:GLN:NE2	11:O:206:TYR:O	2.41	0.46
11:O:225:GLY:H	11:O:231:LYS:HB3	1.79	0.46
12:M:240:THR:HG23	12:M:244:THR:HG21	1.96	0.46
12:M:243:TRP:NE1	12:M:310:ASN:O	2.43	0.46
5:I:3:THR:HA	5:I:6:THR:HG22	1.97	0.46
7:D:23:GLU:O	7:D:25:HIS:ND1	2.48	0.46
8:Y:70:ALA:HB3	8:Y:83:ALA:HB3	1.96	0.46
10:B:393:ASN:HD21	10:B:408:THR:HB	1.80	0.46
10:B:60:LEU:HD23	20:B:602:HEM:HBD1	1.97	0.46
10:B:403:SER:HA	11:C:204:GLY:HA2	1.96	0.46
15:B:604:CDL:H571	15:B:604:CDL:H152	1.95	0.46
11:C:273:MET:SD	21:C:304:MQ9:H3D	2.55	0.46
2:R:161:ILE:HA	11:O:134:LYS:HD3	1.98	0.46
2:R:509:ASP:HB2	6:V:31:VAL:HA	1.97	0.46
15:R:606:CDL:HA32	10:N:428:ARG:HH11	1.79	0.46
9:W:57:ARG:NH1	9:W:116:GLU:O	2.48	0.46
15:M:503:CDL:H551	15:M:503:CDL:H722	1.97	0.46
1:E:47:ARG:HE	1:E:51:ILE:HD11	1.81	0.46
1:E:84:LEU:HD23	1:E:84:LEU:HA	1.79	0.46
9:K:153:PHE:O	9:K:159:GLU:HA	2.16	0.46
2:R:149:PHE:HB3	2:R:157:LEU:HG	1.97	0.46
9:K:57:ARG:NH1	9:K:116:GLU:O	2.48	0.46
10:B:135:ARG:HH21	10:B:358:ASP:HA	1.80	0.46
12:A:127:LEU:HA	12:A:130:PRO:HD2	1.98	0.46
12:A:368:HIS:ND1	23:A:501:FES:S1	2.82	0.46
9:K:37:PRO:HG3	11:C:104:SER:HB3	1.97	0.46
7:P:23:GLU:O	7:P:25:HIS:ND1	2.48	0.46
10:N:222:LEU:O	10:N:226:HIS:CB	2.62	0.46
10:N:393:ASN:HD21	10:N:408:THR:HB	1.81	0.46
2:F:146:ALA:HA	2:F:167:GLY:HA3	1.97	0.46
2:F:161:ILE:HA	11:C:134:LYS:HD3	1.98	0.46
5:I:38:MET:HG3	6:J:137:GLY:HA2	1.97	0.46
8:Y:70:ALA:N	8:Y:83:ALA:O	2.49	0.46
10:B:121:MET:HB3	21:C:304:MQ9:H262	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:235:TRP:CD1	1:Q:242:LYS:HB3	2.49	0.46
2:R:146:ALA:HA	2:R:167:GLY:HA3	1.96	0.46
1:E:213:LEU:HD23	1:E:288:VAL:HG12	1.98	0.46
10:B:99:VAL:HG23	10:B:102:GLY:HA3	1.98	0.46
15:R:606:CDL:H321	15:P:201:CDL:H542	1.98	0.46
10:N:78:GLN:HG3	12:M:116:PRO:HB3	1.98	0.46
2:F:149:PHE:HB3	2:F:157:LEU:HG	1.97	0.46
1:Q:47:ARG:HE	1:Q:51:ILE:HD11	1.81	0.46
2:F:310:VAL:HG11	2:F:333:ILE:HD13	1.98	0.46
3:G:25:VAL:HG12	3:G:180:VAL:HG21	1.98	0.46
7:D:43:MET:H	10:B:372:VAL:HG11	1.79	0.46
1:Q:132:ASP:HB3	1:Q:143:GLY:HA3	1.98	0.46
1:Q:227:SER:HB3	1:Q:245:VAL:HB	1.97	0.46
2:R:215:VAL:HA	2:R:218:ILE:HD12	1.98	0.46
21:O:304:MQ9:H272	21:O:304:MQ9:H503	1.98	0.46
10:N:58:VAL:O	10:N:61:THR:OG1	2.30	0.45
10:N:99:VAL:HG23	10:N:102:GLY:HA3	1.98	0.45
1:E:299:TYR:HD2	1:E:300:ILE:HG13	1.80	0.45
2:F:77:GLU:OE2	11:C:127:GLY:N	2.44	0.45
10:B:38:TRP:HB2	11:C:288:MET:HA	1.99	0.45
10:B:78:GLN:HG3	12:A:116:PRO:HB3	1.98	0.45
10:N:60:LEU:HD23	20:N:603:HEM:HBD1	1.97	0.45
1:E:34:GLY:HA3	2:F:451:TRP:CD1	2.51	0.45
1:E:132:ASP:HB3	1:E:143:GLY:HA3	1.98	0.45
1:E:184:PRO:HD2	1:E:189:THR:HA	1.99	0.45
1:E:227:SER:HB3	1:E:245:VAL:HB	1.97	0.45
9:K:61:GLN:HA	9:K:174:ARG:HH12	1.82	0.45
9:K:172:PRO:HA	11:C:235:ARG:HG3	1.98	0.45
10:B:214:LEU:HD21	21:N:609:MQ9:H352	1.98	0.45
2:R:206:MET:O	2:R:293:TYR:OH	2.25	0.45
2:R:395:ILE:O	2:R:399:HIS:ND1	2.39	0.45
2:R:400:TYR:HA	2:R:442:PHE:HZ	1.81	0.45
3:S:47:TYR:HA	3:S:139:VAL:HG11	1.98	0.45
7:P:43:MET:H	10:N:372:VAL:HG11	1.81	0.45
8:Z:30:SER:OG	8:Z:31:GLU:N	2.49	0.45
8:Z:70:ALA:N	8:Z:83:ALA:O	2.49	0.45
12:M:127:LEU:HA	12:M:130:PRO:HD2	1.98	0.45
1:E:319:PRO:HA	1:E:320:PRO:HD3	1.75	0.45
10:B:20:TYR:HE2	15:B:603:CDL:H612	1.81	0.45
1:Q:34:GLY:HA3	2:R:451:TRP:CD1	2.51	0.45
1:Q:299:TYR:HD2	1:Q:300:ILE:HG13	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:213:ILE:HA	2:R:216:THR:HB	1.98	0.45
2:R:420:LYS:HD2	2:R:519:TRP:CE3	2.51	0.45
9:W:61:GLN:HA	9:W:174:ARG:HH12	1.80	0.45
10:N:38:TRP:HB2	11:O:288:MET:HA	1.99	0.45
1:E:220:ARG:HE	1:E:259:GLN:HB3	1.80	0.45
2:F:139:GLY:O	2:F:142:THR:OG1	2.27	0.45
14:F:601:HEA:HHA	14:F:601:HEA:HAD1	1.72	0.45
10:B:104:PHE:HB2	12:A:129:THR:HG23	1.97	0.45
10:B:381:ILE:HG21	15:B:604:CDL:H151	1.98	0.45
11:C:174:GLY:H	11:C:247:ALA:HB2	1.81	0.45
2:R:38:LYS:NZ	2:R:526:PRO:O	2.42	0.45
10:N:235:HIS:NE2	20:N:602:HEM:O2A	2.37	0.45
15:N:606:CDL:H521	15:N:606:CDL:H321	1.98	0.45
12:M:348:HIS:NE2	12:M:384:PRO:HB2	2.31	0.45
3:G:183:TYR:HA	3:G:186:HIS:HB2	1.98	0.45
2:R:310:VAL:HG11	2:R:333:ILE:HD13	1.98	0.45
1:E:135:ALA:HB1	1:E:232:HIS:NE2	2.32	0.45
10:B:49:SER:O	10:B:52:ILE:HB	2.17	0.45
12:A:418:GLU:CD	19:A:503:9YF:C1	2.90	0.45
9:W:153:PHE:O	9:W:159:GLU:HA	2.16	0.45
10:N:132:ALA:HB1	20:N:602:HEM:HBD2	1.97	0.45
21:N:609:MQ9:H161	21:N:609:MQ9:H122	1.73	0.45
2:F:400:TYR:HA	2:F:442:PHE:HZ	1.82	0.45
3:G:47:TYR:HA	3:G:139:VAL:HG11	1.98	0.45
10:B:328:PRO:HB3	12:A:415:ALA:HB3	1.98	0.45
11:C:130:GLN:NE2	11:C:206:TYR:O	2.41	0.45
11:C:246:VAL:HA	11:C:249:VAL:HG22	1.99	0.45
21:C:304:MQ9:H162	21:C:304:MQ9:H122	1.79	0.45
1:Q:213:LEU:HD23	1:Q:288:VAL:HG12	1.98	0.45
3:S:101:ARG:HG2	10:N:503:LEU:HD12	1.99	0.45
10:N:291:LYS:HA	10:N:292:PRO:HD3	1.84	0.45
10:N:381:ILE:HG21	15:N:605:CDL:H151	1.98	0.45
12:M:283:PHE:HE1	12:M:311:PRO:HB3	1.82	0.45
2:F:215:VAL:HA	2:F:218:ILE:HD12	1.98	0.45
2:F:375:SER:OG	2:F:397:HIS:ND1	2.41	0.45
1:Q:135:ALA:HB1	1:Q:232:HIS:NE2	2.32	0.45
1:Q:184:PRO:HD2	1:Q:189:THR:HA	1.99	0.45
2:R:414:ILE:O	2:R:418:PHE:CB	2.60	0.45
10:N:270:GLY:HA3	12:M:141:LEU:HB2	1.99	0.45
2:F:420:LYS:HD2	2:F:519:TRP:CE3	2.53	0.44
8:Y:30:SER:OG	8:Y:31:GLU:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:B:609:MQ9:H352	10:N:214:LEU:HD21	1.99	0.44
10:N:403:SER:HA	11:O:204:GLY:HA2	1.97	0.44
3:G:101:ARG:HG2	10:B:503:LEU:HD12	1.99	0.44
12:A:370:SER:HB2	12:A:384:PRO:HD2	1.99	0.44
10:N:328:PRO:HB3	12:M:415:ALA:HB3	1.98	0.44
15:B:605:CDL:H521	15:B:605:CDL:H321	1.99	0.44
1:Q:134:THR:HG23	1:Q:141:LYS:HB3	1.99	0.44
14:R:601:HEA:HHA	14:R:601:HEA:HAA2	1.87	0.44
10:N:49:SER:O	10:N:52:ILE:HB	2.16	0.44
10:B:152:MET:HG2	10:B:305:MET:HE3	2.00	0.44
11:O:227:GLN:HE21	22:O:301:HEC:HBD2	1.82	0.44
9:K:54:VAL:HB	9:K:75:PHE:HB3	2.00	0.44
10:B:329:GLN:HE22	12:A:384:PRO:HB3	1.82	0.44
3:S:25:VAL:HG12	3:S:180:VAL:HG21	1.98	0.44
10:N:100:ARG:NH1	12:M:112:TRP:HE1	2.15	0.44
1:E:134:THR:HG23	1:E:141:LYS:HB3	1.99	0.44
1:E:197:ASN:OD1	1:E:197:ASN:N	2.50	0.44
2:F:16:PRO:HB3	5:I:49:TRP:CD2	2.53	0.44
10:B:111:TRP:CD1	10:B:276:GLY:HA2	2.53	0.44
11:C:121:ARG:O	11:C:134:LYS:NZ	2.51	0.44
1:Q:240:LEU:HA	2:R:387:HIS:CD2	2.53	0.44
5:U:53:GLU:HG3	6:V:60:ARG:HG2	2.00	0.44
10:N:111:TRP:CD1	10:N:276:GLY:HA2	2.53	0.44
10:N:152:MET:HG2	10:N:305:MET:HE3	2.00	0.44
1:E:60:VAL:HG11	14:F:601:HEA:H22	2.00	0.44
1:E:240:LEU:HA	2:F:387:HIS:CD2	2.53	0.44
10:B:100:ARG:NH1	12:A:112:TRP:HE1	2.15	0.44
21:C:304:MQ9:H272	21:C:304:MQ9:H503	1.98	0.44
3:S:183:TYR:HA	3:S:186:HIS:HB2	1.98	0.44
2:F:189:MET:O	2:F:192:THR:OG1	2.31	0.44
12:A:283:PHE:HE1	12:A:311:PRO:HB3	1.82	0.44
1:Q:319:PRO:HA	1:Q:320:PRO:HD3	1.75	0.44
9:W:63:ASP:OD1	12:M:400:GLY:N	2.51	0.44
12:M:153:LYS:NZ	15:M:503:CDL:OA4	2.47	0.44
12:M:270:ARG:NH2	12:M:401:TYR:OH	2.50	0.44
7:D:72:GLU:HG2	10:B:409:TRP:CE2	2.53	0.44
9:K:77:ALA:HB3	9:K:112:LEU:HB3	2.00	0.44
11:O:246:VAL:HA	11:O:249:VAL:HG22	1.99	0.44
10:B:270:GLY:HA3	12:A:141:LEU:HB2	1.99	0.43
15:B:603:CDL:H141	15:N:604:CDL:H141	2.00	0.43
7:P:72:GLU:HG2	10:N:409:TRP:CE2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:N:136:PRO:HB3	10:N:360:HIS:CE1	2.52	0.43
10:N:311:LEU:HD13	10:N:387:LEU:HD21	2.00	0.43
7:D:66:ASN:OD1	7:D:66:ASN:N	2.51	0.43
12:A:243:TRP:NE1	12:A:310:ASN:O	2.43	0.43
12:A:270:ARG:NH2	12:A:401:TYR:OH	2.50	0.43
2:R:306:LEU:O	2:R:310:VAL:HB	2.18	0.43
11:O:174:GLY:H	11:O:247:ALA:HB2	1.81	0.43
1:E:141:LYS:HD3	1:E:204:LEU:HD23	2.00	0.43
2:F:306:LEU:HB3	2:F:333:ILE:HG22	2.00	0.43
12:M:319:PRO:HA	12:M:322:MET:HG2	2.00	0.43
2:F:213:ILE:HA	2:F:216:THR:HB	1.98	0.43
2:F:509:ASP:HB2	6:J:31:VAL:HA	1.99	0.43
11:C:121:ARG:HH12	11:C:208:PRO:HG3	1.84	0.43
9:K:63:ASP:OD1	12:A:400:GLY:N	2.52	0.43
10:B:47:LEU:HD22	10:B:227:LEU:HD21	2.01	0.43
12:A:319:PRO:HA	12:A:322:MET:HG2	2.00	0.43
4:T:134:TRP:H	10:N:489:ASN:HD21	1.67	0.43
8:Z:31:GLU:HA	8:Z:32:PRO:HD3	1.85	0.43
9:W:77:ALA:HB3	9:W:112:LEU:HB3	2.00	0.43
9:W:107:PRO:HD3	9:W:112:LEU:HD12	2.00	0.43
12:M:274:ILE:O	12:M:316:ARG:NH2	2.51	0.43
2:F:473:LEU:HA	2:F:476:ILE:HG22	2.00	0.43
3:G:13:THR:H	4:H:84:PHE:HB2	1.83	0.43
10:B:311:LEU:HD13	10:B:387:LEU:HD21	2.00	0.43
12:A:246:ARG:CZ	12:A:286:ARG:HH12	2.31	0.43
12:A:274:ILE:O	12:A:316:ARG:NH2	2.52	0.43
11:O:121:ARG:HH12	11:O:208:PRO:HG3	1.84	0.43
12:M:393:PRO:HB2	12:M:405:ASN:HB3	1.99	0.43
2:F:414:ILE:O	2:F:418:PHE:CB	2.60	0.43
10:B:44:GLU:O	10:B:48:TYR:N	2.47	0.43
10:B:237:GLN:NE2	10:B:247:ASN:O	2.52	0.43
11:C:227:GLN:HE21	22:C:301:HEC:HBD2	1.83	0.43
1:Q:197:ASN:OD1	1:Q:197:ASN:N	2.50	0.43
2:R:473:LEU:HA	2:R:476:ILE:HG22	2.00	0.43
5:U:31:PRO:HB2	6:V:37:LEU:HD21	1.99	0.43
1:E:96:LEU:HA	1:E:99:THR:HG22	2.01	0.43
6:J:76:ASP:N	6:J:76:ASP:OD1	2.52	0.43
10:B:216:PRO:HA	10:B:219:ILE:HB	2.01	0.43
1:Q:96:LEU:HA	1:Q:99:THR:HG22	2.01	0.43
21:O:304:MQ9:H72	21:O:304:MQ9:H101	1.89	0.43
12:M:246:ARG:CZ	12:M:286:ARG:HH12	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:194:VAL:HG22	4:H:4:GLU:HG2	2.01	0.43
2:F:392:TYR:CE1	2:F:459:ARG:HA	2.53	0.43
14:F:601:HEA:HHA	14:F:601:HEA:HAA2	1.87	0.43
15:D:201:CDL:H181	10:B:419:PRO:HB2	2.01	0.43
2:R:289:PRO:HG3	2:R:540:ARG:NH1	2.33	0.43
9:W:62:THR:OG1	9:W:64:TYR:O	2.36	0.43
10:N:237:GLN:NE2	10:N:247:ASN:O	2.52	0.43
12:A:393:PRO:HB2	12:A:405:ASN:HB3	1.99	0.43
1:Q:60:VAL:HG11	14:R:601:HEA:H22	2.00	0.43
1:Q:141:LYS:HD3	1:Q:204:LEU:HD23	2.01	0.43
2:R:306:LEU:HB3	2:R:333:ILE:HG22	2.00	0.43
7:P:66:ASN:OD1	7:P:66:ASN:N	2.51	0.43
10:N:216:PRO:HA	10:N:219:ILE:HB	2.01	0.43
11:O:121:ARG:O	11:O:134:LYS:NZ	2.51	0.43
2:F:156:PRO:HD3	2:F:252:VAL:HG12	2.00	0.42
11:C:122:MET:O	11:C:124:ALA:N	2.52	0.42
2:R:392:TYR:CE1	2:R:459:ARG:HA	2.53	0.42
12:M:370:SER:HB2	12:M:384:PRO:HD2	2.00	0.42
1:E:122:HIS:HB3	1:E:220:ARG:HH22	1.84	0.42
2:F:392:TYR:OH	14:F:602:HEA:O1A	2.32	0.42
21:B:610:MQ9:H253	21:B:610:MQ9:H271	1.87	0.42
5:U:2:SER:O	5:U:5:LEU:N	2.48	0.42
10:N:335:VAL:O	10:N:339:LEU:N	2.53	0.42
15:N:601:CDL:H552	15:N:601:CDL:H581	1.81	0.42
15:N:606:CDL:H571	15:N:606:CDL:H751	2.00	0.42
2:R:445:THR:HG23	2:R:446:PHE:CD2	2.54	0.42
2:F:80:ASN:HA	2:F:83:PHE:CE2	2.55	0.42
3:G:187:PHE:HA	3:G:190:ILE:HG22	2.01	0.42
4:H:134:TRP:H	10:B:489:ASN:HD21	1.66	0.42
10:B:281:ILE:HG13	11:C:271:GLU:CD	2.45	0.42
1:E:98:LEU:HA	1:E:101:ILE:HG22	2.02	0.42
2:F:266:GLU:O	2:F:269:ILE:HG13	2.19	0.42
2:F:289:PRO:HG3	2:F:540:ARG:NH1	2.35	0.42
2:F:306:LEU:O	2:F:310:VAL:HB	2.18	0.42
2:F:445:THR:HG23	2:F:446:PHE:CD2	2.54	0.42
7:D:40:TRP:CG	10:B:355:THR:HG1	2.37	0.42
9:K:62:THR:OG1	9:K:64:TYR:O	2.36	0.42
12:A:230:THR:HG21	12:A:235:LYS:HD3	2.02	0.42
12:A:370:SER:HA	12:A:383:GLY:HA3	2.02	0.42
2:R:266:GLU:O	2:R:269:ILE:HG13	2.19	0.42
3:G:156:VAL:HG11	4:H:122:ILE:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:B:605:CDL:H751	15:B:605:CDL:H571	2.01	0.42
12:A:164:ARG:NH2	12:A:166:ASP:OD2	2.52	0.42
15:P:201:CDL:H181	10:N:419:PRO:HB2	2.01	0.42
11:O:122:MET:O	11:O:124:ALA:N	2.53	0.42
12:M:164:ARG:NH2	12:M:166:ASP:OD2	2.53	0.42
15:T:201:CDL:H532	15:T:201:CDL:H151	2.02	0.42
10:N:47:LEU:HD22	10:N:227:LEU:HD21	2.01	0.42
10:N:207:LEU:O	10:N:211:HIS:CB	2.68	0.42
2:F:448:VAL:HG21	2:F:476:ILE:HG23	2.02	0.42
4:H:134:TRP:N	10:B:489:ASN:HD21	2.18	0.42
10:B:77:TYR:CZ	10:B:285:TRP:HB2	2.55	0.42
10:B:118:ALA:HB2	10:B:303:PHE:HZ	1.85	0.42
10:B:335:VAL:O	10:B:339:LEU:N	2.53	0.42
21:B:608:MQ9:H202	21:B:608:MQ9:H171	1.92	0.42
12:A:371:GLN:N	12:A:382:PHE:O	2.53	0.42
6:V:76:ASP:N	6:V:76:ASP:OD1	2.51	0.42
7:P:64:ARG:O	10:N:318:TRP:NE1	2.46	0.42
2:F:57:LEU:HB3	14:F:602:HEA:H202	2.02	0.42
7:D:48:MET:HB2	15:D:201:CDL:H121	2.01	0.42
10:B:31:ASN:HD22	10:B:252:ARG:HD2	1.84	0.42
19:A:503:9YF:C36	19:A:503:9YF:C40	2.98	0.42
2:R:80:ASN:HA	2:R:83:PHE:CE2	2.55	0.42
2:R:268:TYR:OH	14:R:601:HEA:O11	2.22	0.42
5:U:21:LEU:HA	5:U:24:ILE:HG12	2.02	0.42
6:V:138:ASN:HB3	6:V:141:ASP:HB2	2.02	0.42
12:M:289:ASP:OD1	12:M:289:ASP:N	2.46	0.42
2:F:103:ALA:HB2	2:F:213:ILE:HD13	2.02	0.42
10:B:207:LEU:O	10:B:211:HIS:CB	2.68	0.42
12:A:309:ARG:HD2	12:A:412:VAL:HG13	2.01	0.42
12:A:377:PHE:O	12:A:379:LYS:N	2.47	0.42
1:Q:241:PHE:HZ	1:Q:243:ARG:HH21	1.68	0.42
2:R:103:ALA:HB2	2:R:213:ILE:HD13	2.02	0.42
2:R:156:PRO:HD3	2:R:252:VAL:HG12	2.00	0.42
21:O:304:MQ9:H353	21:O:304:MQ9:H372	1.71	0.42
12:M:230:THR:HG21	12:M:235:LYS:HD3	2.02	0.42
1:E:241:PHE:HZ	1:E:243:ARG:HH21	1.68	0.41
15:H:201:CDL:H532	15:H:201:CDL:H151	2.02	0.41
6:J:138:ASN:HB3	6:J:141:ASP:HB2	2.02	0.41
10:B:136:PRO:HA	10:N:19:ARG:HG3	2.01	0.41
10:B:397:ALA:HB2	10:B:407:THR:HG21	2.02	0.41
1:Q:122:HIS:HB3	1:Q:220:ARG:HH22	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:507:VAL:HB	6:V:30:ALA:HB3	2.02	0.41
10:N:77:TYR:CZ	10:N:285:TRP:HB2	2.55	0.41
1:E:35:TRP:HZ3	2:F:387:HIS:ND1	2.18	0.41
2:F:85:MET:HE1	2:F:171:TRP:CD1	2.55	0.41
1:Q:129:VAL:HG23	1:Q:147:ILE:HG12	2.02	0.41
2:R:85:MET:HE1	2:R:171:TRP:CD1	2.55	0.41
3:S:30:ILE:HD13	3:S:30:ILE:HA	1.88	0.41
3:S:187:PHE:HA	3:S:190:ILE:HG22	2.01	0.41
5:U:70:VAL:HG23	6:V:112:ALA:HB2	2.02	0.41
7:P:83:ILE:HD11	10:N:417:VAL:HG23	2.02	0.41
9:W:172:PRO:HA	11:O:235:ARG:HG3	2.00	0.41
10:N:31:ASN:HD22	10:N:252:ARG:HD2	1.85	0.41
10:N:281:ILE:HG13	11:O:271:GLU:CD	2.45	0.41
11:O:174:GLY:N	11:O:247:ALA:HB2	2.35	0.41
1:E:129:VAL:HG23	1:E:147:ILE:HG12	2.02	0.41
2:F:277:ILE:O	2:F:281:ILE:HG12	2.20	0.41
10:B:19:ARG:NE	10:N:138:GLU:OE2	2.43	0.41
11:C:174:GLY:N	11:C:247:ALA:HB2	2.35	0.41
2:R:88:THR:HG22	2:R:151:TRP:HD1	1.86	0.41
2:R:104:ASN:HD21	2:R:122:ASN:ND2	2.18	0.41
2:R:194:VAL:HG22	4:T:4:GLU:HG2	2.02	0.41
2:R:264:HIS:HA	2:R:267:VAL:HG22	2.02	0.41
3:G:147:HIS:NE2	3:G:192:TRP:HB2	2.35	0.41
4:H:2:HIS:CE1	4:H:57:ARG:HH22	2.39	0.41
10:B:59:TRP:HE3	10:B:60:LEU:HD12	1.85	0.41
9:W:37:PRO:HG3	11:O:104:SER:HB3	2.01	0.41
2:F:104:ASN:HD21	2:F:122:ASN:ND2	2.18	0.41
6:J:130:ALA:HB1	6:J:134:PHE:HE2	1.85	0.41
10:B:37:HIS:NE2	15:B:604:CDL:OB4	2.52	0.41
1:Q:35:TRP:HZ3	2:R:387:HIS:ND1	2.18	0.41
15:R:606:CDL:H331	15:R:606:CDL:H671	2.01	0.41
7:P:48:MET:HB2	15:P:201:CDL:H121	2.01	0.41
9:W:54:VAL:HB	9:W:75:PHE:HB3	2.01	0.41
10:N:29:GLN:NE2	15:N:604:CDL:OB7	2.53	0.41
9:K:107:PRO:HD3	9:K:112:LEU:HD12	2.02	0.41
21:C:304:MQ9:H301	21:C:304:MQ9:H322	1.92	0.41
1:Q:98:LEU:HA	1:Q:101:ILE:HG22	2.02	0.41
4:T:66:ARG:HE	4:T:68:GLU:HB3	1.86	0.41
2:F:121:LEU:HD11	15:F:605:CDL:H342	2.03	0.41
5:I:21:LEU:HA	5:I:24:ILE:HG12	2.02	0.41
17:K:203:PLM:HE1	17:K:203:PLM:HB2	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:41:LEU:O	10:B:44:GLU:HB2	2.20	0.41
15:B:603:CDL:H602	15:B:611:CDL:H531	2.02	0.41
11:C:169:GLN:NE2	11:C:214:ASN:HD21	2.18	0.41
12:A:271:PRO:HG3	12:A:402:LEU:HD21	2.03	0.41
12:A:418:GLU:CD	19:A:503:9YF:O8	2.63	0.41
1:Q:121:MET:HE2	1:Q:123:LYS:HG3	2.02	0.41
1:Q:128:GLU:HG2	1:Q:220:ARG:HB3	2.03	0.41
1:Q:137:GLN:HE21	1:Q:138:TRP:NE1	2.18	0.41
3:S:156:VAL:HG11	4:T:122:ILE:HD12	2.01	0.41
15:T:201:CDL:H342	15:N:606:CDL:H152	2.03	0.41
6:V:130:ALA:HB1	6:V:134:PHE:HE2	1.85	0.41
10:N:213:LEU:O	10:N:217:GLY:N	2.44	0.41
12:M:370:SER:HA	12:M:383:GLY:HA3	2.01	0.41
2:F:117:ALA:O	3:G:15:ARG:NH1	2.53	0.41
3:G:76:VAL:HG11	3:G:112:PHE:HD2	1.86	0.41
10:B:58:VAL:O	10:B:61:THR:OG1	2.30	0.41
10:B:370:VAL:HG22	10:B:373:ARG:HB3	2.03	0.41
12:A:134:LEU:O	12:A:138:LEU:HB2	2.21	0.41
12:A:418:GLU:OE2	19:A:503:9YF:C28	2.69	0.41
2:R:57:LEU:HB3	14:R:602:HEA:H202	2.02	0.41
2:R:68:MET:HE3	2:R:72:GLN:HG3	2.03	0.41
10:N:136:PRO:O	10:N:233:GLN:NE2	2.43	0.41
1:E:55:ILE:HD13	1:E:55:ILE:HA	1.91	0.41
1:E:121:MET:HE2	1:E:123:LYS:HG3	2.02	0.41
1:E:137:GLN:HE21	1:E:138:TRP:NE1	2.18	0.41
7:D:5:GLN:HE21	10:B:467:PRO:HD3	1.86	0.41
10:B:130:THR:HB	10:B:364:LEU:HD13	2.02	0.41
10:B:250:GLY:O	12:A:160:SER:N	2.53	0.41
11:C:215:PRO:HA	11:C:218:ILE:HD12	2.03	0.41
2:R:46:VAL:HG21	15:R:606:CDL:H531	2.03	0.41
2:R:121:LEU:HD11	15:R:605:CDL:H342	2.03	0.41
10:N:37:HIS:NE2	15:N:605:CDL:OB4	2.53	0.41
10:N:130:THR:HB	10:N:364:LEU:HD13	2.03	0.41
10:N:145:SER:O	10:N:149:ILE:HG12	2.21	0.41
12:M:134:LEU:O	12:M:138:LEU:HB2	2.21	0.41
12:M:271:PRO:HG3	12:M:402:LEU:HD21	2.03	0.41
12:M:309:ARG:HD2	12:M:412:VAL:HG13	2.02	0.41
2:F:208:ILE:HB	2:F:293:TYR:HE1	1.86	0.41
2:F:445:THR:HA	2:F:477:SER:HA	2.03	0.41
9:K:35:GLN:HG2	12:A:359:GLN:HB3	2.03	0.41
10:B:291:LYS:HA	10:B:292:PRO:HD3	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:503:9YF:C1	19:A:503:9YF:C28	2.99	0.41
4:T:134:TRP:N	10:N:489:ASN:HD21	2.18	0.41
10:N:370:VAL:HG22	10:N:373:ARG:HB3	2.03	0.41
2:F:33:THR:OG1	4:H:89:SER:N	2.55	0.40
2:F:330:THR:HA	2:F:333:ILE:HG12	2.03	0.40
4:H:66:ARG:HE	4:H:68:GLU:HB3	1.85	0.40
7:D:35:SER:HB2	7:D:38:TRP:CD1	2.57	0.40
9:K:30:SER:O	9:K:34:THR:OG1	2.34	0.40
2:R:208:ILE:HB	2:R:293:TYR:HE1	1.86	0.40
10:N:397:ALA:HB2	10:N:407:THR:HG21	2.02	0.40
7:D:88:GLY:HA3	15:D:201:CDL:H851	2.04	0.40
11:C:177:VAL:O	11:C:181:GLY:N	2.51	0.40
2:R:267:VAL:HA	2:R:270:ILE:HD12	2.04	0.40
2:R:277:ILE:O	2:R:281:ILE:HG12	2.20	0.40
4:T:2:HIS:CE1	4:T:57:ARG:HH22	2.38	0.40
10:N:118:ALA:HB2	10:N:303:PHE:HZ	1.85	0.40
21:N:610:MQ9:H271	21:N:610:MQ9:H253	1.87	0.40
2:F:124:LEU:HD11	4:H:95:ILE:HG21	2.04	0.40
2:F:507:VAL:HB	6:J:30:ALA:HB3	2.03	0.40
15:H:201:CDL:H161	15:A:502:CDL:H752	2.04	0.40
9:K:67:PRO:HB3	9:K:140:THR:HA	2.04	0.40
1:Q:246:LEU:HD22	1:Q:254:SER:HB2	2.03	0.40
14:R:601:HEA:H263	14:R:601:HEA:H132	1.95	0.40
10:N:59:TRP:HE3	10:N:60:LEU:HD12	1.85	0.40
1:E:214:VAL:HG11	1:E:313:LEU:HD21	2.04	0.40
2:F:264:HIS:HA	2:F:267:VAL:HG22	2.03	0.40
10:B:177:GLY:HA3	12:A:349:LEU:HA	2.04	0.40
3:S:147:HIS:NE2	3:S:192:TRP:HB2	2.36	0.40
4:T:108:LEU:O	4:T:110:LEU:N	2.54	0.40
10:N:41:LEU:O	10:N:44:GLU:HB2	2.20	0.40
2:F:242:ALA:O	3:G:138:SER:OG	2.29	0.40
2:F:267:VAL:HA	2:F:270:ILE:HD12	2.04	0.40
10:B:145:SER:O	10:B:149:ILE:HG12	2.21	0.40
21:B:608:MQ9:H201	21:B:608:MQ9:H222	2.01	0.40
12:A:394:ILE:HD13	12:A:394:ILE:HG21	1.91	0.40
2:R:330:THR:HA	2:R:333:ILE:HG12	2.04	0.40
10:N:44:GLU:O	10:N:48:TYR:N	2.47	0.40
10:N:249:VAL:HG23	12:M:161:VAL:HB	2.04	0.40
11:O:98:VAL:HA	11:O:99:PRO:HD3	1.94	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	E	310/341 (91%)	269 (87%)	41 (13%)	0	100	100
1	Q	310/341 (91%)	268 (86%)	42 (14%)	0	100	100
2	F	550/575 (96%)	506 (92%)	44 (8%)	0	100	100
2	R	550/575 (96%)	507 (92%)	43 (8%)	0	100	100
3	G	201/203 (99%)	187 (93%)	13 (6%)	1 (0%)	24	57
3	S	201/203 (99%)	187 (93%)	13 (6%)	1 (0%)	24	57
4	H	137/139 (99%)	125 (91%)	12 (9%)	0	100	100
4	T	137/139 (99%)	125 (91%)	12 (9%)	0	100	100
5	I	63/79 (80%)	57 (90%)	6 (10%)	0	100	100
5	U	63/79 (80%)	57 (90%)	6 (10%)	0	100	100
6	J	143/157 (91%)	129 (90%)	14 (10%)	0	100	100
6	V	143/157 (91%)	129 (90%)	14 (10%)	0	100	100
7	D	88/100 (88%)	84 (96%)	4 (4%)	0	100	100
7	P	88/100 (88%)	83 (94%)	5 (6%)	0	100	100
8	Y	214/236 (91%)	185 (86%)	29 (14%)	0	100	100
8	Z	214/236 (91%)	188 (88%)	26 (12%)	0	100	100
9	K	141/186 (76%)	118 (84%)	22 (16%)	1 (1%)	18	51
9	W	141/186 (76%)	116 (82%)	24 (17%)	1 (1%)	18	51
10	B	533/546 (98%)	492 (92%)	40 (8%)	1 (0%)	43	74
10	N	533/546 (98%)	492 (92%)	40 (8%)	1 (0%)	43	74
11	C	221/294 (75%)	197 (89%)	23 (10%)	1 (0%)	24	57
11	O	221/294 (75%)	196 (89%)	24 (11%)	1 (0%)	24	57
12	A	380/421 (90%)	337 (89%)	43 (11%)	0	100	100
12	M	380/421 (90%)	336 (88%)	44 (12%)	0	100	100
All	All	5962/6554 (91%)	5370 (90%)	584 (10%)	8 (0%)	49	79

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	G	14	SER
3	S	14	SER
11	C	226	PRO
11	O	226	PRO
9	K	117	PRO
9	W	117	PRO
10	B	241	PRO
10	N	241	PRO

5.3.2 Protein sidechains [i](#)

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	E	260/288 (90%)	258 (99%)	2 (1%)	73	77
1	Q	260/288 (90%)	258 (99%)	2 (1%)	73	77
2	F	453/471 (96%)	450 (99%)	3 (1%)	76	78
2	R	453/471 (96%)	449 (99%)	4 (1%)	70	76
3	G	155/161 (96%)	155 (100%)	0	100	100
3	S	155/161 (96%)	155 (100%)	0	100	100
4	H	106/106 (100%)	106 (100%)	0	100	100
4	T	106/106 (100%)	106 (100%)	0	100	100
5	I	52/59 (88%)	52 (100%)	0	100	100
5	U	52/59 (88%)	52 (100%)	0	100	100
6	J	107/114 (94%)	106 (99%)	1 (1%)	70	76
6	V	107/114 (94%)	106 (99%)	1 (1%)	70	76
7	D	76/83 (92%)	76 (100%)	0	100	100
7	P	76/83 (92%)	76 (100%)	0	100	100
8	Y	20/167 (12%)	20 (100%)	0	100	100
8	Z	20/167 (12%)	20 (100%)	0	100	100
9	K	120/146 (82%)	119 (99%)	1 (1%)	73	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	W	120/146 (82%)	119 (99%)	1 (1%)	73	77
10	B	429/438 (98%)	426 (99%)	3 (1%)	76	78
10	N	429/438 (98%)	426 (99%)	3 (1%)	76	78
11	C	163/220 (74%)	163 (100%)	0	100	100
11	O	163/220 (74%)	163 (100%)	0	100	100
12	A	312/343 (91%)	311 (100%)	1 (0%)	86	83
12	M	312/343 (91%)	311 (100%)	1 (0%)	86	83
All	All	4506/5192 (87%)	4483 (100%)	23 (0%)	78	80

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	179	ILE
1	E	263	ILE
2	F	187	VAL
2	F	205	ARG
2	F	452	LEU
6	J	73	LEU
9	K	88	LEU
10	B	134	ARG
10	B	295	VAL
10	B	327	ILE
12	A	138	LEU
1	Q	179	ILE
1	Q	263	ILE
2	R	187	VAL
2	R	205	ARG
2	R	410	THR
2	R	452	LEU
6	V	73	LEU
9	W	88	LEU
10	N	134	ARG
10	N	295	VAL
10	N	327	ILE
12	M	138	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	117	GLN
1	E	137	GLN
1	E	309	ASN
2	F	37	HIS
2	F	76	ASN
2	F	80	ASN
2	F	122	ASN
2	F	474	ASN
3	G	66	ASN
3	G	150	HIS
3	G	186	HIS
4	H	2	HIS
6	J	40	HIS
7	D	5	GLN
9	K	28	GLN
9	K	40	ASN
9	K	43	ASN
10	B	31	ASN
10	B	365	GLN
10	B	393	ASN
10	B	473	HIS
10	B	489	ASN
11	C	94	ASN
11	C	96	GLN
11	C	153	ASN
11	C	164	HIS
11	C	169	GLN
11	C	193	ASN
11	C	227	GLN
12	A	151	GLN
12	A	310	ASN
12	A	369	GLN
1	Q	117	GLN
1	Q	137	GLN
1	Q	309	ASN
2	R	37	HIS
2	R	76	ASN
2	R	80	ASN
2	R	122	ASN
2	R	474	ASN
3	S	66	ASN
3	S	150	HIS
3	S	186	HIS

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Mol	Chain	Res	Type
4	T	2	HIS
6	V	40	HIS
7	P	5	GLN
9	W	28	GLN
9	W	40	ASN
9	W	43	ASN
10	N	31	ASN
10	N	282	ASN
10	N	329	GLN
10	N	360	HIS
10	N	365	GLN
10	N	489	ASN
11	O	94	ASN
11	O	151	GLN
11	O	153	ASN
11	O	164	HIS
11	O	169	GLN
11	O	193	ASN
11	O	227	GLN
12	M	151	GLN
12	M	310	ASN
12	M	359	GLN
12	M	369	GLN

5.3.3 RNA [i](#)

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 74 ligands modelled in this entry, 8 are monoatomic - leaving 66 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$
19	9YF	C	303	-	58,58,58	0.85	4 (6%)	69,71,71	0.94	3 (4%)
15	CDL	F	606	-	80,80,99	1.23	6 (7%)	86,92,111	1.00	5 (5%)
22	HEC	O	302	11	50,50,50	1.70	6 (12%)	68,82,82	2.11	18 (26%)
15	CDL	B	611	-	65,65,99	1.35	8 (12%)	71,77,111	1.15	4 (5%)
15	CDL	N	606	-	78,78,99	1.25	7 (8%)	84,90,111	0.98	5 (5%)
16	9Y0	B	606	15	48,48,48	1.30	5 (10%)	51,53,53	0.89	2 (3%)
19	9YF	M	504	-	58,58,58	1.16	4 (6%)	69,71,71	1.11	5 (7%)
21	MQ9	N	607	-	44,44,59	3.93	15 (34%)	54,57,75	3.23	23 (42%)
18	9XX	K	204	9	41,41,41	1.16	3 (7%)	44,44,44	1.15	3 (6%)
16	9Y0	S	301	-	42,42,48	1.35	5 (11%)	44,47,53	0.85	2 (4%)
17	PLM	Y	301	8	10,10,17	0.56	0	9,9,17	0.56	0
16	9Y0	G	301	-	42,42,48	1.35	5 (11%)	44,47,53	0.85	2 (4%)
15	CDL	F	605	-	75,75,99	1.25	7 (9%)	81,87,111	1.04	4 (4%)
15	CDL	N	601	-	65,65,99	1.35	7 (10%)	71,77,111	1.15	4 (5%)
16	9Y0	B	612	15	48,48,48	1.30	5 (10%)	51,53,53	0.89	2 (3%)
21	MQ9	N	609	-	59,59,59	3.97	19 (32%)	72,75,75	3.44	35 (48%)
19	9YF	W	202	-	58,58,58	0.88	4 (6%)	69,71,71	0.96	3 (4%)
15	CDL	R	606	-	80,80,99	1.22	6 (7%)	86,92,111	1.00	5 (5%)
15	CDL	B	605	-	78,78,99	1.25	7 (8%)	84,90,111	0.98	5 (5%)
20	HEM	B	601	10	49,49,50	1.20	4 (8%)	66,81,82	1.40	9 (13%)
19	9YF	K	202	-	58,58,58	0.88	4 (6%)	69,71,71	0.94	3 (4%)
16	9Y0	W	201	-	37,37,48	1.42	4 (10%)	40,42,53	1.00	2 (5%)
23	FES	M	502	12	0,4,4	-	-	-	-	-
16	9Y0	K	201	-	37,37,48	1.42	3 (8%)	40,42,53	1.02	2 (5%)
14	HEA	R	602	2	66,67,67	5.49	24 (36%)	78,103,103	5.14	56 (71%)
18	9XX	Z	302	8	31,31,41	1.27	3 (9%)	34,34,44	1.13	2 (5%)
17	PLM	Z	301	8	10,10,17	0.57	0	9,9,17	0.56	0
22	HEC	O	301	11	50,50,50	1.78	6 (12%)	68,82,82	1.54	8 (11%)
15	CDL	N	605	-	76,76,99	1.26	7 (9%)	82,88,111	1.08	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	MQ9	C	304	-	59,59,59	3.89	18 (30%)	72,75,75	3.43	31 (43%)
16	9Y0	D	202	-	40,40,48	1.37	4 (10%)	43,45,53	1.00	2 (4%)
19	9YF	A	504	-	58,58,58	0.87	3 (5%)	69,71,71	0.96	4 (5%)
22	HEC	C	302	11	50,50,50	1.70	6 (12%)	68,82,82	2.11	18 (26%)
20	HEM	B	602	10	50,50,50	1.49	7 (14%)	66,82,82	1.13	7 (10%)
15	CDL	D	201	-	87,87,99	1.20	8 (9%)	93,99,111	0.94	5 (5%)
15	CDL	B	604	-	76,76,99	1.25	7 (9%)	82,88,111	1.08	5 (6%)
21	MQ9	B	610	-	44,44,59	3.95	16 (36%)	54,57,75	3.20	22 (40%)
21	MQ9	O	304	-	59,59,59	3.89	18 (30%)	72,75,75	3.43	32 (44%)
16	9Y0	P	202	-	40,40,48	1.38	4 (10%)	43,45,53	0.99	2 (4%)
15	CDL	M	503	-	94,94,99	1.19	6 (6%)	100,106,111	0.93	5 (5%)
17	PLM	K	203	9	16,16,17	0.47	0	15,15,17	0.44	0
21	MQ9	N	610	-	44,44,59	3.95	16 (36%)	54,57,75	3.20	22 (40%)
15	CDL	R	605	-	75,75,99	1.25	7 (9%)	81,87,111	1.04	4 (4%)
19	9YF	M	501	-	58,58,58	0.87	3 (5%)	69,71,71	0.96	4 (5%)
14	HEA	F	602	2	66,67,67	5.49	24 (36%)	78,103,103	5.14	55 (70%)
15	CDL	P	201	-	87,87,99	1.20	8 (9%)	93,99,111	0.95	5 (5%)
15	CDL	N	604	16	73,73,99	1.32	7 (9%)	79,85,111	1.04	5 (6%)
19	9YF	O	303	-	58,58,58	0.85	4 (6%)	69,71,71	0.94	3 (4%)
14	HEA	R	601	2	66,67,67	5.11	20 (30%)	78,103,103	6.59	56 (71%)
19	9YF	A	503	-	58,58,58	1.16	4 (6%)	69,71,71	1.23	7 (10%)
15	CDL	T	201	-	78,78,99	1.25	7 (8%)	84,90,111	0.92	4 (4%)
22	HEC	C	301	11	50,50,50	1.78	6 (12%)	68,82,82	1.54	8 (11%)
15	CDL	B	603	16	73,73,99	1.32	7 (9%)	79,85,111	1.04	4 (5%)
21	MQ9	B	608	-	49,49,59	3.95	16 (32%)	60,63,75	3.30	25 (41%)
15	CDL	A	502	-	94,94,99	1.19	6 (6%)	100,106,111	0.93	5 (5%)
21	MQ9	N	608	-	49,49,59	3.95	16 (32%)	60,63,75	3.31	26 (43%)
18	9XX	W	204	9	41,41,41	1.15	3 (7%)	44,44,44	1.11	3 (6%)
23	FES	A	501	12	0,4,4	-	-	-	-	-
20	HEM	N	602	10	49,49,50	1.20	4 (8%)	66,81,82	1.39	9 (13%)
15	CDL	H	201	-	78,78,99	1.25	7 (8%)	84,90,111	0.92	4 (4%)
18	9XX	Y	302	8	31,31,41	1.27	3 (9%)	34,34,44	1.14	2 (5%)
21	MQ9	B	609	-	59,59,59	3.97	19 (32%)	72,75,75	3.44	35 (48%)
20	HEM	N	603	10	50,50,50	1.49	7 (14%)	66,82,82	1.14	7 (10%)
14	HEA	F	601	2	66,67,67	5.10	20 (30%)	78,103,103	6.59	56 (71%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	MQ9	B	607	-	44,44,59	3.94	17 (38%)	54,57,75	3.23	23 (42%)
17	PLM	W	203	9	16,16,17	0.48	0	15,15,17	0.44	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	9YF	C	303	-	-	33/54/78/78	0/1/1/1
15	CDL	F	606	-	-	51/91/91/110	-
22	HEC	O	302	11	1/1/3/7	4/14/54/54	-
15	CDL	B	611	-	-	44/76/76/110	-
15	CDL	N	606	-	-	41/89/89/110	-
16	9Y0	B	606	15	-	33/52/52/52	-
19	9YF	M	504	-	-	29/54/78/78	0/1/1/1
21	MQ9	N	607	-	-	19/35/55/73	0/2/2/2
18	9XX	K	204	9	-	22/43/43/43	-
16	9Y0	S	301	-	-	23/46/46/52	-
17	PLM	Y	301	8	-	0/7/8/15	-
16	9Y0	G	301	-	-	22/46/46/52	-
15	CDL	F	605	-	-	39/86/86/110	-
15	CDL	N	601	-	-	42/76/76/110	-
16	9Y0	B	612	15	-	34/52/52/52	-
21	MQ9	N	609	-	-	25/53/73/73	0/2/2/2
19	9YF	W	202	-	-	24/54/78/78	0/1/1/1
15	CDL	R	606	-	-	49/91/91/110	-
15	CDL	B	605	-	-	42/89/89/110	-
20	HEM	B	601	10	-	4/12/52/54	-
19	9YF	K	202	-	-	28/54/78/78	0/1/1/1
16	9Y0	W	201	-	-	29/41/41/52	-
23	FES	M	502	12	-	-	0/1/1/1
16	9Y0	K	201	-	-	27/41/41/52	-
14	HEA	R	602	2	-	16/36/76/76	-
18	9XX	Z	302	8	-	13/33/33/43	-
17	PLM	Z	301	8	-	0/7/8/15	-
22	HEC	O	301	11	-	3/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CDL	N	605	-	-	49/87/87/110	-
21	MQ9	C	304	-	-	31/53/73/73	0/2/2/2
16	9Y0	D	202	-	-	26/44/44/52	-
19	9YF	A	504	-	-	21/54/78/78	0/1/1/1
22	HEC	C	302	11	1/1/3/7	4/14/54/54	-
20	HEM	B	602	10	-	5/14/54/54	-
15	CDL	D	201	-	-	56/98/98/110	-
15	CDL	B	604	-	-	49/87/87/110	-
21	MQ9	B	610	-	-	19/35/55/73	0/2/2/2
21	MQ9	O	304	-	-	31/53/73/73	0/2/2/2
16	9Y0	P	202	-	-	26/44/44/52	-
15	CDL	M	503	-	-	61/105/105/110	-
17	PLM	K	203	9	-	4/13/14/15	-
21	MQ9	N	610	-	-	19/35/55/73	0/2/2/2
15	CDL	R	605	-	-	38/86/86/110	-
19	9YF	M	501	-	-	21/54/78/78	0/1/1/1
14	HEA	F	602	2	-	16/36/76/76	-
15	CDL	P	201	-	-	57/98/98/110	-
15	CDL	N	604	16	-	52/84/84/110	-
19	9YF	O	303	-	-	33/54/78/78	0/1/1/1
14	HEA	R	601	2	-	20/36/76/76	-
19	9YF	A	503	-	-	26/54/78/78	0/1/1/1
15	CDL	T	201	-	-	52/89/89/110	-
22	HEC	C	301	11	-	3/14/54/54	-
15	CDL	B	603	16	-	51/84/84/110	-
21	MQ9	B	608	-	-	21/41/61/73	0/2/2/2
15	CDL	A	502	-	-	61/105/105/110	-
21	MQ9	N	608	-	-	21/41/61/73	0/2/2/2
18	9XX	W	204	9	-	24/43/43/43	-
23	FES	A	501	12	-	-	0/1/1/1
20	HEM	N	602	10	-	4/12/52/54	-
15	CDL	H	201	-	-	52/89/89/110	-
18	9XX	Y	302	8	-	13/33/33/43	-
21	MQ9	B	609	-	-	25/53/73/73	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	HEM	N	603	10	-	5/14/54/54	-
14	HEA	F	601	2	-	20/36/76/76	-
21	MQ9	B	607	-	-	19/35/55/73	0/2/2/2
17	PLM	W	203	9	-	4/13/14/15	-

