



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 08:22 AM UTC

PDB ID : 9FTZ / pdb_00009ftz
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:

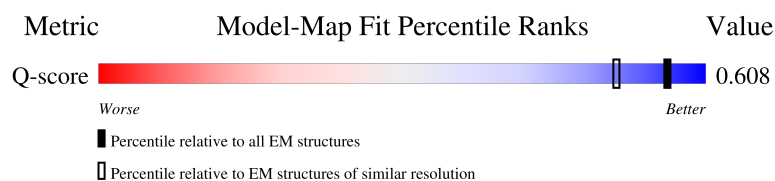
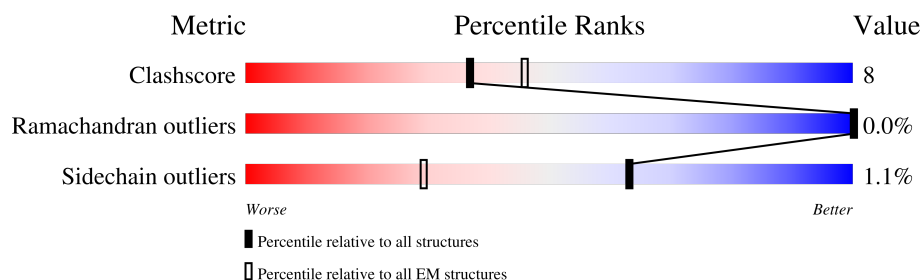
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.60 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.



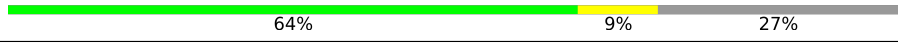
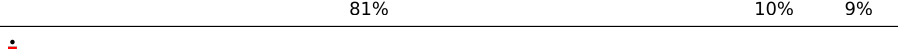
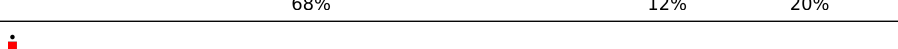
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8728 (2.10 - 3.10)

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	
2	G	408	
2	M	408	
3	H	556	

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Mol	Chain	Length	Quality of chain
3	N	556	
4	P	100	
5	S	203	
6	T	139	
7	R	575	
8	Q	341	
9	U	79	
10	V	157	
11	W	186	
12	Y	236	
12	c	236	

2 Entry composition

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
1	O	223	Total	C	N	O	S	0	0
			1623	1008	289	314	12		

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
2	M	380	Total	C	N	O	S	0	0
			2967	1919	502	535	11		
2	G	380	Total	C	N	O	S	0	0
			2967	1919	502	535	11		

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

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

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
4	P	73	Total	C	N	O	S	0	0
			586	385	107	90	4		

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
5	S	184	Total	C	N	O	S	0	0
			1441	967	229	238	7		

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

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

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

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

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
8	Q	299	Total	C	N	O	S	0	0
			2382	1541	396	435	10		

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

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

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

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

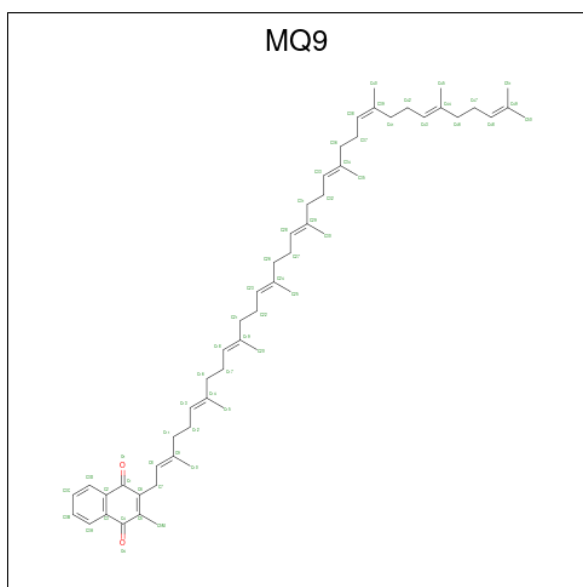
- Molecule 11 is a protein called LpqE protein.

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

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

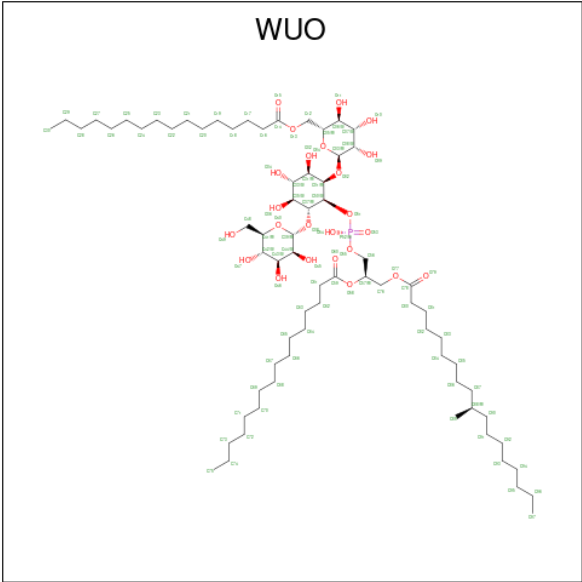
Mol	Chain	Residues	Atoms					AltConf	Trace
12	Y	25	Total	C	N	O	S	0	0
			168	103	26	38	1		
12	c	25	Total	C	N	O	S	0	0
			168	103	26	38	1		

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



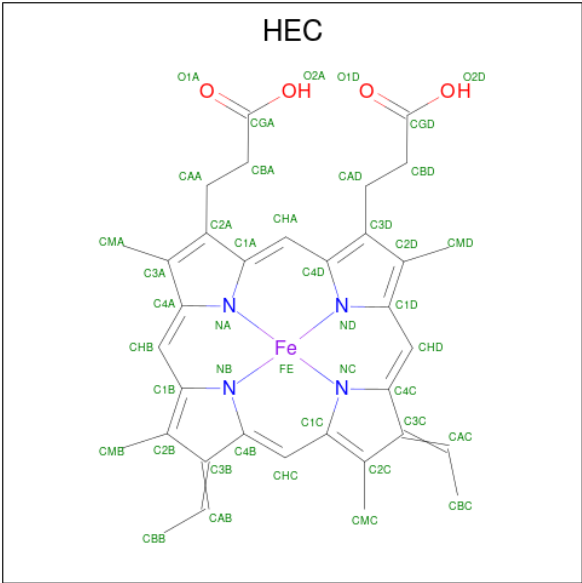
Mol	Chain	Residues	Atoms			AltConf
13	O	1	Total	C	O	0
			58	56	2	
13	O	1	Total	C	O	0
			58	56	2	
13	N	1	Total	C	O	0
			58	56	2	
13	H	1	Total	C	O	0
			58	56	2	
13	H	1	Total	C	O	0
			58	56	2	

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



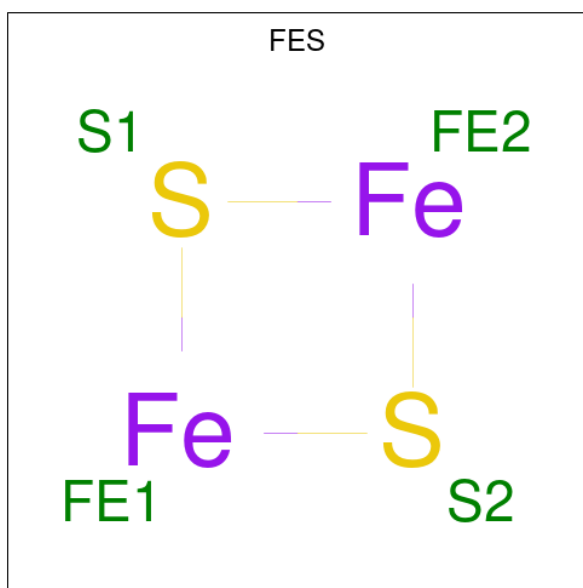
Mol	Chain	Residues	Atoms				AltConf
14	O	1	Total	C	O	P	0
			97	72	24	1	
14	P	1	Total	C	O	P	0
			97	72	24	1	

- Molecule 15 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



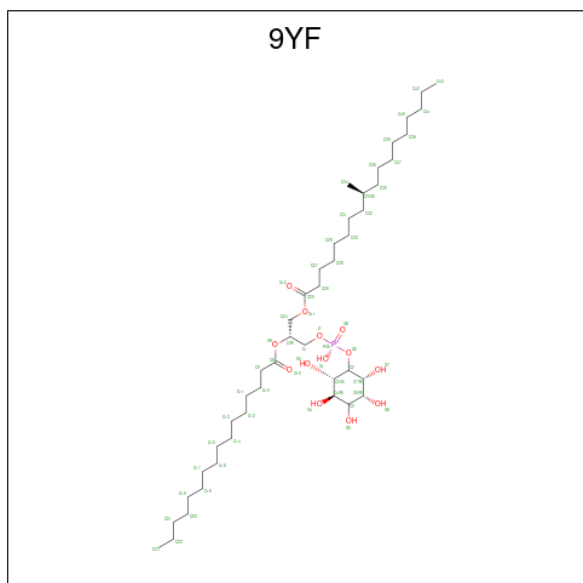
Mol	Chain	Residues	Atoms					AltConf
15	O	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
15	O	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 16 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



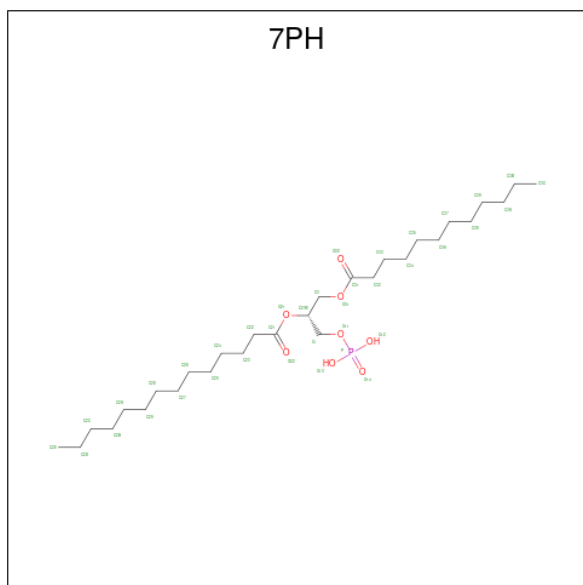
Mol	Chain	Residues	Atoms			AltConf
16	M	1	Total	Fe	S	0
			4	2	2	
16	G	1	Total	Fe	S	0
			4	2	2	

- 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 (CCD ID: 9YF) (formula: $\text{C}_{44}\text{H}_{85}\text{O}_{13}\text{P}$).



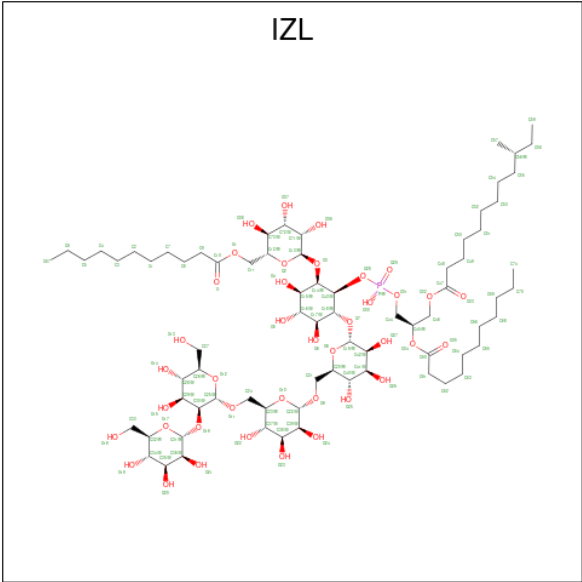
Mol	Chain	Residues	Atoms				AltConf
17	M	1	Total	C	O	P	0
			58	44	13	1	
17	W	1	Total	C	O	P	0
			58	44	13	1	
17	G	1	Total	C	O	P	0
			58	44	13	1	

- Molecule 18 is (1R)-2-(dodecanoyloxy)-1-[(phosphonooxy)methyl]ethyl tetradecanoate (CCD ID: 7PH) (formula: C₂₉H₅₇O₈P).



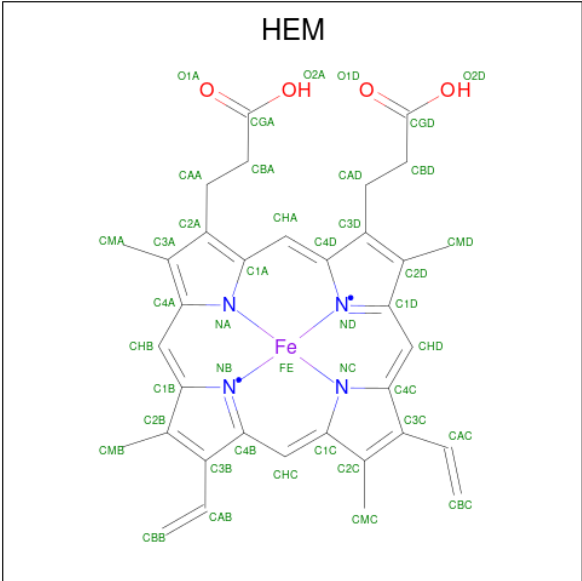
Mol	Chain	Residues	Atoms				AltConf
18	M	1	Total	C	O	P	0
			38	29	8	1	
18	S	1	Total	C	O	P	0
			38	29	8	1	
18	G	1	Total	C	O	P	0
			38	29	8	1	
18	G	1	Total	C	O	P	0
			38	29	8	1	

- 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 (CCD ID: IZL) (formula: C₇₄H₁₃₃O₃₉P).



Mol	Chain	Residues	Atoms				AltConf
19	M	1	Total	C	O	P	0
			114	74	39	1	
19	G	1	Total	C	O	P	0
			114	74	39	1	

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



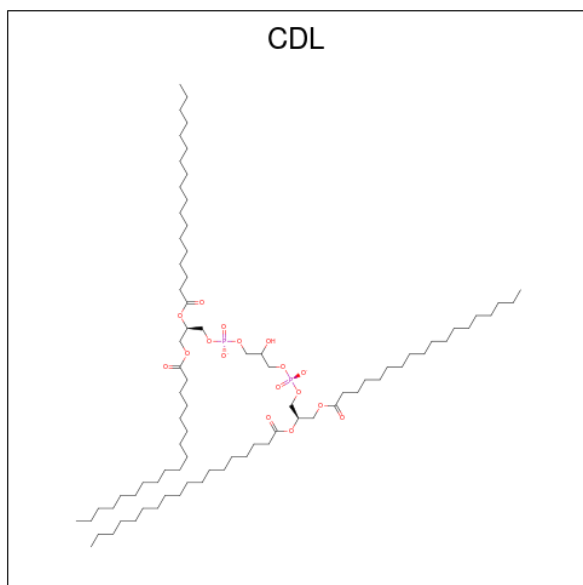
Mol	Chain	Residues	Atoms					AltConf
20	N	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

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

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



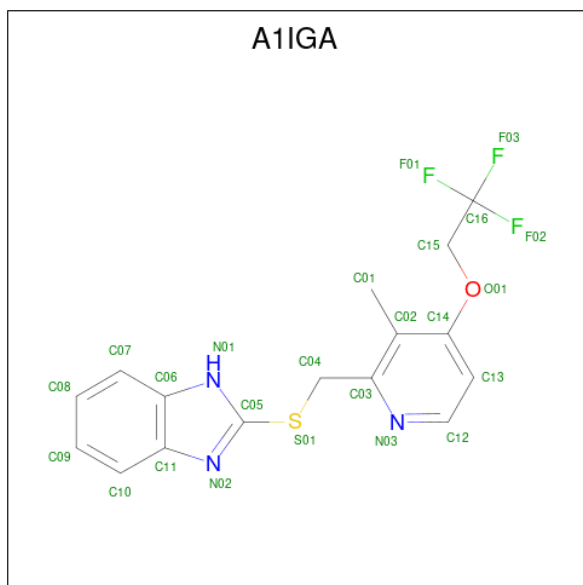
Mol	Chain	Residues	Atoms				AltConf
21	N	1	Total	C	O	P	0
			77	58	17	2	
21	N	1	Total	C	O	P	0
			79	60	17	2	
21	N	1	Total	C	O	P	0
			79	60	17	2	
21	P	1	Total	C	O	P	0
			77	58	17	2	
21	R	1	Total	C	O	P	0
			77	58	17	2	
21	R	1	Total	C	O	P	0
			77	58	17	2	
21	H	1	Total	C	O	P	0
			74	55	17	2	
21	H	1	Total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

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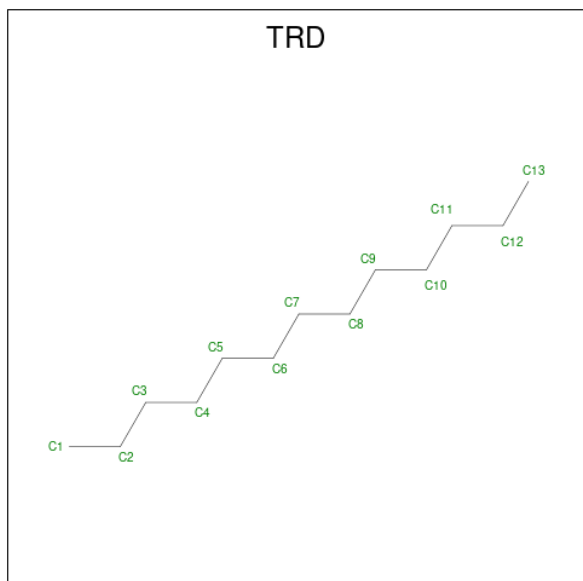
Mol	Chain	Residues	Atoms				AltConf
21	H	1	Total	C	O	P	0
			77	58	17	2	

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



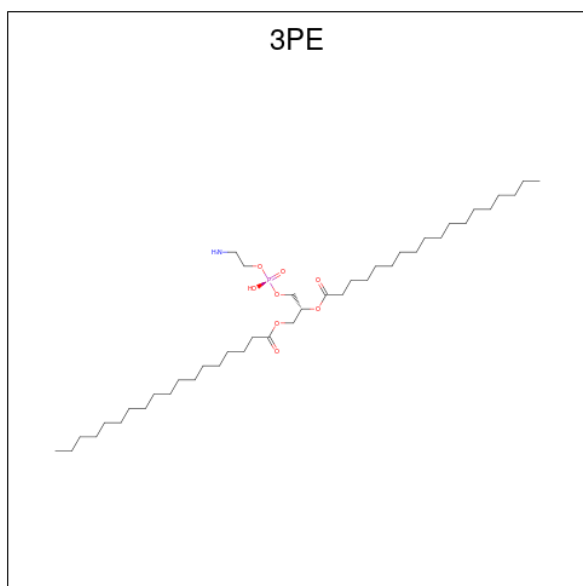
Mol	Chain	Residues	Atoms						AltConf
22	N	1	Total	C	F	N	O	S	0
			24	16	3	3	1	1	

- Molecule 23 is TRIDECANE (CCD ID: TRD) (formula: $C_{13}H_{28}$).



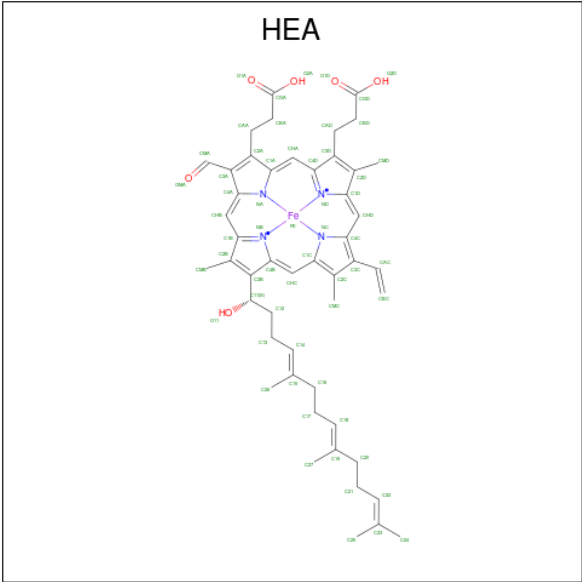
Mol	Chain	Residues	Atoms		AltConf
23	S	1	Total	C	0
			13	13	
23	T	1	Total	C	0
			13	13	
23	R	1	Total	C	0
			13	13	
23	R	1	Total	C	0
			13	13	
23	Q	1	Total	C	0
			13	13	

- Molecule 24 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 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 (CCD ID: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).



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

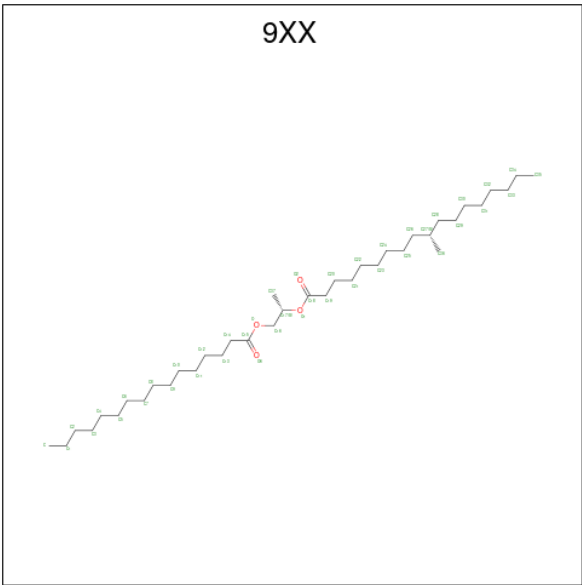
- Molecule 26 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

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

- Molecule 27 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

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

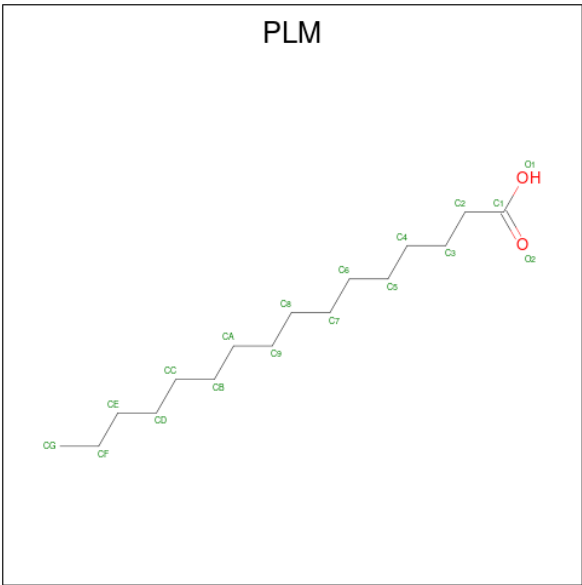


Mol	Chain	Residues	Atoms			AltConf
28	R	1	Total	C	O	0
			42	38	4	
28	Y	1	Total	C	O	0
			32	28	4	
28	c	1	Total	C	O	0
			32	28	4	

- Molecule 29 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 30 is PALMITIC ACID (CCD ID: 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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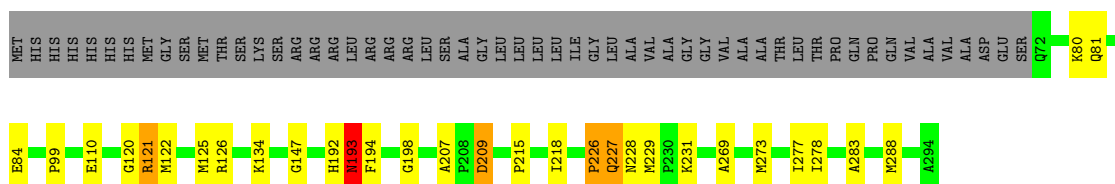
Mol	Chain	Residues	Atoms		AltConf
31	W	2	Total 2	O 2	0
31	Y	2	Total 2	O 2	0
31	H	13	Total 13	O 13	0
31	G	11	Total 11	O 11	0

3 Residue-property plots [i](#)

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

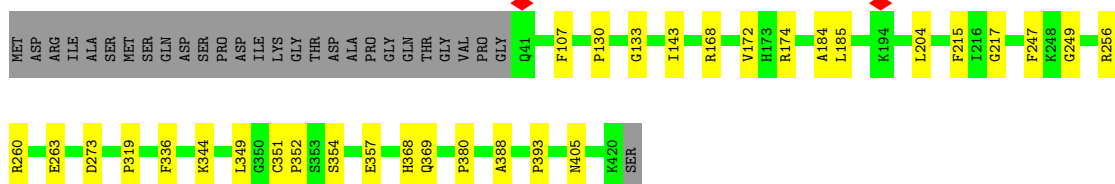
- Molecule 1: Cytochrome bc1 complex cytochrome c subunit

Chain O: 



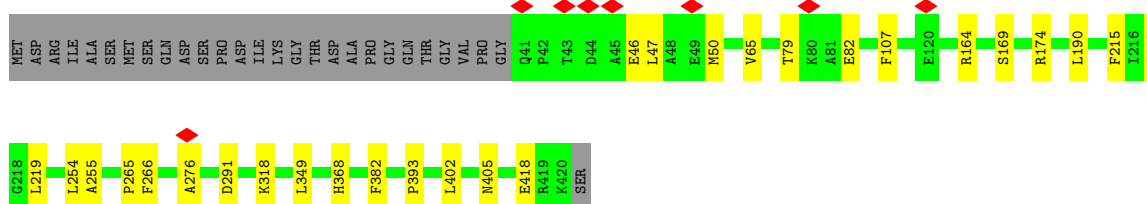
- Molecule 2: Cytochrome bc1 complex cytochrome c subunit

Chain M: 



- Molecule 2: Cytochrome bc1 complex cytochrome c subunit

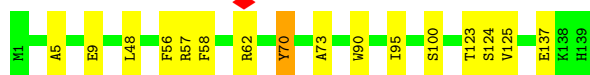
Chain G: 



- Molecule 3: Cytochrome bc1 complex cytochrome b subunit

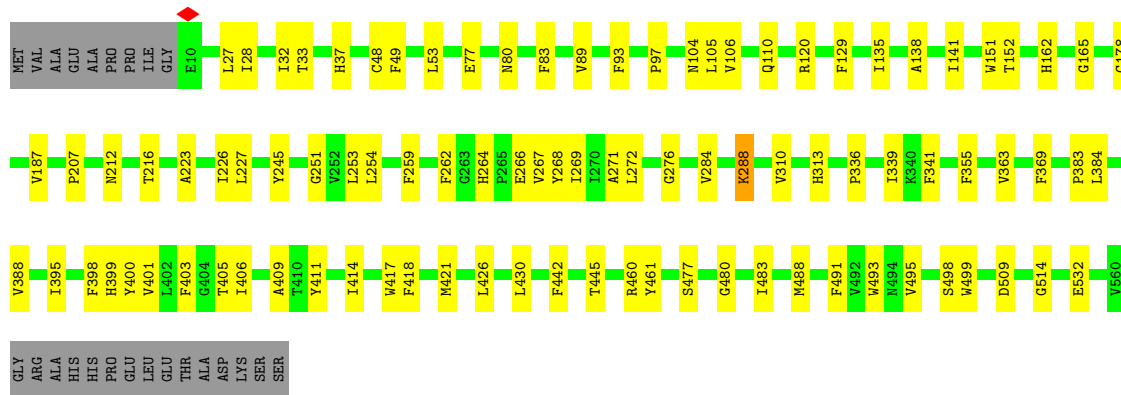
Chain N: 

Chain T:  88% 11%



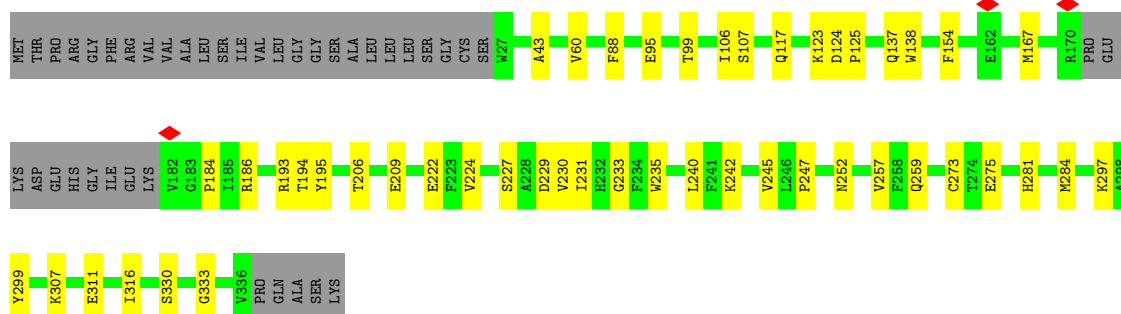
• Molecule 7: Cytochrome c oxidase subunit 1

Chain R:  79% 16%



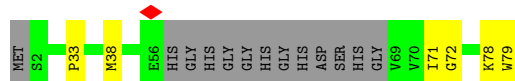
• Molecule 8: cytochrome-c oxidase

Chain Q:  74% 14% 12%



• Molecule 9: Cytochrome c oxidase subunit

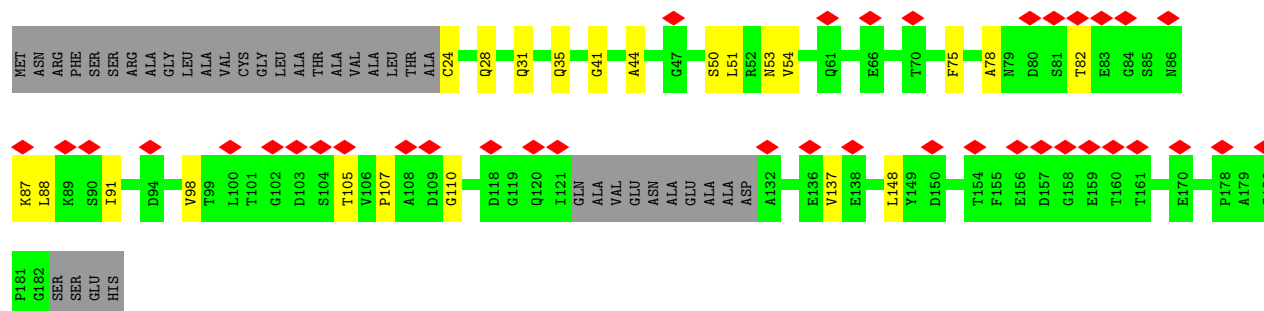
Chain U:  76% 8% 16%



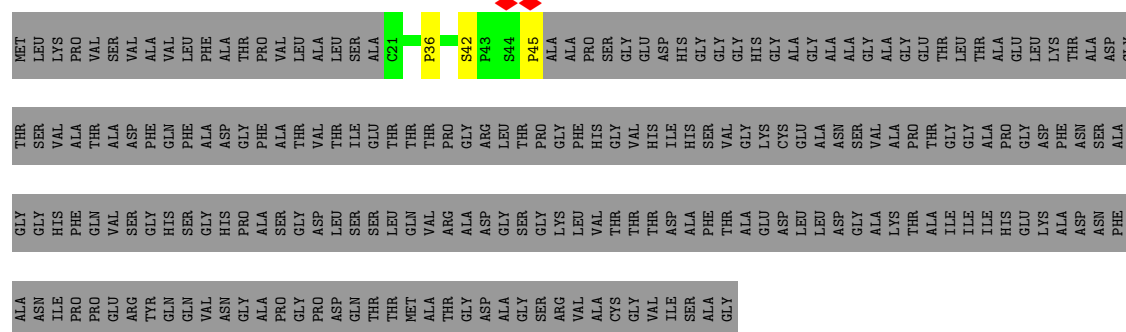
• Molecule 10: Uncharacterized protein MSMEG_4692/MSMEI_4575

Chain V:  73% 17% 9%

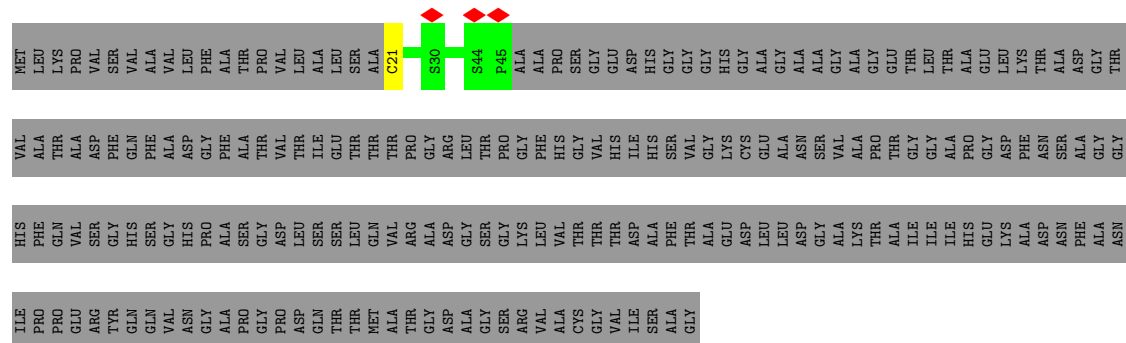
- Molecule 11: LpqE protein



- Molecule 12: Superoxide dismutase [Cu-Zn]



- Molecule 12: Superoxide dismutase [Cu-Zn]



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: A1IGA, WUO, 3PE, HEA, PLM, CA, MG, 9XX, 7PH, HEC, FES, TRD, HEM, MQ9, IZL, 9YF, CDL, CU

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	0.48	2/1660 (0.1%)	0.65	4/2250 (0.2%)
2	G	0.18	0/3046	0.32	0/4129
2	M	0.19	0/3046	0.34	0/4129
3	H	0.32	0/3534	0.46	0/4820
3	N	0.34	1/4299 (0.0%)	0.46	0/5862
4	P	0.14	0/606	0.26	0/825
5	S	0.11	0/1488	0.28	0/2032
6	T	0.22	0/1112	0.34	0/1524
7	R	0.25	0/4529	0.40	0/6187
8	Q	0.28	0/2447	0.41	0/3330
9	U	0.48	0/515	0.48	0/704
10	V	0.44	0/1042	0.65	1/1423 (0.1%)
11	W	0.15	0/1100	0.37	0/1508
12	Y	0.11	0/175	0.30	0/244
12	c	0.09	0/175	0.27	0/244
All	All	0.29	3/28774 (0.0%)	0.42	5/39211 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	236	THR	C-O	-5.37	1.17	1.23
1	O	226	PRO	C-O	-5.12	1.18	1.23
1	O	192	HIS	CE1-NE2	-5.07	1.27	1.32

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	192	HIS	CA-C-O	-7.96	109.66	119.28
10	V	75	ALA	N-CA-C	-5.65	106.43	113.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	192	HIS	CA-CB-CG	-5.64	108.16	113.80
1	O	193	ASN	CA-CB-CG	5.39	117.99	112.60
1	O	209	ASP	CA-C-O	-5.03	115.66	121.19

