



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 07:23 AM UTC

PDB ID : 9GY6 / pdb_00009gy6
EMDB ID : EMD-51689
Title : Mycobacterial cytochrome bc1:aa3 with inhibitor
Authors : lamers, M.H.; Verma, A.K.
Deposited on : 2024-10-01
Resolution : 3.10 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:

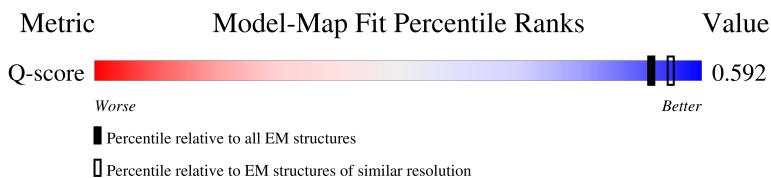
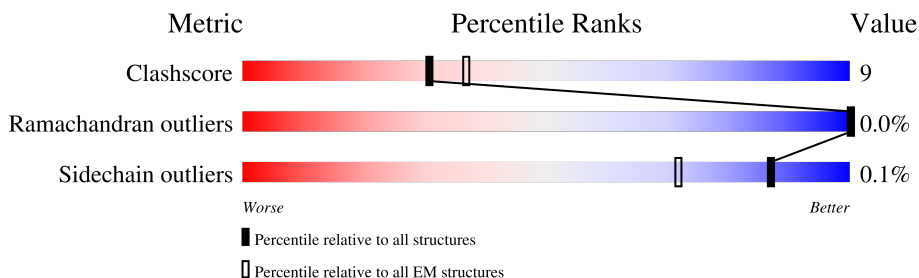
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.10 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.



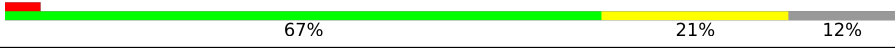
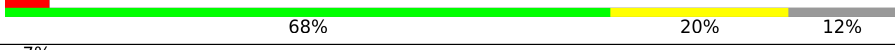
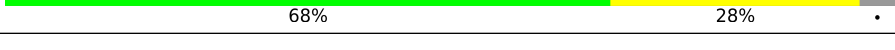
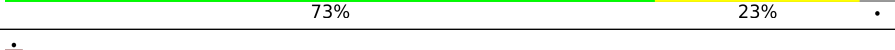
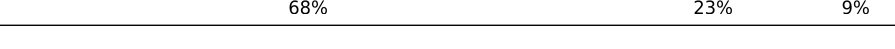
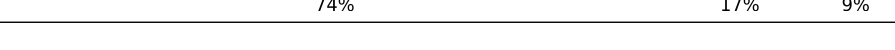
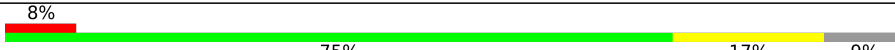
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14724 (2.60 - 3.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	421	 78% 11% 10%
1	M	421	 75% 14% 10%
2	B	546	 79% 19% .
2	N	546	 80% 17% .

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Mol	Chain	Length	Quality of chain
3	C	268	
3	O	268	
4	D	84	
4	P	84	
5	E	341	
5	Q	341	
6	F	575	
6	R	575	
7	G	203	
7	S	203	
8	H	139	
8	T	139	
9	I	79	
9	U	79	
10	J	157	
10	V	157	
11	L	236	
11	X	236	

2 Entry composition

There are 25 unique types of molecules in this entry. The entry contains 43307 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 Rieske iron-sulfur subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	377	Total	C	N	O	S	0	0
			2947	1907	498	531	11		
1	M	377	Total	C	N	O	S	0	0
			2942	1904	496	531	11		

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP A0R051
A	2	ASP	-	expression tag	UNP A0R051
A	3	TYR	-	expression tag	UNP A0R051
A	4	ARG	-	expression tag	UNP A0R051
A	5	ASN	-	expression tag	UNP A0R051
A	6	GLY	-	expression tag	UNP A0R051
A	7	GLY	-	expression tag	UNP A0R051
A	8	ARG	-	expression tag	UNP A0R051
A	9	HIS	-	expression tag	UNP A0R051
A	10	ARG	-	expression tag	UNP A0R051
A	11	CYS	-	expression tag	UNP A0R051
A	12	GLY	-	expression tag	UNP A0R051
A	13	HIS	-	expression tag	UNP A0R051
A	14	VAL	-	expression tag	UNP A0R051
M	1	MET	-	initiating methionine	UNP A0R051
M	2	ASP	-	expression tag	UNP A0R051
M	3	TYR	-	expression tag	UNP A0R051
M	4	ARG	-	expression tag	UNP A0R051
M	5	ASN	-	expression tag	UNP A0R051
M	6	GLY	-	expression tag	UNP A0R051
M	7	GLY	-	expression tag	UNP A0R051
M	8	ARG	-	expression tag	UNP A0R051
M	9	HIS	-	expression tag	UNP A0R051
M	10	ARG	-	expression tag	UNP A0R051
M	11	CYS	-	expression tag	UNP A0R051
M	12	GLY	-	expression tag	UNP A0R051

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Chain	Residue	Modelled	Actual	Comment	Reference
M	13	HIS	-	expression tag	UNP A0R051
M	14	VAL	-	expression tag	UNP A0R051

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	531	Total	C	N	O	S	0	0
			4153	2734	705	696	18		
2	N	534	Total	C	N	O	S	0	0
			4176	2747	710	701	18		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	156	TYR	PHE	engineered mutation	UNP A0R052
B	182	MET	ILE	engineered mutation	UNP A0R052
B	189	LEU	MET	engineered mutation	UNP A0R052
B	309	GLU	ASP	engineered mutation	UNP A0R052
B	312	ALA	ILE	engineered mutation	UNP A0R052
N	156	TYR	PHE	engineered mutation	UNP A0R052
N	182	MET	ILE	engineered mutation	UNP A0R052
N	189	LEU	MET	engineered mutation	UNP A0R052
N	309	GLU	ASP	engineered mutation	UNP A0R052
N	312	ALA	ILE	engineered mutation	UNP A0R052

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

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

- Molecule 4 is a protein called Transmembrane protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	74	Total	C	N	O	S	0	0
			590	387	108	91	4		
4	P	74	Total	C	N	O	S	0	0
			590	387	108	91	4		

- Molecule 5 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	285	Total	C	N	O	S	0	0
			2271	1472	375	415	9		
5	Q	285	Total	C	N	O	S	0	0
			2271	1472	375	415	9		

- Molecule 6 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	551	Total	C	N	O	S	0	0
			4364	2933	694	711	26		
6	R	551	Total	C	N	O	S	0	0
			4364	2933	694	711	26		

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	1	MET	-	initiating methionine	UNP A0A2U9PNL2
F	2	VAL	-	expression tag	UNP A0A2U9PNL2
F	3	ALA	-	expression tag	UNP A0A2U9PNL2
F	4	GLU	-	expression tag	UNP A0A2U9PNL2
F	5	ALA	-	expression tag	UNP A0A2U9PNL2
F	6	PRO	-	expression tag	UNP A0A2U9PNL2
F	7	PRO	-	expression tag	UNP A0A2U9PNL2
F	8	ILE	-	expression tag	UNP A0A2U9PNL2
F	9	GLY	-	expression tag	UNP A0A2U9PNL2
F	10	GLU	-	expression tag	UNP A0A2U9PNL2
F	11	LEU	-	expression tag	UNP A0A2U9PNL2
F	12	GLU	-	expression tag	UNP A0A2U9PNL2
F	13	ALA	-	expression tag	UNP A0A2U9PNL2
F	14	ARG	-	expression tag	UNP A0A2U9PNL2
F	15	ARG	-	expression tag	UNP A0A2U9PNL2
F	16	PRO	-	expression tag	UNP A0A2U9PNL2
F	17	PHE	-	expression tag	UNP A0A2U9PNL2
F	18	PRO	-	expression tag	UNP A0A2U9PNL2
F	19	GLU	-	expression tag	UNP A0A2U9PNL2
F	20	ARG	-	expression tag	UNP A0A2U9PNL2
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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 7 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	185	Total	C	N	O	S	0	0
			1449	973	230	239	7		
7	S	185	Total	C	N	O	S	0	0
			1449	973	230	239	7		

- Molecule 8 is a protein called Cytochrome c oxidase polypeptide 4.

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

- Molecule 9 is a protein called Secreted protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	65	Total	C	N	O	S	0	0
			490	324	83	82	1		
9	U	66	Total	C	N	O	S	0	0
			498	329	84	83	2		

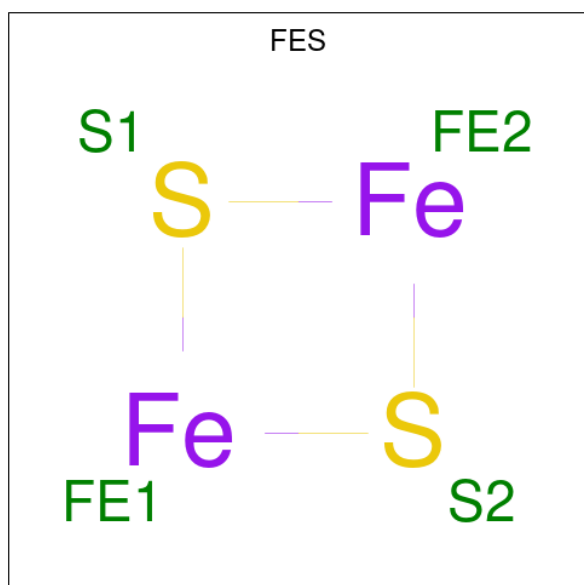
- Molecule 10 is a protein called DUF5130 domain-containing protein.

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

- Molecule 11 is a protein called Superoxide dismutase [Cu-Zn].

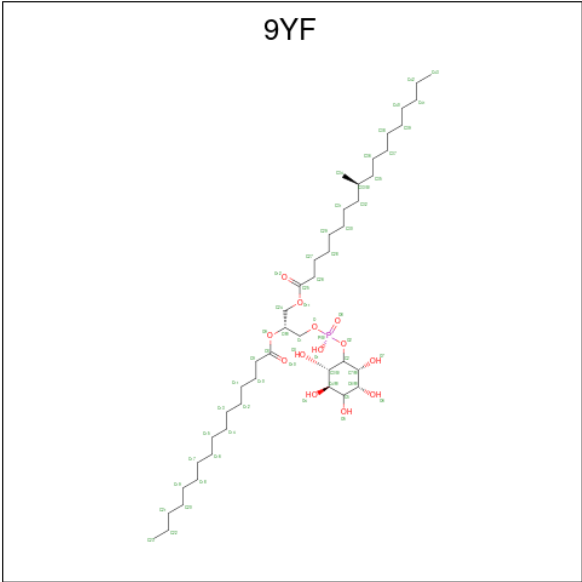
Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	28	Total	C	N	O	S	0	0
			185	113	29	42	1		
11	X	28	Total	C	N	O	S	0	0
			185	113	29	42	1		

- Molecule 12 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



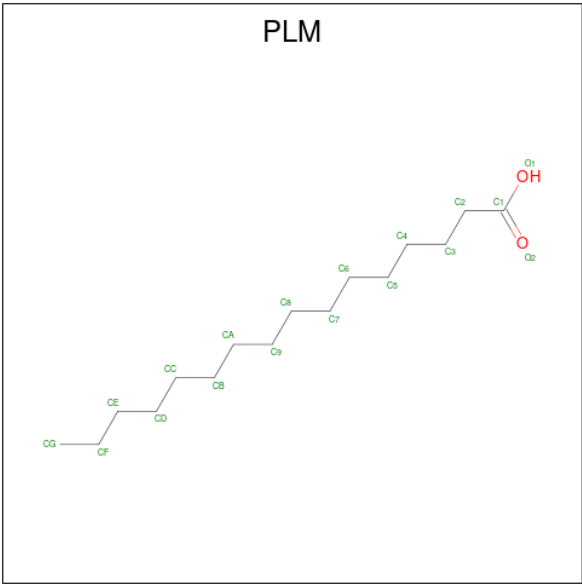
Mol	Chain	Residues	Atoms			AltConf
12	A	1	Total	Fe	S	0
			4	2	2	
12	M	1	Total	Fe	S	0
			4	2	2	

- Molecule 13 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).



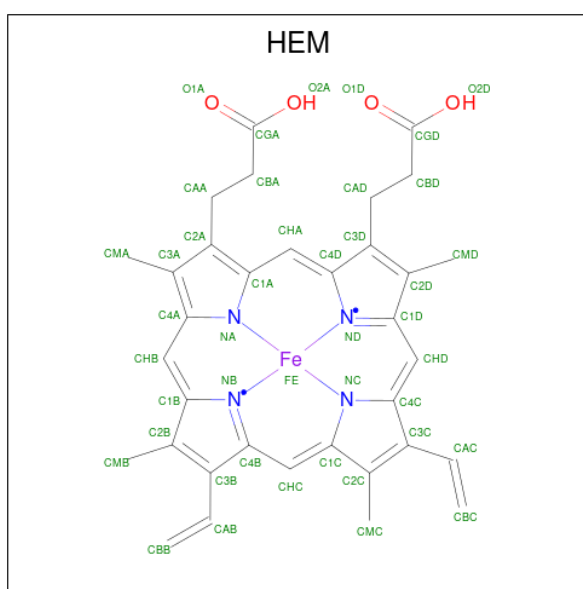
Mol	Chain	Residues	Atoms				AltConf
13	A	1	Total	C	O	P	0
			58	44	13	1	
13	C	1	Total	C	O	P	0
			58	44	13	1	
13	M	1	Total	C	O	P	0
			58	44	13	1	
13	O	1	Total	C	O	P	0
			58	44	13	1	

- Molecule 14 is PALMITIC ACID (CCD ID: PLM) (formula: C₁₆H₃₂O₂).



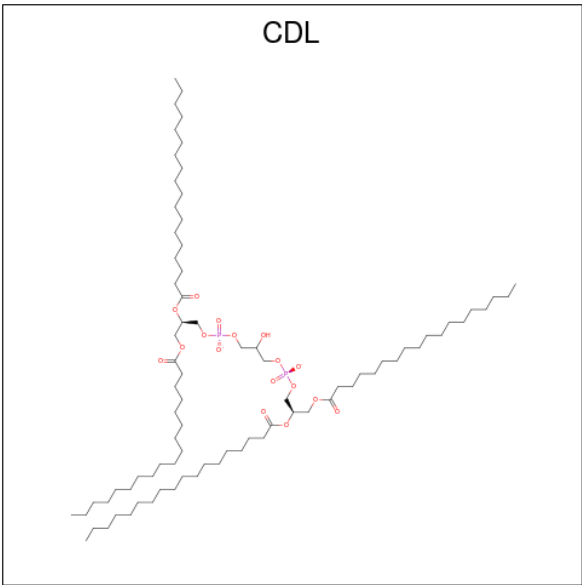
Mol	Chain	Residues	Atoms			AltConf
14	A	1	Total	C	O	0
			17	16	1	
14	G	1	Total	C	O	0
			17	16	1	
14	M	1	Total	C	O	0
			17	16	1	
14	T	1	Total	C	O	0
			17	16	1	

- Molecule 15 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

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



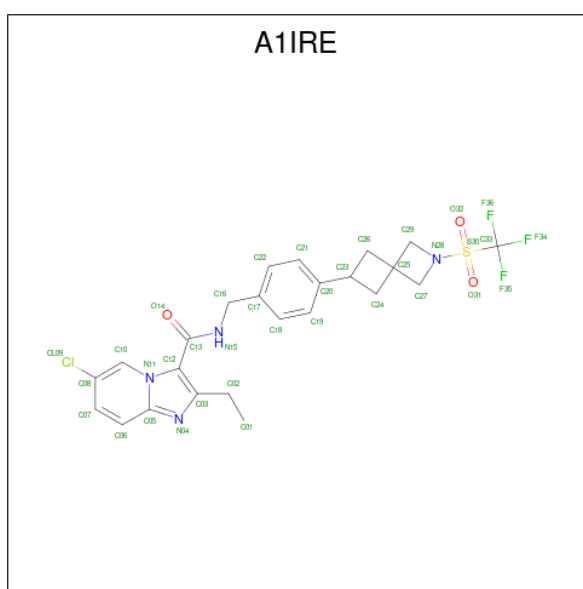
Mol	Chain	Residues	Atoms				AltConf
16	B	1	Total	C	O	P	0
			74	55	17	2	
16	B	1	Total	C	O	P	0
			77	58	17	2	
16	B	1	Total	C	O	P	0
			79	60	17	2	
16	C	1	Total	C	O	P	0
			79	60	17	2	
16	D	1	Total	C	O	P	0
			88	69	17	2	
16	D	1	Total	C	O	P	0
			95	76	17	2	
16	F	1	Total	C	O	P	0
			76	57	17	2	
16	F	1	Total	C	O	P	0
			81	62	17	2	
16	M	1	Total	C	O	P	0
			74	55	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	N	1	Total	C	O	P	0
			79	60	17	2	
16	P	1	Total	C	O	P	0
			88	69	17	2	

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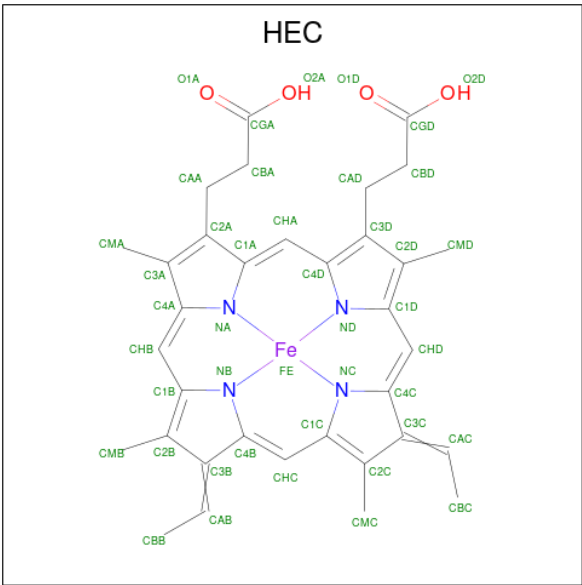
Mol	Chain	Residues	Atoms				AltConf
16	P	1	Total	C	O	P	0
			95	76	17	2	
16	R	1	Total	C	O	P	0
			76	57	17	2	
16	R	1	Total	C	O	P	0
			81	62	17	2	

- Molecule 17 is 6-chloranyl-2-ethyl-N-[[4-[2-(trifluoromethylsulfonyl)-2-azaspiro[3.3]heptan-6-yl]phenyl]methyl]imidazo[1,2-a]pyridine-3-carboxamide (CCD ID: A1IRE) (formula: $C_{24}H_{24}ClF_3N_4O_3S$).



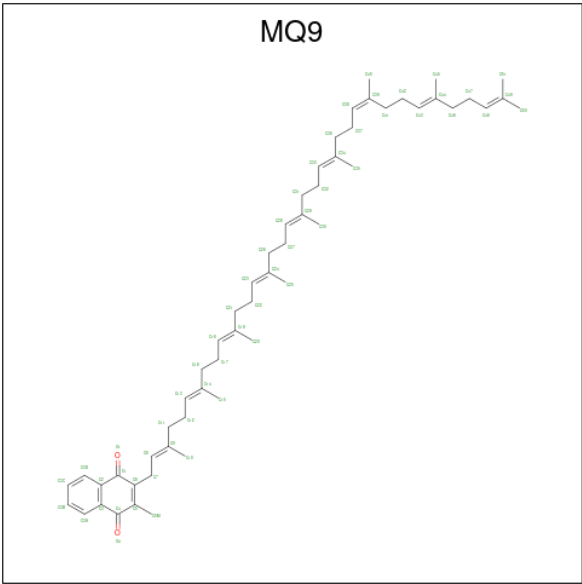
Mol	Chain	Residues	Atoms							AltConf
17	B	1	Total	C	Cl	F	N	O	S	0
			36	24	1	3	4	3	1	
17	N	1	Total	C	Cl	F	N	O	S	0
			36	24	1	3	4	3	1	

- Molecule 18 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



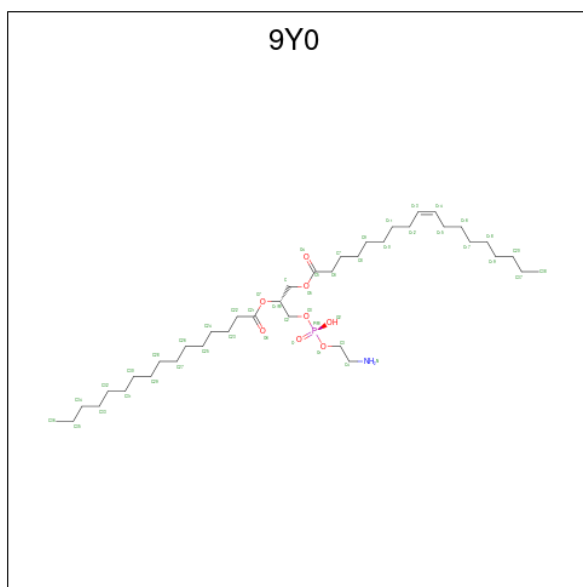
Mol	Chain	Residues	Atoms					AltConf
18	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
18	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
18	O	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
18	O	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 19 is MENAQUINONE-9 (CCD ID: MQ9) (formula: C₅₆H₈₀O₂).



Mol	Chain	Residues	Atoms			AltConf
19	C	1	Total	C	O	0
			58	56	2	
19	O	1	Total	C	O	0
			58	56	2	

- Molecule 20 is (2R)-3-(((2-aminoethoxy)(hydroxy)phosphoryl)oxy)-2-(palmitoyloxy)propyl (E)-octadec-9-enoate (CCD ID: 9Y0) (formula: C₃₉H₇₆NO₈P).



Mol	Chain	Residues	Atoms					AltConf
20	D	1	Total	C	N	O	P	0
			41	31	1	8	1	
20	G	1	Total	C	N	O	P	0
			43	33	1	8	1	
20	P	1	Total	C	N	O	P	0
			41	31	1	8	1	
20	S	1	Total	C	N	O	P	0
			43	33	1	8	1	

- Molecule 21 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

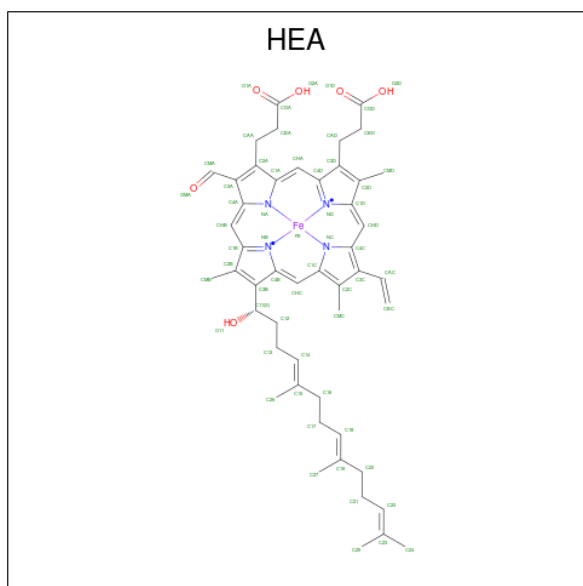
Mol	Chain	Residues	Atoms		AltConf
21	E	2	Total	Cu	0
			2	2	
21	F	2	Total	Cu	0
			2	2	
21	Q	2	Total	Cu	0
			2	2	

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Mol	Chain	Residues	Atoms		AltConf
21	R	2	Total	Cu	0
			2	2	

- Molecule 22 is HEME-A (CCD ID: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).

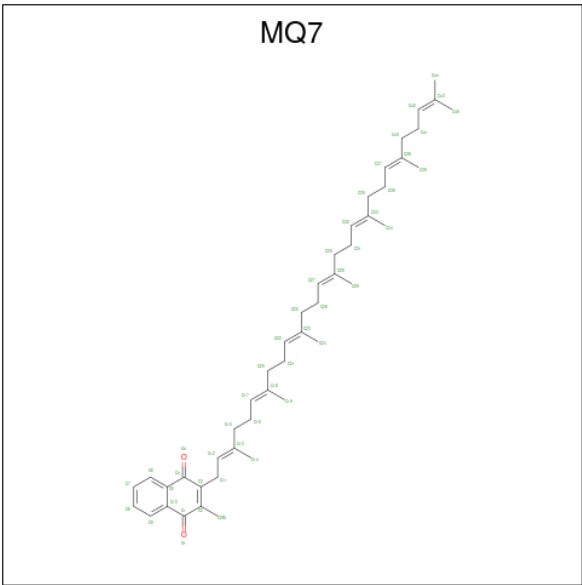


Mol	Chain	Residues	Atoms					AltConf
22	F	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
22	F	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
22	R	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
22	R	1	Total	C	Fe	N	O	0
			60	49	1	4	6	

- Molecule 23 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
23	F	1	Total	Ca	0
			1	1	
23	R	1	Total	Ca	0
			1	1	

- Molecule 24 is MENAQUINONE-7 (CCD ID: MQ7) (formula: $C_{46}H_{64}O_2$).



Mol	Chain	Residues	Atoms			AltConf
24	H	1	Total	C	O	0
			48	46	2	
24	O	1	Total	C	O	0
			48	46	2	

- Molecule 25 is water.

Mol	Chain	Residues	Atoms		AltConf
25	A	25	Total	O	0
			25	25	
25	B	45	Total	O	0
			45	45	
25	C	10	Total	O	0
			10	10	
25	D	4	Total	O	0
			4	4	
25	E	8	Total	O	0
			8	8	
25	F	25	Total	O	0
			25	25	
25	G	1	Total	O	0
			1	1	
25	H	5	Total	O	0
			5	5	
25	J	1	Total	O	0
			1	1	
25	L	1	Total	O	0
			1	1	

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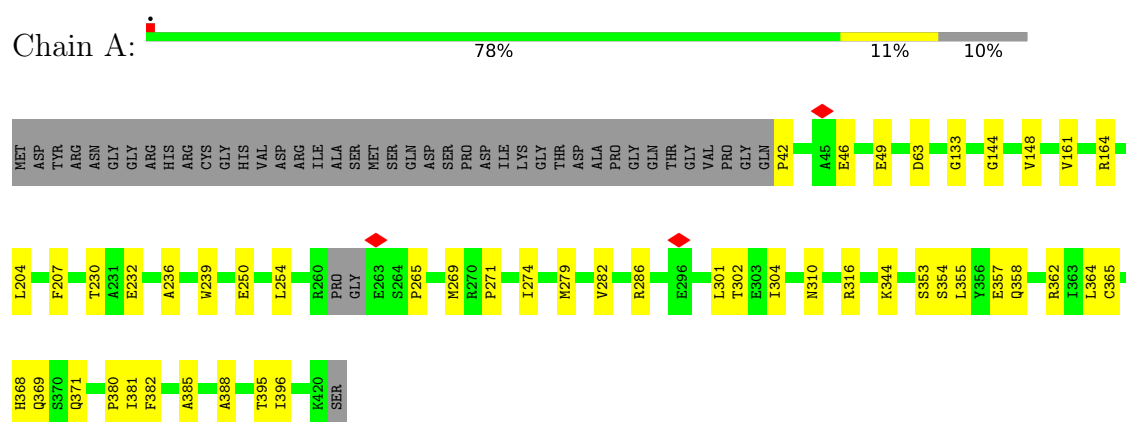
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Mol	Chain	Residues	Atoms		AltConf
25	M	21	Total 21	O 21	0
25	N	43	Total 43	O 43	0
25	O	2	Total 2	O 2	0
25	P	3	Total 3	O 3	0
25	Q	1	Total 1	O 1	0
25	R	11	Total 11	O 11	0
25	S	2	Total 2	O 2	0
25	T	2	Total 2	O 2	0
25	U	1	Total 1	O 1	0

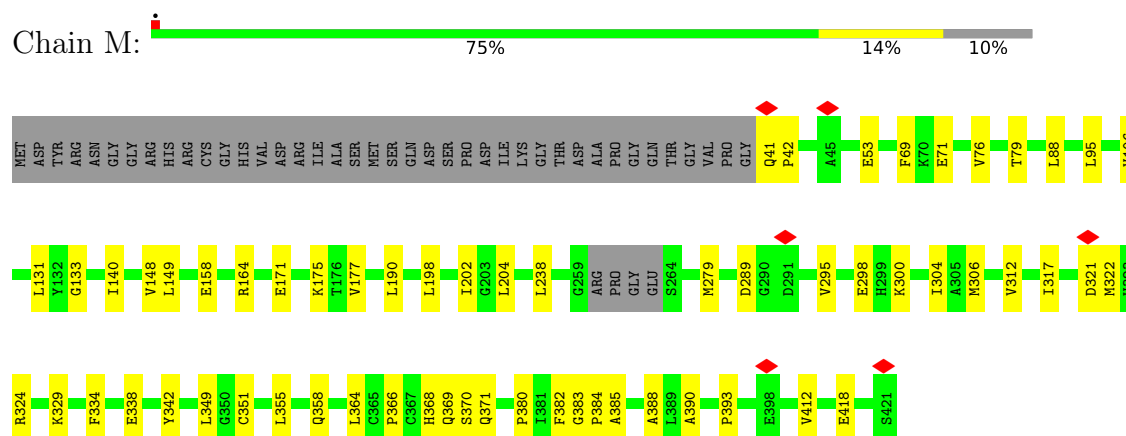
3 Residue-property plots

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.

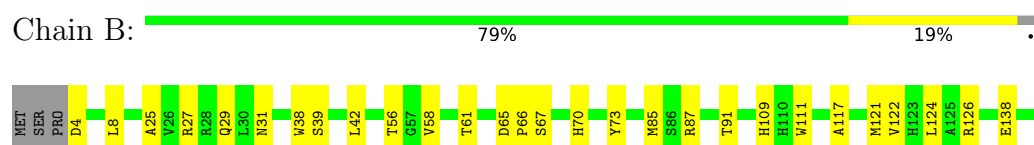
- Molecule 1: Cytochrome bc1 complex Rieske iron-sulfur subunit

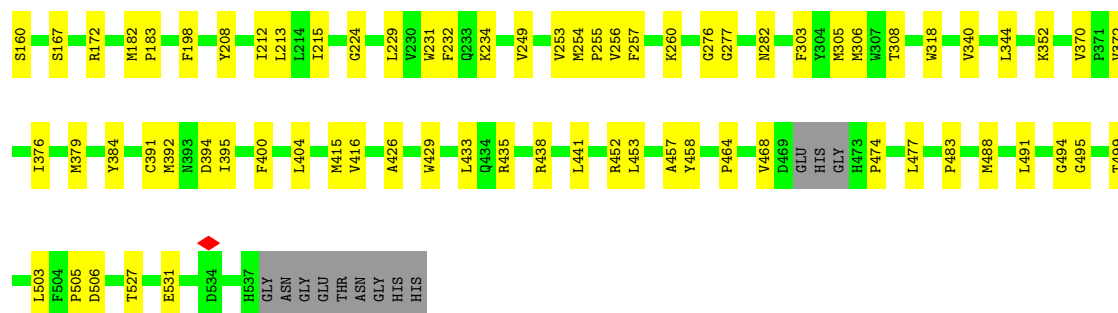


- Molecule 1: Cytochrome bc1 complex Rieske iron-sulfur subunit



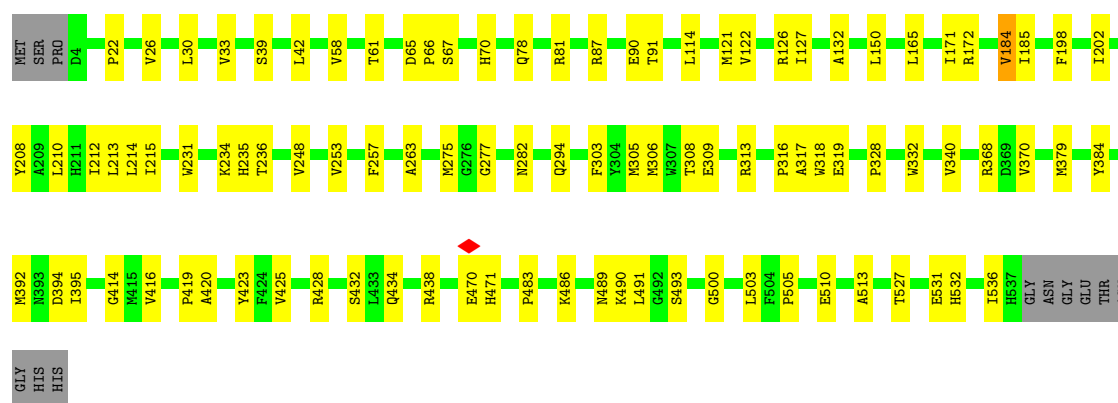
- Molecule 2: Cytochrome bc1 complex cytochrome b subunit





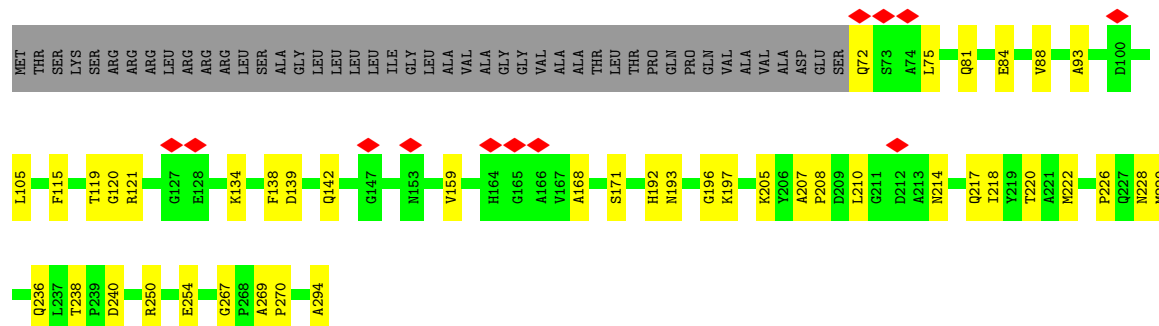
- Molecule 2: Cytochrome bc1 complex cytochrome b subunit

Chain N: 80% 17% .



