



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 08:28 AM UTC

PDB ID : 9FU0 / pdb_00009fu0
EMDB ID : EMD-50753
Title : CIII2/CIV respiratory chain supercomplex from Mycobacterium smegmatis
Authors : Kovalova, T.; Krol, S.; Gamiz-Hernandez, A.; Sjostrand, D.; Kaila, V.;
Brzezinski, P.; Hogbom, M.
Deposited on : 2024-06-25
Resolution : 2.70 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:

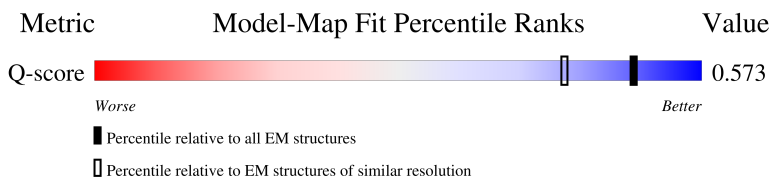
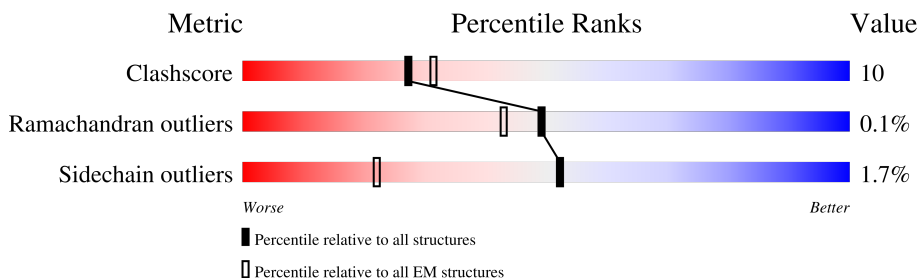
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.70 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.



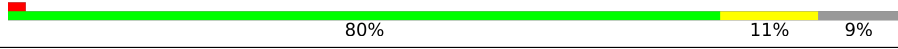
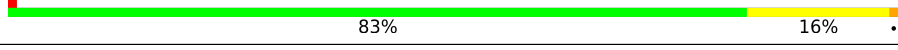
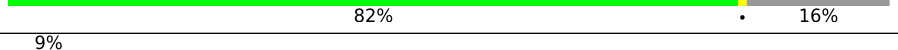
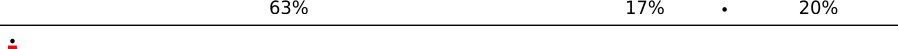
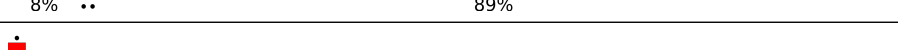
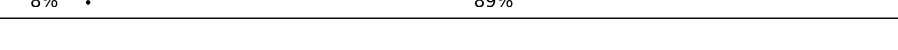
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10327 (2.20 - 3.20)

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	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	MQ9	N	607	-	-	X	-
15	MQ9	N	608	-	-	X	-
15	MQ9	O	304	-	-	X	-
17	FES	G	501	-	-	X	-

2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 30643 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		

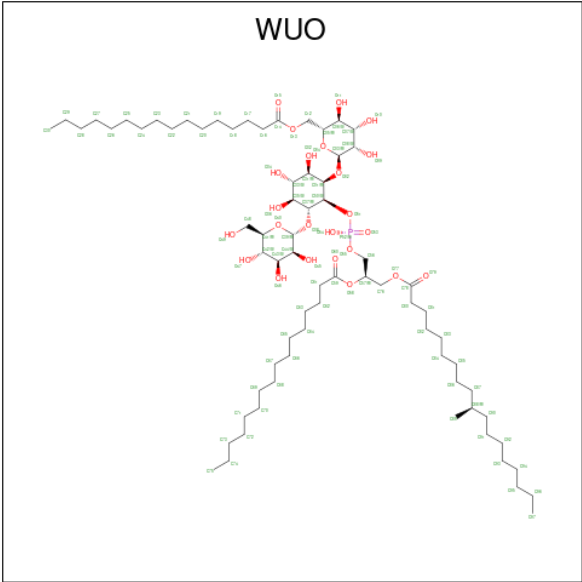
- Molecule 11 is a protein called LpqE protein.

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].

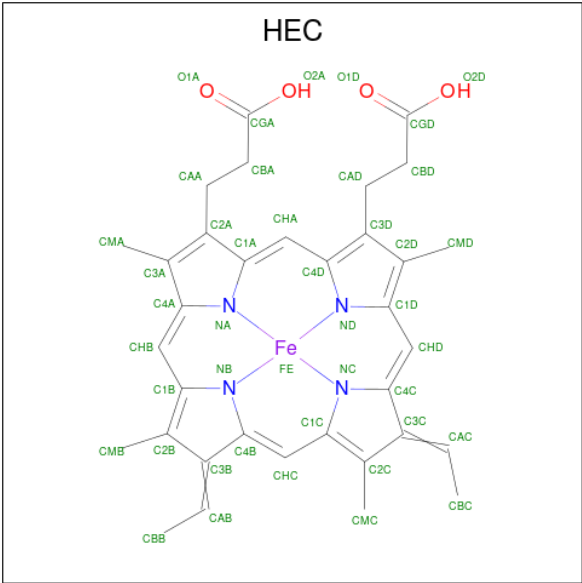
Mol	Chain	Residues	Atoms					AltConf	Trace
12	Y	25	Total	C	N	O	S	0	0
			168	103	26	38	1		
12	c	25	Total	C	N	O	S	0	0
			168	103	26	38	1		

- Molecule 13 is acyl-phosphatidyl-myo-inositol dimannoside (AcPIM2) (CCD ID: WUO) (formula: C₇₂H₁₃₅O₂₄P).



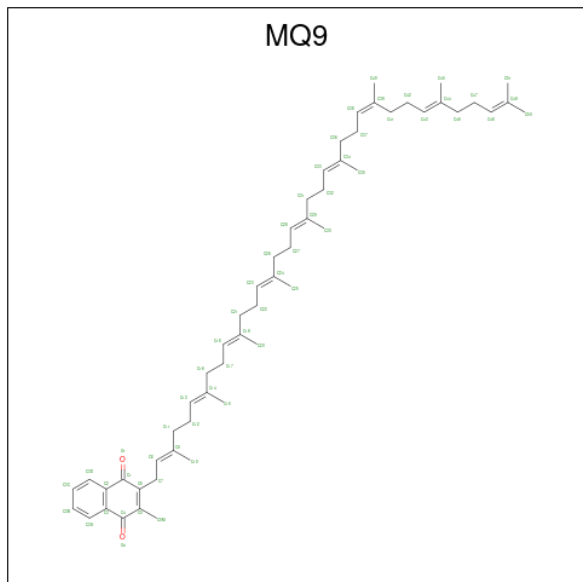
Mol	Chain	Residues	Atoms				AltConf
13	O	1	Total	C	O	P	0
			97	72	24	1	
13	P	1	Total	C	O	P	0
			97	72	24	1	

- Molecule 14 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



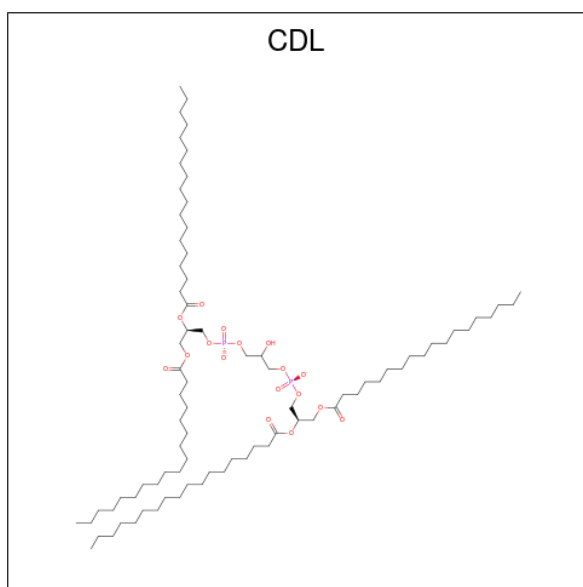
Mol	Chain	Residues	Atoms					AltConf
14	O	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
14	O	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 15 is MENAQUINONE-9 (CCD ID: MQ9) (formula: $C_{56}H_{80}O_2$) (labeled as "Ligand of Interest" by depositor).



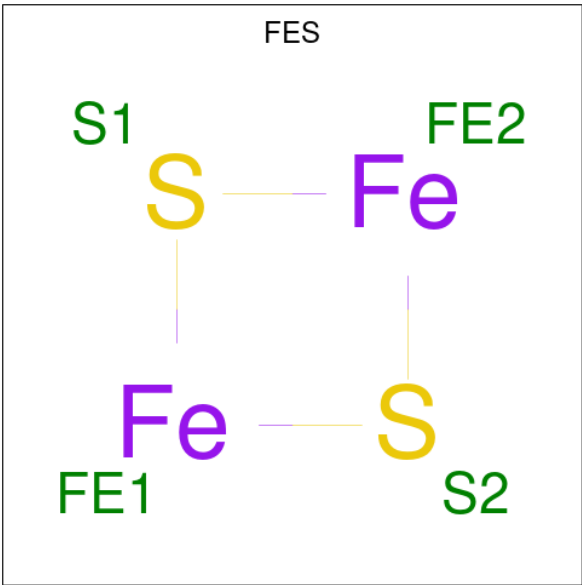
Mol	Chain	Residues	Atoms			AltConf
15	O	1	Total	C	O	0
			58	56	2	
15	N	1	Total	C	O	0
			58	56	2	
15	N	1	Total	C	O	0
			58	56	2	
15	N	1	Total	C	O	0
			58	56	2	
15	H	1	Total	C	O	0
			58	56	2	
15	H	1	Total	C	O	0
			58	56	2	

- Molecule 16 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



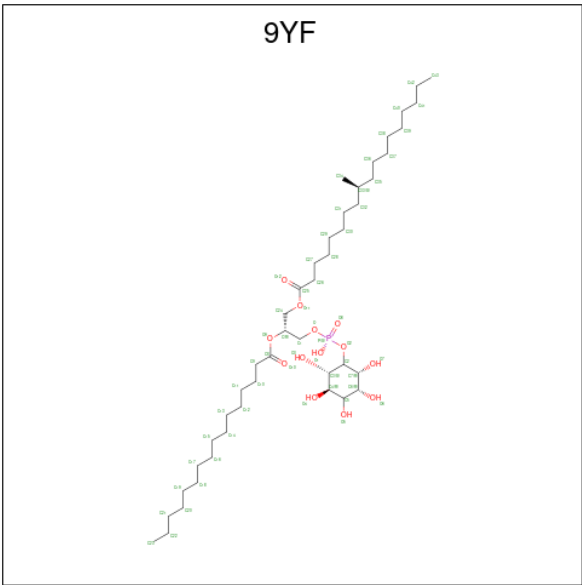
Mol	Chain	Residues	Atoms				AltConf
16	O	1	Total	C	O	P	0
			79	60	17	2	
16	N	1	Total	C	O	P	0
			74	55	17	2	
16	N	1	Total	C	O	P	0
			77	58	17	2	
16	N	1	Total	C	O	P	0
			79	60	17	2	
16	P	1	Total	C	O	P	0
			77	58	17	2	
16	R	1	Total	C	O	P	0
			77	58	17	2	
16	R	1	Total	C	O	P	0
			77	58	17	2	
16	H	1	Total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

- Molecule 17 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



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

- Molecule 18 is (2R)-2-(hexadecanoyloxy)-3-{[(S)-hydroxy{[(1R,2R,3R,4R,5R,6S)-2,3,4,5,6-pentahydroxycyclohexyl]oxy}phosphoryl]oxy}propyl (9S)-9-methyloctadecanoate (CCD ID: 9YF) (formula: C₄₄H₈₅O₁₃P).



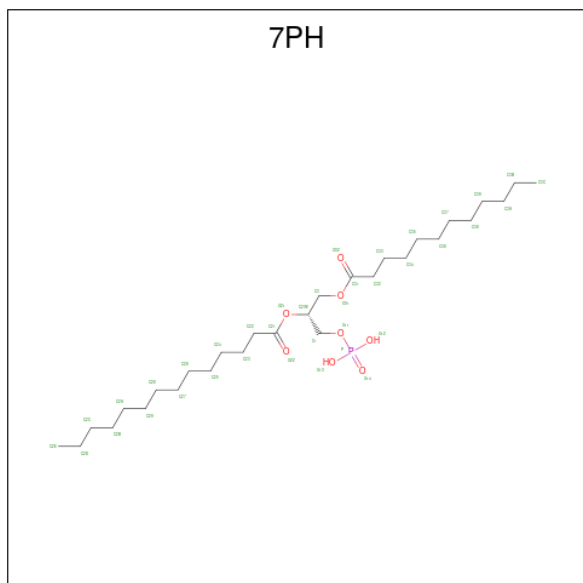
Mol	Chain	Residues	Atoms				AltConf
18	M	1	Total	C	O	P	0
			58	44	13	1	

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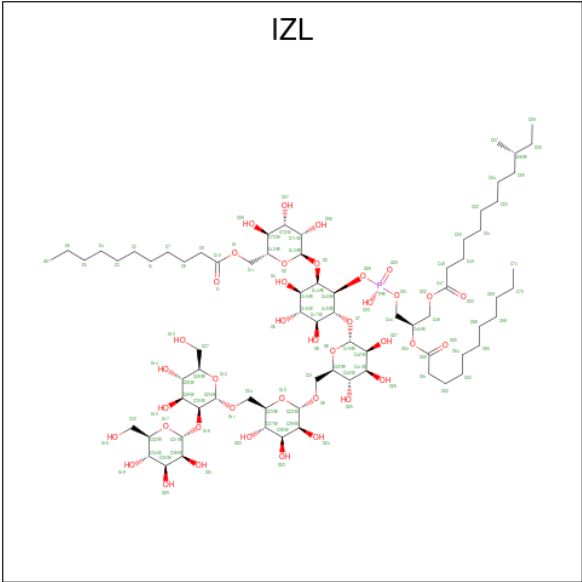
Mol	Chain	Residues	Atoms				AltConf
18	W	1	Total	C	O	P	0
			58	44	13	1	
18	G	1	Total	C	O	P	0
			58	44	13	1	

- Molecule 19 is (1R)-2-(dodecanoyloxy)-1-[(phosphonooxy)methyl]ethyl tetradecanoate (CCD ID: 7PH) (formula: C₂₉H₅₇O₈P).



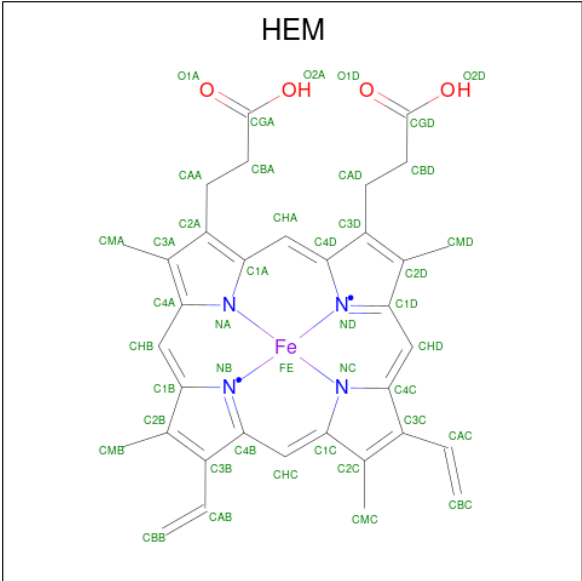
Mol	Chain	Residues	Atoms				AltConf
19	M	1	Total	C	O	P	0
			38	29	8	1	
19	S	1	Total	C	O	P	0
			38	29	8	1	
19	G	1	Total	C	O	P	0
			38	29	8	1	
19	G	1	Total	C	O	P	0
			38	29	8	1	

- Molecule 20 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
20	M	1	Total	C	O	P	0
			114	74	39	1	
20	G	1	Total	C	O	P	0
			114	74	39	1	

- Molecule 21 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



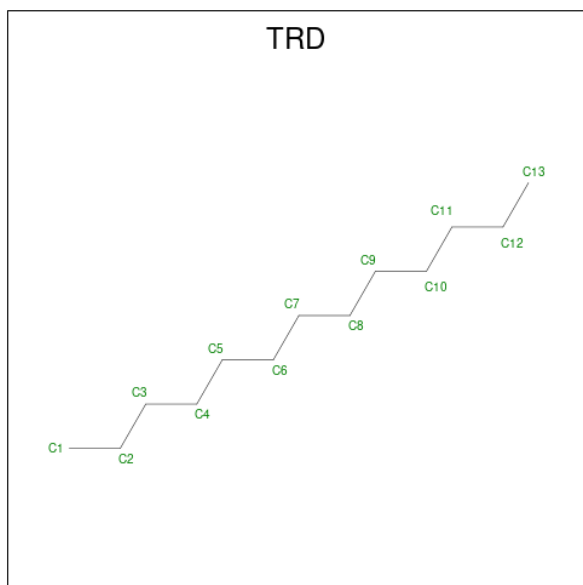
Mol	Chain	Residues	Atoms					AltConf
21	N	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

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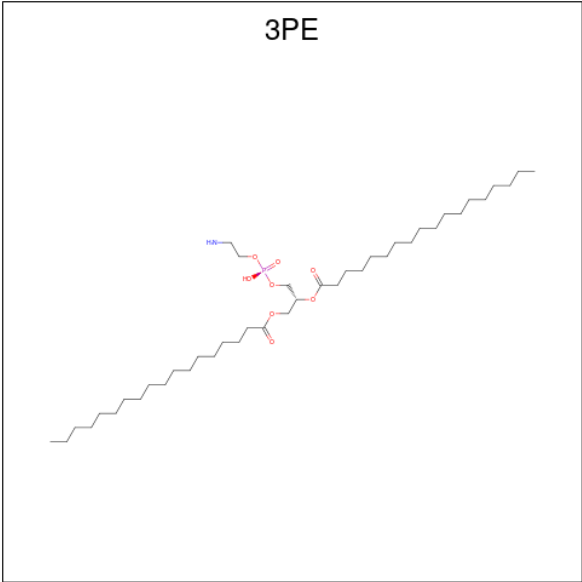
Mol	Chain	Residues	Atoms					AltConf
21	N	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
21	H	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
21	H	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 22 is TRIDECANE (CCD ID: TRD) (formula: $C_{13}H_{28}$).



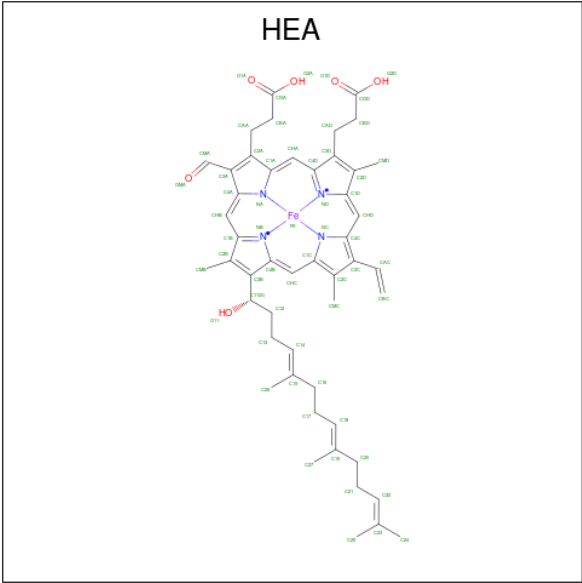
Mol	Chain	Residues	Atoms		AltConf
22	S	1	Total	C	0
			13	13	
22	T	1	Total	C	0
			13	13	
22	R	1	Total	C	0
			13	13	
22	R	1	Total	C	0
			13	13	
22	Q	1	Total	C	0
			13	13	

- Molecule 23 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	
23	S	1	32	22	1	8	1	0

- Molecule 24 is HEME-A (CCD ID: HEA) (formula: C₄₉H₅₆FeN₄O₆).



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

- Molecule 25 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

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

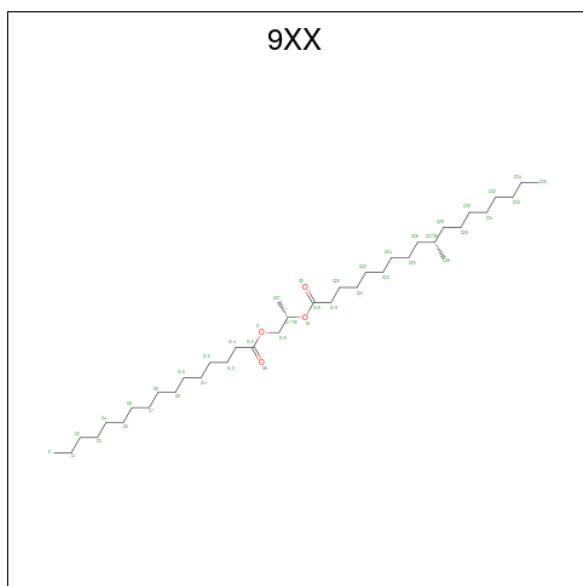
- Molecule 26 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

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

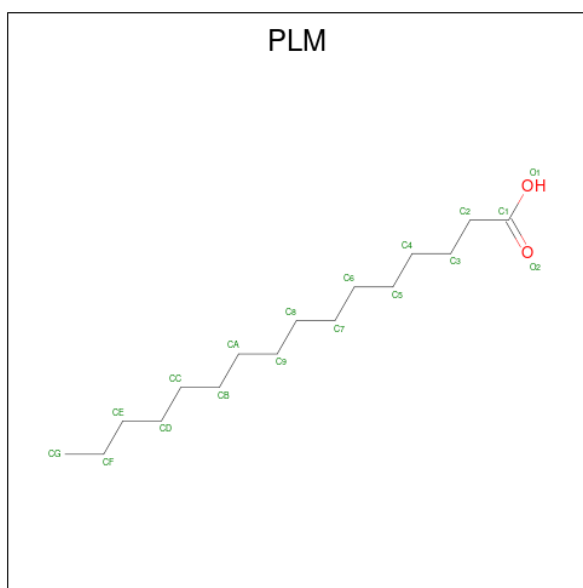
Mol	Chain	Residues	Atoms		AltConf
27	R	1	Total	Mg	0
			1	1	

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



Mol	Chain	Residues	Atoms			AltConf
28	W	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 PALMITIC ACID (CCD ID: PLM) (formula: $C_{16}H_{32}O_2$).



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

- Molecule 30 is water.

Mol	Chain	Residues	Atoms		AltConf
30	O	42	Total	O	0
			42	42	
30	M	37	Total	O	0
			37	37	
30	N	68	Total	O	0
			68	68	
30	P	9	Total	O	0
			9	9	
30	S	6	Total	O	0
			6	6	
30	T	10	Total	O	0
			10	10	
30	R	53	Total	O	0
			53	53	
30	Q	26	Total	O	0
			26	26	

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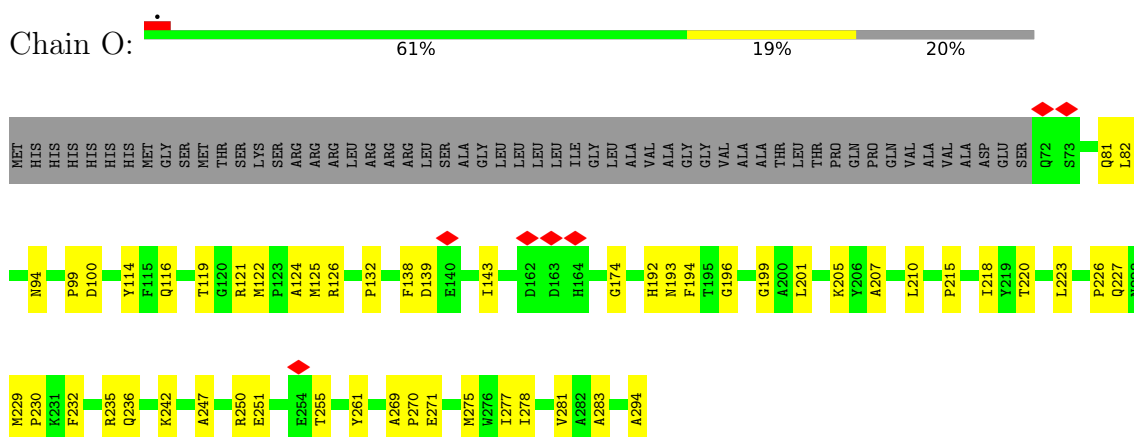
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Mol	Chain	Residues	Atoms		AltConf
30	U	1	Total 1	O 1	0
30	W	8	Total 8	O 8	0
30	Y	1	Total 1	O 1	0
30	H	12	Total 12	O 12	0
30	G	10	Total 10	O 10	0

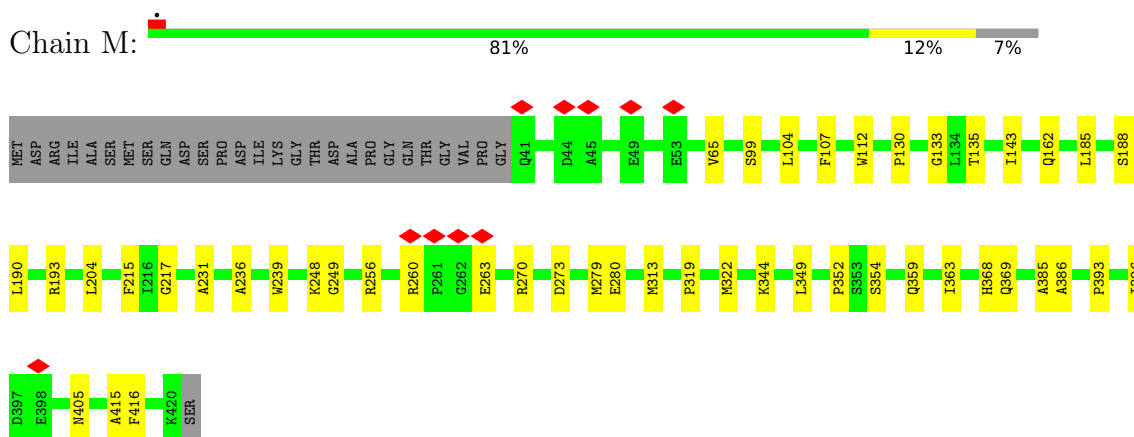
3 Residue-property plots

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

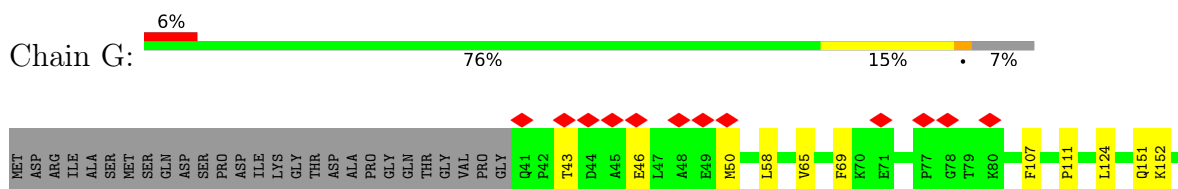
- Molecule 1: Cytochrome bc1 complex cytochrome c subunit



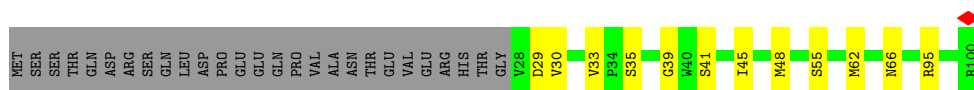
- Molecule 2: Cytochrome bc1 complex cytochrome c subunit



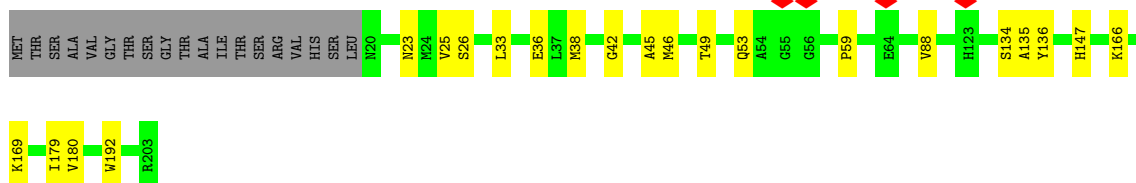
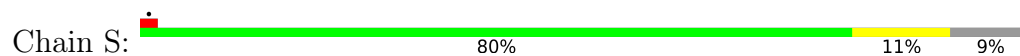
- Molecule 2: Cytochrome bc1 complex cytochrome c subunit



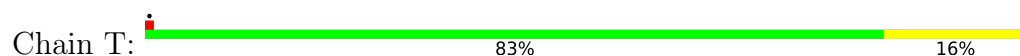




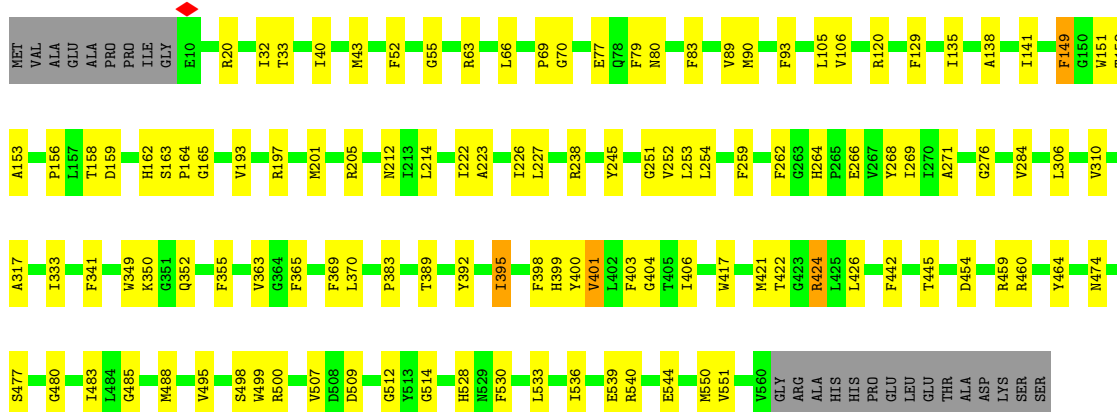
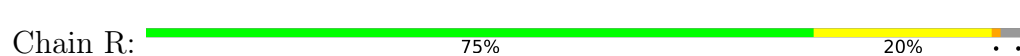
- Molecule 5: Probable cytochrome c oxidase subunit 3



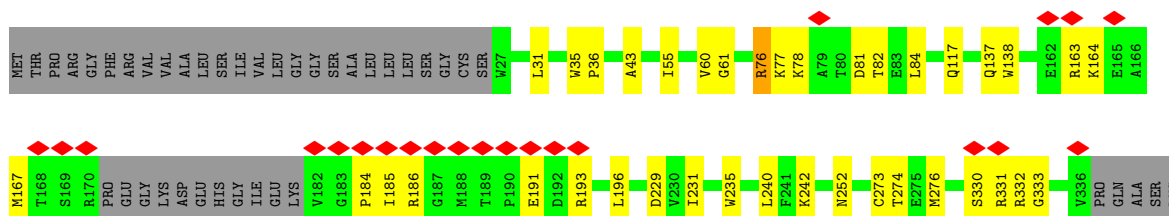
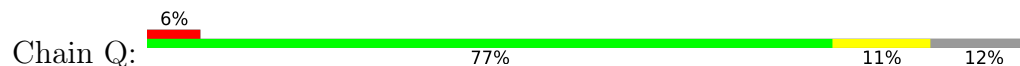
- Molecule 6: Cytochrome c oxidase polypeptide 4



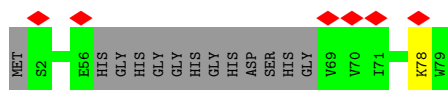
- Molecule 7: Cytochrome c oxidase subunit 1



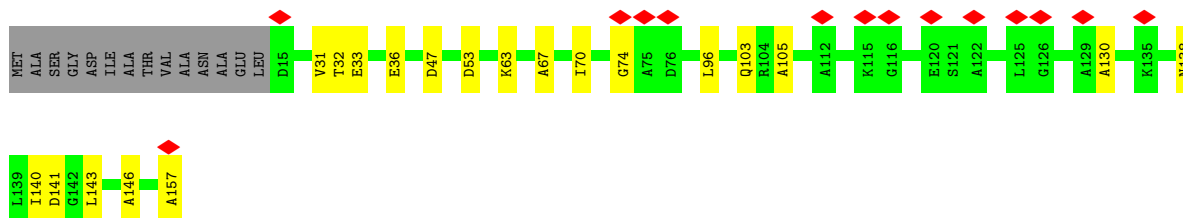
- Molecule 8: cytochrome-c oxidase



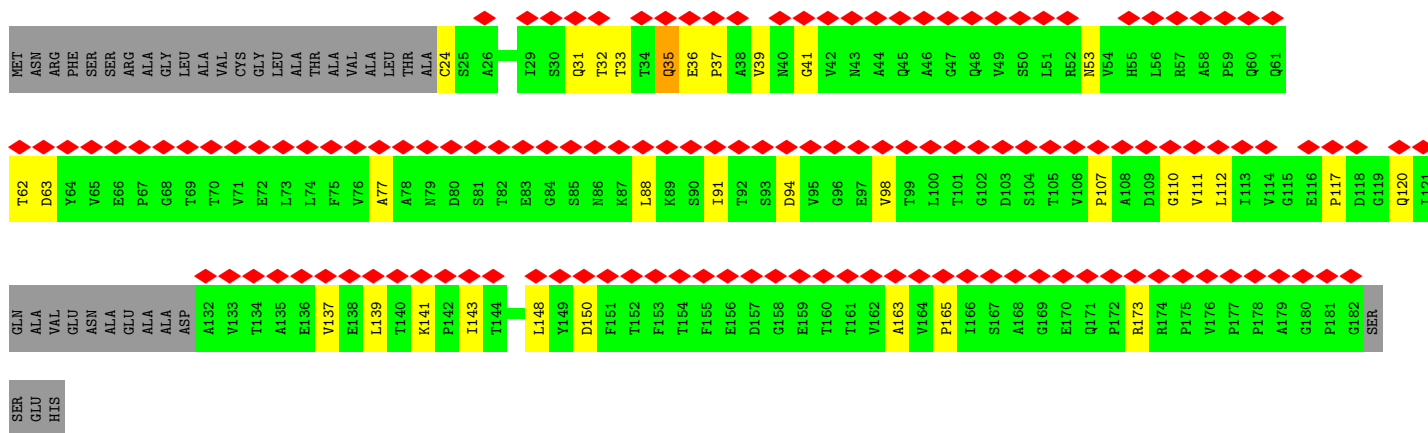
Chain U: 8% 82% 16%



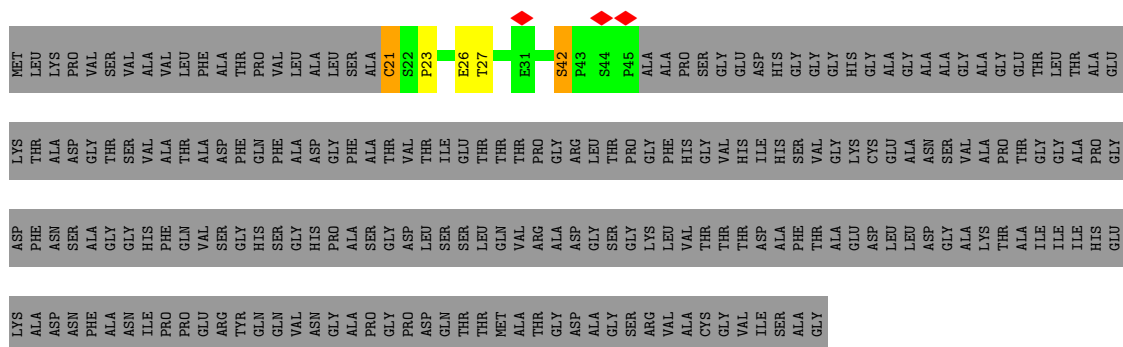
Chain V: 9% 78% 13% 9%



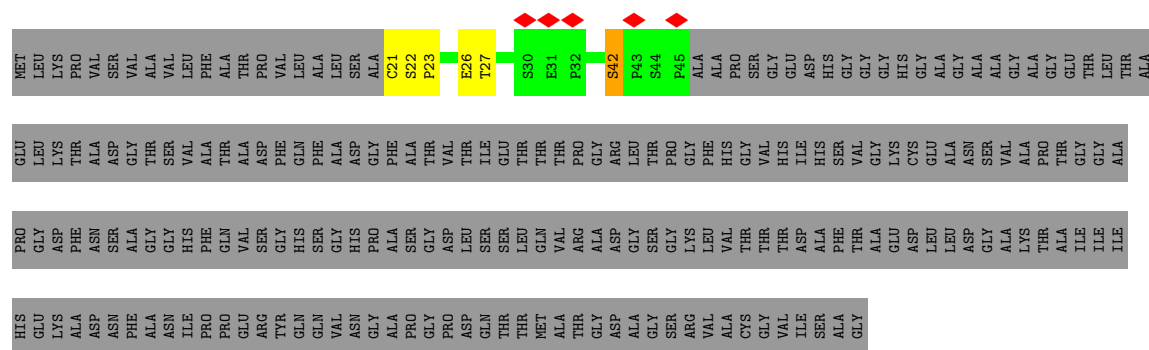
Chain W: 73% 63% 17% 20%



Chain Y: 8% 2% 89%



Chain c: 8% 89%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	51000	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	1.240	Depositor
Minimum map value	-0.656	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.036	Depositor
Recommended contour level	0.204	Depositor
Map size (Å)	444.96, 444.96, 444.96	wwPDB
Map dimensions	540, 540, 540	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.824, 0.824, 0.824	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	O	0.19	0/1660	0.39	0/2250
2	G	0.37	0/3046	0.48	0/4129
2	M	0.22	0/3046	0.33	0/4129
3	H	0.36	0/3534	0.52	3/4820 (0.1%)
3	N	0.42	1/4299 (0.0%)	0.53	1/5862 (0.0%)
4	P	0.18	0/606	0.33	0/825
5	S	0.13	0/1488	0.24	0/2032
6	T	0.37	0/1112	0.52	0/1524
7	R	0.35	0/4529	0.50	2/6187 (0.0%)
8	Q	0.28	0/2447	0.47	1/3330 (0.0%)
9	U	0.08	0/515	0.22	0/704
10	V	0.10	0/1042	0.30	0/1423
11	W	0.32	0/1100	0.44	0/1508
12	Y	0.20	0/175	0.39	0/244
12	c	0.57	0/175	0.69	0/244
All	All	0.32	1/28774 (0.0%)	0.46	7/39211 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	322	PRO	C-O	-6.27	1.19	1.24

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	322	PRO	CB-CA-C	-7.45	105.62	111.87
7	R	400	TYR	N-CA-C	-5.84	106.70	113.88
3	H	20	TYR	CA-C-O	-5.79	112.64	119.48
7	R	70	GLY	CA-C-O	-5.70	118.30	122.23
3	H	172	ARG	N-CA-C	-5.62	106.47	113.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	410	ILE	N-CA-C	-5.20	105.43	110.42
8	Q	81	ASP	CB-CA-C	5.19	120.03	111.31

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	47	0
2	G	2967	0	2976	69	0
2	M	2967	0	2976	43	0
3	H	3425	0	3469	79	0
3	N	4167	0	4192	115	0
4	P	586	0	578	11	0
5	S	1441	0	1439	18	0
6	T	1077	0	1058	19	0
7	R	4369	0	4346	117	0
8	Q	2382	0	2335	46	0
9	U	499	0	504	1	0
10	V	1024	0	1035	13	0
11	W	1083	0	1055	33	0
12	Y	168	0	151	6	0
12	c	168	0	151	4	0
13	O	97	0	0	2	0
13	P	97	0	0	0	0
14	O	86	0	60	6	0
15	H	116	0	160	17	0
15	N	174	0	240	53	0
15	O	58	0	80	24	0
16	H	151	0	190	7	0
16	N	230	0	295	19	0
16	O	79	0	105	5	0
16	P	77	0	98	9	0
16	R	154	0	196	5	0
17	G	4	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	M	4	0	0	1	0
18	G	58	0	0	2	0
18	M	58	0	0	2	0
18	W	58	0	0	2	0
19	G	76	0	110	1	0
19	M	38	0	55	2	0
19	S	38	0	55	3	0
20	G	114	0	0	0	0
20	M	114	0	0	0	0
21	H	86	0	60	8	0
21	N	86	0	60	5	0
22	Q	13	0	28	0	0
22	R	26	0	56	0	0
22	S	13	0	28	0	0
22	T	13	0	28	0	0
23	S	32	0	38	0	0
24	R	120	0	108	22	0
25	Q	2	0	0	1	0
25	R	1	0	0	0	0
26	R	1	0	0	0	0
27	R	1	0	0	0	0
28	W	42	0	0	3	0
28	Y	32	0	0	1	0
28	c	32	0	0	2	0
29	W	11	0	16	3	0
29	Y	11	0	16	0	0
29	c	11	0	16	0	0
30	G	10	0	0	0	0
30	H	12	0	0	0	0
30	M	37	0	0	0	0
30	N	68	0	0	1	0
30	O	42	0	0	0	0
30	P	9	0	0	0	0
30	Q	26	0	0	0	0
30	R	53	0	0	0	0
30	S	6	0	0	0	0
30	T	10	0	0	0	0
30	U	1	0	0	0	0
30	W	8	0	0	0	0
30	Y	1	0	0	0	0
All	All	30643	0	29923	593	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 10.