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	31	0
2	G	2967	0	2976	25	0
2	M	2967	0	2976	33	0
3	H	3425	0	3469	69	0
3	N	4167	0	4192	82	0
4	P	586	0	578	7	0
5	S	1441	0	1439	17	0
6	T	1077	0	1058	12	0
7	R	4369	0	4346	74	0
8	Q	2382	0	2335	38	0
9	U	499	0	504	6	0
10	V	1024	0	1035	26	0
11	W	1083	0	1055	14	0
12	Y	168	0	150	3	0
12	c	168	0	151	6	0
13	H	116	0	160	12	0
13	N	58	0	80	17	0
13	O	116	0	160	16	0
14	O	97	0	0	3	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	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	17	0
20	N	86	0	60	13	0
21	H	225	0	282	14	0
21	N	235	0	308	8	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
25	R	120	0	108	20	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	6	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	2	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	458	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 (458) 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)
12:c:21:CYS:N	30:c:301:PLM:O2	1.81	1.14
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
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
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
3:H:124:LEU:HD12	20:H:605:HEM:HMC1	1.61	0.81
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
12:c:21:CYS:SG	28:c:302:9XX:C37	2.70	0.79
3:N:152:MET:HE3	3:N:305:MET:HE3	1.65	0.79
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
12:c:21:CYS:SG	28:c:302:9XX:C16	2.74	0.74
20:N:605:HEM:HBC2	20:N:605:HEM:HMC2	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
12:c:21:CYS:SG	28:c:302:9XX:C17	2.77	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:CBD	2.20	0.70
3:H:262:GLY:HA3	13:H:606:MQ9:H221	1.73	0.70
3:H:320:PHE:CZ	28:c:302:9XX:C9	2.75	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
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
1:O:218:ILE:HA	15:O:303:HEC:HMA2	1.76	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
12:c:21:CYS:SG	28:c:302:9XX:O1	2.60	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
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
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
3:N:412:ARG:HB3	4:P:62:MET:HE1	1.86	0.57
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:HBC2	20:H:605:HEM:CMC	2.35	0.56
12:c:21:CYS:N	30:c:301:PLM:C1	2.65	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:N:110:HIS:CD2	20:N:601:HEM:HMA2	2.41	0.55
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
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
3:H:304:TYR:C	3:H:304:TYR:CD2	2.86	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
3:H:320:PHE:HZ	28:c:302:9XX:C9	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
7:R:251:GLY:HA2	7:R:254:LEU:HB3	1.92	0.51
7:R:461:TYR:OH	8:Q:273:CYS:O	2.25	0.50
10:V:84:ILE:HG21	10:V:96:LEU:HD21	1.89	0.50
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
1:O:122:MET:HE3	15:O:304:HEC:CHA	2.42	0.49
1:O:215:PRO:HA	1:O:218:ILE:HD12	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
3:H:304:TYR:C	3:H:304:TYR:HD2	2.22	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
1:O:81:GLN:NE2	8:Q:167:MET:HE2	2.30	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:O:193:ASN:HA	3:N:296:SER:HG	1.80	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
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
7:R:264:HIS:NE2	7:R:268:TYR:HE2	2.13	0.46
2:G:418:GLU:CD	2:G:418:GLU:H	2.23	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
7:R:53:LEU:HD23	7:R:488:MET:HE2	1.97	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
3:N:308:THR:HG21	3:N:337:MET:HE2	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
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
2:M:168:ARG:HH12	3:H:14:ASP:CG	2.25	0.44
3:H:116:PHE:O	3:H:120:ILE:HG13	2.17	0.44
1:O:273:MET:HE2	14:O:302:WUO:C89	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:N:68:MET:HE3	3:N:204:ILE:HG12	2.01	0.43
13:N:606:MQ9:H321	13:N:606:MQ9:H303	1.81	0.43
7:R:49:PHE:HZ	7:R:411:TYR:OH	2.01	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
3:H:48:TYR:OH	3:H:261:SER:OG	2.37	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: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
8:Q:231:ILE:HG22	8:Q:275:GLU:HG2	2.01	0.42
1:O:288:MET:HE3	21:N:602:CDL:H712	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
2:G:46:GLU:HB3	2:G:50:MET:HE3	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
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
8:Q:333:GLY:HA3	11:W:28:GLN:CD	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:269:ALA:HA	3:N:306:MET:HE1	2.02	0.41
13:O:301:MQ9:H221	13:O:301:MQ9:H203	1.65	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
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:265:PHE:C	3:H:265:PHE:CD2	2.97	0.41
3:H:271:VAL:O	3:H:275:MET:HG3	2.21	0.41
3:N:126:ARG:O	3:N:130:THR:OG1	2.31	0.41
13:O:301:MQ9:H161	21:N:602:CDL:H571	2.03	0.41
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
2:G:418:GLU:CD	2:G:418:GLU:N	2.78	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	43	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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 ⓘ

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	69
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%)	339 (97%)	12 (3%)	32	60
3	N	428/448 (96%)	422 (99%)	6 (1%)	59	81
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%)	70	87
7	R	453/471 (96%)	451 (100%)	2 (0%)	84	93
8	Q	255/288 (88%)	253 (99%)	2 (1%)	73	88
9	U	51/59 (86%)	50 (98%)	1 (2%)	48	74
10	V	105/114 (92%)	100 (95%)	5 (5%)	23	47
11	W	121/146 (83%)	121 (100%)	0	100	100
12	Y	20/167 (12%)	20 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	c	20/167 (12%)	20 (100%)	0	100	100
All	All	2899/3530 (82%)	2866 (99%)	33 (1%)	63	84

All (33) 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	185	ILE
3	N	187	THR
3	N	234	LYS
3	N	294	GLN
3	N	305	MET
3	N	337	MET
6	T	70	TYR
7	R	129	PHE
7	R	288	LYS
8	Q	206	THR
8	Q	229	ASP
9	U	71	ILE
10	V	82	ARG
10	V	83	GLU
10	V	84	ILE
10	V	85	LEU
10	V	103	GLN
3	H	106	ARG
3	H	138	GLU
3	H	180	MET
3	H	185	ILE
3	H	187	THR
3	H	300	GLN
3	H	302	ASP
3	H	303	PHE
3	H	304	TYR
3	H	305	MET
3	H	306	MET
3	H	374	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	O	187	ASN
2	M	115	GLN
3	N	110	HIS
3	N	140	ASN
7	R	81	GLN
7	R	212	ASN
8	Q	285	ASN
8	Q	302	GLN
3	H	29	GLN
3	H	300	GLN
2	G	115	GLN
2	G	180	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	$\# Z > 2$
25	HEA	R	603	7	67,67,67	2.64	25 (37%)	81,103,103	2.21	35 (43%)
21	CDL	H	601	-	73,73,99	0.30	0	79,85,111	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	9YF	M	502	-	58,58,58	1.37	5 (8%)	68,71,71	1.11	5 (7%)
16	FES	G	501	2	0,4,4	-	-	-		
20	HEM	H	602	3	50,50,50	1.90	13 (26%)	67,82,82	1.76	20 (29%)
14	WUO	O	302	-	99,99,99	1.60	10 (10%)	122,125,125	1.29	13 (10%)
28	9XX	R	609	-	41,41,41	1.17	2 (4%)	44,44,44	0.97	4 (9%)
18	7PH	S	501	-	37,37,37	0.30	0	40,42,42	0.34	0
18	7PH	M	503	-	37,37,37	0.30	0	40,42,42	0.34	0
15	HEC	O	304	1	46,50,50	1.98	7 (15%)	58,82,82	1.61	5 (8%)
28	9XX	Y	302	-	31,31,41	1.29	2 (6%)	34,34,44	1.13	4 (11%)
18	7PH	G	504	-	37,37,37	0.97	4 (10%)	40,42,42	1.17	2 (5%)
19	IZL	M	504	-	119,119,119	1.73	29 (24%)	160,163,163	1.30	19 (11%)
14	WUO	P	302	-	99,99,99	1.61	11 (11%)	122,125,125	1.29	13 (10%)
20	HEM	N	605	3	50,50,50	2.06	19 (38%)	67,82,82	1.68	15 (22%)
30	PLM	W	202	-	9,10,17	0.79	0	8,9,17	0.44	0
13	MQ9	O	301	-	59,59,59	0.37	0	73,75,75	0.43	1 (1%)
20	HEM	N	601	3	50,50,50	1.97	13 (26%)	67,82,82	1.87	13 (19%)
23	TRD	S	502	-	12,12,12	0.10	0	11,11,11	0.05	0
13	MQ9	H	607	-	59,59,59	0.36	0	73,75,75	0.41	1 (1%)
18	7PH	G	505	-	37,37,37	0.97	4 (10%)	40,42,42	1.14	2 (5%)
13	MQ9	N	606	-	59,59,59	0.35	0	73,75,75	0.40	1 (1%)
21	CDL	P	301	-	76,76,99	0.41	0	82,88,111	0.52	0
13	MQ9	H	606	-	59,59,59	0.37	0	73,75,75	0.43	1 (1%)
21	CDL	H	604	-	76,76,99	0.30	0	82,88,111	0.35	0
24	3PE	S	503	-	31,31,50	0.33	0	34,36,55	0.39	0
30	PLM	c	301	-	9,10,17	0.36	0	8,9,17	0.36	0
23	TRD	T	201	-	12,12,12	0.10	0	11,11,11	0.05	0
17	9YF	W	201	-	58,58,58	1.38	4 (6%)	68,71,71	1.11	3 (4%)
21	CDL	H	603	-	73,73,99	0.30	0	79,85,111	0.36	0
30	PLM	Y	301	-	9,10,17	0.79	0	8,9,17	0.45	0
21	CDL	N	602	-	76,76,99	0.30	0	82,88,111	0.35	0
20	HEM	H	605	3	50,50,50	2.06	18 (36%)	67,82,82	1.91	21 (31%)
22	A1IGA	N	604	-	26,26,26	2.36	7 (26%)	37,37,37	2.47	13 (35%)
23	TRD	Q	403	-	12,12,12	0.10	0	11,11,11	0.06	0
25	HEA	R	602	7	67,67,67	2.26	26 (38%)	81,103,103	2.44	29 (35%)
21	CDL	R	605	-	76,76,99	0.30	0	82,88,111	0.35	0
13	MQ9	O	305	-	59,59,59	0.50	0	73,75,75	0.47	1 (1%)
16	FES	M	501	2	0,4,4	-	-	-		
23	TRD	R	608	-	12,12,12	0.10	0	11,11,11	0.05	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	TRD	R	607	-	12,12,12	0.10	0	11,11,11	0.05	0
19	IZL	G	503	-	119,119,119	1.73	29 (24%)	160,163,163	1.30	19 (11%)
15	HEC	O	303	1	46,50,50	2.04	9 (19%)	58,82,82	1.73	7 (12%)
17	9YF	G	502	-	58,58,58	1.38	5 (8%)	68,71,71	1.11	2 (2%)
28	9XX	c	302	-	31,31,41	1.29	2 (6%)	34,34,44	1.10	4 (11%)
21	CDL	R	601	-	76,76,99	0.30	0	82,88,111	0.35	0
21	CDL	N	607	-	78,78,99	0.29	0	84,90,111	0.35	0
21	CDL	N	603	-	78,78,99	0.29	0	84,90,111	0.34	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	HEA	R	603	7	-	15/36/76/76	-
21	CDL	H	601	-	-	35/84/84/110	-
17	9YF	M	502	-	-	26/54/78/78	0/1/1/1
16	FES	G	501	2	-	-	0/1/1/1
20	HEM	H	602	3	-	4/14/54/54	-
14	WUO	O	302	-	-	28/84/148/148	0/3/3/3
28	9XX	R	609	-	-	23/43/43/43	-
18	7PH	S	501	-	-	13/39/39/39	-
18	7PH	M	503	-	-	15/39/39/39	-
15	HEC	O	304	1	-	9/14/54/54	-
28	9XX	Y	302	-	-	11/33/33/43	-
18	7PH	G	504	-	-	10/39/39/39	-
19	IZL	M	504	-	-	37/84/208/208	0/6/6/6
14	WUO	P	302	-	-	43/84/148/148	0/3/3/3
20	HEM	N	605	3	-	9/14/54/54	-
30	PLM	W	202	-	-	2/8/8/15	-
13	MQ9	O	301	-	-	9/53/73/73	0/2/2/2
20	HEM	N	601	3	-	7/14/54/54	-
23	TRD	S	502	-	-	2/10/10/10	-
13	MQ9	H	607	-	-	28/53/73/73	0/2/2/2
18	7PH	G	505	-	-	11/39/39/39	-
13	MQ9	N	606	-	-	27/53/73/73	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CDL	P	301	-	-	45/87/87/110	-
13	MQ9	H	606	-	-	19/53/73/73	0/2/2/2
21	CDL	H	604	-	-	40/87/87/110	-
24	3PE	S	503	-	-	14/35/35/54	-
30	PLM	c	301	-	-	0/8/8/15	-
23	TRD	T	201	-	-	1/10/10/10	-
17	9YF	W	201	-	-	32/54/78/78	0/1/1/1
21	CDL	H	603	-	-	39/84/84/110	-
30	PLM	Y	301	-	-	0/8/8/15	-
21	CDL	N	602	-	-	50/87/87/110	-
20	HEM	H	605	3	-	8/14/54/54	-
22	A1IGA	N	604	-	-	7/11/11/11	0/3/3/3
23	TRD	Q	403	-	-	1/10/10/10	-
25	HEA	R	602	7	-	12/36/76/76	-
21	CDL	R	605	-	-	41/87/87/110	-
13	MQ9	O	305	-	-	20/53/73/73	0/2/2/2
23	TRD	R	608	-	-	2/10/10/10	-
16	FES	M	501	2	-	-	0/1/1/1
23	TRD	R	607	-	-	1/10/10/10	-
19	IZL	G	503	-	-	37/84/208/208	0/6/6/6
15	HEC	O	303	1	-	7/14/54/54	-
17	9YF	G	502	-	-	26/54/78/78	0/1/1/1
28	9XX	c	302	-	-	16/33/33/43	-
21	CDL	R	601	-	-	51/87/87/110	-
21	CDL	N	607	-	-	48/89/89/110	-
21	CDL	N	603	-	-	53/89/89/110	-

All (244) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	O	303	HEC	CAC-C3C	7.62	1.59	1.35
15	O	304	HEC	CAC-C3C	7.54	1.59	1.35
25	R	603	HEA	FE-NB	7.11	2.16	1.94
15	O	304	HEC	CAB-C3B	6.78	1.57	1.35
15	O	303	HEC	CAB-C3B	6.75	1.56	1.35
20	H	602	HEM	FE-NB	6.40	2.14	1.94
25	R	603	HEA	FE-NC	6.38	2.16	1.95
14	O	302	WUO	P52-O51	6.11	1.77	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	P	302	WUO	P52-O51	6.10	1.77	1.59
22	N	604	A1IGA	C05-S01	5.92	1.83	1.75
14	P	302	WUO	C50-C01	5.78	1.64	1.52
14	O	302	WUO	C50-C01	5.64	1.63	1.52
25	R	603	HEA	FE-ND	5.41	2.11	1.94
14	O	302	WUO	P52-O55	5.40	1.80	1.59
22	N	604	A1IGA	C05-N02	5.36	1.41	1.30
14	P	302	WUO	P52-O55	5.36	1.80	1.59
25	R	603	HEA	CHD-C1D	5.32	1.49	1.38
25	R	602	HEA	FE-NB	5.25	2.11	1.94
17	W	201	9YF	P-O2	5.24	1.75	1.59
17	G	502	9YF	P-O2	5.21	1.75	1.59
25	R	603	HEA	C1A-NA	5.06	1.49	1.39
20	N	605	HEM	FE-NB	4.99	2.10	1.94
25	R	602	HEA	FE-NC	4.88	2.11	1.95
25	R	603	HEA	C3B-C2B	4.87	1.45	1.34
17	M	502	9YF	P-O2	4.86	1.74	1.59
20	H	605	HEM	C1B-NB	-4.80	1.31	1.40
19	G	503	IZL	P-O28	4.74	1.73	1.59
25	R	602	HEA	FE-ND	4.74	2.09	1.94
25	R	602	HEA	C3B-C2B	4.74	1.45	1.34
19	M	504	IZL	P-O28	4.72	1.73	1.59
25	R	602	HEA	C3D-C2D	4.67	1.46	1.36
14	P	302	WUO	C56-C57	4.63	1.65	1.50
14	O	302	WUO	C56-C57	4.62	1.65	1.50
19	G	503	IZL	C44-C45	4.58	1.65	1.50
19	M	504	IZL	C44-C45	4.56	1.65	1.50
22	N	604	A1IGA	C02-C03	4.54	1.43	1.39
20	N	601	HEM	FE-NB	4.44	2.08	1.94
25	R	602	HEA	CHC-C4B	4.43	1.47	1.38
17	W	201	9YF	P-O	4.41	1.76	1.59
17	M	502	9YF	P-O	4.40	1.76	1.59
19	G	503	IZL	C43-C14	4.39	1.61	1.52
17	G	502	9YF	P-O	4.38	1.76	1.59
19	M	504	IZL	C43-C14	4.36	1.61	1.52
20	H	605	HEM	FE-NB	4.32	2.08	1.94
28	R	609	9XX	C16-C17	4.28	1.60	1.50
20	N	601	HEM	C3C-C4C	-4.26	1.38	1.46
28	c	302	9XX	C16-C17	4.24	1.60	1.50
22	N	604	A1IGA	C04-C03	4.24	1.54	1.50
28	Y	302	9XX	C16-C17	4.23	1.60	1.50
20	N	601	HEM	FE-NC	4.23	2.09	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	N	601	HEM	C1B-NB	-4.22	1.32	1.40
20	N	605	HEM	FE-NC	4.20	2.09	1.95
25	R	603	HEA	C4B-NB	-4.18	1.33	1.40
20	N	605	HEM	C1B-NB	-4.16	1.33	1.40
25	R	603	HEA	CHC-C4B	4.16	1.46	1.38
20	N	605	HEM	C4D-ND	-4.12	1.33	1.40
20	H	602	HEM	FE-NC	4.09	2.08	1.95
20	N	601	HEM	C4D-ND	-4.08	1.33	1.40
25	R	603	HEA	C11-C3B	-4.06	1.46	1.51
20	H	605	HEM	C4D-ND	-4.06	1.33	1.40
19	M	504	IZL	P-O31	4.04	1.75	1.59
25	R	603	HEA	C3D-C2D	4.04	1.45	1.36
19	G	503	IZL	P-O31	4.03	1.75	1.59
20	H	605	HEM	C1C-C2C	-4.01	1.37	1.45
20	N	605	HEM	C3C-C4C	-3.99	1.39	1.46
25	R	603	HEA	CHD-C4C	3.92	1.48	1.39
25	R	603	HEA	CHA-C1A	3.90	1.46	1.38
25	R	603	HEA	C4A-NA	3.88	1.46	1.39
25	R	602	HEA	CHD-C1D	3.87	1.46	1.38
20	H	602	HEM	C1B-NB	-3.82	1.33	1.40
20	N	601	HEM	C1C-C2C	-3.81	1.37	1.45
22	N	604	A1IGA	C04-S01	3.80	1.92	1.82
14	P	302	WUO	C50-C37	3.80	1.60	1.52
25	R	603	HEA	C1D-ND	-3.79	1.33	1.40
25	R	603	HEA	CHB-C4A	3.76	1.45	1.38
14	O	302	WUO	C50-C37	3.75	1.60	1.52
25	R	603	HEA	C4C-NC	-3.74	1.32	1.39
15	O	303	HEC	CBC-CAC	-3.74	1.35	1.49
25	R	603	HEA	C1C-NC	-3.74	1.32	1.39
20	H	602	HEM	C1C-C2C	-3.64	1.38	1.45
20	H	605	HEM	FE-NC	3.63	2.07	1.95
20	H	602	HEM	C4D-ND	-3.61	1.34	1.40
25	R	603	HEA	C3A-C2A	3.60	1.45	1.37
20	H	605	HEM	C4B-NB	-3.57	1.31	1.38
25	R	602	HEA	C1A-NA	3.54	1.46	1.39
20	N	605	HEM	C1C-C2C	-3.54	1.38	1.45
25	R	602	HEA	C1D-ND	-3.52	1.34	1.40
25	R	602	HEA	CHB-C4A	3.52	1.45	1.38
25	R	602	HEA	C3A-C2A	3.51	1.45	1.37
25	R	602	HEA	C4A-NA	3.49	1.46	1.39
15	O	304	HEC	CBC-CAC	-3.48	1.36	1.49
25	R	603	HEA	CHC-C1C	3.47	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	R	602	HEA	CHC-C1C	3.45	1.47	1.39
20	N	601	HEM	O2D-CGD	-3.38	1.19	1.30
25	R	602	HEA	CHA-C1A	3.32	1.44	1.38
25	R	602	HEA	C4B-NB	-3.28	1.34	1.40
25	R	602	HEA	CHB-C1B	3.26	1.46	1.39
20	H	605	HEM	C3C-C4C	-3.21	1.40	1.46
25	R	603	HEA	CHA-C4D	3.12	1.46	1.39
20	N	601	HEM	C1A-C2A	-3.11	1.38	1.44
25	R	602	HEA	C4C-NC	-3.10	1.33	1.39
14	O	302	WUO	C76-C57	3.10	1.60	1.50
25	R	602	HEA	CHD-C4C	3.09	1.46	1.39
14	P	302	WUO	C76-C57	3.08	1.60	1.50
19	M	504	IZL	C25-C30	2.99	1.59	1.52
20	H	602	HEM	O2D-CGD	-2.99	1.20	1.30
25	R	603	HEA	CHB-C1B	2.99	1.46	1.39
19	G	503	IZL	C25-C30	2.98	1.59	1.52
20	N	601	HEM	C4B-NB	-2.97	1.33	1.38
20	H	605	HEM	FE-ND	-2.96	1.85	1.94
19	G	503	IZL	C31-C36	2.96	1.61	1.52
19	M	504	IZL	C31-C36	2.95	1.61	1.52
20	N	605	HEM	C4B-NB	-2.92	1.33	1.38
20	N	605	HEM	O2A-CGA	-2.89	1.21	1.30
20	H	605	HEM	C1D-ND	-2.87	1.33	1.38
20	N	605	HEM	C1D-ND	-2.86	1.33	1.38
25	R	603	HEA	O2D-CGD	-2.86	1.21	1.30
20	N	605	HEM	C1C-NC	-2.83	1.34	1.39
25	R	603	HEA	O2A-CGA	-2.83	1.21	1.30
20	H	605	HEM	C4A-NA	-2.82	1.34	1.39
20	N	605	HEM	O2D-CGD	-2.81	1.21	1.30
20	N	605	HEM	FE-ND	-2.81	1.86	1.94
20	H	605	HEM	C1A-C2A	-2.80	1.39	1.44
20	H	605	HEM	C2A-C3A	-2.80	1.31	1.38
19	M	504	IZL	O28-C43	-2.80	1.34	1.44
19	G	503	IZL	O28-C43	-2.80	1.34	1.44
19	M	504	IZL	C43-C18	2.78	1.58	1.52
25	R	602	HEA	CHA-C4D	2.75	1.45	1.39
19	G	503	IZL	C43-C18	2.74	1.57	1.52
20	H	602	HEM	C4B-NB	-2.70	1.33	1.38
20	H	602	HEM	O2A-CGA	-2.69	1.21	1.30
20	H	605	HEM	C1C-NC	-2.69	1.34	1.39
18	G	504	7PH	O21-C2	-2.67	1.40	1.46
18	G	505	7PH	O21-C2	-2.66	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	M	504	IZL	C61-C60	2.64	1.58	1.50
19	G	503	IZL	C61-C60	2.63	1.58	1.50
20	N	605	HEM	C1A-C2A	-2.61	1.39	1.44
25	R	603	HEA	C1B-NB	-2.59	1.33	1.38
19	M	504	IZL	C29-C28	2.58	1.59	1.52
20	H	605	HEM	C1B-C2B	-2.58	1.39	1.44
19	G	503	IZL	C29-C28	2.58	1.59	1.52
19	G	503	IZL	O38-C73	-2.57	1.36	1.43
17	M	502	9YF	C1-C	2.56	1.58	1.50
19	M	504	IZL	O38-C73	-2.56	1.36	1.43
19	G	503	IZL	C13-C71	2.55	1.60	1.52
20	H	602	HEM	C3C-C4C	-2.53	1.41	1.46
19	M	504	IZL	C13-C71	2.52	1.59	1.52
17	W	201	9YF	C1-C	2.52	1.58	1.50
20	N	601	HEM	C4C-NC	-2.48	1.35	1.39
15	O	303	HEC	C3D-C2D	-2.47	1.32	1.38
15	O	304	HEC	CMD-C2D	2.46	1.55	1.50
20	H	605	HEM	O2D-CGD	-2.46	1.22	1.30
20	N	605	HEM	C4A-C3A	-2.46	1.37	1.43
20	N	601	HEM	C1D-ND	-2.45	1.34	1.38
22	N	604	A1IGA	C15-C16	2.45	1.58	1.48
19	G	503	IZL	O1-C10	2.44	1.40	1.33
18	G	505	7PH	O31-C31	2.43	1.40	1.33
22	N	604	A1IGA	C06-N01	2.43	1.43	1.38
19	G	503	IZL	C48-C47	2.43	1.57	1.50
19	G	503	IZL	O34-C60	2.43	1.41	1.34
17	G	502	9YF	C1-C	2.42	1.58	1.50
18	G	504	7PH	O31-C31	2.42	1.40	1.33
19	M	504	IZL	C48-C47	2.42	1.57	1.50
19	G	503	IZL	C24-C23	2.41	1.58	1.51
19	M	504	IZL	O34-C60	2.41	1.41	1.34
20	N	605	HEM	C3D-C2D	-2.41	1.31	1.36
19	M	504	IZL	C24-C23	2.41	1.58	1.51
19	M	504	IZL	O1-C10	2.41	1.40	1.33
20	N	601	HEM	O2A-CGA	-2.41	1.22	1.30
20	N	605	HEM	C4C-NC	-2.39	1.35	1.39
20	N	601	HEM	C1C-NC	-2.39	1.35	1.39
15	O	304	HEC	CBB-CAB	-2.37	1.40	1.49
25	R	602	HEA	C1B-NB	-2.36	1.34	1.38
19	G	503	IZL	O24-C39	-2.35	1.37	1.43
20	H	602	HEM	C1A-C2A	-2.35	1.39	1.44
19	M	504	IZL	O24-C39	-2.35	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	N	605	HEM	C1B-C2B	-2.34	1.39	1.44
15	O	303	HEC	CBB-CAB	-2.34	1.40	1.49
15	O	303	HEC	C3C-C4C	-2.34	1.41	1.46
19	G	503	IZL	O37-C72	-2.33	1.37	1.43
25	R	602	HEA	O2D-CGD	-2.32	1.23	1.30
25	R	602	HEA	O2A-CGA	-2.32	1.23	1.30
19	M	504	IZL	O37-C72	-2.31	1.37	1.43
17	M	502	9YF	C24-C	2.29	1.58	1.50
20	H	605	HEM	C4C-NC	-2.27	1.35	1.39
14	P	302	WUO	O77-C78	2.27	1.40	1.33
14	O	302	WUO	O77-C78	2.26	1.39	1.33
25	R	602	HEA	C1C-NC	-2.26	1.35	1.39
17	W	201	9YF	C24-C	2.24	1.57	1.50
25	R	602	HEA	C4D-ND	-2.24	1.34	1.38
20	H	602	HEM	C4A-NA	-2.23	1.35	1.39
14	O	302	WUO	O51-C50	-2.23	1.36	1.44
14	P	302	WUO	O51-C50	-2.23	1.36	1.44
19	G	503	IZL	C35-C34	2.23	1.58	1.52
19	M	504	IZL	C35-C34	2.22	1.58	1.52
19	M	504	IZL	O23-C38	-2.22	1.37	1.43
20	H	602	HEM	C1B-C2B	-2.22	1.40	1.44
20	N	605	HEM	C4A-NA	-2.21	1.35	1.39
25	R	602	HEA	C4B-C3B	2.20	1.48	1.44
19	G	503	IZL	O23-C38	-2.20	1.37	1.43
15	O	303	HEC	C3B-C4B	-2.20	1.42	1.46
15	O	304	HEC	C3D-C2D	-2.19	1.33	1.38
19	M	504	IZL	O6-C17	-2.19	1.37	1.43
20	H	605	HEM	O2A-CGA	-2.18	1.23	1.30
17	G	502	9YF	C24-C	2.18	1.57	1.50
17	M	502	9YF	O2-C2	-2.18	1.36	1.44
19	G	503	IZL	O1-C11	-2.18	1.40	1.45
19	G	503	IZL	C36-C35	2.18	1.58	1.52
14	O	302	WUO	C31-C01	2.18	1.58	1.52
19	M	504	IZL	C36-C35	2.17	1.58	1.52
18	G	504	7PH	O31-C3	-2.17	1.40	1.45
18	G	505	7PH	O21-C21	2.17	1.40	1.34
19	M	504	IZL	O1-C11	-2.16	1.40	1.45
19	G	503	IZL	P-O30	-2.16	1.45	1.55
19	M	504	IZL	P-O30	-2.16	1.45	1.55
19	G	503	IZL	O6-C17	-2.16	1.37	1.43
19	M	504	IZL	O26-C41	-2.16	1.37	1.43
14	P	302	WUO	C06-C05	2.15	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	G	505	7PH	O31-C3	-2.15	1.40	1.45
19	G	503	IZL	O26-C41	-2.14	1.37	1.43
14	P	302	WUO	C31-C01	2.14	1.58	1.52
14	O	302	WUO	C06-C05	2.13	1.57	1.53
15	O	303	HEC	C3B-C2B	-2.13	1.34	1.41
19	G	503	IZL	O9-C21	-2.12	1.40	1.43
18	G	504	7PH	O21-C21	2.12	1.40	1.34
19	M	504	IZL	O9-C21	-2.11	1.40	1.43
20	H	602	HEM	C1A-NA	-2.11	1.35	1.39
28	R	609	9XX	O-C15	2.10	1.39	1.33
19	G	503	IZL	O12-C26	-2.09	1.39	1.44
19	M	504	IZL	O12-C26	-2.09	1.39	1.44
28	c	302	9XX	O-C15	2.08	1.39	1.33
28	Y	302	9XX	O-C15	2.08	1.39	1.33
19	M	504	IZL	C33-C32	2.08	1.58	1.51
20	N	605	HEM	C1A-NA	-2.08	1.35	1.39
20	H	605	HEM	CHA-C1A	-2.07	1.34	1.39
19	G	503	IZL	C33-C32	2.07	1.58	1.51
25	R	603	HEA	C4D-ND	-2.06	1.34	1.38
25	R	602	HEA	C1C-C2C	2.04	1.47	1.43
15	O	303	HEC	C3C-C2C	-2.03	1.34	1.41
17	G	502	9YF	C4-C3	2.02	1.57	1.52
15	O	304	HEC	C3C-C4C	-2.02	1.42	1.46
19	G	503	IZL	C42-C41	2.01	1.57	1.52
14	P	302	WUO	C12-C05	2.01	1.57	1.51
19	M	504	IZL	C42-C41	2.01	1.57	1.52