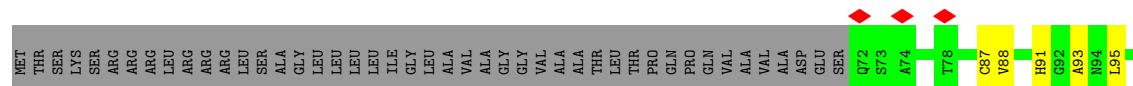
- Molecule 3: Cytochrome bc1 complex cytochrome c subunit

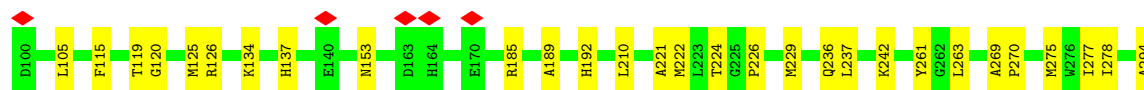
Chain C: 67% 16% 17%



- Molecule 3: Cytochrome bc1 complex cytochrome c subunit

Chain O: 71% 13% 17%





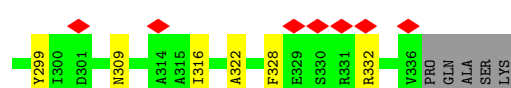
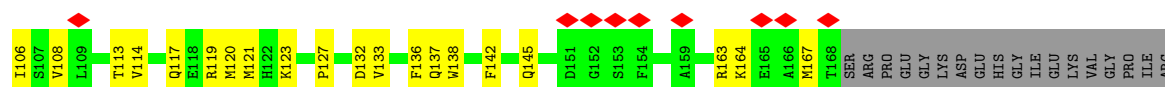
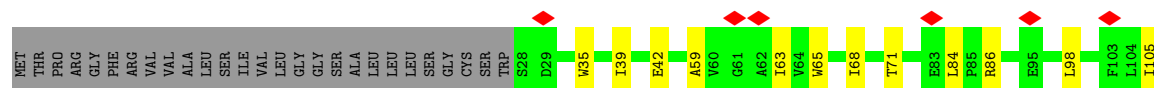
- Molecule 4: Transmembrane protein



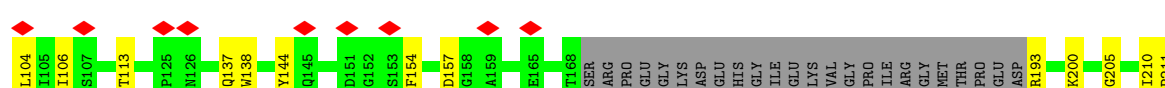
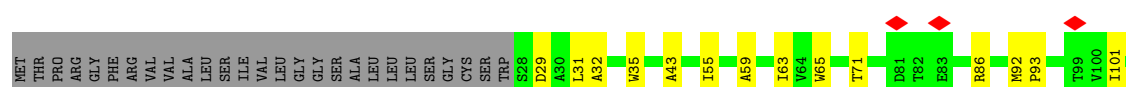
- Molecule 4: Transmembrane protein



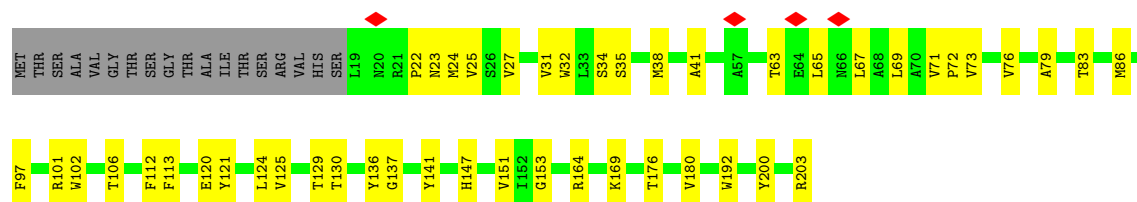
- Molecule 5: Cytochrome c oxidase subunit 2



- Molecule 5: Cytochrome c oxidase subunit 2

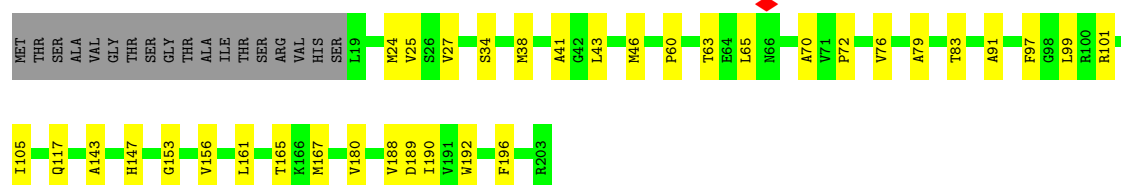


Chain G: 



- Molecule 7: Cytochrome c oxidase subunit 3

Chain S: 



- Molecule 8: Cytochrome c oxidase polypeptide 4

Chain H: 



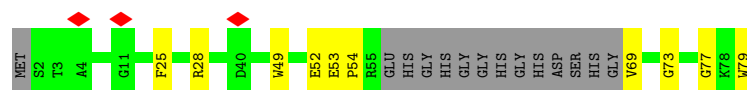
- Molecule 8: Cytochrome c oxidase polypeptide 4

Chain T: 



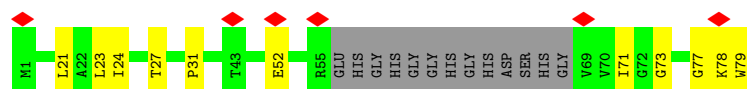
- Molecule 9: Secreted protein

Chain I: 

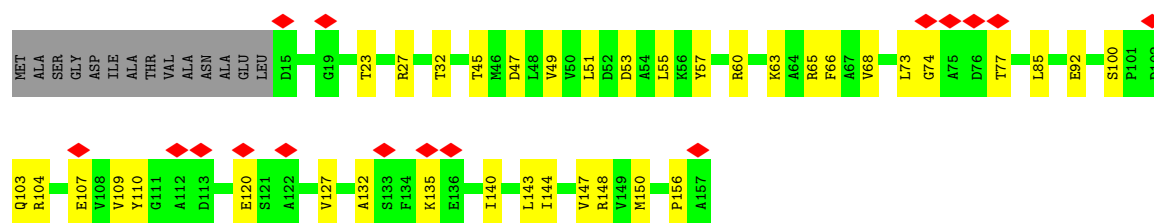


- Molecule 9: Secreted protein

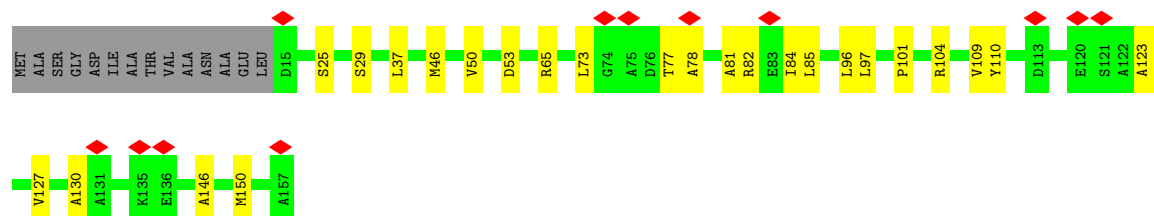
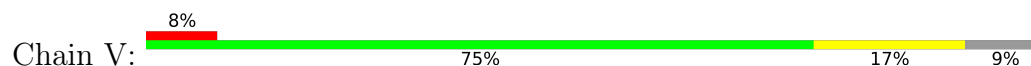
Chain U: 



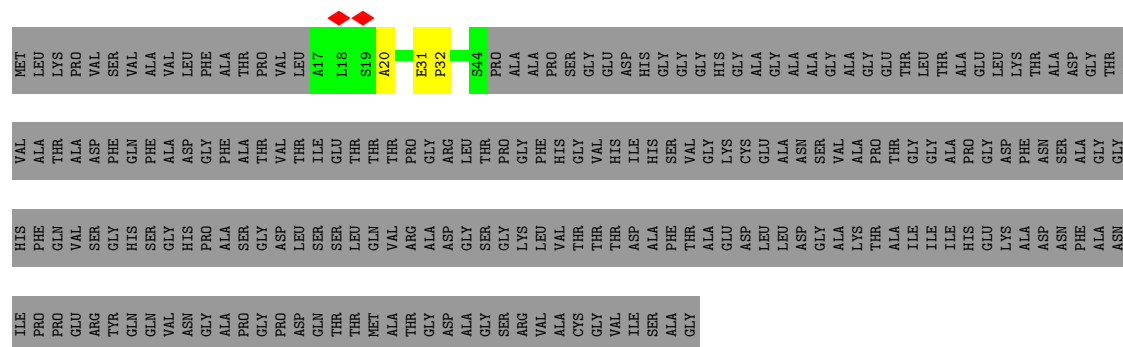
- Molecule 10: DUF5130 domain-containing protein



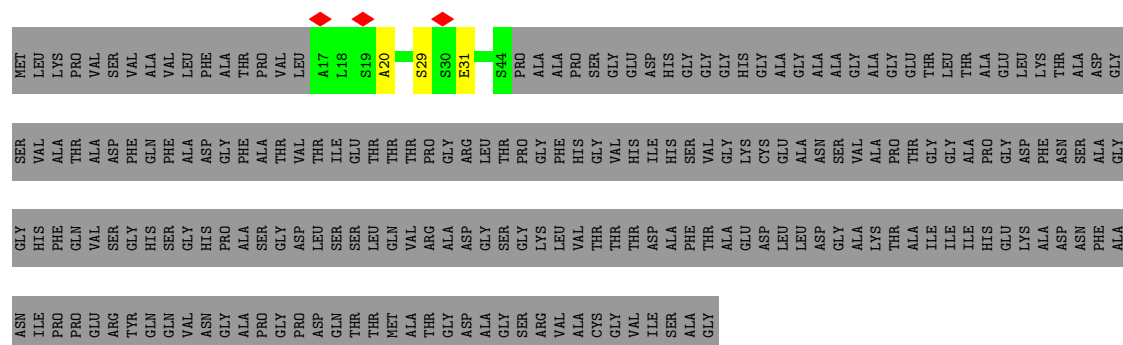
- Molecule 10: DUF5130 domain-containing protein



- Molecule 11: Superoxide dismutase [Cu-Zn]



- Molecule 11: Superoxide dismutase [Cu-Zn]



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	42000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.063	Depositor
Minimum map value	-0.031	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.009	Depositor
Map size (Å)	351.12003, 351.12003, 351.12003	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8360001, 0.8360001, 0.8360001	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CU, CDL, FES, 9YF, MQ7, A1IRE, PLM, HEM, CA, HEC, MQ9, 9Y0, HEA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.16	0/3024	0.34	0/4096
1	M	0.16	0/3019	0.35	0/4091
2	B	0.19	0/4284	0.38	0/5841
2	N	0.20	0/4309	0.37	0/5876
3	C	0.17	0/1660	0.40	0/2250
3	O	0.15	0/1660	0.35	0/2250
4	D	0.15	0/610	0.33	0/830
4	P	0.14	0/610	0.32	0/830
5	E	0.18	0/2332	0.41	0/3173
5	Q	0.16	0/2332	0.39	0/3173
6	F	0.19	0/4524	0.42	0/6180
6	R	0.19	0/4524	0.42	0/6180
7	G	0.18	0/1496	0.37	0/2043
7	S	0.22	0/1496	0.39	0/2043
8	H	0.22	0/1112	0.43	0/1524
8	T	0.16	0/1112	0.35	0/1524
9	I	0.17	0/506	0.41	0/692
9	U	0.17	0/514	0.43	0/702
10	J	0.16	0/1042	0.36	0/1423
10	V	0.14	0/1042	0.33	0/1423
11	L	0.11	0/191	0.31	0/265
11	X	0.12	0/191	0.33	0/265
All	All	0.18	0/41590	0.38	0/56674