All (593) 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:Y:21:CYS:SG	28:Y:302:9XX:C37	2.16	1.32
12:c:21:CYS:SG	28:c:302:9XX:C37	2.20	1.30
3:N:337:MET:HE1	15:N:608:MQ9:C3A	1.66	1.25
3:N:337:MET:HE1	15:N:608:MQ9:C3B	1.76	1.15
11:W:36:GLU:HB3	11:W:37:PRO:HD2	1.36	1.04
15:O:304:MQ9:H101	3:N:392:MET:HE1	1.39	1.01
15:H:605:MQ9:H261	15:H:605:MQ9:H301	1.48	0.94
24:R:602:HEA:H212	8:Q:60:VAL:HG11	1.49	0.93
3:N:337:MET:CE	15:N:608:MQ9:C3A	2.47	0.91
16:N:603:CDL:OB3	16:H:602:CDL:H1	1.68	0.91
11:W:24:CYS:SG	28:W:202:9XX:C37	2.58	0.91
15:O:304:MQ9:C10	3:N:392:MET:HE1	1.99	0.91
15:N:607:MQ9:H251	15:N:607:MQ9:H212	1.53	0.90
15:N:607:MQ9:H5M3	15:N:607:MQ9:H8	1.51	0.89
7:R:550:MET:HE2	8:Q:84:LEU:HD12	1.53	0.89
7:R:153:ALA:HB1	7:R:158:THR:HG21	1.53	0.88
16:N:603:CDL:H721	16:N:603:CDL:H162	1.55	0.88
7:R:395:ILE:HD11	7:R:459:ARG:HB2	1.57	0.87
2:G:268:LYS:HD2	2:G:401:TYR:CD1	2.10	0.86
15:O:304:MQ9:H33	15:O:304:MQ9:H401	1.59	0.84
16:H:603:CDL:HA21	16:H:603:CDL:HB32	1.57	0.84
15:N:608:MQ9:H512	15:N:608:MQ9:H461	1.58	0.84
15:O:304:MQ9:H412	3:N:402:ILE:HD11	1.60	0.84
6:T:70:TYR:HB3	6:T:73:ALA:HB2	1.60	0.84
15:N:607:MQ9:H5M3	15:N:607:MQ9:C8	2.06	0.83
3:H:135:ARG:HB2	3:H:138:GLU:OE1	1.80	0.80
2:G:316:ARG:HG3	2:G:339:LEU:CD2	2.10	0.80
11:W:36:GLU:HB3	11:W:37:PRO:CD	2.12	0.80
7:R:395:ILE:HD11	7:R:459:ARG:CB	2.12	0.79
3:N:337:MET:HE1	15:N:608:MQ9:H3A	1.64	0.79
15:N:607:MQ9:C31	15:N:607:MQ9:H261	2.13	0.78
2:G:254:LEU:HD12	2:G:402:LEU:HB3	1.65	0.78
8:Q:76:ARG:CB	8:Q:76:ARG:HH21	1.98	0.77
15:O:304:MQ9:C10	3:N:392:MET:CE	2.63	0.77
2:M:369:GLN:HG3	3:N:404:LEU:HD21	1.68	0.75
7:R:422:THR:HG22	7:R:424:ARG:HG2	1.66	0.75
2:G:279:MET:CG	2:G:313:MET:HG3	2.16	0.75
3:N:266:ALA:HB2	15:N:607:MQ9:H302	1.67	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:337:MET:CE	15:N:608:MQ9:H3A	2.15	0.74
16:N:603:CDL:H112	16:N:603:CDL:H311	1.68	0.74
15:N:608:MQ9:H8	15:N:608:MQ9:C5M	2.18	0.73
21:H:601:HEM:HHC	21:H:601:HEM:HBB2	1.69	0.73
21:H:601:HEM:HBC2	21:H:601:HEM:HHH	1.69	0.72
2:G:349:LEU:HD12	2:G:368:HIS:CE1	2.24	0.72
3:N:265:PHE:CD2	15:N:607:MQ9:C35	2.73	0.72
7:R:395:ILE:HG12	24:R:603:HEA:HAA2	1.72	0.72
10:V:130:ALA:HB2	10:V:146:ALA:HB2	1.71	0.72
2:G:314:LEU:CD2	2:G:339:LEU:HD22	2.20	0.71
3:H:160:SER:OG	3:H:171:ILE:HD11	1.89	0.71
2:G:316:ARG:HG3	2:G:339:LEU:HD23	1.70	0.71
3:N:193:LEU:HB2	15:N:608:MQ9:H161	1.71	0.71
3:N:370:VAL:HG22	4:P:39:GLY:HA3	1.71	0.71
15:O:304:MQ9:H401	15:O:304:MQ9:C33	2.21	0.70
3:H:231:TRP:HE3	15:H:605:MQ9:H5M2	1.54	0.70
2:M:359:GLN:CG	11:W:35:GLN:HG2	2.21	0.69
15:H:606:MQ9:H48	15:H:606:MQ9:H453	1.74	0.69
7:R:401:VAL:CG1	24:R:602:HEA:C3C	2.70	0.69
3:H:104:PHE:HE2	15:H:605:MQ9:H512	1.56	0.69
7:R:395:ILE:CD1	7:R:459:ARG:HB3	2.23	0.69
3:N:206:ARG:HD3	15:N:608:MQ9:H203	1.74	0.68
7:R:253:LEU:HD23	8:Q:252:ASN:HB3	1.74	0.68
7:R:550:MET:HE2	8:Q:84:LEU:CD1	2.21	0.68
7:R:93:PHE:HA	7:R:129:PHE:HZ	1.58	0.68
1:O:125:MET:HG3	7:R:162:HIS:HA	1.75	0.68
3:H:316:PRO:HA	3:H:412:ARG:NH1	2.09	0.68
3:H:295:VAL:HB	2:G:352:PRO:HG2	1.76	0.68
15:N:608:MQ9:H461	15:N:608:MQ9:C51	2.22	0.67
2:M:359:GLN:HG3	11:W:35:GLN:HG2	1.74	0.67
7:R:395:ILE:CD1	7:R:459:ARG:CB	2.73	0.67
16:H:603:CDL:HA4	16:H:603:CDL:H712	1.75	0.67
3:N:189:MET:HE2	15:N:608:MQ9:H122	1.78	0.66
2:G:254:LEU:O	2:G:269:MET:HG3	1.95	0.66
1:O:81:GLN:HE22	8:Q:163:ARG:HB2	1.59	0.66
3:H:231:TRP:CE3	15:H:605:MQ9:H5M2	2.31	0.66
15:O:304:MQ9:H253	15:O:304:MQ9:H28	1.78	0.66
2:M:143:ILE:HG22	15:N:607:MQ9:H301	1.76	0.66
3:N:67:SER:HB3	3:N:87:ARG:HB2	1.78	0.66
2:M:133:GLY:HA3	3:N:277:GLY:HA3	1.78	0.65
2:M:344:LYS:HE3	2:M:354:SER:HB3	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:126:ARG:HB2	7:R:77:GLU:HG2	1.78	0.65
11:W:88:LEU:HD21	11:W:91:ILE:HD11	1.78	0.65
2:G:169:SER:HB2	2:G:174:ARG:HG3	1.77	0.65
3:N:220:LEU:CD1	16:N:603:CDL:C83	2.75	0.65
15:N:607:MQ9:H8	15:N:607:MQ9:C5M	2.26	0.65
21:H:604:HEM:HBB2	21:H:604:HEM:HHC	1.79	0.65
2:M:393:PRO:HB2	2:M:405:ASN:HB3	1.77	0.65
1:O:132:PRO:HG2	7:R:164:PRO:HB2	1.79	0.64
16:P:301:CDL:H511	16:P:301:CDL:H721	1.79	0.64
15:N:607:MQ9:H212	15:N:607:MQ9:C25	2.27	0.64
3:H:262:GLY:HA3	15:H:605:MQ9:H221	1.78	0.64
3:H:172:ARG:HD2	3:H:172:ARG:O	1.98	0.64
8:Q:273:CYS:SG	25:Q:402:CU:CU	1.87	0.64
3:H:60:LEU:HD13	21:H:601:HEM:HBD1	1.80	0.64
3:N:29:GLN:HE21	16:N:603:CDL:HB4	1.62	0.64
16:P:301:CDL:H111	16:R:605:CDL:HA62	1.80	0.64
3:N:265:PHE:CD2	15:N:607:MQ9:H353	2.33	0.63
11:W:98:VAL:HG22	11:W:137:VAL:HG22	1.80	0.63
2:M:369:GLN:CG	3:N:404:LEU:HD21	2.27	0.63
3:N:265:PHE:HB3	15:N:607:MQ9:H351	1.80	0.63
3:N:253:VAL:HA	3:N:257:PHE:HB3	1.81	0.63
5:S:166:LYS:HE3	19:S:501:7PH:H1A	1.80	0.63
3:H:184:VAL:H	2:G:417:TRP:CG	2.17	0.63
15:N:608:MQ9:H512	15:N:608:MQ9:C46	2.28	0.63
3:H:38:TRP:HZ2	16:H:603:CDL:HB61	1.65	0.62
15:O:304:MQ9:H102	3:N:392:MET:CE	2.29	0.62
15:O:304:MQ9:H452	18:W:201:9YF:C34	2.29	0.62
15:O:304:MQ9:H472	3:N:410:ILE:HG21	1.82	0.62
7:R:266:GLU:HA	7:R:269:ILE:HD12	1.82	0.62
3:H:185:ILE:HD12	18:G:502:9YF:C34	2.29	0.62
3:N:29:GLN:HA	3:N:29:GLN:OE1	2.00	0.61
7:R:152:THR:HA	7:R:259:PHE:CZ	2.34	0.61
7:R:162:HIS:NE2	8:Q:229:ASP:HB2	2.14	0.61
14:O:303:HEC:HMD3	11:W:32:THR:O	2.00	0.61
6:T:26:THR:HG22	6:T:30:ALA:HB2	1.82	0.61
7:R:485:GLY:HA2	24:R:603:HEA:H161	1.81	0.61
21:N:606:HEM:HMC2	21:N:606:HEM:HBC2	1.83	0.61
3:N:232:PHE:CZ	16:N:603:CDL:H712	2.36	0.61
11:W:24:CYS:N	29:W:203:PLM:O2	2.33	0.61
2:G:349:LEU:HD12	2:G:368:HIS:HE1	1.62	0.61
2:M:188:SER:HB2	2:G:155:ILE:HG12	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:230:VAL:HG11	21:H:604:HEM:HAA1	1.83	0.61
7:R:401:VAL:HG11	24:R:602:HEA:C4C	2.30	0.61
3:N:73:TYR:HB2	3:N:85:MET:HE3	1.82	0.61
3:N:230:VAL:CG1	15:N:607:MQ9:H3B	2.31	0.60
7:R:120:ARG:HB2	16:R:601:CDL:PB2	2.40	0.60
15:N:607:MQ9:H261	15:N:607:MQ9:H311	1.81	0.60
15:N:608:MQ9:H8	15:N:608:MQ9:H5M1	1.82	0.60
7:R:539:GLU:HG2	7:R:540:ARG:HG3	1.82	0.60
2:M:319:PRO:HG3	11:W:165:PRO:HG3	1.84	0.60
3:N:230:VAL:HG11	21:N:606:HEM:HAA1	1.83	0.60
7:R:401:VAL:HG13	24:R:602:HEA:C3C	2.31	0.60
3:H:184:VAL:HA	2:G:417:TRP:CD1	2.37	0.60
3:N:227:LEU:O	15:N:607:MQ9:H3C	2.02	0.59
7:R:424:ARG:HH11	7:R:424:ARG:CG	2.14	0.59
2:G:368:HIS:HB2	17:G:501:FES:S1	2.42	0.59
21:H:604:HEM:HBC2	21:H:604:HEM:HMC2	1.84	0.59
12:c:21:CYS:HG	28:c:302:9XX:C37	2.15	0.59
16:O:305:CDL:H161	19:S:501:7PH:H35	1.83	0.59
3:H:56:THR:HG23	15:H:605:MQ9:H453	1.83	0.59
2:G:274:ILE:O	2:G:274:ILE:HG23	2.02	0.59
7:R:355:PHE:HE1	7:R:363:VAL:HG21	1.66	0.59
3:H:171:ILE:O	3:H:171:ILE:HG22	2.02	0.59
3:H:195:GLY:O	2:G:221:LYS:HE2	2.03	0.59
5:S:53:GLN:HB3	8:Q:186:ARG:HH11	1.66	0.59
24:R:602:HEA:HBC1	24:R:602:HEA:HMC3	1.85	0.59
7:R:105:LEU:HB3	7:R:421:MET:HE3	1.85	0.58
5:S:134:SER:HA	8:Q:184:PRO:HA	1.85	0.58
1:O:126:ARG:HH22	7:R:165:GLY:HA3	1.68	0.58
7:R:251:GLY:HA2	7:R:254:LEU:HB3	1.85	0.58
3:H:261:SER:OG	15:H:605:MQ9:H121	2.03	0.58
1:O:192:HIS:CE1	1:O:210:LEU:HD21	2.39	0.58
7:R:32:ILE:HG13	7:R:33:THR:HG23	1.85	0.58
28:W:202:9XX:C15	29:W:203:PLM:H62	2.33	0.58
2:M:107:PHE:HE2	2:G:217:GLY:HA3	1.69	0.58
11:W:41:GLY:HA3	11:W:53:ASN:HA	1.86	0.58
7:R:245:TYR:HA	7:R:251:GLY:HA3	1.85	0.58
15:O:304:MQ9:H412	3:N:402:ILE:CD1	2.34	0.57
2:M:65:VAL:HG22	2:M:162:GLN:HB2	1.86	0.57
1:O:226:PRO:HB2	14:O:302:HEC:HBD1	1.87	0.57
3:H:253:VAL:HA	3:H:257:PHE:HB3	1.86	0.57
3:N:337:MET:HE1	15:N:608:MQ9:H3B	1.82	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:172:ARG:HD2	3:H:172:ARG:C	2.30	0.57
3:H:262:GLY:HA2	15:H:605:MQ9:H201	1.87	0.57
5:S:45:ALA:HB1	6:T:37:ALA:HA	1.85	0.57
24:R:602:HEA:HBC1	24:R:602:HEA:CMC	2.34	0.57
2:G:363:ILE:HB	2:G:372:PHE:HB2	1.86	0.57
3:N:26:VAL:O	3:N:30:LEU:HG	2.05	0.57
15:O:304:MQ9:C20	6:T:113:LEU:HD21	2.35	0.57
7:R:383:PRO:HG3	8:Q:117:GLN:HB3	1.87	0.57
15:N:607:MQ9:H261	15:N:607:MQ9:H312	1.86	0.56
3:N:212:ILE:HD11	3:H:212:ILE:HD11	1.86	0.56
3:N:26:VAL:CG1	3:N:30:LEU:HD11	2.34	0.56
3:N:319:GLU:O	12:Y:21:CYS:HB2	2.04	0.56
24:R:602:HEA:H212	8:Q:60:VAL:CG1	2.30	0.56
3:H:194:PHE:CD2	3:H:203:LEU:HD12	2.41	0.56
3:N:25:ALA:O	3:N:29:GLN:HG2	2.06	0.56
2:G:393:PRO:HB2	2:G:405:ASN:HB3	1.86	0.56
3:N:323:PHE:N	3:N:323:PHE:CD1	2.73	0.56
15:H:605:MQ9:H261	15:H:605:MQ9:C30	2.21	0.56
15:O:304:MQ9:H311	15:O:304:MQ9:C35	2.36	0.56
3:H:31:ASN:HB3	2:G:65:VAL:HG21	1.88	0.56
10:V:138:ASN:HB3	10:V:141:ASP:HB2	1.87	0.56
2:G:328:ARG:HD2	2:G:377:PHE:CD2	2.41	0.56
15:O:304:MQ9:H311	15:O:304:MQ9:H352	1.88	0.56
6:T:128:LEU:HD11	7:R:120:ARG:HD2	1.88	0.56
3:H:194:PHE:HE2	3:H:203:LEU:CD1	2.18	0.56
5:S:23:ASN:HB3	5:S:26:SER:HB2	1.87	0.56
3:N:369:ASP:HA	3:N:434:GLN:HE21	1.69	0.56
7:R:355:PHE:CE2	8:Q:76:ARG:HD3	2.41	0.56
16:H:603:CDL:H162	16:H:603:CDL:H361	1.88	0.55
3:N:136:PRO:HG3	3:N:360:HIS:CE1	2.42	0.55
3:H:411:GLY:O	3:H:415:MET:HG3	2.06	0.55
3:H:104:PHE:CE2	15:H:605:MQ9:H512	2.41	0.55
15:O:304:MQ9:O1	15:O:304:MQ9:H8	2.05	0.55
8:Q:76:ARG:HH21	8:Q:76:ARG:HB2	1.72	0.55
9:U:78:LYS:HA	10:V:105:ALA:HA	1.89	0.55
3:H:194:PHE:CE2	3:H:203:LEU:CD1	2.89	0.55
3:H:314:LEU:O	3:H:412:ARG:HG2	2.07	0.55
8:Q:76:ARG:HH21	8:Q:76:ARG:CG	2.18	0.55
3:H:194:PHE:HE2	3:H:203:LEU:HD11	1.72	0.55
15:O:304:MQ9:H253	15:O:304:MQ9:C28	2.36	0.55
8:Q:43:ALA:HB1	8:Q:240:LEU:HD12	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:V:47:ASP:HB3	10:V:140:ILE:HG21	1.88	0.55
2:G:316:ARG:HG3	2:G:339:LEU:HD21	1.86	0.55
21:N:602:HEM:HMB1	21:N:602:HEM:HBB2	1.89	0.55
3:H:291:LYS:HB2	3:H:294:GLN:HG2	1.87	0.55
2:G:364:LEU:HD13	2:G:371:GLN:NE2	2.22	0.55
2:G:316:ARG:CG	2:G:339:LEU:HD23	2.37	0.55
1:O:235:ARG:HA	11:W:173:ARG:HB2	1.88	0.54
21:N:606:HEM:HMB1	21:N:606:HEM:HBB2	1.89	0.54
2:G:181:LEU:HB3	19:G:505:7PH:H32	1.88	0.54
3:N:412:ARG:HB3	4:P:62:MET:HE1	1.88	0.54
3:H:194:PHE:CE2	3:H:203:LEU:HD12	2.42	0.54
3:N:165:LEU:HD21	3:N:294:GLN:HB3	1.89	0.54
2:M:322:MET:HG3	11:W:148:LEU:HD11	1.90	0.54
2:M:215:PHE:HD2	15:H:605:MQ9:H502	1.73	0.54
7:R:401:VAL:HG11	24:R:602:HEA:C3C	2.36	0.54
2:M:231:ALA:HB1	2:M:248:LYS:HD3	1.89	0.54
2:G:314:LEU:HD22	2:G:339:LEU:HD22	1.88	0.54
7:R:93:PHE:HA	7:R:129:PHE:CZ	2.41	0.54
2:G:279:MET:HG2	2:G:313:MET:HG3	1.89	0.54
2:M:217:GLY:HA3	2:G:107:PHE:HE2	1.72	0.54
6:T:90:TRP:HB3	7:R:33:THR:HG22	1.89	0.54
2:M:359:GLN:HG3	11:W:35:GLN:CG	2.38	0.53
7:R:317:ALA:HB2	7:R:389:THR:HG21	1.89	0.53
7:R:365:PHE:HD1	7:R:404:GLY:O	1.90	0.53
7:R:495:VAL:HG11	16:R:605:CDL:H391	1.90	0.53
15:H:606:MQ9:H453	15:H:606:MQ9:C48	2.33	0.53
2:G:293:THR:HG23	2:G:294:THR:HG23	1.89	0.53
1:O:251:GLU:O	1:O:255:THR:HG23	2.08	0.53
15:O:304:MQ9:H33	15:O:304:MQ9:C40	2.35	0.53
3:N:67:SER:HB2	3:H:67:SER:HB2	1.88	0.53
16:H:602:CDL:OA7	16:H:602:CDL:HA22	2.08	0.53
15:O:304:MQ9:C28	15:O:304:MQ9:C25	2.86	0.53
2:M:204:LEU:HD11	15:H:605:MQ9:H303	1.90	0.53
2:G:249:GLY:HA3	12:c:42:SER:HB2	1.90	0.53
16:P:301:CDL:H411	7:R:500:ARG:HH22	1.74	0.53
7:R:499:TRP:HE1	16:R:605:CDL:HA32	1.73	0.53
7:R:480:GLY:HA2	7:R:483:ILE:HD12	1.90	0.53
1:O:82:LEU:HD22	1:O:138:PHE:CE1	2.43	0.53
2:G:256:ARG:HD3	2:G:280:GLU:HG2	1.91	0.53
2:G:308:VAL:HG13	2:G:309:ARG:HG3	1.89	0.53
1:O:139:ASP:O	1:O:143:ILE:HG13	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:304:MQ9:H352	15:O:304:MQ9:C31	2.39	0.52
24:R:603:HEA:H261	24:R:603:HEA:C18	2.37	0.52
5:S:25:VAL:HG12	5:S:180:VAL:HG11	1.92	0.52
11:W:117:PRO:HD2	11:W:120:GLN:HG3	1.91	0.52
2:G:268:LYS:HE3	2:G:401:TYR:CE1	2.44	0.52
3:N:308:THR:HB	15:N:608:MQ9:H3B	1.92	0.52
8:Q:191:GLU:HB3	8:Q:193:ARG:HH12	1.75	0.52
2:M:107:PHE:CE2	2:G:217:GLY:HA3	2.45	0.52
2:M:359:GLN:CD	11:W:35:GLN:HG2	2.35	0.51
3:H:180:MET:SD	2:G:414:PRO:HB2	2.49	0.51
18:M:502:9YF:C34	3:N:185:ILE:HD12	2.40	0.51
10:V:63:LYS:HB2	10:V:157:ALA:H	1.76	0.51
2:G:380:PRO:HD3	2:G:388:ALA:HA	1.92	0.51
3:H:312:ILE:HG12	3:H:333:VAL:HG21	1.92	0.51
7:R:66:LEU:HD11	7:R:79:PHE:HZ	1.74	0.51
1:O:81:GLN:OE1	8:Q:167:MET:HE2	2.10	0.51
1:O:116:GLN:HB3	1:O:122:MET:HG3	1.93	0.51
3:N:165:LEU:HD13	3:N:291:LYS:H	1.76	0.51
3:N:320:PHE:HZ	3:N:332:TRP:HZ2	1.58	0.51
7:R:395:ILE:CD1	7:R:459:ARG:HB2	2.36	0.51
8:Q:76:ARG:CG	8:Q:76:ARG:NH2	2.73	0.51
3:H:185:ILE:O	3:H:185:ILE:HG13	2.11	0.51
4:P:95:ARG:HG3	4:P:95:ARG:HH11	1.76	0.51
1:O:99:PRO:O	8:Q:330:SER:HB3	2.10	0.50
7:R:80:ASN:HA	7:R:83:PHE:CE1	2.46	0.50
7:R:152:THR:HG22	7:R:259:PHE:HE2	1.76	0.50
1:O:119:THR:HB	1:O:121:ARG:HH22	1.76	0.50
3:N:185:ILE:O	3:N:185:ILE:HG13	2.11	0.50
3:N:220:LEU:HD12	16:N:603:CDL:C83	2.40	0.50
3:N:456:GLY:HA3	7:R:533:LEU:HB2	1.94	0.50
8:Q:235:TRP:CE3	8:Q:274:THR:HG21	2.46	0.50
3:N:320:PHE:CZ	3:N:332:TRP:HZ2	2.30	0.50
7:R:156:PRO:O	7:R:159:ASP:HB2	2.11	0.50
2:G:272:GLU:CD	2:G:272:GLU:H	2.19	0.50
3:N:71:VAL:HG21	3:N:90:GLU:HG3	1.94	0.50
16:N:603:CDL:H511	16:H:602:CDL:H112	1.94	0.50
16:N:604:CDL:HB62	16:N:605:CDL:H311	1.94	0.50
2:G:69:PHE:HB3	2:G:159:ILE:HG22	1.93	0.50
16:O:305:CDL:H132	6:T:123:THR:HG23	1.93	0.50
7:R:512:GLY:HA2	10:V:31:VAL:HB	1.92	0.50
7:R:264:HIS:NE2	7:R:268:TYR:HE2	2.09	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:104:LEU:CD1	2:G:213:VAL:HG11	2.42	0.50
3:N:284:ILE:HA	3:N:287:LEU:HD12	1.94	0.49
5:S:38:MET:HG3	7:R:222:ILE:HA	1.94	0.49
3:H:89:TYR:OH	3:H:288:GLY:CA	2.59	0.49
3:H:195:GLY:HA3	3:H:202:ILE:HD11	1.94	0.49
1:O:261:TYR:CD1	13:O:301:WUO:O09	2.65	0.49
7:R:212:ASN:HD22	7:R:276:GLY:N	2.10	0.49
8:Q:235:TRP:HE3	8:Q:274:THR:CG2	2.26	0.49
12:Y:23:PRO:HG2	12:Y:26:GLU:HB3	1.95	0.49
8:Q:235:TRP:CE3	8:Q:274:THR:CG2	2.95	0.49
3:N:344:LEU:HA	15:N:601:MQ9:H451	1.95	0.49
1:O:119:THR:HB	1:O:121:ARG:NH2	2.27	0.49
5:S:42:GLY:O	5:S:46:MET:HG3	2.13	0.49
3:H:244:THR:HG23	3:H:246:THR:H	1.77	0.49
2:M:396:ILE:HD12	11:W:63:ASP:HB2	1.95	0.49
7:R:152:THR:HA	7:R:259:PHE:CE2	2.48	0.49
3:H:89:TYR:CZ	3:H:288:GLY:C	2.91	0.49
2:G:256:ARG:HD3	2:G:280:GLU:CD	2.38	0.49
7:R:424:ARG:CG	7:R:424:ARG:NH1	2.73	0.48
24:R:603:HEA:O11	24:R:603:HEA:HHC	2.13	0.48
2:G:279:MET:HA	2:G:314:LEU:O	2.12	0.48
2:M:256:ARG:HH12	2:M:273:ASP:HB3	1.78	0.48
3:N:230:VAL:HG12	15:N:607:MQ9:H3B	1.94	0.48
3:N:258:ALA:HB1	15:N:607:MQ9:H202	1.94	0.48
3:N:319:GLU:O	12:Y:21:CYS:CB	2.61	0.48
3:N:420:ALA:HB2	16:P:301:CDL:H771	1.94	0.48
3:H:210:LEU:HD23	3:H:214:LEU:HD12	1.95	0.48
2:G:279:MET:CG	2:G:313:MET:CG	2.91	0.48
6:T:128:LEU:CD1	7:R:120:ARG:HD2	2.43	0.48
14:O:303:HEC:CMD	11:W:32:THR:O	2.61	0.48
2:M:313:MET:HE1	2:M:363:ILE:HG21	1.95	0.48
3:N:15:ALA:HB1	3:N:19:ARG:HH12	1.77	0.48
3:N:265:PHE:HD2	15:N:607:MQ9:H352	1.79	0.48
7:R:460:ARG:N	24:R:603:HEA:O2A	2.46	0.48
1:O:294:ALA:HA	3:N:483:PRO:HG2	1.95	0.48
3:N:497:PRO:HA	5:S:169:LYS:HA	1.96	0.48
15:N:608:MQ9:C51	15:N:608:MQ9:C46	2.88	0.48
3:H:89:TYR:OH	3:H:288:GLY:HA2	2.14	0.48
5:S:49:THR:HG21	7:R:254:LEU:HB2	1.96	0.48
7:R:201:MET:HE2	7:R:536:ILE:HD13	1.96	0.48
3:H:42:LEU:HD13	3:H:122:VAL:HG12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:321:TYR:HE1	12:Y:21:CYS:O	1.96	0.48
15:O:304:MQ9:H272	7:R:135:ILE:HG13	1.96	0.47
4:P:45:ILE:HD12	4:P:48:MET:HE3	1.95	0.47
7:R:355:PHE:CD2	8:Q:76:ARG:HD3	2.49	0.47
3:H:67:SER:HB3	3:H:87:ARG:HB2	1.96	0.47
2:M:260:ARG:HE	2:M:263:GLU:HG3	1.79	0.47
3:N:126:ARG:O	3:N:130:THR:OG1	2.30	0.47
5:S:147:HIS:CE1	5:S:192:TRP:HB2	2.49	0.47
6:T:131:GLU:HB3	7:R:120:ARG:HH22	1.79	0.47
3:N:172:ARG:O	3:N:176:SER:HB3	2.14	0.47
24:R:602:HEA:HMD3	24:R:602:HEA:CBD	2.45	0.47
3:H:156:PHE:CZ	3:H:171:ILE:HD13	2.49	0.47
2:G:256:ARG:HD3	2:G:280:GLU:CG	2.44	0.47
1:O:81:GLN:NE2	8:Q:163:ARG:HB2	2.27	0.47
1:O:124:ALA:HB3	14:O:303:HEC:HBC2	1.96	0.47
1:O:201:LEU:HB2	1:O:205:LYS:HB2	1.95	0.47
1:O:227:GLN:HB3	11:W:35:GLN:HE22	1.79	0.47
16:N:604:CDL:H522	16:N:604:CDL:H722	1.97	0.47
4:P:29:ASP:CG	4:P:30:VAL:H	2.23	0.47
7:R:509:ASP:HB3	10:V:31:VAL:HG12	1.96	0.47
4:P:48:MET:HG2	16:P:301:CDL:H571	1.97	0.47
3:H:160:SER:HA	3:H:167:SER:HB2	1.95	0.47
7:R:370:LEU:HD21	8:Q:61:GLY:HA2	1.96	0.47
7:R:399:HIS:O	7:R:442:PHE:HE1	1.98	0.47
24:R:602:HEA:HMD3	24:R:602:HEA:HBD2	1.97	0.47
5:S:36:GLU:OE1	5:S:36:GLU:HA	2.14	0.47
7:R:544:GLU:HG2	7:R:551:VAL:HG22	1.97	0.47
3:N:327:ILE:HG22	3:N:331:VAL:HG21	1.97	0.46
2:M:415:ALA:HB1	3:N:326:THR:HG21	1.98	0.46
7:R:40:ILE:HA	7:R:43:MET:HE2	1.96	0.46
8:Q:235:TRP:CD1	8:Q:242:LYS:HB3	2.50	0.46
3:H:154:GLU:HB2	3:H:215:ILE:HG21	1.96	0.46
1:O:277:ILE:HG23	1:O:278:ILE:HG13	1.97	0.46
7:R:284:VAL:HG22	7:R:514:GLY:HA2	1.97	0.46
7:R:488:MET:HE3	7:R:488:MET:HA	1.96	0.46
24:R:603:HEA:HMC3	24:R:603:HEA:HBC1	1.97	0.46
3:N:266:ALA:HB2	15:N:607:MQ9:C30	2.41	0.46
7:R:77:GLU:CD	8:Q:332:ARG:HH22	2.23	0.46
3:H:41:LEU:HD22	3:H:44:GLU:OE1	2.16	0.46
2:M:104:LEU:HD12	2:G:213:VAL:HG11	1.97	0.46
3:N:340:VAL:HG22	15:N:601:MQ9:H401	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:55:SER:HB2	16:P:301:CDL:H772	1.98	0.46
11:W:37:PRO:HB2	11:W:39:VAL:HG22	1.97	0.46
3:H:410:ILE:HD13	3:H:410:ILE:HA	1.69	0.46
2:M:249:GLY:HA3	12:Y:42:SER:HB2	1.98	0.46
2:G:279:MET:HE3	2:G:279:MET:HB3	1.67	0.46
1:O:236:GLN:NE2	2:M:280:GLU:HB2	2.30	0.46
3:N:232:PHE:HZ	16:N:603:CDL:H712	1.78	0.46
15:N:608:MQ9:C5M	15:N:608:MQ9:C8	2.86	0.46
2:M:416:PHE:O	3:N:326:THR:HB	2.16	0.46
7:R:52:PHE:CD2	7:R:90:MET:HE1	2.51	0.46
3:H:297:ALA:O	2:G:366:PRO:HB2	2.16	0.46
1:O:81:GLN:HE21	8:Q:163:ARG:HE	1.64	0.46
16:N:605:CDL:H312	16:N:605:CDL:H121	1.98	0.46
7:R:66:LEU:O	7:R:474:ASN:HB3	2.15	0.45
7:R:306:LEU:HB3	7:R:333:ILE:HG12	1.98	0.45
16:P:301:CDL:H552	16:P:301:CDL:H762	1.98	0.45
7:R:310:VAL:HG21	7:R:333:ILE:HD11	1.99	0.45
15:H:606:MQ9:H253	15:H:606:MQ9:H271	1.42	0.45
2:G:151:GLN:NE2	2:G:152:LYS:HG3	2.32	0.45
1:O:271:GLU:CD	3:N:281:ILE:HG13	2.42	0.45
15:N:607:MQ9:H353	15:N:607:MQ9:H372	1.63	0.45
15:N:607:MQ9:H453	15:N:607:MQ9:H471	1.55	0.45
2:G:279:MET:SD	2:G:313:MET:HG3	2.55	0.45
2:M:112:TRP:CZ2	18:G:502:9YF:O6	2.69	0.45
16:P:301:CDL:H512	16:P:301:CDL:H541	1.65	0.45
5:S:166:LYS:HE2	19:S:501:7PH:O22	2.16	0.45
24:R:603:HEA:H271	24:R:603:HEA:H211	1.45	0.45
10:V:74:GLY:O	10:V:103:GLN:NE2	2.50	0.45
2:M:349:LEU:HD12	2:M:368:HIS:CE1	2.51	0.45
3:N:282:ASN:ND2	21:N:602:HEM:O1A	2.50	0.45
15:N:608:MQ9:H172	15:N:608:MQ9:H153	1.60	0.45
28:W:202:9XX:O6	29:W:203:PLM:H62	2.16	0.45
3:H:175:LEU:CD1	15:H:606:MQ9:H3A	2.47	0.45
1:O:100:ASP:O	11:W:33:THR:HB	2.17	0.45
3:N:464:PRO:HB3	3:N:474:PRO:HB3	1.99	0.45
11:W:62:THR:HG22	11:W:63:ASP:H	1.81	0.45
3:H:89:TYR:CE2	3:H:289:PRO:N	2.85	0.45
3:H:143:ILE:HG22	3:H:226:HIS:HD1	1.81	0.45
3:H:362:ASN:ND2	2:G:166:ASP:OD2	2.50	0.45
3:H:136:PRO:HD2	3:H:137:ARG:NH1	2.32	0.45
3:H:254:MET:HA	3:H:255:PRO:HA	1.75	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:R:20:ARG:NH1	10:V:53:ASP:OD2	2.50	0.45
3:H:172:ARG:C	3:H:172:ARG:CD	2.90	0.45
11:W:107:PRO:HG2	11:W:110:GLY:HA3	1.99	0.45
3:H:75:GLY:HA2	3:H:98:GLU:OE2	2.17	0.45
3:H:127:ILE:HG23	3:H:132:ALA:HB3	1.99	0.45
3:H:362:ASN:ND2	2:G:164:ARG:HD2	2.31	0.45
2:G:355:LEU:HD12	2:G:366:PRO:HB3	1.99	0.45
2:M:385:ALA:O	4:P:66:ASN:ND2	2.50	0.44
3:N:218:ILE:HD13	15:N:608:MQ9:H422	1.99	0.44
7:R:349:TRP:CD1	7:R:350:LYS:HG2	2.52	0.44
2:G:274:ILE:HD13	2:G:316:ARG:HB2	2.00	0.44
15:N:601:MQ9:H272	15:N:601:MQ9:H253	1.76	0.44
5:S:59:PRO:HB3	5:S:136:TYR:CZ	2.52	0.44
2:G:43:THR:OG1	2:G:46:GLU:OE1	2.28	0.44
2:M:349:LEU:HB2	17:M:501:FES:S2	2.58	0.44
7:R:352:GLN:HB3	8:Q:77:LYS:HG3	1.99	0.44
2:M:130:PRO:HA	3:N:277:GLY:O	2.17	0.44
16:N:605:CDL:H242	6:T:97:LEU:HB3	2.00	0.44
7:R:55:GLY:HA3	7:R:90:MET:SD	2.58	0.44
7:R:223:ALA:O	7:R:226:ILE:HG22	2.16	0.44
7:R:406:ILE:HD12	7:R:406:ILE:H	1.82	0.44
7:R:422:THR:HG22	7:R:424:ARG:CG	2.41	0.44
7:R:507:VAL:HG11	10:V:32:THR:HG23	1.99	0.44
8:Q:137:GLN:HA	8:Q:138:TRP:HA	1.66	0.44
1:O:275:MET:HE1	3:N:115:MET:HE3	1.99	0.44
7:R:69:PRO:HG3	7:R:464:TYR:CE2	2.53	0.44
7:R:268:TYR:HA	7:R:271:ALA:HB3	2.00	0.44
1:O:218:ILE:HA	14:O:302:HEC:HMA2	2.00	0.44
1:O:269:ALA:HB3	1:O:270:PRO:HD3	1.98	0.44
3:N:447:THR:HA	3:N:488:MET:HG3	2.00	0.44
18:M:502:9YF:C41	15:N:608:MQ9:H151	2.48	0.44
3:N:26:VAL:HG12	3:N:30:LEU:CD1	2.47	0.44
7:R:163:SER:O	7:R:238:ARG:NH2	2.50	0.44
1:O:215:PRO:HG3	1:O:250:ARG:HG3	1.98	0.44
2:M:185:LEU:HB2	19:M:503:7PH:H32A	2.00	0.44
3:N:460:GLU:HB2	7:R:528:HIS:CE1	2.53	0.44
2:G:314:LEU:HD21	2:G:339:LEU:HD22	1.99	0.44
2:G:395:THR:HG23	2:G:403:VAL:HG23	2.00	0.44
1:O:82:LEU:HD22	1:O:138:PHE:CD1	2.53	0.44
1:O:114:TYR:HD2	1:O:220:THR:HG21	1.83	0.44
15:O:304:MQ9:C35	15:O:304:MQ9:C31	2.96	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:234:LYS:HG2	30:N:736:HOH:O	2.16	0.44
8:Q:191:GLU:HB3	8:Q:193:ARG:NH1	2.32	0.43
3:H:89:TYR:CD2	3:H:289:PRO:HB3	2.52	0.43
7:R:77:GLU:OE1	8:Q:332:ARG:NH2	2.50	0.43
1:O:226:PRO:HD2	1:O:229:MET:SD	2.58	0.43
1:O:227:GLN:CG	11:W:35:GLN:HE22	2.30	0.43
16:O:305:CDL:H381	15:N:601:MQ9:H151	2.00	0.43
3:N:193:LEU:HA	15:N:608:MQ9:H201	1.99	0.43
3:N:438:ARG:HD3	3:N:438:ARG:N	2.32	0.43
11:W:62:THR:HG22	11:W:63:ASP:N	2.32	0.43
2:G:279:MET:HG3	2:G:313:MET:CG	2.48	0.43
3:N:85:MET:SD	3:N:89:TYR:HD2	2.41	0.43
6:T:100:SER:HB2	7:R:135:ILE:HD11	2.01	0.43
15:N:607:MQ9:H403	15:N:607:MQ9:H422	1.60	0.43
3:N:227:LEU:HD12	16:N:603:CDL:H801	2.01	0.43
15:N:607:MQ9:H321	15:N:607:MQ9:H303	1.65	0.43
4:P:33:VAL:HG11	4:P:41:SER:HB3	2.01	0.43
5:S:88:VAL:HG13	5:S:179:ILE:HG12	2.01	0.43
7:R:193:VAL:HG11	7:R:214:LEU:HD22	2.01	0.43
7:R:227:LEU:HD22	7:R:262:PHE:CZ	2.54	0.43
8:Q:332:ARG:HD2	11:W:33:THR:HG21	1.99	0.43
1:O:232:PHE:CE1	14:O:302:HEC:HBB2	2.54	0.43
3:N:368:ARG:O	3:N:434:GLN:NE2	2.50	0.43
15:O:304:MQ9:H202	6:T:113:LEU:HD21	1.99	0.43
2:G:254:LEU:CD1	2:G:402:LEU:HB3	2.43	0.43
4:P:95:ARG:HG3	4:P:95:ARG:NH1	2.32	0.43
8:Q:164:LYS:NZ	8:Q:196:LEU:O	2.49	0.43
1:O:174:GLY:H	1:O:247:ALA:HB2	1.84	0.43
2:M:99:SER:OG	2:M:135:THR:O	2.37	0.43
2:G:415:ALA:HA	2:G:419:ARG:HD2	2.00	0.43
3:N:232:PHE:CZ	16:N:603:CDL:C71	3.02	0.42
3:N:499:THR:HG21	3:N:514:LEU:HD12	2.00	0.42
7:R:162:HIS:HD2	8:Q:137:GLN:HE22	1.67	0.42
3:H:106:ARG:NH1	21:H:601:HEM:O1A	2.52	0.42
3:H:184:VAL:N	2:G:417:TRP:CG	2.87	0.42
3:H:193:LEU:HD12	3:H:193:LEU:O	2.19	0.42
3:N:220:LEU:HD11	16:N:603:CDL:C83	2.47	0.42
5:S:166:LYS:O	5:S:166:LYS:HG2	2.19	0.42
7:R:152:THR:HG22	7:R:259:PHE:CE2	2.54	0.42
7:R:341:PHE:CD2	24:R:602:HEA:H171	2.54	0.42
7:R:398:PHE:CD1	24:R:602:HEA:HAD1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:R:426:LEU:HD23	7:R:498:SER:HB2	2.00	0.42
3:H:114:LEU:HD21	3:H:302:ASP:OD1	2.20	0.42
3:H:237:GLN:NE2	3:H:247:ASN:O	2.52	0.42
12:c:23:PRO:HG2	12:c:26:GLU:HB3	2.01	0.42
1:O:227:GLN:HB3	11:W:35:GLN:NE2	2.35	0.42
3:N:400:PHE:HA	6:T:108:LEU:HD13	2.01	0.42
7:R:52:PHE:HE1	7:R:488:MET:SD	2.43	0.42
7:R:401:VAL:HG13	24:R:602:HEA:CAC	2.50	0.42
10:V:33:GLU:HB2	10:V:36:GLU:HG3	2.00	0.42
3:H:234:LYS:O	2:G:164:ARG:NH1	2.52	0.42
1:O:81:GLN:HE21	8:Q:163:ARG:NE	2.18	0.42
1:O:223:LEU:HD23	1:O:242:LYS:HE3	2.00	0.42
7:R:445:THR:HA	7:R:477:SER:HA	2.02	0.42
3:H:175:LEU:HD13	15:H:606:MQ9:H3A	2.00	0.42
3:H:400:PHE:HD2	3:H:402:ILE:H	1.67	0.42
2:M:189:THR:O	2:M:193:ARG:HD3	2.19	0.42
5:S:135:ALA:HB2	8:Q:185:ILE:HG13	2.01	0.42
7:R:149:PHE:CD1	7:R:158:THR:HG22	2.54	0.42
11:W:94:ASP:OD2	11:W:141:LYS:NZ	2.45	0.42
1:O:94:ASN:HB3	11:W:111:VAL:HG12	2.02	0.42
3:N:66:PRO:HG3	3:N:208:TYR:CD2	2.55	0.42
3:N:468:VAL:HA	3:N:474:PRO:HA	2.02	0.42
10:V:70:ILE:HD11	10:V:143:LEU:HD11	2.02	0.42
3:H:385:LEU:HD23	3:H:385:LEU:HA	1.89	0.42
2:G:379:LYS:O	2:G:379:LYS:HG3	2.19	0.42
1:O:193:ASN:OD1	1:O:196:GLY:N	2.53	0.42
1:O:199:GLY:O	1:O:207:ALA:N	2.51	0.42
3:N:283:PRO:O	3:N:287:LEU:HG	2.19	0.42
3:N:458:TYR:HD2	7:R:530:PHE:HB2	1.85	0.42
5:S:33:LEU:HD23	5:S:33:LEU:HA	1.92	0.42
6:T:71:GLU:O	7:R:205:ARG:NH2	2.52	0.42
2:G:50:MET:HE1	2:G:58:LEU:HD22	2.02	0.42
3:N:262:GLY:HA3	15:N:607:MQ9:H222	2.02	0.42
8:Q:36:PRO:HD2	8:Q:240:LEU:HD21	2.02	0.42
3:H:183:PRO:HA	2:G:417:TRP:HB2	2.02	0.42
15:O:304:MQ9:H102	3:N:392:MET:HE2	2.01	0.41
3:N:265:PHE:CD2	15:N:607:MQ9:H352	2.52	0.41
3:N:434:GLN:NE2	4:P:35:SER:HB2	2.35	0.41
3:N:532:HIS:O	3:N:536:ILE:HG12	2.20	0.41
3:N:489:ASN:OD1	3:N:490:LYS:N	2.52	0.41
11:W:77:ALA:HB3	11:W:112:LEU:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:H:604:HEM:HBB2	21:H:604:HEM:CHC	2.47	0.41
11:W:150:ASP:HA	11:W:163:ALA:HA	2.01	0.41
3:N:379:MET:HE1	16:P:301:CDL:H612	2.03	0.41
7:R:52:PHE:HA	7:R:90:MET:HE1	2.02	0.41
7:R:341:PHE:HZ	7:R:369:PHE:CD2	2.38	0.41
11:W:24:CYS:HG	18:W:201:9YF:C24	2.34	0.41
2:G:204:LEU:HD23	2:G:204:LEU:HA	1.96	0.41
3:N:489:ASN:HD22	6:T:133:TYR:N	2.18	0.41
6:T:21:VAL:O	6:T:25:LEU:HB2	2.20	0.41
8:Q:331:ARG:C	8:Q:333:GLY:N	2.77	0.41
3:H:78:GLN:CB	3:H:79:PRO:HD3	2.50	0.41
3:H:222:LEU:HD23	3:H:222:LEU:HA	1.89	0.41
2:G:376:GLU:HG2	2:G:379:LYS:HG2	2.02	0.41
1:O:281:VAL:HG12	16:O:305:CDL:H791	2.01	0.41
7:R:403:PHE:HE1	24:R:603:HEA:HO1	1.67	0.41
7:R:454:ASP:HB3	8:Q:35:TRP:HD1	1.85	0.41
3:H:188:TRP:CZ3	2:G:222:ASN:HA	2.56	0.41
2:G:111:PRO:HG3	2:G:124:LEU:HD13	2.02	0.41
3:N:467:PRO:HG2	3:N:475:ILE:HD11	2.02	0.41
15:N:607:MQ9:H103	15:N:607:MQ9:H121	1.63	0.41
7:R:355:PHE:CE1	7:R:363:VAL:HG21	2.50	0.41
7:R:460:ARG:HD3	8:Q:276:MET:HB2	2.01	0.41
7:R:550:MET:HE2	8:Q:84:LEU:HB2	2.03	0.41
3:H:433:LEU:HD23	3:H:433:LEU:HA	1.91	0.41
2:M:386:ALA:HB2	3:N:317:ALA:HB1	2.03	0.41
7:R:138:ALA:O	7:R:141:ILE:HG12	2.21	0.41
8:Q:31:LEU:HD13	8:Q:55:ILE:HD11	2.01	0.41
1:O:230:PRO:HB3	2:M:279:MET:N	2.35	0.41
3:N:487:ARG:HD2	6:T:131:GLU:O	2.19	0.41
16:N:603:CDL:H712	16:N:603:CDL:HB61	1.64	0.41
6:T:58:PHE:O	6:T:62:ARG:HG2	2.21	0.41
7:R:120:ARG:HB2	16:R:601:CDL:OB4	2.21	0.41
7:R:252:VAL:HG13	8:Q:231:ILE:HD11	2.03	0.41
7:R:403:PHE:HE1	24:R:603:HEA:O11	2.04	0.41
11:W:139:LEU:HD11	11:W:143:ILE:HD13	2.02	0.41
1:O:283:ALA:HB1	3:N:45:ILE:HD13	2.02	0.41
2:M:352:PRO:O	3:N:295:VAL:HG11	2.21	0.41
3:N:47:LEU:HD13	3:N:227:LEU:HD11	2.03	0.41
3:N:512:GLU:HA	3:N:515:THR:HG22	2.03	0.41
7:R:106:VAL:HG11	7:R:417:TRP:CE2	2.56	0.41
3:N:309:ASP:HA	3:N:312:ILE:HD12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:R:193:VAL:O	7:R:197:ARG:HG3	2.20	0.40
7:R:392:TYR:CE1	7:R:459:ARG:HA	2.56	0.40
8:Q:193:ARG:HB3	8:Q:196:LEU:HD12	2.03	0.40
2:G:349:LEU:HB2	17:G:501:FES:S2	2.61	0.40
15:O:304:MQ9:H422	15:O:304:MQ9:H153	2.02	0.40
16:O:305:CDL:H521	16:O:305:CDL:H711	2.03	0.40
2:M:236:ALA:HB3	2:M:239:TRP:CD1	2.56	0.40
3:N:266:ALA:CB	15:N:607:MQ9:H302	2.43	0.40
10:V:67:ALA:HB3	10:V:96:LEU:HA	2.03	0.40
3:H:229:LEU:HD23	3:H:229:LEU:HA	1.91	0.40
3:N:38:TRP:CH2	16:N:604:CDL:H711	2.57	0.40
3:N:68:MET:HE1	3:N:199:PRO:HB2	2.02	0.40
3:H:314:LEU:O	3:H:412:ARG:CG	2.69	0.40
1:O:261:TYR:CE1	13:O:301:WUO:O09	2.74	0.40
2:M:190:LEU:HD22	19:M:503:7PH:H39A	2.04	0.40
16:N:604:CDL:H371	16:N:604:CDL:H171	2.04	0.40
15:N:608:MQ9:H111	15:N:608:MQ9:H251	2.03	0.40
6:T:137:GLU:HG2	6:T:139:HIS:H	1.85	0.40
7:R:89:VAL:HG22	7:R:93:PHE:HD2	1.85	0.40
7:R:262:PHE:CZ	7:R:266:GLU:HG3	2.56	0.40
7:R:445:THR:O	7:R:477:SER:OG	2.39	0.40
3:H:89:TYR:CE2	3:H:289:PRO:HD3	2.57	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%)	213 (96%)	8 (4%)	0	100	100
2	G	378/408 (93%)	358 (95%)	19 (5%)	1 (0%)	36	60
2	M	378/408 (93%)	369 (98%)	9 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	H	433/556 (78%)	413 (95%)	19 (4%)	1 (0%)	43	68
3	N	531/556 (96%)	514 (97%)	16 (3%)	1 (0%)	43	68
4	P	71/100 (71%)	70 (99%)	1 (1%)	0	100	100
5	S	182/203 (90%)	182 (100%)	0	0	100	100
6	T	137/139 (99%)	133 (97%)	4 (3%)	0	100	100
7	R	549/575 (96%)	535 (97%)	14 (3%)	0	100	100
8	Q	295/341 (86%)	284 (96%)	11 (4%)	0	100	100
9	U	62/79 (78%)	62 (100%)	0	0	100	100
10	V	141/157 (90%)	139 (99%)	2 (1%)	0	100	100
11	W	145/186 (78%)	133 (92%)	12 (8%)	0	100	100
12	Y	23/236 (10%)	21 (91%)	2 (9%)	0	100	100
12	c	23/236 (10%)	21 (91%)	2 (9%)	0	100	100
All	All	3569/4458 (80%)	3447 (97%)	119 (3%)	3 (0%)	49	73

