



Full wwPDB EM Validation Report ⓘ

Nov 20, 2024 – 06:49 pm GMT

PDB ID : 9FTZ
EMDB ID : EMD-50752
Title : CIII2/CIV respiratory supercomplex from Mycobacterium smegmatis with lansoprazole sulfide
Authors : Kovalova, T.; Krol, S.; Gamiz-Hernandez, A.; Sjostrand, D.; Kaila, V.; Brzezinski, P.; Hogbom, M.
Deposited on : 2024-06-25
Resolution : 2.60 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.dev113
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

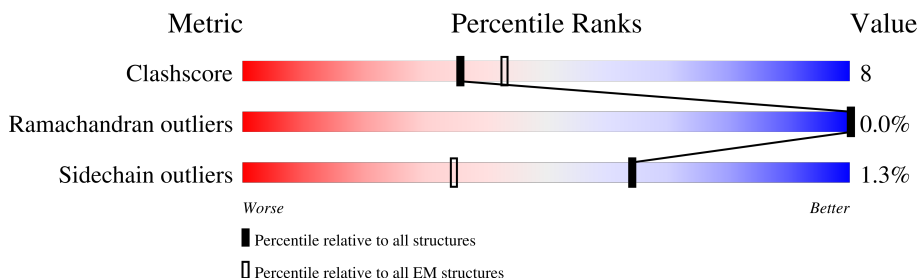
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.60 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	O	278	71% 8% 20%
2	G	408	86% 7% 7%
2	M	408	86% 8% 7%
3	H	556	64% 14% 22%
3	N	556	80% 16%
4	P	100	65% 8% 27%
5	S	203	81% 10% 9%
6	T	139	88% 12%

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Mol	Chain	Length	Quality of chain
7	R	575	 79% 17%
8	Q	341	 74% 14% 12%
9	U	79	 75% 9% 16%
10	V	157	 73% 17% 9%
11	W	186	 20% 68% 12% 20%
12	Y	236	 9% 89%
12	c	236	 11% 89%

2 Entry composition [i](#)

There are 31 unique types of molecules in this entry. The entry contains 30674 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 bc1 complex cytochrome c subunit.

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

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	17	MET	-	initiating methionine	UNP A0R050
O	18	HIS	-	expression tag	UNP A0R050
O	19	HIS	-	expression tag	UNP A0R050
O	20	HIS	-	expression tag	UNP A0R050
O	21	HIS	-	expression tag	UNP A0R050
O	22	HIS	-	expression tag	UNP A0R050
O	23	HIS	-	expression tag	UNP A0R050
O	24	MET	-	expression tag	UNP A0R050
O	25	GLY	-	expression tag	UNP A0R050
O	26	SER	-	expression tag	UNP A0R050

- Molecule 2 is a protein called Cytochrome bc1 complex cytochrome c subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	M	380	2967	1919	502	535	11	0	0
2	G	380	2967	1919	502	535	11	0	0

- Molecule 3 is a protein called Cytochrome bc1 complex cytochrome b subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	N	533	4167	2743	707	699	18	0	0
3	H	435	3425	2274	574	560	17	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	547	LYS	-	expression tag	UNP A0R052
N	548	LEU	-	expression tag	UNP A0R052
N	549	ASP	-	expression tag	UNP A0R052
N	550	TYR	-	expression tag	UNP A0R052
N	551	LYS	-	expression tag	UNP A0R052
N	552	ASP	-	expression tag	UNP A0R052
N	553	ASP	-	expression tag	UNP A0R052
N	554	ASP	-	expression tag	UNP A0R052
N	555	ASP	-	expression tag	UNP A0R052
N	556	LYS	-	expression tag	UNP A0R052
H	547	LYS	-	expression tag	UNP A0R052
H	548	LEU	-	expression tag	UNP A0R052
H	549	ASP	-	expression tag	UNP A0R052
H	550	TYR	-	expression tag	UNP A0R052
H	551	LYS	-	expression tag	UNP A0R052
H	552	ASP	-	expression tag	UNP A0R052
H	553	ASP	-	expression tag	UNP A0R052
H	554	ASP	-	expression tag	UNP A0R052
H	555	ASP	-	expression tag	UNP A0R052
H	556	LYS	-	expression tag	UNP A0R052

- Molecule 4 is a protein called Transmembrane protein.

Mol	Chain	Residues	Atoms				AltConf	Trace	
			Total	C	N	O			S
4	P	73	586	385	107	90	4	0	0

There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	1	MET	-	initiating methionine	UNP A0QVH4
P	2	SER	-	expression tag	UNP A0QVH4
P	3	SER	-	expression tag	UNP A0QVH4
P	4	THR	-	expression tag	UNP A0QVH4
P	5	GLN	-	expression tag	UNP A0QVH4
P	6	ASP	-	expression tag	UNP A0QVH4
P	7	ARG	-	expression tag	UNP A0QVH4
P	8	SER	-	expression tag	UNP A0QVH4
P	9	GLN	-	expression tag	UNP A0QVH4
P	10	LEU	-	expression tag	UNP A0QVH4
P	11	ASP	-	expression tag	UNP A0QVH4

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Chain	Residue	Modelled	Actual	Comment	Reference
P	12	PRO	-	expression tag	UNP A0QVH4
P	13	GLU	-	expression tag	UNP A0QVH4
P	14	GLU	-	expression tag	UNP A0QVH4
P	15	GLN	-	expression tag	UNP A0QVH4
P	16	PRO	-	expression tag	UNP A0QVH4
P	17	VAL	-	expression tag	UNP A0QVH4

- Molecule 5 is a protein called Probable cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	S	184	1441	967	229	238	7	0	0

- Molecule 6 is a protein called Cytochrome c oxidase polypeptide 4.

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

- Molecule 7 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	R	551	4369	2936	694	713	26	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	1	MET	-	initiating methionine	UNP A0A2U9PNL2
R	2	VAL	-	expression tag	UNP A0A2U9PNL2
R	3	ALA	-	expression tag	UNP A0A2U9PNL2
R	4	GLU	-	expression tag	UNP A0A2U9PNL2
R	5	ALA	-	expression tag	UNP A0A2U9PNL2
R	6	PRO	-	expression tag	UNP A0A2U9PNL2
R	7	PRO	-	expression tag	UNP A0A2U9PNL2
R	8	ILE	-	expression tag	UNP A0A2U9PNL2
R	9	GLY	-	expression tag	UNP A0A2U9PNL2
R	10	GLU	-	expression tag	UNP A0A2U9PNL2
R	11	LEU	-	expression tag	UNP A0A2U9PNL2
R	12	GLU	-	expression tag	UNP A0A2U9PNL2
R	13	ALA	-	expression tag	UNP A0A2U9PNL2
R	14	ARG	-	expression tag	UNP A0A2U9PNL2

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Chain	Residue	Modelled	Actual	Comment	Reference
R	15	ARG	-	expression tag	UNP A0A2U9PNL2
R	16	PRO	-	expression tag	UNP A0A2U9PNL2
R	17	PHE	-	expression tag	UNP A0A2U9PNL2
R	18	PRO	-	expression tag	UNP A0A2U9PNL2
R	19	GLU	-	expression tag	UNP A0A2U9PNL2
R	20	ARG	-	expression tag	UNP A0A2U9PNL2

- Molecule 8 is a protein called cytochrome-c oxidase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	Q	299	2382	1541	396	435	10	0	0

- Molecule 9 is a protein called Cytochrome c oxidase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	U	66	499	329	84	85	1	0	0

- Molecule 10 is a protein called Uncharacterized protein MSMEG_4692/MSMEI_4575.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	V	143	1024	647	174	201	2	0	0

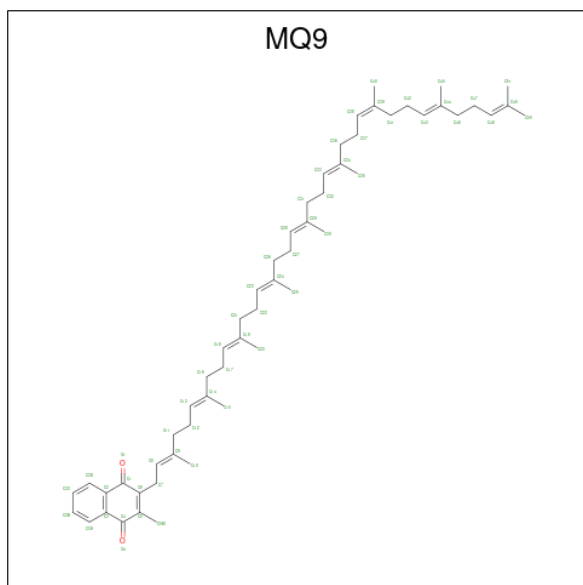
- Molecule 11 is a protein called LpqE protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	W	149	1083	670	181	231	1	0	0

- Molecule 12 is a protein called Superoxide dismutase [Cu-Zn].

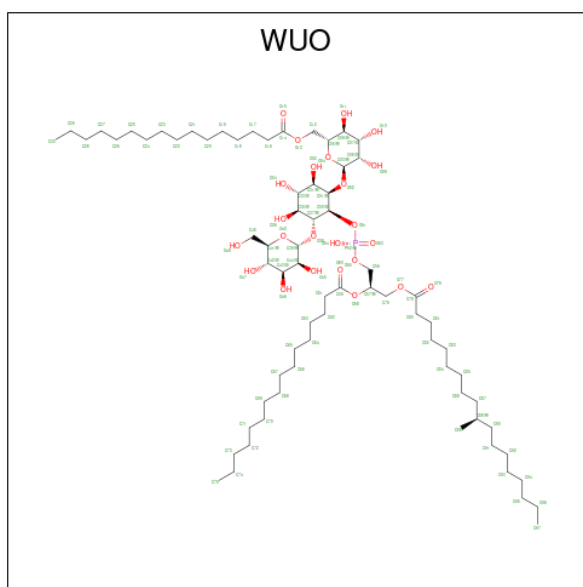
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	Y	25	168	103	26	38	1	0	0
12	c	25	168	103	26	38	1	0	0

- Molecule 13 is MENAQUINONE-9 (three-letter code: MQ9) (formula: C₅₆H₈₀O₂) (labeled as "Ligand of Interest" by depositor).



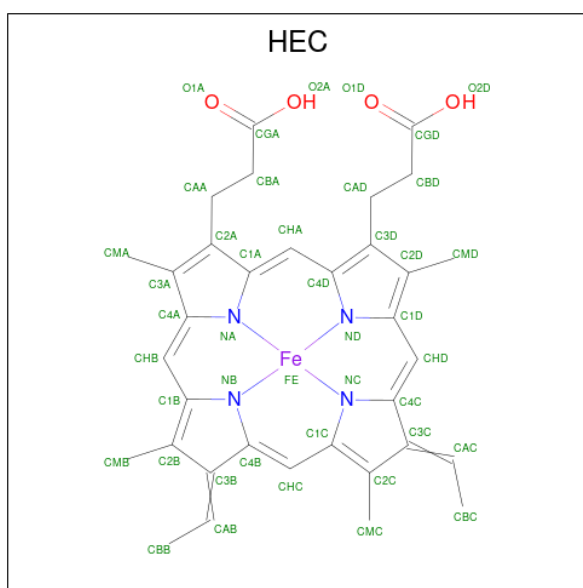
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
13	O	1	58	56	2	0
13	O	1	58	56	2	0
13	N	1	58	56	2	0
13	H	1	58	56	2	0
13	H	1	58	56	2	0

- Molecule 14 is acyl-phosphatidyl-myo-inositol dimannoside (AcPIM2) (three-letter code: WUO) (formula: $C_{72}H_{135}O_{24}P$).



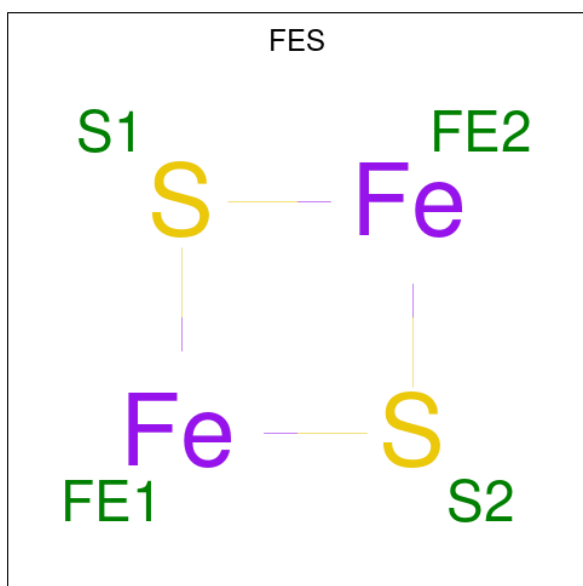
Mol	Chain	Residues	Atoms				AltConf
14	O	1	Total	C	O	P	0
			97	72	24	1	
14	P	1	Total	C	O	P	0
			97	72	24	1	

- Molecule 15 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



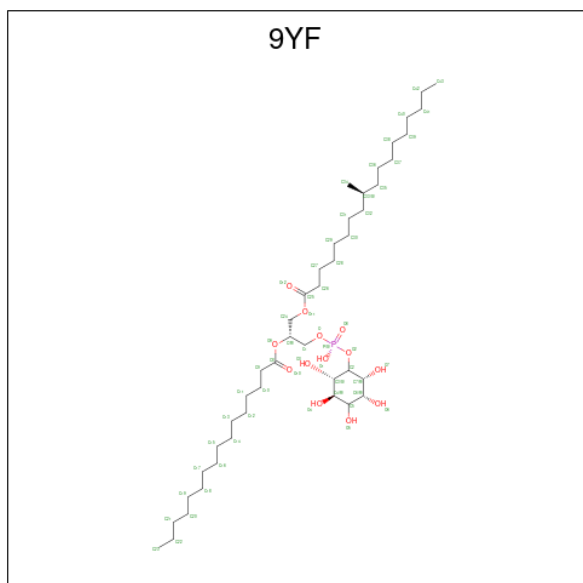
Mol	Chain	Residues	Atoms					AltConf
15	O	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
15	O	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 16 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



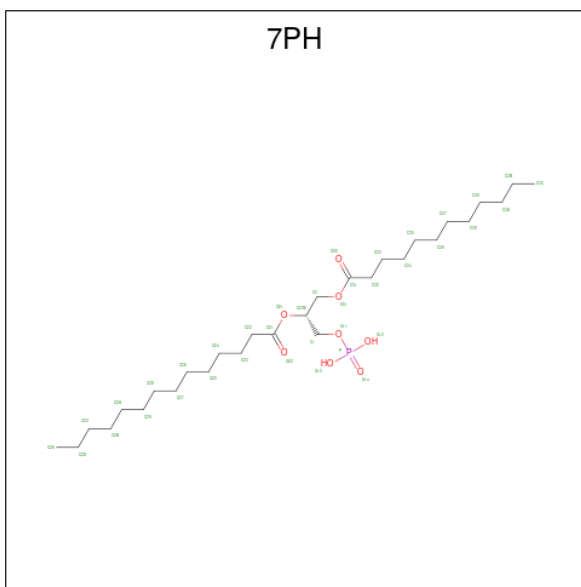
Mol	Chain	Residues	Atoms			AltConf
16	M	1	Total	Fe	S	0
			4	2	2	
16	G	1	Total	Fe	S	0
			4	2	2	

- Molecule 17 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 (three-letter code: 9YF) (formula: C₄₄H₈₅O₁₃P).



Mol	Chain	Residues	Atoms				AltConf
17	M	1	Total	C	O	P	0
			58	44	13	1	
17	W	1	Total	C	O	P	0
			58	44	13	1	
17	G	1	Total	C	O	P	0
			58	44	13	1	

- Molecule 18 is (1R)-2-(dodecanoyloxy)-1-[(phosphonoxy)methyl]ethyl tetradecanoate (three-letter code: 7PH) (formula: C₂₉H₅₇O₈P).



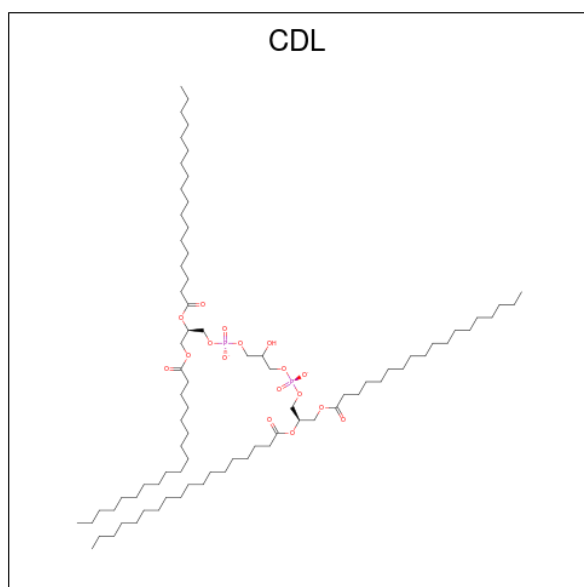
Mol	Chain	Residues	Atoms				AltConf
18	M	1	Total	C	O	P	0
			38	29	8	1	
18	S	1	Total	C	O	P	0
			38	29	8	1	
18	G	1	Total	C	O	P	0
			38	29	8	1	
18	G	1	Total	C	O	P	0
			38	29	8	1	

- Molecule 19 is [(2 {R})-3-[(1 {S},2 {R},3 {S},4 {S},5 {R},6 {R})-2-[(2 {R},3 {S},4 {S},5 {S},6 {R})-6-[(2 {S},3 {S},4 {S},5 {S},6 {R})-6-[(2 {S},3 {S},4 {S},5 {S},6 {R})-6-(hydroxymethyl)-3-[(2 {R},3 {S},4 {S},5 {S},6 {R})-6-(hydroxymethyl)-3,4,5-tris(oxidanyl)oxan-2-yl]oxy-4,5-bis(oxidanyl)oxan-2-yl]oxymethyl]-3,4,5-tris(oxidanyl)oxan-2-yl]oxy-3,4,5-tris(oxidanyl)-6-[(2 {R},3 {S},4 {S},5 {S},6 {R})-3,4,5-tris(oxidanyl)-6-(undecanoyloxymethyl)oxan-2-yl]oxy-cyclohexyl]oxy-oxidanyl-phosphoryl]oxy-2-undecanoyloxy-propyl] (10 {R})-10-methyldodecanoate (three-letter code: IZL) (formula: C₇₄H₁₃₃O₃₉P).

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

- Molecule 21 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



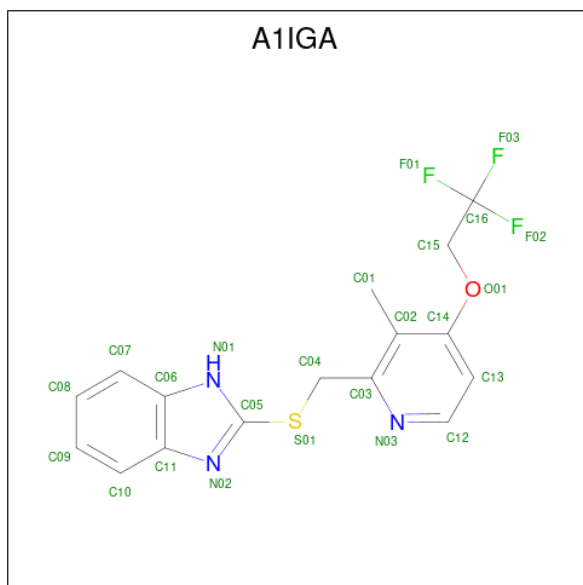
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
21	N	1	Total 77	C 58	O 17	P 2	0
21	N	1	Total 79	C 60	O 17	P 2	0
21	N	1	Total 79	C 60	O 17	P 2	0
21	P	1	Total 77	C 58	O 17	P 2	0
21	R	1	Total 77	C 58	O 17	P 2	0
21	R	1	Total 77	C 58	O 17	P 2	0
21	H	1	Total 74	C 55	O 17	P 2	0
21	H	1	Total 74	C 55	O 17	P 2	0

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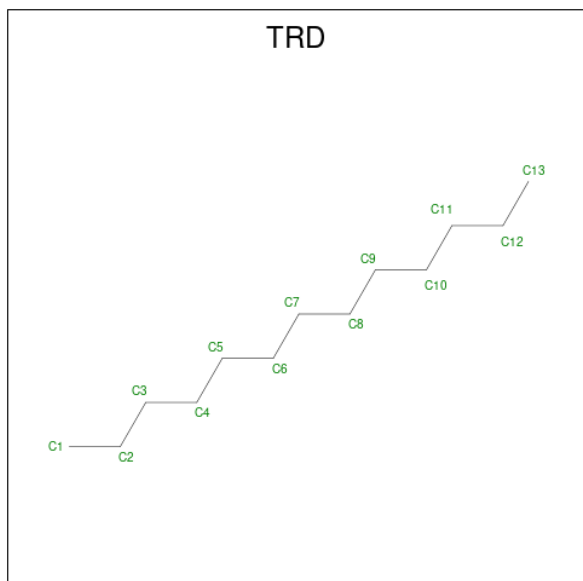
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
21	H	1	77	58	17	2	0

- Molecule 22 is Lansoprazole sulfide (three-letter code: A1IGA) (formula: $C_{16}H_{14}F_3N_3OS$) (labeled as "Ligand of Interest" by depositor).



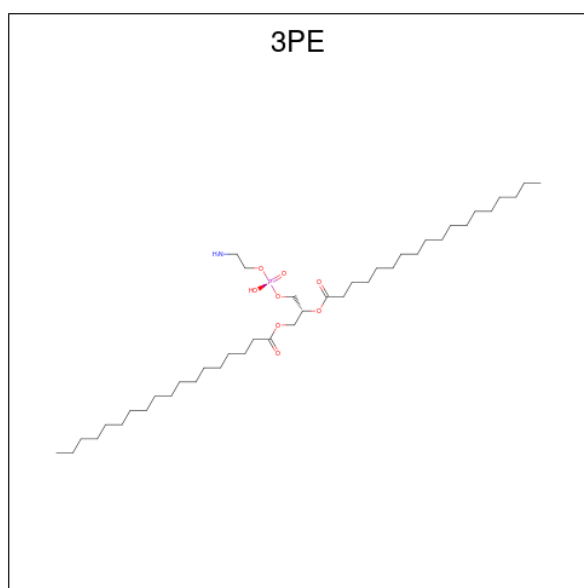
Mol	Chain	Residues	Atoms					AltConf	
			Total	C	F	N	O		S
22	N	1	24	16	3	3	1	1	0

- Molecule 23 is TRIDECANE (three-letter code: TRD) (formula: $C_{13}H_{28}$).



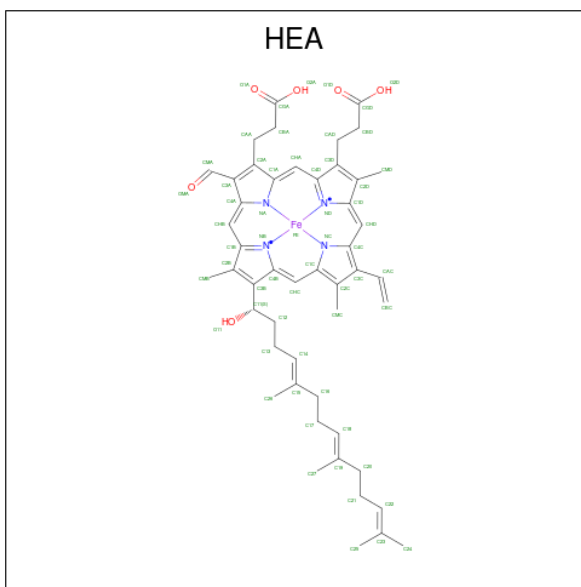
Mol	Chain	Residues	Atoms		AltConf
23	S	1	Total	C	0
			13	13	
23	T	1	Total	C	0
			13	13	
23	R	1	Total	C	0
			13	13	
23	R	1	Total	C	0
			13	13	
23	Q	1	Total	C	0
			13	13	

- Molecule 24 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
24	S	1	32	22	1	8	1	0

- Molecule 25 is HEME-A (three-letter code: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).



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

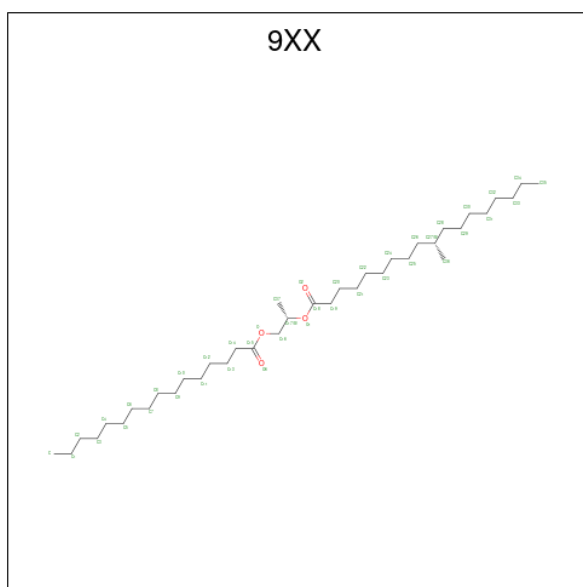
- Molecule 26 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		AltConf
			Total	Cu	
26	R	1	1	1	0
26	Q	2	2	2	0

- Molecule 27 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
			Total	Ca	
27	R	1	1	1	0

- Molecule 28 is (2S)-1-(hexadecanoyloxy)propan-2-yl (10S)-10-methyloctadecanoate (three-letter code: 9XX) (formula: C₃₈H₇₄O₄).

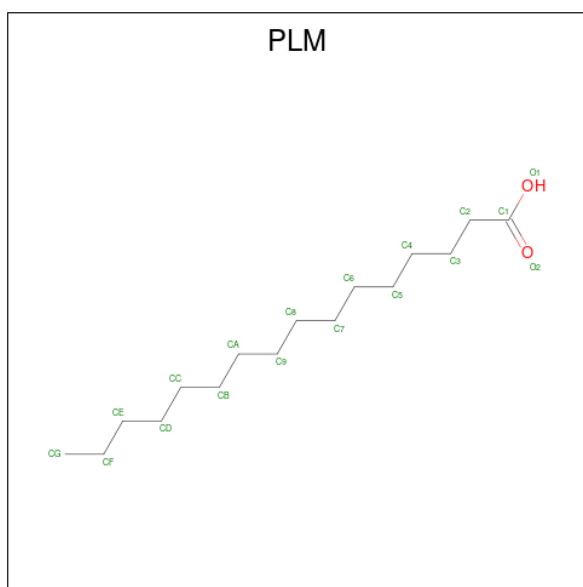


Mol	Chain	Residues	Atoms			AltConf
28	R	1	Total	C	O	0
			42	38	4	
28	Y	1	Total	C	O	0
			32	28	4	
28	c	1	Total	C	O	0
			32	28	4	

- Molecule 29 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
29	R	1	Total	Mg	0
			1	1	

- Molecule 30 is PALMITIC ACID (three-letter code: PLM) (formula: C₁₆H₃₂O₂).



Mol	Chain	Residues	Atoms			AltConf
30	W	1	Total	C	O	0
			11	10	1	
30	Y	1	Total	C	O	0
			11	10	1	
30	c	1	Total	C	O	0
			11	10	1	

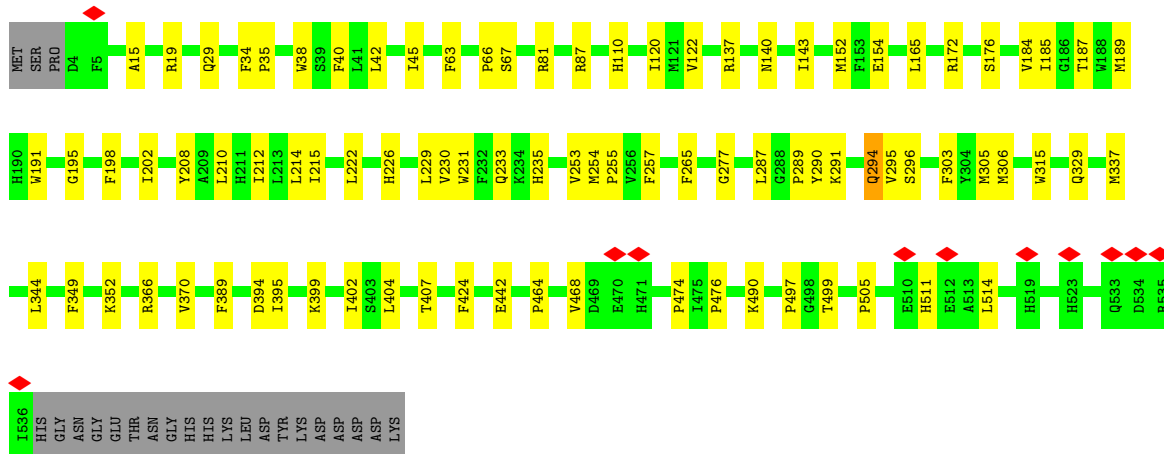
- Molecule 31 is water.

Mol	Chain	Residues	Atoms		AltConf
31	O	50	Total	O	0
			50	50	
31	M	51	Total	O	0
			51	51	
31	N	78	Total	O	0
			78	78	
31	P	8	Total	O	0
			8	8	
31	S	10	Total	O	0
			10	10	
31	T	9	Total	O	0
			9	9	
31	R	67	Total	O	0
			67	67	
31	Q	44	Total	O	0
			44	44	
31	V	3	Total	O	0
			3	3	

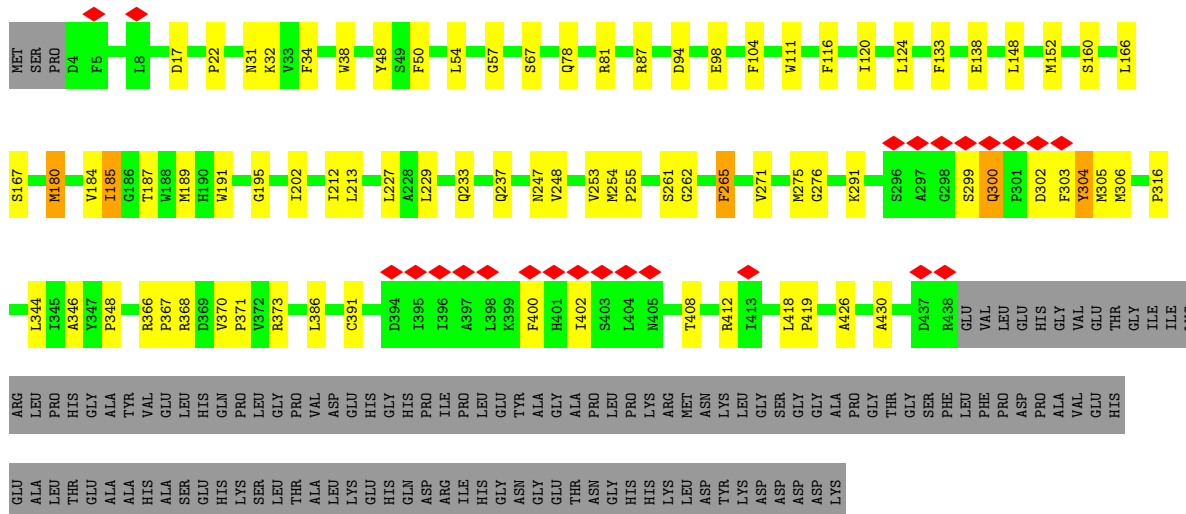
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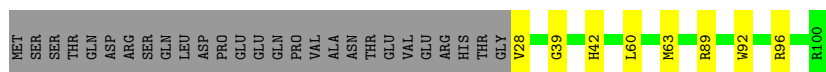
Mol	Chain	Residues	Atoms		AltConf
31	W	2	Total 2	O 2	0
31	Y	2	Total 2	O 2	0
31	H	13	Total 13	O 13	0
31	G	11	Total 11	O 11	0



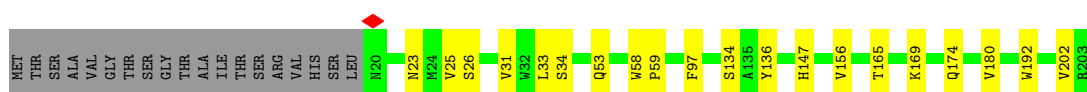
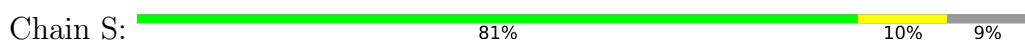
• Molecule 3: Cytochrome bc1 complex cytochrome b subunit



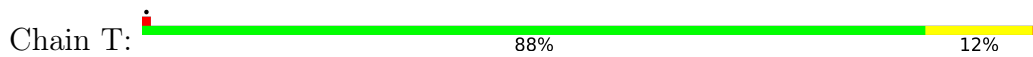
• Molecule 4: Transmembrane protein



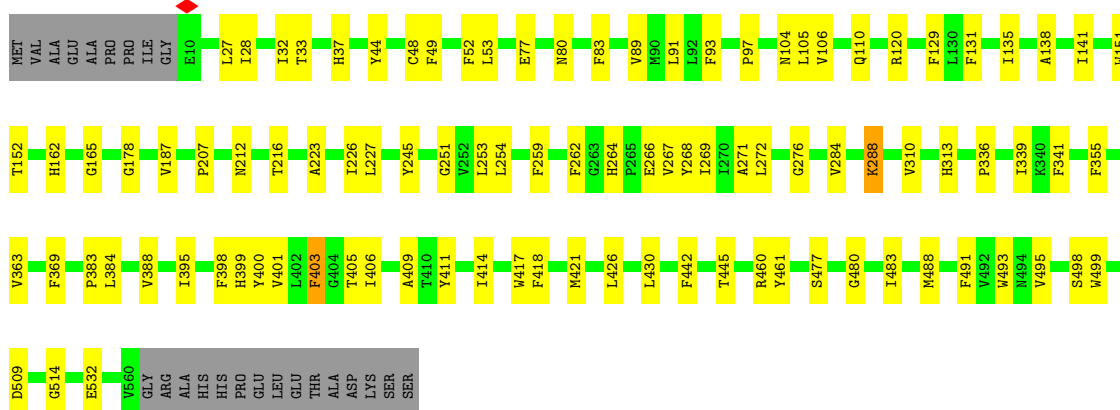
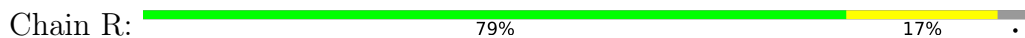
• Molecule 5: Probable cytochrome c oxidase subunit 3



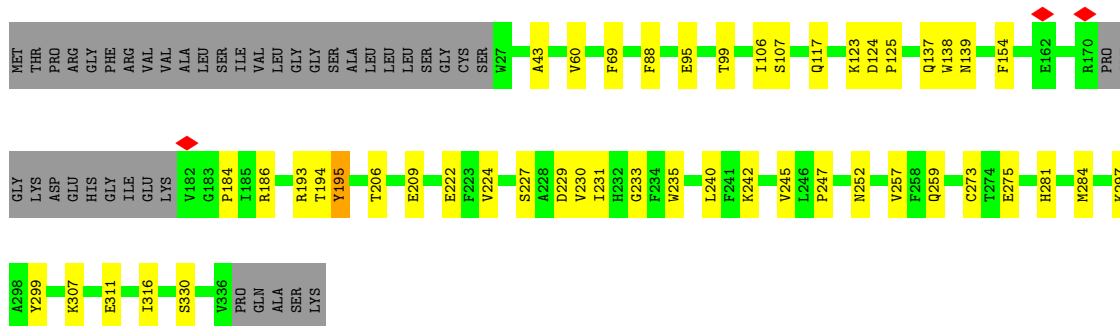
• Molecule 6: Cytochrome c oxidase polypeptide 4



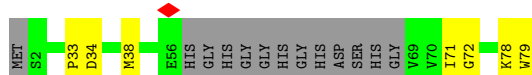
• Molecule 7: Cytochrome c oxidase subunit 1



• Molecule 8: cytochrome-c oxidase



• Molecule 9: Cytochrome c oxidase subunit



• Molecule 10: Uncharacterized protein MSMEG_4692/MSMEI_4575



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	100396	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.166	Depositor
Minimum map value	-0.628	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.033	Depositor
Recommended contour level	0.176	Depositor
Map size (Å)	447.12, 447.12, 447.12	wwPDB
Map dimensions	540, 540, 540	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.828, 0.828, 0.828	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: IZL, 9YF, PLM, 3PE, MG, WUO, HEA, 9XX, CU, A1IGA, FES, CA, CDL, HEM, TRD, MQ9, 7PH, HEC

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	O	0.37	0/1660	0.54	0/2250
2	G	0.26	0/3046	0.42	0/4129
2	M	0.26	0/3046	0.41	0/4129
3	H	0.30	0/3534	0.42	0/4820
3	N	0.31	0/4299	0.42	0/5862
4	P	0.23	0/606	0.36	0/825
5	S	0.25	0/1488	0.36	0/2032
6	T	0.27	0/1112	0.39	0/1524
7	R	0.28	0/4529	0.42	0/6187
8	Q	0.29	0/2447	0.42	0/3330
9	U	0.36	0/515	0.43	0/704
10	V	0.35	0/1042	0.48	0/1423
11	W	0.25	0/1100	0.46	0/1508
12	Y	0.24	0/175	0.43	0/244
12	c	0.25	0/175	0.44	0/244
All	All	0.29	0/28774	0.43	0/39211

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	O	1623	0	1560	26	0
2	G	2967	0	2976	23	0
2	M	2967	0	2976	32	0
3	H	3425	0	3469	66	0
3	N	4167	0	4192	77	0
4	P	586	0	578	6	0
5	S	1441	0	1439	17	0
6	T	1077	0	1058	13	0
7	R	4369	0	4346	77	0
8	Q	2382	0	2335	35	0
9	U	499	0	504	6	0
10	V	1024	0	1035	26	0
11	W	1083	0	1055	15	0
12	Y	168	0	150	3	0
12	c	168	0	151	0	0
13	H	116	0	160	13	0
13	N	58	0	80	17	0
13	O	116	0	160	17	0
14	O	97	0	0	2	0
14	P	97	0	0	3	0
15	O	86	0	60	6	0
16	G	4	0	0	1	0
16	M	4	0	0	1	0
17	G	58	0	0	0	0
17	M	58	0	0	0	0
17	W	58	0	0	2	0
18	G	76	0	110	2	0
18	M	38	0	55	1	0
18	S	38	0	55	1	0
19	G	114	0	0	0	0
19	M	114	0	0	0	0
20	H	86	0	60	19	0
20	N	86	0	60	13	0
21	H	225	0	282	14	0
21	N	235	0	308	7	0
21	P	77	0	98	11	0
21	R	154	0	196	12	0
22	N	24	0	0	0	0
23	Q	13	0	28	0	0
23	R	26	0	56	0	0
23	S	13	0	28	1	0
23	T	13	0	28	0	0
24	S	32	0	38	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	R	120	0	108	23	0
26	Q	2	0	0	0	0
26	R	1	0	0	0	0
27	R	1	0	0	0	0
28	R	42	0	0	1	0
28	Y	32	0	0	0	0
28	c	32	0	0	0	0
29	R	1	0	0	0	0
30	W	11	0	16	1	0
30	Y	11	0	16	0	0
30	c	11	0	16	0	0
31	G	11	0	0	0	0
31	H	13	0	0	0	0
31	M	51	0	0	0	0
31	N	78	0	0	2	0
31	O	50	0	0	1	0
31	P	8	0	0	0	0
31	Q	44	0	0	0	0
31	R	67	0	0	1	0
31	S	10	0	0	0	0
31	T	9	0	0	0	0
31	V	3	0	0	0	0
31	W	2	0	0	0	0
31	Y	2	0	0	0	0
All	All	30674	0	29842	447	0