All (253) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	O	303	HEC	CBB-CAB-C3B	-8.74	109.96	127.43
22	N	604	A1IGA	C04-S01-C05	8.56	118.18	100.44
15	O	304	HEC	CBB-CAB-C3B	-8.37	110.70	127.43
20	N	601	HEM	CHC-C4B-NB	7.03	131.99	124.42
25	R	602	HEA	C3D-C4D-ND	5.98	116.14	110.35
25	R	602	HEA	C3C-C4C-NC	5.81	114.69	109.80
19	G	503	IZL	O10-C23-C24	5.45	117.50	106.69
25	R	602	HEA	C2D-C1D-ND	5.45	116.11	109.84
19	M	504	IZL	O10-C23-C24	5.45	117.49	106.69
25	R	602	HEA	C2B-C1B-NB	5.41	116.15	109.90
22	N	604	A1IGA	C03-C04-S01	5.40	120.23	109.54
25	R	602	HEA	C3C-C2C-C1C	-5.37	100.84	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	R	602	HEA	C3B-C4B-NB	5.29	115.92	109.84
25	R	603	HEA	C3D-C4D-ND	5.14	115.32	110.35
25	R	603	HEA	C2B-C1B-NB	5.13	115.83	109.90
20	H	605	HEM	CHA-C4D-ND	4.92	130.45	124.37
25	R	602	HEA	C1D-C2D-C3D	-4.64	102.10	106.98
20	N	605	HEM	CHD-C1D-ND	4.61	129.38	124.42
25	R	603	HEA	C3B-C4B-NB	4.54	115.06	109.84
25	R	603	HEA	C3C-C2C-C1C	-4.52	101.85	107.17
20	H	605	HEM	CHC-C4B-NB	4.51	129.28	124.42
15	O	304	HEC	CBC-CAC-C3C	-4.39	118.66	127.43
17	W	201	9YF	C7-C2-C3	-4.37	104.79	110.86
20	N	601	HEM	C1B-NB-C4B	4.34	110.35	105.21
20	N	601	HEM	CAD-CBD-CGD	-4.33	102.19	113.67
28	Y	302	9XX	O1-C18-C19	4.30	120.78	111.48
17	G	502	9YF	C7-C2-C3	-4.22	105.00	110.86
17	W	201	9YF	O1-P-O8	4.17	131.86	112.44
17	M	502	9YF	O1-P-O8	4.17	131.82	112.44
17	G	502	9YF	O1-P-O8	4.15	131.76	112.44
28	c	302	9XX	O1-C18-C19	4.15	120.46	111.48
28	R	609	9XX	O1-C18-C19	4.14	120.43	111.48
17	M	502	9YF	C7-C2-C3	-4.11	105.15	110.86
20	H	602	HEM	CBA-CAA-C2A	-4.10	101.19	112.53
20	H	605	HEM	CAD-CBD-CGD	-4.10	102.78	113.67
22	N	604	A1IGA	S01-C05-N01	4.05	130.33	120.37
22	N	604	A1IGA	O01-C14-C02	4.04	120.13	115.37
25	R	603	HEA	C1B-C2B-C3B	-4.01	102.15	106.80
14	O	302	WUO	O58-C59-C61	3.99	120.11	111.48
19	G	503	IZL	O34-C60-C61	3.95	120.04	111.48
19	M	504	IZL	O34-C60-C61	3.95	120.02	111.48
14	P	302	WUO	O58-C59-C61	3.95	120.02	111.48
25	R	602	HEA	C2C-C1C-NC	3.94	116.46	110.14
25	R	603	HEA	C12-C11-C3B	-3.93	105.97	112.12
25	R	602	HEA	C2A-C1A-NA	3.87	114.06	110.32
20	H	605	HEM	CHD-C1D-ND	3.85	128.57	124.42
14	P	302	WUO	O04-C05-C12	3.85	114.33	106.69
14	O	302	WUO	O04-C05-C12	3.83	114.29	106.69
20	N	601	HEM	CHD-C4C-NC	3.79	128.58	124.45
20	N	605	HEM	CHC-C4B-NB	3.78	128.49	124.42
25	R	603	HEA	CBA-CAA-C2A	-3.77	102.11	112.53
20	H	602	HEM	CHC-C4B-NB	3.71	128.41	124.42
18	G	505	7PH	O21-C21-C22	3.68	119.44	111.48
25	R	603	HEA	C2A-C1A-NA	3.67	113.86	110.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	H	605	HEM	CAA-C2A-C1A	3.66	132.09	124.94
25	R	602	HEA	CMB-C2B-C1B	3.64	130.72	125.03
18	G	504	7PH	O21-C21-C22	3.63	119.34	111.48
20	N	605	HEM	CHD-C1D-C2D	-3.63	119.30	125.03
14	P	302	WUO	C03-O04-C05	3.60	120.75	113.72
20	N	601	HEM	C3B-C4B-NB	-3.55	106.92	109.47
14	O	302	WUO	C03-O04-C05	3.55	120.64	113.72
25	R	602	HEA	C3A-C2A-C1A	-3.54	103.70	107.05
20	H	605	HEM	C1B-NB-C4B	3.51	109.36	105.21
25	R	602	HEA	C1B-C2B-C3B	-3.50	102.74	106.80
19	G	503	IZL	O11-C25-C30	3.50	114.93	108.31
19	M	504	IZL	O11-C25-C30	3.48	114.90	108.31
22	N	604	A1IGA	C02-C03-N03	-3.43	120.57	123.92
25	R	603	HEA	CMD-C2D-C1D	3.40	130.35	125.03
25	R	602	HEA	CBA-CAA-C2A	-3.40	103.14	112.53
19	M	504	IZL	C21-O9-C22	3.40	121.08	113.80
19	G	503	IZL	C21-O9-C22	3.38	121.04	113.80
22	N	604	A1IGA	C07-C06-C11	-3.34	118.43	122.10
20	H	605	HEM	O2A-CGA-CBA	3.32	124.48	114.00
14	O	302	WUO	O54-P52-O53	3.31	127.84	112.44
14	P	302	WUO	O54-P52-O53	3.31	127.84	112.44
15	O	303	HEC	O1D-CGD-CBD	-3.26	112.74	123.09
20	H	602	HEM	CAD-CBD-CGD	-3.22	105.12	113.67
14	O	302	WUO	O55-P52-O53	-3.21	96.20	108.94
14	P	302	WUO	C08-C07-C06	-3.21	105.20	110.83
14	P	302	WUO	O55-P52-O53	-3.20	96.27	108.94
15	O	303	HEC	CBC-CAC-C3C	-3.19	121.06	127.43
20	N	605	HEM	CAD-C3D-C4D	3.17	130.22	124.70
14	O	302	WUO	C08-C07-C06	-3.15	105.30	110.83
25	R	602	HEA	CMC-C2C-C1C	3.14	130.20	125.42
20	N	605	HEM	C1B-NB-C4B	3.13	108.92	105.21
20	N	601	HEM	O2A-CGA-CBA	3.12	123.86	114.00
14	O	302	WUO	C33-C31-C01	3.11	116.73	109.68
14	P	302	WUO	C33-C31-C01	3.10	116.71	109.68
25	R	603	HEA	C4D-C3D-C2D	-3.10	102.38	106.89
20	H	605	HEM	CBD-CAD-C3D	-3.09	103.99	112.53
20	N	601	HEM	CHD-C1D-ND	3.07	127.73	124.42
25	R	603	HEA	C27-C19-C20	3.07	120.56	115.23
20	N	605	HEM	CAD-C3D-C2D	-3.07	122.12	127.87
20	H	605	HEM	C1A-CHA-C4D	-3.06	119.06	126.25
19	G	503	IZL	O28-P-O29	-3.03	100.13	109.81
25	R	602	HEA	C13-C12-C11	-3.01	109.58	114.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	N	605	HEM	O2A-CGA-O1A	-3.01	115.59	123.33
19	M	504	IZL	O28-P-O29	-3.01	100.19	109.81
20	H	605	HEM	C3B-C4B-NB	-3.01	107.31	109.47
25	R	602	HEA	C4B-C3B-C2B	-3.01	102.39	107.44
20	H	602	HEM	CHB-C1B-NB	3.00	128.08	124.37
25	R	602	HEA	C27-C19-C20	2.99	120.42	115.23
25	R	603	HEA	CHA-C4D-C3D	-2.99	120.42	124.77
19	M	504	IZL	O11-C24-C23	2.98	116.14	109.42
19	G	503	IZL	O11-C24-C23	2.97	116.11	109.42
25	R	602	HEA	C13-C14-C15	-2.96	120.85	127.62
22	N	604	A1IGA	C11-C06-N01	2.93	109.23	105.71
25	R	603	HEA	OMA-CMA-C3A	-2.92	119.02	125.62
20	H	605	HEM	CAA-C2A-C3A	-2.89	120.60	127.07
25	R	603	HEA	C4A-NA-C1A	-2.88	101.12	105.82
22	N	604	A1IGA	C14-C02-C03	2.88	118.63	116.51
25	R	603	HEA	C3A-C2A-C1A	-2.87	104.33	107.05
22	N	604	A1IGA	S01-C05-N02	-2.86	118.92	125.95
19	G	503	IZL	O1-C11-C12	2.86	114.45	108.41
19	M	504	IZL	O1-C11-C12	2.86	114.44	108.41
20	H	605	HEM	CHB-C1B-NB	2.85	127.89	124.37
25	R	603	HEA	C12-C13-C14	-2.85	104.68	112.16
25	R	602	HEA	C4D-C3D-C2D	-2.84	102.76	106.89
25	R	603	HEA	C17-C18-C19	-2.80	121.22	127.62
20	H	602	HEM	C3B-C4B-NB	-2.80	107.46	109.47
20	H	602	HEM	CHD-C1D-ND	2.79	127.42	124.42
22	N	604	A1IGA	C01-C02-C03	-2.78	120.31	122.70
25	R	602	HEA	C21-C20-C19	-2.78	103.98	113.19
25	R	603	HEA	C2D-C1D-ND	2.78	113.03	109.84
25	R	603	HEA	CMB-C2B-C1B	2.75	129.34	125.03
20	H	602	HEM	CHD-C4C-NC	2.75	127.44	124.45
20	H	602	HEM	CMB-C2B-C1B	2.72	129.29	125.03
20	H	605	HEM	CHD-C1D-C2D	-2.72	120.73	125.03
20	H	602	HEM	C4C-C3C-C2C	2.70	109.16	106.81
25	R	602	HEA	CHA-C4D-C3D	-2.70	120.84	124.77
20	N	605	HEM	O2A-CGA-CBA	2.70	122.52	114.00
20	N	601	HEM	CHB-C1B-NB	2.69	127.69	124.37
25	R	603	HEA	C1D-C2D-C3D	-2.68	104.16	106.98
15	O	303	HEC	CBA-CAA-C2A	-2.68	105.11	112.53
18	G	504	7PH	O31-C31-C32	2.68	120.01	111.83
20	N	605	HEM	C3B-C4B-NB	-2.68	107.54	109.47
20	N	605	HEM	CHB-C1B-NB	2.67	127.67	124.37
25	R	603	HEA	C2C-C1C-NC	2.66	114.40	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	N	601	HEM	CHD-C1D-C2D	-2.63	120.87	125.03
25	R	603	HEA	C4B-C3B-C2B	-2.62	103.04	107.44
25	R	602	HEA	C4A-NA-C1A	-2.61	101.56	105.82
13	O	301	MQ9	C7-C6-C5	-2.61	120.42	124.89
13	H	606	MQ9	C7-C6-C5	-2.59	120.45	124.89
14	P	302	WUO	O04-C05-C06	2.58	114.35	109.70
25	R	603	HEA	CHA-C1A-NA	-2.57	121.65	124.45
19	G	503	IZL	O30-P-O29	2.55	124.30	112.44
19	M	504	IZL	O30-P-O29	2.55	124.30	112.44
14	O	302	WUO	O04-C05-C06	2.54	114.28	109.70
20	N	601	HEM	CBA-CAA-C2A	-2.54	105.51	112.53
20	N	605	HEM	C2A-C1A-NA	-2.53	107.34	110.15
19	G	503	IZL	O32-C47-C48	2.52	119.52	111.83
13	H	607	MQ9	C7-C6-C5	-2.52	120.58	124.89
19	M	504	IZL	O32-C47-C48	2.52	119.51	111.83
15	O	303	HEC	O1A-CGA-CBA	-2.52	115.11	123.09
19	M	504	IZL	C31-O17-C32	2.51	118.62	113.72
19	G	503	IZL	C31-O17-C32	2.51	118.61	113.72
22	N	604	A1IGA	C06-C11-N02	-2.50	106.00	109.42
18	G	505	7PH	O31-C31-C32	2.50	119.46	111.83
25	R	602	HEA	C26-C15-C16	2.50	119.57	115.23
19	G	503	IZL	O1-C10-C9	2.48	119.40	111.83
19	M	504	IZL	O1-C10-C9	2.47	119.37	111.83
15	O	304	HEC	O1D-CGD-CBD	-2.47	115.27	123.09
28	Y	302	9XX	O-C15-C14	2.46	119.34	111.83
25	R	603	HEA	CAD-C3D-C4D	2.45	128.97	124.70
14	P	302	WUO	O02-C01-C50	2.45	113.64	107.42
20	N	605	HEM	C4C-CHD-C1D	-2.44	120.83	126.02
14	O	302	WUO	O02-C01-C50	2.44	113.61	107.42
20	H	602	HEM	CHC-C1C-NC	2.43	127.10	124.45
20	N	601	HEM	CHA-C1A-NA	2.43	128.26	123.86
20	H	602	HEM	CBD-CAD-C3D	2.42	119.23	112.53
25	R	603	HEA	CHC-C4B-NB	-2.42	121.37	124.37
13	N	606	MQ9	C7-C6-C5	-2.42	120.74	124.89
25	R	603	HEA	CHB-C1B-NB	-2.42	121.82	124.42
14	P	302	WUO	O10-C07-C08	-2.42	104.67	110.38
28	R	609	9XX	O-C15-C14	2.42	119.20	111.83
28	c	302	9XX	O-C15-C14	2.41	119.19	111.83
20	H	602	HEM	CAC-C3C-C2C	-2.40	120.63	128.43
14	O	302	WUO	O10-C07-C08	-2.40	104.73	110.38
15	O	304	HEC	CBD-CAD-C3D	2.36	119.07	112.53
20	H	602	HEM	CHA-C4D-ND	2.34	127.27	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	H	602	HEM	C1B-NB-C4B	2.34	107.98	105.21
15	O	303	HEC	CAD-CBD-CGD	2.34	119.86	113.67
19	G	503	IZL	O1-C10-O	-2.33	117.80	123.63
19	M	504	IZL	O1-C10-O	-2.32	117.82	123.63
19	G	503	IZL	C24-O11-C25	2.32	118.76	113.80
14	O	302	WUO	O58-C59-O60	-2.31	118.30	123.70
20	N	605	HEM	CAD-CBD-CGD	-2.31	107.53	113.67
19	M	504	IZL	C24-O11-C25	2.31	118.74	113.80
14	P	302	WUO	O58-C59-O60	-2.30	118.33	123.70
15	O	303	HEC	CHC-C4B-NB	2.30	126.95	124.45
28	Y	302	9XX	O1-C18-O2	-2.29	118.35	123.70
17	M	502	9YF	O6-C6-C7	-2.28	105.00	110.38
20	H	602	HEM	O2A-CGA-O1A	-2.28	117.47	123.33
25	R	602	HEA	CHB-C1B-C2B	-2.28	121.43	125.03
20	H	602	HEM	C2A-C1A-NA	-2.27	107.64	110.15
20	H	602	HEM	CAC-C3C-C4C	2.26	130.21	124.82
20	N	601	HEM	O2A-CGA-O1A	-2.26	117.53	123.33
25	R	603	HEA	C1A-CHA-C4D	-2.25	121.23	126.02
25	R	603	HEA	CAA-C2A-C1A	2.24	129.40	124.85
25	R	603	HEA	O2D-CGD-CBD	2.23	121.06	114.00
25	R	603	HEA	C26-C15-C14	-2.23	117.90	123.63
28	c	302	9XX	O1-C18-O2	-2.23	118.50	123.70
20	N	601	HEM	O2D-CGD-O1D	-2.22	117.61	123.33
25	R	603	HEA	C4A-C3A-C2A	2.22	108.74	106.81
28	R	609	9XX	O1-C18-O2	-2.22	118.53	123.70
25	R	602	HEA	CHD-C1D-C2D	-2.21	120.65	126.95
13	O	305	MQ9	C7-C6-C5	-2.21	121.10	124.89
19	M	504	IZL	O25-C40-C20	-2.20	103.90	109.32
19	G	503	IZL	O25-C40-C20	-2.20	103.91	109.32
15	O	304	HEC	O1A-CGA-CBA	-2.18	116.18	123.09
25	R	603	HEA	O11-C11-C12	-2.18	103.36	109.14
25	R	603	HEA	CAD-CBD-CGD	-2.18	107.89	113.67
20	H	602	HEM	C4D-ND-C1D	2.18	107.78	105.21
22	N	604	A1IGA	N01-C05-N02	-2.17	110.75	113.25
19	M	504	IZL	O17-C32-C33	2.16	111.80	106.44
20	N	605	HEM	CHA-C4D-ND	2.16	127.04	124.37
20	H	605	HEM	C4D-ND-C1D	2.16	107.76	105.21
19	G	503	IZL	O17-C32-C33	2.15	111.78	106.44
19	G	503	IZL	O34-C60-O35	-2.14	118.69	123.70
20	H	605	HEM	C4C-CHD-C1D	-2.14	121.48	126.02
20	H	605	HEM	CMA-C3A-C4A	2.13	128.66	125.42
19	M	504	IZL	O34-C60-O35	-2.13	118.73	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	N	605	HEM	C4A-CHB-C1B	-2.12	121.26	126.25
19	G	503	IZL	O16-C31-O17	-2.12	105.12	110.69
19	G	503	IZL	O16-C31-C36	2.12	113.29	108.09
19	M	504	IZL	O16-C31-C36	2.11	113.29	108.09
20	H	605	HEM	O1A-CGA-CBA	-2.10	116.42	123.09
19	M	504	IZL	O16-C31-O17	-2.10	105.17	110.69
28	Y	302	9XX	O1-C17-C16	2.10	111.04	106.21
20	H	605	HEM	CHA-C4D-C3D	-2.10	121.36	125.23
14	O	302	WUO	O38-C39-O40	-2.09	105.20	110.69
22	N	604	A1IGA	C04-C03-N03	2.07	118.22	116.03
20	H	602	HEM	O2D-CGD-O1D	-2.07	118.00	123.33
14	P	302	WUO	O38-C39-O40	-2.07	105.24	110.69
20	H	605	HEM	CBC-CAC-C3C	-2.06	117.21	127.53
14	O	302	WUO	O40-C39-C44	2.05	114.58	110.37
19	G	503	IZL	O32-C46-C45	2.04	114.29	108.40
14	P	302	WUO	O40-C39-C44	2.04	114.57	110.37
25	R	603	HEA	C25-C23-C24	2.04	119.29	114.59
28	R	609	9XX	O1-C17-C16	2.04	110.90	106.21
25	R	603	HEA	CMC-C2C-C1C	2.04	128.53	125.42
20	H	605	HEM	C1D-C2D-C3D	-2.04	104.84	106.98
28	c	302	9XX	O1-C17-C16	2.03	110.89	106.21
17	W	201	9YF	O6-C6-C7	-2.03	105.58	110.38
19	M	504	IZL	O32-C46-C45	2.03	114.26	108.40
25	R	602	HEA	CHC-C1C-C2C	-2.03	121.53	127.43
25	R	602	HEA	C4B-NB-C1B	-2.03	102.80	105.21
25	R	602	HEA	O1A-CGA-CBA	-2.03	116.66	123.09
20	H	605	HEM	O2D-CGD-CBD	2.03	120.40	114.00
17	M	502	9YF	O2-P-O8	-2.03	103.33	109.81
20	H	602	HEM	CHB-C1B-C2B	-2.01	121.22	126.95
17	M	502	9YF	O11-C25-C26	2.01	117.96	111.83
25	R	602	HEA	CAD-CBD-CGD	-2.01	108.34	113.67

There are no chirality outliers.

All (934) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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

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Mol	Chain	Res	Type	Atoms
13	O	305	MQ9	C41-C42-C43-C44
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	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	C26-C27-C28-C29
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
15	O	303	HEC	C2C-C3C-CAC-CBC
15	O	303	HEC	C4C-C3C-CAC-CBC
15	O	304	HEC	C2B-C3B-CAB-CBB
15	O	304	HEC	C4B-C3B-CAB-CBB
15	O	304	HEC	C2C-C3C-CAC-CBC
15	O	304	HEC	C4C-C3C-CAC-CBC
17	M	502	9YF	C2-O2-P-O1
17	M	502	9YF	C2-O2-P-O
17	M	502	9YF	C1-O-P-O1
17	M	502	9YF	C1-O-P-O2
17	W	201	9YF	C2-O2-P-O
17	W	201	9YF	C1-O-P-O1
17	W	201	9YF	C1-O-P-O2
17	W	201	9YF	C1-O-P-O8

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Mol	Chain	Res	Type	Atoms
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	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	CA2-OA2-PA1-OA5
21	N	602	CDL	CA3-OA5-PA1-OA2
21	N	602	CDL	CA3-OA5-PA1-OA3
21	N	602	CDL	CB2-OB2-PB2-OB4
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
21	N	603	CDL	CB2-OB2-PB2-OB3
21	N	603	CDL	CB2-OB2-PB2-OB5
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

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Mol	Chain	Res	Type	Atoms
21	N	607	CDL	CA3-OA5-PA1-OA3
21	N	607	CDL	CA3-OA5-PA1-OA4
21	N	607	CDL	CB2-OB2-PB2-OB4
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-OA2
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	CA2-OA2-PA1-OA5
21	R	601	CDL	CB2-OB2-PB2-OB3
21	R	601	CDL	CB2-OB2-PB2-OB4
21	R	601	CDL	CB2-OB2-PB2-OB5
21	R	605	CDL	CA2-OA2-PA1-OA3
21	R	605	CDL	CA2-OA2-PA1-OA5
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	CB2-OB2-PB2-OB5
21	R	605	CDL	CB3-OB5-PB2-OB3
21	R	605	CDL	CB3-OB5-PB2-OB4
21	H	601	CDL	CA2-OA2-PA1-OA5
21	H	601	CDL	CA3-OA5-PA1-OA2
21	H	601	CDL	C11-CA5-OA6-CA4
21	H	601	CDL	CB2-OB2-PB2-OB3
21	H	601	CDL	CB2-OB2-PB2-OB4
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	CA3-OA5-PA1-OA2
21	H	603	CDL	CB2-OB2-PB2-OB5
21	H	603	CDL	CB3-OB5-PB2-OB2
21	H	603	CDL	CB3-OB5-PB2-OB4
21	H	604	CDL	CA2-C1-CB2-OB2
21	H	604	CDL	CA2-OA2-PA1-OA3

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Mol	Chain	Res	Type	Atoms
21	H	604	CDL	CA2-OA2-PA1-OA5
21	H	604	CDL	CB2-OB2-PB2-OB4
21	H	604	CDL	CB2-OB2-PB2-OB5
22	N	604	A1IGA	O01-C15-C16-F01
22	N	604	A1IGA	O01-C15-C16-F02
22	N	604	A1IGA	C03-C04-S01-C05
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	602	HEA	C2A-C3A-CMA-OMA
25	R	602	HEA	C4A-C3A-CMA-OMA
25	R	603	HEA	C11-C12-C13-C14
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	C19-C18-O1-C17
28	Y	302	9XX	O2-C18-O1-C17
30	W	202	PLM	O2-C1-C2-C3
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
13	N	606	MQ9	C47-C48-C49-C50
13	N	606	MQ9	C47-C48-C49-C51
21	N	603	CDL	C31-CA7-OA8-CA6
21	H	604	CDL	C31-CA7-OA8-CA6
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
18	G	504	7PH	C32-C31-O31-C3
22	N	604	A1IGA	O01-C15-C16-F03

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Mol	Chain	Res	Type	Atoms
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
13	O	301	MQ9	C20-C19-C21-C22
13	H	606	MQ9	C35-C34-C36-C37
13	H	607	MQ9	C30-C29-C31-C32
25	R	603	HEA	C26-C15-C16-C17
13	O	301	MQ9	C18-C19-C21-C22
25	R	602	HEA	C2D-C3D-CAD-CBD
14	P	302	WUO	C80-C78-O77-C76
21	N	607	CDL	C71-CB7-OB8-CB6
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
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
14	P	302	WUO	O40-C41-C48-O49
17	G	502	9YF	O12-C25-O11-C24
25	R	602	HEA	C4D-C3D-CAD-CBD
25	R	603	HEA	C4D-C3D-CAD-CBD
19	G	503	IZL	O35-C60-O34-C45
21	N	603	CDL	OA7-CA5-OA6-CA4
19	G	503	IZL	C36-C31-O16-C30
14	P	302	WUO	O04-C05-C12-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	O12-C26-C27-O13
19	G	503	IZL	O12-C26-C27-O13
19	M	504	IZL	C36-C31-O16-C30
14	P	302	WUO	C42-C41-C48-O49
21	N	603	CDL	C11-CA5-OA6-CA4
21	R	605	CDL	CB4-CB6-OB8-CB7
17	G	502	9YF	C26-C25-O11-C24

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Mol	Chain	Res	Type	Atoms
19	M	504	IZL	O17-C31-O16-C30
19	G	503	IZL	O17-C31-O16-C30
13	O	301	MQ9	C25-C24-C26-C27
13	O	301	MQ9	C23-C24-C26-C27
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	606	MQ9	C33-C34-C36-C37
19	M	504	IZL	O35-C60-O34-C45
13	O	305	MQ9	C14-C16-C17-C18
13	N	606	MQ9	C14-C16-C17-C18
13	H	606	MQ9	C24-C26-C27-C28
13	H	606	MQ9	C44-C46-C47-C48
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
19	M	504	IZL	O12-C25-O11-C24
19	G	503	IZL	O12-C25-O11-C24
19	M	504	IZL	O17-C32-C33-O18
19	G	503	IZL	O17-C32-C33-O18
13	O	305	MQ9	C47-C48-C49-C50
21	R	605	CDL	C51-C52-C53-C54
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
19	M	504	IZL	C37-C23-C24-O11
19	G	503	IZL	C37-C23-C24-O11
21	R	605	CDL	C71-C72-C73-C74
19	M	504	IZL	C34-C32-C33-O18
19	G	503	IZL	C34-C32-C33-O18
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	H	607	MQ9	C28-C29-C31-C32
13	H	607	MQ9	C43-C44-C46-C47
25	R	603	HEA	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
25	R	603	HEA	C18-C19-C20-C21
19	M	504	IZL	C54-C55-C56-C57
19	G	503	IZL	C54-C55-C56-C57
21	N	603	CDL	O1-C1-CB2-OB2
25	R	603	HEA	C2D-C3D-CAD-CBD
14	P	302	WUO	O55-C56-C57-O58
14	O	302	WUO	C80-C81-C82-C83
21	N	607	CDL	CA7-C31-C32-C33
21	H	604	CDL	C57-C58-C59-C60
21	P	301	CDL	CB5-C51-C52-C53
21	R	601	CDL	CA7-C31-C32-C33
13	N	606	MQ9	C24-C26-C27-C28
13	H	607	MQ9	C9-C11-C12-C13
21	P	301	CDL	C51-C52-C53-C54
28	R	609	9XX	C11-C12-C13-C14
14	O	302	WUO	C59-C61-C62-C63
17	M	502	9YF	C25-C26-C27-C28
21	N	607	CDL	CA5-C11-C12-C13
14	P	302	WUO	O15-C14-O13-C12
28	c	302	9XX	O6-C15-O-C16
20	N	605	HEM	C3D-CAD-CBD-CGD
17	W	201	9YF	C25-C26-C27-C28
17	G	502	9YF	C25-C26-C27-C28
21	P	301	CDL	CA5-C11-C12-C13
21	R	601	CDL	CB7-C71-C72-C73
28	c	302	9XX	C12-C13-C14-C15
14	O	302	WUO	O79-C78-O77-C76
21	R	601	CDL	OA9-CA7-OA8-CA6
20	H	605	HEM	C3A-C2A-CAA-CBA
21	N	602	CDL	O1-C1-CB2-OB2
21	R	601	CDL	O1-C1-CA2-OA2
21	H	604	CDL	O1-C1-CB2-OB2
21	H	604	CDL	C71-CB7-OB8-CB6
21	N	603	CDL	CB5-C51-C52-C53
21	R	601	CDL	CA5-C11-C12-C13
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
14	P	302	WUO	C27-C28-C29-C30
14	P	302	WUO	C59-C61-C62-C63
14	P	302	WUO	C78-C80-C81-C82

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Mol	Chain	Res	Type	Atoms
21	N	607	CDL	C11-CA5-OA6-CA4
21	N	607	CDL	C51-CB5-OB6-CB4
21	N	607	CDL	C34-C35-C36-C37
21	N	607	CDL	OB7-CB5-OB6-CB4
21	P	301	CDL	CB2-C1-CA2-OA2
21	R	601	CDL	CB2-C1-CA2-OA2
21	H	603	CDL	CB2-C1-CA2-OA2
17	G	502	9YF	C33-C35-C36-C37
13	H	607	MQ9	C47-C48-C49-C51
14	O	302	WUO	C88-C90-C91-C92
17	M	502	9YF	C33-C35-C36-C37
17	W	201	9YF	C30-C31-C32-C33
21	N	603	CDL	C77-C78-C79-C80
21	H	603	CDL	C58-C59-C60-C61
21	R	601	CDL	CB5-C51-C52-C53
14	O	302	WUO	C61-C59-O58-C57
24	S	503	3PE	C22-C21-O21-C2
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	C88-C90-C91-C92
13	O	301	MQ9	C14-C16-C17-C18
21	H	601	CDL	O1-C1-CA2-OA2
21	H	603	CDL	O1-C1-CA2-OA2
20	N	601	HEM	C3D-CAD-CBD-CGD
21	R	601	CDL	C51-CB5-OB6-CB4
21	H	604	CDL	C51-CB5-OB6-CB4
21	H	604	CDL	CB5-C51-C52-C53
17	M	502	9YF	C38-C39-C40-C41
17	W	201	9YF	C38-C39-C40-C41
17	G	502	9YF	C38-C39-C40-C41
21	R	605	CDL	C15-C16-C17-C18
21	R	605	CDL	C56-C57-C58-C59
17	W	201	9YF	C13-C14-C15-C16
18	G	505	7PH	C24-C25-C26-C27
21	N	602	CDL	C53-C54-C55-C56
21	R	605	CDL	C72-C73-C74-C75
21	H	601	CDL	C79-C80-C81-C82
17	M	502	9YF	C11-C12-C13-C14
17	G	502	9YF	C11-C12-C13-C14
17	G	502	9YF	C29-C30-C31-C32
21	H	604	CDL	OB9-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
14	O	302	WUO	C24-C25-C26-C27
18	S	501	7PH	C29-C2A-C2B-C2C
21	N	607	CDL	C78-C79-C80-C81
21	P	301	CDL	C11-C12-C13-C14
21	R	605	CDL	C32-C33-C34-C35
21	H	603	CDL	C16-C17-C18-C19
14	P	302	WUO	C24-C25-C26-C27
17	W	201	9YF	C16-C17-C18-C19
21	N	607	CDL	C71-C72-C73-C74
18	M	503	7PH	C21-C22-C23-C24
21	N	602	CDL	CA7-C31-C32-C33
14	O	302	WUO	C22-C23-C24-C25
21	N	607	CDL	C54-C55-C56-C57
23	Q	403	TRD	C2-C3-C4-C5
14	O	302	WUO	C64-C65-C66-C67
21	N	603	CDL	C51-C52-C53-C54
21	H	604	CDL	C51-C52-C53-C54
14	P	302	WUO	C82-C83-C84-C85
24	S	503	3PE	C23-C24-C25-C26
17	M	502	9YF	C31-C32-C33-C35
17	G	502	9YF	C31-C32-C33-C35
17	M	502	9YF	C29-C30-C31-C32
23	R	607	TRD	C7-C8-C9-C10
17	W	201	9YF	C10-C11-C12-C13
21	N	603	CDL	C57-C58-C59-C60
21	N	607	CDL	C13-C14-C15-C16
21	N	607	CDL	C57-C58-C59-C60
17	W	201	9YF	C29-C30-C31-C32
21	N	602	CDL	C17-C18-C19-C20
21	R	605	CDL	C59-C60-C61-C62
21	N	603	CDL	C73-C74-C75-C76
21	H	604	CDL	OB7-CB5-OB6-CB4
19	M	504	IZL	C2-C1-C7-C8
19	G	503	IZL	C2-C1-C7-C8
21	N	603	CDL	C76-C77-C78-C79
21	H	601	CDL	CB2-C1-CA2-OA2
13	O	301	MQ9	C29-C31-C32-C33
21	N	607	CDL	C76-C77-C78-C79
21	R	605	CDL	C17-C18-C19-C20
21	H	604	CDL	CB7-C71-C72-C73
17	M	502	9YF	C13-C14-C15-C16
19	M	504	IZL	C51-C52-C53-C54

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Mol	Chain	Res	Type	Atoms
19	G	503	IZL	C51-C52-C53-C54
21	N	607	CDL	C12-C13-C14-C15
21	N	607	CDL	C74-C75-C76-C77
21	N	607	CDL	C81-C82-C83-C84
21	R	605	CDL	C57-C58-C59-C60
21	H	601	CDL	C74-C75-C76-C77
17	M	502	9YF	C18-C19-C20-C21
21	H	601	CDL	C15-C16-C17-C18
28	R	609	9XX	C6-C7-C8-C9
14	P	302	WUO	C83-C84-C85-C86
17	M	502	9YF	C19-C20-C21-C22
17	W	201	9YF	C39-C40-C41-C42
17	G	502	9YF	C18-C19-C20-C21
18	M	503	7PH	C22-C23-C24-C25
21	H	604	CDL	C71-C72-C73-C74
14	O	302	WUO	C26-C27-C28-C29
21	P	301	CDL	C12-C13-C14-C15
21	H	604	CDL	C32-C33-C34-C35
28	R	609	9XX	C3-C4-C5-C6
18	G	505	7PH	C21-C22-C23-C24
13	O	305	MQ9	C47-C48-C49-C51
28	R	609	9XX	C10-C11-C12-C13
17	G	502	9YF	C13-C14-C15-C16
17	G	502	9YF	C19-C20-C21-C22
21	P	301	CDL	C36-C37-C38-C39
14	P	302	WUO	C64-C65-C66-C67
21	N	602	CDL	C36-C37-C38-C39
21	R	601	CDL	C73-C74-C75-C76
21	H	601	CDL	C76-C77-C78-C79
21	N	602	CDL	C34-C35-C36-C37
21	R	601	CDL	C59-C60-C61-C62
21	H	603	CDL	C74-C75-C76-C77
21	R	601	CDL	OB7-CB5-OB6-CB4
18	M	503	7PH	C25-C26-C27-C28
13	H	607	MQ9	C47-C48-C49-C50
23	R	608	TRD	C5-C6-C7-C8
24	S	503	3PE	C32-C31-O31-C3
14	O	302	WUO	C92-C93-C94-C95
21	H	601	CDL	C59-C60-C61-C62
21	N	602	CDL	C59-C60-C61-C62
21	N	607	CDL	C73-C74-C75-C76
14	O	302	WUO	C81-C82-C83-C84

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Mol	Chain	Res	Type	Atoms
21	H	603	CDL	C55-C56-C57-C58
21	R	605	CDL	CB5-C51-C52-C53
21	N	607	CDL	C32-C33-C34-C35
21	H	604	CDL	C59-C60-C61-C62
14	P	302	WUO	C61-C59-O58-C57
21	H	604	CDL	C11-CA5-OA6-CA4
28	c	302	9XX	C19-C18-O1-C17
21	R	605	CDL	CA7-C31-C32-C33
14	P	302	WUO	O60-C59-O58-C57
17	W	201	9YF	C35-C36-C37-C38
21	R	601	CDL	C57-C58-C59-C60
28	R	609	9XX	C31-C32-C33-C34
14	O	302	WUO	C16-C17-C18-C19
14	P	302	WUO	C25-C26-C27-C28
21	N	603	CDL	C74-C75-C76-C77
13	N	606	MQ9	C5-C6-C7-C8
21	R	605	CDL	C34-C35-C36-C37
13	H	606	MQ9	C40-C39-C41-C42
21	P	301	CDL	C58-C59-C60-C61
21	H	601	CDL	C57-C58-C59-C60
21	R	605	CDL	C37-C38-C39-C40
17	W	201	9YF	C27-C28-C29-C30
18	M	503	7PH	C24-C25-C26-C27
21	R	601	CDL	C74-C75-C76-C77
21	H	604	CDL	C74-C75-C76-C77
21	H	603	CDL	C14-C15-C16-C17
21	N	602	CDL	C54-C55-C56-C57
21	H	601	CDL	C78-C79-C80-C81
13	N	606	MQ9	C1-C6-C7-C8
21	H	604	CDL	CA7-C31-C32-C33
21	N	602	CDL	C52-C53-C54-C55
21	H	603	CDL	C73-C74-C75-C76
21	H	604	CDL	C38-C39-C40-C41
21	H	603	CDL	C13-C14-C15-C16
17	W	201	9YF	C28-C29-C30-C31
21	R	601	CDL	C14-C15-C16-C17
14	P	302	WUO	C91-C92-C93-C94
20	H	602	HEM	C3D-CAD-CBD-CGD
28	c	302	9XX	O2-C18-O1-C17
17	W	201	9YF	C37-C38-C39-C40
21	N	602	CDL	C71-C72-C73-C74
21	N	603	CDL	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
21	H	604	CDL	C55-C56-C57-C58
21	P	301	CDL	C33-C34-C35-C36
21	N	603	CDL	C22-C23-C24-C25
28	c	302	9XX	C22-C23-C24-C25
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
17	W	201	9YF	C9-C10-C11-C12
21	N	602	CDL	C51-C52-C53-C54
21	P	301	CDL	C56-C57-C58-C59
28	Y	302	9XX	C26-C27-C28-C29
21	R	601	CDL	C32-C33-C34-C35
24	S	503	3PE	O32-C31-O31-C3
21	H	601	CDL	C53-C54-C55-C56
28	R	609	9XX	C4-C5-C6-C7
21	H	601	CDL	C51-CB5-OB6-CB4
21	H	601	CDL	C77-C78-C79-C80
18	G	505	7PH	C23-C24-C25-C26
13	H	606	MQ9	C47-C48-C49-C51
17	W	201	9YF	C11-C12-C13-C14
14	P	302	WUO	C56-C57-C76-O77
18	M	503	7PH	C1-C2-C3-O31
21	H	603	CDL	CB3-CB4-CB6-OB8
21	H	604	CDL	C53-C54-C55-C56
18	S	501	7PH	C27-C28-C29-C2A
21	H	601	CDL	C16-C17-C18-C19
19	M	504	IZL	C62-C63-C64-C65
19	G	503	IZL	C62-C63-C64-C65
17	M	502	9YF	C30-C31-C32-C33
21	N	603	CDL	C71-C72-C73-C74
23	S	502	TRD	C7-C8-C9-C10
21	N	603	CDL	C78-C79-C80-C81
21	H	603	CDL	C76-C77-C78-C79
28	R	609	9XX	C1-C2-C3-C4
15	O	304	HEC	C3D-CAD-CBD-CGD
17	W	201	9YF	C19-C20-C21-C22
19	M	504	IZL	C1-C7-C8-C9
19	G	503	IZL	C1-C7-C8-C9
21	N	602	CDL	C16-C17-C18-C19
14	P	302	WUO	C90-C91-C92-C93