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	N	184	VAL
3	H	184	VAL
2	G	274	ILE

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%)	162 (99%)	1 (1%)	78	91
2	G	311/333 (93%)	299 (96%)	12 (4%)	28	57
2	M	311/333 (93%)	310 (100%)	1 (0%)	86	94
3	H	351/448 (78%)	342 (97%)	9 (3%)	40	70
3	N	428/448 (96%)	421 (98%)	7 (2%)	55	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	103 (97%)	3 (3%)	38	68
7	R	453/471 (96%)	447 (99%)	6 (1%)	61	83
8	Q	255/288 (88%)	252 (99%)	3 (1%)	63	84
9	U	51/59 (86%)	51 (100%)	0	100	100
10	V	105/114 (92%)	105 (100%)	0	100	100
11	W	121/146 (83%)	119 (98%)	2 (2%)	53	79
12	Y	20/167 (12%)	17 (85%)	3 (15%)	3	7
12	c	20/167 (12%)	17 (85%)	3 (15%)	3	7
All	All	2899/3530 (82%)	2849 (98%)	50 (2%)	52	79

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	194	PHE
2	M	270	ARG
3	N	28	ARG
3	N	90	GLU
3	N	244	THR
3	N	323	PHE
3	N	327	ILE
3	N	351	GLU
3	N	438	ARG
6	T	26	THR
6	T	28	MET
6	T	31	THR
7	R	63	ARG
7	R	149	PHE
7	R	151	TRP
7	R	395	ILE
7	R	401	VAL
7	R	424	ARG
8	Q	76	ARG
8	Q	78	LYS
8	Q	82	THR
11	W	31	GLN
11	W	35	GLN

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Mol	Chain	Res	Type
12	Y	21	CYS
12	Y	27	THR
12	Y	42	SER
3	H	20	TYR
3	H	78	GLN
3	H	138	GLU
3	H	172	ARG
3	H	352	LYS
3	H	408	THR
3	H	410	ILE
3	H	412	ARG
3	H	413	ILE
2	G	225	LYS
2	G	256	ARG
2	G	269	MET
2	G	270	ARG
2	G	272	GLU
2	G	274	ILE
2	G	279	MET
2	G	314	LEU
2	G	316	ARG
2	G	379	LYS
2	G	381	ILE
2	G	382	PHE
12	c	22	SER
12	c	27	THR
12	c	42	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	O	81	GLN
1	O	130	GLN
1	O	187	ASN
1	O	192	HIS
2	M	371	GLN
3	N	84	GLN
3	N	294	GLN
3	N	401	HIS
7	R	72	GLN
7	R	212	ASN
7	R	239	HIS

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Mol	Chain	Res	Type
7	R	528	HIS
8	Q	137	GLN
8	Q	226	ASN
8	Q	285	ASN
11	W	35	GLN
2	G	115	GLN
2	G	151	GLN
2	G	323	HIS

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	$\# Z > 2$
16	CDL	O	305	-	78,78,99	0.29	0	84,90,111	0.34	0
19	7PH	S	501	-	37,37,37	0.30	0	40,42,42	0.34	0
15	MQ9	O	304	-	59,59,59	0.37	0	73,75,75	0.43	1 (1%)
20	IZL	M	504	-	119,119,119	1.73	29 (24%)	160,163,163	1.30	19 (11%)
16	CDL	N	603	-	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
16	CDL	H	603	-	76,76,99	0.29	0	82,88,111	0.35	0
29	PLM	W	203	-	9,10,17	0.56	0	8,9,17	0.42	0
16	CDL	N	604	-	76,76,99	0.29	0	82,88,111	0.35	0
15	MQ9	N	608	-	59,59,59	0.36	0	73,75,75	0.43	1 (1%)
13	WUO	O	301	-	99,99,99	1.61	11 (11%)	122,125,125	1.29	13 (10%)
22	TRD	R	607	-	12,12,12	0.10	0	11,11,11	0.05	0
19	7PH	M	503	-	37,37,37	0.97	4 (10%)	40,42,42	1.17	2 (5%)
19	7PH	G	505	-	37,37,37	0.97	4 (10%)	40,42,42	1.14	2 (5%)
23	3PE	S	503	-	31,31,50	1.09	4 (12%)	34,36,55	1.13	2 (5%)
15	MQ9	H	605	-	59,59,59	0.36	0	73,75,75	0.42	1 (1%)
21	HEM	N	602	3	50,50,50	1.42	8 (16%)	67,82,82	1.07	4 (5%)
18	9YF	G	502	-	58,58,58	1.38	4 (6%)	68,71,71	1.10	3 (4%)
19	7PH	G	504	-	37,37,37	0.97	4 (10%)	40,42,42	1.17	2 (5%)
16	CDL	R	601	-	76,76,99	1.42	11 (14%)	82,88,111	1.14	4 (4%)
18	9YF	W	201	-	58,58,58	1.39	4 (6%)	68,71,71	1.11	3 (4%)
28	9XX	Y	302	-	31,31,41	1.10	4 (12%)	34,34,44	1.38	3 (8%)
21	HEM	H	604	3	50,50,50	1.46	7 (14%)	67,82,82	1.15	6 (8%)
22	TRD	R	608	-	12,12,12	0.10	0	11,11,11	0.05	0
24	HEA	R	603	7	67,67,67	2.56	25 (37%)	81,103,103	2.49	31 (38%)
15	MQ9	N	601	-	59,59,59	0.36	0	73,75,75	0.43	1 (1%)
21	HEM	H	601	3	50,50,50	1.45	6 (12%)	67,82,82	1.25	5 (7%)
22	TRD	S	502	-	12,12,12	0.29	0	11,11,11	0.86	0
14	HEC	O	302	1	46,50,50	1.84	6 (13%)	58,82,82	1.85	4 (6%)
24	HEA	R	602	-	67,67,67	2.25	25 (37%)	81,103,103	2.54	35 (43%)
16	CDL	H	602	-	73,73,99	0.30	0	79,85,111	0.35	0
15	MQ9	N	607	-	59,59,59	0.36	0	73,75,75	0.41	1 (1%)
14	HEC	O	303	1	46,50,50	1.84	7 (15%)	58,82,82	1.94	4 (6%)
28	9XX	c	302	-	31,31,41	1.11	4 (12%)	34,34,44	1.38	3 (8%)
22	TRD	Q	403	-	12,12,12	0.10	0	11,11,11	0.05	0
29	PLM	c	301	-	9,10,17	0.57	0	8,9,17	0.42	0
22	TRD	T	201	-	12,12,12	0.29	0	11,11,11	0.86	0
16	CDL	R	605	-	76,76,99	0.30	0	82,88,111	0.35	0
18	9YF	M	502	-	58,58,58	1.37	5 (8%)	68,71,71	1.11	3 (4%)
28	9XX	W	202	-	41,41,41	0.98	4 (9%)	44,44,44	1.26	2 (4%)
17	FES	G	501	2	0,4,4	-	-	-	-	-
16	CDL	N	605	-	78,78,99	0.29	0	84,90,111	0.34	0
16	CDL	P	301	-	76,76,99	1.42	11 (14%)	82,88,111	1.11	4 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	HEM	N	606	3	50,50,50	1.48	8 (16%)	67,82,82	1.05	4 (5%)
13	WUO	P	302	-	99,99,99	1.59	9 (9%)	122,125,125	1.30	14 (11%)
29	PLM	Y	301	-	9,10,17	0.57	0	8,9,17	0.42	0
20	IZL	G	503	-	119,119,119	1.73	29 (24%)	160,163,163	1.30	19 (11%)
17	FES	M	501	2	0,4,4	-	-	-	-	-
15	MQ9	H	606	-	59,59,59	0.36	0	73,75,75	0.41	1 (1%)

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
16	CDL	O	305	-	-	38/89/89/110	-
19	7PH	S	501	-	-	11/39/39/39	-
15	MQ9	O	304	-	-	25/53/73/73	0/2/2/2
20	IZL	M	504	-	-	37/84/208/208	0/6/6/6
16	CDL	N	603	-	-	47/84/84/110	-
16	CDL	H	603	-	-	41/87/87/110	-
29	PLM	W	203	-	-	1/8/8/15	-
16	CDL	N	604	-	-	41/87/87/110	-
15	MQ9	N	608	-	-	30/53/73/73	0/2/2/2
13	WUO	O	301	-	-	33/84/148/148	0/3/3/3
22	TRD	R	607	-	-	0/10/10/10	-
19	7PH	M	503	-	-	12/39/39/39	-
19	7PH	G	505	-	-	12/39/39/39	-
23	3PE	S	503	-	-	14/35/35/54	-
15	MQ9	H	605	-	-	23/53/73/73	0/2/2/2
21	HEM	N	602	3	-	1/14/54/54	-
18	9YF	G	502	-	-	31/54/78/78	0/1/1/1
19	7PH	G	504	-	-	18/39/39/39	-
16	CDL	R	601	-	-	54/87/87/110	-
18	9YF	W	201	-	-	30/54/78/78	0/1/1/1
28	9XX	Y	302	-	-	9/33/33/43	-
21	HEM	H	604	3	-	3/14/54/54	-
22	TRD	R	608	-	-	1/10/10/10	-
24	HEA	R	603	7	-	19/36/76/76	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	MQ9	N	601	-	-	8/53/73/73	0/2/2/2
21	HEM	H	601	3	-	3/14/54/54	-
22	TRD	S	502	-	-	1/10/10/10	-
14	HEC	O	302	1	-	4/14/54/54	-
24	HEA	R	602	-	-	7/36/76/76	-
16	CDL	H	602	-	-	36/84/84/110	-
15	MQ9	N	607	-	-	35/53/73/73	0/2/2/2
14	HEC	O	303	1	-	7/14/54/54	-
28	9XX	c	302	-	-	9/33/33/43	-
22	TRD	Q	403	-	-	0/10/10/10	-
29	PLM	c	301	-	-	0/8/8/15	-
22	TRD	T	201	-	-	1/10/10/10	-
16	CDL	R	605	-	-	46/87/87/110	-
18	9YF	M	502	-	-	32/54/78/78	0/1/1/1
28	9XX	W	202	-	-	13/43/43/43	-
17	FES	G	501	2	-	-	0/1/1/1
16	CDL	N	605	-	-	52/89/89/110	-
16	CDL	P	301	-	-	48/87/87/110	-
21	HEM	N	606	3	-	5/14/54/54	-
13	WUO	P	302	-	-	40/84/148/148	0/3/3/3
29	PLM	Y	301	-	-	0/8/8/15	-
20	IZL	G	503	-	-	37/84/208/208	0/6/6/6
17	FES	M	501	2	-	-	0/1/1/1
15	MQ9	H	606	-	-	32/53/73/73	0/2/2/2

All (233) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	R	603	HEA	FE-NB	6.26	2.14	1.94
14	O	302	HEC	CAB-C3B	6.18	1.55	1.35
14	O	303	HEC	CAC-C3C	6.17	1.55	1.35
14	O	302	HEC	CAC-C3C	6.16	1.55	1.35
14	O	303	HEC	CAB-C3B	6.13	1.54	1.35
13	O	301	WUO	P52-O51	6.10	1.77	1.59
13	P	302	WUO	P52-O51	6.03	1.77	1.59
24	R	603	HEA	FE-ND	5.93	2.13	1.94
13	O	301	WUO	C50-C01	5.85	1.64	1.52
14	O	303	HEC	C3D-C2D	5.74	1.53	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	O	302	HEC	C3D-C2D	5.73	1.53	1.38
24	R	603	HEA	FE-NC	5.68	2.13	1.95
13	P	302	WUO	P52-O55	5.44	1.80	1.59
13	O	301	WUO	P52-O55	5.41	1.80	1.59
18	W	201	9YF	P-O2	5.24	1.75	1.59
18	G	502	9YF	P-O2	5.23	1.75	1.59
24	R	603	HEA	C11-C3B	-5.15	1.45	1.51
13	P	302	WUO	C50-C01	5.14	1.62	1.52
18	M	502	9YF	P-O2	5.07	1.74	1.59
24	R	602	HEA	FE-NB	4.95	2.10	1.94
24	R	602	HEA	FE-ND	4.90	2.10	1.94
20	G	503	IZL	P-O28	4.72	1.73	1.59
24	R	603	HEA	CHC-C4B	4.72	1.47	1.38
20	M	504	IZL	P-O28	4.70	1.73	1.59
24	R	603	HEA	C1A-NA	4.68	1.48	1.39
13	O	301	WUO	C56-C57	4.68	1.65	1.50
13	P	302	WUO	C56-C57	4.67	1.65	1.50
20	M	504	IZL	C44-C45	4.58	1.65	1.50
20	G	503	IZL	C44-C45	4.56	1.65	1.50
24	R	602	HEA	C11-C3B	-4.48	1.45	1.51
24	R	603	HEA	C3B-C2B	4.48	1.44	1.34
18	W	201	9YF	P-O	4.44	1.76	1.59
20	M	504	IZL	C43-C14	4.43	1.61	1.52
24	R	603	HEA	C1D-ND	-4.43	1.32	1.40
24	R	602	HEA	FE-NC	4.41	2.09	1.95
18	G	502	9YF	P-O	4.40	1.76	1.59
20	G	503	IZL	C43-C14	4.40	1.61	1.52
18	M	502	9YF	P-O	4.36	1.76	1.59
24	R	603	HEA	C4B-NB	-4.34	1.32	1.40
24	R	602	HEA	C3B-C2B	4.23	1.44	1.34
24	R	602	HEA	C3D-C2D	4.17	1.45	1.36
13	P	302	WUO	C50-C37	4.09	1.60	1.52
20	M	504	IZL	P-O31	4.06	1.75	1.59
20	G	503	IZL	P-O31	4.06	1.75	1.59
24	R	603	HEA	C1C-NC	-4.02	1.32	1.39
24	R	602	HEA	CHD-C1D	4.02	1.46	1.38
28	W	202	9XX	O1-C17	-3.91	1.40	1.47
24	R	603	HEA	CHD-C1D	3.90	1.46	1.38
24	R	602	HEA	CHC-C4B	3.89	1.46	1.38
13	O	301	WUO	C50-C37	3.87	1.60	1.52
28	c	302	9XX	O1-C17	-3.86	1.40	1.47
16	P	301	CDL	OA8-CA7	3.83	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	Y	302	9XX	O1-C17	-3.83	1.40	1.47
24	R	603	HEA	C4C-NC	-3.82	1.32	1.39
16	R	601	CDL	OA8-CA7	3.82	1.44	1.33
24	R	602	HEA	C1D-ND	-3.74	1.33	1.40
21	H	601	HEM	FE-ND	3.73	2.06	1.94
24	R	602	HEA	C4B-NB	-3.71	1.33	1.40
21	N	606	HEM	FE-ND	3.70	2.06	1.94
24	R	603	HEA	CHA-C1A	3.68	1.45	1.38
21	H	604	HEM	FE-ND	3.68	2.06	1.94
24	R	602	HEA	C1A-NA	3.64	1.46	1.39
24	R	603	HEA	C3D-C2D	3.64	1.44	1.36
24	R	603	HEA	CHC-C1C	3.62	1.47	1.39
16	P	301	CDL	OB8-CB7	3.58	1.43	1.33
16	R	601	CDL	OB8-CB7	3.58	1.43	1.33
21	H	604	HEM	FE-NB	3.57	2.05	1.94
24	R	602	HEA	CHB-C4A	3.54	1.45	1.38
21	N	606	HEM	FE-NA	3.45	2.06	1.95
24	R	603	HEA	C4D-ND	-3.40	1.32	1.38
24	R	602	HEA	CHA-C1A	3.40	1.45	1.38
21	N	606	HEM	FE-NB	3.36	2.05	1.94
21	H	601	HEM	FE-NB	3.33	2.05	1.94
21	N	606	HEM	FE-NC	3.33	2.06	1.95
21	N	602	HEM	FE-ND	3.32	2.05	1.94
24	R	603	HEA	CHB-C4A	3.32	1.44	1.38
16	P	301	CDL	OA6-CA5	3.29	1.43	1.34
21	N	602	HEM	FE-NA	3.29	2.06	1.95
16	R	601	CDL	OA6-CA5	3.28	1.43	1.34
21	H	604	HEM	FE-NC	3.26	2.05	1.95
24	R	602	HEA	C4A-NA	3.26	1.45	1.39
21	N	602	HEM	FE-NB	3.23	2.04	1.94
24	R	602	HEA	CHC-C1C	3.18	1.46	1.39
21	H	601	HEM	FE-NA	3.16	2.05	1.95
24	R	603	HEA	C3A-C2A	3.14	1.44	1.37
21	H	601	HEM	FE-NC	3.12	2.05	1.95
13	O	301	WUO	C76-C57	3.11	1.60	1.50
13	P	302	WUO	C76-C57	3.11	1.60	1.50
21	N	602	HEM	CAB-C3B	3.10	1.55	1.47
24	R	602	HEA	C4C-NC	-3.10	1.33	1.39
21	H	604	HEM	FE-NA	3.08	2.05	1.95
21	H	604	HEM	CAC-C3C	3.08	1.55	1.47
21	N	606	HEM	CAB-C3B	3.07	1.55	1.47
21	N	606	HEM	CAC-C3C	3.07	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	R	603	HEA	O2D-CGD	-3.06	1.20	1.30
24	R	602	HEA	C3A-C2A	3.06	1.44	1.37
21	N	602	HEM	CAC-C3C	3.04	1.55	1.47
24	R	602	HEA	CHB-C1B	3.03	1.46	1.39
24	R	603	HEA	C4A-NA	3.02	1.45	1.39
20	G	503	IZL	C25-C30	3.01	1.59	1.52
24	R	603	HEA	CHA-C4D	3.01	1.46	1.39
20	M	504	IZL	C31-C36	2.99	1.61	1.52
24	R	602	HEA	CHD-C4C	2.98	1.46	1.39
20	M	504	IZL	C25-C30	2.97	1.59	1.52
20	G	503	IZL	C31-C36	2.97	1.61	1.52
16	P	301	CDL	OB6-CB4	-2.97	1.39	1.46
21	H	601	HEM	CAB-C3B	2.97	1.55	1.47
21	H	601	HEM	CAC-C3C	2.92	1.55	1.47
24	R	602	HEA	CHA-C4D	2.91	1.45	1.39
21	H	604	HEM	CAB-C3B	2.91	1.55	1.47
16	R	601	CDL	OB6-CB4	-2.88	1.39	1.46
24	R	603	HEA	CHD-C4C	2.85	1.45	1.39
24	R	602	HEA	C1C-NC	-2.85	1.34	1.39
16	R	601	CDL	OB6-CB5	2.84	1.42	1.34
20	G	503	IZL	O28-C43	-2.82	1.34	1.44
21	N	602	HEM	FE-NC	2.80	2.04	1.95
20	M	504	IZL	O28-C43	-2.79	1.34	1.44
16	P	301	CDL	OB6-CB5	2.78	1.42	1.34
20	G	503	IZL	C43-C18	2.72	1.57	1.52
20	M	504	IZL	C43-C18	2.71	1.57	1.52
19	G	505	7PH	O21-C2	-2.69	1.40	1.46
19	G	504	7PH	O21-C2	-2.67	1.40	1.46
20	M	504	IZL	C61-C60	2.65	1.58	1.50
20	G	503	IZL	C61-C60	2.63	1.58	1.50
19	M	503	7PH	O21-C2	-2.60	1.40	1.46
24	R	603	HEA	C1B-NB	-2.59	1.33	1.38
20	G	503	IZL	O38-C73	-2.58	1.36	1.43
20	G	503	IZL	C29-C28	2.57	1.59	1.52
20	M	504	IZL	C29-C28	2.56	1.59	1.52
20	G	503	IZL	C13-C71	2.55	1.60	1.52
20	M	504	IZL	O38-C73	-2.54	1.36	1.43
18	W	201	9YF	C1-C	2.54	1.58	1.50
20	M	504	IZL	C13-C71	2.54	1.60	1.52
24	R	603	HEA	O2A-CGA	-2.48	1.22	1.30
19	M	503	7PH	O31-C31	2.45	1.40	1.33
20	M	504	IZL	C48-C47	2.42	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	G	503	IZL	C48-C47	2.42	1.57	1.50
18	G	502	9YF	C1-C	2.42	1.58	1.50
28	c	302	9XX	O-C15	2.42	1.40	1.33
20	M	504	IZL	O1-C10	2.42	1.40	1.33
16	P	301	CDL	OA6-CA4	-2.42	1.40	1.46
20	G	503	IZL	C24-C23	2.41	1.58	1.51
20	G	503	IZL	O1-C10	2.41	1.40	1.33
28	Y	302	9XX	O-C15	2.41	1.40	1.33
19	G	504	7PH	O31-C31	2.41	1.40	1.33
18	M	502	9YF	C1-C	2.40	1.58	1.50
20	M	504	IZL	O24-C39	-2.40	1.37	1.43
16	R	601	CDL	OA6-CA4	-2.40	1.41	1.46
20	M	504	IZL	C24-C23	2.40	1.58	1.51
19	G	505	7PH	O31-C31	2.40	1.40	1.33
20	M	504	IZL	O34-C60	2.39	1.41	1.34
20	G	503	IZL	O34-C60	2.39	1.41	1.34
20	G	503	IZL	O24-C39	-2.37	1.37	1.43
16	R	601	CDL	C11-CA5	2.37	1.57	1.50
16	P	301	CDL	PB2-OB5	2.36	1.68	1.59
24	R	602	HEA	O2A-CGA	-2.36	1.23	1.30
16	R	601	CDL	PA1-OA5	2.35	1.68	1.59
28	W	202	9XX	O-C15	2.35	1.40	1.33
23	S	503	3PE	O21-C2	-2.34	1.41	1.46
24	R	602	HEA	C4D-ND	-2.34	1.34	1.38
23	S	503	3PE	O31-C31	2.34	1.40	1.33
20	G	503	IZL	O37-C72	-2.32	1.37	1.43
16	P	301	CDL	C11-CA5	2.31	1.57	1.50
16	R	601	CDL	PB2-OB5	2.31	1.68	1.59
20	M	504	IZL	O37-C72	-2.31	1.37	1.43
24	R	602	HEA	O2D-CGD	-2.31	1.23	1.30
16	P	301	CDL	PB2-OB2	2.31	1.68	1.59
28	W	202	9XX	O1-C18	2.31	1.40	1.34
24	R	602	HEA	C1B-NB	-2.29	1.34	1.38
23	S	503	3PE	O21-C21	2.28	1.40	1.34
16	R	601	CDL	PB2-OB2	2.28	1.68	1.59
13	P	302	WUO	O77-C78	2.28	1.40	1.33
16	P	301	CDL	PA1-OA5	2.28	1.68	1.59
13	O	301	WUO	O77-C78	2.27	1.40	1.33
24	R	603	HEA	CHB-C1B	2.26	1.44	1.39
18	W	201	9YF	C24-C	2.25	1.57	1.50
28	W	202	9XX	O-C16	-2.25	1.40	1.45
13	P	302	WUO	O51-C50	-2.25	1.36	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	G	502	9YF	C24-C	2.23	1.57	1.50
23	S	503	3PE	O31-C3	-2.22	1.40	1.45
28	c	302	9XX	O1-C18	2.22	1.40	1.34
20	M	504	IZL	O23-C38	-2.22	1.37	1.43
20	M	504	IZL	C35-C34	2.22	1.58	1.52
19	M	503	7PH	O21-C21	2.21	1.40	1.34
18	M	502	9YF	C24-C	2.20	1.57	1.50
28	Y	302	9XX	O1-C18	2.20	1.40	1.34
20	G	503	IZL	C35-C34	2.20	1.58	1.52
13	O	301	WUO	C31-C01	2.20	1.58	1.52
19	G	505	7PH	O31-C3	-2.19	1.40	1.45
13	O	301	WUO	O51-C50	-2.19	1.36	1.44
20	G	503	IZL	C36-C35	2.18	1.58	1.52
28	Y	302	9XX	O-C16	-2.18	1.40	1.45
19	G	504	7PH	O21-C21	2.18	1.40	1.34
20	G	503	IZL	O26-C41	-2.18	1.37	1.43
20	G	503	IZL	O23-C38	-2.18	1.37	1.43
20	G	503	IZL	O1-C11	-2.18	1.40	1.45
28	c	302	9XX	O-C16	-2.17	1.40	1.45
20	M	504	IZL	O6-C17	-2.17	1.37	1.43
20	M	504	IZL	O26-C41	-2.17	1.37	1.43
19	G	505	7PH	O21-C21	2.16	1.40	1.34
20	G	503	IZL	P-O30	-2.16	1.45	1.55
20	M	504	IZL	P-O30	-2.16	1.45	1.55
20	M	504	IZL	C36-C35	2.15	1.57	1.52
20	G	503	IZL	O6-C17	-2.15	1.37	1.43
20	G	503	IZL	O9-C21	-2.15	1.40	1.43
20	M	504	IZL	O1-C11	-2.14	1.40	1.45
19	M	503	7PH	O31-C3	-2.12	1.40	1.45
21	N	602	HEM	CMB-C2B	2.09	1.55	1.50
20	M	504	IZL	C33-C32	2.09	1.58	1.51
20	M	504	IZL	O12-C26	-2.09	1.39	1.44
21	N	606	HEM	CMB-C2B	2.09	1.55	1.50
20	M	504	IZL	O9-C21	-2.08	1.40	1.43
19	G	504	7PH	O31-C3	-2.08	1.40	1.45
13	O	301	WUO	C06-C05	2.08	1.57	1.53
16	P	301	CDL	C31-CA7	2.07	1.56	1.50
20	G	503	IZL	O12-C26	-2.07	1.39	1.44
14	O	303	HEC	CMC-C2C	2.06	1.55	1.50
14	O	302	HEC	CMC-C2C	2.06	1.55	1.50
20	G	503	IZL	C33-C32	2.06	1.58	1.51
16	R	601	CDL	C31-CA7	2.05	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	O	303	HEC	CMB-C2B	2.05	1.55	1.50
21	N	606	HEM	CMC-C2C	2.05	1.55	1.50
14	O	302	HEC	C3C-C2C	-2.03	1.34	1.41
20	G	503	IZL	C42-C41	2.03	1.57	1.52
20	M	504	IZL	C42-C41	2.02	1.57	1.52
14	O	303	HEC	C3C-C2C	-2.02	1.34	1.41
14	O	302	HEC	CMB-C2B	2.01	1.54	1.50
18	M	502	9YF	O2-C2	-2.01	1.37	1.44
13	P	302	WUO	C06-C05	2.01	1.57	1.53
14	O	303	HEC	C3B-C2B	-2.01	1.34	1.41
13	O	301	WUO	O13-C14	2.01	1.39	1.33
21	N	602	HEM	CMC-C2C	2.01	1.54	1.50
21	H	604	HEM	CMC-C2C	2.01	1.54	1.50