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

All (447) 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)
7:R:406:ILE:HD11	25:R:603:HEA:HAC	1.15	1.12
1:O:273:MET:HG3	14:O:302:WUO:C89	1.93	0.98
21:P:301:CDL:H532	21:P:301:CDL:H742	1.44	0.97
25:R:603:HEA:HBD2	25:R:603:HEA:HHA	1.48	0.93
7:R:406:ILE:HD11	25:R:603:HEA:CAC	1.99	0.92
20:H:602:HEM:HHC	20:H:602:HEM:HBB2	1.52	0.91
3:N:140:ASN:HD21	3:N:230:VAL:CG2	1.85	0.89
21:P:301:CDL:H561	21:P:301:CDL:H782	1.51	0.88
13:H:606:MQ9:H261	13:H:606:MQ9:H301	1.54	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:143:ILE:HG22	13:N:606:MQ9:C30	2.05	0.87
10:V:84:ILE:HG22	10:V:96:LEU:CD2	2.04	0.87
1:O:228:ASN:OD1	2:M:357:GLU:HB3	1.74	0.87
20:H:605:HEM:HBC2	20:H:605:HEM:HMC2	1.56	0.85
7:R:406:ILE:CD1	25:R:603:HEA:HAC	2.04	0.85
25:R:603:HEA:HHD	25:R:603:HEA:HBC1	1.59	0.84
6:T:9:GLU:OE2	6:T:57:ARG:HD2	1.80	0.81
21:P:301:CDL:H552	21:P:301:CDL:H762	1.62	0.81
20:H:602:HEM:HHD	20:H:602:HEM:HBC2	1.60	0.80
21:P:301:CDL:H762	21:P:301:CDL:C55	2.11	0.80
3:N:140:ASN:ND2	3:N:230:VAL:HG22	1.96	0.80
13:N:606:MQ9:H5M3	13:N:606:MQ9:H8	1.66	0.78
3:N:35:PRO:HB2	3:N:40:PHE:CE2	2.19	0.78
3:H:346:ALA:HB2	13:H:607:MQ9:C30	2.14	0.77
1:O:273:MET:CG	14:O:302:WUO:C89	2.63	0.77
21:P:301:CDL:H782	21:P:301:CDL:C56	2.14	0.77
10:V:84:ILE:HG22	10:V:96:LEU:HD21	1.67	0.76
10:V:84:ILE:CG2	10:V:96:LEU:HD21	2.15	0.76
8:Q:193:ARG:HA	8:Q:195:TYR:CE1	2.21	0.76
3:H:166:LEU:HD11	3:H:299:SER:HB3	1.66	0.75
3:N:140:ASN:ND2	3:N:230:VAL:CG2	2.49	0.75
3:N:35:PRO:HB2	3:N:40:PHE:HE2	1.52	0.75
3:N:442:GLU:HG3	3:N:476:PRO:HB3	1.68	0.75
20:N:605:HEM:HBC2	20:N:605:HEM:HMC2	1.68	0.74
3:N:140:ASN:HD21	3:N:230:VAL:HG23	1.51	0.74
21:N:607:CDL:HB22	6:T:137:GLU:HG3	1.68	0.74
14:P:302:WUO:C28	25:R:603:HEA:H241	2.19	0.73
8:Q:193:ARG:HA	8:Q:195:TYR:HE1	1.54	0.73
2:M:143:ILE:CG2	13:N:606:MQ9:C30	2.66	0.72
20:N:605:HEM:HBD2	20:N:605:HEM:HHA	1.69	0.72
3:N:34:PHE:HZ	3:N:231:TRP:CZ3	2.06	0.72
3:H:180:MET:O	3:H:180:MET:HG2	1.89	0.72
13:H:606:MQ9:O1	13:H:606:MQ9:H111	1.90	0.72
2:M:352:PRO:O	3:N:295:VAL:HG11	1.89	0.72
7:R:266:GLU:HA	7:R:269:ILE:HD12	1.72	0.71
1:O:227:GLN:HG2	31:O:427:HOH:O	1.91	0.71
3:N:464:PRO:HB3	3:N:474:PRO:HB3	1.71	0.71
20:N:605:HEM:HHA	20:N:605:HEM:CBF	2.20	0.70
3:H:262:GLY:HA3	13:H:606:MQ9:H221	1.73	0.70
3:N:34:PHE:CZ	3:N:231:TRP:CZ3	2.79	0.69
7:R:253:LEU:HD23	8:Q:252:ASN:HB3	1.72	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:R:398:PHE:HA	7:R:401:VAL:HG12	1.73	0.69
3:H:306:MET:SD	3:H:391:CYS:SG	2.90	0.69
3:N:38:TRP:CH2	21:N:602:CDL:H711	2.28	0.68
25:R:603:HEA:HHA	25:R:603:HEA:CBD	2.22	0.68
2:M:143:ILE:CG2	13:N:606:MQ9:H301	2.23	0.68
2:M:215:PHE:HD2	13:H:606:MQ9:H502	1.58	0.68
6:T:70:TYR:HB3	6:T:73:ALA:HB2	1.75	0.68
2:M:344:LYS:HE3	2:M:354:SER:HB3	1.75	0.67
10:V:84:ILE:HG22	10:V:96:LEU:HD22	1.75	0.67
21:N:602:CDL:H522	21:N:602:CDL:H722	1.75	0.67
10:V:85:LEU:O	10:V:85:LEU:HG	1.92	0.67
2:M:133:GLY:HA3	3:N:277:GLY:HA3	1.77	0.67
21:H:604:CDL:HA22	21:H:604:CDL:HB32	1.77	0.66
3:N:67:SER:HB3	3:N:87:ARG:HB2	1.78	0.65
9:U:38:MET:HG3	10:V:137:GLY:HA2	1.79	0.65
13:N:606:MQ9:H8	13:N:606:MQ9:C5M	2.26	0.64
3:H:346:ALA:HB2	13:H:607:MQ9:H302	1.79	0.64
2:G:349:LEU:HD12	2:G:368:HIS:HE1	1.62	0.64
21:P:301:CDL:H532	21:P:301:CDL:C74	2.23	0.63
5:S:25:VAL:HG12	5:S:180:VAL:HG11	1.80	0.63
2:M:143:ILE:HG22	13:N:606:MQ9:H302	1.81	0.63
3:H:166:LEU:HD11	3:H:299:SER:CB	2.28	0.62
20:N:601:HEM:HBC2	20:N:601:HEM:HMC2	1.81	0.62
3:H:166:LEU:CD1	3:H:299:SER:HB3	2.30	0.62
7:R:49:PHE:HZ	7:R:411:TYR:HH	1.48	0.62
3:N:253:VAL:HA	3:N:257:PHE:HB3	1.80	0.62
11:W:88:LEU:HD21	11:W:91:ILE:HD11	1.81	0.62
2:M:369:GLN:HG3	3:N:404:LEU:HD21	1.81	0.61
1:O:231:LYS:O	1:O:231:LYS:HG2	2.00	0.61
20:N:605:HEM:HBD2	20:N:605:HEM:CHA	2.27	0.61
2:G:169:SER:HB2	2:G:174:ARG:HG3	1.81	0.61
7:R:395:ILE:HD13	25:R:603:HEA:HAA1	1.81	0.61
7:R:32:ILE:HG13	7:R:33:THR:HG23	1.83	0.61
2:G:276:ALA:HB1	2:G:318:LYS:HG2	1.82	0.60
13:N:606:MQ9:H5M3	13:N:606:MQ9:C8	2.32	0.60
7:R:461:TYR:HE1	8:Q:281:HIS:CE1	2.20	0.59
3:H:265:PHE:HD2	3:H:265:PHE:O	1.85	0.59
20:H:605:HEM:HBD2	20:H:605:HEM:HMD2	1.84	0.59
3:N:230:VAL:O	13:N:606:MQ9:H3C	2.02	0.59
7:R:355:PHE:HE1	7:R:363:VAL:HG21	1.66	0.59
7:R:400:TYR:HA	7:R:442:PHE:HZ	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:R:495:VAL:HG11	21:R:605:CDL:H371	1.84	0.59
3:H:195:GLY:HA3	3:H:202:ILE:HD11	1.84	0.59
3:H:367:PRO:HG2	21:H:604:CDL:CA3	2.33	0.59
7:R:383:PRO:HG3	8:Q:117:GLN:HB3	1.84	0.59
3:H:367:PRO:HG2	21:H:604:CDL:HA31	1.85	0.59
13:H:606:MQ9:H261	13:H:606:MQ9:C30	2.26	0.58
7:R:105:LEU:HD22	7:R:421:MET:HG3	1.85	0.58
3:H:31:ASN:HB3	2:G:65:VAL:HG21	1.84	0.58
20:H:605:HEM:HMC2	20:H:605:HEM:CBC	2.32	0.58
13:O:305:MQ9:H502	3:N:407:THR:O	2.02	0.58
25:R:603:HEA:O11	25:R:603:HEA:HHC	2.04	0.58
1:O:198:GLY:HA2	1:O:207:ALA:O	2.04	0.57
2:M:349:LEU:HD12	2:M:368:HIS:CE1	2.39	0.57
8:Q:195:TYR:HD1	8:Q:195:TYR:H	1.50	0.57
2:M:107:PHE:HE2	2:G:217:GLY:HA3	1.68	0.56
21:R:605:CDL:OB9	21:R:605:CDL:HB4	2.05	0.56
3:N:67:SER:HB2	3:H:67:SER:HB2	1.85	0.56
20:H:605:HEM:HBA1	20:H:605:HEM:HHA	1.86	0.56
3:H:34:PHE:HE2	3:H:253:VAL:HG22	1.71	0.56
3:H:316:PRO:HA	3:H:412:ARG:HH11	1.70	0.56
13:N:606:MQ9:H8	13:N:606:MQ9:H13	1.88	0.56
9:U:79:TRP:HZ3	10:V:105:ALA:O	1.88	0.56
8:Q:284:MET:O	8:Q:284:MET:HG3	2.04	0.56
13:O:305:MQ9:C41	13:O:305:MQ9:H451	2.36	0.56
1:O:277:ILE:HG23	1:O:278:ILE:HG13	1.87	0.56
20:N:601:HEM:HBC2	20:N:601:HEM:CMC	2.35	0.56
2:G:349:LEU:HD12	2:G:368:HIS:CE1	2.40	0.55
3:H:67:SER:HB3	3:H:87:ARG:HB2	1.87	0.55
7:R:336:PRO:HA	7:R:339:ILE:HD12	1.88	0.55
3:N:34:PHE:HZ	3:N:231:TRP:CE3	2.24	0.55
3:N:265:PHE:CD2	13:N:606:MQ9:H353	2.42	0.55
2:M:215:PHE:CD2	13:H:606:MQ9:H502	2.41	0.55
9:U:79:TRP:CZ3	10:V:105:ALA:O	2.59	0.55
3:N:185:ILE:HD12	3:N:189:MET:SD	2.47	0.55
7:R:28:ILE:HD13	21:R:605:CDL:CB7	2.37	0.55
20:H:605:HEM:HBD2	20:H:605:HEM:CMD	2.36	0.55
13:O:305:MQ9:C41	13:O:305:MQ9:C45	2.85	0.55
5:S:34:SER:HB3	6:T:48:LEU:HG	1.88	0.54
2:M:172:VAL:HA	2:G:47:LEU:HD21	1.89	0.54
10:V:138:ASN:HB3	10:V:141:ASP:HB3	1.89	0.54
1:O:229:MET:HG3	15:O:303:HEC:NC	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:126:ARG:HH22	7:R:165:GLY:HA3	1.73	0.54
10:V:33:GLU:HB2	10:V:36:GLU:HG3	1.89	0.54
7:R:80:ASN:HA	7:R:83:PHE:CE1	2.42	0.54
7:R:110:GLN:HB3	7:R:207:PRO:HG2	1.90	0.54
4:P:92:TRP:CZ2	4:P:96:ARG:HD3	2.43	0.54
13:N:606:MQ9:H211	13:N:606:MQ9:C25	2.38	0.53
3:N:143:ILE:HG23	3:N:222:LEU:HD22	1.90	0.53
3:N:226:HIS:O	3:N:230:VAL:HG23	2.09	0.53
7:R:151:TRP:HD1	25:R:603:HEA:O2D	1.91	0.53
13:O:305:MQ9:H38	3:N:402:ILE:HD11	1.90	0.53
25:R:603:HEA:HBD2	25:R:603:HEA:CHA	2.32	0.53
7:R:399:HIS:O	7:R:403:PHE:HB2	2.08	0.53
20:N:605:HEM:CBD	20:N:605:HEM:CHA	2.85	0.53
7:R:27:LEU:HD21	21:R:605:CDL:H121	1.90	0.53
28:R:609:9XX:C37	11:W:24:CYS:SG	2.97	0.53
10:V:70:ILE:HD11	10:V:143:LEU:HD11	1.90	0.53
2:G:254:LEU:HD12	2:G:402:LEU:HB3	1.89	0.53
20:H:605:HEM:CMD	20:H:605:HEM:CBD	2.86	0.52
2:G:393:PRO:HB2	2:G:405:ASN:HB3	1.90	0.52
3:N:212:ILE:HD11	3:H:212:ILE:HD11	1.92	0.52
5:S:165:THR:HA	5:S:174:GLN:NE2	2.24	0.52
7:R:288:LYS:HE3	8:Q:88:PHE:CE2	2.45	0.52
9:U:78:LYS:HA	10:V:105:ALA:HA	1.91	0.52
2:M:256:ARG:HH12	2:M:273:ASP:HB3	1.75	0.52
7:R:28:ILE:HD13	21:R:605:CDL:OB9	2.08	0.52
13:N:606:MQ9:C8	13:N:606:MQ9:H13	2.40	0.52
8:Q:230:VAL:O	8:Q:247:PRO:HD3	2.09	0.52
3:N:198:PHE:HE2	3:N:290:TYR:HH	1.58	0.52
7:R:288:LYS:HE3	8:Q:88:PHE:CZ	2.45	0.52
13:O:305:MQ9:H5M2	3:N:399:LYS:HG3	1.92	0.51
10:V:73:LEU:O	10:V:77:THR:HA	2.10	0.51
6:T:58:PHE:O	6:T:62:ARG:HG2	2.10	0.51
3:H:57:GLY:O	20:H:602:HEM:HBC2	2.10	0.51
3:N:468:VAL:HA	3:N:474:PRO:HA	1.91	0.51
5:S:147:HIS:CE1	5:S:192:TRP:HB2	2.45	0.51
7:R:91:LEU:HG	25:R:603:HEA:HMD3	1.92	0.51
3:H:104:PHE:HE2	13:H:606:MQ9:H512	1.75	0.51
13:N:606:MQ9:C5M	13:N:606:MQ9:C8	2.89	0.51
3:N:110:HIS:CD2	20:N:601:HEM:HMA3	2.46	0.51
7:R:251:GLY:HA2	7:R:254:LEU:HB3	1.92	0.51
10:V:84:ILE:HG21	10:V:96:LEU:HD21	1.89	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:R:445:THR:HA	7:R:477:SER:HA	1.93	0.50
3:H:227:LEU:HB2	21:H:603:CDL:H771	1.93	0.50
1:O:229:MET:HG3	15:O:303:HEC:C1C	2.42	0.50
1:O:283:ALA:HB1	3:N:45:ILE:HD13	1.93	0.50
10:V:130:ALA:HB2	10:V:146:ALA:HB2	1.94	0.50
3:N:42:LEU:HD13	3:N:122:VAL:HG12	1.94	0.50
3:H:227:LEU:HD12	21:H:603:CDL:H782	1.92	0.50
3:N:15:ALA:HB1	3:N:19:ARG:HH12	1.77	0.50
1:O:121:ARG:NE	15:O:303:HEC:O2D	2.45	0.49
6:T:100:SER:HB2	7:R:135:ILE:HD11	1.93	0.49
7:R:499:TRP:HD1	7:R:499:TRP:O	1.95	0.49
1:O:126:ARG:HB2	7:R:77:GLU:HG2	1.93	0.49
2:M:260:ARG:HE	2:M:263:GLU:HG3	1.77	0.49
7:R:216:THR:HG23	7:R:269:ILE:HA	1.95	0.49
7:R:245:TYR:HA	7:R:251:GLY:HA3	1.95	0.49
2:M:130:PRO:HA	3:N:277:GLY:O	2.12	0.49
3:H:304:TYR:C	3:H:304:TYR:CD2	2.86	0.49
1:O:215:PRO:HA	1:O:218:ILE:HD12	1.95	0.49
13:O:305:MQ9:H151	3:N:389:PHE:CE2	2.47	0.49
5:S:59:PRO:HB3	5:S:136:TYR:CZ	2.47	0.49
8:Q:235:TRP:CD1	8:Q:242:LYS:HB3	2.48	0.49
10:V:106:ILE:HG22	10:V:127:VAL:HG22	1.93	0.49
3:H:386:LEU:HD21	3:H:418:LEU:HD13	1.95	0.49
3:N:34:PHE:CZ	3:N:231:TRP:HZ3	2.30	0.49
13:O:301:MQ9:H451	3:N:344:LEU:HA	1.95	0.48
4:P:28:VAL:HG13	4:P:42:HIS:HB2	1.94	0.48
7:R:212:ASN:HD22	7:R:276:GLY:N	2.10	0.48
3:H:152:MET:SD	3:H:304:TYR:O	2.71	0.48
3:N:370:VAL:HG22	4:P:39:GLY:HA3	1.95	0.48
14:P:302:WUO:C94	21:R:605:CDL:H572	2.43	0.48
3:H:54:LEU:HD23	20:H:602:HEM:HMC3	1.95	0.48
13:O:305:MQ9:C45	13:O:305:MQ9:H412	2.43	0.48
5:S:134:SER:HA	8:Q:184:PRO:HA	1.94	0.48
3:H:34:PHE:HE2	3:H:253:VAL:CG2	2.26	0.48
3:N:120:ILE:HG12	20:N:605:HEM:HAB	1.95	0.48
14:P:302:WUO:C29	25:R:603:HEA:H241	2.44	0.48
11:W:24:CYS:N	30:W:202:PLM:O2	2.46	0.48
2:M:352:PRO:HG2	3:N:295:VAL:HB	1.96	0.48
3:N:230:VAL:O	3:N:230:VAL:HG12	2.13	0.48
13:N:606:MQ9:H48	2:G:215:PHE:HD2	1.78	0.48
4:P:89:ARG:NH2	21:P:301:CDL:OA3	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:50:PHE:HE1	20:H:602:HEM:HBB1	1.78	0.48
3:N:40:PHE:CD1	3:N:235:HIS:HE1	2.32	0.48
7:R:152:THR:HA	7:R:259:PHE:CZ	2.49	0.48
25:R:602:HEA:HBD2	25:R:602:HEA:HMD1	1.96	0.48
10:V:73:LEU:HB3	10:V:77:THR:HA	1.95	0.48
3:H:50:PHE:CE1	20:H:602:HEM:HBB1	2.48	0.48
7:R:414:ILE:HG21	7:R:491:PHE:HZ	1.78	0.47
3:N:184:VAL:HG12	3:N:185:ILE:HG23	1.96	0.47
13:N:606:MQ9:H403	13:N:606:MQ9:H422	1.67	0.47
25:R:603:HEA:H211	25:R:603:HEA:H271	1.68	0.47
8:Q:123:LYS:HG2	8:Q:259:GLN:HG3	1.95	0.47
3:N:35:PRO:CB	3:N:40:PHE:HE2	2.26	0.47
7:R:480:GLY:HA2	7:R:483:ILE:HD12	1.95	0.47
7:R:509:ASP:HB3	10:V:31:VAL:HG12	1.95	0.47
1:O:226:PRO:HB2	15:O:303:HEC:O1D	2.14	0.47
3:N:137:ARG:HG2	31:N:753:HOH:O	2.14	0.47
3:N:349:PHE:HA	3:N:352:LYS:HG2	1.95	0.47
2:M:204:LEU:HD11	13:H:606:MQ9:H303	1.96	0.47
8:Q:137:GLN:HA	8:Q:138:TRP:HA	1.68	0.47
1:O:218:ILE:HG23	15:O:303:HEC:HMA1	1.96	0.47
7:R:426:LEU:HD23	7:R:498:SER:HB2	1.95	0.47
8:Q:307:LYS:HB3	8:Q:311:GLU:HG3	1.97	0.47
9:U:72:GLY:O	10:V:115:LYS:HD3	2.14	0.47
3:H:32:LYS:HG2	3:H:34:PHE:CZ	2.49	0.47
3:N:254:MET:HA	3:N:255:PRO:HA	1.73	0.47
8:Q:222:GLU:OE1	8:Q:259:GLN:NE2	2.40	0.47
10:V:70:ILE:HD11	10:V:143:LEU:CD1	2.45	0.47
11:W:24:CYS:HG	17:W:201:9YF:C24	2.28	0.47
2:M:351:CYS:HB2	16:M:501:FES:S2	2.55	0.47
6:T:90:TRP:HB3	7:R:33:THR:HG22	1.96	0.47
2:M:217:GLY:HA3	2:G:107:PHE:HE2	1.80	0.46
3:N:66:PRO:HG3	3:N:208:TYR:CD2	2.50	0.46
7:R:138:ALA:O	7:R:141:ILE:HG12	2.16	0.46
11:W:87:LYS:HG3	11:W:105:THR:HG22	1.97	0.46
3:H:400:PHE:HD2	3:H:402:ILE:H	1.62	0.46
3:N:394:ASP:OD1	3:N:395:ILE:N	2.49	0.46
7:R:395:ILE:HA	7:R:398:PHE:CE1	2.50	0.46
1:O:125:MET:HG3	7:R:162:HIS:HA	1.97	0.46
7:R:268:TYR:HA	7:R:271:ALA:HB3	1.97	0.46
8:Q:227:SER:HB2	8:Q:245:VAL:HG12	1.97	0.46
2:M:247:PHE:CE1	12:Y:45:PRO:HA	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:R:264:HIS:NE2	7:R:268:TYR:HE2	2.13	0.46
13:O:301:MQ9:H71	13:O:301:MQ9:H5M3	1.79	0.46
6:T:96:SER:HG	7:R:131:PHE:HD2	1.62	0.46
5:S:202:VAL:HG11	23:S:502:TRD:H62	1.98	0.46
3:H:160:SER:HA	3:H:167:SER:HB2	1.98	0.46
3:H:229:LEU:O	3:H:233:GLN:HB2	2.15	0.46
10:V:114:VAL:HA	10:V:117:ARG:HD3	1.97	0.46
3:H:120:ILE:HG22	3:H:148:LEU:HD12	1.97	0.46
2:G:265:PRO:HB3	2:G:291:ASP:HB2	1.98	0.46
3:N:35:PRO:HB2	3:N:40:PHE:CD2	2.50	0.46
18:G:504:7PH:H2D	18:G:504:7PH:H2AA	1.79	0.46
3:N:295:VAL:HG13	3:N:295:VAL:O	2.16	0.46
1:O:120:GLY:HA3	1:O:134:LYS:O	2.16	0.45
7:R:52:PHE:HE2	25:R:603:HEA:HMC3	1.79	0.45
3:H:124:LEU:HD12	20:H:605:HEM:HMC2	1.98	0.45
3:N:366:ARG:HE	21:N:602:CDL:H1O1	1.61	0.45
4:P:89:ARG:NH1	21:P:301:CDL:H381	2.30	0.45
7:R:405:THR:O	7:R:409:ALA:HB3	2.16	0.45
10:V:76:ASP:OD1	10:V:76:ASP:N	2.49	0.45
3:H:254:MET:HA	3:H:255:PRO:HA	1.72	0.45
20:H:605:HEM:HMA2	20:H:605:HEM:HAA2	1.83	0.45
8:Q:154:PHE:CD1	8:Q:297:LYS:HG2	2.51	0.45
8:Q:231:ILE:CG2	8:Q:275:GLU:HG2	2.46	0.45
2:M:249:GLY:HA3	12:Y:42:SER:HB2	1.99	0.45
1:O:273:MET:SD	13:O:301:MQ9:H3D	2.56	0.45
3:N:140:ASN:HD22	3:N:230:VAL:HG22	1.78	0.45
3:N:229:LEU:O	3:N:233:GLN:HB2	2.17	0.45
8:Q:209:GLU:OE1	11:W:82:THR:HG21	2.17	0.45
3:N:172:ARG:O	3:N:176:SER:HB3	2.16	0.45
21:P:301:CDL:H762	21:P:301:CDL:C54	2.46	0.45
7:R:53:LEU:HD23	7:R:488:MET:HE2	1.97	0.45
21:N:607:CDL:H151	6:T:123:THR:HG23	1.98	0.45
2:G:368:HIS:HB2	16:G:501:FES:S1	2.57	0.45
3:N:165:LEU:HD21	3:N:294:GLN:HB3	1.99	0.45
21:P:301:CDL:H762	21:P:301:CDL:C56	2.47	0.45
6:T:95:ILE:HG12	6:T:124:SER:HB3	1.99	0.45
7:R:532:GLU:HG3	10:V:23:THR:HB	1.99	0.45
11:W:44:ALA:HB3	11:W:51:LEU:HB2	1.99	0.45
20:N:601:HEM:CMB	20:N:601:HEM:HBB2	2.46	0.45
13:O:305:MQ9:H151	3:N:389:PHE:HE2	1.82	0.44
3:N:63:PHE:HZ	2:G:219:LEU:HG	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:W:54:VAL:HG22	11:W:75:PHE:HB2	1.99	0.44
21:H:601:CDL:H112	21:H:603:CDL:H511	1.99	0.44
1:O:99:PRO:O	8:Q:330:SER:HB3	2.16	0.44
1:O:218:ILE:HA	15:O:303:HEC:HMA2	1.98	0.44
3:H:116:PHE:O	3:H:120:ILE:HG13	2.17	0.44
13:H:606:MQ9:H5M3	13:H:606:MQ9:H72	1.77	0.44
25:R:602:HEA:H212	8:Q:60:VAL:HG11	1.99	0.44
3:H:366:ARG:HG2	3:H:368:ARG:HG2	1.98	0.44
3:H:418:LEU:HB3	3:H:419:PRO:HD3	2.00	0.44
7:R:267:VAL:HB	25:R:602:HEA:HAC	1.98	0.44
8:Q:194:THR:HG22	8:Q:194:THR:O	2.18	0.44
21:R:605:CDL:HA31	21:R:605:CDL:OA7	2.18	0.44
20:H:602:HEM:HBC2	20:H:602:HEM:CHD	2.34	0.44
5:S:23:ASN:HB3	5:S:26:SER:HB2	1.98	0.44
7:R:212:ASN:ND2	7:R:276:GLY:N	2.66	0.44
8:Q:124:ASP:OD2	8:Q:125:PRO:HD2	2.18	0.44
13:H:606:MQ9:H422	13:H:606:MQ9:H403	1.77	0.44
11:W:107:PRO:HG2	11:W:110:GLY:HA3	2.00	0.44
3:H:371:PRO:HB3	3:H:430:ALA:HB3	1.99	0.44
21:N:603:CDL:H801	21:N:603:CDL:H772	1.59	0.44
11:W:50:SER:HB2	11:W:78:ALA:HB3	1.99	0.44
7:R:48:CYS:SG	7:R:97:PRO:HG2	2.58	0.43
11:W:98:VAL:HG22	11:W:137:VAL:HG22	2.00	0.43
3:H:185:ILE:HD12	3:H:189:MET:SD	2.57	0.43
7:R:414:ILE:O	7:R:418:PHE:HB2	2.18	0.43
3:H:367:PRO:HG2	21:H:604:CDL:HA32	1.99	0.43
13:O:305:MQ9:H422	13:O:305:MQ9:H403	1.74	0.43
2:M:185:LEU:HB2	18:M:503:7PH:H35	2.00	0.43
3:N:497:PRO:HA	5:S:169:LYS:HA	2.00	0.43
5:S:165:THR:HA	5:S:174:GLN:HE22	1.84	0.43
3:N:29:GLN:HG3	3:N:231:TRP:HZ2	1.82	0.43
21:R:605:CDL:H711	21:R:605:CDL:H741	1.71	0.43
13:N:606:MQ9:H321	13:N:606:MQ9:H303	1.81	0.43
2:G:46:GLU:O	2:G:50:MET:HG3	2.18	0.43
2:M:336:PHE:HD1	12:Y:36:PRO:HG2	1.83	0.43
3:N:490:LYS:HA	3:N:490:LYS:HD2	1.92	0.43
25:R:603:HEA:HBC1	25:R:603:HEA:CHD	2.36	0.43
3:H:426:ALA:HB2	21:H:604:CDL:H361	2.00	0.43
2:M:352:PRO:HD2	3:N:295:VAL:CG2	2.49	0.43
3:N:154:GLU:HB2	3:N:215:ILE:HG21	2.01	0.43
8:Q:43:ALA:HB1	8:Q:240:LEU:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:305:MQ9:H451	13:O:305:MQ9:H411	2.00	0.43
7:R:151:TRP:NE1	25:R:602:HEA:O2D	2.52	0.43
7:R:227:LEU:HD22	7:R:262:PHE:CZ	2.53	0.43
7:R:495:VAL:CG1	21:R:605:CDL:H371	2.48	0.43
21:R:601:CDL:H182	21:R:601:CDL:H372	2.00	0.43
21:H:601:CDL:H511	21:H:603:CDL:CA5	2.48	0.43
5:S:147:HIS:NE2	5:S:192:TRP:HB2	2.34	0.43
8:Q:95:GLU:O	8:Q:99:THR:HG23	2.18	0.43
3:H:38:TRP:HZ2	21:H:604:CDL:HB61	1.83	0.43
3:H:304:TYR:C	3:H:304:TYR:HD2	2.22	0.43
11:W:31:GLN:O	11:W:35:GLN:HG3	2.19	0.43
3:H:166:LEU:HD21	3:H:300:GLN:H	1.83	0.43
2:M:319:PRO:HB3	11:W:148:LEU:HD21	2.00	0.42
3:N:424:PHE:HB2	21:P:301:CDL:H521	2.01	0.42
6:T:70:TYR:CB	6:T:73:ALA:HB2	2.47	0.42
7:R:37:HIS:O	7:R:104:ASN:HB3	2.19	0.42
3:H:111:TRP:HD1	3:H:276:GLY:HA2	1.84	0.42
3:H:133:PHE:HD1	3:H:348:PRO:HB3	1.84	0.42
2:G:79:THR:HG23	2:G:82:GLU:H	1.83	0.42
2:M:184:ALA:HB1	3:H:255:PRO:HB3	2.00	0.42
3:N:499:THR:HB	3:N:511:HIS:HB2	2.01	0.42
7:R:499:TRP:O	7:R:499:TRP:CD1	2.72	0.42
3:H:48:TYR:OH	3:H:261:SER:OG	2.37	0.42
13:H:607:MQ9:H321	13:H:607:MQ9:H303	1.65	0.42
7:R:212:ASN:HD22	7:R:276:GLY:H	1.68	0.42
3:N:230:VAL:HG13	31:N:701:HOH:O	2.19	0.42
20:H:602:HEM:HHD	20:H:602:HEM:CBC	2.42	0.42
13:O:305:MQ9:H451	13:O:305:MQ9:H412	1.99	0.42
20:N:601:HEM:HBC1	3:H:213:LEU:HD21	2.01	0.42
7:R:212:ASN:ND2	7:R:272:LEU:O	2.52	0.42
25:R:603:HEA:CBD	25:R:603:HEA:CHA	2.91	0.42
1:O:110:GLU:HG3	1:O:147:GLY:HA3	2.02	0.42
21:H:604:CDL:H311	21:H:604:CDL:HA61	1.58	0.42
13:O:305:MQ9:H303	17:W:201:9YF:C37	2.49	0.42
5:S:53:GLN:HB3	8:Q:186:ARG:HH11	1.85	0.42
7:R:460:ARG:O	8:Q:281:HIS:HD2	2.02	0.42
3:H:22:PRO:HB3	21:H:601:CDL:HA62	2.02	0.42
3:H:124:LEU:HD12	20:H:605:HEM:CMC	2.49	0.42
3:H:367:PRO:CG	21:H:604:CDL:HA31	2.49	0.42
4:P:60:LEU:O	4:P:63:MET:HG3	2.20	0.42
5:S:33:LEU:HD23	5:S:33:LEU:HA	1.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Q:231:ILE:HG22	8:Q:275:GLU:HG2	2.01	0.42
3:H:408:THR:HB	2:G:382:PHE:HZ	1.84	0.42
2:M:393:PRO:HB2	2:M:405:ASN:HB3	2.02	0.42
20:N:605:HEM:HMC2	20:N:605:HEM:CBC	2.44	0.42
6:T:125:VAL:HG11	21:R:601:CDL:H362	2.02	0.42
3:H:94:ASP:HA	3:H:98:GLU:OE1	2.20	0.42
3:H:124:LEU:HD11	3:H:344:LEU:HD11	2.02	0.42
5:S:31:VAL:HG12	7:R:187:VAL:HG22	2.01	0.41
5:S:156:VAL:HG22	18:S:501:7PH:H3B	2.02	0.41
3:H:120:ILE:HG12	20:H:605:HEM:HAB	2.00	0.41
3:N:505:PRO:HB3	5:S:97:PHE:CE2	2.55	0.41
8:Q:224:VAL:HG22	8:Q:257:VAL:HG22	2.03	0.41
11:W:144:THR:H	11:W:149:TYR:HH	1.67	0.41
3:H:78:GLN:HA	3:H:81:ARG:HG3	2.01	0.41
3:H:370:VAL:HG12	3:H:373:ARG:H	1.86	0.41
3:N:195:GLY:HA3	3:N:202:ILE:HD11	2.02	0.41
7:R:106:VAL:HG11	7:R:417:TRP:CE2	2.55	0.41
7:R:178:GLY:HA3	31:R:761:HOH:O	2.21	0.41
2:G:418:GLU:H	2:G:418:GLU:CD	2.23	0.41
13:O:301:MQ9:H221	13:O:301:MQ9:H203	1.65	0.41
7:R:49:PHE:HZ	7:R:411:TYR:OH	2.01	0.41
7:R:89:VAL:HG22	7:R:93:PHE:HD2	1.86	0.41
8:Q:284:MET:O	8:Q:284:MET:CG	2.69	0.41
10:V:68:VAL:HG11	10:V:143:LEU:HD13	2.01	0.41
3:H:248:VAL:HG22	2:G:164:ARG:NH2	2.35	0.41
21:H:601:CDL:H182	21:H:601:CDL:H152	1.86	0.41
3:N:289:PRO:HG2	3:N:291:LYS:HE2	2.02	0.41
7:R:310:VAL:O	7:R:313:HIS:ND1	2.54	0.41
10:V:106:ILE:HG22	10:V:106:ILE:O	2.20	0.41
2:M:174:ARG:NH1	3:H:17:ASP:OD2	2.48	0.41
3:N:110:HIS:HB2	20:N:601:HEM:HBA1	2.02	0.41
3:N:152:MET:HE2	3:N:152:MET:HB3	1.85	0.41
7:R:264:HIS:O	7:R:267:VAL:HG22	2.21	0.41
8:Q:106:ILE:HG13	8:Q:107:SER:N	2.36	0.41
8:Q:233:GLY:O	8:Q:273:CYS:HA	2.21	0.41
3:H:291:LYS:HD3	3:H:291:LYS:HA	1.89	0.41
1:O:227:GLN:HB3	1:O:228:ASN:H	1.68	0.41
13:N:606:MQ9:H211	13:N:606:MQ9:H252	2.02	0.41
8:Q:195:TYR:CD1	8:Q:195:TYR:N	2.86	0.41
3:H:271:VAL:O	3:H:275:MET:HG3	2.21	0.41
13:O:301:MQ9:H161	21:N:602:CDL:H571	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:107:PHE:CE2	2:G:217:GLY:HA3	2.53	0.41
2:M:380:PRO:HD3	2:M:388:ALA:HA	2.03	0.41
3:N:303:PHE:HA	3:N:306:MET:SD	2.60	0.41
3:N:499:THR:HG21	3:N:514:LEU:HD12	2.02	0.41
7:R:227:LEU:HB2	7:R:262:PHE:CG	2.56	0.41
9:U:33:PRO:HG2	10:V:41:TYR:O	2.21	0.41
11:W:41:GLY:HA3	11:W:53:ASN:HA	2.01	0.41
3:H:248:VAL:HG22	2:G:164:ARG:HH21	1.85	0.41
2:G:255:ALA:HB1	2:G:266:PHE:HB3	2.02	0.41
7:R:284:VAL:HG22	7:R:514:GLY:HA2	2.02	0.41
25:R:603:HEA:H261	25:R:603:HEA:H172	1.25	0.41
3:H:237:GLN:NE2	3:H:247:ASN:O	2.53	0.41
1:O:194:PHE:CD2	3:N:287:LEU:HD22	2.56	0.40
7:R:430:LEU:HD21	7:R:493:TRP:HD1	1.85	0.40
20:H:602:HEM:HBB2	20:H:602:HEM:CHC	2.29	0.40
1:O:193:ASN:HA	3:N:296:SER:OG	2.20	0.40
5:S:58:TRP:HA	5:S:59:PRO:HA	1.96	0.40
6:T:5:ALA:HB2	6:T:56:PHE:CB	2.51	0.40
7:R:384:LEU:O	7:R:388:VAL:HG22	2.21	0.40
25:R:603:HEA:O11	25:R:603:HEA:CHC	2.70	0.40
2:G:190:LEU:HD22	18:G:505:7PH:H3BA	2.03	0.40
3:N:210:LEU:HD23	3:N:214:LEU:HD12	2.02	0.40
7:R:223:ALA:O	7:R:226:ILE:HG22	2.20	0.40
7:R:341:PHE:HE1	7:R:369:PHE:HD2	1.68	0.40
1:O:80:LYS:O	1:O:84:GLU:HG3	2.21	0.40
3:N:315:TRP:HB3	3:N:329:GLN:NE2	2.36	0.40
7:R:120:ARG:NE	21:R:601:CDL:OB3	2.40	0.40
8:Q:299:TYR:HB2	8:Q:316:ILE:HD13	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [\(i\)](#)

5.3.1 Protein backbone [\(i\)](#)

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	O	221/278 (80%)	211 (96%)	10 (4%)	0	100	100
2	G	378/408 (93%)	365 (97%)	13 (3%)	0	100	100
2	M	378/408 (93%)	370 (98%)	8 (2%)	0	100	100
3	H	433/556 (78%)	422 (98%)	10 (2%)	1 (0%)	44	66
3	N	531/556 (96%)	518 (98%)	13 (2%)	0	100	100
4	P	71/100 (71%)	70 (99%)	1 (1%)	0	100	100
5	S	182/203 (90%)	181 (100%)	1 (0%)	0	100	100
6	T	137/139 (99%)	134 (98%)	3 (2%)	0	100	100
7	R	549/575 (96%)	544 (99%)	5 (1%)	0	100	100
8	Q	295/341 (86%)	287 (97%)	8 (3%)	0	100	100
9	U	62/79 (78%)	62 (100%)	0	0	100	100
10	V	141/157 (90%)	137 (97%)	4 (3%)	0	100	100
11	W	145/186 (78%)	132 (91%)	13 (9%)	0	100	100
12	Y	23/236 (10%)	20 (87%)	3 (13%)	0	100	100
12	c	23/236 (10%)	22 (96%)	1 (4%)	0	100	100
All	All	3569/4458 (80%)	3475 (97%)	93 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	H	184	VAL

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	O	163/206 (79%)	159 (98%)	4 (2%)	42	68
2	G	311/333 (93%)	311 (100%)	0	100	100
2	M	311/333 (93%)	311 (100%)	0	100	100
3	H	351/448 (78%)	340 (97%)	11 (3%)	35	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	N	428/448 (96%)	422 (99%)	6 (1%)	62	82
4	P	58/83 (70%)	58 (100%)	0	100	100
5	S	146/161 (91%)	146 (100%)	0	100	100
6	T	106/106 (100%)	105 (99%)	1 (1%)	75	90
7	R	453/471 (96%)	449 (99%)	4 (1%)	75	90
8	Q	255/288 (88%)	250 (98%)	5 (2%)	50	74
9	U	51/59 (86%)	49 (96%)	2 (4%)	27	53
10	V	105/114 (92%)	100 (95%)	5 (5%)	21	44
11	W	121/146 (83%)	121 (100%)	0	100	100
12	Y	20/167 (12%)	20 (100%)	0	100	100
12	c	20/167 (12%)	20 (100%)	0	100	100
All	All	2899/3530 (82%)	2861 (99%)	38 (1%)	64	84

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	121	ARG
1	O	193	ASN
1	O	209	ASP
1	O	227	GLN
3	N	81	ARG
3	N	187	THR
3	N	191	TRP
3	N	294	GLN
3	N	305	MET
3	N	337	MET
6	T	70	TYR
7	R	44	TYR
7	R	129	PHE
7	R	288	LYS
7	R	403	PHE
8	Q	69	PHE
8	Q	139	ASN
8	Q	195	TYR
8	Q	206	THR
8	Q	229	ASP
9	U	34	ASP
9	U	71	ILE

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Mol	Chain	Res	Type
10	V	82	ARG
10	V	83	GLU
10	V	84	ILE
10	V	85	LEU
10	V	103	GLN
3	H	138	GLU
3	H	180	MET
3	H	185	ILE
3	H	187	THR
3	H	191	TRP
3	H	265	PHE
3	H	300	GLN
3	H	302	ASP
3	H	303	PHE
3	H	304	TYR
3	H	305	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
3	N	140	ASN