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2947	0	2958	32	0
1	M	2942	0	2951	45	0
2	B	4153	0	4176	76	0
2	N	4176	0	4195	75	0
3	C	1623	0	1560	37	0
3	O	1623	0	1560	31	0
4	D	590	0	581	15	0
4	P	590	0	581	15	0
5	E	2271	0	2228	60	0
5	Q	2271	0	2228	44	0
6	F	4364	0	4343	128	0
6	R	4364	0	4343	109	0
7	G	1449	0	1450	40	0
7	S	1449	0	1450	27	0
8	H	1077	0	1058	18	0
8	T	1077	0	1058	16	0
9	I	490	0	498	11	0
9	U	498	0	510	11	0
10	J	1024	0	1035	30	0
10	V	1024	0	1035	21	0
11	L	185	0	170	3	0
11	X	185	0	170	3	0
12	A	4	0	0	1	0
12	M	4	0	0	1	0
13	A	58	0	0	0	0
13	C	58	0	0	1	0
13	M	58	0	0	0	0
13	O	58	0	0	0	0
14	A	17	0	31	0	0
14	G	17	0	31	1	0
14	M	17	0	31	1	0
14	T	17	0	31	4	0
15	B	85	0	57	5	0
15	N	85	0	57	5	0
16	B	230	0	294	13	0
16	C	79	0	105	3	0
16	D	183	0	269	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	F	157	0	205	15	0
16	M	74	0	92	6	0
16	N	309	0	400	12	0
16	P	183	0	269	12	0
16	R	157	0	208	6	0
17	B	36	0	0	0	0
17	N	36	0	0	1	0
18	C	86	0	60	2	0
18	O	86	0	60	2	0
19	C	58	0	80	7	0
19	O	58	0	80	7	0
20	D	41	0	0	0	0
20	G	43	0	0	0	0
20	P	41	0	0	1	0
20	S	43	0	0	0	0
21	E	2	0	0	0	0
21	F	2	0	0	0	0
21	Q	2	0	0	0	0
21	R	2	0	0	0	0
22	F	120	0	108	16	0
22	R	120	0	108	8	0
23	F	1	0	0	0	0
23	R	1	0	0	0	0
24	H	48	0	64	2	0
24	O	48	0	64	3	0
25	A	25	0	0	0	0
25	B	45	0	0	0	0
25	C	10	0	0	0	0
25	D	4	0	0	0	0
25	E	8	0	0	0	0
25	F	25	0	0	2	0
25	G	1	0	0	0	0
25	H	5	0	0	0	0
25	J	1	0	0	0	0
25	L	1	0	0	0	0
25	M	21	0	0	0	0
25	N	43	0	0	1	0
25	O	2	0	0	0	0
25	P	3	0	0	0	0
25	Q	1	0	0	0	0
25	R	11	0	0	0	0
25	S	2	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	T	2	0	0	0	0
25	U	1	0	0	0	0
All	All	43307	0	42842	762	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (762) 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)
6:F:406:ILE:HD11	22:F:602:HEA:HBC2	1.31	1.07
6:F:406:ILE:HD11	22:F:602:HEA:CBC	1.91	0.99
6:F:402:LEU:HD13	22:F:602:HEA:HAC	1.45	0.98
6:F:406:ILE:CD1	22:F:602:HEA:HBC2	2.02	0.89
1:A:133:GLY:HA3	2:B:277:GLY:HA3	1.63	0.80
7:G:25:VAL:HG12	7:G:180:VAL:HG11	1.66	0.76
1:A:358:GLN:NE2	3:C:229:MET:O	2.19	0.75
2:N:184:VAL:HG23	2:N:185:ILE:HG23	1.69	0.74
6:R:211:TRP:HZ3	8:T:7:LEU:HD21	1.53	0.73
6:R:20:ARG:NH2	10:V:53:ASP:OD1	2.22	0.73
6:F:80:ASN:HA	6:F:83:PHE:CE2	2.25	0.72
6:R:267:VAL:HB	22:R:601:HEA:HAC	1.71	0.72
6:F:19:GLU:O	6:F:424:ARG:NH2	2.22	0.72
10:J:132:ALA:HA	10:J:135:LYS:HD2	1.71	0.72
2:N:67:SER:HB3	2:N:87:ARG:HB3	1.72	0.71
16:D:101:CDL:H711	16:F:606:CDL:H721	1.72	0.71
6:R:271:ALA:HA	6:R:405:THR:HG21	1.72	0.71
1:A:271:PRO:O	1:A:316:ARG:NH1	2.23	0.70
6:F:310:VAL:O	6:F:313:HIS:ND1	2.24	0.70
6:R:470:PHE:O	6:R:474:ASN:ND2	2.24	0.69
6:F:203:MET:HE2	8:H:4:GLU:HG3	1.73	0.69
1:M:321:ASP:OD1	1:M:324:ARG:NH1	2.26	0.69
1:M:279:MET:O	3:O:236:GLN:NE2	2.26	0.68
3:O:126:ARG:HH22	6:R:163:SER:HA	1.58	0.68
6:F:509:ASP:HB2	6:F:519:TRP:HB3	1.76	0.67
7:S:167:MET:HG2	14:T:201:PLM:H41	1.76	0.67
10:J:140:ILE:O	10:J:144:ILE:HG12	1.95	0.67
6:F:267:VAL:HB	22:F:601:HEA:HAC	1.74	0.67
6:F:33:THR:HG22	8:H:90:TRP:HB3	1.77	0.66
2:N:438:ARG:HH12	4:P:19:SER:HB3	1.60	0.66
6:F:341:PHE:HZ	6:F:369:PHE:HD1	1.43	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:101:CDL:H182	16:P:101:CDL:H331	1.77	0.66
6:R:546:HIS:HE2	10:V:29:SER:HG	1.43	0.66
1:A:362:ARG:HD3	1:A:381:ILE:HD11	1.76	0.66
6:R:288:LYS:NZ	6:R:349:TRP:O	2.23	0.66
6:F:470:PHE:O	6:F:474:ASN:ND2	2.29	0.66
6:F:544:GLU:HG2	6:F:554:MET:HE1	1.78	0.65
3:C:121:ARG:HH12	3:C:208:PRO:HG3	1.61	0.65
7:G:65:LEU:HB2	7:G:203:ARG:HH11	1.61	0.65
5:Q:220:ARG:NH1	5:Q:259:GLN:OE1	2.29	0.65
6:F:35:THR:HB	6:F:119:PRO:HB2	1.78	0.65
1:M:79:THR:HG22	2:N:510:GLU:HG2	1.78	0.65
6:F:18:PRO:O	6:F:20:ARG:NH1	2.29	0.65
6:R:206:MET:O	6:R:293:TYR:OH	2.09	0.65
7:S:25:VAL:HG12	7:S:180:VAL:HG11	1.77	0.65
6:R:402:LEU:HD13	22:R:602:HEA:HAC	1.78	0.65
6:F:97:PRO:HG3	6:F:129:PHE:CE1	2.33	0.64
5:Q:71:THR:HG21	6:R:348:MET:HB3	1.78	0.64
2:N:500:GLY:HA3	2:N:505:PRO:HA	1.79	0.64
3:O:137:HIS:O	5:Q:193:ARG:NH2	2.30	0.64
4:D:69:ALA:HA	16:D:103:CDL:H582	1.79	0.64
1:M:133:GLY:HA3	2:N:277:GLY:HA3	1.79	0.63
5:Q:32:ALA:HB1	5:Q:35:TRP:HB2	1.80	0.63
5:Q:243:ARG:NH1	5:Q:255:ASP:O	2.31	0.63
1:A:355:LEU:HD22	1:A:364:LEU:HD23	1.80	0.63
2:B:213:LEU:HD21	15:N:602:HEM:HBC1	1.79	0.63
6:R:532:GLU:HB3	10:V:25:SER:HB3	1.80	0.63
2:B:379:MET:HE1	16:D:101:CDL:H392	1.79	0.63
5:Q:272:ARG:NH1	6:R:456:GLY:O	2.31	0.63
9:I:52:GLU:HA	10:J:65:ARG:HH11	1.64	0.62
5:E:252:ASN:HB3	6:F:253:LEU:HD23	1.81	0.62
7:G:24:MET:HA	7:G:27:VAL:HG22	1.82	0.62
24:O:301:MQ7:H142	24:O:301:MQ7:H2M3	1.80	0.62
5:E:106:ILE:HB	6:F:331:PHE:HB3	1.80	0.62
6:R:104:ASN:OD1	6:R:122:ASN:ND2	2.29	0.62
6:R:173:MET:HE2	8:T:106:ALA:HB3	1.82	0.62
10:J:85:LEU:HD12	10:J:109:VAL:HG23	1.82	0.62
2:B:305:MET:O	2:B:308:THR:OG1	2.16	0.61
7:G:34:SER:HB2	8:H:48:LEU:HG	1.81	0.61
6:R:110:GLN:NE2	6:R:280:GLU:OE2	2.32	0.61
7:S:34:SER:HB3	8:T:48:LEU:HG	1.81	0.61
5:E:117:GLN:HB3	6:F:383:PRO:HD3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:221:LEU:HD22	7:G:35:SER:HB3	1.81	0.61
5:Q:252:ASN:HB3	6:R:253:LEU:HD23	1.82	0.61
2:N:87:ARG:NH1	2:N:90:GLU:OE2	2.33	0.61
2:N:486:LYS:NZ	16:N:605:CDL:OB3	2.34	0.61
6:R:264:HIS:CD2	6:R:268:TYR:HE2	2.18	0.61
10:J:74:GLY:O	10:J:103:GLN:NE2	2.33	0.61
7:S:147:HIS:CE1	7:S:192:TRP:HB2	2.36	0.60
3:C:214:ASN:OD1	3:C:217:GLN:NE2	2.32	0.60
2:B:182:MET:HE3	2:B:183:PRO:HD3	1.83	0.60
6:F:398:PHE:HA	6:F:401:VAL:HG22	1.81	0.60
16:C:305:CDL:H522	14:G:302:PLM:H81	1.84	0.60
5:E:123:LYS:NZ	5:E:255:ASP:OD1	2.26	0.60
7:G:27:VAL:HG12	8:H:55:PHE:HE2	1.66	0.60
6:F:153:ALA:O	6:F:255:TRP:NE1	2.34	0.60
7:G:120:GLU:OE2	7:G:200:TYR:OH	2.19	0.60
2:B:384:TYR:HB2	19:C:304:MQ9:H362	1.84	0.60
7:S:24:MET:HA	7:S:27:VAL:HG22	1.83	0.59
9:U:52:GLU:HA	10:V:65:ARG:HE	1.66	0.59
6:F:507:VAL:HG21	10:J:32:THR:HG23	1.84	0.59
15:N:601:HEM:HBB2	15:N:601:HEM:HMB2	1.83	0.59
6:R:303:ILE:HG13	6:R:336:PRO:HB2	1.85	0.59
10:V:130:ALA:HB2	10:V:146:ALA:HB2	1.85	0.59
2:B:212:ILE:HD11	2:N:212:ILE:HD11	1.84	0.59
15:B:601:HEM:HMB2	15:B:601:HEM:HBB2	1.85	0.59
15:B:602:HEM:HBB2	15:B:602:HEM:HMB2	1.83	0.59
10:J:63:LYS:HG3	10:J:156:PRO:HB3	1.85	0.59
1:A:164:ARG:O	2:B:234:LYS:NZ	2.36	0.59
6:R:544:GLU:HB2	6:R:551:VAL:HG22	1.83	0.59
9:U:23:LEU:O	9:U:27:THR:OG1	2.19	0.59
2:B:527:THR:O	2:B:531:GLU:HG2	2.03	0.58
10:J:23:THR:OG1	10:J:27:ARG:O	2.20	0.58
1:M:390:ALA:HB3	1:M:412:VAL:HG12	1.84	0.58
8:H:118:VAL:O	8:H:122:ILE:HG12	2.04	0.58
6:R:33:THR:HG22	8:T:90:TRP:HB3	1.83	0.58
2:B:65:ASP:HB3	2:B:91:THR:HG21	1.83	0.58
5:Q:280:PHE:HB3	5:Q:283:MET:HB2	1.86	0.58
10:J:144:ILE:O	10:J:148:ARG:HG3	2.03	0.58
16:P:103:CDL:H272	6:R:492:VAL:HG21	1.85	0.58
1:A:269:MET:HE2	1:A:274:ILE:HD11	1.85	0.58
2:N:394:ASP:OD1	2:N:395:ILE:N	2.36	0.57
16:P:103:CDL:H761	16:P:103:CDL:H342	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:218:ILE:HG22	3:C:222:MET:HE2	1.86	0.57
9:I:54:PRO:O	10:J:65:ARG:NH2	2.33	0.57
5:Q:138:TRP:CD1	5:Q:280:PHE:HB2	2.40	0.57
7:G:125:VAL:HG13	7:G:130:THR:HG22	1.86	0.57
10:J:55:LEU:HD23	10:J:147:VAL:HG11	1.85	0.57
3:C:88:VAL:HG12	3:C:93:ALA:HA	1.85	0.57
2:N:379:MET:HG2	2:N:419:PRO:HB3	1.86	0.57
3:C:121:ARG:NH2	18:C:302:HEC:O2A	2.35	0.57
2:N:65:ASP:HB3	2:N:91:THR:HG21	1.86	0.57
4:P:17:VAL:HG11	4:P:25:SER:HB2	1.86	0.57
7:S:43:LEU:HD13	7:S:143:ALA:HA	1.86	0.57
2:B:468:VAL:HA	2:B:474:PRO:HA	1.87	0.57
4:P:75:TRP:O	20:P:102:9Y0:N	2.37	0.57
2:B:253:VAL:HA	2:B:257:PHE:HB3	1.87	0.57
6:R:97:PRO:HG3	6:R:129:PHE:CE1	2.40	0.57
24:H:201:MQ7:H242	24:H:201:MQ7:H393	1.87	0.57
2:B:435:ARG:NH1	4:D:16:ASP:O	2.37	0.56
6:F:499:TRP:HE1	16:F:606:CDL:HB4	1.70	0.56
1:M:295:VAL:O	1:M:298:GLU:HG3	2.05	0.56
2:N:42:LEU:HD13	2:N:122:VAL:HG12	1.87	0.56
3:O:95:LEU:HD13	3:O:153:ASN:ND2	2.19	0.56
2:B:224:GLY:HA2	16:B:603:CDL:H791	1.87	0.56
6:R:398:PHE:HA	6:R:401:VAL:HG22	1.88	0.56
10:V:73:LEU:HD13	10:V:77:THR:HB	1.87	0.56
2:B:303:PHE:HB2	19:C:304:MQ9:H3A	1.86	0.56
6:F:349:TRP:CD1	6:F:350:LYS:HG2	2.39	0.56
6:R:341:PHE:HZ	6:R:369:PHE:HD1	1.53	0.56
2:B:494:GLY:O	7:G:169:LYS:HG2	2.05	0.56
10:J:100:SER:O	10:J:104:ARG:N	2.39	0.56
1:M:95:LEU:HD22	16:M:503:CDL:H771	1.88	0.56
6:F:16:PRO:HD3	9:I:49:TRP:HB3	1.88	0.56
9:I:69:VAL:N	10:J:92:GLU:OE2	2.38	0.56
1:M:385:ALA:O	4:P:50:ASN:ND2	2.38	0.56
2:N:234:LYS:NZ	25:N:701:HOH:O	2.36	0.56
7:G:147:HIS:CE1	7:G:192:TRP:HB2	2.40	0.56
6:F:355:PHE:HE1	6:F:363:VAL:HG21	1.72	0.55
2:B:318:TRP:HD1	11:L:20:ALA:HB2	1.71	0.55
6:R:80:ASN:HA	6:R:83:PHE:CE2	2.42	0.55
6:R:276:GLY:O	6:R:280:GLU:HG2	2.06	0.55
7:S:167:MET:HA	14:T:201:PLM:H22	1.87	0.55
1:A:357:GLU:OE1	3:C:205:LYS:NZ	2.34	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:438:ARG:HH12	4:D:19:SER:HB2	1.71	0.55
16:F:605:CDL:H571	8:H:125:VAL:HG11	1.89	0.55
5:E:136:PHE:O	5:E:138:TRP:N	2.40	0.55
6:R:536:ILE:O	6:R:537:ARG:NH1	2.37	0.55
6:R:87:GLY:HA3	22:R:602:HEA:HBD1	1.88	0.55
6:F:420:LYS:NZ	6:F:522:SER:O	2.37	0.55
7:G:23:ASN:HD21	7:G:176:THR:HG23	1.72	0.55
9:I:73:GLY:HA3	10:J:110:TYR:CZ	2.41	0.55
2:N:370:VAL:HG22	4:P:23:GLY:HA3	1.89	0.55
16:P:103:CDL:H331	16:P:103:CDL:H582	1.89	0.55
2:B:372:VAL:O	2:B:376:ILE:HG12	2.06	0.55
6:F:26:ASN:O	6:F:30:LYS:HE3	2.07	0.55
6:F:434:HIS:CD2	6:F:491:PHE:HB2	2.42	0.54
6:R:95:ALA:O	6:R:98:ILE:HG22	2.06	0.54
1:M:76:VAL:HG21	2:N:513:ALA:HB1	1.88	0.54
2:N:78:GLN:HA	2:N:81:ARG:HG3	1.88	0.54
25:F:702:HOH:O	7:G:164:ARG:NH2	2.39	0.54
9:I:52:GLU:HA	10:J:65:ARG:NH1	2.23	0.54
5:Q:235:TRP:CD1	5:Q:242:LYS:HB3	2.42	0.54
2:B:392:MET:HE3	3:C:269:ALA:HB1	1.90	0.54
3:O:115:PHE:O	3:O:119:THR:OG1	2.17	0.54
6:R:118:PHE:HB3	16:R:605:CDL:HA31	1.89	0.54
10:J:110:TYR:OH	10:J:120:GLU:OE1	2.15	0.54
3:C:226:PRO:HD2	3:C:229:MET:SD	2.48	0.54
6:F:532:GLU:HG3	10:J:23:THR:HB	1.90	0.54
6:R:284:VAL:HG22	6:R:514:GLY:HA2	1.88	0.54
5:E:263:ILE:HG21	5:E:290:VAL:HG21	1.90	0.54
6:F:206:MET:O	6:F:293:TYR:OH	2.12	0.54
2:N:236:THR:OG1	15:N:601:HEM:O1D	2.25	0.54
6:F:268:TYR:OH	22:F:601:HEA:O11	2.20	0.53
6:F:59:ALA:HB2	6:F:86:HIS:CE1	2.42	0.53
16:N:604:CDL:H522	16:N:604:CDL:H722	1.90	0.53
9:U:21:LEU:HA	9:U:24:ILE:HG22	1.89	0.53
6:F:200:GLY:HA3	6:F:536:ILE:HB	1.91	0.53
6:R:190:ILE:HG12	6:R:214:LEU:HD12	1.91	0.53
2:N:33:VAL:HG12	2:N:248:VAL:HG12	1.90	0.53
2:N:275:MET:HE1	3:O:275:MET:HE2	1.90	0.53
2:B:42:LEU:HD13	2:B:122:VAL:HG12	1.89	0.53
5:E:272:ARG:NH1	6:F:456:GLY:O	2.41	0.53
2:B:138:GLU:OE2	2:B:352:LYS:NZ	2.38	0.53
2:N:282:ASN:ND2	15:N:602:HEM:O2A	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:80:ARG:NH2	16:P:103:CDL:OB4	2.41	0.53
16:B:603:CDL:HA4	16:N:603:CDL:H521	1.90	0.53
3:C:193:ASN:ND2	3:C:197:LYS:HB2	2.24	0.53
5:E:133:VAL:HB	5:E:225:LEU:HD23	1.90	0.53
2:N:416:VAL:HG13	4:P:39:SER:HB2	1.91	0.53
1:M:355:LEU:HB2	1:M:364:LEU:O	2.09	0.53
6:R:59:ALA:HB2	6:R:86:HIS:CE1	2.44	0.53
6:R:544:GLU:HB3	6:R:554:MET:HE1	1.90	0.53
5:E:42:GLU:HG2	5:E:120:MET:HA	1.91	0.52
2:B:340:VAL:HG13	19:C:304:MQ9:H412	1.91	0.52
4:D:73:ARG:NH1	16:D:103:CDL:OA7	2.42	0.52
3:O:95:LEU:HD13	3:O:153:ASN:HD22	1.74	0.52
5:Q:238:GLU:HG3	5:Q:269:PHE:HD1	1.73	0.52
6:R:153:ALA:HB1	6:R:158:THR:HG21	1.92	0.52
6:F:187:VAL:HG22	7:G:31:VAL:HG23	1.92	0.52
10:J:47:ASP:HB3	10:J:140:ILE:HG21	1.90	0.52
2:B:483:PRO:HG2	3:C:294:ALA:HA	1.91	0.52
6:R:81:GLN:HG3	6:R:148:ASP:HB3	1.91	0.52
6:R:441:GLY:O	6:R:445:THR:HG22	2.10	0.52
1:A:355:LEU:HB2	1:A:364:LEU:HB3	1.91	0.52
4:D:12:VAL:HG13	4:D:26:HIS:HB2	1.90	0.52
1:M:355:LEU:HD13	1:M:366:PRO:HD3	1.91	0.52
5:Q:137:GLN:HB3	5:Q:138:TRP:CE3	2.45	0.52
2:B:27:ARG:HB2	1:M:177:VAL:HG22	1.91	0.52
5:E:114:VAL:HA	5:E:117:GLN:HG2	1.92	0.52
5:E:138:TRP:HA	5:E:284:MET:SD	2.50	0.52
5:E:332:ARG:NH2	6:F:77:GLU:OE1	2.41	0.52
2:N:39:SER:HB2	2:N:126:ARG:HG3	1.92	0.52
6:R:384:LEU:O	6:R:388:VAL:HG22	2.10	0.52
4:D:78:ARG:NH2	16:D:101:CDL:OA4	2.42	0.52
2:B:66:PRO:HG3	2:B:208:TYR:CD2	2.46	0.51
2:B:370:VAL:HG22	4:D:23:GLY:HA3	1.92	0.51
6:F:445:THR:HG23	6:F:446:PHE:CD2	2.45	0.51
8:T:54:THR:HG22	8:T:58:PHE:CE2	2.45	0.51
5:E:137:GLN:HG2	5:E:229:ASP:OD2	2.10	0.51
2:N:309:GLU:HG3	17:N:606:A1IRE:N04	2.25	0.51
6:R:420:LYS:HG3	6:R:421:MET:HE2	1.93	0.51
7:S:147:HIS:NE2	7:S:192:TRP:HB2	2.25	0.51
2:B:318:TRP:CD1	11:L:20:ALA:HB2	2.46	0.51
16:D:103:CDL:HA31	6:F:496:PHE:HE2	1.76	0.51
5:E:264:GLN:HB2	5:E:265:GLN:OE1	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:148:VAL:HG23	2:N:263:ALA:HB1	1.93	0.51
10:V:46:MET:O	10:V:50:VAL:HG23	2.11	0.51
2:B:282:ASN:ND2	15:B:602:HEM:O2A	2.42	0.51
3:C:269:ALA:HB3	3:C:270:PRO:HD3	1.93	0.51
1:M:418:GLU:OE1	1:M:418:GLU:N	2.44	0.51
6:F:405:THR:O	6:F:409:ALA:HB3	2.11	0.51
3:O:269:ALA:HB3	3:O:270:PRO:HD3	1.92	0.51
6:R:48:CYS:SG	6:R:97:PRO:HB2	2.51	0.51
6:R:426:LEU:HD23	6:R:498:SER:HB2	1.93	0.51
6:F:480:GLY:HA2	6:F:483:ILE:HD12	1.92	0.51
16:F:605:CDL:H402	7:G:32:TRP:CZ2	2.46	0.51
2:N:253:VAL:HA	2:N:257:PHE:HB3	1.93	0.51
5:Q:59:ALA:O	5:Q:63:ILE:HG12	2.11	0.51
6:R:537:ARG:CZ	8:T:72:ASP:HA	2.40	0.51
1:A:161:VAL:HG22	2:B:249:VAL:HG22	1.93	0.51
6:F:264:HIS:NE2	6:F:268:TYR:HE2	2.09	0.51
6:R:400:TYR:HA	6:R:442:PHE:HZ	1.76	0.50
2:B:452:ARG:NH2	2:B:458:TYR:OH	2.45	0.50
3:O:222:MET:HE2	3:O:242:LYS:HG2	1.94	0.50
6:R:392:TYR:CE1	6:R:459:ARG:HA	2.46	0.50
9:U:78:LYS:HG3	10:V:104:ARG:O	2.12	0.50
6:R:341:PHE:HZ	6:R:369:PHE:CD1	2.28	0.50
6:F:104:ASN:CG	6:F:122:ASN:HD21	2.20	0.50
6:R:402:LEU:CD1	22:R:602:HEA:HAC	2.42	0.50
6:R:420:LYS:NZ	6:R:521:THR:O	2.45	0.50
3:C:192:HIS:CE1	3:C:207:ALA:HB1	2.46	0.50
1:M:149:LEU:HD21	16:M:503:CDL:HA22	1.94	0.50
16:D:103:CDL:H201	16:F:606:CDL:H772	1.94	0.50
5:E:71:THR:HG21	6:F:348:MET:HB3	1.93	0.50
5:E:84:LEU:HD13	6:F:543:PHE:HZ	1.77	0.50
5:E:215:LEU:HD13	5:E:221:ILE:HD13	1.94	0.50
6:F:172:ILE:HG23	6:F:231:LEU:HD22	1.93	0.50
6:F:531:THR:OG1	6:F:532:GLU:OE1	2.28	0.50
2:N:527:THR:O	2:N:531:GLU:HG2	2.11	0.50
3:O:275:MET:HE2	3:O:275:MET:HA	1.93	0.50
1:M:53:GLU:OE2	1:M:53:GLU:N	2.43	0.49
5:Q:248:GLU:O	5:Q:252:ASN:ND2	2.35	0.49
6:R:445:THR:HG23	6:R:446:PHE:CD2	2.48	0.49
2:B:499:THR:HG23	2:B:506:ASP:HB2	1.94	0.49
3:C:197:LYS:HE3	13:C:303:9YF:O7	2.11	0.49
10:J:51:LEU:HD13	10:J:144:ILE:HD13	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:202:ILE:HG13	2:N:202:ILE:O	2.11	0.49
6:R:264:HIS:O	6:R:267:VAL:HG22	2.12	0.49
6:R:284:VAL:HG21	6:R:416:PHE:HZ	1.77	0.49
7:S:70:ALA:HB1	7:S:196:PHE:HE1	1.77	0.49
3:O:125:MET:HG3	6:R:162:HIS:HA	1.93	0.49
9:U:73:GLY:HA3	10:V:110:TYR:CZ	2.48	0.49
3:C:168:ALA:HB1	3:C:171:SER:HB3	1.95	0.49
5:E:235:TRP:CD1	5:E:242:LYS:HB3	2.47	0.49
6:F:106:VAL:HG11	6:F:417:TRP:CE2	2.47	0.49
7:S:60:PRO:O	7:S:63:THR:HG22	2.12	0.49
10:V:78:ALA:O	10:V:82:ARG:HD3	2.12	0.49
1:A:279:MET:O	3:C:236:GLN:NE2	2.45	0.49
5:E:164:LYS:NZ	5:E:194:THR:O	2.39	0.49
2:N:340:VAL:HA	19:O:305:MQ9:H401	1.94	0.49
6:F:199:PRO:HG3	8:H:78:GLY:HA3	1.95	0.49
2:B:426:ALA:HA	16:B:604:CDL:H332	1.95	0.49
3:C:121:ARG:NH1	3:C:208:PRO:HG3	2.27	0.49
5:E:138:TRP:CD1	5:E:280:PHE:HB2	2.47	0.49
6:F:95:ALA:O	6:F:98:ILE:HG22	2.13	0.49
6:F:310:VAL:HG12	6:F:329:MET:HB3	1.95	0.49
7:G:22:PRO:HD3	8:H:66:ARG:HD3	1.94	0.49
5:Q:235:TRP:CH2	6:R:456:GLY:HA2	2.47	0.49
7:S:117:GLN:NE2	25:S:401:HOH:O	2.35	0.49
2:B:435:ARG:NH1	6:F:23:PRO:HB2	2.27	0.49
6:F:152:THR:HA	6:F:259:PHE:CZ	2.47	0.49
7:S:156:VAL:HG22	14:T:201:PLM:HG1	1.93	0.49
5:E:65:TRP:CD1	6:F:370:LEU:HD23	2.48	0.49
2:N:503:LEU:HD22	7:S:101:ARG:HG2	1.94	0.49
6:R:200:GLY:HA3	6:R:536:ILE:HB	1.93	0.49
10:J:77:THR:OG1	10:J:107:GLU:OE2	2.30	0.48
3:O:185:ARG:HA	3:O:189:ALA:HB3	1.94	0.48
5:Q:218:GLY:HA2	5:Q:262:GLU:HB2	1.95	0.48
6:F:155:SER:HB2	6:F:255:TRP:HB3	1.95	0.48
2:N:150:LEU:HD22	2:N:215:ILE:HG23	1.96	0.48
2:N:489:ASN:OD1	2:N:490:LYS:N	2.46	0.48
6:R:155:SER:HB2	6:R:255:TRP:HB3	1.96	0.48
2:B:154:GLU:HB2	2:B:215:ILE:HG21	1.95	0.48
2:B:400:PHE:HA	8:H:108:LEU:HD13	1.95	0.48
16:D:101:CDL:H152	16:D:101:CDL:H311	1.95	0.48
9:U:79:TRP:CH2	10:V:104:ARG:HA	2.48	0.48
5:E:316:ILE:HG22	5:E:316:ILE:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:182:MET:HE3	2:B:183:PRO:CD	2.43	0.48
6:F:30:LYS:O	6:F:34:THR:HB	2.13	0.48
6:F:330:THR:O	6:F:333:ILE:HG22	2.14	0.48
2:N:532:HIS:O	2:N:536:ILE:HG12	2.13	0.48
2:B:67:SER:HB3	2:B:87:ARG:HB3	1.95	0.48
5:E:98:LEU:HB3	6:F:342:PHE:CD2	2.48	0.48
7:G:83:THR:OG1	7:G:106:THR:OG1	2.27	0.48
24:O:301:MQ7:H241	24:O:301:MQ7:H261	1.72	0.48
2:N:318:TRP:CD1	11:X:20:ALA:HB2	2.49	0.48
3:O:87:CYS:O	3:O:91:HIS:HB2	2.13	0.48
3:O:134:LYS:HD3	6:R:164:PRO:HG3	1.96	0.48
10:V:85:LEU:HD13	10:V:109:VAL:HG12	1.94	0.48
6:F:460:ARG:H	22:F:602:HEA:CGA	2.27	0.48
2:N:210:LEU:HA	2:N:214:LEU:HB2	1.96	0.48
3:C:250:ARG:NH2	3:C:254:GLU:OE2	2.47	0.48
6:F:264:HIS:HE2	6:F:268:TYR:HE2	1.61	0.48
7:G:23:ASN:HD21	7:G:176:THR:CG2	2.26	0.48
2:N:66:PRO:HG3	2:N:208:TYR:CD2	2.49	0.48
5:Q:222:GLU:HG3	5:Q:259:GLN:HG2	1.96	0.48
3:C:81:GLN:HB2	5:E:163:ARG:HH11	1.78	0.47
7:S:91:ALA:HB2	7:S:99:LEU:HD13	1.95	0.47
6:F:459:ARG:HG3	6:F:460:ARG:HG3	1.96	0.47
7:G:69:LEU:HD23	7:G:120:GLU:HB2	1.95	0.47
10:J:53:ASP:O	10:J:57:TYR:HD2	1.97	0.47
1:M:306:MET:SD	2:N:70:HIS:NE2	2.85	0.47
2:N:491:LEU:O	2:N:493:SER:N	2.42	0.47
4:P:74:ASN:O	4:P:78:ARG:HG3	2.14	0.47
6:R:434:HIS:HB2	6:R:490:PRO:HB2	1.95	0.47
3:C:138:PHE:HB3	3:C:142:GLN:HB2	1.96	0.47
10:V:81:ALA:HA	10:V:84:ILE:HG12	1.96	0.47
1:A:265:PRO:HG2	1:A:301:LEU:HD23	1.95	0.47
3:O:277:ILE:HG23	3:O:278:ILE:HG13	1.96	0.47
5:Q:157:ASP:O	5:Q:200:LYS:NZ	2.47	0.47
6:R:371:LEU:HD23	6:R:400:TYR:CE2	2.49	0.47
7:S:161:LEU:O	7:S:165:THR:HG23	2.14	0.47
2:B:495:GLY:HA3	7:G:169:LYS:HE3	1.97	0.47
3:C:72:GLN:HG3	3:C:75:LEU:H	1.79	0.47
5:E:229:ASP:OD1	5:E:230:VAL:N	2.46	0.47
6:F:102:PHE:O	6:F:106:VAL:HG22	2.13	0.47
8:H:47:GLY:O	8:H:51:ILE:HG12	2.14	0.47
3:O:120:GLY:O	3:O:134:LYS:HE3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:264:HIS:O	6:F:267:VAL:HG22	2.15	0.47
2:N:22:PRO:HB2	2:N:26:VAL:HG23	1.96	0.47
1:A:207:PHE:CE1	1:M:140:ILE:HB	2.49	0.47
2:B:56:THR:HG1	2:B:109:HIS:HD1	1.60	0.47
2:B:453:LEU:HB2	2:B:457:ALA:HB3	1.96	0.47
3:C:139:ASP:OD2	3:C:142:GLN:NE2	2.47	0.47
6:F:112:GLY:HA2	6:F:530:PHE:CE2	2.50	0.47
6:F:173:MET:HE2	8:H:106:ALA:HB3	1.96	0.47
6:F:499:TRP:NE1	16:F:606:CDL:HB4	2.30	0.47
16:F:605:CDL:H392	16:F:605:CDL:H151	1.96	0.47
1:M:358:GLN:NE2	3:O:229:MET:O	2.39	0.47
6:F:288:LYS:HB3	6:F:288:LYS:HE2	1.65	0.47
6:F:452:LEU:HD13	6:F:473:LEU:HB2	1.96	0.47
7:G:121:TYR:O	7:G:125:VAL:HG23	2.14	0.47
3:O:237:LEU:O	3:O:242:LYS:NZ	2.44	0.47
5:Q:233:GLY:HA3	5:Q:274:THR:H	1.80	0.47
16:C:305:CDL:HB22	8:H:137:GLU:HG3	1.97	0.47
6:F:37:HIS:ND1	6:F:104:ASN:O	2.37	0.47
7:G:86:MET:HE3	7:G:102:TRP:CZ2	2.49	0.47
16:M:503:CDL:H542	16:M:503:CDL:HA61	1.97	0.47
3:O:229:MET:HE3	18:O:303:HEC:C4B	2.45	0.47
5:Q:231:ILE:HD11	6:R:252:VAL:HG13	1.97	0.47
15:B:602:HEM:HBC1	2:N:213:LEU:HD21	1.96	0.47
4:D:76:TRP:CD1	16:D:103:CDL:H511	2.50	0.47
5:E:113:THR:CG2	6:F:382:PRO:HD2	2.45	0.47
6:F:55:GLY:O	6:F:86:HIS:ND1	2.44	0.47
1:M:370:SER:HA	1:M:383:GLY:HA3	1.96	0.47
2:N:428:ARG:HH22	16:P:101:CDL:H1	1.80	0.47
2:B:441:LEU:HD22	2:B:477:LEU:HB2	1.97	0.46
6:F:227:LEU:HD22	6:F:262:PHE:CZ	2.50	0.46
19:C:304:MQ9:H43	19:C:304:MQ9:H471	1.65	0.46
5:E:240:LEU:HA	6:F:387:HIS:ND1	2.30	0.46
8:H:91:TRP:O	8:H:95:ILE:HG13	2.16	0.46
3:O:88:VAL:HG23	3:O:93:ALA:HB2	1.97	0.46
5:Q:235:TRP:CE3	5:Q:274:THR:HG21	2.50	0.46
6:R:30:LYS:O	6:R:34:THR:HB	2.16	0.46
4:D:78:ARG:NH1	4:D:84:ARG:O	2.46	0.46
6:F:105:LEU:HB3	6:F:421:MET:HE3	1.97	0.46
22:F:602:HEA:H261	22:F:602:HEA:H172	1.57	0.46
16:M:503:CDL:HA62	16:N:607:CDL:H571	1.97	0.46
16:B:605:CDL:HA61	8:H:90:TRP:HZ2	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:81:GLN:HG3	6:F:148:ASP:HB3	1.97	0.46
6:F:371:LEU:HD23	6:F:400:TYR:CE1	2.50	0.46
6:F:379:LEU:HD21	6:F:394:VAL:HG22	1.97	0.46
7:G:79:ALA:O	7:G:83:THR:HG23	2.16	0.46
2:N:231:TRP:CG	16:N:603:CDL:H731	2.51	0.46
16:D:101:CDL:H341	16:D:101:CDL:H312	1.43	0.46
19:O:305:MQ9:H253	19:O:305:MQ9:H271	1.65	0.46
6:R:211:TRP:CZ3	8:T:7:LEU:HD21	2.43	0.46
6:R:226:ILE:HG13	7:S:38:MET:HG3	1.97	0.46
1:M:106:VAL:HG11	1:M:131:LEU:HB3	1.98	0.46
9:U:79:TRP:HH2	10:V:101:PRO:HA	1.81	0.46
7:G:129:THR:O	7:G:141:TYR:OH	2.30	0.46
1:M:69:PHE:CE1	1:M:71:GLU:HG2	2.51	0.46
2:N:384:TYR:HB2	19:O:305:MQ9:H362	1.97	0.46
19:O:305:MQ9:H353	19:O:305:MQ9:H412	1.97	0.46
16:R:606:CDL:H612	16:R:606:CDL:H581	1.55	0.46
19:C:304:MQ9:H253	19:C:304:MQ9:H271	1.65	0.46
6:F:479:VAL:O	6:F:483:ILE:HG13	2.16	0.46
15:N:602:HEM:HMB1	15:N:602:HEM:HBB2	1.97	0.46
5:Q:263:ILE:HG21	5:Q:290:VAL:HG21	1.98	0.46
1:A:304:ILE:O	1:A:310:ASN:ND2	2.44	0.46
1:A:369:GLN:HG3	2:B:404:LEU:HD11	1.98	0.46
19:C:304:MQ9:H372	19:C:304:MQ9:H411	1.71	0.46
16:C:305:CDL:H542	16:C:305:CDL:H572	1.62	0.46
5:E:195:TYR:CD2	5:E:248:GLU:HG2	2.50	0.46
5:Q:144:TYR:OH	5:Q:214:VAL:O	2.32	0.46
1:A:344:LYS:HE2	1:A:354:SER:HB3	1.99	0.45
4:D:42:PHE:HA	4:D:45:VAL:HG12	1.98	0.45
1:M:349:LEU:HD12	1:M:368:HIS:CE1	2.50	0.45
3:O:115:PHE:CE1	3:O:221:ALA:HB2	2.51	0.45
16:B:605:CDL:HA61	16:B:605:CDL:H312	1.82	0.45
6:F:420:LYS:O	6:F:525:PRO:HD3	2.16	0.45
2:N:420:ALA:HB2	16:P:101:CDL:H191	1.97	0.45
16:N:607:CDL:H592	14:T:201:PLM:H71	1.98	0.45
1:M:371:GLN:HB2	1:M:382:PHE:HB3	1.99	0.45
2:N:309:GLU:CD	2:N:313:ARG:HH22	2.23	0.45
5:E:231:ILE:HG22	5:E:275:GLU:HG2	1.99	0.45
2:N:505:PRO:HB3	7:S:97:PHE:CE2	2.51	0.45
3:O:192:HIS:CE1	3:O:210:LEU:HD21	2.52	0.45
5:Q:86:ARG:HH21	6:R:560:VAL:HA	1.81	0.45
2:B:39:SER:HB2	2:B:126:ARG:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:503:LEU:HD22	7:G:101:ARG:HG2	1.97	0.45
6:R:156:PRO:O	6:R:162:HIS:ND1	2.48	0.45
2:B:117:ALA:O	2:B:121:MET:HG3	2.17	0.45
2:B:160:SER:HA	2:B:167:SER:HB2	1.98	0.45
16:D:101:CDL:H732	16:F:606:CDL:H721	1.98	0.45
5:E:35:TRP:HD1	6:F:454:ASP:HB3	1.81	0.45
6:F:403:PHE:HZ	22:F:602:HEA:O11	1.99	0.45
6:R:310:VAL:O	6:R:313:HIS:ND1	2.50	0.45
3:C:134:LYS:HD2	6:F:161:ILE:HA	1.98	0.45
5:E:227:SER:HB2	5:E:245:VAL:HG12	1.97	0.45
16:N:607:CDL:H831	16:N:607:CDL:H801	1.61	0.45
6:R:172:ILE:HG23	6:R:231:LEU:HD22	1.98	0.45
16:R:605:CDL:H761	7:S:153:GLY:HA3	1.98	0.45
16:D:101:CDL:H151	16:D:101:CDL:H181	1.67	0.45
5:E:119:ARG:HE	5:E:119:ARG:HA	1.81	0.45
5:E:235:TRP:CE3	5:E:274:THR:HG21	2.51	0.45
3:O:229:MET:HG3	18:O:303:HEC:NC	2.32	0.45
6:R:59:ALA:HA	6:R:62:MET:HE2	1.98	0.45
6:R:152:THR:HA	6:R:259:PHE:CZ	2.51	0.45
16:D:103:CDL:OA3	6:F:500:ARG:NH1	2.45	0.45
5:E:299:TYR:OH	5:E:309:ASN:OD1	2.17	0.45
5:Q:154:PHE:HZ	5:Q:300:ILE:HG21	1.80	0.45
7:S:72:PRO:O	7:S:76:VAL:HG23	2.16	0.45
7:S:79:ALA:O	7:S:83:THR:HG23	2.15	0.45
5:E:59:ALA:O	5:E:63:ILE:HG12	2.17	0.45
7:G:147:HIS:NE2	7:G:192:TRP:HB2	2.32	0.45
8:H:71:GLU:O	8:H:72:ASP:C	2.59	0.45
5:Q:238:GLU:HG3	5:Q:269:PHE:CD1	2.51	0.45
6:R:449:GLN:HA	6:R:452:LEU:HB2	1.97	0.45
4:D:17:VAL:HG11	4:D:25:SER:HB2	1.99	0.44
16:D:103:CDL:H151	16:D:103:CDL:H182	1.81	0.44
6:F:285:PHE:CZ	6:F:358:PRO:HG2	2.52	0.44
6:F:445:THR:HA	6:F:477:SER:HA	1.98	0.44
3:O:115:PHE:CE2	3:O:226:PRO:HB3	2.52	0.44
2:B:254:MET:HA	2:B:255:PRO:HA	1.65	0.44
2:N:121:MET:HB3	19:O:305:MQ9:H262	1.98	0.44
2:N:379:MET:HE2	2:N:423:TYR:CD2	2.52	0.44
1:A:368:HIS:HB2	12:A:501:FES:S2	2.57	0.44
1:A:385:ALA:O	4:D:50:ASN:ND2	2.49	0.44
6:F:90:MET:HE3	22:F:602:HEA:HHC	1.98	0.44
10:J:73:LEU:HG	10:J:100:SER:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:380:PRO:HD3	1:M:388:ALA:HA	1.99	0.44
2:B:58:VAL:O	2:B:61:THR:OG1	2.33	0.44
2:B:124:LEU:HD11	2:B:344:LEU:HD11	1.99	0.44
6:F:148:ASP:OD2	25:F:701:HOH:O	2.20	0.44
6:F:306:LEU:HD21	6:F:332:LEU:HG	1.99	0.44
5:Q:106:ILE:HB	6:R:331:PHE:HB3	1.99	0.44
2:B:488:MET:HE2	2:B:491:LEU:HD12	1.99	0.44
5:E:113:THR:HG23	6:F:383:PRO:HD2	2.00	0.44
5:E:137:GLN:HB3	5:E:138:TRP:CE3	2.52	0.44
6:F:57:LEU:HD13	22:F:602:HEA:H202	1.99	0.44
5:Q:101:ILE:O	5:Q:104:LEU:HG	2.18	0.44
5:Q:299:TYR:OH	5:Q:303:ARG:NH2	2.48	0.44
3:C:193:ASN:OD1	3:C:196:GLY:N	2.51	0.44
5:E:132:ASP:OD2	5:E:145:GLN:HB2	2.17	0.44
6:F:253:LEU:HD11	6:F:318:THR:HG21	1.98	0.44
24:H:201:MQ7:H212	24:H:201:MQ7:H191	1.83	0.44
1:M:317:ILE:HB	1:M:322:MET:HE2	2.00	0.44
5:Q:43:ALA:HB1	5:Q:240:LEU:HD12	1.99	0.44
5:Q:113:THR:HG23	6:R:383:PRO:HD2	2.00	0.44
1:A:236:ALA:HB3	1:A:239:TRP:CD1	2.51	0.44
1:A:380:PRO:HD3	1:A:388:ALA:HA	2.00	0.44
16:F:605:CDL:H112	16:F:605:CDL:H372	1.99	0.44
7:G:69:LEU:C	7:G:72:PRO:HD2	2.42	0.44
2:N:470:GLU:HG2	2:N:471:HIS:H	1.83	0.44
16:P:101:CDL:H831	16:P:101:CDL:H862	1.51	0.44
16:B:604:CDL:H381	16:B:605:CDL:H591	2.00	0.44
6:F:18:PRO:HG2	6:F:504:PRO:HB3	2.00	0.44
2:N:368:ARG:O	2:N:434:GLN:NE2	2.33	0.44
16:N:605:CDL:H791	16:R:606:CDL:H661	2.00	0.44
8:T:54:THR:HG22	8:T:58:PHE:HE2	1.82	0.44
3:C:267:GLY:O	3:C:270:PRO:HD2	2.18	0.44
16:D:103:CDL:H841	16:D:103:CDL:H872	1.82	0.44
8:H:3:ILE:O	8:H:7:LEU:HD23	2.18	0.44
1:M:289:ASP:HA	1:M:300:LYS:HE3	2.00	0.44
16:M:503:CDL:HB4	16:M:503:CDL:H512	1.77	0.44
2:N:316:PRO:HG2	2:N:318:TRP:CZ2	2.53	0.44
3:O:91:HIS:CE1	3:O:105:LEU:HG	2.52	0.44
5:Q:233:GLY:O	5:Q:273:CYS:HA	2.18	0.44
6:R:121:LEU:HB2	16:R:605:CDL:HA32	1.99	0.44
2:B:232:PHE:HZ	16:B:603:CDL:HB61	1.83	0.43
7:G:67:LEU:HD13	7:G:200:TYR:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:25:PHE:HA	9:I:28:ARG:HD2	2.00	0.43
9:I:77:GLY:HA3	10:J:127:VAL:HG11	2.00	0.43
6:R:211:TRP:O	6:R:215:VAL:HG23	2.18	0.43
3:C:238:THR:OG1	3:C:240:ASP:OD1	2.34	0.43
2:N:483:PRO:HG2	3:O:294:ALA:HA	2.01	0.43
2:B:38:TRP:CH2	16:B:604:CDL:H711	2.54	0.43
5:E:121:MET:HE2	5:E:121:MET:HB3	1.93	0.43
6:F:552:GLU:HB2	6:F:553:ARG:NH2	2.33	0.43
7:G:76:VAL:HG21	7:G:112:PHE:CE2	2.53	0.43
5:Q:65:TRP:HH2	6:R:371:LEU:HD13	1.84	0.43
2:N:26:VAL:O	2:N:30:LEU:HG	2.17	0.43
16:N:605:CDL:H132	16:N:607:CDL:HA4	2.00	0.43
6:R:58:MET:HG2	6:R:82:LEU:HD22	2.00	0.43
6:R:395:ILE:HA	6:R:398:PHE:CE2	2.54	0.43
2:B:415:MET:HE3	4:D:42:PHE:HE2	1.83	0.43
5:E:227:SER:OG	5:E:230:VAL:O	2.21	0.43
7:G:71:VAL:HB	7:G:72:PRO:HD3	2.00	0.43
7:G:147:HIS:O	7:G:151:VAL:HG23	2.19	0.43
1:M:88:LEU:HD13	16:M:503:CDL:H712	2.01	0.43
1:M:384:PRO:HA	2:N:317:ALA:HB2	1.99	0.43
6:R:365:PHE:HD1	6:R:404:GLY:O	2.01	0.43
6:R:405:THR:O	6:R:409:ALA:HB3	2.18	0.43
6:R:420:LYS:O	6:R:525:PRO:HD3	2.19	0.43
16:D:103:CDL:H221	16:D:103:CDL:H192	1.51	0.43
1:M:190:LEU:HD22	14:M:504:PLM:HC1	2.00	0.43
2:N:58:VAL:O	2:N:61:THR:OG1	2.31	0.43
6:R:257:HIS:NE2	8:T:35:GLU:OE2	2.51	0.43
2:B:73:TYR:HB2	2:B:85:MET:HE3	2.00	0.43
5:E:119:ARG:HA	5:E:119:ARG:NE	2.34	0.43
6:F:400:TYR:HA	6:F:442:PHE:HZ	1.82	0.43
7:G:63:THR:HG21	7:G:136:TYR:CE1	2.54	0.43
7:G:137:GLY:O	7:G:141:TYR:HD2	2.01	0.43
10:J:143:LEU:O	10:J:147:VAL:HG23	2.19	0.43
2:N:303:PHE:HA	2:N:306:MET:HG3	2.00	0.43
2:N:432:SER:OG	6:R:29:TYR:HB2	2.18	0.43
6:R:203:MET:HE2	8:T:4:GLU:HG3	2.01	0.43
6:R:267:VAL:HB	22:R:601:HEA:CAC	2.45	0.43
6:R:390:ASP:HA	6:R:459:ARG:HD3	1.99	0.43
6:R:402:LEU:HB3	22:R:602:HEA:HAC	1.99	0.43
9:U:77:GLY:HA3	10:V:127:VAL:HG11	2.01	0.43
1:A:144:GLY:O	1:A:148:VAL:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:D:103:CDL:H412	16:D:103:CDL:H821	2.01	0.43
6:F:418:PHE:CD2	6:F:426:LEU:HG	2.54	0.43
1:M:131:LEU:HD23	1:M:131:LEU:HA	1.87	0.43
2:N:184:VAL:HG23	2:N:185:ILE:N	2.34	0.43
2:N:425:VAL:HG13	6:R:28:ILE:HD11	1.99	0.43
6:R:226:ILE:HD11	7:S:38:MET:SD	2.59	0.43
5:E:235:TRP:HZ2	6:F:387:HIS:CE1	2.37	0.43
16:N:605:CDL:H571	16:N:605:CDL:H601	1.69	0.43
5:Q:29:ASP:OD1	5:Q:29:ASP:N	2.49	0.43
6:R:355:PHE:HE1	6:R:363:VAL:HG21	1.83	0.43
10:V:123:ALA:HB3	10:V:124:PRO:HD3	2.01	0.43
2:B:4:ASP:O	2:B:8:LEU:HG	2.19	0.43
5:E:279:THR:O	6:F:76:ASN:HB3	2.19	0.43
1:M:334:PHE:CE2	1:M:393:PRO:HG3	2.54	0.43
5:Q:241:PHE:HZ	5:Q:243:ARG:HH21	1.64	0.43
5:Q:272:ARG:HB3	6:R:461:TYR:OH	2.19	0.43
22:R:602:HEA:H261	22:R:602:HEA:H172	1.75	0.43
2:B:156:TYR:HA	2:B:159:TYR:CE2	2.54	0.42
1:A:230:THR:HG22	1:A:232:GLU:H	1.84	0.42
16:D:103:CDL:H181	16:F:606:CDL:H752	2.01	0.42
11:L:31:GLU:OE2	11:L:32:PRO:HD2	2.19	0.42
1:M:164:ARG:NH1	2:N:235:HIS:O	2.49	0.42
6:R:155:SER:OG	6:R:245:TYR:HB3	2.19	0.42
3:C:120:GLY:HA3	3:C:134:LYS:O	2.19	0.42
3:C:208:PRO:HG2	18:C:302:HEC:HBA1	2.01	0.42
6:F:15:ARG:HD2	9:I:52:GLU:OE2	2.20	0.42
16:F:605:CDL:H771	7:G:153:GLY:HA3	2.01	0.42
9:I:53:GLU:HG2	10:J:60:ARG:HB2	2.00	0.42
3:O:126:ARG:NH2	6:R:163:SER:HA	2.31	0.42
5:Q:331:ARG:NE	5:Q:333:GLY:O	2.52	0.42
6:R:375:SER:OG	6:R:397:HIS:ND1	2.50	0.42
3:C:159:VAL:HG12	3:C:220:THR:HG21	2.02	0.42
5:E:167:MET:SD	5:E:193:ARG:HB2	2.60	0.42
2:N:172:ARG:HB2	2:N:198:PHE:CZ	2.54	0.42
6:R:227:LEU:HD22	6:R:262:PHE:CZ	2.54	0.42
6:R:345:ILE:HD13	6:R:345:ILE:HA	1.88	0.42
16:D:101:CDL:H782	16:D:103:CDL:H222	2.01	0.42
5:E:138:TRP:HZ2	5:E:278:GLY:HA3	1.85	0.42
2:N:114:LEU:HB3	3:O:275:MET:HG2	2.00	0.42
2:N:171:ILE:HG22	2:N:198:PHE:HE1	1.84	0.42
6:R:222:ILE:O	7:S:38:MET:HG2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:T:13:ALA:O	8:T:17:LEU:HD23	2.20	0.42
2:B:111:TRP:HD1	2:B:276:GLY:HA2	1.84	0.42
3:C:119:THR:HG21	3:C:121:ARG:NH2	2.35	0.42
3:C:134:LYS:HD3	6:F:164:PRO:HG3	2.01	0.42
6:F:121:LEU:HD11	6:F:184:LEU:HD13	2.01	0.42
16:F:606:CDL:H871	16:F:606:CDL:H841	1.82	0.42
2:N:319:GLU:OE1	2:N:328:PRO:HA	2.20	0.42
5:Q:205:GLY:HA3	5:Q:211:PRO:HD3	2.01	0.42
6:R:392:TYR:CD1	6:R:395:ILE:HG13	2.55	0.42
10:V:85:LEU:HD12	10:V:96:LEU:HB3	2.00	0.42
5:Q:92:MET:HB2	5:Q:93:PRO:HD3	2.01	0.42
7:S:38:MET:O	7:S:41:ALA:HB3	2.20	0.42
3:C:205:LYS:HD2	3:C:228:ASN:ND2	2.34	0.42
5:E:65:TRP:HD1	5:E:68:ILE:HD12	1.85	0.42
1:M:69:PHE:O	1:M:158:GLU:HA	2.20	0.42
1:M:366:PRO:O	1:M:369:GLN:NE2	2.52	0.42
2:N:416:VAL:CG1	4:P:39:SER:HB2	2.49	0.42
2:B:429:TRP:HH2	16:B:605:CDL:H742	1.85	0.42
5:E:86:ARG:HG3	6:F:557:GLU:OE1	2.19	0.42
16:N:603:CDL:H771	16:N:603:CDL:H741	1.70	0.42
4:P:80:ARG:HB2	4:P:82:TRP:CD1	2.55	0.42
6:R:55:GLY:O	6:R:86:HIS:ND1	2.49	0.42
6:R:285:PHE:CZ	6:R:358:PRO:HG2	2.55	0.42
6:R:341:PHE:CZ	6:R:369:PHE:HD1	2.35	0.42
1:A:204:LEU:HD23	1:A:204:LEU:HA	1.87	0.42
1:A:250:GLU:CD	1:A:286:ARG:HE	2.28	0.42
2:B:505:PRO:HB3	7:G:97:PHE:CE2	2.54	0.42
3:C:192:HIS:CE1	3:C:210:LEU:HD21	2.55	0.42
3:O:261:TYR:CE2	3:O:263:LEU:HD23	2.54	0.42
7:S:167:MET:HE1	8:T:130:PHE:HB3	2.01	0.42
3:C:84:GLU:HA	3:C:88:VAL:HG13	2.02	0.41
5:E:265:GLN:OE1	5:E:265:GLN:N	2.53	0.41
6:F:149:PHE:HE1	6:F:153:ALA:HB2	1.84	0.41
2:N:470:GLU:HG2	2:N:471:HIS:N	2.35	0.41
5:Q:299:TYR:O	5:Q:303:ARG:HG2	2.20	0.41
8:T:112:TRP:CD1	8:T:112:TRP:H	2.37	0.41
1:A:353:SER:HA	1:A:365:CYS:HA	2.01	0.41
5:E:39:ILE:HD11	5:E:239:PHE:CE1	2.55	0.41
5:E:289:ARG:HH12	5:E:322:ALA:HA	1.83	0.41
6:F:419:PRO:HG3	6:F:425:LEU:HD23	2.02	0.41
6:F:445:THR:HB	6:F:480:GLY:C	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:171:GLU:O	1:M:175:LYS:HG2	2.20	0.41
3:O:224:THR:O	3:O:224:THR:OG1	2.35	0.41
1:A:371:GLN:HB2	1:A:382:PHE:HB3	2.03	0.41
4:D:28:PRO:HG2	4:D:31:VAL:HG23	2.02	0.41
6:F:495:VAL:HG11	16:F:606:CDL:H812	2.02	0.41
10:J:45:THR:O	10:J:49:VAL:HG23	2.20	0.41
10:J:73:LEU:HD13	10:J:77:THR:HB	2.01	0.41
19:O:305:MQ9:H153	19:O:305:MQ9:H172	1.65	0.41
4:P:27:MET:HE3	16:P:101:CDL:H371	2.02	0.41
6:R:537:ARG:HA	6:R:537:ARG:HD3	1.86	0.41
7:S:65:LEU:HD23	7:S:65:LEU:HA	1.89	0.41
1:A:46:GLU:HA	1:A:49:GLU:HG2	2.01	0.41
1:A:254:LEU:HD23	1:A:282:VAL:HG21	2.02	0.41
5:E:284:MET:O	5:E:284:MET:HG2	2.21	0.41
6:F:195:CYS:SG	7:G:24:MET:HB3	2.60	0.41
1:M:329:LYS:HA	11:X:29:SER:HB3	2.03	0.41
2:N:165:LEU:HD11	2:N:294:GLN:O	2.21	0.41
2:N:318:TRP:O	2:N:332:TRP:NE1	2.47	0.41
4:P:19:SER:HB2	4:P:22:TRP:CD1	2.56	0.41
2:B:306:MET:HG2	2:B:391:CYS:SG	2.60	0.41
5:E:113:THR:HG21	6:F:382:PRO:HD2	2.03	0.41
6:F:89:VAL:HG22	6:F:93:PHE:HD2	1.85	0.41
6:F:267:VAL:HB	22:F:601:HEA:CAC	2.46	0.41
9:I:79:TRP:CD2	10:J:104:ARG:HG3	2.55	0.41
1:M:289:ASP:OD2	1:M:304:ILE:HD11	2.20	0.41
1:M:312:VAL:HG13	1:M:342:TYR:O	2.21	0.41
4:P:43:LEU:O	4:P:60:LEU:HD22	2.21	0.41
1:A:63:ASP:OD2	2:B:31:ASN:ND2	2.44	0.41
1:A:302:THR:HG21	2:B:70:HIS:CD2	2.56	0.41
3:C:115:PHE:CE2	3:C:226:PRO:HG3	2.55	0.41
6:F:43:MET:HB3	6:F:126:PHE:CZ	2.56	0.41
16:F:606:CDL:H591	16:F:606:CDL:H562	1.79	0.41
6:R:330:THR:O	6:R:333:ILE:HG22	2.20	0.41
9:U:79:TRP:CH2	10:V:101:PRO:HA	2.56	0.41
1:A:395:THR:OG1	1:A:396:ILE:N	2.53	0.41
2:B:256:VAL:HG12	2:B:260:LYS:HE2	2.03	0.41
3:C:115:PHE:HE2	3:C:226:PRO:HG3	1.85	0.41
5:E:248:GLU:OE1	6:F:248:ALA:HA	2.20	0.41
6:F:403:PHE:HZ	22:F:602:HEA:HO1	1.68	0.41
6:F:532:GLU:OE1	6:F:532:GLU:N	2.54	0.41
6:R:263:GLY:O	6:R:267:VAL:HG13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:V:97:LEU:HB2	10:V:150:MET:HE1	2.02	0.41
2:B:416:VAL:HG13	4:D:39:SER:HB2	2.02	0.41
6:F:287:ARG:HD3	6:F:352:GLN:O	2.20	0.41
6:F:290:ILE:HD12	6:F:347:THR:OG1	2.20	0.41
6:F:365:PHE:HD1	6:F:404:GLY:O	2.03	0.41
6:F:398:PHE:CD2	22:F:601:HEA:HAD1	2.55	0.41
2:N:489:ASN:HD22	8:T:132:TYR:C	2.29	0.41
6:R:229:ALA:O	7:S:46:MET:HE1	2.19	0.41
8:T:9:GLU:OE2	8:T:57:ARG:NH1	2.43	0.41
2:B:231:TRP:CE2	16:B:603:CDL:H712	2.56	0.41
2:B:394:ASP:OD1	2:B:395:ILE:N	2.53	0.41
2:B:433:LEU:HD11	16:B:605:CDL:OB7	2.20	0.41
2:B:464:PRO:HB3	2:B:474:PRO:HB3	2.02	0.41
5:E:65:TRP:HE1	6:F:367:ILE:HA	1.86	0.41
6:F:245:TYR:CZ	6:F:255:TRP:HE3	2.39	0.41
6:F:406:ILE:CD1	22:F:602:HEA:CBC	2.74	0.41
16:F:605:CDL:H402	7:G:32:TRP:HZ2	1.85	0.41
10:J:68:VAL:HG11	10:J:143:LEU:HD13	2.02	0.41
1:M:204:LEU:HD23	1:M:204:LEU:HA	1.92	0.41
1:M:238:LEU:HD23	1:M:238:LEU:HA	1.89	0.41
16:N:604:CDL:H341	16:N:605:CDL:H552	2.03	0.41
16:P:101:CDL:H811	16:P:101:CDL:H842	1.74	0.41
7:S:101:ARG:O	7:S:105:ILE:HG12	2.20	0.41
9:U:31:PRO:HB2	10:V:37:LEU:CD2	2.51	0.41
10:V:123:ALA:O	10:V:127:VAL:HG23	2.21	0.41
1:A:42:PRO:HA	1:A:46:GLU:OE2	2.21	0.41
2:B:38:TRP:HZ2	16:B:604:CDL:HB4	1.86	0.41
3:C:105:LEU:HD23	3:C:105:LEU:HA	1.94	0.41
8:H:5:ALA:O	8:H:9:GLU:OE1	2.38	0.41
10:J:66:PHE:HE2	10:J:150:MET:HB3	1.86	0.41
2:N:127:ILE:HG23	2:N:132:ALA:HB3	2.03	0.41
16:P:101:CDL:H152	16:P:101:CDL:H311	2.03	0.41
2:B:124:LEU:HD12	15:B:601:HEM:HMC2	2.02	0.40
5:E:65:TRP:CE2	6:F:367:ILE:HG23	2.57	0.40
5:E:127:PRO:HG3	5:E:222:GLU:OE1	2.20	0.40
6:F:278:VAL:HG21	6:F:365:PHE:CE2	2.55	0.40
7:G:73:VAL:HB	7:G:113:PHE:CD1	2.56	0.40
8:H:6:ARG:HA	8:H:9:GLU:CD	2.47	0.40
2:N:316:PRO:HG3	4:P:46:MET:HG2	2.03	0.40
6:R:445:THR:HA	6:R:477:SER:HA	2.03	0.40
2:B:503:LEU:O	7:G:101:ARG:NH1	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:105:ILE:O	5:E:108:VAL:HG12	2.20	0.40
5:E:142:PHE:CE2	5:E:213:LEU:HB2	2.56	0.40
5:E:283:MET:HG2	5:E:328:PHE:CG	2.57	0.40
6:F:384:LEU:O	6:F:388:VAL:HG22	2.21	0.40
6:F:403:PHE:HA	6:F:407:VAL:HB	2.03	0.40
3:O:126:ARG:HH12	6:R:163:SER:HA	1.86	0.40
19:O:305:MQ9:H412	19:O:305:MQ9:H372	1.84	0.40
5:Q:253:ASN:HB3	8:T:31:THR:HB	2.03	0.40
11:X:31:GLU:N	11:X:31:GLU:OE1	2.53	0.40
2:B:25:ALA:O	2:B:29:GLN:HG2	2.21	0.40
5:E:71:THR:HG22	6:F:353:LEU:HD11	2.04	0.40
6:F:314:HIS:ND1	22:F:601:HEA:HAA2	2.36	0.40
7:G:124:LEU:HD23	7:G:124:LEU:HA	1.92	0.40
1:M:41:GLN:HA	1:M:42:PRO:HD3	1.90	0.40
2:N:305:MET:O	2:N:308:THR:OG1	2.18	0.40
6:R:56:GLY:HA3	22:R:602:HEA:H161	2.03	0.40
6:R:91:LEU:HA	6:R:91:LEU:HD23	1.81	0.40
6:R:392:TYR:HB3	6:R:449:GLN:HB3	2.03	0.40
2:B:229:LEU:HD23	16:B:603:CDL:H121	2.03	0.40
7:G:38:MET:O	7:G:41:ALA:HB3	2.20	0.40
1:M:198:LEU:O	1:M:202:ILE:HG12	2.21	0.40
1:M:351:CYS:HB2	12:M:501:FES:S1	2.62	0.40
2:N:414:GLY:C	2:N:416:VAL:H	2.29	0.40
5:Q:31:LEU:HD13	5:Q:55:ILE:HD11	2.04	0.40
5:Q:331:ARG:NH2	5:Q:334:GLU:HA	2.36	0.40
9:U:71:ILE:HD11	9:U:73:GLY:O	2.20	0.40
2:B:121:MET:HB3	19:C:304:MQ9:H262	2.03	0.40
2:B:172:ARG:HB2	2:B:198:PHE:CZ	2.57	0.40
1:M:322:MET:CE	1:M:338:GLU:HA	2.51	0.40
2:N:392:MET:HE3	24:O:301:MQ7:H143	2.03	0.40
2:N:425:VAL:HG22	16:R:606:CDL:H122	2.03	0.40
4:P:73:ARG:HH12	16:P:103:CDL:HA32	1.87	0.40
5:Q:210:ILE:HG23	5:Q:286:PHE:HA	2.03	0.40
6:R:266:GLU:HA	6:R:269:ILE:HD12	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	373/421 (89%)	362 (97%)	11 (3%)	0	100	100
1	M	373/421 (89%)	362 (97%)	11 (3%)	0	100	100
2	B	527/546 (96%)	508 (96%)	19 (4%)	0	100	100
2	N	532/546 (97%)	513 (96%)	18 (3%)	1 (0%)	43	73
3	C	221/268 (82%)	210 (95%)	11 (5%)	0	100	100
3	O	221/268 (82%)	210 (95%)	11 (5%)	0	100	100
4	D	72/84 (86%)	71 (99%)	1 (1%)	0	100	100
4	P	72/84 (86%)	70 (97%)	2 (3%)	0	100	100
5	E	281/341 (82%)	267 (95%)	14 (5%)	0	100	100
5	Q	281/341 (82%)	269 (96%)	12 (4%)	0	100	100
6	F	549/575 (96%)	536 (98%)	13 (2%)	0	100	100
6	R	549/575 (96%)	528 (96%)	21 (4%)	0	100	100
7	G	183/203 (90%)	182 (100%)	1 (0%)	0	100	100
7	S	183/203 (90%)	180 (98%)	3 (2%)	0	100	100
8	H	137/139 (99%)	133 (97%)	4 (3%)	0	100	100
8	T	137/139 (99%)	133 (97%)	4 (3%)	0	100	100
9	I	61/79 (77%)	58 (95%)	3 (5%)	0	100	100
9	U	62/79 (78%)	57 (92%)	5 (8%)	0	100	100
10	J	141/157 (90%)	138 (98%)	3 (2%)	0	100	100
10	V	141/157 (90%)	138 (98%)	3 (2%)	0	100	100
11	L	26/236 (11%)	25 (96%)	1 (4%)	0	100	100
11	X	26/236 (11%)	24 (92%)	2 (8%)	0	100	100
All	All	5148/6098 (84%)	4974 (97%)	173 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	N	184	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	309/343 (90%)	309 (100%)	0	100	100
1	M	309/343 (90%)	309 (100%)	0	100	100
2	B	426/437 (98%)	426 (100%)	0	100	100
2	N	428/437 (98%)	428 (100%)	0	100	100
3	C	163/197 (83%)	163 (100%)	0	100	100
3	O	163/197 (83%)	163 (100%)	0	100	100
4	D	58/67 (87%)	58 (100%)	0	100	100
4	P	58/67 (87%)	58 (100%)	0	100	100
5	E	243/288 (84%)	243 (100%)	0	100	100
5	Q	243/288 (84%)	243 (100%)	0	100	100
6	F	452/471 (96%)	452 (100%)	0	100	100
6	R	452/471 (96%)	452 (100%)	0	100	100
7	G	147/161 (91%)	147 (100%)	0	100	100
7	S	147/161 (91%)	144 (98%)	3 (2%)	48	72
8	H	106/106 (100%)	106 (100%)	0	100	100
8	T	106/106 (100%)	106 (100%)	0	100	100
9	I	50/59 (85%)	50 (100%)	0	100	100
9	U	51/59 (86%)	51 (100%)	0	100	100
10	J	105/114 (92%)	105 (100%)	0	100	100
10	V	105/114 (92%)	105 (100%)	0	100	100
11	L	21/167 (13%)	21 (100%)	0	100	100
11	X	21/167 (13%)	21 (100%)	0	100	100
All	All	4163/4820 (86%)	4160 (100%)	3 (0%)	87	90