All (197) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	O	303	HEC	CBB-CAB-C3B	-8.80	109.84	127.43
14	O	303	HEC	CBC-CAC-C3C	-8.29	110.86	127.43
14	O	302	HEC	CBC-CAC-C3C	-8.12	111.21	127.43
14	O	302	HEC	CBB-CAB-C3B	-8.11	111.22	127.43
24	R	602	HEA	C3D-C4D-ND	6.56	116.69	110.35
24	R	603	HEA	C2B-C1B-NB	5.78	116.58	109.90
24	R	603	HEA	C12-C11-C3B	-5.63	103.33	112.12
20	M	504	IZL	O10-C23-C24	5.48	117.55	106.69
20	G	503	IZL	O10-C23-C24	5.47	117.54	106.69
24	R	602	HEA	C13-C12-C11	-5.37	105.81	114.39
24	R	603	HEA	C1D-C2D-C3D	-5.22	101.49	106.98
24	R	602	HEA	C2B-C1B-NB	5.20	115.92	109.90
24	R	602	HEA	C3C-C2C-C1C	-5.16	101.08	107.17
24	R	602	HEA	C13-C14-C15	-5.14	115.85	127.62
24	R	602	HEA	C3B-C4B-NB	5.07	115.67	109.84
24	R	602	HEA	C3C-C4C-NC	4.99	114.00	109.80
24	R	602	HEA	C2D-C1D-ND	4.90	115.47	109.84
24	R	603	HEA	C3A-C2A-C1A	-4.77	102.53	107.05
24	R	603	HEA	C3C-C2C-C1C	-4.73	101.59	107.17
24	R	603	HEA	C1B-C2B-C3B	-4.43	101.67	106.80
28	W	202	9XX	O1-C18-C19	4.41	121.02	111.48
24	R	602	HEA	C1D-C2D-C3D	-4.40	102.36	106.98
24	R	603	HEA	OMA-CMA-C3A	-4.24	116.06	125.62
24	R	602	HEA	C2A-C1A-NA	4.23	114.40	110.32
18	W	201	9YF	O1-P-O8	4.20	131.97	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	G	502	9YF	O1-P-O8	4.17	131.82	112.44
24	R	603	HEA	C4A-C3A-C2A	4.13	110.40	106.81
18	W	201	9YF	C7-C2-C3	-4.13	105.13	110.86
18	M	502	9YF	O1-P-O8	4.13	131.64	112.44
24	R	603	HEA	C3D-C4D-ND	4.09	114.31	110.35
24	R	603	HEA	C2A-C1A-NA	4.08	114.26	110.32
13	P	302	WUO	O58-C59-C61	4.04	120.21	111.48
28	Y	302	9XX	O1-C18-C19	4.02	120.19	111.48
24	R	603	HEA	CHA-C1A-NA	-4.02	120.08	124.45
28	c	302	9XX	O1-C18-C19	4.01	120.17	111.48
16	R	601	CDL	OA6-CA5-C11	3.98	120.09	111.48
20	G	503	IZL	O34-C60-C61	3.97	120.08	111.48
18	G	502	9YF	C7-C2-C3	-3.97	105.35	110.86
19	M	503	7PH	O21-C21-C22	3.96	120.05	111.48
13	O	301	WUO	O04-C05-C12	3.94	114.51	106.69
20	M	504	IZL	O34-C60-C61	3.93	119.99	111.48
13	O	301	WUO	O58-C59-C61	3.93	119.98	111.48
16	R	601	CDL	OB6-CB5-C51	3.92	119.96	111.48
18	M	502	9YF	C7-C2-C3	-3.90	105.45	110.86
24	R	602	HEA	C26-C15-C16	3.89	121.98	115.23
24	R	603	HEA	C2D-C1D-ND	3.86	114.28	109.84
24	R	603	HEA	C3C-C4C-NC	3.77	112.97	109.80
24	R	603	HEA	C3B-C4B-NB	3.77	114.17	109.84
19	G	504	7PH	O21-C21-C22	3.77	119.63	111.48
13	P	302	WUO	O04-C05-C12	3.76	114.15	106.69
23	S	503	3PE	O21-C21-C22	3.76	119.61	111.48
24	R	602	HEA	C2C-C1C-NC	3.75	116.16	110.14
16	P	301	CDL	OB6-CB5-C51	3.75	119.59	111.48
24	R	603	HEA	C17-C18-C19	-3.74	119.06	127.62
24	R	602	HEA	CHA-C4D-C3D	-3.72	119.35	124.77
24	R	603	HEA	CMD-C2D-C1D	3.66	130.76	125.03
13	P	302	WUO	C03-O04-C05	3.66	120.87	113.72
16	P	301	CDL	OA6-CA5-C11	3.65	119.39	111.48
19	G	505	7PH	O21-C21-C22	3.65	119.39	111.48
13	O	301	WUO	C03-O04-C05	3.63	120.81	113.72
24	R	603	HEA	CAD-CBD-CGD	-3.62	104.06	113.67
24	R	602	HEA	C1B-C2B-C3B	-3.61	102.61	106.80
14	O	303	HEC	C4D-ND-C1D	3.56	111.63	105.82
24	R	602	HEA	OMA-CMA-C3A	-3.52	117.67	125.62
14	O	302	HEC	C4D-ND-C1D	3.51	111.55	105.82
20	G	503	IZL	O11-C25-C30	3.50	114.94	108.31
20	M	504	IZL	O11-C25-C30	3.49	114.92	108.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	G	503	IZL	C21-O9-C22	3.40	121.08	113.80
20	M	504	IZL	C21-O9-C22	3.37	121.02	113.80
24	R	602	HEA	CBA-CAA-C2A	-3.36	103.25	112.53
24	R	603	HEA	CAA-C2A-C1A	3.35	131.67	124.85
13	P	302	WUO	O54-P52-O53	3.35	128.01	112.44
13	O	301	WUO	O54-P52-O53	3.29	127.76	112.44
24	R	602	HEA	C3A-C2A-C1A	-3.29	103.93	107.05
24	R	603	HEA	O11-C11-C3B	-3.22	105.35	111.26
13	P	302	WUO	O55-P52-O53	-3.22	96.16	108.94
13	O	301	WUO	C33-C31-C01	3.19	116.93	109.68
13	O	301	WUO	C08-C07-C06	-3.18	105.25	110.83
13	O	301	WUO	O55-P52-O53	-3.17	96.35	108.94
24	R	603	HEA	CHA-C4D-C3D	-3.09	120.27	124.77
24	R	603	HEA	CMC-C2C-C1C	3.02	130.02	125.42
20	M	504	IZL	O28-P-O29	-3.01	100.19	109.81
20	G	503	IZL	O28-P-O29	-3.00	100.22	109.81
24	R	602	HEA	C4A-NA-C1A	-2.99	100.94	105.82
20	G	503	IZL	O11-C24-C23	2.95	116.08	109.42
24	R	602	HEA	CAD-C3D-C2D	2.95	133.39	127.87
20	M	504	IZL	O11-C24-C23	2.95	116.06	109.42
24	R	603	HEA	C4A-NA-C1A	-2.94	101.03	105.82
21	H	601	HEM	C3B-C2B-C1B	2.90	108.59	106.41
20	G	503	IZL	O1-C11-C12	2.87	114.46	108.41
13	P	302	WUO	C08-C07-C06	-2.86	105.80	110.83
20	M	504	IZL	O1-C11-C12	2.85	114.43	108.41
21	H	604	HEM	C3B-C2B-C1B	2.84	108.55	106.41
16	R	601	CDL	OA8-CA7-C31	2.84	120.50	111.83
24	R	602	HEA	C4D-C3D-C2D	-2.81	102.80	106.89
28	Y	302	9XX	O-C15-C14	2.78	120.30	111.83
28	c	302	9XX	O-C15-C14	2.77	120.29	111.83
24	R	603	HEA	C25-C23-C24	2.77	120.95	114.59
19	G	504	7PH	O31-C31-C32	2.74	120.18	111.83
13	P	302	WUO	C31-C01-C50	-2.71	105.63	111.72
23	S	503	3PE	O31-C31-C32	2.70	120.08	111.83
16	P	301	CDL	OB8-CB7-C71	2.70	120.07	111.83
16	P	301	CDL	OA8-CA7-C31	2.70	120.06	111.83
16	R	601	CDL	OB8-CB7-C71	2.70	120.05	111.83
24	R	602	HEA	CMB-C2B-C1B	2.68	129.23	125.03
19	M	503	7PH	O31-C31-C32	2.65	119.91	111.83
28	Y	302	9XX	C17-O1-C18	-2.63	113.99	117.78
28	c	302	9XX	C17-O1-C18	-2.63	113.99	117.78
24	R	602	HEA	C4B-C3B-C2B	-2.63	103.02	107.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	N	601	MQ9	C7-C6-C5	-2.62	120.40	124.89
21	H	604	HEM	C3B-C4B-NB	-2.62	107.59	109.47
28	W	202	9XX	O-C15-C14	2.61	119.78	111.83
15	O	304	MQ9	C7-C6-C5	-2.61	120.42	124.89
24	R	603	HEA	CHB-C1B-C2B	-2.60	120.92	125.03
19	G	505	7PH	O31-C31-C32	2.60	119.76	111.83
13	P	302	WUO	C33-C31-C01	2.59	115.57	109.68
15	N	608	MQ9	C7-C6-C5	-2.58	120.47	124.89
21	H	604	HEM	C1B-NB-C4B	2.58	108.26	105.21
24	R	603	HEA	C27-C19-C20	2.57	119.69	115.23
24	R	603	HEA	C12-C13-C14	-2.56	105.43	112.16
20	M	504	IZL	O30-P-O29	2.55	124.29	112.44
20	G	503	IZL	O30-P-O29	2.55	124.29	112.44
15	H	605	MQ9	C7-C6-C5	-2.54	120.54	124.89
21	H	601	HEM	C1B-NB-C4B	2.53	108.20	105.21
13	P	302	WUO	O02-C01-C50	2.52	113.83	107.42
13	O	301	WUO	O02-C01-C50	2.52	113.83	107.42
14	O	303	HEC	C2A-C1A-NA	-2.52	107.89	110.32
20	M	504	IZL	O32-C47-C48	2.52	119.51	111.83
20	G	503	IZL	O32-C47-C48	2.52	119.51	111.83
20	M	504	IZL	C31-O17-C32	2.50	118.60	113.72
13	P	302	WUO	O10-C07-C08	-2.50	104.49	110.38
24	R	602	HEA	CAD-CBD-CGD	-2.49	107.06	113.67
13	O	301	WUO	O04-C05-C06	2.49	114.18	109.70
20	G	503	IZL	O1-C10-C9	2.48	119.41	111.83
24	R	602	HEA	C26-C15-C14	-2.48	117.26	123.63
20	G	503	IZL	C31-O17-C32	2.48	118.56	113.72
20	M	504	IZL	O1-C10-C9	2.46	119.35	111.83
15	N	607	MQ9	C7-C6-C5	-2.46	120.67	124.89
15	H	606	MQ9	C7-C6-C5	-2.45	120.69	124.89
24	R	603	HEA	CHC-C4B-NB	-2.44	121.35	124.37
24	R	602	HEA	CMD-C2D-C1D	2.43	128.84	125.03
21	H	601	HEM	C3B-C4B-NB	-2.42	107.73	109.47
13	O	301	WUO	O10-C07-C08	-2.41	104.69	110.38
24	R	602	HEA	C27-C19-C20	2.34	119.29	115.23
20	G	503	IZL	C24-O11-C25	2.33	118.79	113.80
20	G	503	IZL	O1-C10-O	-2.32	117.82	123.63
21	N	606	HEM	C4D-ND-C1D	2.31	107.95	105.21
24	R	603	HEA	CMB-C2B-C1B	2.31	128.64	125.03
20	M	504	IZL	O1-C10-O	-2.31	117.86	123.63
13	P	302	WUO	O58-C59-O60	-2.30	118.32	123.70
20	M	504	IZL	C24-O11-C25	2.30	118.73	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	P	302	WUO	C33-C35-C37	2.30	114.90	109.68
24	R	602	HEA	CHC-C1C-C2C	-2.28	120.80	127.43
13	O	301	WUO	O58-C59-O60	-2.28	118.38	123.70
21	H	601	HEM	C4D-ND-C1D	2.27	107.90	105.21
14	O	302	HEC	C2A-C1A-NA	-2.27	108.13	110.32
21	N	602	HEM	C4D-ND-C1D	2.26	107.89	105.21
21	N	606	HEM	C2A-C1A-NA	-2.25	107.66	110.15
21	N	602	HEM	C1B-NB-C4B	2.24	107.86	105.21
21	H	604	HEM	C4D-ND-C1D	2.24	107.86	105.21
21	H	604	HEM	C2A-C1A-NA	-2.22	107.69	110.15
24	R	602	HEA	CHB-C1B-C2B	-2.22	121.52	125.03
24	R	602	HEA	CHA-C1A-C2A	-2.21	121.37	124.86
20	M	504	IZL	O25-C40-C20	-2.21	103.88	109.32
20	G	503	IZL	O25-C40-C20	-2.20	103.90	109.32
24	R	603	HEA	C17-C16-C15	-2.20	105.90	113.19
13	P	302	WUO	O40-C39-C44	2.19	114.87	110.37
24	R	602	HEA	CMC-C2C-C1C	2.19	128.75	125.42
13	P	302	WUO	O04-C05-C06	2.19	113.64	109.70
24	R	603	HEA	C4B-C3B-C2B	-2.18	103.77	107.44
21	H	601	HEM	CHC-C1C-NC	2.18	126.82	124.45
20	G	503	IZL	O17-C32-C33	2.18	111.83	106.44
21	N	606	HEM	C3D-C4D-ND	-2.17	107.79	110.17
20	M	504	IZL	O17-C32-C33	2.16	111.80	106.44
18	M	502	9YF	O6-C6-C7	-2.16	105.29	110.38
20	G	503	IZL	O34-C60-O35	-2.15	118.68	123.70
24	R	602	HEA	C25-C23-C24	2.15	119.53	114.59
24	R	602	HEA	C1D-ND-C4D	-2.13	102.68	105.21
21	N	606	HEM	C1B-NB-C4B	2.13	107.73	105.21
24	R	603	HEA	C2C-C1C-NC	2.13	113.55	110.14
20	G	503	IZL	O16-C31-O17	-2.13	105.10	110.69
24	R	602	HEA	CAA-C2A-C1A	2.11	129.15	124.85
20	M	504	IZL	O34-C60-O35	-2.11	118.77	123.70
20	G	503	IZL	O16-C31-C36	2.11	113.28	108.09
20	M	504	IZL	O16-C31-O17	-2.10	105.18	110.69
24	R	602	HEA	C25-C23-C22	-2.09	116.37	122.66
20	M	504	IZL	O16-C31-C36	2.09	113.24	108.09
13	O	301	WUO	O40-C39-C44	2.07	114.62	110.37
13	O	301	WUO	O38-C39-O40	-2.07	105.25	110.69
24	R	602	HEA	C4B-NB-C1B	-2.06	102.77	105.21
18	W	201	9YF	O11-C25-C26	2.05	118.09	111.83
21	N	602	HEM	C2A-C1A-NA	-2.04	107.89	110.15
21	H	604	HEM	C3D-C4D-ND	-2.04	107.93	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	G	503	IZL	O32-C46-C45	2.04	114.28	108.40
20	M	504	IZL	O32-C46-C45	2.04	114.27	108.40
21	N	602	HEM	C3D-C4D-ND	-2.01	107.96	110.17
18	G	502	9YF	O11-C25-C26	2.00	117.94	111.83

There are no chirality outliers.

All (947) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	P	302	WUO	C06-C05-C12-O13
13	P	302	WUO	O55-C56-C57-O58
14	O	302	HEC	C2B-C3B-CAB-CBB
14	O	302	HEC	C4B-C3B-CAB-CBB
14	O	302	HEC	C2C-C3C-CAC-CBC
14	O	303	HEC	C2B-C3B-CAB-CBB
14	O	303	HEC	C4B-C3B-CAB-CBB
14	O	303	HEC	C2C-C3C-CAC-CBC
15	O	304	MQ9	C1-C6-C7-C8
15	O	304	MQ9	C7-C8-C9-C10
15	O	304	MQ9	C7-C8-C9-C11
15	O	304	MQ9	C22-C23-C24-C25
15	O	304	MQ9	C22-C23-C24-C26
15	O	304	MQ9	C31-C32-C33-C34
15	O	304	MQ9	C32-C33-C34-C35
15	O	304	MQ9	C32-C33-C34-C36
15	O	304	MQ9	C42-C43-C44-C45
15	O	304	MQ9	C42-C43-C44-C46
15	N	607	MQ9	C12-C13-C14-C15
15	N	607	MQ9	C12-C13-C14-C16
15	N	607	MQ9	C21-C22-C23-C24
15	N	607	MQ9	C26-C27-C28-C29
15	N	607	MQ9	C27-C28-C29-C30
15	N	607	MQ9	C27-C28-C29-C31
15	N	607	MQ9	C43-C44-C46-C47
15	N	607	MQ9	C45-C44-C46-C47
15	N	608	MQ9	C7-C8-C9-C10
15	N	608	MQ9	C7-C8-C9-C11
15	N	608	MQ9	C30-C29-C31-C32
15	N	608	MQ9	C32-C33-C34-C35
15	N	608	MQ9	C32-C33-C34-C36
15	N	608	MQ9	C42-C43-C44-C45
15	N	608	MQ9	C42-C43-C44-C46

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Mol	Chain	Res	Type	Atoms
15	N	608	MQ9	C46-C47-C48-C49
15	H	605	MQ9	C7-C8-C9-C10
15	H	605	MQ9	C7-C8-C9-C11
15	H	605	MQ9	C12-C13-C14-C15
15	H	605	MQ9	C12-C13-C14-C16
15	H	605	MQ9	C22-C23-C24-C25
15	H	605	MQ9	C22-C23-C24-C26
15	H	605	MQ9	C26-C27-C28-C29
15	H	606	MQ9	C7-C8-C9-C10
15	H	606	MQ9	C7-C8-C9-C11
15	H	606	MQ9	C17-C18-C19-C20
15	H	606	MQ9	C17-C18-C19-C21
15	H	606	MQ9	C27-C28-C29-C30
15	H	606	MQ9	C27-C28-C29-C31
15	H	606	MQ9	C36-C37-C38-C39
15	H	606	MQ9	C37-C38-C39-C40
15	H	606	MQ9	C37-C38-C39-C41
15	H	606	MQ9	C42-C43-C44-C45
15	H	606	MQ9	C42-C43-C44-C46
16	O	305	CDL	CA2-OA2-PA1-OA3
16	O	305	CDL	CA2-OA2-PA1-OA5
16	O	305	CDL	CA3-OA5-PA1-OA2
16	O	305	CDL	CA3-OA5-PA1-OA4
16	N	603	CDL	CA2-OA2-PA1-OA3
16	N	603	CDL	CA2-OA2-PA1-OA5
16	N	603	CDL	CA3-OA5-PA1-OA3
16	N	603	CDL	CA3-OA5-PA1-OA4
16	N	603	CDL	C11-CA5-OA6-CA4
16	N	603	CDL	CB2-OB2-PB2-OB3
16	N	603	CDL	CB3-OB5-PB2-OB2
16	N	603	CDL	CB3-OB5-PB2-OB4
16	N	604	CDL	CA3-OA5-PA1-OA2
16	N	604	CDL	CA3-OA5-PA1-OA3
16	N	604	CDL	CA3-OA5-PA1-OA4
16	N	604	CDL	CB2-OB2-PB2-OB4
16	N	604	CDL	CB2-OB2-PB2-OB5
16	N	605	CDL	CA2-OA2-PA1-OA3
16	N	605	CDL	CA2-OA2-PA1-OA4
16	N	605	CDL	CA2-OA2-PA1-OA5
16	N	605	CDL	CA3-OA5-PA1-OA2
16	N	605	CDL	CA3-OA5-PA1-OA3
16	N	605	CDL	CA3-OA5-PA1-OA4

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Mol	Chain	Res	Type	Atoms
16	N	605	CDL	CB2-OB2-PB2-OB3
16	N	605	CDL	CB2-OB2-PB2-OB4
16	N	605	CDL	CB2-OB2-PB2-OB5
16	N	605	CDL	CB3-OB5-PB2-OB2
16	N	605	CDL	CB3-OB5-PB2-OB3
16	P	301	CDL	CA2-OA2-PA1-OA3
16	P	301	CDL	CA2-OA2-PA1-OA4
16	P	301	CDL	CA2-OA2-PA1-OA5
16	P	301	CDL	OA7-CA5-OA6-CA4
16	P	301	CDL	CB2-OB2-PB2-OB3
16	P	301	CDL	CB2-OB2-PB2-OB4
16	P	301	CDL	CB2-OB2-PB2-OB5
16	P	301	CDL	CB3-OB5-PB2-OB2
16	P	301	CDL	CB3-OB5-PB2-OB3
16	P	301	CDL	C51-CB5-OB6-CB4
16	R	601	CDL	CA2-OA2-PA1-OA3
16	R	601	CDL	CA2-OA2-PA1-OA4
16	R	601	CDL	CA2-OA2-PA1-OA5
16	R	601	CDL	CB2-OB2-PB2-OB3
16	R	601	CDL	CB2-OB2-PB2-OB4
16	R	601	CDL	CB2-OB2-PB2-OB5
16	R	601	CDL	CB3-OB5-PB2-OB4
16	R	605	CDL	CA2-C1-CB2-OB2
16	R	605	CDL	CA3-OA5-PA1-OA2
16	R	605	CDL	CB2-OB2-PB2-OB4
16	R	605	CDL	CB3-OB5-PB2-OB2
16	R	605	CDL	C51-CB5-OB6-CB4
16	H	602	CDL	CA3-OA5-PA1-OA2
16	H	602	CDL	C11-CA5-OA6-CA4
16	H	602	CDL	CB3-OB5-PB2-OB2
16	H	602	CDL	CB3-OB5-PB2-OB3
16	H	602	CDL	CB3-OB5-PB2-OB4
16	H	603	CDL	CA2-OA2-PA1-OA3
16	H	603	CDL	CB2-OB2-PB2-OB3
16	H	603	CDL	CB2-OB2-PB2-OB4
16	H	603	CDL	CB2-OB2-PB2-OB5
16	H	603	CDL	CB3-OB5-PB2-OB3
18	M	502	9YF	C2-O2-P-O1
18	M	502	9YF	C2-O2-P-O
18	M	502	9YF	C1-O-P-O2
18	W	201	9YF	C2-O2-P-O1
18	W	201	9YF	C9-C8-O9-C

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Mol	Chain	Res	Type	Atoms
18	G	502	9YF	C2-O2-P-O1
18	G	502	9YF	C1-O-P-O2
19	M	503	7PH	C1-O11-P-O12
19	M	503	7PH	C1-O11-P-O13
19	M	503	7PH	C1-O11-P-O14
20	M	504	IZL	O31-C44-C45-O34
20	M	504	IZL	C48-C47-O32-C46
20	M	504	IZL	C43-O28-P-O30
20	G	503	IZL	O31-C44-C45-O34
20	G	503	IZL	C48-C47-O32-C46
20	G	503	IZL	C43-O28-P-O30
21	N	606	HEM	C1A-C2A-CAA-CBA
23	S	503	3PE	C1-O11-P-O12
23	S	503	3PE	C1-O11-P-O13
23	S	503	3PE	C1-O11-P-O14
23	S	503	3PE	C22-C21-O21-C2
24	R	602	HEA	C2D-C3D-CAD-CBD
24	R	603	HEA	C2A-C3A-CMA-OMA
24	R	603	HEA	C4A-C3A-CMA-OMA
24	R	603	HEA	C11-C12-C13-C14
28	W	202	9XX	O-C16-C17-O1
28	W	202	9XX	C19-C18-O1-C17
28	W	202	9XX	O2-C18-O1-C17
28	Y	302	9XX	C19-C18-O1-C17
28	Y	302	9XX	O2-C18-O1-C17
28	c	302	9XX	C19-C18-O1-C17
28	c	302	9XX	O2-C18-O1-C17
29	W	203	PLM	O2-C1-C2-C3
16	N	603	CDL	OB9-CB7-OB8-CB6
20	M	504	IZL	O33-C47-O32-C46
20	G	503	IZL	O33-C47-O32-C46
20	M	504	IZL	O10-C23-C24-O11
20	G	503	IZL	O10-C23-C24-O11
15	O	304	MQ9	C47-C48-C49-C50
15	O	304	MQ9	C47-C48-C49-C51
15	N	607	MQ9	C47-C48-C49-C50
15	N	607	MQ9	C47-C48-C49-C51
16	N	603	CDL	C71-CB7-OB8-CB6
16	H	603	CDL	C31-CA7-OA8-CA6
13	P	302	WUO	O79-C78-O77-C76
16	N	605	CDL	OA9-CA7-OA8-CA6
16	H	603	CDL	OA9-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
19	G	504	7PH	O32-C31-O31-C3
28	W	202	9XX	O6-C15-O-C16
16	N	603	CDL	OA7-CA5-OA6-CA4
16	P	301	CDL	OB7-CB5-OB6-CB4
16	H	602	CDL	OA7-CA5-OA6-CA4
18	W	201	9YF	O10-C8-O9-C
23	S	503	3PE	O22-C21-O21-C2
16	N	605	CDL	C31-CA7-OA8-CA6
16	P	301	CDL	C11-CA5-OA6-CA4
20	M	504	IZL	C61-C60-O34-C45
20	G	503	IZL	C61-C60-O34-C45
15	N	601	MQ9	C20-C19-C21-C22
15	N	607	MQ9	C30-C29-C31-C32
15	N	607	MQ9	C35-C34-C36-C37
15	N	607	MQ9	C40-C39-C41-C42
15	N	608	MQ9	C15-C14-C16-C17
15	H	605	MQ9	C35-C34-C36-C37
15	H	606	MQ9	C15-C14-C16-C17
24	R	603	HEA	C26-C15-C16-C17
24	R	603	HEA	C27-C19-C20-C21
15	N	607	MQ9	C28-C29-C31-C32
15	N	607	MQ9	C38-C39-C41-C42
15	N	608	MQ9	C13-C14-C16-C17
15	N	608	MQ9	C28-C29-C31-C32
24	R	603	HEA	C14-C15-C16-C17
13	P	302	WUO	C80-C78-O77-C76
16	R	605	CDL	C31-CA7-OA8-CA6
18	M	502	9YF	C26-C25-O11-C24
18	G	502	9YF	C26-C25-O11-C24
19	G	504	7PH	C32-C31-O31-C3
28	W	202	9XX	C14-C15-O-C16
15	O	304	MQ9	C12-C13-C14-C15
15	N	607	MQ9	C7-C8-C9-C10
15	N	608	MQ9	C27-C28-C29-C30
15	H	606	MQ9	C22-C23-C24-C25
15	O	304	MQ9	C12-C13-C14-C16
15	N	607	MQ9	C7-C8-C9-C11
15	N	608	MQ9	C27-C28-C29-C31
16	R	605	CDL	OA9-CA7-OA8-CA6
24	R	602	HEA	C4D-C3D-CAD-CBD
16	R	605	CDL	OB7-CB5-OB6-CB4
20	M	504	IZL	O35-C60-O34-C45

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Mol	Chain	Res	Type	Atoms
20	G	503	IZL	O35-C60-O34-C45
16	P	301	CDL	O1-C1-CA2-OA2
20	M	504	IZL	O12-C26-C27-O13
20	G	503	IZL	O12-C26-C27-O13
20	M	504	IZL	C36-C31-O16-C30
20	G	503	IZL	C36-C31-O16-C30
16	N	605	CDL	C11-CA5-OA6-CA4
19	G	504	7PH	C22-C21-O21-C2
18	G	502	9YF	O12-C25-O11-C24
20	M	504	IZL	O17-C31-O16-C30
20	G	503	IZL	O17-C31-O16-C30
15	N	607	MQ9	C12-C11-C9-C10
15	N	608	MQ9	C25-C24-C26-C27
15	H	606	MQ9	C25-C24-C26-C27
15	N	601	MQ9	C18-C19-C21-C22
15	N	607	MQ9	C12-C11-C9-C8
15	N	608	MQ9	C23-C24-C26-C27
15	H	605	MQ9	C33-C34-C36-C37
15	H	606	MQ9	C23-C24-C26-C27
15	H	606	MQ9	C28-C29-C31-C32
24	R	603	HEA	C18-C19-C20-C21
15	N	601	MQ9	C19-C21-C22-C23
15	N	608	MQ9	C29-C31-C32-C33
15	N	608	MQ9	C34-C36-C37-C38
15	H	605	MQ9	C24-C26-C27-C28
15	H	605	MQ9	C44-C46-C47-C48
15	H	606	MQ9	C14-C16-C17-C18
15	H	606	MQ9	C19-C21-C22-C23
24	R	603	HEA	C19-C20-C21-C22
18	M	502	9YF	O12-C25-O11-C24
20	M	504	IZL	O12-C25-O11-C24
20	G	503	IZL	O12-C25-O11-C24
15	N	607	MQ9	C37-C38-C39-C40
20	M	504	IZL	O17-C32-C33-O18
20	G	503	IZL	O17-C32-C33-O18
15	N	607	MQ9	C17-C18-C19-C21
15	H	606	MQ9	C22-C23-C24-C26
15	H	606	MQ9	C47-C48-C49-C51
19	G	504	7PH	O22-C21-O21-C2
16	N	605	CDL	CB2-C1-CA2-OA2
16	R	601	CDL	CA2-C1-CB2-OB2
16	O	305	CDL	C71-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
16	R	601	CDL	C31-CA7-OA8-CA6
20	M	504	IZL	C37-C23-C24-O11
20	G	503	IZL	C37-C23-C24-O11
20	M	504	IZL	C34-C32-C33-O18
20	G	503	IZL	C34-C32-C33-O18
16	N	605	CDL	C57-C58-C59-C60
15	N	601	MQ9	C25-C24-C26-C27
15	H	606	MQ9	C30-C29-C31-C32
15	N	601	MQ9	C23-C24-C26-C27
15	N	607	MQ9	C33-C34-C36-C37
15	H	606	MQ9	C13-C14-C16-C17
13	O	301	WUO	C89-C88-C90-C91
13	P	302	WUO	C86-C87-C88-C89
18	W	201	9YF	C31-C32-C33-C34
20	M	504	IZL	C54-C55-C56-C57
20	G	503	IZL	C54-C55-C56-C57
16	O	305	CDL	OB9-CB7-OB8-CB6
16	R	605	CDL	C11-CA5-OA6-CA4
18	G	502	9YF	C14-C15-C16-C17
15	N	607	MQ9	C17-C18-C19-C20
18	M	502	9YF	C14-C15-C16-C17
16	R	601	CDL	CA7-C31-C32-C33
18	M	502	9YF	C31-C32-C33-C35
18	G	502	9YF	C31-C32-C33-C35
16	N	603	CDL	CA5-C11-C12-C13
18	M	502	9YF	C11-C10-C9-C8
13	P	302	WUO	O04-C05-C12-O13
16	N	605	CDL	OA7-CA5-OA6-CA4
15	N	608	MQ9	C39-C41-C42-C43
15	H	606	MQ9	C24-C26-C27-C28
24	R	602	HEA	C19-C20-C21-C22
24	R	603	HEA	C15-C16-C17-C18
13	P	302	WUO	C85-C86-C87-C88
16	N	603	CDL	CB7-C71-C72-C73
16	N	604	CDL	CB5-C51-C52-C53
16	R	601	CDL	CB7-C71-C72-C73
14	O	303	HEC	C3D-CAD-CBD-CGD
21	N	602	HEM	C3D-CAD-CBD-CGD
21	H	601	HEM	C3D-CAD-CBD-CGD
13	O	301	WUO	C59-C61-C62-C63
13	P	302	WUO	C59-C61-C62-C63
16	O	305	CDL	CB5-C51-C52-C53

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Mol	Chain	Res	Type	Atoms
18	G	502	9YF	C11-C10-C9-C8
18	G	502	9YF	C25-C26-C27-C28
16	R	601	CDL	OA9-CA7-OA8-CA6
13	O	301	WUO	C80-C81-C82-C83
16	P	301	CDL	C11-C12-C13-C14
16	N	605	CDL	O1-C1-CA2-OA2
16	N	605	CDL	O1-C1-CB2-OB2
16	P	301	CDL	O1-C1-CB2-OB2
16	R	601	CDL	O1-C1-CB2-OB2
16	R	601	CDL	CA5-C11-C12-C13
18	M	502	9YF	C25-C26-C27-C28
16	R	605	CDL	OA7-CA5-OA6-CA4
20	M	504	IZL	C28-C26-C27-O13
20	G	503	IZL	C28-C26-C27-O13
20	M	504	IZL	C53-C54-C55-C56
20	G	503	IZL	C53-C54-C55-C56
18	W	201	9YF	C30-C31-C32-C33
13	P	302	WUO	C16-C14-O13-C12
16	O	305	CDL	C51-CB5-OB6-CB4
16	N	605	CDL	C51-CB5-OB6-CB4
13	P	302	WUO	C23-C24-C25-C26
18	W	201	9YF	C25-C26-C27-C28
16	N	605	CDL	OB7-CB5-OB6-CB4
16	N	605	CDL	CA2-C1-CB2-OB2
16	P	301	CDL	CA2-C1-CB2-OB2
18	G	502	9YF	C33-C35-C36-C37
16	N	605	CDL	C77-C78-C79-C80
16	R	605	CDL	C74-C75-C76-C77
18	M	502	9YF	C33-C35-C36-C37
18	M	502	9YF	C9-C8-O9-C
18	G	502	9YF	C9-C8-O9-C
16	O	305	CDL	OB7-CB5-OB6-CB4
18	M	502	9YF	O10-C8-O9-C
18	G	502	9YF	O10-C8-O9-C
15	N	601	MQ9	C14-C16-C17-C18
15	N	601	MQ9	C29-C31-C32-C33
15	H	606	MQ9	C9-C11-C12-C13
16	R	605	CDL	O1-C1-CB2-OB2
16	N	603	CDL	C31-CA7-OA8-CA6
13	P	302	WUO	O15-C14-O13-C12
16	N	605	CDL	CA7-C31-C32-C33
23	S	503	3PE	C3-C2-O21-C21

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Mol	Chain	Res	Type	Atoms
15	H	606	MQ9	C47-C48-C49-C50
13	O	301	WUO	C93-C94-C95-C96
13	O	301	WUO	C61-C59-O58-C57
19	S	501	7PH	C22-C21-O21-C2
16	O	305	CDL	C57-C58-C59-C60
16	N	603	CDL	C55-C56-C57-C58
18	W	201	9YF	C35-C36-C37-C38
16	O	305	CDL	C76-C77-C78-C79
16	R	601	CDL	C36-C37-C38-C39
16	H	603	CDL	C36-C37-C38-C39
18	M	502	9YF	C11-C12-C13-C14
18	G	502	9YF	C11-C12-C13-C14
19	S	501	7PH	C27-C28-C29-C2A
16	H	603	CDL	CB5-C51-C52-C53
13	P	302	WUO	C82-C83-C84-C85
16	R	601	CDL	C32-C33-C34-C35
18	W	201	9YF	C16-C17-C18-C19
13	O	301	WUO	C24-C25-C26-C27
13	P	302	WUO	C90-C91-C92-C93
16	N	605	CDL	C55-C56-C57-C58
16	P	301	CDL	C32-C33-C34-C35
16	R	605	CDL	C35-C36-C37-C38
18	M	502	9YF	C29-C30-C31-C32
18	M	502	9YF	C38-C39-C40-C41
18	G	502	9YF	C29-C30-C31-C32
18	G	502	9YF	C38-C39-C40-C41
19	S	501	7PH	O22-C21-O21-C2
13	P	302	WUO	C64-C65-C66-C67
16	N	605	CDL	C52-C53-C54-C55
16	R	605	CDL	C16-C17-C18-C19
16	H	602	CDL	C18-C19-C20-C21
18	W	201	9YF	C29-C30-C31-C32
19	G	505	7PH	C21-C22-C23-C24
13	O	301	WUO	C64-C65-C66-C67
16	N	605	CDL	C22-C23-C24-C25
16	R	601	CDL	C59-C60-C61-C62
16	H	603	CDL	C13-C14-C15-C16
18	M	502	9YF	C18-C19-C20-C21
18	G	502	9YF	C18-C19-C20-C21
16	N	604	CDL	C51-CB5-OB6-CB4
16	H	602	CDL	C51-CB5-OB6-CB4
16	H	603	CDL	C11-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
16	R	601	CDL	C53-C54-C55-C56
16	N	604	CDL	O1-C1-CA2-OA2
19	S	501	7PH	C21-C22-C23-C24
16	R	605	CDL	C57-C58-C59-C60
16	H	602	CDL	C55-C56-C57-C58
18	M	502	9YF	C13-C14-C15-C16
18	W	201	9YF	C13-C14-C15-C16
16	P	301	CDL	C71-C72-C73-C74
16	H	602	CDL	C78-C79-C80-C81
16	H	603	CDL	C32-C33-C34-C35
16	N	603	CDL	C79-C80-C81-C82
16	N	605	CDL	C71-C72-C73-C74
19	S	501	7PH	C26-C27-C28-C29
13	O	301	WUO	O60-C59-O58-C57
16	R	605	CDL	C53-C54-C55-C56
20	M	504	IZL	C2-C1-C7-C8
20	G	503	IZL	C2-C1-C7-C8
13	P	302	WUO	C24-C25-C26-C27
16	N	603	CDL	C17-C18-C19-C20
16	N	604	CDL	C32-C33-C34-C35
16	N	604	CDL	C54-C55-C56-C57
18	G	502	9YF	C19-C20-C21-C22
13	P	302	WUO	C83-C84-C85-C86
16	O	305	CDL	C55-C56-C57-C58
16	N	604	CDL	C71-C72-C73-C74
16	N	605	CDL	C20-C21-C22-C23
16	N	605	CDL	C74-C75-C76-C77
16	R	605	CDL	C32-C33-C34-C35
16	H	603	CDL	C53-C54-C55-C56
18	M	502	9YF	C19-C20-C21-C22
18	G	502	9YF	C13-C14-C15-C16
20	M	504	IZL	C51-C52-C53-C54
20	G	503	IZL	C51-C52-C53-C54
18	W	201	9YF	C39-C40-C41-C42
16	H	602	CDL	C13-C14-C15-C16
13	P	302	WUO	C19-C20-C21-C22
16	R	601	CDL	C33-C34-C35-C36
16	H	602	CDL	C76-C77-C78-C79
19	S	501	7PH	C2A-C2B-C2C-C2D
15	N	607	MQ9	C22-C23-C24-C25
16	R	605	CDL	CA7-C31-C32-C33
16	N	603	CDL	OA9-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
16	R	601	CDL	C51-CB5-OB6-CB4
16	R	601	CDL	C34-C35-C36-C37
13	P	302	WUO	C61-C62-C63-C64
16	N	605	CDL	C76-C77-C78-C79
19	G	504	7PH	C32-C33-C34-C35
18	G	502	9YF	C39-C40-C41-C42
16	N	604	CDL	OB7-CB5-OB6-CB4
15	O	304	MQ9	C30-C29-C31-C32
15	H	605	MQ9	C40-C39-C41-C42
16	N	603	CDL	C53-C54-C55-C56
15	N	607	MQ9	C37-C38-C39-C41
16	H	603	CDL	C15-C16-C17-C18
18	M	502	9YF	C39-C40-C41-C42
18	W	201	9YF	C10-C11-C12-C13
22	R	608	TRD	C5-C6-C7-C8
16	H	602	CDL	CA5-C11-C12-C13
13	O	301	WUO	C80-C78-O77-C76
16	N	605	CDL	C71-CB7-OB8-CB6
13	P	302	WUO	C27-C28-C29-C30
16	N	604	CDL	C36-C37-C38-C39
16	N	604	CDL	C35-C36-C37-C38
16	R	605	CDL	C59-C60-C61-C62
16	N	603	CDL	CA7-C31-C32-C33
16	P	301	CDL	CB5-C51-C52-C53
15	N	608	MQ9	C47-C48-C49-C50
16	N	603	CDL	C16-C17-C18-C19
22	S	502	TRD	C4-C5-C6-C7
16	R	605	CDL	O1-C1-CA2-OA2
16	N	603	CDL	C72-C73-C74-C75
19	G	504	7PH	C35-C36-C37-C38
16	N	603	CDL	C51-CB5-OB6-CB4
16	N	604	CDL	C11-CA5-OA6-CA4
16	R	601	CDL	C11-CA5-OA6-CA4
16	H	603	CDL	C51-CB5-OB6-CB4
16	N	604	CDL	CA7-C31-C32-C33
24	R	603	HEA	C1A-C2A-CAA-CBA
18	M	502	9YF	C30-C31-C32-C33
16	N	603	CDL	OB7-CB5-OB6-CB4
16	H	603	CDL	OB7-CB5-OB6-CB4
16	N	603	CDL	C12-C13-C14-C15
16	H	602	CDL	C73-C74-C75-C76
16	O	305	CDL	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
16	O	305	CDL	C32-C33-C34-C35
16	O	305	CDL	C74-C75-C76-C77
16	O	305	CDL	C80-C81-C82-C83
16	N	603	CDL	C74-C75-C76-C77
15	N	608	MQ9	C20-C19-C21-C22
16	H	603	CDL	C16-C17-C18-C19
16	O	305	CDL	C13-C14-C15-C16
16	N	603	CDL	C71-C72-C73-C74
19	M	503	7PH	C29-C2A-C2B-C2C
16	R	601	CDL	CB5-C51-C52-C53
16	H	602	CDL	OB7-CB5-OB6-CB4
16	H	603	CDL	OA7-CA5-OA6-CA4
16	O	305	CDL	C81-C82-C83-C84
15	O	304	MQ9	C29-C31-C32-C33
15	N	607	MQ9	C44-C46-C47-C48
15	H	606	MQ9	C29-C31-C32-C33
21	H	604	HEM	C4B-C3B-CAB-CBB
13	P	302	WUO	C84-C85-C86-C87
16	H	602	CDL	C54-C55-C56-C57
16	H	603	CDL	C57-C58-C59-C60
19	G	505	7PH	C23-C24-C25-C26
13	O	301	WUO	C81-C82-C83-C84
16	N	605	CDL	C73-C74-C75-C76
16	R	605	CDL	C56-C57-C58-C59
16	H	602	CDL	C79-C80-C81-C82
13	P	302	WUO	C91-C92-C93-C94
16	P	301	CDL	C55-C56-C57-C58
16	R	605	CDL	C31-C32-C33-C34
16	N	603	CDL	C52-C53-C54-C55
16	N	605	CDL	C53-C54-C55-C56
19	G	505	7PH	C22-C23-C24-C25
13	P	302	WUO	C25-C26-C27-C28
16	P	301	CDL	CA5-C11-C12-C13
15	N	608	MQ9	C18-C19-C21-C22
18	G	502	9YF	C30-C31-C32-C33
16	P	301	CDL	C53-C54-C55-C56
18	G	502	9YF	C12-C13-C14-C15
19	M	503	7PH	C2A-C2B-C2C-C2D
16	N	604	CDL	C57-C58-C59-C60
15	H	605	MQ9	C47-C48-C49-C51
16	O	305	CDL	C73-C74-C75-C76
18	M	502	9YF	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
28	W	202	9XX	C6-C7-C8-C9
16	N	605	CDL	OB9-CB7-OB8-CB6
16	H	603	CDL	OB5-CB3-CB4-CB6
19	G	504	7PH	O11-C1-C2-C3
20	M	504	IZL	O31-C44-C45-C46
20	G	503	IZL	O31-C44-C45-C46
23	S	503	3PE	O11-C1-C2-C3
16	R	601	CDL	OB7-CB5-OB6-CB4
28	Y	302	9XX	C26-C27-C28-C29
28	c	302	9XX	C26-C27-C28-C29
16	N	604	CDL	C55-C56-C57-C58
13	O	301	WUO	O79-C78-O77-C76
13	O	301	WUO	C85-C86-C87-C88
16	H	603	CDL	C59-C60-C61-C62
13	P	302	WUO	C88-C90-C91-C92
16	H	603	CDL	C31-C32-C33-C34
23	S	503	3PE	C32-C31-O31-C3
16	N	604	CDL	C51-C52-C53-C54
16	H	602	CDL	C51-C52-C53-C54
16	R	605	CDL	CA3-CA4-CA6-OA8
16	H	602	CDL	CB3-CB4-CB6-OB8
18	W	201	9YF	C1-C-C24-O11
19	M	503	7PH	C1-C2-C3-O31
18	W	201	9YF	C33-C35-C36-C37
16	R	601	CDL	O1-C1-CA2-OA2
13	O	301	WUO	C65-C66-C67-C68
18	W	201	9YF	C38-C39-C40-C41
19	G	504	7PH	C34-C35-C36-C37
20	M	504	IZL	C62-C63-C64-C65
20	G	503	IZL	C62-C63-C64-C65
16	P	301	CDL	C58-C59-C60-C61
15	H	605	MQ9	C38-C39-C41-C42
19	G	504	7PH	C33-C34-C35-C36
16	N	603	CDL	C18-C19-C20-C21
16	O	305	CDL	C34-C35-C36-C37
16	N	604	CDL	C73-C74-C75-C76
21	N	606	HEM	C2A-CAA-CBA-CGA
20	M	504	IZL	C1-C7-C8-C9
20	G	503	IZL	C1-C7-C8-C9
28	W	202	9XX	C9-C10-C11-C12
16	P	301	CDL	C38-C39-C40-C41
16	R	601	CDL	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
16	N	604	CDL	C53-C54-C55-C56
18	M	502	9YF	C37-C38-C39-C40
16	H	603	CDL	OA5-CA3-CA4-OA6
18	W	201	9YF	O9-C-C1-O
16	O	305	CDL	C78-C79-C80-C81
16	R	605	CDL	C33-C34-C35-C36
19	S	501	7PH	C29-C2A-C2B-C2C
18	M	502	9YF	C16-C17-C18-C19
24	R	603	HEA	O11-C11-C12-C13
15	N	607	MQ9	C13-C14-C16-C17
16	R	605	CDL	C60-C61-C62-C63
13	P	302	WUO	C81-C82-C83-C84
16	P	301	CDL	C13-C14-C15-C16
16	H	602	CDL	C15-C16-C17-C18
28	W	202	9XX	C4-C5-C6-C7
16	H	603	CDL	C76-C77-C78-C79
13	O	301	WUO	C91-C92-C93-C94
18	G	502	9YF	C16-C17-C18-C19
16	N	605	CDL	C78-C79-C80-C81
13	O	301	WUO	C27-C28-C29-C30
20	M	504	IZL	C4-C5-C6-C67
20	G	503	IZL	C4-C5-C6-C67
16	N	605	CDL	C51-C52-C53-C54
16	H	603	CDL	C18-C19-C20-C21
28	Y	302	9XX	C19-C20-C21-C22
28	c	302	9XX	C19-C20-C21-C22
16	H	603	CDL	C60-C61-C62-C63
24	R	602	HEA	C3B-C11-C12-C13
24	R	603	HEA	C3B-C11-C12-C13
16	O	305	CDL	C83-C84-C85-C86
23	S	503	3PE	O32-C31-O31-C3
20	M	504	IZL	C7-C8-C9-C10
20	G	503	IZL	C7-C8-C9-C10
16	P	301	CDL	C73-C74-C75-C76
18	W	201	9YF	C15-C16-C17-C18
16	N	604	CDL	C60-C61-C62-C63
16	N	605	CDL	C34-C35-C36-C37
16	H	602	CDL	C32-C33-C34-C35
18	G	502	9YF	C37-C38-C39-C40
16	H	602	CDL	C59-C60-C61-C62
19	G	504	7PH	C31-C32-C33-C34
20	G	503	IZL	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
16	N	605	CDL	C79-C80-C81-C82
15	H	606	MQ9	C40-C39-C41-C42
16	P	301	CDL	C18-C19-C20-C21
20	M	504	IZL	C1-C2-C3-C4
18	W	201	9YF	C27-C28-C29-C30
16	R	601	CDL	OA7-CA5-OA6-CA4
28	Y	302	9XX	C36-C27-C28-C29
28	c	302	9XX	C36-C27-C28-C29
16	N	605	CDL	CA4-CA3-OA5-PA1
13	P	302	WUO	C94-C95-C96-C97
13	O	301	WUO	C90-C91-C92-C93
16	N	604	CDL	C76-C77-C78-C79
16	N	605	CDL	C31-C32-C33-C34
16	R	605	CDL	C76-C77-C78-C79
16	N	604	CDL	OB5-CB3-CB4-CB6
16	P	301	CDL	OB5-CB3-CB4-CB6
16	R	601	CDL	OB5-CB3-CB4-CB6
19	G	505	7PH	O11-C1-C2-C3
16	N	603	CDL	C14-C15-C16-C17
16	N	604	CDL	C37-C38-C39-C40
13	P	302	WUO	C86-C87-C88-C90
15	N	608	MQ9	C47-C48-C49-C51
16	O	305	CDL	CA7-C31-C32-C33
19	M	503	7PH	C22-C23-C24-C25
16	R	605	CDL	C18-C19-C20-C21
15	N	607	MQ9	C15-C14-C16-C17
15	N	607	MQ9	C25-C24-C26-C27
15	O	304	MQ9	C28-C29-C31-C32
15	N	607	MQ9	C23-C24-C26-C27
21	N	606	HEM	C3A-C2A-CAA-CBA
18	W	201	9YF	C11-C12-C13-C14
28	Y	302	9XX	O-C16-C17-C37
28	c	302	9XX	O-C16-C17-C37
16	R	601	CDL	C71-CB7-OB8-CB6
16	O	305	CDL	C79-C80-C81-C82
28	W	202	9XX	C10-C11-C12-C13
13	O	301	WUO	C94-C95-C96-C97
16	R	601	CDL	C18-C19-C20-C21
18	M	502	9YF	C10-C11-C12-C13
19	G	505	7PH	C26-C27-C28-C29
16	N	604	CDL	OA7-CA5-OA6-CA4
16	R	601	CDL	CB2-C1-CA2-OA2