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 53 ligands modelled in this entry, 5 are monoatomic - leaving 48 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
20	HEM	N	601	3	41,50,50	1.67	10 (24%)	45,82,82	2.16	11 (24%)
23	TRD	R	608	-	12,12,12	0.09	0	11,11,11	0.05	0
24	3PE	S	503	-	31,31,50	0.33	0	34,36,55	0.38	0
13	MQ9	N	606	-	59,59,59	0.34	0	72,75,75	0.31	0
23	TRD	S	502	-	12,12,12	0.09	0	11,11,11	0.06	0
18	7PH	M	503	-	37,37,37	0.30	0	41,42,42	0.34	0
16	FES	M	501	2	0,4,4	-	-	-	-	-
14	WUO	O	302	-	99,99,99	1.60	10 (10%)	123,125,125	1.29	12 (9%)
30	PLM	W	202	-	10,10,17	0.78	0	9,9,17	0.60	0
21	CDL	H	604	-	76,76,99	0.30	0	82,88,111	0.34	0
23	TRD	Q	403	-	12,12,12	0.09	0	11,11,11	0.06	0
15	HEC	O	303	1	32,50,50	2.02	4 (12%)	24,82,82	2.28	12 (50%)
25	HEA	R	603	7	57,67,67	2.09	16 (28%)	61,103,103	2.25	25 (40%)
18	7PH	G	504	-	37,37,37	0.95	4 (10%)	41,42,42	1.14	2 (4%)
18	7PH	S	501	-	37,37,37	0.30	0	41,42,42	0.34	0
13	MQ9	O	305	-	59,59,59	0.48	0	72,75,75	0.41	0
13	MQ9	H	607	-	59,59,59	0.35	0	72,75,75	0.31	0
13	MQ9	O	301	-	59,59,59	0.36	0	72,75,75	0.32	0
13	MQ9	H	606	-	59,59,59	0.35	0	72,75,75	0.32	0
17	9YF	W	201	-	58,58,58	1.40	5 (8%)	69,71,71	1.08	3 (4%)
20	HEM	H	602	3	41,50,50	1.70	10 (24%)	45,82,82	2.05	15 (33%)
18	7PH	G	505	-	37,37,37	0.96	4 (10%)	41,42,42	1.11	2 (4%)
30	PLM	c	301	-	10,10,17	0.41	0	9,9,17	0.45	0
23	TRD	T	201	-	12,12,12	0.09	0	11,11,11	0.05	0
21	CDL	N	603	-	78,78,99	0.29	0	84,90,111	0.34	0
21	CDL	R	605	-	76,76,99	0.29	0	82,88,111	0.34	0
14	WUO	P	302	-	99,99,99	1.61	10 (10%)	123,125,125	1.30	12 (9%)
25	HEA	R	602	7	57,67,67	1.92	16 (28%)	61,103,103	2.47	24 (39%)
19	IZL	M	504	-	119,119,119	1.75	30 (25%)	161,163,163	1.31	18 (11%)
19	IZL	G	503	-	119,119,119	1.75	30 (25%)	161,163,163	1.31	18 (11%)
20	HEM	H	605	3	41,50,50	1.81	13 (31%)	45,82,82	2.12	15 (33%)
17	9YF	M	502	-	58,58,58	1.38	5 (8%)	69,71,71	1.08	3 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CDL	N	602	-	76,76,99	0.29	0	82,88,111	0.34	0
15	HEC	O	304	1	32,50,50	1.96	5 (15%)	24,82,82	2.10	9 (37%)
21	CDL	H	601	-	73,73,99	0.30	0	79,85,111	0.35	0
30	PLM	Y	301	-	10,10,17	0.79	0	9,9,17	0.60	0
21	CDL	R	601	-	76,76,99	0.29	0	82,88,111	0.34	0
21	CDL	H	603	-	73,73,99	0.30	0	79,85,111	0.35	0
28	9XX	R	609	-	41,41,41	1.14	2 (4%)	44,44,44	0.96	4 (9%)
21	CDL	N	607	-	78,78,99	0.29	0	84,90,111	0.35	0
28	9XX	c	302	-	31,31,41	1.25	2 (6%)	34,34,44	1.09	4 (11%)
21	CDL	P	301	-	76,76,99	0.40	0	82,88,111	0.52	0
22	A1IGA	N	604	-	24,26,26	1.99	5 (20%)	30,37,37	3.14	7 (23%)
20	HEM	N	605	3	41,50,50	1.74	12 (29%)	45,82,82	1.96	13 (28%)
16	FES	G	501	2	0,4,4	-	-	-	-	-
28	9XX	Y	302	-	31,31,41	1.25	2 (6%)	34,34,44	1.12	4 (11%)
23	TRD	R	607	-	12,12,12	0.09	0	11,11,11	0.06	0
17	9YF	G	502	-	58,58,58	1.39	5 (8%)	69,71,71	1.07	3 (4%)

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
20	HEM	N	601	3	-	7/12/54/54	-
23	TRD	R	608	-	-	2/10/10/10	-
24	3PE	S	503	-	-	14/35/35/54	-
13	MQ9	N	606	-	-	27/53/73/73	0/2/2/2
23	TRD	S	502	-	-	2/10/10/10	-
18	7PH	M	503	-	-	16/39/39/39	-
30	PLM	W	202	-	-	1/7/8/15	-
14	WUO	O	302	-	-	29/84/148/148	0/3/3/3
16	FES	M	501	2	-	-	0/1/1/1
21	CDL	H	604	-	-	41/87/87/110	-
23	TRD	Q	403	-	-	1/10/10/10	-
15	HEC	O	303	1	-	3/10/54/54	-
25	HEA	R	603	7	-	14/32/76/76	-
18	7PH	G	504	-	-	10/39/39/39	-
18	7PH	S	501	-	-	13/39/39/39	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	MQ9	O	305	-	-	20/53/73/73	0/2/2/2
13	MQ9	H	607	-	-	28/53/73/73	0/2/2/2
13	MQ9	O	301	-	-	9/53/73/73	0/2/2/2
13	MQ9	H	606	-	-	21/53/73/73	0/2/2/2
17	9YF	W	201	-	-	33/54/78/78	0/1/1/1
20	HEM	H	602	3	-	4/12/54/54	-
18	7PH	G	505	-	-	11/39/39/39	-
30	PLM	c	301	-	-	0/7/8/15	-
23	TRD	T	201	-	-	1/10/10/10	-
21	CDL	N	603	-	-	53/89/89/110	-
21	CDL	R	605	-	-	42/87/87/110	-
14	WUO	P	302	-	-	42/84/148/148	0/3/3/3
25	HEA	R	602	7	-	10/32/76/76	-
19	IZL	M	504	-	-	38/84/208/208	0/6/6/6
19	IZL	G	503	-	-	38/84/208/208	0/6/6/6
20	HEM	H	605	3	-	8/12/54/54	-
17	9YF	M	502	-	-	28/54/78/78	0/1/1/1
21	CDL	N	602	-	-	51/87/87/110	-
15	HEC	O	304	1	-	5/10/54/54	-
21	CDL	H	601	-	-	37/84/84/110	-
30	PLM	Y	301	-	-	0/7/8/15	-
21	CDL	R	601	-	-	53/87/87/110	-
21	CDL	H	603	-	-	41/84/84/110	-
28	9XX	R	609	-	-	24/43/43/43	-
21	CDL	N	607	-	-	48/89/89/110	-
28	9XX	c	302	-	-	16/33/33/43	-
21	CDL	P	301	-	-	47/87/87/110	-
22	A1IGA	N	604	-	-	5/9/11/11	0/3/3/3
20	HEM	N	605	3	-	8/12/54/54	-
16	FES	G	501	2	-	-	0/1/1/1
28	9XX	Y	302	-	-	11/33/33/43	-
23	TRD	R	607	-	-	1/10/10/10	-
17	9YF	G	502	-	-	28/54/78/78	0/1/1/1

All (200) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	O	302	WUO	P52-O51	6.61	1.77	1.60
14	P	302	WUO	P52-O51	6.60	1.77	1.60
15	O	303	HEC	C2B-C3B	-6.50	1.34	1.40
15	O	303	HEC	C3C-C2C	-6.17	1.34	1.40
15	O	304	HEC	C3C-C2C	-5.92	1.34	1.40
15	O	304	HEC	C2B-C3B	-5.90	1.34	1.40
14	P	302	WUO	C50-C01	5.73	1.64	1.52
17	W	201	9YF	P-O2	5.60	1.75	1.60
14	O	302	WUO	C50-C01	5.59	1.63	1.52
17	G	502	9YF	P-O2	5.56	1.75	1.60
25	R	603	HEA	CHD-C1D	5.53	1.49	1.35
14	O	302	WUO	P52-O55	5.25	1.80	1.59
14	P	302	WUO	P52-O55	5.20	1.80	1.59
17	M	502	9YF	P-O2	5.16	1.74	1.60
19	G	503	IZL	P-O28	5.02	1.73	1.60
19	M	504	IZL	P-O28	5.00	1.73	1.60
25	R	603	HEA	C3B-C2B	4.92	1.45	1.34
20	H	605	HEM	C1B-NB	-4.85	1.31	1.40
25	R	602	HEA	CHC-C4B	4.83	1.47	1.35
25	R	602	HEA	C3B-C2B	4.78	1.45	1.34
25	R	602	HEA	C3D-C2D	4.76	1.46	1.36
14	P	302	WUO	C56-C57	4.76	1.65	1.50
14	O	302	WUO	C56-C57	4.75	1.65	1.50
19	G	503	IZL	C44-C45	4.71	1.65	1.50
19	M	504	IZL	C44-C45	4.68	1.65	1.50
25	R	603	HEA	CHC-C4B	4.62	1.46	1.35
22	N	604	A1IGA	C04-S01	4.61	1.92	1.82
22	N	604	A1IGA	C02-C03	4.48	1.43	1.39
22	N	604	A1IGA	C05-S01	4.42	1.83	1.75
25	R	602	HEA	CHD-C1D	4.40	1.46	1.35
19	G	503	IZL	C43-C14	4.36	1.61	1.52
19	M	504	IZL	C43-C14	4.33	1.61	1.52
17	W	201	9YF	P-O	4.29	1.76	1.59
20	N	601	HEM	C1B-NB	-4.28	1.32	1.40
17	M	502	9YF	P-O	4.27	1.76	1.59
17	G	502	9YF	P-O	4.26	1.76	1.59
25	R	603	HEA	C4B-NB	-4.23	1.33	1.40
20	N	605	HEM	C1B-NB	-4.21	1.33	1.40
28	R	609	9XX	C16-C17	4.17	1.60	1.50
20	N	605	HEM	C4D-ND	-4.17	1.33	1.40
28	c	302	9XX	C16-C17	4.14	1.60	1.50
20	N	601	HEM	C4D-ND	-4.13	1.33	1.40
28	Y	302	9XX	C16-C17	4.13	1.60	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	R	603	HEA	C3D-C2D	4.12	1.45	1.36
20	H	605	HEM	C4D-ND	-4.11	1.33	1.40
25	R	603	HEA	FE-NB	4.03	2.16	1.96
22	N	604	A1IGA	C04-C03	3.96	1.54	1.50
19	M	504	IZL	P-O31	3.93	1.75	1.59
19	G	503	IZL	P-O31	3.92	1.75	1.59
20	H	602	HEM	C1B-NB	-3.87	1.33	1.40
25	R	603	HEA	C1D-ND	-3.84	1.33	1.40
14	P	302	WUO	C50-C37	3.77	1.60	1.52
14	O	302	WUO	C50-C37	3.72	1.60	1.52
15	O	303	HEC	CBC-CAC	-3.69	1.35	1.49
20	H	602	HEM	C4D-ND	-3.66	1.34	1.40
20	H	602	HEM	C3C-C2C	-3.66	1.35	1.40
25	R	603	HEA	C3A-C2A	3.61	1.45	1.40
20	H	602	HEM	FE-NB	3.59	2.14	1.96
25	R	602	HEA	C1D-ND	-3.57	1.34	1.40
25	R	602	HEA	C3A-C2A	3.46	1.45	1.40
15	O	304	HEC	CBC-CAC	-3.43	1.36	1.49
20	H	605	HEM	C4B-NB	-3.38	1.31	1.38
25	R	602	HEA	C4B-NB	-3.33	1.34	1.40
20	N	601	HEM	O2D-CGD	-3.30	1.19	1.30
25	R	602	HEA	C3C-C2C	3.28	1.44	1.40
14	O	302	WUO	C76-C57	3.19	1.60	1.50
14	P	302	WUO	C76-C57	3.18	1.60	1.50
19	G	503	IZL	C31-C36	3.02	1.61	1.52
19	M	504	IZL	C31-C36	3.01	1.61	1.52
25	R	603	HEA	FE-ND	2.97	2.11	1.96
19	M	504	IZL	C25-C30	2.93	1.59	1.52
19	G	503	IZL	C25-C30	2.92	1.59	1.52
20	H	602	HEM	O2D-CGD	-2.92	1.20	1.30
25	R	602	HEA	FE-NB	2.87	2.11	1.96
20	N	605	HEM	O2A-CGA	-2.81	1.21	1.30
20	N	601	HEM	C4B-NB	-2.81	1.33	1.38
25	R	603	HEA	O2D-CGD	-2.78	1.21	1.30
19	M	504	IZL	C43-C18	2.76	1.58	1.52
20	N	605	HEM	C4B-NB	-2.76	1.33	1.38
25	R	603	HEA	O2A-CGA	-2.75	1.21	1.30
20	N	605	HEM	O2D-CGD	-2.74	1.21	1.30
20	H	605	HEM	C1B-C2B	-2.73	1.39	1.44
19	G	503	IZL	C43-C18	2.73	1.57	1.52
20	H	605	HEM	C1D-ND	-2.72	1.33	1.38
19	G	503	IZL	O38-C73	-2.71	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	N	605	HEM	FE-NB	2.71	2.10	1.96
20	N	605	HEM	C1D-ND	-2.70	1.33	1.38
19	M	504	IZL	O38-C73	-2.70	1.36	1.43
25	R	603	HEA	C3C-C2C	2.69	1.44	1.40
17	M	502	9YF	C1-C	2.65	1.58	1.50
19	M	504	IZL	C29-C28	2.63	1.59	1.52
19	G	503	IZL	C29-C28	2.63	1.59	1.52
19	M	504	IZL	O28-C43	-2.63	1.34	1.44
19	G	503	IZL	O28-C43	-2.63	1.34	1.44
19	M	504	IZL	C61-C60	2.62	1.58	1.50
20	H	602	HEM	O2A-CGA	-2.62	1.21	1.30
19	G	503	IZL	C61-C60	2.61	1.58	1.50
17	W	201	9YF	C1-C	2.61	1.58	1.50
19	G	503	IZL	C13-C71	2.60	1.60	1.52
25	R	603	HEA	C4C-CHD	2.60	1.48	1.41
19	M	504	IZL	C13-C71	2.58	1.59	1.52
25	R	602	HEA	FE-ND	2.55	2.09	1.96
20	H	602	HEM	C4B-NB	-2.55	1.33	1.38
17	G	502	9YF	C1-C	2.50	1.58	1.50
18	G	504	7PH	O21-C2	-2.50	1.40	1.46
18	G	505	7PH	O21-C2	-2.50	1.40	1.46
19	G	503	IZL	O24-C39	-2.48	1.37	1.43
20	N	605	HEM	C1B-C2B	-2.48	1.39	1.44
19	M	504	IZL	O24-C39	-2.48	1.37	1.43
19	G	503	IZL	O37-C72	-2.46	1.37	1.43
25	R	603	HEA	C1B-NB	-2.44	1.33	1.38
19	M	504	IZL	O37-C72	-2.44	1.37	1.43
19	G	503	IZL	O1-C10	2.44	1.40	1.33
18	G	505	7PH	O31-C31	2.44	1.40	1.33
25	R	603	HEA	CAA-C2A	-2.42	1.48	1.52
18	G	504	7PH	O31-C31	2.42	1.40	1.33
19	G	503	IZL	O34-C60	2.42	1.41	1.34
19	M	504	IZL	O1-C10	2.41	1.40	1.33
19	G	503	IZL	C48-C47	2.41	1.57	1.50
19	M	504	IZL	O34-C60	2.40	1.41	1.34
20	N	605	HEM	C3D-C2D	-2.40	1.31	1.36
19	M	504	IZL	C48-C47	2.40	1.57	1.50
20	H	605	HEM	O2D-CGD	-2.39	1.22	1.30
22	N	604	A1IGA	C15-C16	2.39	1.58	1.48
25	R	602	HEA	C4B-C3B	2.38	1.48	1.44
20	N	601	HEM	FE-NB	2.37	2.08	1.96
17	M	502	9YF	C24-C	2.37	1.58	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	H	602	HEM	C1B-C2B	-2.35	1.40	1.44
15	O	304	HEC	CBB-CAB	-2.35	1.40	1.49
20	N	601	HEM	O2A-CGA	-2.35	1.22	1.30
19	M	504	IZL	O23-C38	-2.34	1.37	1.43
20	N	601	HEM	C3C-C2C	-2.33	1.37	1.40
19	G	503	IZL	O23-C38	-2.32	1.37	1.43
17	W	201	9YF	C24-C	2.32	1.57	1.50
20	N	601	HEM	C1D-ND	-2.31	1.34	1.38
19	G	503	IZL	C24-C23	2.31	1.58	1.51
15	O	303	HEC	CBB-CAB	-2.31	1.40	1.49
19	M	504	IZL	C24-C23	2.31	1.58	1.51
19	M	504	IZL	O6-C17	-2.31	1.37	1.43
20	N	605	HEM	C3C-C2C	-2.31	1.37	1.40
20	H	605	HEM	FE-NB	2.29	2.08	1.96
20	H	605	HEM	C2C-C1C	-2.28	1.37	1.42
19	G	503	IZL	O6-C17	-2.28	1.37	1.43
19	G	503	IZL	C35-C34	2.28	1.58	1.52
19	M	504	IZL	O26-C41	-2.28	1.37	1.43
19	M	504	IZL	C35-C34	2.27	1.58	1.52
14	P	302	WUO	O77-C78	2.27	1.40	1.33
14	O	302	WUO	O77-C78	2.27	1.39	1.33
19	G	503	IZL	O26-C41	-2.26	1.37	1.43
25	R	602	HEA	O2D-CGD	-2.26	1.23	1.30
17	G	502	9YF	C24-C	2.26	1.57	1.50
25	R	602	HEA	O2A-CGA	-2.25	1.23	1.30
20	H	605	HEM	FE-ND	-2.25	1.85	1.96
20	H	605	HEM	C1A-CHA	-2.24	1.34	1.41
25	R	603	HEA	C1C-CHC	2.23	1.47	1.41
25	R	602	HEA	C1B-NB	-2.23	1.34	1.38
19	G	503	IZL	C36-C35	2.22	1.58	1.52
19	M	504	IZL	C36-C35	2.22	1.58	1.52
20	H	602	HEM	CAA-C2A	-2.22	1.48	1.52
25	R	602	HEA	C1C-CHC	2.22	1.47	1.41
14	O	302	WUO	C31-C01	2.18	1.58	1.52
14	P	302	WUO	C06-C05	2.17	1.57	1.53
18	G	505	7PH	O21-C21	2.16	1.40	1.34
14	O	302	WUO	C06-C05	2.16	1.57	1.53
14	P	302	WUO	C31-C01	2.15	1.58	1.52
20	N	605	HEM	FE-ND	-2.15	1.86	1.96
19	G	503	IZL	P-O30	-2.13	1.45	1.55
19	M	504	IZL	P-O30	-2.13	1.45	1.55
19	G	503	IZL	O1-C11	-2.13	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	H	605	HEM	O2A-CGA	-2.12	1.23	1.30
18	G	504	7PH	O31-C3	-2.12	1.40	1.45
19	M	504	IZL	O1-C11	-2.11	1.40	1.45
25	R	602	HEA	C4D-ND	-2.11	1.34	1.38
20	N	601	HEM	C2C-C1C	-2.11	1.37	1.42
19	M	504	IZL	O4-C15	-2.11	1.38	1.43
18	G	504	7PH	O21-C21	2.11	1.40	1.34
28	R	609	9XX	O-C15	2.11	1.39	1.33
18	G	505	7PH	O31-C3	-2.10	1.40	1.45
14	O	302	WUO	O51-C50	-2.10	1.36	1.44
14	P	302	WUO	O51-C50	-2.10	1.36	1.44
19	G	503	IZL	O12-C26	-2.10	1.39	1.44
19	M	504	IZL	O12-C26	-2.09	1.39	1.44
28	c	302	9XX	O-C15	2.09	1.39	1.33
28	Y	302	9XX	O-C15	2.08	1.39	1.33
20	H	605	HEM	CAA-C2A	-2.08	1.49	1.52
19	G	503	IZL	O4-C15	-2.07	1.38	1.43
19	M	504	IZL	C33-C32	2.07	1.58	1.51
20	N	601	HEM	C1B-C2B	-2.07	1.40	1.44
17	G	502	9YF	C4-C3	2.06	1.57	1.52
19	G	503	IZL	C33-C32	2.06	1.58	1.51
19	G	503	IZL	C42-C41	2.05	1.57	1.52
19	M	504	IZL	C42-C41	2.05	1.57	1.52
20	H	605	HEM	C2A-C3A	-2.05	1.31	1.37
17	M	502	9YF	O2-C2	-2.05	1.36	1.44
17	W	201	9YF	C4-C3	2.04	1.57	1.52
19	M	504	IZL	C46-C45	2.04	1.56	1.50
20	N	605	HEM	CAA-C2A	-2.03	1.49	1.52
19	G	503	IZL	O9-C21	-2.01	1.40	1.43
15	O	304	HEC	CMD-C2D	2.00	1.55	1.51
20	H	602	HEM	C3B-C2B	-2.00	1.33	1.37

All (216) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	N	604	A1IGA	C04-S01-C05	14.33	118.18	102.42
20	N	601	HEM	CHC-C4B-NB	6.96	131.99	124.43
20	H	602	HEM	CBA-CAA-C2A	-6.70	101.19	112.62
25	R	603	HEA	CBA-CAA-C2A	-6.23	102.11	112.60
25	R	602	HEA	C3D-C4D-ND	5.97	116.14	110.36
25	R	602	HEA	CBA-CAA-C2A	-5.62	103.14	112.60
19	G	503	IZL	O10-C23-C24	5.37	117.50	106.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	M	504	IZL	O10-C23-C24	5.36	117.49	106.67
20	N	601	HEM	CAD-CBD-CGD	-5.30	102.19	113.60
25	R	602	HEA	C2D-C1D-ND	5.29	116.11	109.84
25	R	602	HEA	C2B-C1B-NB	5.23	116.15	109.88
25	R	602	HEA	C3B-C4B-NB	5.13	115.92	109.84
25	R	603	HEA	C3D-C4D-ND	5.12	115.32	110.36
20	N	601	HEM	C1B-NB-C4B	5.11	110.35	105.07
20	H	605	HEM	CAD-CBD-CGD	-5.03	102.78	113.60
25	R	603	HEA	C2B-C1B-NB	4.96	115.83	109.88
20	H	605	HEM	CHA-C4D-ND	4.91	130.45	124.38
22	N	604	A1IGA	O01-C14-C02	4.65	120.13	115.33
22	N	604	A1IGA	C03-C04-S01	4.63	120.23	109.96
25	R	602	HEA	C1D-C2D-C3D	-4.62	102.10	106.96
20	N	605	HEM	CHD-C1D-ND	4.56	129.38	124.43
20	H	605	HEM	CHC-C4B-NB	4.46	129.28	124.43
15	O	303	HEC	CBA-CAA-C2A	-4.44	105.11	112.60
25	R	603	HEA	C3B-C4B-NB	4.41	115.06	109.84
28	Y	302	9XX	O1-C18-C19	4.30	120.78	111.50
25	R	602	HEA	C3C-C4C-NC	4.24	114.69	109.21
17	W	201	9YF	C7-C2-C3	-4.20	104.79	110.85
20	N	601	HEM	CBA-CAA-C2A	-4.17	105.51	112.62
28	c	302	9XX	O1-C18-C19	4.16	120.46	111.50
20	H	605	HEM	C1B-NB-C4B	4.15	109.36	105.07
28	R	609	9XX	O1-C18-C19	4.14	120.43	111.50
17	G	502	9YF	C7-C2-C3	-4.06	105.00	110.85
14	O	302	WUO	O58-C59-C61	3.99	120.11	111.50
17	W	201	9YF	O1-P-O8	3.97	131.86	112.24
17	M	502	9YF	O1-P-O8	3.96	131.82	112.24
19	G	503	IZL	O34-C60-C61	3.96	120.04	111.50
19	M	504	IZL	O34-C60-C61	3.95	120.02	111.50
14	P	302	WUO	O58-C59-C61	3.95	120.02	111.50
17	M	502	9YF	C7-C2-C3	-3.95	105.15	110.85
17	G	502	9YF	O1-P-O8	3.95	131.76	112.24
20	H	602	HEM	CAD-CBD-CGD	-3.94	105.12	113.60
25	R	603	HEA	C1B-C2B-C3B	-3.89	102.15	106.80
19	M	504	IZL	O11-C24-C23	3.83	116.14	109.05
19	G	503	IZL	O11-C24-C23	3.82	116.11	109.05
20	H	605	HEM	CHD-C1D-ND	3.81	128.57	124.43
14	P	302	WUO	O04-C05-C12	3.80	114.33	106.67
15	O	304	HEC	CBD-CAD-C3D	3.78	119.07	112.62
14	O	302	WUO	O04-C05-C12	3.78	114.29	106.67
19	M	504	IZL	C21-O9-C22	3.76	121.08	113.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	G	503	IZL	C21-O9-C22	3.74	121.04	113.74
20	N	605	HEM	CHC-C4B-NB	3.73	128.49	124.43
25	R	602	HEA	CMB-C2B-C1B	3.73	130.72	125.04
20	N	605	HEM	C1B-NB-C4B	3.72	108.92	105.07
18	G	505	7PH	O21-C21-C22	3.68	119.44	111.50
20	H	602	HEM	CHC-C4B-NB	3.67	128.41	124.43
18	G	504	7PH	O21-C21-C22	3.64	119.34	111.50
20	N	605	HEM	CHD-C1D-C2D	-3.63	119.30	124.98
15	O	303	HEC	CMD-C2D-C1D	-3.62	122.90	128.46
14	P	302	WUO	C03-O04-C05	3.60	120.75	113.69
15	O	304	HEC	CMD-C2D-C1D	-3.56	122.99	128.46
14	O	302	WUO	C03-O04-C05	3.54	120.64	113.69
25	R	603	HEA	CMD-C2D-C1D	3.49	130.35	125.04
15	O	304	HEC	CMB-C2B-C1B	-3.49	123.11	128.46
19	G	503	IZL	O11-C25-C30	3.48	114.93	108.22
19	M	504	IZL	O11-C25-C30	3.46	114.90	108.22
22	N	604	A1IGA	C02-C03-N03	-3.45	120.57	123.95
15	O	304	HEC	CMB-C2B-C3B	3.43	129.86	125.82
25	R	602	HEA	C1B-C2B-C3B	-3.40	102.74	106.80
14	O	302	WUO	O55-P52-O53	-3.29	96.20	109.07
14	P	302	WUO	O55-P52-O53	-3.27	96.27	109.07
20	H	605	HEM	O2A-CGA-CBA	3.25	124.48	114.03
20	H	602	HEM	C2C-C3C-C4C	3.23	109.16	106.90
14	P	302	WUO	C08-C07-C06	-3.22	105.20	110.82
15	O	303	HEC	O1D-CGD-CBD	-3.22	112.74	123.08
20	N	605	HEM	CAD-C3D-C4D	3.18	130.22	124.66
25	R	602	HEA	C13-C12-C11	-3.18	109.58	114.35
14	O	302	WUO	C08-C07-C06	-3.16	105.30	110.82
14	O	302	WUO	O54-P52-O53	3.16	127.84	112.24
14	P	302	WUO	O54-P52-O53	3.16	127.84	112.24
25	R	603	HEA	C27-C19-C20	3.14	120.56	115.27
20	H	605	HEM	CBD-CAD-C3D	-3.11	103.99	112.63
25	R	603	HEA	C4D-C3D-C2D	-3.10	102.38	106.90
20	N	605	HEM	O2A-CGA-O1A	-3.09	115.59	123.30
20	N	605	HEM	CAD-C3D-C2D	-3.09	122.12	127.88
14	O	302	WUO	C33-C31-C01	3.09	116.73	109.68
14	P	302	WUO	C33-C31-C01	3.08	116.71	109.68
25	R	602	HEA	C27-C19-C20	3.06	120.42	115.27
20	N	601	HEM	O2A-CGA-CBA	3.06	123.86	114.03
20	N	601	HEM	CHD-C1D-ND	3.03	127.73	124.43
25	R	603	HEA	CHA-C4D-C3D	-3.01	120.42	124.84
20	H	602	HEM	CHB-C1B-NB	3.00	128.08	124.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	R	602	HEA	C4B-C3B-C2B	-2.94	102.39	107.41
22	N	604	A1IGA	C14-C02-C03	2.88	118.63	116.51
25	R	603	HEA	C12-C13-C14	-2.86	104.68	112.23
15	O	303	HEC	C1D-C2D-C3D	2.85	108.98	107.00
20	H	605	HEM	CHB-C1B-NB	2.84	127.89	124.38
25	R	602	HEA	C4D-C3D-C2D	-2.84	102.76	106.90
19	G	503	IZL	O1-C11-C12	2.84	114.45	108.43
19	M	504	IZL	O1-C11-C12	2.84	114.44	108.43
15	O	303	HEC	C2B-C3B-C4B	2.83	109.41	106.35
25	R	602	HEA	C13-C14-C15	-2.83	120.85	127.66
25	R	603	HEA	CMB-C2B-C1B	2.82	129.34	125.04
20	N	605	HEM	CAD-CBD-CGD	-2.82	107.53	113.60
20	H	602	HEM	C1B-NB-C4B	2.81	107.98	105.07
15	O	304	HEC	C4C-C3C-C2C	2.81	109.39	106.35
15	O	303	HEC	CMC-C2C-C3C	2.80	129.12	125.82
20	H	602	HEM	CMB-C2B-C1B	2.79	129.29	125.04
15	O	303	HEC	CMB-C2B-C3B	2.78	129.09	125.82
20	N	605	HEM	CMA-C3A-C4A	-2.77	124.20	128.46
20	H	602	HEM	CHD-C1D-ND	2.75	127.42	124.43
15	O	303	HEC	CMB-C2B-C1B	-2.75	124.23	128.46
25	R	602	HEA	C21-C20-C19	-2.74	103.98	112.98
20	H	602	HEM	C3C-C4C-NC	-2.73	105.79	110.94
22	N	604	A1IGA	C01-C02-C03	-2.73	120.31	122.69
20	H	605	HEM	CHD-C1D-C2D	-2.72	120.73	124.98
25	R	602	HEA	CHA-C4D-C3D	-2.72	120.84	124.84
25	R	603	HEA	OMA-CMA-C3A	-2.70	119.02	124.91
25	R	603	HEA	C2D-C1D-ND	2.70	113.03	109.84
20	N	601	HEM	CHB-C1B-NB	2.68	127.69	124.38
25	R	603	HEA	C17-C18-C19	-2.67	121.22	127.66
20	N	605	HEM	CHB-C1B-NB	2.67	127.67	124.38
25	R	603	HEA	C1D-C2D-C3D	-2.66	104.16	106.96
25	R	603	HEA	CAD-CBD-CGD	-2.66	107.89	113.60
25	R	603	HEA	CMC-C2C-C3C	2.65	129.63	124.68
20	N	605	HEM	O2A-CGA-CBA	2.64	122.52	114.03
20	N	601	HEM	CHD-C1D-C2D	-2.63	120.87	124.98
20	H	602	HEM	C4D-ND-C1D	2.62	107.78	105.07
20	H	605	HEM	C4D-ND-C1D	2.60	107.76	105.07
14	P	302	WUO	P52-O51-C50	2.60	128.88	119.41
15	O	303	HEC	CMC-C2C-C1C	-2.58	124.49	128.46
18	G	504	7PH	O31-C31-C32	2.58	120.01	111.91
19	G	503	IZL	C24-O11-C25	2.57	118.76	113.74
14	P	302	WUO	O04-C05-C06	2.56	114.35	109.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	M	504	IZL	C24-O11-C25	2.56	118.74	113.74
25	R	603	HEA	C4B-C3B-C2B	-2.56	103.04	107.41
25	R	602	HEA	C26-C15-C16	2.55	119.57	115.27
15	O	304	HEC	C1D-C2D-C3D	2.55	108.77	107.00
14	O	302	WUO	P52-O51-C50	2.54	128.65	119.41
14	O	302	WUO	O04-C05-C06	2.53	114.28	109.69
19	M	504	IZL	C31-O17-C32	2.51	118.62	113.69
19	G	503	IZL	C31-O17-C32	2.51	118.61	113.69
19	G	503	IZL	O28-P-O29	-2.49	100.13	109.47
15	O	303	HEC	O1A-CGA-CBA	-2.48	115.11	123.08
19	M	504	IZL	O28-P-O29	-2.47	100.19	109.47
25	R	603	HEA	CAD-C3D-C4D	2.47	128.97	124.66
14	P	302	WUO	O10-C07-C08	-2.46	104.67	110.35
25	R	602	HEA	CAD-CBD-CGD	-2.45	108.34	113.60
19	G	503	IZL	O30-P-O29	2.44	124.30	112.24
19	M	504	IZL	O30-P-O29	2.44	124.30	112.24
25	R	603	HEA	CHC-C4B-NB	-2.44	121.37	124.38
15	O	304	HEC	O1D-CGD-CBD	-2.43	115.27	123.08
14	O	302	WUO	O10-C07-C08	-2.43	104.73	110.35
14	P	302	WUO	O02-C01-C50	2.43	113.64	107.48
19	G	503	IZL	O32-C47-C48	2.43	119.52	111.91
19	M	504	IZL	O32-C47-C48	2.42	119.51	111.91
14	O	302	WUO	O02-C01-C50	2.41	113.61	107.48
18	G	505	7PH	O31-C31-C32	2.41	119.46	111.91
25	R	603	HEA	CHB-C1B-NB	-2.41	121.82	124.43
19	G	503	IZL	O1-C10-C9	2.39	119.40	111.91
19	M	504	IZL	O1-C10-C9	2.38	119.37	111.91
20	H	602	HEM	CBD-CAD-C3D	2.38	119.23	112.63
28	Y	302	9XX	O-C15-C14	2.37	119.34	111.91
20	H	602	HEM	O2A-CGA-O1A	-2.34	117.47	123.30
20	H	602	HEM	CHA-C4D-ND	2.34	127.27	124.38
28	R	609	9XX	O-C15-C14	2.32	119.20	111.91
28	c	302	9XX	O-C15-C14	2.32	119.19	111.91
17	M	502	9YF	O6-C6-C7	-2.31	105.00	110.35
20	N	601	HEM	O2A-CGA-O1A	-2.31	117.53	123.30
20	H	605	HEM	CAA-C2A-C3A	-2.31	120.60	127.25
20	H	605	HEM	CMC-C2C-C3C	2.31	129.00	124.68
19	G	503	IZL	O1-C10-O	-2.29	117.80	123.59
19	M	504	IZL	O1-C10-O	-2.29	117.82	123.59
20	N	601	HEM	O2D-CGD-O1D	-2.28	117.61	123.30
25	R	602	HEA	CMC-C2C-C3C	2.28	128.94	124.68
15	O	303	HEC	C4C-C3C-C2C	2.28	108.81	106.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	N	601	HEM	CHC-C4B-C3B	-2.27	121.09	124.57
25	R	602	HEA	CHB-C1B-C2B	-2.27	121.43	124.98
25	R	603	HEA	C26-C15-C14	-2.25	117.90	123.68
14	O	302	WUO	O58-C59-O60	-2.24	118.30	123.70
14	P	302	WUO	O58-C59-O60	-2.22	118.33	123.70
28	Y	302	9XX	O1-C18-O2	-2.21	118.35	123.70
25	R	602	HEA	C4B-NB-C1B	-2.20	102.80	105.07
25	R	602	HEA	CHD-C1D-C2D	-2.19	120.65	126.72
25	R	603	HEA	O2D-CGD-CBD	2.19	121.06	114.03
15	O	303	HEC	CAD-CBD-CGD	2.18	119.86	113.76
19	M	504	IZL	O25-C40-C20	-2.17	103.90	109.30
19	G	503	IZL	O25-C40-C20	-2.17	103.91	109.30
25	R	603	HEA	O11-C11-C12	-2.17	103.36	109.42
19	M	504	IZL	O17-C32-C33	2.16	111.80	106.44
20	N	605	HEM	CHA-C4D-ND	2.15	127.04	124.38
28	c	302	9XX	O1-C18-O2	-2.15	118.50	123.70
15	O	304	HEC	O1A-CGA-CBA	-2.15	116.18	123.08
15	O	304	HEC	CMC-C2C-C3C	2.15	128.35	125.82
19	G	503	IZL	O17-C32-C33	2.15	111.78	106.44
28	R	609	9XX	O1-C18-O2	-2.14	118.53	123.70
20	H	602	HEM	O2D-CGD-O1D	-2.13	118.00	123.30
25	R	603	HEA	C25-C23-C24	2.12	119.29	114.60
28	Y	302	9XX	O1-C17-C16	2.12	111.04	106.13
20	H	605	HEM	CHA-C4D-C3D	-2.11	121.36	125.33
20	H	602	HEM	CMA-C3A-C4A	-2.10	125.23	128.46
25	R	602	HEA	C1D-ND-C4D	-2.10	102.90	105.07
20	N	605	HEM	CBA-CAA-C2A	-2.08	109.07	112.62
22	N	604	A1IGA	C04-C03-N03	2.07	118.22	116.03
20	H	605	HEM	O1A-CGA-CBA	-2.07	116.42	123.08
19	G	503	IZL	O34-C60-O35	-2.07	118.69	123.70
25	R	602	HEA	C25-C23-C22	-2.07	116.68	122.65
17	W	201	9YF	O6-C6-C7	-2.06	105.58	110.35
19	M	504	IZL	O34-C60-O35	-2.06	118.73	123.70
28	R	609	9XX	O1-C17-C16	2.06	110.90	106.13
28	c	302	9XX	O1-C17-C16	2.05	110.89	106.13
17	G	502	9YF	O6-C6-C7	-2.02	105.68	110.35
20	H	605	HEM	C1D-C2D-C3D	-2.01	104.84	106.96
19	G	503	IZL	O32-C46-C45	2.01	114.29	108.43
19	G	503	IZL	O16-C31-C36	2.00	113.29	108.10
19	M	504	IZL	O16-C31-C36	2.00	113.29	108.10
19	M	504	IZL	O32-C46-C45	2.00	114.26	108.43

There are no chirality outliers.