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Mol	Chain	Res	Type	Atoms
17	M	502	9YF	C37-C38-C39-C40
21	N	603	CDL	C20-C21-C22-C23
21	R	601	CDL	C51-C52-C53-C54
21	R	605	CDL	C33-C34-C35-C36
21	N	603	CDL	CA6-CA4-OA6-CA5
21	P	301	CDL	CA3-CA4-OA6-CA5
21	P	301	CDL	C52-C53-C54-C55
21	H	601	CDL	C71-C72-C73-C74
14	P	302	WUO	C61-C62-C63-C64
21	N	602	CDL	C72-C73-C74-C75
21	H	603	CDL	C51-C52-C53-C54
21	H	601	CDL	C54-C55-C56-C57
21	H	603	CDL	C53-C54-C55-C56
21	P	301	CDL	OB5-CB3-CB4-OB6
21	N	607	CDL	C51-C52-C53-C54
18	M	503	7PH	C27-C28-C29-C2A
13	N	606	MQ9	C12-C11-C9-C8
13	N	606	MQ9	C18-C19-C21-C22
21	N	602	CDL	C33-C34-C35-C36
21	N	603	CDL	C13-C14-C15-C16
21	N	607	CDL	C15-C16-C17-C18
21	P	301	CDL	C14-C15-C16-C17
17	G	502	9YF	C16-C17-C18-C19
21	P	301	CDL	C15-C16-C17-C18
21	P	301	CDL	C60-C61-C62-C63
28	c	302	9XX	C5-C6-C7-C8
19	M	504	IZL	C7-C8-C9-C10
21	N	602	CDL	C35-C36-C37-C38
17	M	502	9YF	O9-C-C24-O11
21	P	301	CDL	C18-C19-C20-C21
17	M	502	9YF	C16-C17-C18-C19
19	G	503	IZL	C4-C5-C6-C67
21	H	603	CDL	C59-C60-C61-C62
21	R	601	CDL	C71-C72-C73-C74
19	M	504	IZL	C4-C5-C6-C67
25	R	602	HEA	C3B-C11-C12-C13
19	G	503	IZL	C7-C8-C9-C10
21	N	603	CDL	C11-C12-C13-C14
21	N	607	CDL	C79-C80-C81-C82
21	R	601	CDL	C11-C12-C13-C14
18	G	505	7PH	C22-C23-C24-C25
19	G	503	IZL	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
19	M	504	IZL	C1-C2-C3-C4
24	S	503	3PE	C32-C33-C34-C35
14	O	302	WUO	C27-C28-C29-C30
17	G	502	9YF	C30-C31-C32-C33
13	N	606	MQ9	C12-C11-C9-C10
21	N	603	CDL	C79-C80-C81-C82
21	P	301	CDL	CB4-CB6-OB8-CB7
14	P	302	WUO	C62-C63-C64-C65
21	H	604	CDL	OA7-CA5-OA6-CA4
28	Y	302	9XX	C25-C26-C27-C36
28	Y	302	9XX	C36-C27-C28-C29
17	G	502	9YF	C26-C27-C28-C29
21	N	607	CDL	C16-C17-C18-C19
21	P	301	CDL	C37-C38-C39-C40
28	R	609	9XX	C22-C23-C24-C25
21	R	605	CDL	C60-C61-C62-C63
18	G	504	7PH	O11-C1-C2-C3
18	G	505	7PH	O11-C1-C2-C3
18	S	501	7PH	C22-C21-O21-C2
17	W	201	9YF	C40-C41-C42-C43
21	N	602	CDL	C76-C77-C78-C79
21	N	602	CDL	C39-C40-C41-C42
21	H	603	CDL	C19-C20-C21-C22
21	N	602	CDL	C57-C58-C59-C60
13	N	606	MQ9	C20-C19-C21-C22
28	c	302	9XX	O1-C18-C19-C20
28	Y	302	9XX	O-C16-C17-C37
28	c	302	9XX	O-C16-C17-C37
21	H	604	CDL	C76-C77-C78-C79
21	P	301	CDL	C38-C39-C40-C41
18	G	504	7PH	C22-C23-C24-C25
21	N	602	CDL	CB3-CB4-CB6-OB8
14	O	302	WUO	C83-C84-C85-C86
14	P	302	WUO	C19-C20-C21-C22
19	M	504	IZL	C66-C68-C69-C70
19	G	503	IZL	C66-C68-C69-C70
28	c	302	9XX	C11-C10-C9-C8
21	N	603	CDL	C55-C56-C57-C58
28	Y	302	9XX	O-C16-C17-O1
28	c	302	9XX	O-C16-C17-O1
17	G	502	9YF	C37-C38-C39-C40
17	W	201	9YF	O9-C-C1-O

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Mol	Chain	Res	Type	Atoms
18	G	504	7PH	O11-C1-C2-O21
21	H	601	CDL	OA5-CA3-CA4-OA6
21	H	604	CDL	C1-CA2-OA2-PA1
21	H	604	CDL	C39-C40-C41-C42
28	R	609	9XX	C19-C20-C21-C22
14	O	302	WUO	C84-C85-C86-C87
21	N	602	CDL	C73-C74-C75-C76
28	R	609	9XX	C21-C22-C23-C24
17	G	502	9YF	C20-C21-C22-C23
21	N	602	CDL	CB5-C51-C52-C53
17	M	502	9YF	C20-C21-C22-C23
18	M	503	7PH	C28-C29-C2A-C2B
21	N	607	CDL	C31-C32-C33-C34
21	P	301	CDL	C39-C40-C41-C42
28	c	302	9XX	C7-C8-C9-C10
13	N	606	MQ9	C44-C46-C47-C48
21	R	601	CDL	C13-C14-C15-C16
21	H	603	CDL	C57-C58-C59-C60
14	O	302	WUO	C65-C66-C67-C68
14	O	302	WUO	C94-C95-C96-C97
21	N	607	CDL	C12-C11-CA5-OA6
21	H	603	CDL	C18-C19-C20-C21
21	P	301	CDL	OB5-CB3-CB4-CB6
24	S	503	3PE	O11-C1-C2-C3
14	P	302	WUO	C86-C87-C88-C90
21	R	601	CDL	C12-C13-C14-C15
14	P	302	WUO	C66-C67-C68-C69
19	M	504	IZL	C23-C24-O11-C25
19	G	503	IZL	C23-C24-O11-C25
21	N	602	CDL	C60-C61-C62-C63
21	H	601	CDL	OB7-CB5-OB6-CB4
20	H	605	HEM	C2B-C3B-CAB-CBB
21	N	603	CDL	C56-C57-C58-C59
21	N	602	CDL	C71-CB7-OB8-CB6
18	S	501	7PH	O22-C21-O21-C2
21	R	601	CDL	OB5-CB3-CB4-OB6
21	H	603	CDL	OA5-CA3-CA4-OA6
21	P	301	CDL	C16-C17-C18-C19
17	W	201	9YF	C1-C-C24-O11
21	R	601	CDL	CB3-CB4-CB6-OB8
20	H	602	HEM	C4B-C3B-CAB-CBB
21	H	604	CDL	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
28	R	609	9XX	C9-C10-C11-C12
13	H	606	MQ9	C38-C39-C41-C42
21	N	603	CDL	C31-C32-C33-C34
21	N	607	CDL	C53-C54-C55-C56
21	P	301	CDL	C59-C60-C61-C62
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	H	604	CDL	C54-C55-C56-C57
21	R	605	CDL	C36-C37-C38-C39
18	S	501	7PH	C36-C37-C38-C39
18	G	505	7PH	C29-C2A-C2B-C2C
21	R	601	CDL	C16-C17-C18-C19
21	H	604	CDL	C15-C16-C17-C18
21	P	301	CDL	C53-C54-C55-C56
28	R	609	9XX	C24-C25-C26-C27
21	N	603	CDL	CA4-CA3-OA5-PA1
17	M	502	9YF	C2-O2-P-O8
17	W	201	9YF	C2-O2-P-O1
28	R	609	9XX	C23-C24-C25-C26
21	P	301	CDL	CA2-C1-CB2-OB2
14	O	302	WUO	C31-C01-O02-C03
21	H	601	CDL	C18-C19-C20-C21
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	OB9-CB7-OB8-CB6
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	N	602	CDL	C74-C75-C76-C77
21	N	607	CDL	C55-C56-C57-C58
21	N	603	CDL	C58-C59-C60-C61
21	R	601	CDL	C33-C34-C35-C36
28	Y	302	9XX	C19-C20-C21-C22
15	O	303	HEC	C4B-C3B-CAB-CBB
14	P	302	WUO	C93-C94-C95-C96
21	R	605	CDL	C75-C76-C77-C78
14	P	302	WUO	C50-C37-O38-C39
21	H	604	CDL	C60-C61-C62-C63
18	S	501	7PH	O11-C1-C2-O21

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Mol	Chain	Res	Type	Atoms
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
21	R	605	CDL	C11-CA5-OA6-CA4
21	N	603	CDL	C24-C25-C26-C27
25	R	603	HEA	C4A-C3A-CMA-OMA
21	R	605	CDL	C73-C74-C75-C76
21	R	605	CDL	OA7-CA5-OA6-CA4
14	P	302	WUO	O58-C57-C76-O77
17	G	502	9YF	O9-C-C24-O11
17	W	201	9YF	C15-C16-C17-C18
17	M	502	9YF	C1-C-C24-O11
25	R	603	HEA	O11-C11-C3B-C4B
21	H	603	CDL	C31-C32-C33-C34
13	H	606	MQ9	C47-C48-C49-C50
18	M	503	7PH	C23-C24-C25-C26
14	O	302	WUO	C56-O55-P52-O51
15	O	303	HEC	C2B-C3B-CAB-CBB
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-OB5
21	N	602	CDL	CB3-OB5-PB2-OB2
21	N	602	CDL	CB3-OB5-PB2-OB3
21	N	602	CDL	CB3-OB5-PB2-OB4
21	N	603	CDL	CA2-OA2-PA1-OA5
21	N	603	CDL	CB2-OB2-PB2-OB4
21	N	603	CDL	CB3-OB5-PB2-OB2
21	N	607	CDL	CA2-OA2-PA1-OA4
21	N	607	CDL	CA2-OA2-PA1-OA5
21	N	607	CDL	CB2-OB2-PB2-OB5
21	N	607	CDL	CB3-OB5-PB2-OB2
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	605	CDL	CA2-OA2-PA1-OA4
21	R	605	CDL	CB2-OB2-PB2-OB3
21	R	605	CDL	CB3-OB5-PB2-OB2
21	H	601	CDL	CA2-OA2-PA1-OA3

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Mol	Chain	Res	Type	Atoms
21	H	601	CDL	CB2-OB2-PB2-OB5
21	H	603	CDL	CA3-OA5-PA1-OA3
21	H	603	CDL	CB2-OB2-PB2-OB3
21	H	604	CDL	CA2-OA2-PA1-OA4
25	R	603	HEA	O11-C11-C3B-C2B
28	c	302	9XX	C16-C17-O1-C18
17	M	502	9YF	C26-C27-C28-C29
21	P	301	CDL	C72-C73-C74-C75
21	H	603	CDL	C32-C33-C34-C35
21	H	601	CDL	CB4-CB3-OB5-PB2
14	O	302	WUO	C50-C01-O02-C03
18	S	501	7PH	C33-C34-C35-C36
24	S	503	3PE	C25-C26-C27-C28
17	M	502	9YF	C11-C10-C9-C8
14	O	302	WUO	C93-C94-C95-C96
21	R	601	CDL	CB3-CB4-OB6-CB5
24	S	503	3PE	C3-C2-O21-C21
18	G	504	7PH	C37-C38-C39-C3A
14	O	302	WUO	C89-C88-C90-C91
28	R	609	9XX	C36-C27-C28-C29
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	H	603	CDL	C15-C16-C17-C18
21	R	601	CDL	C34-C35-C36-C37
21	N	602	CDL	CA5-C11-C12-C13
28	Y	302	9XX	C13-C14-C15-O
14	P	302	WUO	C17-C18-C19-C20
21	N	603	CDL	C1-CA2-OA2-PA1
13	H	606	MQ9	C46-C47-C48-C49
15	O	304	HEC	CAD-CBD-CGD-O2D
15	O	303	HEC	CAA-CBA-CGA-O2A
21	H	603	CDL	OA5-CA3-CA4-CA6
20	H	605	HEM	C4B-C3B-CAB-CBB
21	N	607	CDL	C14-C15-C16-C17
23	R	608	TRD	C6-C7-C8-C9
21	N	607	CDL	C36-C37-C38-C39
18	S	501	7PH	C34-C35-C36-C37
21	N	603	CDL	C71-CB7-OB8-CB6
21	H	603	CDL	C54-C55-C56-C57
13	O	301	MQ9	C15-C14-C16-C17
18	G	504	7PH	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
21	N	603	CDL	C16-C17-C18-C19
21	R	601	CDL	C55-C56-C57-C58
13	O	305	MQ9	C13-C14-C16-C17
22	N	604	A1IGA	C13-C14-O01-C15
13	O	305	MQ9	C25-C24-C26-C27
13	H	606	MQ9	C30-C29-C31-C32
25	R	602	HEA	CAA-CBA-CGA-O1A
13	O	305	MQ9	C34-C36-C37-C38
20	H	602	HEM	CAA-CBA-CGA-O1A
19	M	504	IZL	C46-C45-O34-C60
19	G	503	IZL	C46-C45-O34-C60
21	R	601	CDL	CB6-CB4-OB6-CB5
14	P	302	WUO	C23-C24-C25-C26
28	R	609	9XX	C30-C31-C32-C33
13	H	606	MQ9	C28-C29-C31-C32
21	N	603	CDL	OB9-CB7-OB8-CB6
15	O	304	HEC	CAD-CBD-CGD-O1D
20	N	605	HEM	CAA-CBA-CGA-O1A
20	H	602	HEM	CAA-CBA-CGA-O2A
28	c	302	9XX	C27-C28-C29-C30
25	R	603	HEA	CAD-CBD-CGD-O2D
25	R	602	HEA	O11-C11-C12-C13
13	O	305	MQ9	C15-C14-C16-C17
21	R	601	CDL	C53-C54-C55-C56
13	O	305	MQ9	C23-C24-C26-C27
21	R	601	CDL	C54-C55-C56-C57
18	G	505	7PH	C32-C33-C34-C35
22	N	604	A1IGA	N01-C05-S01-C04
20	N	601	HEM	C4D-C3D-CAD-CBD
25	R	602	HEA	CAA-CBA-CGA-O2A
25	R	603	HEA	CAD-CBD-CGD-O1D
21	H	604	CDL	O1-C1-CA2-OA2
13	O	301	MQ9	C45-C44-C46-C47
13	O	305	MQ9	C12-C11-C9-C10
13	H	607	MQ9	C25-C24-C26-C27
21	P	301	CDL	CB7-C71-C72-C73
21	H	604	CDL	C35-C36-C37-C38
21	N	602	CDL	C31-CA7-OA8-CA6
13	H	607	MQ9	C20-C19-C21-C22
20	N	605	HEM	CAA-CBA-CGA-O2A
18	S	501	7PH	O31-C31-C32-C33
14	P	302	WUO	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
21	R	601	CDL	C76-C77-C78-C79
21	N	602	CDL	OA9-CA7-OA8-CA6
20	H	605	HEM	CAD-CBD-CGD-O1D
28	c	302	9XX	O2-C18-C19-C20
21	R	605	CDL	C18-C19-C20-C21
21	R	601	CDL	C32-C31-CA7-OA8
21	R	605	CDL	C16-C17-C18-C19
19	G	503	IZL	C3-C4-C5-C6
20	H	605	HEM	CAD-CBD-CGD-O2D
19	M	504	IZL	C3-C4-C5-C6
19	M	504	IZL	C15-C14-O3-C13
21	P	301	CDL	C34-C35-C36-C37
21	N	603	CDL	OA6-CA4-CA6-OA8
21	P	301	CDL	OA6-CA4-CA6-OA8
15	O	303	HEC	CAA-CBA-CGA-O1A
21	H	604	CDL	C52-C53-C54-C55
13	O	305	MQ9	C12-C11-C9-C8
21	R	601	CDL	CB4-CB3-OB5-PB2
21	N	602	CDL	C55-C56-C57-C58
21	R	605	CDL	C31-C32-C33-C34
19	G	503	IZL	C15-C14-O3-C13
21	N	602	CDL	C32-C31-CA7-OA8
14	O	302	WUO	C91-C92-C93-C94
17	G	502	9YF	C35-C36-C37-C38
28	R	609	9XX	C25-C26-C27-C36
25	R	602	HEA	CAD-CBD-CGD-O2D
21	R	601	CDL	C18-C19-C20-C21
21	N	607	CDL	C35-C36-C37-C38
21	R	601	CDL	C52-C51-CB5-OB6
20	N	601	HEM	CAA-CBA-CGA-O2A
25	R	603	HEA	C2A-C3A-CMA-OMA
21	R	605	CDL	C12-C13-C14-C15
21	H	601	CDL	C12-C13-C14-C15
28	R	609	9XX	C2-C3-C4-C5
21	N	603	CDL	C1-CB2-OB2-PB2
22	N	604	A1IGA	C02-C14-O01-C15
21	N	602	CDL	OB5-CB3-CB4-OB6
21	R	601	CDL	C17-C18-C19-C20
13	O	305	MQ9	C24-C26-C27-C28
17	G	502	9YF	C1-C-C24-O11
17	W	201	9YF	C12-C13-C14-C15
20	N	605	HEM	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
21	R	601	CDL	C31-C32-C33-C34
15	O	304	HEC	CAA-CBA-CGA-O1A
17	W	201	9YF	O12-C25-O11-C24
13	N	606	MQ9	C25-C24-C26-C27
20	N	601	HEM	CAA-CBA-CGA-O1A
25	R	602	HEA	CAD-CBD-CGD-O1D
19	M	504	IZL	C43-C14-O3-C13
14	P	302	WUO	C71-C72-C73-C74
20	N	601	HEM	CAD-CBD-CGD-O2D
21	R	605	CDL	C76-C77-C78-C79
19	G	503	IZL	C43-C14-O3-C13
28	R	609	9XX	C7-C8-C9-C10
21	N	602	CDL	OB5-CB3-CB4-CB6
21	N	607	CDL	C12-C11-CA5-OA7
21	N	602	CDL	OB7-CB5-OB6-CB4
21	N	603	CDL	C15-C16-C17-C18
21	H	601	CDL	CA4-CA3-OA5-PA1
17	W	201	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
18	G	505	7PH	C28-C29-C2A-C2B
21	R	601	CDL	OB9-CB7-OB8-CB6
21	N	602	CDL	C51-CB5-OB6-CB4
18	G	504	7PH	O21-C21-C22-C23
19	M	504	IZL	O1-C10-C9-C8
19	G	503	IZL	O1-C10-C9-C8
14	P	302	WUO	C20-C21-C22-C23
18	G	505	7PH	O21-C21-C22-C23
21	N	602	CDL	C18-C19-C20-C21
13	O	301	MQ9	C13-C14-C16-C17
21	N	607	CDL	C83-C84-C85-C86
21	R	601	CDL	C71-CB7-OB8-CB6
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
14	P	302	WUO	C81-C82-C83-C84
13	H	606	MQ9	C25-C24-C26-C27
13	H	607	MQ9	C15-C14-C16-C17
25	R	602	HEA	C27-C19-C20-C21
17	W	201	9YF	O9-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
28	Y	302	9XX	O1-C18-C19-C20
21	H	603	CDL	C12-C13-C14-C15
14	P	302	WUO	C18-C19-C20-C21
24	S	503	3PE	C33-C34-C35-C36
17	G	502	9YF	C15-C16-C17-C18
17	W	201	9YF	C26-C25-O11-C24
17	M	502	9YF	C36-C37-C38-C39
15	O	304	HEC	CAA-CBA-CGA-O2A
19	G	503	IZL	C49-C50-C51-C52
19	M	504	IZL	C44-C45-O34-C60
19	G	503	IZL	C44-C45-O34-C60
21	N	602	CDL	C12-C13-C14-C15
18	M	503	7PH	C29-C2A-C2B-C2C
20	N	605	HEM	CAD-CBD-CGD-O1D
19	M	504	IZL	C49-C50-C51-C52
21	P	301	CDL	C74-C75-C76-C77
14	P	302	WUO	C31-C01-O02-C03
23	T	201	TRD	C5-C6-C7-C8
23	S	502	TRD	C1-C2-C3-C4
21	P	301	CDL	C12-C11-CA5-OA6
21	R	605	CDL	C55-C56-C57-C58
18	M	503	7PH	O21-C21-C22-C23
21	H	601	CDL	C32-C31-CA7-OA8
21	H	603	CDL	C32-C31-CA7-OA8
28	Y	302	9XX	O2-C18-C19-C20
18	M	503	7PH	C32-C33-C34-C35
14	P	302	WUO	O58-C59-C61-C62
15	O	303	HEC	CAD-CBD-CGD-O2D
28	c	302	9XX	C37-C17-O1-C18
20	N	601	HEM	C2D-C3D-CAD-CBD
21	R	601	CDL	C75-C76-C77-C78
19	G	503	IZL	O-C10-C9-C8
19	M	504	IZL	O-C10-C9-C8
20	N	601	HEM	CAD-CBD-CGD-O1D
20	N	605	HEM	CAD-CBD-CGD-O2D
20	N	605	HEM	C2B-C3B-CAB-CBB
18	G	505	7PH	O22-C21-C22-C23
21	N	602	CDL	C38-C39-C40-C41
21	H	604	CDL	C72-C71-CB7-OB8
21	N	607	CDL	O1-C1-CB2-OB2
17	G	502	9YF	C27-C28-C29-C30
25	R	603	HEA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
21	N	607	CDL	C32-C31-CA7-OA8
21	P	301	CDL	C52-C51-CB5-OB6
21	R	601	CDL	C72-C71-CB7-OB8
14	P	302	WUO	O60-C59-C61-C62

There are no ring outliers.

36 monomers are involved in 165 short contacts:

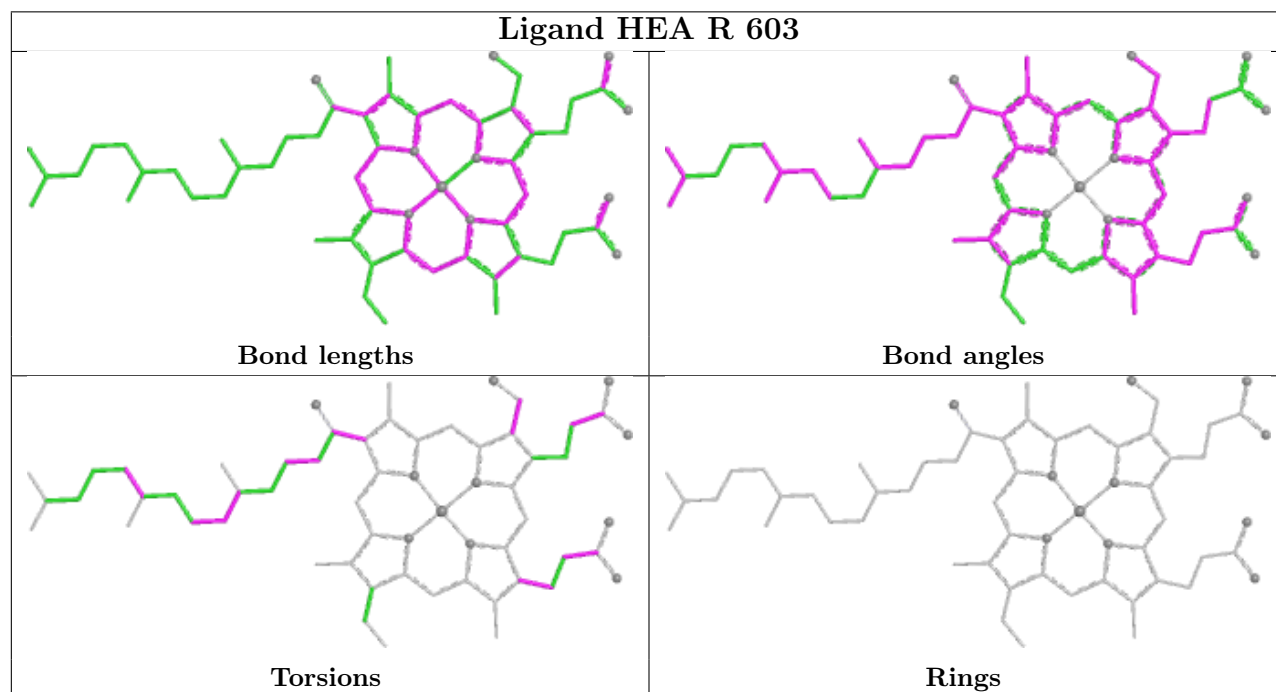
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	R	603	HEA	17	0
21	H	601	CDL	4	0
16	G	501	FES	1	0
20	H	602	HEM	9	0
14	O	302	WUO	3	0
28	R	609	9XX	1	0
18	S	501	7PH	1	0
18	M	503	7PH	1	0
15	O	304	HEC	1	0
18	G	504	7PH	1	0
14	P	302	WUO	3	0
20	N	605	HEM	7	0
30	W	202	PLM	1	0
13	O	301	MQ9	4	0
20	N	601	HEM	6	0
23	S	502	TRD	1	0
13	H	607	MQ9	3	0
18	G	505	7PH	1	0
13	N	606	MQ9	17	0
21	P	301	CDL	11	0
13	H	606	MQ9	9	0
21	H	604	CDL	8	0
30	c	301	PLM	2	0
17	W	201	9YF	1	0
21	H	603	CDL	4	0
21	N	602	CDL	5	0
20	H	605	HEM	8	0
25	R	602	HEA	3	0
21	R	605	CDL	9	0
13	O	305	MQ9	12	0
16	M	501	FES	1	0
15	O	303	HEC	5	0
28	c	302	9XX	6	0