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	S	188	VAL
7	S	189	ASP
7	S	190	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	162	GLN
2	B	519	HIS
5	E	145	GLN
5	E	226	ASN
6	F	104	ASN
6	F	122	ASN
6	F	434	HIS
7	G	23	ASN
7	G	127	HIS
1	M	115	GLN
1	M	369	GLN
3	O	130	GLN
3	O	151	GLN
3	O	153	ASN
3	O	192	HIS
5	Q	226	ASN
6	R	78	GLN
6	R	249	ASN
6	R	387	HIS
6	R	549	HIS
10	V	93	ASN
10	V	138	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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 59 ligands modelled in this entry, 10 are monoatomic - leaving 49 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$
14	PLM	M	504	-	15,16,17	0.46	0	14,15,17	0.34	0
13	9YF	C	303	-	58,58,58	0.88	4 (6%)	68,71,71	1.03	2 (2%)
22	HEA	F	601	-	67,67,67	2.43	24 (35%)	81,103,103	2.49	31 (38%)
16	CDL	P	103	-	94,94,99	1.33	11 (11%)	100,106,111	1.10	4 (4%)
16	CDL	D	103	-	94,94,99	1.33	10 (10%)	100,106,111	1.10	4 (4%)
13	9YF	M	502	-	58,58,58	0.90	5 (8%)	68,71,71	1.18	5 (7%)
15	HEM	N	601	2	49,49,50	1.47	6 (12%)	67,81,82	1.06	4 (5%)
17	A1IRE	N	606	-	40,40,40	2.74	14 (35%)	49,63,63	2.87	14 (28%)
19	MQ9	O	305	-	59,59,59	1.58	5 (8%)	73,75,75	1.64	20 (27%)
13	9YF	A	502	-	58,58,58	0.89	4 (6%)	68,71,71	1.13	6 (8%)
20	9Y0	S	301	-	42,42,48	0.96	4 (9%)	45,47,53	1.12	2 (4%)
18	HEC	O	302	3	46,50,50	1.84	6 (13%)	58,82,82	1.97	5 (8%)
16	CDL	F	605	-	75,75,99	1.41	10 (13%)	81,87,111	1.16	4 (4%)
16	CDL	R	605	-	75,75,99	1.42	11 (14%)	81,87,111	1.14	4 (4%)
16	CDL	M	503	-	73,73,99	1.44	12 (16%)	79,85,111	1.18	5 (6%)
16	CDL	N	607	-	78,78,99	1.38	11 (14%)	84,90,111	1.15	4 (4%)
16	CDL	D	101	-	87,87,99	1.34	10 (11%)	93,99,111	1.11	4 (4%)
18	HEC	C	302	3	46,50,50	1.82	5 (10%)	58,82,82	1.93	5 (8%)
18	HEC	O	303	3	46,50,50	1.82	5 (10%)	58,82,82	1.95	4 (6%)
20	9Y0	D	102	-	40,40,48	0.97	4 (10%)	43,45,53	1.11	2 (4%)
19	MQ9	C	304	-	59,59,59	1.57	5 (8%)	73,75,75	1.65	20 (27%)
13	9YF	O	304	-	58,58,58	0.89	5 (8%)	68,71,71	1.08	3 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	HEA	F	602	6	67,67,67	2.51	26 (38%)	81,103,103	2.44	34 (41%)
22	HEA	R	601	6	67,67,67	2.42	26 (38%)	81,103,103	2.54	34 (41%)
12	FES	M	501	1	0,4,4	-	-	-	-	-
15	HEM	B	602	2	50,50,50	1.38	7 (14%)	67,82,82	1.04	2 (2%)
17	A1IRE	B	606	-	40,40,40	2.69	14 (35%)	49,63,63	2.68	16 (32%)
16	CDL	N	605	-	78,78,99	1.37	10 (12%)	84,90,111	1.11	4 (4%)
16	CDL	B	605	-	78,78,99	1.37	10 (12%)	84,90,111	1.14	4 (4%)
16	CDL	N	603	-	73,73,99	1.42	10 (13%)	79,85,111	1.13	4 (5%)
24	MQ7	H	201	-	49,49,49	1.74	5 (10%)	61,63,63	1.62	14 (22%)
16	CDL	C	305	-	78,78,99	1.39	11 (14%)	84,90,111	1.14	4 (4%)
22	HEA	R	602	6	67,67,67	2.46	28 (41%)	81,103,103	2.44	33 (40%)
16	CDL	R	606	-	80,80,99	1.37	11 (13%)	86,92,111	1.07	4 (4%)
14	PLM	T	201	-	15,16,17	0.48	0	14,15,17	0.33	0
14	PLM	A	503	-	15,16,17	0.45	0	14,15,17	0.33	0
24	MQ7	O	301	-	49,49,49	1.70	5 (10%)	61,63,63	1.64	16 (26%)
16	CDL	B	604	-	76,76,99	1.40	10 (13%)	82,88,111	1.17	4 (4%)
12	FES	A	501	1	0,4,4	-	-	-	-	-
16	CDL	N	604	-	76,76,99	1.39	10 (13%)	82,88,111	1.18	4 (4%)
16	CDL	F	606	-	80,80,99	1.37	10 (12%)	86,92,111	1.09	4 (4%)
20	9Y0	P	102	-	40,40,48	0.97	3 (7%)	43,45,53	1.04	2 (4%)
16	CDL	P	101	-	87,87,99	1.34	10 (11%)	93,99,111	1.11	5 (5%)
14	PLM	G	302	-	15,16,17	0.47	0	14,15,17	0.32	0
15	HEM	N	602	2	50,50,50	1.39	9 (18%)	67,82,82	1.03	2 (2%)
20	9Y0	G	301	-	42,42,48	0.96	4 (9%)	45,47,53	1.08	2 (4%)
18	HEC	C	301	3	46,50,50	1.85	5 (10%)	58,82,82	1.89	4 (6%)
15	HEM	B	601	2	49,49,50	1.47	6 (12%)	67,81,82	1.06	4 (5%)
16	CDL	B	603	-	73,73,99	1.42	10 (13%)	79,85,111	1.18	4 (5%)

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
14	PLM	M	504	-	-	5/14/14/15	-
13	9YF	C	303	-	-	34/54/78/78	0/1/1/1
22	HEA	F	601	-	-	7/36/76/76	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CDL	P	103	-	-	61/105/105/110	-
16	CDL	D	103	-	-	62/105/105/110	-
13	9YF	M	502	-	-	21/54/78/78	0/1/1/1
15	HEM	N	601	2	-	4/12/52/54	-
17	A1IRE	N	606	-	-	13/28/50/50	0/5/5/5
19	MQ9	O	305	-	-	22/53/73/73	0/2/2/2
13	9YF	A	502	-	-	26/54/78/78	0/1/1/1
20	9Y0	S	301	-	-	18/46/46/52	-
18	HEC	O	302	3	-	5/14/54/54	-
16	CDL	F	605	-	-	45/86/86/110	-
16	CDL	R	605	-	-	40/86/86/110	-
16	CDL	M	503	-	-	41/84/84/110	-
16	CDL	N	607	-	-	57/89/89/110	-
16	CDL	D	101	-	-	54/98/98/110	-
18	HEC	C	302	3	-	9/14/54/54	-
18	HEC	O	303	3	-	5/14/54/54	-
20	9Y0	D	102	-	-	20/44/44/52	-
19	MQ9	C	304	-	-	17/53/73/73	0/2/2/2
13	9YF	O	304	-	-	36/54/78/78	0/1/1/1
22	HEA	F	602	6	-	8/36/76/76	-
22	HEA	R	601	6	-	7/36/76/76	-
12	FES	M	501	1	-	-	0/1/1/1
15	HEM	B	602	2	-	2/14/54/54	-
17	A1IRE	B	606	-	-	14/28/50/50	0/5/5/5
16	CDL	N	605	-	-	51/89/89/110	-
16	CDL	B	605	-	-	50/89/89/110	-
16	CDL	N	603	-	-	38/84/84/110	-
24	MQ7	H	201	-	-	12/41/61/61	0/2/2/2
16	CDL	C	305	-	-	45/89/89/110	-
22	HEA	R	602	6	-	8/36/76/76	-
16	CDL	R	606	-	-	56/91/91/110	-
14	PLM	T	201	-	-	6/14/14/15	-
14	PLM	A	503	-	-	1/14/14/15	-
24	MQ7	O	301	-	-	11/41/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CDL	B	604	-	-	43/87/87/110	-
12	FES	A	501	1	-	-	0/1/1/1
16	CDL	N	604	-	-	43/87/87/110	-
16	CDL	F	606	-	-	42/91/91/110	-
20	9Y0	P	102	-	-	22/44/44/52	-
16	CDL	P	101	-	-	59/98/98/110	-
14	PLM	G	302	-	-	5/14/14/15	-
15	HEM	N	602	2	-	1/14/54/54	-
20	9Y0	G	301	-	-	21/46/46/52	-
18	HEC	C	301	3	-	5/14/54/54	-
15	HEM	B	601	2	-	2/12/52/54	-
16	CDL	B	603	-	-	41/84/84/110	-