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Mol	Chain	Res	Type	Atoms
16	N	604	CDL	C31-C32-C33-C34
16	N	604	CDL	CB3-CB4-CB6-OB8
19	G	504	7PH	C1-C2-C3-O31
20	M	504	IZL	C66-C68-C69-C70
20	G	503	IZL	C66-C68-C69-C70
15	H	605	MQ9	C15-C14-C16-C17
28	Y	302	9XX	O-C16-C17-O1
28	c	302	9XX	O-C16-C17-O1
16	N	604	CDL	OB5-CB3-CB4-OB6
16	H	603	CDL	OB5-CB3-CB4-OB6
19	G	504	7PH	O11-C1-C2-O21
23	S	503	3PE	O11-C1-C2-O21
16	N	605	CDL	C1-CA2-OA2-PA1
16	N	603	CDL	C78-C79-C80-C81
16	R	605	CDL	C37-C38-C39-C40
18	G	502	9YF	C10-C11-C12-C13
24	R	603	HEA	C3A-C2A-CAA-CBA
21	H	604	HEM	C2A-CAA-CBA-CGA
16	R	605	CDL	C55-C56-C57-C58
23	S	503	3PE	C32-C33-C34-C35
13	P	302	WUO	C62-C63-C64-C65
13	P	302	WUO	O58-C57-C76-O77
16	H	602	CDL	C52-C53-C54-C55
15	H	605	MQ9	C47-C48-C49-C50
16	R	601	CDL	C51-C52-C53-C54
16	P	301	CDL	C74-C75-C76-C77
16	O	305	CDL	C71-C72-C73-C74
16	N	604	CDL	C16-C17-C18-C19
15	O	304	MQ9	C9-C11-C12-C13
15	N	607	MQ9	C9-C11-C12-C13
16	R	605	CDL	C12-C13-C14-C15
18	W	201	9YF	C37-C38-C39-C40
15	H	605	MQ9	C13-C14-C16-C17
15	H	606	MQ9	C38-C39-C41-C42
16	R	605	CDL	C36-C37-C38-C39
16	P	301	CDL	CB2-C1-CA2-OA2
16	H	603	CDL	C37-C38-C39-C40
16	P	301	CDL	C34-C35-C36-C37
13	P	302	WUO	O55-C56-C57-C76
16	H	603	CDL	OA5-CA3-CA4-CA6
13	O	301	WUO	C70-C71-C72-C73
13	O	301	WUO	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
16	H	603	CDL	C73-C74-C75-C76
16	N	605	CDL	C11-C12-C13-C14
15	O	304	MQ9	C5-C6-C7-C8
15	N	608	MQ9	C5-C6-C7-C8
20	M	504	IZL	C23-C24-O11-C25
20	G	503	IZL	C23-C24-O11-C25
16	P	301	CDL	C59-C60-C61-C62
16	N	604	CDL	C33-C34-C35-C36
16	R	601	CDL	C12-C13-C14-C15
18	W	201	9YF	C19-C20-C21-C22
16	N	605	CDL	CA6-CA4-OA6-CA5
16	R	601	CDL	OB9-CB7-OB8-CB6
16	N	604	CDL	C38-C39-C40-C41
16	N	603	CDL	C77-C78-C79-C80
16	P	301	CDL	OB5-CB3-CB4-OB6
16	R	601	CDL	OB5-CB3-CB4-OB6
19	G	505	7PH	O11-C1-C2-O21
15	N	607	MQ9	C24-C26-C27-C28
16	R	601	CDL	CA3-CA4-CA6-OA8
21	H	601	HEM	C4B-C3B-CAB-CBB
21	H	601	HEM	C4C-C3C-CAC-CBC
15	N	607	MQ9	C1-C6-C7-C8
15	N	608	MQ9	C1-C6-C7-C8
16	N	605	CDL	OA6-CA4-CA6-OA8
16	R	605	CDL	OA6-CA4-CA6-OA8
19	M	503	7PH	O21-C2-C3-O31
19	G	504	7PH	O21-C2-C3-O31
13	P	302	WUO	C89-C88-C90-C91
16	R	601	CDL	C74-C75-C76-C77
28	W	202	9XX	C2-C3-C4-C5
16	N	603	CDL	C32-C33-C34-C35
28	W	202	9XX	C19-C20-C21-C22
16	O	305	CDL	C15-C16-C17-C18
16	H	603	CDL	C33-C34-C35-C36
18	M	502	9YF	C2-O2-P-O8
16	N	605	CDL	C24-C25-C26-C27
16	N	603	CDL	C51-C52-C53-C54
19	S	501	7PH	O11-C1-C2-C3
13	O	301	WUO	C25-C26-C27-C28
16	H	602	CDL	C16-C17-C18-C19
16	R	601	CDL	C39-C40-C41-C42
16	H	603	CDL	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
14	O	302	HEC	C4C-C3C-CAC-CBC
14	O	303	HEC	C4C-C3C-CAC-CBC
15	O	304	MQ9	C15-C14-C16-C17
15	O	304	MQ9	C20-C19-C21-C22
16	H	602	CDL	OB5-CB3-CB4-OB6
19	S	501	7PH	O11-C1-C2-O21
13	O	301	WUO	C92-C93-C94-C95
18	M	502	9YF	C31-C32-C33-C34
18	G	502	9YF	C31-C32-C33-C34
18	M	502	9YF	C20-C21-C22-C23
16	N	603	CDL	C57-C58-C59-C60
16	N	603	CDL	C31-C32-C33-C34
13	O	301	WUO	O58-C57-C76-O77
16	N	604	CDL	OB6-CB4-CB6-OB8
16	R	601	CDL	OA6-CA4-CA6-OA8
16	H	602	CDL	OB6-CB4-CB6-OB8
18	W	201	9YF	O9-C-C24-O11
16	R	601	CDL	C75-C76-C77-C78
13	P	302	WUO	C56-C57-C76-O77
16	N	605	CDL	CA3-CA4-CA6-OA8
24	R	603	HEA	O11-C11-C3B-C4B
18	W	201	9YF	C36-C37-C38-C39
16	O	305	CDL	CA2-OA2-PA1-OA4
16	O	305	CDL	CA3-OA5-PA1-OA3
16	O	305	CDL	CB2-OB2-PB2-OB3
16	O	305	CDL	CB3-OB5-PB2-OB2
16	O	305	CDL	CB3-OB5-PB2-OB3
16	O	305	CDL	CB3-OB5-PB2-OB4
16	N	603	CDL	CA2-OA2-PA1-OA4
16	N	603	CDL	CA3-OA5-PA1-OA2
16	N	603	CDL	CB2-OB2-PB2-OB4
16	N	603	CDL	CB2-OB2-PB2-OB5
16	N	604	CDL	CB2-OB2-PB2-OB3
16	N	605	CDL	CB3-OB5-PB2-OB4
16	P	301	CDL	CA3-OA5-PA1-OA2
16	P	301	CDL	CA3-OA5-PA1-OA4
16	P	301	CDL	CB3-OB5-PB2-OB4
16	R	601	CDL	CB3-OB5-PB2-OB2
16	R	601	CDL	CB3-OB5-PB2-OB3
16	R	605	CDL	CA3-OA5-PA1-OA3
16	R	605	CDL	CB2-OB2-PB2-OB3
16	R	605	CDL	CB2-OB2-PB2-OB5

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Mol	Chain	Res	Type	Atoms
16	R	605	CDL	CB3-OB5-PB2-OB3
16	H	602	CDL	CA3-OA5-PA1-OA3
16	H	603	CDL	CA2-OA2-PA1-OA5
16	H	603	CDL	CB3-OB5-PB2-OB2
18	M	502	9YF	C1-O-P-O8
18	W	201	9YF	C1-O-P-O1
18	W	201	9YF	C1-O-P-O2
18	W	201	9YF	C1-O-P-O8
18	G	502	9YF	C1-O-P-O8
23	S	503	3PE	C11-O13-P-O14
13	O	301	WUO	C67-C68-C69-C70
16	R	601	CDL	C52-C51-CB5-OB6
16	H	603	CDL	C1-CB2-OB2-PB2
16	P	301	CDL	C51-C52-C53-C54
16	P	301	CDL	C76-C77-C78-C79
16	N	605	CDL	C32-C33-C34-C35
16	N	603	CDL	CA4-CA6-OA8-CA7
16	N	603	CDL	C11-C12-C13-C14
16	P	301	CDL	C60-C61-C62-C63
19	G	505	7PH	C37-C38-C39-C3A
16	N	604	CDL	C18-C19-C20-C21
16	R	605	CDL	C58-C59-C60-C61
19	G	504	7PH	C27-C28-C29-C2A
16	N	604	CDL	C14-C15-C16-C17
16	O	305	CDL	CB2-C1-CA2-OA2
16	R	605	CDL	C73-C74-C75-C76
19	G	504	7PH	C23-C24-C25-C26
18	G	502	9YF	C20-C21-C22-C23
16	R	601	CDL	C71-C72-C73-C74
15	H	605	MQ9	C46-C47-C48-C49
16	N	604	CDL	C74-C75-C76-C77
16	N	605	CDL	C18-C19-C20-C21
16	R	601	CDL	OB6-CB4-CB6-OB8
16	H	602	CDL	O1-C1-CB2-OB2
23	S	503	3PE	C23-C24-C25-C26
16	N	604	CDL	CA5-C11-C12-C13
13	P	302	WUO	C21-C22-C23-C24
15	H	605	MQ9	C19-C21-C22-C23
16	H	603	CDL	CA7-C31-C32-C33
19	G	504	7PH	C24-C25-C26-C27
16	O	305	CDL	C51-C52-C53-C54
16	R	601	CDL	C32-C31-CA7-OA8

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Mol	Chain	Res	Type	Atoms
15	N	607	MQ9	C5-C6-C7-C8
13	P	302	WUO	C66-C67-C68-C69
21	H	604	HEM	C1A-C2A-CAA-CBA
16	H	602	CDL	CA7-C31-C32-C33
16	H	603	CDL	C71-CB7-OB8-CB6
16	P	301	CDL	C54-C55-C56-C57
15	N	608	MQ9	C22-C23-C24-C25
13	O	301	WUO	C88-C90-C91-C92
24	R	603	HEA	C2A-CAA-CBA-CGA
16	R	601	CDL	C31-C32-C33-C34
16	N	603	CDL	C58-C59-C60-C61
19	G	505	7PH	C24-C25-C26-C27
16	H	603	CDL	OB9-CB7-OB8-CB6
13	P	302	WUO	C71-C72-C73-C74
19	M	503	7PH	C28-C29-C2A-C2B
16	P	301	CDL	OB6-CB4-CB6-OB8
15	O	304	MQ9	C13-C14-C16-C17
13	P	302	WUO	C65-C66-C67-C68
19	S	501	7PH	C34-C35-C36-C37
16	P	301	CDL	C14-C15-C16-C17
16	R	605	CDL	C13-C14-C15-C16
22	T	201	TRD	C3-C4-C5-C6
13	O	301	WUO	C23-C24-C25-C26
15	O	304	MQ9	C18-C19-C21-C22
15	O	304	MQ9	C19-C21-C22-C23
18	W	201	9YF	C28-C29-C30-C31
28	W	202	9XX	C21-C22-C23-C24
16	H	602	CDL	CB6-CB4-OB6-CB5
20	M	504	IZL	C46-C45-O34-C60
20	G	503	IZL	C46-C45-O34-C60
13	P	302	WUO	C31-C01-O02-C03
15	N	608	MQ9	C45-C44-C46-C47
15	H	605	MQ9	C30-C29-C31-C32
16	H	602	CDL	C53-C54-C55-C56
19	M	503	7PH	O11-C1-C2-O21
24	R	602	HEA	O11-C11-C12-C13
15	N	601	MQ9	C45-C44-C46-C47
13	O	301	WUO	C87-C88-C90-C91
15	H	606	MQ9	C39-C41-C42-C43
15	H	606	MQ9	C44-C46-C47-C48
16	O	305	CDL	C35-C36-C37-C38
16	P	301	CDL	C56-C57-C58-C59

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Mol	Chain	Res	Type	Atoms
16	R	605	CDL	C15-C16-C17-C18
16	N	604	CDL	C52-C53-C54-C55
14	O	303	HEC	CAD-CBD-CGD-O2D
15	N	608	MQ9	C35-C34-C36-C37
15	H	605	MQ9	C28-C29-C31-C32
16	H	602	CDL	C31-C32-C33-C34
15	H	606	MQ9	C12-C11-C9-C10
16	P	301	CDL	C1-CA2-OA2-PA1
16	R	601	CDL	CB4-CB3-OB5-PB2
18	M	502	9YF	C36-C37-C38-C39
19	M	503	7PH	C26-C27-C28-C29
14	O	303	HEC	CAD-CBD-CGD-O1D
15	N	608	MQ9	C22-C23-C24-C26
15	N	607	MQ9	C19-C21-C22-C23
16	P	301	CDL	CB3-CB4-CB6-OB8
16	R	601	CDL	CB3-CB4-CB6-OB8
23	S	503	3PE	C33-C34-C35-C36
16	N	605	CDL	OA5-CA3-CA4-OA6
13	O	301	WUO	C20-C21-C22-C23
16	R	601	CDL	C37-C38-C39-C40
16	H	602	CDL	C57-C58-C59-C60
20	M	504	IZL	C3-C4-C5-C6
20	G	503	IZL	C3-C4-C5-C6
13	P	302	WUO	O60-C59-O58-C57
18	G	502	9YF	C36-C37-C38-C39
16	N	604	CDL	C32-C31-CA7-OA8
13	O	301	WUO	C83-C84-C85-C86
13	P	302	WUO	C93-C94-C95-C96
16	H	602	CDL	OB5-CB3-CB4-CB6
18	W	201	9YF	C24-C-C1-O
20	G	503	IZL	C15-C14-O3-C13
19	G	504	7PH	O21-C21-C22-C23
28	Y	302	9XX	C13-C14-C15-O
28	c	302	9XX	C13-C14-C15-O
16	R	605	CDL	C34-C35-C36-C37
16	N	604	CDL	C39-C40-C41-C42
19	G	505	7PH	C25-C26-C27-C28
20	M	504	IZL	C15-C14-O3-C13
16	R	605	CDL	C51-C52-C53-C54
24	R	603	HEA	CAA-CBA-CGA-O2A
19	S	501	7PH	C1-O11-P-O12
16	R	605	CDL	C54-C55-C56-C57

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Mol	Chain	Res	Type	Atoms
16	P	301	CDL	C37-C38-C39-C40
18	M	502	9YF	C26-C27-C28-C29
15	N	608	MQ9	C33-C34-C36-C37
21	N	606	HEM	CAD-CBD-CGD-O2D
16	H	603	CDL	C51-C52-C53-C54
24	R	603	HEA	CAA-CBA-CGA-O1A
13	O	301	WUO	C71-C72-C73-C74
13	O	301	WUO	C31-C01-O02-C03
13	O	301	WUO	C56-C57-C76-O77
20	M	504	IZL	C44-C45-C46-O32
28	W	202	9XX	C18-C19-C20-C21
15	O	304	MQ9	C35-C34-C36-C37
15	H	606	MQ9	C35-C34-C36-C37
20	G	503	IZL	C43-C14-O3-C13
16	R	605	CDL	C72-C71-CB7-OB8
18	G	502	9YF	C26-C27-C28-C29
28	Y	302	9XX	C10-C11-C12-C13
28	c	302	9XX	C10-C11-C12-C13
20	M	504	IZL	C43-C14-O3-C13
16	N	605	CDL	OA5-CA3-CA4-CA6
16	N	603	CDL	C59-C60-C61-C62
19	G	505	7PH	O21-C21-C22-C23
16	N	603	CDL	C15-C16-C17-C18
24	R	603	HEA	CAD-CBD-CGD-O2D
13	O	301	WUO	C06-C05-C12-O13
18	M	502	9YF	O9-C8-C9-C10
18	W	201	9YF	C2-O2-P-O8
18	G	502	9YF	C2-O2-P-O8
20	M	504	IZL	C43-O28-P-O29
20	G	503	IZL	C43-O28-P-O29
16	H	602	CDL	C32-C31-CA7-OA8
13	P	302	WUO	C61-C59-O58-C57
21	N	606	HEM	CAD-CBD-CGD-O1D
13	O	301	WUO	C50-C01-O02-C03
18	G	502	9YF	O9-C8-C9-C10
20	M	504	IZL	O1-C10-C9-C8
20	G	503	IZL	O1-C10-C9-C8
20	G	503	IZL	C44-C45-C46-O32
19	M	503	7PH	C23-C24-C25-C26
15	H	605	MQ9	C12-C11-C9-C10
15	H	605	MQ9	C25-C24-C26-C27
16	N	603	CDL	C72-C71-CB7-OB8

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Mol	Chain	Res	Type	Atoms
16	R	601	CDL	C72-C71-CB7-OB8
16	H	603	CDL	OB6-CB4-CB6-OB8
16	O	305	CDL	C14-C15-C16-C17
16	O	305	CDL	C12-C11-CA5-OA6
16	R	601	CDL	C35-C36-C37-C38
16	H	603	CDL	C35-C36-C37-C38
20	M	504	IZL	C44-C45-O34-C60
20	G	503	IZL	C44-C45-O34-C60
20	M	504	IZL	C49-C50-C51-C52
20	G	503	IZL	C49-C50-C51-C52
24	R	602	HEA	CAA-CBA-CGA-O1A
19	G	504	7PH	C25-C26-C27-C28
16	R	601	CDL	C12-C11-CA5-OA6
18	G	502	9YF	O10-C8-C9-C10
19	G	505	7PH	C32-C33-C34-C35
16	N	603	CDL	C72-C71-CB7-OB9
16	R	605	CDL	C72-C71-CB7-OB9
16	H	602	CDL	C32-C31-CA7-OA9
15	N	608	MQ9	C43-C44-C46-C47
18	M	502	9YF	O10-C8-C9-C10
19	G	505	7PH	O22-C21-C22-C23
16	R	605	CDL	C11-C12-C13-C14
20	G	503	IZL	O-C10-C9-C8
24	R	603	HEA	CAD-CBD-CGD-O1D
13	P	302	WUO	C63-C64-C65-C66
16	O	305	CDL	C12-C11-CA5-OA7
16	R	601	CDL	C72-C71-CB7-OB9
20	M	504	IZL	O-C10-C9-C8
16	P	301	CDL	CA7-C31-C32-C33
24	R	602	HEA	CAA-CBA-CGA-O2A
16	P	301	CDL	C32-C31-CA7-OA8
18	W	201	9YF	C18-C19-C20-C21

There are no ring outliers.

36 monomers are involved in 197 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	O	305	CDL	5	0
19	S	501	7PH	3	0
15	O	304	MQ9	24	0
16	N	603	CDL	13	0
16	H	603	CDL	4	0

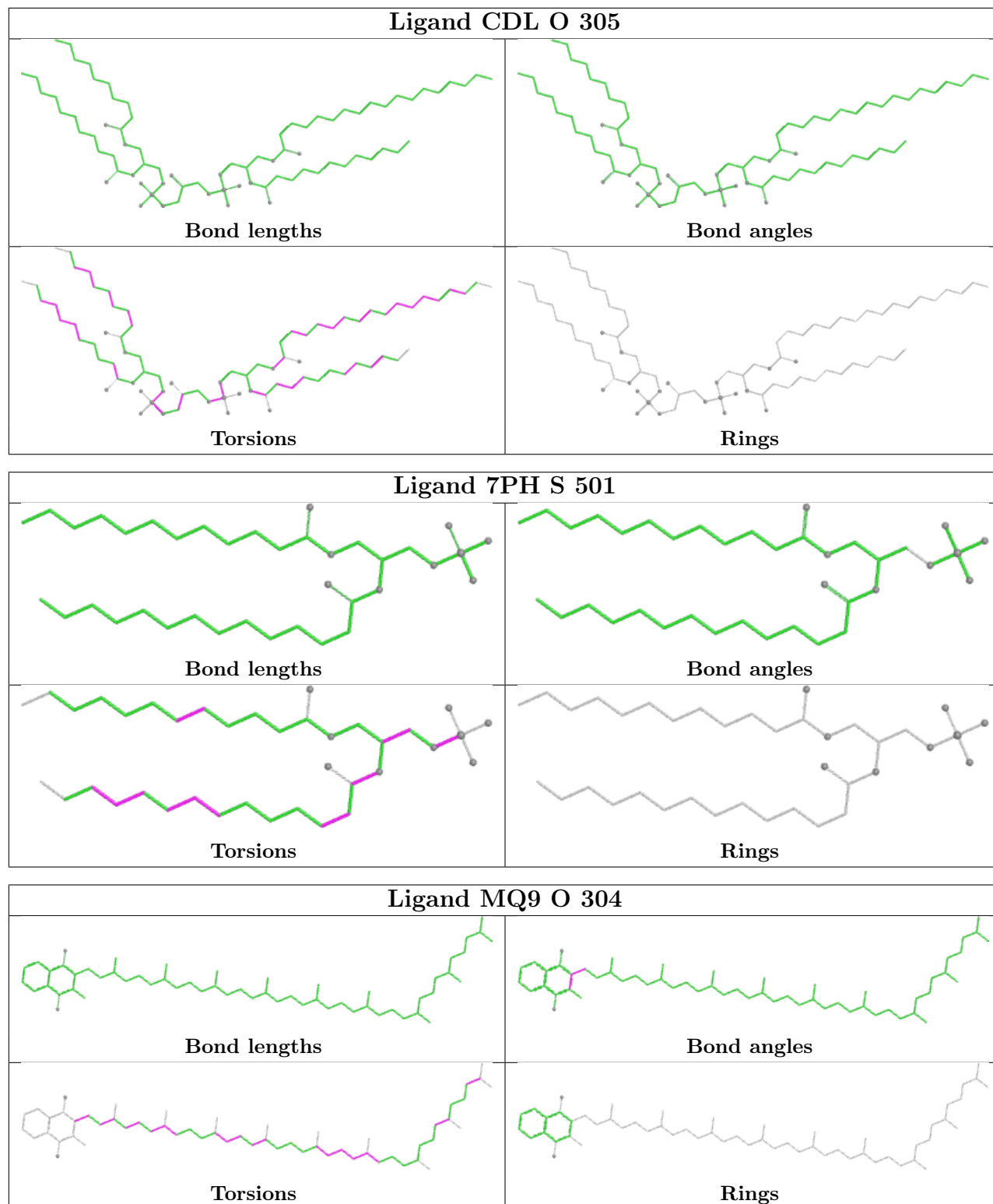
Continued on next page...

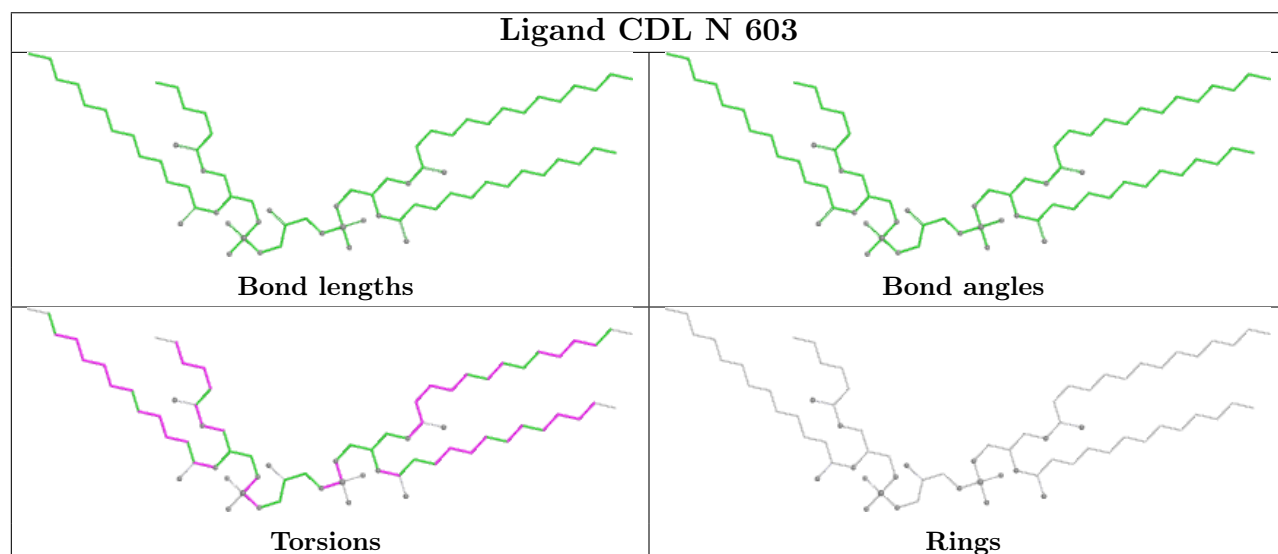
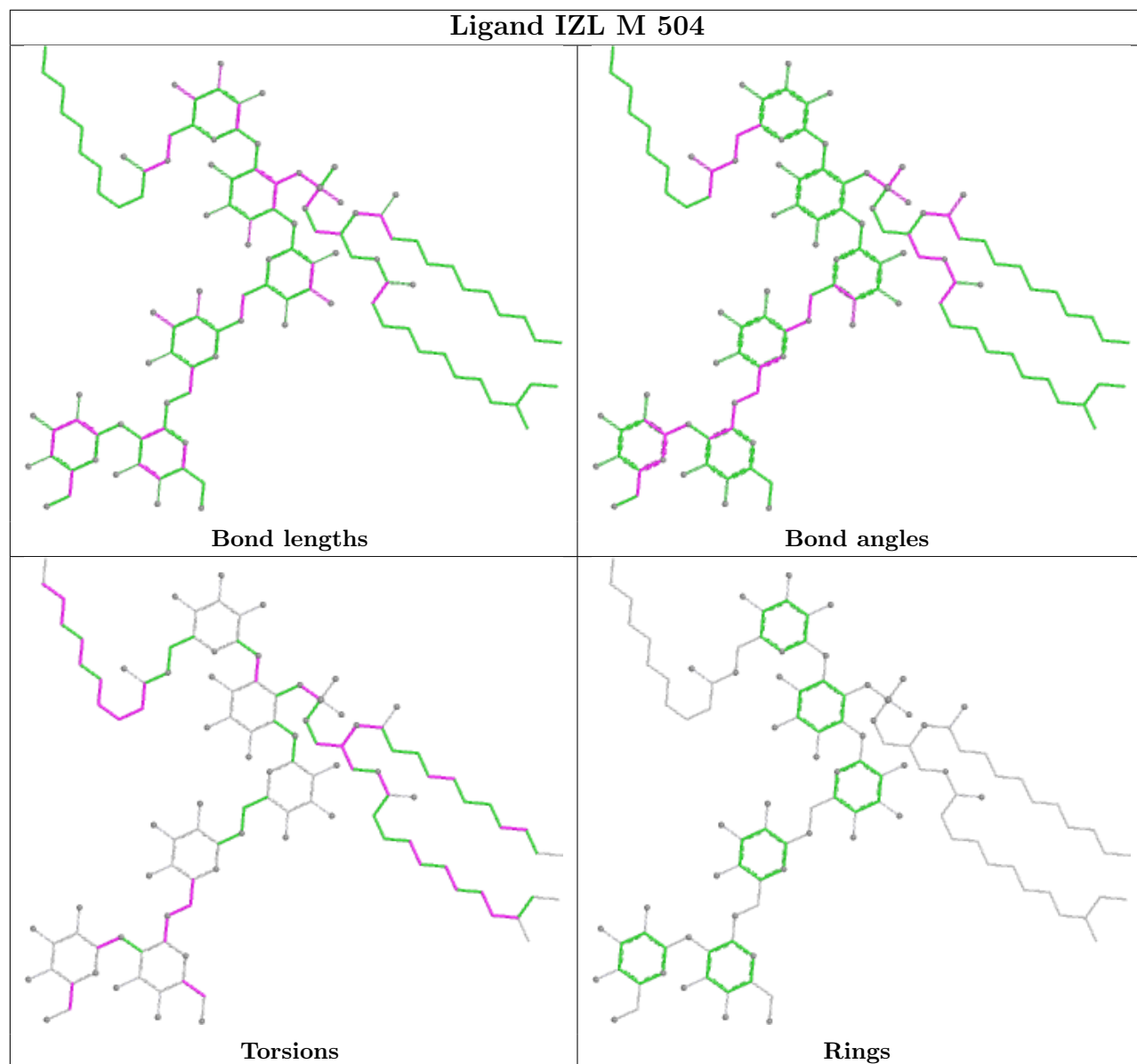
Continued from previous page...

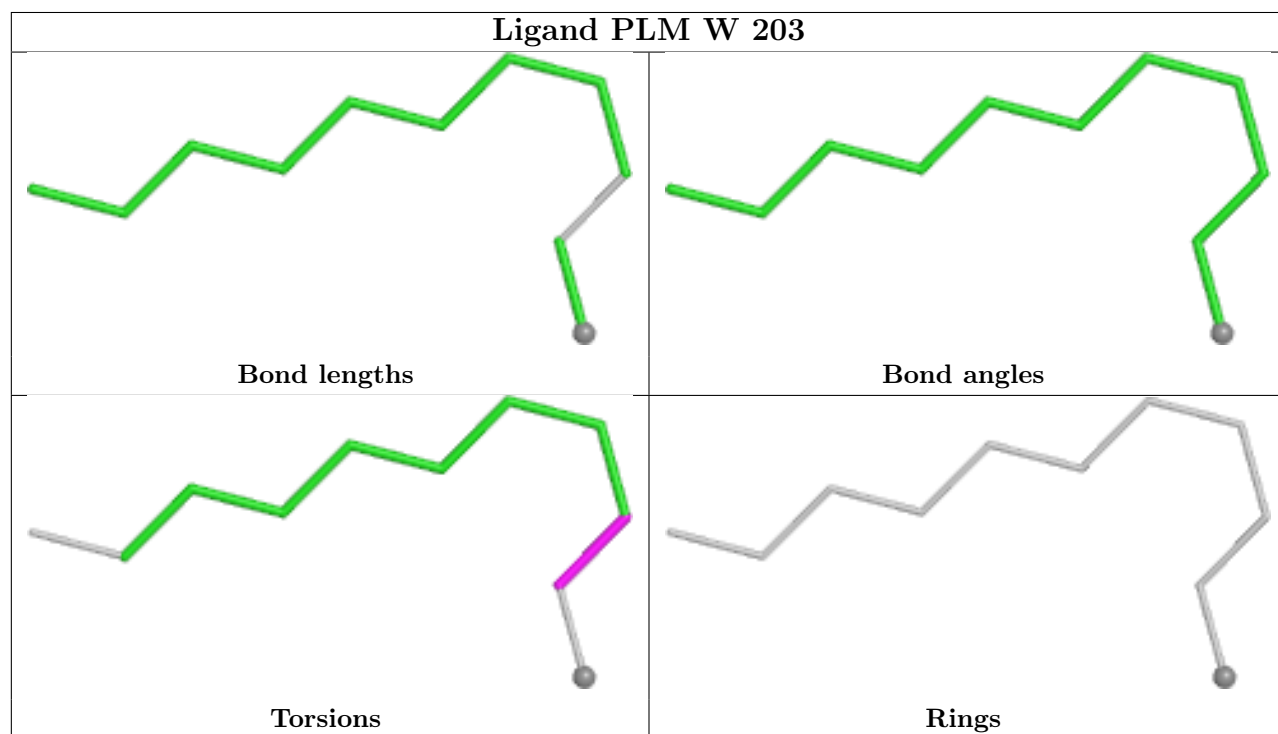
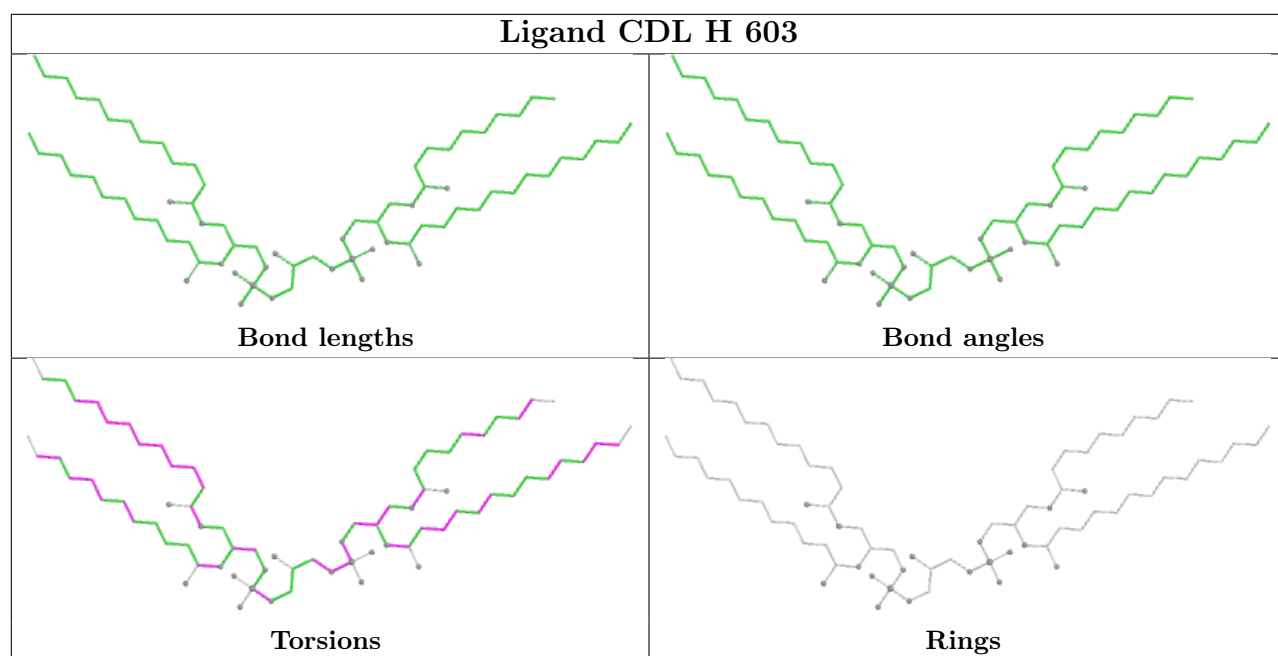
Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	W	203	PLM	3	0
16	N	604	CDL	4	0
15	N	608	MQ9	22	0
13	O	301	WUO	2	0
19	M	503	7PH	2	0
19	G	505	7PH	1	0
15	H	605	MQ9	12	0
21	N	602	HEM	2	0
18	G	502	9YF	2	0
16	R	601	CDL	2	0
18	W	201	9YF	2	0
28	Y	302	9XX	1	0
21	H	604	HEM	4	0
24	R	603	HEA	9	0
15	N	601	MQ9	4	0
21	H	601	HEM	4	0
14	O	302	HEC	3	0
24	R	602	HEA	13	0
16	H	602	CDL	3	0
15	N	607	MQ9	27	0
14	O	303	HEC	3	0
28	c	302	9XX	2	0
16	R	605	CDL	3	0
18	M	502	9YF	2	0
28	W	202	9XX	3	0
17	G	501	FES	2	0
16	N	605	CDL	3	0
16	P	301	CDL	9	0
21	N	606	HEM	3	0
17	M	501	FES	1	0
15	H	606	MQ9	5	0