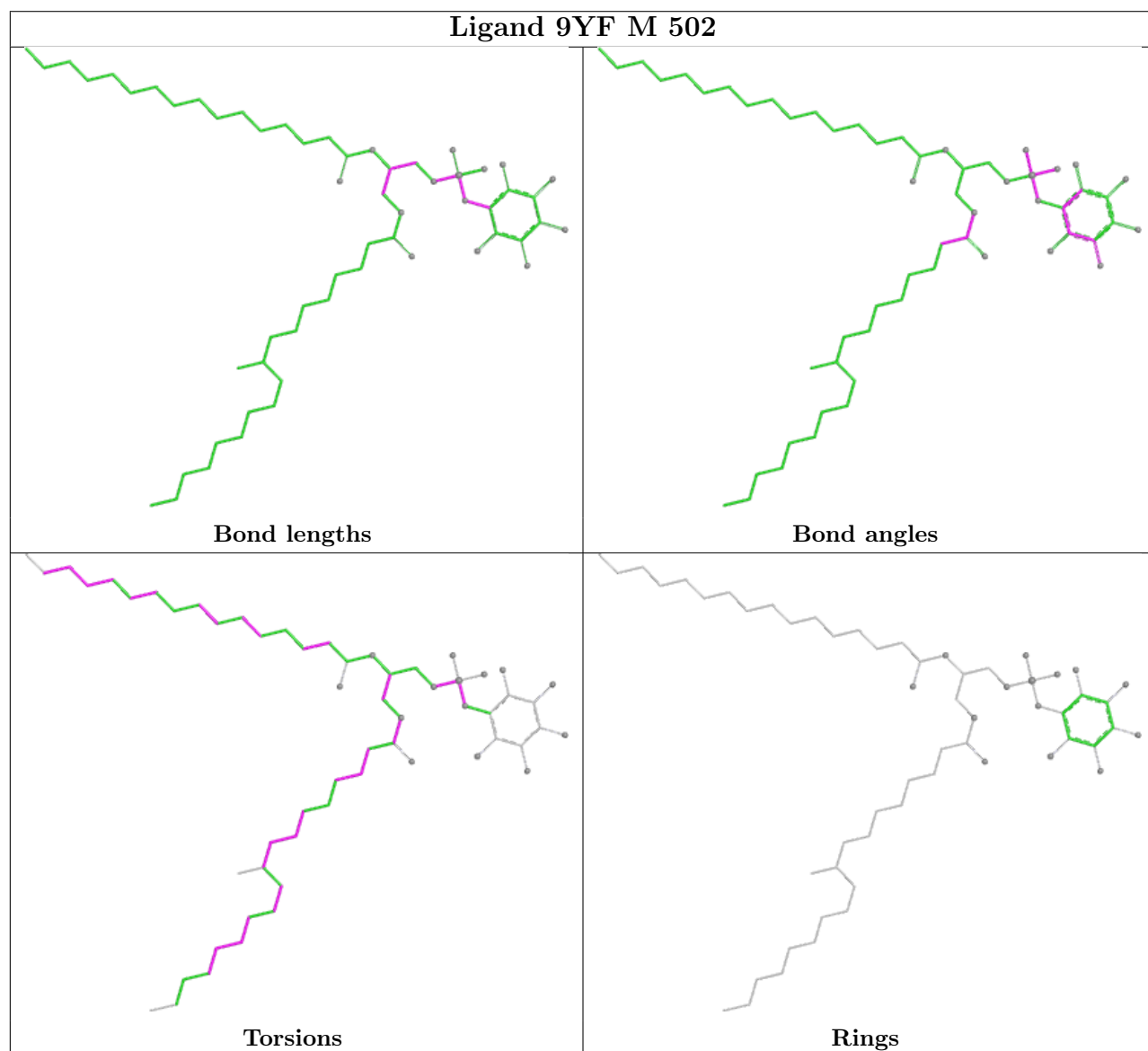
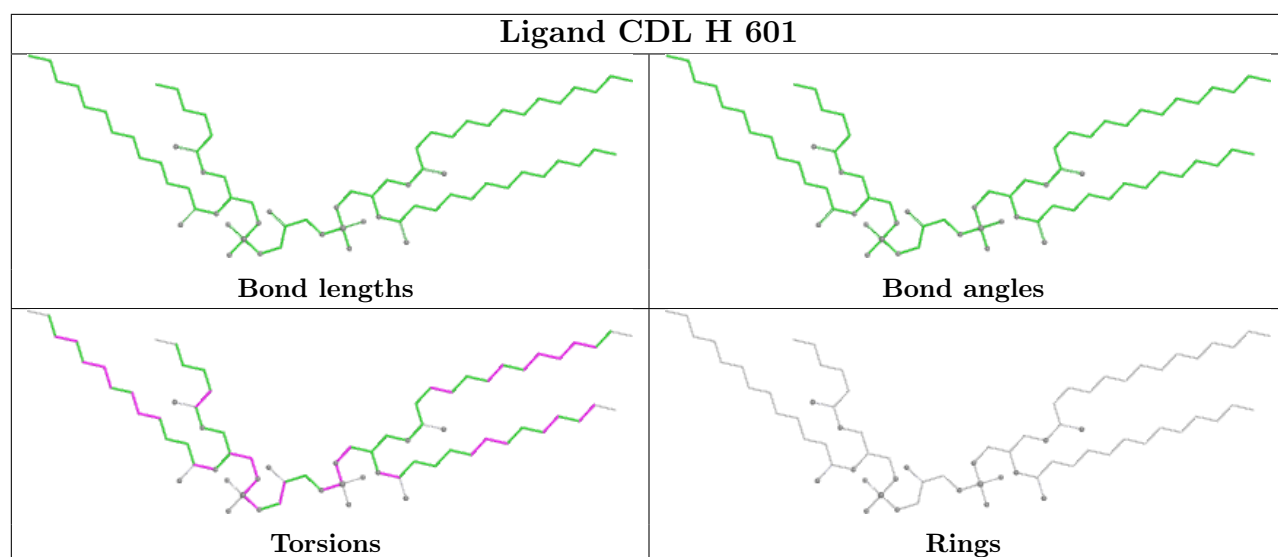
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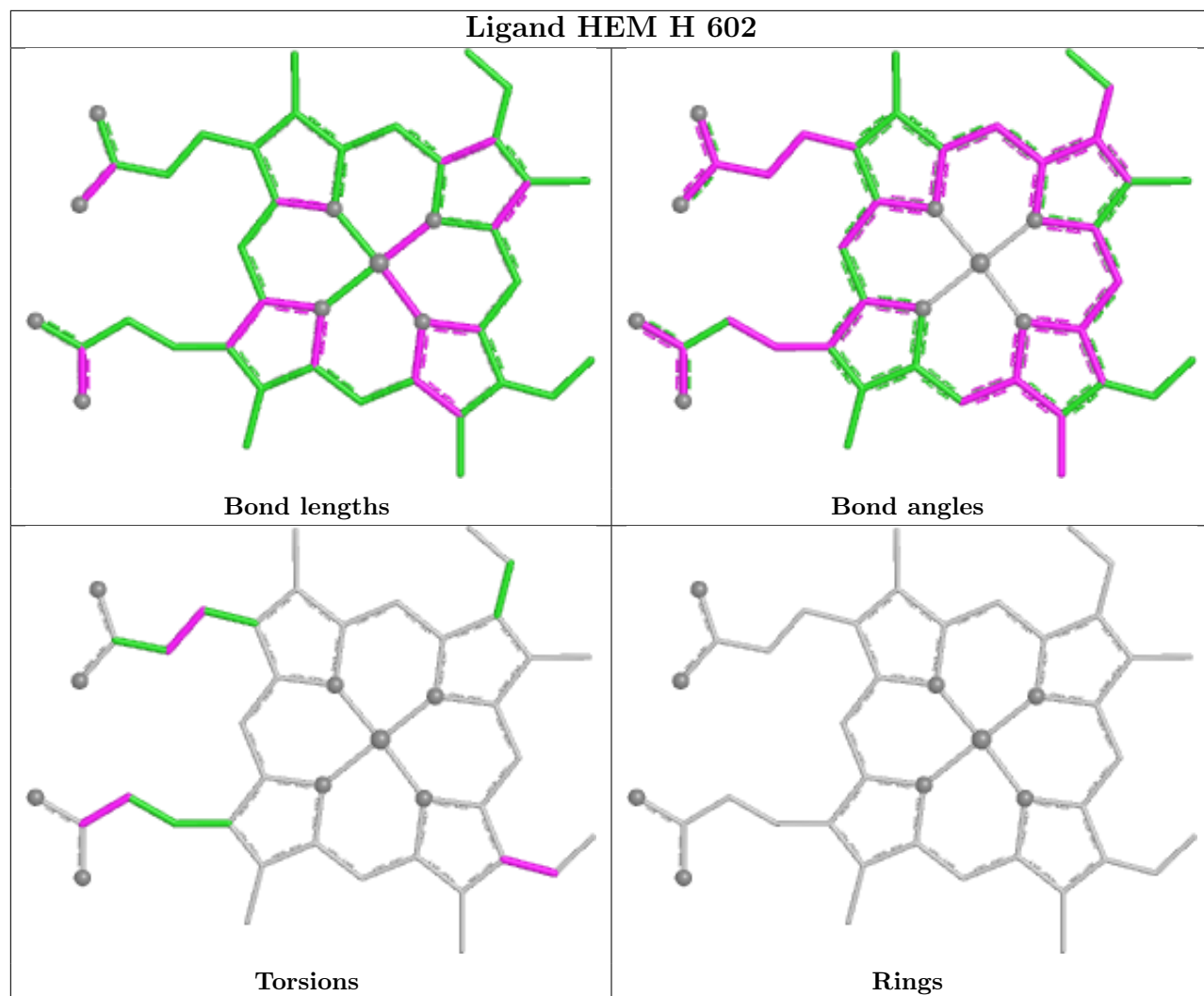
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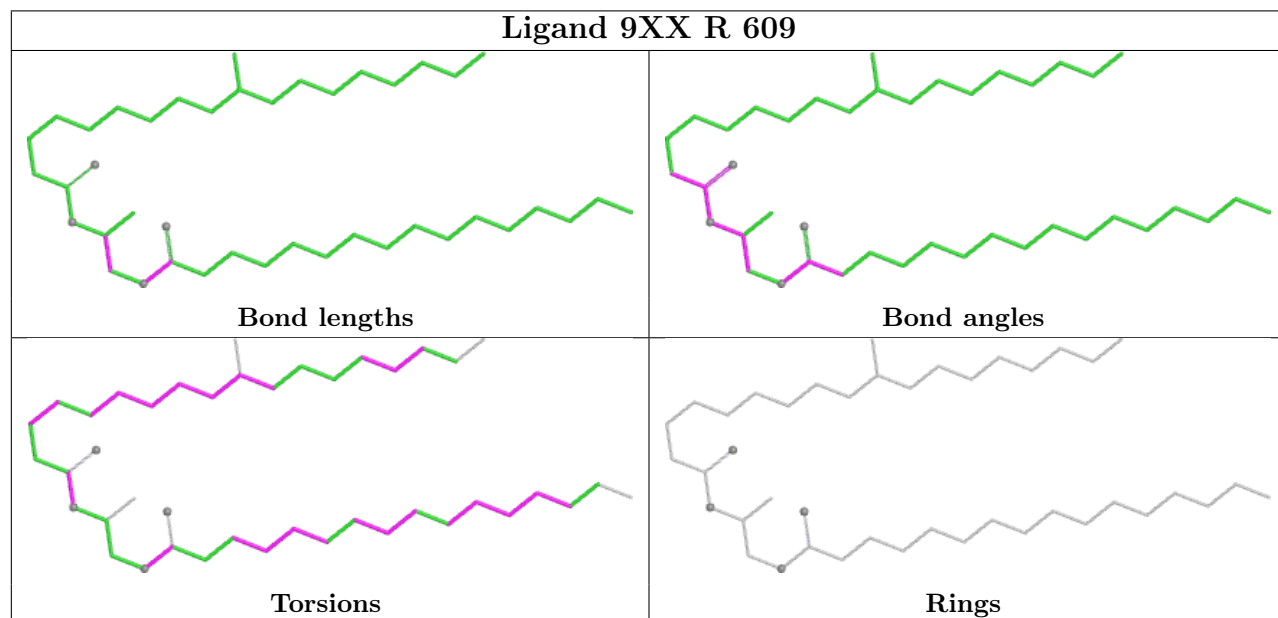
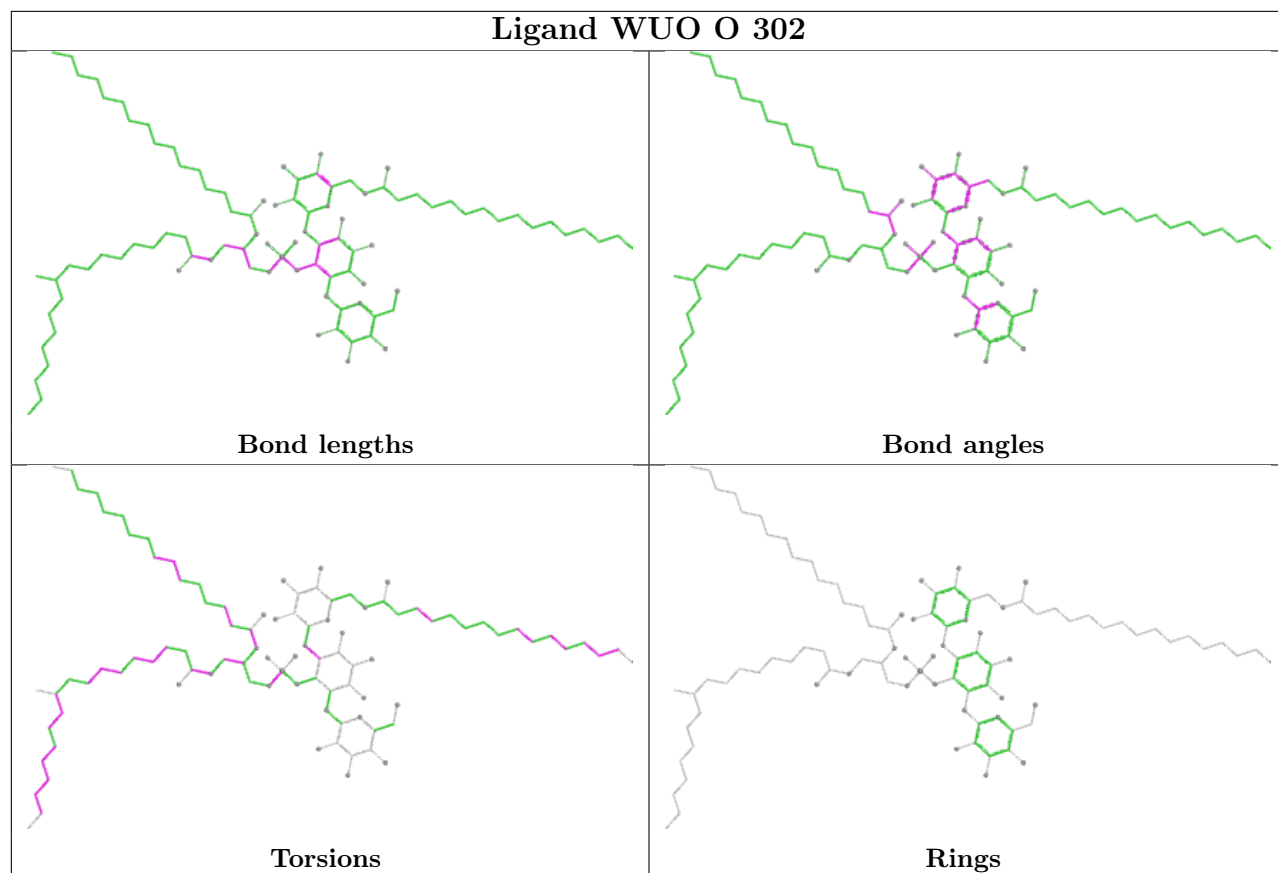
Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	R	601	CDL	3	0
21	N	607	CDL	2	0
21	N	603	CDL	1	0

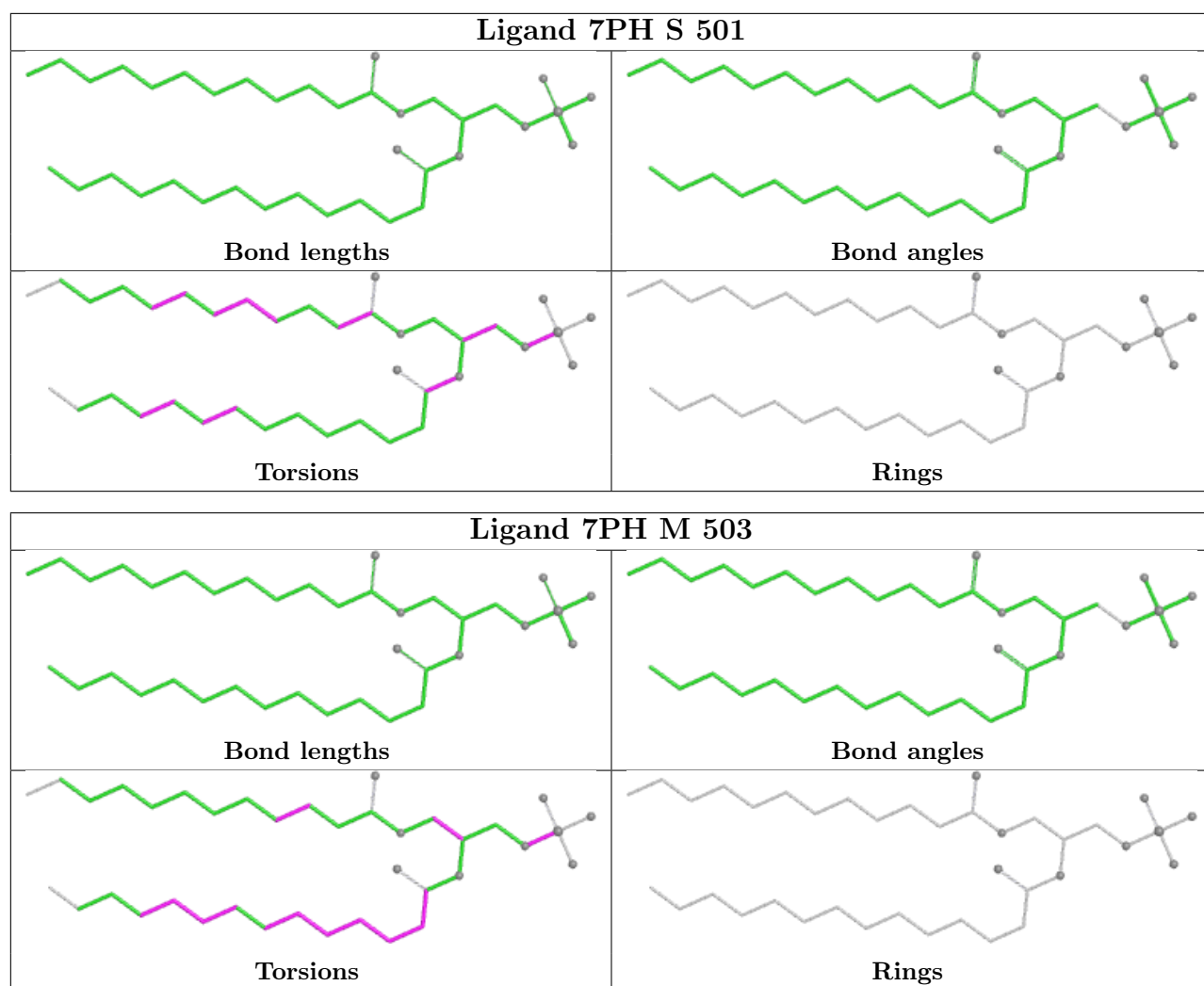
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

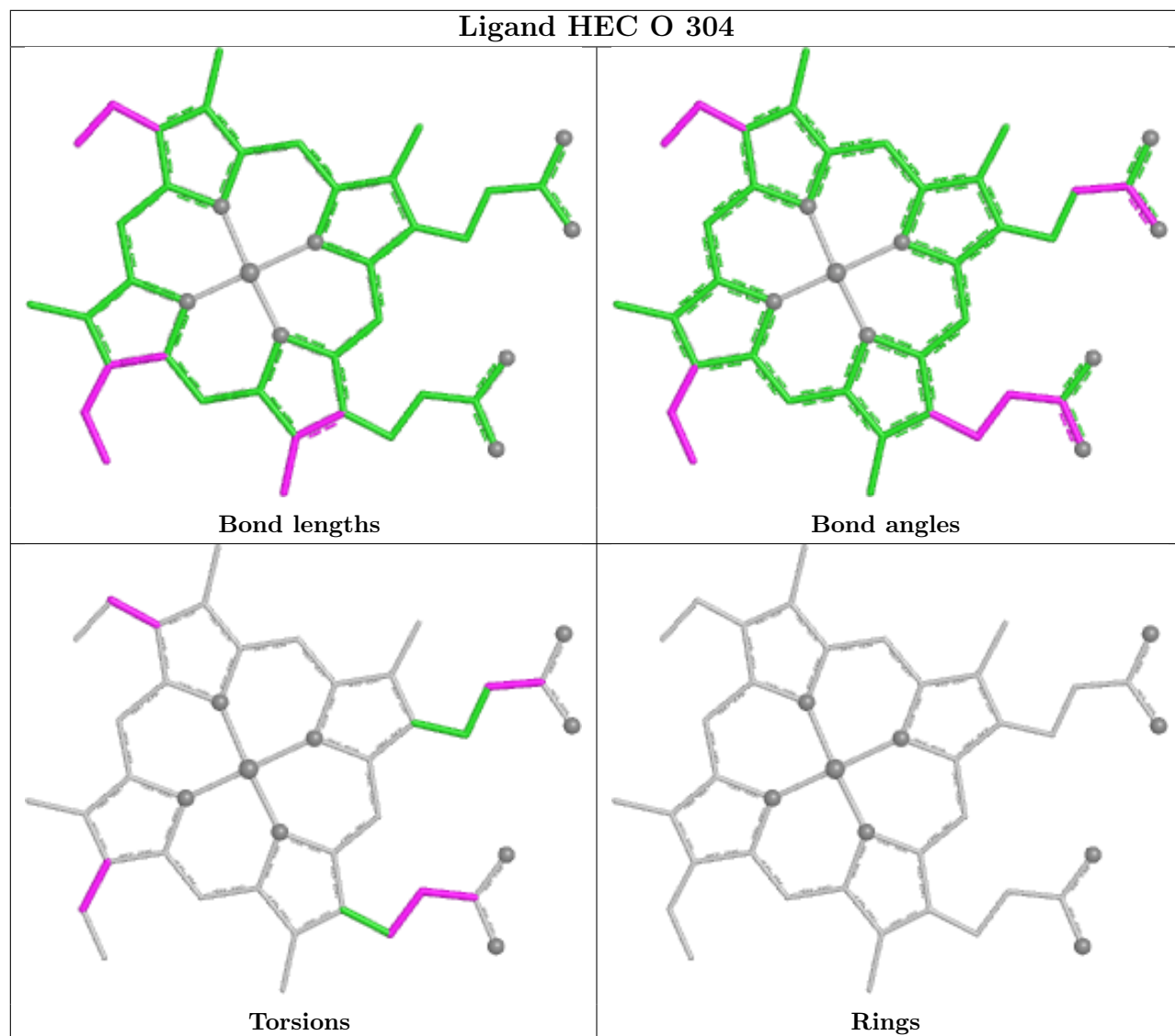


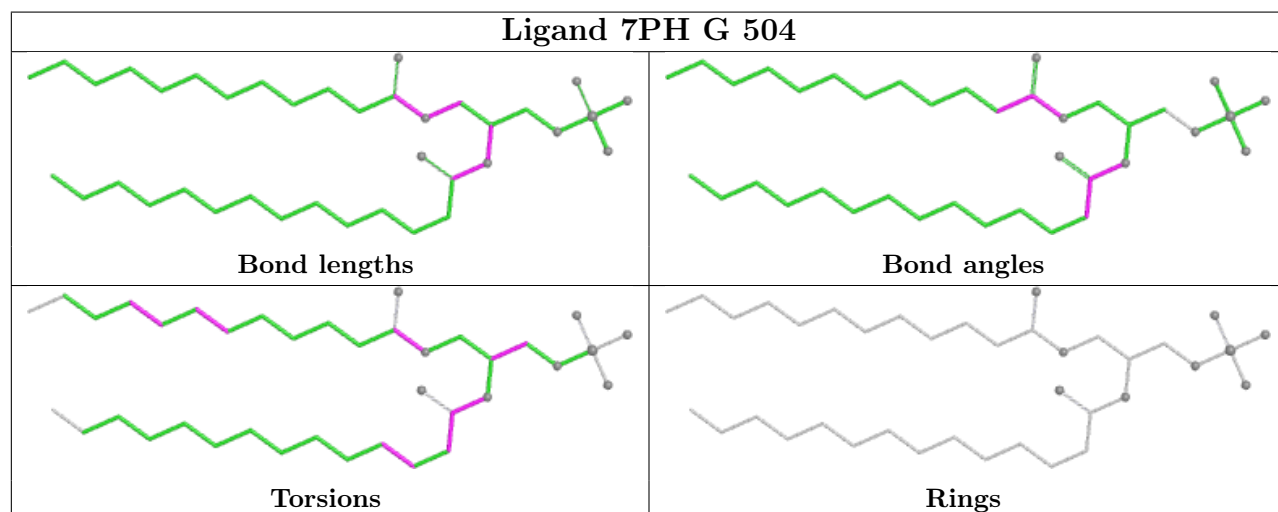
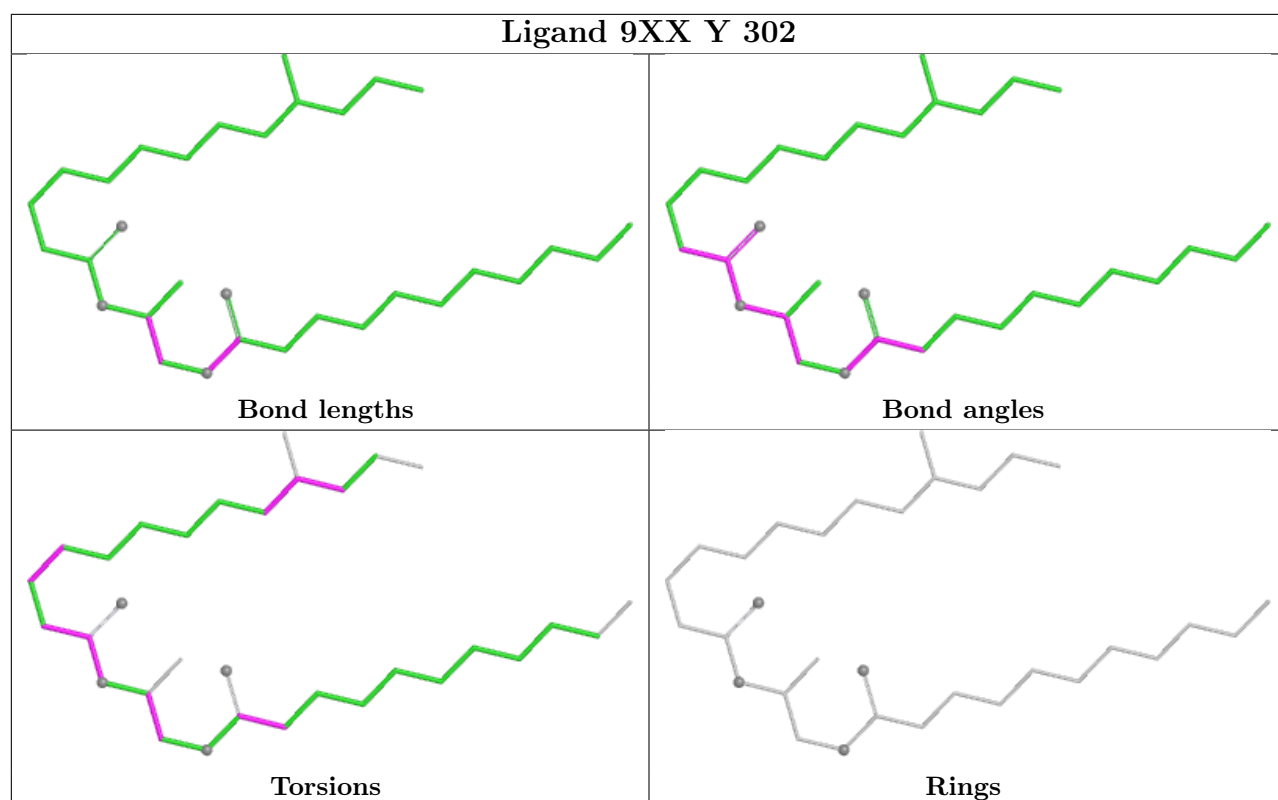


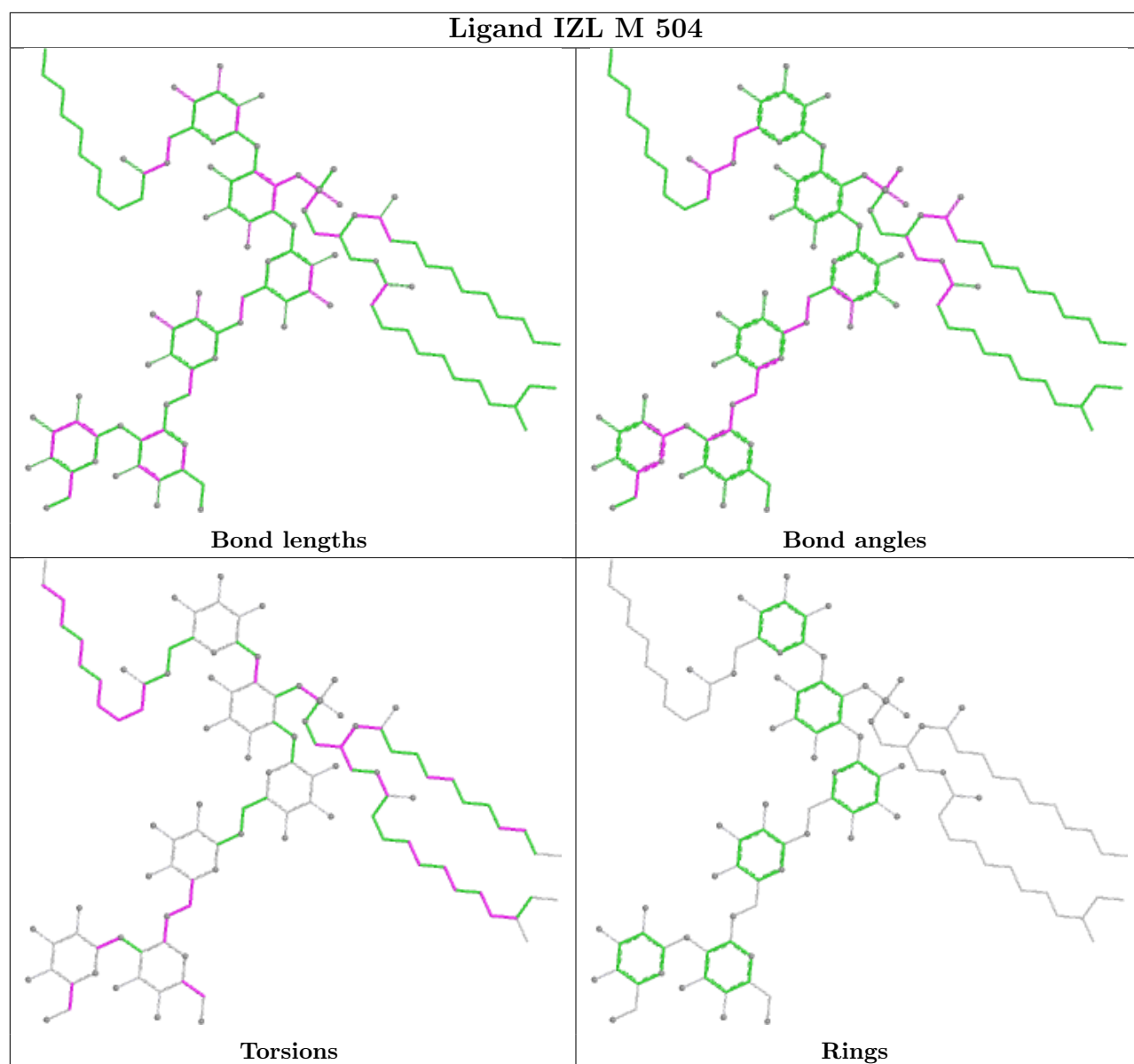


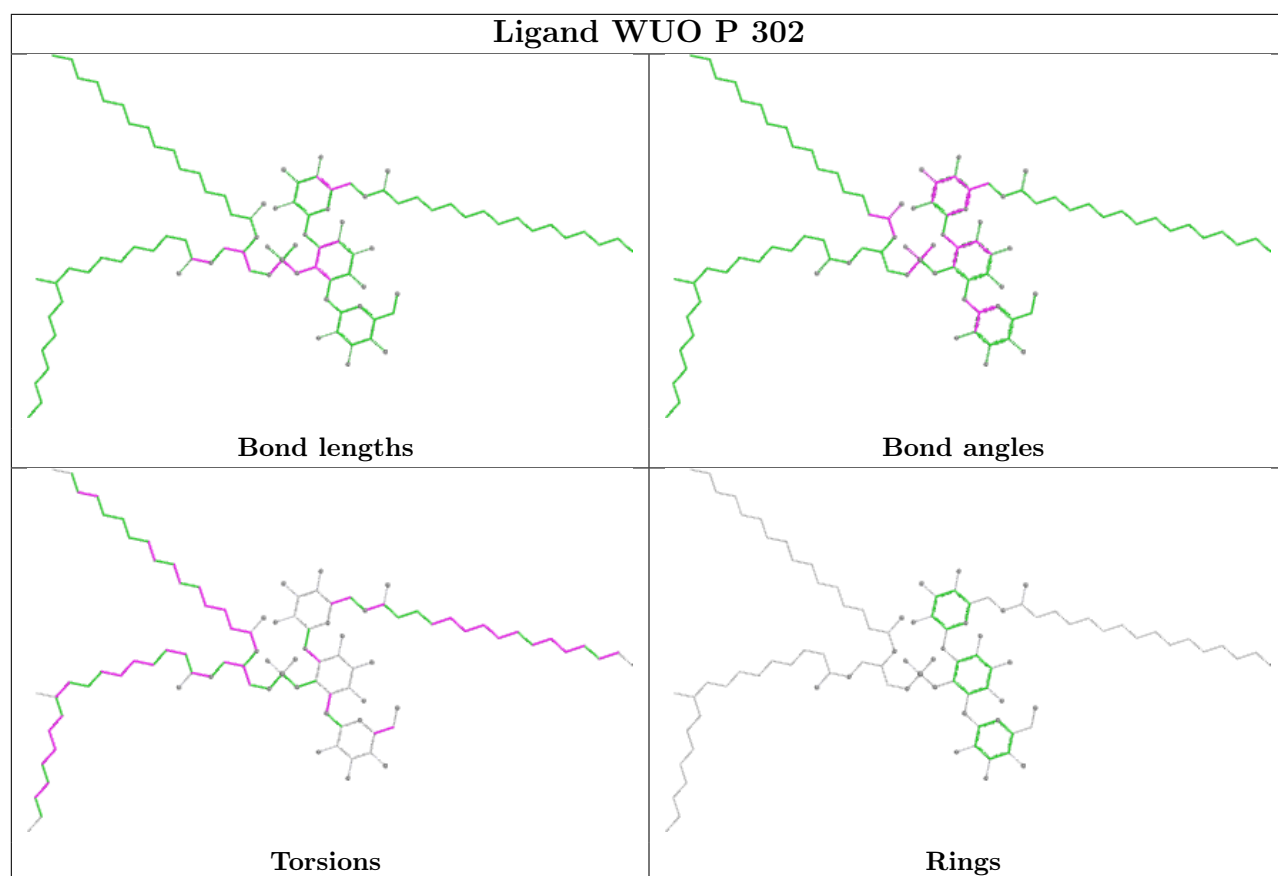


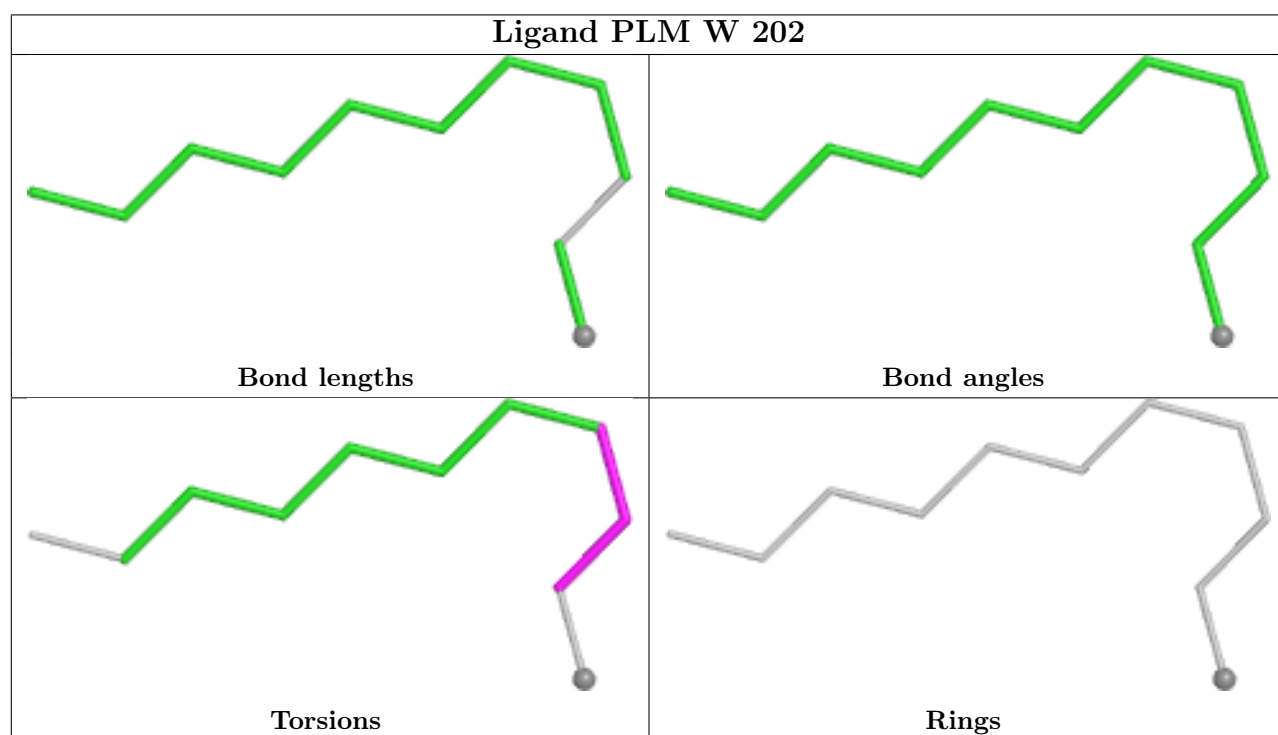
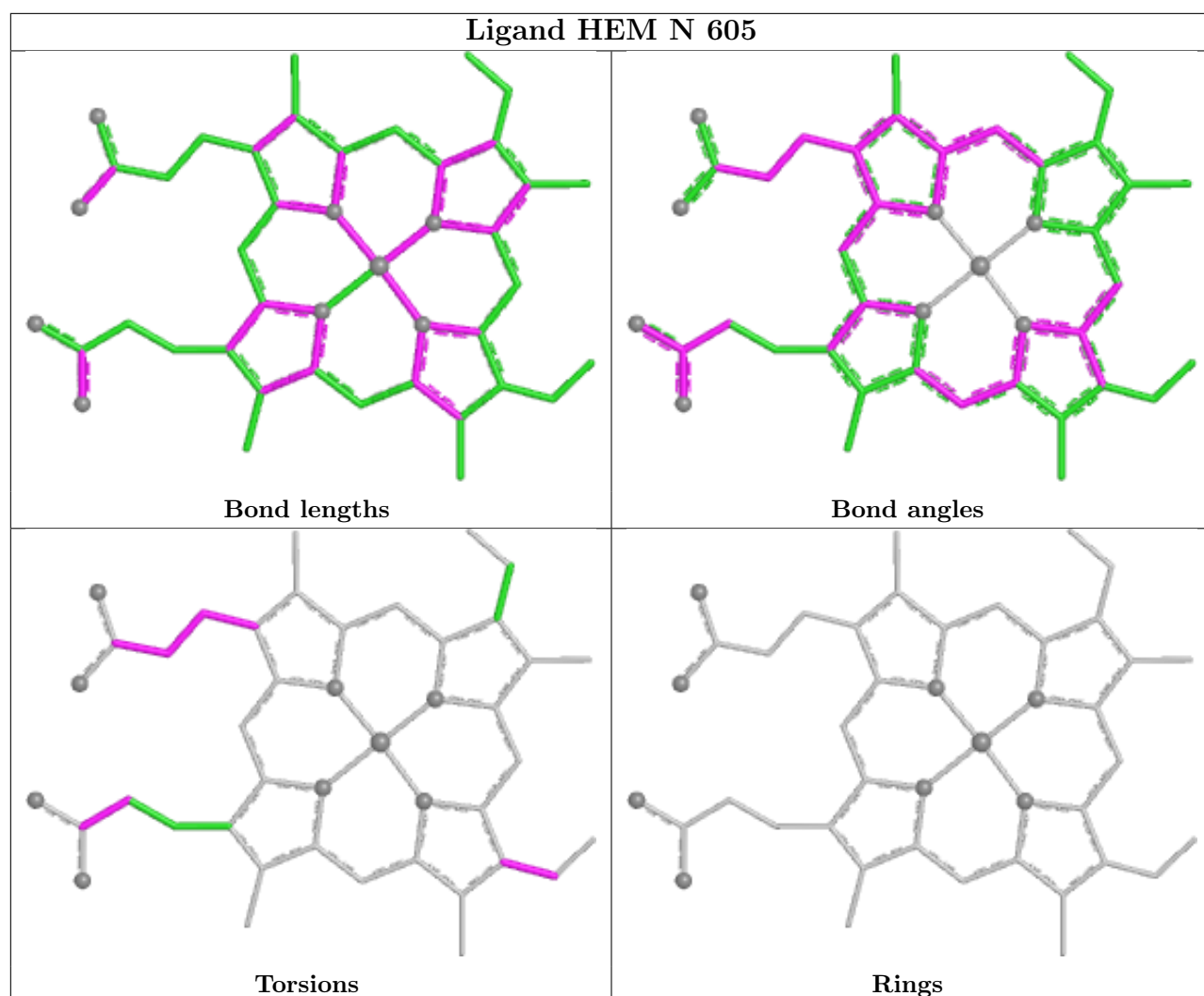