All (941) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	O	301	MQ9	C18-C19-C21-C22
13	O	301	MQ9	C20-C19-C21-C22
13	O	305	MQ9	C12-C13-C14-C15
13	O	305	MQ9	C12-C13-C14-C16
13	O	305	MQ9	C22-C23-C24-C25
13	O	305	MQ9	C22-C23-C24-C26
13	O	305	MQ9	C27-C28-C29-C30
13	O	305	MQ9	C27-C28-C29-C31
13	O	305	MQ9	C41-C42-C43-C44
13	N	606	MQ9	C5-C6-C7-C8
13	N	606	MQ9	C1-C6-C7-C8
13	N	606	MQ9	C7-C8-C9-C10
13	N	606	MQ9	C7-C8-C9-C11
13	N	606	MQ9	C12-C13-C14-C15
13	N	606	MQ9	C12-C13-C14-C16
13	N	606	MQ9	C14-C16-C17-C18
13	N	606	MQ9	C21-C22-C23-C24
13	N	606	MQ9	C27-C28-C29-C31
13	N	606	MQ9	C32-C33-C34-C35
13	N	606	MQ9	C32-C33-C34-C36
13	H	606	MQ9	C7-C8-C9-C10
13	H	606	MQ9	C7-C8-C9-C11
13	H	606	MQ9	C22-C23-C24-C25
13	H	606	MQ9	C24-C26-C27-C28
13	H	606	MQ9	C26-C27-C28-C29
13	H	606	MQ9	C35-C34-C36-C37
13	H	606	MQ9	C44-C46-C47-C48
13	H	607	MQ9	C12-C13-C14-C15
13	H	607	MQ9	C12-C13-C14-C16
13	H	607	MQ9	C22-C23-C24-C25
13	H	607	MQ9	C22-C23-C24-C26
13	H	607	MQ9	C27-C28-C29-C30
13	H	607	MQ9	C27-C28-C29-C31
13	H	607	MQ9	C32-C33-C34-C35
13	H	607	MQ9	C32-C33-C34-C36
13	H	607	MQ9	C37-C38-C39-C40
13	H	607	MQ9	C42-C43-C44-C45
13	H	607	MQ9	C42-C43-C44-C46
13	H	607	MQ9	C44-C46-C47-C48
14	O	302	WUO	C56-O55-P52-O53
14	P	302	WUO	C06-C05-C12-O13
14	P	302	WUO	C86-C87-C88-C89

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Mol	Chain	Res	Type	Atoms
17	M	502	9YF	C2-O2-P-O1
17	M	502	9YF	C1-O-P-O1
17	W	201	9YF	C2-O2-P-O1
17	W	201	9YF	C2-O2-P-O8
17	W	201	9YF	C1-O-P-O1
17	W	201	9YF	C1-O-P-O2
17	W	201	9YF	C1-O-P-O8
17	W	201	9YF	C9-C8-O9-C
17	W	201	9YF	O10-C8-O9-C
17	G	502	9YF	C2-O2-P-O1
17	G	502	9YF	C1-O-P-O1
17	G	502	9YF	C1-O-P-O2
17	G	502	9YF	C1-O-P-O8
18	M	503	7PH	C1-O11-P-O12
18	M	503	7PH	C1-O11-P-O13
18	M	503	7PH	C1-O11-P-O14
18	S	501	7PH	C1-O11-P-O12
18	S	501	7PH	C1-O11-P-O13
18	S	501	7PH	C1-O11-P-O14
18	G	504	7PH	C22-C21-O21-C2
19	M	504	IZL	O31-C44-C45-O34
19	M	504	IZL	C48-C47-O32-C46
19	M	504	IZL	C43-O28-P-O30
19	G	503	IZL	O31-C44-C45-O34
19	G	503	IZL	C48-C47-O32-C46
19	G	503	IZL	C43-O28-P-O30
20	N	605	HEM	C2D-C3D-CAD-CBD
20	N	605	HEM	C4D-C3D-CAD-CBD
20	H	605	HEM	C1A-C2A-CAA-CBA
20	H	605	HEM	C3A-C2A-CAA-CBA
20	H	605	HEM	C2D-C3D-CAD-CBD
20	H	605	HEM	C4D-C3D-CAD-CBD
21	N	602	CDL	CA2-C1-CB2-OB2
21	N	602	CDL	CA2-OA2-PA1-OA3
21	N	602	CDL	CA3-OA5-PA1-OA3
21	N	602	CDL	CB2-OB2-PB2-OB5
21	N	603	CDL	CB2-C1-CA2-OA2
21	N	603	CDL	CA2-OA2-PA1-OA3
21	N	603	CDL	CA2-OA2-PA1-OA4
21	N	603	CDL	CA3-OA5-PA1-OA2
21	N	603	CDL	CA3-OA5-PA1-OA3
21	N	603	CDL	CA3-OA5-PA1-OA4

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Mol	Chain	Res	Type	Atoms
21	N	603	CDL	CB2-OB2-PB2-OB3
21	N	603	CDL	CB3-OB5-PB2-OB3
21	N	603	CDL	CB3-OB5-PB2-OB4
21	N	607	CDL	CA2-OA2-PA1-OA3
21	N	607	CDL	CA3-OA5-PA1-OA2
21	N	607	CDL	CA3-OA5-PA1-OA3
21	N	607	CDL	CA3-OA5-PA1-OA4
21	N	607	CDL	CB2-OB2-PB2-OB5
21	P	301	CDL	CA2-OA2-PA1-OA3
21	P	301	CDL	CA2-OA2-PA1-OA4
21	P	301	CDL	CA2-OA2-PA1-OA5
21	P	301	CDL	CA3-OA5-PA1-OA3
21	P	301	CDL	C11-CA5-OA6-CA4
21	P	301	CDL	CB3-OB5-PB2-OB2
21	R	601	CDL	CA2-C1-CB2-OB2
21	R	601	CDL	CA2-OA2-PA1-OA4
21	R	601	CDL	CB2-OB2-PB2-OB4
21	R	605	CDL	CA2-OA2-PA1-OA3
21	R	605	CDL	CA3-OA5-PA1-OA2
21	R	605	CDL	CA3-OA5-PA1-OA3
21	R	605	CDL	CA3-OA5-PA1-OA4
21	R	605	CDL	CB2-OB2-PB2-OB4
21	R	605	CDL	CB3-OB5-PB2-OB3
21	R	605	CDL	CB3-OB5-PB2-OB4
21	H	601	CDL	C11-CA5-OA6-CA4
21	H	601	CDL	CB2-OB2-PB2-OB3
21	H	601	CDL	CB3-OB5-PB2-OB2
21	H	601	CDL	CB3-OB5-PB2-OB3
21	H	601	CDL	CB3-OB5-PB2-OB4
21	H	603	CDL	CA2-OA2-PA1-OA3
21	H	603	CDL	CA2-OA2-PA1-OA4
21	H	603	CDL	CA2-OA2-PA1-OA5
21	H	603	CDL	CB3-OB5-PB2-OB4
21	H	604	CDL	CA2-C1-CB2-OB2
21	H	604	CDL	CA2-OA2-PA1-OA3
21	H	604	CDL	CB2-OB2-PB2-OB4
22	N	604	A1IGA	O01-C15-C16-F01
22	N	604	A1IGA	O01-C15-C16-F02
24	S	503	3PE	C1-O11-P-O12
24	S	503	3PE	C1-O11-P-O13
24	S	503	3PE	C1-O11-P-O14
25	R	603	HEA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
25	R	603	HEA	C26-C15-C16-C17
28	R	609	9XX	C14-C15-O-C16
28	R	609	9XX	C19-C18-O1-C17
28	R	609	9XX	O2-C18-O1-C17
28	R	609	9XX	C25-C26-C27-C28
28	Y	302	9XX	O-C16-C17-C37
28	Y	302	9XX	O-C16-C17-O1
28	Y	302	9XX	C19-C18-O1-C17
28	Y	302	9XX	O2-C18-O1-C17
30	W	202	PLM	C1-C2-C3-C4
19	M	504	IZL	O33-C47-O32-C46
19	G	503	IZL	O33-C47-O32-C46
21	H	604	CDL	OA9-CA7-OA8-CA6
28	R	609	9XX	O6-C15-O-C16
19	M	504	IZL	O10-C23-C24-O11
19	G	503	IZL	O10-C23-C24-O11
21	N	603	CDL	C31-CA7-OA8-CA6
21	H	604	CDL	C31-CA7-OA8-CA6
13	N	606	MQ9	C47-C48-C49-C50
13	N	606	MQ9	C47-C48-C49-C51
14	P	302	WUO	O79-C78-O77-C76
18	G	504	7PH	O32-C31-O31-C3
21	N	603	CDL	OA9-CA7-OA8-CA6
21	N	607	CDL	OB9-CB7-OB8-CB6
18	G	504	7PH	O22-C21-O21-C2
21	N	603	CDL	OB7-CB5-OB6-CB4
21	P	301	CDL	OA7-CA5-OA6-CA4
21	R	605	CDL	OB7-CB5-OB6-CB4
21	H	601	CDL	OA7-CA5-OA6-CA4
21	H	603	CDL	OA7-CA5-OA6-CA4
22	N	604	A1IGA	O01-C15-C16-F03
18	G	504	7PH	C32-C31-O31-C3
19	M	504	IZL	C61-C60-O34-C45
19	G	503	IZL	C61-C60-O34-C45
21	N	603	CDL	C51-CB5-OB6-CB4
21	R	605	CDL	C51-CB5-OB6-CB4
21	H	603	CDL	C11-CA5-OA6-CA4
17	M	502	9YF	O12-C25-O11-C24
14	P	302	WUO	O04-C05-C12-O13
25	R	602	HEA	C2D-C3D-CAD-CBD
13	H	607	MQ9	C30-C29-C31-C32
13	H	606	MQ9	C33-C34-C36-C37

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Mol	Chain	Res	Type	Atoms
14	P	302	WUO	C80-C78-O77-C76
21	N	607	CDL	C71-CB7-OB8-CB6
14	P	302	WUO	O40-C41-C48-O49
25	R	602	HEA	C4D-C3D-CAD-CBD
25	R	603	HEA	C4D-C3D-CAD-CBD
13	N	606	MQ9	C17-C18-C19-C20
13	N	606	MQ9	C27-C28-C29-C30
13	H	606	MQ9	C12-C13-C14-C15
13	H	607	MQ9	C7-C8-C9-C10
19	M	504	IZL	O17-C31-O16-C30
19	G	503	IZL	O17-C31-O16-C30
19	G	503	IZL	O35-C60-O34-C45
21	N	603	CDL	OA7-CA5-OA6-CA4
13	N	606	MQ9	C17-C18-C19-C21
13	H	606	MQ9	C12-C13-C14-C16
13	H	606	MQ9	C22-C23-C24-C26
13	H	607	MQ9	C7-C8-C9-C11
13	H	607	MQ9	C37-C38-C39-C41
17	G	502	9YF	O12-C25-O11-C24
19	G	503	IZL	C36-C31-O16-C30
19	M	504	IZL	O12-C26-C27-O13
19	G	503	IZL	O12-C26-C27-O13
21	N	603	CDL	O1-C1-CA2-OA2
21	P	301	CDL	O1-C1-CA2-OA2
21	R	601	CDL	O1-C1-CB2-OB2
17	M	502	9YF	C26-C25-O11-C24
19	M	504	IZL	C36-C31-O16-C30
21	N	603	CDL	C11-CA5-OA6-CA4
14	P	302	WUO	C42-C41-C48-O49
21	R	605	CDL	CB4-CB6-OB8-CB7
21	R	605	CDL	C51-C52-C53-C54
21	R	605	CDL	C71-C72-C73-C74
17	G	502	9YF	C26-C25-O11-C24
19	M	504	IZL	O35-C60-O34-C45
13	O	305	MQ9	C47-C48-C49-C50
13	O	301	MQ9	C25-C24-C26-C27
13	O	305	MQ9	C40-C39-C41-C42
13	N	606	MQ9	C30-C29-C31-C32
13	N	606	MQ9	C40-C39-C41-C42
13	H	607	MQ9	C45-C44-C46-C47
25	R	603	HEA	C27-C19-C20-C21
13	O	301	MQ9	C23-C24-C26-C27

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Mol	Chain	Res	Type	Atoms
13	O	305	MQ9	C38-C39-C41-C42
13	N	606	MQ9	C28-C29-C31-C32
13	N	606	MQ9	C38-C39-C41-C42
13	H	607	MQ9	C43-C44-C46-C47
25	R	603	HEA	C14-C15-C16-C17
25	R	603	HEA	C18-C19-C20-C21
19	M	504	IZL	C37-C23-C24-O11
19	G	503	IZL	C37-C23-C24-O11
19	M	504	IZL	O17-C32-C33-O18
19	G	503	IZL	O17-C32-C33-O18
19	M	504	IZL	O12-C25-O11-C24
19	G	503	IZL	O12-C25-O11-C24
13	O	305	MQ9	C14-C16-C17-C18
13	H	607	MQ9	C14-C16-C17-C18
13	H	607	MQ9	C19-C21-C22-C23
13	H	607	MQ9	C29-C31-C32-C33
25	R	602	HEA	C19-C20-C21-C22
25	R	603	HEA	C15-C16-C17-C18
14	O	302	WUO	C80-C81-C82-C83
21	N	603	CDL	CA2-C1-CB2-OB2
14	O	302	WUO	C80-C78-O77-C76
14	P	302	WUO	C16-C14-O13-C12
21	R	601	CDL	C31-CA7-OA8-CA6
28	c	302	9XX	C14-C15-O-C16
21	H	604	CDL	C57-C58-C59-C60
19	M	504	IZL	C34-C32-C33-O18
19	G	503	IZL	C34-C32-C33-O18
25	R	603	HEA	C2D-C3D-CAD-CBD
21	P	301	CDL	C51-C52-C53-C54
14	P	302	WUO	O55-C56-C57-O58
28	R	609	9XX	C11-C12-C13-C14
21	N	603	CDL	O1-C1-CB2-OB2
13	H	607	MQ9	C28-C29-C31-C32
19	M	504	IZL	C54-C55-C56-C57
19	G	503	IZL	C54-C55-C56-C57
21	N	607	CDL	CA7-C31-C32-C33
21	P	301	CDL	CA5-C11-C12-C13
15	O	304	HEC	C3D-CAD-CBD-CGD
21	N	607	CDL	CA5-C11-C12-C13
21	P	301	CDL	CB5-C51-C52-C53
21	R	601	CDL	CA7-C31-C32-C33
21	N	607	CDL	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
13	H	607	MQ9	C47-C48-C49-C51
14	O	302	WUO	C59-C61-C62-C63
14	P	302	WUO	C59-C61-C62-C63
17	M	502	9YF	C25-C26-C27-C28
17	W	201	9YF	C25-C26-C27-C28
17	G	502	9YF	C25-C26-C27-C28
28	c	302	9XX	C12-C13-C14-C15
19	M	504	IZL	C28-C26-C27-O13
19	G	503	IZL	C28-C26-C27-O13
19	M	504	IZL	C53-C54-C55-C56
19	G	503	IZL	C53-C54-C55-C56
21	N	603	CDL	CB5-C51-C52-C53
21	R	601	CDL	CA5-C11-C12-C13
21	R	601	CDL	CB7-C71-C72-C73
20	N	605	HEM	C3D-CAD-CBD-CGD
14	P	302	WUO	O15-C14-O13-C12
28	c	302	9XX	O6-C15-O-C16
21	N	603	CDL	C77-C78-C79-C80
21	H	603	CDL	C58-C59-C60-C61
14	O	302	WUO	O79-C78-O77-C76
21	R	601	CDL	OA9-CA7-OA8-CA6
13	O	301	MQ9	C14-C16-C17-C18
13	N	606	MQ9	C24-C26-C27-C28
13	H	607	MQ9	C9-C11-C12-C13
14	P	302	WUO	C78-C80-C81-C82
21	N	602	CDL	O1-C1-CB2-OB2
21	R	601	CDL	O1-C1-CA2-OA2
21	H	604	CDL	O1-C1-CB2-OB2
17	G	502	9YF	C33-C35-C36-C37
21	H	604	CDL	C71-CB7-OB8-CB6
14	O	302	WUO	C88-C90-C91-C92
14	P	302	WUO	C27-C28-C29-C30
21	N	607	CDL	C11-CA5-OA6-CA4
21	N	607	CDL	C51-CB5-OB6-CB4
17	M	502	9YF	C33-C35-C36-C37
17	W	201	9YF	C30-C31-C32-C33
17	M	502	9YF	C1-O-P-O2
21	N	602	CDL	CA2-OA2-PA1-OA5
21	N	602	CDL	CB3-OB5-PB2-OB2
21	N	603	CDL	CA2-OA2-PA1-OA5
21	N	603	CDL	CB2-OB2-PB2-OB5
21	N	603	CDL	CB3-OB5-PB2-OB2

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Mol	Chain	Res	Type	Atoms
21	N	607	CDL	CB3-OB5-PB2-OB2
21	P	301	CDL	CA3-OA5-PA1-OA2
21	R	601	CDL	CA2-OA2-PA1-OA5
21	R	601	CDL	CB2-OB2-PB2-OB5
21	R	605	CDL	CA2-OA2-PA1-OA5
21	R	605	CDL	CB2-OB2-PB2-OB5
21	R	605	CDL	CB3-OB5-PB2-OB2
21	H	601	CDL	CA2-OA2-PA1-OA5
21	H	601	CDL	CB2-OB2-PB2-OB5
21	H	603	CDL	CA3-OA5-PA1-OA2
21	H	603	CDL	CB2-OB2-PB2-OB5
21	H	603	CDL	CB3-OB5-PB2-OB2
21	H	604	CDL	CB2-OB2-PB2-OB5
21	R	601	CDL	CB5-C51-C52-C53
21	P	301	CDL	CB2-C1-CA2-OA2
21	R	601	CDL	CB2-C1-CA2-OA2
21	H	603	CDL	CB2-C1-CA2-OA2
21	N	607	CDL	OB7-CB5-OB6-CB4
14	P	302	WUO	C88-C90-C91-C92
17	W	201	9YF	C2-O2-P-O
17	M	502	9YF	C38-C39-C40-C41
17	W	201	9YF	C38-C39-C40-C41
21	R	605	CDL	C56-C57-C58-C59
14	O	302	WUO	C61-C59-O58-C57
24	S	503	3PE	C22-C21-O21-C2
14	O	302	WUO	C24-C25-C26-C27
17	M	502	9YF	C11-C12-C13-C14
17	G	502	9YF	C38-C39-C40-C41
18	G	505	7PH	C24-C25-C26-C27
21	N	602	CDL	C53-C54-C55-C56
21	R	605	CDL	C15-C16-C17-C18
21	R	605	CDL	C72-C73-C74-C75
21	H	601	CDL	C79-C80-C81-C82
13	O	305	MQ9	C47-C48-C49-C51
14	O	302	WUO	C22-C23-C24-C25
14	O	302	WUO	C64-C65-C66-C67
17	W	201	9YF	C13-C14-C15-C16
17	G	502	9YF	C29-C30-C31-C32
21	N	607	CDL	C54-C55-C56-C57
21	N	607	CDL	C78-C79-C80-C81
21	P	301	CDL	C11-C12-C13-C14
21	H	604	CDL	C51-C52-C53-C54

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Mol	Chain	Res	Type	Atoms
23	Q	403	TRD	C2-C3-C4-C5
14	O	302	WUO	O60-C59-O58-C57
21	N	607	CDL	OA7-CA5-OA6-CA4
24	S	503	3PE	O22-C21-O21-C2
14	P	302	WUO	C24-C25-C26-C27
17	M	502	9YF	C29-C30-C31-C32
17	W	201	9YF	C16-C17-C18-C19
18	S	501	7PH	C29-C2A-C2B-C2C
21	N	603	CDL	C51-C52-C53-C54
21	N	607	CDL	C57-C58-C59-C60
17	W	201	9YF	C29-C30-C31-C32
17	G	502	9YF	C11-C12-C13-C14
21	N	602	CDL	C17-C18-C19-C20
21	N	603	CDL	C57-C58-C59-C60
21	N	607	CDL	C13-C14-C15-C16
21	H	603	CDL	C16-C17-C18-C19
24	S	503	3PE	C23-C24-C25-C26
21	H	601	CDL	O1-C1-CA2-OA2
21	H	603	CDL	O1-C1-CA2-OA2
20	N	601	HEM	C3D-CAD-CBD-CGD
17	M	502	9YF	C13-C14-C15-C16
19	M	504	IZL	C2-C1-C7-C8
19	G	503	IZL	C2-C1-C7-C8
21	N	607	CDL	C71-C72-C73-C74
21	N	607	CDL	C76-C77-C78-C79
21	R	605	CDL	C32-C33-C34-C35
21	R	605	CDL	C59-C60-C61-C62
18	M	503	7PH	C21-C22-C23-C24
21	N	602	CDL	CA7-C31-C32-C33
21	H	604	CDL	CB5-C51-C52-C53
14	P	302	WUO	C82-C83-C84-C85
23	R	607	TRD	C7-C8-C9-C10
13	H	607	MQ9	C47-C48-C49-C50
17	W	201	9YF	C10-C11-C12-C13
21	N	607	CDL	C74-C75-C76-C77
21	R	605	CDL	C17-C18-C19-C20
21	H	601	CDL	C74-C75-C76-C77
28	R	609	9XX	C25-C26-C27-C36
14	O	302	WUO	C92-C93-C94-C95
14	P	302	WUO	C64-C65-C66-C67
14	P	302	WUO	C83-C84-C85-C86
17	M	502	9YF	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
17	W	201	9YF	C39-C40-C41-C42
17	G	502	9YF	C13-C14-C15-C16
17	G	502	9YF	C19-C20-C21-C22
21	P	301	CDL	C12-C13-C14-C15
21	R	601	CDL	C73-C74-C75-C76
21	H	601	CDL	C76-C77-C78-C79
21	H	604	CDL	C32-C33-C34-C35
21	H	604	CDL	C71-C72-C73-C74
21	N	603	CDL	C73-C74-C75-C76
21	N	603	CDL	C76-C77-C78-C79
21	H	603	CDL	C74-C75-C76-C77
21	R	601	CDL	C51-CB5-OB6-CB4
21	H	604	CDL	C51-CB5-OB6-CB4
18	M	503	7PH	C25-C26-C27-C28
21	R	601	CDL	C59-C60-C61-C62
21	H	601	CDL	C15-C16-C17-C18
21	H	604	CDL	CB7-C71-C72-C73
19	M	504	IZL	C51-C52-C53-C54
19	G	503	IZL	C51-C52-C53-C54
21	N	602	CDL	C59-C60-C61-C62
21	N	607	CDL	C32-C33-C34-C35
21	N	607	CDL	C73-C74-C75-C76
21	R	605	CDL	C57-C58-C59-C60
21	H	603	CDL	C55-C56-C57-C58
21	H	604	CDL	C59-C60-C61-C62
14	O	302	WUO	C81-C82-C83-C84
21	N	607	CDL	C81-C82-C83-C84
14	O	302	WUO	C26-C27-C28-C29
14	P	302	WUO	C25-C26-C27-C28
17	M	502	9YF	C18-C19-C20-C21
17	G	502	9YF	C18-C19-C20-C21
21	P	301	CDL	C58-C59-C60-C61
21	R	601	CDL	C57-C58-C59-C60
21	R	605	CDL	C34-C35-C36-C37
21	H	601	CDL	C57-C58-C59-C60
28	R	609	9XX	C6-C7-C8-C9
18	G	505	7PH	C21-C22-C23-C24
17	W	201	9YF	C27-C28-C29-C30
21	N	603	CDL	C74-C75-C76-C77
21	R	601	CDL	C74-C75-C76-C77
28	R	609	9XX	C3-C4-C5-C6
18	M	503	7PH	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
18	M	503	7PH	C24-C25-C26-C27
21	H	603	CDL	C14-C15-C16-C17
21	H	604	CDL	C74-C75-C76-C77
28	R	609	9XX	C10-C11-C12-C13
21	N	607	CDL	C12-C13-C14-C15
21	H	601	CDL	C78-C79-C80-C81
21	H	604	CDL	C38-C39-C40-C41
21	H	604	CDL	OB9-CB7-OB8-CB6
21	N	602	CDL	C36-C37-C38-C39
21	P	301	CDL	C36-C37-C38-C39
21	H	604	CDL	OB7-CB5-OB6-CB4
21	N	602	CDL	C34-C35-C36-C37
21	R	601	CDL	C14-C15-C16-C17
14	P	302	WUO	C91-C92-C93-C94
23	R	608	TRD	C5-C6-C7-C8
21	R	605	CDL	CB5-C51-C52-C53
21	H	601	CDL	CB2-C1-CA2-OA2
17	W	201	9YF	C37-C38-C39-C40
21	H	604	CDL	C55-C56-C57-C58
28	R	609	9XX	C31-C32-C33-C34
21	R	601	CDL	OB7-CB5-OB6-CB4
17	W	201	9YF	C35-C36-C37-C38
28	c	302	9XX	C22-C23-C24-C25
21	R	605	CDL	CA7-C31-C32-C33
14	O	302	WUO	C16-C17-C18-C19
21	N	603	CDL	C22-C23-C24-C25
21	R	605	CDL	C37-C38-C39-C40
21	H	601	CDL	C59-C60-C61-C62
17	W	201	9YF	C9-C10-C11-C12
21	N	602	CDL	C51-C52-C53-C54
13	N	606	MQ9	C18-C19-C21-C22
17	M	502	9YF	C31-C32-C33-C35
17	G	502	9YF	C31-C32-C33-C35
14	P	302	WUO	O60-C59-O58-C57
24	S	503	3PE	C32-C31-O31-C3
28	R	609	9XX	C4-C5-C6-C7
21	N	602	CDL	C52-C53-C54-C55
21	N	602	CDL	C54-C55-C56-C57
21	H	601	CDL	C77-C78-C79-C80
21	H	603	CDL	C73-C74-C75-C76
21	H	604	CDL	CA7-C31-C32-C33
17	W	201	9YF	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
21	H	603	CDL	C13-C14-C15-C16
17	W	201	9YF	C11-C12-C13-C14
13	O	301	MQ9	C29-C31-C32-C33
18	S	501	7PH	C27-C28-C29-C2A
21	N	602	CDL	C71-C72-C73-C74
21	N	603	CDL	C18-C19-C20-C21
21	H	601	CDL	C16-C17-C18-C19
14	P	302	WUO	C61-C59-O58-C57
21	H	604	CDL	C11-CA5-OA6-CA4
28	c	302	9XX	C19-C18-O1-C17
23	S	502	TRD	C7-C8-C9-C10
28	c	302	9XX	O2-C18-O1-C17
28	R	609	9XX	C1-C2-C3-C4
17	W	201	9YF	C19-C20-C21-C22
21	N	602	CDL	C16-C17-C18-C19
21	P	301	CDL	C33-C34-C35-C36
21	H	603	CDL	C76-C77-C78-C79
14	P	302	WUO	C90-C91-C92-C93
21	N	603	CDL	C20-C21-C22-C23
21	R	601	CDL	C51-C52-C53-C54
13	N	606	MQ9	C20-C19-C21-C22
13	H	606	MQ9	C40-C39-C41-C42
13	N	606	MQ9	C12-C11-C9-C8
13	H	606	MQ9	C47-C48-C49-C51
21	P	301	CDL	C56-C57-C58-C59
21	R	605	CDL	C33-C34-C35-C36
14	P	302	WUO	C61-C62-C63-C64
21	R	601	CDL	C32-C33-C34-C35
21	H	601	CDL	C53-C54-C55-C56
21	N	602	CDL	C72-C73-C74-C75
21	P	301	CDL	C52-C53-C54-C55
21	H	601	CDL	C71-C72-C73-C74
21	N	602	CDL	CA3-OA5-PA1-OA2
21	N	607	CDL	CA2-OA2-PA1-OA5
21	H	601	CDL	CA3-OA5-PA1-OA2
21	H	604	CDL	CA2-OA2-PA1-OA5
21	H	603	CDL	C51-C52-C53-C54
14	P	302	WUO	O55-C56-C57-C76
19	M	504	IZL	O31-C44-C45-C46
19	G	503	IZL	O31-C44-C45-C46
21	N	607	CDL	OA5-CA3-CA4-CA6
21	R	601	CDL	OB5-CB3-CB4-CB6

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Mol	Chain	Res	Type	Atoms
21	N	607	CDL	C51-C52-C53-C54
18	G	505	7PH	C23-C24-C25-C26
20	H	602	HEM	C3D-CAD-CBD-CGD
21	N	603	CDL	C13-C14-C15-C16
21	N	602	CDL	C35-C36-C37-C38
21	N	607	CDL	C15-C16-C17-C18
21	H	604	CDL	C53-C54-C55-C56
13	N	606	MQ9	C12-C11-C9-C10
21	N	602	CDL	C33-C34-C35-C36
21	P	301	CDL	C14-C15-C16-C17
21	P	301	CDL	C15-C16-C17-C18
17	G	502	9YF	C16-C17-C18-C19
14	P	302	WUO	C56-C57-C76-O77
18	M	503	7PH	C1-C2-C3-O31
19	M	504	IZL	C62-C63-C64-C65
19	G	503	IZL	C62-C63-C64-C65
21	N	602	CDL	CB3-CB4-CB6-OB8
21	H	603	CDL	CB3-CB4-CB6-OB8
21	H	603	CDL	C53-C54-C55-C56
17	M	502	9YF	C16-C17-C18-C19
21	P	301	CDL	C60-C61-C62-C63
19	M	504	IZL	C23-C24-O11-C25
19	G	503	IZL	C23-C24-O11-C25
21	N	603	CDL	C71-C72-C73-C74
28	c	302	9XX	C5-C6-C7-C8
21	N	603	CDL	C78-C79-C80-C81
21	P	301	CDL	C18-C19-C20-C21
21	R	601	CDL	C71-C72-C73-C74
21	H	603	CDL	C59-C60-C61-C62
24	S	503	3PE	O32-C31-O31-C3
14	O	302	WUO	C27-C28-C29-C30
17	M	502	9YF	C37-C38-C39-C40
19	M	504	IZL	C1-C7-C8-C9
19	G	503	IZL	C1-C7-C8-C9
17	M	502	9YF	C2-O2-P-O
17	G	502	9YF	C2-O2-P-O
19	M	504	IZL	C43-O28-P-O31
19	G	503	IZL	C43-O28-P-O31
21	N	603	CDL	C11-C12-C13-C14
21	N	607	CDL	C79-C80-C81-C82
21	R	601	CDL	C11-C12-C13-C14
21	H	601	CDL	C54-C55-C56-C57

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Mol	Chain	Res	Type	Atoms
17	M	502	9YF	C30-C31-C32-C33
21	H	601	CDL	C51-CB5-OB6-CB4
18	G	505	7PH	C22-C23-C24-C25
21	N	603	CDL	C79-C80-C81-C82
18	M	503	7PH	C27-C28-C29-C2A
19	G	503	IZL	C4-C5-C6-C67
19	M	504	IZL	C4-C5-C6-C67
21	N	603	CDL	CA6-CA4-OA6-CA5
21	P	301	CDL	CA3-CA4-OA6-CA5
14	P	302	WUO	C62-C63-C64-C65
17	W	201	9YF	C40-C41-C42-C43
21	N	607	CDL	C16-C17-C18-C19
21	P	301	CDL	OB5-CB3-CB4-OB6
28	R	609	9XX	C22-C23-C24-C25
19	M	504	IZL	C7-C8-C9-C10
17	G	502	9YF	C26-C27-C28-C29
17	M	502	9YF	O9-C-C24-O11
19	G	503	IZL	C1-C2-C3-C4
24	S	503	3PE	C32-C33-C34-C35
21	H	604	CDL	OA7-CA5-OA6-CA4
19	M	504	IZL	C1-C2-C3-C4
21	N	602	CDL	C76-C77-C78-C79
19	G	503	IZL	C7-C8-C9-C10
28	Y	302	9XX	C26-C27-C28-C29
28	c	302	9XX	O1-C18-C19-C20
21	N	602	CDL	C39-C40-C41-C42
28	Y	302	9XX	C25-C26-C27-C36
28	Y	302	9XX	C36-C27-C28-C29
21	P	301	CDL	C38-C39-C40-C41
21	R	605	CDL	C60-C61-C62-C63
18	G	504	7PH	C22-C23-C24-C25
21	P	301	CDL	C37-C38-C39-C40
21	H	603	CDL	C19-C20-C21-C22
21	P	301	CDL	CB4-CB6-OB8-CB7
21	H	604	CDL	C76-C77-C78-C79
17	G	502	9YF	C30-C31-C32-C33
21	N	602	CDL	C57-C58-C59-C60
18	G	504	7PH	O11-C1-C2-C3
18	G	505	7PH	O11-C1-C2-C3
19	G	503	IZL	C66-C68-C69-C70
19	M	504	IZL	C66-C68-C69-C70
28	c	302	9XX	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
14	O	302	WUO	C83-C84-C85-C86
18	S	501	7PH	C22-C21-O21-C2
21	N	602	CDL	CB5-C51-C52-C53
28	R	609	9XX	C19-C20-C21-C22
14	P	302	WUO	C19-C20-C21-C22
21	N	603	CDL	C55-C56-C57-C58
14	O	302	WUO	C84-C85-C86-C87
17	G	502	9YF	C37-C38-C39-C40
17	W	201	9YF	C1-C-C24-O11
28	c	302	9XX	O-C16-C17-C37
28	R	609	9XX	C21-C22-C23-C24
21	N	602	CDL	C73-C74-C75-C76
17	M	502	9YF	C2-O2-P-O8
17	G	502	9YF	C2-O2-P-O8
19	M	504	IZL	C43-O28-P-O29
19	G	503	IZL	C43-O28-P-O29
14	O	302	WUO	C56-O55-P52-O51
18	M	503	7PH	C28-C29-C2A-C2B
21	P	301	CDL	C39-C40-C41-C42
17	W	201	9YF	O9-C-C1-O
18	G	504	7PH	O11-C1-C2-O21
21	H	601	CDL	OA5-CA3-CA4-OA6
21	N	607	CDL	C12-C11-CA5-OA6
21	N	607	CDL	C31-C32-C33-C34
21	H	603	CDL	C57-C58-C59-C60
28	c	302	9XX	C7-C8-C9-C10
14	O	302	WUO	C94-C95-C96-C97
21	R	601	CDL	C13-C14-C15-C16
28	c	302	9XX	O-C16-C17-O1
14	O	302	WUO	C65-C66-C67-C68
21	H	604	CDL	C39-C40-C41-C42
13	N	606	MQ9	C44-C46-C47-C48
21	H	603	CDL	C18-C19-C20-C21
21	H	601	CDL	OB7-CB5-OB6-CB4
21	N	602	CDL	C60-C61-C62-C63
21	N	603	CDL	CA4-CA3-OA5-PA1
21	H	601	CDL	CB4-CB3-OB5-PB2
21	H	604	CDL	C1-CA2-OA2-PA1
17	G	502	9YF	C20-C21-C22-C23
21	R	601	CDL	C12-C13-C14-C15
18	S	501	7PH	O22-C21-O21-C2
14	P	302	WUO	C66-C67-C68-C69

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Mol	Chain	Res	Type	Atoms
17	M	502	9YF	C20-C21-C22-C23
21	N	603	CDL	C56-C57-C58-C59
21	P	301	CDL	OB5-CB3-CB4-CB6
24	S	503	3PE	O11-C1-C2-C3
21	P	301	CDL	C16-C17-C18-C19
21	H	604	CDL	C16-C17-C18-C19
21	N	607	CDL	C53-C54-C55-C56
18	G	505	7PH	C29-C2A-C2B-C2C
28	R	609	9XX	C9-C10-C11-C12
21	P	301	CDL	C53-C54-C55-C56
21	H	604	CDL	C15-C16-C17-C18
20	H	605	HEM	C2B-C3B-CAB-CBB
28	R	609	9XX	C24-C25-C26-C27
18	S	501	7PH	C36-C37-C38-C39
21	N	603	CDL	C31-C32-C33-C34
21	R	605	CDL	C36-C37-C38-C39
21	H	604	CDL	C54-C55-C56-C57
21	P	301	CDL	C59-C60-C61-C62
21	R	601	CDL	C16-C17-C18-C19
21	R	601	CDL	CB3-CB4-CB6-OB8
21	R	601	CDL	OB5-CB3-CB4-OB6
21	H	603	CDL	OA5-CA3-CA4-OA6
20	H	602	HEM	C4B-C3B-CAB-CBB
21	P	301	CDL	CA2-C1-CB2-OB2
28	R	609	9XX	C23-C24-C25-C26
18	M	503	7PH	O21-C2-C3-O31
21	R	601	CDL	OB6-CB4-CB6-OB8
21	H	603	CDL	OB6-CB4-CB6-OB8
21	N	602	CDL	C71-CB7-OB8-CB6
21	N	603	CDL	C58-C59-C60-C61
21	H	601	CDL	C18-C19-C20-C21
13	O	305	MQ9	C13-C14-C16-C17
21	N	603	CDL	C23-C24-C25-C26
21	H	601	CDL	C13-C14-C15-C16
21	N	603	CDL	C19-C20-C21-C22
21	N	602	CDL	C74-C75-C76-C77
21	N	607	CDL	C55-C56-C57-C58
21	H	604	CDL	C60-C61-C62-C63
21	R	601	CDL	C33-C34-C35-C36
28	Y	302	9XX	C19-C20-C21-C22
14	P	302	WUO	C93-C94-C95-C96
13	O	305	MQ9	C15-C14-C16-C17

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Mol	Chain	Res	Type	Atoms
21	N	603	CDL	C1-CA2-OA2-PA1
13	H	606	MQ9	C38-C39-C41-C42
21	R	605	CDL	C75-C76-C77-C78
17	M	502	9YF	C1-O-P-O8
21	N	602	CDL	CA2-OA2-PA1-OA4
21	N	602	CDL	CA3-OA5-PA1-OA4
21	N	602	CDL	CB2-OB2-PB2-OB4
21	N	602	CDL	CB3-OB5-PB2-OB3
21	N	602	CDL	CB3-OB5-PB2-OB4
21	N	603	CDL	CB2-OB2-PB2-OB4
21	N	607	CDL	CA2-OA2-PA1-OA4
21	N	607	CDL	CB2-OB2-PB2-OB4
21	N	607	CDL	CB3-OB5-PB2-OB3
21	N	607	CDL	CB3-OB5-PB2-OB4
21	P	301	CDL	CA3-OA5-PA1-OA4
21	P	301	CDL	CB3-OB5-PB2-OB4
21	R	601	CDL	CB2-OB2-PB2-OB3
21	R	605	CDL	CA2-OA2-PA1-OA4
21	R	605	CDL	CB2-OB2-PB2-OB3
21	H	601	CDL	CA2-OA2-PA1-OA3
21	H	601	CDL	CB2-OB2-PB2-OB4
21	H	603	CDL	CA3-OA5-PA1-OA3
21	H	603	CDL	CB2-OB2-PB2-OB3
21	H	604	CDL	CA2-OA2-PA1-OA4
18	S	501	7PH	O11-C1-C2-C3
21	H	601	CDL	OA5-CA3-CA4-CA6
21	H	603	CDL	OB5-CB3-CB4-CB6
21	H	604	CDL	OB5-CB3-CB4-CB6
21	R	605	CDL	OA7-CA5-OA6-CA4
13	H	606	MQ9	C47-C48-C49-C50
25	R	602	HEA	C3B-C11-C12-C13
21	N	602	CDL	OB9-CB7-OB8-CB6
21	R	605	CDL	C73-C74-C75-C76
17	W	201	9YF	C15-C16-C17-C18
21	N	603	CDL	C24-C25-C26-C27
14	P	302	WUO	C86-C87-C88-C90
18	S	501	7PH	O11-C1-C2-O21
18	G	505	7PH	O11-C1-C2-O21
21	N	607	CDL	OA5-CA3-CA4-OA6
21	H	603	CDL	OB5-CB3-CB4-OB6
21	H	604	CDL	OB5-CB3-CB4-OB6
24	S	503	3PE	O11-C1-C2-O21

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Mol	Chain	Res	Type	Atoms
14	O	302	WUO	C31-C01-O02-C03
21	H	603	CDL	C31-C32-C33-C34
21	R	605	CDL	C11-CA5-OA6-CA4
18	M	503	7PH	C23-C24-C25-C26
17	M	502	9YF	C11-C10-C9-C8
17	M	502	9YF	C1-C-C24-O11
21	P	301	CDL	C72-C73-C74-C75
25	R	603	HEA	O11-C11-C3B-C4B
14	P	302	WUO	O58-C57-C76-O77
17	G	502	9YF	O9-C-C24-O11
18	S	501	7PH	C33-C34-C35-C36
17	M	502	9YF	C26-C27-C28-C29
24	S	503	3PE	C25-C26-C27-C28
28	c	302	9XX	C16-C17-O1-C18
21	H	603	CDL	C32-C33-C34-C35
14	O	302	WUO	C89-C88-C90-C91
28	R	609	9XX	C36-C27-C28-C29
18	G	504	7PH	C37-C38-C39-C3A
14	O	302	WUO	C93-C94-C95-C96
14	P	302	WUO	C50-C37-O38-C39
21	N	602	CDL	CA5-C11-C12-C13
21	R	601	CDL	C34-C35-C36-C37
21	R	601	CDL	CB3-CB4-OB6-CB5
24	S	503	3PE	C3-C2-O21-C21
28	Y	302	9XX	C13-C14-C15-O
21	H	603	CDL	C15-C16-C17-C18
14	P	302	WUO	C17-C18-C19-C20
14	O	302	WUO	C50-C01-O02-C03
13	O	305	MQ9	C34-C36-C37-C38
14	O	302	WUO	O58-C57-C76-O77
17	W	201	9YF	O9-C-C24-O11
21	N	602	CDL	OB6-CB4-CB6-OB8
21	R	601	CDL	CB3-OB5-PB2-OB2
23	R	608	TRD	C6-C7-C8-C9
21	N	607	CDL	C14-C15-C16-C17
18	S	501	7PH	C34-C35-C36-C37
21	H	603	CDL	C54-C55-C56-C57
21	N	603	CDL	C16-C17-C18-C19
18	G	504	7PH	C35-C36-C37-C38
21	N	607	CDL	C36-C37-C38-C39
21	N	603	CDL	C71-CB7-OB8-CB6
21	H	603	CDL	OA5-CA3-CA4-CA6