All (506) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	F	602	HEA	CHA-C1A	16.63	1.70	1.38
14	R	602	HEA	CHA-C1A	16.58	1.70	1.38
14	F	602	HEA	CHD-C1D	16.08	1.71	1.38
14	R	602	HEA	CHD-C1D	16.04	1.71	1.38
14	R	601	HEA	CHD-C1D	16.00	1.71	1.38
14	F	601	HEA	CHD-C1D	15.98	1.71	1.38
14	R	601	HEA	CHA-C1A	15.46	1.68	1.38
14	F	601	HEA	CHA-C1A	15.46	1.68	1.38
14	R	602	HEA	CHC-C4B	15.00	1.69	1.38
14	F	602	HEA	CHC-C4B	14.96	1.68	1.38
14	R	602	HEA	CHB-C4A	14.45	1.66	1.38
14	F	602	HEA	CHB-C4A	14.44	1.66	1.38
14	R	602	HEA	CHB-C1B	13.80	1.70	1.39
14	F	602	HEA	CHB-C1B	13.76	1.70	1.39
14	R	601	HEA	CHB-C4A	13.73	1.65	1.38
14	F	601	HEA	CHB-C4A	13.72	1.65	1.38
14	R	601	HEA	CHC-C4B	13.66	1.66	1.38
14	F	601	HEA	CHC-C4B	13.64	1.66	1.38
14	R	601	HEA	CHB-C1B	12.17	1.67	1.39
14	F	601	HEA	CHB-C1B	12.15	1.67	1.39
14	R	602	HEA	CHC-C1C	11.89	1.66	1.39
14	F	602	HEA	CHC-C1C	11.88	1.66	1.39
14	R	602	HEA	CHD-C4C	11.64	1.65	1.39
14	F	602	HEA	CHD-C4C	11.61	1.65	1.39
14	F	601	HEA	CHD-C4C	11.45	1.65	1.39
14	R	601	HEA	CHD-C4C	11.43	1.65	1.39
14	R	601	HEA	CHC-C1C	10.85	1.63	1.39
14	F	601	HEA	CHC-C1C	10.85	1.63	1.39
14	F	602	HEA	CHA-C4D	10.79	1.63	1.39
14	R	602	HEA	CHA-C4D	10.78	1.63	1.39
14	R	601	HEA	CHA-C4D	9.97	1.62	1.39
14	F	601	HEA	CHA-C4D	9.94	1.61	1.39
14	F	602	HEA	C14-C15	9.66	1.56	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	R	602	HEA	C14-C15	9.64	1.56	1.33
21	N	610	MQ9	C18-C19	9.31	1.55	1.33
21	B	610	MQ9	C18-C19	9.30	1.55	1.33
21	N	609	MQ9	C23-C24	9.27	1.55	1.33
21	B	609	MQ9	C23-C24	9.27	1.55	1.33
21	B	609	MQ9	C18-C19	9.24	1.55	1.33
21	N	609	MQ9	C18-C19	9.22	1.55	1.33
21	B	607	MQ9	C18-C19	9.21	1.55	1.33
21	N	607	MQ9	C18-C19	9.21	1.55	1.33
21	C	304	MQ9	C33-C34	9.18	1.55	1.33
21	B	610	MQ9	C28-C29	9.14	1.54	1.33
21	B	608	MQ9	C28-C29	9.13	1.54	1.33
21	N	608	MQ9	C28-C29	9.13	1.54	1.33
21	O	304	MQ9	C33-C34	9.12	1.54	1.33
21	B	609	MQ9	C33-C34	9.10	1.54	1.33
21	B	610	MQ9	C23-C24	9.10	1.54	1.33
21	N	610	MQ9	C23-C24	9.09	1.54	1.33
21	N	609	MQ9	C33-C34	9.09	1.54	1.33
21	N	610	MQ9	C28-C29	9.08	1.54	1.33
21	N	608	MQ9	C33-C34	9.04	1.54	1.33
21	N	607	MQ9	C23-C24	9.02	1.54	1.33
21	O	304	MQ9	C28-C29	9.02	1.54	1.33
21	B	608	MQ9	C33-C34	9.02	1.54	1.33
21	C	304	MQ9	C28-C29	9.01	1.54	1.33
21	B	608	MQ9	C23-C24	9.01	1.54	1.33
21	B	609	MQ9	C28-C29	9.01	1.54	1.33
21	N	608	MQ9	C23-C24	9.00	1.54	1.33
21	B	607	MQ9	C23-C24	8.99	1.54	1.33
21	B	608	MQ9	C18-C19	8.98	1.54	1.33
21	N	608	MQ9	C18-C19	8.97	1.54	1.33
21	N	609	MQ9	C28-C29	8.97	1.54	1.33
21	O	304	MQ9	C23-C24	8.93	1.54	1.33
21	C	304	MQ9	C23-C24	8.91	1.54	1.33
21	C	304	MQ9	C38-C39	8.90	1.54	1.33
21	N	609	MQ9	C38-C39	8.89	1.54	1.33
21	B	609	MQ9	C38-C39	8.88	1.54	1.33
21	O	304	MQ9	C38-C39	8.88	1.54	1.33
14	R	601	HEA	C14-C15	8.88	1.54	1.33
14	F	601	HEA	C14-C15	8.88	1.54	1.33
21	B	607	MQ9	C28-C29	8.86	1.54	1.33
21	N	607	MQ9	C28-C29	8.84	1.54	1.33
21	B	609	MQ9	C13-C14	8.78	1.54	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	N	609	MQ9	C13-C14	8.77	1.54	1.33
14	R	601	HEA	C18-C19	8.75	1.54	1.33
21	B	610	MQ9	C13-C14	8.73	1.53	1.33
21	B	607	MQ9	C13-C14	8.72	1.53	1.33
21	N	610	MQ9	C13-C14	8.71	1.53	1.33
21	C	304	MQ9	C18-C19	8.70	1.53	1.33
14	F	601	HEA	C18-C19	8.69	1.53	1.33
21	N	607	MQ9	C13-C14	8.69	1.53	1.33
21	O	304	MQ9	C18-C19	8.68	1.53	1.33
21	N	608	MQ9	C13-C14	8.55	1.53	1.33
21	B	608	MQ9	C13-C14	8.55	1.53	1.33
21	B	609	MQ9	C43-C44	8.46	1.53	1.33
14	F	602	HEA	C18-C19	8.45	1.53	1.33
21	B	609	MQ9	C8-C9	8.43	1.53	1.33
21	N	609	MQ9	C43-C44	8.43	1.53	1.33
21	N	609	MQ9	C8-C9	8.42	1.53	1.33
14	R	602	HEA	C18-C19	8.39	1.53	1.33
21	B	610	MQ9	C8-C9	8.35	1.53	1.33
21	N	610	MQ9	C8-C9	8.35	1.53	1.33
21	B	607	MQ9	C8-C9	8.35	1.53	1.33
21	N	607	MQ9	C8-C9	8.32	1.52	1.33
21	C	304	MQ9	C43-C44	8.31	1.52	1.33
21	O	304	MQ9	C13-C14	8.30	1.52	1.33
21	O	304	MQ9	C43-C44	8.28	1.52	1.33
21	C	304	MQ9	C13-C14	8.28	1.52	1.33
21	B	608	MQ9	C8-C9	8.22	1.52	1.33
21	N	607	MQ9	O1-C1	8.19	1.40	1.23
21	N	608	MQ9	C8-C9	8.19	1.52	1.33
21	O	304	MQ9	C8-C9	8.19	1.52	1.33
21	C	304	MQ9	C8-C9	8.19	1.52	1.33
21	B	607	MQ9	O1-C1	8.17	1.40	1.23
21	B	607	MQ9	O4-C4	8.14	1.40	1.23
21	N	607	MQ9	O4-C4	8.11	1.40	1.23
21	N	609	MQ9	O4-C4	8.01	1.40	1.23
21	B	609	MQ9	O4-C4	8.01	1.40	1.23
21	N	608	MQ9	O4-C4	8.00	1.40	1.23
21	B	608	MQ9	O4-C4	7.99	1.40	1.23
21	B	609	MQ9	O1-C1	7.98	1.40	1.23
21	N	609	MQ9	O1-C1	7.96	1.40	1.23
21	C	304	MQ9	O1-C1	7.96	1.40	1.23
21	O	304	MQ9	O1-C1	7.96	1.40	1.23
21	N	610	MQ9	O1-C1	7.94	1.40	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	608	MQ9	O1-C1	7.91	1.40	1.23
21	N	608	MQ9	O1-C1	7.90	1.39	1.23
21	B	610	MQ9	O1-C1	7.90	1.39	1.23
21	N	610	MQ9	O4-C4	7.87	1.39	1.23
21	B	610	MQ9	O4-C4	7.84	1.39	1.23
21	O	304	MQ9	O4-C4	7.80	1.39	1.23
21	C	304	MQ9	O4-C4	7.80	1.39	1.23
21	B	610	MQ9	C33-C34	7.79	1.54	1.32
21	N	610	MQ9	C33-C34	7.76	1.54	1.32
21	N	608	MQ9	C38-C39	7.69	1.54	1.32
22	O	301	HEC	C3D-C2D	7.67	1.53	1.36
21	B	608	MQ9	C38-C39	7.65	1.54	1.32
22	C	301	HEC	C3D-C2D	7.63	1.53	1.36
22	C	302	HEC	C3D-C2D	7.50	1.52	1.36
22	O	302	HEC	C3D-C2D	7.49	1.52	1.36
21	N	607	MQ9	C33-C34	7.44	1.53	1.32
21	B	607	MQ9	C33-C34	7.39	1.53	1.32
14	R	602	HEA	C22-C23	7.26	1.53	1.32
14	F	602	HEA	C22-C23	7.25	1.53	1.32
21	C	304	MQ9	C48-C49	7.24	1.53	1.32
21	O	304	MQ9	C48-C49	7.24	1.53	1.32
21	N	609	MQ9	C48-C49	7.22	1.53	1.32
21	B	609	MQ9	C48-C49	7.21	1.53	1.32
14	R	601	HEA	C22-C23	7.10	1.52	1.32
14	F	601	HEA	C22-C23	7.09	1.52	1.32
14	R	602	HEA	C4A-NA	-5.12	1.29	1.39
14	F	602	HEA	C4A-NA	-5.08	1.29	1.39
20	B	602	HEM	FE-ND	4.76	2.09	1.94
20	N	603	HEM	FE-ND	4.75	2.09	1.94
22	C	301	HEC	FE-ND	4.65	2.09	1.94
22	O	301	HEC	FE-ND	4.64	2.09	1.94
14	F	602	HEA	FE-NC	-4.46	1.79	1.95
14	R	602	HEA	FE-NC	-4.44	1.80	1.95
14	F	602	HEA	C1C-NC	-4.38	1.31	1.39
21	O	304	MQ9	C5-C4	-4.38	1.38	1.48
21	N	608	MQ9	C5-C4	-4.35	1.38	1.48
14	R	602	HEA	C1C-NC	-4.34	1.31	1.39
21	C	304	MQ9	C5-C4	-4.34	1.38	1.48
21	B	608	MQ9	C5-C4	-4.32	1.38	1.48
14	R	602	HEA	CMA-C3A	4.29	1.54	1.45
14	F	602	HEA	C1A-C2A	-4.29	1.37	1.45
14	R	602	HEA	C1A-C2A	-4.27	1.37	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	F	602	HEA	C4D-ND	-4.26	1.30	1.38
14	R	602	HEA	C4D-ND	-4.24	1.30	1.38
14	F	602	HEA	CMA-C3A	4.23	1.54	1.45
21	N	610	MQ9	C5-C4	-4.22	1.39	1.48
21	B	610	MQ9	C5-C4	-4.22	1.39	1.48
14	R	601	HEA	C4A-NA	-4.21	1.31	1.39
14	F	601	HEA	C4A-NA	-4.19	1.31	1.39
14	R	601	HEA	C1A-C2A	-4.15	1.37	1.45
14	F	601	HEA	C1A-C2A	-4.11	1.37	1.45
21	N	609	MQ9	C5-C4	-4.04	1.39	1.48
21	B	609	MQ9	C5-C4	-4.02	1.39	1.48
20	B	602	HEM	FE-NA	4.02	2.08	1.95
21	B	607	MQ9	C5-C4	-4.02	1.39	1.48
21	N	607	MQ9	C5-C4	-4.01	1.39	1.48
20	N	603	HEM	FE-NA	4.01	2.08	1.95
16	K	201	9Y0	O7-C21	4.00	1.45	1.34
16	W	201	9Y0	O7-C21	3.99	1.45	1.34
16	D	202	9Y0	O7-C21	3.86	1.45	1.34
16	P	202	9Y0	O7-C21	3.83	1.45	1.34
14	R	601	HEA	CMA-C3A	3.77	1.53	1.45
14	F	601	HEA	CMA-C3A	3.74	1.53	1.45
16	B	612	9Y0	O7-C21	3.73	1.44	1.34
16	B	606	9Y0	O7-C21	3.70	1.44	1.34
14	R	601	HEA	C1C-NC	-3.68	1.32	1.39
16	G	301	9Y0	O7-C21	3.66	1.44	1.34
16	S	301	9Y0	O7-C21	3.64	1.44	1.34
14	F	601	HEA	C1C-NC	-3.63	1.32	1.39
22	C	301	HEC	FE-NB	3.61	2.06	1.94
15	B	611	CDL	OA6-CA5	3.61	1.44	1.34
15	N	601	CDL	OA6-CA5	3.60	1.44	1.34
16	P	202	9Y0	O5-C5	3.59	1.43	1.33
16	D	202	9Y0	O5-C5	3.59	1.43	1.33
22	C	302	HEC	FE-NB	3.59	2.06	1.94
15	B	603	CDL	OB8-CB7	3.59	1.43	1.33
14	F	602	HEA	C3B-C2B	3.58	1.42	1.34
14	R	602	HEA	C3B-C2B	3.58	1.42	1.34
16	W	201	9Y0	O5-C5	3.57	1.43	1.33
15	N	604	CDL	OB8-CB7	3.56	1.43	1.33
22	O	301	HEC	FE-NB	3.56	2.05	1.94
22	O	302	HEC	FE-NB	3.54	2.05	1.94
15	N	605	CDL	OB8-CB7	3.53	1.43	1.33
16	K	201	9Y0	O5-C5	3.50	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	N	601	CDL	OB8-CB7	3.49	1.43	1.33
15	B	611	CDL	OB8-CB7	3.49	1.43	1.33
15	A	502	CDL	OB8-CB7	3.48	1.43	1.33
15	B	604	CDL	OB8-CB7	3.48	1.43	1.33
15	M	503	CDL	OB8-CB7	3.48	1.43	1.33
15	D	201	CDL	OB8-CB7	3.48	1.43	1.33
15	P	201	CDL	OB8-CB7	3.47	1.43	1.33
16	G	301	9Y0	O5-C5	3.47	1.43	1.33
16	B	612	9Y0	O5-C5	3.47	1.43	1.33
16	S	301	9Y0	O5-C5	3.46	1.43	1.33
15	T	201	CDL	OB8-CB7	3.46	1.43	1.33
15	H	201	CDL	OB8-CB7	3.46	1.43	1.33
21	C	304	MQ9	C3-C4	-3.44	1.41	1.48
15	F	605	CDL	OB8-CB7	3.44	1.43	1.33
14	R	602	HEA	FE-ND	-3.44	1.84	1.94
14	R	602	HEA	C4C-NC	-3.43	1.33	1.39
16	B	606	9Y0	O5-C5	3.43	1.43	1.33
18	W	204	9XX	O1-C17	-3.43	1.41	1.47
21	O	304	MQ9	C3-C4	-3.41	1.41	1.48
15	R	605	CDL	OB8-CB7	3.40	1.43	1.33
14	F	602	HEA	FE-ND	-3.39	1.84	1.94
15	B	605	CDL	OA6-CA5	3.38	1.43	1.34
15	R	606	CDL	OB8-CB7	3.38	1.43	1.33
15	N	606	CDL	OB8-CB7	3.38	1.43	1.33
15	N	606	CDL	OA6-CA5	3.38	1.43	1.34
14	F	602	HEA	C4C-NC	-3.37	1.33	1.39
15	F	606	CDL	OB8-CB7	3.37	1.43	1.33
15	B	605	CDL	OB8-CB7	3.37	1.43	1.33
18	K	204	9XX	O1-C17	-3.36	1.41	1.47
21	B	608	MQ9	C3-C4	-3.35	1.41	1.48
21	N	608	MQ9	C3-C4	-3.35	1.41	1.48
15	B	603	CDL	OA8-CA7	3.32	1.43	1.33
15	N	604	CDL	OA8-CA7	3.32	1.43	1.33
21	B	608	MQ9	C6-C1	-3.30	1.38	1.47
21	N	608	MQ9	C6-C1	-3.30	1.38	1.47
15	A	502	CDL	OA6-CA5	3.26	1.43	1.34
21	C	304	MQ9	C6-C1	-3.26	1.39	1.47
15	M	503	CDL	OA6-CA5	3.26	1.43	1.34
15	B	603	CDL	OA6-CA5	3.25	1.43	1.34
21	O	304	MQ9	C6-C1	-3.24	1.39	1.47
15	R	605	CDL	OA6-CA5	3.24	1.43	1.34
15	N	604	CDL	OA6-CA5	3.23	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	F	605	CDL	OA6-CA5	3.21	1.43	1.34
15	R	606	CDL	OA6-CA5	3.21	1.43	1.34
15	F	606	CDL	OA6-CA5	3.21	1.43	1.34
18	Y	302	9XX	O-C15	3.20	1.42	1.33
18	Z	302	9XX	O-C15	3.19	1.42	1.33
18	K	204	9XX	O-C15	3.19	1.42	1.33
18	W	204	9XX	O-C15	3.18	1.42	1.33
15	F	606	CDL	OA8-CA7	3.18	1.42	1.33
22	O	302	HEC	FE-NC	3.18	2.05	1.95
21	O	304	MQ9	C2-C3	-3.17	1.35	1.40
15	R	606	CDL	OA8-CA7	3.17	1.42	1.33
15	H	201	CDL	OA6-CA5	3.15	1.43	1.34
21	B	610	MQ9	C6-C1	-3.14	1.39	1.47
22	C	302	HEC	FE-NC	3.14	2.05	1.95
21	N	610	MQ9	C6-C1	-3.14	1.39	1.47
15	N	601	CDL	OB6-CB5	3.13	1.43	1.34
15	B	605	CDL	OA8-CA7	3.13	1.42	1.33
15	B	611	CDL	OB6-CB5	3.12	1.43	1.34
15	T	201	CDL	OA6-CA5	3.12	1.43	1.34
15	N	606	CDL	OA8-CA7	3.11	1.42	1.33
15	M	503	CDL	OA8-CA7	3.11	1.42	1.33
15	B	605	CDL	OB6-CB5	3.10	1.43	1.34
21	C	304	MQ9	C2-C3	-3.10	1.35	1.40
19	A	503	9YF	O11-C25	3.10	1.42	1.33
15	A	502	CDL	OA8-CA7	3.09	1.42	1.33
14	R	601	HEA	C4D-ND	-3.08	1.32	1.38
21	B	607	MQ9	C6-C5	3.08	1.40	1.35
22	C	301	HEC	FE-NA	3.07	2.05	1.95
22	O	301	HEC	FE-NA	3.07	2.05	1.95
15	F	605	CDL	OA8-CA7	3.06	1.42	1.33
15	H	201	CDL	OA8-CA7	3.06	1.42	1.33
21	B	609	MQ9	C3-C4	-3.06	1.42	1.48
15	D	201	CDL	OA8-CA7	3.06	1.42	1.33
15	N	606	CDL	OB6-CB5	3.06	1.42	1.34
14	F	601	HEA	FE-NC	-3.06	1.84	1.95
21	N	609	MQ9	C3-C4	-3.06	1.42	1.48
15	B	611	CDL	OA8-CA7	3.05	1.42	1.33
15	N	601	CDL	OA8-CA7	3.05	1.42	1.33
21	N	607	MQ9	C6-C5	3.05	1.40	1.35
14	R	601	HEA	FE-NC	-3.05	1.84	1.95
15	N	604	CDL	OB6-CB5	3.04	1.42	1.34
15	P	201	CDL	OA8-CA7	3.04	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	T	201	CDL	OA8-CA7	3.04	1.42	1.33
15	R	605	CDL	OA8-CA7	3.03	1.42	1.33
15	B	603	CDL	OB6-CB5	3.02	1.42	1.34
15	B	604	CDL	OA6-CA5	3.01	1.42	1.34
19	M	504	9YF	O11-C25	3.01	1.42	1.33
21	B	608	MQ9	C2-C1	-3.01	1.42	1.48
15	N	605	CDL	OA6-CA5	3.00	1.42	1.34
14	F	601	HEA	C4D-ND	-3.00	1.32	1.38
21	N	608	MQ9	C2-C1	-2.99	1.42	1.48
15	N	605	CDL	OA8-CA7	2.98	1.42	1.33
21	C	304	MQ9	C2-C1	-2.97	1.42	1.48
21	O	304	MQ9	C2-C1	-2.97	1.42	1.48
15	M	503	CDL	OB6-CB5	2.97	1.42	1.34
15	B	604	CDL	OA8-CA7	2.96	1.42	1.33
15	D	201	CDL	OA6-CA5	2.95	1.42	1.34
15	A	502	CDL	OB6-CB5	2.95	1.42	1.34
21	B	609	MQ9	C6-C1	-2.95	1.39	1.47
21	N	609	MQ9	C6-C1	-2.93	1.39	1.47
15	P	201	CDL	OA6-CA5	2.92	1.42	1.34
18	Z	302	9XX	O1-C17	-2.92	1.42	1.47
21	N	609	MQ9	C6-C5	2.92	1.40	1.35
21	B	607	MQ9	C3-C4	-2.89	1.42	1.48
18	Y	302	9XX	O1-C17	-2.88	1.42	1.47
21	B	609	MQ9	C6-C5	2.87	1.40	1.35
21	N	607	MQ9	C3-C4	-2.84	1.42	1.48
21	N	610	MQ9	C2-C1	-2.83	1.42	1.48
21	N	607	MQ9	C7-C8	2.81	1.54	1.50
15	F	605	CDL	OB6-CB5	2.79	1.42	1.34
21	B	607	MQ9	C2-C1	-2.79	1.42	1.48
21	N	607	MQ9	C2-C1	-2.79	1.42	1.48
21	B	610	MQ9	C2-C1	-2.78	1.42	1.48
15	R	605	CDL	OB6-CB5	2.77	1.42	1.34
15	R	606	CDL	OB6-CB5	2.76	1.42	1.34
15	F	606	CDL	OB6-CB5	2.75	1.42	1.34
21	B	607	MQ9	C7-C8	2.75	1.54	1.50
19	A	504	9YF	O9-C	-2.74	1.39	1.46
21	B	609	MQ9	C2-C1	-2.73	1.43	1.48
18	Y	302	9XX	O1-C18	2.73	1.42	1.34
21	N	609	MQ9	C2-C1	-2.73	1.43	1.48
19	M	501	9YF	O9-C	-2.71	1.39	1.46
18	Z	302	9XX	O1-C18	2.71	1.42	1.34
21	N	610	MQ9	C6-C5	2.71	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	601	HEM	CAB-C3B	2.70	1.54	1.47
21	N	608	MQ9	C2-C3	-2.70	1.36	1.40
15	P	201	CDL	OB6-CB5	2.70	1.41	1.34
21	N	608	MQ9	C6-C5	2.69	1.40	1.35
21	N	610	MQ9	C3-C4	-2.69	1.43	1.48
15	D	201	CDL	OB6-CB5	2.68	1.41	1.34
21	B	607	MQ9	C6-C1	-2.68	1.40	1.47
21	B	610	MQ9	C3-C4	-2.68	1.43	1.48
21	B	608	MQ9	C6-C5	2.68	1.40	1.35
21	B	610	MQ9	C6-C5	2.68	1.40	1.35
15	H	201	CDL	OB6-CB5	2.67	1.41	1.34
15	T	201	CDL	OB6-CB5	2.67	1.41	1.34
21	N	607	MQ9	C6-C1	-2.67	1.40	1.47
22	C	302	HEC	FE-NA	2.67	2.04	1.95
21	B	608	MQ9	C2-C3	-2.66	1.36	1.40
15	B	604	CDL	OA6-CA4	-2.65	1.40	1.46
15	N	605	CDL	OB6-CB5	2.65	1.41	1.34
20	N	602	HEM	CAB-C3B	2.65	1.54	1.47
22	O	302	HEC	FE-NA	2.65	2.04	1.95
15	N	605	CDL	OA6-CA4	-2.64	1.40	1.46
15	B	604	CDL	OB6-CB5	2.63	1.41	1.34
21	B	607	MQ9	C2-C3	-2.62	1.36	1.40
21	N	607	MQ9	C2-C3	-2.62	1.36	1.40
14	R	602	HEA	C1D-C2D	-2.62	1.39	1.44
14	F	602	HEA	C1D-C2D	-2.61	1.39	1.44
15	D	201	CDL	OA6-CA4	-2.61	1.40	1.46
21	N	610	MQ9	C2-C3	-2.60	1.36	1.40
21	N	609	MQ9	C2-C3	-2.59	1.36	1.40
15	P	201	CDL	OA6-CA4	-2.58	1.40	1.46
19	M	504	9YF	P-O2	2.58	1.67	1.60
21	B	609	MQ9	C2-C3	-2.57	1.36	1.40
21	B	610	MQ9	C2-C3	-2.55	1.36	1.40
19	K	202	9YF	O9-C	-2.55	1.40	1.46
22	C	301	HEC	FE-NC	2.54	2.03	1.95
20	B	602	HEM	CAC-C3C	2.53	1.54	1.47
20	N	603	HEM	CAC-C3C	2.53	1.54	1.47
15	F	606	CDL	OA6-CA4	-2.52	1.40	1.46
21	C	304	MQ9	C6-C5	2.51	1.39	1.35
19	C	303	9YF	O9-C	-2.51	1.40	1.46
22	O	301	HEC	FE-NC	2.51	2.03	1.95
19	O	303	9YF	O9-C	-2.50	1.40	1.46
19	W	202	9YF	O9-C	-2.50	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	R	606	CDL	OA6-CA4	-2.48	1.40	1.46
15	H	201	CDL	OA6-CA4	-2.47	1.40	1.46
15	B	603	CDL	OA6-CA4	-2.47	1.40	1.46
15	N	604	CDL	OA6-CA4	-2.47	1.40	1.46
15	T	201	CDL	OA6-CA4	-2.47	1.40	1.46
14	R	601	HEA	CAC-C3C	2.46	1.54	1.47
21	O	304	MQ9	C6-C5	2.46	1.39	1.35
15	F	605	CDL	OA6-CA4	-2.46	1.40	1.46
15	A	502	CDL	OA6-CA4	-2.45	1.40	1.46
15	M	503	CDL	OA6-CA4	-2.45	1.40	1.46
14	F	601	HEA	CAC-C3C	2.45	1.54	1.47
20	N	603	HEM	CAB-C3B	2.43	1.54	1.47
15	R	605	CDL	OA6-CA4	-2.43	1.40	1.46
18	K	204	9XX	O1-C18	2.43	1.41	1.34
20	B	602	HEM	CAB-C3B	2.42	1.54	1.47
19	K	202	9YF	O11-C25	2.42	1.40	1.33
18	W	204	9XX	O1-C18	2.40	1.41	1.34
21	B	610	MQ9	C7-C8	2.38	1.54	1.50
21	N	610	MQ9	C7-C8	2.38	1.54	1.50
19	M	501	9YF	O11-C25	2.38	1.40	1.33
14	R	602	HEA	FE-NA	-2.38	1.87	1.95
14	F	602	HEA	FE-NA	-2.36	1.87	1.95
19	W	202	9YF	O11-C25	2.36	1.40	1.33
16	W	201	9Y0	C22-C21	2.36	1.57	1.50
19	A	503	9YF	P-O2	2.35	1.66	1.60
16	B	606	9Y0	C22-C21	2.35	1.57	1.50
16	P	202	9Y0	C22-C21	2.35	1.57	1.50
19	A	504	9YF	O11-C25	2.35	1.40	1.33
14	R	601	HEA	C4C-NC	-2.34	1.35	1.39
16	B	612	9Y0	C22-C21	2.34	1.57	1.50
19	O	303	9YF	O11-C24	-2.34	1.39	1.45
16	D	202	9Y0	C22-C21	2.32	1.57	1.50
19	C	303	9YF	O11-C24	-2.32	1.39	1.45
14	F	601	HEA	C4C-NC	-2.31	1.35	1.39
16	K	201	9Y0	C22-C21	2.30	1.57	1.50
20	B	601	HEM	FE-NA	2.30	2.02	1.95
20	N	602	HEM	C3C-C2C	-2.29	1.32	1.36
15	N	605	CDL	C71-CB7	2.28	1.57	1.50
15	B	604	CDL	C71-CB7	2.27	1.57	1.50
20	B	601	HEM	C3C-C2C	-2.27	1.32	1.36
16	S	301	9Y0	C22-C21	2.27	1.57	1.50
21	N	609	MQ9	C21-C19	2.27	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	N	602	HEM	FE-NA	2.27	2.02	1.95
20	B	602	HEM	C2A-C3A	-2.26	1.32	1.38
20	N	603	HEM	C2A-C3A	-2.26	1.32	1.38
21	B	609	MQ9	C21-C19	2.26	1.56	1.51
16	G	301	9Y0	C22-C21	2.25	1.57	1.50
16	G	301	9Y0	C6-C5	2.23	1.57	1.50
21	B	609	MQ9	C7-C8	2.23	1.53	1.50
21	N	609	MQ9	C7-C8	2.23	1.53	1.50
16	S	301	9Y0	C6-C5	2.23	1.57	1.50
15	N	604	CDL	C71-CB7	2.21	1.57	1.50
15	B	603	CDL	C71-CB7	2.21	1.57	1.50
19	A	503	9YF	O9-C8	2.20	1.40	1.34
19	K	202	9YF	O11-C24	-2.20	1.40	1.45
14	F	601	HEA	C3A-C4A	-2.19	1.42	1.46
14	R	601	HEA	C3A-C4A	-2.19	1.42	1.46
19	A	504	9YF	O11-C24	-2.19	1.40	1.45
19	M	501	9YF	O11-C24	-2.19	1.40	1.45
19	W	202	9YF	O11-C24	-2.18	1.40	1.45
19	C	303	9YF	O11-C25	2.18	1.39	1.33
15	B	611	CDL	PA1-OA5	2.17	1.68	1.59
19	O	303	9YF	O11-C25	2.17	1.39	1.33
22	O	301	HEC	C3C-C2C	-2.17	1.33	1.38
21	N	608	MQ9	C21-C19	2.17	1.55	1.51
19	M	504	9YF	O9-C	-2.16	1.41	1.46
15	N	606	CDL	PA1-OA5	2.16	1.68	1.59
21	B	608	MQ9	C21-C19	2.16	1.55	1.51
15	B	605	CDL	PA1-OA5	2.16	1.68	1.59
22	C	301	HEC	C3C-C2C	-2.16	1.33	1.38
15	T	201	CDL	C71-CB7	2.16	1.57	1.50
15	N	601	CDL	PA1-OA5	2.15	1.68	1.59
19	W	202	9YF	O9-C8	2.15	1.40	1.34
15	H	201	CDL	C71-CB7	2.15	1.57	1.50
16	B	606	9Y0	C6-C5	2.14	1.57	1.50
22	O	302	HEC	CAC-C3C	2.13	1.56	1.51
15	B	605	CDL	C71-CB7	2.13	1.56	1.50
19	K	202	9YF	O9-C8	2.12	1.40	1.34
16	B	612	9Y0	C6-C5	2.12	1.56	1.50
15	F	606	CDL	OB6-CB4	-2.12	1.41	1.46
19	A	503	9YF	O9-C	-2.11	1.41	1.46
22	C	302	HEC	CAC-C3C	2.11	1.56	1.51
15	R	606	CDL	OB6-CB4	-2.11	1.41	1.46
15	N	606	CDL	C71-CB7	2.11	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	502	CDL	PA1-OA5	2.11	1.67	1.59
15	M	503	CDL	PA1-OA5	2.11	1.67	1.59
15	H	201	CDL	OB6-CB4	-2.10	1.41	1.46
15	N	605	CDL	OB6-CB4	-2.10	1.41	1.46
15	D	201	CDL	PA1-OA5	2.09	1.67	1.59
15	P	201	CDL	PA1-OA5	2.08	1.67	1.59
15	B	604	CDL	OB6-CB4	-2.08	1.41	1.46
15	B	605	CDL	OA6-CA4	-2.07	1.41	1.46
15	D	201	CDL	OB6-CB4	-2.06	1.41	1.46
15	B	611	CDL	PA1-OA2	2.06	1.67	1.59
21	O	304	MQ9	C7-C8	2.06	1.53	1.50
15	T	201	CDL	OB6-CB4	-2.06	1.41	1.46
14	F	602	HEA	C3C-C2C	-2.06	1.34	1.41
15	N	606	CDL	OA6-CA4	-2.06	1.41	1.46
14	R	602	HEA	C3C-C2C	-2.05	1.34	1.41
22	C	302	HEC	C3C-C2C	-2.05	1.33	1.38
15	D	201	CDL	C71-CB7	2.05	1.56	1.50
15	B	603	CDL	PA1-OA5	2.05	1.67	1.59
15	N	601	CDL	PA1-OA2	2.05	1.67	1.59
19	M	504	9YF	O9-C8	2.05	1.40	1.34
20	B	602	HEM	C3B-C2B	-2.05	1.33	1.37
20	N	603	HEM	C3B-C2B	-2.05	1.33	1.37
16	G	301	9Y0	O7-C1	-2.05	1.41	1.46
15	P	201	CDL	OB6-CB4	-2.05	1.41	1.46
22	O	302	HEC	C3C-C2C	-2.04	1.33	1.38
15	F	605	CDL	OB6-CB4	-2.04	1.41	1.46
15	P	201	CDL	C71-CB7	2.04	1.56	1.50
15	N	604	CDL	PA1-OA5	2.04	1.67	1.59
16	P	202	9Y0	C6-C5	2.04	1.56	1.50
16	S	301	9Y0	O7-C1	-2.03	1.41	1.46
19	C	303	9YF	O9-C8	2.03	1.40	1.34
19	O	303	9YF	O9-C8	2.03	1.40	1.34
21	B	610	MQ9	C3A-C3	2.03	1.43	1.39
21	N	610	MQ9	C3A-C3	2.03	1.43	1.39
21	B	607	MQ9	C7-C6	2.03	1.54	1.51
20	B	601	HEM	C2A-C3A	-2.03	1.33	1.38
20	B	602	HEM	CMC-C2C	2.02	1.55	1.50
21	B	607	MQ9	C3D-C2	2.02	1.43	1.39
15	N	601	CDL	PB2-OB2	2.02	1.67	1.59
16	D	202	9Y0	C6-C5	2.02	1.56	1.50
15	B	611	CDL	PB2-OB2	2.02	1.67	1.59
16	B	612	9Y0	O7-C1	-2.02	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	606	9Y0	O7-C1	-2.02	1.41	1.46
21	C	304	MQ9	C7-C8	2.01	1.53	1.50
16	W	201	9Y0	C6-C5	2.01	1.56	1.50
20	N	603	HEM	CMC-C2C	2.01	1.55	1.50
20	N	602	HEM	C2A-C3A	-2.01	1.33	1.38
15	F	605	CDL	PA1-OA5	2.00	1.67	1.59
15	B	611	CDL	C71-CB7	2.00	1.56	1.50
14	F	602	HEA	C3A-C4A	-2.00	1.42	1.46
15	R	605	CDL	PA1-OA5	2.00	1.67	1.59
15	R	605	CDL	OB6-CB4	-2.00	1.41	1.46
14	R	602	HEA	C3A-C4A	-2.00	1.42	1.46