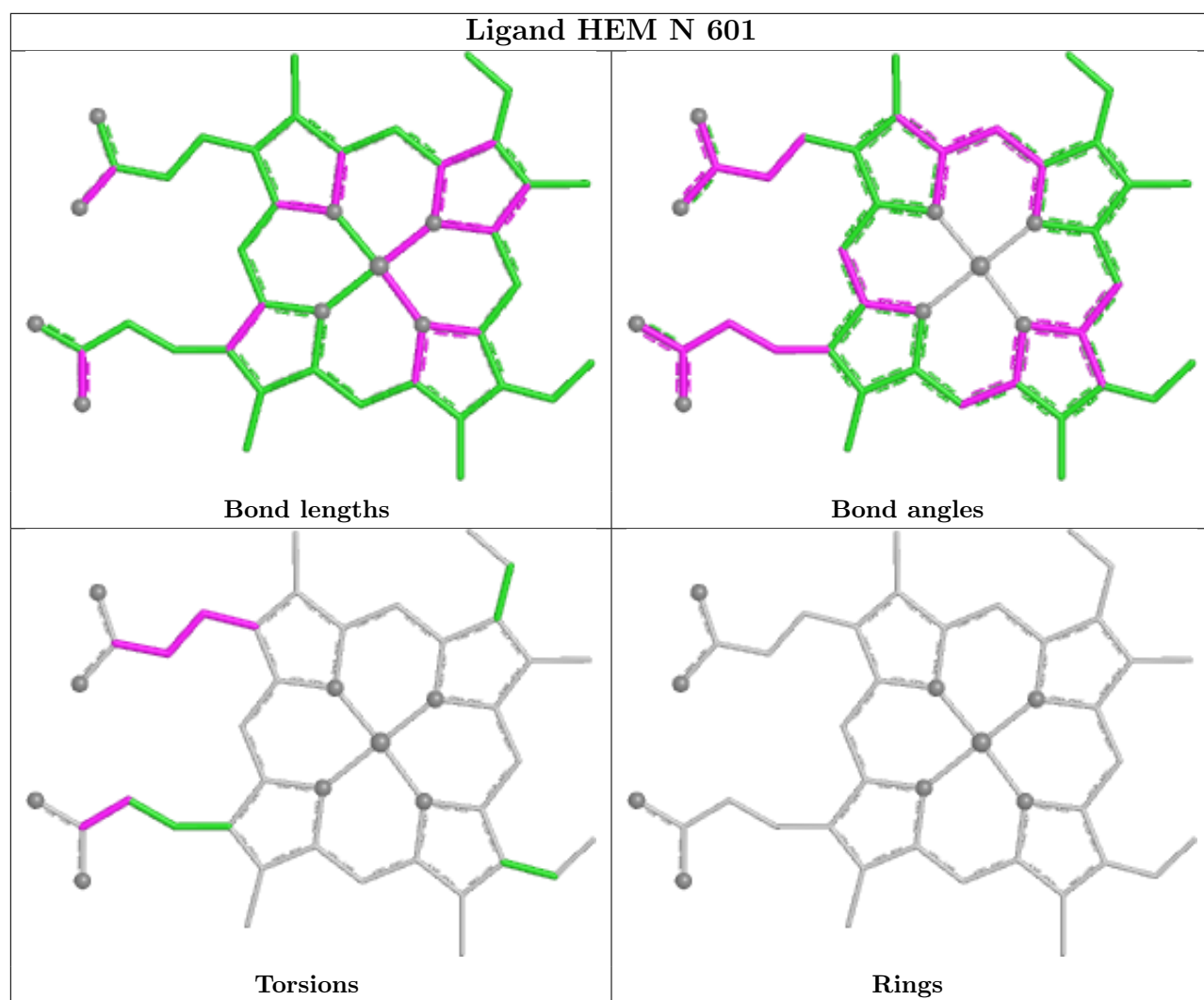
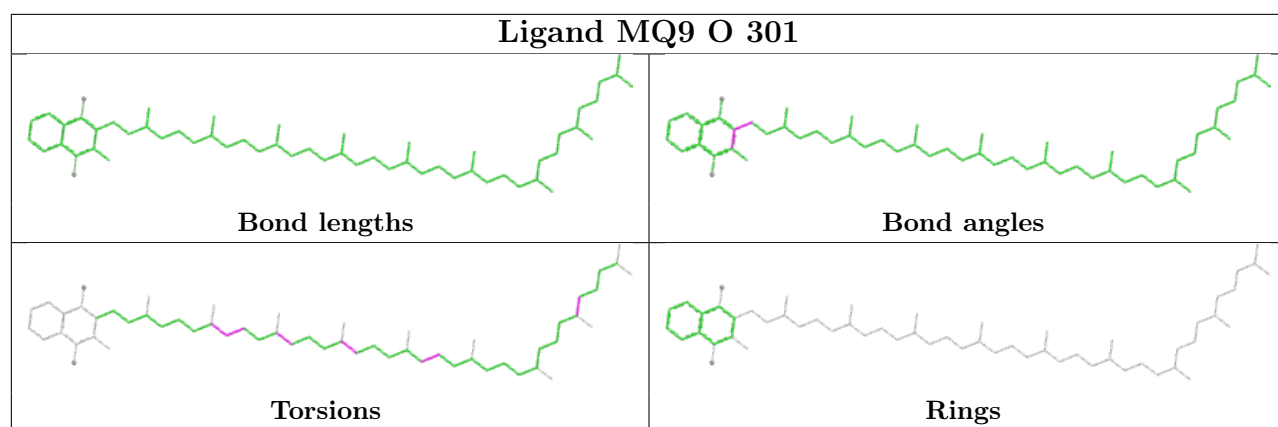


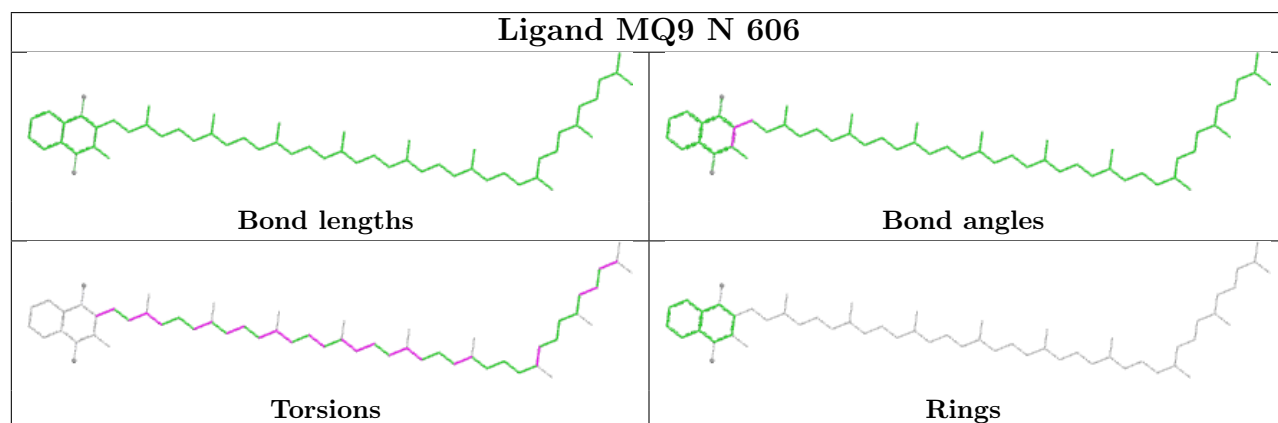
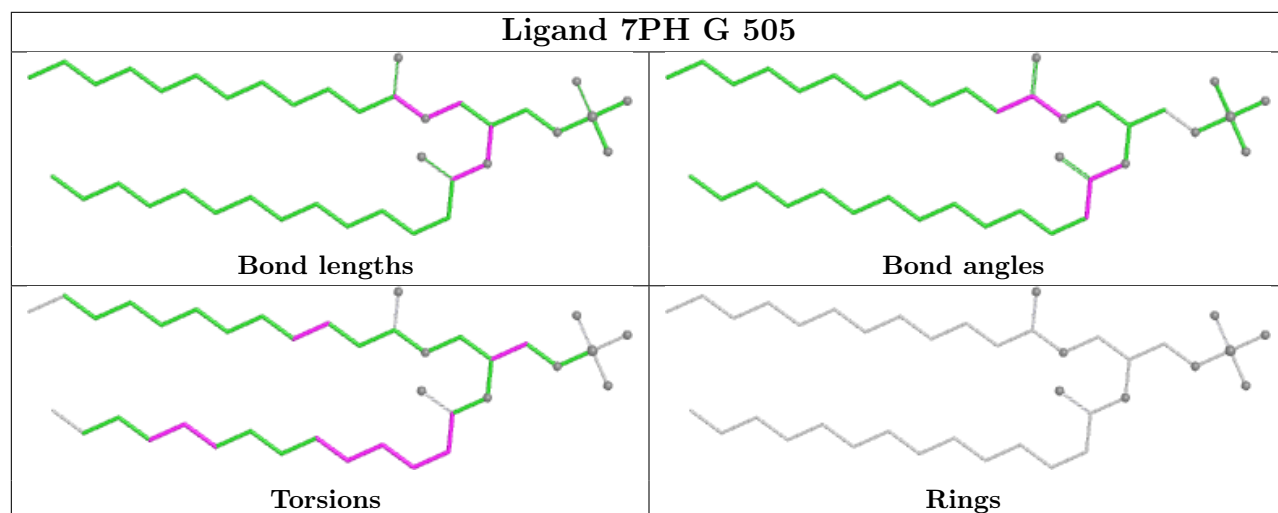
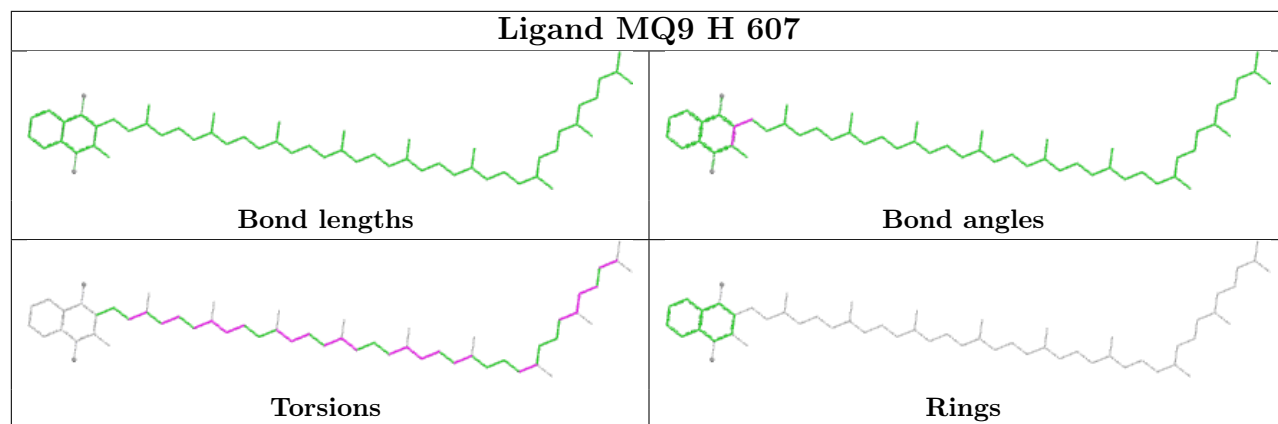


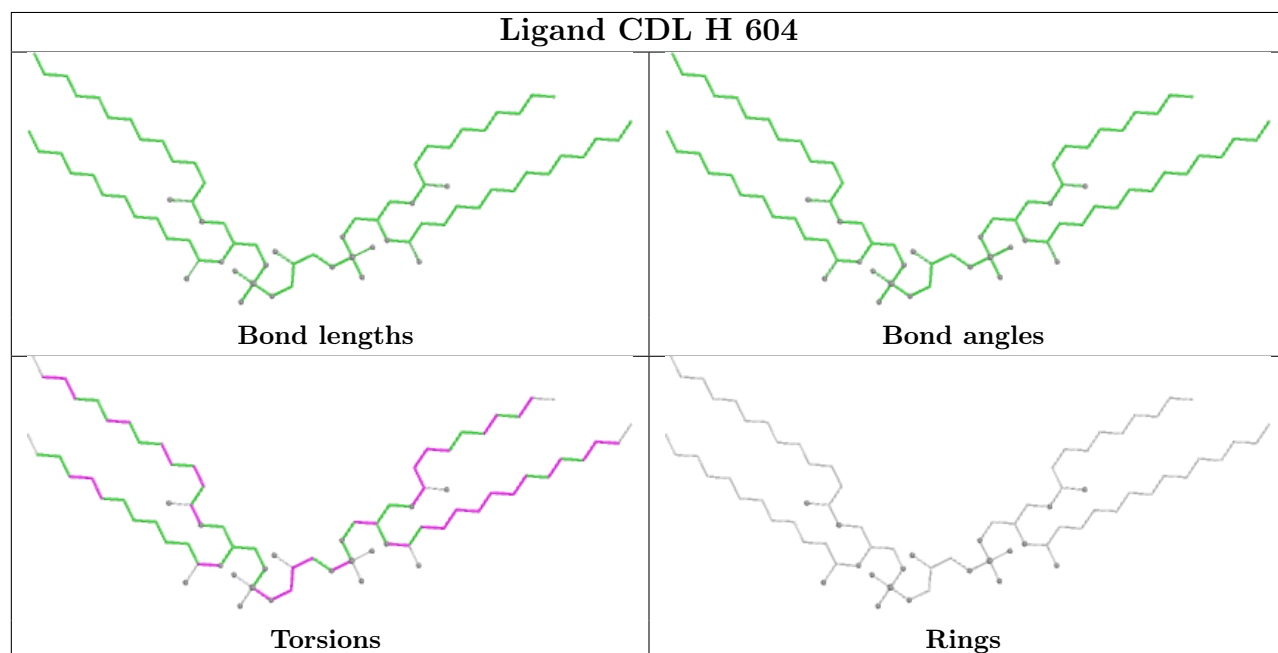
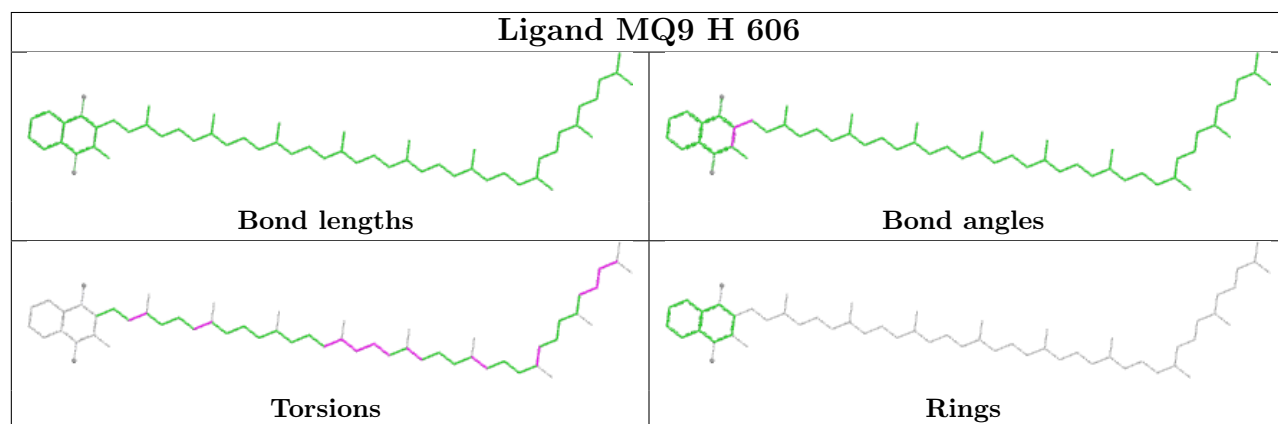
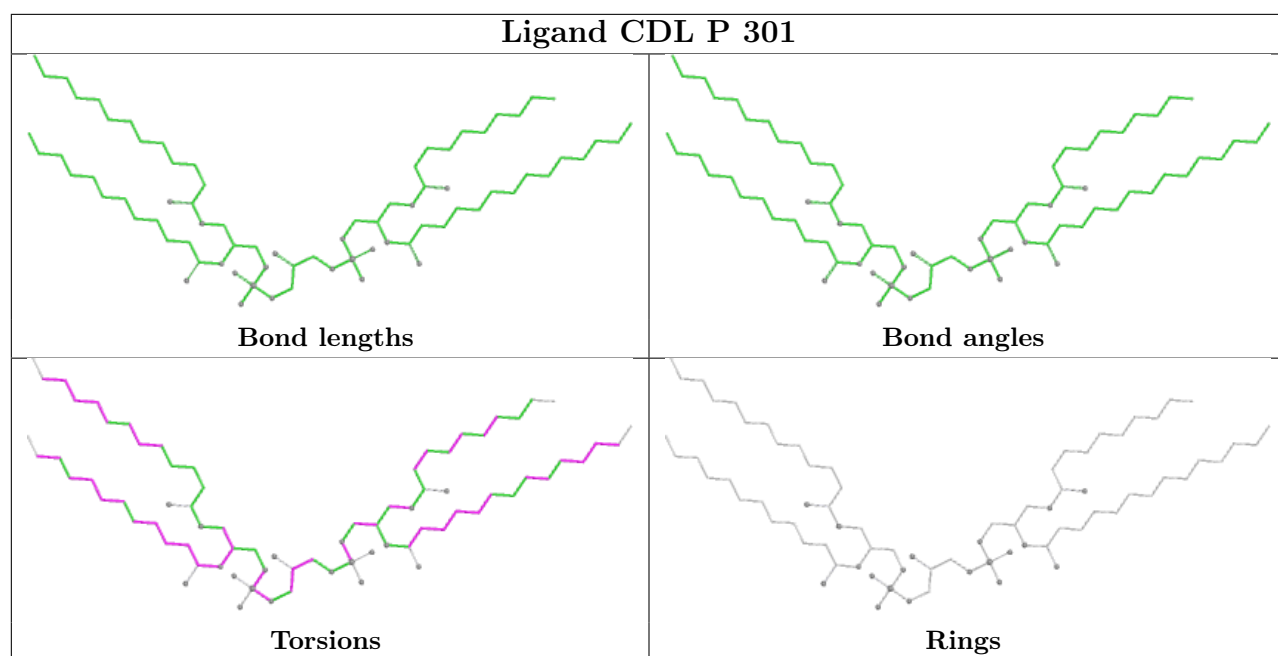


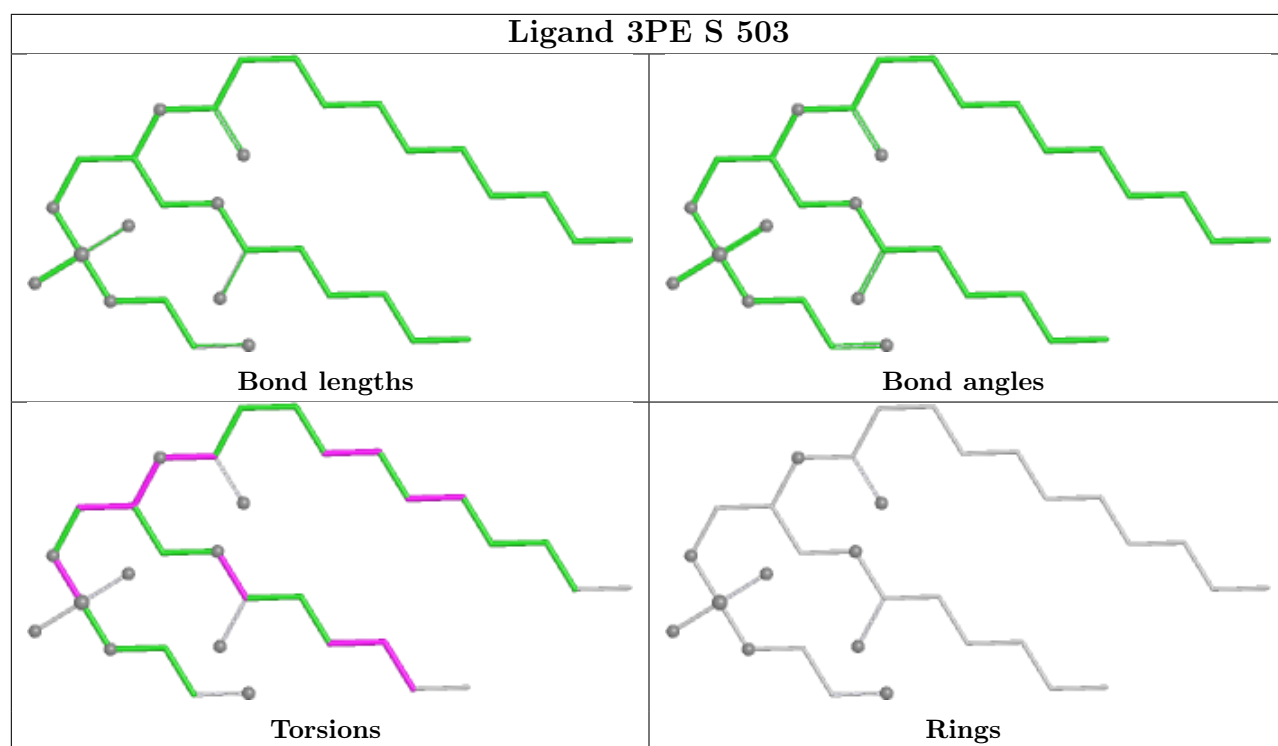


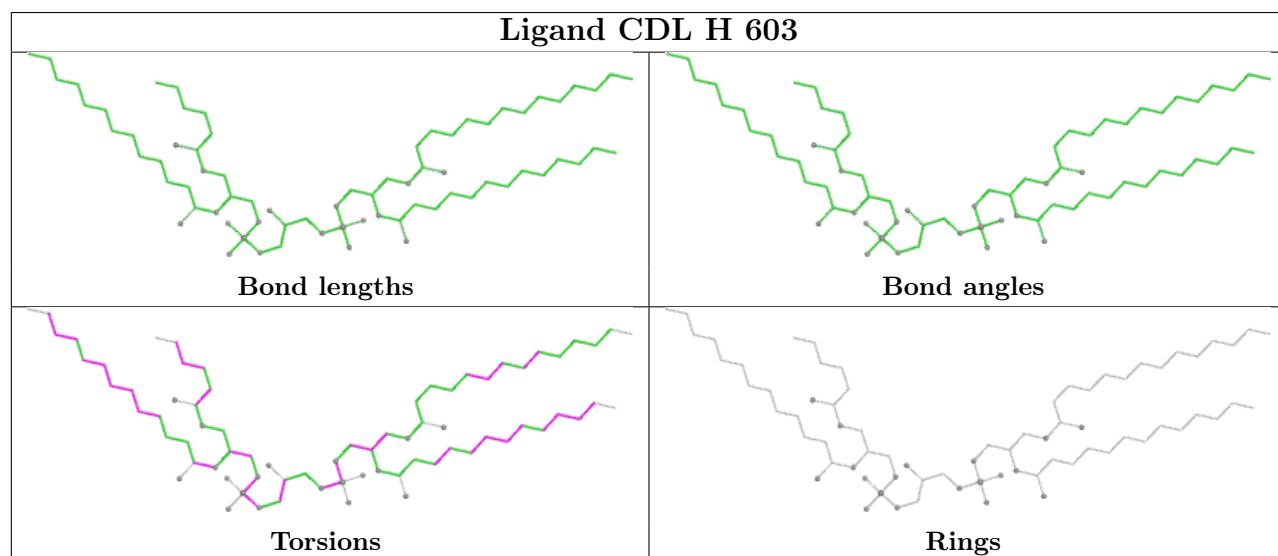
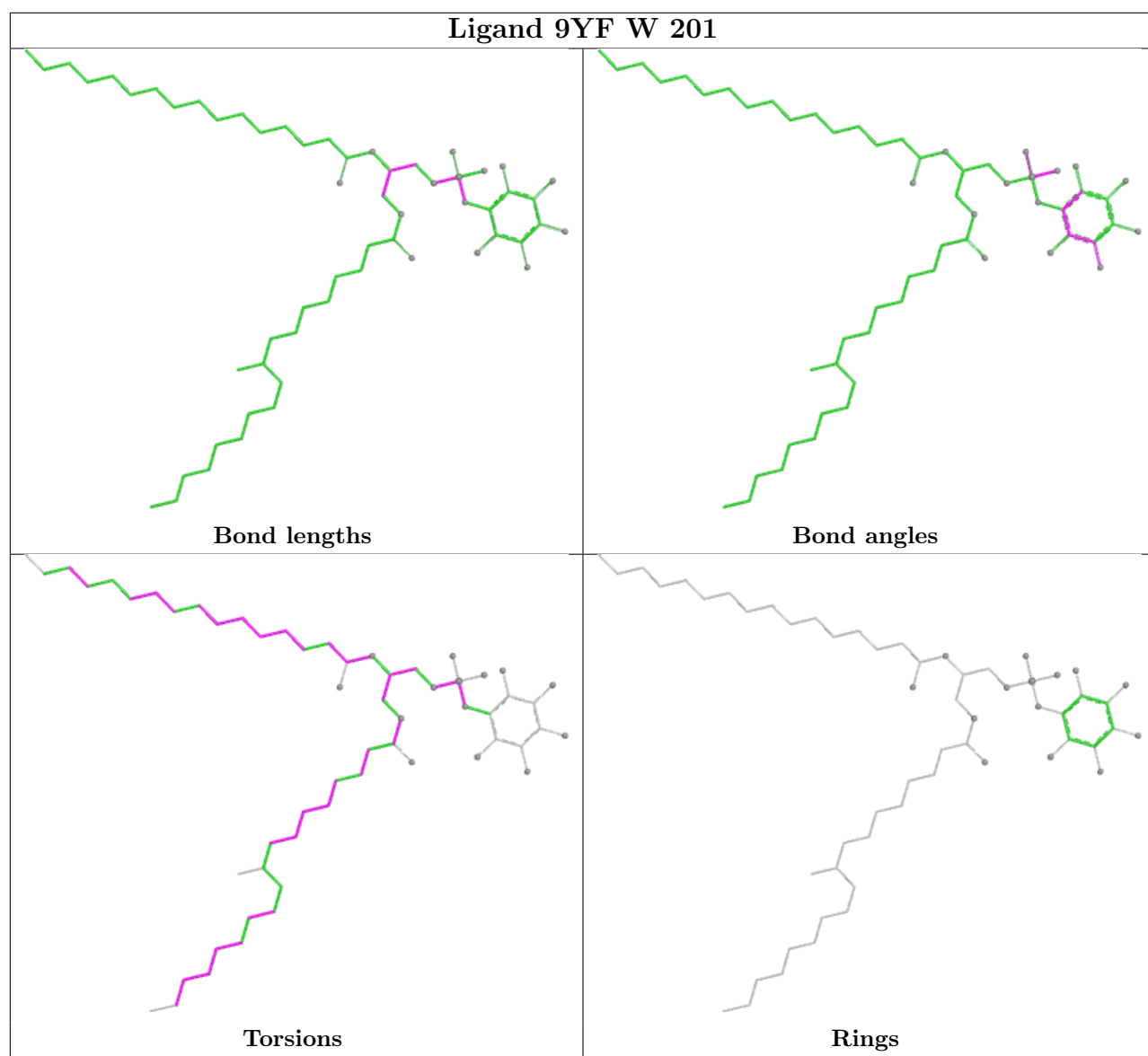


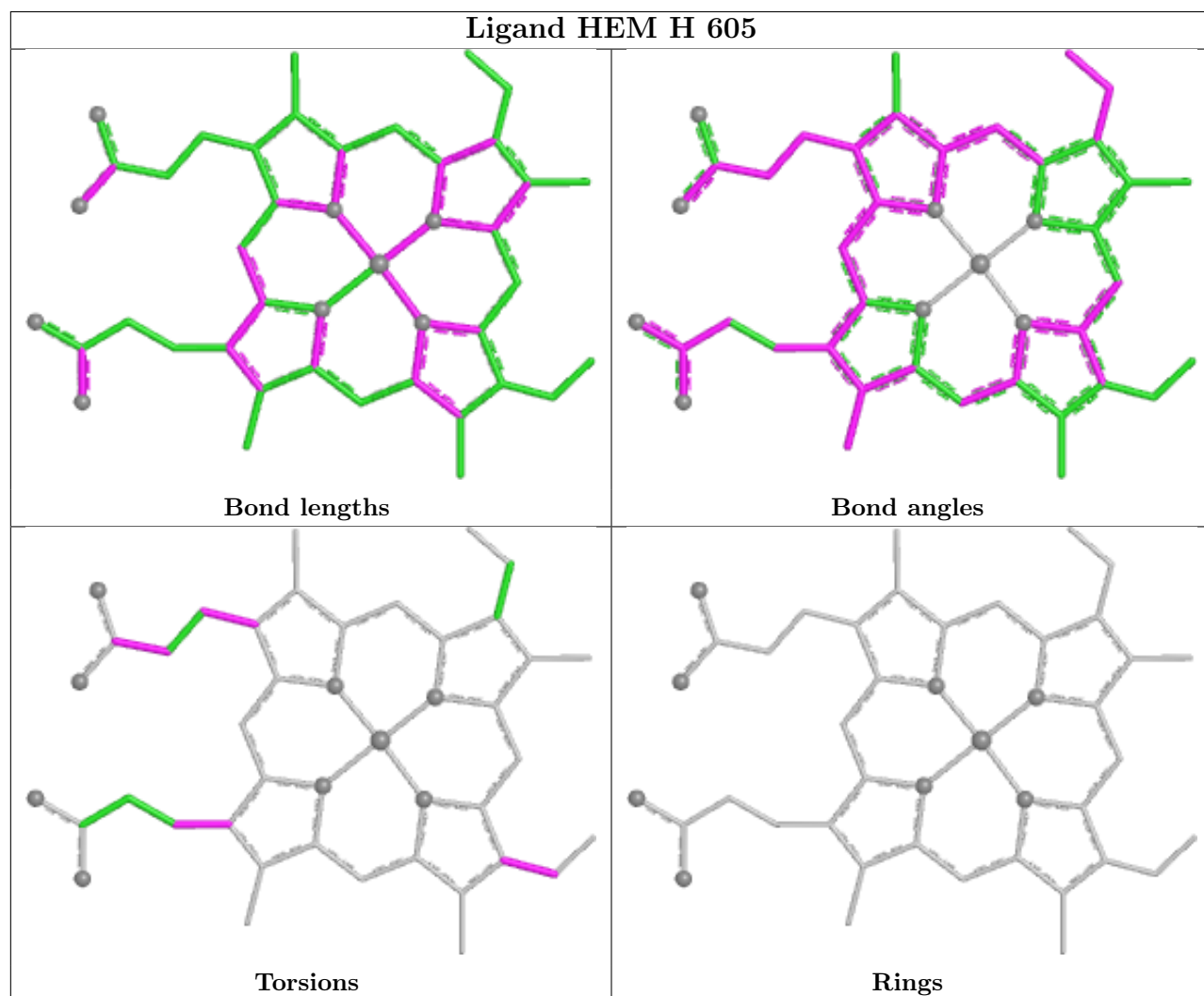
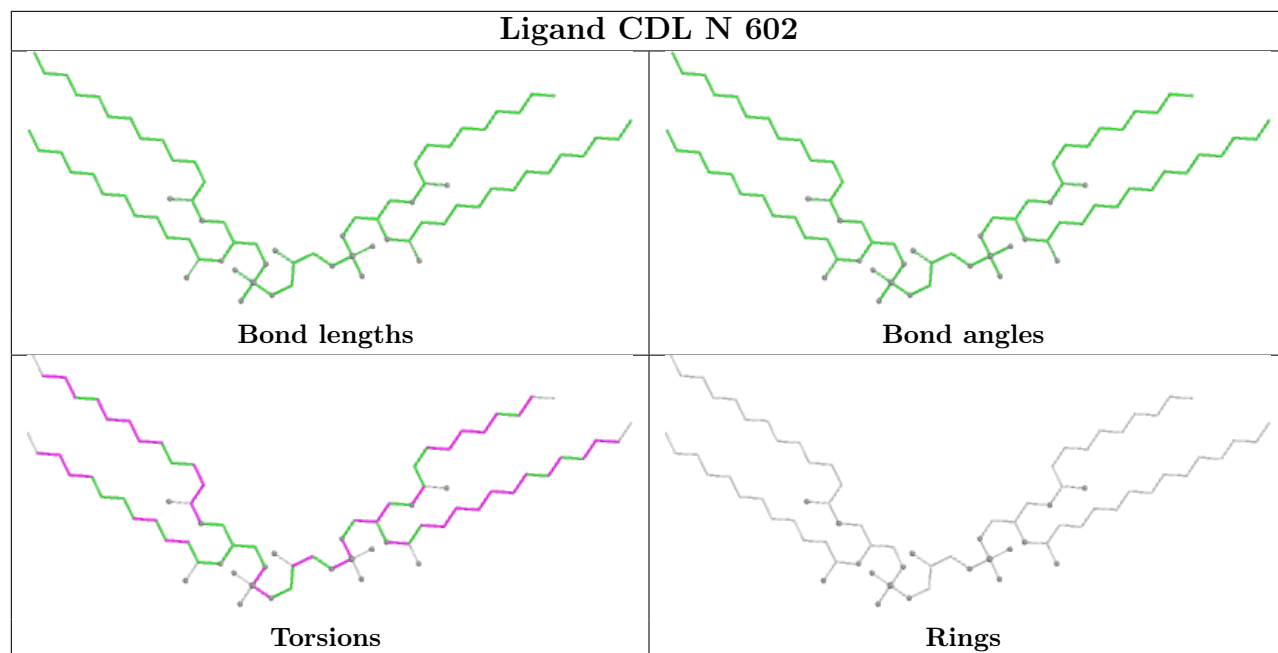