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Mol	Chain	Res	Type	Atoms
21	R	601	CDL	C55-C56-C57-C58
13	H	606	MQ9	C46-C47-C48-C49
20	H	605	HEM	C4B-C3B-CAB-CBB
21	H	604	CDL	O1-C1-CA2-OA2
20	N	605	HEM	CAA-CBA-CGA-O1A
25	R	602	HEA	CAA-CBA-CGA-O1A
28	R	609	9XX	C30-C31-C32-C33
21	R	601	CDL	CB4-CB3-OB5-PB2
20	H	602	HEM	CAA-CBA-CGA-O2A
22	N	604	A1IGA	C13-C14-O01-C15
15	O	304	HEC	CAD-CBD-CGD-O2D
20	H	602	HEM	CAA-CBA-CGA-O1A
14	P	302	WUO	C23-C24-C25-C26
21	R	601	CDL	C53-C54-C55-C56
21	R	601	CDL	C54-C55-C56-C57
15	O	303	HEC	CAA-CBA-CGA-O2A
21	P	301	CDL	CB7-C71-C72-C73
20	H	605	HEM	CAD-CBD-CGD-O1D
20	N	601	HEM	C4D-C3D-CAD-CBD
19	M	504	IZL	C46-C45-O34-C60
19	G	503	IZL	C46-C45-O34-C60
21	R	601	CDL	CB6-CB4-OB6-CB5
13	O	301	MQ9	C15-C14-C16-C17
28	c	302	9XX	C27-C28-C29-C30
21	N	603	CDL	OB9-CB7-OB8-CB6
18	G	505	7PH	C32-C33-C34-C35
25	R	602	HEA	CAA-CBA-CGA-O2A
25	R	603	HEA	CAD-CBD-CGD-O2D
15	O	304	HEC	CAD-CBD-CGD-O1D
20	H	605	HEM	CAD-CBD-CGD-O2D
14	P	302	WUO	C21-C22-C23-C24
13	O	305	MQ9	C24-C26-C27-C28
20	N	605	HEM	CAA-CBA-CGA-O2A
25	R	603	HEA	CAD-CBD-CGD-O1D
21	R	601	CDL	C76-C77-C78-C79
21	R	605	CDL	C16-C17-C18-C19
21	N	602	CDL	C31-CA7-OA8-CA6
21	R	605	CDL	C18-C19-C20-C21
21	H	604	CDL	C35-C36-C37-C38
21	P	301	CDL	C34-C35-C36-C37
21	H	604	CDL	C52-C53-C54-C55
21	N	602	CDL	OA9-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
18	S	501	7PH	O31-C31-C32-C33
21	R	601	CDL	C32-C31-CA7-OA8
21	N	602	CDL	C55-C56-C57-C58
28	c	302	9XX	O2-C18-C19-C20
19	G	503	IZL	C3-C4-C5-C6
13	O	305	MQ9	C25-C24-C26-C27
13	H	606	MQ9	C30-C29-C31-C32
17	G	502	9YF	C35-C36-C37-C38
19	M	504	IZL	C3-C4-C5-C6
14	O	302	WUO	C91-C92-C93-C94
21	R	605	CDL	C31-C32-C33-C34
21	N	602	CDL	C32-C31-CA7-OA8
21	N	607	CDL	C35-C36-C37-C38
21	R	601	CDL	C18-C19-C20-C21
13	H	606	MQ9	C13-C14-C16-C17
13	H	606	MQ9	C28-C29-C31-C32
15	O	303	HEC	CAA-CBA-CGA-O1A
21	N	603	CDL	C1-CB2-OB2-PB2
21	N	603	CDL	OA6-CA4-CA6-OA8
21	P	301	CDL	OA6-CA4-CA6-OA8
21	R	605	CDL	C12-C13-C14-C15
21	H	601	CDL	C12-C13-C14-C15
13	O	301	MQ9	C45-C44-C46-C47
13	H	607	MQ9	C25-C24-C26-C27
28	R	609	9XX	C2-C3-C4-C5
13	O	305	MQ9	C23-C24-C26-C27
21	R	601	CDL	C17-C18-C19-C20
17	W	201	9YF	C12-C13-C14-C15
21	R	601	CDL	C31-C32-C33-C34
21	R	601	CDL	C52-C51-CB5-OB6
21	R	605	CDL	C76-C77-C78-C79
25	R	602	HEA	CAD-CBD-CGD-O2D
21	N	602	CDL	OB7-CB5-OB6-CB4
17	W	201	9YF	O12-C25-O11-C24
20	N	601	HEM	CAA-CBA-CGA-O2A
14	P	302	WUO	C71-C72-C73-C74
13	O	305	MQ9	C12-C11-C9-C10
13	H	607	MQ9	C20-C19-C21-C22
18	G	505	7PH	O21-C21-C22-C23
19	M	504	IZL	O1-C10-C9-C8
19	G	503	IZL	O1-C10-C9-C8
17	G	502	9YF	C1-C-C24-O11

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Mol	Chain	Res	Type	Atoms
21	H	601	CDL	CA4-CA3-OA5-PA1
21	N	602	CDL	OB5-CB3-CB4-OB6
21	N	603	CDL	C15-C16-C17-C18
28	R	609	9XX	C7-C8-C9-C10
20	N	605	HEM	C4B-C3B-CAB-CBB
21	N	607	CDL	C12-C11-CA5-OA7
20	N	601	HEM	CAD-CBD-CGD-O2D
19	M	504	IZL	C15-C14-O3-C13
20	N	601	HEM	CAA-CBA-CGA-O1A
25	R	602	HEA	CAD-CBD-CGD-O1D
22	N	604	A1IGA	C02-C14-O01-C15
21	N	602	CDL	OB5-CB3-CB4-CB6
28	c	302	9XX	C37-C17-O1-C18
15	O	304	HEC	CAA-CBA-CGA-O1A
21	R	601	CDL	OB9-CB7-OB8-CB6
14	P	302	WUO	C20-C21-C22-C23
18	G	505	7PH	C28-C29-C2A-C2B
19	G	503	IZL	C15-C14-O3-C13
20	N	605	HEM	CAD-CBD-CGD-O1D
28	Y	302	9XX	O1-C18-C19-C20
21	R	601	CDL	C71-CB7-OB8-CB6
17	W	201	9YF	O9-C8-C9-C10
21	N	602	CDL	C18-C19-C20-C21
21	N	607	CDL	C83-C84-C85-C86
13	O	305	MQ9	C12-C11-C9-C8
17	M	502	9YF	C31-C32-C33-C34
17	G	502	9YF	C31-C32-C33-C34
17	W	201	9YF	C26-C25-O11-C24
14	P	302	WUO	C81-C82-C83-C84
21	N	602	CDL	C51-CB5-OB6-CB4
18	G	504	7PH	O21-C21-C22-C23
21	H	603	CDL	C12-C13-C14-C15
14	P	302	WUO	C18-C19-C20-C21
13	N	606	MQ9	C25-C24-C26-C27
24	S	503	3PE	C33-C34-C35-C36
17	G	502	9YF	C15-C16-C17-C18
23	S	502	TRD	C1-C2-C3-C4
19	M	504	IZL	C43-C14-O3-C13
14	O	302	WUO	C56-C57-C76-O77
19	M	504	IZL	C44-C45-C46-O32
19	G	503	IZL	C44-C45-C46-O32
21	P	301	CDL	CA3-CA4-CA6-OA8

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Mol	Chain	Res	Type	Atoms
19	G	503	IZL	C43-C14-O3-C13
21	N	602	CDL	C12-C13-C14-C15
13	H	606	MQ9	C15-C14-C16-C17
18	M	503	7PH	O21-C21-C22-C23
21	P	301	CDL	C74-C75-C76-C77
28	Y	302	9XX	O2-C18-C19-C20
15	O	303	HEC	CAD-CBD-CGD-O2D
20	N	605	HEM	CAD-CBD-CGD-O2D
17	M	502	9YF	C36-C37-C38-C39
14	O	302	WUO	C56-O55-P52-O54
21	H	601	CDL	CA3-OA5-PA1-OA3
21	H	603	CDL	CA3-OA5-PA1-OA4
19	G	503	IZL	C49-C50-C51-C52
21	P	301	CDL	C12-C11-CA5-OA6
15	O	304	HEC	CAA-CBA-CGA-O2A
19	G	503	IZL	O-C10-C9-C8
23	T	201	TRD	C5-C6-C7-C8
25	R	602	HEA	O11-C11-C12-C13
19	M	504	IZL	O-C10-C9-C8
19	M	504	IZL	C49-C50-C51-C52
21	R	605	CDL	C55-C56-C57-C58
14	P	302	WUO	O58-C59-C61-C62
18	M	503	7PH	C29-C2A-C2B-C2C
19	M	504	IZL	C44-C45-O34-C60
19	G	503	IZL	C44-C45-O34-C60
18	G	505	7PH	O22-C21-C22-C23
21	N	607	CDL	O1-C1-CB2-OB2
21	H	604	CDL	C72-C71-CB7-OB8
21	N	602	CDL	C38-C39-C40-C41
21	N	607	CDL	C32-C31-CA7-OA8
21	H	601	CDL	C32-C31-CA7-OA8
20	N	601	HEM	C2D-C3D-CAD-CBD
25	R	603	HEA	CAA-CBA-CGA-O2A
17	G	502	9YF	C27-C28-C29-C30
13	H	606	MQ9	C25-C24-C26-C27
13	H	607	MQ9	C15-C14-C16-C17
25	R	602	HEA	C27-C19-C20-C21
13	O	301	MQ9	C13-C14-C16-C17
25	R	603	HEA	O11-C11-C3B-C2B
20	N	601	HEM	CAD-CBD-CGD-O1D
21	P	301	CDL	C52-C51-CB5-OB6
21	R	601	CDL	C72-C71-CB7-OB8

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Mol	Chain	Res	Type	Atoms
21	R	601	CDL	C75-C76-C77-C78
21	R	601	CDL	C72-C71-CB7-OB9
25	R	603	HEA	CAA-CBA-CGA-O1A
21	H	603	CDL	C32-C31-CA7-OA8
28	R	609	9XX	C13-C14-C15-O
17	W	201	9YF	O10-C8-C9-C10
21	P	301	CDL	C52-C51-CB5-OB7
18	M	503	7PH	C32-C33-C34-C35
21	H	601	CDL	C52-C51-CB5-OB6
21	R	605	CDL	C13-C14-C15-C16
18	M	503	7PH	O22-C21-C22-C23
21	P	301	CDL	C12-C11-CA5-OA7
21	N	602	CDL	C31-C32-C33-C34
21	H	603	CDL	CA5-C11-C12-C13
14	P	302	WUO	O60-C59-C61-C62
17	M	502	9YF	C35-C36-C37-C38
21	H	604	CDL	C12-C11-CA5-OA6

There are no ring outliers.

33 monomers are involved in 163 short contacts:

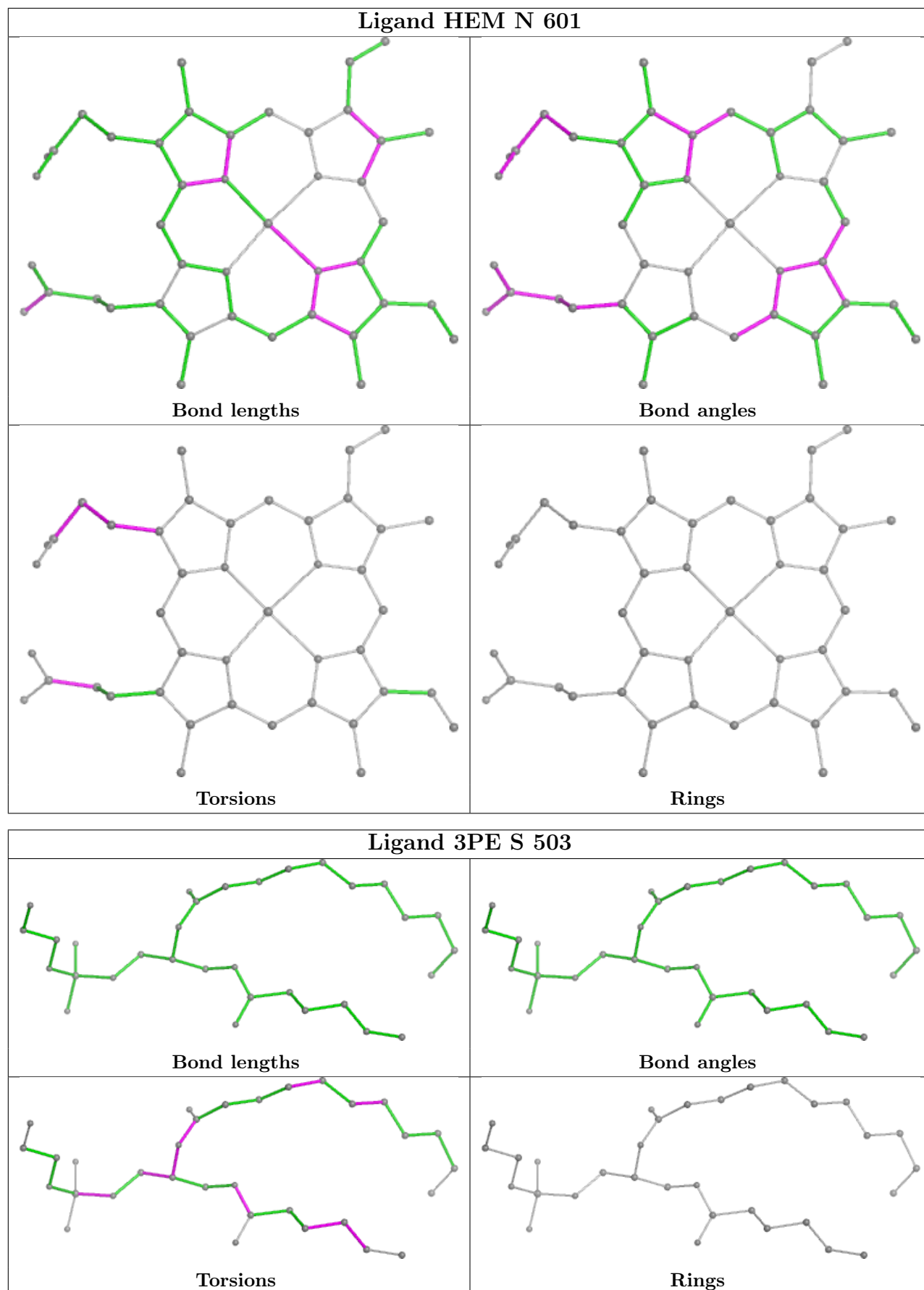
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	N	601	HEM	6	0
13	N	606	MQ9	17	0
23	S	502	TRD	1	0
18	M	503	7PH	1	0
16	M	501	FES	1	0
14	O	302	WUO	2	0
30	W	202	PLM	1	0
21	H	604	CDL	8	0
15	O	303	HEC	6	0
25	R	603	HEA	19	0
18	G	504	7PH	1	0
18	S	501	7PH	1	0
13	O	305	MQ9	12	0
13	H	607	MQ9	3	0
13	O	301	MQ9	5	0
13	H	606	MQ9	10	0
17	W	201	9YF	2	0
20	H	602	HEM	9	0
18	G	505	7PH	1	0
21	N	603	CDL	1	0

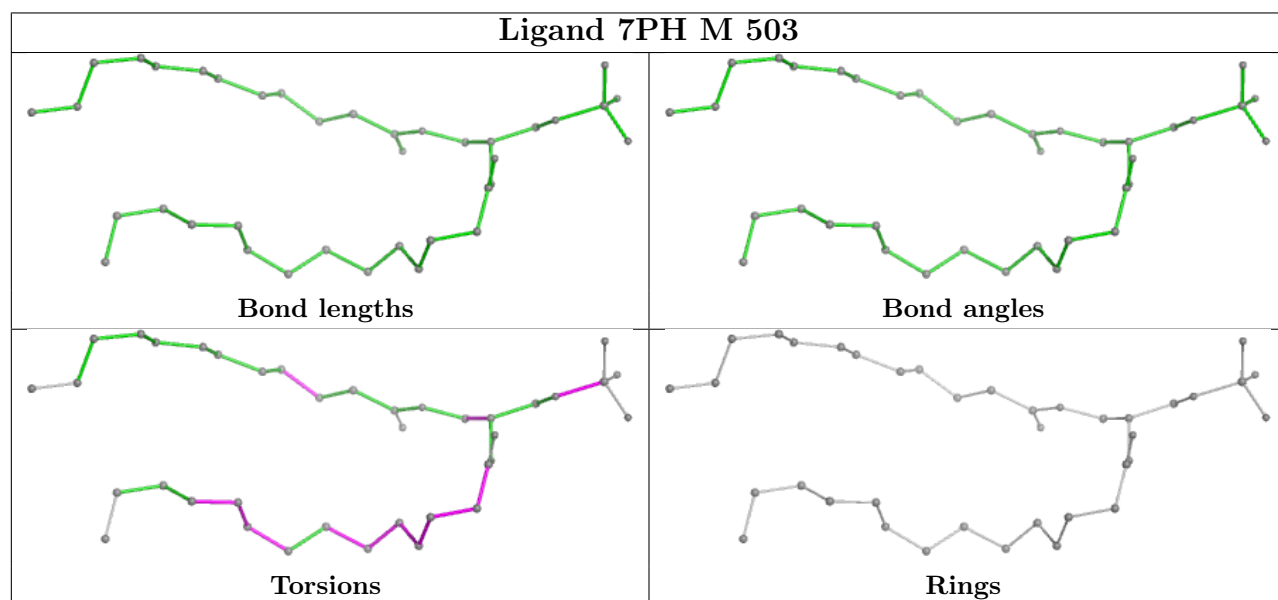
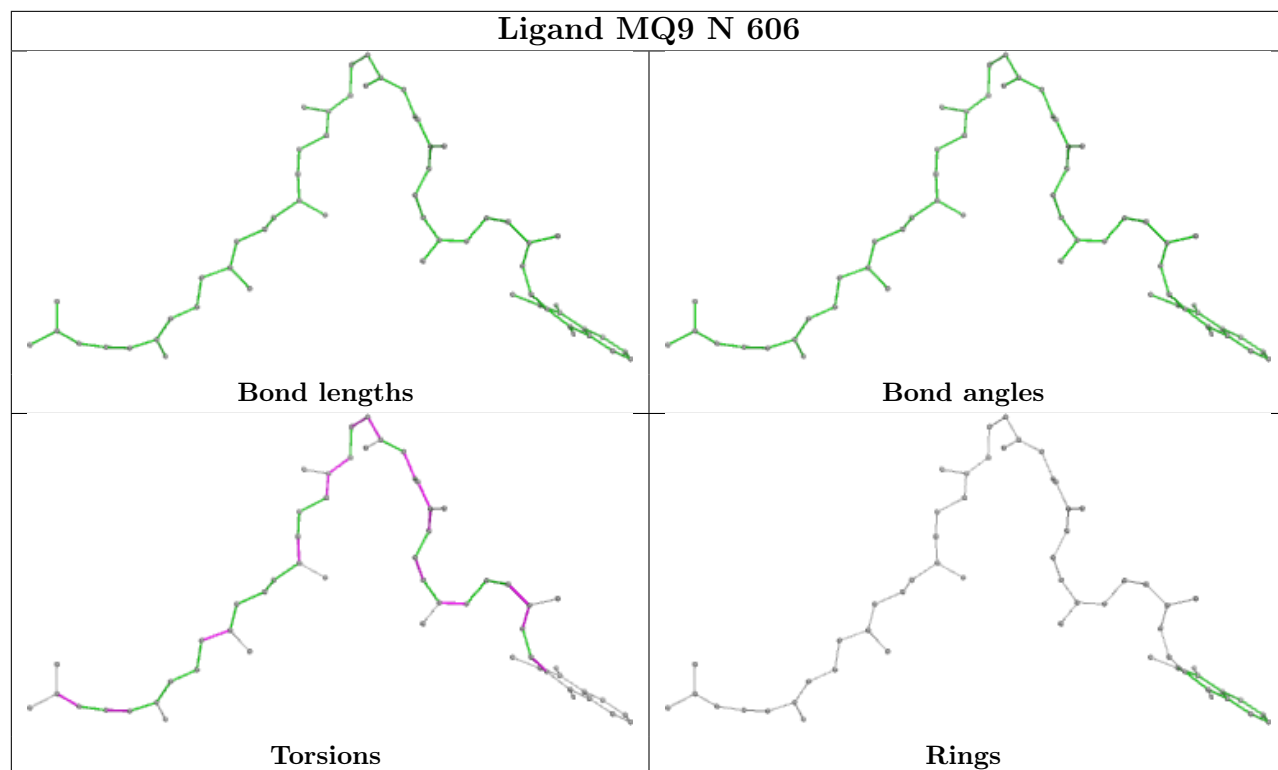
Continued on next page...

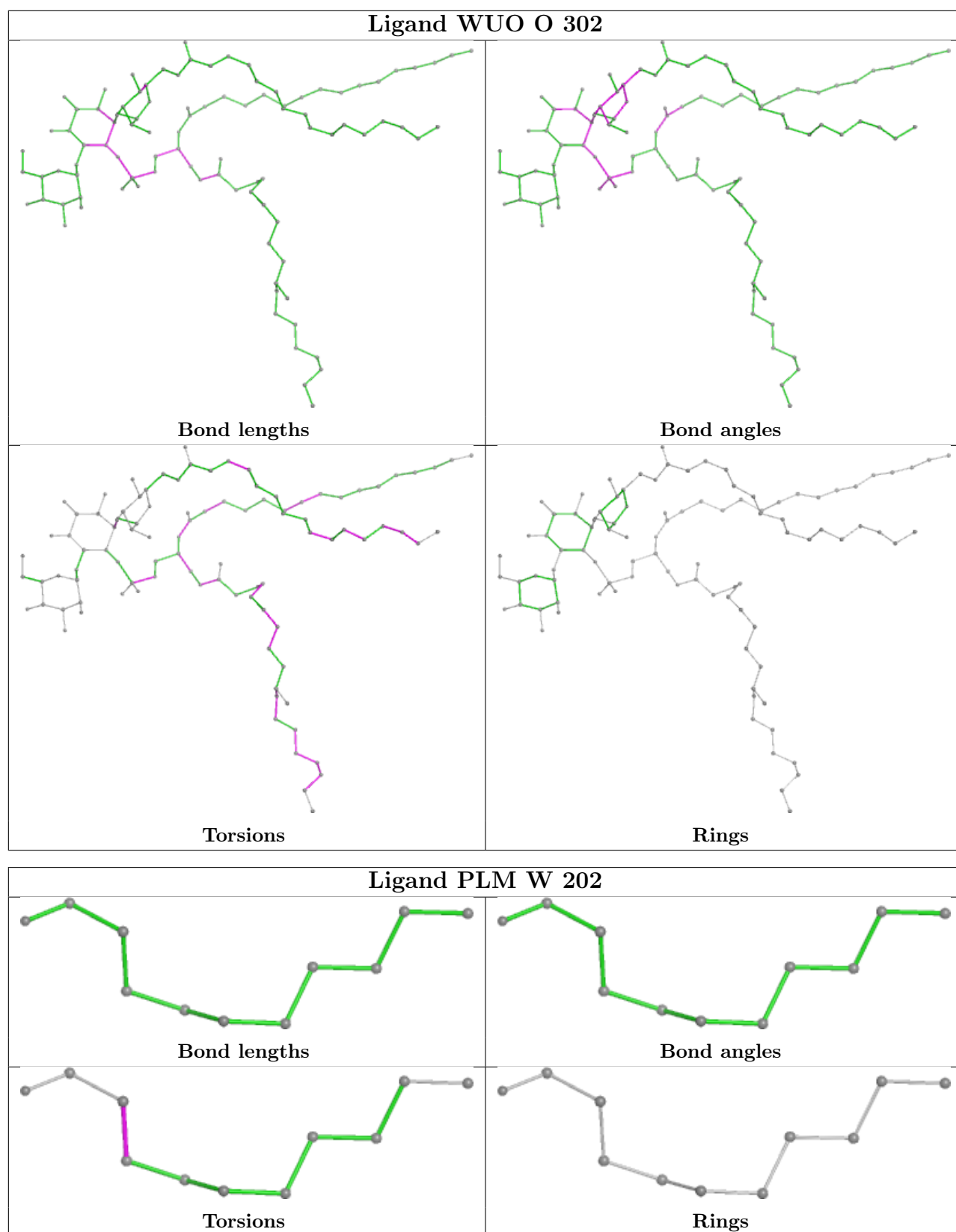
Continued from previous page...

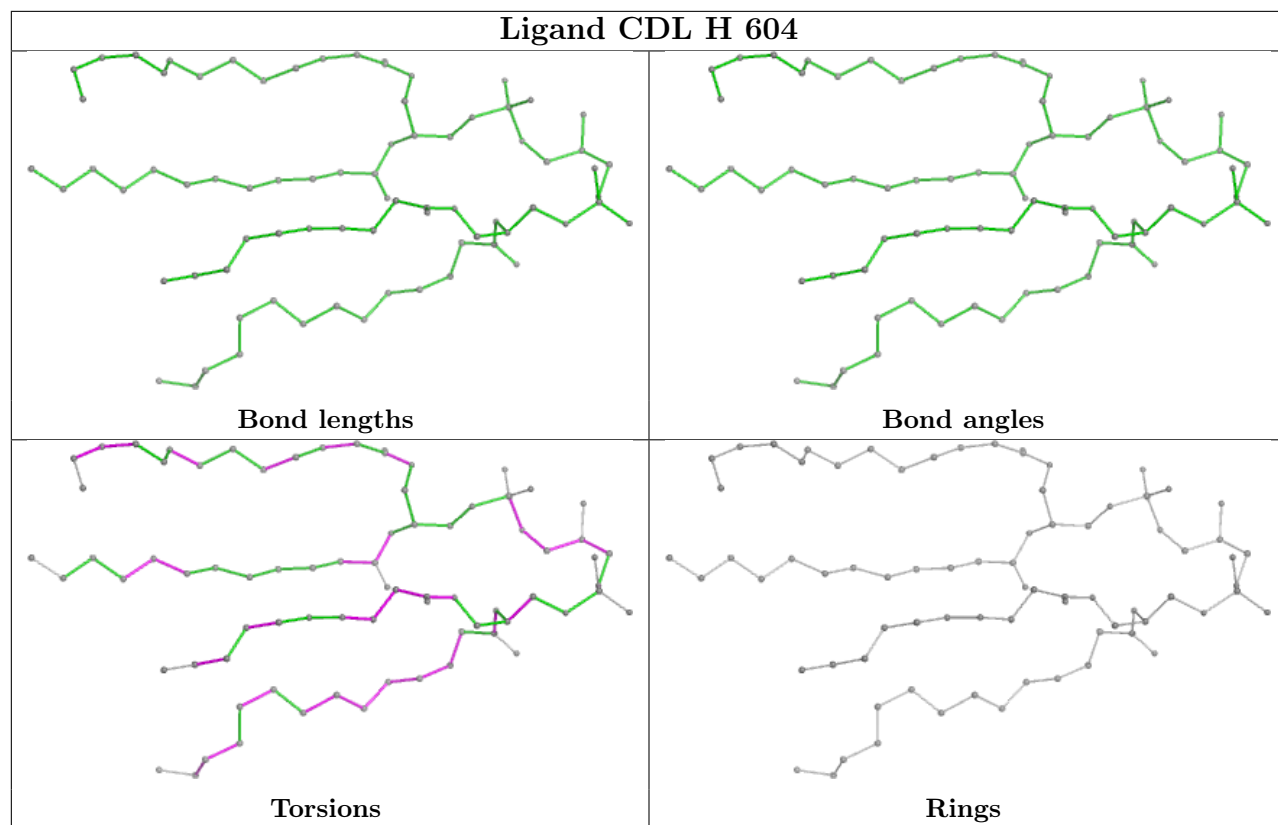
Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	R	605	CDL	9	0
14	P	302	WUO	3	0
25	R	602	HEA	4	0
20	H	605	HEM	10	0
21	N	602	CDL	4	0
21	H	601	CDL	4	0
21	R	601	CDL	3	0
21	H	603	CDL	4	0
28	R	609	9XX	1	0
21	N	607	CDL	2	0
21	P	301	CDL	11	0
20	N	605	HEM	7	0
16	G	501	FES	1	0

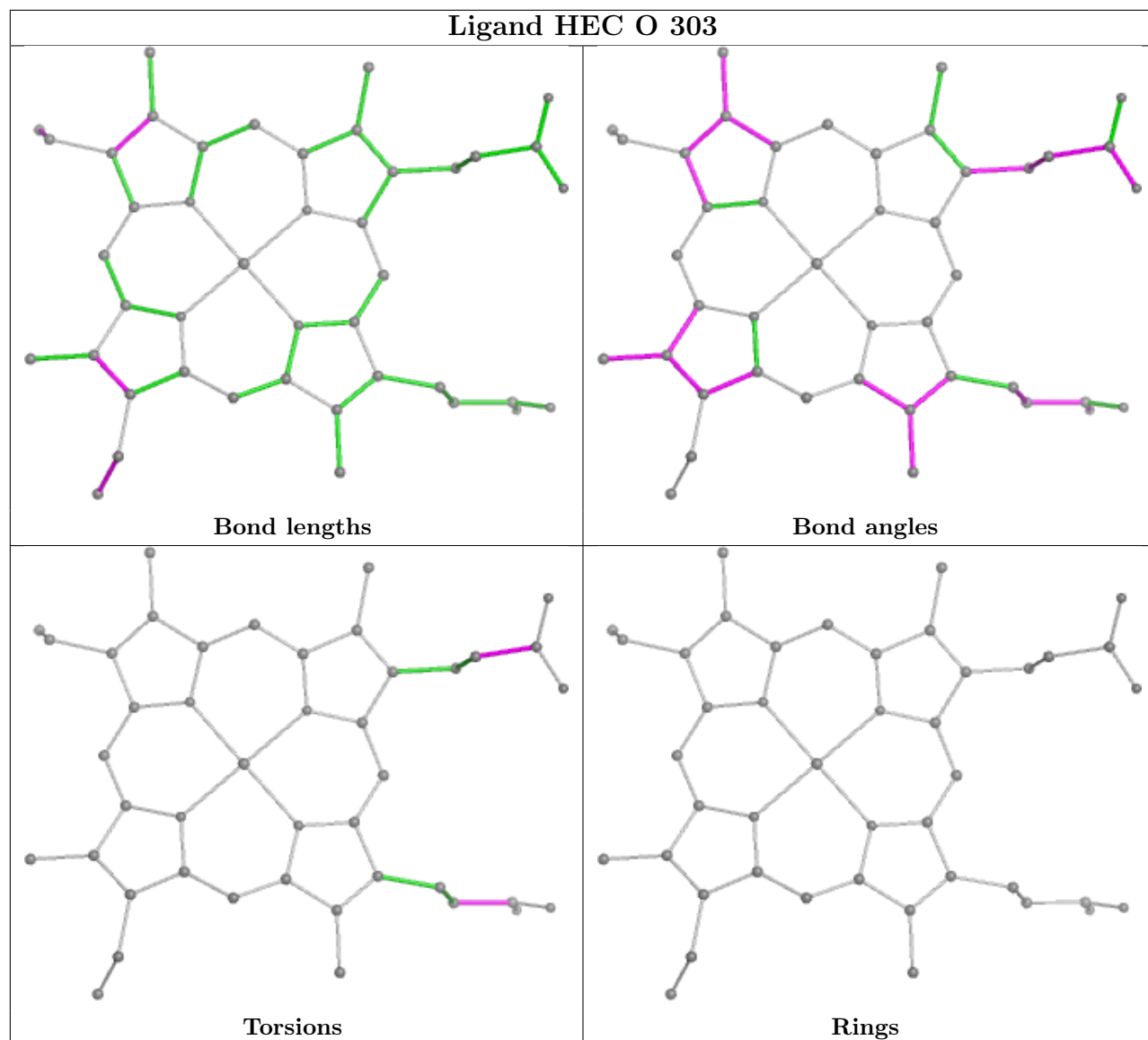
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

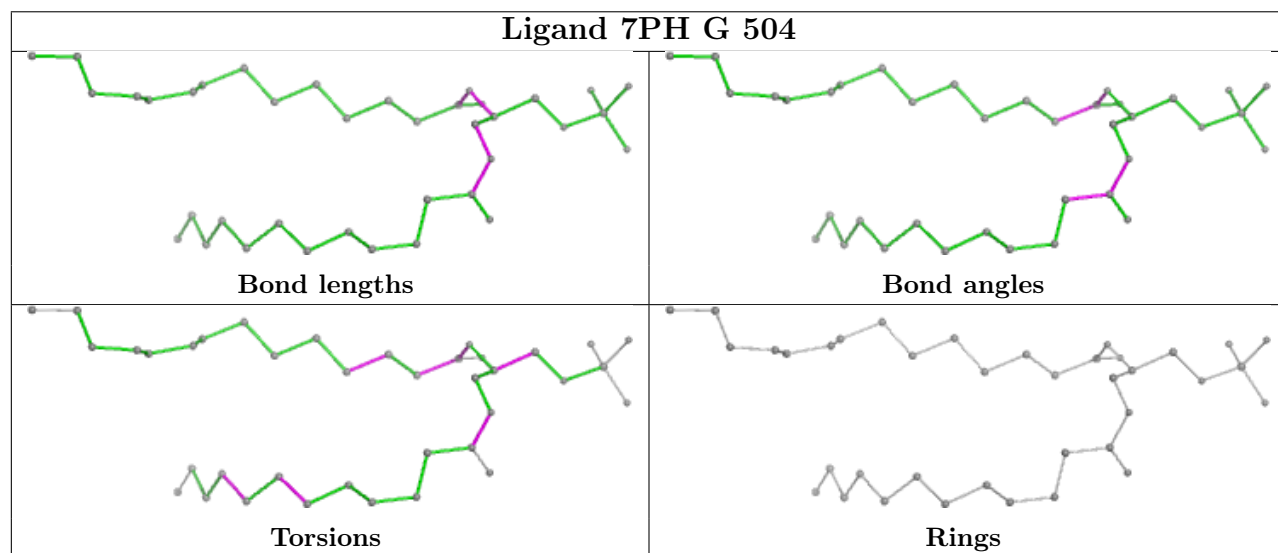
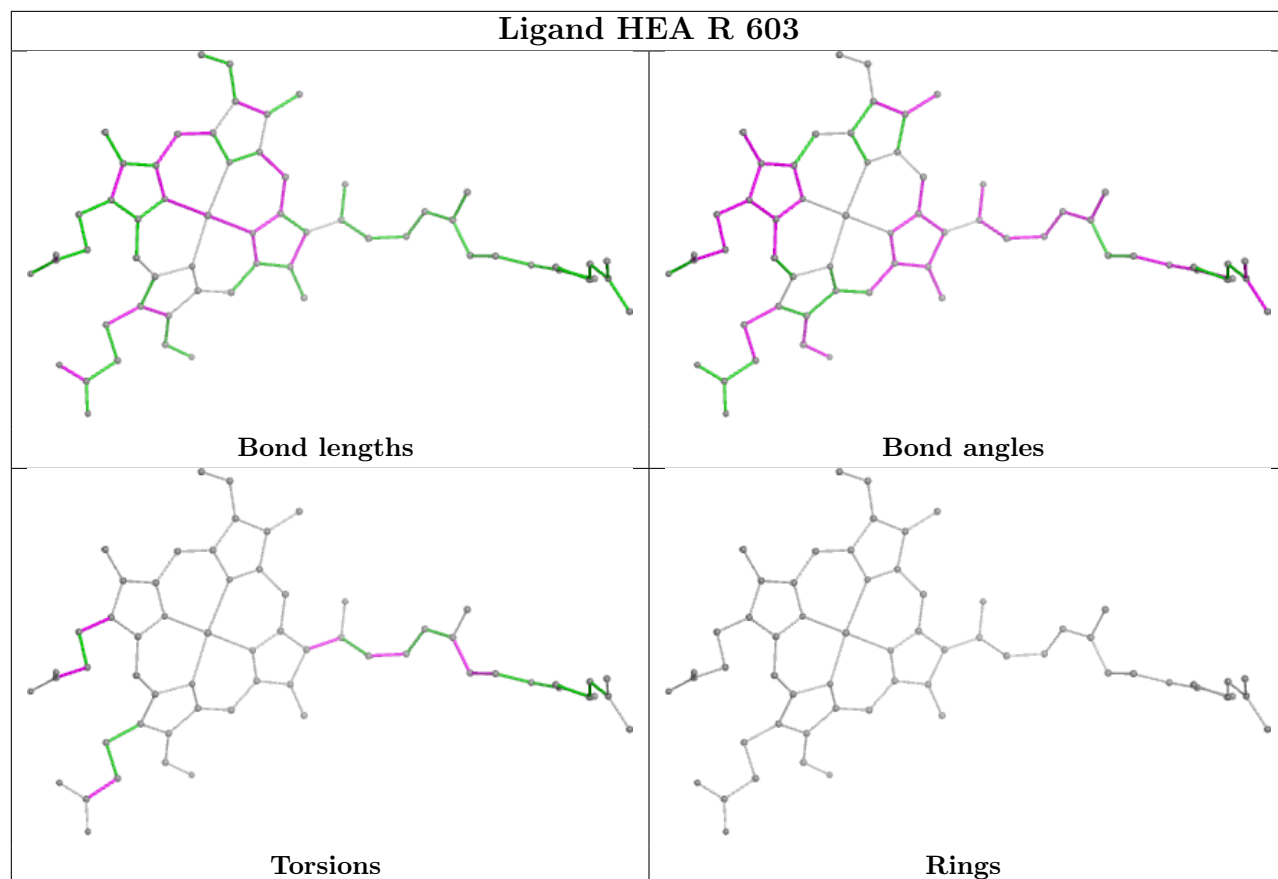