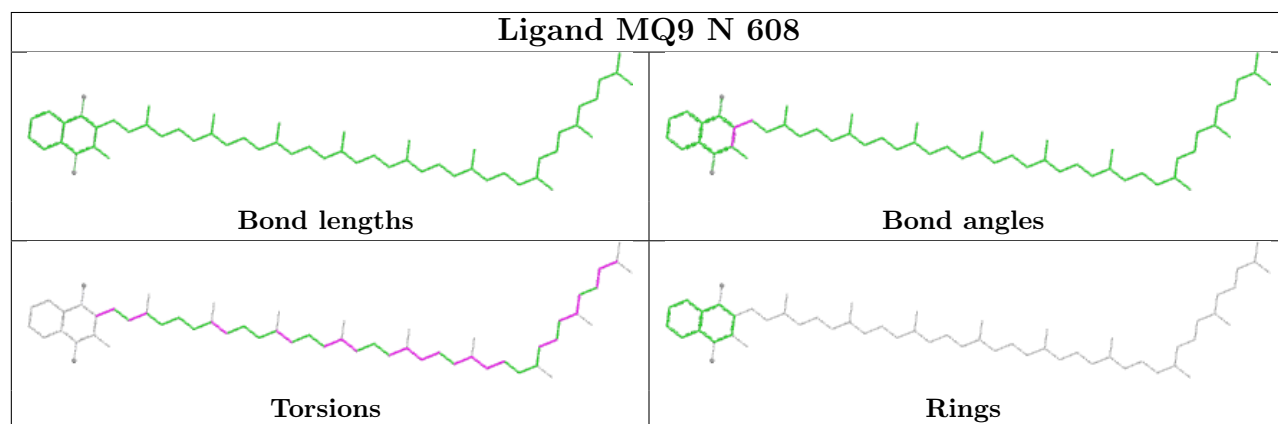
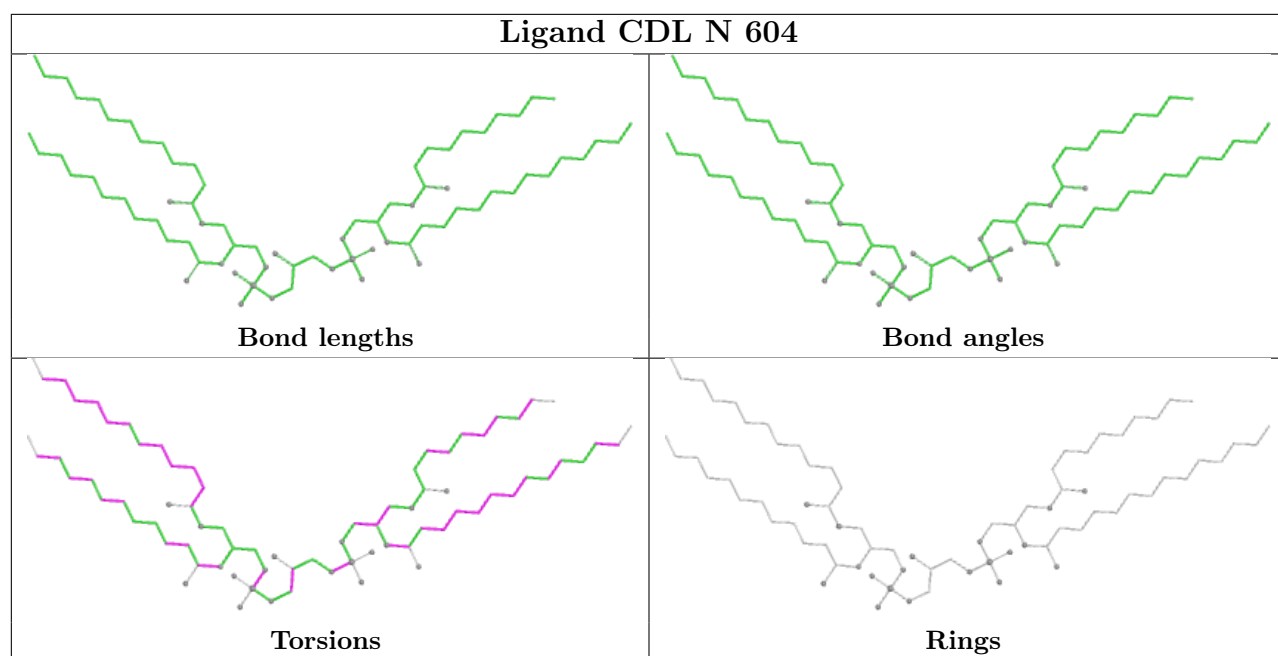
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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

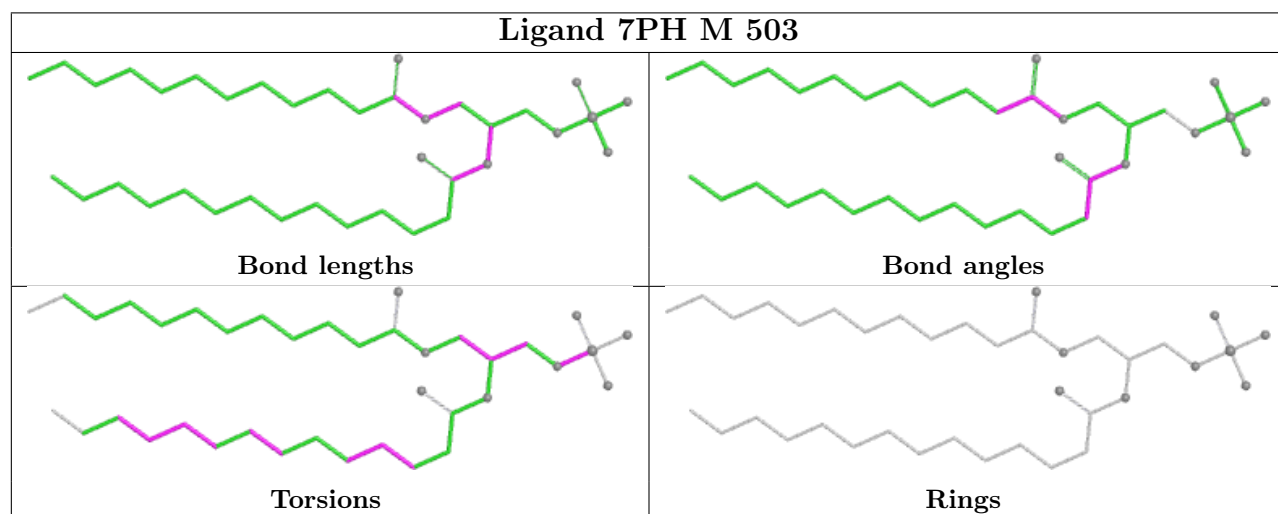
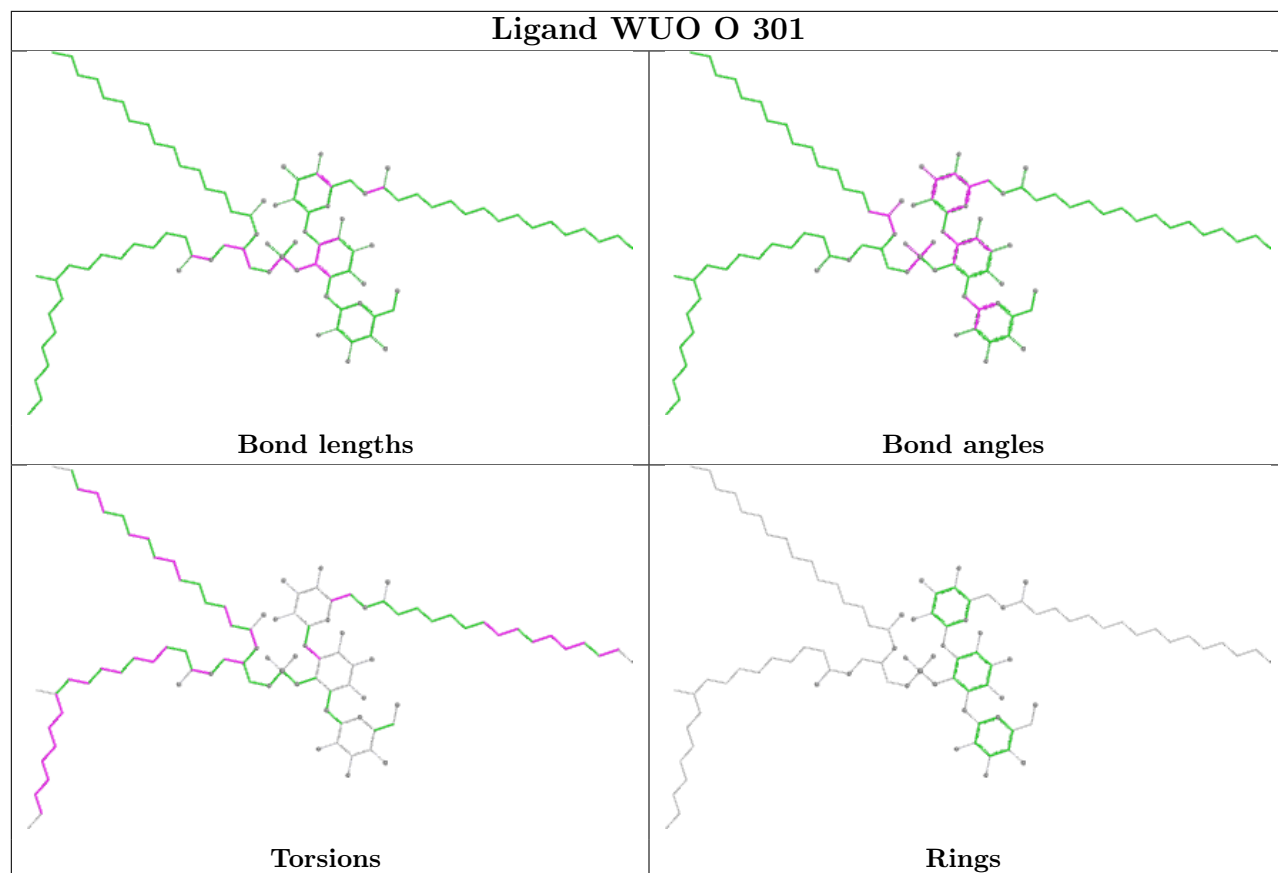
equivalents in the CSD to analyse the geometry.

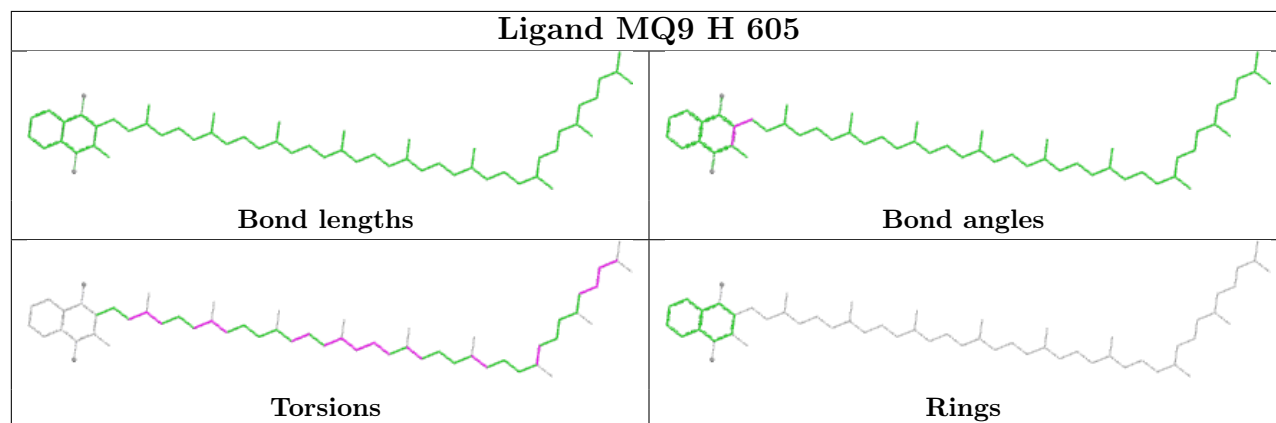
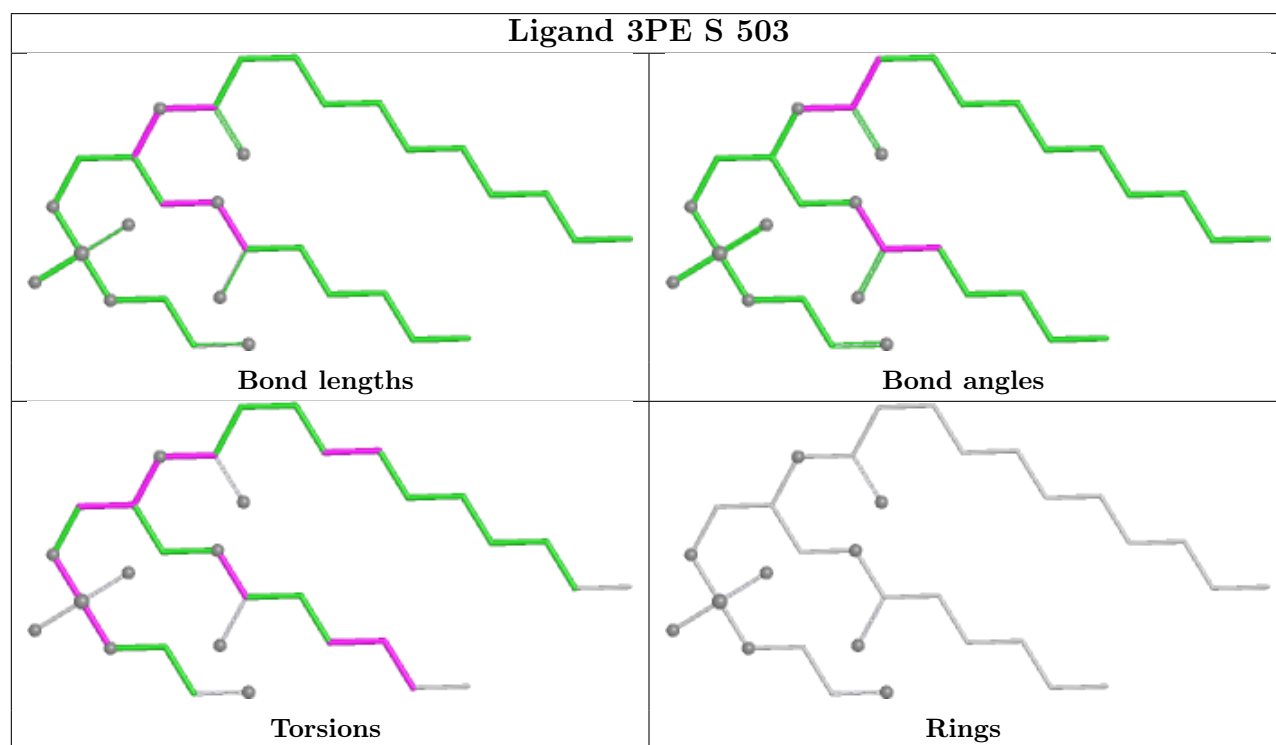
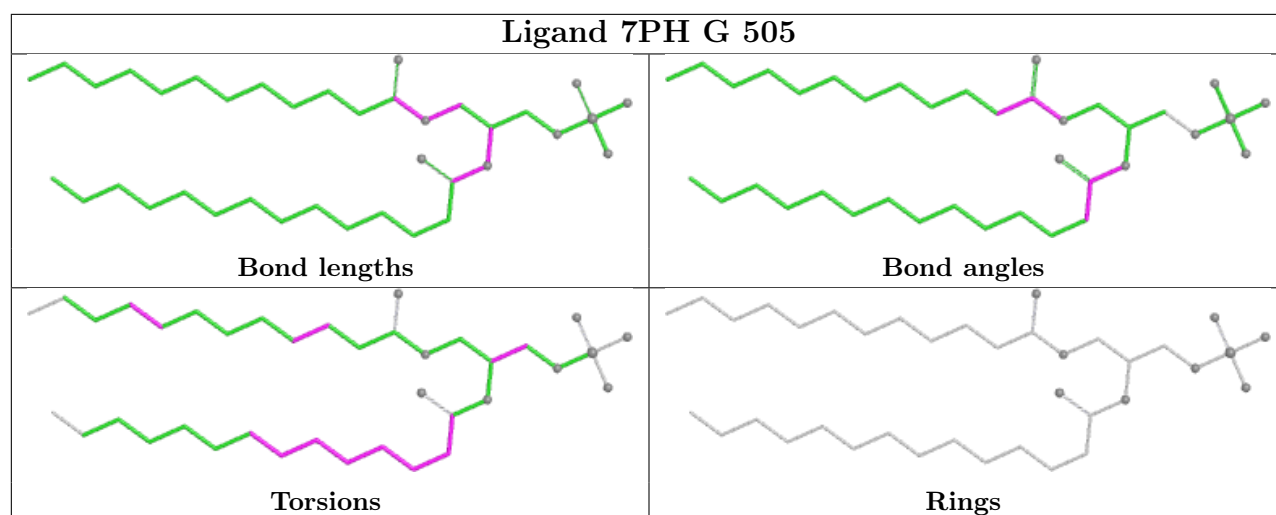


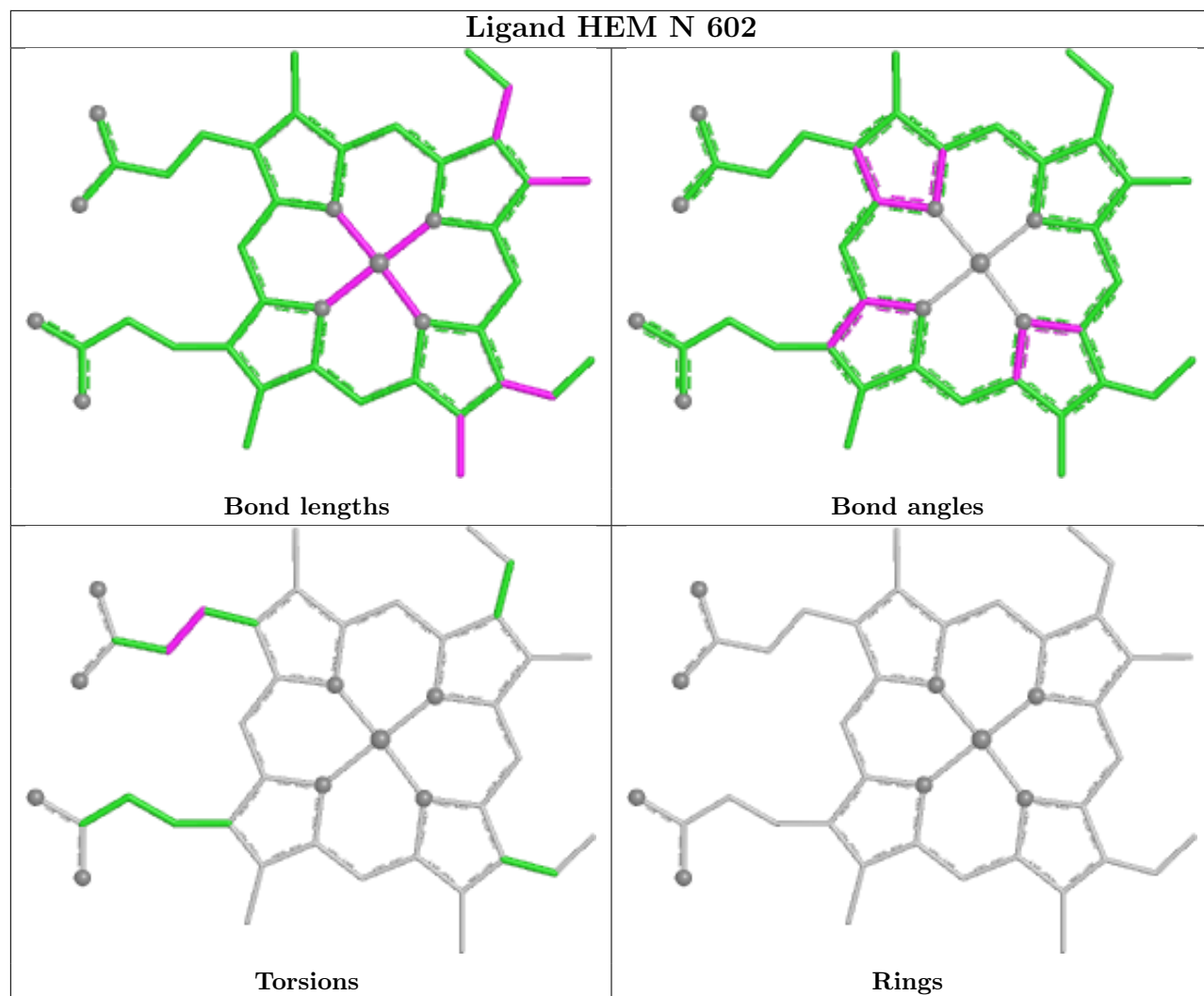


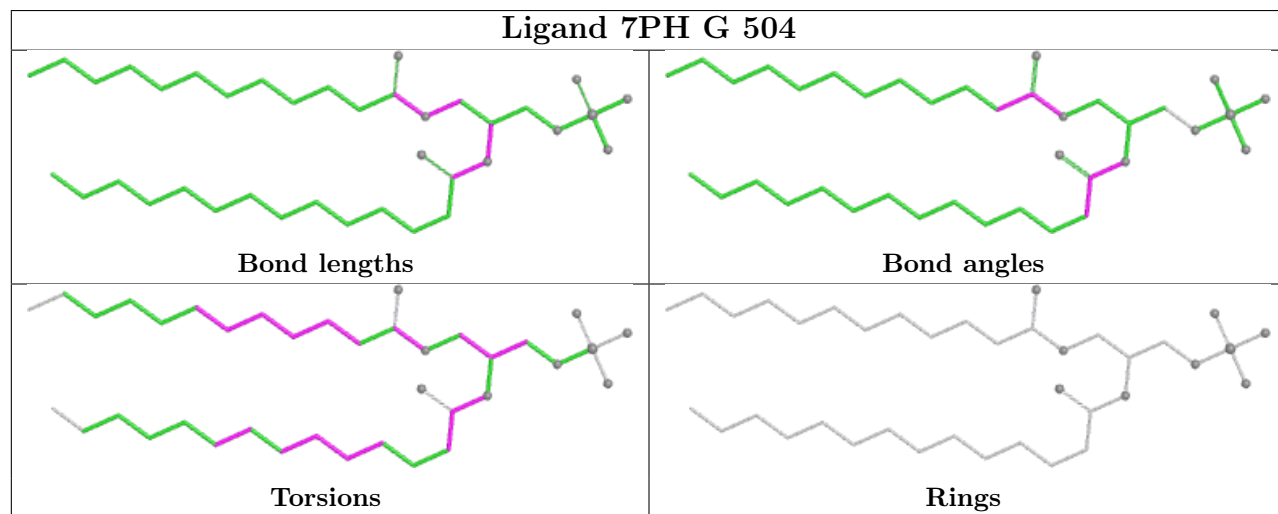
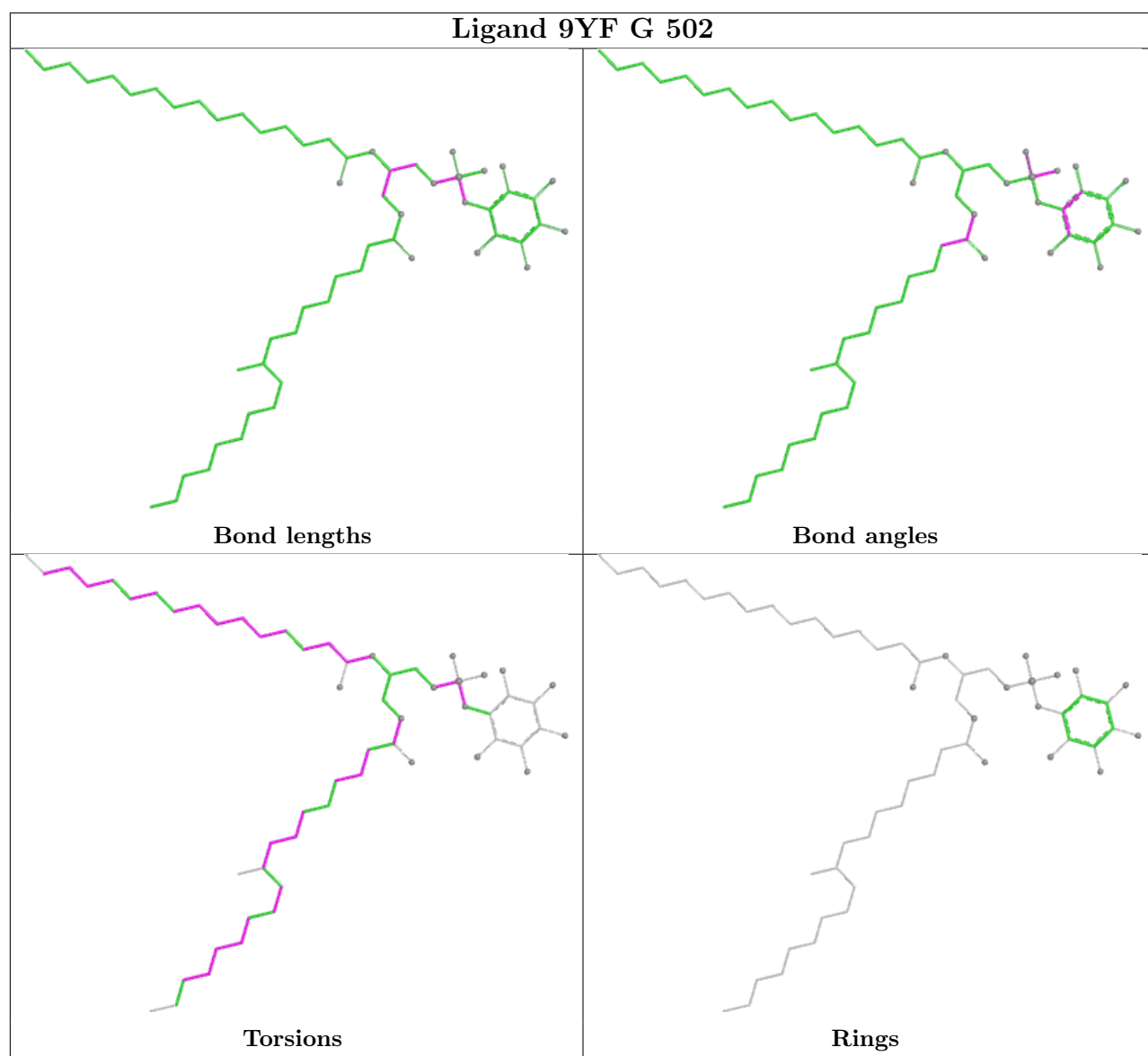


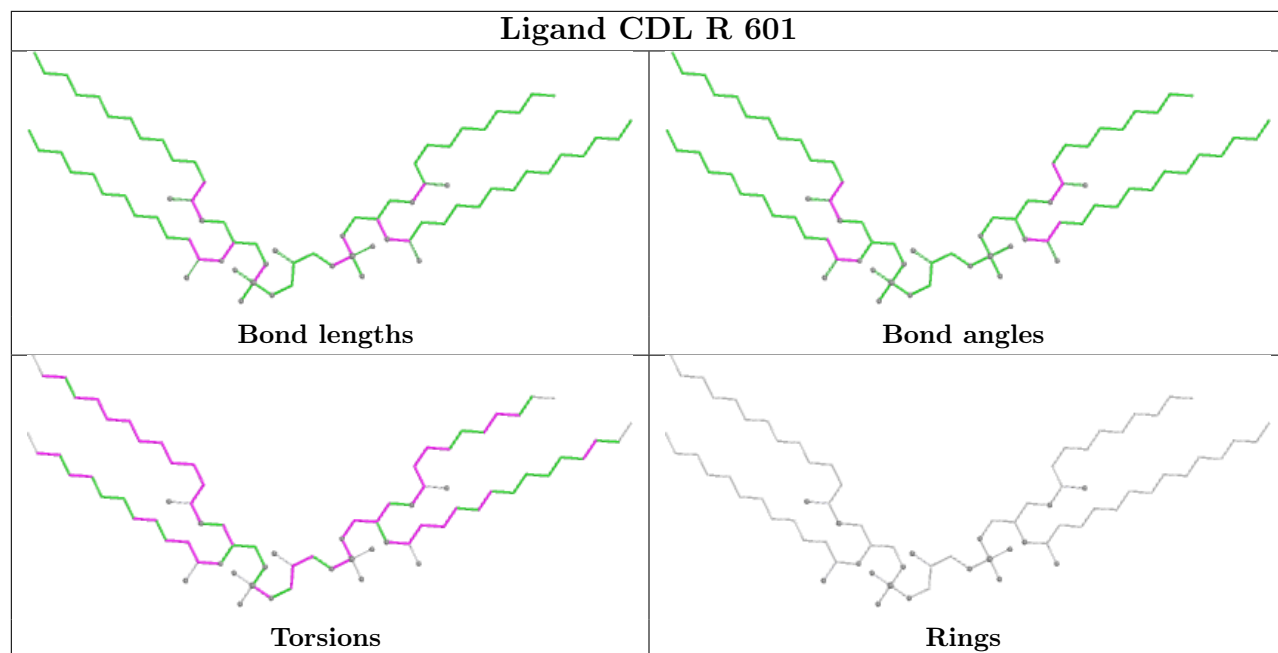


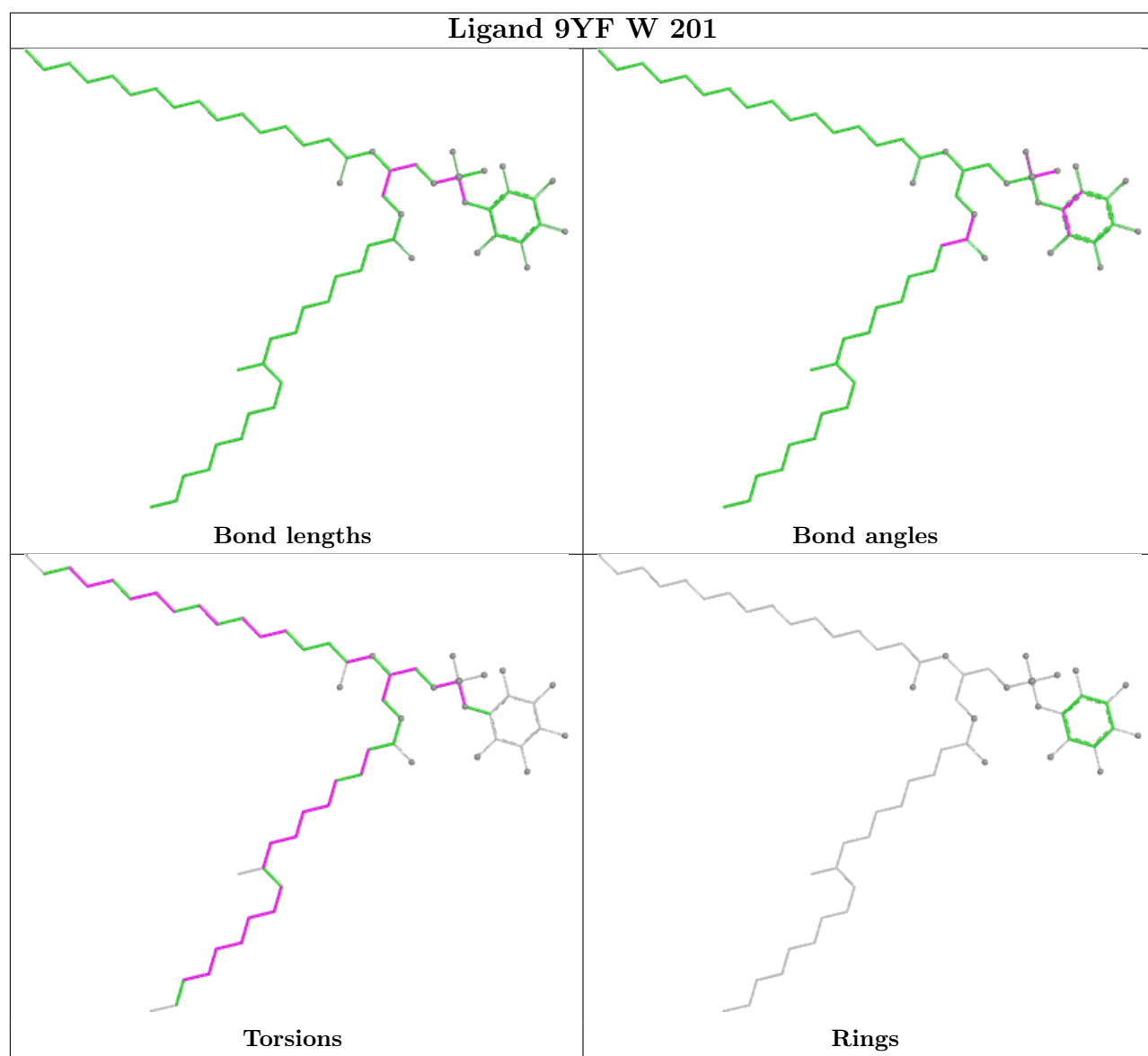


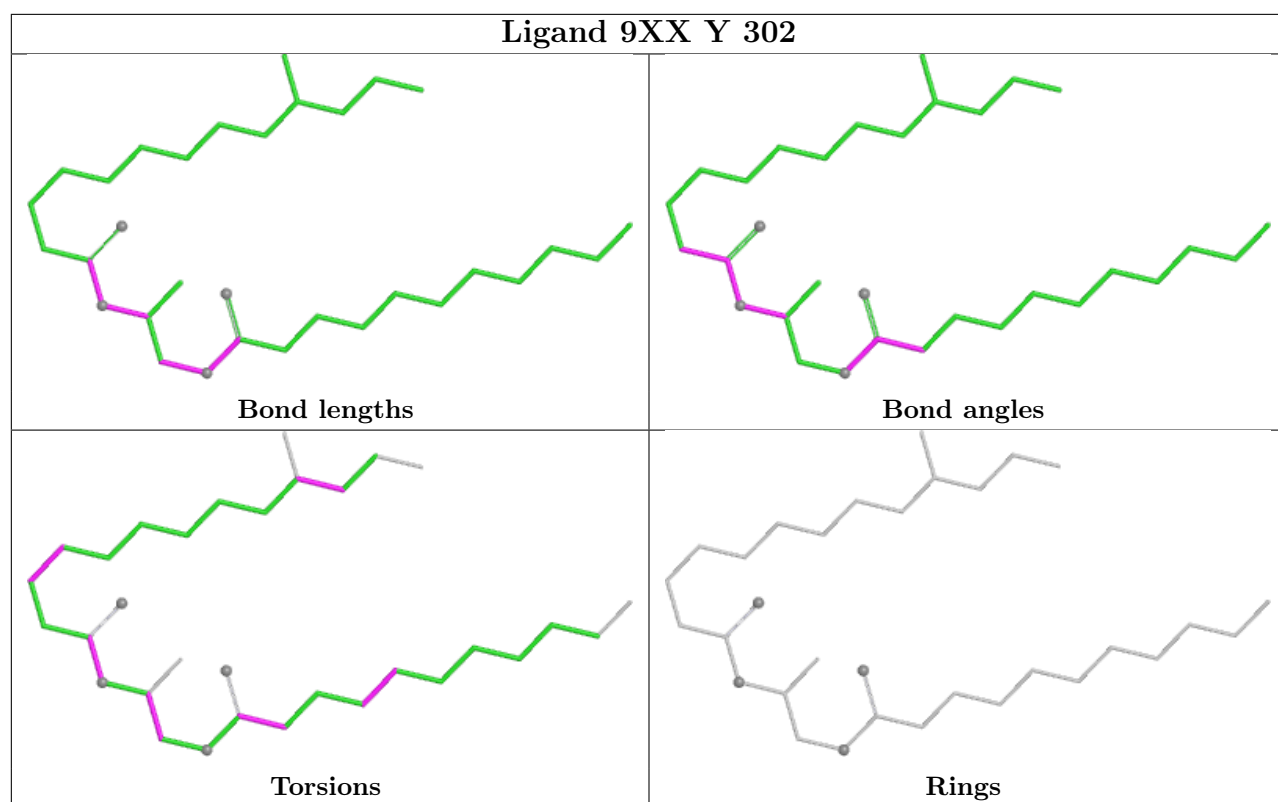


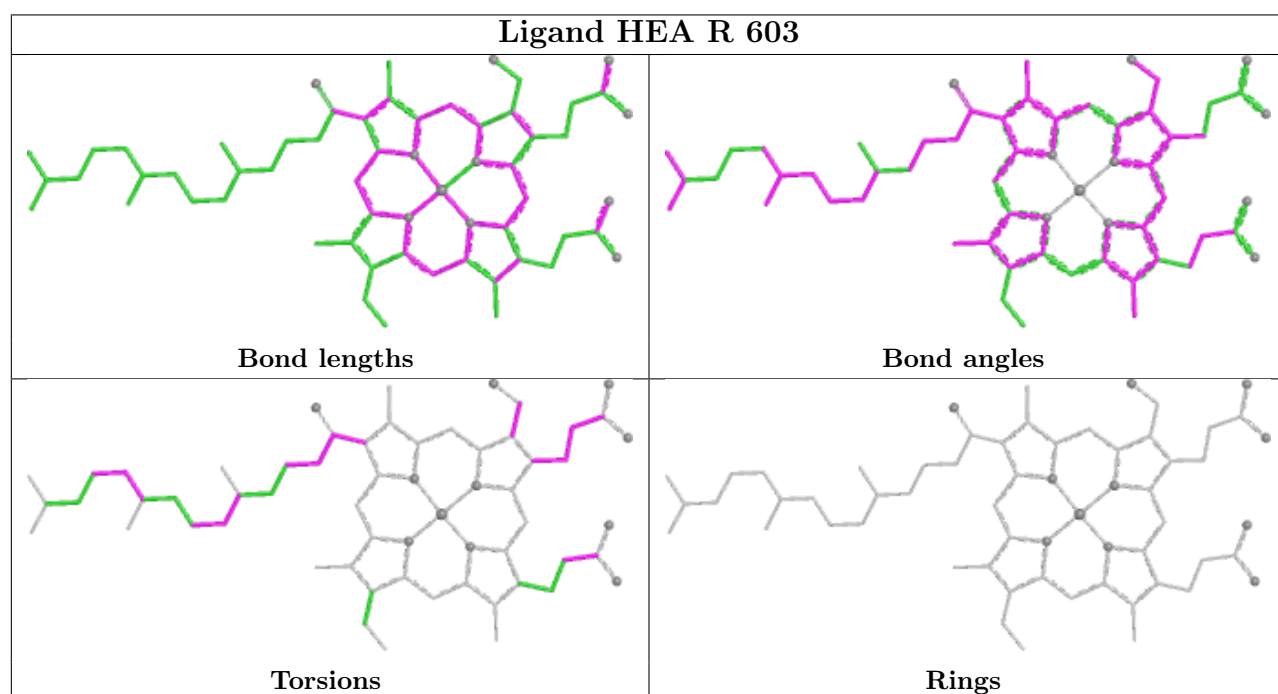
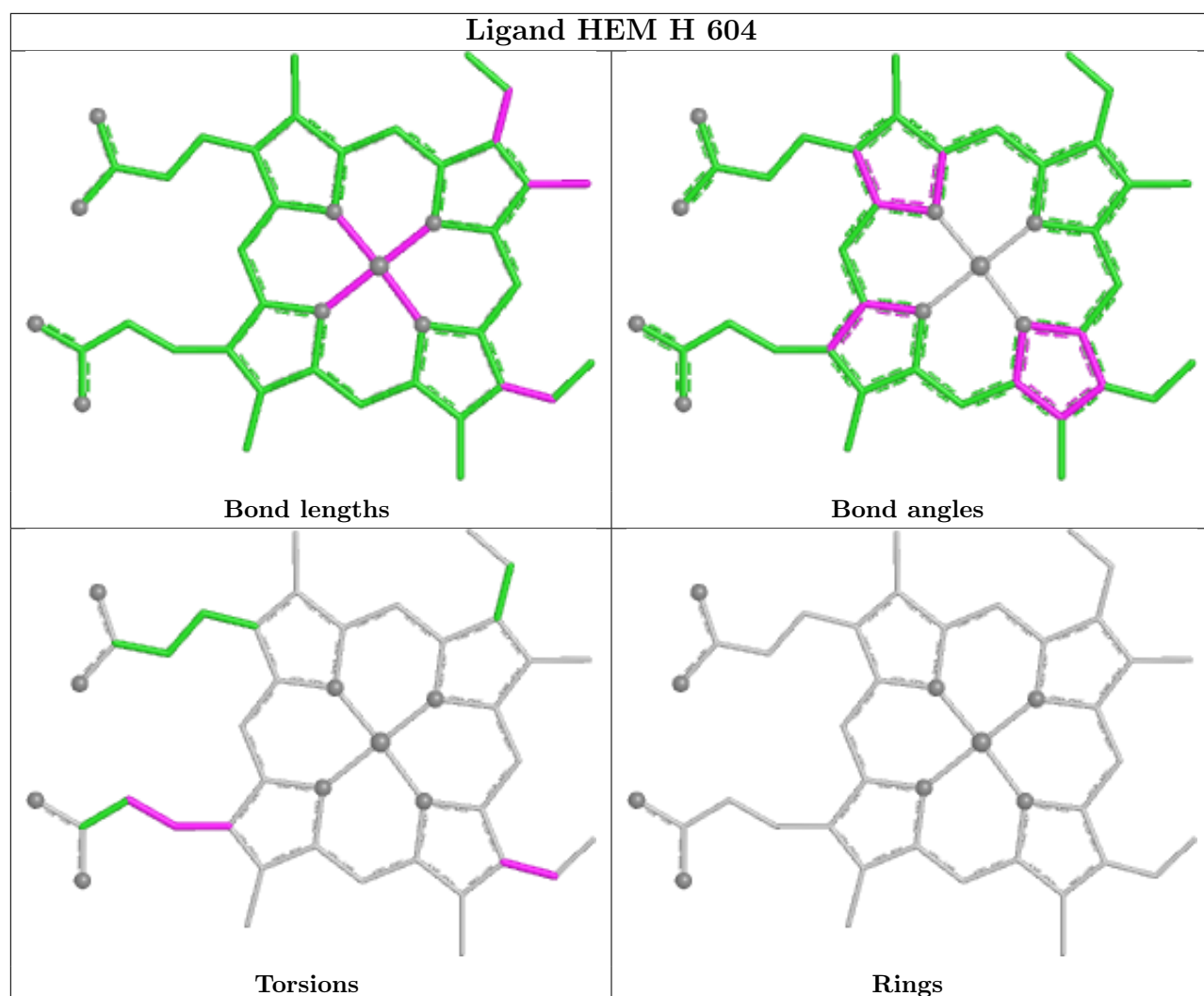