All (722) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	F	601	HEA	C3C-C4C-NC	18.72	121.77	110.25
14	R	601	HEA	C3C-C4C-NC	18.61	121.70	110.25
14	R	601	HEA	CHA-C4D-C3D	-14.29	103.83	124.84
14	F	601	HEA	CHA-C4D-C3D	-14.23	103.92	124.84
14	R	602	HEA	C1A-CHA-C4D	-14.20	95.42	126.06
14	F	602	HEA	C1A-CHA-C4D	-14.16	95.52	126.06
14	F	601	HEA	C4C-NC-C1C	-13.96	91.68	105.35
14	R	601	HEA	C4C-NC-C1C	-13.90	91.73	105.35
14	R	602	HEA	C4C-CHD-C1D	-13.82	93.57	126.34
14	F	602	HEA	C4C-CHD-C1D	-13.80	93.60	126.34
14	F	602	HEA	C1C-CHC-C4B	-13.33	94.72	126.34
14	R	602	HEA	C1C-CHC-C4B	-13.28	94.83	126.34
14	R	601	HEA	CHB-C4A-C3A	-12.68	103.58	125.26
14	F	601	HEA	CHB-C4A-C3A	-12.67	103.59	125.26
14	F	601	HEA	C4C-CHD-C1D	-12.52	96.65	126.34
14	R	601	HEA	C4C-CHD-C1D	-12.52	96.65	126.34
14	R	601	HEA	C3D-C4D-ND	12.18	122.16	110.36
14	F	601	HEA	C3D-C4D-ND	12.15	122.12	110.36
14	R	601	HEA	C1A-CHA-C4D	-11.95	100.28	126.06
14	F	601	HEA	C4A-CHB-C1B	-11.94	100.29	126.06
14	R	601	HEA	C4A-CHB-C1B	-11.93	100.31	126.06
14	F	601	HEA	C1A-CHA-C4D	-11.93	100.32	126.06
14	F	601	HEA	C4A-NA-C1A	-11.75	93.84	105.35
14	R	601	HEA	C4A-NA-C1A	-11.70	93.89	105.35
14	R	601	HEA	C1D-ND-C4D	-11.50	93.19	105.07
14	F	601	HEA	C1D-ND-C4D	-11.50	93.19	105.07
14	R	602	HEA	C3C-C4C-NC	11.37	117.24	110.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	F	602	HEA	C3C-C4C-NC	11.30	117.20	110.25
14	R	601	HEA	C1C-CHC-C4B	-10.62	101.15	126.34
14	F	601	HEA	C1C-CHC-C4B	-10.60	101.19	126.34
14	R	601	HEA	C4B-NB-C1B	-10.60	94.12	105.07
14	F	601	HEA	C4B-NB-C1B	-10.58	94.15	105.07
14	F	602	HEA	C4A-CHB-C1B	-9.88	104.74	126.06
14	R	602	HEA	C4A-CHB-C1B	-9.83	104.86	126.06
14	R	601	HEA	CHB-C4A-NA	9.71	134.94	124.44
14	F	601	HEA	CHB-C4A-NA	9.67	134.90	124.44
21	B	609	MQ9	C7-C8-C9	-9.21	111.46	126.79
14	F	601	HEA	C2A-C1A-NA	9.20	119.27	110.32
21	N	609	MQ9	C7-C8-C9	-9.19	111.49	126.79
14	R	601	HEA	C2A-C1A-NA	9.15	119.23	110.32
14	R	602	HEA	CHA-C4D-C3D	-9.09	111.48	124.84
21	N	608	MQ9	C7-C8-C9	-9.04	111.74	126.79
14	R	601	HEA	CHC-C1C-C2C	-9.02	101.77	127.24
14	F	601	HEA	CHC-C1C-C2C	-9.00	101.80	127.24
21	B	608	MQ9	C7-C8-C9	-8.98	111.84	126.79
14	F	602	HEA	CHA-C4D-C3D	-8.93	111.71	124.84
14	R	601	HEA	CHA-C4D-ND	8.79	133.97	124.42
14	F	601	HEA	CHA-C4D-ND	8.74	133.91	124.42
14	F	602	HEA	C4C-NC-C1C	-8.60	96.93	105.35
14	R	602	HEA	C4C-NC-C1C	-8.56	96.96	105.35
14	R	601	HEA	C2D-C1D-ND	8.55	119.97	109.84
14	F	601	HEA	C2D-C1D-ND	8.54	119.95	109.84
21	B	610	MQ9	C7-C8-C9	-8.42	112.78	126.79
21	N	610	MQ9	C7-C8-C9	-8.40	112.81	126.79
14	F	601	HEA	C2C-C1C-NC	8.38	122.84	110.08
14	R	601	HEA	C2C-C1C-NC	8.36	122.81	110.08
21	O	304	MQ9	C7-C8-C9	-8.35	112.89	126.79
21	C	304	MQ9	C7-C8-C9	-8.35	112.90	126.79
14	R	601	HEA	C3B-C4B-NB	8.29	119.66	109.84
14	F	601	HEA	C3B-C4B-NB	8.27	119.64	109.84
14	F	601	HEA	CHA-C1A-C2A	-8.05	111.90	124.94
14	R	601	HEA	CHA-C1A-C2A	-8.02	111.94	124.94
14	F	602	HEA	CHB-C4A-C3A	-7.92	111.72	125.26
14	R	602	HEA	C3D-C4D-ND	7.91	118.02	110.36
14	R	602	HEA	CHB-C4A-C3A	-7.89	111.75	125.26
14	R	601	HEA	CHB-C1B-C2B	-7.84	112.73	124.98
14	F	602	HEA	C3D-C4D-ND	7.84	117.95	110.36
14	F	601	HEA	CHB-C1B-C2B	-7.83	112.74	124.98
22	C	302	HEC	CAC-C3C-C4C	7.64	135.51	124.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	O	302	HEC	CAC-C3C-C4C	7.61	135.48	124.92
21	O	304	MQ9	C17-C18-C19	-7.39	109.87	127.66
21	C	304	MQ9	C17-C18-C19	-7.39	109.88	127.66
14	R	601	HEA	C2B-C1B-NB	7.31	118.63	109.88
14	F	601	HEA	C2B-C1B-NB	7.27	118.59	109.88
22	C	302	HEC	C1D-ND-C4D	7.06	112.36	105.07
14	F	602	HEA	CHC-C1C-C2C	-7.05	107.32	127.24
14	R	602	HEA	CHC-C1C-C2C	-7.05	107.33	127.24
14	R	602	HEA	C4A-C3A-C2A	-7.03	100.98	106.75
22	O	302	HEC	C1D-ND-C4D	7.02	112.32	105.07
14	F	602	HEA	C26-C15-C16	-7.00	103.50	115.27
14	R	602	HEA	C26-C15-C16	-6.99	103.51	115.27
14	F	602	HEA	C4A-C3A-C2A	-6.94	101.06	106.75
21	N	607	MQ9	C12-C13-C14	-6.91	111.02	127.66
21	B	607	MQ9	C12-C13-C14	-6.90	111.05	127.66
21	B	608	MQ9	C17-C18-C19	-6.81	111.27	127.66
21	N	608	MQ9	C17-C18-C19	-6.79	111.31	127.66
14	R	602	HEA	C1D-ND-C4D	-6.66	98.19	105.07
21	B	609	MQ9	C17-C18-C19	-6.64	111.66	127.66
21	N	609	MQ9	C17-C18-C19	-6.63	111.71	127.66
14	F	602	HEA	C1D-ND-C4D	-6.56	98.29	105.07
21	N	607	MQ9	C22-C23-C24	-6.54	111.90	127.66
21	B	607	MQ9	C22-C23-C24	-6.54	111.92	127.66
21	C	304	MQ9	C42-C43-C44	-6.47	112.07	127.66
21	O	304	MQ9	C42-C43-C44	-6.47	112.08	127.66
21	B	607	MQ9	C10-C9-C8	-6.46	107.11	123.68
21	N	607	MQ9	C10-C9-C8	-6.45	107.12	123.68
21	O	304	MQ9	C12-C13-C14	-6.43	112.18	127.66
21	C	304	MQ9	C12-C13-C14	-6.43	112.19	127.66
21	N	607	MQ9	C7-C8-C9	-6.42	116.11	126.79
21	N	609	MQ9	C27-C28-C29	-6.40	112.24	127.66
21	B	607	MQ9	C7-C8-C9	-6.40	116.13	126.79
21	B	609	MQ9	C27-C28-C29	-6.38	112.30	127.66
14	R	601	HEA	CHD-C1D-C2D	-6.34	109.12	126.73
14	F	601	HEA	CHD-C1D-C2D	-6.34	109.13	126.73
21	C	304	MQ9	C22-C23-C24	-6.32	112.45	127.66
21	O	304	MQ9	C22-C23-C24	-6.32	112.45	127.66
21	B	609	MQ9	C42-C43-C44	-6.31	112.47	127.66
14	F	602	HEA	C17-C18-C19	-6.28	112.54	127.66
21	N	608	MQ9	C15-C14-C13	-6.28	107.58	123.68
21	N	609	MQ9	C42-C43-C44	-6.27	112.56	127.66
21	B	608	MQ9	C15-C14-C13	-6.26	107.62	123.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	R	602	HEA	C17-C18-C19	-6.25	112.60	127.66
21	O	304	MQ9	C15-C14-C13	-6.19	107.80	123.68
21	B	608	MQ9	C11-C9-C8	-6.18	108.61	121.12
14	R	601	HEA	C4A-C3A-C2A	-6.18	101.68	106.75
21	C	304	MQ9	C15-C14-C13	-6.16	107.87	123.68
14	R	601	HEA	CHC-C1C-NC	6.15	135.16	123.85
21	O	304	MQ9	C11-C9-C8	-6.15	108.67	121.12
21	C	304	MQ9	C11-C9-C8	-6.14	108.70	121.12
21	N	608	MQ9	C11-C9-C8	-6.14	108.70	121.12
14	F	601	HEA	C4A-C3A-C2A	-6.13	101.72	106.75
14	F	601	HEA	CHC-C1C-NC	6.12	135.11	123.85
21	N	608	MQ9	C22-C23-C24	-6.12	112.93	127.66
21	B	610	MQ9	C12-C13-C14	-6.11	112.94	127.66
21	N	610	MQ9	C12-C13-C14	-6.11	112.95	127.66
21	B	608	MQ9	C22-C23-C24	-6.09	112.99	127.66
21	O	304	MQ9	C46-C44-C43	-6.07	108.83	121.12
21	C	304	MQ9	C46-C44-C43	-6.07	108.83	121.12
14	F	602	HEA	C20-C19-C18	-6.05	108.88	121.12
21	N	610	MQ9	C22-C23-C24	-6.04	113.12	127.66
21	B	610	MQ9	C22-C23-C24	-6.04	113.12	127.66
14	R	602	HEA	C2D-C1D-ND	6.02	116.97	109.84
14	F	602	HEA	C2D-C1D-ND	6.02	116.97	109.84
14	F	602	HEA	C2C-C1C-NC	6.01	119.23	110.08
21	B	609	MQ9	C12-C13-C14	-6.01	113.19	127.66
21	N	609	MQ9	C11-C9-C8	-6.00	108.98	121.12
14	R	602	HEA	C20-C19-C18	-6.00	108.98	121.12
21	N	609	MQ9	C12-C13-C14	-5.99	113.24	127.66
22	C	301	HEC	C1D-ND-C4D	5.97	111.24	105.07
21	B	609	MQ9	C11-C9-C8	-5.97	109.05	121.12
14	R	602	HEA	C13-C14-C15	-5.96	113.32	127.66
14	R	602	HEA	C2C-C1C-NC	5.95	119.15	110.08
14	F	602	HEA	C13-C14-C15	-5.93	113.38	127.66
22	O	301	HEC	C1D-ND-C4D	5.93	111.19	105.07
21	N	608	MQ9	C27-C28-C29	-5.92	113.39	127.66
21	B	610	MQ9	C10-C9-C8	-5.89	108.57	123.68
21	N	610	MQ9	C10-C9-C8	-5.89	108.58	123.68
21	N	608	MQ9	C10-C9-C8	-5.88	108.60	123.68
21	B	608	MQ9	C27-C28-C29	-5.88	113.51	127.66
21	B	607	MQ9	C31-C29-C28	-5.83	109.31	121.12
21	B	608	MQ9	C10-C9-C8	-5.83	108.72	123.68
14	F	601	HEA	C27-C19-C18	-5.82	108.74	123.68
21	C	304	MQ9	C16-C14-C13	-5.82	109.35	121.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	N	607	MQ9	C31-C29-C28	-5.81	109.35	121.12
21	O	304	MQ9	C16-C14-C13	-5.81	109.35	121.12
21	B	607	MQ9	C15-C14-C13	-5.81	108.77	123.68
14	R	601	HEA	C27-C19-C18	-5.81	108.79	123.68
21	N	607	MQ9	C15-C14-C13	-5.80	108.80	123.68
22	C	302	HEC	CAC-C3C-C2C	-5.78	117.60	126.86
22	O	302	HEC	CAC-C3C-C2C	-5.78	117.61	126.86
21	B	608	MQ9	C12-C13-C14	-5.77	113.78	127.66
21	N	608	MQ9	C12-C13-C14	-5.76	113.80	127.66
21	B	610	MQ9	C27-C28-C29	-5.73	113.86	127.66
21	B	610	MQ9	C15-C14-C13	-5.72	109.00	123.68
21	N	610	MQ9	C27-C28-C29	-5.72	113.88	127.66
21	B	609	MQ9	C15-C14-C13	-5.72	109.00	123.68
21	N	610	MQ9	C15-C14-C13	-5.72	109.01	123.68
21	N	609	MQ9	C15-C14-C13	-5.72	109.02	123.68
21	N	609	MQ9	C22-C23-C24	-5.66	114.04	127.66
14	R	602	HEA	CHD-C4C-NC	5.64	134.23	123.85
14	R	601	HEA	C16-C15-C14	-5.64	109.70	121.12
21	B	607	MQ9	C11-C9-C8	-5.64	109.70	121.12
14	F	602	HEA	CHD-C4C-NC	5.64	134.22	123.85
21	B	609	MQ9	C22-C23-C24	-5.63	114.10	127.66
21	N	607	MQ9	C11-C9-C8	-5.63	109.73	121.12
21	B	609	MQ9	C37-C38-C39	-5.62	114.12	127.66
14	F	601	HEA	C16-C15-C14	-5.62	109.74	121.12
14	R	601	HEA	CHD-C4C-NC	5.62	134.18	123.85
21	N	610	MQ9	C11-C9-C8	-5.61	109.75	121.12
21	B	610	MQ9	C11-C9-C8	-5.60	109.79	121.12
21	N	609	MQ9	C37-C38-C39	-5.59	114.21	127.66
14	F	601	HEA	CHD-C4C-NC	5.58	134.12	123.85
21	C	304	MQ9	C10-C9-C8	-5.58	109.37	123.68
21	B	609	MQ9	C45-C44-C43	-5.57	109.38	123.68
21	O	304	MQ9	C10-C9-C8	-5.57	109.40	123.68
21	N	609	MQ9	C45-C44-C43	-5.56	109.42	123.68
21	O	304	MQ9	C45-C44-C43	-5.55	109.45	123.68
14	R	602	HEA	C27-C19-C18	-5.54	109.48	123.68
21	C	304	MQ9	C45-C44-C43	-5.53	109.48	123.68
14	F	602	HEA	C27-C19-C18	-5.51	109.55	123.68
14	F	602	HEA	C3B-C4B-NB	5.51	116.36	109.84
21	O	304	MQ9	C25-C24-C23	-5.50	109.56	123.68
21	B	607	MQ9	C27-C28-C29	-5.49	114.44	127.66
21	B	608	MQ9	C36-C34-C33	-5.48	110.02	121.12
21	N	607	MQ9	C27-C28-C29	-5.48	114.46	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	C	304	MQ9	C25-C24-C23	-5.48	109.62	123.68
14	R	602	HEA	CHA-C4D-ND	5.47	130.36	124.42
21	B	610	MQ9	C16-C14-C13	-5.44	110.10	121.12
21	N	608	MQ9	C36-C34-C33	-5.44	110.10	121.12
14	R	602	HEA	C3B-C4B-NB	5.44	116.28	109.84
21	C	304	MQ9	C37-C38-C39	-5.43	114.58	127.66
21	N	609	MQ9	C10-C9-C8	-5.43	109.75	123.68
21	N	610	MQ9	C16-C14-C13	-5.42	110.14	121.12
21	B	609	MQ9	C10-C9-C8	-5.42	109.77	123.68
21	O	304	MQ9	C37-C38-C39	-5.42	114.61	127.66
21	B	609	MQ9	C36-C34-C33	-5.39	110.22	121.12
21	N	609	MQ9	C36-C34-C33	-5.38	110.23	121.12
21	C	304	MQ9	C40-C39-C38	-5.37	109.89	123.68
14	F	602	HEA	C4A-NA-C1A	-5.37	100.09	105.35
21	O	304	MQ9	C40-C39-C38	-5.36	109.92	123.68
14	F	601	HEA	CHD-C4C-C3C	-5.36	103.85	127.71
14	R	601	HEA	CHD-C4C-C3C	-5.36	103.86	127.71
14	F	602	HEA	CHA-C4D-ND	5.34	130.22	124.42
14	R	602	HEA	C4A-NA-C1A	-5.33	100.13	105.35
21	N	609	MQ9	C46-C44-C43	-5.32	110.36	121.12
14	F	602	HEA	CHB-C4A-NA	5.31	130.19	124.44
21	B	609	MQ9	C46-C44-C43	-5.29	110.41	121.12
21	B	608	MQ9	C16-C14-C13	-5.24	110.52	121.12
14	R	602	HEA	CHB-C4A-NA	5.23	130.10	124.44
21	N	608	MQ9	C25-C24-C23	-5.23	110.27	123.68
21	N	608	MQ9	C16-C14-C13	-5.23	110.54	121.12
21	B	608	MQ9	C25-C24-C23	-5.21	110.32	123.68
14	F	601	HEA	CHD-C1D-ND	5.20	130.79	124.37
14	R	601	HEA	CHD-C1D-ND	5.20	130.78	124.37
21	B	607	MQ9	C17-C18-C19	-5.18	115.19	127.66
21	B	610	MQ9	C31-C29-C28	-5.17	110.66	121.12
21	N	609	MQ9	C16-C14-C13	-5.16	110.67	121.12
21	N	607	MQ9	C17-C18-C19	-5.16	115.22	127.66
21	B	609	MQ9	C16-C14-C13	-5.16	110.68	121.12
21	N	610	MQ9	C31-C29-C28	-5.15	110.70	121.12
21	B	608	MQ9	C20-C19-C18	-5.15	110.48	123.68
14	F	602	HEA	C2A-C1A-NA	5.13	115.31	110.32
21	N	608	MQ9	C20-C19-C18	-5.12	110.55	123.68
14	R	601	HEA	C3C-C2C-C1C	-5.10	101.00	107.16
14	F	601	HEA	C3C-C2C-C1C	-5.09	101.01	107.16
21	N	610	MQ9	C17-C18-C19	-5.09	115.41	127.66
21	B	607	MQ9	C30-C29-C28	-5.09	110.63	123.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	R	602	HEA	CHC-C1C-NC	5.08	133.20	123.85
21	B	610	MQ9	C17-C18-C19	-5.08	115.43	127.66
14	F	601	HEA	C21-C22-C23	-5.07	110.42	127.75
21	N	607	MQ9	C30-C29-C28	-5.07	110.68	123.68
14	R	601	HEA	C21-C22-C23	-5.06	110.45	127.75
21	B	610	MQ9	C25-C24-C23	-5.05	110.72	123.68
14	F	602	HEA	CHC-C1C-NC	5.05	133.14	123.85
14	R	602	HEA	C2A-C1A-NA	5.04	115.23	110.32
21	N	610	MQ9	C25-C24-C23	-5.03	110.78	123.68
21	C	304	MQ9	C31-C29-C28	-4.94	111.12	121.12
21	O	304	MQ9	C31-C29-C28	-4.93	111.14	121.12
21	N	609	MQ9	C32-C33-C34	-4.92	115.82	127.66
21	N	607	MQ9	C26-C24-C23	-4.92	111.17	121.12
21	B	609	MQ9	C32-C33-C34	-4.92	115.82	127.66
21	B	609	MQ9	C40-C39-C38	-4.90	111.10	123.68
21	N	609	MQ9	C40-C39-C38	-4.90	111.10	123.68
21	N	608	MQ9	C32-C33-C34	-4.89	115.88	127.66
21	B	607	MQ9	C26-C24-C23	-4.89	111.22	121.12
21	N	610	MQ9	C26-C24-C23	-4.88	111.23	121.12
21	B	610	MQ9	C26-C24-C23	-4.88	111.24	121.12
21	C	304	MQ9	C36-C34-C33	-4.88	111.24	121.12
21	O	304	MQ9	C36-C34-C33	-4.88	111.24	121.12
21	B	608	MQ9	C32-C33-C34	-4.86	115.95	127.66
14	R	601	HEA	CHC-C4B-C3B	-4.85	113.32	125.80
14	F	601	HEA	CHC-C4B-C3B	-4.84	113.34	125.80
14	F	602	HEA	CHD-C1D-C2D	-4.81	113.36	126.73
21	N	607	MQ9	C16-C14-C13	-4.80	111.41	121.12
14	R	602	HEA	CHD-C1D-C2D	-4.80	113.41	126.73
14	R	601	HEA	C17-C18-C19	-4.79	116.13	127.66
14	F	601	HEA	C17-C18-C19	-4.78	116.14	127.66
21	B	607	MQ9	C16-C14-C13	-4.78	111.44	121.12
14	R	601	HEA	C24-C23-C22	-4.78	108.84	122.65
14	F	601	HEA	C24-C23-C22	-4.77	108.87	122.65
21	N	609	MQ9	C41-C39-C38	-4.76	111.48	121.12
21	B	609	MQ9	C41-C39-C38	-4.73	111.55	121.12
15	B	603	CDL	OB6-CB5-C51	4.69	121.60	111.50
14	F	602	HEA	C3C-C2C-C1C	-4.68	101.51	107.16
14	R	602	HEA	C3C-C2C-C1C	-4.66	101.54	107.16
21	O	304	MQ9	C32-C33-C34	-4.66	116.45	127.66
21	C	304	MQ9	C32-C33-C34	-4.65	116.47	127.66
21	N	609	MQ9	C20-C19-C18	-4.64	111.76	123.68
14	F	602	HEA	CBD-CAD-C3D	4.64	125.50	112.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	R	602	HEA	CBD-CAD-C3D	4.63	125.50	112.63
18	Y	302	9XX	O1-C18-C19	4.62	121.47	111.50
21	B	609	MQ9	C20-C19-C18	-4.62	111.82	123.68
21	N	610	MQ9	C30-C29-C28	-4.61	111.84	123.68
21	B	610	MQ9	C30-C29-C28	-4.61	111.86	123.68
21	N	607	MQ9	C32-C33-C34	-4.61	112.01	127.75
15	N	604	CDL	OB6-CB5-C51	4.60	121.42	111.50
21	B	609	MQ9	C30-C29-C28	-4.60	111.88	123.68
21	C	304	MQ9	C20-C19-C18	-4.60	111.88	123.68
21	B	607	MQ9	C32-C33-C34	-4.60	112.04	127.75
18	Z	302	9XX	O1-C18-C19	4.59	121.40	111.50
21	O	304	MQ9	C20-C19-C18	-4.58	111.92	123.68
22	O	301	HEC	CAD-C3D-C4D	4.58	132.66	124.66
21	N	609	MQ9	C30-C29-C28	-4.58	111.94	123.68
22	C	301	HEC	CAD-C3D-C4D	4.55	132.61	124.66
21	C	304	MQ9	C26-C24-C23	-4.54	111.93	121.12
15	N	601	CDL	OB6-CB5-C51	4.54	121.28	111.50
14	F	601	HEA	C26-C15-C14	-4.53	112.06	123.68
15	B	611	CDL	OB6-CB5-C51	4.53	121.25	111.50
14	R	601	HEA	C26-C15-C14	-4.52	112.07	123.68
15	R	606	CDL	OA6-CA5-C11	4.52	121.24	111.50
21	N	609	MQ9	C26-C24-C23	-4.52	111.98	121.12
21	O	304	MQ9	C26-C24-C23	-4.52	111.98	121.12
15	F	606	CDL	OA6-CA5-C11	4.51	121.22	111.50
21	N	608	MQ9	C35-C34-C33	-4.51	112.12	123.68
21	B	608	MQ9	C35-C34-C33	-4.50	112.14	123.68
15	N	605	CDL	OA6-CA5-C11	4.49	121.17	111.50
21	B	609	MQ9	C26-C24-C23	-4.47	112.06	121.12
15	B	604	CDL	OA6-CA5-C11	4.45	121.10	111.50
14	R	601	HEA	C13-C14-C15	-4.45	116.94	127.66
14	F	601	HEA	C13-C14-C15	-4.45	116.95	127.66
14	F	602	HEA	CMC-C2C-C1C	4.44	132.13	125.37
18	K	204	9XX	O1-C18-C19	4.44	121.07	111.50
14	F	602	HEA	C4B-NB-C1B	-4.43	100.49	105.07
14	F	602	HEA	C21-C22-C23	-4.42	112.65	127.75
14	R	602	HEA	C21-C22-C23	-4.40	112.71	127.75
21	B	609	MQ9	C25-C24-C23	-4.40	112.39	123.68
21	N	609	MQ9	C25-C24-C23	-4.40	112.40	123.68
14	R	602	HEA	CMC-C2C-C1C	4.40	132.06	125.37
15	B	604	CDL	OB6-CB5-C51	4.39	120.96	111.50
15	N	605	CDL	OB6-CB5-C51	4.38	120.94	111.50
14	R	602	HEA	C4B-NB-C1B	-4.37	100.56	105.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	N	601	CDL	OA6-CA5-C11	4.34	120.84	111.50
21	N	609	MQ9	C31-C29-C28	-4.33	112.35	121.12
15	B	611	CDL	OA6-CA5-C11	4.33	120.83	111.50
21	B	609	MQ9	C31-C29-C28	-4.32	112.37	121.12
21	N	607	MQ9	C36-C34-C33	-4.32	110.17	122.65
14	R	602	HEA	CHD-C4C-C3C	-4.32	108.51	127.71
21	B	607	MQ9	C36-C34-C33	-4.31	110.19	122.65
14	F	602	HEA	CHD-C4C-C3C	-4.30	108.56	127.71
19	A	503	9YF	O9-C8-C9	4.27	120.71	111.50
14	F	602	HEA	CHD-C1D-ND	4.27	129.64	124.37
21	C	304	MQ9	C27-C28-C29	-4.26	117.41	127.66
21	C	304	MQ9	C41-C39-C38	-4.25	112.51	121.12
21	O	304	MQ9	C27-C28-C29	-4.25	117.43	127.66
14	R	602	HEA	CHD-C1D-ND	4.23	129.59	124.37
21	O	304	MQ9	C41-C39-C38	-4.22	112.57	121.12
16	W	201	9Y0	O7-C21-C22	4.20	120.56	111.50
15	R	605	CDL	OA6-CA5-C11	4.20	120.55	111.50
15	R	605	CDL	OB6-CB5-C51	4.20	120.54	111.50
21	N	610	MQ9	C21-C19-C18	-4.19	112.64	121.12
21	B	610	MQ9	C21-C19-C18	-4.19	112.64	121.12
21	B	607	MQ9	C15-C14-C16	-4.18	108.23	115.27
21	C	304	MQ9	C21-C19-C18	-4.18	112.66	121.12
16	K	201	9Y0	O7-C21-C22	4.18	120.51	111.50
15	F	605	CDL	OA6-CA5-C11	4.17	120.50	111.50
15	F	605	CDL	OB6-CB5-C51	4.17	120.50	111.50
16	D	202	9Y0	O7-C21-C22	4.17	120.49	111.50
21	O	304	MQ9	C21-C19-C18	-4.17	112.68	121.12
14	R	601	HEA	C4D-C3D-C2D	-4.17	100.82	106.90
21	N	607	MQ9	C15-C14-C16	-4.17	108.26	115.27
21	B	607	MQ9	C35-C34-C33	-4.15	110.65	122.65
14	F	601	HEA	C4D-C3D-C2D	-4.15	100.85	106.90
21	N	607	MQ9	C35-C34-C33	-4.15	110.67	122.65
16	P	202	9Y0	O7-C21-C22	4.14	120.43	111.50
21	N	609	MQ9	C47-C48-C49	-4.13	113.63	127.75
14	F	602	HEA	C25-C23-C22	-4.13	110.72	122.65
21	B	609	MQ9	C47-C48-C49	-4.13	113.65	127.75
14	R	602	HEA	C25-C23-C22	-4.12	110.74	122.65
16	B	612	9Y0	O7-C21-C22	4.12	120.37	111.50
19	C	303	9YF	O9-C8-C9	4.11	120.36	111.50
16	B	606	9Y0	O7-C21-C22	4.11	120.36	111.50
15	B	603	CDL	OA6-CA5-C11	4.11	120.36	111.50
21	N	607	MQ9	C25-C24-C23	-4.10	113.15	123.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	O	303	9YF	O9-C8-C9	4.10	120.34	111.50
14	R	602	HEA	C24-C23-C22	-4.09	110.83	122.65
15	N	606	CDL	OA6-CA5-C11	4.08	120.29	111.50
14	F	602	HEA	C24-C23-C22	-4.08	110.87	122.65
15	D	201	CDL	OA6-CA5-C11	4.08	120.28	111.50
15	P	201	CDL	OA6-CA5-C11	4.07	120.28	111.50
21	B	607	MQ9	C25-C24-C23	-4.07	113.23	123.68
18	W	204	9XX	O1-C18-C19	4.07	120.27	111.50
15	B	605	CDL	OA6-CA5-C11	4.07	120.27	111.50
14	R	601	HEA	CBD-CAD-C3D	4.06	123.91	112.63
15	N	604	CDL	OA6-CA5-C11	4.06	120.25	111.50
14	F	601	HEA	CBD-CAD-C3D	4.05	123.88	112.63
15	M	503	CDL	OA6-CA5-C11	4.05	120.23	111.50
19	K	202	9YF	O9-C8-C9	4.04	120.22	111.50
19	W	202	9YF	O9-C8-C9	4.04	120.21	111.50
15	A	502	CDL	OA6-CA5-C11	4.04	120.20	111.50
15	P	201	CDL	OB6-CB5-C51	4.03	120.19	111.50
14	R	601	HEA	CHA-C1A-NA	4.03	128.80	124.44
14	F	601	HEA	CHA-C1A-NA	4.02	128.79	124.44
21	B	609	MQ9	C35-C34-C33	-4.00	113.43	123.68
15	H	201	CDL	OB6-CB5-C51	3.99	120.11	111.50
15	T	201	CDL	OB6-CB5-C51	3.98	120.09	111.50
21	N	609	MQ9	C35-C34-C33	-3.96	113.51	123.68
21	O	304	MQ9	C45-C44-C46	-3.96	108.61	115.27
14	F	601	HEA	C27-C19-C20	-3.96	108.61	115.27
14	R	601	HEA	C27-C19-C20	-3.96	108.61	115.27
15	D	201	CDL	OB6-CB5-C51	3.96	120.03	111.50
21	C	304	MQ9	C45-C44-C46	-3.95	108.62	115.27
21	C	304	MQ9	C10-C9-C11	-3.93	108.66	115.27
14	F	601	HEA	C26-C15-C16	-3.93	108.66	115.27
21	N	608	MQ9	C35-C34-C36	-3.93	108.66	115.27
21	B	609	MQ9	C51-C49-C48	-3.93	111.30	122.65
21	N	609	MQ9	C51-C49-C48	-3.92	111.31	122.65
14	R	601	HEA	C26-C15-C16	-3.92	108.67	115.27
21	O	304	MQ9	C10-C9-C11	-3.91	108.69	115.27
21	B	608	MQ9	C35-C34-C36	-3.90	108.71	115.27
14	R	601	HEA	C20-C19-C18	-3.88	113.27	121.12
15	R	606	CDL	OB6-CB5-C51	3.87	119.84	111.50
15	F	606	CDL	OB6-CB5-C51	3.87	119.84	111.50
21	B	608	MQ9	C26-C24-C23	-3.86	113.31	121.12
14	F	601	HEA	C20-C19-C18	-3.86	113.31	121.12
19	A	504	9YF	O9-C8-C9	3.85	119.81	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	M	501	9YF	O9-C8-C9	3.85	119.81	111.50
21	N	608	MQ9	C26-C24-C23	-3.85	113.33	121.12
15	M	503	CDL	OB6-CB5-C51	3.83	119.75	111.50
21	N	608	MQ9	C15-C14-C16	-3.83	108.83	115.27
21	N	608	MQ9	C21-C19-C18	-3.82	113.38	121.12
21	B	608	MQ9	C15-C14-C16	-3.82	108.84	115.27
14	F	601	HEA	CHB-C1B-NB	3.81	128.56	124.42
21	B	608	MQ9	C21-C19-C18	-3.81	113.40	121.12
15	A	502	CDL	OB6-CB5-C51	3.81	119.71	111.50
21	N	610	MQ9	C20-C19-C18	-3.81	113.91	123.68
21	N	607	MQ9	C21-C19-C18	-3.80	113.42	121.12
21	N	608	MQ9	C37-C38-C39	-3.80	114.76	127.75
21	B	610	MQ9	C20-C19-C18	-3.80	113.93	123.68
14	R	601	HEA	CHB-C1B-NB	3.79	128.54	124.42
21	B	607	MQ9	C21-C19-C18	-3.79	113.45	121.12
21	N	608	MQ9	C30-C29-C28	-3.78	113.98	123.68
21	N	610	MQ9	C36-C34-C33	-3.78	111.73	122.65
14	F	601	HEA	C25-C23-C22	-3.77	111.74	122.65
21	B	608	MQ9	C30-C29-C28	-3.77	114.00	123.68
14	R	601	HEA	C25-C23-C22	-3.77	111.75	122.65
21	C	304	MQ9	C35-C34-C33	-3.77	114.01	123.68
21	B	608	MQ9	C37-C38-C39	-3.77	114.87	127.75
21	B	610	MQ9	C36-C34-C33	-3.77	111.76	122.65
21	O	304	MQ9	C35-C34-C33	-3.75	114.05	123.68
21	B	609	MQ9	C50-C49-C48	-3.73	111.86	122.65
21	N	609	MQ9	C50-C49-C48	-3.73	111.87	122.65
19	A	503	9YF	O2-C2-C7	3.72	117.33	108.66
21	N	608	MQ9	C40-C39-C38	-3.72	111.90	122.65
14	F	602	HEA	CAD-CBD-CGD	-3.71	105.61	113.60
14	R	602	HEA	CAD-CBD-CGD	-3.70	105.64	113.60
21	B	608	MQ9	C40-C39-C38	-3.67	112.03	122.65
15	T	201	CDL	OA6-CA5-C11	3.65	119.36	111.50
15	H	201	CDL	OA6-CA5-C11	3.64	119.35	111.50
22	O	301	HEC	CAD-CBD-CGD	-3.63	105.78	113.60
21	B	609	MQ9	C21-C19-C18	-3.63	113.77	121.12
21	N	609	MQ9	C21-C19-C18	-3.63	113.77	121.12
14	F	601	HEA	C3A-C2A-C1A	-3.62	103.62	107.08
22	C	301	HEC	CAD-CBD-CGD	-3.62	105.82	113.60
21	B	610	MQ9	C15-C14-C16	-3.61	109.19	115.27
16	G	301	9Y0	O7-C21-C22	3.61	119.27	111.50
21	N	610	MQ9	C15-C14-C16	-3.60	109.21	115.27
16	S	301	9Y0	O7-C21-C22	3.60	119.26	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	F	602	HEA	C26-C15-C14	-3.58	114.50	123.68
21	O	304	MQ9	C47-C48-C49	-3.57	115.54	127.75
21	C	304	MQ9	C47-C48-C49	-3.57	115.55	127.75
14	R	601	HEA	C3A-C2A-C1A	-3.57	103.67	107.08
14	R	602	HEA	C26-C15-C14	-3.55	114.56	123.68
21	C	304	MQ9	C30-C29-C28	-3.53	114.63	123.68
21	O	304	MQ9	C30-C29-C28	-3.52	114.64	123.68
21	O	304	MQ9	C51-C49-C48	-3.52	112.47	122.65
21	C	304	MQ9	C51-C49-C48	-3.51	112.49	122.65
15	N	606	CDL	OB6-CB5-C51	3.51	119.06	111.50
20	B	601	HEM	CMB-C2B-C1B	-3.49	119.72	125.04
22	C	302	HEC	CMC-C2C-C1C	-3.49	120.06	125.37
21	N	610	MQ9	C32-C33-C34	-3.47	115.88	127.75
18	K	204	9XX	C17-O1-C18	-3.47	113.41	117.88
21	B	610	MQ9	C32-C33-C34	-3.47	115.88	127.75
22	O	302	HEC	CMC-C2C-C1C	-3.47	120.08	125.37
15	B	605	CDL	OB6-CB5-C51	3.47	118.98	111.50
14	R	602	HEA	C27-C19-C20	-3.47	109.44	115.27
21	B	609	MQ9	C45-C44-C46	-3.46	109.45	115.27
14	F	602	HEA	C27-C19-C20	-3.45	109.46	115.27
21	N	609	MQ9	C45-C44-C46	-3.45	109.47	115.27
14	R	602	HEA	C16-C15-C14	-3.44	114.15	121.12
20	N	602	HEM	CMB-C2B-C1B	-3.43	119.81	125.04
21	B	609	MQ9	C15-C14-C16	-3.43	109.50	115.27
14	F	602	HEA	C2B-C1B-NB	3.42	113.98	109.88
19	A	503	9YF	C7-C2-C3	3.42	115.78	110.85
18	W	204	9XX	C17-O1-C18	-3.41	113.49	117.88
21	C	304	MQ9	C15-C14-C16	-3.41	109.53	115.27
21	O	304	MQ9	C15-C14-C16	-3.41	109.54	115.27
21	N	609	MQ9	C15-C14-C16	-3.39	109.56	115.27
14	F	602	HEA	C16-C15-C14	-3.39	114.26	121.12
14	R	602	HEA	C2B-C1B-NB	3.38	113.93	109.88
19	M	504	9YF	C7-C2-C3	3.38	115.73	110.85
19	M	504	9YF	O9-C8-C9	3.35	118.73	111.50
22	O	302	HEC	CHD-C4C-C3C	3.31	132.59	125.36
22	C	302	HEC	CHD-C4C-C3C	3.29	132.55	125.36
14	R	601	HEA	CBA-CAA-C2A	3.28	121.73	112.63
14	F	601	HEA	CBA-CAA-C2A	3.27	121.71	112.63
21	N	610	MQ9	C10-C9-C11	-3.27	109.78	115.27
21	N	607	MQ9	C20-C19-C18	-3.26	115.32	123.68
21	B	610	MQ9	C10-C9-C11	-3.26	109.79	115.27
21	B	607	MQ9	C20-C19-C18	-3.23	115.38	123.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	609	MQ9	C10-C9-C11	-3.21	109.87	115.27
21	N	609	MQ9	C10-C9-C11	-3.20	109.89	115.27
14	R	601	HEA	C4B-C3B-C2B	-3.17	101.99	107.41
14	F	601	HEA	C4B-C3B-C2B	-3.16	102.00	107.41
20	B	601	HEM	C4D-ND-C1D	3.14	108.32	105.07
14	F	602	HEA	C1D-C2D-C3D	-3.13	103.67	106.96
14	R	601	HEA	C1D-C2D-C3D	-3.12	103.67	106.96
14	F	601	HEA	C1D-C2D-C3D	-3.11	103.69	106.96
14	R	602	HEA	C1D-C2D-C3D	-3.10	103.70	106.96
20	N	602	HEM	C4D-ND-C1D	3.08	108.26	105.07
14	R	602	HEA	CAA-CBA-CGA	-3.08	106.98	113.60
14	F	602	HEA	CAD-C3D-C4D	3.07	130.03	124.66
14	F	602	HEA	C13-C12-C11	3.05	118.93	114.35
14	R	602	HEA	C13-C12-C11	3.05	118.93	114.35
22	O	302	HEC	CMB-C2B-C1B	-3.04	120.41	125.04
19	W	202	9YF	O11-C25-C26	3.04	121.45	111.91
22	C	302	HEC	CMB-C2B-C1B	-3.03	120.43	125.04
14	F	602	HEA	C12-C13-C14	3.02	120.21	112.23
21	B	608	MQ9	C41-C39-C38	-3.02	113.92	122.65
14	F	602	HEA	CAA-CBA-CGA	-3.02	107.11	113.60
21	N	610	MQ9	C35-C34-C33	-2.99	114.00	122.65
14	R	602	HEA	C12-C13-C14	2.99	120.13	112.23
21	B	610	MQ9	C35-C34-C33	-2.99	114.00	122.65
15	B	604	CDL	OA8-CA7-C31	2.99	121.29	111.91
15	N	605	CDL	OA8-CA7-C31	2.99	121.29	111.91
14	R	602	HEA	CAD-C3D-C4D	2.99	129.88	124.66
21	N	608	MQ9	C41-C39-C38	-2.98	114.02	122.65
14	F	601	HEA	CMC-C2C-C1C	2.98	129.91	125.37
19	K	202	9YF	O11-C25-C26	2.98	121.26	111.91
16	K	201	9Y0	O5-C5-C6	2.96	121.19	111.91
14	R	601	HEA	CMC-C2C-C1C	2.95	129.86	125.37
15	R	605	CDL	OA8-CA7-C31	2.94	121.15	111.91
15	F	605	CDL	OA8-CA7-C31	2.94	121.14	111.91
14	F	601	HEA	OMA-CMA-C3A	-2.93	119.07	125.69
19	M	501	9YF	C7-C6-C5	2.92	115.91	110.82
21	C	304	MQ9	C50-C49-C48	-2.90	114.25	122.65
21	O	304	MQ9	C50-C49-C48	-2.90	114.26	122.65
21	N	608	MQ9	C31-C29-C28	-2.89	115.27	121.12
14	R	601	HEA	OMA-CMA-C3A	-2.89	119.16	125.69
19	A	504	9YF	C7-C6-C5	2.87	115.84	110.82
21	B	608	MQ9	C31-C29-C28	-2.87	115.31	121.12
19	M	504	9YF	C6-C5-C4	2.85	115.79	110.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	502	CDL	OB8-CB7-C71	2.85	120.84	111.91
19	A	503	9YF	C6-C5-C4	2.84	115.78	110.82
22	O	302	HEC	CBB-CAB-C3B	2.84	120.25	112.43
22	C	302	HEC	CBB-CAB-C3B	2.83	120.24	112.43
22	O	301	HEC	CAD-C3D-C2D	-2.82	122.62	127.88
21	B	608	MQ9	C10-C9-C11	-2.82	110.53	115.27
15	M	503	CDL	OB8-CB7-C71	2.81	120.74	111.91
20	B	601	HEM	C4C-NC-C1C	2.81	108.10	105.35
21	N	607	MQ9	C10-C9-C11	-2.80	110.55	115.27
14	R	601	HEA	CMB-C2B-C1B	2.80	129.31	125.04
14	R	602	HEA	CHA-C1A-C2A	-2.80	120.41	124.94
15	P	201	CDL	OA8-CA7-C31	2.79	120.68	111.91
22	C	301	HEC	CAD-C3D-C2D	-2.79	122.69	127.88
15	N	604	CDL	OB8-CB7-C71	2.78	120.64	111.91
14	F	601	HEA	CMB-C2B-C1B	2.78	129.27	125.04
15	D	201	CDL	OA8-CA7-C31	2.78	120.63	111.91
16	P	202	9Y0	O5-C5-C6	2.78	120.62	111.91
20	N	602	HEM	C4C-NC-C1C	2.77	108.06	105.35
20	N	602	HEM	CAA-CBA-CGA	-2.76	107.65	113.60
16	W	201	9Y0	O5-C5-C6	2.76	120.58	111.91
16	D	202	9Y0	O5-C5-C6	2.76	120.57	111.91
21	B	607	MQ9	C10-C9-C11	-2.76	110.63	115.27
21	N	608	MQ9	C10-C9-C11	-2.75	110.64	115.27
15	B	603	CDL	OB8-CB7-C71	2.75	120.53	111.91
15	N	601	CDL	OB8-CB7-C71	2.74	120.49	111.91
20	B	601	HEM	CAA-CBA-CGA	-2.73	107.72	113.60
15	B	611	CDL	OB8-CB7-C71	2.73	120.48	111.91
15	B	604	CDL	OB8-CB7-C71	2.73	120.47	111.91
14	F	602	HEA	CHA-C1A-C2A	-2.73	120.52	124.94
14	F	602	HEA	CHC-C4B-C3B	-2.72	118.80	125.80
14	F	602	HEA	C4B-C3B-C2B	-2.71	102.78	107.41
15	N	605	CDL	OB8-CB7-C71	2.71	120.42	111.91
15	B	605	CDL	OA8-CA7-C31	2.70	120.37	111.91
21	N	609	MQ9	C40-C39-C41	-2.69	110.75	115.27
18	W	204	9XX	O-C15-C14	2.68	120.33	111.91
15	N	606	CDL	OA8-CA7-C31	2.68	120.33	111.91
14	R	602	HEA	C4D-C3D-C2D	-2.68	102.99	106.90
14	R	602	HEA	C4B-C3B-C2B	-2.68	102.84	107.41
14	F	602	HEA	C4D-C3D-C2D	-2.67	103.00	106.90
21	B	609	MQ9	C40-C39-C41	-2.67	110.77	115.27
18	K	204	9XX	O-C15-C14	2.67	120.29	111.91
14	R	602	HEA	CHC-C4B-C3B	-2.66	118.96	125.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	S	301	9Y0	O5-C5-C6	2.64	120.20	111.91
22	O	301	HEC	CHA-C4D-C3D	2.64	128.72	124.84
14	R	601	HEA	CMB-C2B-C3B	-2.64	125.31	130.34
16	G	301	9Y0	O5-C5-C6	2.64	120.18	111.91
14	F	601	HEA	CMB-C2B-C3B	-2.63	125.33	130.34
22	C	301	HEC	CHA-C4D-C3D	2.62	128.69	124.84
16	B	612	9Y0	O5-C5-C6	2.61	120.11	111.91
19	M	501	9YF	O11-C25-C26	2.61	120.10	111.91
19	W	202	9YF	C7-C2-C3	-2.60	107.10	110.85
19	A	504	9YF	O11-C25-C26	2.60	120.07	111.91
16	B	606	9Y0	O5-C5-C6	2.60	120.06	111.91
20	B	601	HEM	CBD-CAD-C3D	-2.58	105.46	112.63
15	D	201	CDL	OB8-CB7-C71	2.57	119.97	111.91
19	A	503	9YF	C24-C-C1	-2.57	105.72	111.79
21	N	609	MQ9	C7-C6-C1	2.56	121.25	118.50
15	P	201	CDL	OB8-CB7-C71	2.56	119.94	111.91
14	R	602	HEA	CBA-CAA-C2A	2.56	119.74	112.63
21	B	609	MQ9	C7-C6-C1	2.55	121.23	118.50
15	T	201	CDL	OB8-CB7-C71	2.54	119.89	111.91
15	B	611	CDL	OA8-CA7-C31	2.54	119.87	111.91
15	N	601	CDL	OA8-CA7-C31	2.54	119.87	111.91
15	M	503	CDL	OA8-CA7-C31	2.54	119.87	111.91
15	H	201	CDL	OB8-CB7-C71	2.53	119.85	111.91
22	O	302	HEC	CHA-C1A-C2A	2.53	129.03	124.94
15	A	502	CDL	OA8-CA7-C31	2.53	119.84	111.91
22	C	302	HEC	CHA-C1A-C2A	2.53	129.03	124.94
22	C	301	HEC	CHB-C1B-NB	2.53	127.16	124.42
21	B	609	MQ9	C25-C24-C26	-2.52	111.04	115.27
22	O	301	HEC	CHB-C1B-NB	2.51	127.15	124.42
19	M	504	9YF	C-O9-C8	-2.50	111.63	117.79
15	N	606	CDL	CB4-OB6-CB5	2.50	123.95	117.79
14	F	602	HEA	CBA-CAA-C2A	2.49	119.55	112.63
20	N	602	HEM	CBD-CAD-C3D	-2.49	105.71	112.63
19	C	303	9YF	O11-C25-C26	2.49	119.72	111.91
21	N	609	MQ9	C25-C24-C26	-2.49	111.08	115.27
19	O	303	9YF	O11-C25-C26	2.48	119.70	111.91
15	F	606	CDL	OA8-CA7-C31	2.48	119.69	111.91
15	B	605	CDL	CB4-OB6-CB5	2.48	123.89	117.79
15	T	201	CDL	OA8-CA7-C31	2.47	119.65	111.91
15	H	201	CDL	OA8-CA7-C31	2.47	119.64	111.91
21	B	609	MQ9	C35-C34-C36	-2.46	111.13	115.27
21	N	609	MQ9	C35-C34-C36	-2.45	111.15	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	N	607	MQ9	C7-C6-C1	2.45	121.12	118.50
15	F	605	CDL	OB8-CB7-C71	2.44	119.57	111.91
15	B	605	CDL	OB8-CB7-C71	2.44	119.56	111.91
15	R	605	CDL	OB8-CB7-C71	2.43	119.54	111.91
15	R	606	CDL	OA8-CA7-C31	2.43	119.54	111.91
20	N	602	HEM	C1C-CHC-C4B	-2.43	120.81	126.06
20	N	603	HEM	C1B-NB-C4B	2.43	107.58	105.07
15	N	606	CDL	OB8-CB7-C71	2.43	119.52	111.91
22	O	302	HEC	C3C-C4C-NC	-2.42	107.44	110.15
22	O	301	HEC	CAA-CBA-CGA	-2.41	108.41	113.60
21	B	610	MQ9	C20-C19-C21	-2.41	111.22	115.27
22	C	301	HEC	CAA-CBA-CGA	-2.41	108.43	113.60
20	B	601	HEM	CAC-C3C-C4C	2.40	128.95	124.71
21	N	610	MQ9	C20-C19-C21	-2.40	111.24	115.27
21	N	607	MQ9	O1-C1-C2	-2.39	117.70	121.56
21	B	607	MQ9	C7-C6-C1	2.38	121.05	118.50
20	N	602	HEM	CAC-C3C-C4C	2.38	128.91	124.71
18	Y	302	9XX	O-C15-C14	2.38	119.37	111.91
18	Z	302	9XX	O-C15-C14	2.38	119.36	111.91
20	B	602	HEM	C1B-NB-C4B	2.37	107.52	105.07
15	F	606	CDL	OB8-CB7-C71	2.37	119.33	111.91
21	B	607	MQ9	O1-C1-C2	-2.35	117.75	121.56
15	R	606	CDL	OB8-CB7-C71	2.35	119.28	111.91
20	B	602	HEM	CAC-C3C-C4C	-2.34	119.24	124.90
20	N	603	HEM	CAC-C3C-C4C	-2.34	119.24	124.90
19	K	202	9YF	C7-C2-C3	-2.34	107.48	110.85
22	C	302	HEC	CBC-CAC-C3C	2.34	118.88	112.43
22	O	302	HEC	CBC-CAC-C3C	2.33	118.87	112.43
22	C	302	HEC	C3C-C4C-NC	-2.33	107.54	110.15
20	B	601	HEM	C1C-CHC-C4B	-2.33	121.03	126.06
14	R	601	HEA	CAD-C3D-C4D	2.33	128.73	124.66
22	C	302	HEC	C3D-C4D-ND	-2.33	108.10	110.36
22	O	302	HEC	CHA-C4D-ND	2.33	126.95	124.42
22	C	302	HEC	CHA-C4D-ND	2.33	126.95	124.42
20	N	603	HEM	CMC-C2C-C1C	-2.33	120.61	124.71
15	P	201	CDL	CA4-OA6-CA5	-2.32	112.08	117.79
14	F	601	HEA	CAD-C3D-C4D	2.31	128.70	124.66
20	B	602	HEM	CMC-C2C-C1C	-2.31	120.64	124.71
22	O	301	HEC	CAB-C3B-C4B	2.31	127.80	124.81
20	B	602	HEM	C4C-NC-C1C	2.30	107.60	105.35
22	O	302	HEC	CAD-CBD-CGD	-2.30	108.66	113.60
22	C	302	HEC	C1B-C2B-C3B	2.29	109.36	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	302	HEC	CAD-CBD-CGD	-2.29	108.68	113.60
22	C	301	HEC	CAB-C3B-C4B	2.28	127.77	124.81
15	D	201	CDL	CA4-OA6-CA5	-2.28	112.17	117.79
22	O	302	HEC	C3D-C4D-ND	-2.28	108.15	110.36
20	N	603	HEM	C4C-NC-C1C	2.27	107.58	105.35
21	N	610	MQ9	C30-C29-C31	-2.27	111.45	115.27
22	O	302	HEC	C1B-C2B-C3B	2.26	109.34	106.96
21	N	608	MQ9	C25-C24-C26	-2.26	111.46	115.27
21	B	610	MQ9	C30-C29-C31	-2.26	111.46	115.27
15	R	606	CDL	CB6-CB4-CB3	-2.25	106.47	111.79
14	F	602	HEA	O2D-CGD-CBD	2.24	121.22	114.03
21	B	608	MQ9	C25-C24-C26	-2.24	111.51	115.27
19	A	503	9YF	O11-C25-C26	2.23	118.92	111.91
20	B	602	HEM	CHC-C1C-NC	2.22	126.84	124.44
14	F	602	HEA	CAA-C2A-C1A	-2.21	120.73	124.89
21	N	609	MQ9	C5M-C5-C6	-2.21	120.80	124.40
14	R	602	HEA	O2D-CGD-CBD	2.20	121.11	114.03
14	R	601	HEA	O2D-CGD-CBD	2.20	121.08	114.03
22	C	302	HEC	CHD-C4C-NC	-2.19	119.81	123.85
20	N	603	HEM	CHC-C1C-NC	2.19	126.81	124.44
15	A	502	CDL	CB6-CB4-CB3	-2.19	106.61	111.79
14	F	601	HEA	O2D-CGD-CBD	2.19	121.05	114.03
14	R	602	HEA	CAA-C2A-C1A	-2.19	120.78	124.89
15	F	606	CDL	CB6-CB4-CB3	-2.18	106.64	111.79
15	M	503	CDL	CB6-CB4-CB3	-2.17	106.64	111.79
21	B	609	MQ9	C5M-C5-C6	-2.17	120.85	124.40
20	B	601	HEM	C3D-C4D-ND	-2.17	107.75	110.17
22	O	302	HEC	CHD-C4C-NC	-2.17	119.86	123.85
22	O	302	HEC	CHB-C1B-NB	2.16	126.77	124.42
15	N	604	CDL	OA8-CA7-C31	2.16	118.68	111.91
22	C	302	HEC	CHB-C1B-NB	2.15	126.75	124.42
19	O	303	9YF	C7-C2-C3	2.15	113.95	110.85
22	C	302	HEC	CHD-C1D-ND	2.14	127.02	124.37
19	C	303	9YF	C7-C2-C3	2.14	113.94	110.85
19	A	503	9YF	C-O9-C8	-2.12	112.56	117.79
15	B	603	CDL	OA8-CA7-C31	2.12	118.57	111.91
22	C	302	HEC	C4A-NA-C1A	2.12	107.42	105.35
21	O	304	MQ9	C35-C34-C36	-2.11	111.72	115.27
21	C	304	MQ9	C35-C34-C36	-2.10	111.74	115.27
20	N	602	HEM	C3D-C4D-ND	-2.10	107.83	110.17
14	F	602	HEA	CHB-C1B-C2B	-2.10	121.70	124.98
22	O	302	HEC	CHD-C1D-ND	2.10	126.96	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	607	MQ9	C5M-C5-C6	-2.09	120.99	124.40
19	M	501	9YF	C6-C5-C4	2.09	114.47	110.82
22	O	302	HEC	C4A-NA-C1A	2.08	107.39	105.35
21	N	607	MQ9	C5M-C5-C6	-2.08	121.01	124.40
20	N	602	HEM	C2D-C1D-ND	-2.08	107.39	109.88
20	B	601	HEM	C2D-C1D-ND	-2.07	107.40	109.88
14	F	601	HEA	CHC-C4B-NB	2.07	126.92	124.37
14	R	601	HEA	CHC-C4B-NB	2.07	126.92	124.37
19	A	504	9YF	C6-C5-C4	2.07	114.43	110.82
15	B	604	CDL	CB4-OB6-CB5	-2.06	112.72	117.79
14	R	602	HEA	CMB-C2B-C3B	-2.06	126.42	130.34
19	M	504	9YF	O11-C25-C26	2.06	118.36	111.91
14	R	602	HEA	CHB-C1B-C2B	-2.06	121.77	124.98
20	N	603	HEM	CAD-CBD-CGD	-2.05	109.18	113.60
20	B	602	HEM	CAA-CBA-CGA	-2.04	109.21	113.60
20	N	603	HEM	CAA-CBA-CGA	-2.04	109.21	113.60
15	N	605	CDL	CB4-OB6-CB5	-2.04	112.77	117.79
21	N	608	MQ9	C5M-C5-C6	-2.04	121.07	124.40
14	F	602	HEA	CMB-C2B-C3B	-2.03	126.47	130.34
15	N	604	CDL	CA4-OA6-CA5	-2.03	112.79	117.79
20	B	602	HEM	CAD-CBD-CGD	-2.02	109.25	113.60
14	R	602	HEA	CMD-C2D-C1D	2.01	128.09	125.04
21	O	304	MQ9	C5M-C5-C6	-2.01	121.13	124.40

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	C	302	HEC	NA
22	O	302	HEC	NA

All (1735) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	F	601	HEA	C1A-C2A-CAA-CBA
14	F	601	HEA	C3A-C2A-CAA-CBA
14	F	601	HEA	C2A-C3A-CMA-OMA
14	F	601	HEA	C4A-C3A-CMA-OMA
14	F	601	HEA	C17-C18-C19-C20
14	F	602	HEA	C1A-C2A-CAA-CBA
14	F	602	HEA	C2A-C3A-CMA-OMA
14	F	602	HEA	C4A-C3A-CMA-OMA
14	F	602	HEA	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
14	F	602	HEA	C4C-C3C-CAC-CBC
14	F	602	HEA	C3B-C11-C12-C13
14	F	602	HEA	O11-C11-C12-C13
14	F	602	HEA	C13-C14-C15-C16
14	F	602	HEA	C14-C15-C16-C17
14	F	602	HEA	C15-C16-C17-C18
14	R	601	HEA	C1A-C2A-CAA-CBA
14	R	601	HEA	C3A-C2A-CAA-CBA
14	R	601	HEA	C2A-C3A-CMA-OMA
14	R	601	HEA	C4A-C3A-CMA-OMA
14	R	601	HEA	C17-C18-C19-C20
14	R	602	HEA	C2A-C3A-CMA-OMA
14	R	602	HEA	C4A-C3A-CMA-OMA
14	R	602	HEA	C2C-C3C-CAC-CBC
14	R	602	HEA	C4C-C3C-CAC-CBC
14	R	602	HEA	C3B-C11-C12-C13
14	R	602	HEA	O11-C11-C12-C13
14	R	602	HEA	C13-C14-C15-C16
14	R	602	HEA	C14-C15-C16-C17
14	R	602	HEA	C15-C16-C17-C18
15	F	605	CDL	OA6-CA4-CA6-OA8
15	F	605	CDL	CB2-OB2-PB2-OB3
15	F	605	CDL	CB2-OB2-PB2-OB4
15	F	605	CDL	CB2-OB2-PB2-OB5
15	F	605	CDL	CB3-OB5-PB2-OB4
15	F	605	CDL	C51-CB5-OB6-CB4
15	F	606	CDL	CA2-OA2-PA1-OA4
15	F	606	CDL	CA3-OA5-PA1-OA3
15	F	606	CDL	CB2-OB2-PB2-OB3
15	F	606	CDL	CB2-OB2-PB2-OB4
15	F	606	CDL	CB2-OB2-PB2-OB5
15	F	606	CDL	CB3-OB5-PB2-OB4
15	H	201	CDL	CA2-C1-CB2-OB2
15	H	201	CDL	CA2-OA2-PA1-OA3
15	H	201	CDL	CA2-OA2-PA1-OA4
15	H	201	CDL	CB2-OB2-PB2-OB3
15	H	201	CDL	CB3-OB5-PB2-OB3
15	D	201	CDL	CA3-OA5-PA1-OA3
15	D	201	CDL	C11-CA5-OA6-CA4
15	D	201	CDL	CB2-OB2-PB2-OB3
15	D	201	CDL	CB3-OB5-PB2-OB3
15	D	201	CDL	CB3-OB5-PB2-OB4

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Mol	Chain	Res	Type	Atoms
15	B	603	CDL	O1-C1-CA2-OA2
15	B	603	CDL	OA5-CA3-CA4-OA6
15	B	603	CDL	OA7-CA5-OA6-CA4
15	B	603	CDL	C11-CA5-OA6-CA4
15	B	603	CDL	CB3-OB5-PB2-OB3
15	B	603	CDL	CB3-OB5-PB2-OB4
15	B	604	CDL	C11-CA5-OA6-CA4
15	B	604	CDL	CB2-OB2-PB2-OB3
15	B	604	CDL	CB2-OB2-PB2-OB4
15	B	605	CDL	CA2-OA2-PA1-OA3
15	B	611	CDL	C11-CA5-OA6-CA4
15	B	611	CDL	C51-CB5-OB6-CB4
15	A	502	CDL	CA2-OA2-PA1-OA3
15	A	502	CDL	CA2-OA2-PA1-OA4
15	A	502	CDL	CA2-OA2-PA1-OA5
15	A	502	CDL	CA3-OA5-PA1-OA3
15	A	502	CDL	C11-CA5-OA6-CA4
15	A	502	CDL	CB2-OB2-PB2-OB3
15	A	502	CDL	CB2-OB2-PB2-OB4
15	A	502	CDL	CB2-OB2-PB2-OB5
15	A	502	CDL	CB3-OB5-PB2-OB4
15	A	502	CDL	C51-CB5-OB6-CB4
15	R	605	CDL	OA6-CA4-CA6-OA8
15	R	605	CDL	CB2-OB2-PB2-OB3
15	R	605	CDL	CB2-OB2-PB2-OB4
15	R	605	CDL	CB2-OB2-PB2-OB5
15	R	605	CDL	CB3-OB5-PB2-OB4
15	R	605	CDL	C51-CB5-OB6-CB4
15	R	606	CDL	CA2-OA2-PA1-OA4
15	R	606	CDL	CB2-OB2-PB2-OB3
15	R	606	CDL	CB2-OB2-PB2-OB4
15	R	606	CDL	CB2-OB2-PB2-OB5
15	R	606	CDL	CB3-OB5-PB2-OB4
15	T	201	CDL	CA2-C1-CB2-OB2
15	T	201	CDL	CA2-OA2-PA1-OA3
15	T	201	CDL	CA2-OA2-PA1-OA4
15	T	201	CDL	CB2-OB2-PB2-OB3
15	T	201	CDL	CB3-OB5-PB2-OB3
15	P	201	CDL	CA3-OA5-PA1-OA3
15	P	201	CDL	C11-CA5-OA6-CA4
15	P	201	CDL	CB2-OB2-PB2-OB3
15	P	201	CDL	CB3-OB5-PB2-OB3

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Mol	Chain	Res	Type	Atoms
15	P	201	CDL	CB3-OB5-PB2-OB4
15	N	601	CDL	C11-CA5-OA6-CA4
15	N	601	CDL	C51-CB5-OB6-CB4
15	N	604	CDL	O1-C1-CA2-OA2
15	N	604	CDL	CA3-OA5-PA1-OA4
15	N	604	CDL	OA5-CA3-CA4-OA6
15	N	604	CDL	OA7-CA5-OA6-CA4
15	N	604	CDL	C11-CA5-OA6-CA4
15	N	604	CDL	CB3-OB5-PB2-OB3
15	N	604	CDL	CB3-OB5-PB2-OB4
15	N	605	CDL	C11-CA5-OA6-CA4
15	N	605	CDL	CB2-OB2-PB2-OB3
15	N	605	CDL	CB2-OB2-PB2-OB4
15	N	606	CDL	CA2-OA2-PA1-OA3
15	M	503	CDL	CA2-OA2-PA1-OA3
15	M	503	CDL	CA2-OA2-PA1-OA4
15	M	503	CDL	CA2-OA2-PA1-OA5
15	M	503	CDL	CA3-OA5-PA1-OA3
15	M	503	CDL	C11-CA5-OA6-CA4
15	M	503	CDL	CB2-OB2-PB2-OB3
15	M	503	CDL	CB2-OB2-PB2-OB4
15	M	503	CDL	CB2-OB2-PB2-OB5
15	M	503	CDL	CB3-OB5-PB2-OB4
15	M	503	CDL	C51-CB5-OB6-CB4
16	G	301	9Y0	O5-C-C1-O7
16	G	301	9Y0	C13-C14-C15-C16
16	D	202	9Y0	O7-C1-C2-O3
16	D	202	9Y0	C22-C21-O7-C1
16	D	202	9Y0	O6-C21-O7-C1
16	D	202	9Y0	O1-C3-C4-N
16	D	202	9Y0	C3-O1-P-O
16	D	202	9Y0	C3-O1-P-O2
16	D	202	9Y0	C3-O1-P-O3
16	K	201	9Y0	C22-C21-O7-C1
16	K	201	9Y0	C3-O1-P-O
16	K	201	9Y0	C3-O1-P-O3
16	K	201	9Y0	C2-O3-P-O2
16	B	606	9Y0	O1-C3-C4-N
16	B	606	9Y0	C2-O3-P-O
16	B	612	9Y0	O1-C3-C4-N
16	B	612	9Y0	C2-O3-P-O
16	S	301	9Y0	O5-C-C1-O7

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Mol	Chain	Res	Type	Atoms
16	S	301	9Y0	C13-C14-C15-C16
16	P	202	9Y0	O7-C1-C2-O3
16	P	202	9Y0	C22-C21-O7-C1
16	P	202	9Y0	O6-C21-O7-C1
16	P	202	9Y0	O1-C3-C4-N
16	P	202	9Y0	C3-O1-P-O
16	P	202	9Y0	C3-O1-P-O2
16	P	202	9Y0	C3-O1-P-O3
16	W	201	9Y0	C22-C21-O7-C1
16	W	201	9Y0	C6-C5-O5-C
16	W	201	9Y0	O4-C5-O5-C
16	W	201	9Y0	C3-O1-P-O
16	W	201	9Y0	C3-O1-P-O3
16	W	201	9Y0	C2-O3-P-O
16	W	201	9Y0	C2-O3-P-O2
18	Y	302	9XX	O-C16-C17-C37
18	Y	302	9XX	O-C16-C17-O1
18	Y	302	9XX	C19-C18-O1-C17
18	Y	302	9XX	O2-C18-O1-C17
18	K	204	9XX	O-C16-C17-C37
18	K	204	9XX	O-C16-C17-O1
18	Z	302	9XX	O-C16-C17-C37
18	Z	302	9XX	O-C16-C17-O1
18	Z	302	9XX	C19-C18-O1-C17
18	Z	302	9XX	O2-C18-O1-C17
18	W	204	9XX	O-C16-C17-C37
18	W	204	9XX	O-C16-C17-O1
19	K	202	9YF	O9-C-C24-O11
19	C	303	9YF	C2-O2-P-O
19	C	303	9YF	C1-O-P-O1
19	C	303	9YF	C1-O-P-O8
19	C	303	9YF	C9-C8-O9-C
19	A	503	9YF	C9-C8-O9-C
19	A	503	9YF	O10-C8-O9-C
19	A	504	9YF	C2-O2-P-O1
19	W	202	9YF	O9-C-C24-O11
19	O	303	9YF	C2-O2-P-O
19	O	303	9YF	C1-O-P-O1
19	O	303	9YF	C1-O-P-O8
19	O	303	9YF	C9-C8-O9-C
19	M	501	9YF	C2-O2-P-O1
19	M	504	9YF	C1-O-P-O1

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Mol	Chain	Res	Type	Atoms
19	M	504	9YF	C1-O-P-O2
19	M	504	9YF	C1-O-P-O8
19	M	504	9YF	C9-C8-O9-C
21	B	607	MQ9	C7-C8-C9-C11
21	B	607	MQ9	C9-C11-C12-C13
21	B	607	MQ9	C18-C19-C21-C22
21	B	607	MQ9	C22-C23-C24-C25
21	B	607	MQ9	C22-C23-C24-C26
21	B	607	MQ9	C27-C28-C29-C30
21	B	607	MQ9	C28-C29-C31-C32
21	B	607	MQ9	C32-C33-C34-C36
21	B	608	MQ9	C7-C8-C9-C10
21	B	608	MQ9	C7-C8-C9-C11
21	B	608	MQ9	C12-C13-C14-C16
21	B	608	MQ9	C13-C14-C16-C17
21	B	608	MQ9	C14-C16-C17-C18
21	B	608	MQ9	C20-C19-C21-C22
21	B	608	MQ9	C19-C21-C22-C23
21	B	608	MQ9	C22-C23-C24-C25
21	B	608	MQ9	C22-C23-C24-C26
21	B	608	MQ9	C27-C28-C29-C30
21	B	608	MQ9	C32-C33-C34-C35
21	B	608	MQ9	C33-C34-C36-C37
21	B	608	MQ9	C34-C36-C37-C38
21	B	608	MQ9	C37-C38-C39-C40
21	B	609	MQ9	C7-C8-C9-C10
21	B	609	MQ9	C7-C8-C9-C11
21	B	609	MQ9	C12-C13-C14-C16
21	B	609	MQ9	C17-C18-C19-C20
21	B	609	MQ9	C20-C19-C21-C22
21	B	609	MQ9	C19-C21-C22-C23
21	B	609	MQ9	C22-C23-C24-C25
21	B	609	MQ9	C33-C34-C36-C37
21	B	609	MQ9	C42-C43-C44-C45
21	B	609	MQ9	C42-C43-C44-C46
21	B	610	MQ9	C7-C8-C9-C11
21	B	610	MQ9	C12-C11-C9-C8
21	B	610	MQ9	C12-C13-C14-C15
21	B	610	MQ9	C12-C13-C14-C16
21	B	610	MQ9	C17-C18-C19-C21
21	B	610	MQ9	C19-C21-C22-C23
21	B	610	MQ9	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
21	B	610	MQ9	C22-C23-C24-C26
21	B	610	MQ9	C27-C28-C29-C30
21	B	610	MQ9	C32-C33-C34-C36
21	C	304	MQ9	C9-C11-C12-C13
21	C	304	MQ9	C12-C13-C14-C16
21	C	304	MQ9	C17-C18-C19-C20
21	C	304	MQ9	C25-C24-C26-C27
21	C	304	MQ9	C29-C31-C32-C33
21	C	304	MQ9	C32-C33-C34-C36
21	C	304	MQ9	C33-C34-C36-C37
21	C	304	MQ9	C37-C38-C39-C41
21	C	304	MQ9	C40-C39-C41-C42
21	C	304	MQ9	C47-C48-C49-C51
21	N	607	MQ9	C7-C8-C9-C11
21	N	607	MQ9	C12-C11-C9-C8
21	N	607	MQ9	C9-C11-C12-C13
21	N	607	MQ9	C18-C19-C21-C22
21	N	607	MQ9	C22-C23-C24-C25
21	N	607	MQ9	C22-C23-C24-C26
21	N	607	MQ9	C27-C28-C29-C30
21	N	607	MQ9	C28-C29-C31-C32
21	N	607	MQ9	C32-C33-C34-C36
21	N	608	MQ9	C7-C8-C9-C10
21	N	608	MQ9	C7-C8-C9-C11
21	N	608	MQ9	C12-C13-C14-C16
21	N	608	MQ9	C13-C14-C16-C17
21	N	608	MQ9	C14-C16-C17-C18
21	N	608	MQ9	C20-C19-C21-C22
21	N	608	MQ9	C19-C21-C22-C23
21	N	608	MQ9	C22-C23-C24-C25
21	N	608	MQ9	C22-C23-C24-C26
21	N	608	MQ9	C27-C28-C29-C30
21	N	608	MQ9	C32-C33-C34-C35
21	N	608	MQ9	C33-C34-C36-C37
21	N	608	MQ9	C34-C36-C37-C38
21	N	608	MQ9	C37-C38-C39-C40
21	N	609	MQ9	C7-C8-C9-C10
21	N	609	MQ9	C7-C8-C9-C11
21	N	609	MQ9	C12-C13-C14-C16
21	N	609	MQ9	C17-C18-C19-C20
21	N	609	MQ9	C20-C19-C21-C22
21	N	609	MQ9	C19-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
21	N	609	MQ9	C22-C23-C24-C25
21	N	609	MQ9	C33-C34-C36-C37
21	N	609	MQ9	C42-C43-C44-C45
21	N	609	MQ9	C42-C43-C44-C46
21	N	610	MQ9	C7-C8-C9-C11
21	N	610	MQ9	C12-C11-C9-C8
21	N	610	MQ9	C12-C13-C14-C15
21	N	610	MQ9	C12-C13-C14-C16
21	N	610	MQ9	C17-C18-C19-C21
21	N	610	MQ9	C19-C21-C22-C23
21	N	610	MQ9	C22-C23-C24-C25
21	N	610	MQ9	C22-C23-C24-C26
21	N	610	MQ9	C27-C28-C29-C30
21	N	610	MQ9	C32-C33-C34-C36
21	O	304	MQ9	C9-C11-C12-C13
21	O	304	MQ9	C12-C13-C14-C16
21	O	304	MQ9	C17-C18-C19-C20
21	O	304	MQ9	C25-C24-C26-C27
21	O	304	MQ9	C29-C31-C32-C33
21	O	304	MQ9	C32-C33-C34-C36
21	O	304	MQ9	C33-C34-C36-C37
21	O	304	MQ9	C37-C38-C39-C41
21	O	304	MQ9	C40-C39-C41-C42
21	O	304	MQ9	C47-C48-C49-C51
22	C	302	HEC	C2C-C3C-CAC-CBC
22	O	302	HEC	C2C-C3C-CAC-CBC
22	C	302	HEC	C4C-C3C-CAC-CBC
22	O	302	HEC	C4C-C3C-CAC-CBC
14	F	601	HEA	C21-C22-C23-C24
14	F	602	HEA	C21-C22-C23-C24
14	R	601	HEA	C21-C22-C23-C24
14	R	602	HEA	C21-C22-C23-C24
16	K	201	9Y0	O4-C5-O5-C
15	F	605	CDL	OB7-CB5-OB6-CB4
15	D	201	CDL	OA7-CA5-OA6-CA4
15	B	604	CDL	OA7-CA5-OA6-CA4
15	B	605	CDL	OA7-CA5-OA6-CA4
15	B	611	CDL	OA7-CA5-OA6-CA4
15	A	502	CDL	OB7-CB5-OB6-CB4
15	R	605	CDL	OB7-CB5-OB6-CB4
15	P	201	CDL	OA7-CA5-OA6-CA4
15	N	601	CDL	OA7-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
15	N	605	CDL	OA7-CA5-OA6-CA4
15	N	606	CDL	OA7-CA5-OA6-CA4
15	M	503	CDL	OB7-CB5-OB6-CB4
16	K	201	9Y0	O6-C21-O7-C1
16	W	201	9Y0	O6-C21-O7-C1
19	C	303	9YF	O10-C8-O9-C
19	O	303	9YF	O10-C8-O9-C
19	M	504	9YF	O10-C8-O9-C
16	K	201	9Y0	C6-C5-O5-C
21	B	607	MQ9	C30-C29-C31-C32
21	N	607	MQ9	C30-C29-C31-C32
21	B	607	MQ9	C12-C11-C9-C8
15	D	201	CDL	OA9-CA7-OA8-CA6
15	P	201	CDL	OA9-CA7-OA8-CA6
15	D	201	CDL	C31-CA7-OA8-CA6
15	D	201	CDL	C71-CB7-OB8-CB6
15	P	201	CDL	C31-CA7-OA8-CA6
15	P	201	CDL	C71-CB7-OB8-CB6
19	C	303	9YF	C26-C25-O11-C24
19	O	303	9YF	C26-C25-O11-C24
19	M	504	9YF	C27-C28-C29-C30
14	R	602	HEA	C1A-C2A-CAA-CBA
21	B	609	MQ9	C47-C48-C49-C50
21	N	609	MQ9	C47-C48-C49-C50
14	F	601	HEA	C17-C18-C19-C27
14	F	602	HEA	C17-C18-C19-C27
14	R	601	HEA	C17-C18-C19-C27
14	R	602	HEA	C17-C18-C19-C27
21	B	607	MQ9	C12-C13-C14-C15
21	B	608	MQ9	C17-C18-C19-C20
21	B	609	MQ9	C27-C28-C29-C30
21	B	609	MQ9	C32-C33-C34-C35
21	B	609	MQ9	C37-C38-C39-C40
21	C	304	MQ9	C7-C8-C9-C10
21	C	304	MQ9	C12-C13-C14-C15
21	C	304	MQ9	C22-C23-C24-C25
21	C	304	MQ9	C42-C43-C44-C45
21	N	607	MQ9	C12-C13-C14-C15
21	N	608	MQ9	C17-C18-C19-C20
21	N	609	MQ9	C27-C28-C29-C30
21	N	609	MQ9	C32-C33-C34-C35
21	N	609	MQ9	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
21	O	304	MQ9	C7-C8-C9-C10
21	O	304	MQ9	C12-C13-C14-C15
21	O	304	MQ9	C22-C23-C24-C25
21	O	304	MQ9	C42-C43-C44-C45
15	B	611	CDL	OB7-CB5-OB6-CB4
15	A	502	CDL	OA7-CA5-OA6-CA4
15	N	601	CDL	OB7-CB5-OB6-CB4
15	M	503	CDL	OA7-CA5-OA6-CA4
14	F	601	HEA	C13-C14-C15-C16
14	R	601	HEA	C13-C14-C15-C16
21	B	607	MQ9	C17-C18-C19-C21
21	C	304	MQ9	C17-C18-C19-C21
21	N	607	MQ9	C17-C18-C19-C21
21	O	304	MQ9	C17-C18-C19-C21
15	D	201	CDL	O1-C1-CB2-OB2
15	B	603	CDL	O1-C1-CB2-OB2
15	B	605	CDL	O1-C1-CA2-OA2
15	A	502	CDL	O1-C1-CA2-OA2
15	P	201	CDL	O1-C1-CB2-OB2
15	N	604	CDL	O1-C1-CB2-OB2
15	N	606	CDL	O1-C1-CA2-OA2
15	M	503	CDL	O1-C1-CA2-OA2
15	B	605	CDL	C11-CA5-OA6-CA4
15	N	606	CDL	C11-CA5-OA6-CA4
21	B	607	MQ9	C32-C33-C34-C35
21	N	607	MQ9	C32-C33-C34-C35
19	A	503	9YF	C28-C29-C30-C31
14	F	602	HEA	C3A-C2A-CAA-CBA
15	D	201	CDL	OB9-CB7-OB8-CB6
19	O	303	9YF	O12-C25-O11-C24
14	F	602	HEA	C2A-CAA-CBA-CGA
14	R	602	HEA	C2A-CAA-CBA-CGA
20	B	601	HEM	C3D-CAD-CBD-CGD
20	N	602	HEM	C3D-CAD-CBD-CGD
14	F	602	HEA	C18-C19-C20-C21
14	R	602	HEA	C18-C19-C20-C21
21	B	609	MQ9	C23-C24-C26-C27
21	B	610	MQ9	C13-C14-C16-C17
21	B	610	MQ9	C23-C24-C26-C27
21	B	610	MQ9	C28-C29-C31-C32
21	C	304	MQ9	C13-C14-C16-C17
21	N	609	MQ9	C23-C24-C26-C27