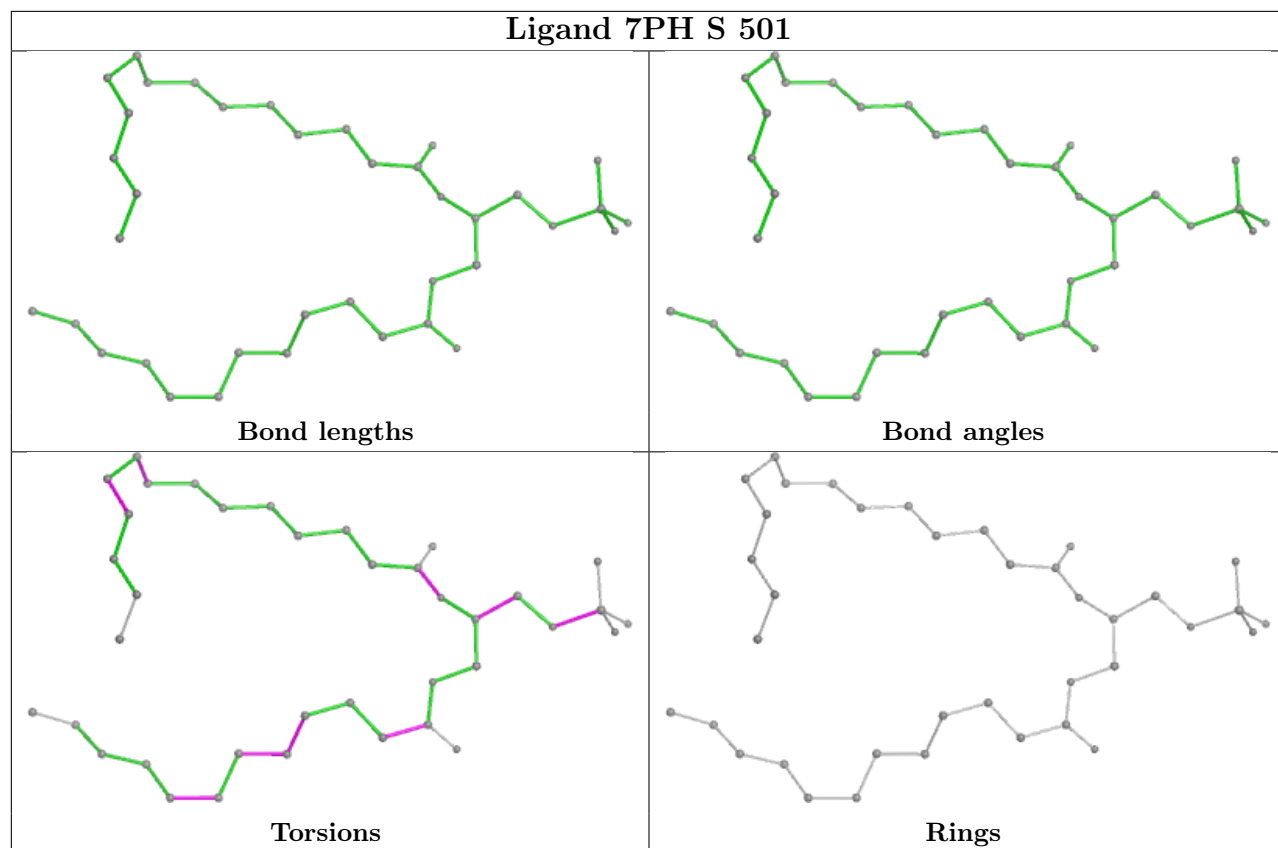


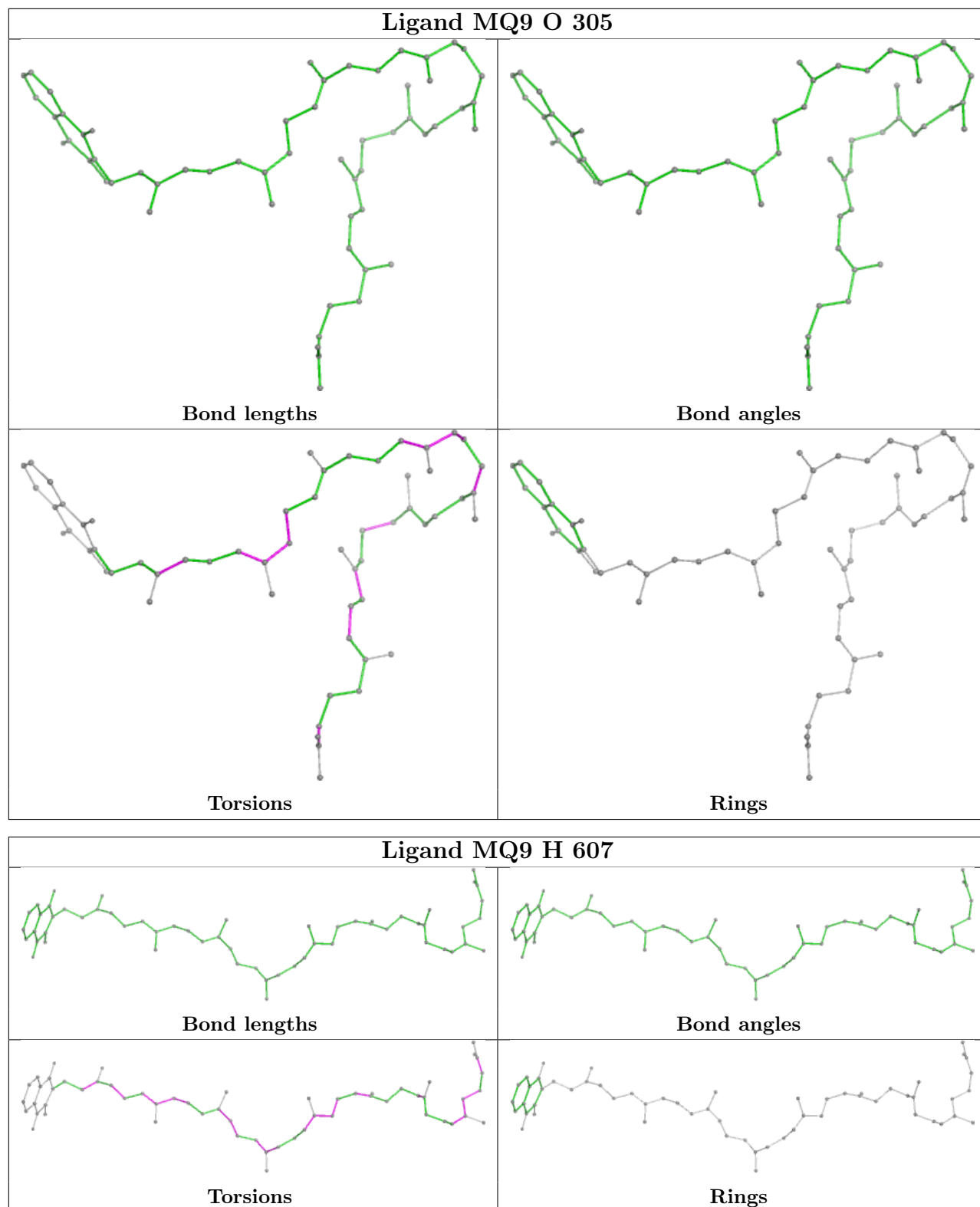


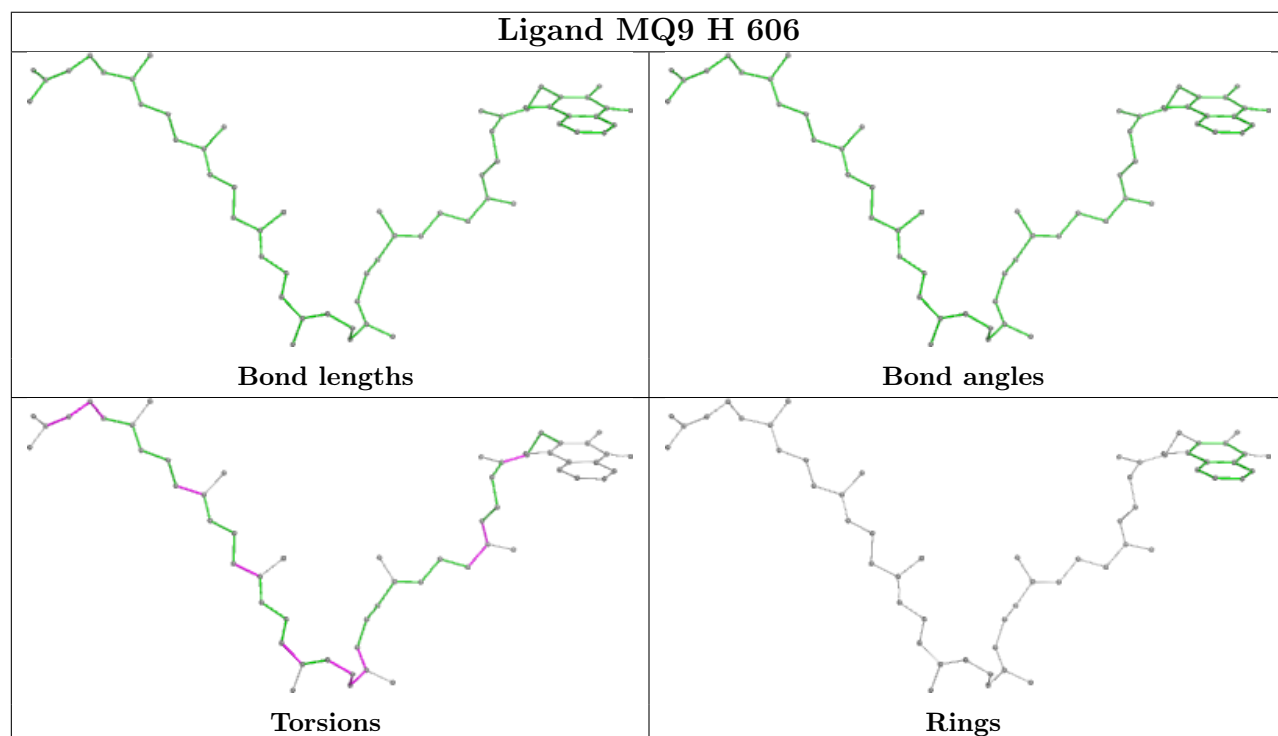
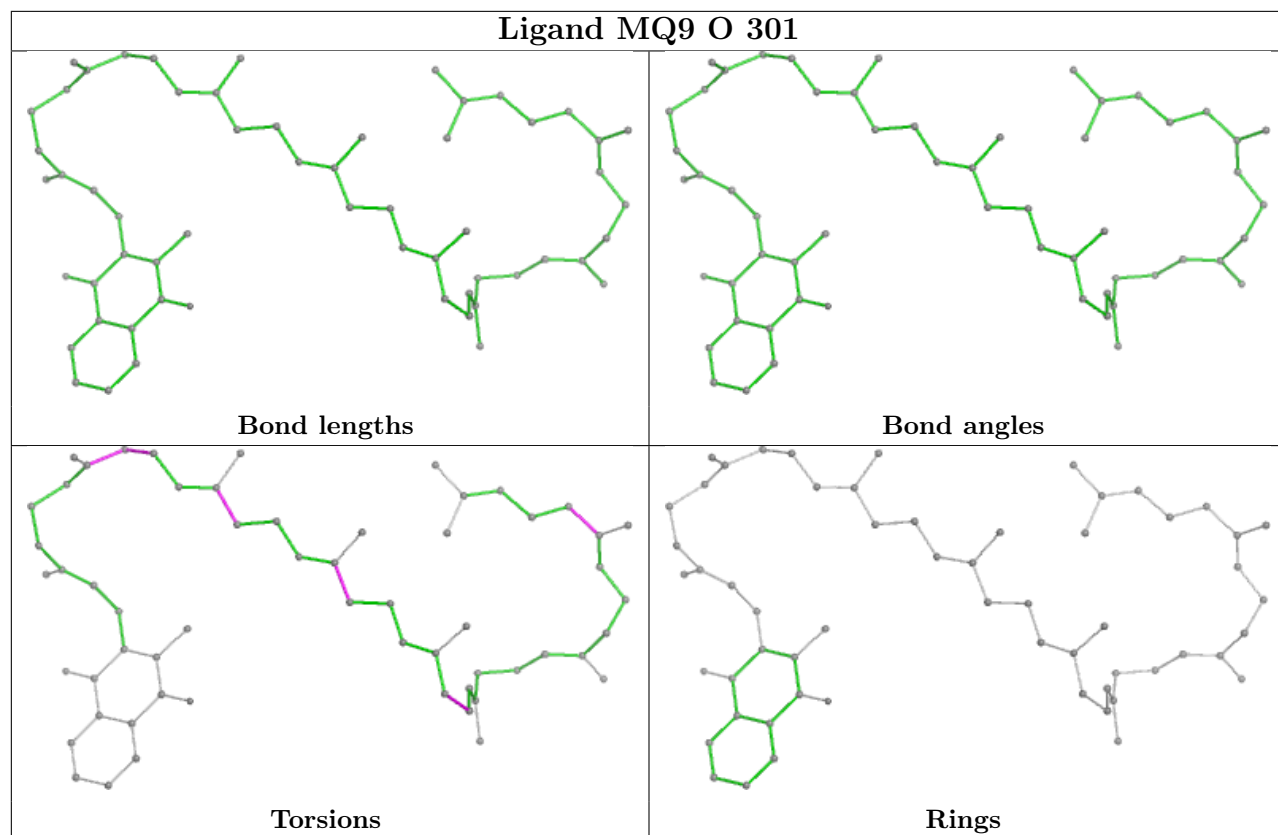


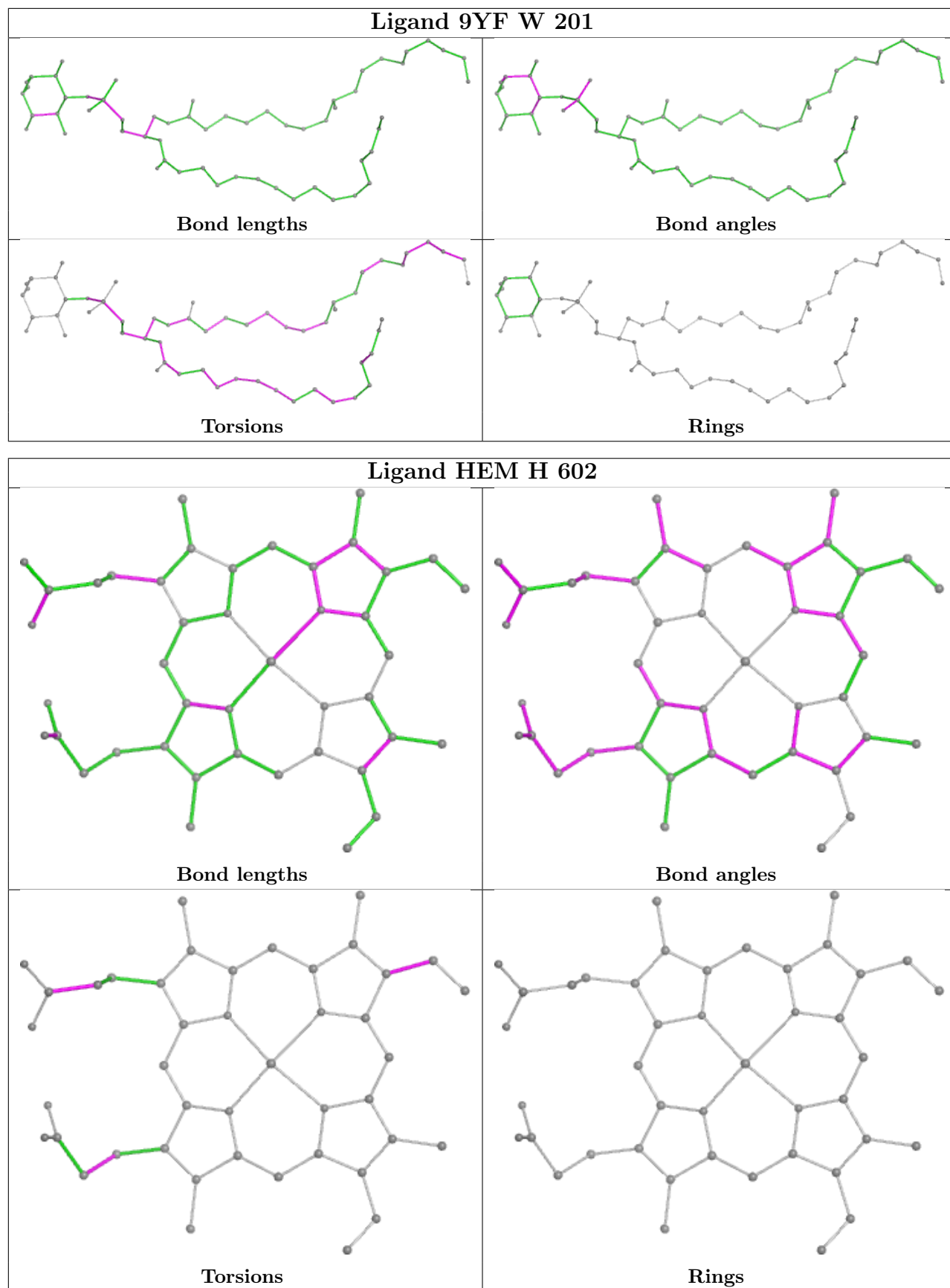


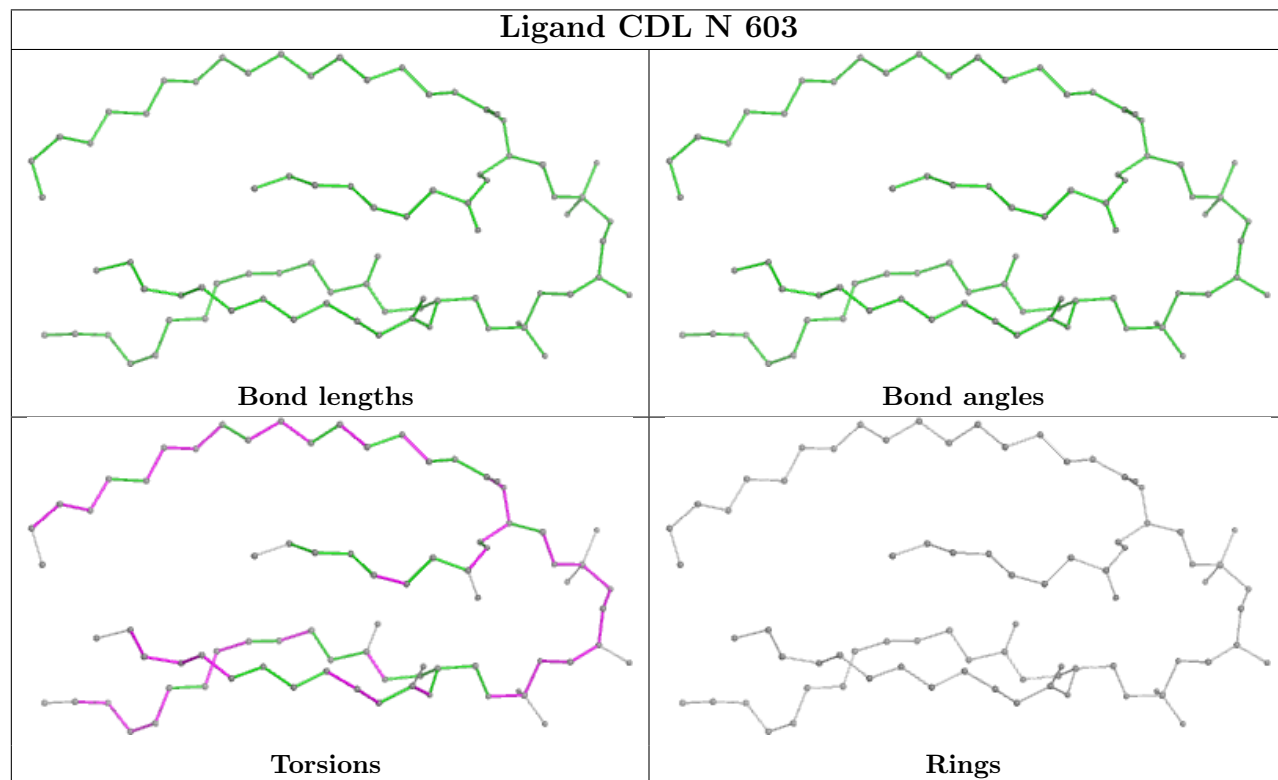
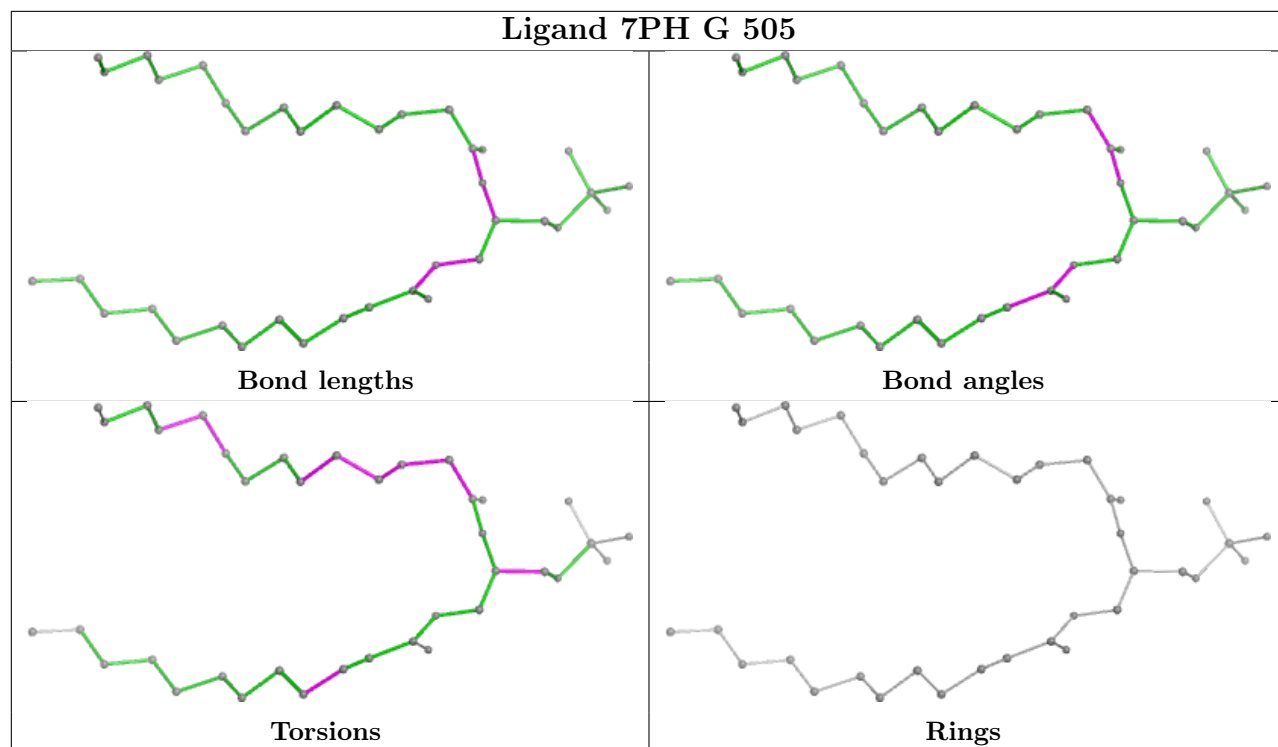


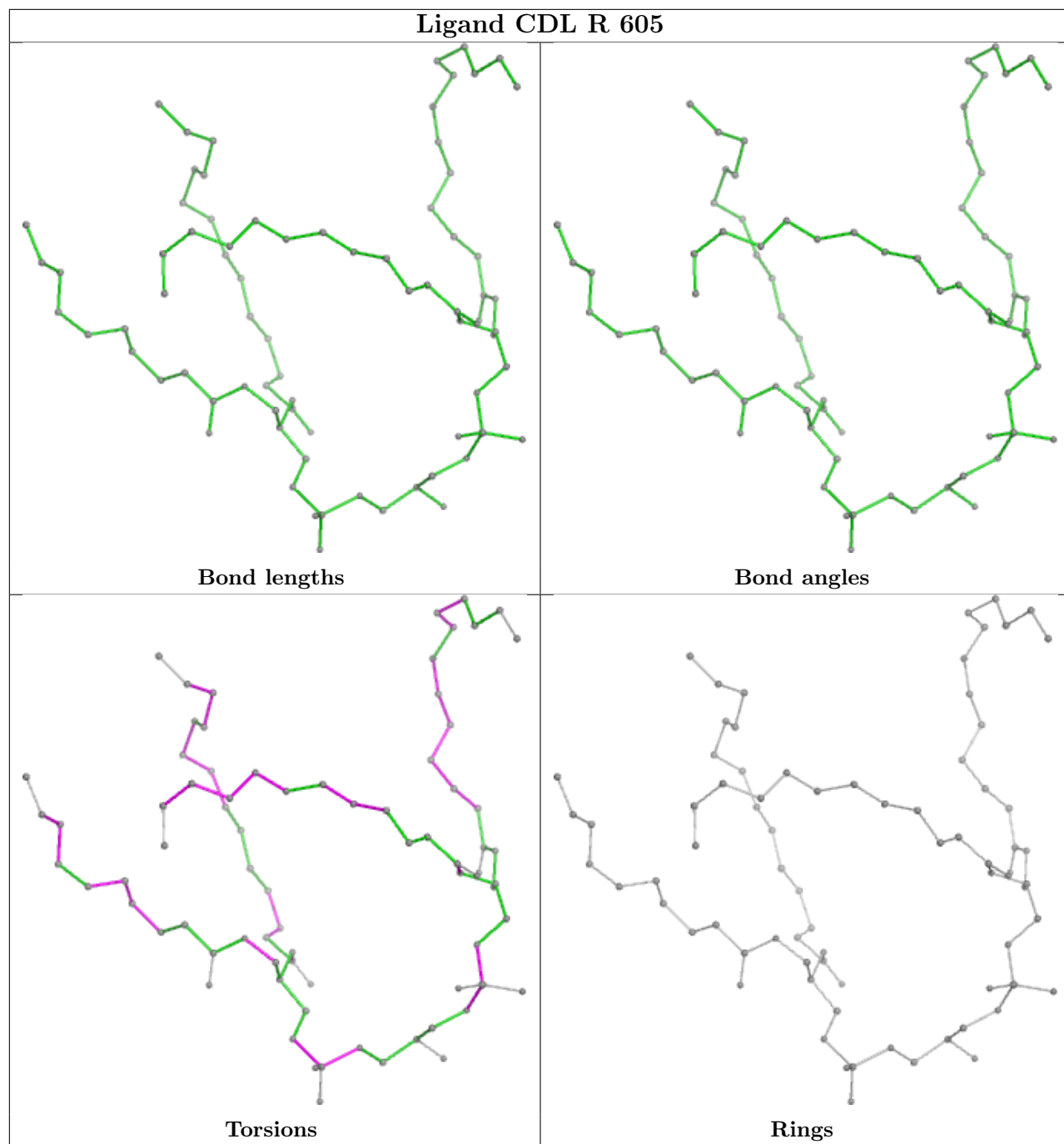


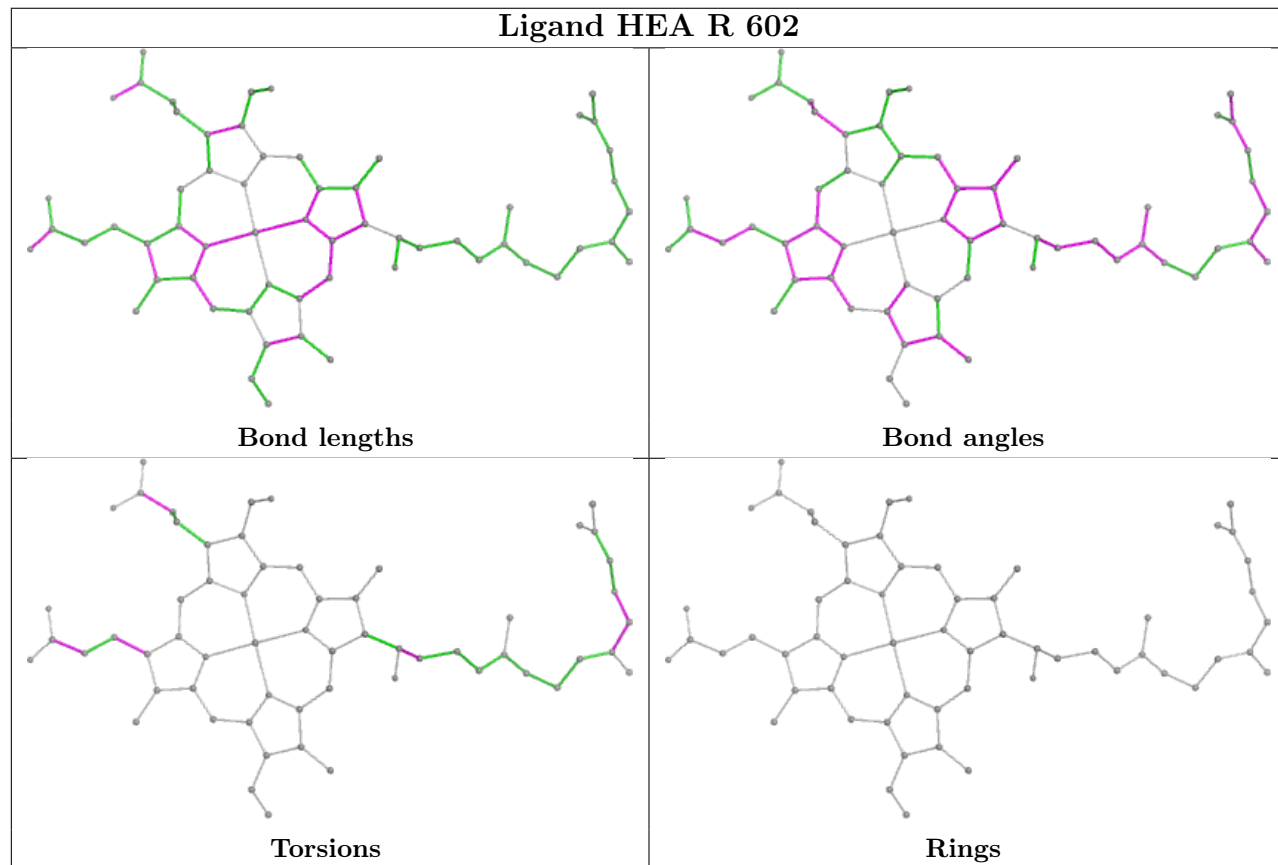
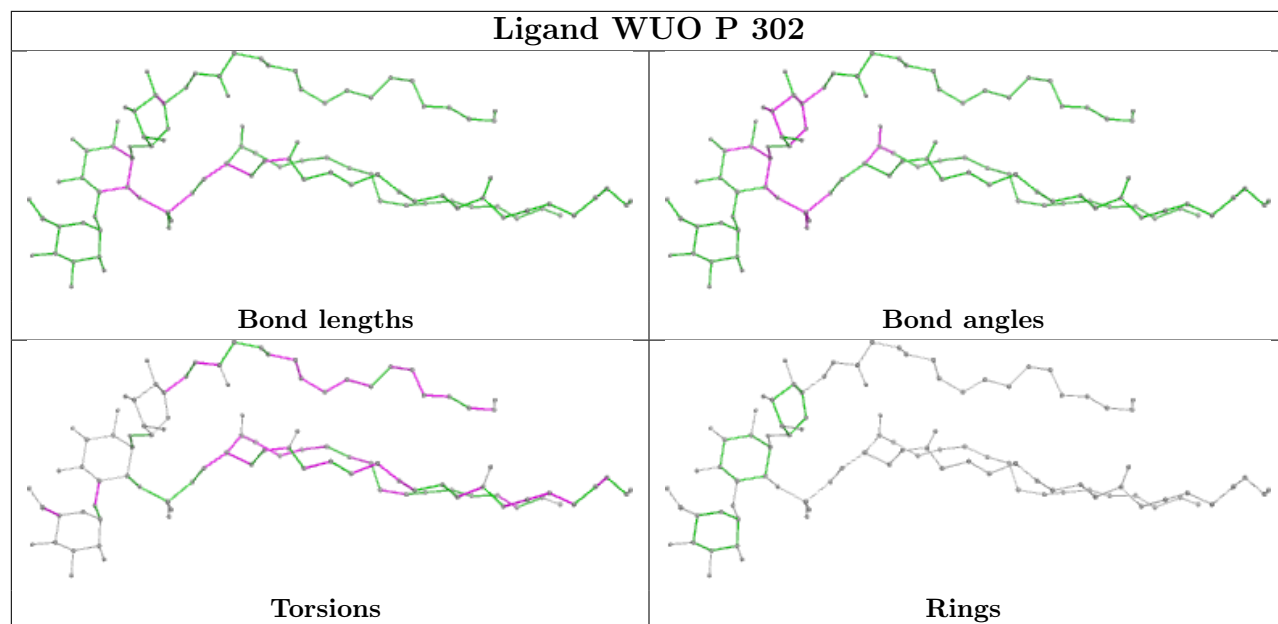