All (411) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	H	201	MQ7	C3-C2	7.89	1.49	1.35
19	O	305	MQ9	C6-C5	7.56	1.48	1.35
24	O	301	MQ7	C3-C2	7.55	1.48	1.35
19	C	304	MQ9	C6-C5	7.54	1.48	1.35
17	B	606	A1IRE	C13-N15	6.97	1.45	1.33
17	N	606	A1IRE	C13-N15	6.93	1.45	1.33
17	N	606	A1IRE	S30-N28	6.85	1.71	1.59
17	B	606	A1IRE	S30-N28	6.73	1.70	1.59
17	N	606	A1IRE	C05-N11	-6.60	1.30	1.39
17	B	606	A1IRE	C05-N11	-6.35	1.30	1.39
18	C	301	HEC	CAC-C3C	6.32	1.55	1.35
18	O	302	HEC	CAC-C3C	6.27	1.55	1.35
17	N	606	A1IRE	C27-C25	-6.27	1.48	1.54
18	C	302	HEC	CAC-C3C	6.17	1.55	1.35
18	C	302	HEC	CAB-C3B	6.15	1.55	1.35
18	O	302	HEC	CAB-C3B	6.15	1.55	1.35
18	C	301	HEC	CAB-C3B	6.11	1.54	1.35
18	O	303	HEC	CAC-C3C	6.10	1.54	1.35
18	O	303	HEC	CAB-C3B	6.07	1.54	1.35
17	B	606	A1IRE	C27-C25	-6.06	1.49	1.54
17	B	606	A1IRE	C29-C25	-5.94	1.49	1.54
17	N	606	A1IRE	C29-C25	-5.91	1.49	1.54
18	C	301	HEC	C3D-C2D	5.83	1.54	1.38
18	O	303	HEC	C3D-C2D	5.69	1.53	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	O	302	HEC	C3D-C2D	5.69	1.53	1.38
22	F	602	HEA	C3B-C2B	5.65	1.47	1.34
18	C	302	HEC	C3D-C2D	5.62	1.53	1.38
22	R	601	HEA	FE-ND	5.56	2.12	1.94
22	R	601	HEA	FE-NB	5.54	2.12	1.94
22	F	601	HEA	FE-NB	5.52	2.11	1.94
22	R	602	HEA	C3B-C2B	5.52	1.47	1.34
22	F	601	HEA	FE-ND	5.46	2.11	1.94
22	F	601	HEA	C3B-C2B	5.36	1.46	1.34
22	R	601	HEA	C3B-C2B	5.35	1.46	1.34
22	R	602	HEA	FE-ND	5.31	2.11	1.94
22	R	602	HEA	FE-NB	5.26	2.11	1.94
22	F	602	HEA	FE-ND	5.23	2.11	1.94
22	F	602	HEA	FE-NB	5.07	2.10	1.94
22	F	602	HEA	C3D-C2D	5.07	1.47	1.36
22	R	602	HEA	C3D-C2D	5.01	1.47	1.36
22	F	601	HEA	C3D-C2D	4.99	1.47	1.36
22	F	601	HEA	FE-NC	4.95	2.11	1.95
22	R	601	HEA	FE-NC	4.93	2.11	1.95
22	R	601	HEA	C3D-C2D	4.88	1.47	1.36
22	F	602	HEA	CHD-C1D	4.87	1.48	1.38
22	F	602	HEA	C3A-C2A	4.83	1.48	1.37
22	R	602	HEA	CHD-C1D	4.80	1.48	1.38
19	C	304	MQ9	C3-C4	4.79	1.57	1.48
22	F	602	HEA	CHB-C4A	4.77	1.47	1.38
19	O	305	MQ9	C3-C4	4.75	1.57	1.48
22	R	602	HEA	FE-NC	4.72	2.10	1.95
24	O	301	MQ7	C5-C4	4.70	1.57	1.48
22	R	602	HEA	C3A-C2A	4.69	1.47	1.37
24	H	201	MQ7	C5-C4	4.69	1.57	1.48
22	F	602	HEA	CHC-C4B	4.67	1.47	1.38
19	O	305	MQ9	C2-C1	4.66	1.57	1.48
24	O	301	MQ7	C10-C1	4.64	1.57	1.48
24	H	201	MQ7	C10-C1	4.61	1.57	1.48
22	R	601	HEA	C3A-C2A	4.57	1.47	1.37
22	F	601	HEA	C3A-C2A	4.53	1.47	1.37
22	F	602	HEA	FE-NC	4.50	2.10	1.95
19	C	304	MQ9	C2-C1	4.49	1.56	1.48
15	N	601	HEM	FE-ND	4.48	2.08	1.94
22	R	602	HEA	CHB-C4A	4.45	1.47	1.38
22	F	602	HEA	CHA-C1A	4.45	1.47	1.38
22	R	602	HEA	CHC-C4B	4.39	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	F	601	HEA	CHD-C1D	4.36	1.47	1.38
22	F	601	HEA	CHC-C4B	4.34	1.47	1.38
22	R	601	HEA	CHB-C4A	4.30	1.46	1.38
22	R	601	HEA	CHD-C1D	4.28	1.47	1.38
22	R	601	HEA	C1A-NA	4.23	1.47	1.39
22	R	602	HEA	CHA-C1A	4.22	1.46	1.38
22	R	601	HEA	CHA-C1A	4.20	1.46	1.38
22	R	601	HEA	CHC-C4B	4.19	1.46	1.38
22	F	601	HEA	CHA-C1A	4.19	1.46	1.38
22	F	601	HEA	C1A-NA	4.19	1.47	1.39
22	F	601	HEA	CHB-C4A	4.16	1.46	1.38
15	B	601	HEM	FE-ND	4.10	2.07	1.94
22	F	601	HEA	C4A-NA	4.09	1.47	1.39
22	R	602	HEA	C1A-NA	4.02	1.47	1.39
22	R	602	HEA	C4A-NA	3.98	1.47	1.39
22	R	601	HEA	C4A-NA	3.91	1.47	1.39
16	R	606	CDL	OA8-CA7	3.89	1.44	1.33
22	F	602	HEA	C1A-NA	3.89	1.46	1.39
15	B	601	HEM	FE-NC	3.87	2.07	1.95
22	F	602	HEA	CHC-C1C	3.82	1.48	1.39
16	B	603	CDL	OA8-CA7	3.82	1.44	1.33
16	D	103	CDL	OA8-CA7	3.81	1.44	1.33
16	N	603	CDL	OA8-CA7	3.80	1.44	1.33
16	F	606	CDL	OA8-CA7	3.80	1.44	1.33
16	D	101	CDL	OA8-CA7	3.79	1.44	1.33
22	F	602	HEA	C4A-NA	3.79	1.46	1.39
16	P	103	CDL	OA8-CA7	3.77	1.44	1.33
22	F	602	HEA	CHD-C4C	3.76	1.47	1.39
16	B	605	CDL	OA8-CA7	3.76	1.44	1.33
16	R	605	CDL	OA8-CA7	3.74	1.44	1.33
22	R	602	HEA	CHD-C4C	3.74	1.47	1.39
16	M	503	CDL	OA8-CA7	3.73	1.44	1.33
16	C	305	CDL	OA8-CA7	3.72	1.44	1.33
15	N	601	HEM	FE-NA	3.71	2.07	1.95
16	P	101	CDL	OA8-CA7	3.71	1.44	1.33
16	N	607	CDL	OA8-CA7	3.70	1.44	1.33
16	F	605	CDL	OA8-CA7	3.69	1.44	1.33
16	N	605	CDL	OA8-CA7	3.69	1.44	1.33
16	M	503	CDL	OB8-CB7	3.68	1.44	1.33
16	B	604	CDL	OA8-CA7	3.67	1.44	1.33
15	N	602	HEM	FE-NB	3.67	2.06	1.94
22	F	602	HEA	CHB-C1B	3.66	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	P	101	CDL	OB8-CB7	3.62	1.43	1.33
16	D	103	CDL	OB8-CB7	3.60	1.43	1.33
16	F	606	CDL	OB8-CB7	3.60	1.43	1.33
16	B	604	CDL	OB8-CB7	3.59	1.43	1.33
16	C	305	CDL	OB8-CB7	3.59	1.43	1.33
16	D	101	CDL	OB8-CB7	3.59	1.43	1.33
16	F	606	CDL	OA6-CA5	3.58	1.44	1.34
16	N	604	CDL	OA8-CA7	3.57	1.43	1.33
16	D	103	CDL	OA6-CA5	3.55	1.44	1.34
16	N	607	CDL	OB8-CB7	3.55	1.43	1.33
16	F	605	CDL	OB8-CB7	3.55	1.43	1.33
16	R	606	CDL	OA6-CA5	3.55	1.44	1.34
16	P	103	CDL	OB8-CB7	3.54	1.43	1.33
16	N	604	CDL	OB8-CB7	3.54	1.43	1.33
22	F	602	HEA	CHA-C4D	3.54	1.47	1.39
22	F	601	HEA	CHD-C4C	3.52	1.47	1.39
16	R	605	CDL	OB8-CB7	3.51	1.43	1.33
16	R	606	CDL	OB8-CB7	3.50	1.43	1.33
16	B	605	CDL	OB8-CB7	3.49	1.43	1.33
22	R	602	HEA	CHC-C1C	3.49	1.47	1.39
16	B	603	CDL	OB8-CB7	3.48	1.43	1.33
16	N	603	CDL	OB8-CB7	3.45	1.43	1.33
22	R	602	HEA	CHA-C4D	3.41	1.47	1.39
16	P	103	CDL	OA6-CA5	3.41	1.43	1.34
22	R	602	HEA	CHB-C1B	3.40	1.46	1.39
16	N	605	CDL	OA6-CA5	3.39	1.43	1.34
16	B	605	CDL	OA6-CA5	3.37	1.43	1.34
15	B	602	HEM	FE-ND	3.35	2.05	1.94
16	N	605	CDL	OB8-CB7	3.35	1.43	1.33
16	F	605	CDL	OA6-CA5	3.33	1.43	1.34
22	F	601	HEA	CHC-C1C	3.33	1.46	1.39
22	R	601	HEA	CHC-C1C	3.31	1.46	1.39
16	P	101	CDL	OA6-CA5	3.31	1.43	1.34
22	R	601	HEA	CHD-C4C	3.30	1.46	1.39
16	R	605	CDL	OA6-CA5	3.30	1.43	1.34
16	D	101	CDL	OA6-CA5	3.29	1.43	1.34
22	R	601	HEA	CHB-C1B	3.28	1.46	1.39
22	F	601	HEA	CHB-C1B	3.28	1.46	1.39
16	M	503	CDL	OA6-CA5	3.26	1.43	1.34
16	B	604	CDL	OA6-CA5	3.26	1.43	1.34
17	N	606	A1IRE	C12-C13	3.23	1.54	1.46
22	F	601	HEA	CHA-C4D	3.20	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	R	601	HEA	CHA-C4D	3.20	1.46	1.39
16	C	305	CDL	OA6-CA5	3.20	1.43	1.34
16	N	603	CDL	OA6-CA5	3.19	1.43	1.34
15	N	602	HEM	FE-ND	3.18	2.04	1.94
16	B	603	CDL	OA6-CA5	3.18	1.43	1.34
15	B	601	HEM	FE-NA	3.17	2.05	1.95
16	N	607	CDL	OA6-CA5	3.17	1.43	1.34
15	B	602	HEM	FE-NB	3.16	2.04	1.94
16	N	604	CDL	OA6-CA5	3.15	1.43	1.34
15	N	601	HEM	FE-NC	3.14	2.05	1.95
22	F	602	HEA	C4B-NB	-3.08	1.34	1.40
22	R	602	HEA	C4B-NB	-3.06	1.34	1.40
15	B	601	HEM	FE-NB	3.06	2.04	1.94
17	B	606	A1IRE	C12-C13	3.03	1.53	1.46
16	F	606	CDL	OB6-CB4	-3.03	1.39	1.46
16	B	604	CDL	OB6-CB4	-3.02	1.39	1.46
15	B	601	HEM	CAB-C3B	3.02	1.55	1.47
16	N	603	CDL	OB6-CB4	-3.01	1.39	1.46
13	A	502	9YF	O9-C	-3.01	1.39	1.46
16	P	103	CDL	OB6-CB4	-3.01	1.39	1.46
15	N	601	HEM	CAB-C3B	3.00	1.55	1.47
16	P	101	CDL	OB6-CB4	-2.99	1.39	1.46
16	N	604	CDL	OB6-CB4	-2.99	1.39	1.46
16	F	605	CDL	OB6-CB5	2.98	1.42	1.34
16	D	103	CDL	OB6-CB4	-2.97	1.39	1.46
16	R	606	CDL	OB6-CB4	-2.96	1.39	1.46
16	B	605	CDL	OB6-CB4	-2.95	1.39	1.46
16	N	607	CDL	OB6-CB4	-2.95	1.39	1.46
15	B	602	HEM	CAB-C3B	2.95	1.55	1.47
15	N	602	HEM	CAB-C3B	2.94	1.55	1.47
17	N	606	A1IRE	O31-S30	2.94	1.46	1.42
15	B	602	HEM	FE-NC	2.93	2.04	1.95
16	D	101	CDL	OB6-CB4	-2.93	1.39	1.46
16	R	605	CDL	OB6-CB4	-2.93	1.39	1.46
16	M	503	CDL	OB6-CB4	-2.92	1.39	1.46
16	B	603	CDL	OB6-CB4	-2.92	1.39	1.46
16	C	305	CDL	OB6-CB4	-2.91	1.39	1.46
17	B	606	A1IRE	O31-S30	2.90	1.46	1.42
16	D	103	CDL	OB6-CB5	2.89	1.42	1.34
16	F	606	CDL	OB6-CB5	2.89	1.42	1.34
17	B	606	A1IRE	C08-CL09	2.89	1.79	1.73
16	N	605	CDL	OB6-CB5	2.88	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	M	503	CDL	OB6-CB5	2.88	1.42	1.34
22	R	602	HEA	C1D-ND	-2.87	1.35	1.40
16	R	606	CDL	OB6-CB5	2.86	1.42	1.34
17	N	606	A1IRE	C03-N04	-2.85	1.32	1.38
13	M	502	9YF	O9-C	-2.85	1.39	1.46
17	N	606	A1IRE	C08-CL09	2.84	1.78	1.73
16	N	605	CDL	OB6-CB4	-2.83	1.39	1.46
17	N	606	A1IRE	O32-S30	2.82	1.46	1.42
20	G	301	9Y0	O7-C1	-2.82	1.40	1.46
15	B	602	HEM	CAC-C3C	2.82	1.54	1.47
22	F	602	HEA	C1D-ND	-2.81	1.35	1.40
16	D	101	CDL	OB6-CB5	2.80	1.42	1.34
13	C	303	9YF	O9-C	-2.80	1.40	1.46
16	B	604	CDL	OB6-CB5	2.79	1.42	1.34
16	B	603	CDL	OB6-CB5	2.79	1.42	1.34
15	N	602	HEM	FE-NA	2.79	2.04	1.95
15	N	601	HEM	FE-NB	2.79	2.03	1.94
22	R	601	HEA	C1D-ND	-2.79	1.35	1.40
16	N	607	CDL	OB6-CB5	2.78	1.42	1.34
16	C	305	CDL	OB6-CB5	2.78	1.42	1.34
16	N	604	CDL	OB6-CB5	2.78	1.42	1.34
16	R	605	CDL	OB6-CB5	2.76	1.42	1.34
16	B	605	CDL	OB6-CB5	2.76	1.42	1.34
16	N	603	CDL	OB6-CB5	2.74	1.42	1.34
22	F	602	HEA	C11-C3B	-2.74	1.48	1.51
15	N	602	HEM	CAC-C3C	2.73	1.54	1.47
16	P	101	CDL	OB6-CB5	2.73	1.42	1.34
20	S	301	9Y0	O7-C1	-2.73	1.40	1.46
16	P	103	CDL	OB6-CB5	2.72	1.42	1.34
22	F	601	HEA	C1D-ND	-2.72	1.35	1.40
16	F	605	CDL	OB6-CB4	-2.71	1.40	1.46
13	O	304	9YF	O9-C	-2.68	1.40	1.46
17	B	606	A1IRE	C03-N04	-2.66	1.32	1.38
22	F	601	HEA	C4B-NB	-2.66	1.35	1.40
22	R	601	HEA	C4B-NB	-2.65	1.35	1.40
17	B	606	A1IRE	C26-C23	-2.64	1.52	1.55
17	N	606	A1IRE	C26-C23	-2.61	1.52	1.55
20	D	102	9Y0	O7-C1	-2.60	1.40	1.46
17	B	606	A1IRE	O32-S30	2.59	1.46	1.42
15	B	602	HEM	FE-NA	2.59	2.03	1.95
22	F	602	HEA	C4C-NC	-2.59	1.34	1.39
22	F	601	HEA	C1C-C2C	2.59	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	P	102	9Y0	O5-C5	2.58	1.40	1.33
22	F	602	HEA	C1C-C2C	2.55	1.49	1.43
16	N	603	CDL	OA6-CA4	-2.54	1.40	1.46
16	N	604	CDL	OA6-CA4	-2.54	1.40	1.46
16	N	607	CDL	OA6-CA4	-2.51	1.40	1.46
20	P	102	9Y0	O7-C21	2.50	1.41	1.34
16	M	503	CDL	OA6-CA4	-2.47	1.40	1.46
13	O	304	9YF	O11-C25	2.45	1.40	1.33
16	F	606	CDL	C11-CA5	2.44	1.57	1.50
20	S	301	9Y0	O5-C5	2.44	1.40	1.33
13	C	303	9YF	O11-C25	2.42	1.40	1.33
13	M	502	9YF	O11-C25	2.42	1.40	1.33
16	B	603	CDL	OA6-CA4	-2.42	1.40	1.46
20	D	102	9Y0	O5-C5	2.42	1.40	1.33
16	B	604	CDL	OA6-CA4	-2.42	1.40	1.46
16	M	503	CDL	PB2-OB5	2.42	1.68	1.59
17	N	606	A1IRE	C24-C23	-2.42	1.53	1.55
22	F	601	HEA	C4B-C3B	2.41	1.49	1.44
16	R	605	CDL	OA6-CA4	-2.41	1.40	1.46
17	N	606	A1IRE	O14-C13	-2.41	1.19	1.23
17	B	606	A1IRE	O14-C13	-2.41	1.19	1.23
17	B	606	A1IRE	C10-C08	2.41	1.39	1.35
16	F	605	CDL	C11-CA5	2.41	1.57	1.50
16	P	101	CDL	OA6-CA4	-2.40	1.40	1.46
16	C	305	CDL	OA6-CA4	-2.40	1.41	1.46
22	R	602	HEA	C11-C3B	-2.40	1.48	1.51
16	R	606	CDL	C11-CA5	2.40	1.57	1.50
16	R	605	CDL	C11-CA5	2.39	1.57	1.50
22	R	601	HEA	C4B-C3B	2.39	1.48	1.44
20	G	301	9Y0	O5-C5	2.38	1.40	1.33
22	R	601	HEA	C1C-C2C	2.38	1.48	1.43
16	P	103	CDL	C11-CA5	2.38	1.57	1.50
17	N	606	A1IRE	C10-C08	2.38	1.39	1.35
16	D	101	CDL	OA6-CA4	-2.37	1.41	1.46
16	D	101	CDL	PB2-OB5	2.37	1.68	1.59
16	D	101	CDL	C11-CA5	2.37	1.57	1.50
22	F	601	HEA	C11-C3B	-2.37	1.48	1.51
22	R	602	HEA	C1C-C2C	2.37	1.48	1.43
16	N	604	CDL	C11-CA5	2.37	1.57	1.50
16	P	101	CDL	C11-CA5	2.36	1.57	1.50
16	D	103	CDL	C11-CA5	2.36	1.57	1.50
16	F	605	CDL	OA6-CA4	-2.35	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	C	305	CDL	PB2-OB5	2.35	1.68	1.59
22	F	602	HEA	C4D-C3D	2.34	1.49	1.45
16	M	503	CDL	C11-CA5	2.34	1.57	1.50
16	N	605	CDL	PB2-OB5	2.34	1.68	1.59
16	F	605	CDL	PB2-OB5	2.34	1.68	1.59
16	B	603	CDL	C11-CA5	2.34	1.57	1.50
16	M	503	CDL	PB2-OB2	2.33	1.68	1.59
16	R	605	CDL	PB2-OB5	2.33	1.68	1.59
22	R	602	HEA	C4B-C3B	2.32	1.48	1.44
16	D	103	CDL	PB2-OB2	2.32	1.68	1.59
15	N	602	HEM	FE-NC	2.32	2.02	1.95
24	O	301	MQ7	O1-C1	-2.32	1.18	1.23
16	R	605	CDL	PA1-OA5	2.32	1.68	1.59
16	P	101	CDL	PB2-OB2	2.32	1.68	1.59
13	A	502	9YF	O11-C25	2.31	1.40	1.33
16	P	103	CDL	PA1-OA5	2.31	1.68	1.59
22	F	602	HEA	C1A-C2A	2.31	1.49	1.45
16	N	607	CDL	PB2-OB5	2.31	1.68	1.59
16	B	603	CDL	PB2-OB5	2.31	1.68	1.59
16	P	101	CDL	PA1-OA5	2.30	1.68	1.59
16	D	103	CDL	PB2-OB5	2.30	1.68	1.59
16	B	605	CDL	C11-CA5	2.30	1.57	1.50
16	N	603	CDL	C11-CA5	2.30	1.57	1.50
16	B	605	CDL	PB2-OB5	2.30	1.68	1.59
16	P	103	CDL	OA6-CA4	-2.30	1.41	1.46
16	M	503	CDL	PA1-OA5	2.29	1.68	1.59
13	A	502	9YF	O11-C24	-2.29	1.40	1.45
16	F	605	CDL	PA1-OA5	2.29	1.68	1.59
22	R	602	HEA	C4C-NC	-2.29	1.35	1.39
16	D	101	CDL	PA1-OA5	2.29	1.68	1.59
16	P	103	CDL	PB2-OB5	2.28	1.68	1.59
16	D	103	CDL	PA1-OA5	2.28	1.68	1.59
16	N	603	CDL	PA1-OA5	2.28	1.68	1.59
16	P	103	CDL	PB2-OB2	2.28	1.68	1.59
19	C	304	MQ9	O1-C1	-2.28	1.18	1.23
16	C	305	CDL	PB2-OB2	2.27	1.68	1.59
16	R	605	CDL	PB2-OB2	2.27	1.68	1.59
16	P	101	CDL	PB2-OB5	2.27	1.68	1.59
16	N	603	CDL	PB2-OB2	2.27	1.68	1.59
16	N	605	CDL	PA1-OA5	2.27	1.68	1.59
19	O	305	MQ9	O4-C4	-2.26	1.18	1.23
16	B	604	CDL	PB2-OB5	2.26	1.68	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	N	605	CDL	C11-CA5	2.26	1.57	1.50
22	F	602	HEA	C4B-C3B	2.26	1.48	1.44
16	F	606	CDL	PB2-OB2	2.26	1.68	1.59
22	R	601	HEA	C11-C3B	-2.26	1.48	1.51
20	G	301	9Y0	O5-C	-2.25	1.40	1.45
16	B	604	CDL	C11-CA5	2.25	1.57	1.50
16	N	607	CDL	PB2-OB2	2.25	1.68	1.59
16	N	603	CDL	PB2-OB5	2.25	1.68	1.59
16	C	305	CDL	C11-CA5	2.25	1.57	1.50
22	F	602	HEA	C1D-C2D	2.25	1.49	1.44
16	B	603	CDL	PA1-OA5	2.25	1.68	1.59
16	N	607	CDL	C11-CA5	2.24	1.57	1.50
19	O	305	MQ9	O1-C1	-2.24	1.18	1.23
16	N	604	CDL	PB2-OB5	2.24	1.68	1.59
16	C	305	CDL	PA1-OA5	2.24	1.68	1.59
13	C	303	9YF	O9-C8	2.24	1.40	1.34
16	R	606	CDL	PA1-OA5	2.24	1.68	1.59
16	N	607	CDL	PA1-OA5	2.24	1.68	1.59
16	F	605	CDL	PB2-OB2	2.23	1.68	1.59
16	R	606	CDL	PB2-OB5	2.23	1.68	1.59
16	D	101	CDL	PB2-OB2	2.22	1.68	1.59
16	B	604	CDL	PB2-OB2	2.22	1.68	1.59
17	B	606	A1IRE	C24-C23	-2.22	1.53	1.55
24	H	201	MQ7	O1-C1	-2.21	1.18	1.23
13	O	304	9YF	O9-C8	2.21	1.40	1.34
16	N	605	CDL	PB2-OB2	2.21	1.68	1.59
22	R	601	HEA	C4C-NC	-2.20	1.35	1.39
16	B	603	CDL	PB2-OB2	2.20	1.68	1.59
16	F	606	CDL	PA1-OA5	2.20	1.68	1.59
22	R	602	HEA	C1A-C2A	2.20	1.49	1.45
13	C	303	9YF	O11-C24	-2.19	1.40	1.45
24	O	301	MQ7	O4-C4	-2.19	1.18	1.23
20	D	102	9Y0	O5-C	-2.18	1.40	1.45
16	B	605	CDL	OA6-CA4	-2.18	1.41	1.46
16	B	605	CDL	PA1-OA5	2.18	1.67	1.59
20	S	301	9Y0	O5-C	-2.18	1.40	1.45
16	B	604	CDL	PA1-OA5	2.17	1.67	1.59
18	O	303	HEC	C3C-C2C	-2.17	1.33	1.41
13	M	502	9YF	O11-C24	-2.17	1.40	1.45
16	N	604	CDL	PB2-OB2	2.17	1.67	1.59
16	R	606	CDL	PB2-OB2	2.17	1.67	1.59
24	H	201	MQ7	O4-C4	-2.16	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	F	601	HEA	C1A-C2A	2.16	1.49	1.45
13	M	502	9YF	O9-C8	2.16	1.40	1.34
22	F	601	HEA	C1D-C2D	2.16	1.48	1.44
19	C	304	MQ9	O4-C4	-2.15	1.18	1.23
16	B	605	CDL	PB2-OB2	2.15	1.67	1.59
20	D	102	9Y0	O7-C21	2.14	1.40	1.34
16	F	606	CDL	PB2-OB5	2.14	1.67	1.59
18	C	302	HEC	C3C-C2C	-2.14	1.33	1.41
20	S	301	9Y0	O7-C21	2.14	1.40	1.34
13	O	304	9YF	O11-C24	-2.13	1.40	1.45
16	N	604	CDL	PA1-OA5	2.13	1.67	1.59
22	R	601	HEA	C4D-C3D	2.13	1.48	1.45
22	R	602	HEA	C1D-C2D	2.12	1.48	1.44
16	M	503	CDL	PA1-OA2	2.12	1.67	1.59
20	G	301	9Y0	O7-C21	2.11	1.40	1.34
15	N	602	HEM	CMB-C2B	2.11	1.55	1.50
18	C	301	HEC	CMB-C2B	2.10	1.55	1.50
18	C	301	HEC	C3B-C2B	-2.09	1.34	1.41
22	R	602	HEA	C4D-C3D	2.09	1.48	1.45
13	A	502	9YF	O9-C8	2.09	1.40	1.34
22	R	601	HEA	C1A-C2A	2.09	1.48	1.45
16	N	605	CDL	OA6-CA4	-2.09	1.41	1.46
20	P	102	9Y0	O7-C1	-2.08	1.41	1.46
22	R	601	HEA	C1B-C2B	2.08	1.48	1.44
22	R	602	HEA	C1C-NC	-2.07	1.35	1.39
15	N	602	HEM	CMC-C2C	2.07	1.55	1.50
22	R	601	HEA	C1D-C2D	2.07	1.48	1.44
16	C	305	CDL	C31-CA7	2.06	1.56	1.50
16	R	605	CDL	C31-CA7	2.06	1.56	1.50
22	R	602	HEA	C3C-C4C	2.06	1.48	1.42
15	N	602	HEM	C2A-C3A	-2.05	1.33	1.38
16	P	103	CDL	C31-CA7	2.05	1.56	1.50
18	O	302	HEC	CMB-C2B	2.05	1.55	1.50
16	F	606	CDL	C31-CA7	2.05	1.56	1.50
13	O	304	9YF	P-O2	2.05	1.65	1.59
16	R	606	CDL	OA6-CA4	-2.04	1.41	1.46
15	B	602	HEM	CMB-C2B	2.04	1.55	1.50
16	N	607	CDL	C31-CA7	2.04	1.56	1.50
15	N	601	HEM	CMB-C2B	2.03	1.54	1.50
18	C	302	HEC	C3B-C2B	-2.03	1.34	1.41
22	F	602	HEA	C1B-C2B	2.03	1.48	1.44
22	F	601	HEA	C4C-NC	-2.02	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	O	302	HEC	C3C-C2C	-2.02	1.34	1.41
16	M	503	CDL	C31-CA7	2.02	1.56	1.50
18	O	302	HEC	C3B-C2B	-2.02	1.34	1.41
18	O	303	HEC	C3B-C2B	-2.02	1.34	1.41
13	M	502	9YF	P-O2	2.02	1.65	1.59
16	D	103	CDL	C71-CB7	2.01	1.56	1.50
15	B	601	HEM	CMB-C2B	2.01	1.54	1.50
16	R	606	CDL	C31-CA7	2.01	1.56	1.50
22	R	602	HEA	C1B-NB	-2.01	1.34	1.38