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Mol	Chain	Res	Type	Atoms
21	N	610	MQ9	C13-C14-C16-C17
21	N	610	MQ9	C23-C24-C26-C27
21	N	610	MQ9	C28-C29-C31-C32
21	O	304	MQ9	C13-C14-C16-C17
15	P	201	CDL	C31-C32-C33-C34
18	W	204	9XX	C23-C24-C25-C26
15	P	201	CDL	OB9-CB7-OB8-CB6
19	C	303	9YF	O12-C25-O11-C24
21	B	607	MQ9	C19-C21-C22-C23
21	B	607	MQ9	C29-C31-C32-C33
21	B	608	MQ9	C9-C11-C12-C13
21	B	610	MQ9	C9-C11-C12-C13
21	B	610	MQ9	C14-C16-C17-C18
21	C	304	MQ9	C14-C16-C17-C18
21	C	304	MQ9	C39-C41-C42-C43
21	N	607	MQ9	C19-C21-C22-C23
21	N	607	MQ9	C29-C31-C32-C33
21	N	608	MQ9	C9-C11-C12-C13
21	N	610	MQ9	C9-C11-C12-C13
21	N	610	MQ9	C14-C16-C17-C18
21	O	304	MQ9	C14-C16-C17-C18
21	O	304	MQ9	C39-C41-C42-C43
15	B	611	CDL	C55-C56-C57-C58
15	N	601	CDL	C55-C56-C57-C58
19	M	504	9YF	C37-C38-C39-C40
15	D	201	CDL	C31-C32-C33-C34
18	K	204	9XX	C28-C29-C30-C31
21	B	610	MQ9	C7-C8-C9-C10
21	N	610	MQ9	C7-C8-C9-C10
15	B	605	CDL	CB2-C1-CA2-OA2
15	N	606	CDL	CB2-C1-CA2-OA2
15	B	611	CDL	C31-CA7-OA8-CA6
15	N	601	CDL	C31-CA7-OA8-CA6
15	N	604	CDL	C31-CA7-OA8-CA6
16	K	201	9Y0	C21-C22-C23-C24
16	W	201	9Y0	C21-C22-C23-C24
15	R	606	CDL	C57-C58-C59-C60
14	R	602	HEA	C3A-C2A-CAA-CBA
15	H	201	CDL	O1-C1-CB2-OB2
15	T	201	CDL	O1-C1-CB2-OB2
18	K	204	9XX	C18-C19-C20-C21
18	W	204	9XX	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
19	C	303	9YF	C25-C26-C27-C28
19	O	303	9YF	C25-C26-C27-C28
15	B	603	CDL	C31-CA7-OA8-CA6
19	M	504	9YF	C31-C32-C33-C34
15	F	606	CDL	C51-CB5-OB6-CB4
15	R	606	CDL	C51-CB5-OB6-CB4
16	G	301	9Y0	C22-C21-O7-C1
16	S	301	9Y0	C22-C21-O7-C1
16	K	201	9Y0	C6-C7-C8-C9
19	A	503	9YF	C10-C11-C12-C13
15	F	605	CDL	CA5-C11-C12-C13
15	F	605	CDL	CB7-C71-C72-C73
15	R	605	CDL	CA5-C11-C12-C13
15	R	605	CDL	CB7-C71-C72-C73
15	P	201	CDL	CB7-C71-C72-C73
15	B	611	CDL	OA9-CA7-OA8-CA6
15	N	601	CDL	OA9-CA7-OA8-CA6
19	O	303	9YF	C30-C31-C32-C33
16	D	202	9Y0	C22-C23-C24-C25
16	P	202	9Y0	C22-C23-C24-C25
15	N	601	CDL	C71-CB7-OB8-CB6
15	H	201	CDL	CB5-C51-C52-C53
15	D	201	CDL	CB7-C71-C72-C73
15	B	611	CDL	CB7-C71-C72-C73
15	T	201	CDL	CB5-C51-C52-C53
16	D	202	9Y0	C21-C22-C23-C24
16	P	202	9Y0	C21-C22-C23-C24
16	W	201	9Y0	C5-C6-C7-C8
15	F	605	CDL	C32-C33-C34-C35
19	C	303	9YF	C30-C31-C32-C33
21	B	609	MQ9	C12-C13-C14-C15
21	N	609	MQ9	C12-C13-C14-C15
15	F	606	CDL	CA7-C31-C32-C33
15	B	603	CDL	CB7-C71-C72-C73
15	B	604	CDL	CB7-C71-C72-C73
15	R	606	CDL	CA7-C31-C32-C33
15	P	201	CDL	CB5-C51-C52-C53
15	N	601	CDL	CB7-C71-C72-C73
15	N	604	CDL	CB7-C71-C72-C73
15	N	605	CDL	CB7-C71-C72-C73
18	K	204	9XX	C12-C13-C14-C15
19	W	202	9YF	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
19	A	503	9YF	C17-C18-C19-C20
15	R	605	CDL	C32-C33-C34-C35
19	A	503	9YF	C37-C38-C39-C40
19	M	504	9YF	C17-C18-C19-C20
18	W	204	9XX	C27-C28-C29-C30
15	B	604	CDL	CB5-C51-C52-C53
15	N	605	CDL	CB5-C51-C52-C53
15	M	503	CDL	CA5-C11-C12-C13
19	A	504	9YF	C11-C10-C9-C8
19	M	501	9YF	C11-C10-C9-C8
18	Y	302	9XX	C27-C28-C29-C30
18	Z	302	9XX	C27-C28-C29-C30
19	K	202	9YF	C14-C15-C16-C17
14	F	601	HEA	C2A-CAA-CBA-CGA
14	F	601	HEA	C3D-CAD-CBD-CGD
14	R	601	HEA	C2A-CAA-CBA-CGA
14	R	601	HEA	C3D-CAD-CBD-CGD
18	W	204	9XX	C19-C18-O1-C17
21	B	610	MQ9	C32-C33-C34-C35
21	N	610	MQ9	C32-C33-C34-C35
19	A	504	9YF	C31-C32-C33-C35
19	M	501	9YF	C31-C32-C33-C35
19	M	504	9YF	C31-C32-C33-C35
15	B	603	CDL	OA9-CA7-OA8-CA6
15	N	604	CDL	OA9-CA7-OA8-CA6
21	B	607	MQ9	C14-C16-C17-C18
21	B	608	MQ9	C24-C26-C27-C28
21	B	609	MQ9	C9-C11-C12-C13
21	B	609	MQ9	C29-C31-C32-C33
21	B	609	MQ9	C34-C36-C37-C38
21	C	304	MQ9	C34-C36-C37-C38
21	N	607	MQ9	C14-C16-C17-C18
21	N	608	MQ9	C24-C26-C27-C28
21	N	609	MQ9	C9-C11-C12-C13
21	N	609	MQ9	C29-C31-C32-C33
21	O	304	MQ9	C34-C36-C37-C38
15	A	502	CDL	CA5-C11-C12-C13
16	B	606	9Y0	C5-C6-C7-C8
16	B	612	9Y0	C5-C6-C7-C8
15	D	201	CDL	O1-C1-CA2-OA2
15	B	605	CDL	O1-C1-CB2-OB2
15	N	606	CDL	O1-C1-CB2-OB2

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Mol	Chain	Res	Type	Atoms
15	M	503	CDL	O1-C1-CB2-OB2
16	G	301	9Y0	O6-C21-O7-C1
16	S	301	9Y0	O6-C21-O7-C1
15	F	605	CDL	C31-CA7-OA8-CA6
15	R	605	CDL	C31-CA7-OA8-CA6
15	N	606	CDL	C71-CB7-OB8-CB6
16	B	606	9Y0	C16-C17-C18-C19
16	B	612	9Y0	C16-C17-C18-C19
19	A	504	9YF	C33-C35-C36-C37
19	M	501	9YF	C33-C35-C36-C37
19	M	504	9YF	C35-C36-C37-C38
22	C	301	HEC	C4D-C3D-CAD-CBD
22	O	301	HEC	C4D-C3D-CAD-CBD
15	F	606	CDL	C57-C58-C59-C60
15	F	606	CDL	CA2-OA2-PA1-OA5
15	H	201	CDL	CA2-OA2-PA1-OA5
15	D	201	CDL	CB3-OB5-PB2-OB2
15	B	603	CDL	CA3-OA5-PA1-OA2
15	B	603	CDL	CB3-OB5-PB2-OB2
15	B	604	CDL	CB2-OB2-PB2-OB5
15	B	604	CDL	CB3-OB5-PB2-OB2
15	B	605	CDL	CA2-OA2-PA1-OA5
15	B	611	CDL	CA3-OA5-PA1-OA2
15	B	611	CDL	CB3-OB5-PB2-OB2
15	A	502	CDL	CB3-OB5-PB2-OB2
15	R	606	CDL	CA2-OA2-PA1-OA5
15	T	201	CDL	CA2-OA2-PA1-OA5
15	P	201	CDL	CB3-OB5-PB2-OB2
15	N	601	CDL	CA3-OA5-PA1-OA2
15	N	601	CDL	CB3-OB5-PB2-OB2
15	N	604	CDL	CA3-OA5-PA1-OA2
15	N	604	CDL	CB3-OB5-PB2-OB2
15	N	605	CDL	CB2-OB2-PB2-OB5
15	N	605	CDL	CB3-OB5-PB2-OB2
15	N	606	CDL	CA2-OA2-PA1-OA5
15	M	503	CDL	CB3-OB5-PB2-OB2
16	K	201	9Y0	C2-O3-P-O1
16	B	606	9Y0	C2-O3-P-O1
16	B	612	9Y0	C2-O3-P-O1
16	W	201	9Y0	C2-O3-P-O1
19	C	303	9YF	C1-O-P-O2
19	O	303	9YF	C1-O-P-O2

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Mol	Chain	Res	Type	Atoms
15	H	201	CDL	CA7-C31-C32-C33
15	D	201	CDL	CB5-C51-C52-C53
15	B	605	CDL	CB5-C51-C52-C53
15	T	201	CDL	CA7-C31-C32-C33
15	B	605	CDL	C71-CB7-OB8-CB6
15	B	611	CDL	C71-CB7-OB8-CB6
15	N	606	CDL	CB5-C51-C52-C53
15	B	603	CDL	CB2-C1-CA2-OA2
15	B	603	CDL	CA2-C1-CB2-OB2
15	B	605	CDL	CA2-C1-CB2-OB2
15	P	201	CDL	CA2-C1-CB2-OB2
15	N	604	CDL	CB2-C1-CA2-OA2
15	N	604	CDL	CA2-C1-CB2-OB2
15	N	606	CDL	CA2-C1-CB2-OB2
15	F	606	CDL	OB7-CB5-OB6-CB4
15	R	606	CDL	OB7-CB5-OB6-CB4
18	W	204	9XX	O2-C18-O1-C17
21	B	609	MQ9	C30-C29-C31-C32
18	K	204	9XX	C14-C15-O-C16
19	A	504	9YF	C2-O2-P-O
19	M	501	9YF	C2-O2-P-O
15	F	605	CDL	C31-C32-C33-C34
15	B	611	CDL	C33-C34-C35-C36
15	R	605	CDL	C31-C32-C33-C34
15	R	606	CDL	C76-C77-C78-C79
15	P	201	CDL	C14-C15-C16-C17
19	A	503	9YF	C19-C20-C21-C22
19	K	202	9YF	C9-C8-O9-C
19	W	202	9YF	C9-C8-O9-C
15	F	605	CDL	C72-C73-C74-C75
15	F	606	CDL	C76-C77-C78-C79
15	H	201	CDL	C34-C35-C36-C37
15	D	201	CDL	C14-C15-C16-C17
15	D	201	CDL	C54-C55-C56-C57
15	D	201	CDL	C75-C76-C77-C78
15	B	611	CDL	C52-C53-C54-C55
15	A	502	CDL	C18-C19-C20-C21
15	R	605	CDL	C72-C73-C74-C75
15	T	201	CDL	C34-C35-C36-C37
15	P	201	CDL	C81-C82-C83-C84
15	N	606	CDL	C73-C74-C75-C76
15	M	503	CDL	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
15	M	503	CDL	C18-C19-C20-C21
15	M	503	CDL	C79-C80-C81-C82
16	B	612	9Y0	C31-C32-C33-C34
16	W	201	9Y0	C11-C10-C9-C8
18	K	204	9XX	C5-C6-C7-C8
19	C	303	9YF	C29-C30-C31-C32
22	C	301	HEC	C2D-C3D-CAD-CBD
22	O	301	HEC	C2D-C3D-CAD-CBD
15	D	201	CDL	C81-C82-C83-C84
15	B	605	CDL	C73-C74-C75-C76
15	A	502	CDL	C14-C15-C16-C17
15	A	502	CDL	C79-C80-C81-C82
15	P	201	CDL	C36-C37-C38-C39
15	P	201	CDL	C75-C76-C77-C78
15	N	604	CDL	C51-C52-C53-C54
15	N	604	CDL	C56-C57-C58-C59
15	N	605	CDL	C11-C12-C13-C14
19	K	202	9YF	C28-C29-C30-C31
19	A	504	9YF	C27-C28-C29-C30
19	O	303	9YF	C29-C30-C31-C32
19	M	501	9YF	C26-C27-C28-C29
19	M	504	9YF	C19-C20-C21-C22
19	K	202	9YF	O10-C8-O9-C
19	W	202	9YF	O10-C8-O9-C
15	B	611	CDL	CA7-C31-C32-C33
15	N	601	CDL	CA7-C31-C32-C33
15	D	201	CDL	C36-C37-C38-C39
15	B	604	CDL	C11-C12-C13-C14
15	P	201	CDL	C54-C55-C56-C57
15	N	601	CDL	C33-C34-C35-C36
15	N	601	CDL	C52-C53-C54-C55
18	K	204	9XX	C10-C11-C12-C13
19	A	504	9YF	C26-C27-C28-C29
15	N	605	CDL	C37-C38-C39-C40
18	W	204	9XX	C10-C11-C12-C13
19	K	202	9YF	C29-C30-C31-C32
19	A	504	9YF	C16-C17-C18-C19
19	W	202	9YF	C28-C29-C30-C31
19	M	501	9YF	C27-C28-C29-C30
19	M	501	9YF	C38-C39-C40-C41
15	A	502	CDL	O1-C1-CB2-OB2
15	P	201	CDL	O1-C1-CA2-OA2

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Mol	Chain	Res	Type	Atoms
20	B	602	HEM	C3D-CAD-CBD-CGD
20	N	603	HEM	C3D-CAD-CBD-CGD
15	F	606	CDL	C83-C84-C85-C86
15	D	201	CDL	C35-C36-C37-C38
15	B	604	CDL	C37-C38-C39-C40
15	B	604	CDL	C72-C73-C74-C75
15	B	605	CDL	C19-C20-C21-C22
15	B	611	CDL	C73-C74-C75-C76
15	A	502	CDL	C78-C79-C80-C81
15	T	201	CDL	C32-C33-C34-C35
15	P	201	CDL	C35-C36-C37-C38
15	N	601	CDL	C53-C54-C55-C56
15	N	605	CDL	C72-C73-C74-C75
15	M	503	CDL	C73-C74-C75-C76
16	B	606	9Y0	C31-C32-C33-C34
16	B	612	9Y0	C9-C10-C11-C12
19	A	504	9YF	C38-C39-C40-C41
19	K	202	9YF	C25-C26-C27-C28
15	H	201	CDL	C32-C33-C34-C35
15	B	605	CDL	C54-C55-C56-C57
15	B	611	CDL	C53-C54-C55-C56
15	A	502	CDL	C73-C74-C75-C76
15	P	201	CDL	C71-C72-C73-C74
15	N	606	CDL	C54-C55-C56-C57
15	M	503	CDL	C78-C79-C80-C81
16	G	301	9Y0	C29-C30-C31-C32
18	W	204	9XX	C19-C20-C21-C22
19	K	202	9YF	C16-C17-C18-C19
19	M	501	9YF	C16-C17-C18-C19
15	B	611	CDL	OB9-CB7-OB8-CB6
18	K	204	9XX	O6-C15-O-C16
15	F	606	CDL	C71-C72-C73-C74
15	H	201	CDL	C75-C76-C77-C78
15	D	201	CDL	C71-C72-C73-C74
15	B	611	CDL	C71-C72-C73-C74
15	R	606	CDL	C83-C84-C85-C86
15	T	201	CDL	C75-C76-C77-C78
15	N	601	CDL	C71-C72-C73-C74
15	N	601	CDL	C73-C74-C75-C76
15	N	604	CDL	C31-C32-C33-C34
16	B	606	9Y0	C28-C29-C30-C31
16	B	612	9Y0	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
16	S	301	9Y0	C29-C30-C31-C32
19	C	303	9YF	C11-C12-C13-C14
19	A	503	9YF	C39-C40-C41-C42
19	M	504	9YF	C16-C17-C18-C19
19	A	503	9YF	C31-C32-C33-C34
15	H	201	CDL	CA5-C11-C12-C13
15	A	502	CDL	CB5-C51-C52-C53
15	M	503	CDL	CB5-C51-C52-C53
15	B	603	CDL	C31-C32-C33-C34
15	R	606	CDL	C61-C62-C63-C64
15	R	606	CDL	C71-C72-C73-C74
15	N	604	CDL	C57-C58-C59-C60
15	N	604	CDL	C73-C74-C75-C76
15	N	605	CDL	C36-C37-C38-C39
16	B	606	9Y0	C9-C10-C11-C12
19	W	202	9YF	C14-C15-C16-C17
19	O	303	9YF	C11-C12-C13-C14
19	O	303	9YF	C15-C16-C17-C18
15	N	601	CDL	OB9-CB7-OB8-CB6
15	B	603	CDL	C73-C74-C75-C76
15	N	606	CDL	C77-C78-C79-C80
19	A	503	9YF	C16-C17-C18-C19
19	W	202	9YF	C16-C17-C18-C19
15	F	606	CDL	C11-CA5-OA6-CA4
15	F	605	CDL	C59-C60-C61-C62
15	F	606	CDL	C53-C54-C55-C56
15	B	603	CDL	C52-C53-C54-C55
15	B	603	CDL	C57-C58-C59-C60
15	B	604	CDL	C36-C37-C38-C39
16	D	202	9Y0	C23-C24-C25-C26
16	B	612	9Y0	C22-C23-C24-C25
16	B	612	9Y0	C27-C28-C29-C30
16	P	202	9Y0	C23-C24-C25-C26
19	C	303	9YF	C39-C40-C41-C42
19	O	303	9YF	C16-C17-C18-C19
16	K	201	9Y0	C10-C11-C12-C13
16	K	201	9Y0	C14-C15-C16-C17
15	H	201	CDL	C13-C14-C15-C16
15	D	201	CDL	C23-C24-C25-C26
15	B	603	CDL	C51-C52-C53-C54
15	B	604	CDL	C13-C14-C15-C16
15	B	604	CDL	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
15	B	604	CDL	C35-C36-C37-C38
15	B	604	CDL	C55-C56-C57-C58
15	B	605	CDL	C11-C12-C13-C14
15	B	605	CDL	C21-C22-C23-C24
15	B	605	CDL	C53-C54-C55-C56
15	B	605	CDL	C77-C78-C79-C80
15	B	611	CDL	C56-C57-C58-C59
15	A	502	CDL	C21-C22-C23-C24
15	R	605	CDL	C59-C60-C61-C62
15	R	606	CDL	C53-C54-C55-C56
15	R	606	CDL	C59-C60-C61-C62
15	T	201	CDL	C13-C14-C15-C16
15	T	201	CDL	C53-C54-C55-C56
15	P	201	CDL	C23-C24-C25-C26
15	P	201	CDL	C80-C81-C82-C83
15	N	601	CDL	C56-C57-C58-C59
15	N	604	CDL	C52-C53-C54-C55
15	N	605	CDL	C55-C56-C57-C58
15	N	606	CDL	C53-C54-C55-C56
18	W	204	9XX	C5-C6-C7-C8
19	C	303	9YF	C10-C11-C12-C13
19	C	303	9YF	C13-C14-C15-C16
19	C	303	9YF	C15-C16-C17-C18
15	N	606	CDL	OB9-CB7-OB8-CB6
21	N	609	MQ9	C34-C36-C37-C38
15	F	606	CDL	C62-C63-C64-C65
15	H	201	CDL	C53-C54-C55-C56
15	H	201	CDL	C57-C58-C59-C60
15	D	201	CDL	C80-C81-C82-C83
15	B	603	CDL	C16-C17-C18-C19
15	A	502	CDL	C77-C78-C79-C80
15	P	201	CDL	C72-C73-C74-C75
15	N	605	CDL	C13-C14-C15-C16
15	N	605	CDL	C16-C17-C18-C19
15	N	605	CDL	C35-C36-C37-C38
15	M	503	CDL	C21-C22-C23-C24
15	M	503	CDL	C77-C78-C79-C80
16	B	606	9Y0	C22-C23-C24-C25
19	C	303	9YF	C16-C17-C18-C19
19	A	504	9YF	C13-C14-C15-C16
19	O	303	9YF	C10-C11-C12-C13
19	O	303	9YF	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
19	O	303	9YF	C39-C40-C41-C42
19	M	501	9YF	C13-C14-C15-C16
15	A	502	CDL	C80-C81-C82-C83
15	R	605	CDL	C35-C36-C37-C38
15	R	606	CDL	C55-C56-C57-C58
15	T	201	CDL	C57-C58-C59-C60
15	M	503	CDL	C80-C81-C82-C83
16	B	606	9Y0	C27-C28-C29-C30
16	W	201	9Y0	C7-C8-C9-C10
19	C	303	9YF	C27-C28-C29-C30
19	O	303	9YF	C27-C28-C29-C30
15	T	201	CDL	CA5-C11-C12-C13
15	B	605	CDL	OB9-CB7-OB8-CB6
15	F	606	CDL	C55-C56-C57-C58
15	D	201	CDL	C72-C73-C74-C75
15	D	201	CDL	C76-C77-C78-C79
15	B	603	CDL	C12-C13-C14-C15
15	A	502	CDL	C52-C53-C54-C55
15	N	606	CDL	C11-C12-C13-C14
15	M	503	CDL	C52-C53-C54-C55
19	K	202	9YF	C15-C16-C17-C18
15	F	605	CDL	C35-C36-C37-C38
15	F	606	CDL	C59-C60-C61-C62
18	K	204	9XX	C27-C28-C29-C30
15	B	603	CDL	C18-C19-C20-C21
15	B	605	CDL	C74-C75-C76-C77
15	P	201	CDL	C76-C77-C78-C79
15	N	606	CDL	C19-C20-C21-C22
15	N	606	CDL	C74-C75-C76-C77
18	K	204	9XX	C19-C20-C21-C22
15	R	605	CDL	OA9-CA7-OA8-CA6
15	F	605	CDL	C60-C61-C62-C63
15	B	604	CDL	C75-C76-C77-C78
15	R	605	CDL	C60-C61-C62-C63
15	T	201	CDL	C55-C56-C57-C58
16	S	301	9Y0	C6-C7-C8-C9
18	K	204	9XX	C9-C10-C11-C12
15	H	201	CDL	CA3-CA4-CA6-OA8
15	T	201	CDL	CA3-CA4-CA6-OA8
15	F	605	CDL	C11-C12-C13-C14
15	N	605	CDL	C75-C76-C77-C78
15	N	606	CDL	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
19	W	202	9YF	C15-C16-C17-C18
14	F	601	HEA	C4D-C3D-CAD-CBD
14	R	601	HEA	C4D-C3D-CAD-CBD
15	N	605	CDL	CA7-C31-C32-C33
15	H	201	CDL	C55-C56-C57-C58
15	N	604	CDL	C16-C17-C18-C19
15	N	605	CDL	C58-C59-C60-C61
15	N	606	CDL	C21-C22-C23-C24
19	O	303	9YF	C38-C39-C40-C41
15	F	605	CDL	OA9-CA7-OA8-CA6
21	C	304	MQ9	C12-C11-C9-C10
21	C	304	MQ9	C45-C44-C46-C47
21	O	304	MQ9	C12-C11-C9-C10
21	O	304	MQ9	C45-C44-C46-C47
19	A	504	9YF	C9-C8-O9-C
19	M	501	9YF	C9-C8-O9-C
15	B	604	CDL	C31-C32-C33-C34
15	B	604	CDL	C58-C59-C60-C61
15	R	605	CDL	C11-C12-C13-C14
15	R	605	CDL	C34-C35-C36-C37
15	F	605	CDL	C34-C35-C36-C37
15	F	606	CDL	C56-C57-C58-C59
15	A	502	CDL	C72-C73-C74-C75
15	T	201	CDL	C54-C55-C56-C57
18	W	204	9XX	C20-C21-C22-C23
19	C	303	9YF	C38-C39-C40-C41
15	B	603	CDL	C56-C57-C58-C59
15	A	502	CDL	C22-C23-C24-C25
15	H	201	CDL	C54-C55-C56-C57
15	T	201	CDL	C14-C15-C16-C17
19	M	504	9YF	C36-C37-C38-C39
15	D	201	CDL	CA2-C1-CB2-OB2
15	F	606	CDL	C61-C62-C63-C64
15	M	503	CDL	C72-C73-C74-C75
15	F	606	CDL	OA7-CA5-OA6-CA4
19	A	504	9YF	O10-C8-O9-C
19	M	501	9YF	O10-C8-O9-C
15	H	201	CDL	C14-C15-C16-C17
15	B	605	CDL	C23-C24-C25-C26
15	B	611	CDL	C32-C33-C34-C35
15	A	502	CDL	C33-C34-C35-C36
16	D	202	9Y0	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
16	P	202	9Y0	C28-C29-C30-C31
15	P	201	CDL	C18-C19-C20-C21
15	N	601	CDL	C32-C33-C34-C35
15	N	605	CDL	C12-C13-C14-C15
15	N	605	CDL	C31-C32-C33-C34
16	S	301	9Y0	C22-C23-C24-C25
18	Y	302	9XX	C22-C23-C24-C25
18	Z	302	9XX	C22-C23-C24-C25
15	D	201	CDL	C18-C19-C20-C21
15	N	604	CDL	C12-C13-C14-C15
15	N	606	CDL	C23-C24-C25-C26
15	M	503	CDL	C33-C34-C35-C36
16	G	301	9Y0	C22-C23-C24-C25
15	A	502	CDL	C31-CA7-OA8-CA6
19	O	303	9YF	C33-C35-C36-C37
19	M	504	9YF	C33-C35-C36-C37
22	C	301	HEC	C3D-CAD-CBD-CGD
22	O	301	HEC	C3D-CAD-CBD-CGD
15	N	601	CDL	C75-C76-C77-C78
15	M	503	CDL	C22-C23-C24-C25
18	K	204	9XX	C11-C12-C13-C14
21	C	304	MQ9	C47-C48-C49-C50
21	O	304	MQ9	C47-C48-C49-C50
15	B	604	CDL	C12-C13-C14-C15
19	W	202	9YF	C29-C30-C31-C32
21	B	608	MQ9	C23-C24-C26-C27
21	N	608	MQ9	C23-C24-C26-C27
15	M	503	CDL	C34-C35-C36-C37
19	A	503	9YF	C40-C41-C42-C43
16	W	201	9Y0	C14-C15-C16-C17
15	R	606	CDL	OA7-CA5-OA6-CA4
16	B	606	9Y0	O6-C21-O7-C1
16	B	612	9Y0	O6-C21-O7-C1
18	K	204	9XX	O2-C18-O1-C17
15	B	604	CDL	CA7-C31-C32-C33
15	H	201	CDL	C71-CB7-OB8-CB6
15	T	201	CDL	C71-CB7-OB8-CB6
15	M	503	CDL	C31-CA7-OA8-CA6
16	D	202	9Y0	C6-C5-O5-C
16	P	202	9Y0	C6-C5-O5-C
15	A	502	CDL	C34-C35-C36-C37
16	G	301	9Y0	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
15	B	611	CDL	C74-C75-C76-C77
15	N	606	CDL	C15-C16-C17-C18
16	K	201	9Y0	C7-C8-C9-C10
15	B	605	CDL	C15-C16-C17-C18
15	T	201	CDL	C80-C81-C82-C83
16	S	301	9Y0	C24-C25-C26-C27
17	W	203	PLM	CB-CC-CD-CE
15	B	604	CDL	C53-C54-C55-C56
15	N	601	CDL	C74-C75-C76-C77
15	N	605	CDL	C53-C54-C55-C56
16	G	301	9Y0	C24-C25-C26-C27
19	M	504	9YF	C38-C39-C40-C41
20	B	602	HEM	C2B-C3B-CAB-CBB
20	N	603	HEM	C2B-C3B-CAB-CBB
15	B	605	CDL	C57-C58-C59-C60
15	B	611	CDL	C75-C76-C77-C78
18	K	204	9XX	C30-C31-C32-C33
19	C	303	9YF	C14-C15-C16-C17
18	W	204	9XX	C14-C15-O-C16
19	K	202	9YF	C26-C25-O11-C24
15	B	605	CDL	C13-C14-C15-C16
15	N	606	CDL	C57-C58-C59-C60
19	M	504	9YF	C13-C14-C15-C16
15	B	604	CDL	CA5-C11-C12-C13
15	N	605	CDL	CA5-C11-C12-C13
15	H	201	CDL	C51-CB5-OB6-CB4
15	R	606	CDL	C11-CA5-OA6-CA4
15	T	201	CDL	C51-CB5-OB6-CB4
16	B	606	9Y0	C22-C21-O7-C1
16	B	612	9Y0	C22-C21-O7-C1
18	K	204	9XX	C19-C18-O1-C17
15	F	606	CDL	OB5-CB3-CB4-OB6
15	R	606	CDL	OB5-CB3-CB4-OB6
16	W	201	9Y0	O7-C1-C2-O3
15	F	606	CDL	C72-C73-C74-C75
15	R	606	CDL	C62-C63-C64-C65
16	G	301	9Y0	C27-C28-C29-C30
16	K	201	9Y0	C15-C16-C17-C18
16	S	301	9Y0	C27-C28-C29-C30
19	C	303	9YF	C18-C19-C20-C21
20	B	602	HEM	C4B-C3B-CAB-CBB
20	N	603	HEM	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
15	H	201	CDL	C80-C81-C82-C83
15	N	604	CDL	C53-C54-C55-C56
15	N	606	CDL	C14-C15-C16-C17
15	B	603	CDL	C14-C15-C16-C17
15	N	604	CDL	C18-C19-C20-C21
15	D	201	CDL	OB6-CB4-CB6-OB8
15	P	201	CDL	OB6-CB4-CB6-OB8
16	B	606	9Y0	O5-C-C1-O7
16	B	612	9Y0	O5-C-C1-O7
19	A	504	9YF	O9-C-C24-O11
19	M	501	9YF	O9-C-C24-O11
15	R	606	CDL	C72-C73-C74-C75
18	Z	302	9XX	C7-C8-C9-C10
19	O	303	9YF	C14-C15-C16-C17
19	O	303	9YF	C18-C19-C20-C21
16	S	301	9Y0	C7-C8-C9-C10
18	Y	302	9XX	C7-C8-C9-C10
16	B	606	9Y0	C14-C15-C16-C17
21	C	304	MQ9	C35-C34-C36-C37
21	N	609	MQ9	C30-C29-C31-C32
21	O	304	MQ9	C35-C34-C36-C37
21	C	304	MQ9	C18-C19-C21-C22
21	O	304	MQ9	C18-C19-C21-C22
15	A	502	CDL	C54-C55-C56-C57
15	T	201	CDL	C76-C77-C78-C79
16	G	301	9Y0	C7-C8-C9-C10
15	H	201	CDL	C76-C77-C78-C79
15	M	503	CDL	C54-C55-C56-C57
15	B	603	CDL	C53-C54-C55-C56
19	A	503	9YF	C13-C14-C15-C16
15	A	502	CDL	OA9-CA7-OA8-CA6
15	T	201	CDL	C11-CA5-OA6-CA4
15	B	611	CDL	C34-C35-C36-C37
15	N	601	CDL	C34-C35-C36-C37
15	N	604	CDL	C54-C55-C56-C57
16	B	606	9Y0	C24-C25-C26-C27
16	B	606	9Y0	C7-C8-C9-C10
16	B	612	9Y0	C7-C8-C9-C10
19	A	503	9YF	C33-C35-C36-C37
15	F	606	CDL	CB3-OB5-PB2-OB2
15	H	201	CDL	CB3-OB5-PB2-OB2
15	B	603	CDL	CA2-OA2-PA1-OA5

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Mol	Chain	Res	Type	Atoms
15	R	606	CDL	CB3-OB5-PB2-OB2
15	T	201	CDL	CB3-OB5-PB2-OB2
15	N	604	CDL	CA2-OA2-PA1-OA5
15	F	606	CDL	C78-C79-C80-C81
19	K	202	9YF	C27-C28-C29-C30
15	D	201	CDL	C21-C22-C23-C24
16	G	301	9Y0	C-C1-C2-O3
16	D	202	9Y0	C-C1-C2-O3
16	S	301	9Y0	C-C1-C2-O3
16	P	202	9Y0	C-C1-C2-O3
15	P	201	CDL	C21-C22-C23-C24
15	R	606	CDL	C56-C57-C58-C59
15	N	604	CDL	C14-C15-C16-C17
15	H	201	CDL	C16-C17-C18-C19
15	T	201	CDL	C16-C17-C18-C19
16	D	202	9Y0	C14-C15-C16-C17
16	W	201	9Y0	C10-C11-C12-C13
18	W	204	9XX	C21-C22-C23-C24
15	D	201	CDL	CB2-C1-CA2-OA2
15	P	201	CDL	CB2-C1-CA2-OA2
21	O	304	MQ9	C23-C24-C26-C27
15	F	606	CDL	C13-C14-C15-C16
15	R	605	CDL	C73-C74-C75-C76
15	P	201	CDL	C11-C12-C13-C14
16	G	301	9Y0	C26-C27-C28-C29
16	B	606	9Y0	C19-C20-C37-C38
18	W	204	9XX	C22-C23-C24-C25
15	D	201	CDL	C11-C12-C13-C14
15	D	201	CDL	C77-C78-C79-C80
15	R	606	CDL	C13-C14-C15-C16
15	R	606	CDL	C78-C79-C80-C81
16	S	301	9Y0	C26-C27-C28-C29
15	B	605	CDL	CB7-C71-C72-C73
15	N	606	CDL	CB7-C71-C72-C73
15	H	201	CDL	C11-CA5-OA6-CA4
15	M	503	CDL	OA9-CA7-OA8-CA6
16	D	202	9Y0	O4-C5-O5-C
16	B	606	9Y0	C18-C19-C20-C37
16	B	612	9Y0	C18-C19-C20-C37
16	B	612	9Y0	C19-C20-C37-C38
18	K	204	9XX	C7-C8-C9-C10
18	W	204	9XX	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
15	F	605	CDL	CA3-CA4-CA6-OA8
15	F	605	CDL	CB3-CB4-CB6-OB8
15	F	606	CDL	CA3-CA4-CA6-OA8
15	B	611	CDL	CA3-CA4-CA6-OA8
15	R	605	CDL	CA3-CA4-CA6-OA8
15	R	605	CDL	CB3-CB4-CB6-OB8
15	N	601	CDL	CA3-CA4-CA6-OA8
16	D	202	9Y0	O5-C-C1-C2
16	P	202	9Y0	O5-C-C1-C2
21	B	608	MQ9	C37-C38-C39-C41
19	C	303	9YF	C33-C35-C36-C37
15	F	605	CDL	C73-C74-C75-C76
15	D	201	CDL	C13-C14-C15-C16
15	B	605	CDL	C14-C15-C16-C17
15	P	201	CDL	C77-C78-C79-C80
15	H	201	CDL	OB9-CB7-OB8-CB6
15	T	201	CDL	OB9-CB7-OB8-CB6
16	P	202	9Y0	O4-C5-O5-C
15	F	606	CDL	C64-C65-C66-C67
15	R	606	CDL	C63-C64-C65-C66
15	P	201	CDL	C13-C14-C15-C16
17	W	203	PLM	C2-C3-C4-C5
18	W	204	9XX	C18-C19-C20-C21
18	W	204	9XX	O6-C15-O-C16
15	R	605	CDL	C39-C40-C41-C42
16	W	201	9Y0	C6-C7-C8-C9
16	B	612	9Y0	C17-C18-C19-C20
15	N	604	CDL	C58-C59-C60-C61
16	B	612	9Y0	C33-C34-C35-C36
16	B	612	9Y0	C14-C15-C16-C17
16	P	202	9Y0	C14-C15-C16-C17
21	B	607	MQ9	C7-C8-C9-C10
19	K	202	9YF	O12-C25-O11-C24
15	B	603	CDL	C54-C55-C56-C57
15	A	502	CDL	C23-C24-C25-C26
15	M	503	CDL	C24-C25-C26-C27
16	B	612	9Y0	C24-C25-C26-C27
15	F	605	CDL	C39-C40-C41-C42
15	A	502	CDL	C24-C25-C26-C27
15	M	503	CDL	C11-C12-C13-C14
21	C	304	MQ9	C23-C24-C26-C27
19	W	202	9YF	C26-C25-O11-C24

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Mol	Chain	Res	Type	Atoms
21	N	608	MQ9	C37-C38-C39-C41
15	B	603	CDL	C58-C59-C60-C61
16	G	301	9Y0	C11-C10-C9-C8
18	W	204	9XX	C9-C10-C11-C12
15	A	502	CDL	CB6-CB4-OB6-CB5
15	M	503	CDL	CB6-CB4-OB6-CB5
16	W	201	9Y0	C-C1-O7-C21
15	B	611	CDL	C11-C12-C13-C14
15	M	503	CDL	C23-C24-C25-C26
15	A	502	CDL	C11-C12-C13-C14
16	B	606	9Y0	C6-C5-O5-C
16	K	201	9Y0	O7-C1-C2-O3
15	D	201	CDL	C79-C80-C81-C82
15	N	601	CDL	C11-C12-C13-C14
15	T	201	CDL	O1-C1-CA2-OA2
15	A	502	CDL	C51-C52-C53-C54
15	N	605	CDL	C14-C15-C16-C17
19	M	504	9YF	C20-C21-C22-C23
19	A	503	9YF	C11-C10-C9-C8
15	P	201	CDL	C79-C80-C81-C82
15	F	606	CDL	C72-C71-CB7-OB8
15	R	606	CDL	C72-C71-CB7-OB8
15	F	606	CDL	OA6-CA4-CA6-OA8
15	D	201	CDL	OA6-CA4-CA6-OA8
15	H	201	CDL	C79-C80-C81-C82
15	B	611	CDL	C13-C14-C15-C16
16	B	606	9Y0	C33-C34-C35-C36
15	H	201	CDL	OB7-CB5-OB6-CB4
15	T	201	CDL	OA7-CA5-OA6-CA4
15	T	201	CDL	OB7-CB5-OB6-CB4
21	N	607	MQ9	C7-C8-C9-C10
18	K	204	9XX	C25-C26-C27-C28
19	W	202	9YF	C32-C33-C35-C36
15	B	604	CDL	C14-C15-C16-C17
15	T	201	CDL	C79-C80-C81-C82
15	N	601	CDL	C13-C14-C15-C16
15	N	604	CDL	C59-C60-C61-C62
15	M	503	CDL	C51-C52-C53-C54
19	A	503	9YF	C34-C33-C35-C36
19	A	504	9YF	C31-C32-C33-C34
19	M	501	9YF	C31-C32-C33-C34
15	T	201	CDL	C31-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
16	B	612	9Y0	C6-C5-O5-C
15	R	606	CDL	C64-C65-C66-C67
17	K	203	PLM	C2-C3-C4-C5
19	A	503	9YF	C20-C21-C22-C23
17	K	203	PLM	CB-CC-CD-CE
15	B	604	CDL	C76-C77-C78-C79
15	A	502	CDL	C56-C57-C58-C59
15	N	605	CDL	C76-C77-C78-C79
16	B	606	9Y0	C17-C18-C19-C20
15	B	604	CDL	CB2-C1-CA2-OA2
15	A	502	CDL	CB2-C1-CA2-OA2
15	N	605	CDL	CB2-C1-CA2-OA2
15	A	502	CDL	C35-C36-C37-C38
15	H	201	CDL	C31-CA7-OA8-CA6
15	N	601	CDL	C57-C58-C59-C60
15	M	503	CDL	C35-C36-C37-C38
15	M	503	CDL	C56-C57-C58-C59
18	K	204	9XX	C22-C23-C24-C25
15	B	611	CDL	C57-C58-C59-C60
15	A	502	CDL	C81-C82-C83-C84
15	R	606	CDL	C75-C76-C77-C78
22	C	302	HEC	C4B-C3B-CAB-CBB
15	F	605	CDL	OA5-CA3-CA4-CA6
15	F	606	CDL	OB5-CB3-CB4-CB6
15	B	603	CDL	OA5-CA3-CA4-CA6
15	R	605	CDL	OA5-CA3-CA4-CA6
15	R	606	CDL	OB5-CB3-CB4-CB6
15	N	604	CDL	OA5-CA3-CA4-CA6
16	W	201	9Y0	C-C1-C2-O3
19	C	303	9YF	C24-C-C1-O
19	O	303	9YF	C24-C-C1-O
21	C	304	MQ9	C19-C21-C22-C23
21	O	304	MQ9	C19-C21-C22-C23
15	A	502	CDL	C13-C14-C15-C16
22	O	302	HEC	C4B-C3B-CAB-CBB
19	A	503	9YF	C25-C26-C27-C28
19	O	303	9YF	C37-C38-C39-C40
15	F	606	CDL	C75-C76-C77-C78
21	B	607	MQ9	C13-C14-C16-C17
21	N	607	MQ9	C13-C14-C16-C17
15	M	503	CDL	C13-C14-C15-C16
15	H	201	CDL	OA7-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
15	T	201	CDL	C74-C75-C76-C77
18	W	204	9XX	C28-C29-C30-C31
18	W	204	9XX	C-C1-C2-C3
19	C	303	9YF	C37-C38-C39-C40
19	M	504	9YF	C26-C25-O11-C24
15	H	201	CDL	C74-C75-C76-C77
16	P	202	9Y0	C24-C25-C26-C27
16	W	201	9Y0	C16-C17-C18-C19
15	M	503	CDL	C81-C82-C83-C84
16	D	202	9Y0	C24-C25-C26-C27
15	H	201	CDL	CB3-CB4-CB6-OB8
15	D	201	CDL	CB3-CB4-CB6-OB8
15	T	201	CDL	CB3-CB4-CB6-OB8
15	P	201	CDL	CB3-CB4-CB6-OB8
16	B	606	9Y0	O5-C-C1-C2
16	B	612	9Y0	O5-C-C1-C2
16	K	201	9Y0	C16-C17-C18-C19
15	B	603	CDL	C71-C72-C73-C74
15	N	604	CDL	C71-C72-C73-C74
18	Z	302	9XX	C5-C6-C7-C8
19	K	202	9YF	C2-O2-P-O8
19	A	504	9YF	C2-O2-P-O8
19	W	202	9YF	C2-O2-P-O8
19	M	501	9YF	C2-O2-P-O8
15	B	604	CDL	C17-C18-C19-C20
15	M	503	CDL	C57-C58-C59-C60
18	Y	302	9XX	C5-C6-C7-C8
15	A	502	CDL	C57-C58-C59-C60
18	W	204	9XX	C30-C31-C32-C33
15	N	605	CDL	C17-C18-C19-C20
15	F	605	CDL	OA5-CA3-CA4-OA6
15	R	605	CDL	OA5-CA3-CA4-OA6
16	G	301	9Y0	O7-C1-C2-O3
16	S	301	9Y0	O7-C1-C2-O3
15	N	606	CDL	C31-C32-C33-C34
19	W	202	9YF	O12-C25-O11-C24
15	B	605	CDL	CA7-C31-C32-C33
15	A	502	CDL	C36-C37-C38-C39
15	H	201	CDL	O1-C1-CA2-OA2
15	B	605	CDL	C31-C32-C33-C34
16	W	201	9Y0	C15-C16-C17-C18
15	T	201	CDL	OA9-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
16	B	606	9Y0	O4-C5-O5-C
16	B	612	9Y0	O4-C5-O5-C
15	R	606	CDL	C82-C83-C84-C85
15	M	503	CDL	C36-C37-C38-C39
15	F	606	CDL	C82-C83-C84-C85
15	H	201	CDL	OB6-CB4-CB6-OB8
15	B	603	CDL	OB6-CB4-CB6-OB8
15	B	605	CDL	OB6-CB4-CB6-OB8
15	B	611	CDL	OA6-CA4-CA6-OA8
15	T	201	CDL	OB6-CB4-CB6-OB8
15	N	601	CDL	OA6-CA4-CA6-OA8
15	N	604	CDL	OB6-CB4-CB6-OB8
15	N	606	CDL	OB6-CB4-CB6-OB8
16	K	201	9Y0	O5-C-C1-O7
15	B	603	CDL	C19-C20-C21-C22
15	N	601	CDL	C72-C73-C74-C75
14	R	601	HEA	C2D-C3D-CAD-CBD
15	B	605	CDL	C51-CB5-OB6-CB4
15	B	611	CDL	C72-C73-C74-C75
15	H	201	CDL	CB2-C1-CA2-OA2
15	B	611	CDL	CA2-C1-CB2-OB2
15	T	201	CDL	CB2-C1-CA2-OA2
15	M	503	CDL	CB2-C1-CA2-OA2
15	N	605	CDL	C33-C34-C35-C36
15	N	606	CDL	C55-C56-C57-C58
19	K	202	9YF	C-C1-O-P
15	H	201	CDL	OA9-CA7-OA8-CA6
15	F	605	CDL	C71-C72-C73-C74
15	D	201	CDL	C52-C53-C54-C55
15	B	605	CDL	C55-C56-C57-C58
15	N	605	CDL	C34-C35-C36-C37
18	K	204	9XX	C4-C5-C6-C7
15	N	604	CDL	C76-C77-C78-C79
16	D	202	9Y0	C11-C10-C9-C8
16	S	301	9Y0	C23-C24-C25-C26
15	R	605	CDL	C71-C72-C73-C74
15	B	605	CDL	OB7-CB5-OB6-CB4
15	N	606	CDL	OB7-CB5-OB6-CB4
15	B	604	CDL	C51-CB5-OB6-CB4
15	N	605	CDL	C51-CB5-OB6-CB4
15	N	606	CDL	C51-CB5-OB6-CB4
15	B	603	CDL	C76-C77-C78-C79

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Mol	Chain	Res	Type	Atoms
15	A	502	CDL	C60-C61-C62-C63
16	G	301	9Y0	C23-C24-C25-C26
14	F	601	HEA	C2D-C3D-CAD-CBD
15	R	606	CDL	CB5-C51-C52-C53
15	N	606	CDL	CA7-C31-C32-C33
16	K	201	9Y0	C-C1-C2-O3
16	B	606	9Y0	C-C1-C2-O3
16	B	612	9Y0	C-C1-C2-O3
19	A	503	9YF	C32-C33-C35-C36
19	O	303	9YF	C31-C32-C33-C35
21	B	609	MQ9	C38-C39-C41-C42
19	A	503	9YF	C2-O2-P-O
16	S	301	9Y0	C11-C10-C9-C8
18	W	204	9XX	C2-C3-C4-C5
15	B	604	CDL	C34-C35-C36-C37
15	M	503	CDL	C60-C61-C62-C63
15	F	606	CDL	CB5-C51-C52-C53
16	D	202	9Y0	C26-C27-C28-C29
16	P	202	9Y0	C26-C27-C28-C29
15	H	201	CDL	C83-C84-C85-C86
16	B	612	9Y0	C21-C22-C23-C24
15	T	201	CDL	C73-C74-C75-C76
15	F	606	CDL	C71-CB7-OB8-CB6
15	H	201	CDL	C73-C74-C75-C76
15	N	604	CDL	C17-C18-C19-C20
15	N	604	CDL	C19-C20-C21-C22
19	A	503	9YF	C9-C10-C11-C12
15	F	605	CDL	C61-C62-C63-C64
15	T	201	CDL	C83-C84-C85-C86
15	R	605	CDL	C61-C62-C63-C64
15	B	605	CDL	CA6-CA4-OA6-CA5
15	B	611	CDL	CA3-CA4-OA6-CA5
15	N	601	CDL	CA3-CA4-OA6-CA5
15	N	606	CDL	CA6-CA4-OA6-CA5
16	K	201	9Y0	C-C1-O7-C21
15	B	604	CDL	C33-C34-C35-C36
15	N	605	CDL	C57-C58-C59-C60
16	D	202	9Y0	C25-C26-C27-C28
15	B	603	CDL	C71-CB7-OB8-CB6
15	N	604	CDL	C71-CB7-OB8-CB6
15	R	605	CDL	C55-C56-C57-C58
16	P	202	9Y0	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
21	N	609	MQ9	C38-C39-C41-C42
15	B	604	CDL	C57-C58-C59-C60
16	W	201	9Y0	C24-C25-C26-C27
15	N	604	CDL	CB3-CB4-CB6-OB8
19	K	202	9YF	C1-C-C24-O11
19	A	504	9YF	C1-C-C24-O11
19	W	202	9YF	C1-C-C24-O11
19	M	501	9YF	C1-C-C24-O11
19	M	504	9YF	C1-C-C24-O11
19	M	504	9YF	O12-C25-O11-C24
19	C	303	9YF	O9-C-C1-O
19	O	303	9YF	O9-C-C1-O
15	A	502	CDL	C75-C76-C77-C78
16	G	301	9Y0	C28-C29-C30-C31
15	M	503	CDL	C75-C76-C77-C78
15	B	604	CDL	OB7-CB5-OB6-CB4
15	N	605	CDL	OB7-CB5-OB6-CB4
15	R	606	CDL	CA5-C11-C12-C13
15	B	603	CDL	C59-C60-C61-C62
15	P	201	CDL	C22-C23-C24-C25
15	F	605	CDL	OB6-CB4-CB6-OB8
15	R	605	CDL	OB6-CB4-CB6-OB8
15	P	201	CDL	OA6-CA4-CA6-OA8
16	D	202	9Y0	O5-C-C1-O7
16	P	202	9Y0	O5-C-C1-O7
16	W	201	9Y0	O5-C-C1-O7
19	M	504	9YF	O9-C-C24-O11
15	N	604	CDL	OB9-CB7-OB8-CB6
15	F	605	CDL	C55-C56-C57-C58
16	D	202	9Y0	C9-C10-C11-C12
15	B	605	CDL	C78-C79-C80-C81
16	S	301	9Y0	C28-C29-C30-C31
15	N	604	CDL	C51-CB5-OB6-CB4
16	B	606	9Y0	C10-C11-C12-C13
16	B	612	9Y0	C10-C11-C12-C13
15	D	201	CDL	C22-C23-C24-C25
16	P	202	9Y0	C9-C10-C11-C12
19	W	202	9YF	C38-C39-C40-C41
15	B	603	CDL	OB9-CB7-OB8-CB6
19	K	202	9YF	C38-C39-C40-C41
15	N	604	CDL	OB7-CB5-OB6-CB4
19	C	303	9YF	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
15	N	605	CDL	C18-C19-C20-C21
18	W	204	9XX	C13-C14-C15-O
15	R	606	CDL	C71-CB7-OB8-CB6
15	B	604	CDL	C18-C19-C20-C21
15	M	503	CDL	C32-C33-C34-C35
15	B	603	CDL	OB7-CB5-OB6-CB4
17	W	203	PLM	C4-C5-C6-C7
19	K	202	9YF	C2-O2-P-O
19	W	202	9YF	C2-O2-P-O
15	P	201	CDL	C19-C20-C21-C22
15	H	201	CDL	CB2-OB2-PB2-OB5
15	D	201	CDL	CA3-OA5-PA1-OA2
15	A	502	CDL	CA3-OA5-PA1-OA2
15	T	201	CDL	CB2-OB2-PB2-OB5
15	P	201	CDL	CA3-OA5-PA1-OA2
15	M	503	CDL	CA3-OA5-PA1-OA2
15	A	502	CDL	C32-C33-C34-C35
15	N	605	CDL	C73-C74-C75-C76
15	B	604	CDL	C73-C74-C75-C76
19	A	503	9YF	C29-C30-C31-C32
21	C	304	MQ9	C30-C29-C31-C32
21	O	304	MQ9	C30-C29-C31-C32
15	F	605	CDL	C1-CB2-OB2-PB2
15	H	201	CDL	C1-CB2-OB2-PB2
15	B	605	CDL	CA4-CA3-OA5-PA1
15	A	502	CDL	C1-CA2-OA2-PA1
15	T	201	CDL	C1-CB2-OB2-PB2
15	N	606	CDL	CA4-CA3-OA5-PA1
15	N	605	CDL	C56-C57-C58-C59
17	K	203	PLM	C4-C5-C6-C7
15	F	605	CDL	CB3-OB5-PB2-OB3
15	F	606	CDL	CB3-OB5-PB2-OB3
15	D	201	CDL	CA3-OA5-PA1-OA4
15	B	603	CDL	CA2-OA2-PA1-OA3
15	B	603	CDL	CA3-OA5-PA1-OA4
15	B	604	CDL	CB3-OB5-PB2-OB3
15	B	604	CDL	CB3-OB5-PB2-OB4
15	B	611	CDL	CA3-OA5-PA1-OA4
15	B	611	CDL	CB2-OB2-PB2-OB4
15	B	611	CDL	CB3-OB5-PB2-OB4
15	A	502	CDL	CB3-OB5-PB2-OB3
15	R	605	CDL	CB3-OB5-PB2-OB3

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Mol	Chain	Res	Type	Atoms
15	R	606	CDL	CB3-OB5-PB2-OB3
15	P	201	CDL	CA3-OA5-PA1-OA4
15	N	601	CDL	CA3-OA5-PA1-OA4
15	N	601	CDL	CB3-OB5-PB2-OB4
15	N	604	CDL	CA2-OA2-PA1-OA3
15	N	604	CDL	CA2-OA2-PA1-OA4
15	N	605	CDL	CB3-OB5-PB2-OB3
15	N	605	CDL	CB3-OB5-PB2-OB4
15	M	503	CDL	CB3-OB5-PB2-OB3
16	K	201	9Y0	C3-O1-P-O2
16	W	201	9Y0	C3-O1-P-O2
19	A	503	9YF	C1-O-P-O8
19	W	202	9YF	C1-O-P-O8
15	D	201	CDL	C34-C35-C36-C37
19	A	504	9YF	C39-C40-C41-C42
15	D	201	CDL	OA5-CA3-CA4-CA6
15	P	201	CDL	OA5-CA3-CA4-CA6
15	D	201	CDL	C19-C20-C21-C22
15	F	606	CDL	OB9-CB7-OB8-CB6
18	Y	302	9XX	C13-C14-C15-O
18	Z	302	9XX	C13-C14-C15-O
15	B	604	CDL	C56-C57-C58-C59
19	M	501	9YF	C39-C40-C41-C42
15	N	606	CDL	C78-C79-C80-C81
15	T	201	CDL	C78-C79-C80-C81
15	F	606	CDL	CA5-C11-C12-C13
15	D	201	CDL	OA5-CA3-CA4-OA6
15	B	611	CDL	OB5-CB3-CB4-OB6
15	P	201	CDL	OA5-CA3-CA4-OA6
15	N	601	CDL	OB5-CB3-CB4-OB6
19	K	202	9YF	C32-C33-C35-C36
19	C	303	9YF	C31-C32-C33-C35
19	M	501	9YF	C37-C38-C39-C40
16	B	606	9Y0	C21-C22-C23-C24
15	B	603	CDL	C51-CB5-OB6-CB4
15	T	201	CDL	C35-C36-C37-C38
15	H	201	CDL	C35-C36-C37-C38
15	H	201	CDL	C78-C79-C80-C81
15	N	605	CDL	C32-C31-CA7-OA8
15	B	603	CDL	CB3-CB4-CB6-OB8
15	B	605	CDL	C32-C33-C34-C35
16	G	301	9Y0	O5-C-C1-C2

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Mol	Chain	Res	Type	Atoms
16	K	201	9Y0	O5-C-C1-C2
16	S	301	9Y0	O5-C-C1-C2
15	R	606	CDL	OB9-CB7-OB8-CB6
15	H	201	CDL	OA6-CA4-CA6-OA8
15	T	201	CDL	OA6-CA4-CA6-OA8
15	N	606	CDL	C76-C77-C78-C79
15	B	604	CDL	C32-C31-CA7-OA8
19	C	303	9YF	C19-C20-C21-C22
15	F	605	CDL	C1-CA2-OA2-PA1
15	H	201	CDL	C1-CA2-OA2-PA1
15	R	605	CDL	C1-CB2-OB2-PB2
15	T	201	CDL	C1-CA2-OA2-PA1
15	M	503	CDL	C1-CA2-OA2-PA1
14	F	602	HEA	C21-C22-C23-C25
18	K	204	9XX	C1-C2-C3-C4
21	B	609	MQ9	C43-C44-C46-C47
19	O	303	9YF	C19-C20-C21-C22
19	W	202	9YF	C34-C33-C35-C36
19	O	303	9YF	C31-C32-C33-C34
15	R	606	CDL	C31-C32-C33-C34
21	B	609	MQ9	C14-C16-C17-C18
21	N	609	MQ9	C14-C16-C17-C18
19	M	504	9YF	O11-C25-C26-C27
15	B	605	CDL	C51-C52-C53-C54
15	B	605	CDL	C76-C77-C78-C79
15	N	601	CDL	C31-C32-C33-C34
15	N	606	CDL	C51-C52-C53-C54
15	M	503	CDL	C71-C72-C73-C74
16	B	606	9Y0	C11-C10-C9-C8
15	B	611	CDL	C31-C32-C33-C34
19	W	202	9YF	C9-C10-C11-C12
15	N	606	CDL	C32-C33-C34-C35
21	B	609	MQ9	C12-C11-C9-C8
21	N	609	MQ9	C12-C11-C9-C8
16	K	201	9Y0	C5-C6-C7-C8
19	A	504	9YF	C37-C38-C39-C40
14	R	601	HEA	C21-C22-C23-C25
15	B	603	CDL	C17-C18-C19-C20
15	B	605	CDL	CB6-CB4-OB6-CB5
15	N	606	CDL	CB6-CB4-OB6-CB5
16	G	301	9Y0	C2-C1-O7-C21
16	S	301	9Y0	C2-C1-O7-C21