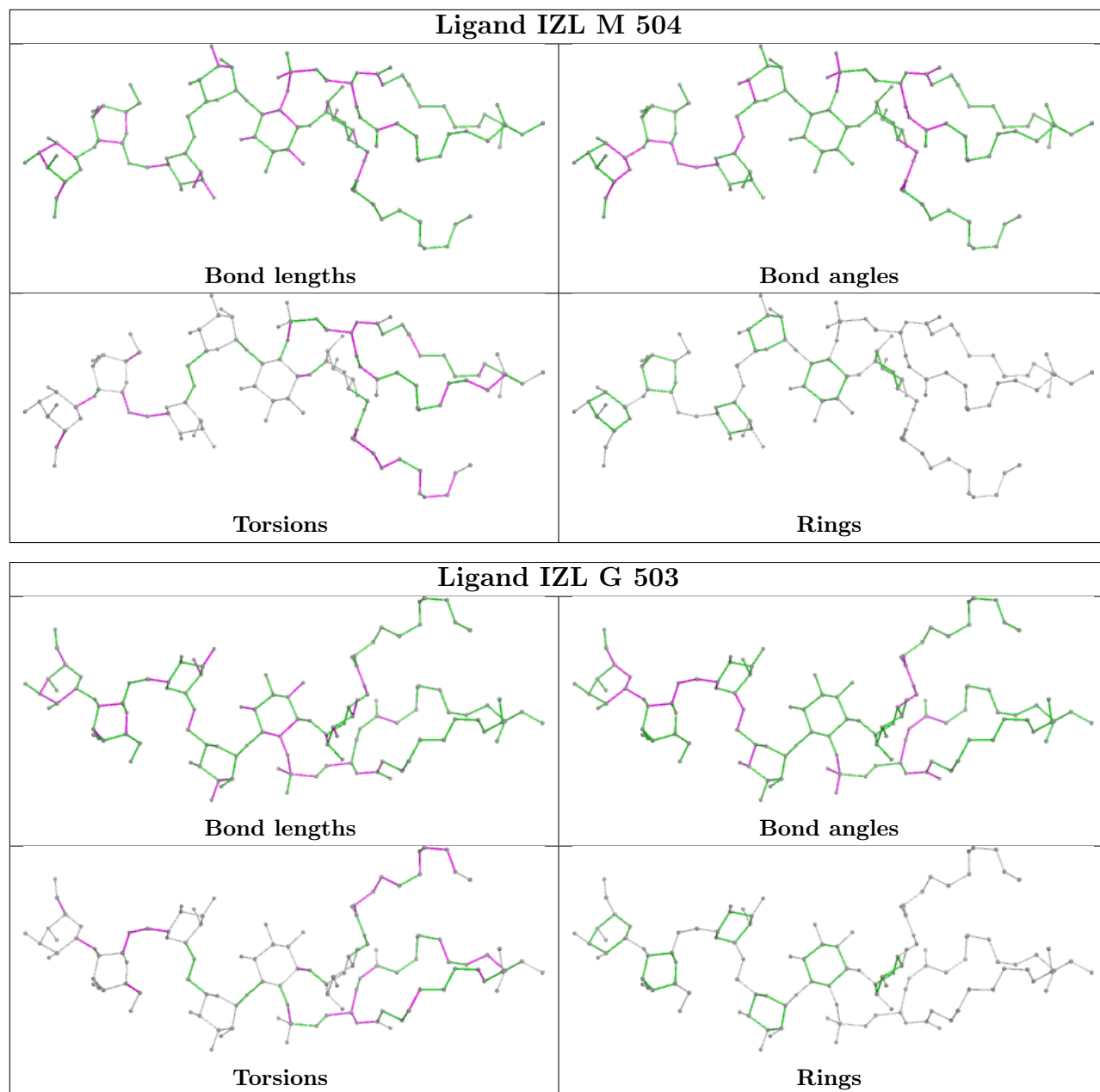


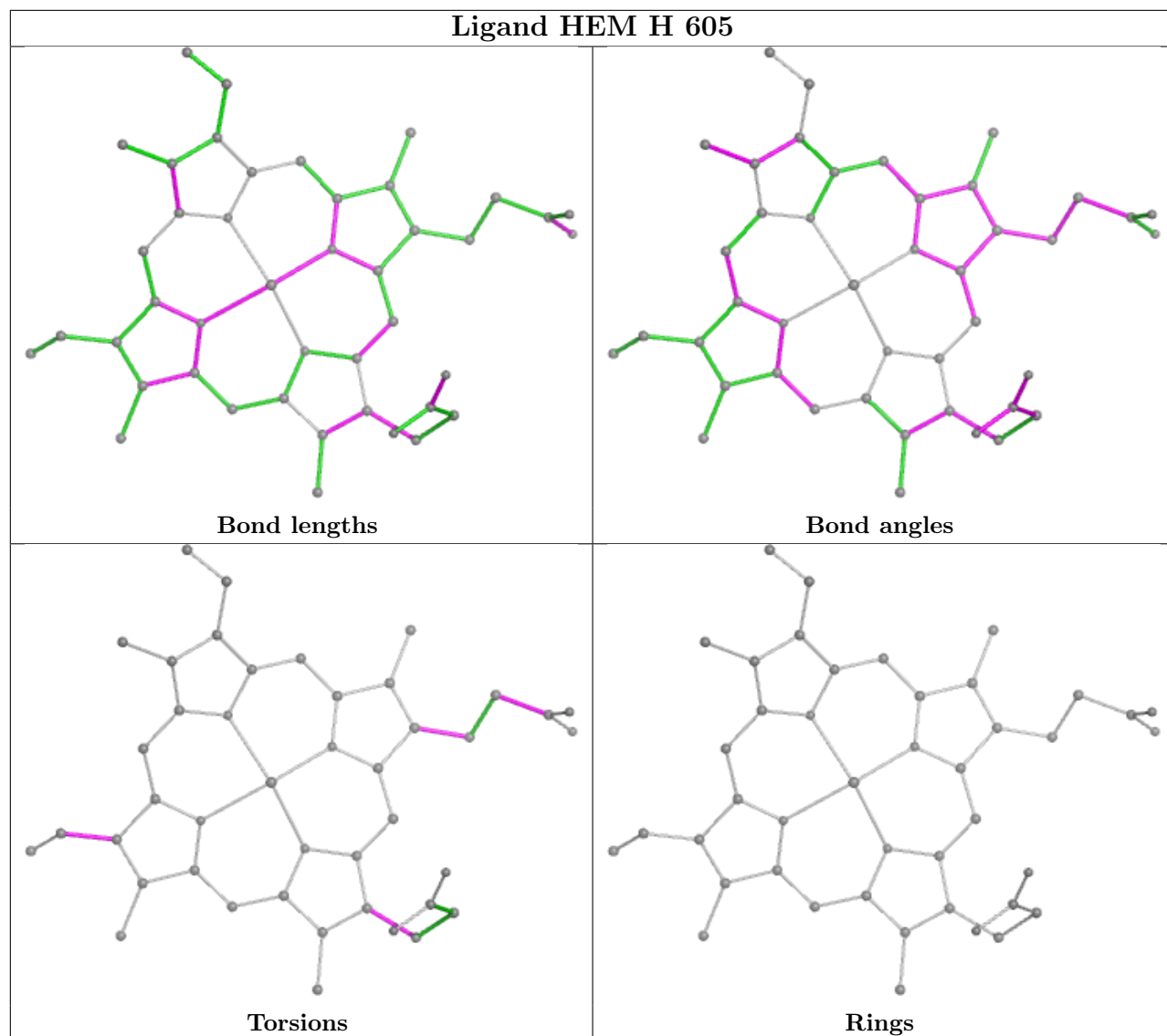


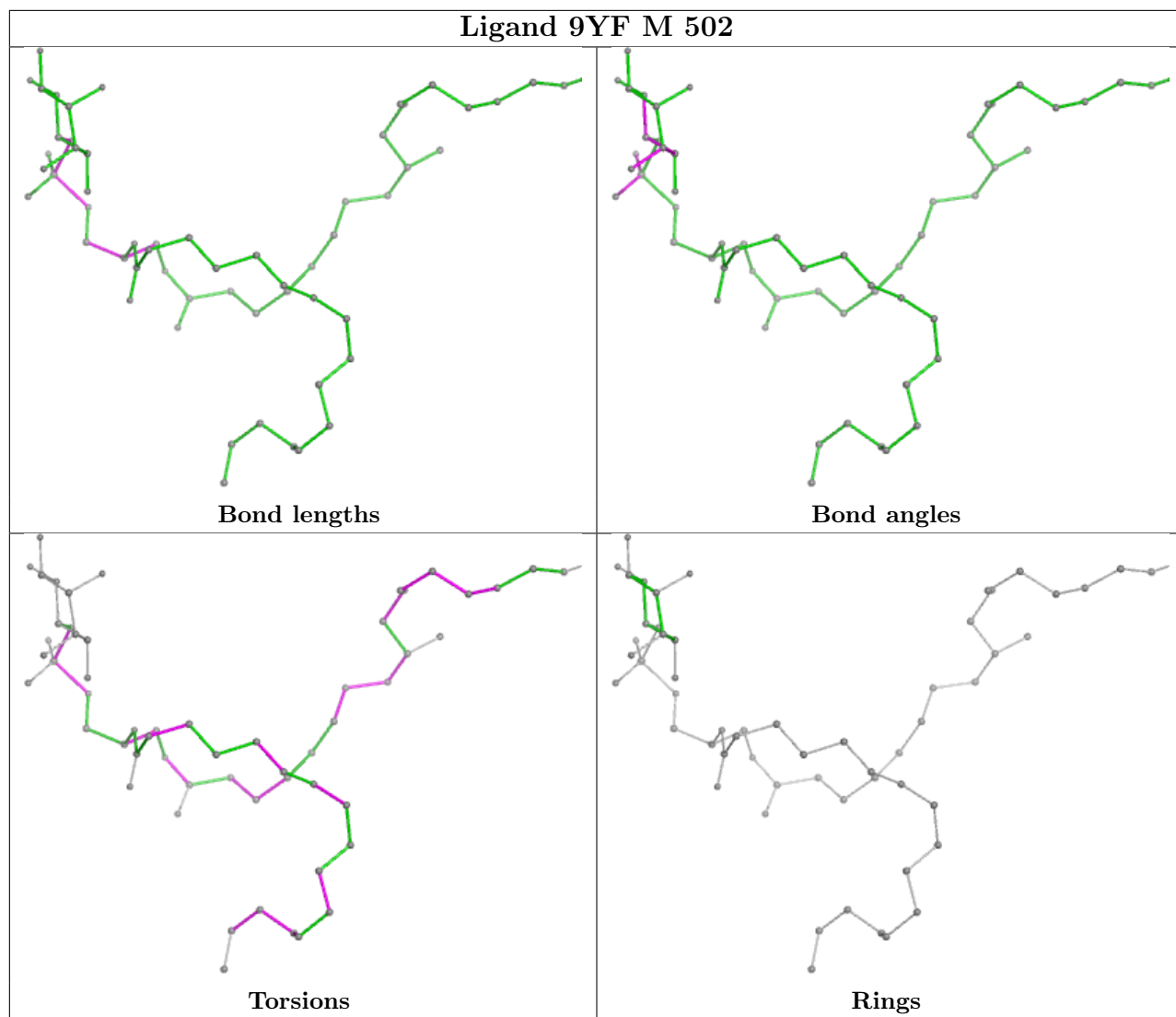


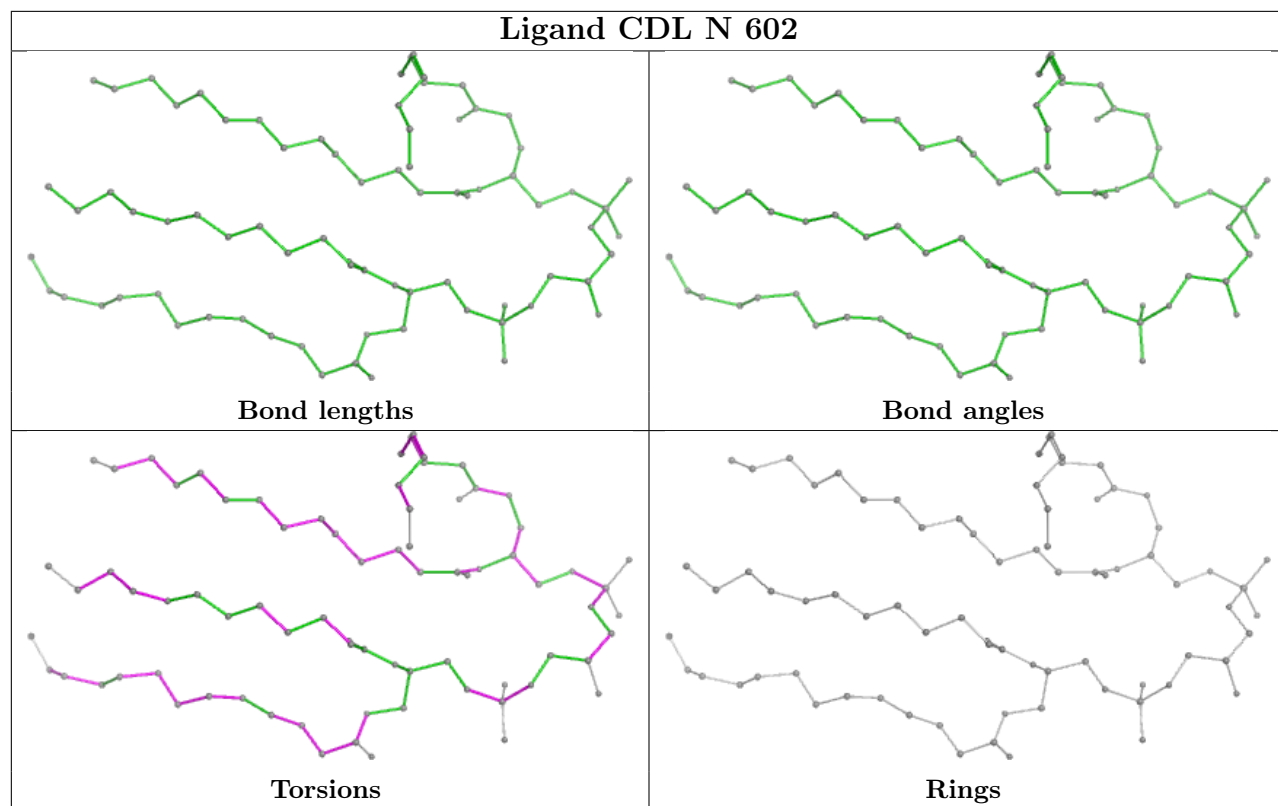


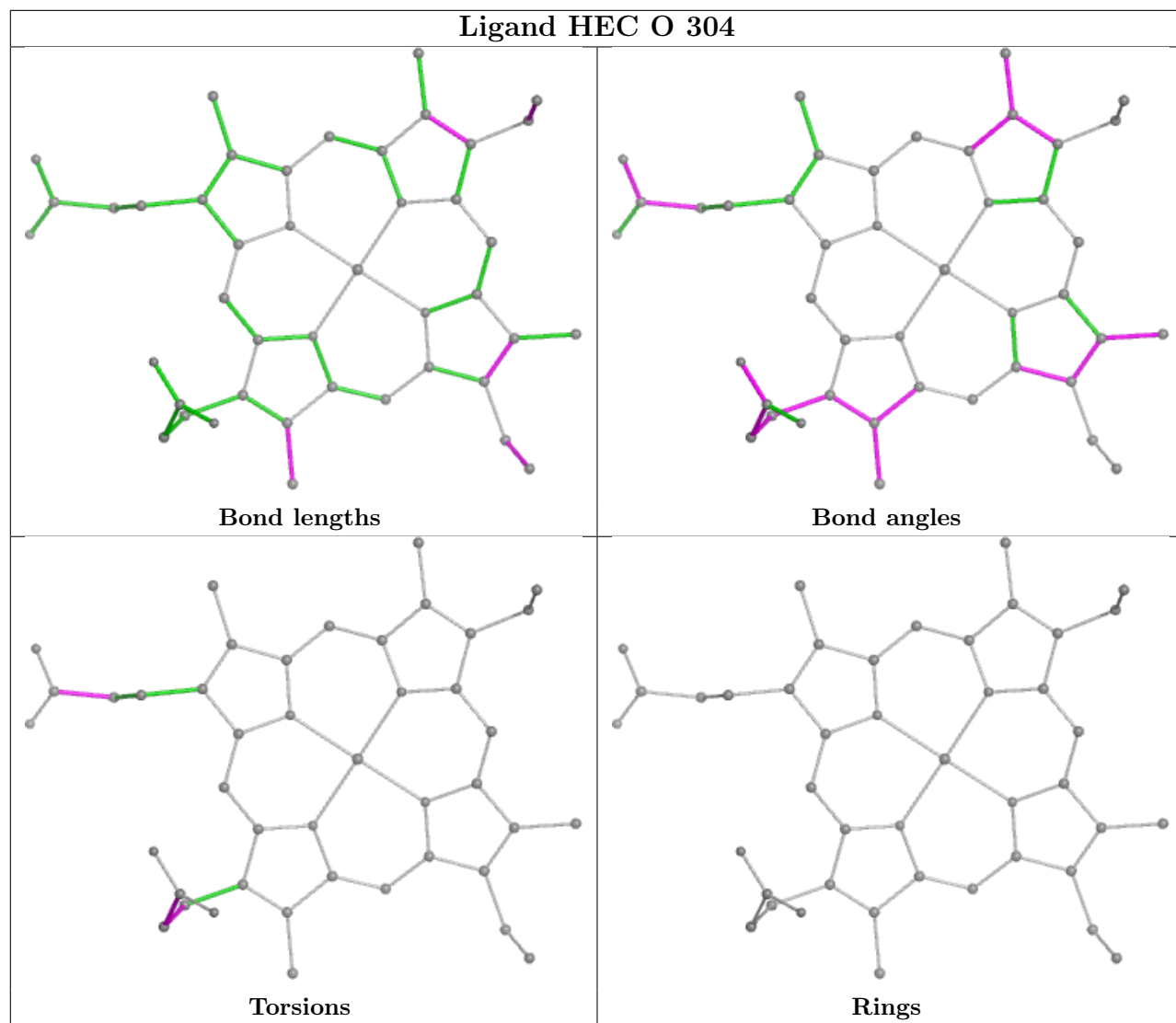


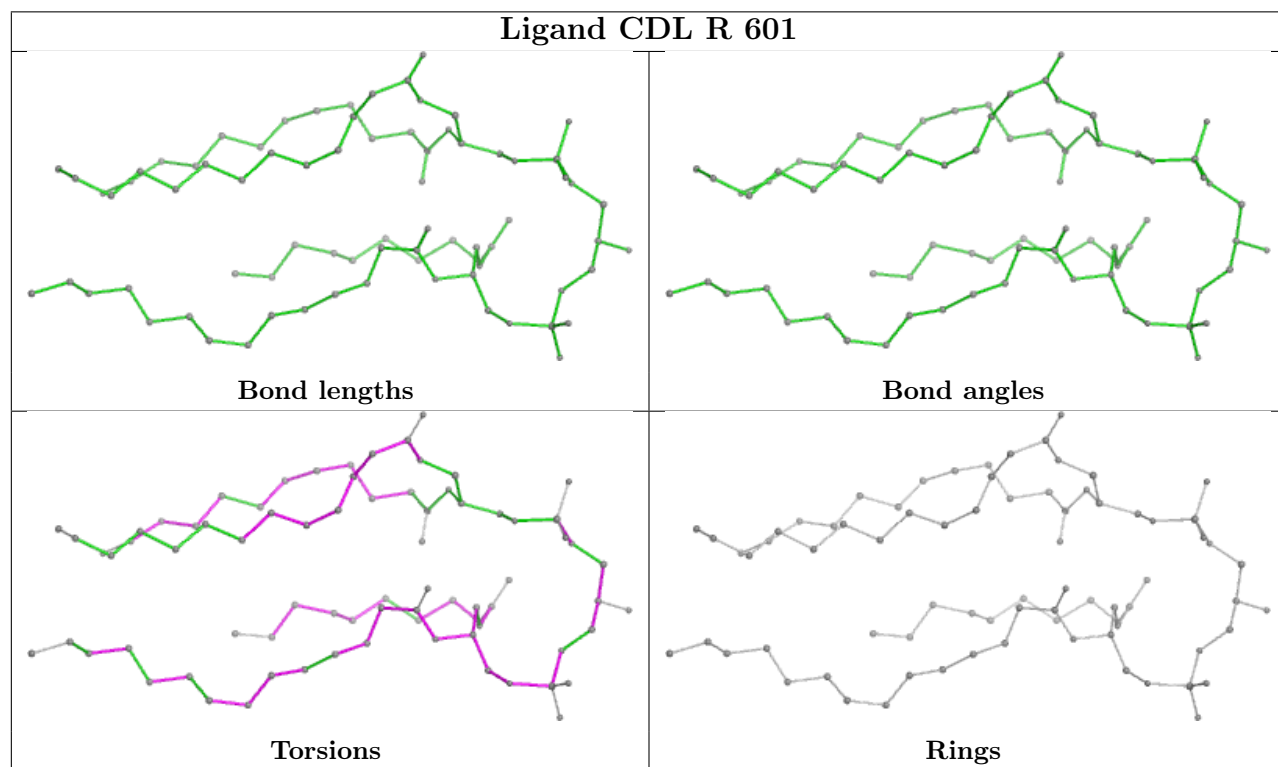
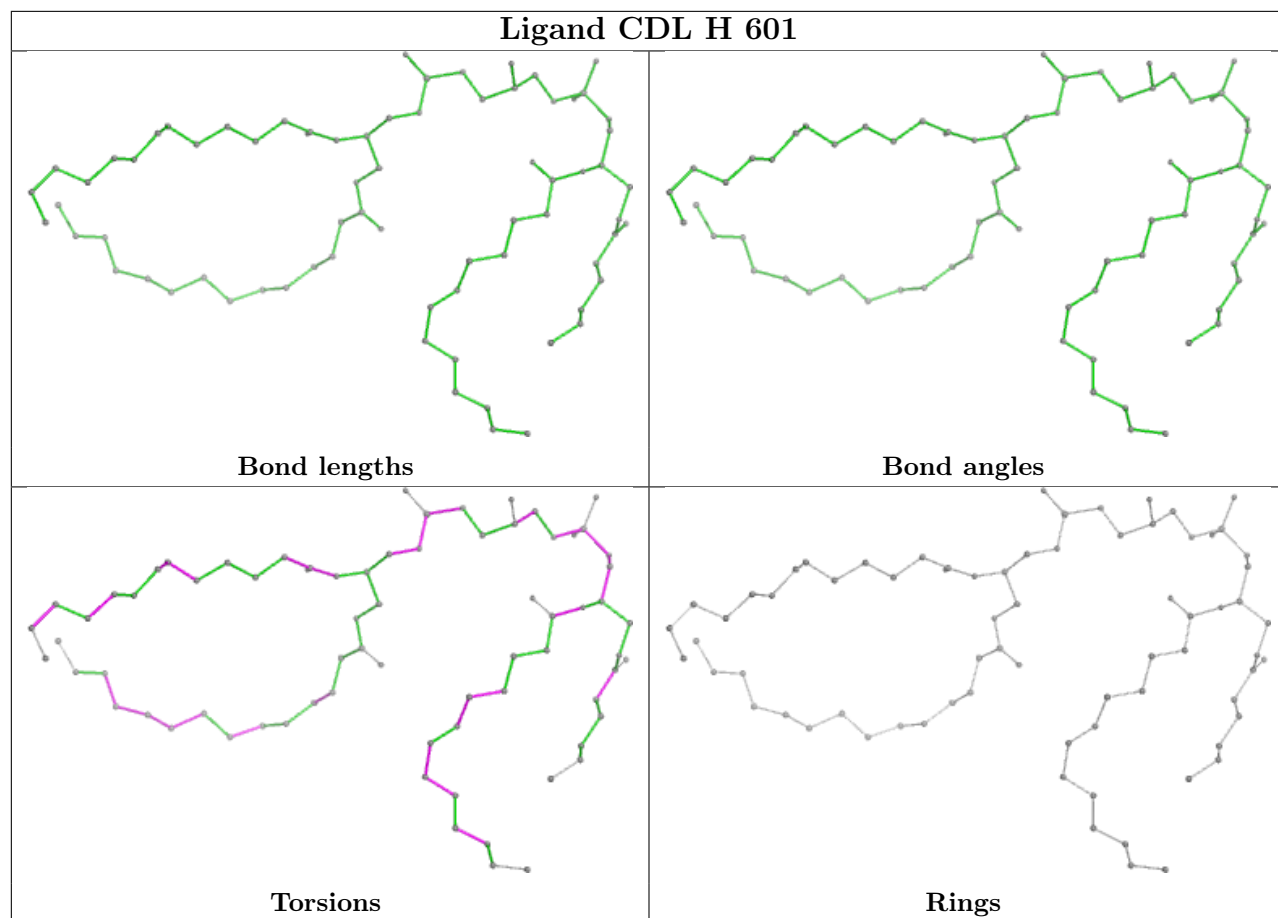


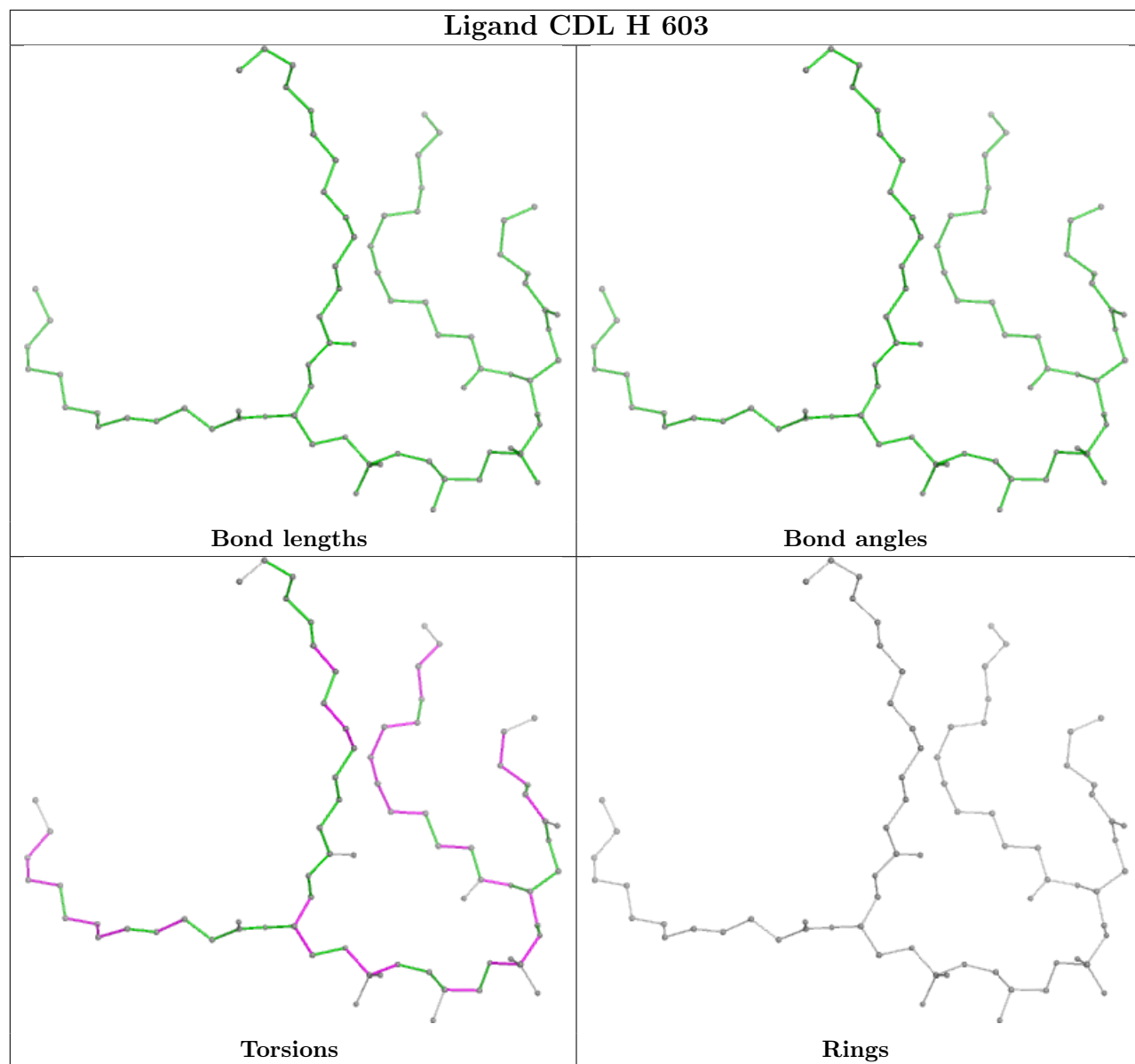


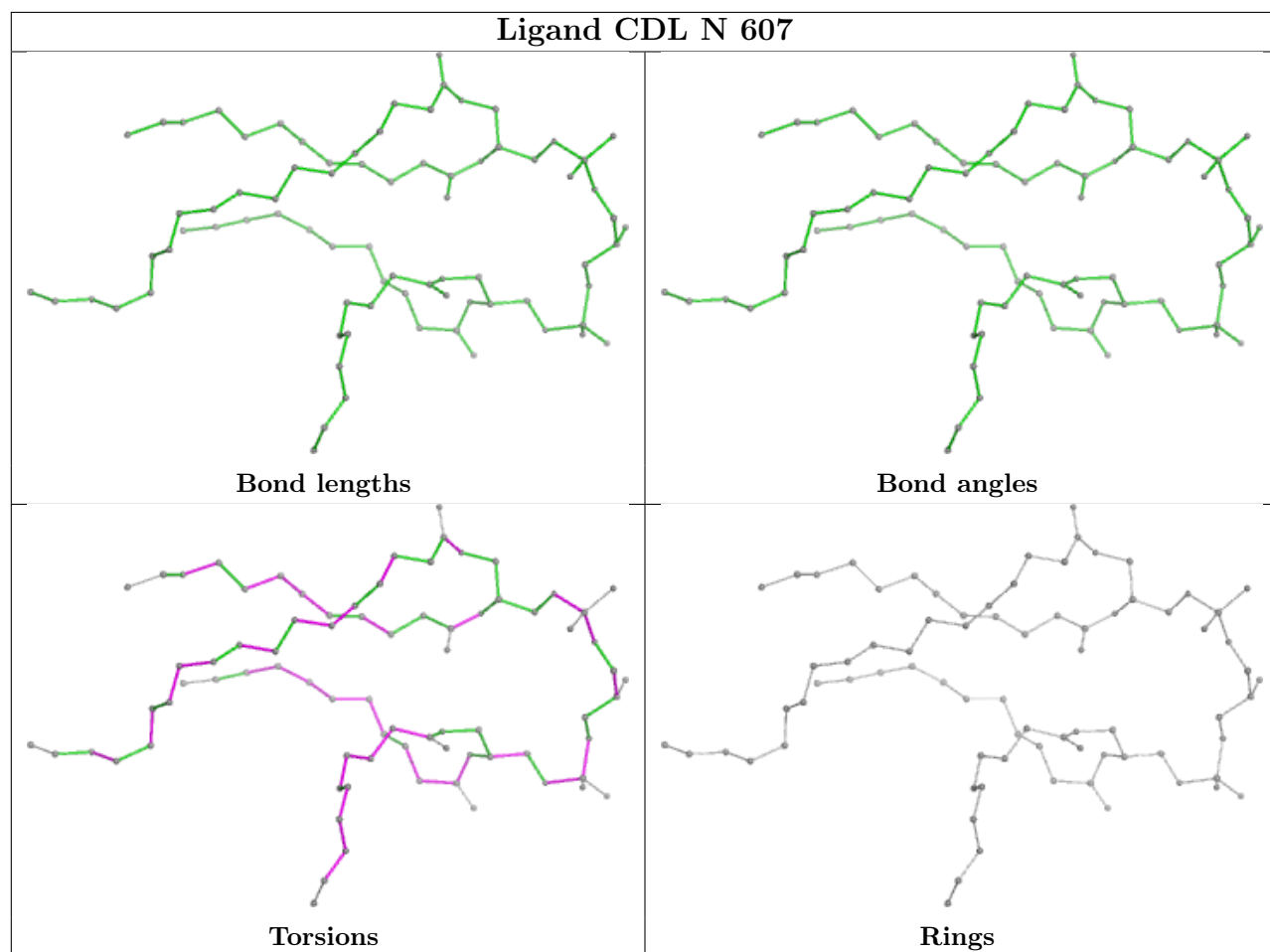
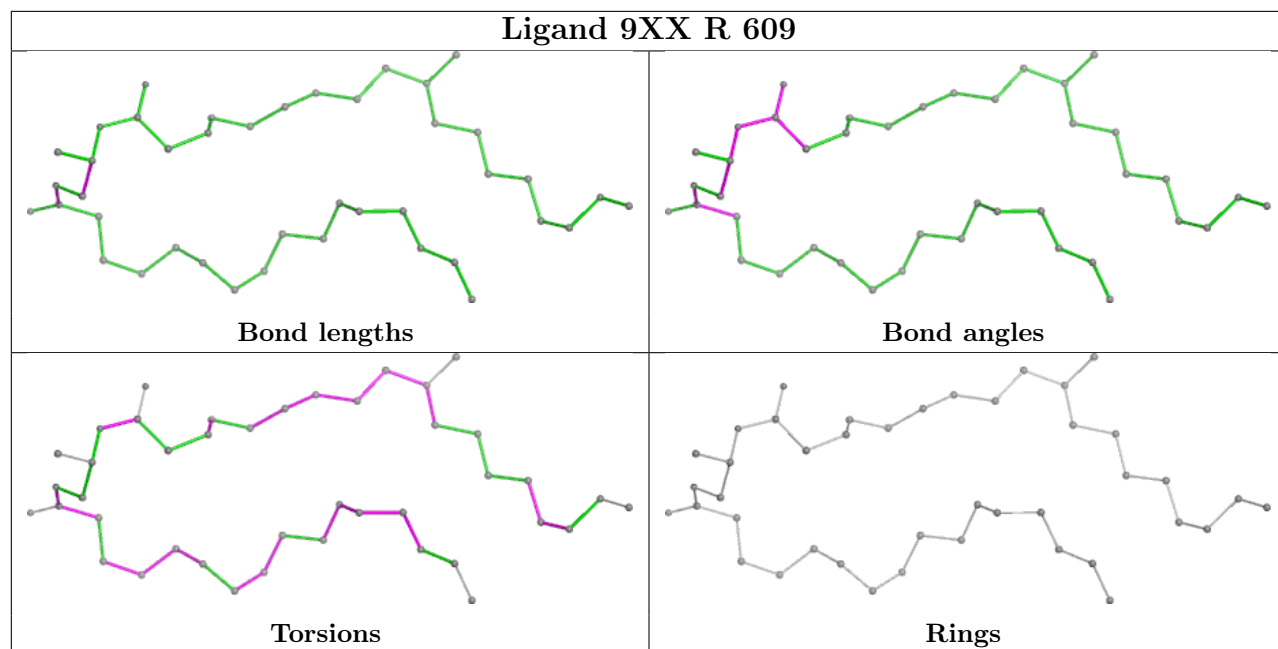


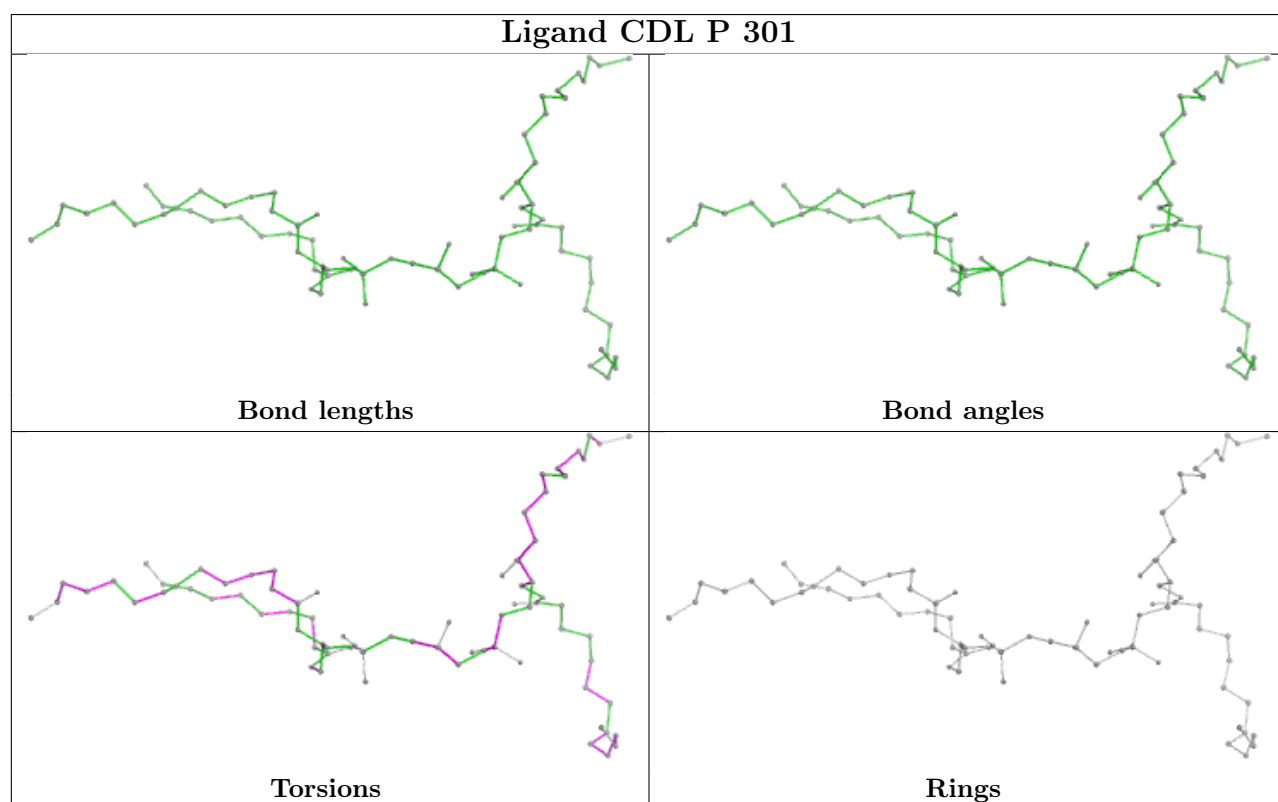
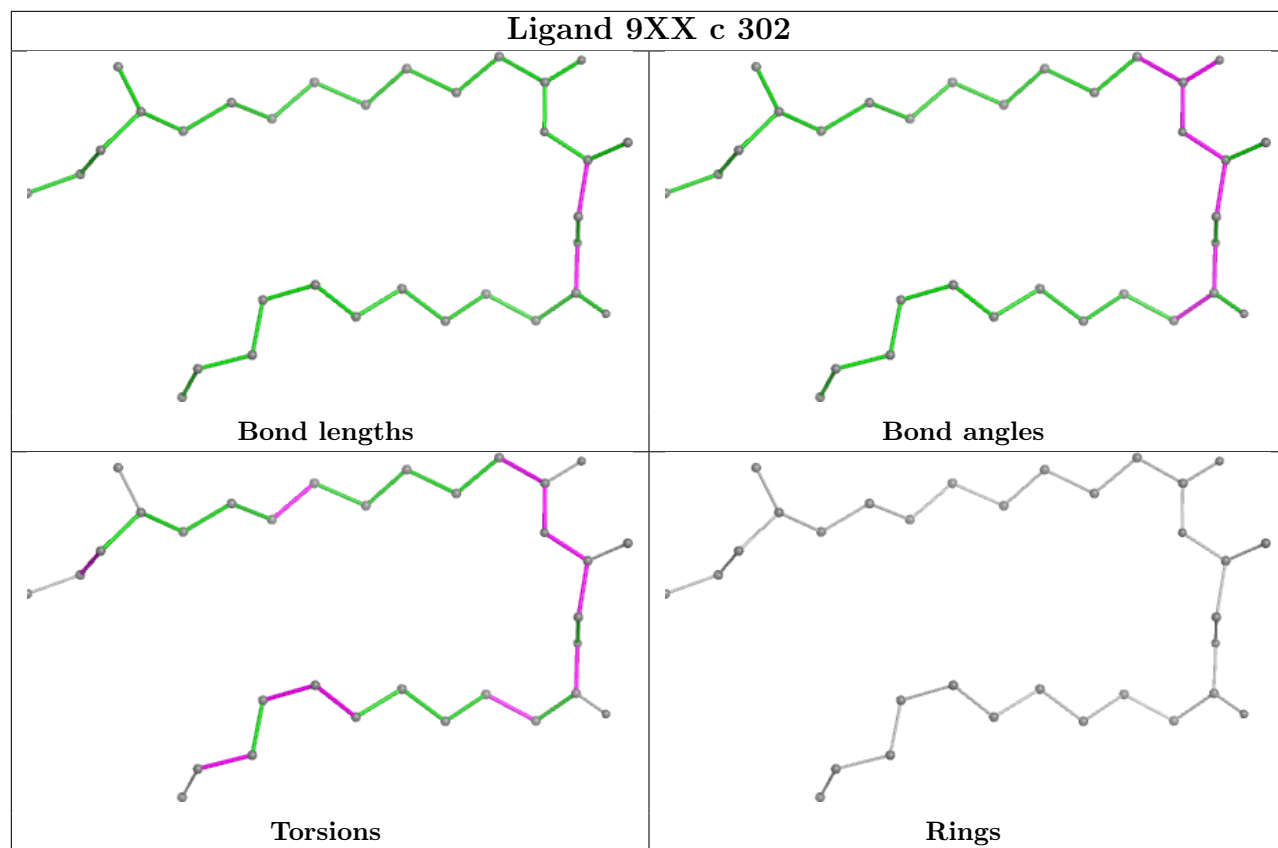


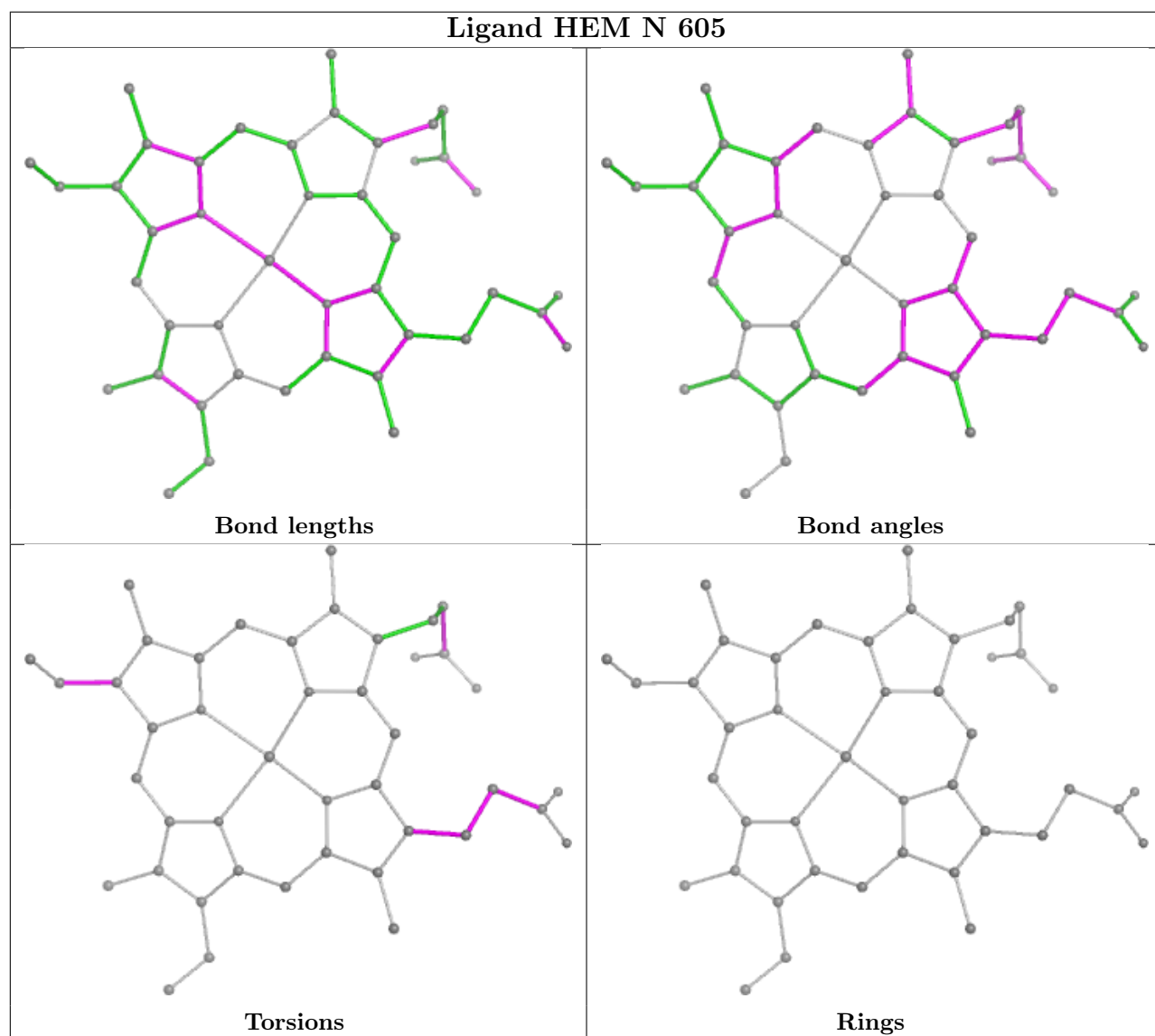
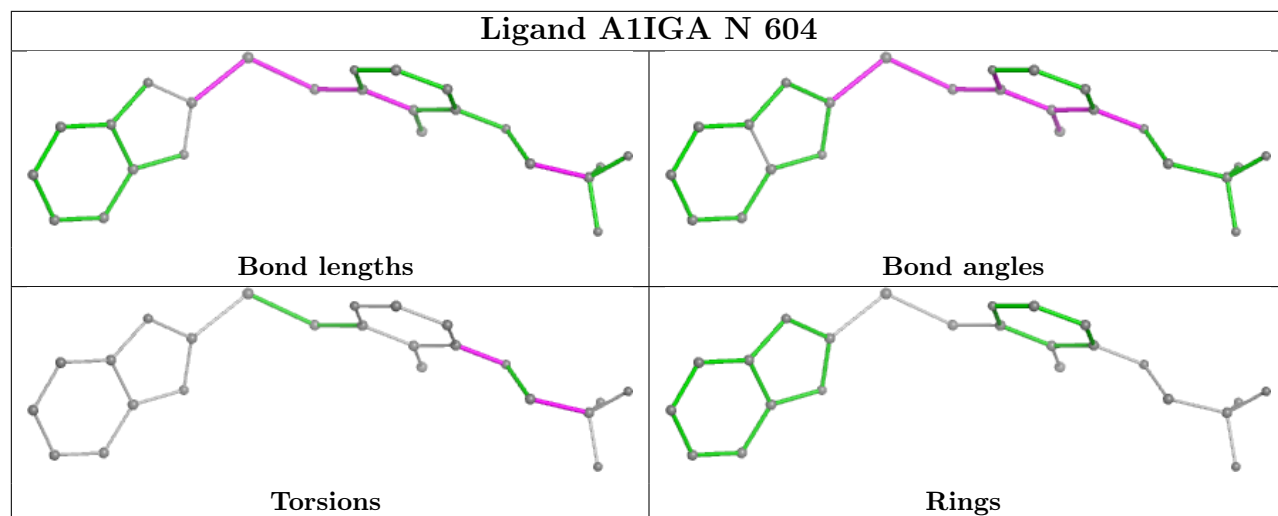


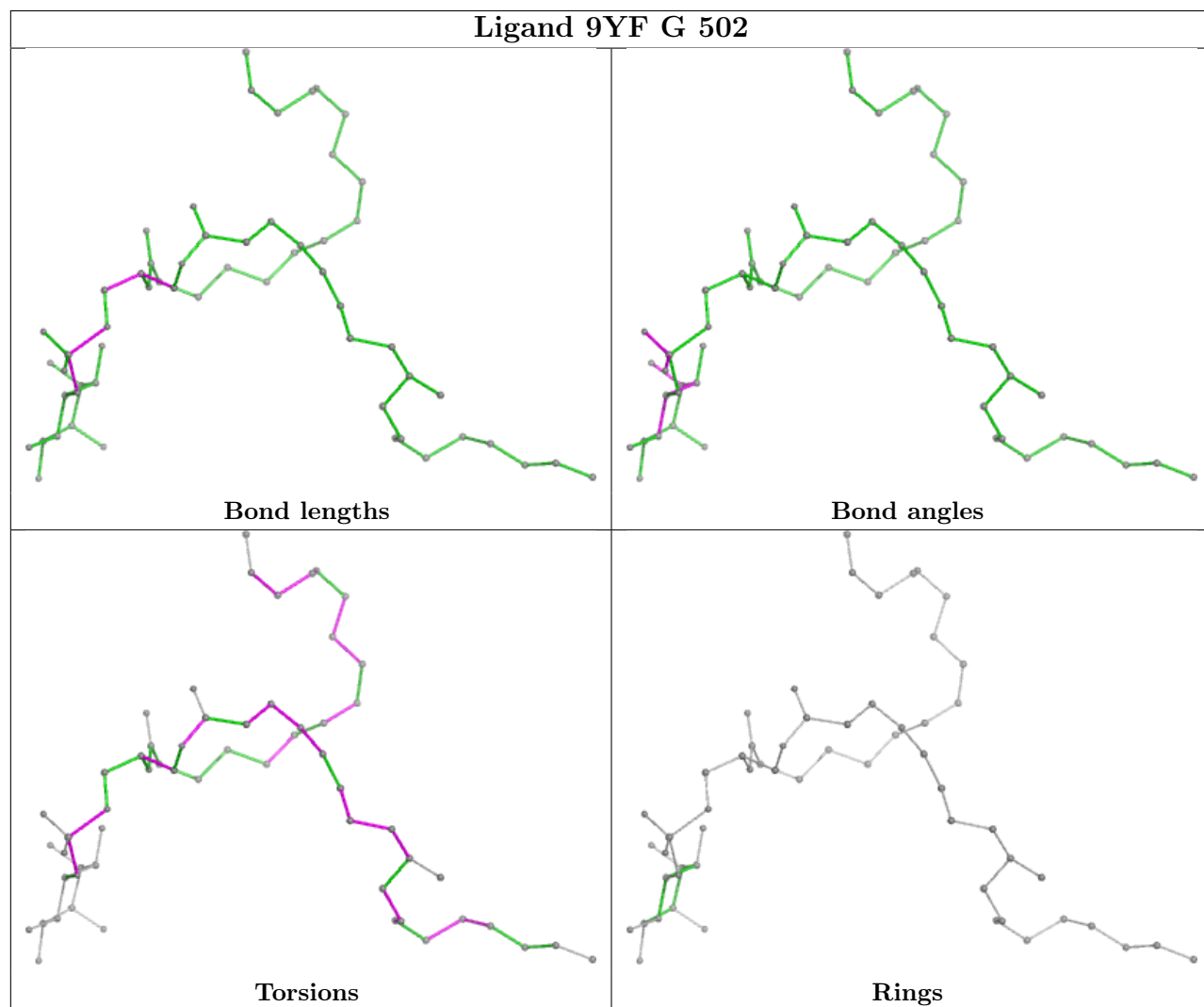
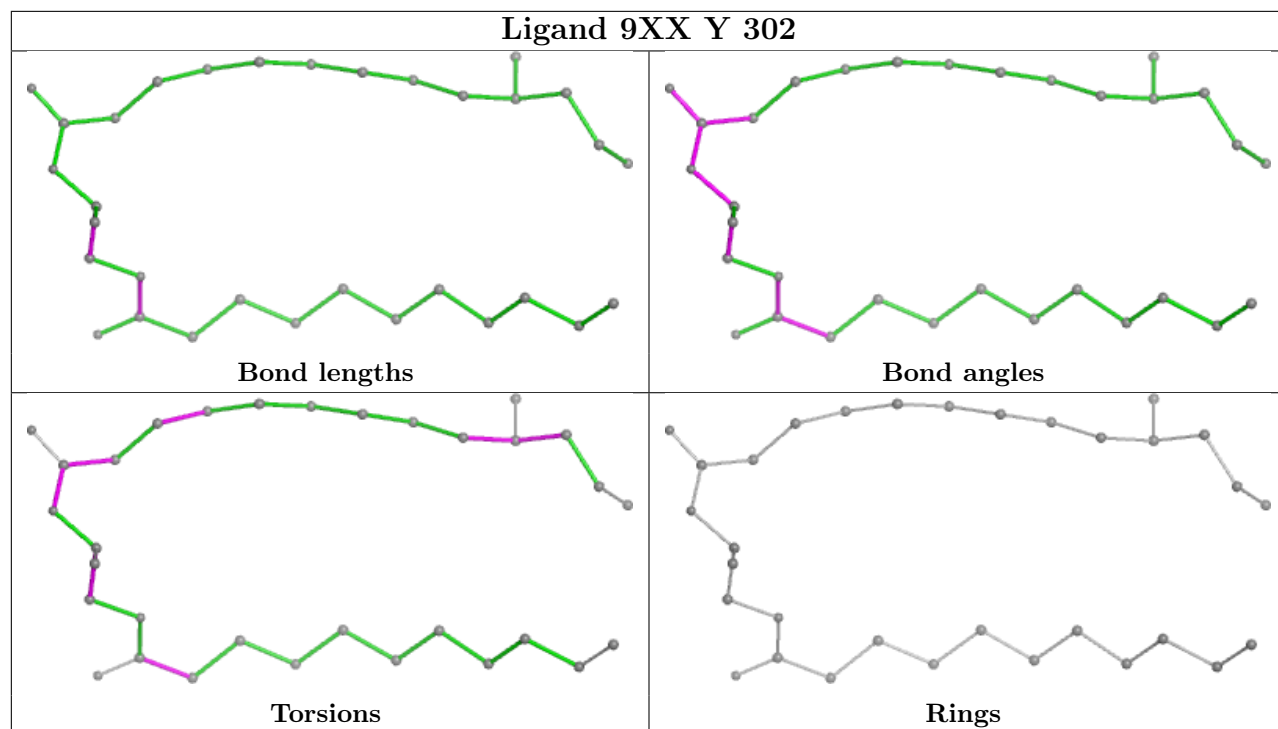












5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

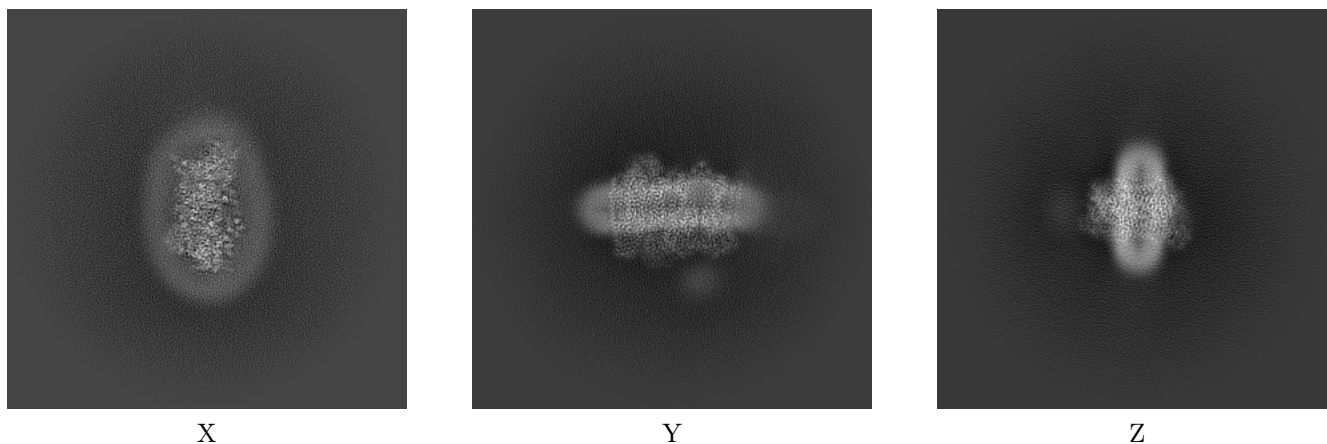
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50752. These allow visual inspection of the internal detail of the map and identification of artifacts.