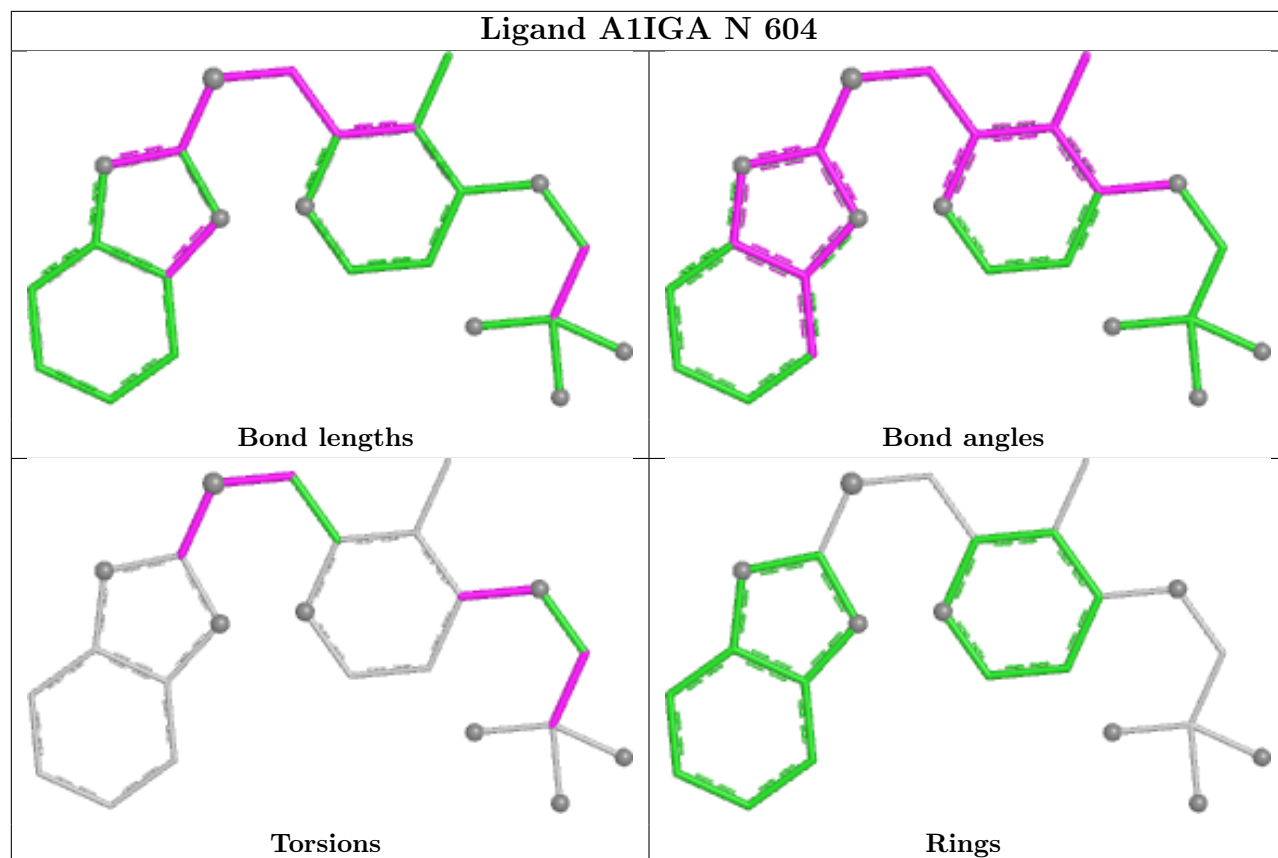




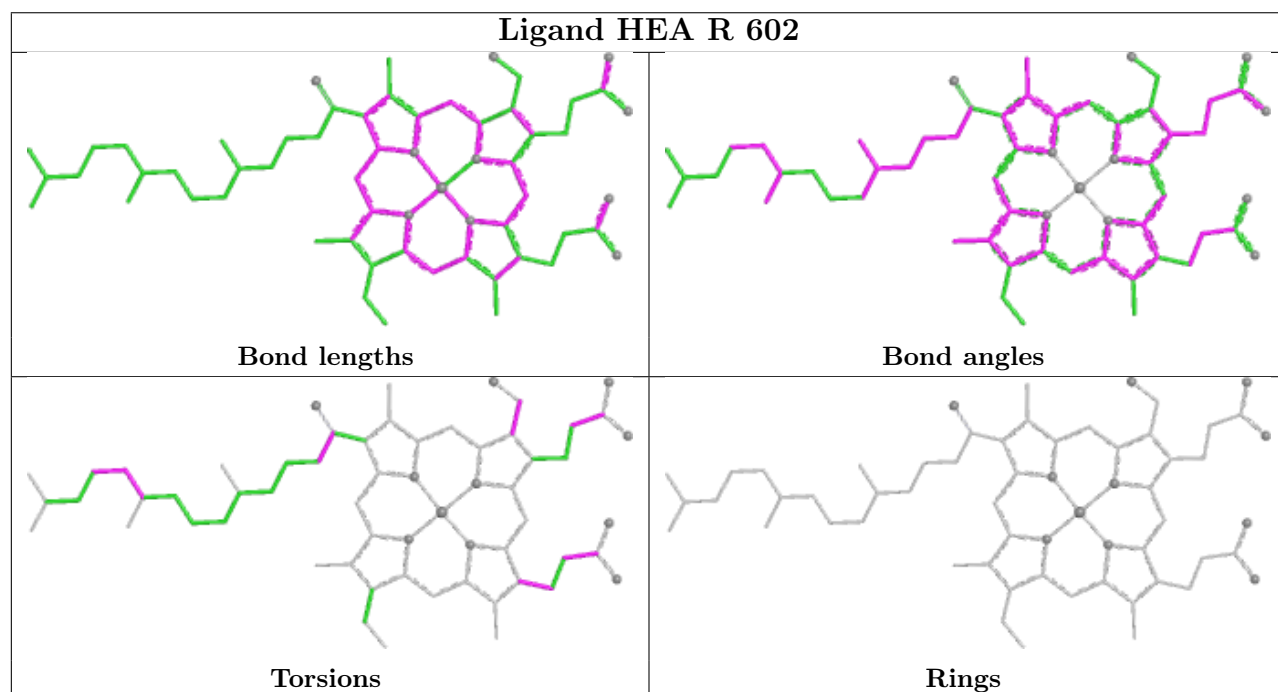


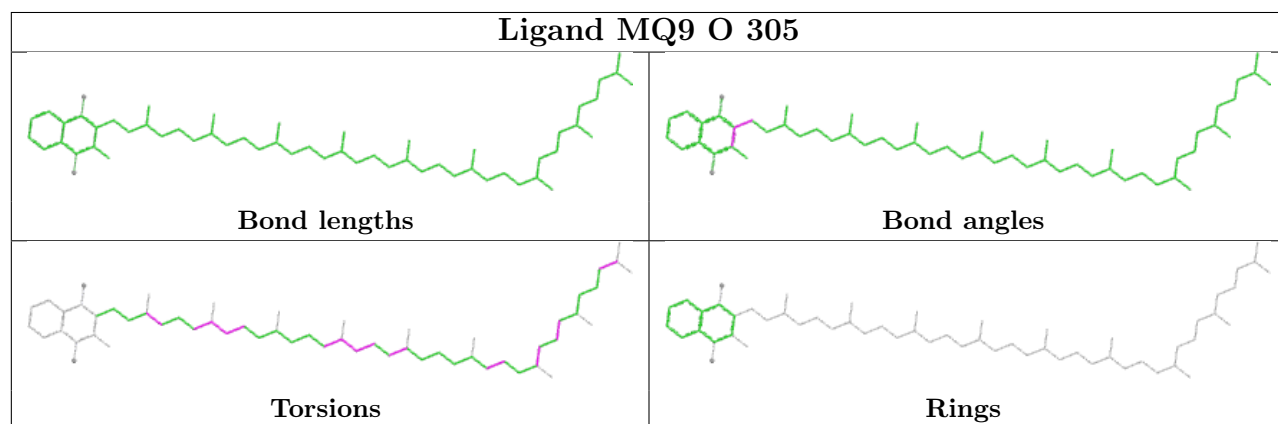
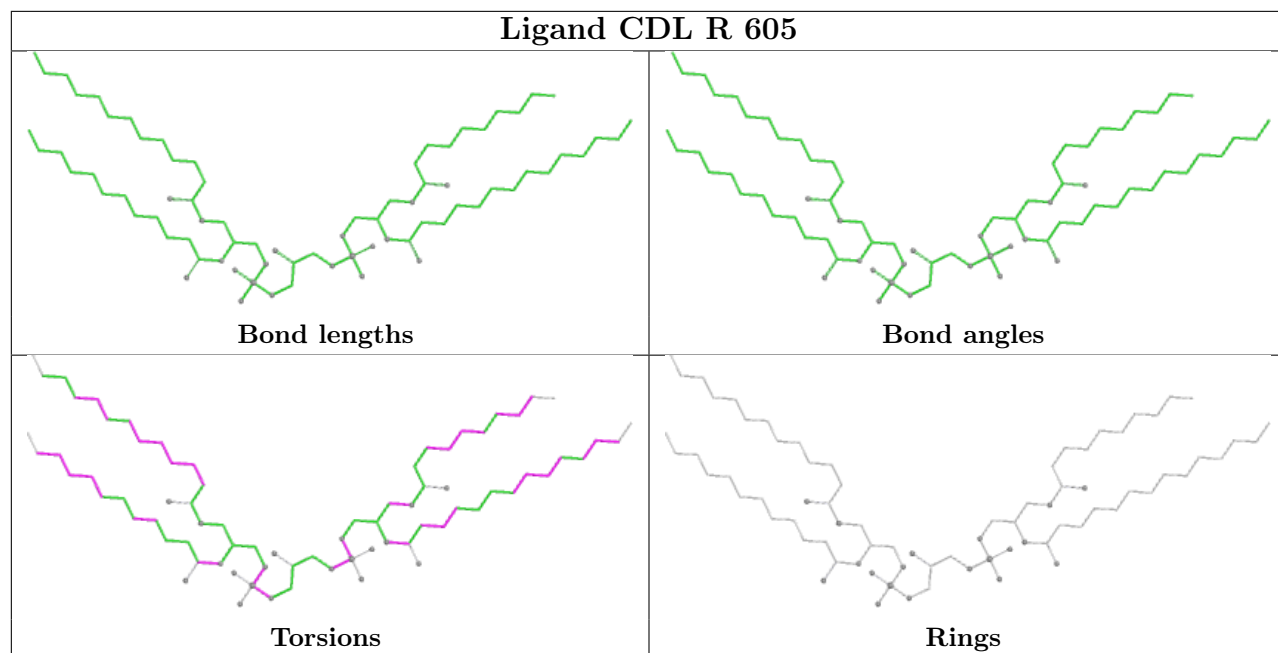


Ligand A1IGA N 604

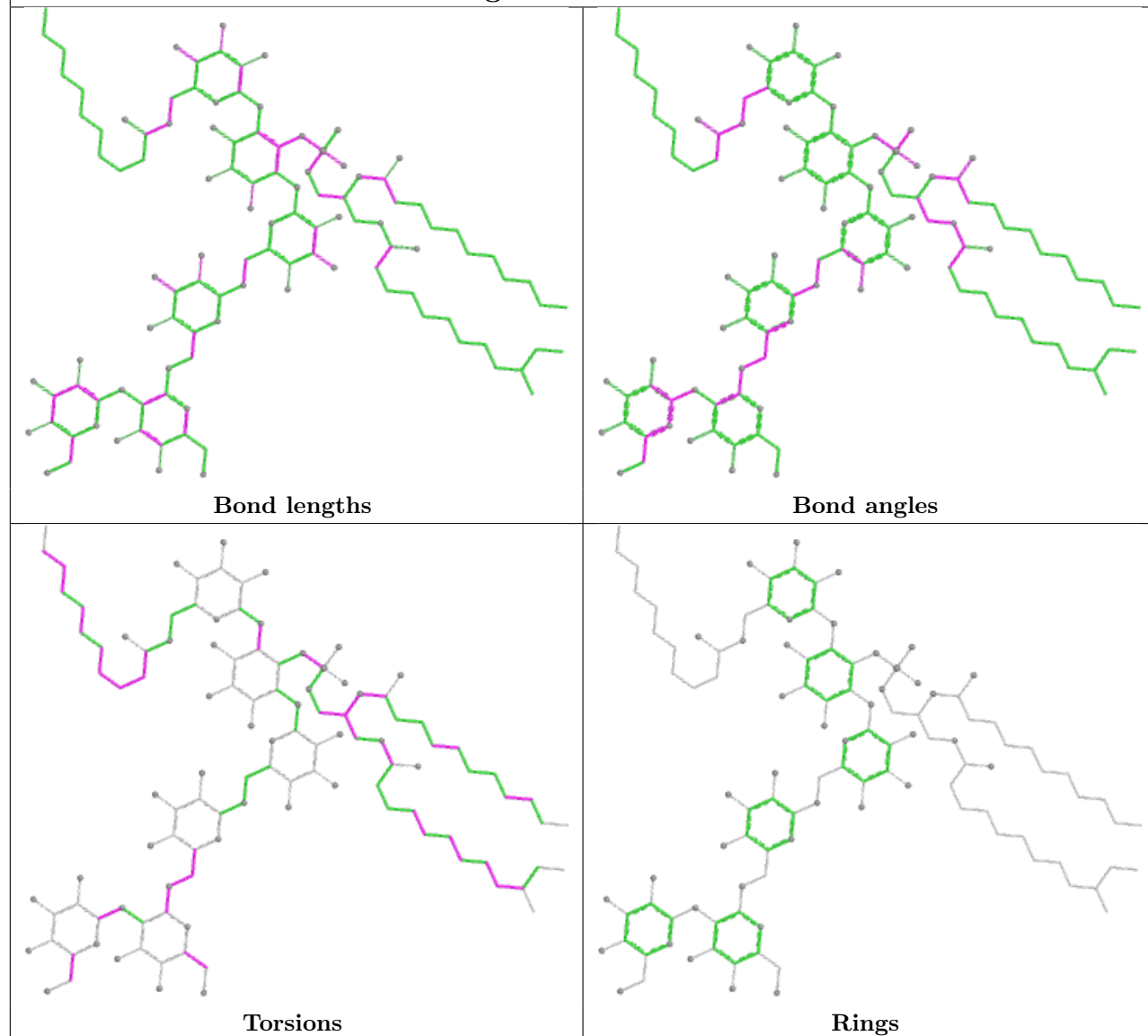


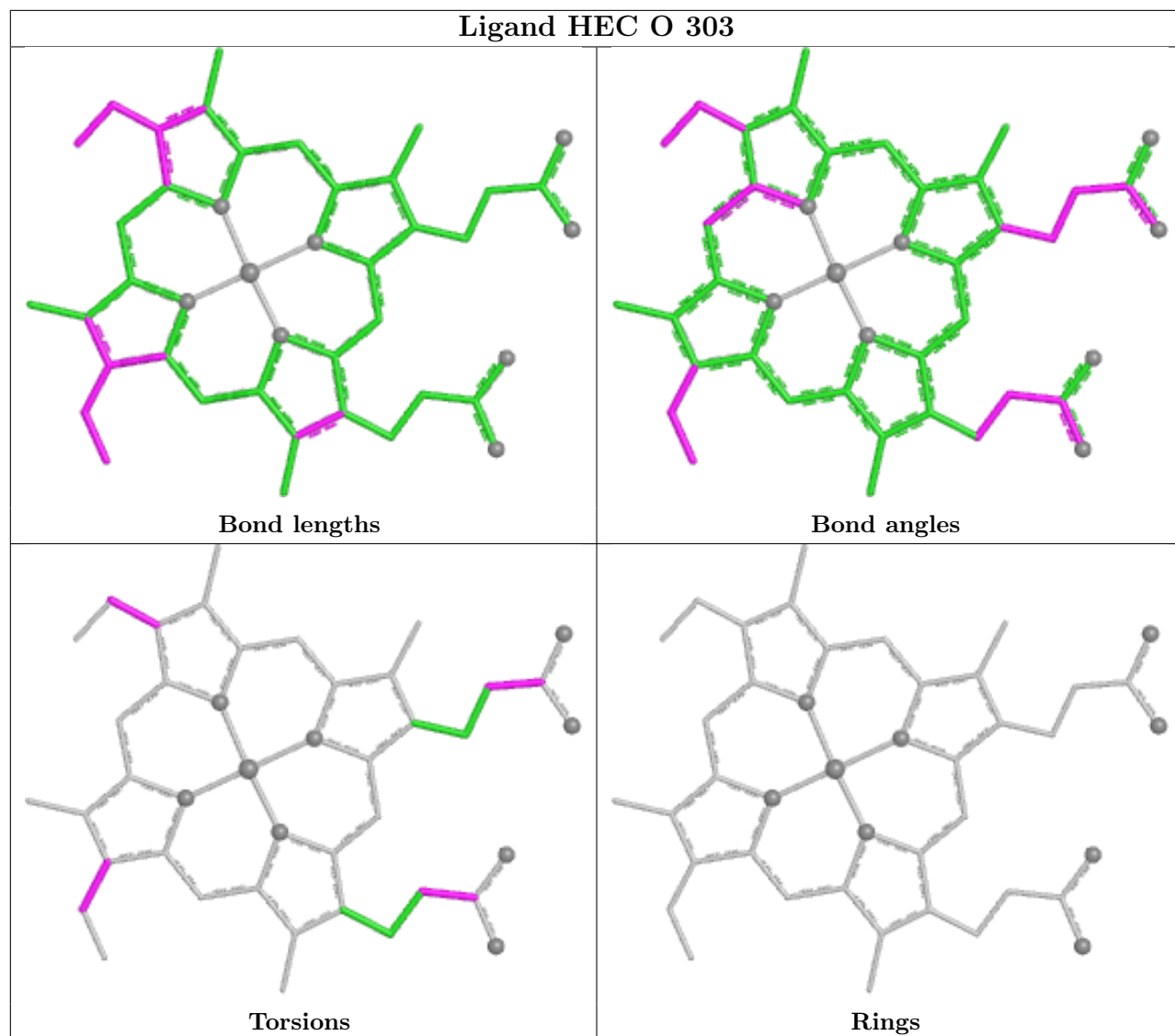
Ligand HEA R 602

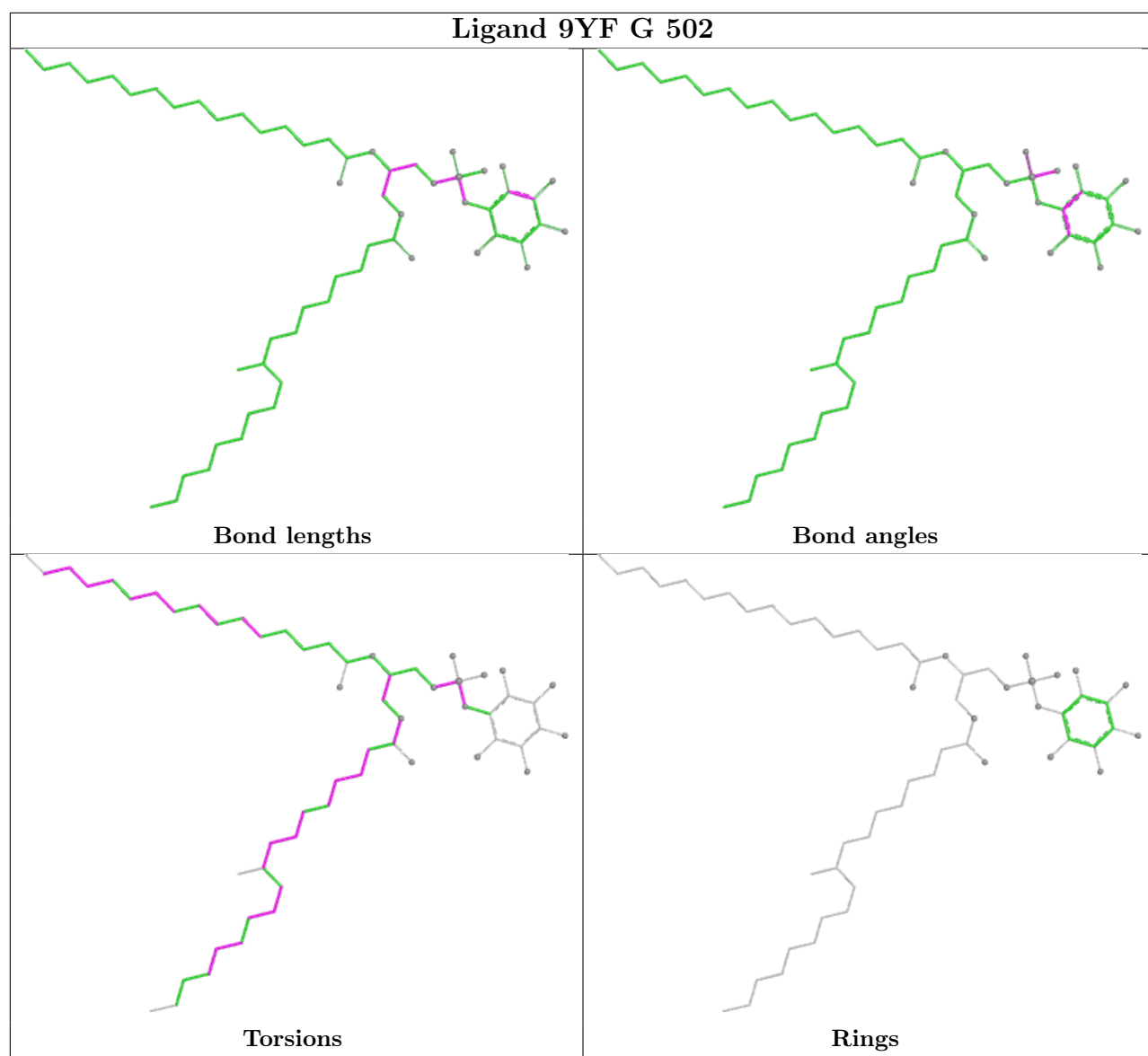


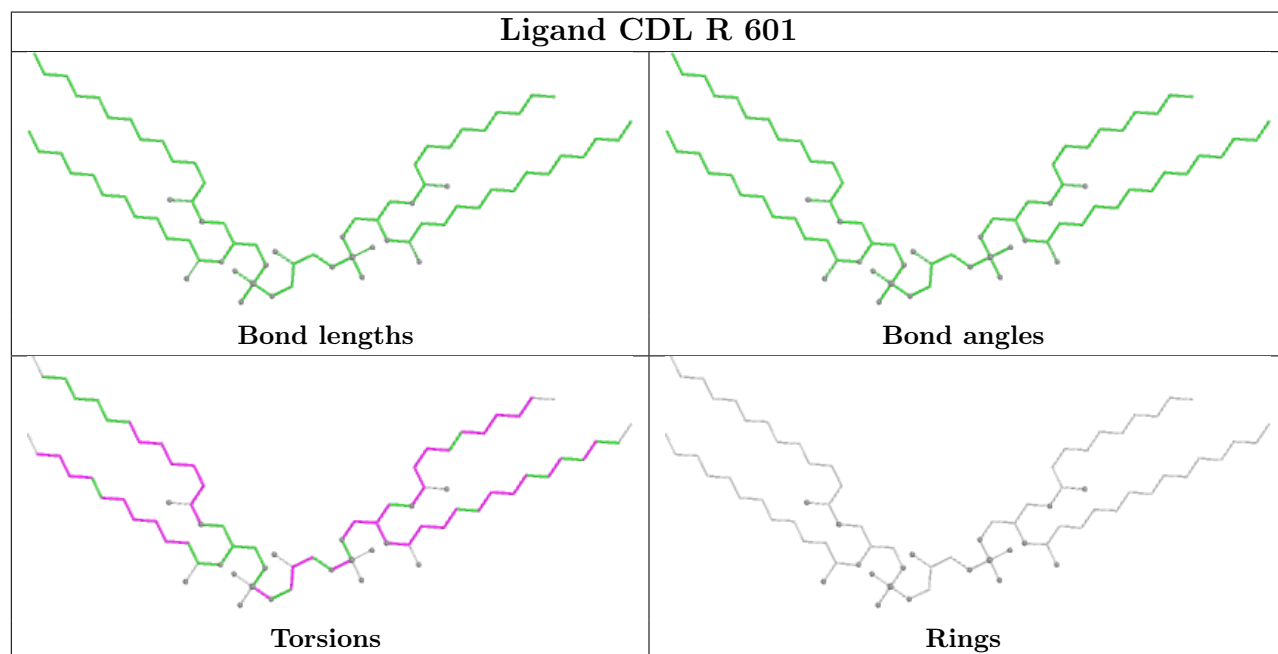
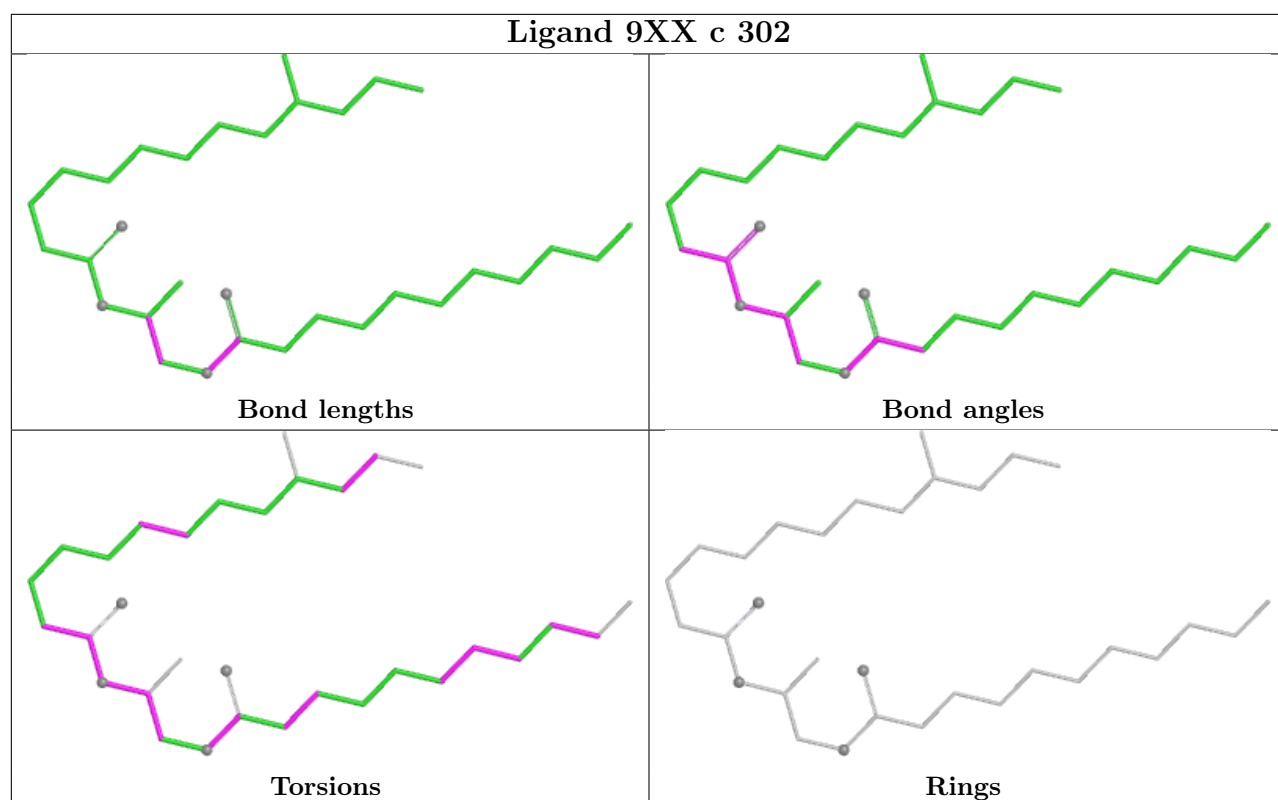


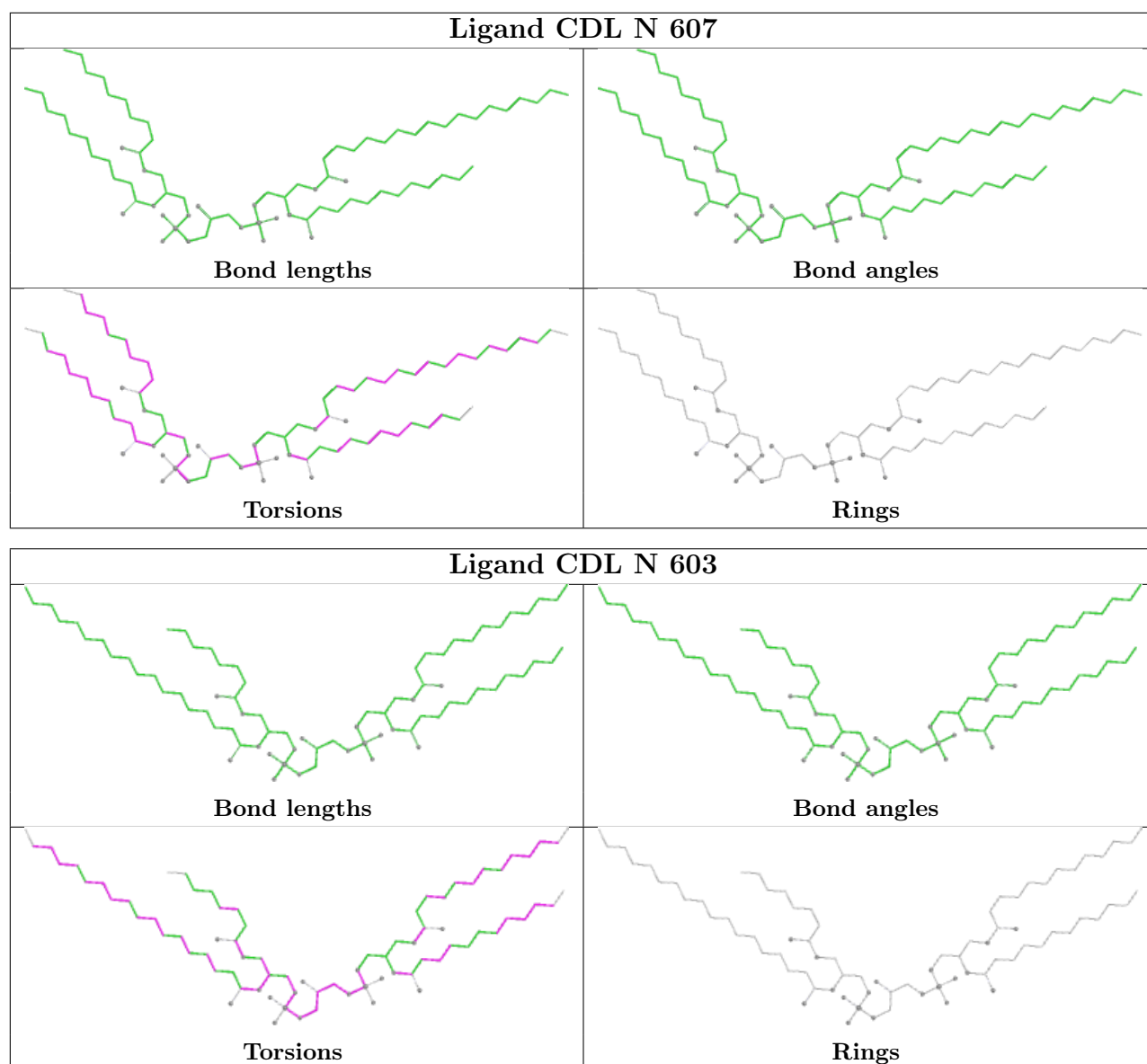
Ligand IZL G 503











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

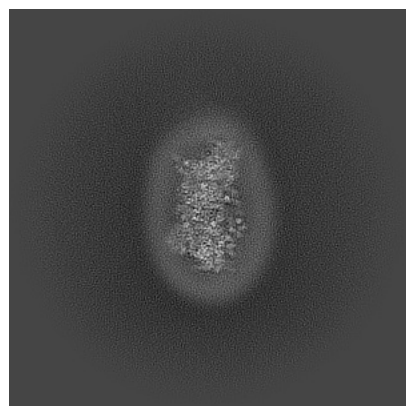
6 Map visualisation [i](#)

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

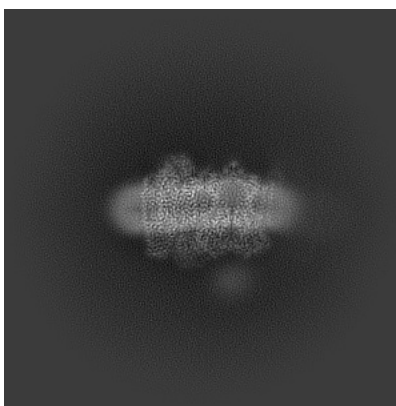
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

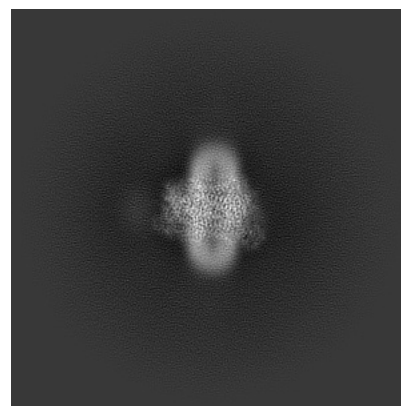
6.1.1 Primary map



X

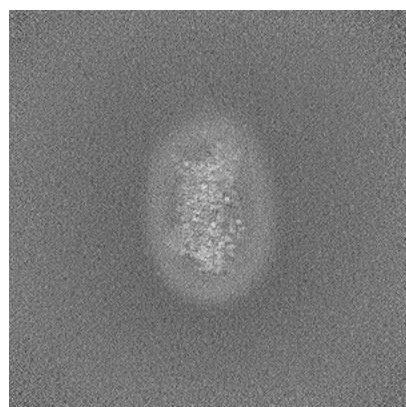


Y

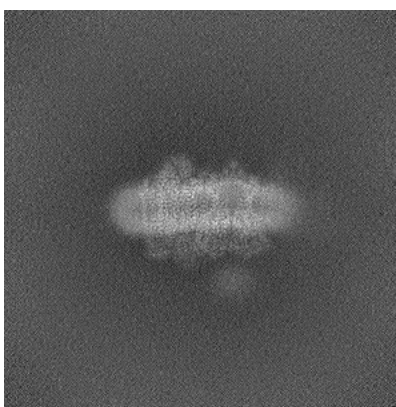


Z

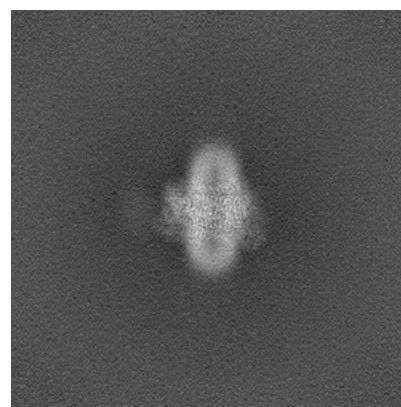
6.1.2 Raw map



X



Y

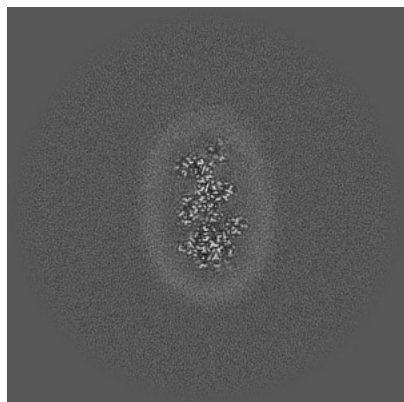


Z

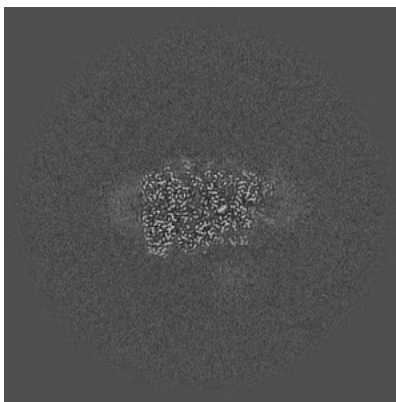
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