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Mol	Chain	Res	Type	Atoms
14	F	601	HEA	C11-C12-C13-C14
14	R	601	HEA	C11-C12-C13-C14
15	N	604	CDL	CA7-C31-C32-C33
16	P	202	9Y0	C11-C10-C9-C8
15	R	605	CDL	C1-CA2-OA2-PA1
15	N	604	CDL	C1-CB2-OB2-PB2
19	W	202	9YF	C-C1-O-P
16	K	201	9Y0	C24-C25-C26-C27
22	O	302	HEC	C2B-C3B-CAB-CBB
21	N	609	MQ9	C43-C44-C46-C47
18	K	204	9XX	C13-C14-C15-O
15	F	605	CDL	C74-C75-C76-C77
16	B	612	9Y0	C11-C10-C9-C8
22	C	302	HEC	C2B-C3B-CAB-CBB
15	A	502	CDL	C71-C72-C73-C74
18	Z	302	9XX	C21-C22-C23-C24
15	D	201	CDL	CB2-OB2-PB2-OB5
15	B	603	CDL	CB2-OB2-PB2-OB5
15	B	604	CDL	CA2-OA2-PA1-OA5
15	B	605	CDL	CA3-OA5-PA1-OA2
15	B	605	CDL	CB2-OB2-PB2-OB5
15	B	611	CDL	CA2-OA2-PA1-OA5
15	P	201	CDL	CB2-OB2-PB2-OB5
15	N	601	CDL	CA2-OA2-PA1-OA5
15	N	604	CDL	CB2-OB2-PB2-OB5
15	N	605	CDL	CA2-OA2-PA1-OA5
15	N	606	CDL	CA3-OA5-PA1-OA2
15	N	606	CDL	CB2-OB2-PB2-OB5
16	G	301	9Y0	C3-O1-P-O3
16	D	202	9Y0	C2-O3-P-O1
16	S	301	9Y0	C3-O1-P-O3
16	P	202	9Y0	C2-O3-P-O1
19	K	202	9YF	C11-C10-C9-C8
18	Y	302	9XX	C21-C22-C23-C24
14	F	601	HEA	C21-C22-C23-C25
15	P	201	CDL	C20-C21-C22-C23
15	D	201	CDL	C52-C51-CB5-OB6
17	W	203	PLM	CD-CE-CF-CG
15	D	201	CDL	CA3-CA4-CA6-OA8
15	P	201	CDL	CA3-CA4-CA6-OA8
19	A	503	9YF	C31-C32-C33-C35
15	N	604	CDL	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
15	T	201	CDL	C17-C18-C19-C20
15	D	201	CDL	C20-C21-C22-C23
15	D	201	CDL	C24-C25-C26-C27
15	P	201	CDL	C24-C25-C26-C27
14	R	602	HEA	C21-C22-C23-C25
15	A	502	CDL	C71-CB7-OB8-CB6
15	M	503	CDL	C71-CB7-OB8-CB6
15	B	604	CDL	CB4-CB3-OB5-PB2
15	N	605	CDL	CB4-CB3-OB5-PB2
15	M	503	CDL	C1-CB2-OB2-PB2
16	W	201	9Y0	C13-C14-C15-C16
15	R	606	CDL	C54-C55-C56-C57
15	N	601	CDL	C12-C13-C14-C15
19	M	504	9YF	C10-C11-C12-C13
19	A	503	9YF	C36-C37-C38-C39
19	C	303	9YF	C28-C29-C30-C31
19	A	503	9YF	O11-C25-C26-C27
16	S	301	9Y0	C30-C31-C32-C33
16	G	301	9Y0	O1-C3-C4-N
16	S	301	9Y0	O1-C3-C4-N
15	P	201	CDL	C52-C53-C54-C55
15	B	604	CDL	OB5-CB3-CB4-OB6
15	N	605	CDL	OB5-CB3-CB4-OB6
15	H	201	CDL	C17-C18-C19-C20
15	H	201	CDL	C51-C52-C53-C54
15	A	502	CDL	OB9-CB7-OB8-CB6
15	M	503	CDL	OB9-CB7-OB8-CB6
21	B	608	MQ9	C30-C29-C31-C32
21	N	608	MQ9	C30-C29-C31-C32
15	T	201	CDL	C52-C53-C54-C55
17	K	203	PLM	CD-CE-CF-CG
19	O	303	9YF	C28-C29-C30-C31
15	B	611	CDL	C12-C13-C14-C15
15	T	201	CDL	C51-C52-C53-C54
16	B	606	9Y0	C29-C30-C31-C32
16	G	301	9Y0	C30-C31-C32-C33
15	R	606	CDL	OA6-CA4-CA6-OA8
15	A	502	CDL	C1-CB2-OB2-PB2
16	D	202	9Y0	C13-C14-C15-C16
16	P	202	9Y0	C13-C14-C15-C16
18	W	204	9XX	C1-C2-C3-C4
21	N	610	MQ9	C20-C19-C21-C22

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Mol	Chain	Res	Type	Atoms
14	R	601	HEA	CAA-CBA-CGA-O1A
15	N	605	CDL	C52-C53-C54-C55
15	B	604	CDL	CA3-CA4-CA6-OA8
15	N	605	CDL	CA3-CA4-CA6-OA8
15	D	201	CDL	C37-C38-C39-C40
15	B	604	CDL	C52-C53-C54-C55
15	R	606	CDL	C74-C75-C76-C77
15	B	611	CDL	O1-C1-CB2-OB2
14	F	601	HEA	CAA-CBA-CGA-O1A
19	K	202	9YF	C2-O2-P-O1
19	W	202	9YF	C2-O2-P-O1
15	B	611	CDL	CA5-C11-C12-C13
15	T	201	CDL	C31-C32-C33-C34
15	B	611	CDL	CB3-CB4-OB6-CB5
15	N	601	CDL	CB3-CB4-OB6-CB5
21	B	610	MQ9	C20-C19-C21-C22
15	H	201	CDL	C31-C32-C33-C34
15	B	603	CDL	C80-C81-C82-C83
15	B	604	CDL	C60-C61-C62-C63
15	N	604	CDL	C80-C81-C82-C83
15	F	606	CDL	C31-C32-C33-C34
19	K	202	9YF	C9-C10-C11-C12
15	F	606	CDL	C54-C55-C56-C57
15	F	606	CDL	C74-C75-C76-C77
19	C	303	9YF	O9-C8-C9-C10
15	B	603	CDL	C11-C12-C13-C14
15	N	606	CDL	OB5-CB3-CB4-CB6
21	B	610	MQ9	C17-C18-C19-C20
21	N	610	MQ9	C17-C18-C19-C20
15	P	201	CDL	C34-C35-C36-C37
15	N	601	CDL	CA5-C11-C12-C13
18	Y	302	9XX	C18-C19-C20-C21
14	F	601	HEA	C18-C19-C20-C21
21	B	608	MQ9	C12-C11-C9-C8
21	N	608	MQ9	C12-C11-C9-C8
15	N	605	CDL	C60-C61-C62-C63
15	H	201	CDL	C52-C53-C54-C55
15	R	606	CDL	C72-C71-CB7-OB9
15	P	201	CDL	C52-C51-CB5-OB6
15	A	502	CDL	CA2-C1-CB2-OB2
15	N	601	CDL	CA2-C1-CB2-OB2
15	M	503	CDL	CA2-C1-CB2-OB2

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Mol	Chain	Res	Type	Atoms
18	Z	302	9XX	C18-C19-C20-C21
21	B	609	MQ9	C15-C14-C16-C17
21	N	609	MQ9	C15-C14-C16-C17
16	B	612	9Y0	C29-C30-C31-C32
14	R	601	HEA	C18-C19-C20-C21
16	K	201	9Y0	O7-C21-C22-C23
15	B	603	CDL	C72-C73-C74-C75
15	N	604	CDL	C72-C73-C74-C75
15	R	606	CDL	C52-C53-C54-C55
15	P	201	CDL	C37-C38-C39-C40
19	M	504	9YF	C25-C26-C27-C28
15	P	201	CDL	C38-C39-C40-C41
18	Z	302	9XX	C9-C10-C11-C12
18	Y	302	9XX	C9-C10-C11-C12
15	B	604	CDL	C72-C71-CB7-OB8
15	N	605	CDL	C72-C71-CB7-OB8
19	O	303	9YF	O9-C8-C9-C10
15	B	603	CDL	CA7-C31-C32-C33
15	F	606	CDL	C72-C71-CB7-OB9
15	M	503	CDL	C83-C84-C85-C86
15	A	502	CDL	C83-C84-C85-C86
16	B	606	9Y0	O7-C1-C2-O3
16	B	612	9Y0	O7-C1-C2-O3
16	W	201	9Y0	O7-C21-C22-C23
15	B	604	CDL	OB5-CB3-CB4-CB6
15	B	611	CDL	OB5-CB3-CB4-CB6
15	N	601	CDL	OB5-CB3-CB4-CB6
15	N	605	CDL	OB5-CB3-CB4-CB6
14	F	601	HEA	C26-C15-C16-C17
14	R	601	HEA	C26-C15-C16-C17
21	C	304	MQ9	C44-C46-C47-C48
21	O	304	MQ9	C44-C46-C47-C48
19	M	504	9YF	C11-C12-C13-C14
20	B	602	HEM	CAA-CBA-CGA-O2A
20	N	603	HEM	CAA-CBA-CGA-O2A
15	F	606	CDL	C52-C51-CB5-OB6
15	R	606	CDL	C52-C51-CB5-OB6
15	F	605	CDL	C14-C15-C16-C17
19	K	202	9YF	C18-C19-C20-C21
21	B	607	MQ9	C15-C14-C16-C17
15	N	605	CDL	C32-C33-C34-C35
19	K	202	9YF	C34-C33-C35-C36

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Mol	Chain	Res	Type	Atoms
20	B	601	HEM	CAA-CBA-CGA-O1A
15	B	604	CDL	O1-C1-CA2-OA2
15	N	605	CDL	O1-C1-CA2-OA2
15	N	604	CDL	C72-C71-CB7-OB8
19	A	504	9YF	O11-C25-C26-C27
19	M	501	9YF	O11-C25-C26-C27
16	K	201	9Y0	C11-C12-C13-C14
15	N	604	CDL	C79-C80-C81-C82
19	W	202	9YF	C18-C19-C20-C21
21	C	304	MQ9	C27-C28-C29-C31
21	O	304	MQ9	C27-C28-C29-C31
14	R	601	HEA	CAA-CBA-CGA-O2A
20	N	602	HEM	CAA-CBA-CGA-O1A
20	N	602	HEM	CAA-CBA-CGA-O2A
16	B	612	9Y0	C15-C16-C17-C18
19	W	202	9YF	C11-C10-C9-C8
15	P	201	CDL	C32-C31-CA7-OA8
15	F	606	CDL	C52-C53-C54-C55
16	D	202	9Y0	C27-C28-C29-C30
21	N	607	MQ9	C15-C14-C16-C17
14	F	601	HEA	CAA-CBA-CGA-O2A
15	B	603	CDL	C79-C80-C81-C82
16	K	201	9Y0	C13-C14-C15-C16
16	P	202	9Y0	C27-C28-C29-C30
20	B	601	HEM	CAA-CBA-CGA-O2A
15	F	605	CDL	OB5-CB3-CB4-OB6
15	R	605	CDL	OB5-CB3-CB4-OB6
15	R	606	CDL	OA5-CA3-CA4-OA6
19	K	202	9YF	O9-C-C1-O
15	F	605	CDL	C72-C71-CB7-OB8
15	R	605	CDL	C72-C71-CB7-OB8
16	B	606	9Y0	O7-C21-C22-C23
16	B	612	9Y0	O7-C21-C22-C23
19	C	303	9YF	O11-C25-C26-C27
15	B	604	CDL	C32-C33-C34-C35
19	O	303	9YF	C36-C37-C38-C39
15	D	201	CDL	C32-C31-CA7-OA8
20	B	602	HEM	CAA-CBA-CGA-O1A
20	N	603	HEM	CAA-CBA-CGA-O1A
16	B	612	9Y0	C11-C12-C13-C14
15	R	605	CDL	C14-C15-C16-C17
19	O	303	9YF	O11-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
15	B	605	CDL	OB5-CB3-CB4-CB6
19	K	202	9YF	C24-C-C1-O
15	M	503	CDL	C72-C71-CB7-OB8
19	W	202	9YF	C37-C38-C39-C40
15	P	201	CDL	OB7-CB5-OB6-CB4
15	A	502	CDL	C72-C71-CB7-OB8
15	D	201	CDL	C38-C39-C40-C41
15	A	502	CDL	C17-C18-C19-C20
19	M	504	9YF	C40-C41-C42-C43
21	O	304	MQ9	C38-C39-C41-C42
19	A	503	9YF	C-C1-O-P
15	A	502	CDL	C82-C83-C84-C85
16	B	606	9Y0	C11-C12-C13-C14
16	S	301	9Y0	C11-C12-C13-C14
16	W	201	9Y0	C11-C12-C13-C14
21	C	304	MQ9	C24-C26-C27-C28
21	O	304	MQ9	C24-C26-C27-C28
15	N	601	CDL	C12-C11-CA5-OA6
15	P	201	CDL	C78-C79-C80-C81
15	F	606	CDL	C63-C64-C65-C66
15	T	201	CDL	C58-C59-C60-C61
15	H	201	CDL	C58-C59-C60-C61
15	M	503	CDL	C17-C18-C19-C20
15	B	603	CDL	C72-C71-CB7-OB8
15	B	611	CDL	C12-C11-CA5-OA6
15	M	503	CDL	C82-C83-C84-C85
16	G	301	9Y0	C11-C12-C13-C14
16	B	612	9Y0	C6-C7-C8-C9
21	C	304	MQ9	C38-C39-C41-C42
19	A	504	9YF	C14-C15-C16-C17
19	M	501	9YF	C14-C15-C16-C17
15	B	605	CDL	C20-C21-C22-C23
15	F	606	CDL	C52-C51-CB5-OB7
15	D	201	CDL	C32-C31-CA7-OA9
15	B	603	CDL	C72-C71-CB7-OB9
15	R	606	CDL	C52-C51-CB5-OB7
15	P	201	CDL	C32-C31-CA7-OA9
19	C	303	9YF	O12-C25-C26-C27
15	R	606	CDL	CA3-CA4-CA6-OA8
16	W	201	9Y0	O5-C-C1-C2
19	O	303	9YF	O12-C25-C26-C27
15	F	606	CDL	CA2-OA2-PA1-OA3

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Mol	Chain	Res	Type	Atoms
15	B	603	CDL	CA2-OA2-PA1-OA4
15	B	611	CDL	CA2-OA2-PA1-OA3
15	R	606	CDL	CA3-OA5-PA1-OA3
15	N	601	CDL	CA2-OA2-PA1-OA3
16	D	202	9Y0	C2-O3-P-O
16	P	202	9Y0	C2-O3-P-O
19	K	202	9YF	C1-O-P-O8
19	C	303	9YF	C36-C37-C38-C39
19	M	501	9YF	O12-C25-C26-C27
15	R	605	CDL	C32-C31-CA7-OA8
15	N	604	CDL	C72-C71-CB7-OB9
19	A	504	9YF	O12-C25-C26-C27
15	F	605	CDL	C32-C31-CA7-OA8
15	N	605	CDL	C74-C75-C76-C77
15	F	605	CDL	C72-C71-CB7-OB9
19	K	202	9YF	C36-C37-C38-C39
19	M	504	9YF	O9-C8-C9-C10
15	M	503	CDL	C72-C71-CB7-OB9
16	B	606	9Y0	O6-C21-C22-C23
15	B	604	CDL	C74-C75-C76-C77
14	F	601	HEA	C3B-C11-C12-C13
14	R	601	HEA	C3B-C11-C12-C13
16	K	201	9Y0	C4-C3-O1-P
16	S	301	9Y0	C4-C3-O1-P
16	W	201	9Y0	C4-C3-O1-P
15	A	502	CDL	C72-C71-CB7-OB9
15	R	605	CDL	C72-C71-CB7-OB9
16	B	612	9Y0	O6-C21-C22-C23
19	K	202	9YF	C37-C38-C39-C40
16	B	606	9Y0	C6-C7-C8-C9
15	T	201	CDL	C52-C51-CB5-OB6
15	F	606	CDL	C14-C15-C16-C17
15	H	201	CDL	C52-C51-CB5-OB6
14	F	601	HEA	C20-C21-C22-C23
15	R	606	CDL	C33-C34-C35-C36
15	F	606	CDL	OA5-CA3-CA4-OA6
19	M	504	9YF	O10-C8-C9-C10
20	B	601	HEM	CAD-CBD-CGD-O1D
18	Y	302	9XX	O1-C18-C19-C20
15	F	605	CDL	C77-C78-C79-C80
15	F	606	CDL	C33-C34-C35-C36
15	D	201	CDL	C78-C79-C80-C81

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Mol	Chain	Res	Type	Atoms
14	R	601	HEA	C20-C21-C22-C23
18	Z	302	9XX	O1-C18-C19-C20
15	R	605	CDL	C32-C31-CA7-OA9
20	N	602	HEM	CAD-CBD-CGD-O1D

There are no ring outliers.

49 monomers are involved in 152 short contacts:

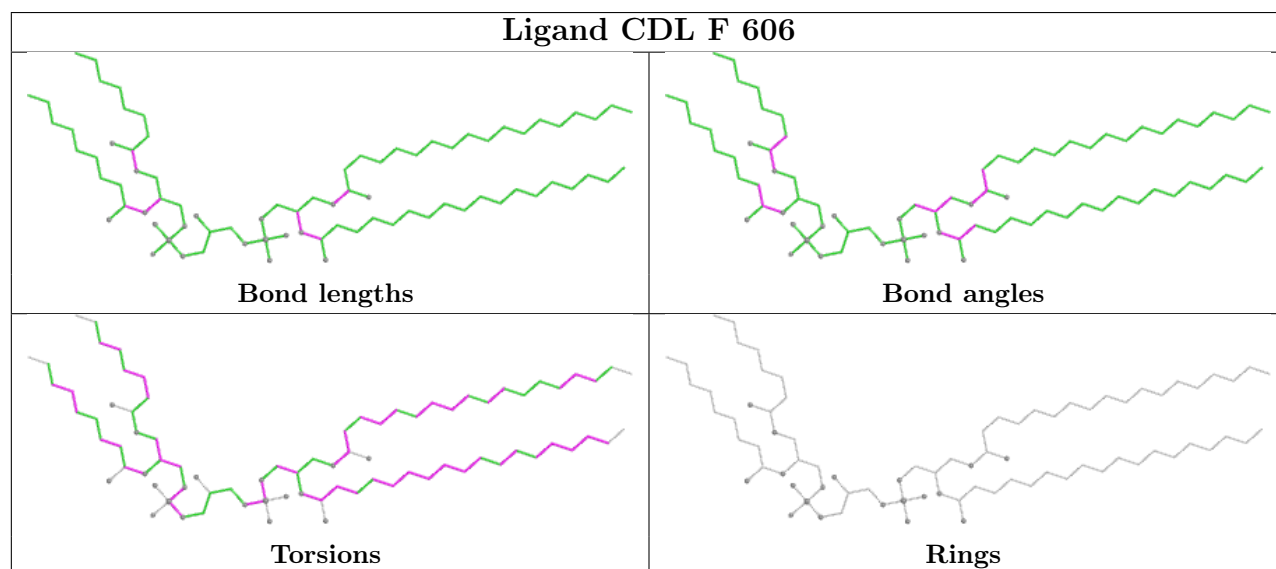
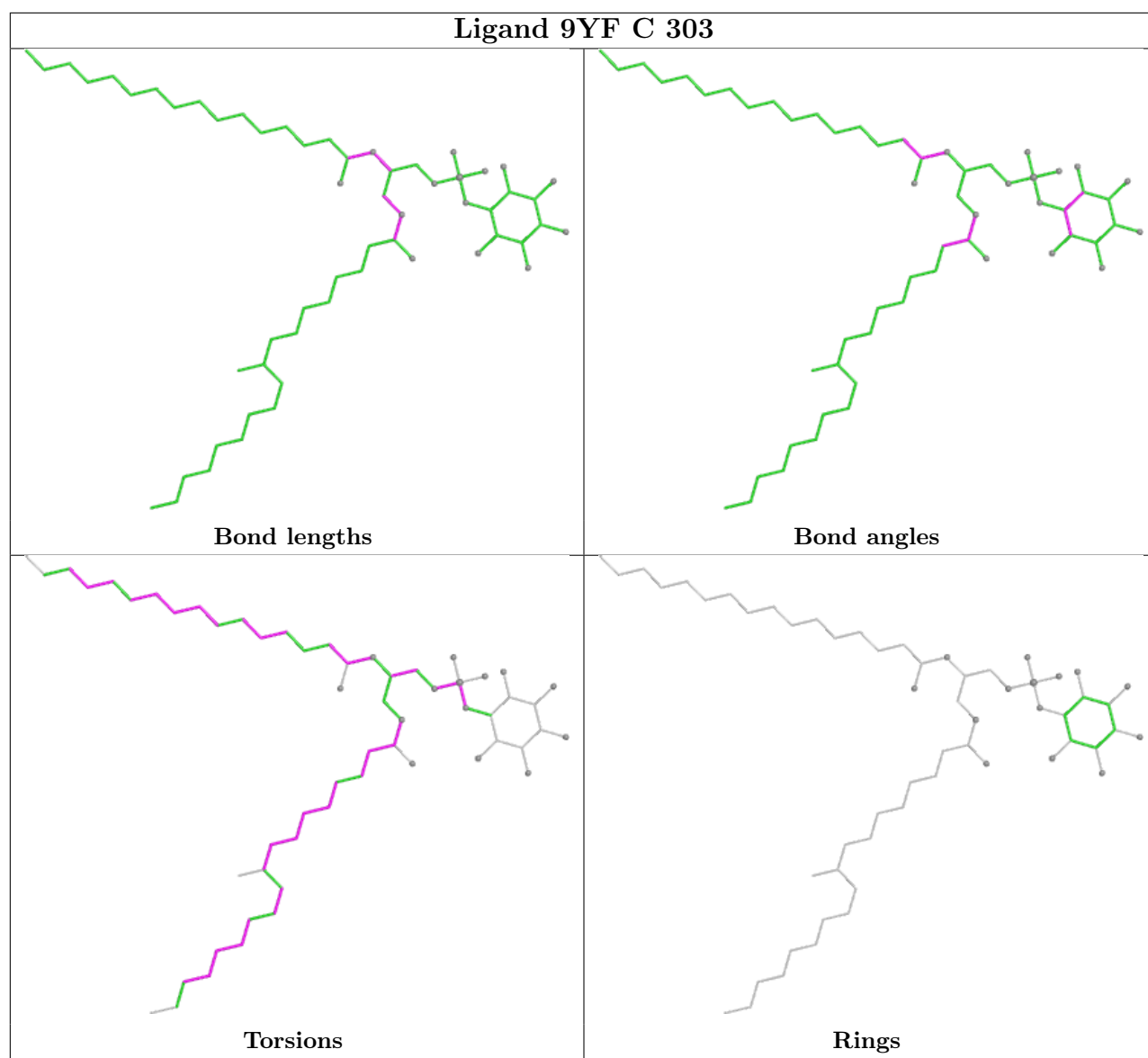
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	C	303	9YF	1	0
15	F	606	CDL	4	0
22	O	302	HEC	3	0
15	B	611	CDL	2	0
15	N	606	CDL	3	0
19	M	504	9YF	6	0
21	N	607	MQ9	1	0
15	F	605	CDL	2	0
15	N	601	CDL	2	0
21	N	609	MQ9	3	0
19	W	202	9YF	1	0
15	R	606	CDL	6	0
15	B	605	CDL	2	0
20	B	601	HEM	2	0
19	K	202	9YF	1	0
23	M	502	FES	2	0
14	R	602	HEA	5	0
22	O	301	HEC	2	0
15	N	605	CDL	4	0
21	C	304	MQ9	7	0
22	C	302	HEC	3	0
20	B	602	HEM	1	0
15	D	201	CDL	6	0
15	B	604	CDL	4	0
21	B	610	MQ9	1	0
21	O	304	MQ9	7	0
15	M	503	CDL	3	0
17	K	203	PLM	1	0
21	N	610	MQ9	1	0
15	R	605	CDL	2	0
14	F	602	HEA	6	0
15	P	201	CDL	5	0
15	N	604	CDL	8	0

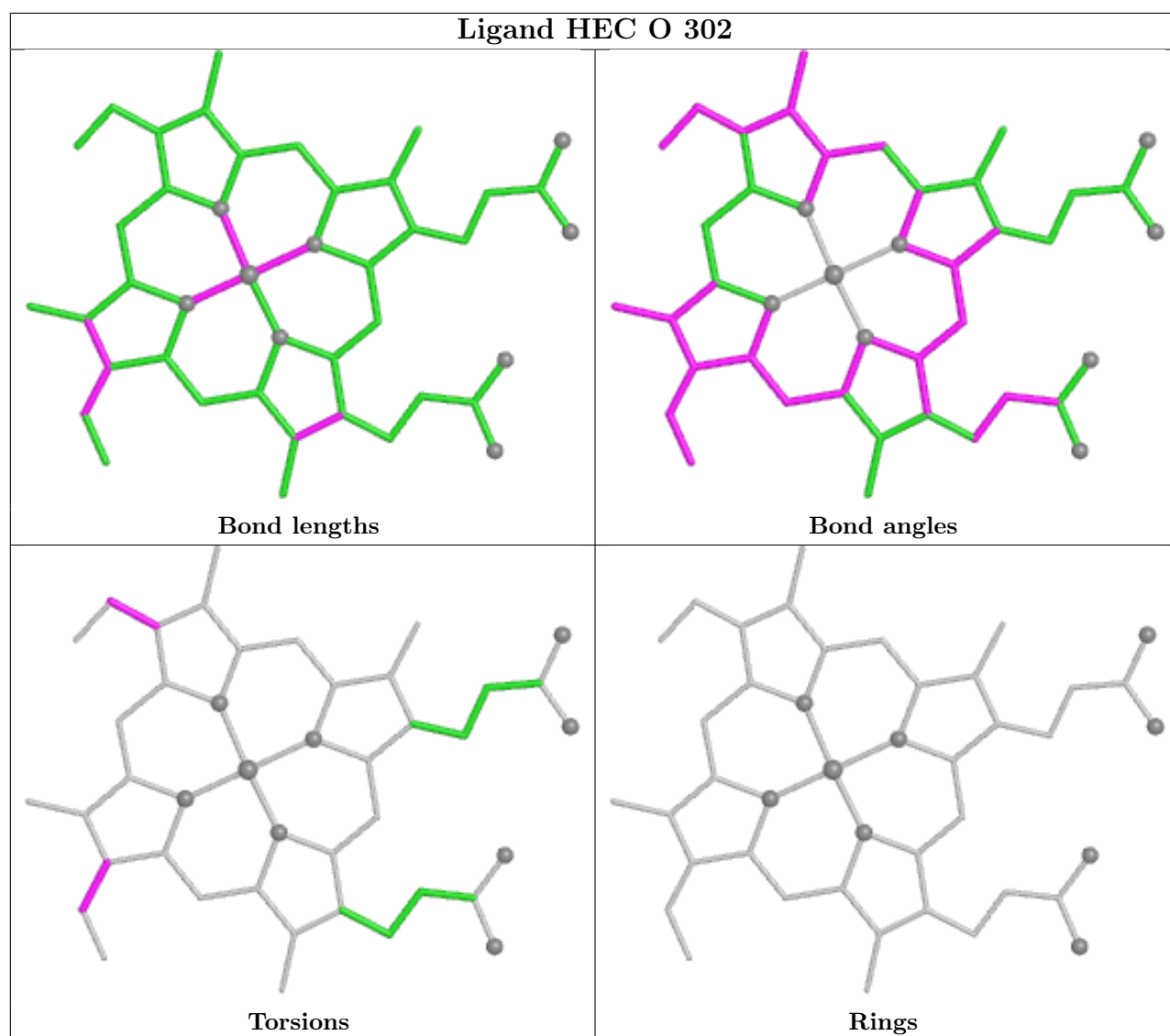
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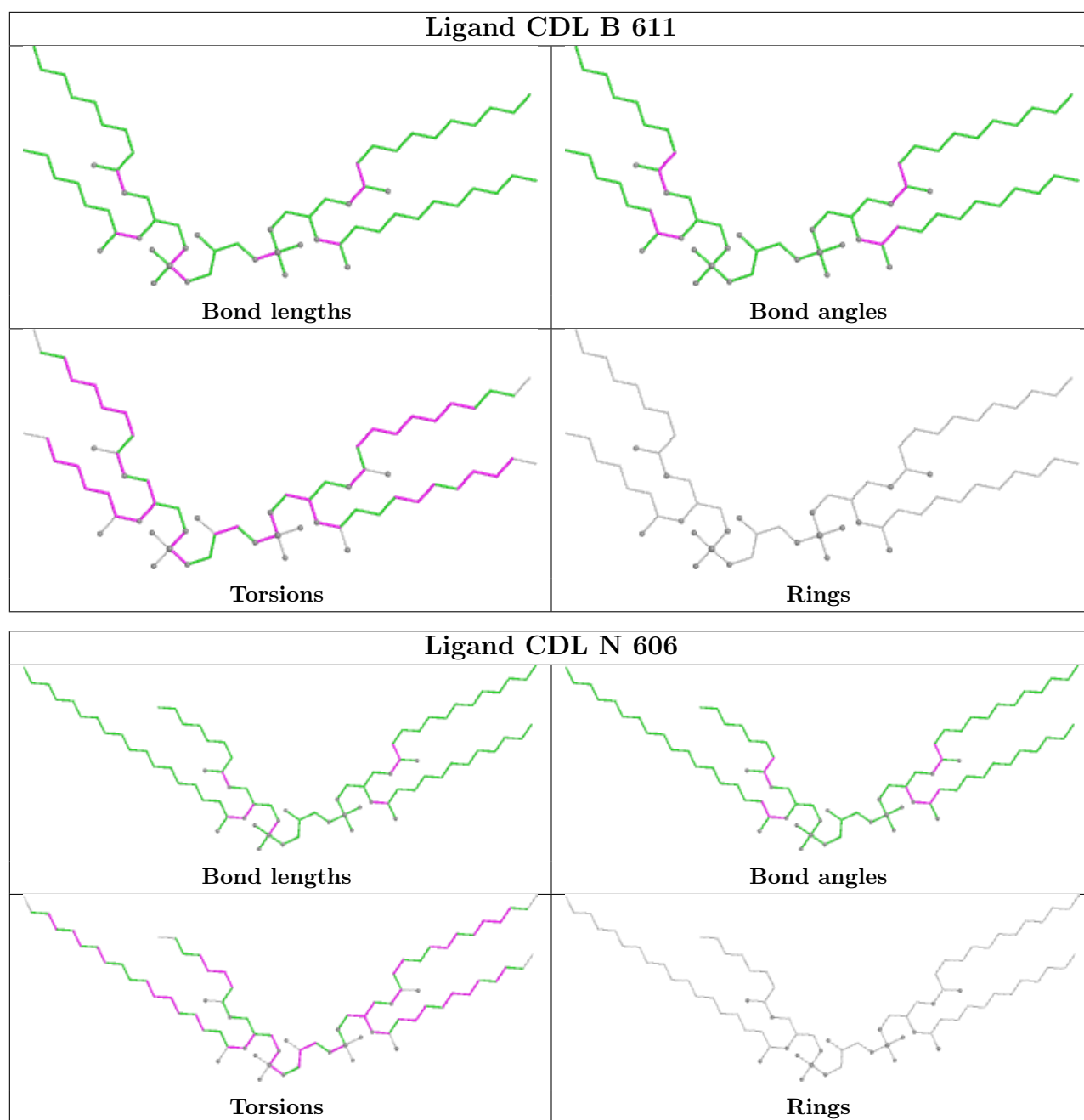
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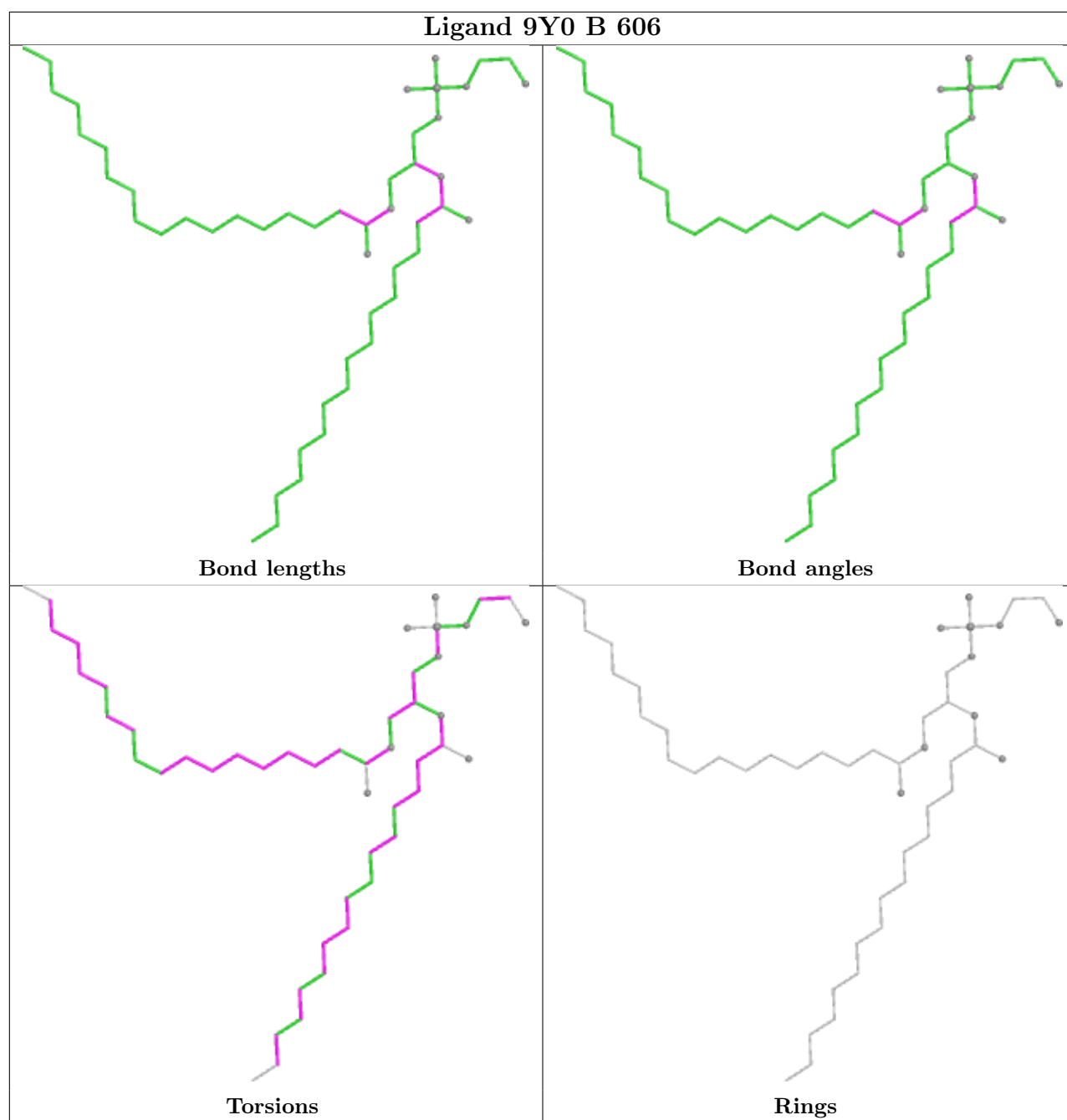
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	O	303	9YF	1	0
14	R	601	HEA	6	0
19	A	503	9YF	17	0
15	T	201	CDL	2	0
22	C	301	HEC	2	0
15	B	603	CDL	7	0
21	B	608	MQ9	3	0
15	A	502	CDL	3	0
21	N	608	MQ9	1	0
23	A	501	FES	1	0
20	N	602	HEM	2	0
15	H	201	CDL	2	0
21	B	609	MQ9	2	0
20	N	603	HEM	1	0
14	F	601	HEA	5	0
21	B	607	MQ9	1	0

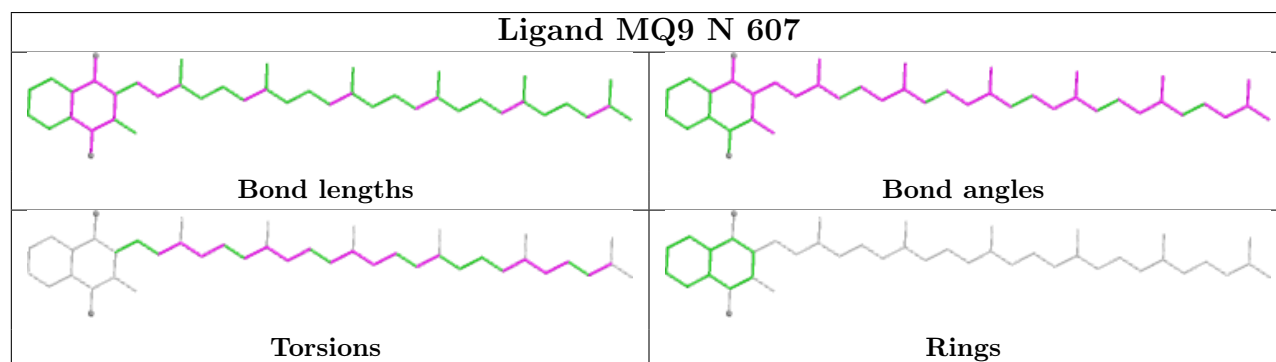
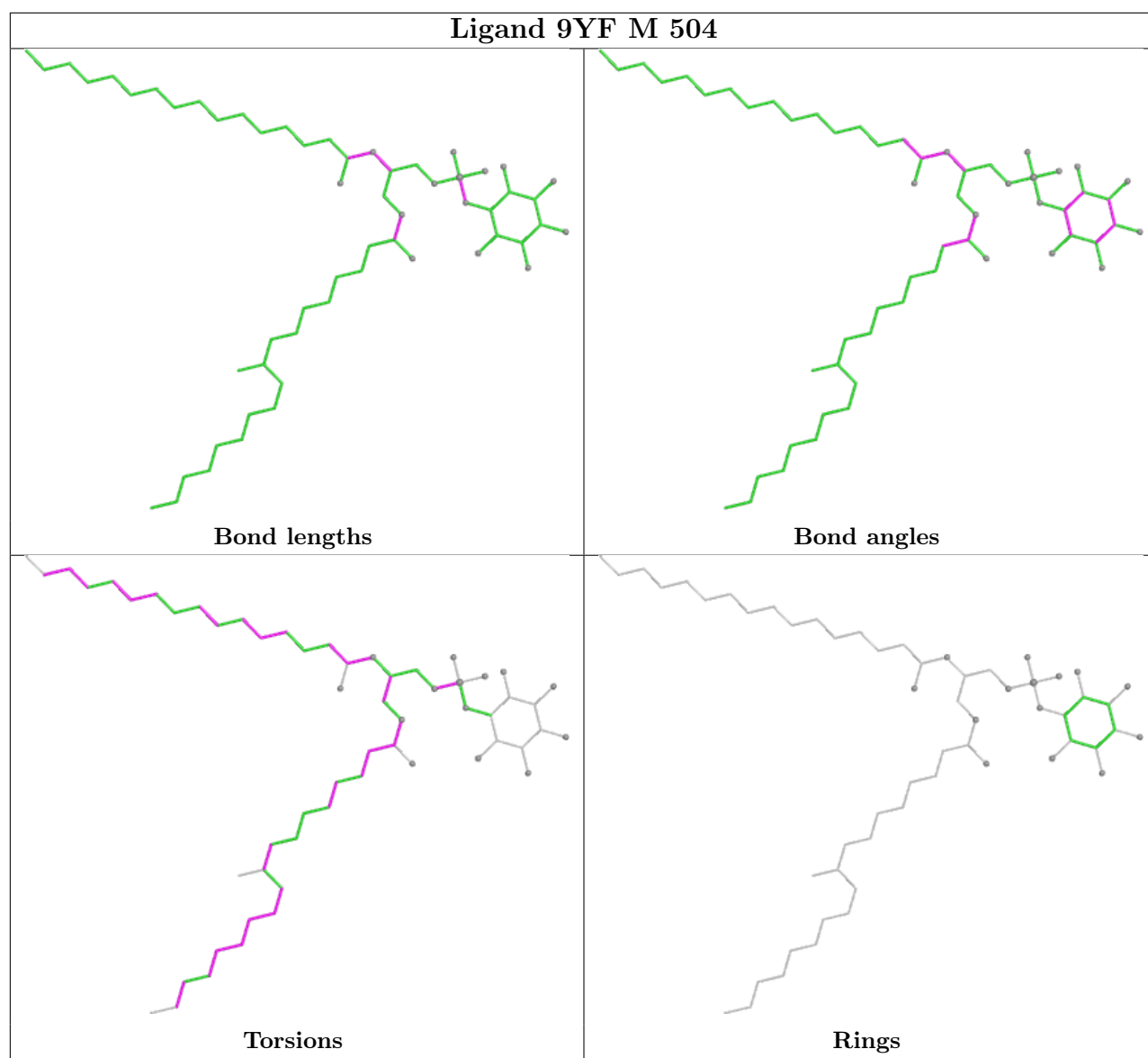
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

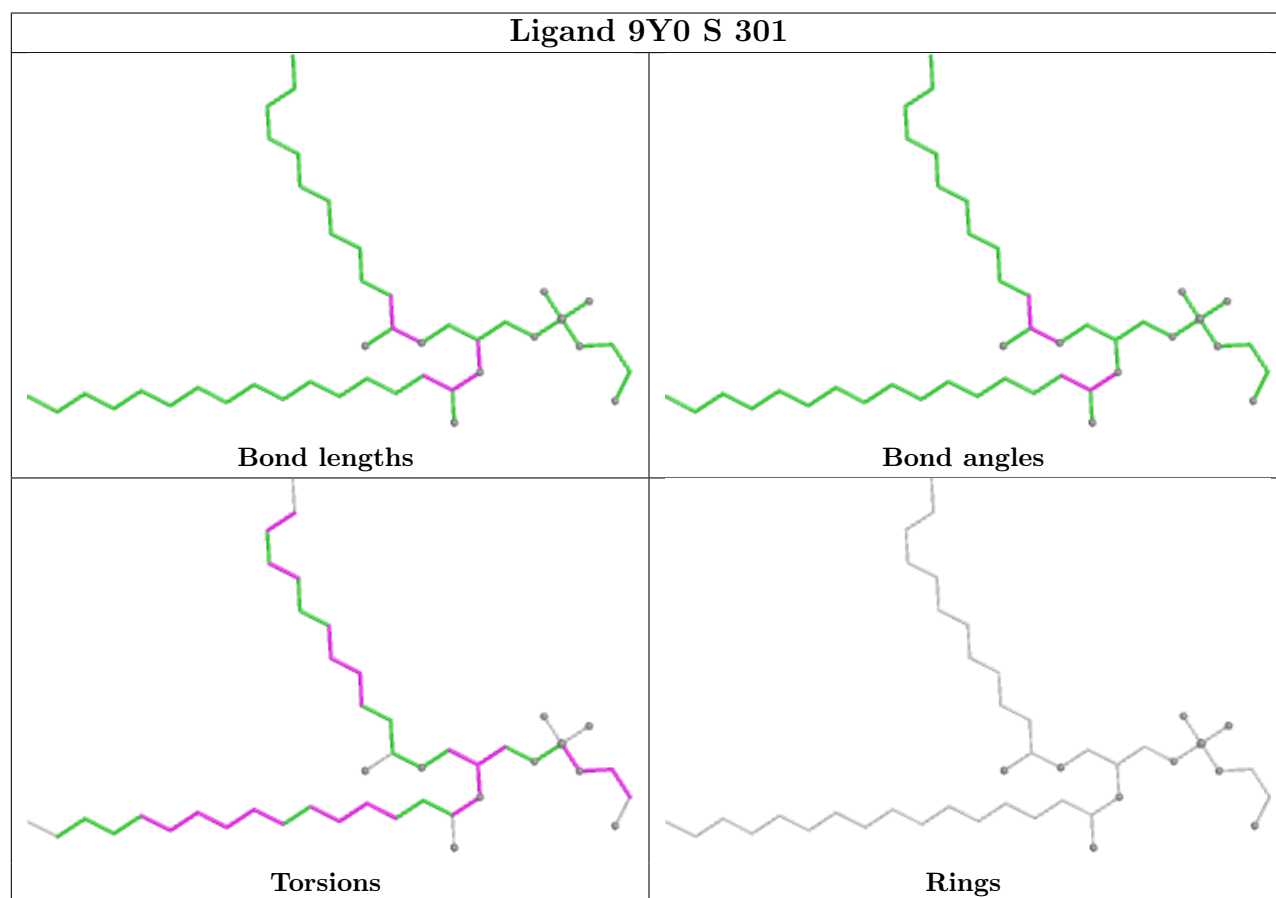
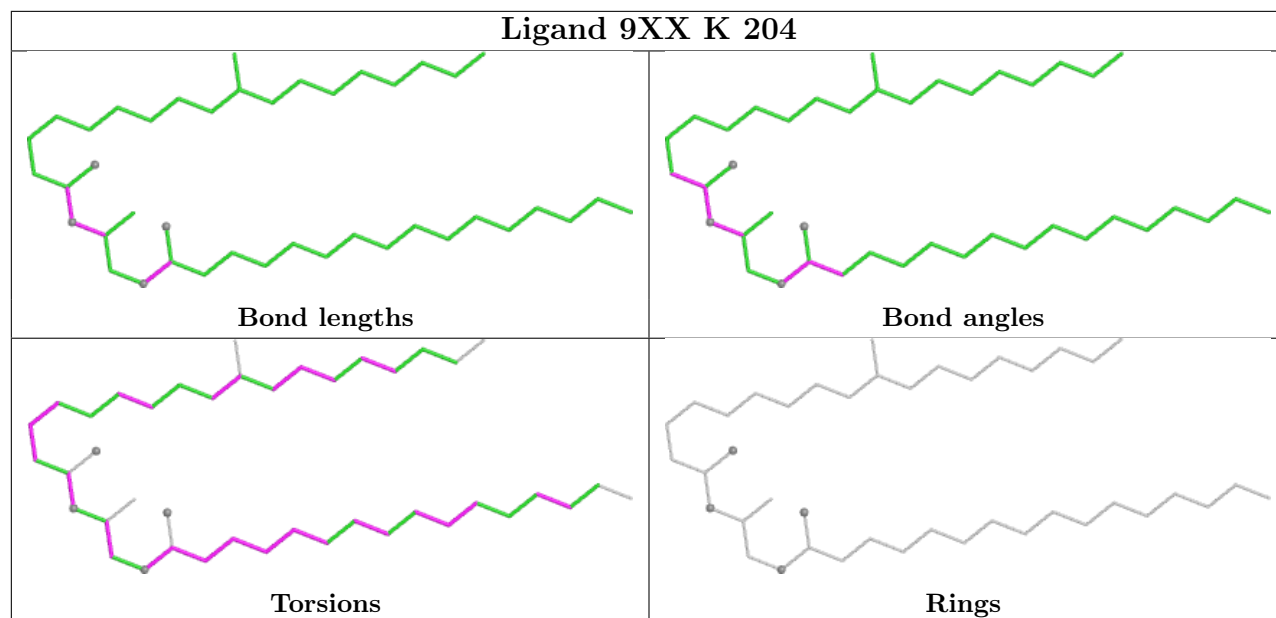


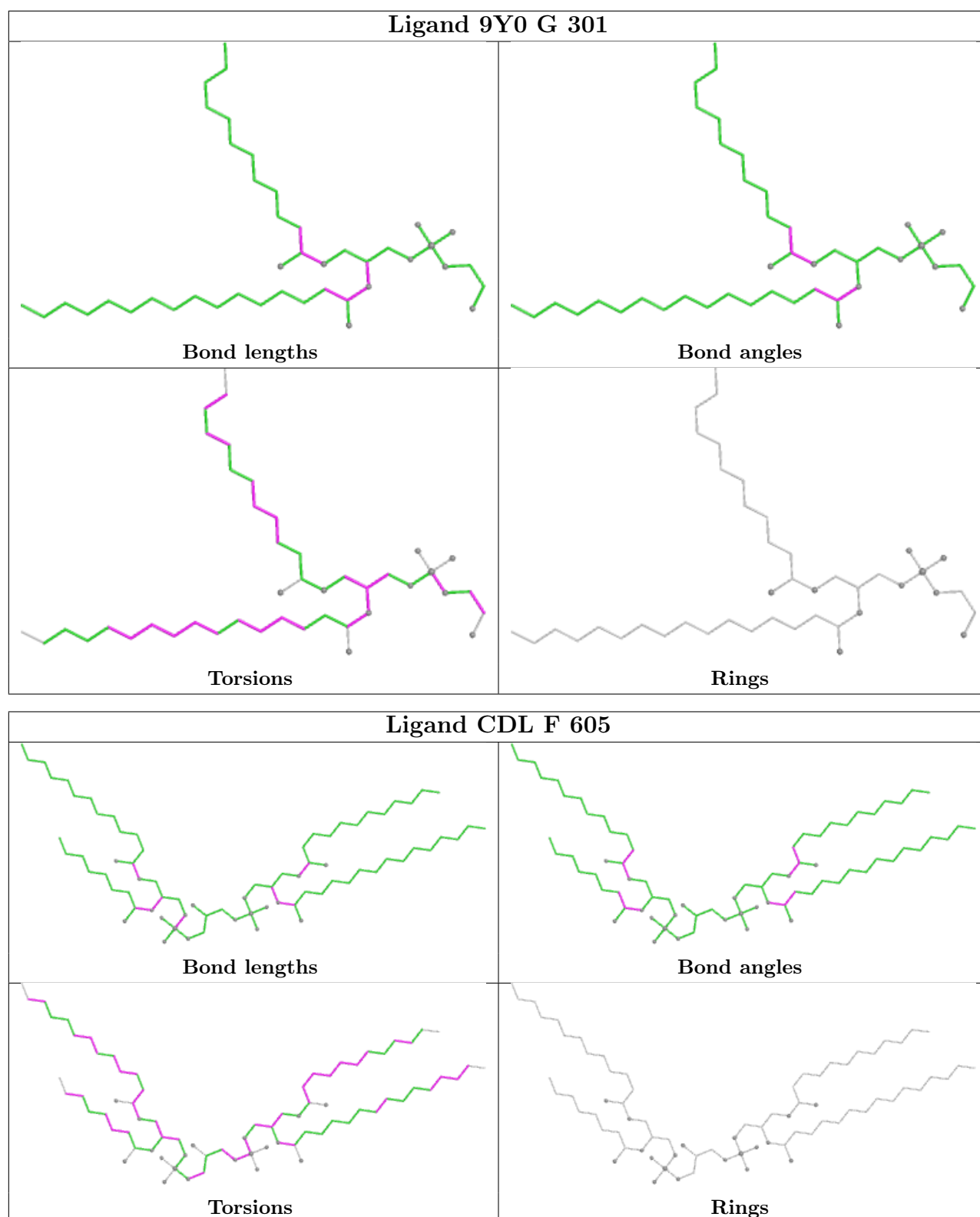


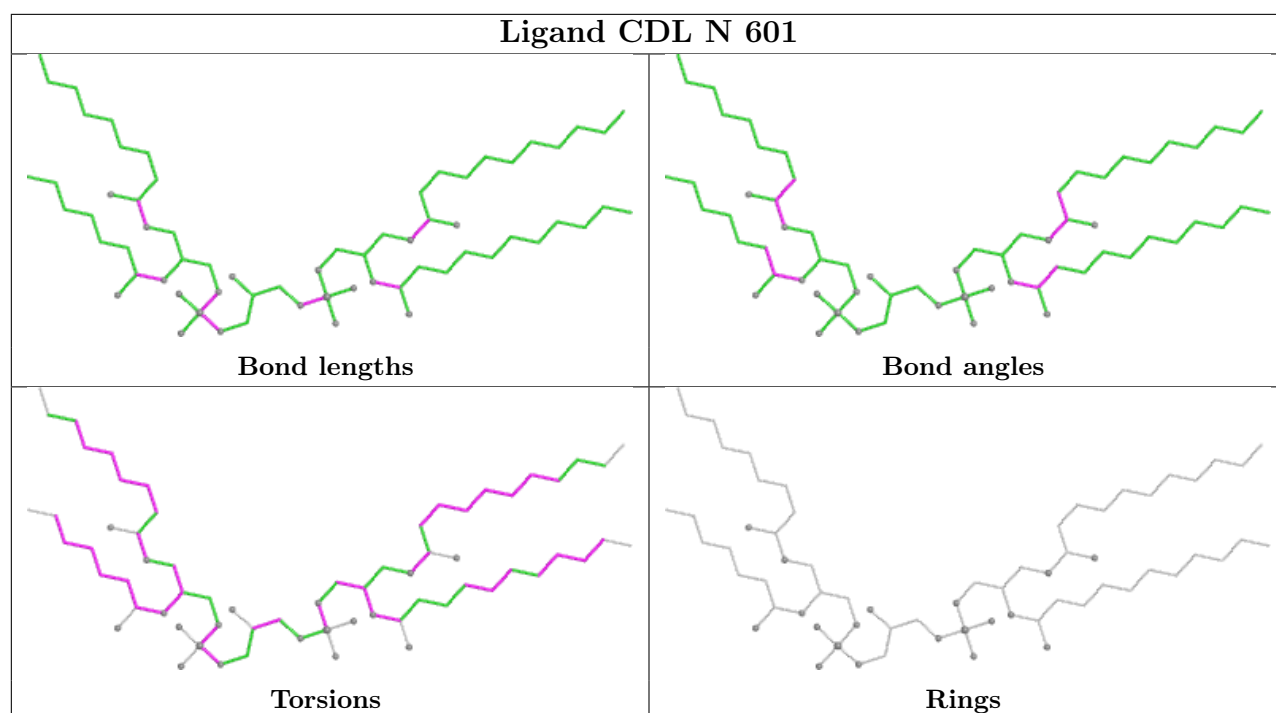


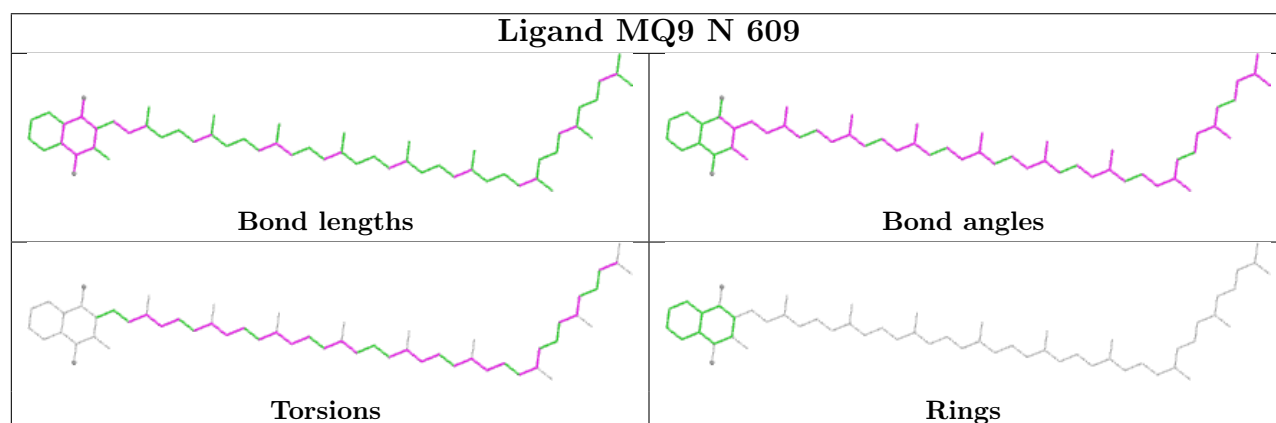
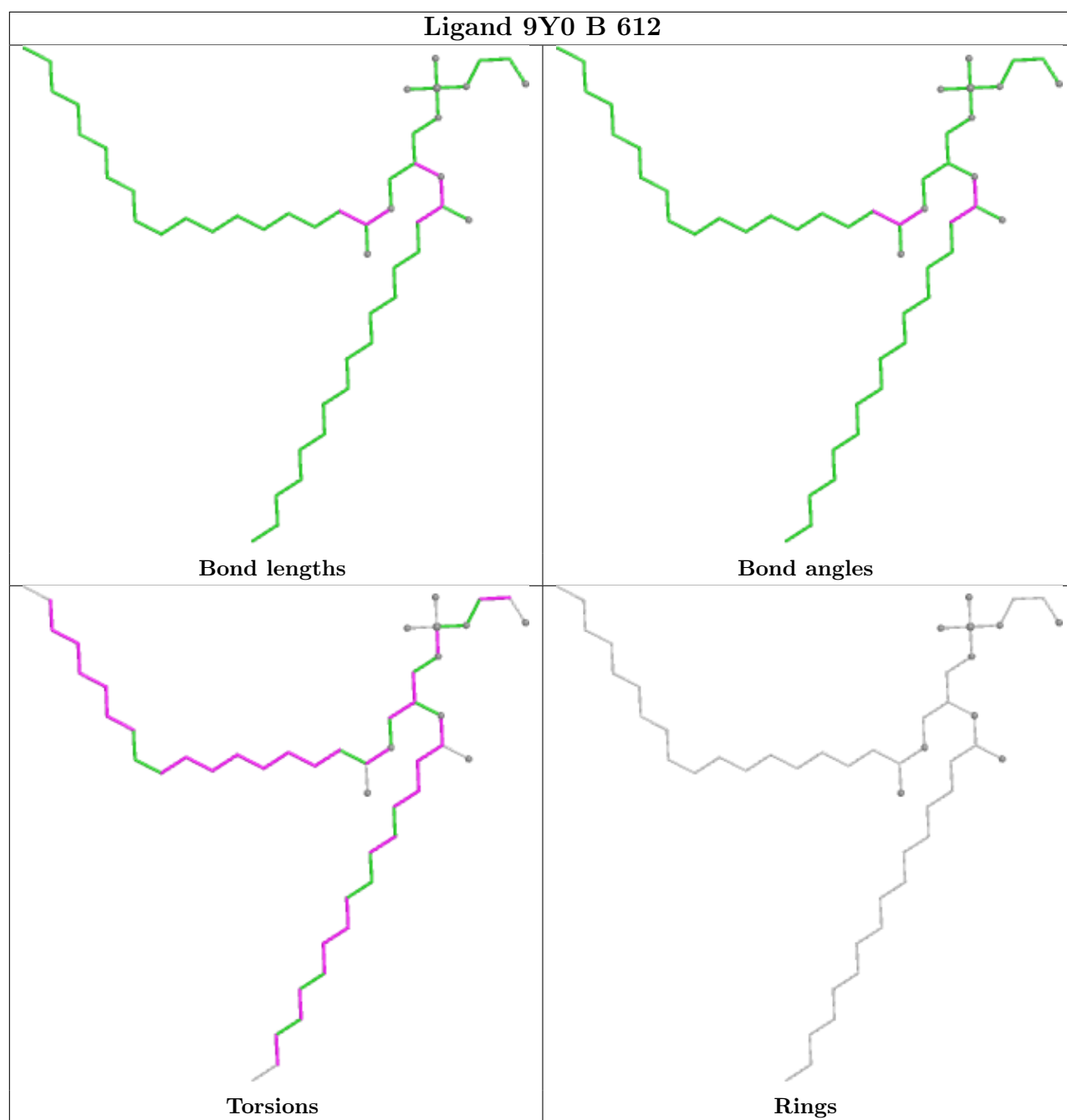