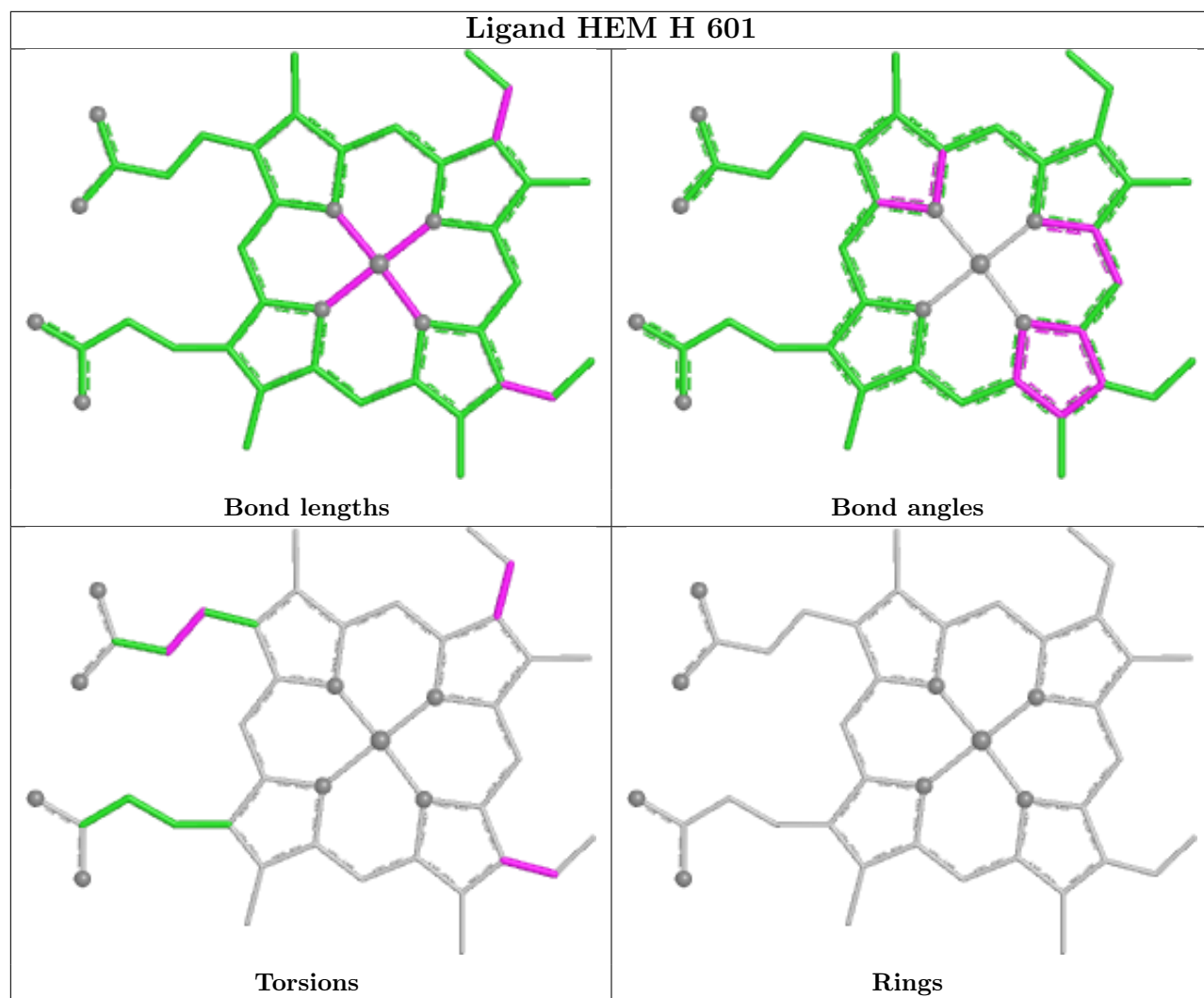
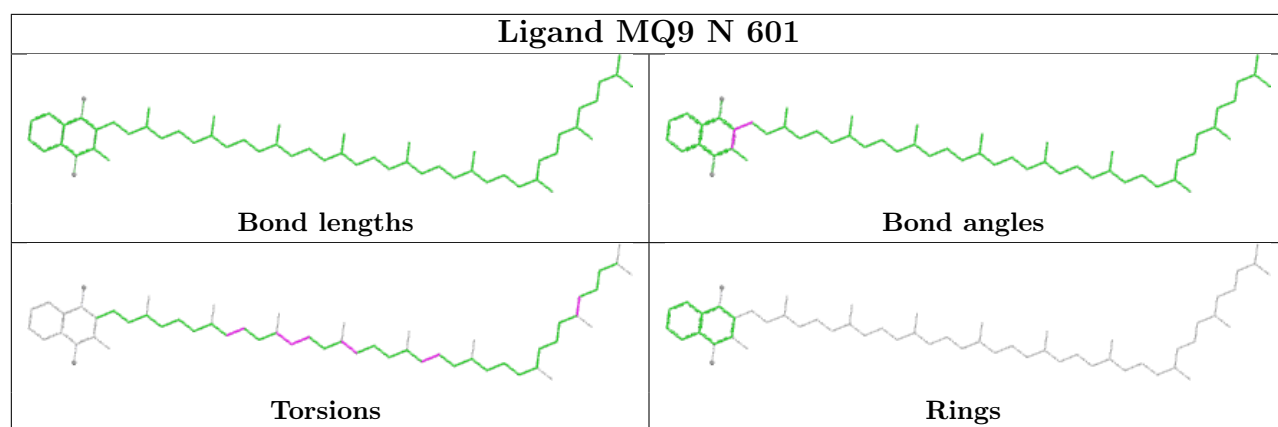


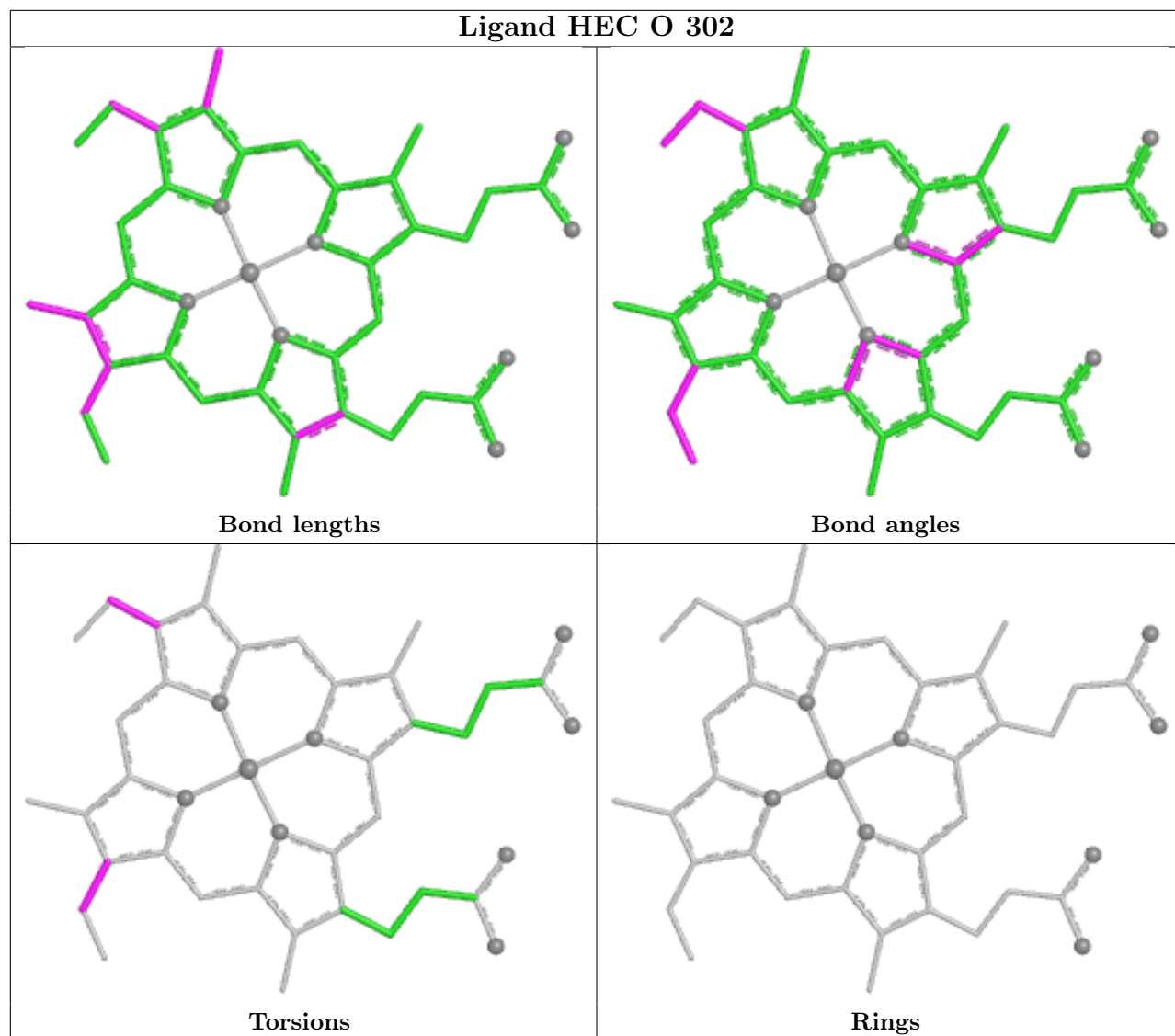


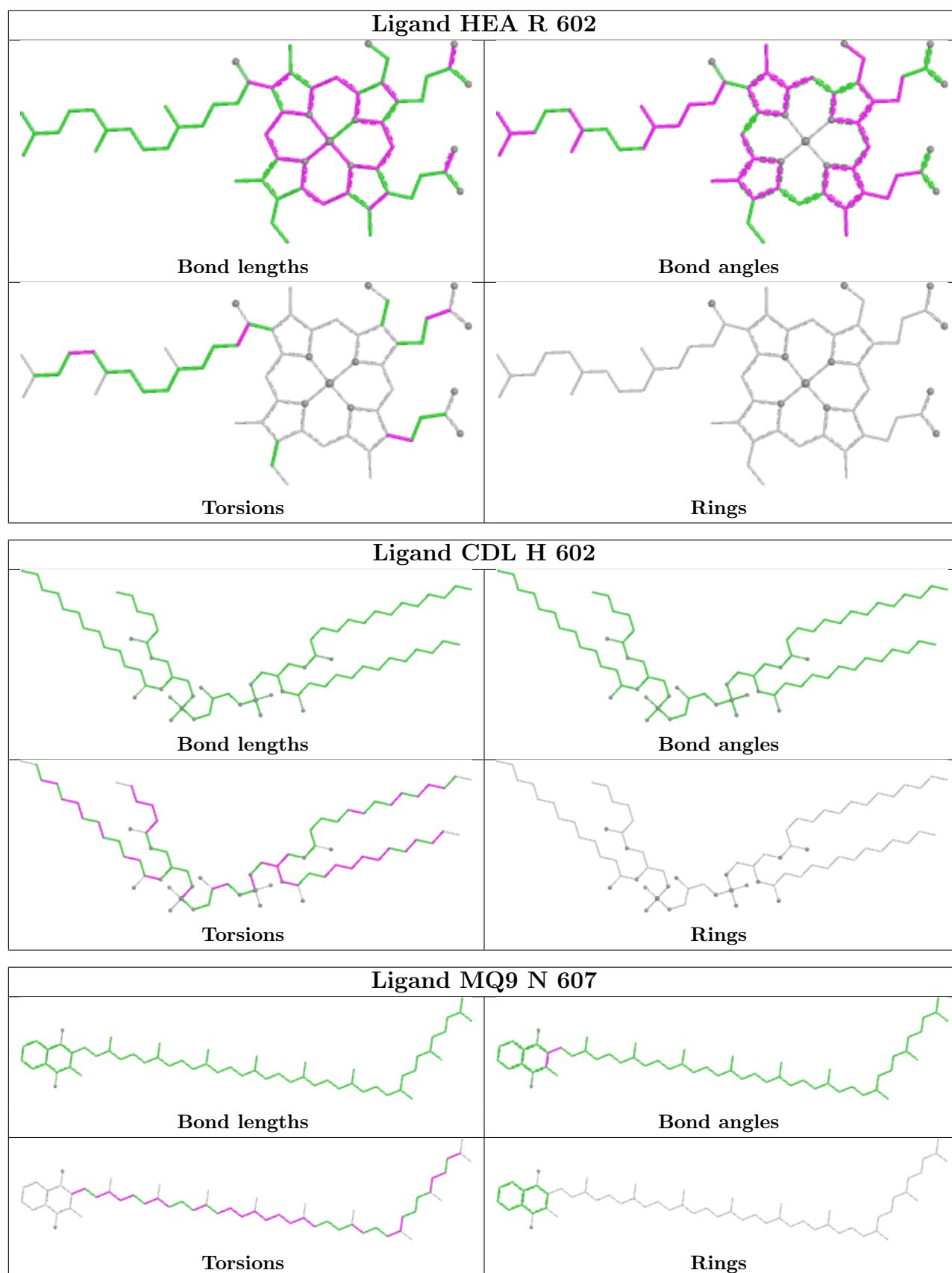


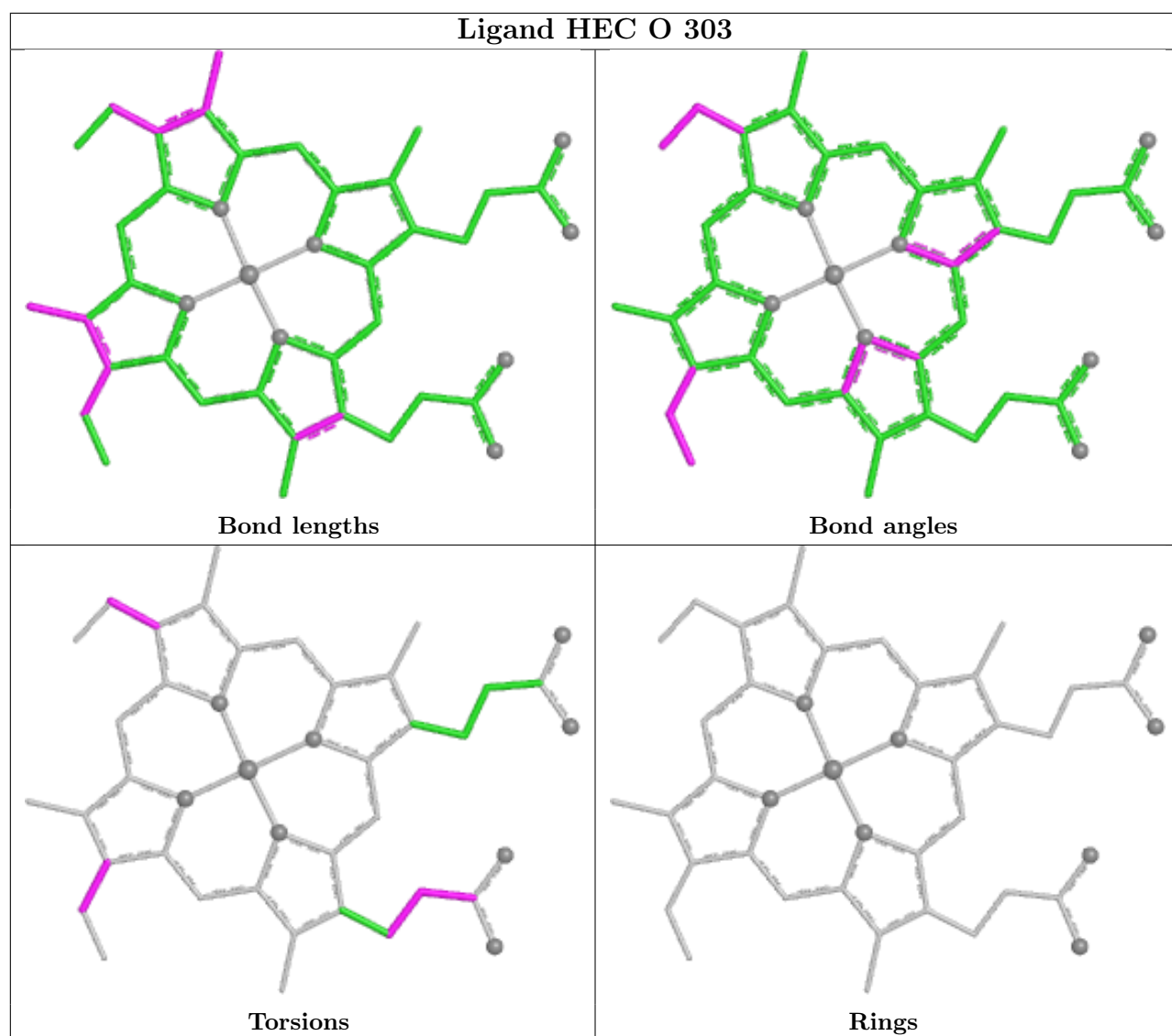


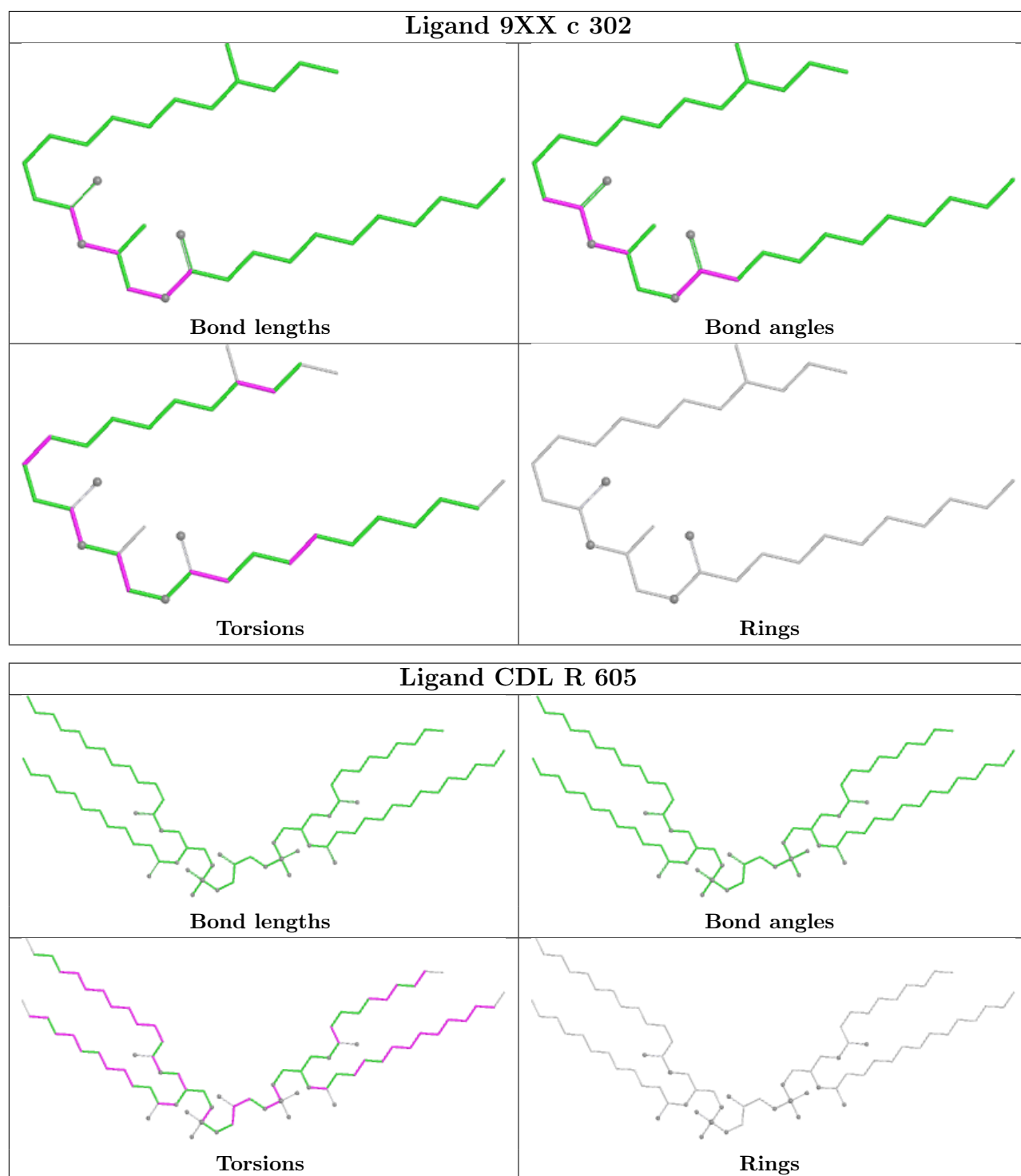


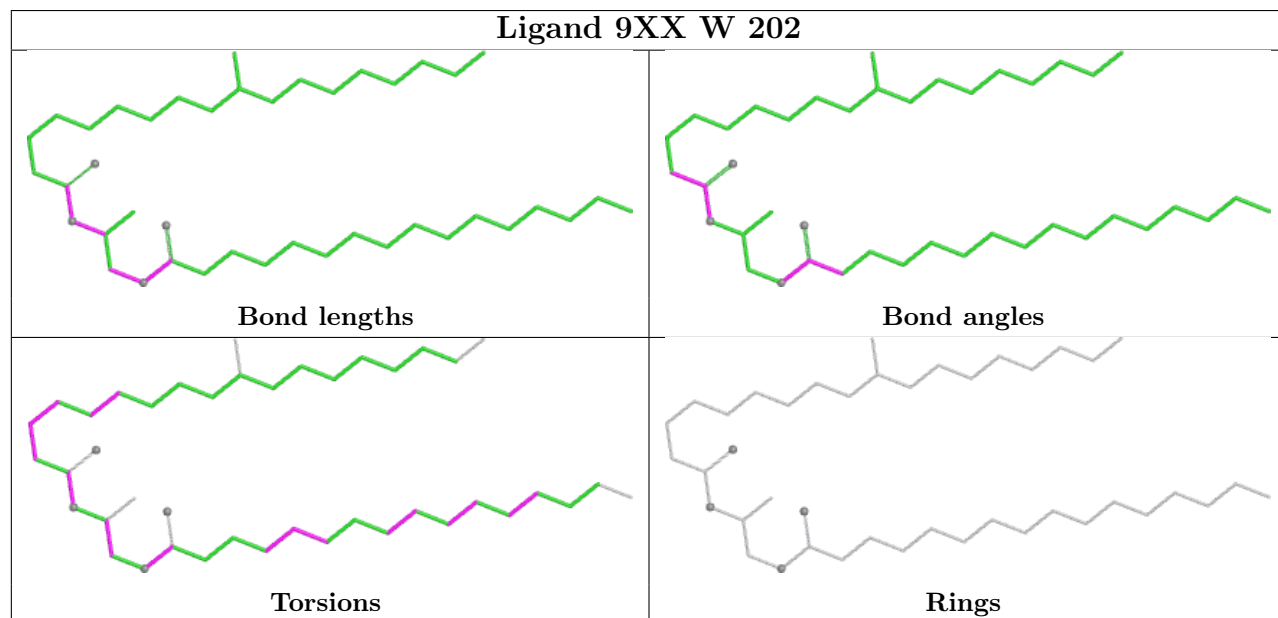
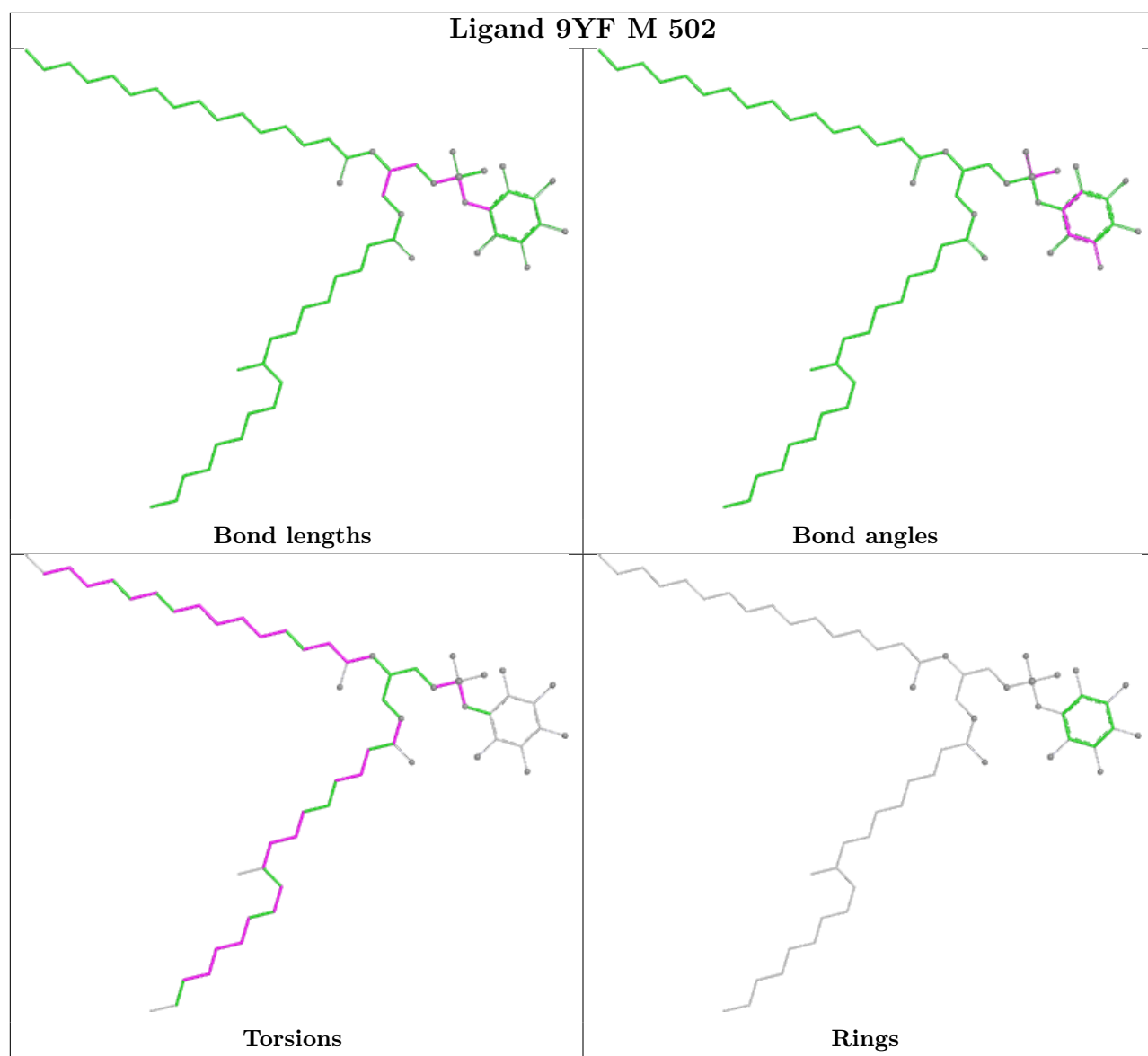


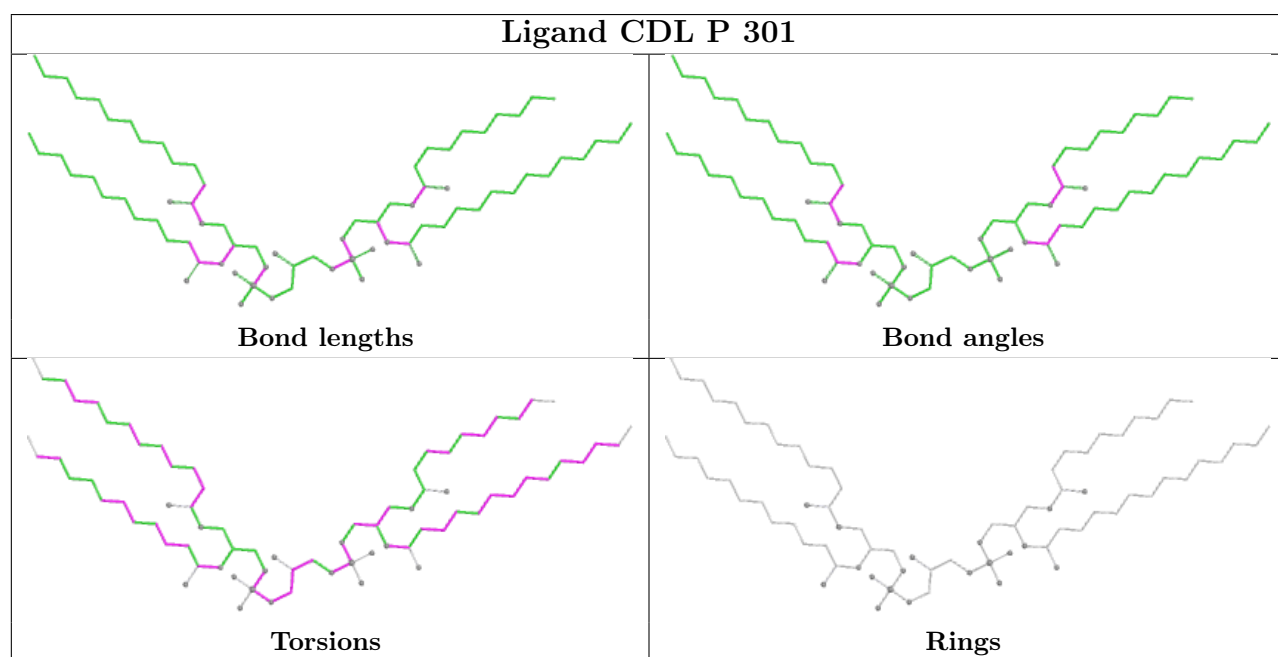
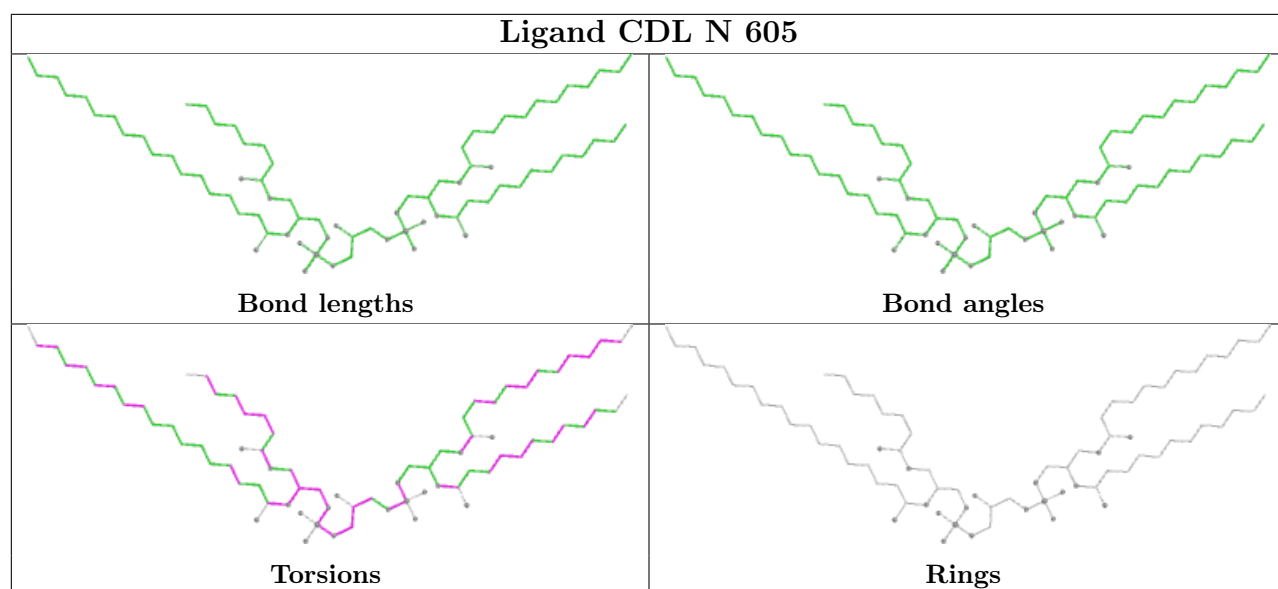


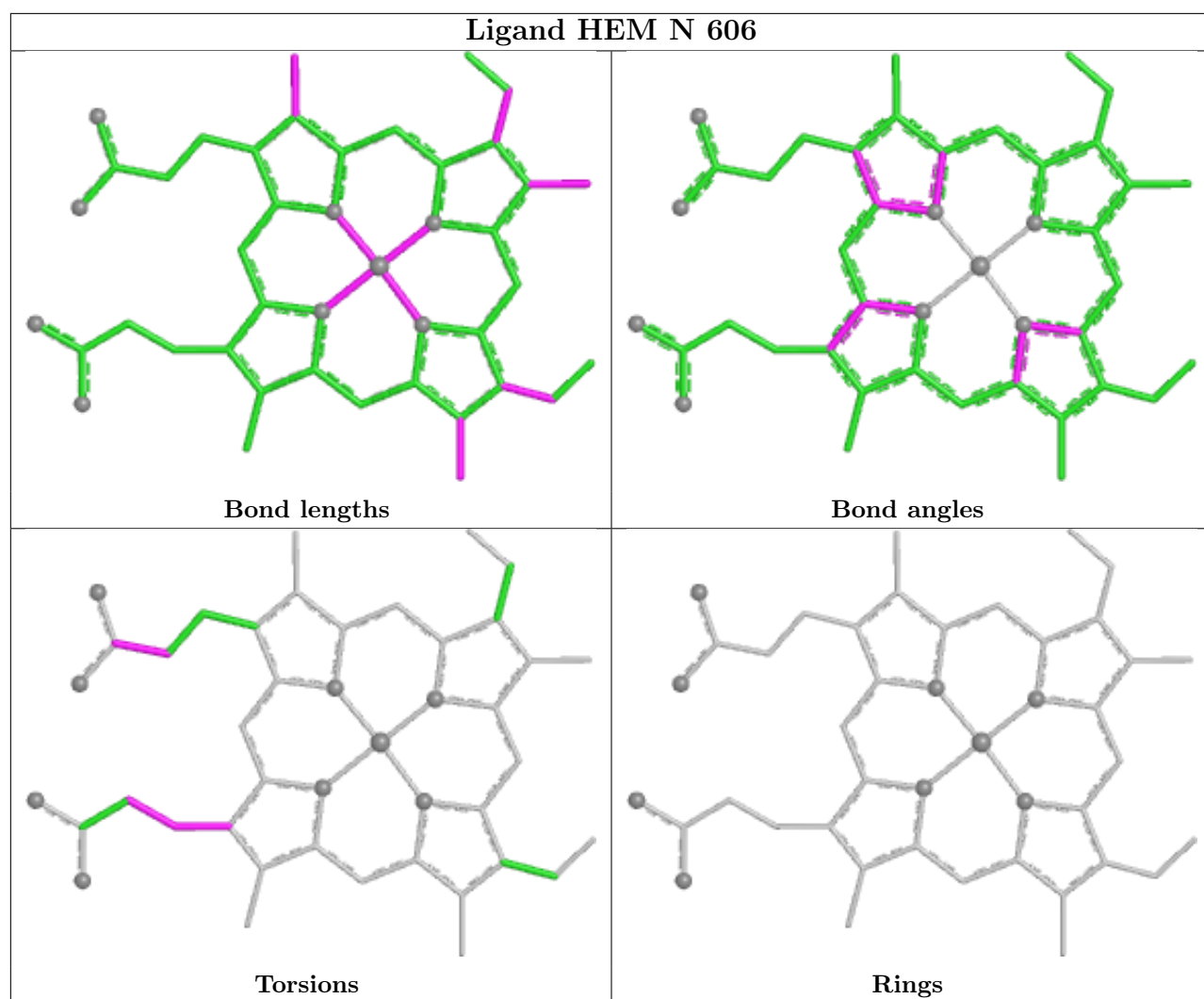


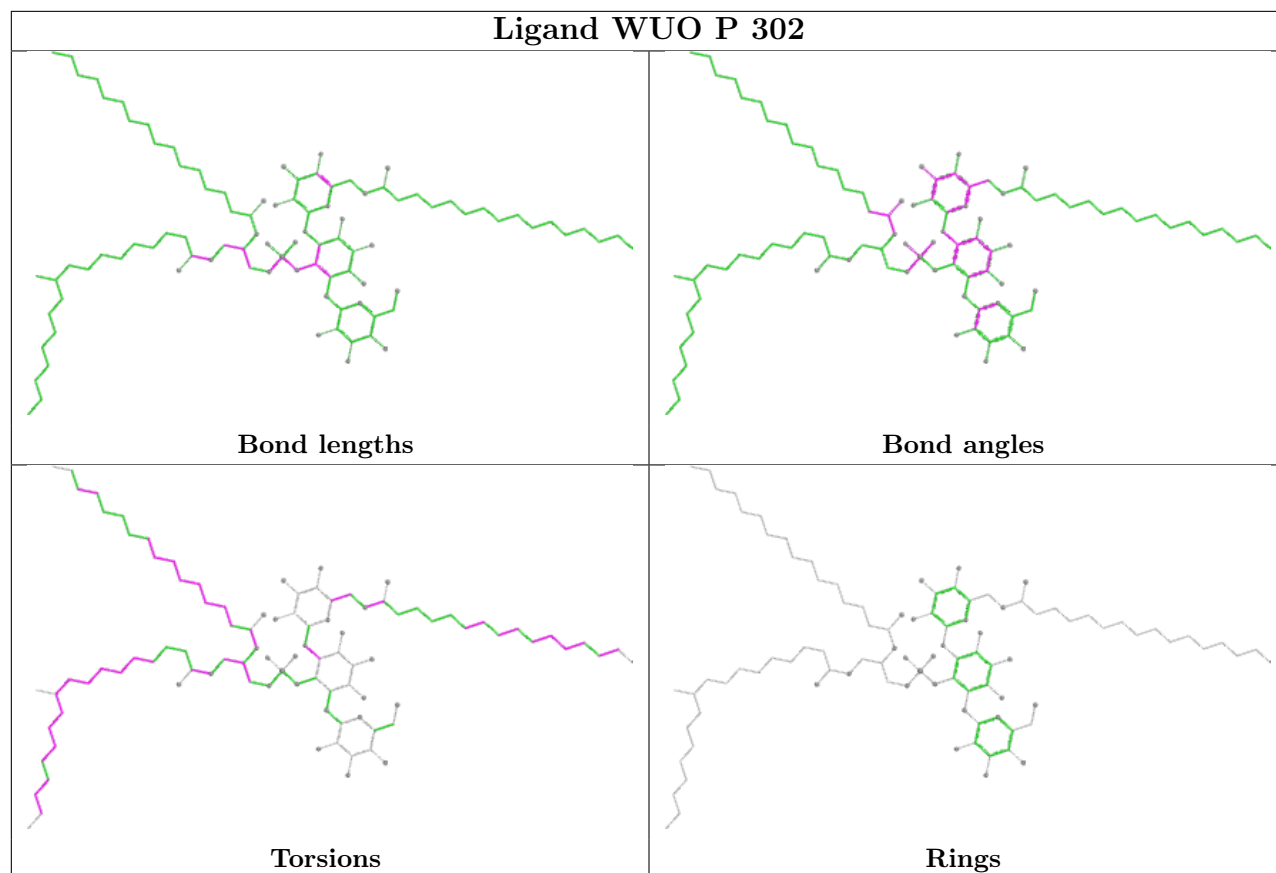


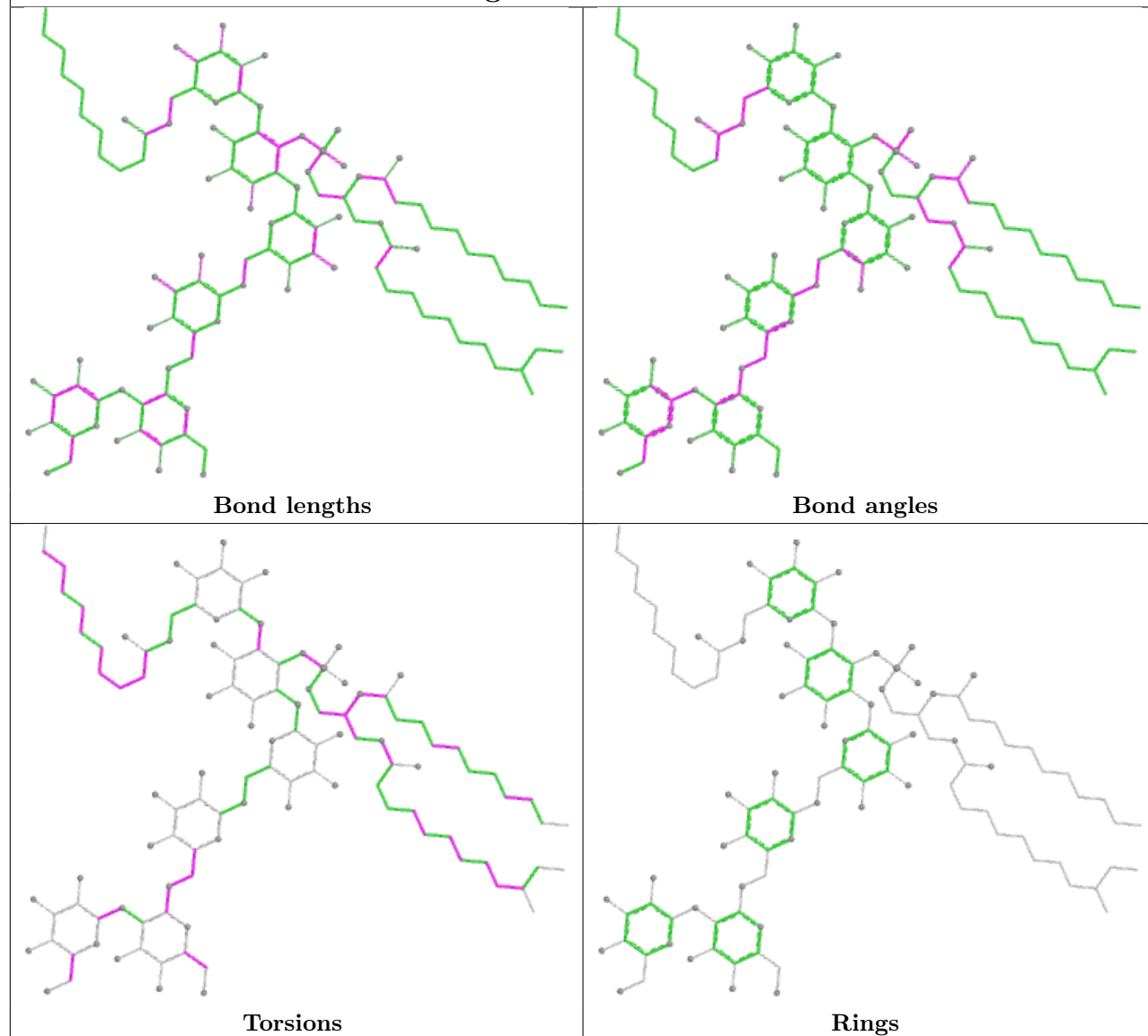
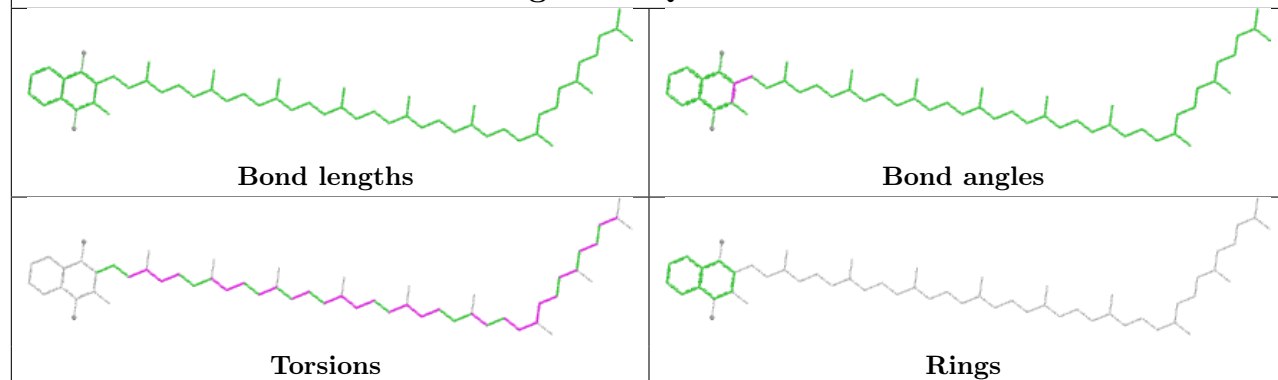










Ligand IZL G 503**Ligand MQ9 H 606**

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.