All (356) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	N	606	A1IRE	O32-S30-O31	-10.65	100.97	120.84
17	B	606	A1IRE	O32-S30-O31	-10.27	101.67	120.84
18	O	303	HEC	CBB-CAB-C3B	-8.70	110.05	127.43
18	C	302	HEC	CBC-CAC-C3C	-8.68	110.09	127.43
18	O	302	HEC	CBB-CAB-C3B	-8.64	110.16	127.43
18	C	301	HEC	CBB-CAB-C3B	-8.59	110.26	127.43
18	O	303	HEC	CBC-CAC-C3C	-8.44	110.56	127.43
17	N	606	A1IRE	C24-C23-C20	-8.22	105.47	119.57
18	O	302	HEC	CBC-CAC-C3C	-8.14	111.16	127.43
18	C	302	HEC	CBB-CAB-C3B	-7.96	111.53	127.43
18	C	301	HEC	CBC-CAC-C3C	-7.59	112.25	127.43
17	B	606	A1IRE	C24-C23-C20	-7.15	107.30	119.57
22	R	601	HEA	C3D-C4D-ND	6.73	116.85	110.35
22	F	601	HEA	C3D-C4D-ND	6.68	116.81	110.35
17	N	606	A1IRE	C26-C23-C20	6.63	130.94	119.57
22	R	602	HEA	C3D-C4D-ND	5.91	116.06	110.35
22	R	601	HEA	C2D-C1D-ND	5.83	116.54	109.84
22	R	601	HEA	C2B-C1B-NB	5.75	116.55	109.90
22	R	601	HEA	C3B-C4B-NB	5.73	116.43	109.84
22	F	601	HEA	C2B-C1B-NB	5.72	116.52	109.90
22	F	602	HEA	CHA-C4D-ND	-5.64	118.35	124.42
22	F	602	HEA	C3C-C2C-C1C	-5.61	100.56	107.17
17	B	606	A1IRE	C26-C23-C20	5.61	129.18	119.57
22	F	601	HEA	C3C-C2C-C1C	-5.53	100.64	107.17
22	F	601	HEA	C2D-C1D-ND	5.49	116.15	109.84
22	R	602	HEA	C3C-C2C-C1C	-5.49	100.69	107.17
22	F	601	HEA	C3B-C4B-NB	5.45	116.11	109.84
22	F	602	HEA	C3D-C4D-ND	5.45	115.62	110.35
22	R	601	HEA	C3C-C2C-C1C	-5.43	100.77	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	R	601	HEA	C3C-C4C-NC	5.42	114.37	109.80
22	F	601	HEA	C3C-C4C-NC	5.41	114.36	109.80
22	R	602	HEA	C3B-C4B-NB	5.29	115.92	109.84
22	R	602	HEA	C2B-C1B-NB	5.24	115.96	109.90
22	F	601	HEA	C2A-C1A-NA	5.04	115.18	110.32
22	R	601	HEA	C2A-C1A-NA	5.03	115.17	110.32
17	N	606	A1IRE	C29-N28-C27	-4.87	88.19	92.16
22	R	602	HEA	C2A-C1A-NA	4.86	115.01	110.32
17	N	606	A1IRE	C17-C16-N15	-4.72	103.13	113.07
22	R	602	HEA	CHA-C4D-ND	-4.69	119.37	124.42
16	M	503	CDL	OB6-CB5-C51	4.69	121.62	111.48
22	F	602	HEA	CHA-C1A-NA	-4.68	119.36	124.45
22	F	602	HEA	C2B-C1B-NB	4.68	115.31	109.90
22	R	602	HEA	C2D-C1D-ND	4.62	115.15	109.84
16	D	103	CDL	OB6-CB5-C51	4.56	121.35	111.48
22	F	602	HEA	C3B-C4B-NB	4.56	115.08	109.84
17	B	606	A1IRE	O31-S30-C33	4.52	111.52	104.31
16	B	603	CDL	OB6-CB5-C51	4.48	121.17	111.48
16	N	605	CDL	OB6-CB5-C51	4.46	121.12	111.48
16	F	605	CDL	OB6-CB5-C51	4.43	121.06	111.48
17	N	606	A1IRE	O31-S30-C33	4.41	111.34	104.31
22	R	601	HEA	C1D-C2D-C3D	-4.39	102.36	106.98
22	F	602	HEA	C2D-C1D-ND	4.34	114.83	109.84
22	F	602	HEA	C2A-C1A-NA	4.29	114.46	110.32
22	F	601	HEA	C1D-C2D-C3D	-4.28	102.47	106.98
17	B	606	A1IRE	C29-N28-C27	-4.26	88.69	92.16
22	F	601	HEA	C2C-C1C-NC	4.22	116.90	110.14
16	N	604	CDL	OB6-CB5-C51	4.20	120.58	111.48
16	C	305	CDL	OB6-CB5-C51	4.20	120.56	111.48
16	B	605	CDL	OB6-CB5-C51	4.19	120.55	111.48
24	O	301	MQ7	C11-C12-C13	-4.19	119.61	126.83
16	B	604	CDL	OA6-CA5-C11	4.19	120.54	111.48
16	M	503	CDL	OA6-CA5-C11	4.18	120.52	111.48
17	B	606	A1IRE	C33-S30-N28	4.16	110.40	104.78
16	P	103	CDL	OA6-CA5-C11	4.15	120.46	111.48
17	N	606	A1IRE	O32-S30-C33	4.14	110.91	104.31
22	R	601	HEA	C2C-C1C-NC	4.12	116.74	110.14
17	N	606	A1IRE	C33-S30-N28	4.10	110.32	104.78
22	R	602	HEA	C3C-C4C-NC	4.09	113.24	109.80
16	N	607	CDL	OA6-CA5-C11	4.06	120.26	111.48
17	B	606	A1IRE	O32-S30-C33	4.05	110.77	104.31
16	C	305	CDL	OA6-CA5-C11	4.04	120.21	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	R	605	CDL	OB6-CB5-C51	4.02	120.19	111.48
22	R	602	HEA	CHA-C1A-NA	-4.02	120.08	124.45
22	F	602	HEA	C1A-CHA-C4D	-4.02	117.48	126.02
13	M	502	9YF	O9-C8-C9	4.01	120.16	111.48
16	P	101	CDL	OA6-CA5-C11	4.01	120.16	111.48
16	P	103	CDL	OB6-CB5-C51	4.01	120.15	111.48
22	R	602	HEA	C3A-C2A-C1A	-4.01	103.25	107.05
16	N	607	CDL	OB6-CB5-C51	4.00	120.14	111.48
16	N	603	CDL	OB6-CB5-C51	3.97	120.08	111.48
20	D	102	9Y0	O7-C21-C22	3.97	120.07	111.48
16	F	605	CDL	OA6-CA5-C11	3.96	120.06	111.48
16	B	604	CDL	OB6-CB5-C51	3.94	120.02	111.48
16	R	605	CDL	OA6-CA5-C11	3.94	120.01	111.48
22	F	602	HEA	C13-C12-C11	-3.94	108.10	114.39
22	F	602	HEA	C3A-C2A-C1A	-3.93	103.33	107.05
24	H	201	MQ7	C11-C12-C13	-3.92	120.08	126.83
16	D	101	CDL	OA6-CA5-C11	3.91	119.94	111.48
22	R	602	HEA	C2C-C1C-NC	3.91	116.41	110.14
19	O	305	MQ9	C7-C8-C9	-3.91	120.09	126.83
16	R	606	CDL	OB6-CB5-C51	3.88	119.88	111.48
16	D	103	CDL	OA6-CA5-C11	3.88	119.87	111.48
16	N	604	CDL	OA6-CA5-C11	3.86	119.83	111.48
16	D	101	CDL	OB6-CB5-C51	3.84	119.80	111.48
16	P	101	CDL	OB6-CB5-C51	3.83	119.76	111.48
16	B	603	CDL	OA6-CA5-C11	3.83	119.76	111.48
16	B	605	CDL	OA6-CA5-C11	3.79	119.68	111.48
16	N	603	CDL	OA6-CA5-C11	3.79	119.67	111.48
22	R	601	HEA	C3A-C2A-C1A	-3.78	103.47	107.05
22	F	601	HEA	C1B-C2B-C3B	-3.78	102.42	106.80
13	O	304	9YF	O9-C8-C9	3.77	119.63	111.48
18	O	303	HEC	C4D-ND-C1D	3.75	111.94	105.82
20	S	301	9Y0	O7-C21-C22	3.74	119.58	111.48
22	F	602	HEA	C13-C14-C15	-3.73	119.08	127.62
22	R	601	HEA	C1B-C2B-C3B	-3.73	102.48	106.80
18	C	302	HEC	C4D-ND-C1D	3.72	111.88	105.82
22	F	602	HEA	C3C-C4C-NC	3.72	112.93	109.80
19	C	304	MQ9	C7-C8-C9	-3.71	120.44	126.83
22	F	602	HEA	C1B-C2B-C3B	-3.67	102.54	106.80
22	R	602	HEA	C1D-C2D-C3D	-3.63	103.16	106.98
22	R	602	HEA	C1B-C2B-C3B	-3.63	102.59	106.80
13	A	502	9YF	O9-C8-C9	3.63	119.33	111.48
22	F	601	HEA	C3A-C2A-C1A	-3.62	103.62	107.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	F	602	HEA	C1D-C2D-C3D	-3.62	103.17	106.98
18	O	302	HEC	C4D-ND-C1D	3.60	111.70	105.82
19	O	305	MQ9	C17-C18-C19	-3.59	119.41	127.62
16	N	605	CDL	OA6-CA5-C11	3.58	119.23	111.48
18	C	301	HEC	C4D-ND-C1D	3.56	111.62	105.82
16	F	606	CDL	OB6-CB5-C51	3.53	119.12	111.48
22	R	602	HEA	C1A-CHA-C4D	-3.50	118.58	126.02
24	O	301	MQ7	C36-C37-C38	-3.48	119.65	127.62
13	C	303	9YF	O9-C8-C9	3.47	119.00	111.48
22	R	602	HEA	C17-C18-C19	-3.43	119.78	127.62
24	H	201	MQ7	C36-C37-C38	-3.41	119.82	127.62
22	F	601	HEA	C13-C14-C15	-3.39	119.86	127.62
22	F	602	HEA	C2C-C1C-NC	3.39	115.57	110.14
24	O	301	MQ7	C31-C32-C33	-3.37	119.92	127.62
19	C	304	MQ9	C32-C33-C34	-3.36	119.94	127.62
20	G	301	9Y0	O7-C21-C22	3.35	118.72	111.48
16	F	606	CDL	OA6-CA5-C11	3.33	118.69	111.48
22	R	602	HEA	C4D-C3D-C2D	-3.33	102.04	106.89
22	F	602	HEA	CMC-C2C-C1C	3.32	130.48	125.42
22	R	602	HEA	C13-C14-C15	-3.31	120.04	127.62
24	H	201	MQ7	C24-C23-C25	3.31	120.97	115.23
22	R	601	HEA	C4D-C3D-C2D	-3.27	102.13	106.89
22	R	601	HEA	C13-C14-C15	-3.27	120.14	127.62
22	F	601	HEA	C4D-C3D-C2D	-3.26	102.15	106.89
24	H	201	MQ7	C21-C22-C23	-3.25	120.18	127.62
22	R	601	HEA	C13-C12-C11	-3.24	109.22	114.39
22	R	602	HEA	C13-C12-C11	-3.23	109.23	114.39
24	H	201	MQ7	C26-C27-C28	-3.22	120.26	127.62
22	R	601	HEA	CHA-C4D-ND	-3.21	120.97	124.42
22	F	602	HEA	C17-C18-C19	-3.20	120.29	127.62
16	R	606	CDL	OA6-CA5-C11	3.20	118.41	111.48
22	F	602	HEA	C4D-C3D-C2D	-3.20	102.23	106.89
24	O	301	MQ7	C24-C23-C25	3.18	120.75	115.23
24	O	301	MQ7	C26-C27-C28	-3.15	120.41	127.62
22	F	601	HEA	C4A-NA-C1A	-3.15	100.69	105.82
19	C	304	MQ9	C37-C38-C39	-3.14	120.43	127.62
22	F	602	HEA	CAD-C3D-C4D	3.14	130.17	124.70
20	P	102	9Y0	O7-C21-C22	3.13	118.26	111.48
22	R	601	HEA	CHB-C1B-NB	-3.12	121.06	124.42
22	F	602	HEA	CHB-C1B-NB	-3.12	121.07	124.42
19	O	305	MQ9	C32-C33-C34	-3.12	120.49	127.62
22	F	601	HEA	C27-C19-C20	3.09	120.59	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	C	304	MQ9	C25-C24-C26	3.09	120.59	115.23
19	C	304	MQ9	C45-C44-C46	3.09	120.58	115.23
19	O	305	MQ9	C15-C14-C16	3.08	120.57	115.23
17	N	606	A1IRE	C06-C05-N11	3.08	121.31	118.41
22	R	602	HEA	C4B-C3B-C2B	-3.04	102.33	107.44
22	R	601	HEA	C4B-C3B-C2B	-3.04	102.33	107.44
24	H	201	MQ7	C31-C32-C33	-3.03	120.69	127.62
22	R	601	HEA	C4A-NA-C1A	-3.02	100.91	105.82
19	C	304	MQ9	C7-C6-C5	-2.98	119.78	124.89
19	C	304	MQ9	C22-C23-C24	-2.98	120.81	127.62
19	O	305	MQ9	C12-C13-C14	-2.97	120.82	127.62
19	C	304	MQ9	C12-C13-C14	-2.97	120.83	127.62
17	B	606	A1IRE	C17-C16-N15	-2.92	106.92	113.07
22	F	601	HEA	C4B-C3B-C2B	-2.91	102.54	107.44
24	H	201	MQ7	C14-C13-C15	2.90	120.27	115.23
19	O	305	MQ9	C25-C24-C26	2.89	120.25	115.23
19	O	305	MQ9	C42-C43-C44	-2.89	121.00	127.62
19	O	305	MQ9	C22-C23-C24	-2.87	121.06	127.62
13	M	502	9YF	C7-C6-C5	2.86	115.84	110.83
22	R	601	HEA	CMB-C2B-C1B	2.84	129.48	125.03
16	M	503	CDL	OA8-CA7-C31	2.84	120.49	111.83
22	R	602	HEA	CHB-C1B-NB	-2.84	121.37	124.42
13	M	502	9YF	O11-C25-C26	2.82	120.44	111.83
24	O	301	MQ7	C21-C22-C23	-2.82	121.17	127.62
19	C	304	MQ9	C5M-C5-C6	-2.81	119.83	124.45
17	B	606	A1IRE	C06-C05-N11	2.81	121.06	118.41
24	O	301	MQ7	C29-C28-C30	2.81	120.10	115.23
19	C	304	MQ9	C15-C14-C16	2.81	120.10	115.23
16	B	603	CDL	OA8-CA7-C31	2.81	120.39	111.83
16	M	503	CDL	OB8-CB7-C71	2.80	120.39	111.83
16	B	604	CDL	OB8-CB7-C71	2.80	120.37	111.83
22	F	601	HEA	CMC-C2C-C1C	2.80	129.68	125.42
16	F	605	CDL	OA8-CA7-C31	2.78	120.32	111.83
24	H	201	MQ7	C34-C33-C35	2.77	120.03	115.23
16	R	605	CDL	OA8-CA7-C31	2.75	120.23	111.83
16	N	607	CDL	OA8-CA7-C31	2.75	120.22	111.83
13	O	304	9YF	O11-C25-C26	2.75	120.22	111.83
16	B	603	CDL	OB8-CB7-C71	2.75	120.22	111.83
17	N	606	A1IRE	C12-N11-C05	2.75	108.88	106.66
16	N	603	CDL	OB8-CB7-C71	2.74	120.17	111.83
16	C	305	CDL	OA8-CA7-C31	2.73	120.17	111.83
16	D	101	CDL	OA8-CA7-C31	2.73	120.17	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	O	305	MQ9	C37-C38-C39	-2.73	121.37	127.62
16	C	305	CDL	OB8-CB7-C71	2.73	120.16	111.83
16	D	103	CDL	OA8-CA7-C31	2.73	120.15	111.83
22	F	602	HEA	C4B-C3B-C2B	-2.73	102.86	107.44
16	N	604	CDL	OB8-CB7-C71	2.73	120.15	111.83
20	G	301	9Y0	O5-C5-C6	2.72	120.14	111.83
24	H	201	MQ7	C16-C17-C18	-2.72	121.40	127.62
22	R	602	HEA	C4A-NA-C1A	-2.72	101.39	105.82
17	N	606	A1IRE	N11-C05-N04	-2.71	108.81	111.26
16	P	103	CDL	OB8-CB7-C71	2.70	120.08	111.83
18	O	303	HEC	C2A-C1A-NA	-2.70	107.71	110.32
16	R	605	CDL	OB8-CB7-C71	2.70	120.07	111.83
22	F	601	HEA	CHB-C1B-NB	-2.70	121.52	124.42
16	N	607	CDL	OB8-CB7-C71	2.70	120.05	111.83
16	P	103	CDL	OA8-CA7-C31	2.69	120.04	111.83
24	H	201	MQ7	C29-C28-C30	2.69	119.90	115.23
13	A	502	9YF	O11-C25-C26	2.69	120.04	111.83
18	C	302	HEC	C2A-C1A-NA	-2.69	107.73	110.32
16	B	604	CDL	OA8-CA7-C31	2.69	120.03	111.83
16	N	603	CDL	OA8-CA7-C31	2.69	120.03	111.83
18	O	302	HEC	C2A-C1A-NA	-2.69	107.73	110.32
19	O	305	MQ9	C7-C6-C5	-2.69	120.29	124.89
16	N	604	CDL	OA8-CA7-C31	2.69	120.02	111.83
24	H	201	MQ7	C19-C18-C20	2.68	119.89	115.23
16	R	606	CDL	OB8-CB7-C71	2.68	120.01	111.83
16	D	103	CDL	OB8-CB7-C71	2.68	120.01	111.83
19	C	304	MQ9	C17-C18-C19	-2.67	121.50	127.62
18	C	301	HEC	C2A-C1A-NA	-2.67	107.75	110.32
22	R	601	HEA	C25-C23-C24	2.67	120.73	114.59
20	S	301	9Y0	O5-C5-C6	2.66	119.96	111.83
16	F	606	CDL	OA8-CA7-C31	2.66	119.94	111.83
16	F	605	CDL	OB8-CB7-C71	2.65	119.92	111.83
22	R	601	HEA	C27-C19-C20	2.64	119.81	115.23
13	O	304	9YF	C7-C2-C3	2.63	114.51	110.86
22	R	602	HEA	CBA-CAA-C2A	-2.63	105.27	112.53
22	F	601	HEA	CMB-C2B-C1B	2.63	129.14	125.03
16	B	605	CDL	OB8-CB7-C71	2.62	119.83	111.83
22	R	602	HEA	CMC-C2C-C1C	2.62	129.41	125.42
16	P	101	CDL	OA8-CA7-C31	2.61	119.81	111.83
24	O	301	MQ7	C34-C33-C35	2.61	119.76	115.23
22	R	601	HEA	C1D-ND-C4D	-2.61	102.12	105.21
13	C	303	9YF	O11-C25-C26	2.61	119.79	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	606	A1IRE	N11-C05-N04	-2.60	108.91	111.26
22	R	602	HEA	CAD-C3D-C4D	2.59	129.22	124.70
22	F	601	HEA	C25-C23-C24	2.59	120.56	114.59
20	P	102	9Y0	O5-C5-C6	2.59	119.74	111.83
22	R	602	HEA	C27-C19-C20	2.59	119.73	115.23
19	O	305	MQ9	C45-C44-C46	2.58	119.72	115.23
17	B	606	A1IRE	C12-N11-C05	2.58	108.75	106.66
16	D	101	CDL	OB8-CB7-C71	2.58	119.70	111.83
17	B	606	A1IRE	C03-C12-N11	2.58	106.45	104.83
19	O	305	MQ9	C27-C28-C29	-2.58	121.73	127.62
19	C	304	MQ9	C42-C43-C44	-2.57	121.73	127.62
20	D	102	9Y0	O5-C5-C6	2.57	119.67	111.83
22	R	601	HEA	CHC-C1C-C2C	-2.57	119.97	127.43
22	F	601	HEA	C26-C15-C16	2.56	119.68	115.23
24	O	301	MQ7	C11-C3-C2	-2.56	120.50	124.89
19	O	305	MQ9	C35-C34-C36	2.56	119.67	115.23
16	P	101	CDL	OB8-CB7-C71	2.56	119.64	111.83
16	R	606	CDL	OA8-CA7-C31	2.55	119.62	111.83
19	C	304	MQ9	C35-C34-C36	2.54	119.64	115.23
22	F	602	HEA	C27-C19-C20	2.54	119.64	115.23
19	O	305	MQ9	C5M-C5-C6	-2.53	120.29	124.45
19	C	304	MQ9	C40-C39-C41	2.53	119.61	115.23
22	R	601	HEA	C4B-NB-C1B	-2.53	102.22	105.21
24	O	301	MQ7	C16-C17-C18	-2.53	121.84	127.62
24	H	201	MQ7	C39-C38-C40	2.52	119.60	115.23
24	O	301	MQ7	C19-C18-C20	2.52	119.60	115.23
22	F	602	HEA	C26-C15-C16	2.51	119.58	115.23
22	R	601	HEA	CMC-C2C-C1C	2.50	129.22	125.42
22	R	601	HEA	C17-C18-C19	-2.49	121.92	127.62
16	F	606	CDL	OB8-CB7-C71	2.49	119.43	111.83
16	N	605	CDL	OA8-CA7-C31	2.49	119.42	111.83
22	F	601	HEA	CHC-C1C-C2C	-2.48	120.22	127.43
19	O	305	MQ9	C10-C9-C11	2.47	119.52	115.23
13	M	502	9YF	C6-C5-C4	2.47	115.17	110.83
22	F	601	HEA	C13-C12-C11	-2.46	110.46	114.39
24	O	301	MQ7	C2M-C2-C3	-2.45	120.42	124.45
22	F	602	HEA	CAD-CBD-CGD	-2.44	107.18	113.67
16	B	605	CDL	OA8-CA7-C31	2.43	119.24	111.83
19	O	305	MQ9	C30-C29-C31	2.42	119.43	115.23
24	O	301	MQ7	C41-C42-C43	-2.42	119.57	127.64
15	N	601	HEM	C4D-ND-C1D	2.42	108.07	105.21
22	F	601	HEA	CHA-C4D-ND	-2.41	121.83	124.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	R	601	HEA	CHA-C1A-NA	-2.40	121.84	124.45
22	F	602	HEA	CMB-C2B-C1B	2.39	128.77	125.03
24	O	301	MQ7	C45-C43-C44	2.39	120.09	114.59
19	C	304	MQ9	C27-C28-C29	-2.38	122.18	127.62
16	N	605	CDL	OB8-CB7-C71	2.38	119.08	111.83
22	F	601	HEA	C4B-NB-C1B	-2.36	102.41	105.21
22	F	601	HEA	C1D-ND-C4D	-2.36	102.42	105.21
22	R	601	HEA	CHD-C1D-C2D	-2.35	120.26	126.95
19	O	305	MQ9	C47-C48-C49	-2.34	119.83	127.64
19	O	305	MQ9	C40-C39-C41	2.34	119.30	115.23
22	F	601	HEA	CHA-C4D-C3D	-2.34	121.36	124.77
19	C	304	MQ9	C10-C9-C11	2.33	119.27	115.23
22	F	602	HEA	C25-C23-C24	2.33	119.94	114.59
15	B	602	HEM	C1B-NB-C4B	2.32	107.96	105.21
24	H	201	MQ7	C45-C43-C44	2.31	119.92	114.59
17	B	606	A1IRE	O14-C13-N15	-2.31	119.17	123.35
15	B	601	HEM	C4D-ND-C1D	2.31	107.94	105.21
19	C	304	MQ9	C20-C19-C21	2.31	119.24	115.23
22	R	602	HEA	C25-C23-C24	2.31	119.90	114.59
22	F	602	HEA	CHC-C4B-NB	-2.31	121.52	124.37
19	O	305	MQ9	C51-C49-C50	2.30	119.88	114.59
22	R	602	HEA	C26-C15-C16	2.30	119.22	115.23
15	B	601	HEM	C1B-NB-C4B	2.29	107.91	105.21
17	N	606	A1IRE	C10-N11-C05	-2.28	120.61	122.33
22	R	602	HEA	OMA-CMA-C3A	-2.28	120.47	125.62
22	R	601	HEA	C26-C15-C16	2.28	119.19	115.23
22	F	602	HEA	OMA-CMA-C3A	-2.28	120.48	125.62
22	R	601	HEA	C21-C22-C23	-2.27	120.06	127.64
22	F	602	HEA	CMD-C2D-C1D	2.27	128.58	125.03
15	N	602	HEM	C4D-ND-C1D	2.24	107.86	105.21
15	N	601	HEM	C1B-NB-C4B	2.24	107.86	105.21
19	O	305	MQ9	C20-C19-C21	2.24	119.11	115.23
13	A	502	9YF	C7-C6-C5	2.23	114.75	110.83
24	O	301	MQ7	C39-C38-C40	2.23	119.10	115.23
22	R	602	HEA	CHC-C4B-NB	-2.23	121.61	124.37
15	B	602	HEM	C2A-C1A-NA	-2.22	107.69	110.15
22	F	601	HEA	CAD-CBD-CGD	-2.21	107.80	113.67
17	N	606	A1IRE	C03-C12-N11	2.21	106.22	104.83
22	F	601	HEA	CHD-C1D-C2D	-2.20	120.68	126.95
24	H	201	MQ7	C41-C42-C43	-2.19	120.34	127.64
24	O	301	MQ7	C14-C13-C15	2.19	119.03	115.23
22	R	601	HEA	CHB-C4A-NA	-2.18	122.08	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	F	601	HEA	C17-C18-C19	-2.18	122.64	127.62
16	P	101	CDL	CB4-OB6-CB5	-2.17	112.59	117.80
18	O	302	HEC	CAA-CBA-CGA	-2.17	107.90	113.67
15	N	601	HEM	C3D-C4D-ND	-2.17	107.79	110.17
17	N	606	A1IRE	O14-C13-N15	-2.17	119.43	123.35
22	F	602	HEA	C4A-NA-C1A	-2.17	102.29	105.82
13	A	502	9YF	C31-C32-C33	-2.15	108.81	115.97
22	F	602	HEA	CBA-CAA-C2A	-2.15	106.59	112.53
19	C	304	MQ9	C47-C48-C49	-2.14	120.50	127.64
15	B	601	HEM	C3D-C4D-ND	-2.14	107.83	110.17
18	C	302	HEC	CAD-C3D-C4D	2.14	129.11	124.94
22	R	602	HEA	CMB-C2B-C1B	2.13	128.35	125.03
22	R	601	HEA	CAD-C3D-C4D	2.12	128.40	124.70
17	B	606	A1IRE	C02-C03-N04	2.12	125.39	119.17
16	M	503	CDL	OB6-CB5-OB7	-2.09	118.81	123.70
22	R	602	HEA	C21-C22-C23	-2.09	120.69	127.64
13	A	502	9YF	C6-C5-C4	2.09	114.49	110.83
15	B	601	HEM	C3B-C2B-C1B	2.08	107.97	106.41
22	R	602	HEA	CHC-C1C-C2C	-2.07	121.43	127.43
22	F	602	HEA	C21-C22-C23	-2.06	120.76	127.64
22	R	601	HEA	CHC-C4B-C3B	-2.06	120.60	125.80
19	C	304	MQ9	C51-C49-C50	2.06	119.32	114.59
15	N	602	HEM	C2A-C1A-NA	-2.06	107.87	110.15
22	R	601	HEA	OMA-CMA-C3A	-2.06	120.98	125.62
13	M	502	9YF	C31-C32-C33	-2.05	109.14	115.97
17	B	606	A1IRE	C26-C25-C24	2.05	90.35	88.14
19	C	304	MQ9	C5M-C5-C4	2.05	120.45	116.68
17	B	606	A1IRE	C10-C08-CL09	2.05	120.92	119.03
22	F	601	HEA	CHA-C1A-NA	-2.04	122.23	124.45
22	F	602	HEA	CAA-C2A-C1A	2.03	128.97	124.85
13	A	502	9YF	C36-C35-C33	-2.02	109.27	115.97
15	N	601	HEM	C3B-C2B-C1B	2.01	107.92	106.41
22	R	602	HEA	CAA-C2A-C1A	2.01	128.93	124.85

There are no chirality outliers.

All (1195) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	A	502	9YF	C1-O-P-O1
13	A	502	9YF	C1-O-P-O2
13	A	502	9YF	C1-O-P-O8
13	A	502	9YF	O9-C-C1-O

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Mol	Chain	Res	Type	Atoms
13	C	303	9YF	C2-O2-P-O
13	C	303	9YF	C1-O-P-O1
13	C	303	9YF	C1-O-P-O2
13	C	303	9YF	C1-O-P-O8
13	M	502	9YF	C1-O-P-O1
13	M	502	9YF	C1-O-P-O2
13	M	502	9YF	C1-O-P-O8
13	M	502	9YF	O9-C-C1-O
13	O	304	9YF	C1-O-P-O1
13	O	304	9YF	C1-O-P-O2
13	O	304	9YF	C1-O-P-O8
14	G	302	PLM	O2-C1-C2-C3
16	B	603	CDL	CA2-OA2-PA1-OA3
16	B	603	CDL	CA2-OA2-PA1-OA4
16	B	603	CDL	CA2-OA2-PA1-OA5
16	B	603	CDL	CA3-OA5-PA1-OA4
16	B	603	CDL	C11-CA5-OA6-CA4
16	B	604	CDL	CA2-OA2-PA1-OA4
16	B	604	CDL	CB2-OB2-PB2-OB3
16	B	604	CDL	CB2-OB2-PB2-OB4
16	B	604	CDL	CB2-OB2-PB2-OB5
16	B	604	CDL	CB3-OB5-PB2-OB2
16	B	604	CDL	CB3-OB5-PB2-OB4
16	B	604	CDL	C51-CB5-OB6-CB4
16	B	605	CDL	CA2-OA2-PA1-OA3
16	B	605	CDL	CA2-OA2-PA1-OA4
16	B	605	CDL	CA2-OA2-PA1-OA5
16	B	605	CDL	CA3-OA5-PA1-OA2
16	B	605	CDL	CA3-OA5-PA1-OA4
16	B	605	CDL	CB3-OB5-PB2-OB2
16	B	605	CDL	CB3-OB5-PB2-OB3
16	B	605	CDL	CB3-OB5-PB2-OB4
16	B	605	CDL	OB7-CB5-OB6-CB4
16	C	305	CDL	CA2-OA2-PA1-OA3
16	C	305	CDL	CA3-OA5-PA1-OA2
16	C	305	CDL	CA3-OA5-PA1-OA3
16	C	305	CDL	CB3-OB5-PB2-OB4
16	D	101	CDL	CB2-C1-CA2-OA2
16	D	101	CDL	CA2-OA2-PA1-OA3
16	D	101	CDL	CA2-OA2-PA1-OA4
16	D	101	CDL	CA3-OA5-PA1-OA2
16	D	101	CDL	CA3-OA5-PA1-OA3

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Mol	Chain	Res	Type	Atoms
16	D	101	CDL	CA3-OA5-PA1-OA4
16	D	101	CDL	C51-CB5-OB6-CB4
16	D	103	CDL	CB2-OB2-PB2-OB4
16	D	103	CDL	CB2-OB2-PB2-OB5
16	D	103	CDL	CB3-OB5-PB2-OB2
16	D	103	CDL	CB3-OB5-PB2-OB3
16	D	103	CDL	OB7-CB5-OB6-CB4
16	D	103	CDL	C51-CB5-OB6-CB4
16	F	605	CDL	CA2-OA2-PA1-OA3
16	F	605	CDL	CA2-OA2-PA1-OA4
16	F	605	CDL	CA2-OA2-PA1-OA5
16	F	605	CDL	CB2-OB2-PB2-OB3
16	F	605	CDL	CB2-OB2-PB2-OB4
16	F	605	CDL	CB2-OB2-PB2-OB5
16	F	605	CDL	CB3-OB5-PB2-OB2
16	F	605	CDL	CB3-OB5-PB2-OB3
16	F	605	CDL	CB3-OB5-PB2-OB4
16	F	605	CDL	C51-CB5-OB6-CB4
16	F	606	CDL	O1-C1-CB2-OB2
16	F	606	CDL	CB2-OB2-PB2-OB3
16	F	606	CDL	CB2-OB2-PB2-OB5
16	F	606	CDL	CB3-OB5-PB2-OB3
16	M	503	CDL	CA2-OA2-PA1-OA3
16	M	503	CDL	CA2-OA2-PA1-OA4
16	M	503	CDL	CA2-OA2-PA1-OA5
16	M	503	CDL	CA3-OA5-PA1-OA2
16	M	503	CDL	CA3-OA5-PA1-OA3
16	M	503	CDL	CA3-OA5-PA1-OA4
16	M	503	CDL	C11-CA5-OA6-CA4
16	M	503	CDL	CB2-OB2-PB2-OB3
16	M	503	CDL	CB2-OB2-PB2-OB4
16	M	503	CDL	CB2-OB2-PB2-OB5
16	M	503	CDL	OB6-CB4-CB6-OB8
16	M	503	CDL	OB7-CB5-OB6-CB4
16	M	503	CDL	C51-CB5-OB6-CB4
16	M	503	CDL	OB9-CB7-OB8-CB6
16	M	503	CDL	C71-CB7-OB8-CB6
16	N	603	CDL	CB3-OB5-PB2-OB3
16	N	603	CDL	CB3-OB5-PB2-OB4
16	N	604	CDL	O1-C1-CA2-OA2
16	N	604	CDL	CA2-OA2-PA1-OA3
16	N	604	CDL	CA3-OA5-PA1-OA2

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Mol	Chain	Res	Type	Atoms
16	N	604	CDL	CA3-OA5-PA1-OA3
16	N	604	CDL	CB3-OB5-PB2-OB3
16	N	604	CDL	OB7-CB5-OB6-CB4
16	N	604	CDL	C51-CB5-OB6-CB4
16	N	605	CDL	O1-C1-CB2-OB2
16	N	605	CDL	CB3-OB5-PB2-OB4
16	N	605	CDL	OB7-CB5-OB6-CB4
16	N	605	CDL	C51-CB5-OB6-CB4
16	N	607	CDL	CA3-OA5-PA1-OA2
16	N	607	CDL	CB2-OB2-PB2-OB4
16	N	607	CDL	CB2-OB2-PB2-OB5
16	N	607	CDL	OB9-CB7-OB8-CB6
16	P	101	CDL	O1-C1-CB2-OB2
16	P	101	CDL	CA2-C1-CB2-OB2
16	P	101	CDL	CA3-OA5-PA1-OA2
16	P	101	CDL	CA3-OA5-PA1-OA3
16	P	101	CDL	OA5-CA3-CA4-OA6
16	P	101	CDL	CB2-OB2-PB2-OB3
16	P	101	CDL	CB2-OB2-PB2-OB4
16	P	101	CDL	CB2-OB2-PB2-OB5
16	P	101	CDL	C51-CB5-OB6-CB4
16	P	103	CDL	O1-C1-CA2-OA2
16	P	103	CDL	C11-CA5-OA6-CA4
16	P	103	CDL	CB2-OB2-PB2-OB3
16	P	103	CDL	CB2-OB2-PB2-OB5
16	R	605	CDL	CA2-C1-CB2-OB2
16	R	605	CDL	CA3-OA5-PA1-OA3
16	R	605	CDL	CB3-OB5-PB2-OB3
16	R	606	CDL	CA2-C1-CB2-OB2
16	R	606	CDL	CA2-OA2-PA1-OA3
16	R	606	CDL	CA2-OA2-PA1-OA4
16	R	606	CDL	CA2-OA2-PA1-OA5
16	R	606	CDL	CB2-OB2-PB2-OB3
16	R	606	CDL	CB2-OB2-PB2-OB4
16	R	606	CDL	CB2-OB2-PB2-OB5
16	R	606	CDL	CB3-OB5-PB2-OB2
16	R	606	CDL	CB3-OB5-PB2-OB3
16	R	606	CDL	CB3-OB5-PB2-OB4
16	R	606	CDL	OB5-CB3-CB4-OB6
17	B	606	A1IRE	C01-C02-C03-C12
17	B	606	A1IRE	C01-C02-C03-N04
17	B	606	A1IRE	C27-N28-S30-O32

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Mol	Chain	Res	Type	Atoms
17	N	606	A1IRE	C01-C02-C03-C12
18	C	301	HEC	C2B-C3B-CAB-CBB
18	C	301	HEC	C4B-C3B-CAB-CBB
18	C	301	HEC	C2C-C3C-CAC-CBC
18	C	301	HEC	C4C-C3C-CAC-CBC
18	C	302	HEC	C2B-C3B-CAB-CBB
18	C	302	HEC	C4B-C3B-CAB-CBB
18	C	302	HEC	C2C-C3C-CAC-CBC
18	C	302	HEC	C4C-C3C-CAC-CBC
18	O	302	HEC	C2B-C3B-CAB-CBB
18	O	302	HEC	C4B-C3B-CAB-CBB
18	O	302	HEC	C2C-C3C-CAC-CBC
18	O	303	HEC	C2B-C3B-CAB-CBB
18	O	303	HEC	C4B-C3B-CAB-CBB
18	O	303	HEC	C2C-C3C-CAC-CBC
18	O	303	HEC	C4C-C3C-CAC-CBC
19	C	304	MQ9	C14-C16-C17-C18
19	O	305	MQ9	C9-C11-C12-C13
19	O	305	MQ9	C13-C14-C16-C17
19	O	305	MQ9	C15-C14-C16-C17
20	D	102	9Y0	C22-C21-O7-C1
20	D	102	9Y0	O1-C3-C4-N
20	D	102	9Y0	C3-O1-P-O
20	D	102	9Y0	C3-O1-P-O3
20	G	301	9Y0	O5-C-C1-O7
20	G	301	9Y0	C3-O1-P-O
20	G	301	9Y0	C3-O1-P-O2
20	G	301	9Y0	C3-O1-P-O3
20	P	102	9Y0	O1-C3-C4-N
20	P	102	9Y0	C3-O1-P-O
20	P	102	9Y0	C3-O1-P-O3
20	P	102	9Y0	C2-O3-P-O
20	P	102	9Y0	C2-O3-P-O2
20	S	301	9Y0	O1-C3-C4-N
13	C	303	9YF	O12-C25-O11-C24
16	B	605	CDL	OA9-CA7-OA8-CA6
16	D	101	CDL	OB9-CB7-OB8-CB6
13	C	303	9YF	C26-C25-O11-C24
16	B	603	CDL	C31-CA7-OA8-CA6
16	B	605	CDL	C31-CA7-OA8-CA6
16	D	101	CDL	C71-CB7-OB8-CB6
16	B	603	CDL	OA9-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
16	D	103	CDL	OA9-CA7-OA8-CA6
16	B	603	CDL	OA7-CA5-OA6-CA4
16	B	604	CDL	OB7-CB5-OB6-CB4
16	D	101	CDL	OB7-CB5-OB6-CB4
16	F	605	CDL	OB7-CB5-OB6-CB4
16	M	503	CDL	OA7-CA5-OA6-CA4
16	P	103	CDL	OA7-CA5-OA6-CA4
20	D	102	9Y0	O6-C21-O7-C1
13	O	304	9YF	C26-C25-O11-C24
16	C	305	CDL	C71-CB7-OB8-CB6
16	N	607	CDL	C71-CB7-OB8-CB6
16	P	103	CDL	C31-CA7-OA8-CA6
16	B	605	CDL	C51-CB5-OB6-CB4
19	O	305	MQ9	C40-C39-C41-C42
22	F	602	HEA	C26-C15-C16-C17
24	H	201	MQ7	C14-C13-C15-C16
24	H	201	MQ7	C19-C18-C20-C21
24	H	201	MQ7	C24-C23-C25-C26
24	O	301	MQ7	C24-C23-C25-C26
19	O	305	MQ9	C38-C39-C41-C42
22	F	602	HEA	C14-C15-C16-C17
24	H	201	MQ7	C12-C13-C15-C16
24	H	201	MQ7	C17-C18-C20-C21
24	H	201	MQ7	C22-C23-C25-C26
16	D	103	CDL	C31-CA7-OA8-CA6
16	R	606	CDL	C71-CB7-OB8-CB6
20	P	102	9Y0	C6-C5-O5-C
13	O	304	9YF	O12-C25-O11-C24
16	C	305	CDL	OB9-CB7-OB8-CB6
16	P	103	CDL	OA9-CA7-OA8-CA6
16	R	606	CDL	OB9-CB7-OB8-CB6
16	P	101	CDL	OB7-CB5-OB6-CB4
16	D	103	CDL	C15-C16-C17-C18
16	B	603	CDL	O1-C1-CA2-OA2
16	B	604	CDL	O1-C1-CA2-OA2
16	B	604	CDL	O1-C1-CB2-OB2
16	D	101	CDL	O1-C1-CA2-OA2
16	D	101	CDL	O1-C1-CB2-OB2
16	D	103	CDL	O1-C1-CA2-OA2
16	N	603	CDL	O1-C1-CB2-OB2
16	R	606	CDL	O1-C1-CB2-OB2
13	O	304	9YF	C9-C8-O9-C