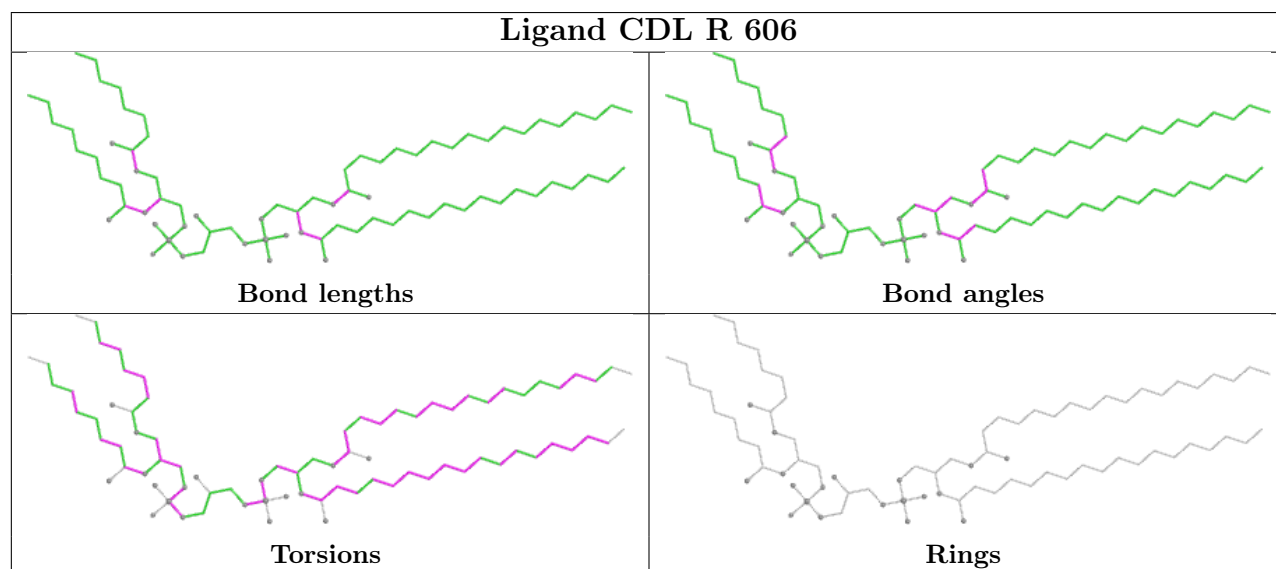
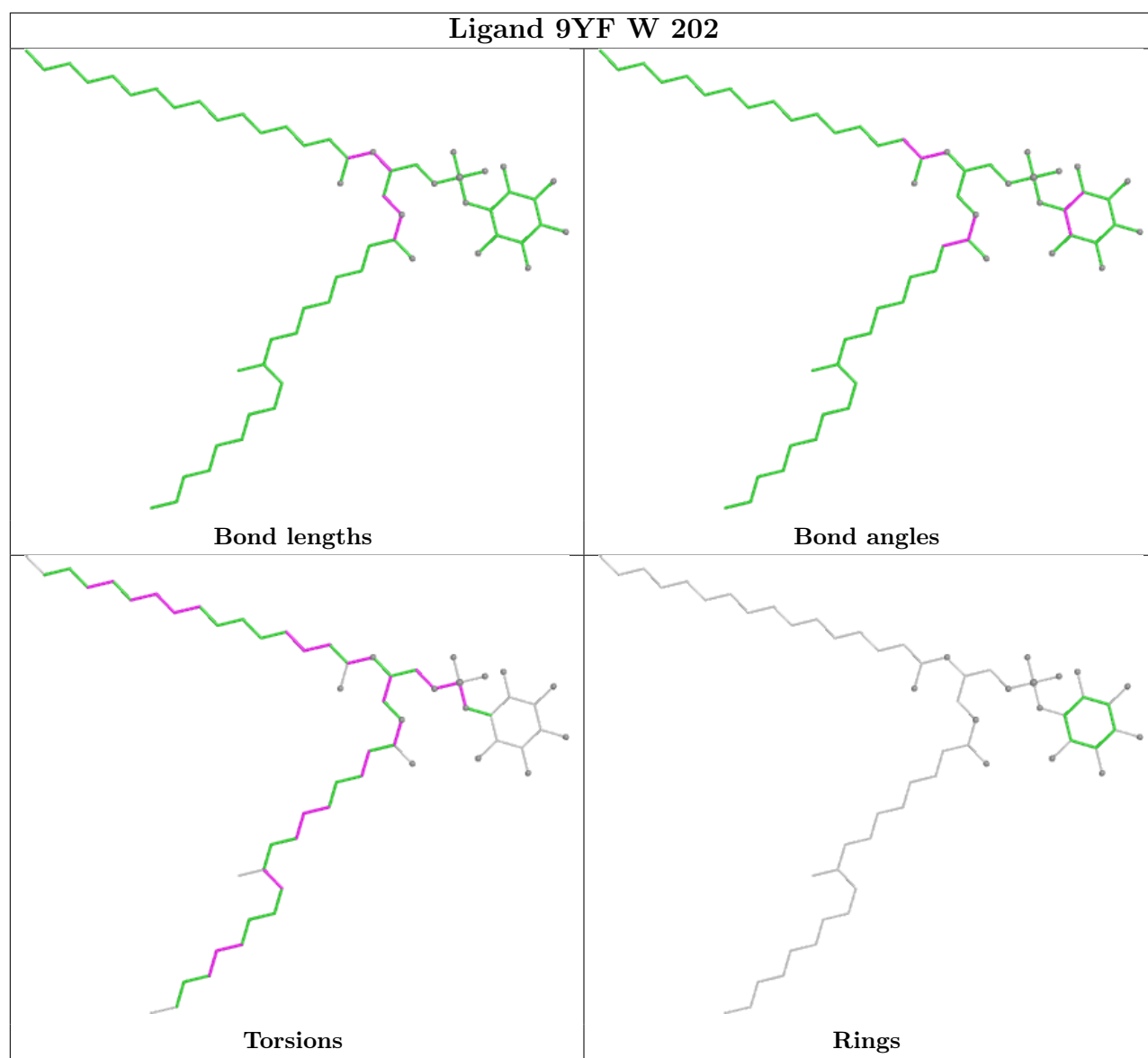


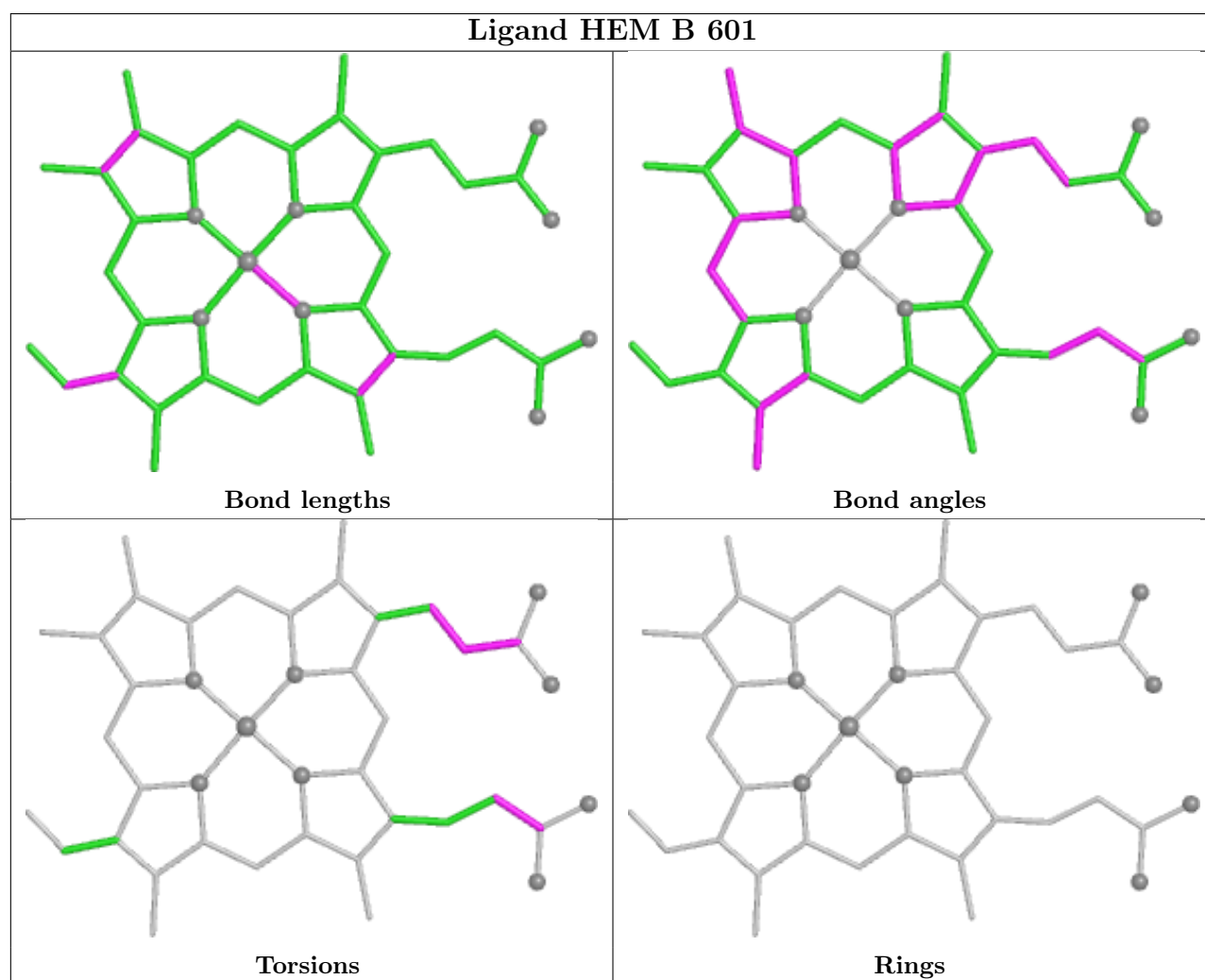
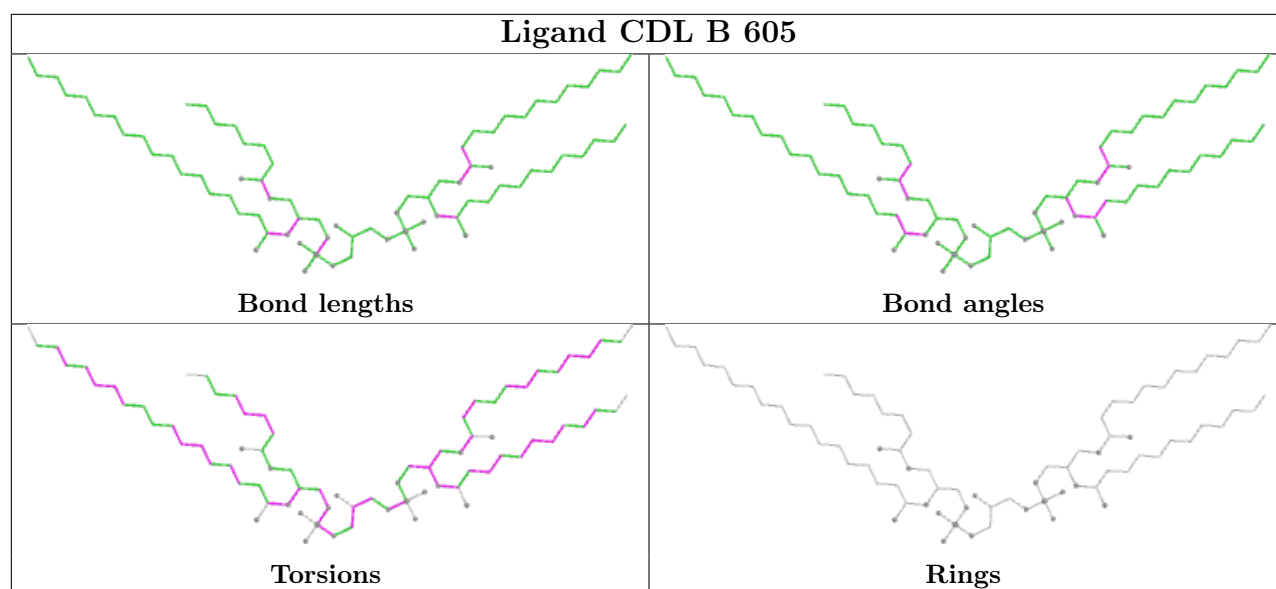


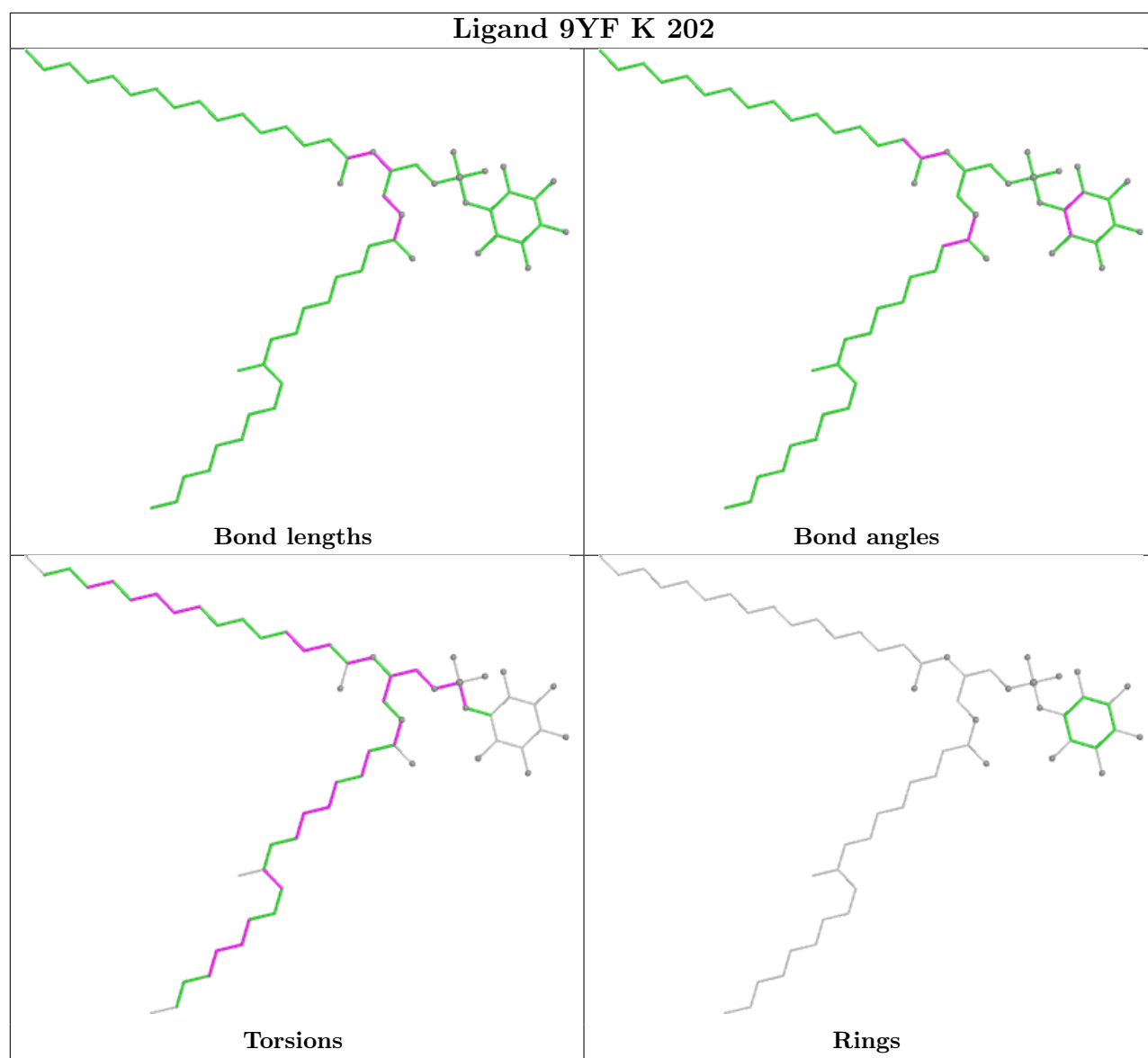


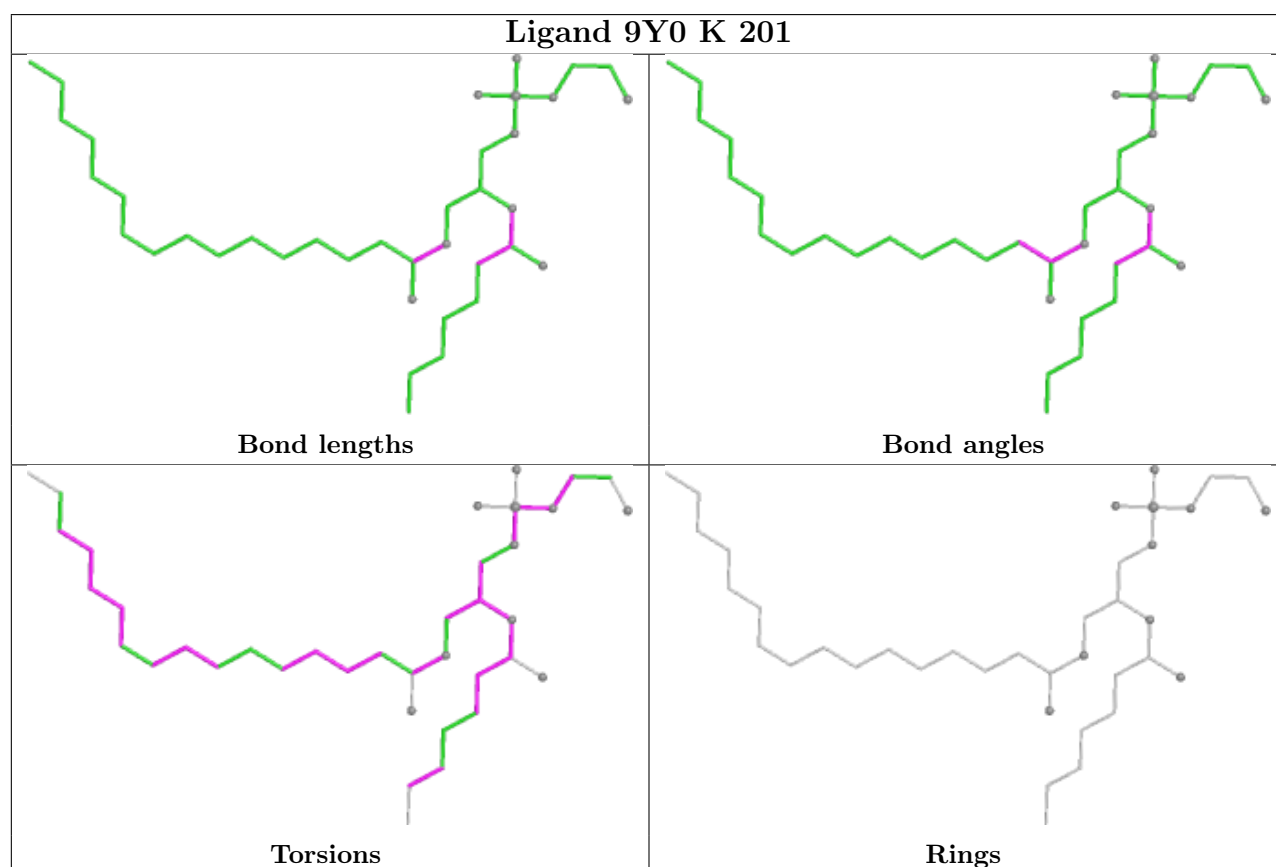
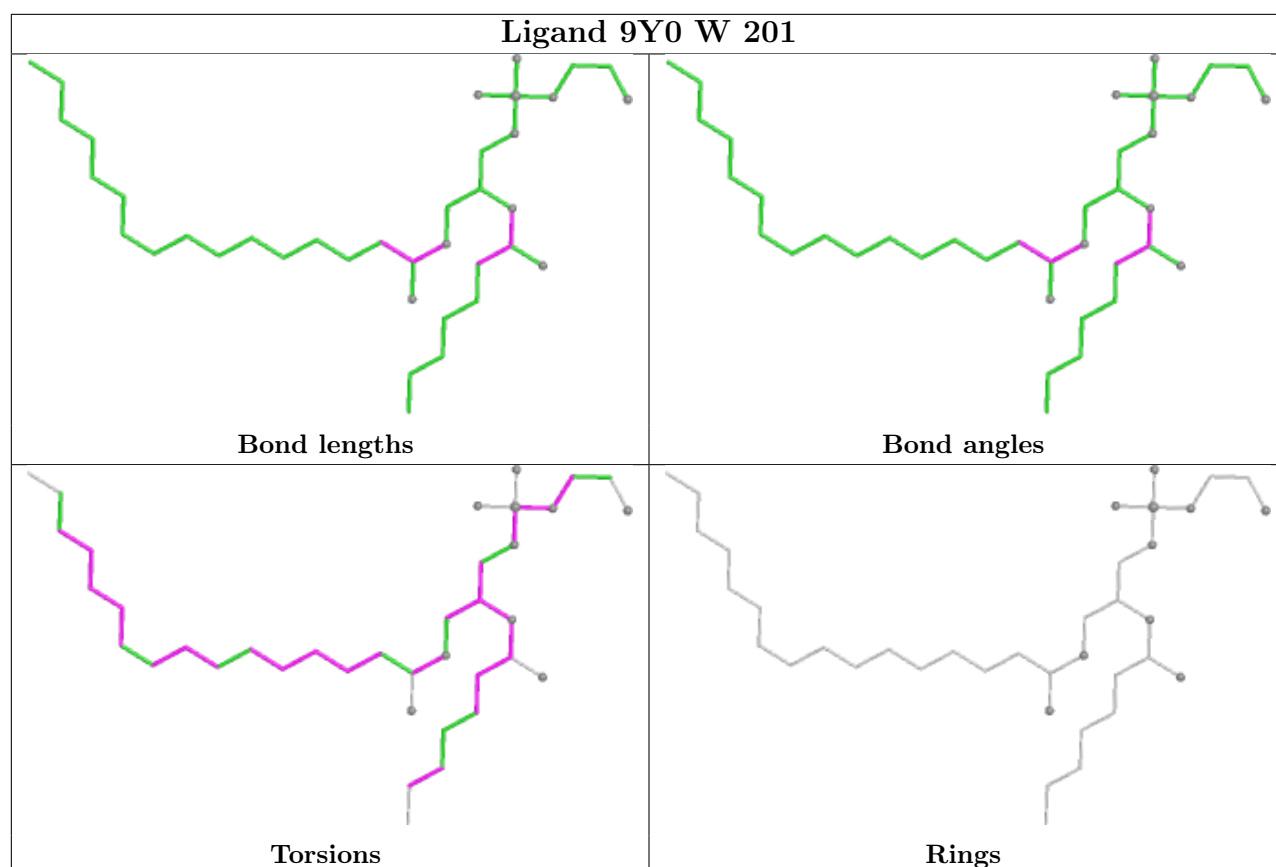


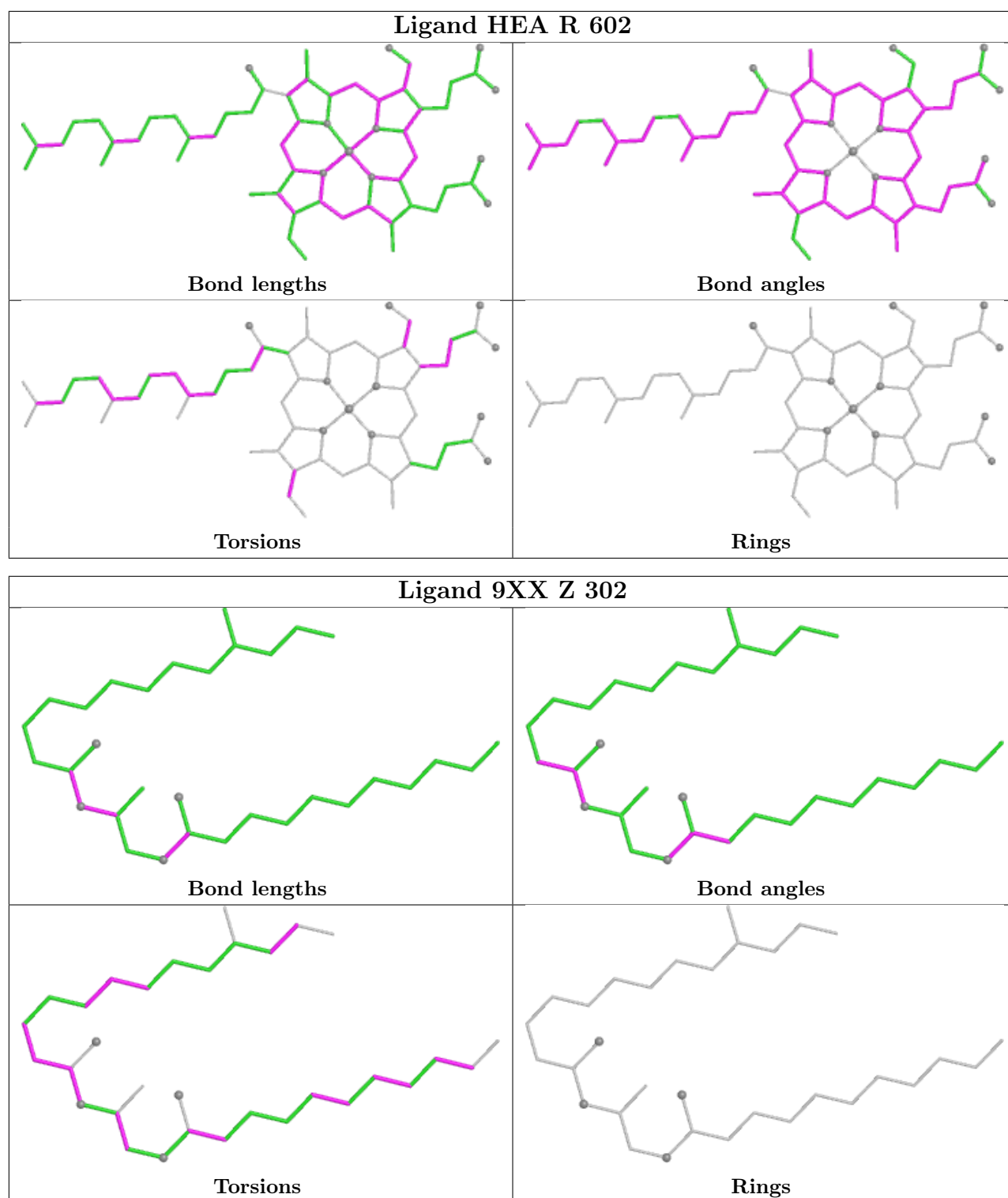


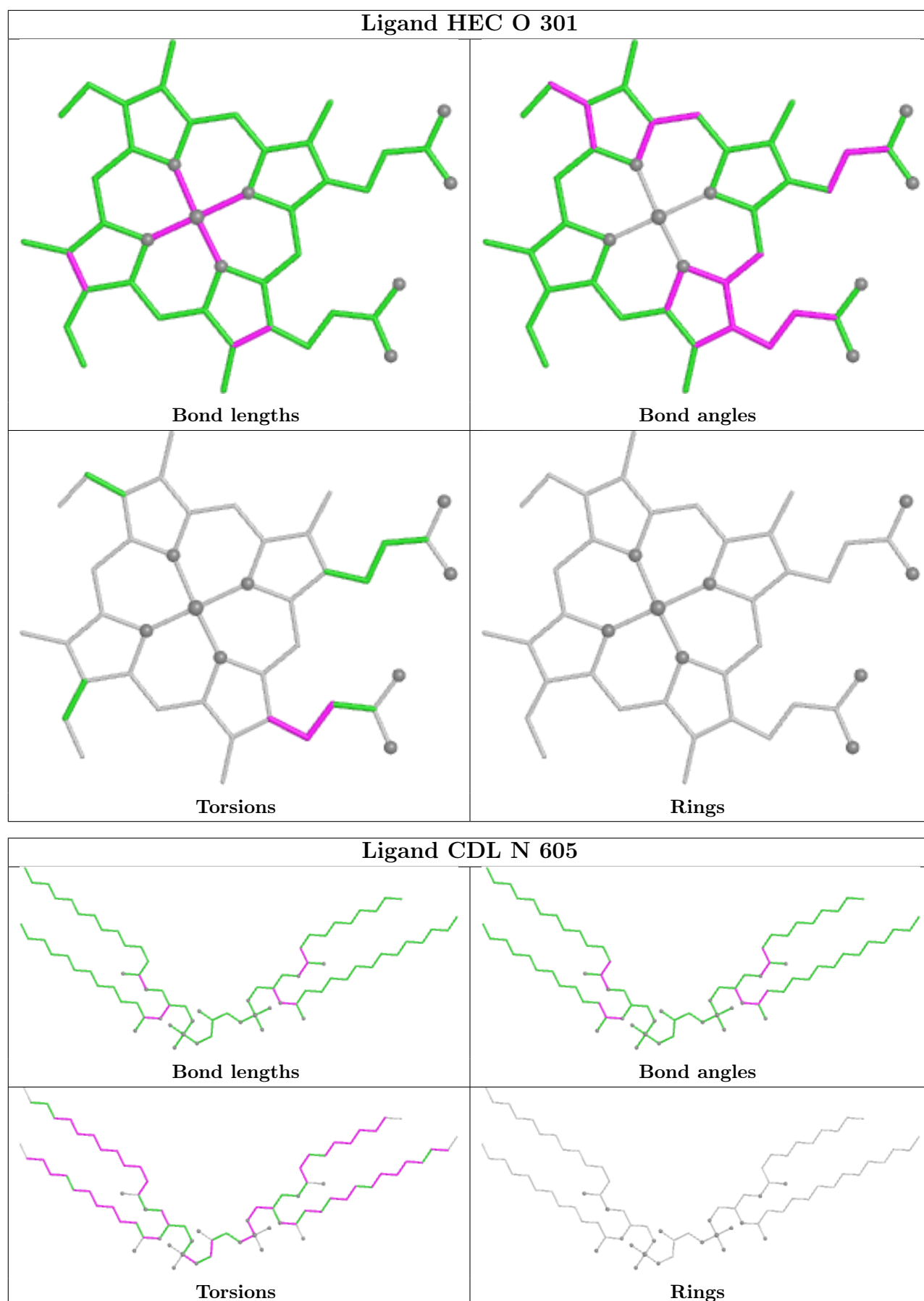


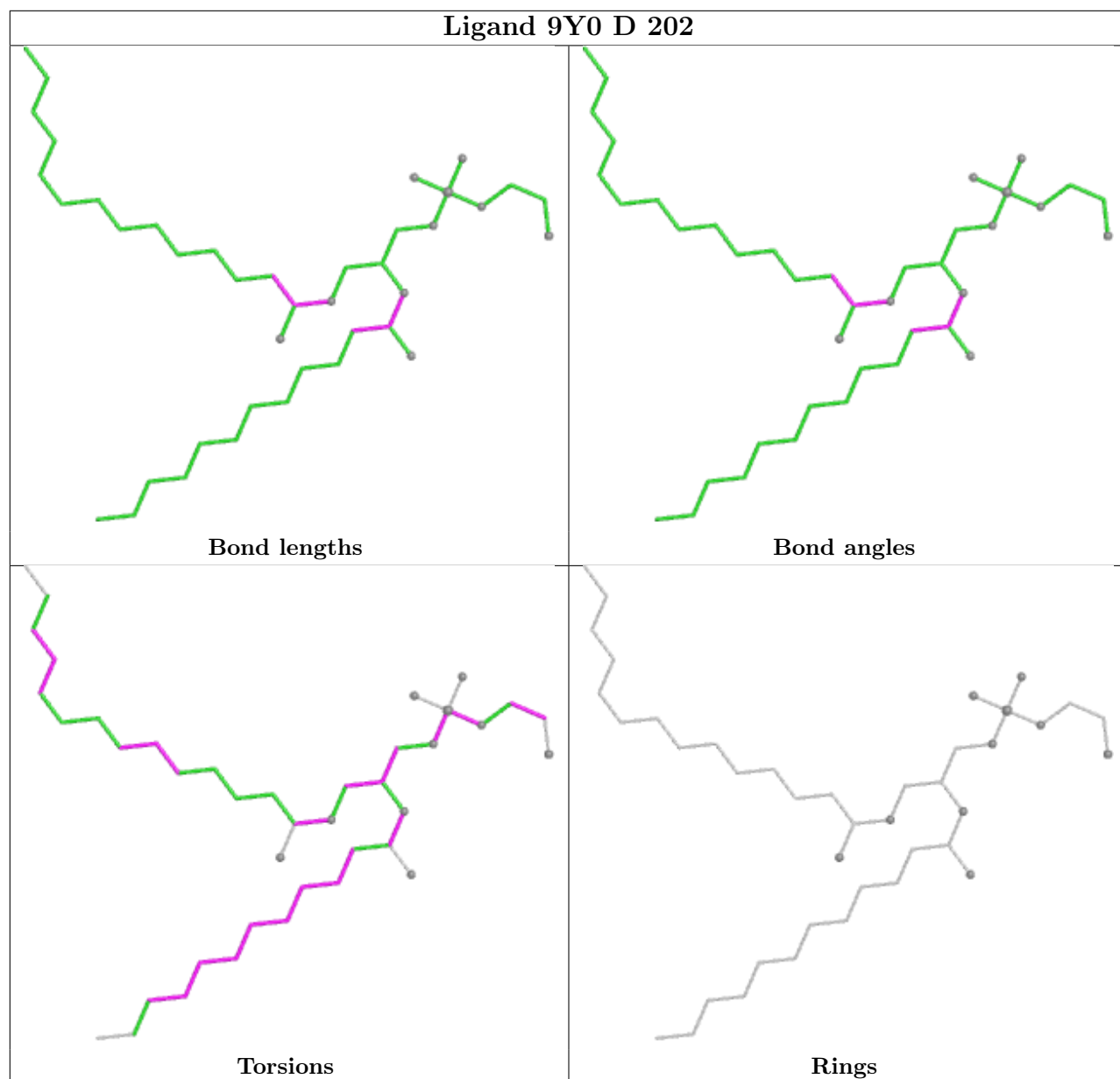
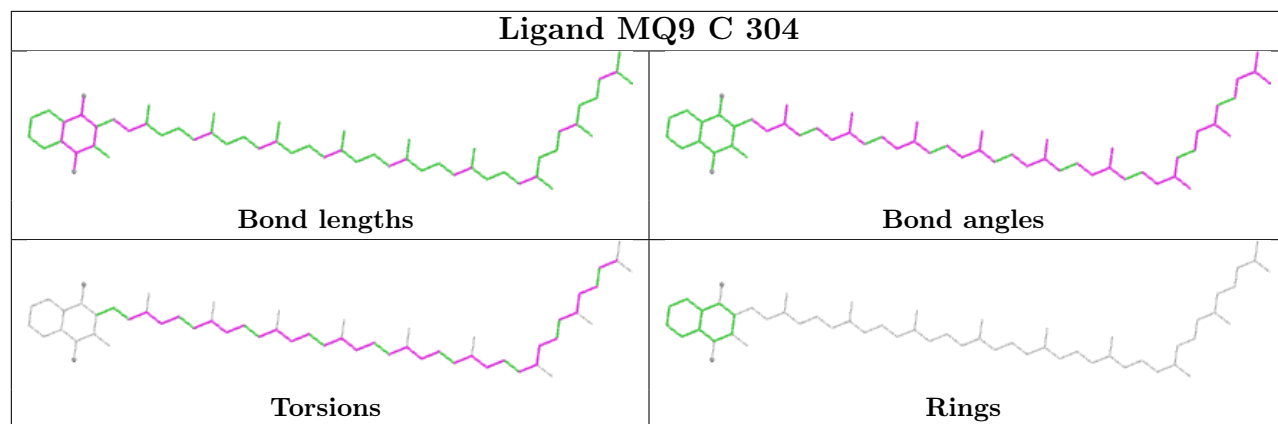


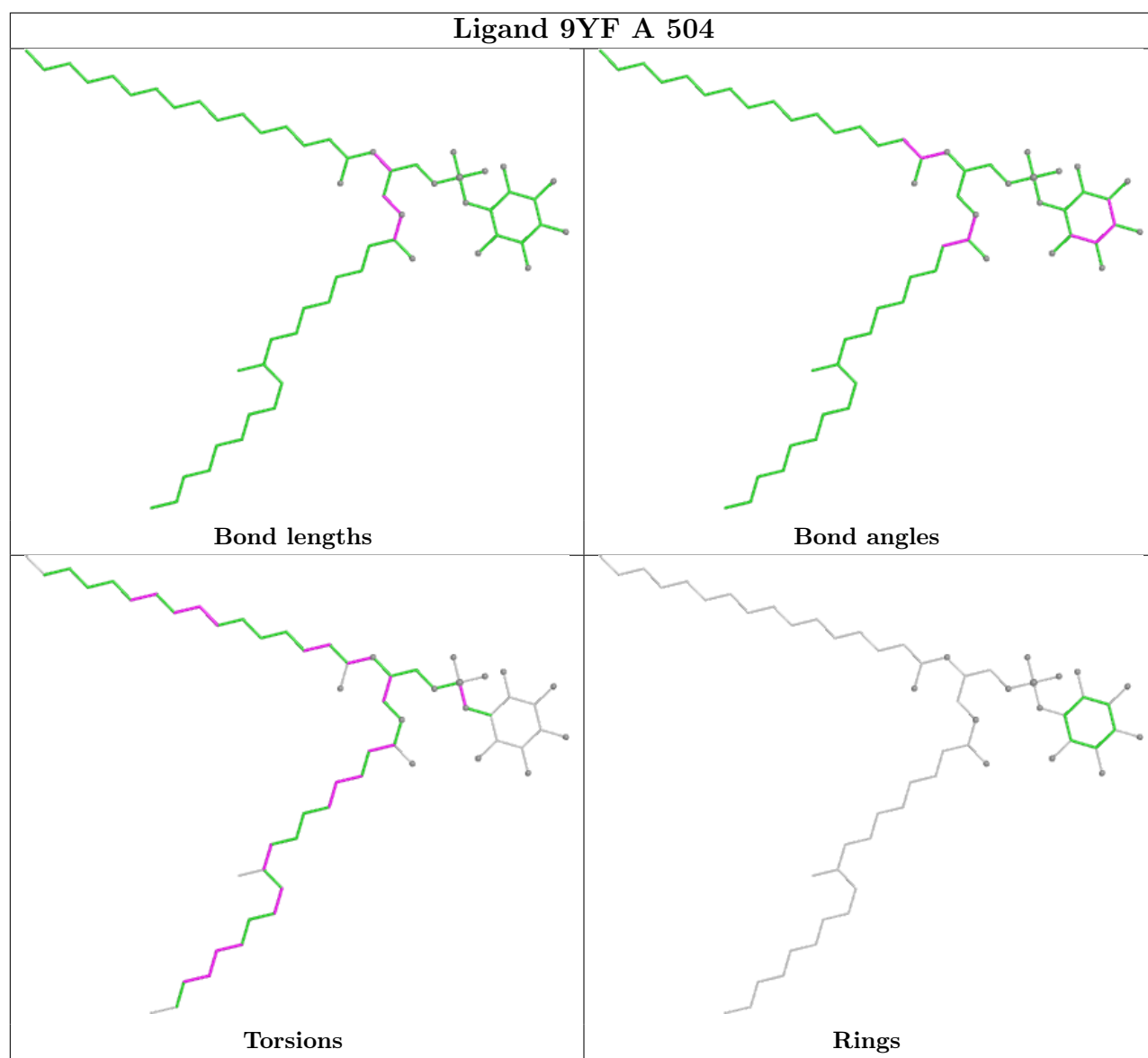


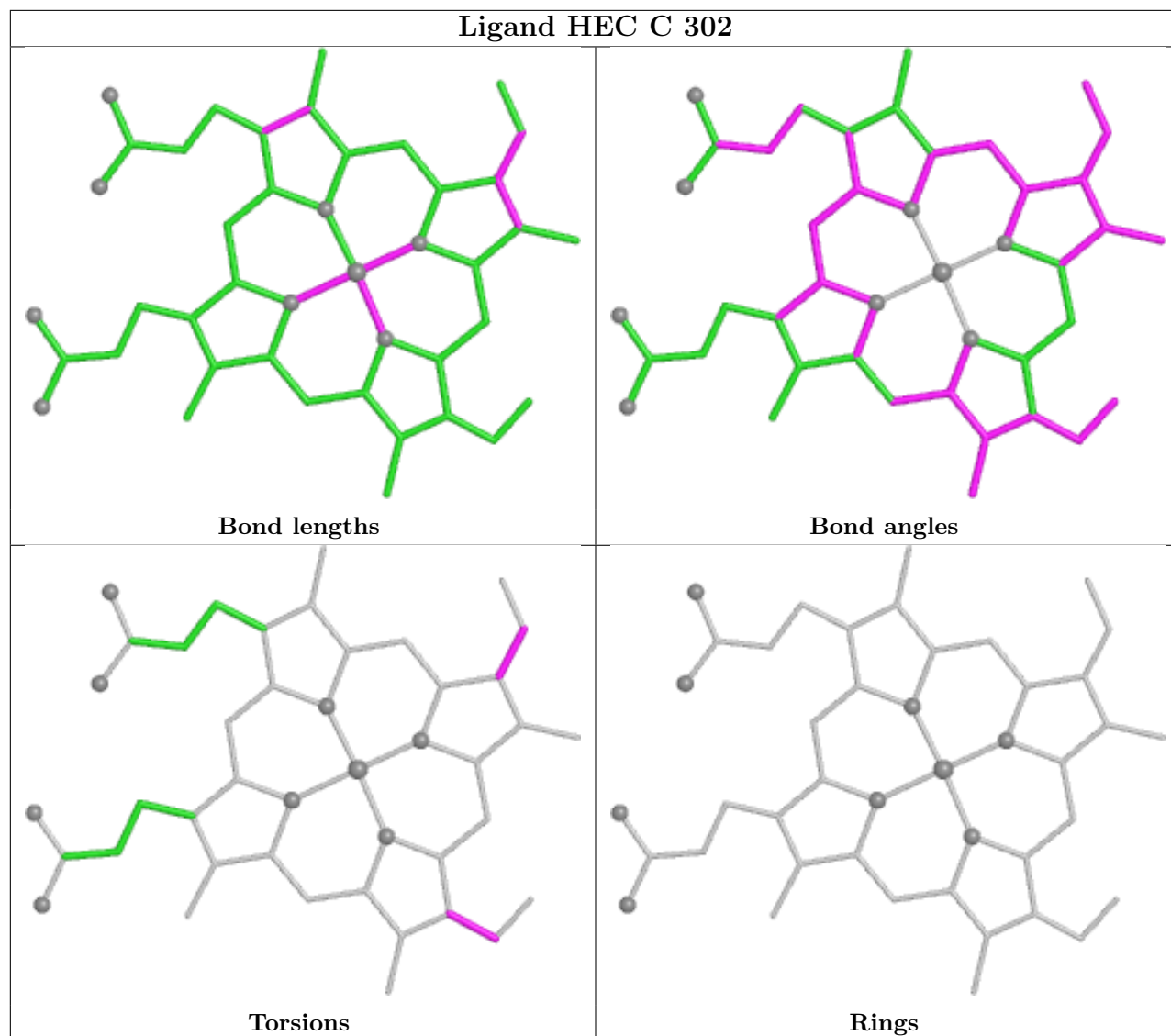


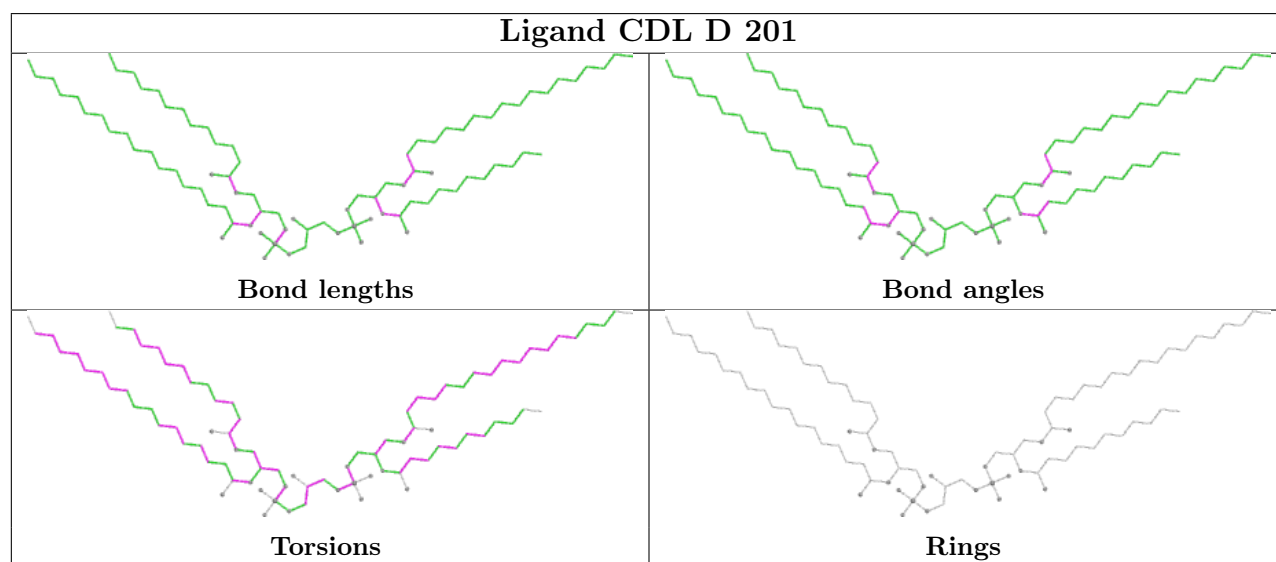
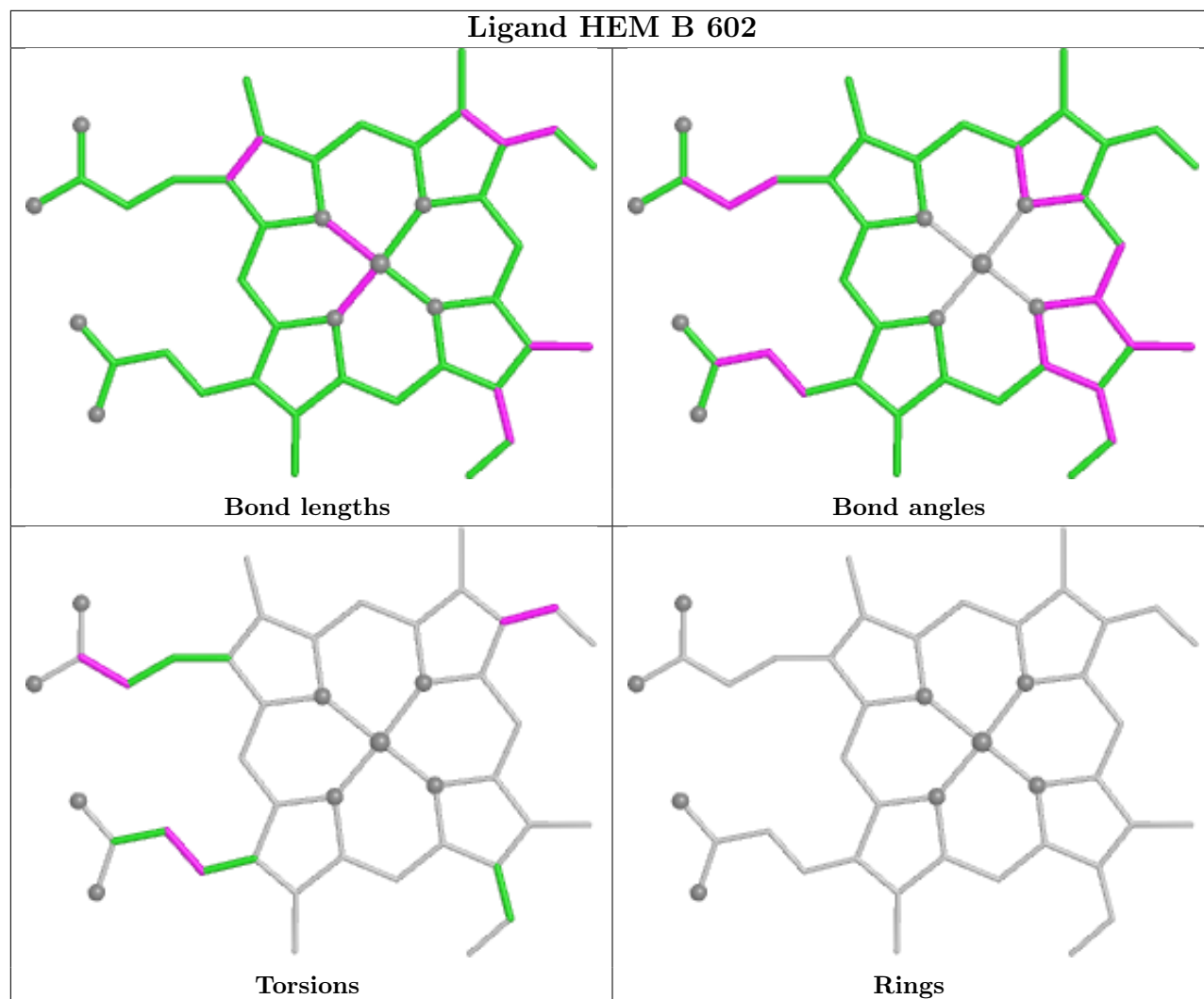