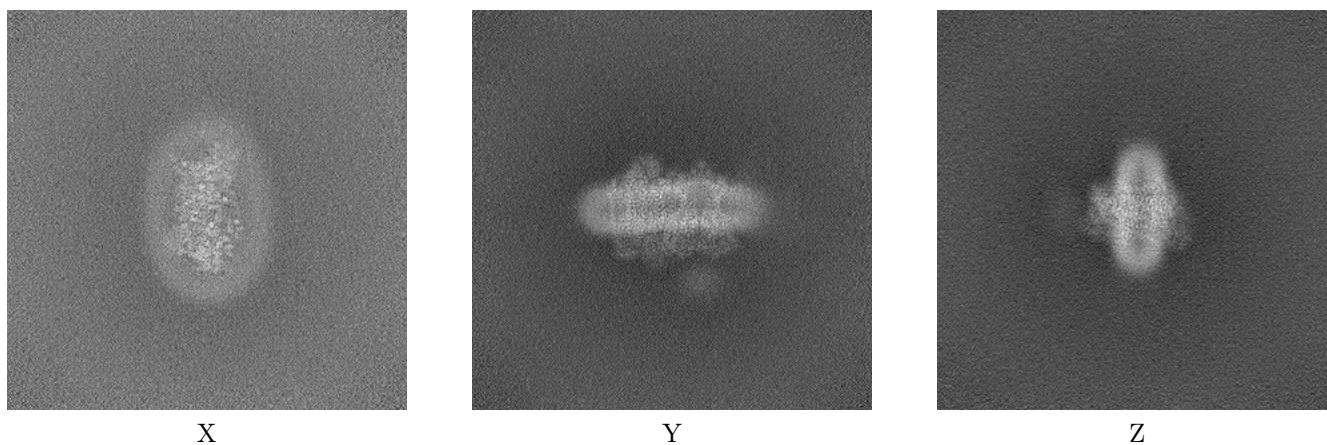
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



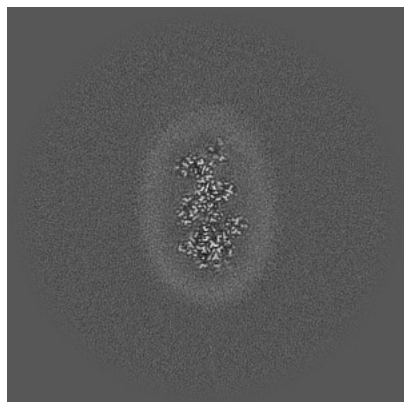
6.1.2 Raw map



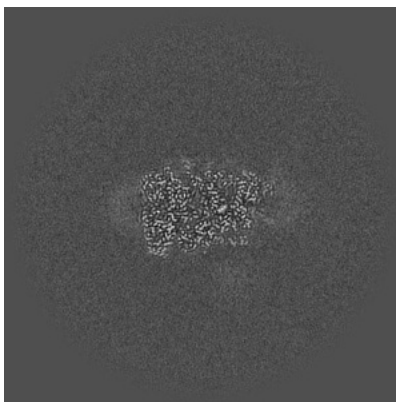
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

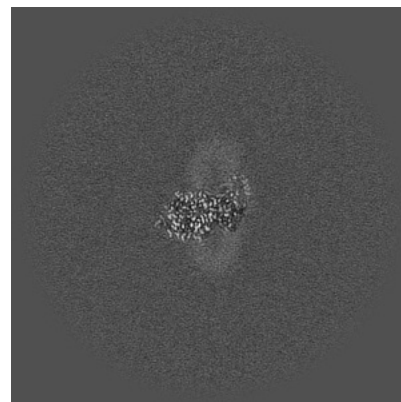
6.2.1 Primary map



X Index: 270

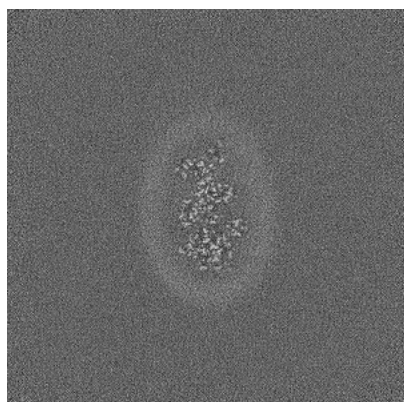


Y Index: 270

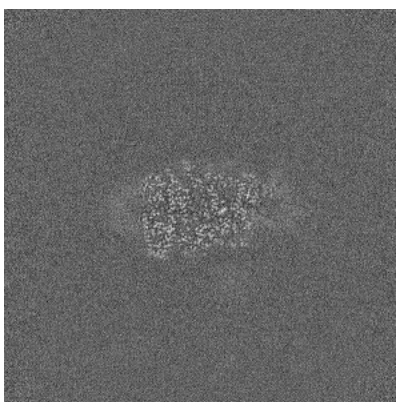


Z Index: 270

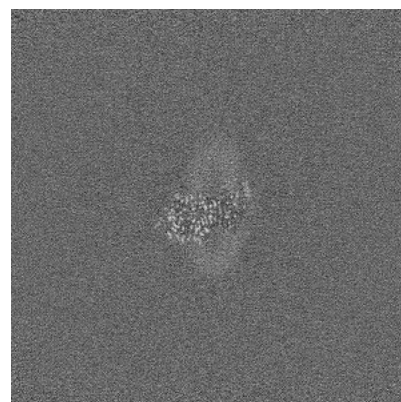
6.2.2 Raw map



X Index: 270



Y Index: 270

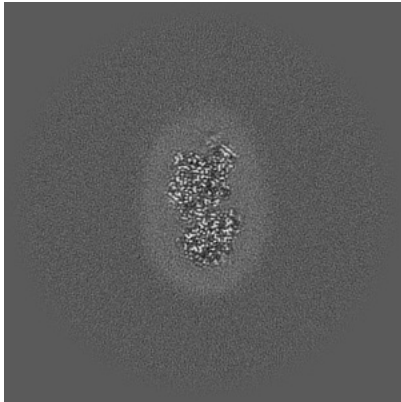


Z Index: 270

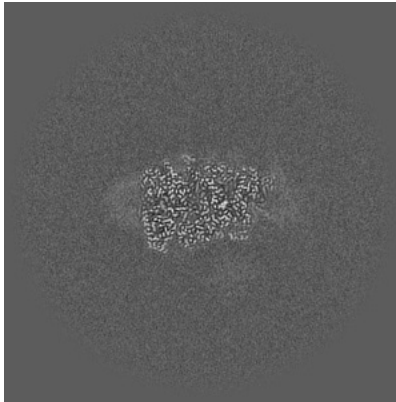
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

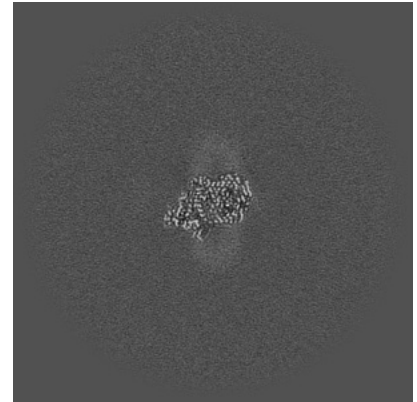
6.3.1 Primary map



X Index: 255

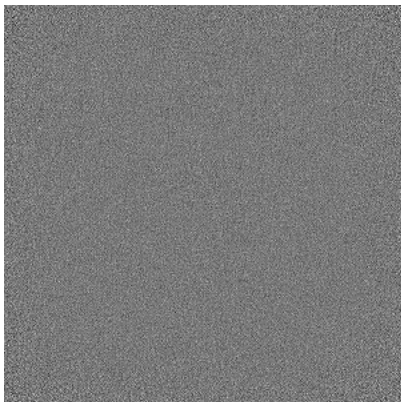


Y Index: 271

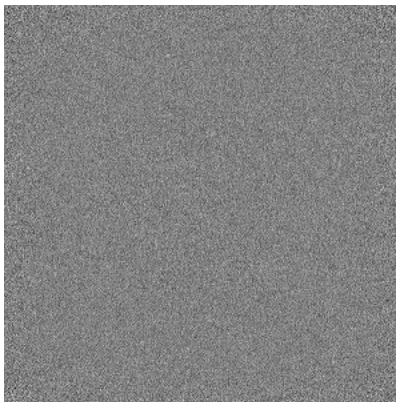


Z Index: 283

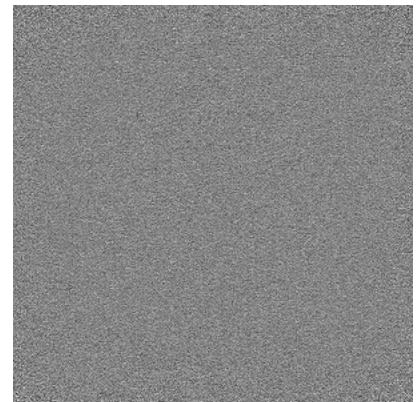
6.3.2 Raw map



X Index: 0



Y Index: 0

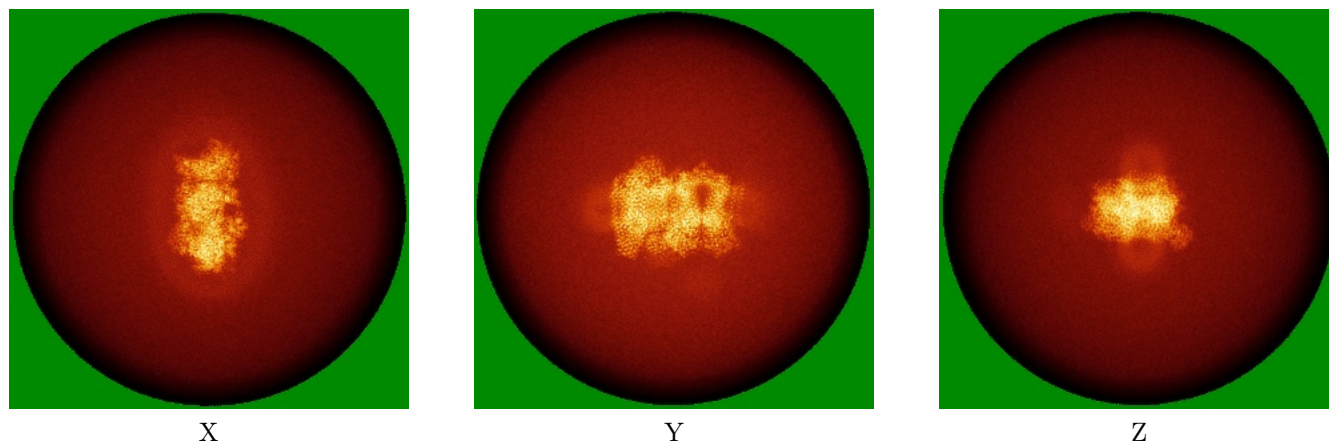


Z Index: 539

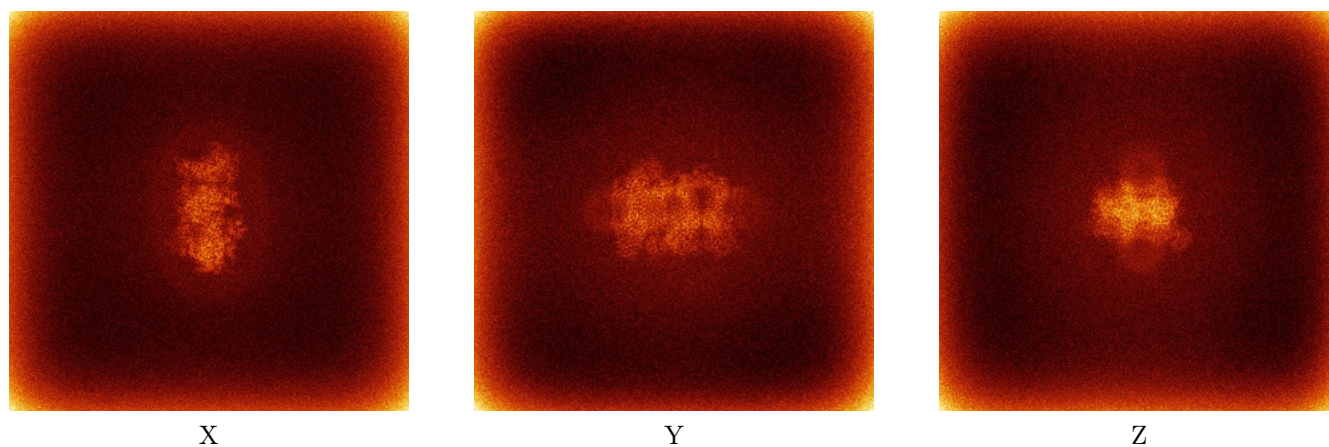
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



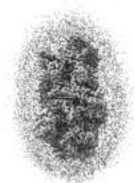
6.4.2 Raw map



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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



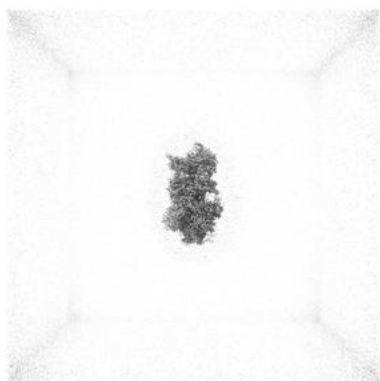
Y



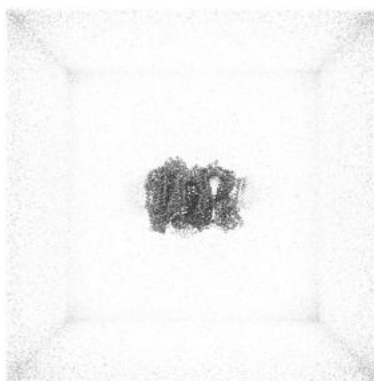
Z

The images above show the 3D surface view of the map at the recommended contour level 0.176. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

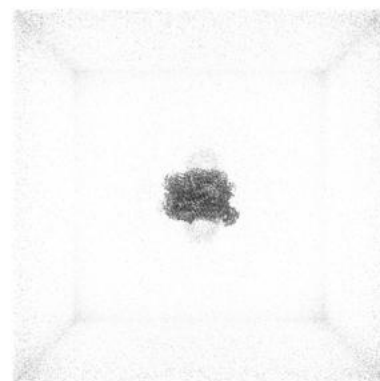
6.5.2 Raw map



X



Y



Z

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

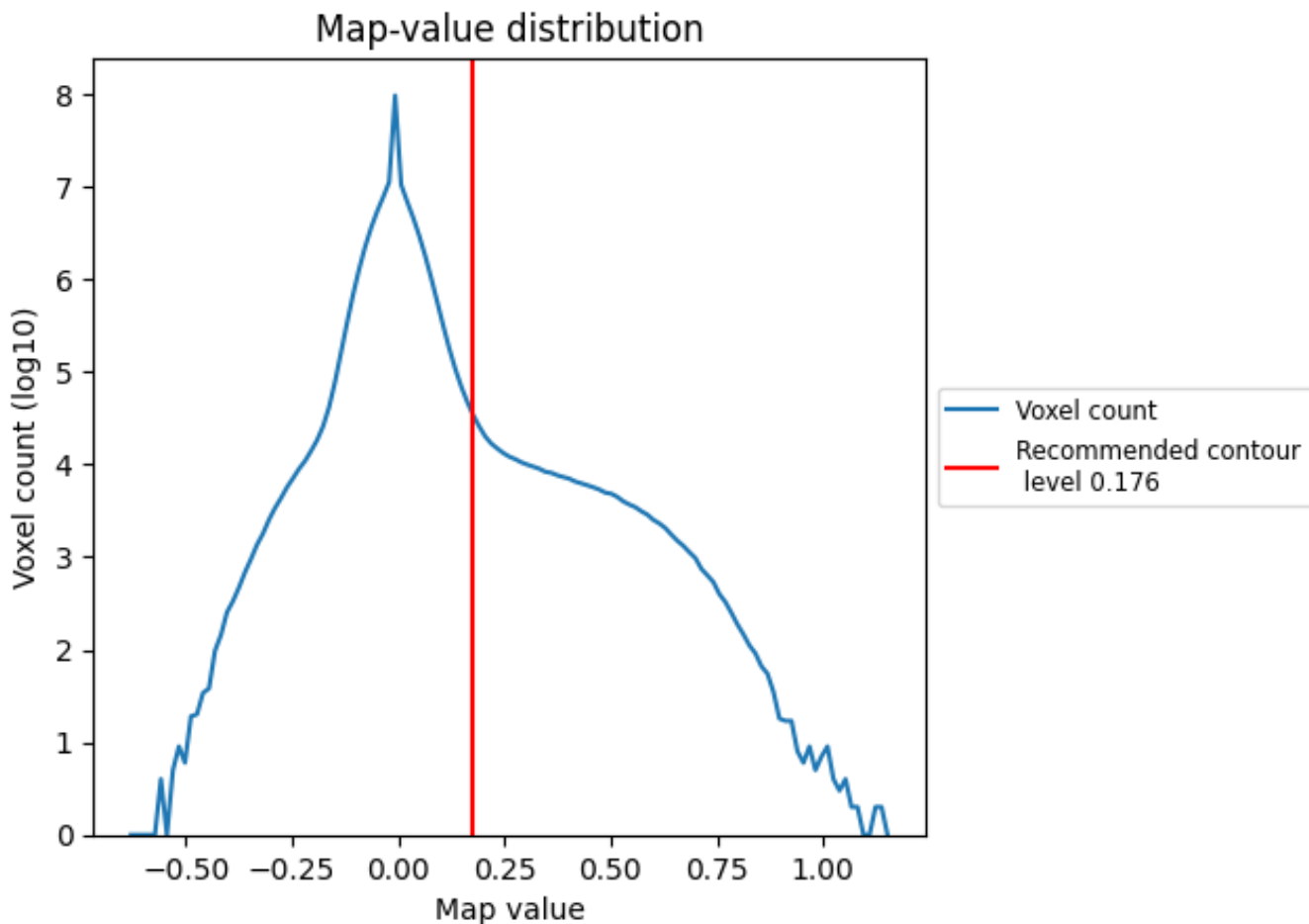
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

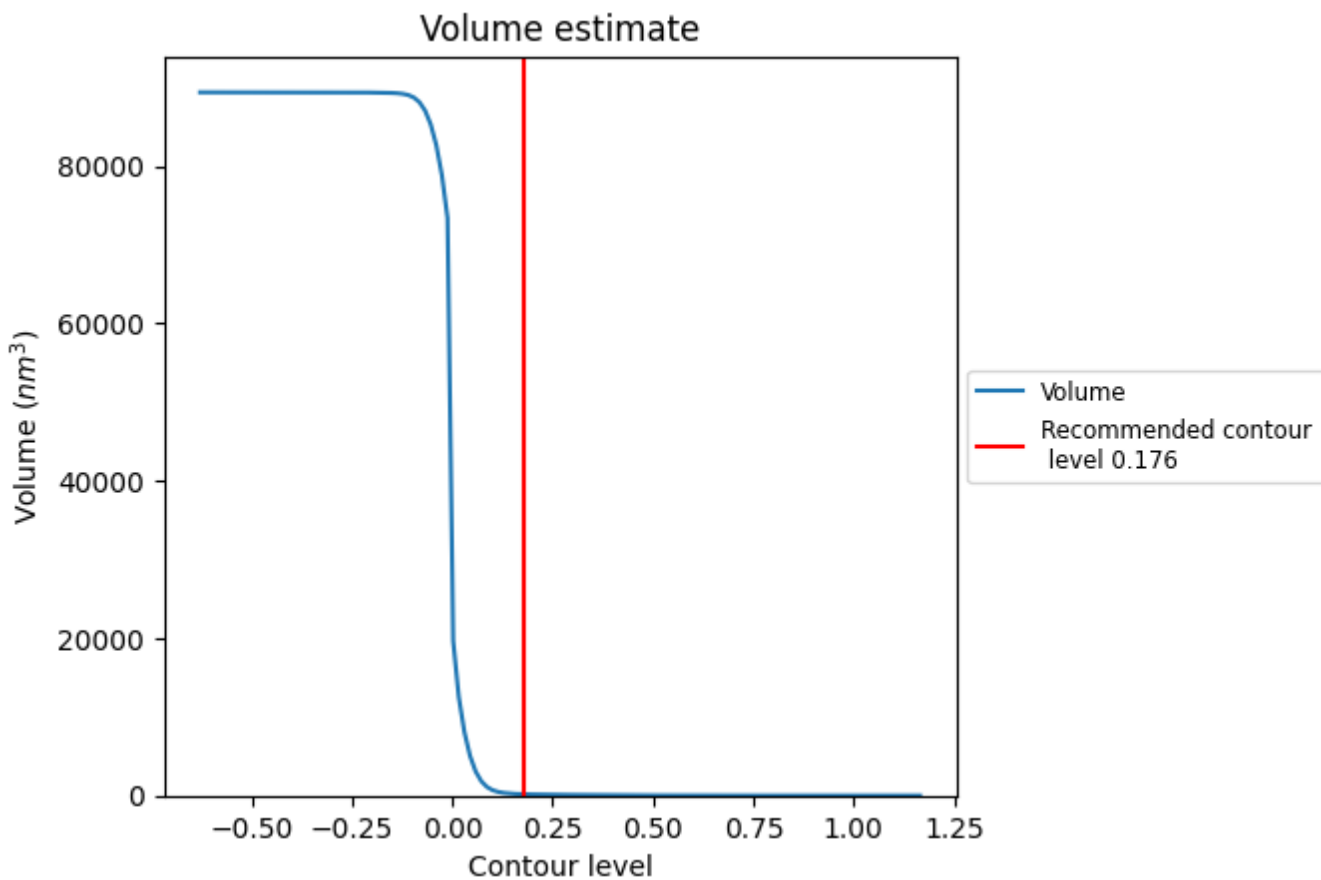
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

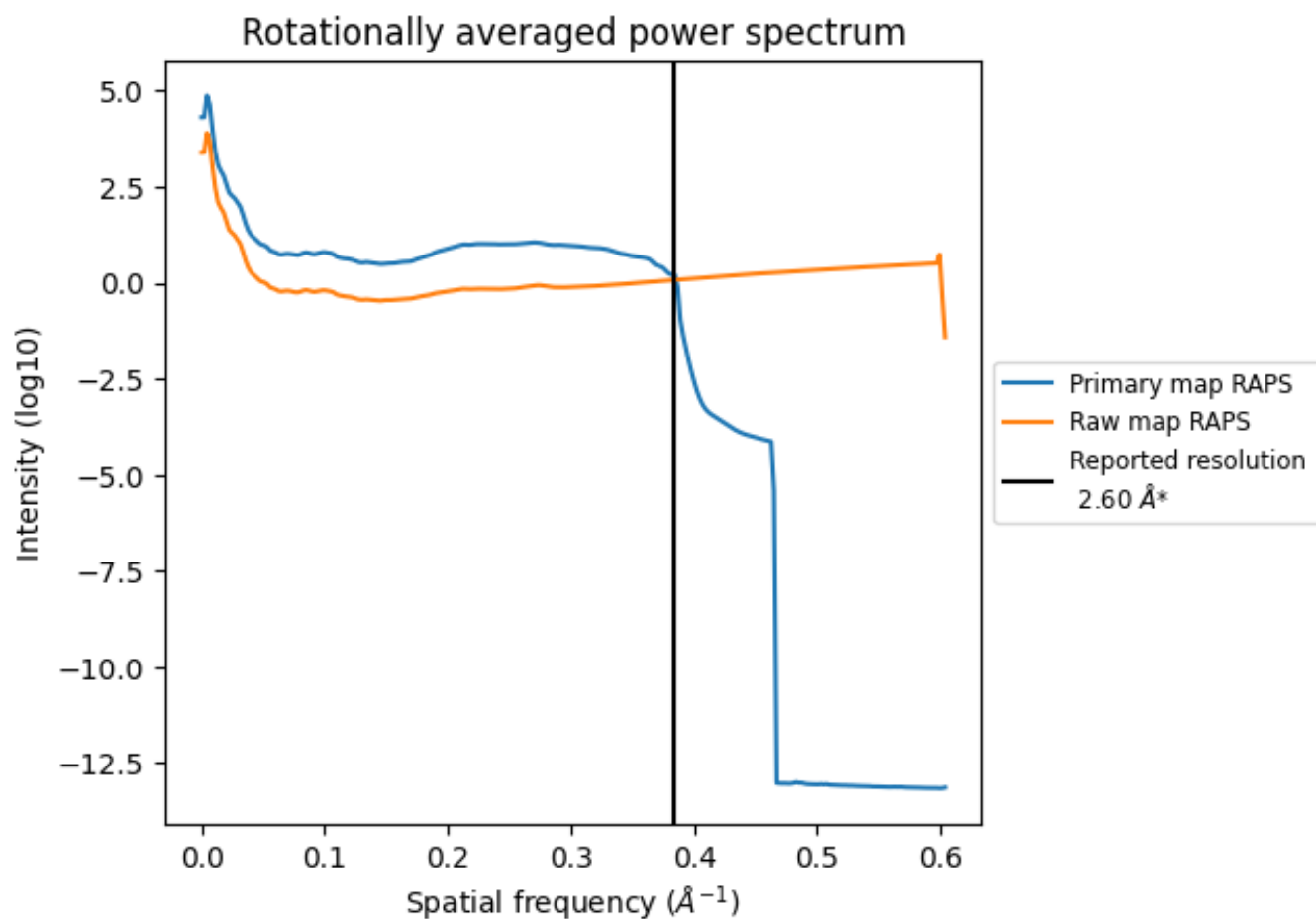
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 174 nm^3 ; this corresponds to an approximate mass of 158 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 [i](#)

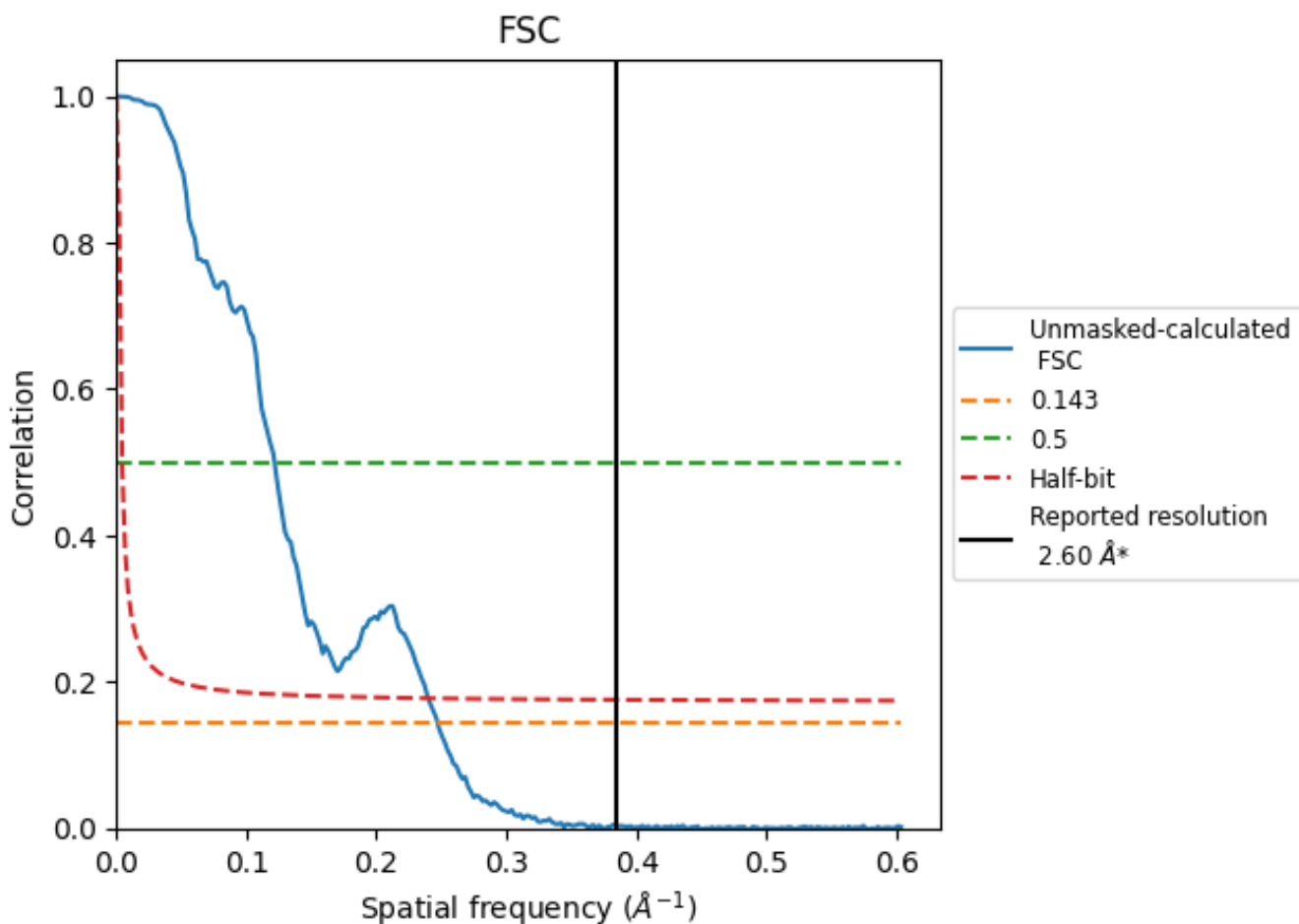


*Reported resolution corresponds to spatial frequency of 0.385 Å⁻¹

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 0.385 Å⁻¹

8.2 Resolution estimates [i](#)

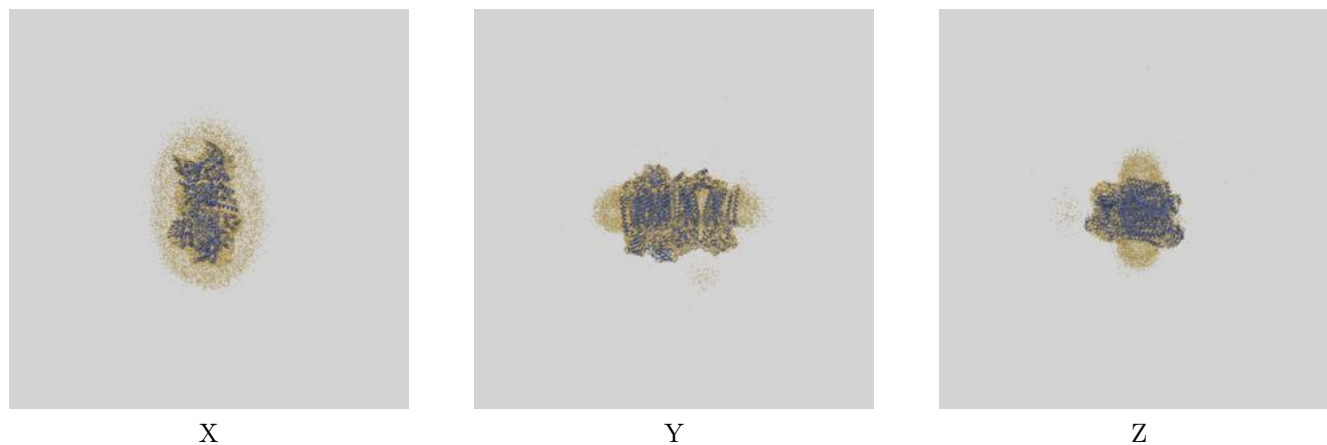
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.05	8.22	4.17

*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 4.05 differs from the reported value 2.6 by more than 10 %

9 Map-model fit [i](#)

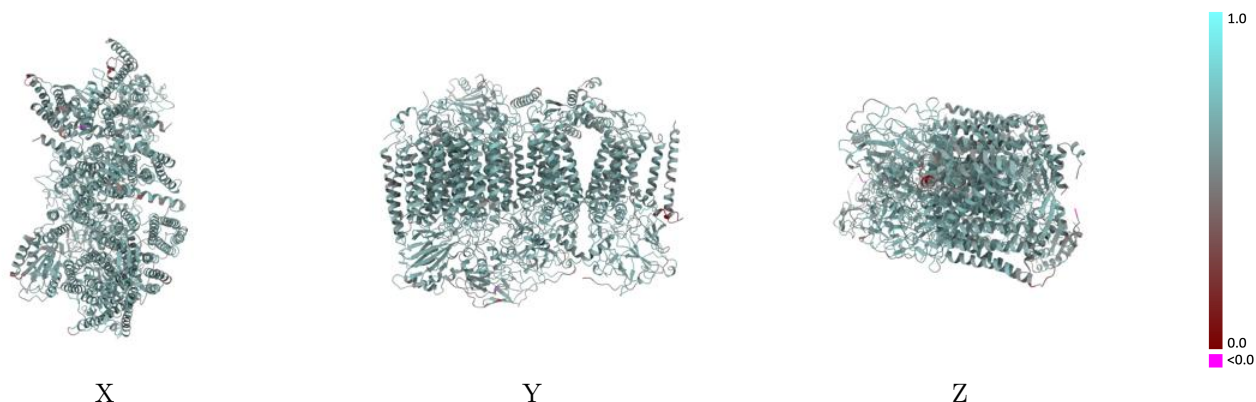
This section contains information regarding the fit between EMDB map EMD-50752 and PDB model 9FTZ. Per-residue inclusion information can be found in section 3 on page 20.

9.1 Map-model overlay [i](#)



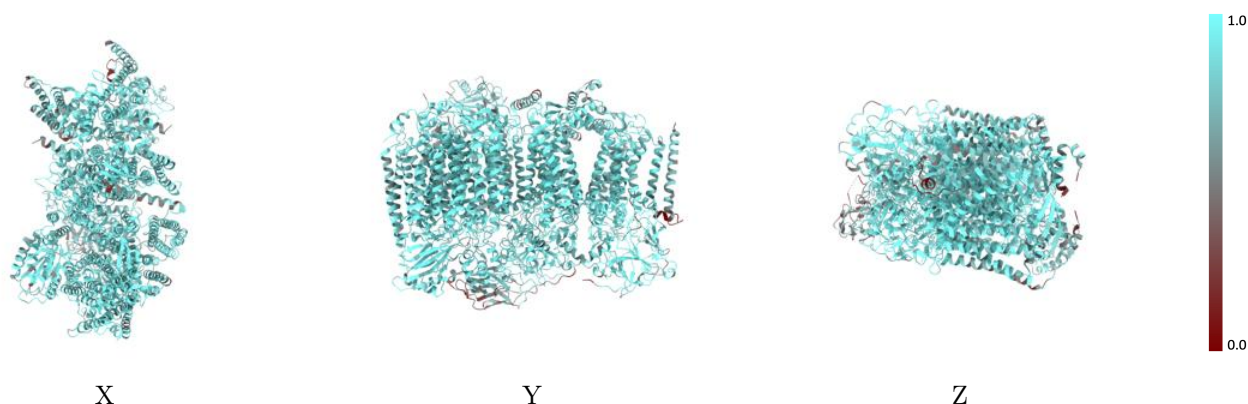
The images above show the 3D surface view of the map at the recommended contour level 0.176 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



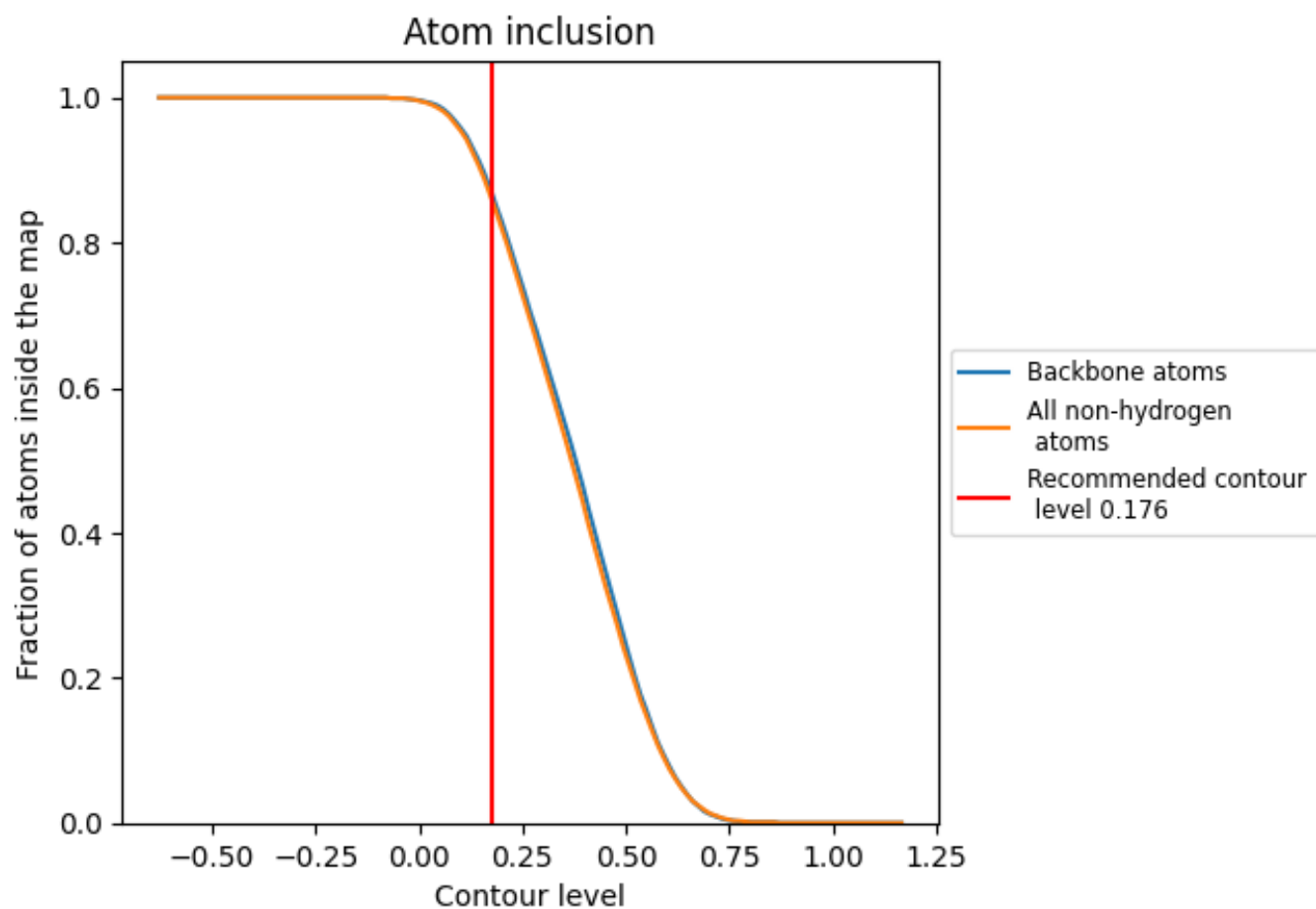
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.176).

































9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 86% 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 (0.176) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8590	 0.6080
G	 0.8170	 0.5840
H	 0.8320	 0.5930
M	 0.8750	 0.6110
N	 0.9070	 0.6320
O	 0.8950	 0.6260
P	 0.8530	 0.6170
Q	 0.8670	 0.6050
R	 0.9280	 0.6360
S	 0.8760	 0.6200
T	 0.8780	 0.6130
U	 0.8230	 0.5720
V	 0.8340	 0.5880
W	 0.5750	 0.5390
Y	 0.7380	 0.5430
c	 0.6240	 0.4640