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Mol	Chain	Res	Type	Atoms
16	D	101	CDL	C11-CA5-OA6-CA4
16	F	606	CDL	C51-CB5-OB6-CB4
16	R	606	CDL	C51-CB5-OB6-CB4
19	O	305	MQ9	C35-C34-C36-C37
24	O	301	MQ7	C19-C18-C20-C21
19	C	304	MQ9	C23-C24-C26-C27
20	P	102	9Y0	O4-C5-O5-C
19	C	304	MQ9	C9-C11-C12-C13
19	C	304	MQ9	C39-C41-C42-C43
19	O	305	MQ9	C14-C16-C17-C18
19	O	305	MQ9	C19-C21-C22-C23
19	O	305	MQ9	C39-C41-C42-C43
22	F	602	HEA	C15-C16-C17-C18
22	F	602	HEA	C19-C20-C21-C22
22	R	602	HEA	C19-C20-C21-C22
24	H	201	MQ7	C13-C15-C16-C17
24	H	201	MQ7	C38-C40-C41-C42
13	O	304	9YF	C14-C15-C16-C17
22	R	601	HEA	C2A-CAA-CBA-CGA
16	P	101	CDL	C31-CA7-OA8-CA6
16	R	605	CDL	C71-CB7-OB8-CB6
16	R	605	CDL	OB9-CB7-OB8-CB6
13	M	502	9YF	C17-C18-C19-C20
16	M	503	CDL	C18-C19-C20-C21
16	N	603	CDL	C74-C75-C76-C77
13	O	304	9YF	O10-C8-O9-C
16	D	101	CDL	OA7-CA5-OA6-CA4
16	R	606	CDL	OB7-CB5-OB6-CB4
16	D	103	CDL	CA2-C1-CB2-OB2
16	F	605	CDL	CB2-C1-CA2-OA2
16	F	606	CDL	CA2-C1-CB2-OB2
16	N	603	CDL	CA2-C1-CB2-OB2
16	N	604	CDL	CB2-C1-CA2-OA2
16	N	605	CDL	CB2-C1-CA2-OA2
16	N	605	CDL	CA2-C1-CB2-OB2
16	N	607	CDL	CB2-C1-CA2-OA2
16	P	101	CDL	CB2-C1-CA2-OA2
16	P	103	CDL	CA2-C1-CB2-OB2
16	R	606	CDL	CB2-C1-CA2-OA2
13	M	502	9YF	C26-C25-O11-C24
20	S	301	9Y0	C6-C5-O5-C
13	C	303	9YF	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
16	P	103	CDL	C19-C20-C21-C22
16	M	503	CDL	C51-C52-C53-C54
19	C	304	MQ9	C25-C24-C26-C27
19	O	305	MQ9	C25-C24-C26-C27
19	O	305	MQ9	C23-C24-C26-C27
19	O	305	MQ9	C33-C34-C36-C37
24	O	301	MQ7	C17-C18-C20-C21
24	O	301	MQ7	C22-C23-C25-C26
13	O	304	9YF	C34-C33-C35-C36
16	D	103	CDL	C31-C32-C33-C34
16	D	101	CDL	C15-C16-C17-C18
16	B	605	CDL	O1-C1-CA2-OA2
16	D	103	CDL	O1-C1-CB2-OB2
16	N	603	CDL	O1-C1-CA2-OA2
16	N	604	CDL	O1-C1-CB2-OB2
16	N	605	CDL	O1-C1-CA2-OA2
16	P	101	CDL	O1-C1-CA2-OA2
16	P	103	CDL	O1-C1-CB2-OB2
16	R	606	CDL	O1-C1-CA2-OA2
16	N	603	CDL	C76-C77-C78-C79
13	A	502	9YF	C11-C10-C9-C8
16	N	605	CDL	CB7-C71-C72-C73
17	N	606	A1IRE	F34-C33-S30-O31
20	S	301	9Y0	O4-C5-O5-C
16	B	605	CDL	OB5-CB3-CB4-OB6
16	D	101	CDL	OA5-CA3-CA4-OA6
16	B	605	CDL	C11-CA5-OA6-CA4
16	N	607	CDL	C11-CA5-OA6-CA4
16	P	103	CDL	OB6-CB4-CB6-OB8
16	N	607	CDL	CA5-C11-C12-C13
16	R	606	CDL	CA5-C11-C12-C13
16	M	503	CDL	CA7-C31-C32-C33
16	F	606	CDL	OB7-CB5-OB6-CB4
19	C	304	MQ9	C34-C36-C37-C38
19	C	304	MQ9	C44-C46-C47-C48
19	O	305	MQ9	C44-C46-C47-C48
22	R	602	HEA	C15-C16-C17-C18
24	O	301	MQ7	C13-C15-C16-C17
24	O	301	MQ7	C38-C40-C41-C42
16	F	605	CDL	CB7-C71-C72-C73
16	F	606	CDL	CB5-C51-C52-C53
16	M	503	CDL	CA5-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
16	R	605	CDL	CB7-C71-C72-C73
16	R	606	CDL	CB5-C51-C52-C53
20	S	301	9Y0	C21-C22-C23-C24
20	S	301	9Y0	C5-C6-C7-C8
17	B	606	A1IRE	F35-C33-S30-O32
13	A	502	9YF	C25-C26-C27-C28
16	B	605	CDL	CB7-C71-C72-C73
16	D	101	CDL	CB5-C51-C52-C53
16	D	103	CDL	CA5-C11-C12-C13
16	F	605	CDL	CA7-C31-C32-C33
16	M	503	CDL	CB7-C71-C72-C73
16	N	607	CDL	CB7-C71-C72-C73
13	M	502	9YF	O12-C25-O11-C24
13	C	303	9YF	C9-C10-C11-C12
16	D	103	CDL	C19-C20-C21-C22
17	B	606	A1IRE	F34-C33-S30-O32
17	N	606	A1IRE	F35-C33-S30-O31
17	N	606	A1IRE	F36-C33-S30-O31
14	G	302	PLM	C7-C8-C9-CA
16	D	101	CDL	C31-C32-C33-C34
16	P	103	CDL	C76-C77-C78-C79
17	B	606	A1IRE	F36-C33-S30-N28
17	N	606	A1IRE	F36-C33-S30-N28
16	B	603	CDL	O1-C1-CB2-OB2
16	F	606	CDL	O1-C1-CA2-OA2
16	R	605	CDL	O1-C1-CB2-OB2
16	F	605	CDL	C71-CB7-OB8-CB6
16	P	101	CDL	OA9-CA7-OA8-CA6
16	B	605	CDL	OA7-CA5-OA6-CA4
17	B	606	A1IRE	F36-C33-S30-O32
13	A	502	9YF	C33-C35-C36-C37
16	C	305	CDL	C11-CA5-OA6-CA4
16	F	606	CDL	CA5-C11-C12-C13
16	N	605	CDL	C57-C58-C59-C60
16	C	305	CDL	OA7-CA5-OA6-CA4
16	D	103	CDL	OA7-CA5-OA6-CA4
16	N	607	CDL	OA7-CA5-OA6-CA4
16	B	603	CDL	CA2-C1-CB2-OB2
16	B	604	CDL	CB2-C1-CA2-OA2
16	B	605	CDL	CB2-C1-CA2-OA2
16	N	605	CDL	C77-C78-C79-C80
16	R	606	CDL	C58-C59-C60-C61

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Mol	Chain	Res	Type	Atoms
16	D	103	CDL	C11-CA5-OA6-CA4
16	N	605	CDL	C11-CA5-OA6-CA4
16	P	101	CDL	C11-CA5-OA6-CA4
16	D	101	CDL	C74-C75-C76-C77
16	N	607	CDL	C80-C81-C82-C83
16	R	606	CDL	C51-C52-C53-C54
17	B	606	A1IRE	F35-C33-S30-O31
17	N	606	A1IRE	F34-C33-S30-O32
16	N	605	CDL	OA7-CA5-OA6-CA4
19	C	304	MQ9	C24-C26-C27-C28
19	O	305	MQ9	C24-C26-C27-C28
24	O	301	MQ7	C28-C30-C31-C32
17	B	606	A1IRE	F34-C33-S30-N28
17	B	606	A1IRE	F35-C33-S30-N28
17	N	606	A1IRE	F34-C33-S30-N28
16	F	605	CDL	O1-C1-CA2-OA2
16	N	607	CDL	O1-C1-CA2-OA2
16	C	305	CDL	C74-C75-C76-C77
15	N	602	HEM	C3D-CAD-CBD-CGD
16	R	606	CDL	C73-C74-C75-C76
16	N	603	CDL	CB5-C51-C52-C53
20	G	301	9Y0	C5-C6-C7-C8
17	B	606	A1IRE	F34-C33-S30-O31
17	N	606	A1IRE	F35-C33-S30-O32
16	B	603	CDL	C57-C58-C59-C60
16	P	101	CDL	C22-C23-C24-C25
16	P	101	CDL	OA7-CA5-OA6-CA4
16	R	605	CDL	C51-CB5-OB6-CB4
16	D	103	CDL	C13-C14-C15-C16
16	R	605	CDL	C31-CA7-OA8-CA6
16	N	604	CDL	CA7-C31-C32-C33
13	C	303	9YF	C26-C27-C28-C29
13	M	502	9YF	C13-C14-C15-C16
16	B	603	CDL	C16-C17-C18-C19
16	B	605	CDL	C14-C15-C16-C17
16	F	605	CDL	C13-C14-C15-C16
16	F	605	CDL	C52-C53-C54-C55
16	N	604	CDL	C13-C14-C15-C16
16	N	607	CDL	C74-C75-C76-C77
17	B	606	A1IRE	F36-C33-S30-O31
17	N	606	A1IRE	F36-C33-S30-O32
14	G	302	PLM	C8-C9-CA-CB

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Mol	Chain	Res	Type	Atoms
16	C	305	CDL	C71-C72-C73-C74
16	N	603	CDL	C55-C56-C57-C58
16	N	605	CDL	C20-C21-C22-C23
16	P	103	CDL	C32-C33-C34-C35
13	C	303	9YF	C10-C11-C12-C13
16	C	305	CDL	C83-C84-C85-C86
16	D	103	CDL	C79-C80-C81-C82
16	N	603	CDL	C78-C79-C80-C81
16	P	101	CDL	C53-C54-C55-C56
16	P	101	CDL	C76-C77-C78-C79
16	P	103	CDL	C11-C12-C13-C14
16	P	103	CDL	C13-C14-C15-C16
16	P	103	CDL	C35-C36-C37-C38
16	P	103	CDL	C51-C52-C53-C54
16	B	604	CDL	C71-CB7-OB8-CB6
13	C	303	9YF	C27-C28-C29-C30
16	B	604	CDL	C51-C52-C53-C54
16	B	605	CDL	C11-C12-C13-C14
16	C	305	CDL	C51-C52-C53-C54
16	D	101	CDL	C13-C14-C15-C16
16	D	101	CDL	C20-C21-C22-C23
16	D	101	CDL	C55-C56-C57-C58
16	D	103	CDL	C21-C22-C23-C24
16	F	605	CDL	C51-C52-C53-C54
16	M	503	CDL	C75-C76-C77-C78
16	R	606	CDL	C60-C61-C62-C63
20	P	102	9Y0	C7-C8-C9-C10
20	S	301	9Y0	C27-C28-C29-C30
13	M	502	9YF	C15-C16-C17-C18
16	B	603	CDL	C76-C77-C78-C79
16	B	604	CDL	C55-C56-C57-C58
16	N	603	CDL	C51-C52-C53-C54
16	N	607	CDL	C76-C77-C78-C79
16	P	103	CDL	C55-C56-C57-C58
20	G	301	9Y0	C7-C8-C9-C10
13	C	303	9YF	C11-C10-C9-C8
13	A	502	9YF	C12-C13-C14-C15
16	D	103	CDL	C61-C62-C63-C64
16	F	605	CDL	C55-C56-C57-C58
16	F	605	CDL	OB9-CB7-OB8-CB6
16	F	605	CDL	C60-C61-C62-C63
16	N	603	CDL	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
16	N	604	CDL	C36-C37-C38-C39
20	D	102	9Y0	C24-C25-C26-C27
13	A	502	9YF	C30-C31-C32-C33
16	N	607	CDL	OA5-CA3-CA4-CA6
16	B	605	CDL	C18-C19-C20-C21
16	P	103	CDL	C16-C17-C18-C19
20	D	102	9Y0	C7-C8-C9-C10
20	P	102	9Y0	C22-C23-C24-C25
14	T	201	PLM	C8-C9-CA-CB
16	B	604	CDL	C74-C75-C76-C77
16	D	103	CDL	C56-C57-C58-C59
16	F	606	CDL	C76-C77-C78-C79
16	N	603	CDL	C79-C80-C81-C82
16	P	103	CDL	C78-C79-C80-C81
16	R	605	CDL	C59-C60-C61-C62
16	C	305	CDL	C31-C32-C33-C34
16	D	103	CDL	C62-C63-C64-C65
16	P	101	CDL	C11-C12-C13-C14
20	P	102	9Y0	C25-C26-C27-C28
16	B	604	CDL	C17-C18-C19-C20
16	D	103	CDL	CB5-C51-C52-C53
16	D	101	CDL	C79-C80-C81-C82
14	T	201	PLM	C7-C8-C9-CA
16	P	103	CDL	C58-C59-C60-C61
16	R	605	CDL	OB7-CB5-OB6-CB4
16	N	605	CDL	CB3-CB4-CB6-OB8
19	O	305	MQ9	C34-C36-C37-C38
13	C	303	9YF	C17-C18-C19-C20
16	B	605	CDL	C21-C22-C23-C24
16	D	101	CDL	C52-C53-C54-C55
16	D	103	CDL	C34-C35-C36-C37
16	F	606	CDL	C12-C13-C14-C15
16	P	101	CDL	C83-C84-C85-C86
16	B	604	CDL	CA5-C11-C12-C13
16	D	101	CDL	CB7-C71-C72-C73
16	N	607	CDL	CB5-C51-C52-C53
13	O	304	9YF	C13-C14-C15-C16
16	B	604	CDL	C59-C60-C61-C62
16	F	606	CDL	C78-C79-C80-C81
16	N	603	CDL	C58-C59-C60-C61
16	R	606	CDL	C33-C34-C35-C36
16	R	606	CDL	C76-C77-C78-C79

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Mol	Chain	Res	Type	Atoms
16	B	603	CDL	C72-C73-C74-C75
16	D	101	CDL	C17-C18-C19-C20
16	D	103	CDL	C16-C17-C18-C19
16	F	606	CDL	C31-C32-C33-C34
16	M	503	CDL	C73-C74-C75-C76
16	N	607	CDL	C77-C78-C79-C80
16	B	605	CDL	C19-C20-C21-C22
13	A	502	9YF	C38-C39-C40-C41
16	F	605	CDL	C36-C37-C38-C39
16	P	103	CDL	C57-C58-C59-C60
16	P	103	CDL	C79-C80-C81-C82
16	P	103	CDL	C81-C82-C83-C84
13	O	304	9YF	C11-C12-C13-C14
16	R	606	CDL	C62-C63-C64-C65
16	B	603	CDL	C59-C60-C61-C62
16	N	604	CDL	C12-C13-C14-C15
15	B	602	HEM	C3D-CAD-CBD-CGD
16	B	604	CDL	C52-C53-C54-C55
16	M	503	CDL	C11-C12-C13-C14
16	R	606	CDL	C53-C54-C55-C56
16	B	604	CDL	C13-C14-C15-C16
16	P	101	CDL	C38-C39-C40-C41
16	B	604	CDL	OB9-CB7-OB8-CB6
16	R	605	CDL	OA9-CA7-OA8-CA6
16	B	603	CDL	C79-C80-C81-C82
16	D	103	CDL	C18-C19-C20-C21
16	D	103	CDL	C22-C23-C24-C25
16	N	607	CDL	C16-C17-C18-C19
16	N	604	CDL	C72-C73-C74-C75
16	B	604	CDL	C57-C58-C59-C60
16	B	605	CDL	C51-C52-C53-C54
16	D	103	CDL	C60-C61-C62-C63
16	F	605	CDL	C31-C32-C33-C34
16	N	605	CDL	C15-C16-C17-C18
16	N	607	CDL	C55-C56-C57-C58
16	P	101	CDL	C71-CB7-OB8-CB6
13	O	304	9YF	C38-C39-C40-C41
16	N	607	CDL	C14-C15-C16-C17
16	P	103	CDL	C18-C19-C20-C21
16	R	606	CDL	C59-C60-C61-C62
13	A	502	9YF	C13-C14-C15-C16
13	A	502	9YF	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
16	D	101	CDL	C80-C81-C82-C83
16	F	605	CDL	C57-C58-C59-C60
16	N	604	CDL	C14-C15-C16-C17
16	N	607	CDL	C34-C35-C36-C37
16	P	103	CDL	C74-C75-C76-C77
16	N	605	CDL	C74-C75-C76-C77
16	P	101	CDL	C51-C52-C53-C54
14	T	201	PLM	C2-C3-C4-C5
16	F	605	CDL	C35-C36-C37-C38
17	N	606	A1IRE	F35-C33-S30-N28
20	G	301	9Y0	C13-C14-C15-C16
16	C	305	CDL	C52-C53-C54-C55
16	B	603	CDL	C74-C75-C76-C77
16	B	603	CDL	C51-CB5-OB6-CB4
16	C	305	CDL	C51-CB5-OB6-CB4
16	N	603	CDL	C51-CB5-OB6-CB4
16	N	607	CDL	C51-CB5-OB6-CB4
16	R	606	CDL	C11-CA5-OA6-CA4
16	N	607	CDL	CA7-C31-C32-C33
16	P	101	CDL	C57-C58-C59-C60
16	C	305	CDL	C80-C81-C82-C83
16	R	606	CDL	C55-C56-C57-C58
16	C	305	CDL	OB7-CB5-OB6-CB4
16	R	606	CDL	OA7-CA5-OA6-CA4
16	N	605	CDL	C11-C12-C13-C14
16	N	605	CDL	C75-C76-C77-C78
16	C	305	CDL	C81-C82-C83-C84
16	R	605	CDL	CA7-C31-C32-C33
17	B	606	A1IRE	C21-C20-C23-C26
14	M	504	PLM	CA-CB-CC-CD
16	N	607	CDL	C81-C82-C83-C84
20	P	102	9Y0	C24-C25-C26-C27
16	D	101	CDL	C37-C38-C39-C40
16	P	101	CDL	C23-C24-C25-C26
16	N	604	CDL	C57-C58-C59-C60
16	N	605	CDL	C18-C19-C20-C21
16	R	606	CDL	C12-C13-C14-C15
16	P	103	CDL	C21-C22-C23-C24
16	F	605	CDL	C76-C77-C78-C79
16	B	603	CDL	OB7-CB5-OB6-CB4
20	D	102	9Y0	O7-C1-C2-O3
16	P	101	CDL	C78-C79-C80-C81

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Mol	Chain	Res	Type	Atoms
16	B	603	CDL	C18-C19-C20-C21
16	N	607	CDL	C71-C72-C73-C74
16	N	607	CDL	C57-C58-C59-C60
16	B	603	CDL	C15-C16-C17-C18
16	R	605	CDL	OA6-CA4-CA6-OA8
16	B	605	CDL	C57-C58-C59-C60
16	F	605	CDL	C34-C35-C36-C37
16	F	606	CDL	C83-C84-C85-C86
16	N	607	CDL	C72-C73-C74-C75
16	P	103	CDL	C59-C60-C61-C62
20	G	301	9Y0	C32-C33-C34-C35
13	C	303	9YF	C15-C16-C17-C18
16	N	607	CDL	C52-C53-C54-C55
16	R	606	CDL	C83-C84-C85-C86
20	D	102	9Y0	C9-C10-C11-C12
16	B	605	CDL	C75-C76-C77-C78
16	D	101	CDL	C18-C19-C20-C21
16	N	604	CDL	C74-C75-C76-C77
16	P	103	CDL	C60-C61-C62-C63
16	B	605	CDL	CA4-CA3-OA5-PA1
16	N	604	CDL	C52-C53-C54-C55
20	P	102	9Y0	C27-C28-C29-C30
16	D	103	CDL	CB2-C1-CA2-OA2
16	P	103	CDL	CB2-C1-CA2-OA2
13	O	304	9YF	C10-C11-C12-C13
16	B	604	CDL	C36-C37-C38-C39
16	R	605	CDL	C56-C57-C58-C59
16	C	305	CDL	C35-C36-C37-C38
16	D	101	CDL	C82-C83-C84-C85
16	N	604	CDL	C55-C56-C57-C58
16	N	607	CDL	C78-C79-C80-C81
16	R	605	CDL	C71-C72-C73-C74
14	G	302	PLM	C6-C7-C8-C9
16	B	605	CDL	C15-C16-C17-C18
16	D	103	CDL	C58-C59-C60-C61
16	M	503	CDL	C76-C77-C78-C79
16	B	603	CDL	CB5-C51-C52-C53
16	B	605	CDL	C22-C23-C24-C25
16	P	101	CDL	OB9-CB7-OB8-CB6
16	C	305	CDL	C72-C73-C74-C75
16	N	604	CDL	C53-C54-C55-C56
16	B	605	CDL	C76-C77-C78-C79

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Mol	Chain	Res	Type	Atoms
16	D	101	CDL	C22-C23-C24-C25
16	M	503	CDL	C16-C17-C18-C19
16	F	606	CDL	C81-C82-C83-C84
16	R	606	CDL	C71-C72-C73-C74
16	N	607	CDL	C33-C34-C35-C36
16	R	605	CDL	C74-C75-C76-C77
13	A	502	9YF	C24-C-C1-O
13	M	502	9YF	C24-C-C1-O
13	O	304	9YF	C24-C-C1-O
16	B	603	CDL	OB5-CB3-CB4-CB6
16	B	605	CDL	OB5-CB3-CB4-CB6
16	C	305	CDL	OA5-CA3-CA4-CA6
16	D	101	CDL	OA5-CA3-CA4-CA6
16	N	603	CDL	OB5-CB3-CB4-CB6
16	P	101	CDL	OA5-CA3-CA4-CA6
16	R	605	CDL	OA5-CA3-CA4-CA6
16	N	607	CDL	OB7-CB5-OB6-CB4
16	D	103	CDL	C53-C54-C55-C56
16	N	603	CDL	C18-C19-C20-C21
16	R	606	CDL	C32-C33-C34-C35
16	M	503	CDL	C74-C75-C76-C77
13	O	304	9YF	C35-C36-C37-C38
13	M	502	9YF	C25-C26-C27-C28
16	C	305	CDL	C16-C17-C18-C19
16	P	101	CDL	C81-C82-C83-C84
16	D	101	CDL	C35-C36-C37-C38
13	A	502	9YF	C34-C33-C35-C36
13	O	304	9YF	C9-C10-C11-C12
16	B	605	CDL	C52-C53-C54-C55
16	D	103	CDL	C11-C12-C13-C14
16	N	605	CDL	C55-C56-C57-C58
16	D	101	CDL	C31-CA7-OA8-CA6
16	N	603	CDL	C31-CA7-OA8-CA6
13	O	304	9YF	C17-C18-C19-C20
16	C	305	CDL	C76-C77-C78-C79
16	P	103	CDL	C71-C72-C73-C74
16	B	603	CDL	CB3-CB4-CB6-OB8
16	B	605	CDL	CB3-CB4-CB6-OB8
16	N	603	CDL	CA3-CA4-CA6-OA8
16	P	103	CDL	CB3-CB4-CB6-OB8
16	R	605	CDL	CB3-CB4-CB6-OB8
20	G	301	9Y0	O5-C-C1-C2

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Mol	Chain	Res	Type	Atoms
16	C	305	CDL	C53-C54-C55-C56
16	D	103	CDL	C35-C36-C37-C38
20	G	301	9Y0	C25-C26-C27-C28
13	A	502	9YF	C19-C20-C21-C22
13	M	502	9YF	C36-C37-C38-C39
16	B	605	CDL	C73-C74-C75-C76
13	M	502	9YF	C35-C36-C37-C38
16	B	605	CDL	C16-C17-C18-C19
16	R	606	CDL	C78-C79-C80-C81
16	R	606	CDL	C81-C82-C83-C84
16	D	103	CDL	C83-C84-C85-C86
16	N	605	CDL	C33-C34-C35-C36
16	N	605	CDL	C51-C52-C53-C54
16	N	607	CDL	C83-C84-C85-C86
16	M	503	CDL	C14-C15-C16-C17
20	D	102	9Y0	C22-C23-C24-C25
16	C	305	CDL	CA7-C31-C32-C33
16	F	605	CDL	C74-C75-C76-C77
16	F	606	CDL	C73-C74-C75-C76
13	C	303	9YF	C29-C30-C31-C32
16	D	103	CDL	C76-C77-C78-C79
16	N	605	CDL	C16-C17-C18-C19
16	N	607	CDL	C15-C16-C17-C18
16	P	101	CDL	C18-C19-C20-C21
16	R	606	CDL	C79-C80-C81-C82
13	A	502	9YF	C15-C16-C17-C18
13	C	303	9YF	C16-C17-C18-C19
16	D	103	CDL	C17-C18-C19-C20
16	M	503	CDL	C53-C54-C55-C56
16	R	605	CDL	CA5-C11-C12-C13
16	D	103	CDL	C37-C38-C39-C40
16	N	605	CDL	C22-C23-C24-C25
16	N	607	CDL	C53-C54-C55-C56
16	D	103	CDL	CA3-CA4-OA6-CA5
16	N	605	CDL	CA6-CA4-OA6-CA5
16	P	103	CDL	CA6-CA4-OA6-CA5
20	S	301	9Y0	C6-C7-C8-C9
20	G	301	9Y0	C10-C11-C12-C13
20	S	301	9Y0	C10-C11-C12-C13
14	G	302	PLM	CB-CC-CD-CE
16	N	607	CDL	C32-C33-C34-C35
16	R	605	CDL	C77-C78-C79-C80

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Mol	Chain	Res	Type	Atoms
16	N	605	CDL	CB5-C51-C52-C53
22	F	601	HEA	C4D-C3D-CAD-CBD
22	F	602	HEA	C4D-C3D-CAD-CBD
16	B	603	CDL	OA5-CA3-CA4-OA6
16	B	604	CDL	OB5-CB3-CB4-OB6
16	B	604	CDL	C11-C12-C13-C14
16	N	605	CDL	C23-C24-C25-C26
16	N	605	CDL	C78-C79-C80-C81
16	P	101	CDL	C37-C38-C39-C40
16	N	604	CDL	C34-C35-C36-C37
19	C	304	MQ9	C33-C34-C36-C37
13	C	303	9YF	C20-C21-C22-C23
16	D	103	CDL	C64-C65-C66-C67
13	C	303	9YF	C39-C40-C41-C42
16	F	606	CDL	C62-C63-C64-C65
16	D	101	CDL	C71-C72-C73-C74
16	D	103	CDL	C20-C21-C22-C23
16	P	101	CDL	C79-C80-C81-C82
16	R	605	CDL	C38-C39-C40-C41
16	R	605	CDL	C60-C61-C62-C63
16	N	603	CDL	C59-C60-C61-C62
16	C	305	CDL	C79-C80-C81-C82
13	O	304	9YF	C20-C21-C22-C23
16	D	103	CDL	C74-C75-C76-C77
16	F	605	CDL	C56-C57-C58-C59
16	R	605	CDL	C76-C77-C78-C79
16	R	606	CDL	C34-C35-C36-C37
13	A	502	9YF	C29-C30-C31-C32
16	B	604	CDL	C18-C19-C20-C21
16	B	604	CDL	C76-C77-C78-C79
24	O	301	MQ7	C33-C35-C36-C37
16	D	101	CDL	OA9-CA7-OA8-CA6
16	M	503	CDL	C57-C58-C59-C60
16	N	607	CDL	C12-C13-C14-C15
16	P	101	CDL	C20-C21-C22-C23
16	F	606	CDL	C31-CA7-OA8-CA6
16	F	605	CDL	C54-C55-C56-C57
16	D	103	CDL	C57-C58-C59-C60
16	N	603	CDL	OA9-CA7-OA8-CA6
16	R	606	CDL	C15-C16-C17-C18
16	F	605	CDL	C59-C60-C61-C62
16	F	606	CDL	C51-C52-C53-C54

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Mol	Chain	Res	Type	Atoms
16	F	606	CDL	C15-C16-C17-C18
19	C	304	MQ9	C35-C34-C36-C37
19	O	305	MQ9	C45-C44-C46-C47
16	D	101	CDL	C23-C24-C25-C26
16	D	101	CDL	C51-C52-C53-C54
16	B	604	CDL	C58-C59-C60-C61
16	N	603	CDL	OB7-CB5-OB6-CB4
16	P	103	CDL	C12-C13-C14-C15
16	N	605	CDL	CA4-CA3-OA5-PA1
22	R	602	HEA	C4C-C3C-CAC-CBC
20	D	102	9Y0	C27-C28-C29-C30
16	N	604	CDL	C76-C77-C78-C79
13	C	303	9YF	C19-C20-C21-C22
16	N	604	CDL	C16-C17-C18-C19
20	P	102	9Y0	C11-C10-C9-C8
16	B	604	CDL	OB5-CB3-CB4-CB6
16	R	606	CDL	OB5-CB3-CB4-CB6
20	D	102	9Y0	C-C1-C2-O3
20	S	301	9Y0	C-C1-C2-O3
16	M	503	CDL	C79-C80-C81-C82
16	B	605	CDL	C79-C80-C81-C82
16	F	606	CDL	C58-C59-C60-C61
13	A	502	9YF	C32-C33-C35-C36
13	O	304	9YF	C31-C32-C33-C35
16	D	101	CDL	C57-C58-C59-C60
16	N	605	CDL	C79-C80-C81-C82
16	C	305	CDL	C14-C15-C16-C17
16	P	101	CDL	C15-C16-C17-C18
16	B	605	CDL	C34-C35-C36-C37
16	D	101	CDL	C11-C12-C13-C14
16	C	305	CDL	C54-C55-C56-C57
13	C	303	9YF	C35-C36-C37-C38
16	C	305	CDL	C15-C16-C17-C18
16	B	604	CDL	CB3-CB4-CB6-OB8
16	C	305	CDL	CA3-CA4-CA6-OA8
16	D	101	CDL	CA3-CA4-CA6-OA8
16	N	604	CDL	CB3-CB4-CB6-OB8
16	N	607	CDL	CA3-CA4-CA6-OA8
16	N	607	CDL	CB3-CB4-CB6-OB8
16	P	101	CDL	CA3-CA4-CA6-OA8
16	R	605	CDL	CA3-CA4-CA6-OA8
19	O	305	MQ9	C29-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
24	H	201	MQ7	C23-C25-C26-C27
24	H	201	MQ7	C33-C35-C36-C37
16	P	101	CDL	C39-C40-C41-C42
13	A	502	9YF	C9-C10-C11-C12
16	P	101	CDL	C16-C17-C18-C19
16	N	607	CDL	C11-C12-C13-C14
16	P	103	CDL	C36-C37-C38-C39
14	T	201	PLM	C9-CA-CB-CC
16	F	605	CDL	C12-C13-C14-C15
19	O	305	MQ9	C43-C44-C46-C47
13	C	303	9YF	O9-C-C1-O
13	O	304	9YF	O9-C-C1-O
16	C	305	CDL	OA5-CA3-CA4-OA6
16	F	605	CDL	OA5-CA3-CA4-OA6
16	N	603	CDL	OA5-CA3-CA4-OA6
16	N	607	CDL	OA5-CA3-CA4-OA6
16	R	605	CDL	OA5-CA3-CA4-OA6
16	R	606	CDL	OA5-CA3-CA4-OA6
16	P	103	CDL	C72-C73-C74-C75
16	F	606	CDL	C52-C53-C54-C55
20	P	102	9Y0	C10-C11-C12-C13
16	D	103	CDL	C71-C72-C73-C74
16	R	606	CDL	CB7-C71-C72-C73
20	S	301	9Y0	C7-C8-C9-C10
22	F	601	HEA	C2D-C3D-CAD-CBD
16	B	604	CDL	C37-C38-C39-C40
16	N	603	CDL	C73-C74-C75-C76
16	R	605	CDL	C52-C51-CB5-OB6
16	N	603	CDL	OA6-CA4-CA6-OA8
16	P	101	CDL	OA6-CA4-CA6-OA8
16	R	606	CDL	C13-C14-C15-C16
16	P	103	CDL	C33-C34-C35-C36
14	A	503	PLM	C8-C9-CA-CB
20	G	301	9Y0	C11-C10-C9-C8
16	B	605	CDL	C78-C79-C80-C81
20	S	301	9Y0	C25-C26-C27-C28
16	C	305	CDL	CB5-C51-C52-C53
13	O	304	9YF	C19-C20-C21-C22
16	P	103	CDL	C77-C78-C79-C80
16	B	605	CDL	C71-C72-C73-C74
16	M	503	CDL	C71-C72-C73-C74
16	R	606	CDL	C61-C62-C63-C64