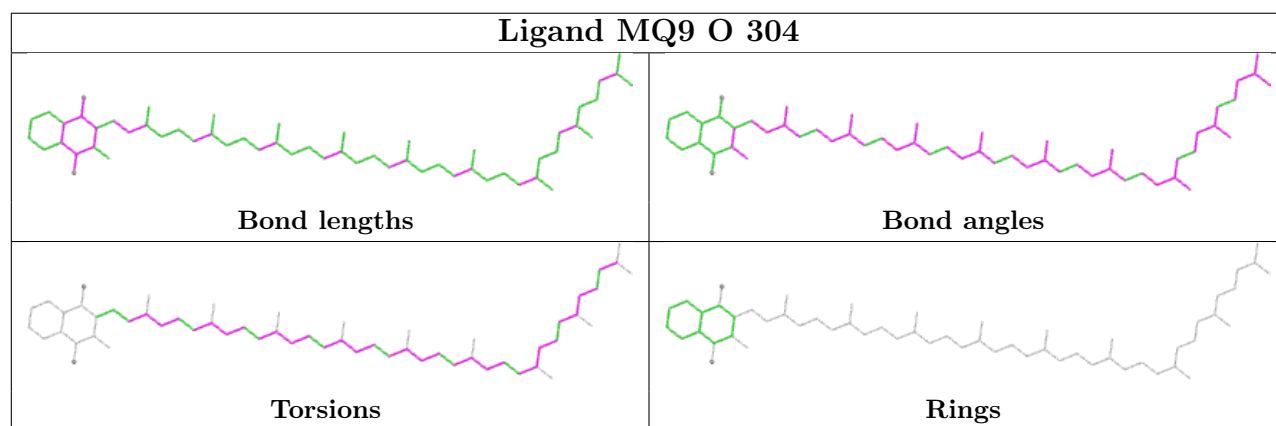
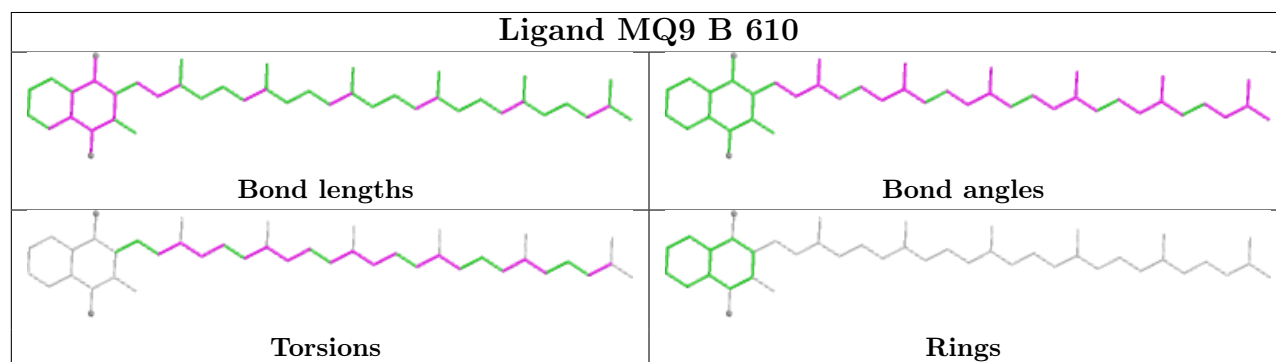
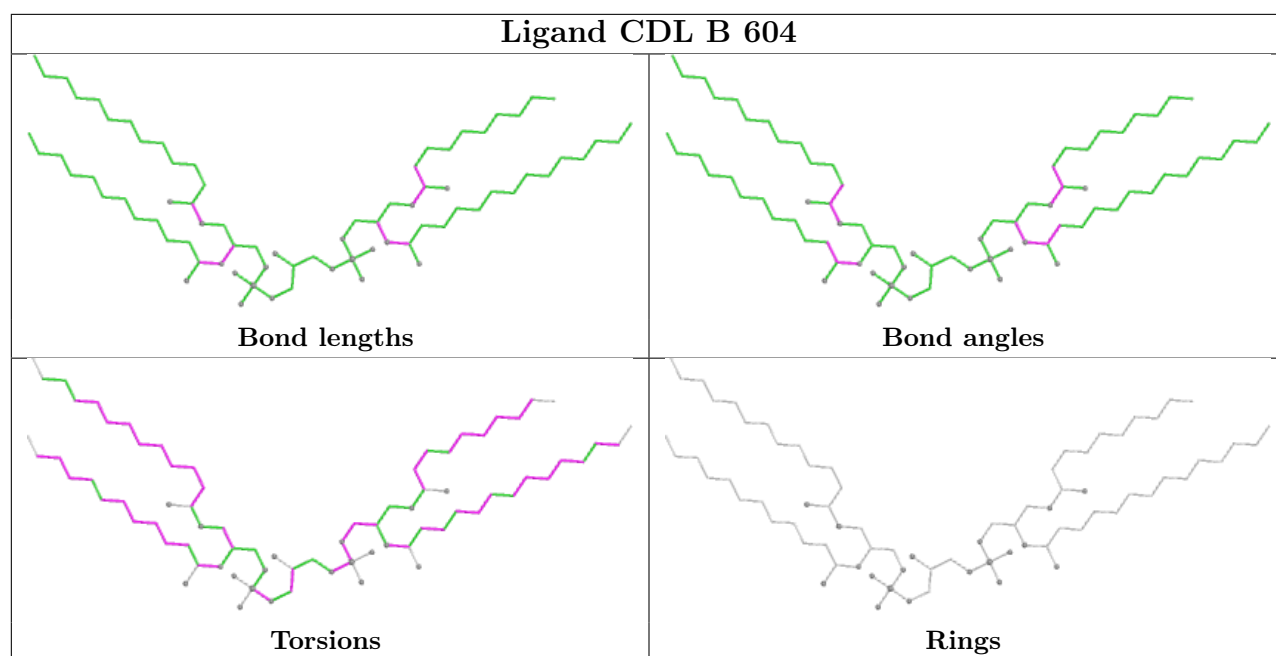


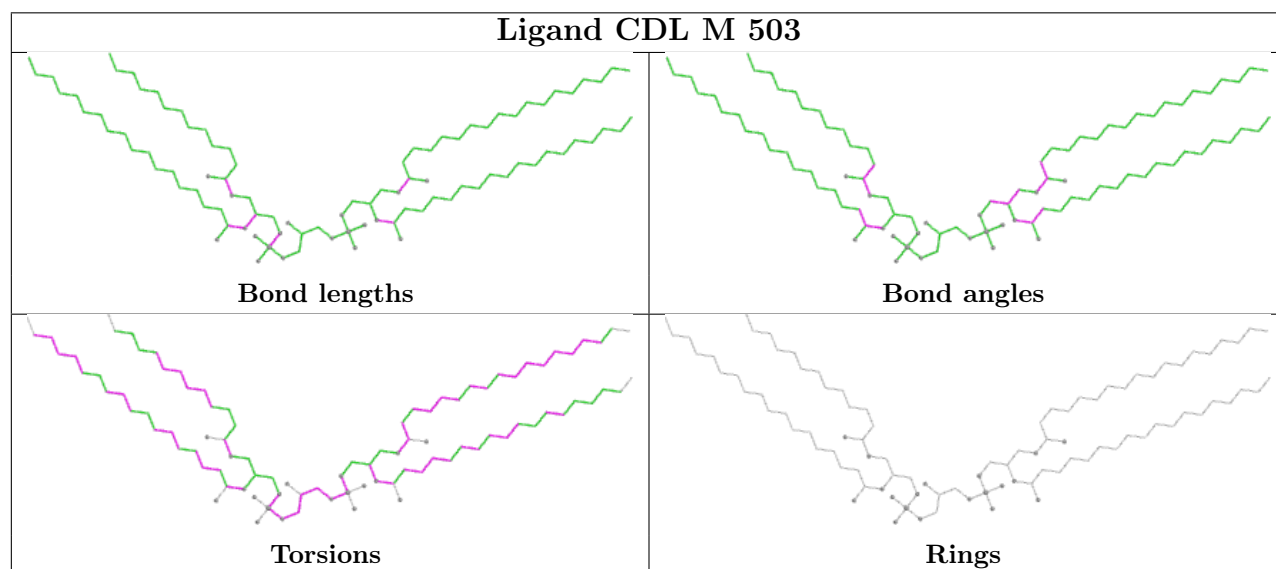
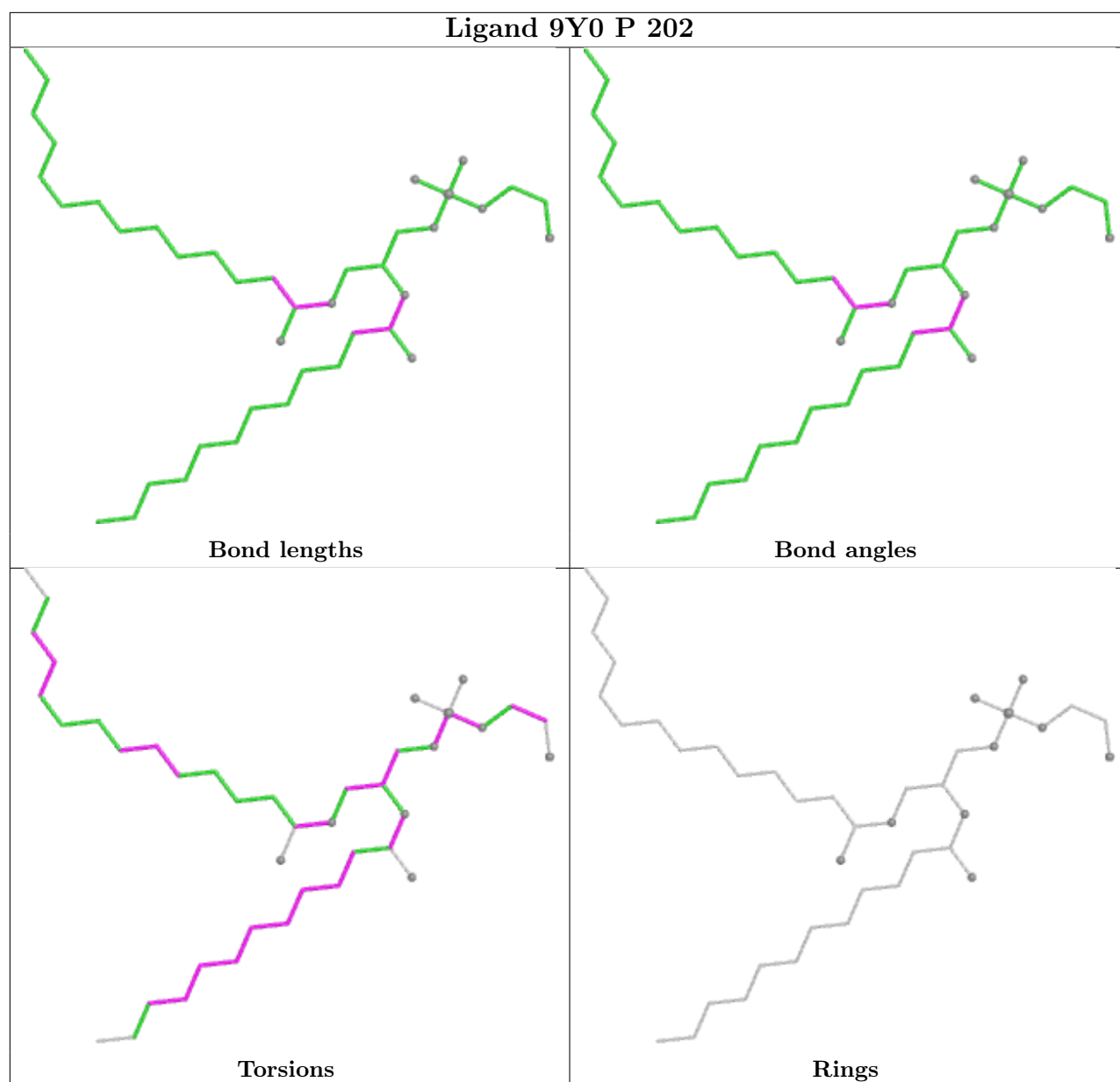


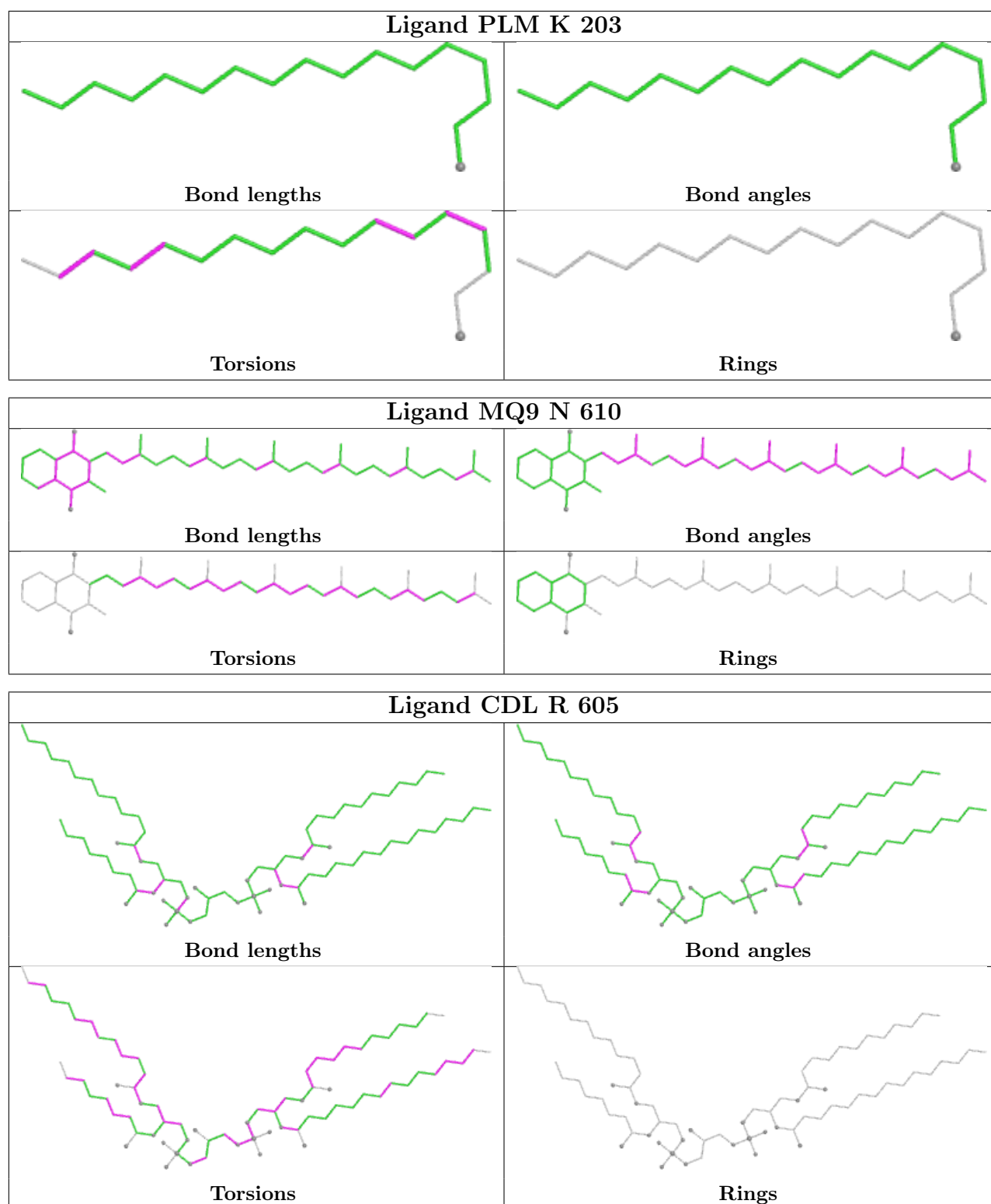


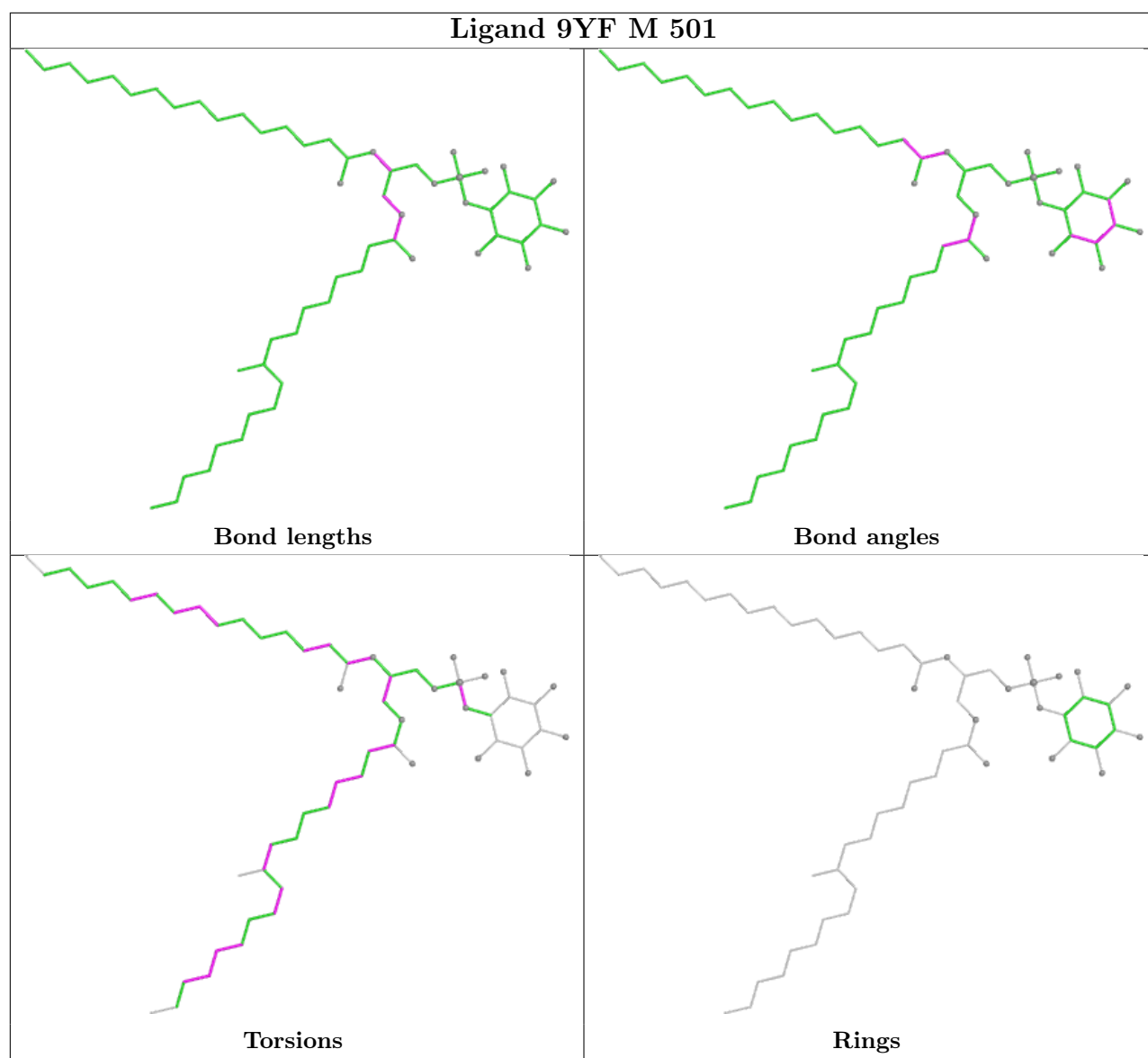


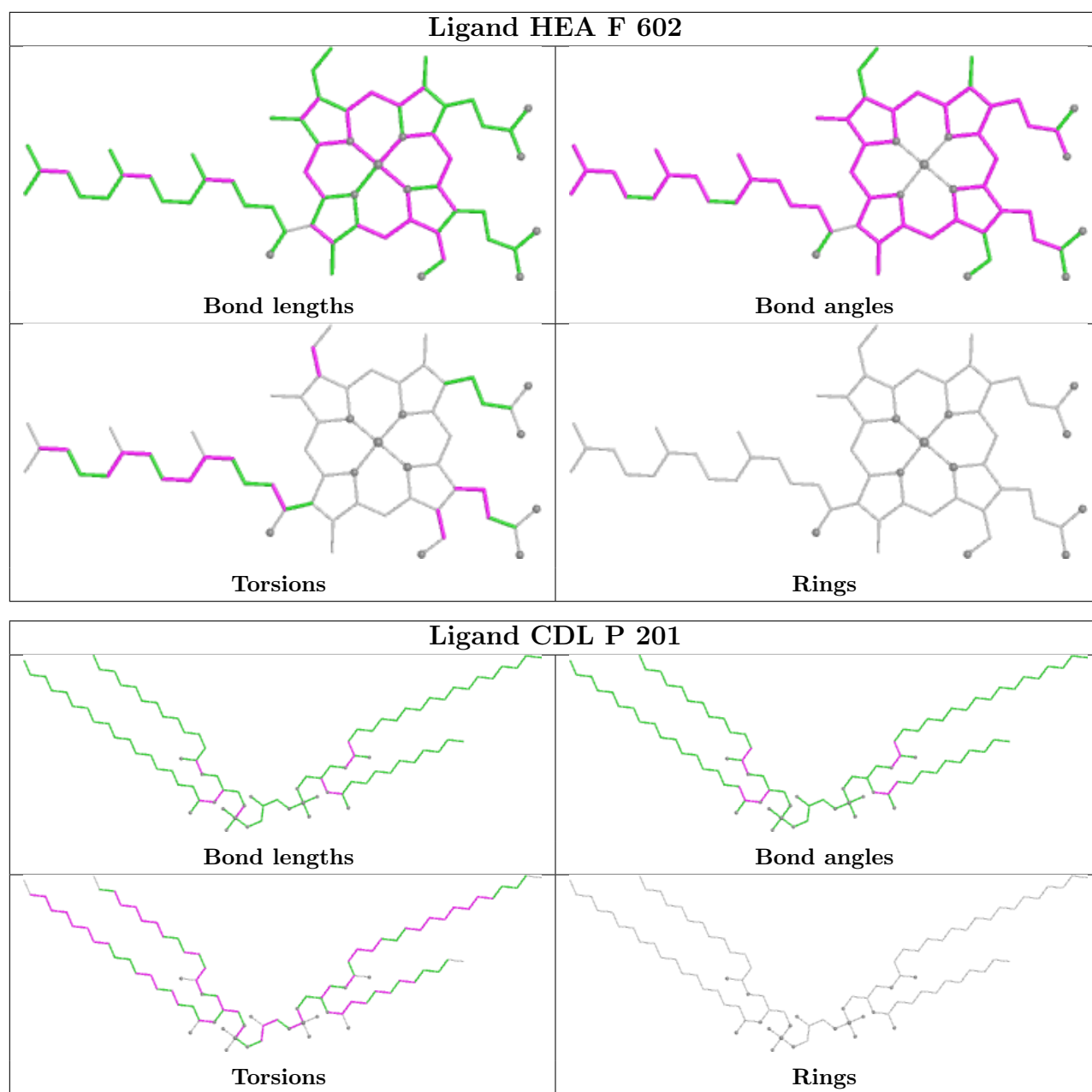


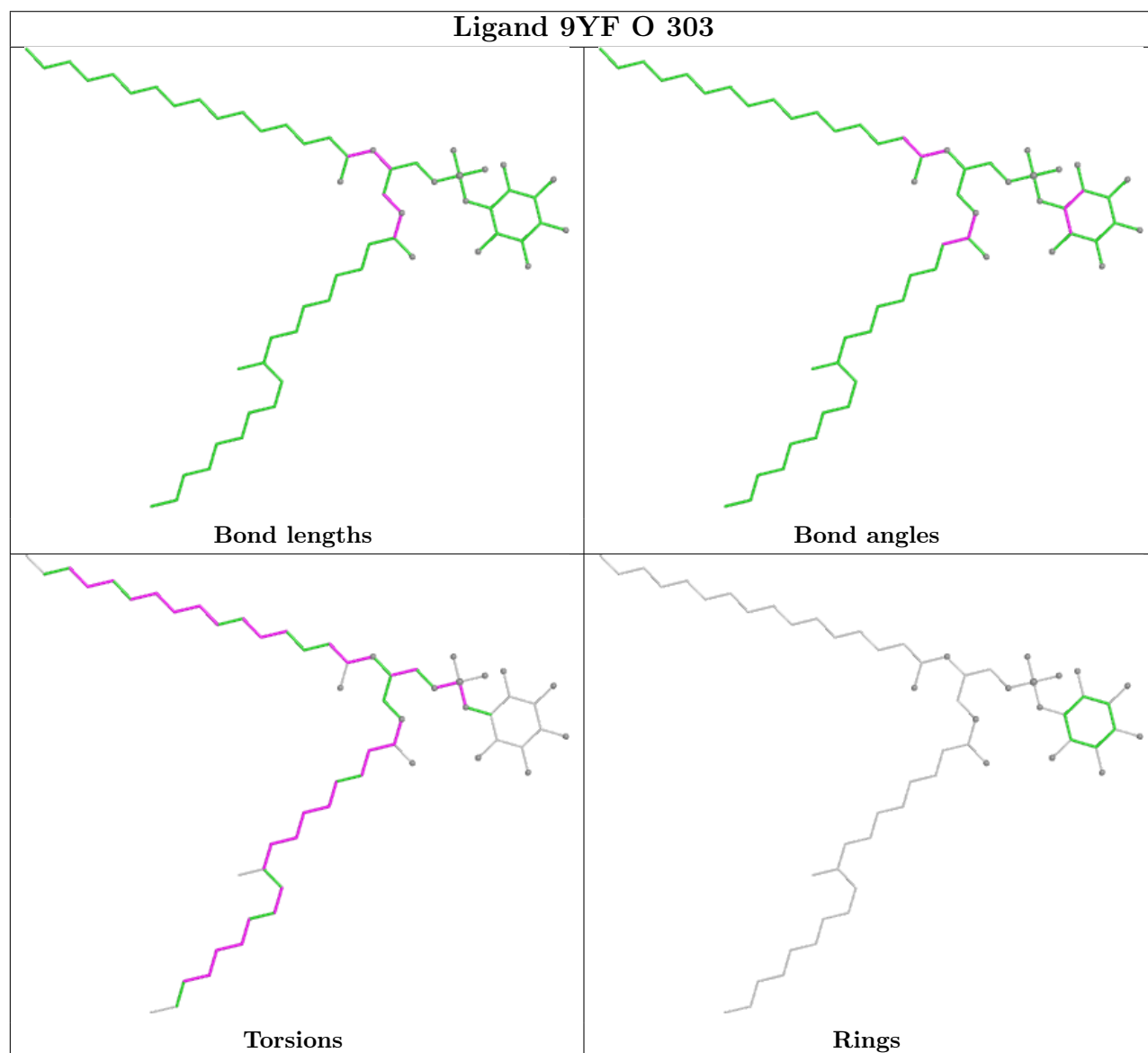
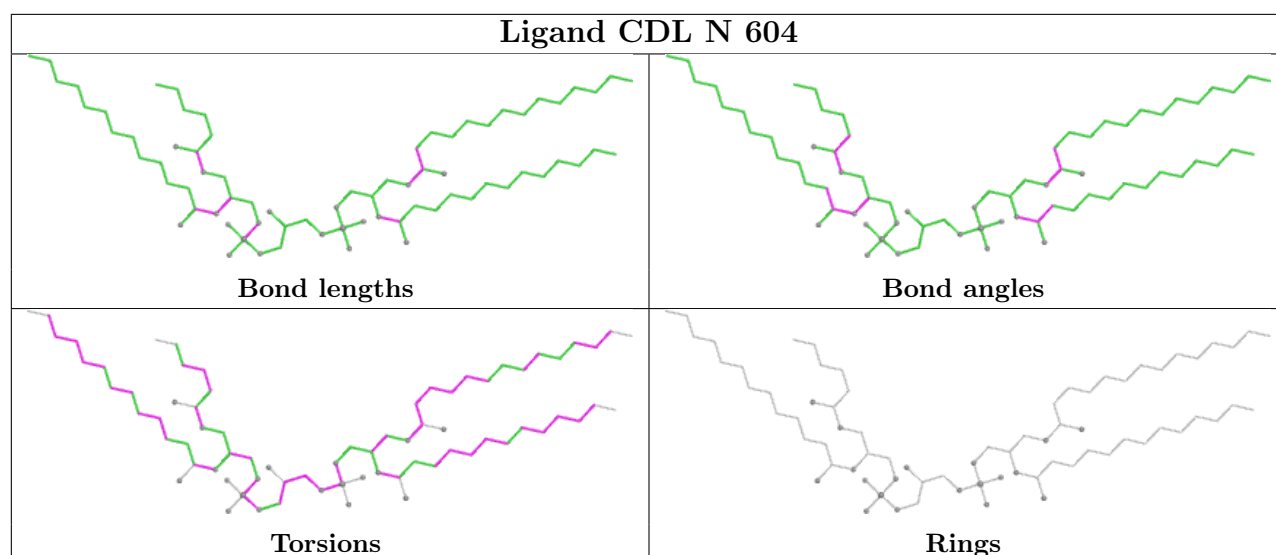


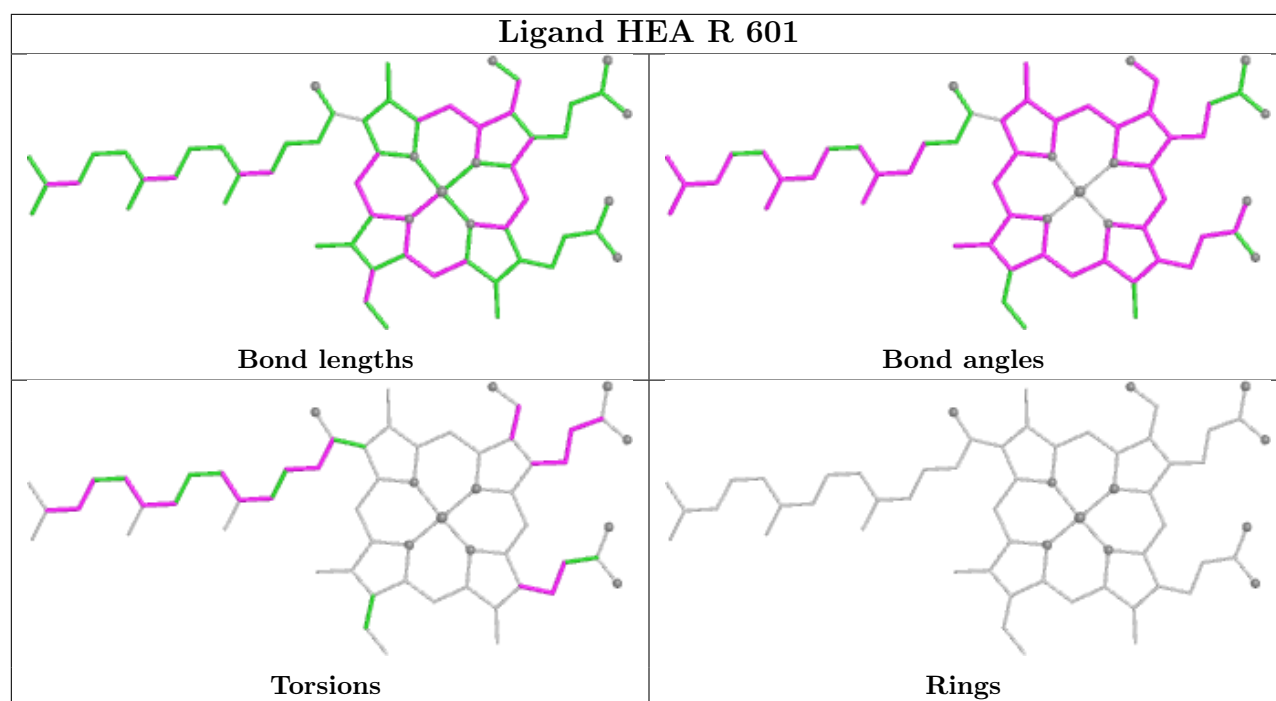


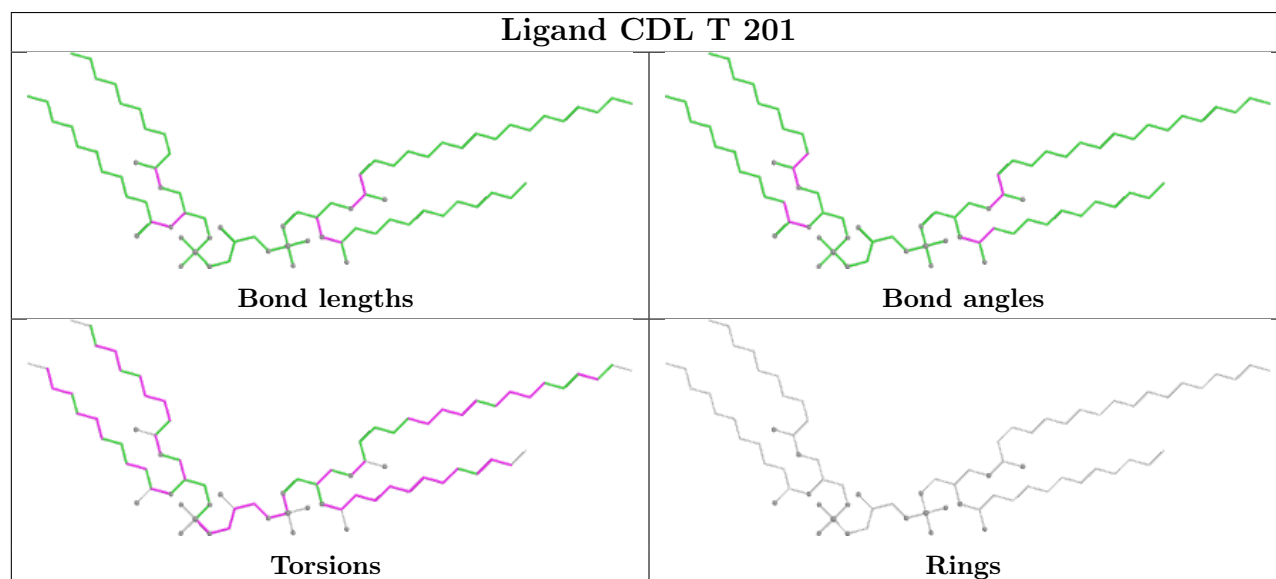
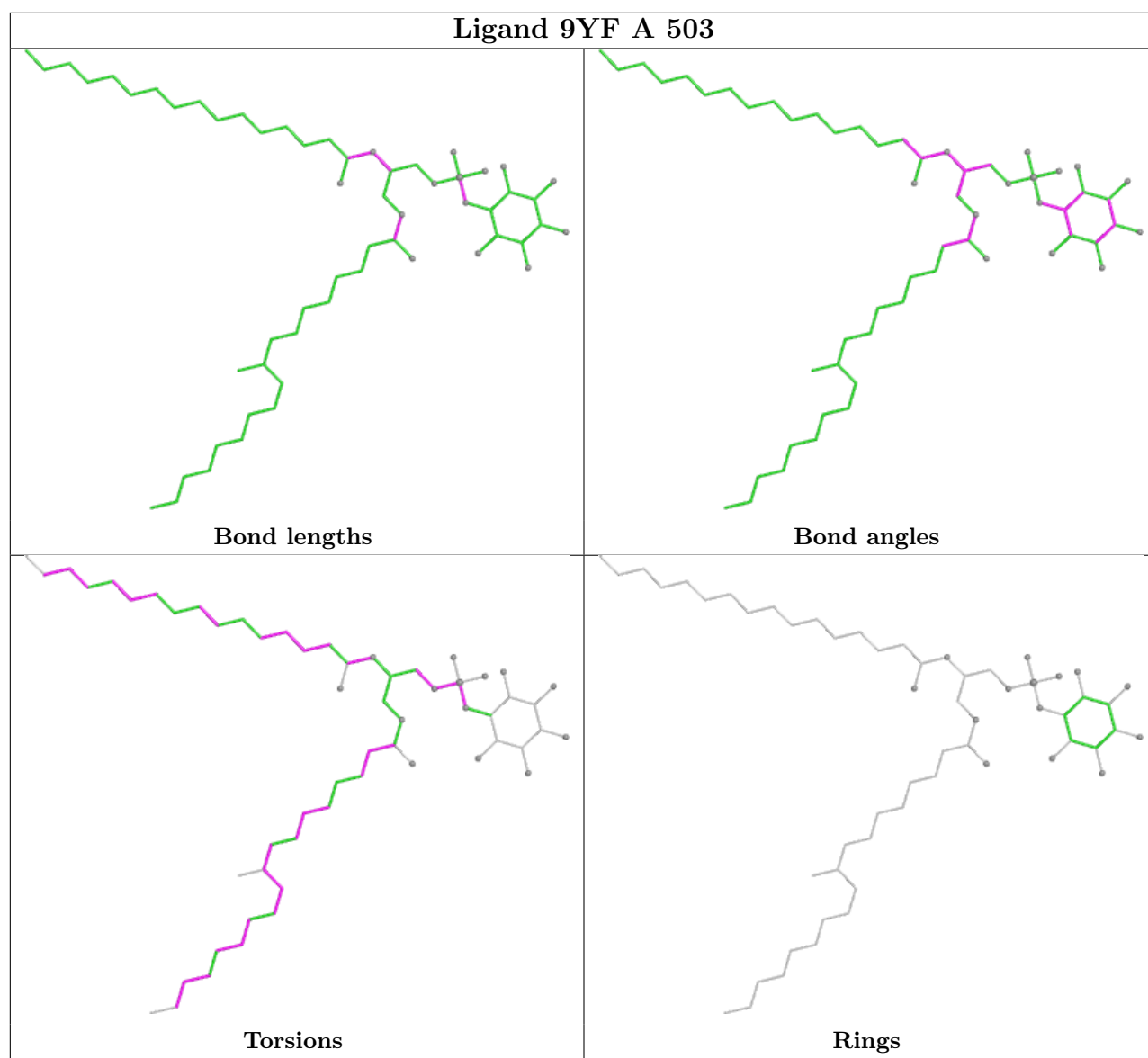




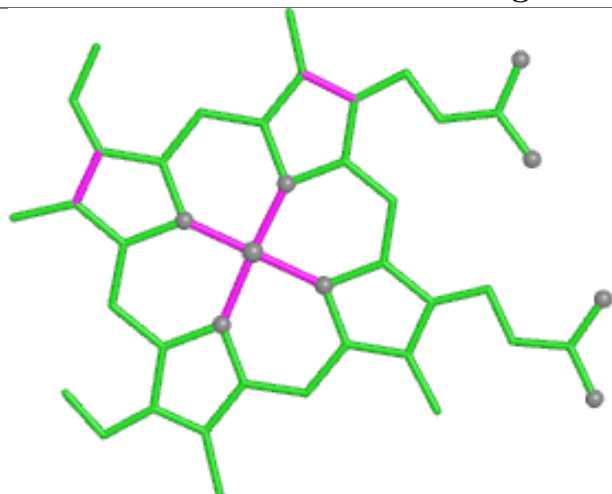




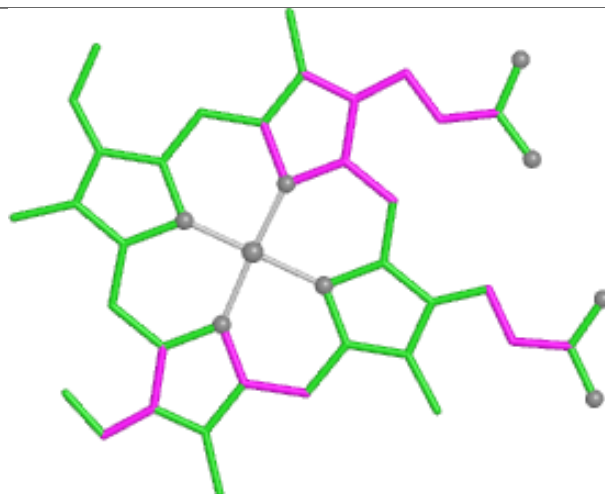




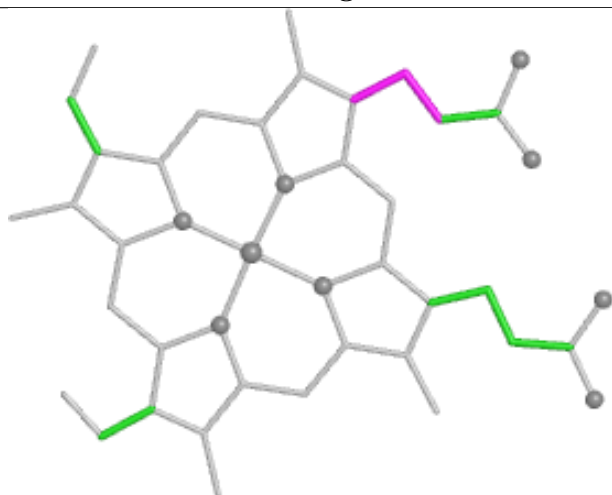
Ligand HEC C 301



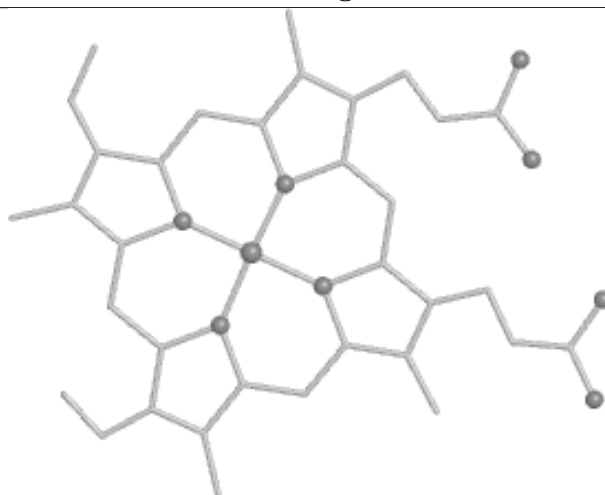
Bond lengths



Bond angles

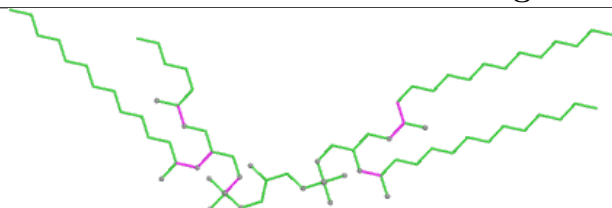


Torsions

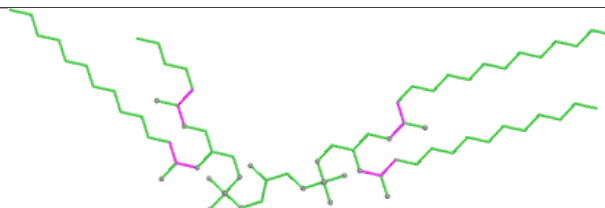


Rings

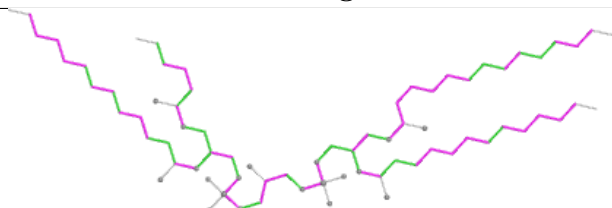
Ligand CDL B 603



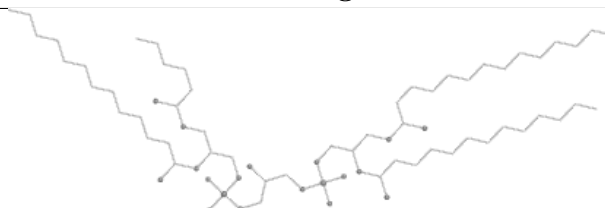
Bond lengths



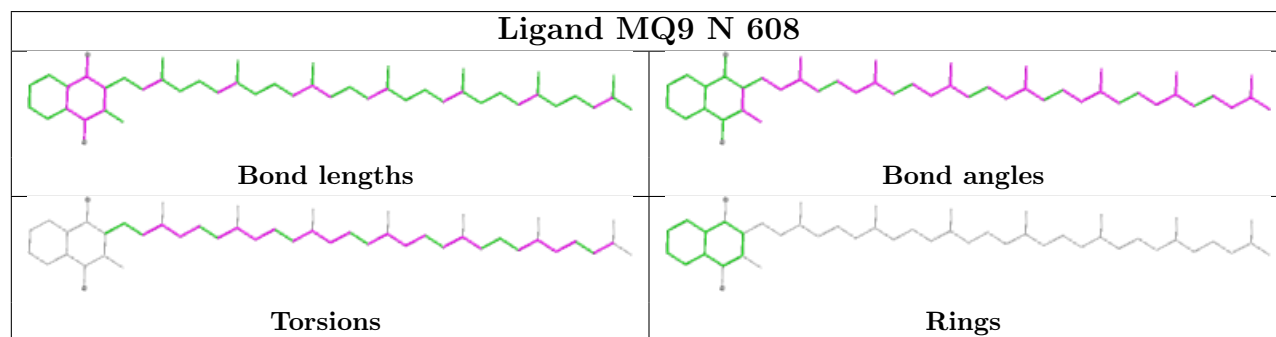
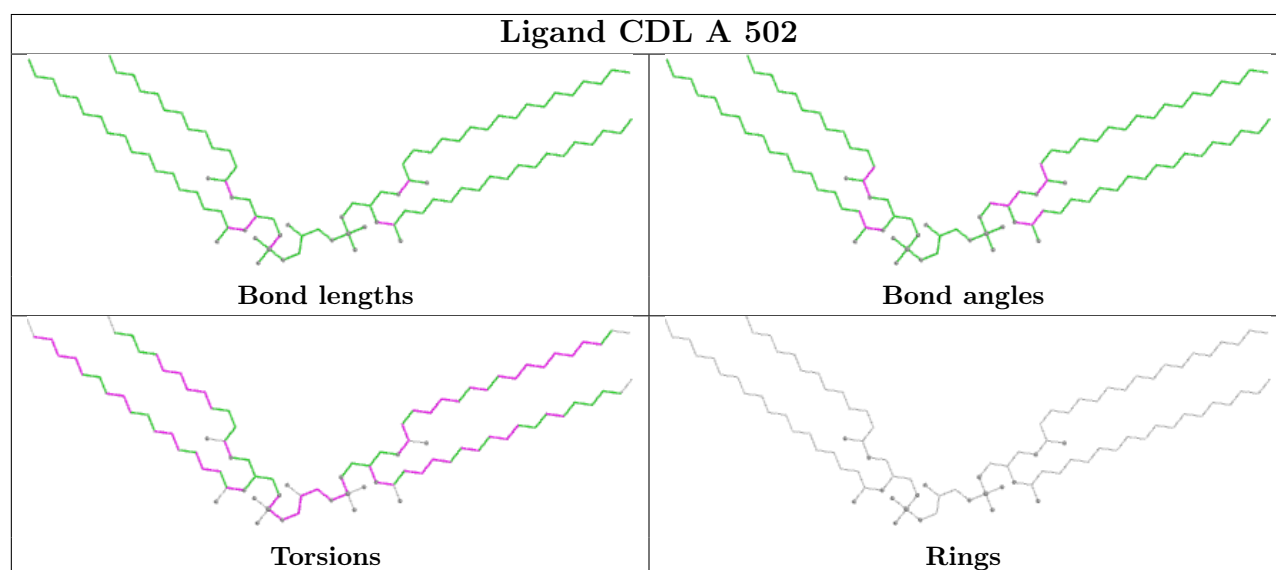
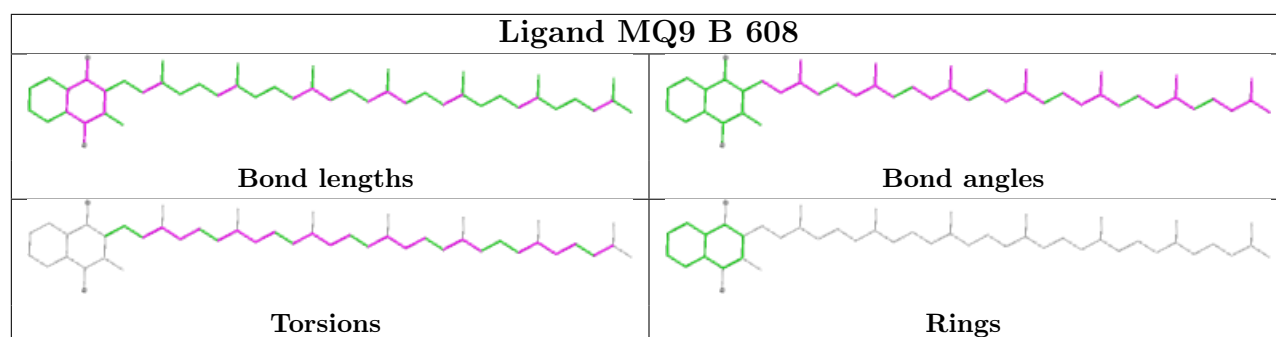
Bond angles

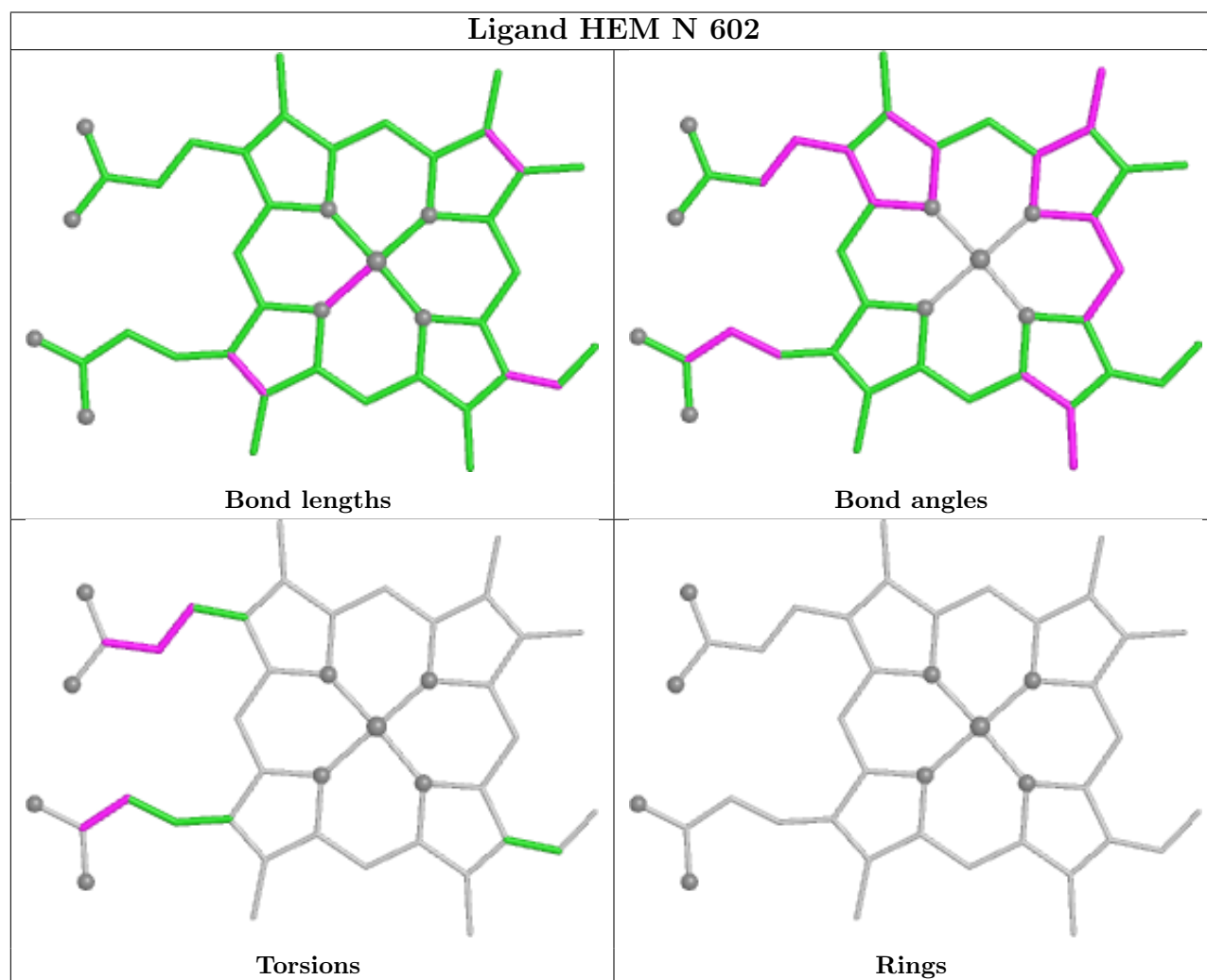
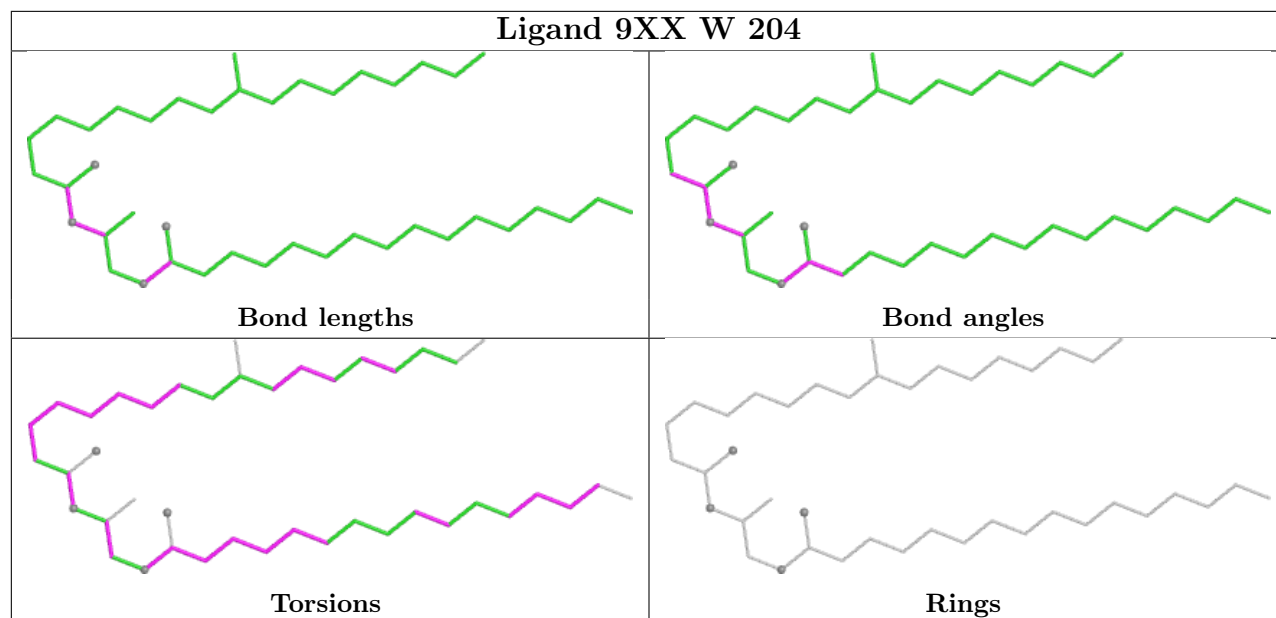