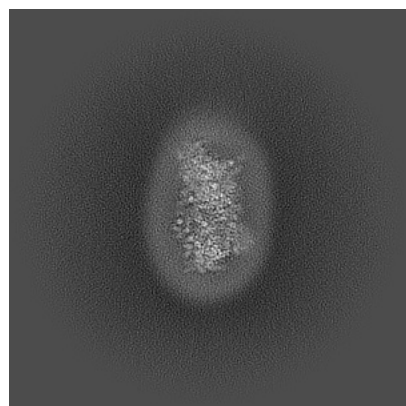
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50753. These allow visual inspection of the internal detail of the map and identification of artifacts.

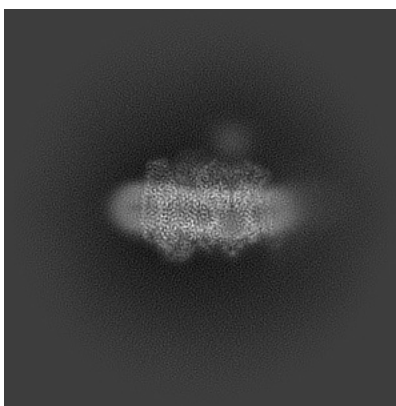
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

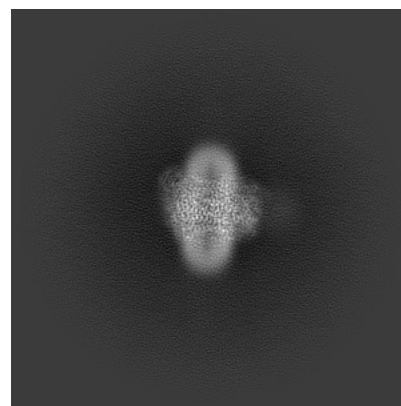
6.1.1 Primary map



X

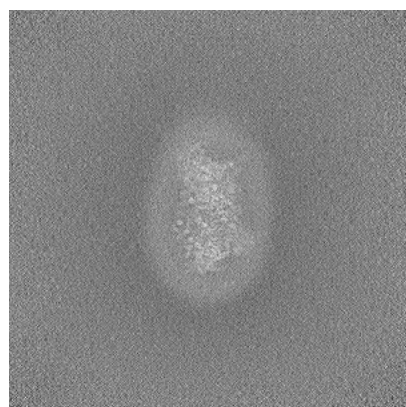


Y

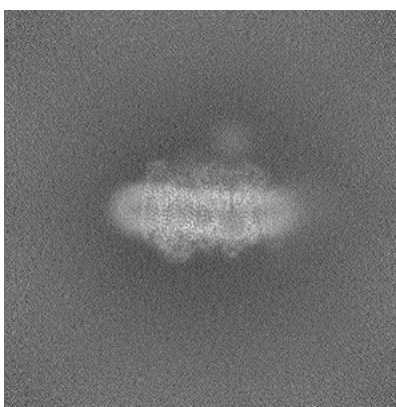


Z

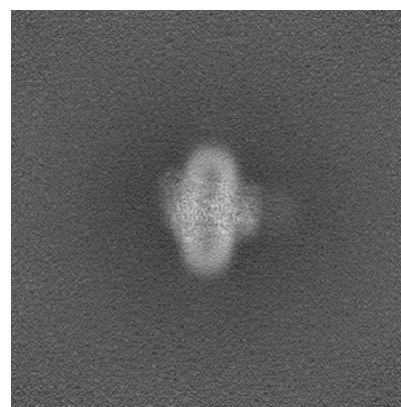
6.1.2 Raw map



X



Y

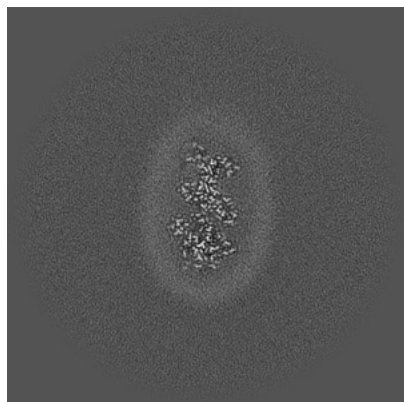


Z

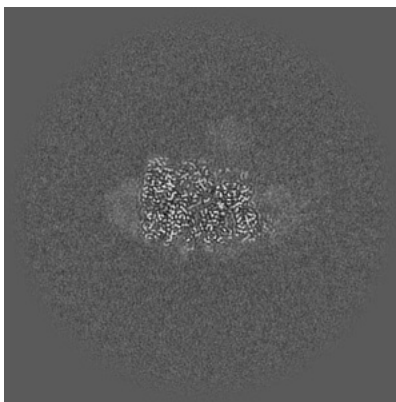
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

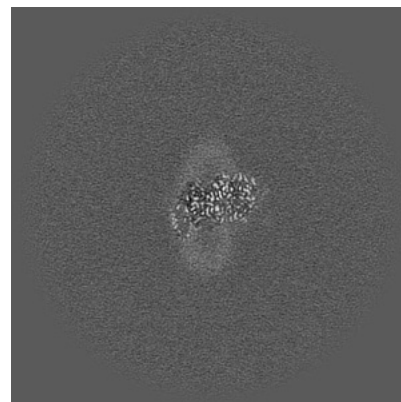
6.2.1 Primary map



X Index: 270

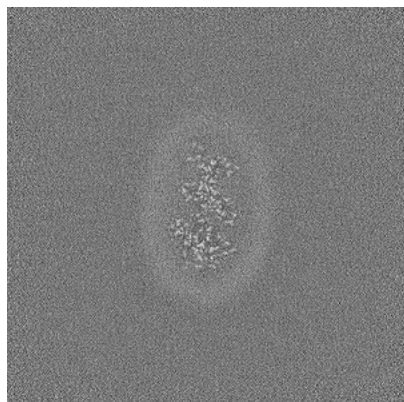


Y Index: 270

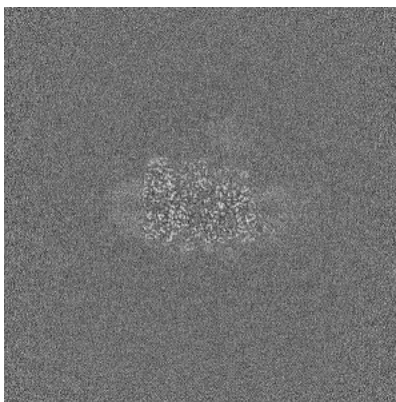


Z Index: 270

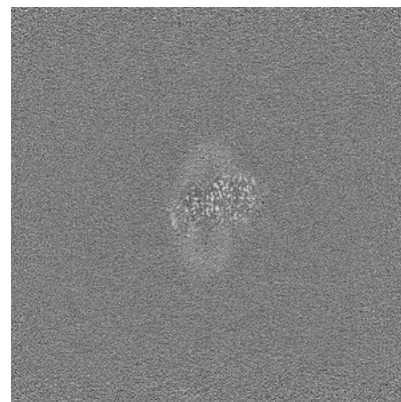
6.2.2 Raw map



X Index: 270



Y Index: 270

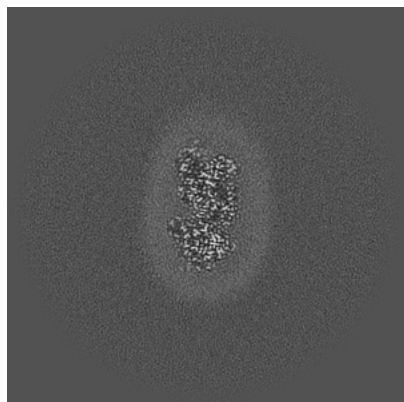


Z Index: 270

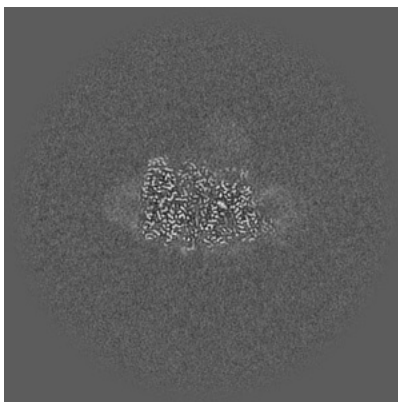
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

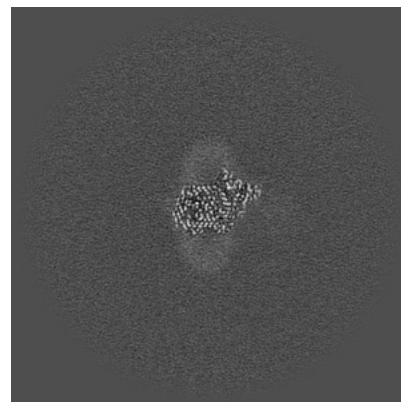
6.3.1 Primary map



X Index: 279

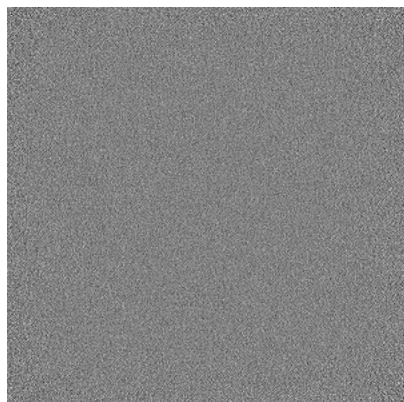


Y Index: 269

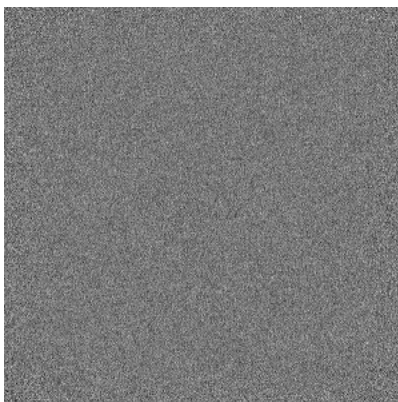


Z Index: 283

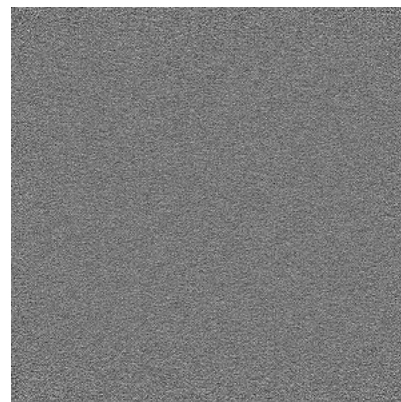
6.3.2 Raw map



X Index: 0



Y Index: 0

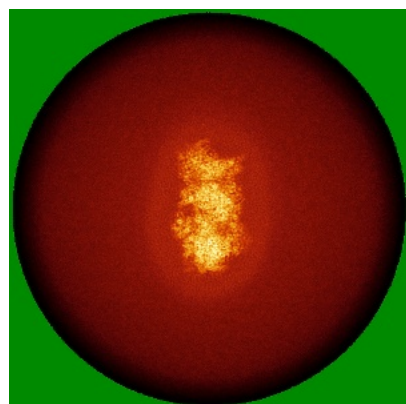


Z Index: 539

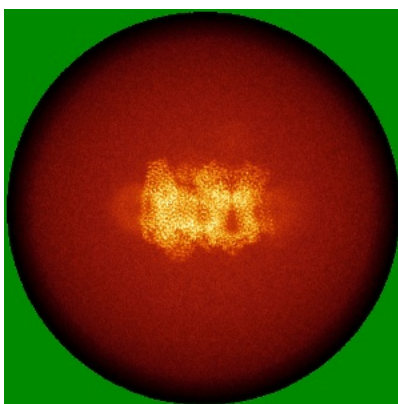
The images above show the largest variance slices of the map in three orthogonal directions.

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

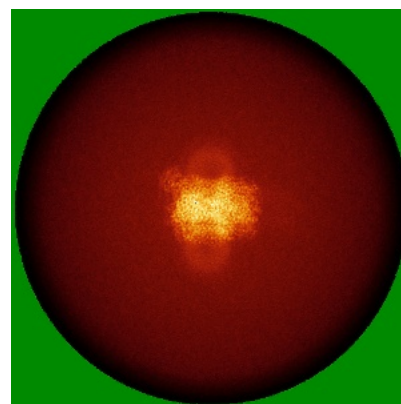
6.4.1 Primary map



X

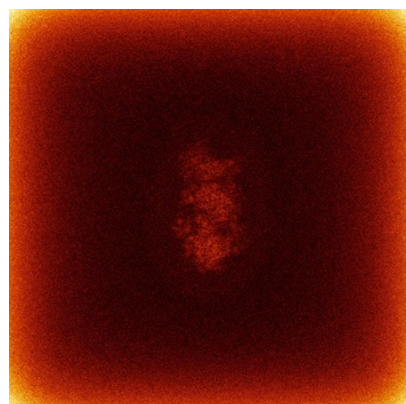


Y

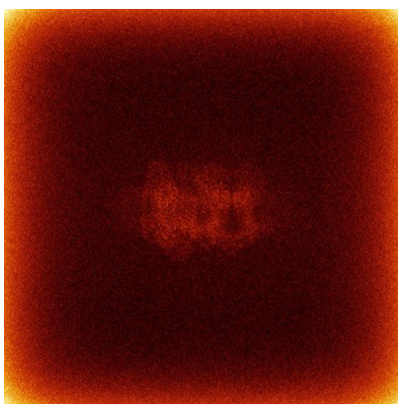


Z

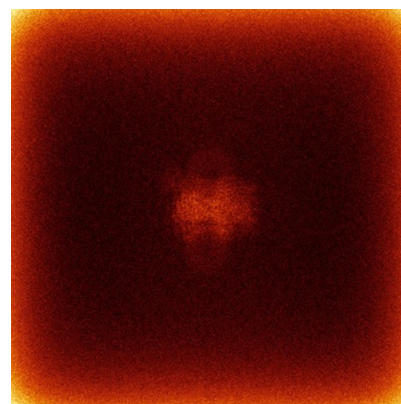
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.204. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

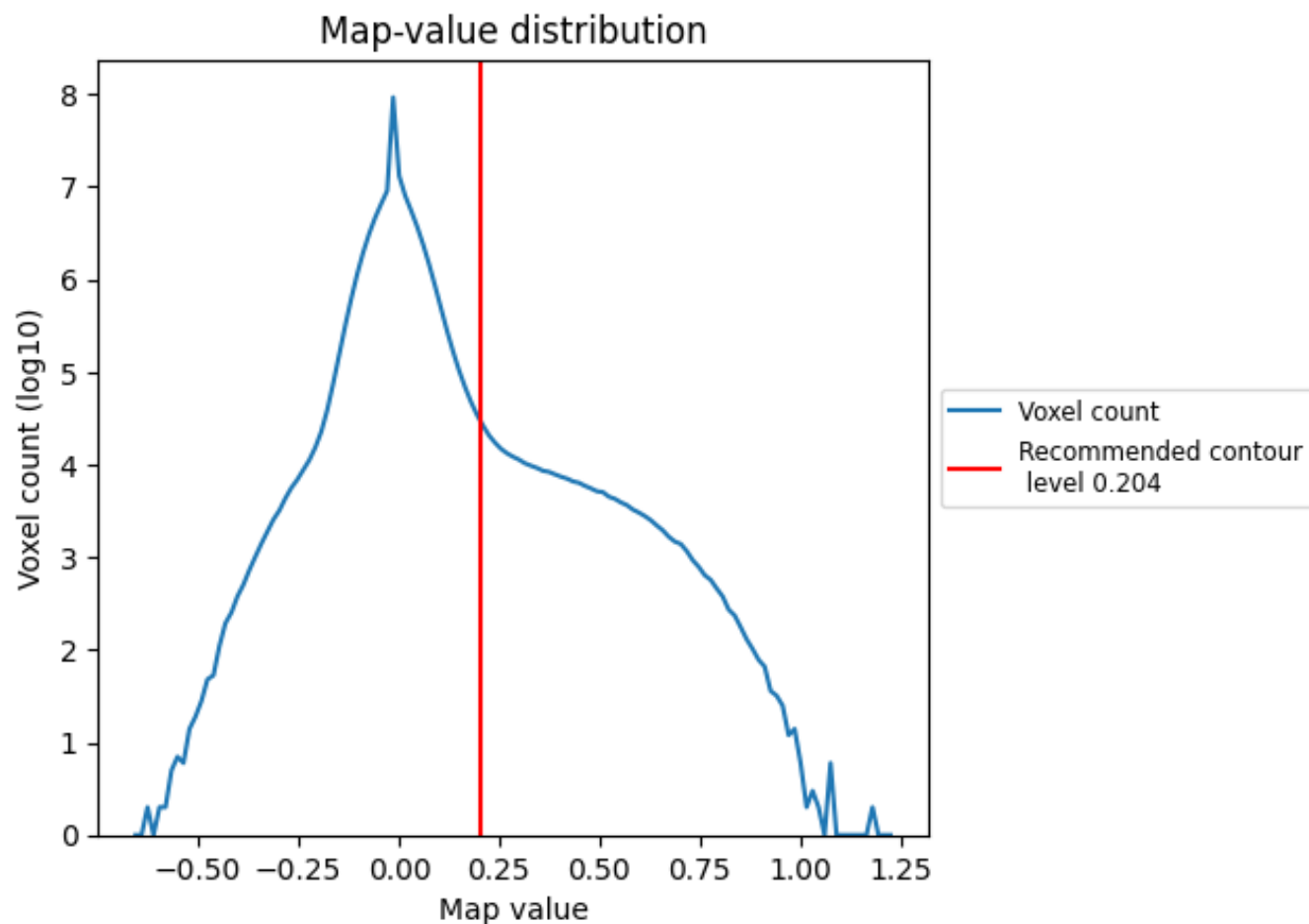
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

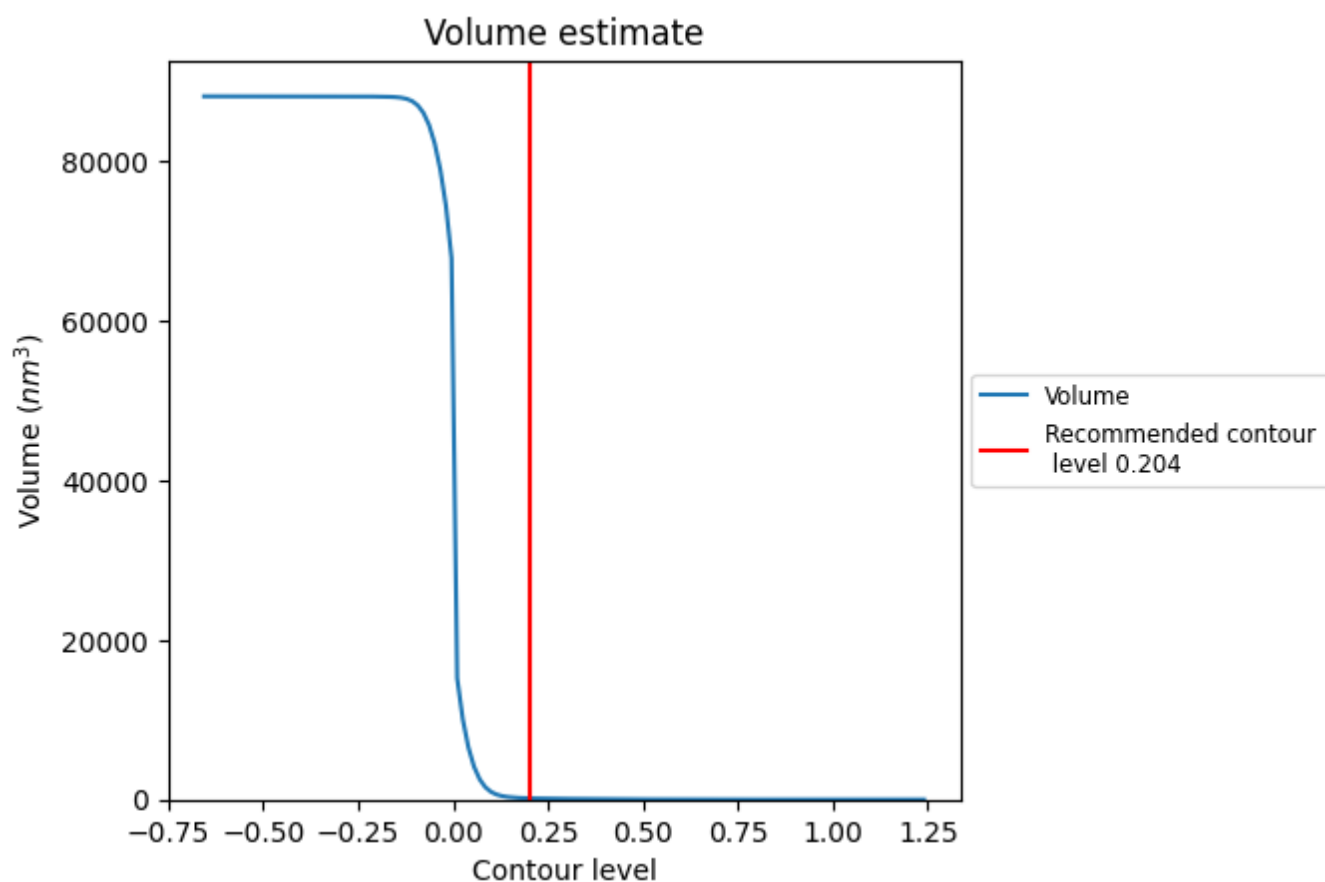
This section contains the results of statistical analysis of the map.

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.

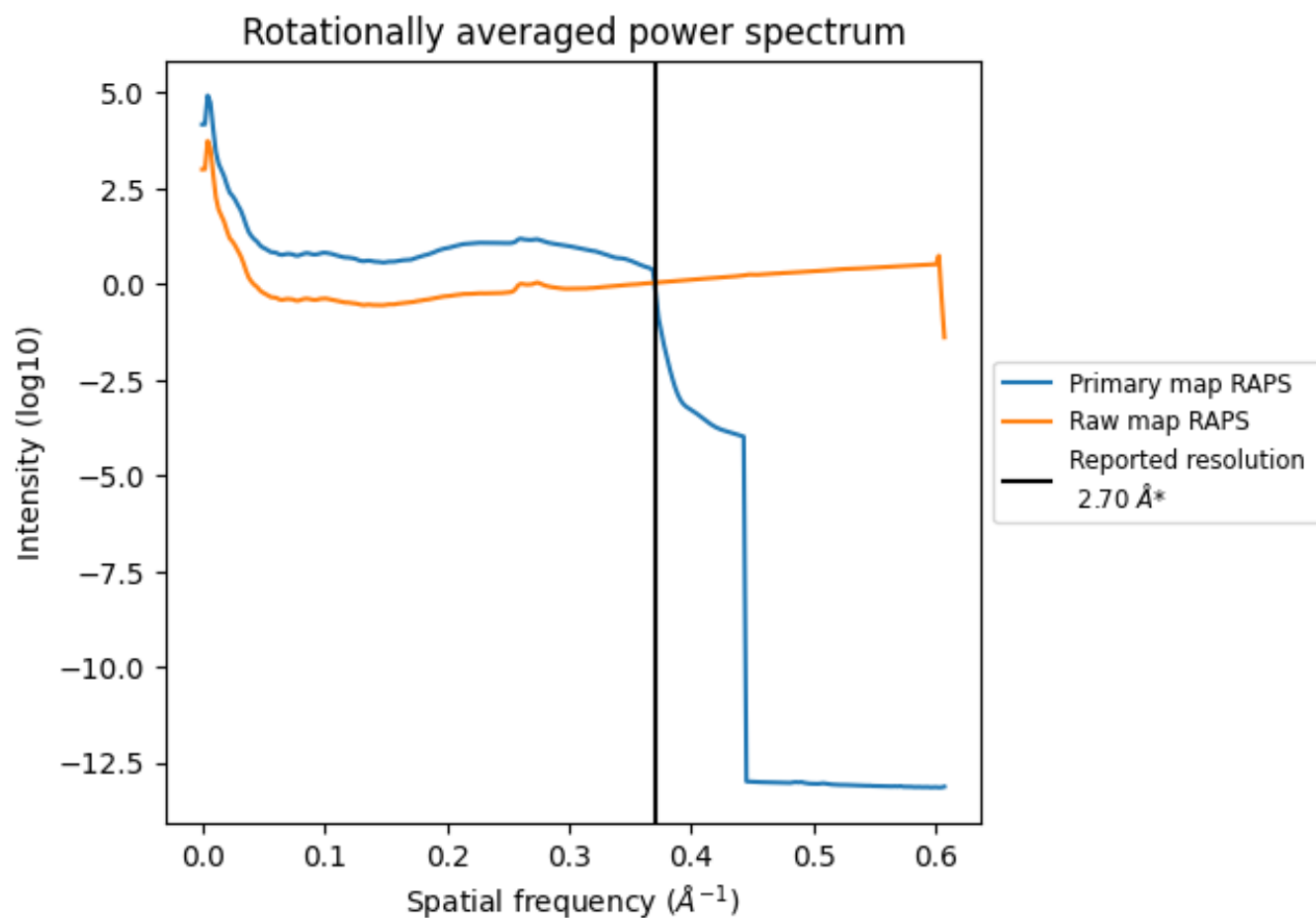
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 154 nm³; this corresponds to an approximate mass of 139 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 ⓘ

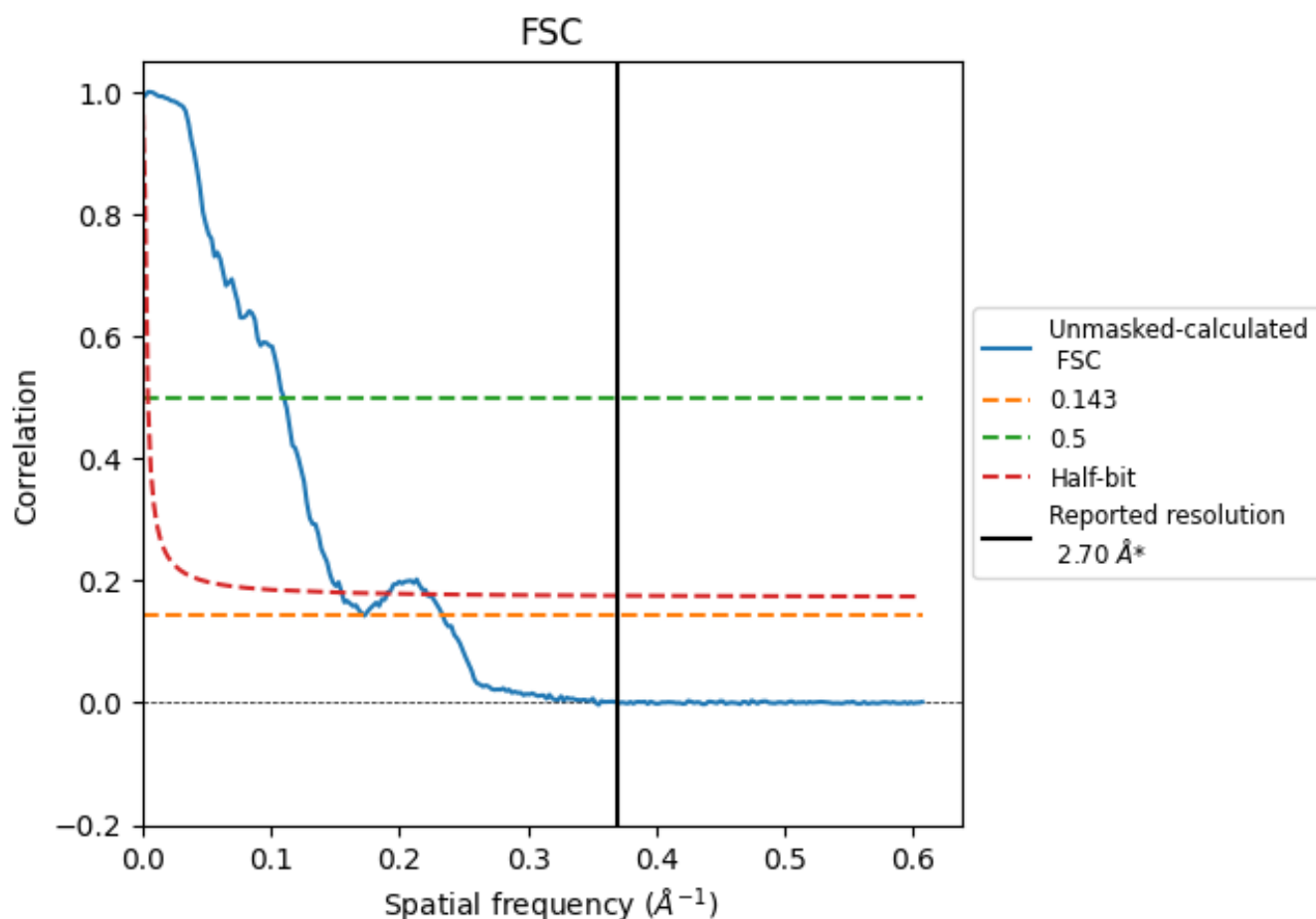


*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

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 0.370 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	5.79	9.08	6.45

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 5.79 differs from the reported value 2.7 by more than 10 %

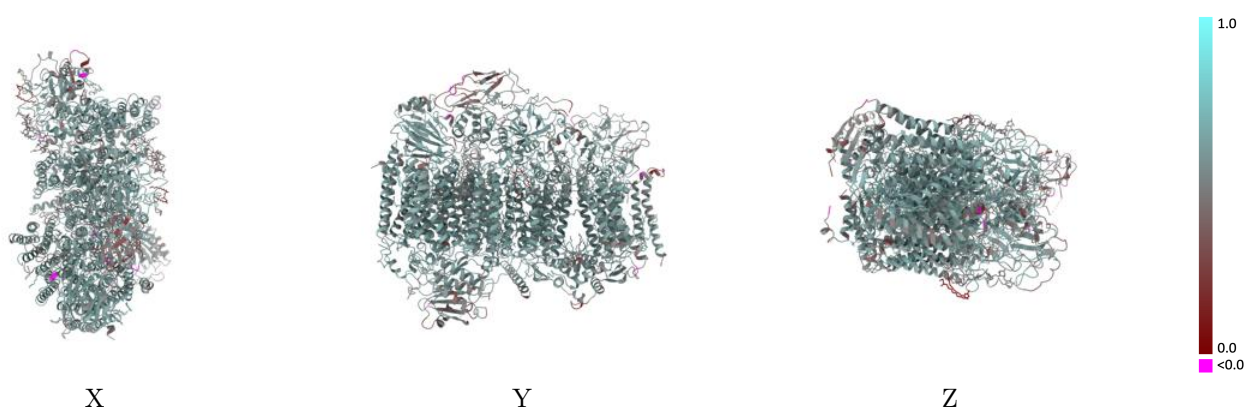
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-50753 and PDB model 9FU0. Per-residue inclusion information can be found in section 3 on page 19.

9.1 Map-model overlay [i](#)

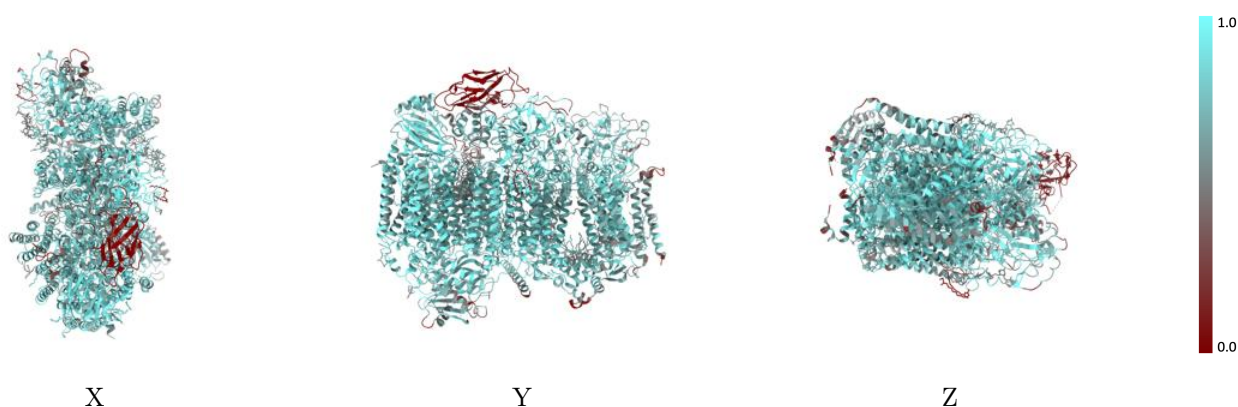
This section was not generated.

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



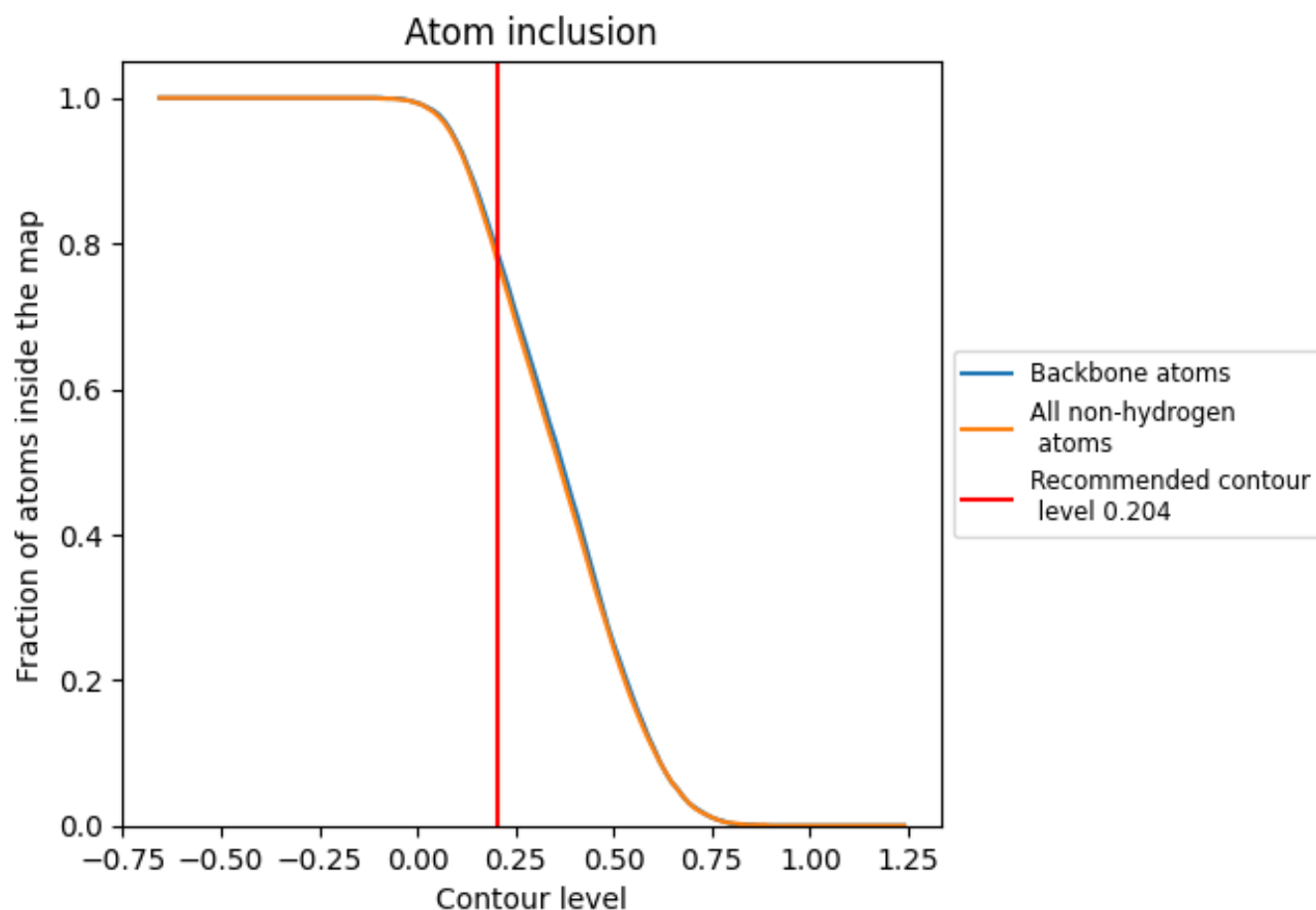
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.204).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 78% 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 (0.204) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7760	0.5730
G	0.7270	0.5410
H	0.7760	0.5700
M	0.8130	0.5820
N	0.8610	0.6080
O	0.7620	0.5800
P	0.7690	0.5750
Q	0.7730	0.5660
R	0.8930	0.6130
S	0.8190	0.5940
T	0.8590	0.6060
U	0.7210	0.5300
V	0.7060	0.5250
W	0.1560	0.4220
Y	0.6140	0.4480
c	0.4860	0.3980

1.0

0.0

<0.0