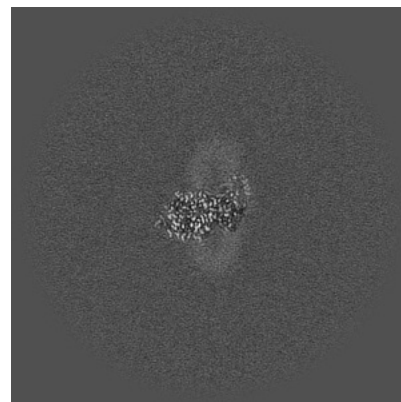
6.2.1 Primary map



X Index: 270

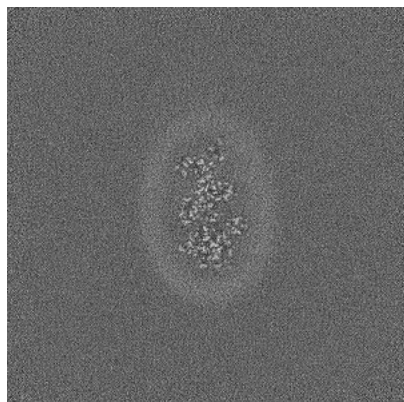


Y Index: 270

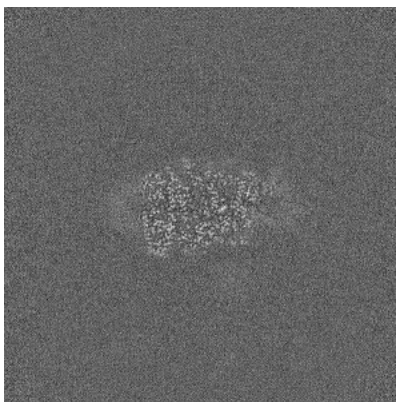


Z Index: 270

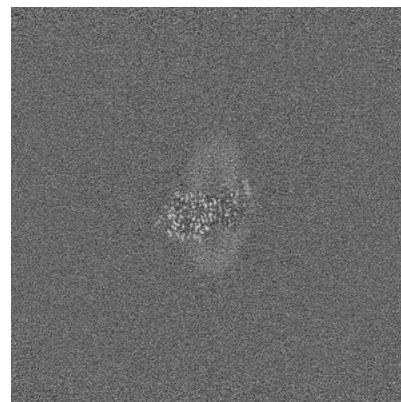
6.2.2 Raw map



X Index: 270



Y Index: 270

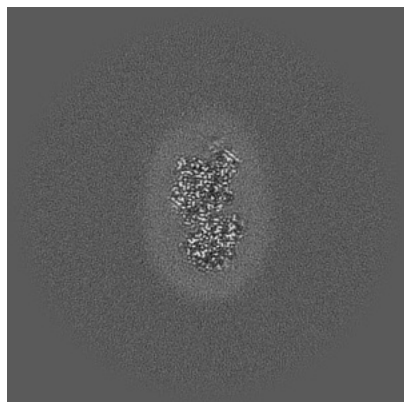


Z Index: 270

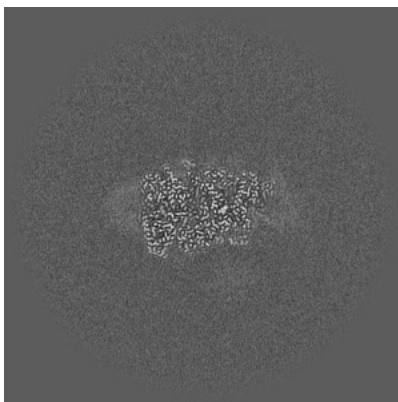
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

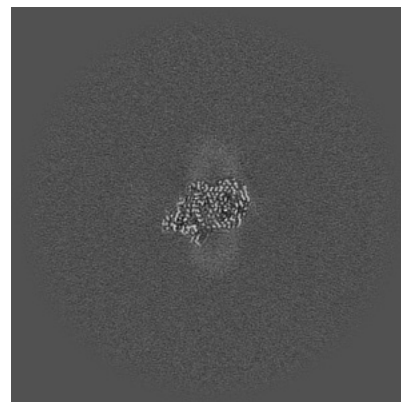
6.3.1 Primary map



X Index: 255

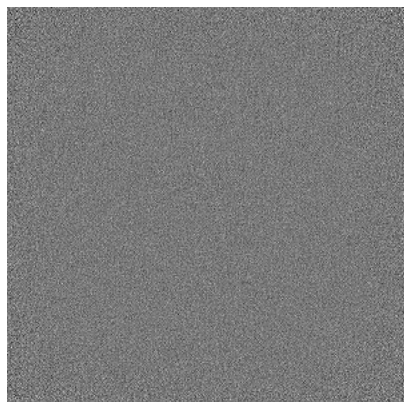


Y Index: 271

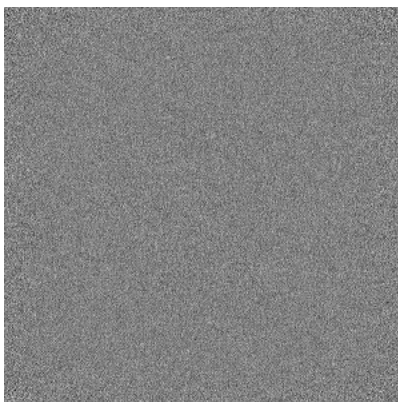


Z Index: 283

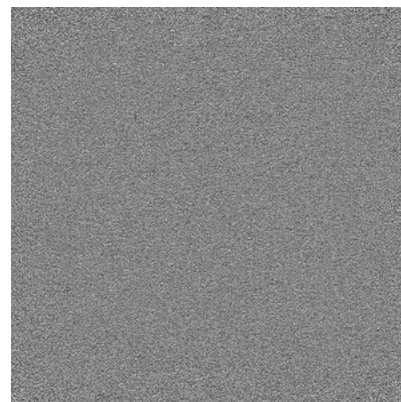
6.3.2 Raw map



X Index: 0



Y Index: 0

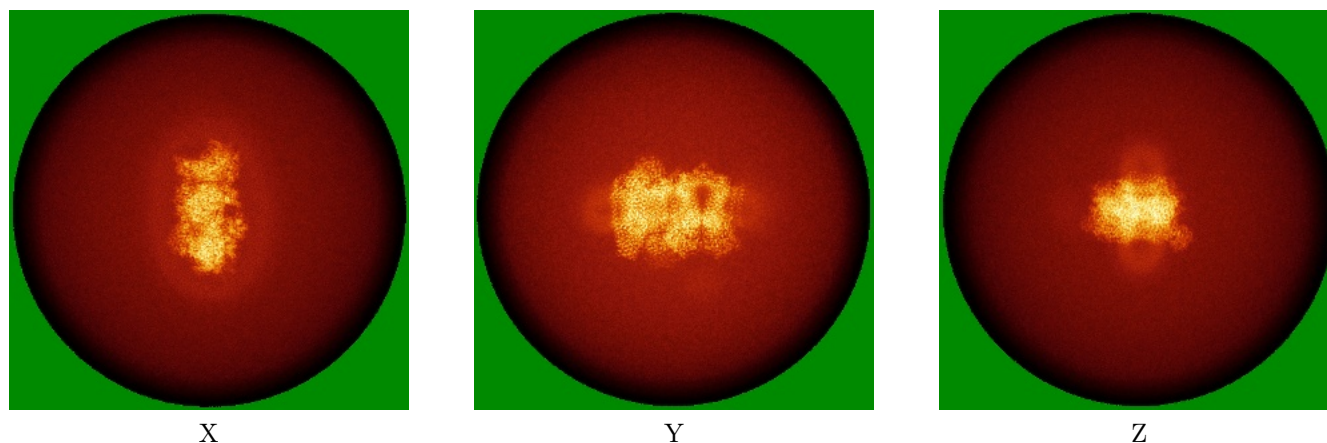


Z Index: 539

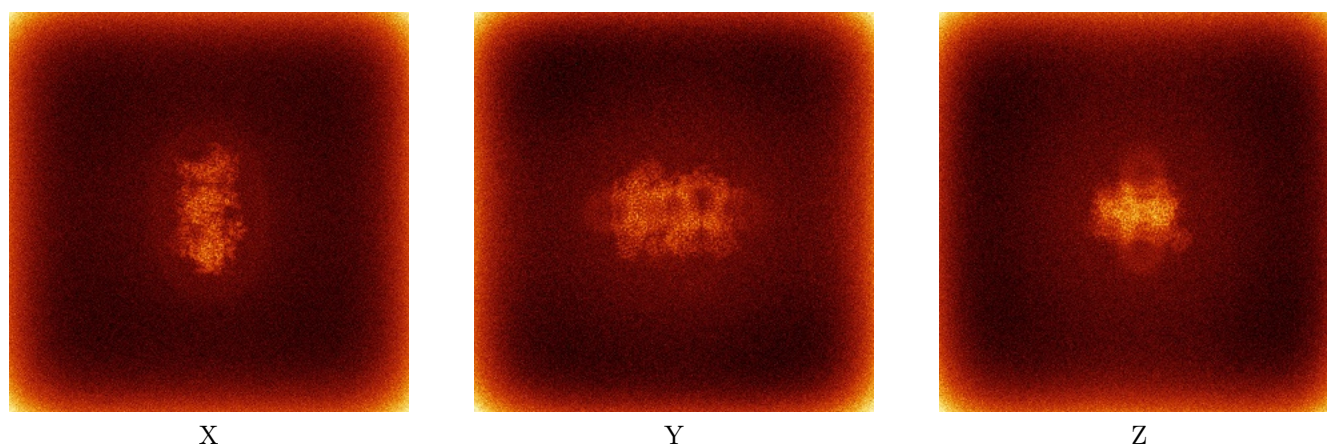
The images above show the largest variance slices of the map in three orthogonal directions.

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](#)

This section was not generated.

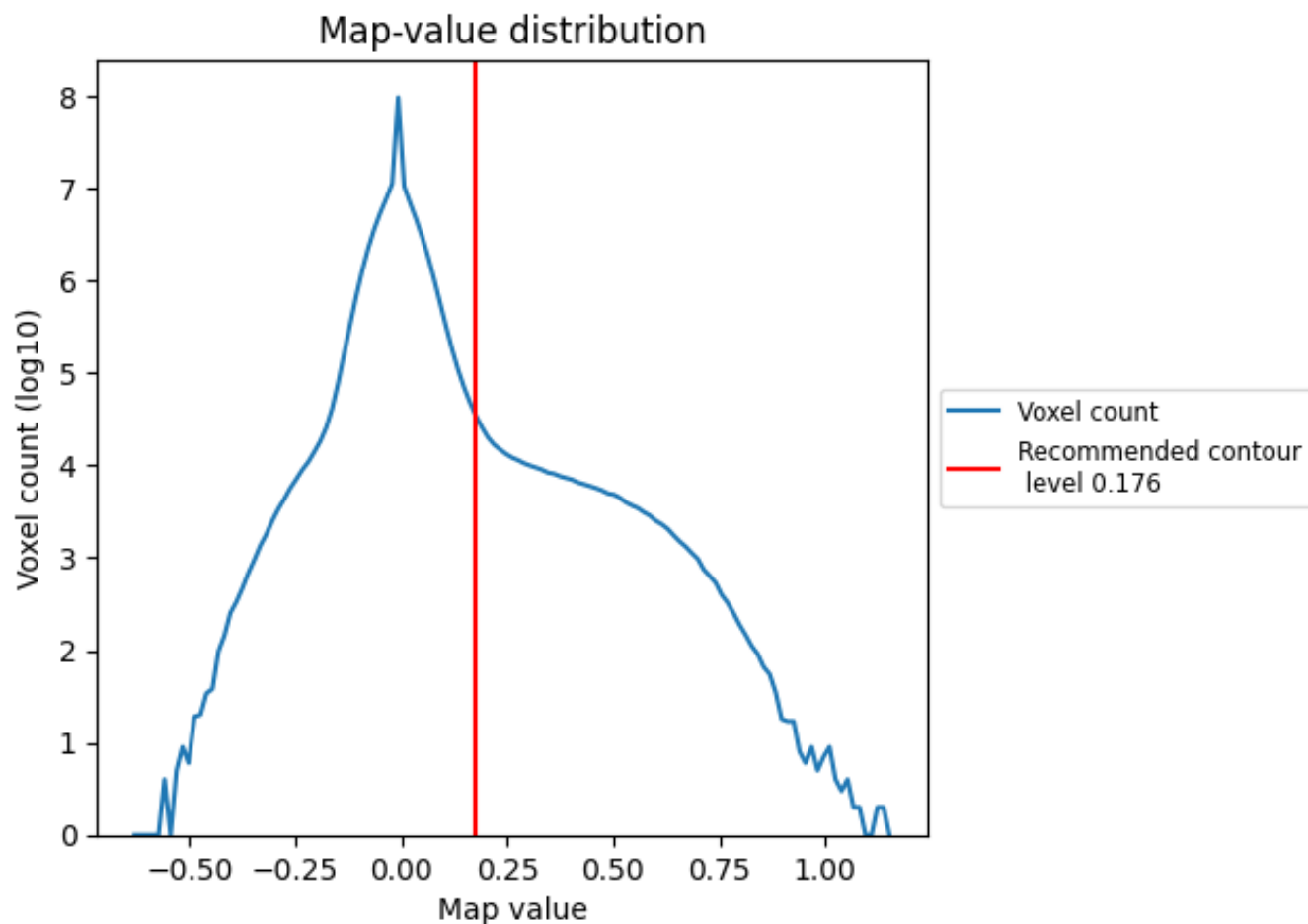
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

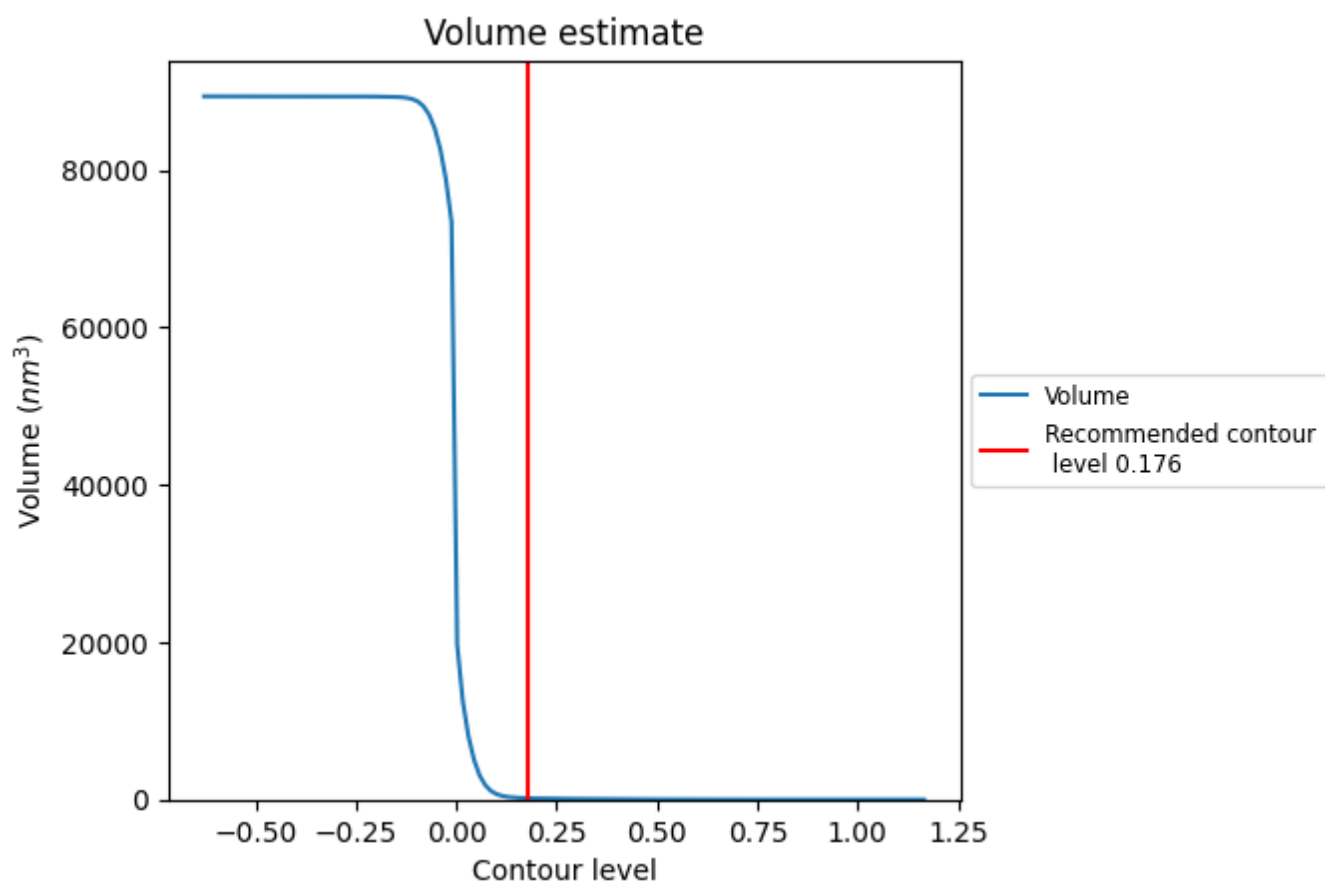
This section contains the results of statistical analysis of the map.

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.

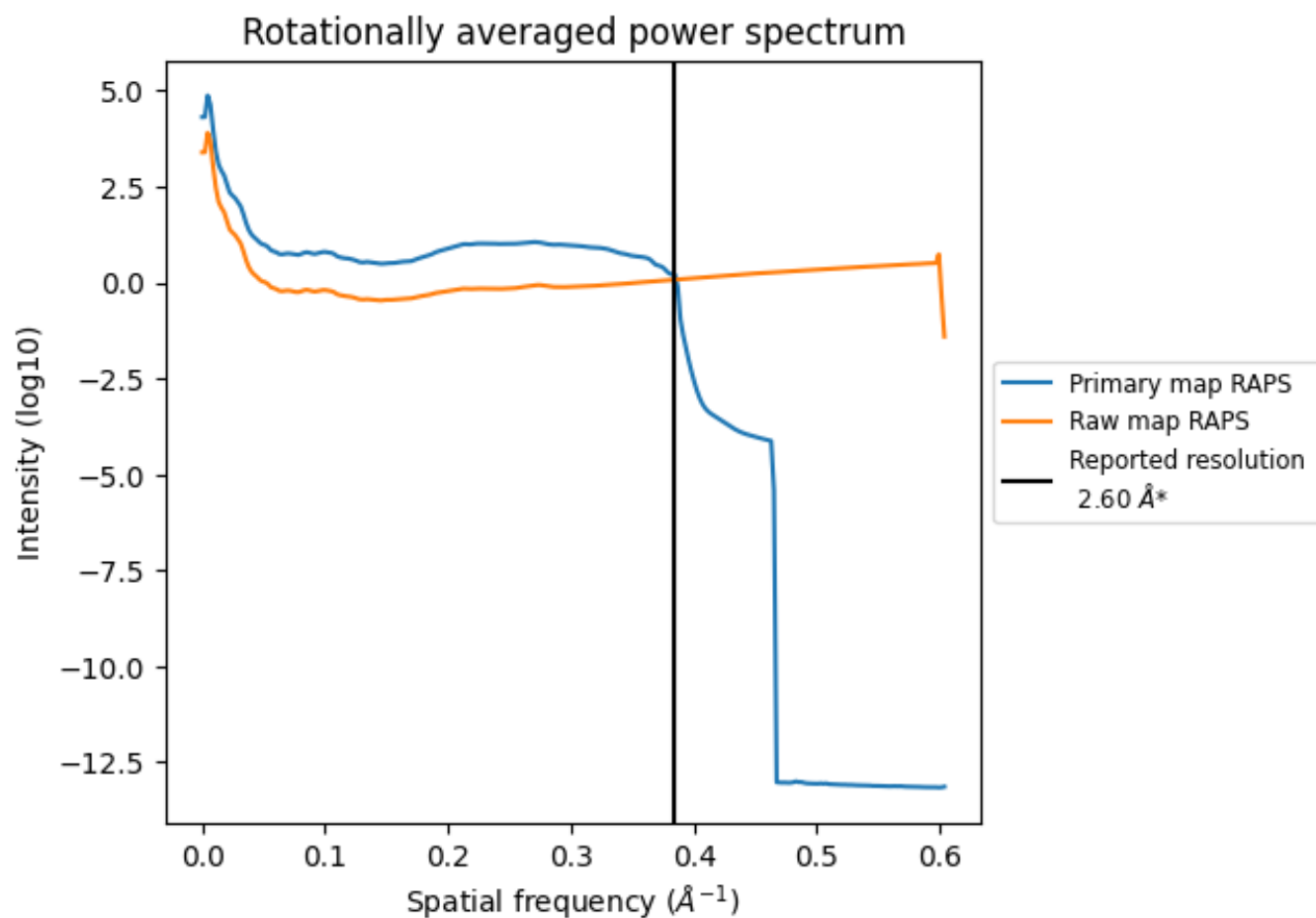
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 174 nm³; 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 ⓘ

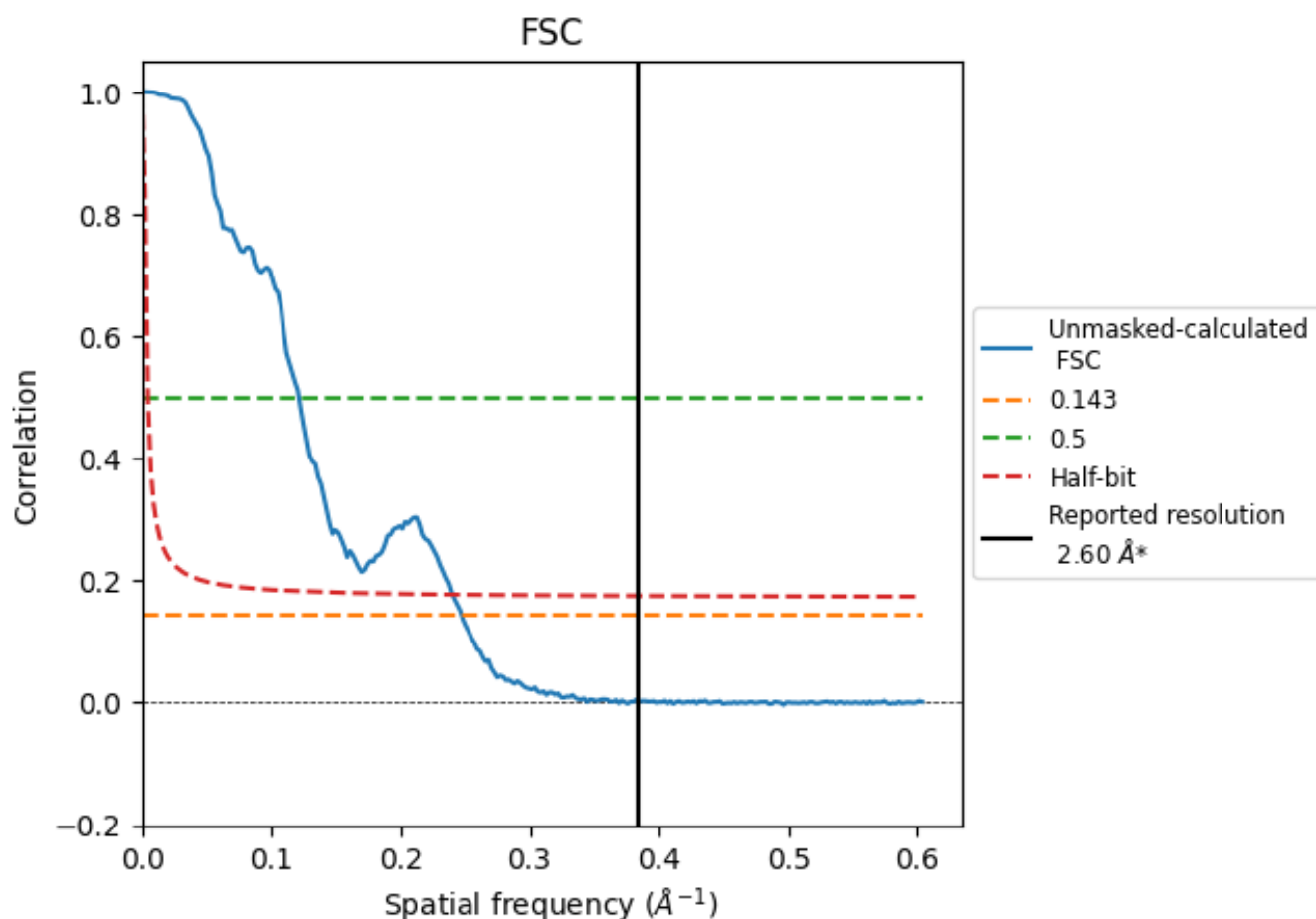


*Reported resolution corresponds to spatial frequency of 0.385 Å⁻¹

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

8.2 Resolution estimates [i](#)

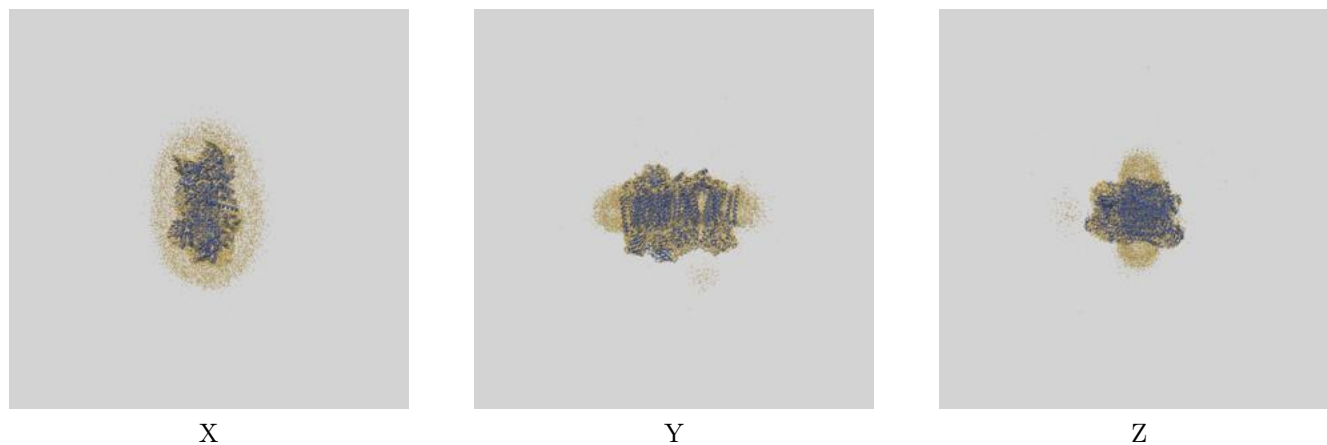
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.05	8.22	4.17

*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](#)

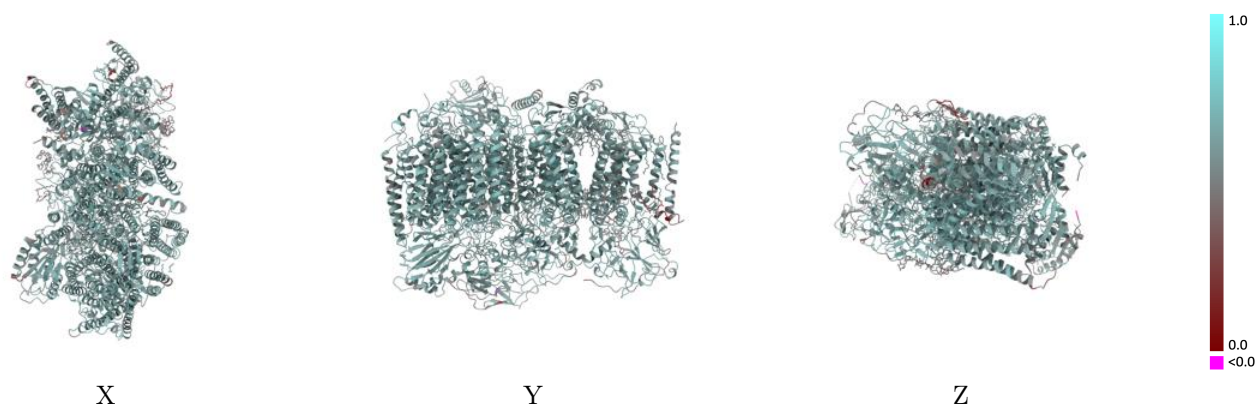
This section contains information regarding the fit between EMDB map EMD-50752 and PDB model 9FTZ. Per-residue inclusion information can be found in [section 3](#) on [page 20](#).

9.1 Map-model overlay [i](#)



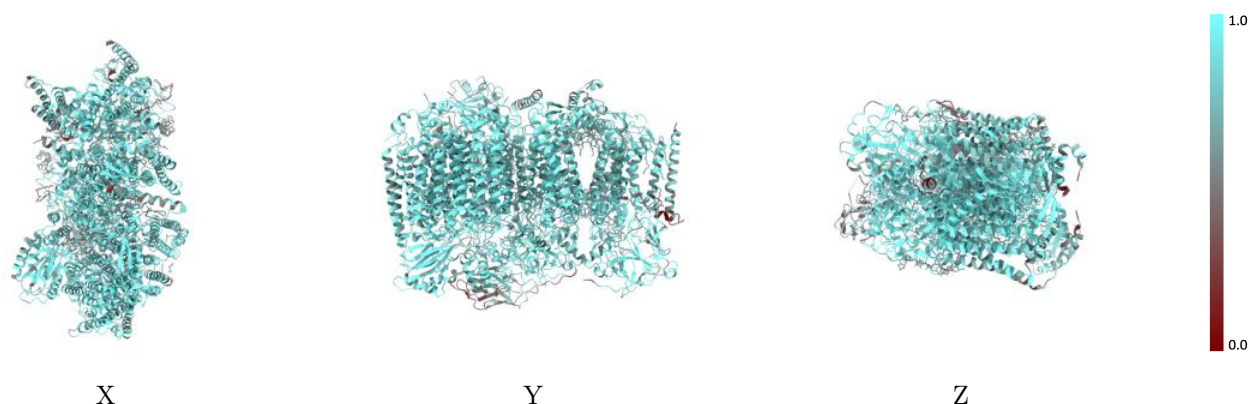
The images above show the 3D surface view of the map at the recommended contour level 0.176 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



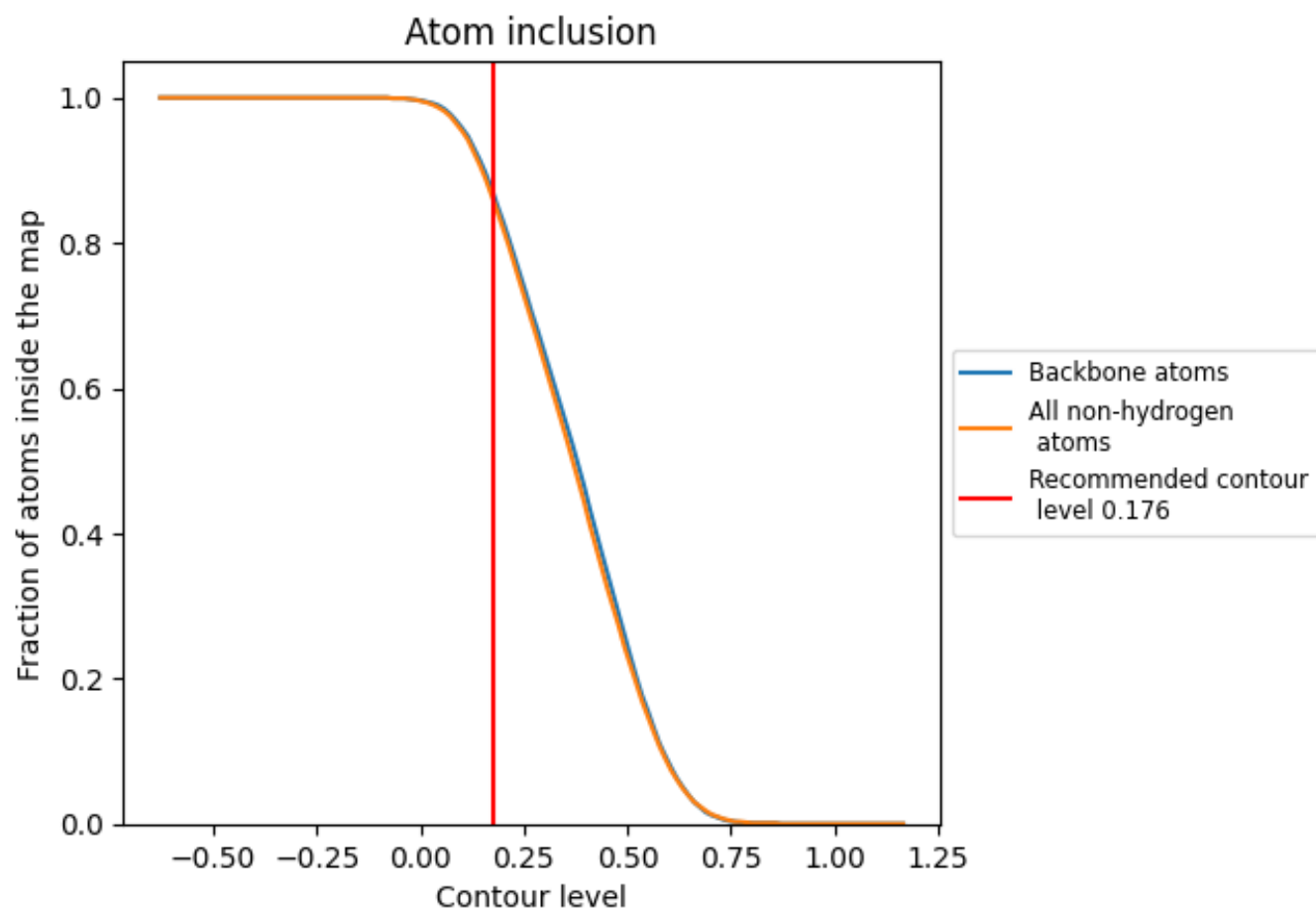
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

1.0

0.0

<0.0