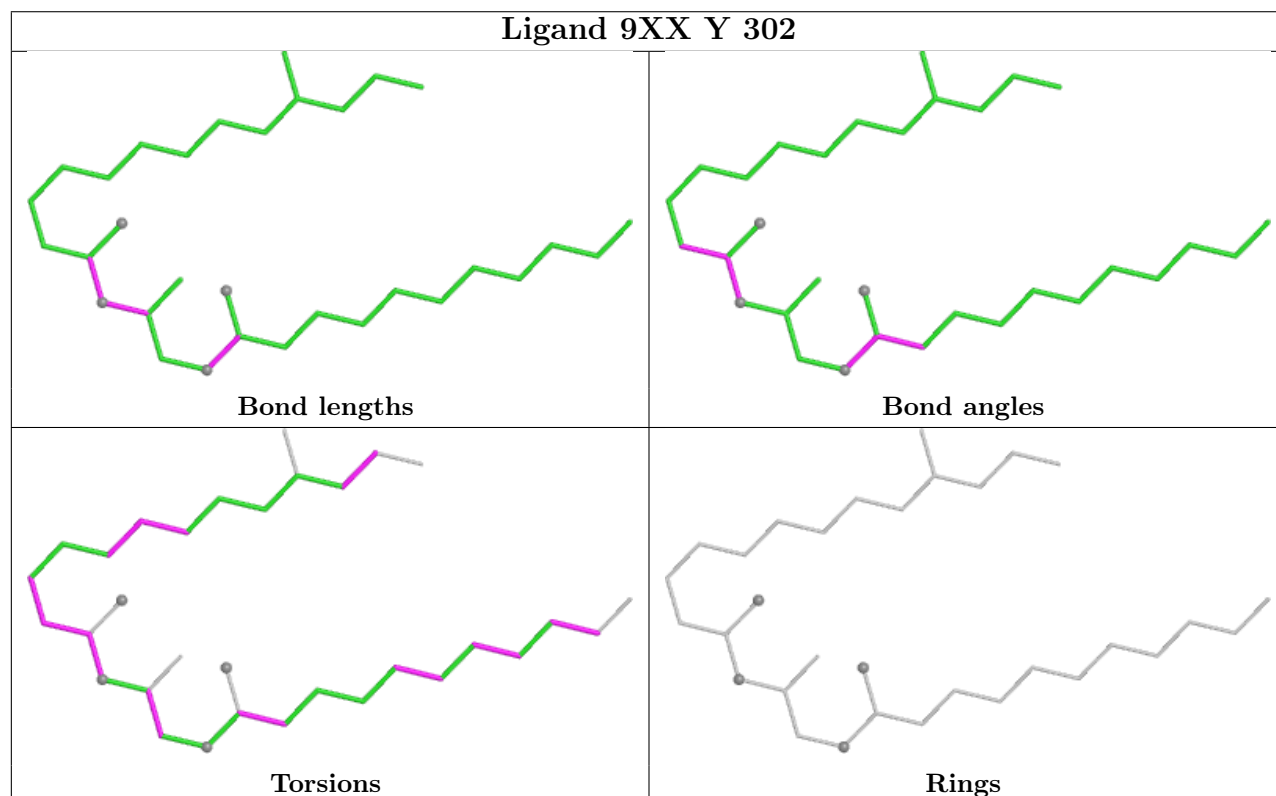
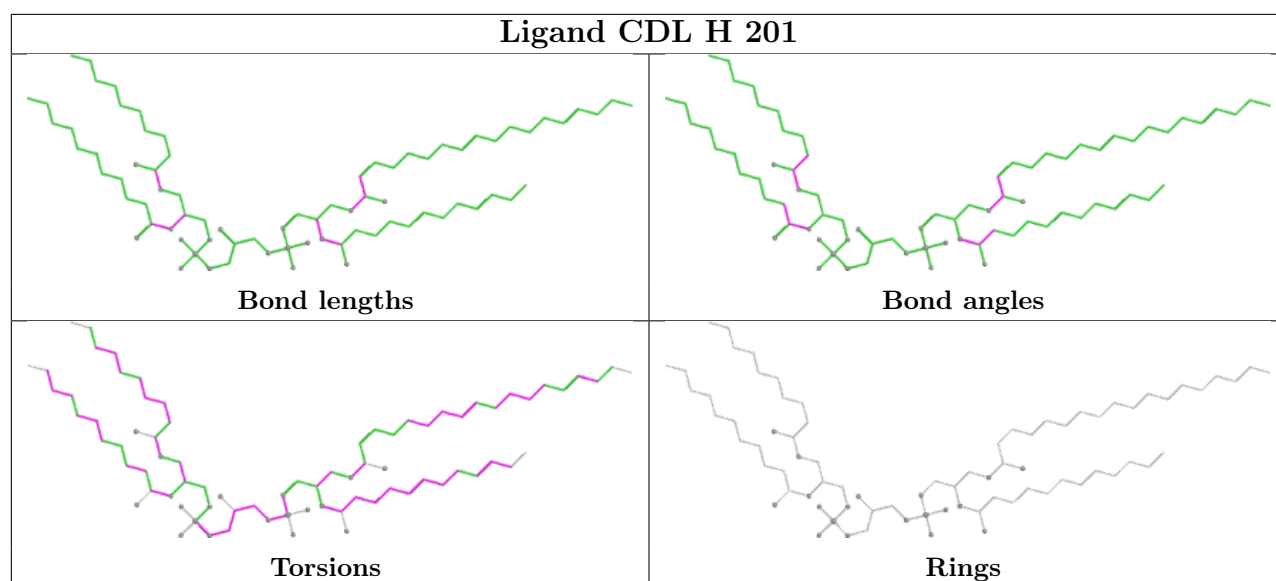
Torsions

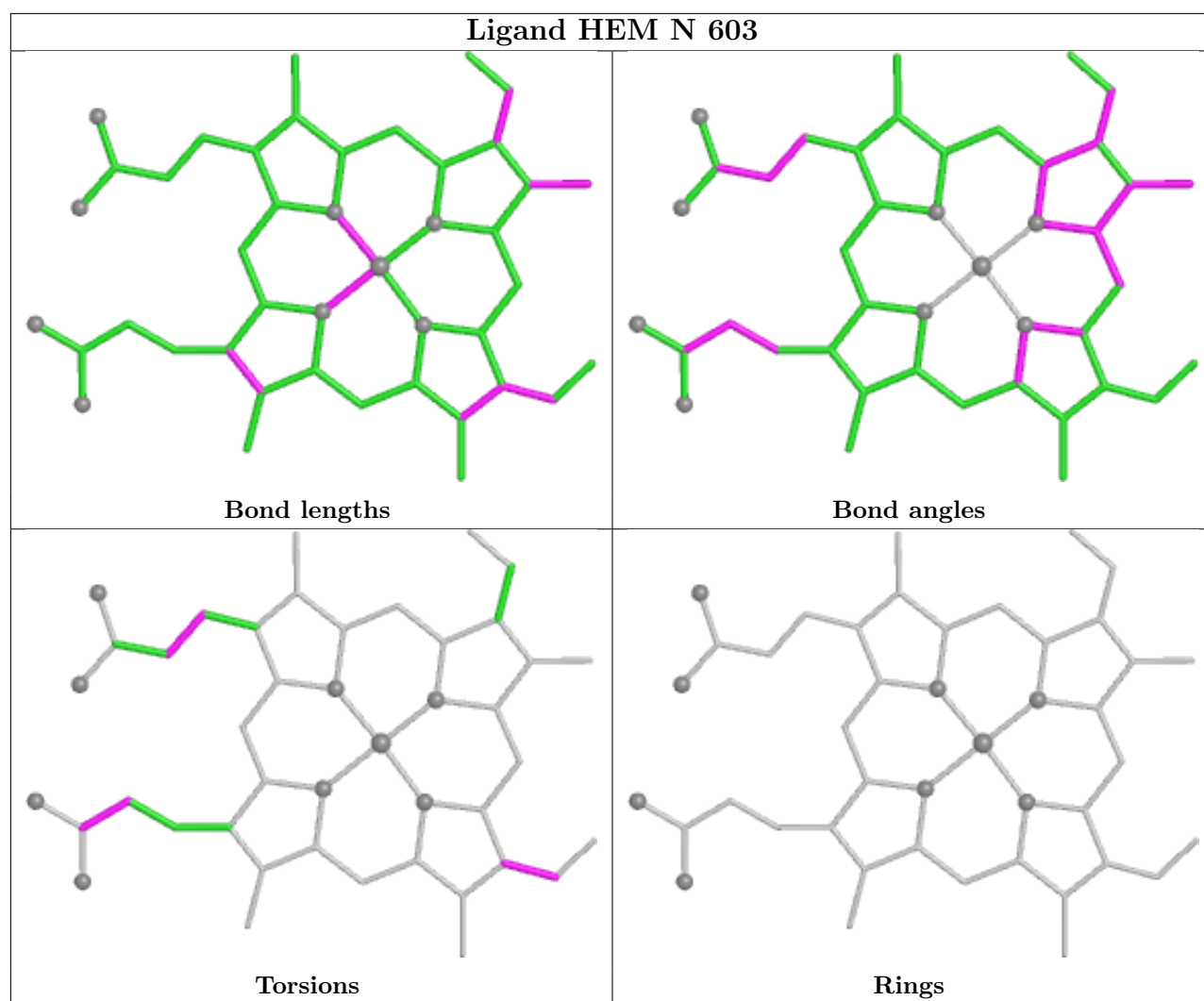
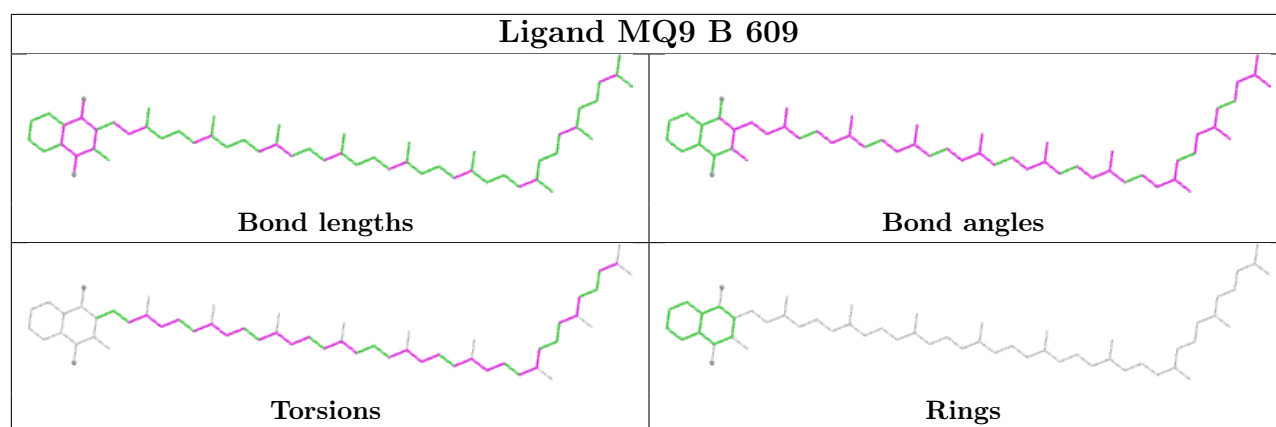


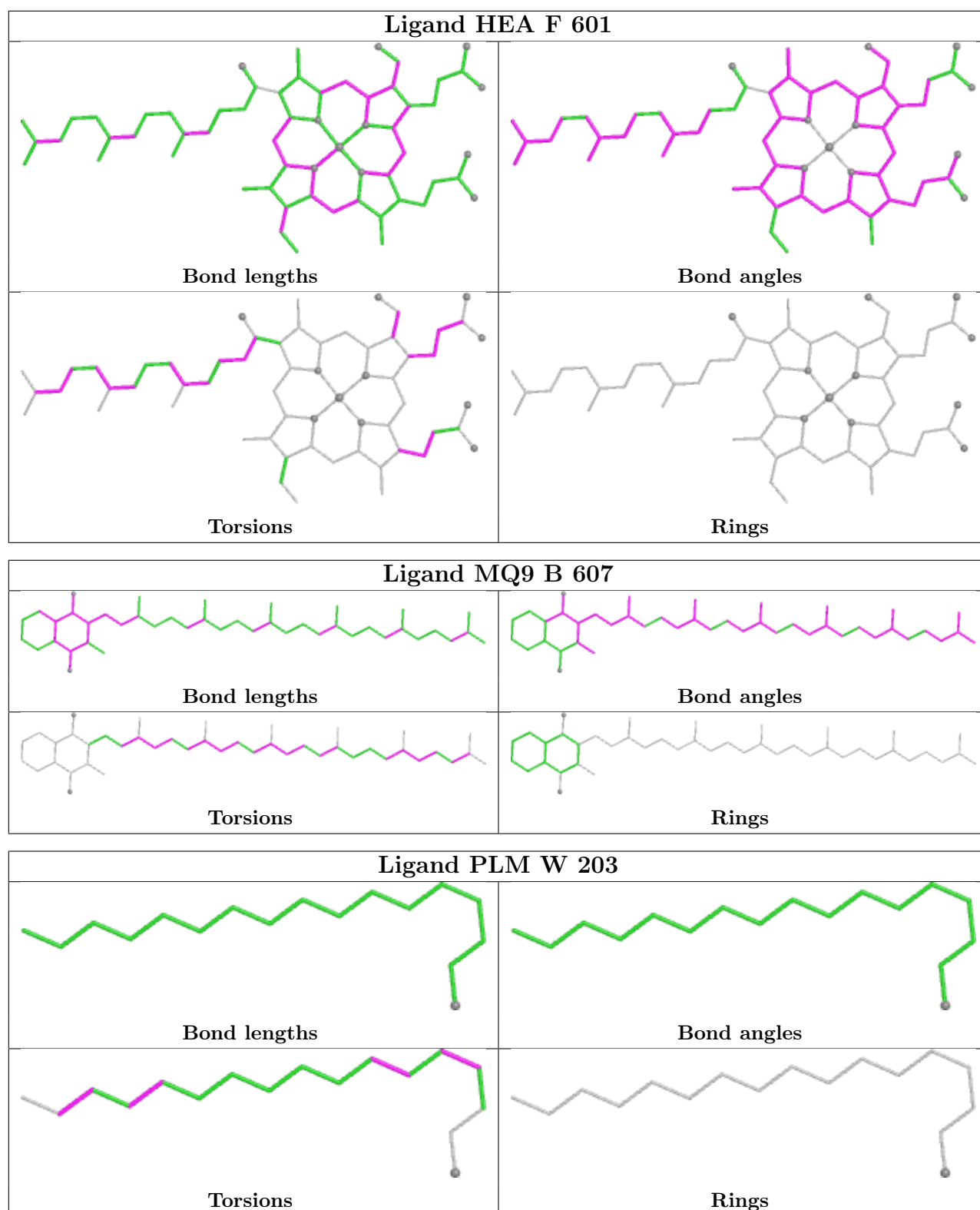
Rings











5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

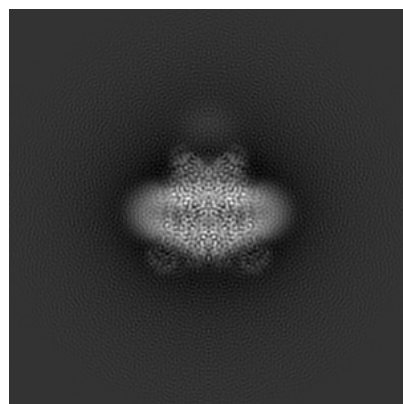
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9610. These allow visual inspection of the internal detail of the map and identification of artifacts.

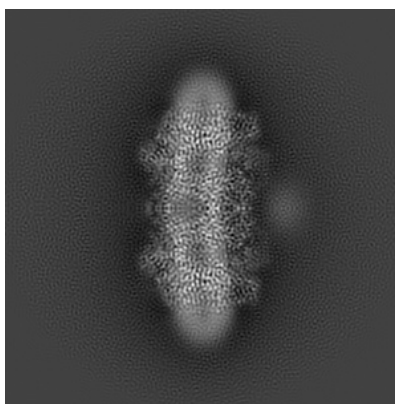
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

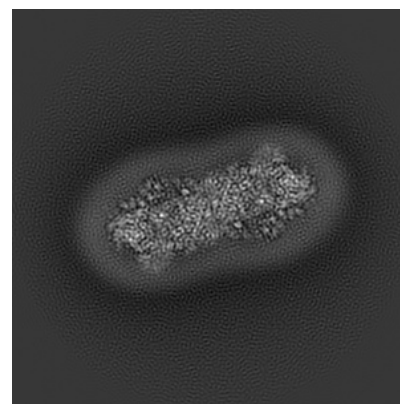
6.1.1 Primary map



X

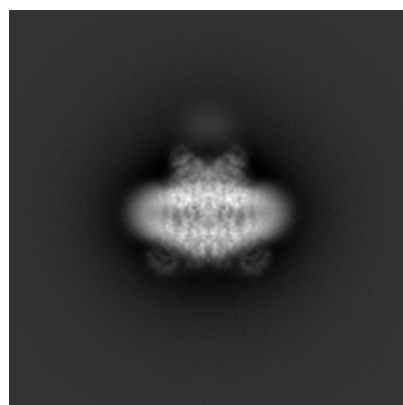


Y

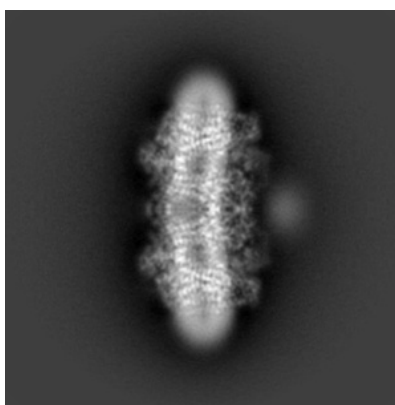


Z

6.1.2 Raw map



X



Y

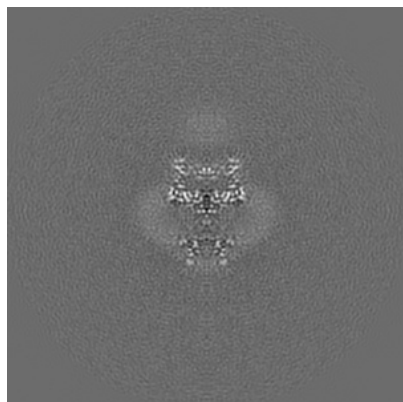


Z

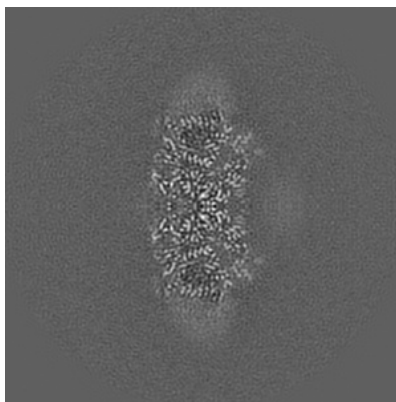
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

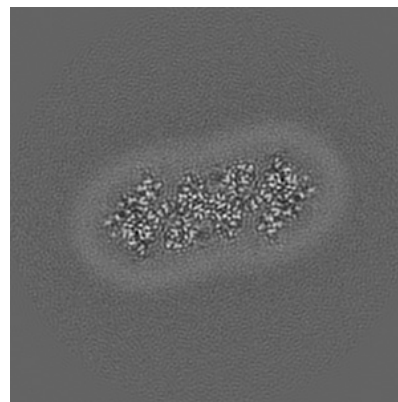
6.2.1 Primary map



X Index: 146

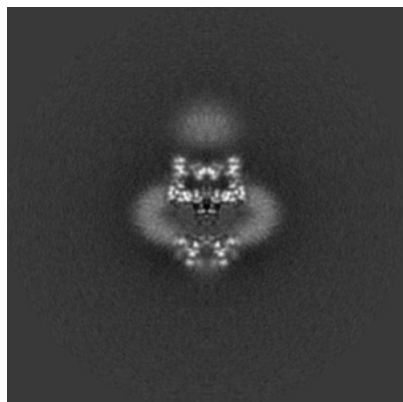


Y Index: 146

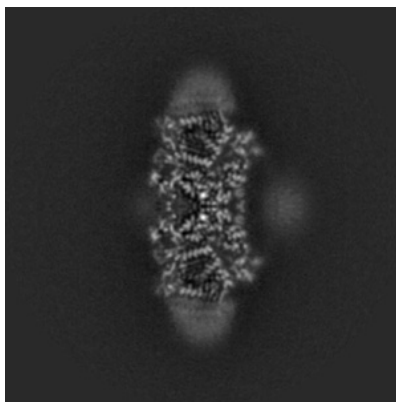


Z Index: 146

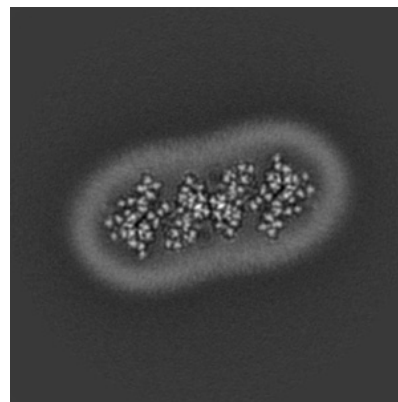
6.2.2 Raw map



X Index: 146



Y Index: 146

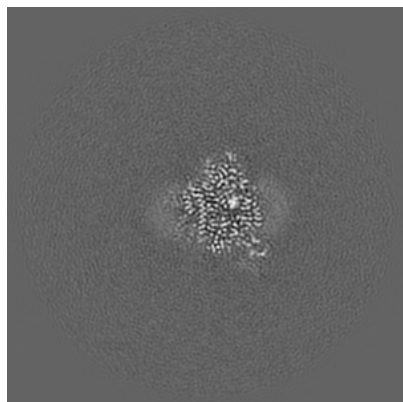


Z Index: 146

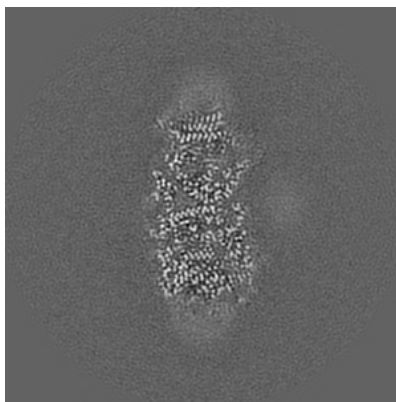
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

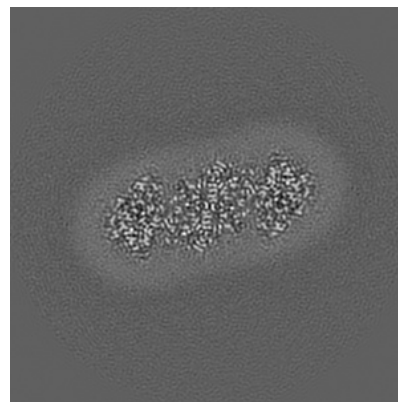
6.3.1 Primary map



X Index: 197

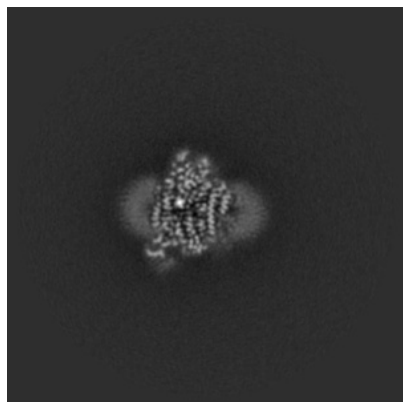


Y Index: 142

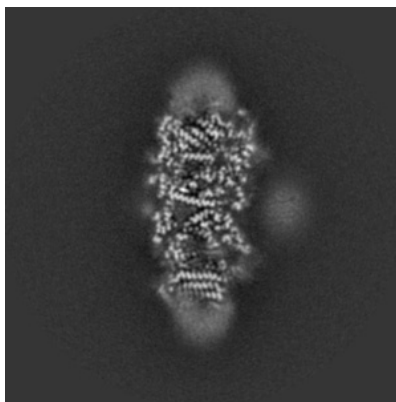


Z Index: 153

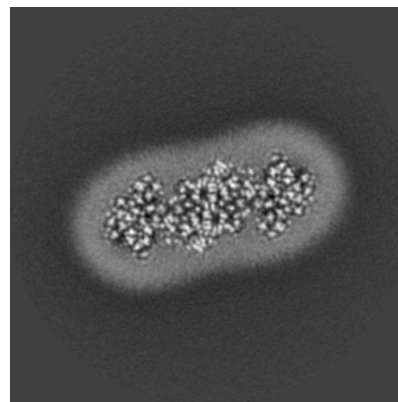
6.3.2 Raw map



X Index: 95



Y Index: 150

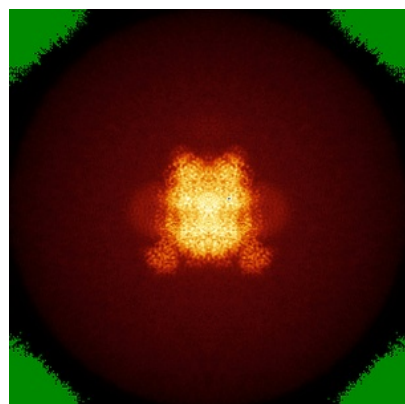


Z Index: 153

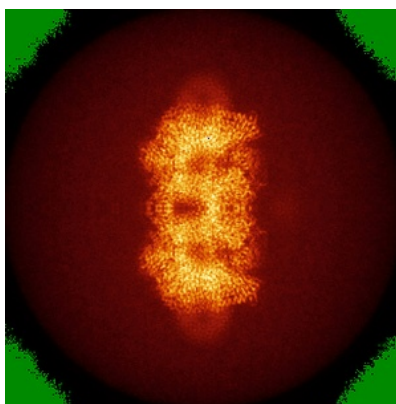
The images above show the largest variance slices of the map in three orthogonal directions.

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

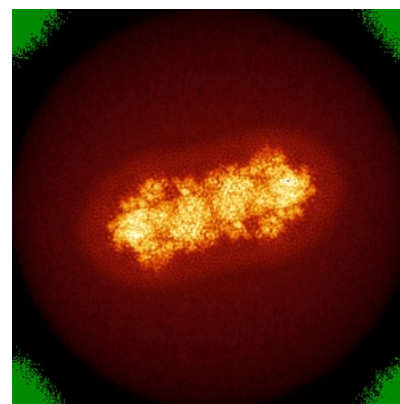
6.4.1 Primary map



X

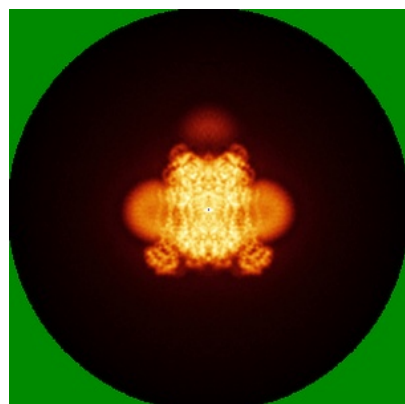


Y

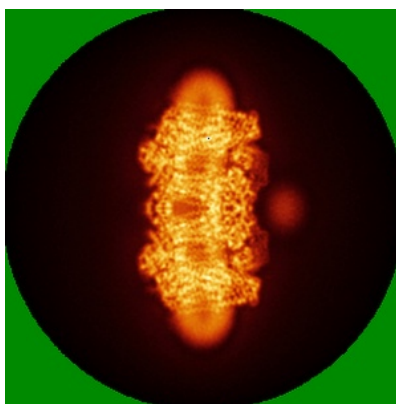


Z

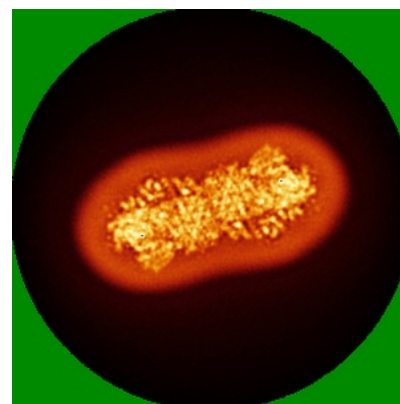
6.4.2 Raw map



X



Y

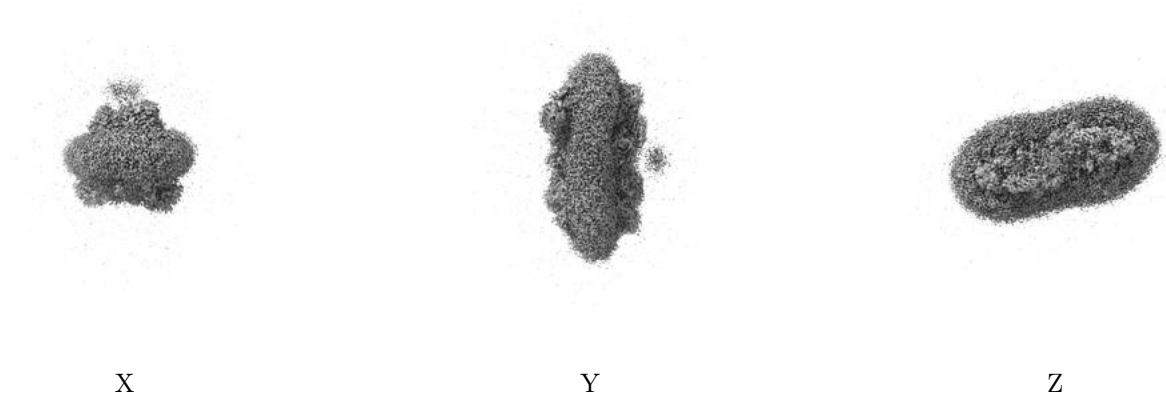


Z

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.

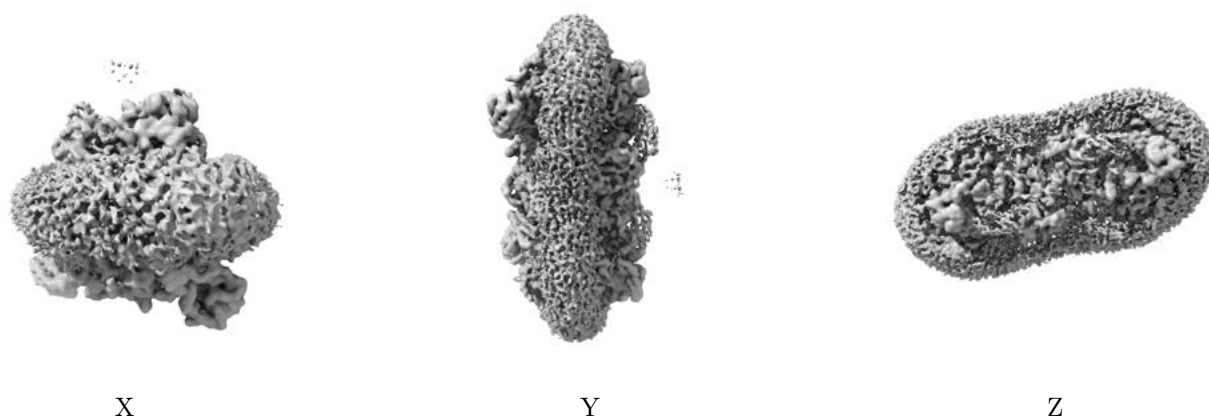
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0452. 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.

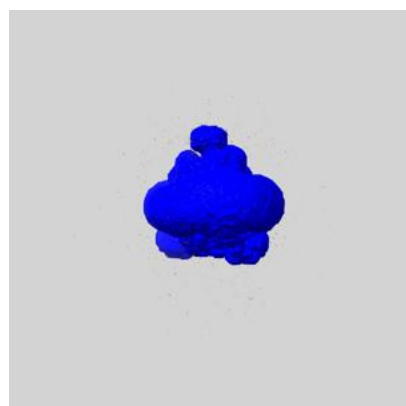
6.6 Mask visualisation [i](#)

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

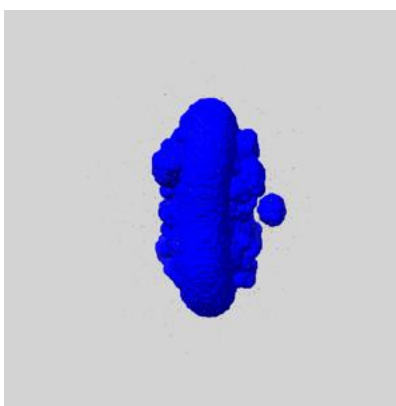
A mask typically either:

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

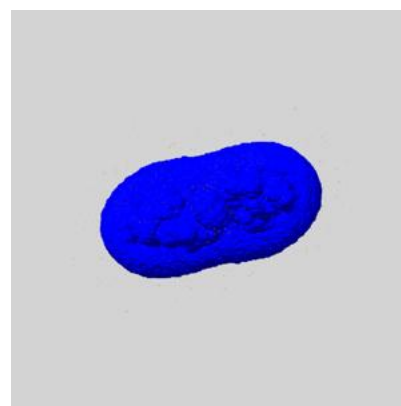
6.6.1 emd_9610_msk_1.map [i](#)



X



Y

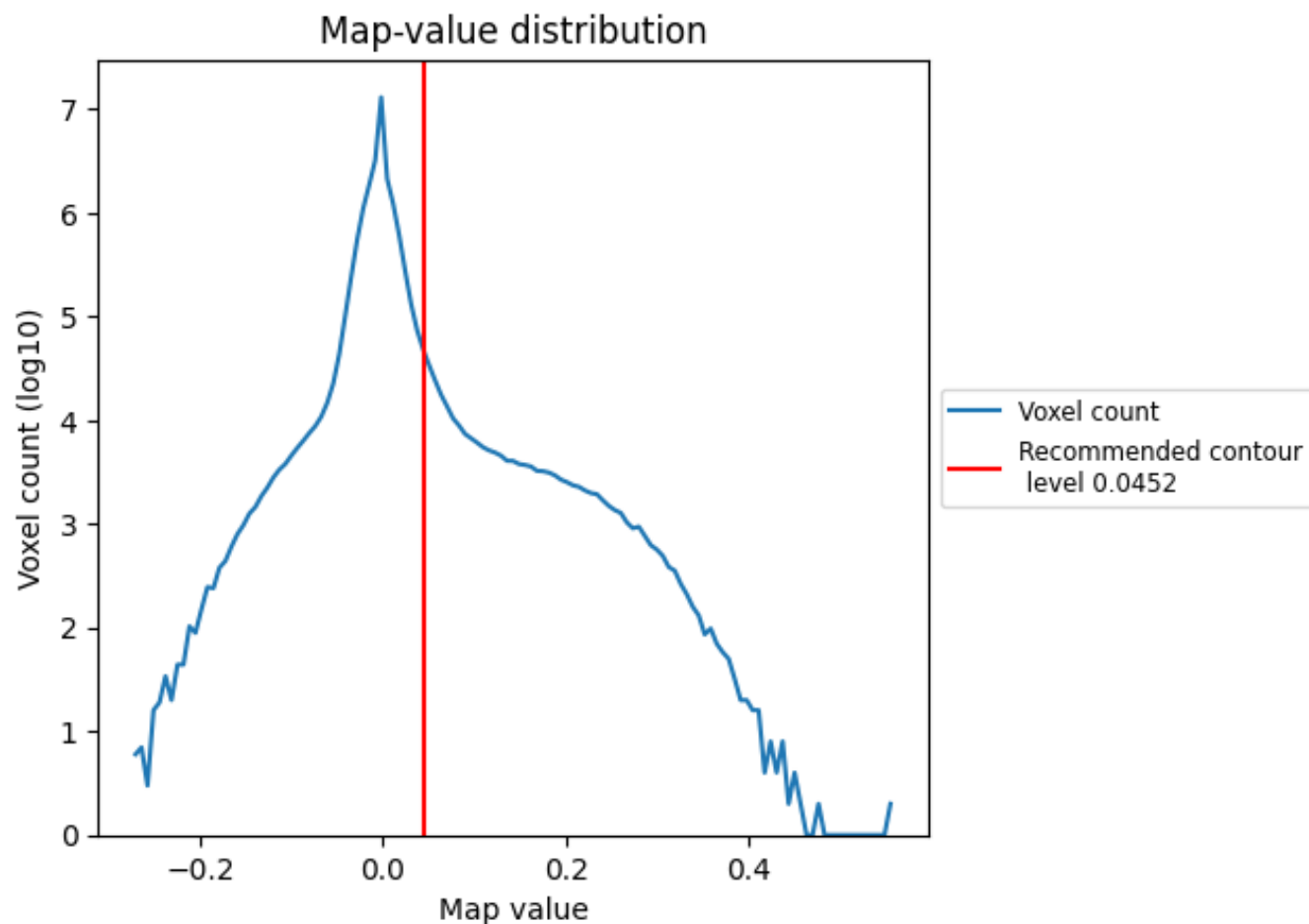


Z

7 Map analysis [i](#)

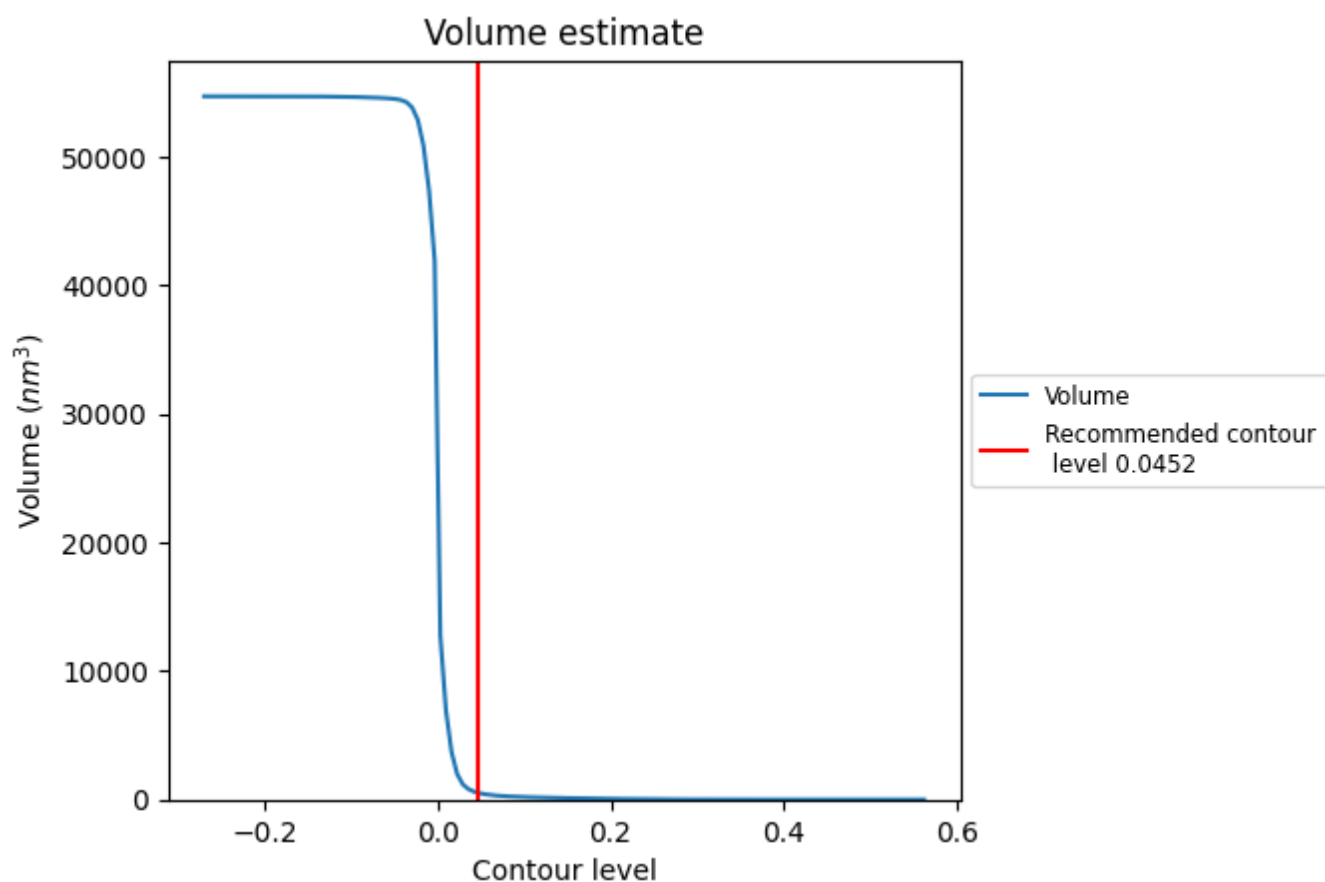
This section contains the results of statistical analysis of the map.

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.

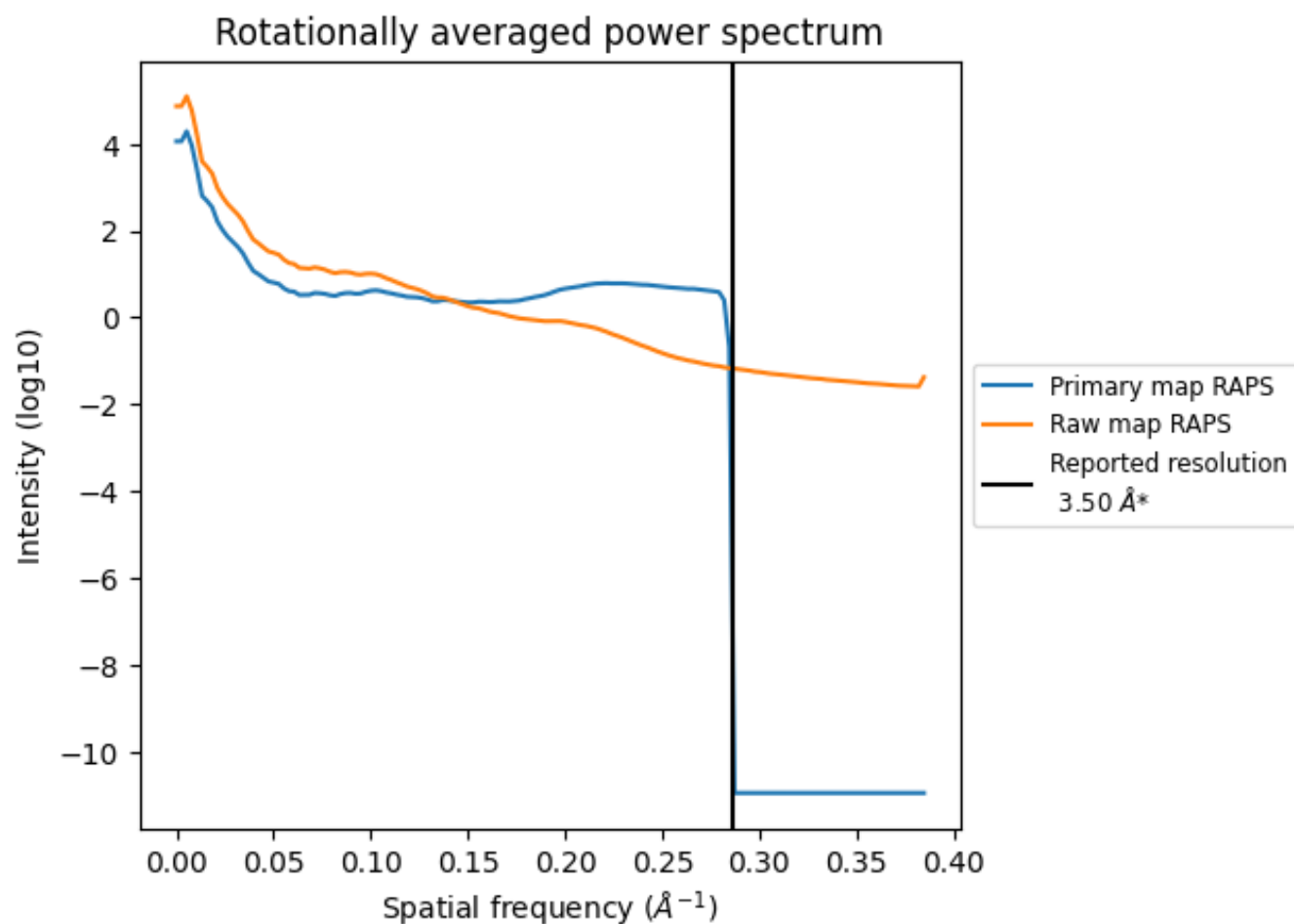
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 554 nm³; this corresponds to an approximate mass of 500 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 ⓘ

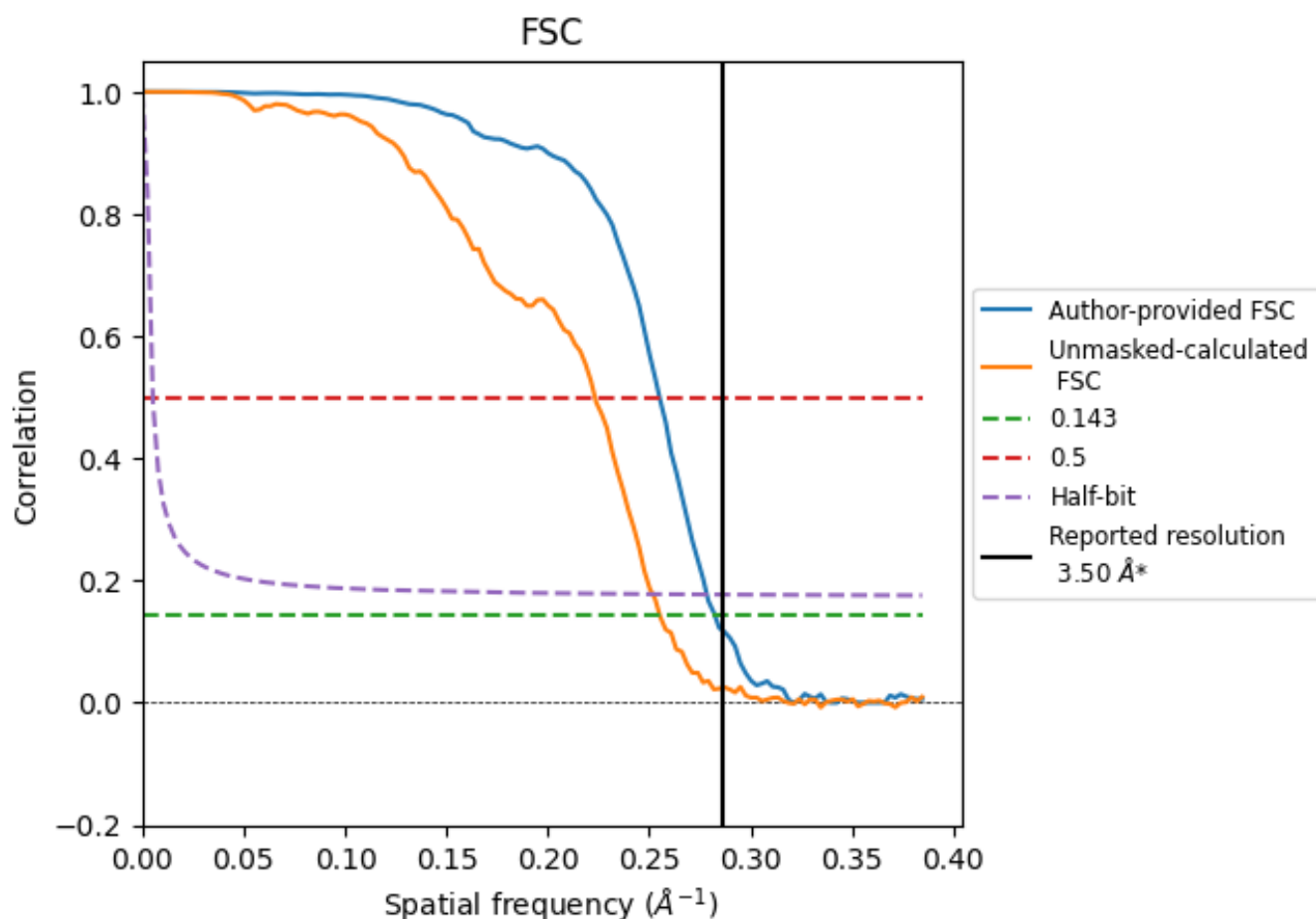


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

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 0.286 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

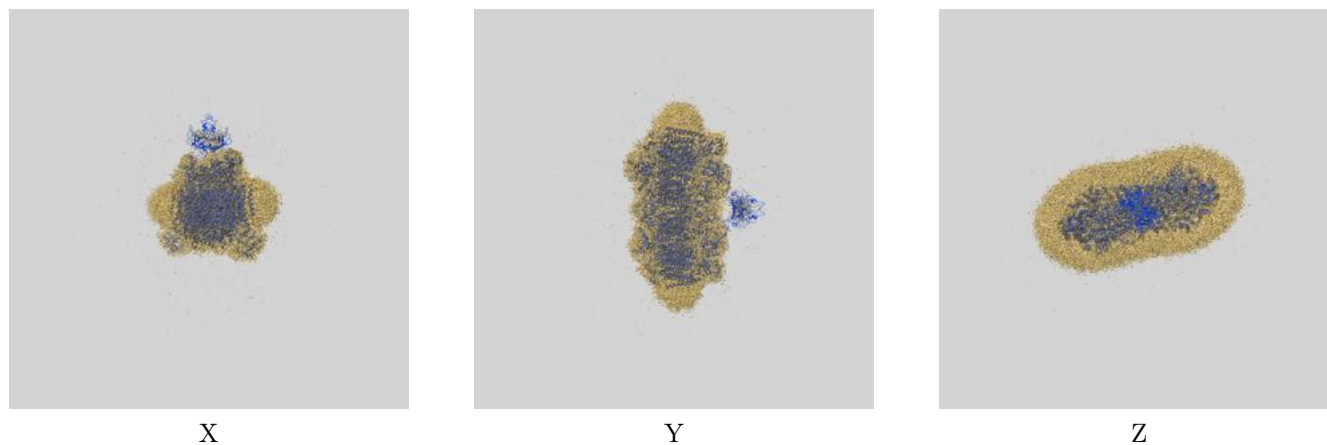
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.54	3.92	3.59
Unmasked-calculated*	3.92	4.48	3.97

*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 3.92 differs from the reported value 3.5 by more than 10 %

9 Map-model fit [i](#)

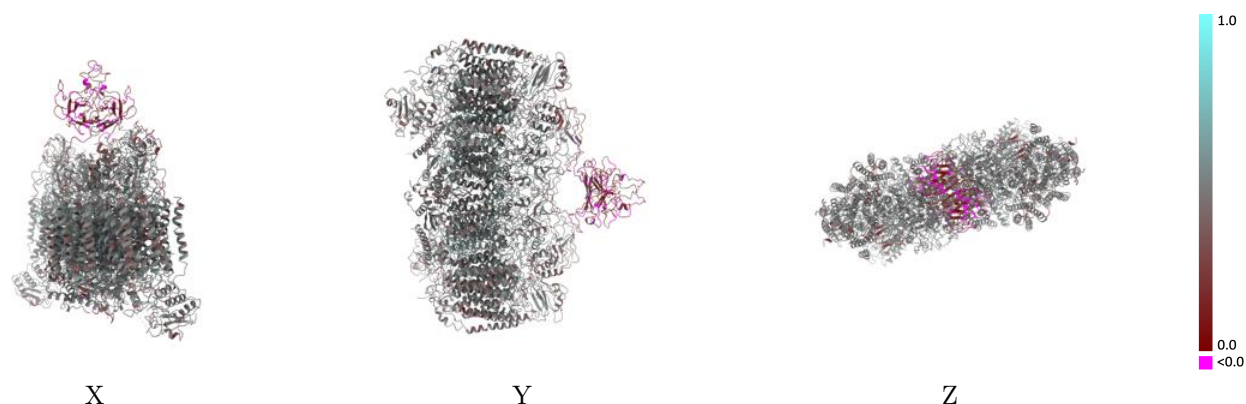
This section contains information regarding the fit between EMDB map EMD-9610 and PDB model 6ADQ. Per-residue inclusion information can be found in [section 3](#) on [page 16](#).

9.1 Map-model overlay [i](#)



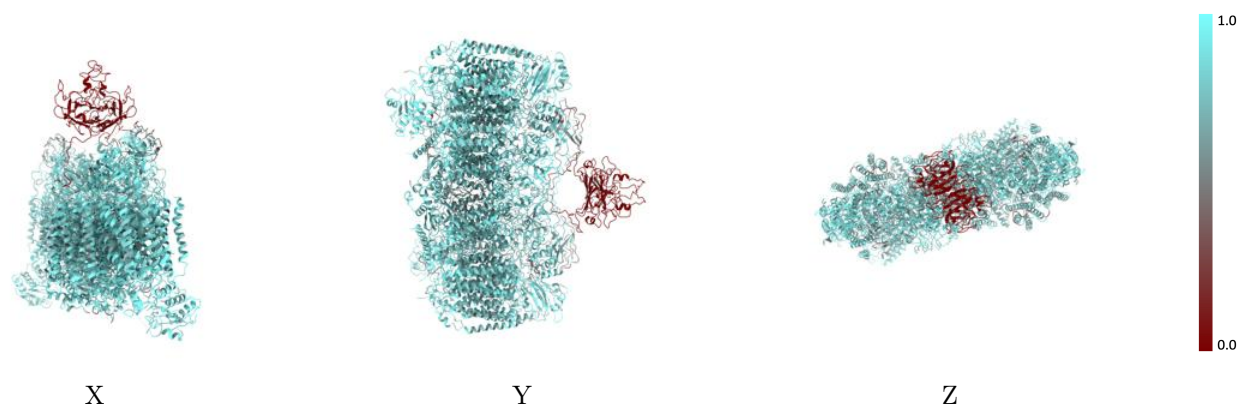
The images above show the 3D surface view of the map at the recommended contour level 0.0452 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



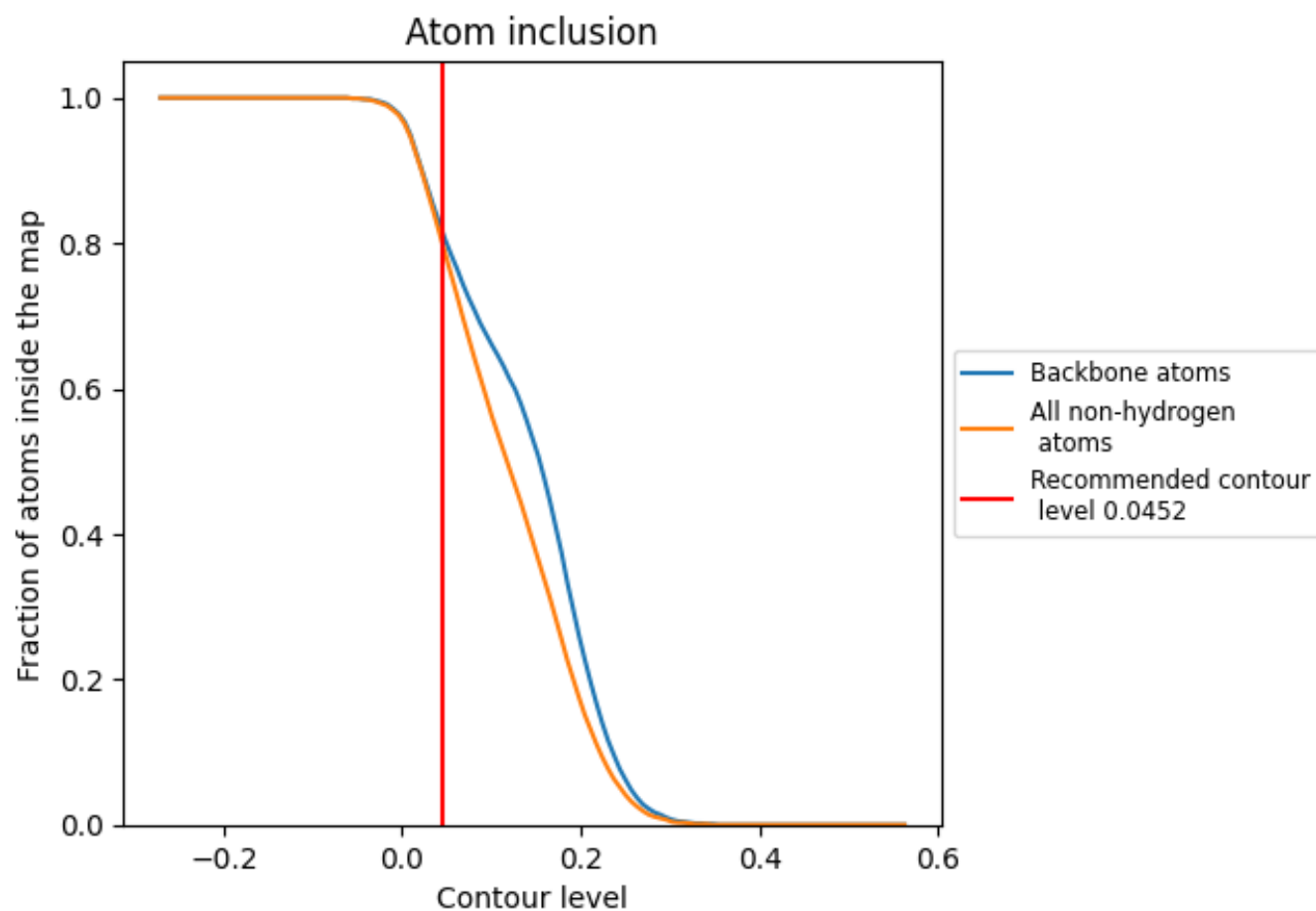
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0452).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 80% 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 (0.0452) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7990	 0.4580
A	 0.8490	 0.4820
B	 0.8400	 0.4890
C	 0.8610	 0.4760
D	 0.7920	 0.4690
E	 0.8090	 0.4410
F	 0.8570	 0.4800
G	 0.8020	 0.4460
H	 0.8280	 0.4710
I	 0.8820	 0.4670
J	 0.8600	 0.4500
K	 0.6380	 0.4380
M	 0.8490	 0.4820
N	 0.8450	 0.4910
O	 0.8610	 0.4770
P	 0.7920	 0.4690
Q	 0.8090	 0.4380
R	 0.8570	 0.4810
S	 0.8020	 0.4460
T	 0.8280	 0.4700
U	 0.8760	 0.4620
V	 0.8640	 0.4540
W	 0.6420	 0.4380
Y	 0.1850	 0.1980
Z	 0.1850	 0.2010