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Mol	Chain	Res	Type	Atoms
20	G	301	9Y0	C27-C28-C29-C30
16	C	305	CDL	C36-C37-C38-C39
24	H	201	MQ7	C28-C30-C31-C32
16	F	606	CDL	C11-C12-C13-C14
13	A	502	9YF	C11-C12-C13-C14
13	O	304	9YF	C11-C10-C9-C8
20	S	301	9Y0	C13-C14-C15-C16
13	M	502	9YF	C26-C27-C28-C29
16	N	604	CDL	C33-C34-C35-C36
13	O	304	9YF	C15-C16-C17-C18
16	F	605	CDL	C78-C79-C80-C81
16	B	603	CDL	CB2-C1-CA2-OA2
16	D	101	CDL	CA2-C1-CB2-OB2
16	P	101	CDL	C33-C34-C35-C36
16	N	604	CDL	C60-C61-C62-C63
16	N	605	CDL	C72-C73-C74-C75
16	F	605	CDL	OA5-CA3-CA4-CA6
16	P	103	CDL	OB5-CB3-CB4-CB6
18	C	302	HEC	C4D-C3D-CAD-CBD
13	O	304	9YF	C39-C40-C41-C42
16	M	503	CDL	C15-C16-C17-C18
13	O	304	9YF	C32-C33-C35-C36
20	D	102	9Y0	C26-C27-C28-C29
17	B	606	A1IRE	C19-C20-C23-C26
16	C	305	CDL	C57-C58-C59-C60
16	N	605	CDL	C14-C15-C16-C17
16	F	606	CDL	C57-C58-C59-C60
16	F	605	CDL	C32-C31-CA7-OA8
16	B	605	CDL	CA6-CA4-OA6-CA5
16	N	605	CDL	CB6-CB4-OB6-CB5
16	F	606	CDL	OA9-CA7-OA8-CA6
16	N	603	CDL	C80-C81-C82-C83
16	R	605	CDL	C78-C79-C80-C81
16	P	103	CDL	OB5-CB3-CB4-OB6
20	S	301	9Y0	O7-C1-C2-O3
16	M	503	CDL	CB3-CB4-CB6-OB8
16	N	603	CDL	CB3-CB4-CB6-OB8
16	R	606	CDL	CB3-CB4-CB6-OB8
20	D	102	9Y0	O5-C-C1-C2
16	R	606	CDL	C56-C57-C58-C59
16	N	603	CDL	C13-C14-C15-C16
20	G	301	9Y0	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
13	C	303	9YF	O9-C-C24-O11
16	B	603	CDL	OB6-CB4-CB6-OB8
16	B	604	CDL	OB6-CB4-CB6-OB8
16	B	605	CDL	OB6-CB4-CB6-OB8
16	C	305	CDL	OB6-CB4-CB6-OB8
16	D	101	CDL	OA6-CA4-CA6-OA8
16	N	603	CDL	OB6-CB4-CB6-OB8
16	N	604	CDL	OB6-CB4-CB6-OB8
16	N	605	CDL	OB6-CB4-CB6-OB8
16	N	607	CDL	OB6-CB4-CB6-OB8
16	R	605	CDL	OB6-CB4-CB6-OB8
20	P	102	9Y0	O5-C-C1-O7
16	B	604	CDL	C35-C36-C37-C38
16	F	606	CDL	C79-C80-C81-C82
16	M	503	CDL	C72-C73-C74-C75
16	N	605	CDL	C76-C77-C78-C79
16	B	605	CDL	C32-C33-C34-C35
16	N	604	CDL	C35-C36-C37-C38
16	D	101	CDL	C32-C33-C34-C35
16	R	605	CDL	C57-C58-C59-C60
15	B	602	HEM	C1A-C2A-CAA-CBA
20	D	102	9Y0	C11-C10-C9-C8
22	F	602	HEA	C2D-C3D-CAD-CBD
16	D	101	CDL	C36-C37-C38-C39
16	D	103	CDL	CA7-C31-C32-C33
16	B	604	CDL	CA2-C1-CB2-OB2
16	F	606	CDL	CB2-C1-CA2-OA2
16	F	606	CDL	C32-C33-C34-C35
16	N	605	CDL	C13-C14-C15-C16
16	N	607	CDL	C56-C57-C58-C59
16	P	103	CDL	C22-C23-C24-C25
16	D	101	CDL	C54-C55-C56-C57
16	R	606	CDL	C32-C31-CA7-OA8
16	N	607	CDL	C51-C52-C53-C54
16	N	605	CDL	C71-C72-C73-C74
20	P	102	9Y0	C14-C15-C16-C17
13	C	303	9YF	C24-C-C1-O
16	D	103	CDL	OA5-CA3-CA4-CA6
16	F	606	CDL	OA5-CA3-CA4-CA6
16	R	605	CDL	OB5-CB3-CB4-CB6
16	R	606	CDL	OA5-CA3-CA4-CA6
16	B	604	CDL	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
20	S	301	9Y0	C32-C33-C34-C35
13	M	502	9YF	C32-C33-C35-C36
13	A	502	9YF	C26-C27-C28-C29
13	O	304	9YF	C37-C38-C39-C40
16	B	604	CDL	C72-C73-C74-C75
16	N	604	CDL	C71-C72-C73-C74
16	N	607	CDL	O1-C1-CB2-OB2
16	D	103	CDL	C51-C52-C53-C54
16	B	605	CDL	C1-CA2-OA2-PA1
16	P	101	CDL	CA4-CA3-OA5-PA1
13	A	502	9YF	C10-C11-C12-C13
18	O	302	HEC	C4C-C3C-CAC-CBC
13	A	502	9YF	C17-C18-C19-C20
16	B	603	CDL	OB5-CB3-CB4-OB6
16	D	103	CDL	OA5-CA3-CA4-OA6
16	F	606	CDL	OA5-CA3-CA4-OA6
16	N	603	CDL	OB5-CB3-CB4-OB6
16	P	101	CDL	C84-C85-C86-C87
13	C	303	9YF	C30-C31-C32-C33
16	N	605	CDL	C53-C54-C55-C56
17	N	606	A1IRE	C01-C02-C03-N04
17	N	606	A1IRE	C29-N28-S30-O32
13	O	304	9YF	C29-C30-C31-C32
16	B	605	CDL	OA6-CA4-CA6-OA8
16	C	305	CDL	OA6-CA4-CA6-OA8
16	N	607	CDL	OA6-CA4-CA6-OA8
16	R	606	CDL	OB6-CB4-CB6-OB8
20	D	102	9Y0	O5-C-C1-O7
13	C	303	9YF	C1-C-C24-O11
16	B	605	CDL	CA3-CA4-CA6-OA8
16	C	305	CDL	CB3-CB4-CB6-OB8
16	N	603	CDL	C19-C20-C21-C22
16	F	606	CDL	C54-C55-C56-C57
16	F	606	CDL	C34-C35-C36-C37
16	D	101	CDL	C14-C15-C16-C17
16	R	606	CDL	C31-C32-C33-C34
16	B	605	CDL	C58-C59-C60-C61
13	M	502	9YF	C18-C19-C20-C21
16	F	606	CDL	C64-C65-C66-C67
16	D	103	CDL	C80-C81-C82-C83
16	B	603	CDL	CA3-OA5-PA1-OA2
16	B	603	CDL	CA3-OA5-PA1-OA3

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Mol	Chain	Res	Type	Atoms
16	B	603	CDL	CB3-OB5-PB2-OB2
16	B	604	CDL	CA2-OA2-PA1-OA3
16	B	604	CDL	CA2-OA2-PA1-OA5
16	B	604	CDL	CA3-OA5-PA1-OA4
16	B	604	CDL	CB3-OB5-PB2-OB3
16	C	305	CDL	CA2-OA2-PA1-OA5
16	C	305	CDL	CB3-OB5-PB2-OB2
16	C	305	CDL	CB3-OB5-PB2-OB3
16	D	101	CDL	CA2-OA2-PA1-OA5
16	D	103	CDL	CA3-OA5-PA1-OA2
16	D	103	CDL	CA3-OA5-PA1-OA3
16	D	103	CDL	CA3-OA5-PA1-OA4
16	N	603	CDL	CB3-OB5-PB2-OB2
16	N	604	CDL	CA2-OA2-PA1-OA4
16	N	604	CDL	CA2-OA2-PA1-OA5
16	N	604	CDL	CA3-OA5-PA1-OA4
16	N	605	CDL	CA3-OA5-PA1-OA3
16	N	605	CDL	CB2-OB2-PB2-OB3
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	N	607	CDL	CB2-OB2-PB2-OB3
16	N	607	CDL	CB3-OB5-PB2-OB2
16	N	607	CDL	CB3-OB5-PB2-OB3
16	N	607	CDL	CB3-OB5-PB2-OB4
16	P	101	CDL	CA2-OA2-PA1-OA3
16	P	101	CDL	CA3-OA5-PA1-OA4
16	P	103	CDL	CA2-OA2-PA1-OA3
16	P	103	CDL	CA2-OA2-PA1-OA4
16	P	103	CDL	CA2-OA2-PA1-OA5
16	P	103	CDL	CB3-OB5-PB2-OB2
16	P	103	CDL	CB3-OB5-PB2-OB4
20	D	102	9Y0	C2-O3-P-O
20	D	102	9Y0	C2-O3-P-O1
20	D	102	9Y0	C2-O3-P-O2
20	G	301	9Y0	O1-C3-C4-N
20	P	102	9Y0	C2-O3-P-O1
19	C	304	MQ9	C40-C39-C41-C42
19	O	305	MQ9	C12-C11-C9-C10
16	B	603	CDL	CB4-CB3-OB5-PB2
16	B	604	CDL	CB4-CB3-OB5-PB2
16	N	604	CDL	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
16	C	305	CDL	CA5-C11-C12-C13
16	C	305	CDL	C13-C14-C15-C16
16	F	606	CDL	CA7-C31-C32-C33
16	M	503	CDL	CB5-C51-C52-C53
16	R	605	CDL	C51-C52-C53-C54
16	P	103	CDL	C37-C38-C39-C40
13	O	304	9YF	C1-C-O9-C8
16	B	605	CDL	CB6-CB4-OB6-CB5
16	D	101	CDL	CA3-CA4-OA6-CA5
16	F	606	CDL	CA6-CA4-OA6-CA5
16	R	606	CDL	CA6-CA4-OA6-CA5
16	N	603	CDL	C15-C16-C17-C18
13	A	502	9YF	C16-C17-C18-C19
16	M	503	CDL	C59-C60-C61-C62
16	B	603	CDL	OA5-CA3-CA4-CA6
13	M	502	9YF	C34-C33-C35-C36
13	O	304	9YF	C31-C32-C33-C34
20	P	102	9Y0	C13-C14-C15-C16
16	R	606	CDL	C52-C53-C54-C55
16	M	503	CDL	OA5-CA3-CA4-OA6
16	R	605	CDL	OB5-CB3-CB4-OB6
16	P	103	CDL	C51-CB5-OB6-CB4
16	P	103	CDL	OB7-CB5-OB6-CB4
20	D	102	9Y0	C1-C2-O3-P
16	F	605	CDL	C52-C51-CB5-OB6
16	P	101	CDL	C74-C75-C76-C77
16	F	605	CDL	CB5-C51-C52-C53
13	M	502	9YF	C29-C30-C31-C32
20	G	301	9Y0	C30-C31-C32-C33
16	P	103	CDL	CB5-C51-C52-C53
16	P	103	CDL	C52-C53-C54-C55
22	R	601	HEA	C3B-C11-C12-C13
13	O	304	9YF	C33-C35-C36-C37
13	C	303	9YF	C11-C12-C13-C14
13	O	304	9YF	C36-C37-C38-C39
16	F	606	CDL	C72-C71-CB7-OB8
16	B	603	CDL	C19-C20-C21-C22
22	R	602	HEA	C26-C15-C16-C17
16	B	605	CDL	C72-C73-C74-C75
20	G	301	9Y0	C23-C24-C25-C26
13	O	304	9YF	C26-C27-C28-C29
16	N	603	CDL	CB2-C1-CA2-OA2

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Mol	Chain	Res	Type	Atoms
16	N	607	CDL	CA2-C1-CB2-OB2
16	P	101	CDL	C1-CB2-OB2-PB2
16	P	103	CDL	CB4-CB3-OB5-PB2
16	N	603	CDL	C53-C54-C55-C56
16	R	605	CDL	C55-C56-C57-C58
19	C	304	MQ9	C12-C11-C9-C10
19	O	305	MQ9	C20-C19-C21-C22
24	O	301	MQ7	C29-C28-C30-C31
16	C	305	CDL	C78-C79-C80-C81
16	P	101	CDL	C56-C57-C58-C59
16	F	605	CDL	C39-C40-C41-C42
14	T	201	PLM	C6-C7-C8-C9
16	D	103	CDL	OA6-CA4-CA6-OA8
22	F	601	HEA	CAD-CBD-CGD-O2D
16	N	603	CDL	C16-C17-C18-C19
19	O	305	MQ9	C12-C11-C9-C8
16	N	607	CDL	C82-C83-C84-C85
16	N	607	CDL	C73-C74-C75-C76
16	R	605	CDL	C13-C14-C15-C16
22	F	601	HEA	CAD-CBD-CGD-O1D
14	M	504	PLM	C7-C8-C9-CA
16	P	101	CDL	CB3-CB4-CB6-OB8
16	P	101	CDL	C73-C74-C75-C76
13	A	502	9YF	C40-C41-C42-C43
16	P	103	CDL	C14-C15-C16-C17
13	C	303	9YF	C38-C39-C40-C41
20	G	301	9Y0	C28-C29-C30-C31
16	P	103	CDL	C34-C35-C36-C37
22	R	601	HEA	CAD-CBD-CGD-O2D
16	N	607	CDL	C79-C80-C81-C82
15	N	601	HEM	CAA-CBA-CGA-O1A
16	M	503	CDL	C77-C78-C79-C80
22	F	601	HEA	C2C-C3C-CAC-CBC
14	M	504	PLM	C2-C3-C4-C5
16	B	603	CDL	C1-CA2-OA2-PA1
16	F	606	CDL	C53-C54-C55-C56
16	F	606	CDL	C77-C78-C79-C80
16	M	503	CDL	OA5-CA3-CA4-CA6
13	C	303	9YF	C7-C2-O2-P
18	C	302	HEC	C3D-CAD-CBD-CGD
18	O	302	HEC	C2A-CAA-CBA-CGA
22	R	601	HEA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
13	C	303	9YF	C31-C32-C33-C35
16	F	605	CDL	OA6-CA4-CA6-OA8
16	P	101	CDL	C36-C37-C38-C39
13	C	303	9YF	C18-C19-C20-C21
16	F	605	CDL	CA2-C1-CB2-OB2
16	N	604	CDL	CA2-C1-CB2-OB2
16	F	605	CDL	C61-C62-C63-C64
19	C	304	MQ9	C12-C11-C9-C8
19	O	305	MQ9	C18-C19-C21-C22
24	O	301	MQ7	C27-C28-C30-C31
16	R	605	CDL	C39-C40-C41-C42
16	D	101	CDL	C81-C82-C83-C84
16	P	103	CDL	C61-C62-C63-C64
13	A	502	9YF	C20-C21-C22-C23
16	D	103	CDL	C1-CA2-OA2-PA1
16	F	606	CDL	C59-C60-C61-C62
16	R	606	CDL	C82-C83-C84-C85
16	D	101	CDL	CA7-C31-C32-C33
16	P	101	CDL	CB5-C51-C52-C53
16	N	604	CDL	C71-CB7-OB8-CB6
16	N	604	CDL	OB9-CB7-OB8-CB6
16	P	101	CDL	C14-C15-C16-C17
16	R	606	CDL	C63-C64-C65-C66
16	D	101	CDL	C56-C57-C58-C59
15	N	601	HEM	CAD-CBD-CGD-O2D
16	N	604	CDL	C32-C31-CA7-OA8
16	N	605	CDL	OB9-CB7-OB8-CB6
22	R	602	HEA	CAD-CBD-CGD-O2D
15	N	601	HEM	CAA-CBA-CGA-O2A
16	D	103	CDL	C38-C39-C40-C41
18	C	302	HEC	CAA-CBA-CGA-O1A
16	P	101	CDL	C54-C55-C56-C57
16	N	605	CDL	C19-C20-C21-C22
20	G	301	9Y0	C-C1-C2-O3
16	D	103	CDL	OB6-CB4-CB6-OB8
16	F	605	CDL	C53-C54-C55-C56
16	N	605	CDL	C58-C59-C60-C61
16	N	605	CDL	C71-CB7-OB8-CB6
13	M	502	9YF	C12-C13-C14-C15
20	S	301	9Y0	C28-C29-C30-C31
16	B	603	CDL	C31-C32-C33-C34
16	R	605	CDL	C52-C51-CB5-OB7

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Mol	Chain	Res	Type	Atoms
22	R	601	HEA	C2D-C3D-CAD-CBD
16	B	604	CDL	C38-C39-C40-C41
16	N	604	CDL	C59-C60-C61-C62
18	O	303	HEC	C2A-CAA-CBA-CGA
16	B	605	CDL	C55-C56-C57-C58
15	N	601	HEM	CAD-CBD-CGD-O1D
13	C	303	9YF	C3-C2-O2-P
18	C	302	HEC	C2D-C3D-CAD-CBD
22	R	602	HEA	CAD-CBD-CGD-O1D
16	B	603	CDL	C12-C13-C14-C15
16	D	101	CDL	CA6-CA4-OA6-CA5
16	N	605	CDL	C1-CA2-OA2-PA1
16	R	605	CDL	C12-C11-CA5-OA6
16	D	103	CDL	CA3-CA4-CA6-OA8
19	C	304	MQ9	C19-C21-C22-C23
16	D	103	CDL	C72-C73-C74-C75
20	P	102	9Y0	C23-C24-C25-C26
20	S	301	9Y0	C9-C10-C11-C12
19	C	304	MQ9	C38-C39-C41-C42
14	T	201	PLM	C5-C6-C7-C8
16	D	103	CDL	CB7-C71-C72-C73
16	B	604	CDL	C32-C31-CA7-OA8
18	C	301	HEC	C2D-C3D-CAD-CBD
20	G	301	9Y0	C6-C7-C8-C9
22	R	601	HEA	C4D-C3D-CAD-CBD
13	C	303	9YF	C31-C32-C33-C34
16	N	603	CDL	OA5-CA3-CA4-CA6
13	M	502	9YF	C38-C39-C40-C41
20	P	102	9Y0	O7-C21-C22-C23
22	R	602	HEA	C14-C15-C16-C17
16	P	101	CDL	C72-C73-C74-C75
16	F	606	CDL	C63-C64-C65-C66
22	R	602	HEA	C2C-C3C-CAC-CBC
16	F	606	CDL	C32-C31-CA7-OA8
16	N	604	CDL	C51-C52-C53-C54
13	C	303	9YF	C2-O2-P-O8
19	C	304	MQ9	C45-C44-C46-C47
13	O	304	9YF	O11-C25-C26-C27
16	N	607	CDL	C52-C51-CB5-OB6
16	P	103	CDL	C12-C11-CA5-OA6
19	C	304	MQ9	C43-C44-C46-C47
16	P	103	CDL	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
16	B	603	CDL	C55-C56-C57-C58
20	S	301	9Y0	C29-C30-C31-C32
16	P	101	CDL	C24-C25-C26-C27
14	M	504	PLM	C9-CA-CB-CC
16	B	603	CDL	C75-C76-C77-C78
22	F	602	HEA	CAD-CBD-CGD-O2D
15	B	601	HEM	CAA-CBA-CGA-O1A
22	F	601	HEA	C4C-C3C-CAC-CBC
18	C	302	HEC	CAA-CBA-CGA-O2A
24	H	201	MQ7	C39-C38-C40-C41
16	D	103	CDL	C84-C85-C86-C87
16	P	103	CDL	C54-C55-C56-C57
16	M	503	CDL	C80-C81-C82-C83
13	O	304	9YF	O9-C8-C9-C10
16	P	101	CDL	C32-C31-CA7-OA8
16	B	605	CDL	C13-C14-C15-C16
24	O	301	MQ7	C30-C31-C32-C33
16	F	605	CDL	C32-C31-CA7-OA9
16	C	305	CDL	C52-C51-CB5-OB6
16	D	103	CDL	C32-C33-C34-C35
16	N	605	CDL	C52-C53-C54-C55
16	B	603	CDL	C53-C54-C55-C56
20	P	102	9Y0	C-C1-O7-C21
20	S	301	9Y0	C11-C10-C9-C8
16	C	305	CDL	C82-C83-C84-C85
15	B	601	HEM	CAA-CBA-CGA-O2A
16	N	604	CDL	C11-C12-C13-C14
16	R	605	CDL	CA4-CA3-OA5-PA1
22	R	601	HEA	C26-C15-C16-C17
16	N	605	CDL	C32-C31-CA7-OA8
20	G	301	9Y0	O7-C1-C2-O3
13	M	502	9YF	C40-C41-C42-C43
16	R	605	CDL	C61-C62-C63-C64
16	N	603	CDL	C72-C73-C74-C75
16	P	101	CDL	CB7-C71-C72-C73
17	N	606	A1IRE	C27-N28-S30-O32
16	P	103	CDL	C12-C11-CA5-OA7
20	P	102	9Y0	O6-C21-C22-C23
16	D	101	CDL	C38-C39-C40-C41
16	P	103	CDL	C83-C84-C85-C86
16	P	101	CDL	C32-C31-CA7-OA9
16	P	101	CDL	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
13	O	304	9YF	O12-C25-C26-C27
16	N	607	CDL	C52-C51-CB5-OB7
16	N	607	CDL	C32-C31-CA7-OA8
16	N	607	CDL	C72-C71-CB7-OB8
22	F	602	HEA	CAD-CBD-CGD-O1D
14	M	504	PLM	C3-C4-C5-C6
16	N	604	CDL	C75-C76-C77-C78
13	C	303	9YF	C37-C38-C39-C40
16	N	604	CDL	C56-C57-C58-C59
22	F	601	HEA	CAA-CBA-CGA-O2A
16	N	604	CDL	C72-C71-CB7-OB8
16	D	103	CDL	C33-C34-C35-C36
16	N	605	CDL	C32-C31-CA7-OA9
16	P	103	CDL	C52-C51-CB5-OB6
13	O	304	9YF	O10-C8-C9-C10

There are no ring outliers.

39 monomers are involved in 145 short contacts:

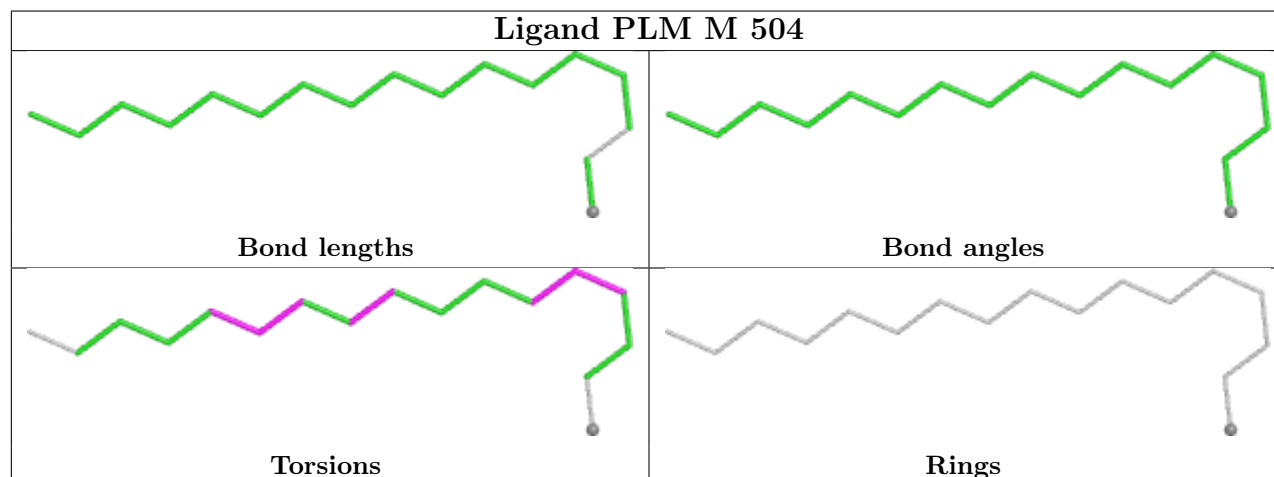
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	M	504	PLM	1	0
13	C	303	9YF	1	0
22	F	601	HEA	5	0
16	P	103	CDL	5	0
16	D	103	CDL	12	0
15	N	601	HEM	2	0
17	N	606	A1IRE	1	0
19	O	305	MQ9	7	0
16	F	605	CDL	6	0
16	R	605	CDL	3	0
16	M	503	CDL	6	0
16	N	607	CDL	4	0
16	D	101	CDL	8	0
18	C	302	HEC	2	0
18	O	303	HEC	2	0
19	C	304	MQ9	7	0
22	F	602	HEA	11	0
22	R	601	HEA	2	0
12	M	501	FES	1	0
15	B	602	HEM	3	0
16	N	605	CDL	5	0
16	B	605	CDL	5	0

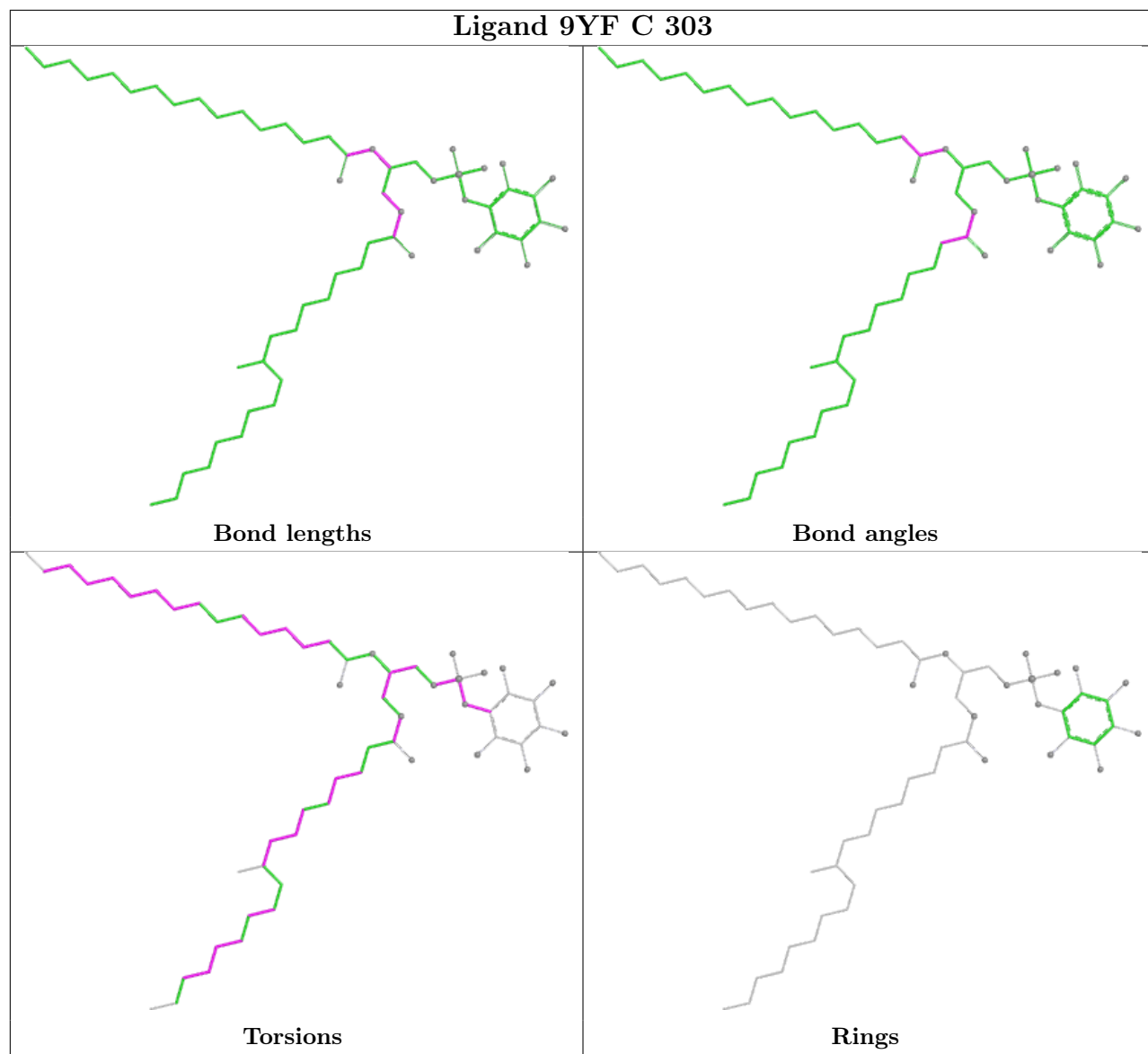
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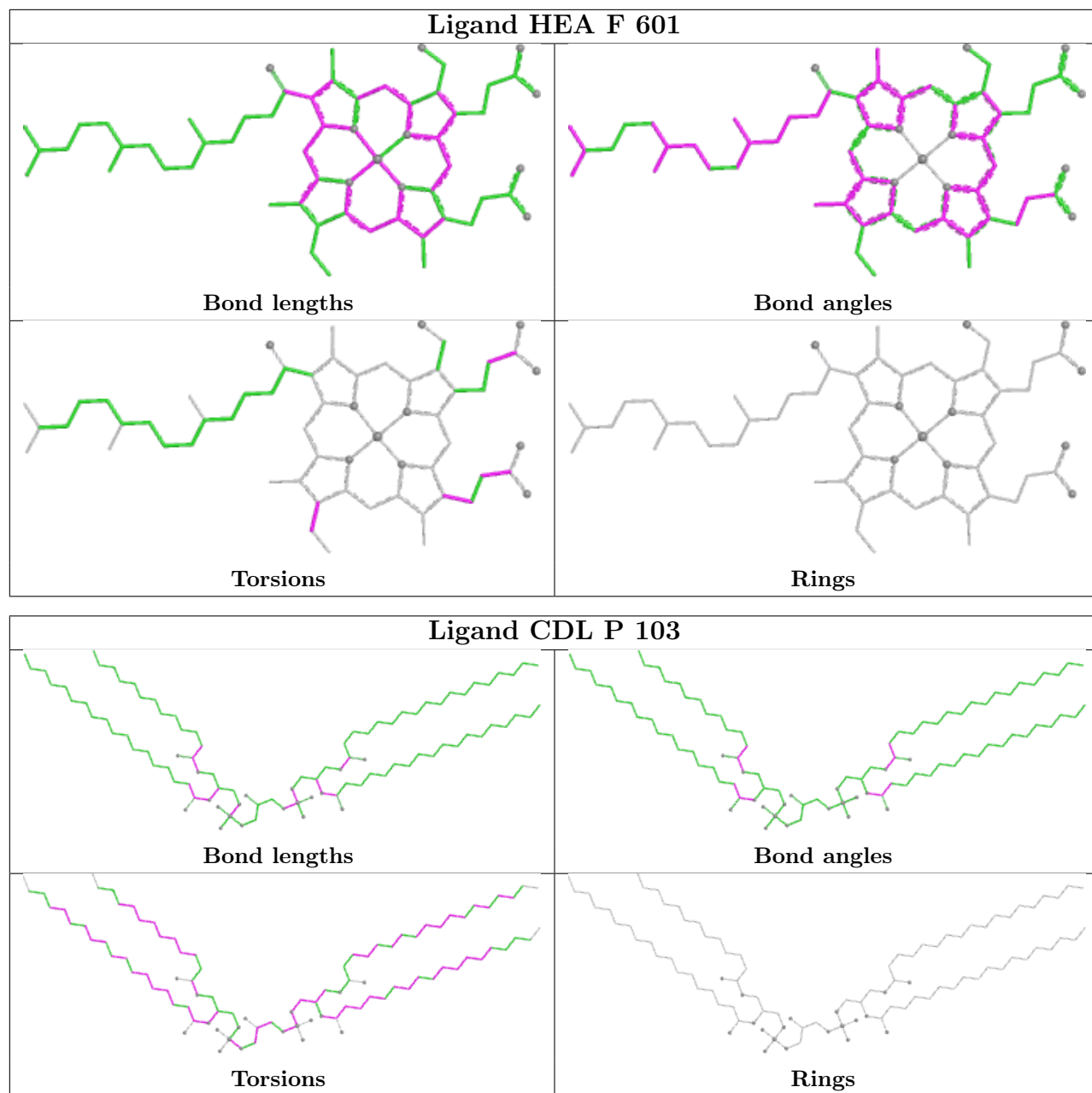
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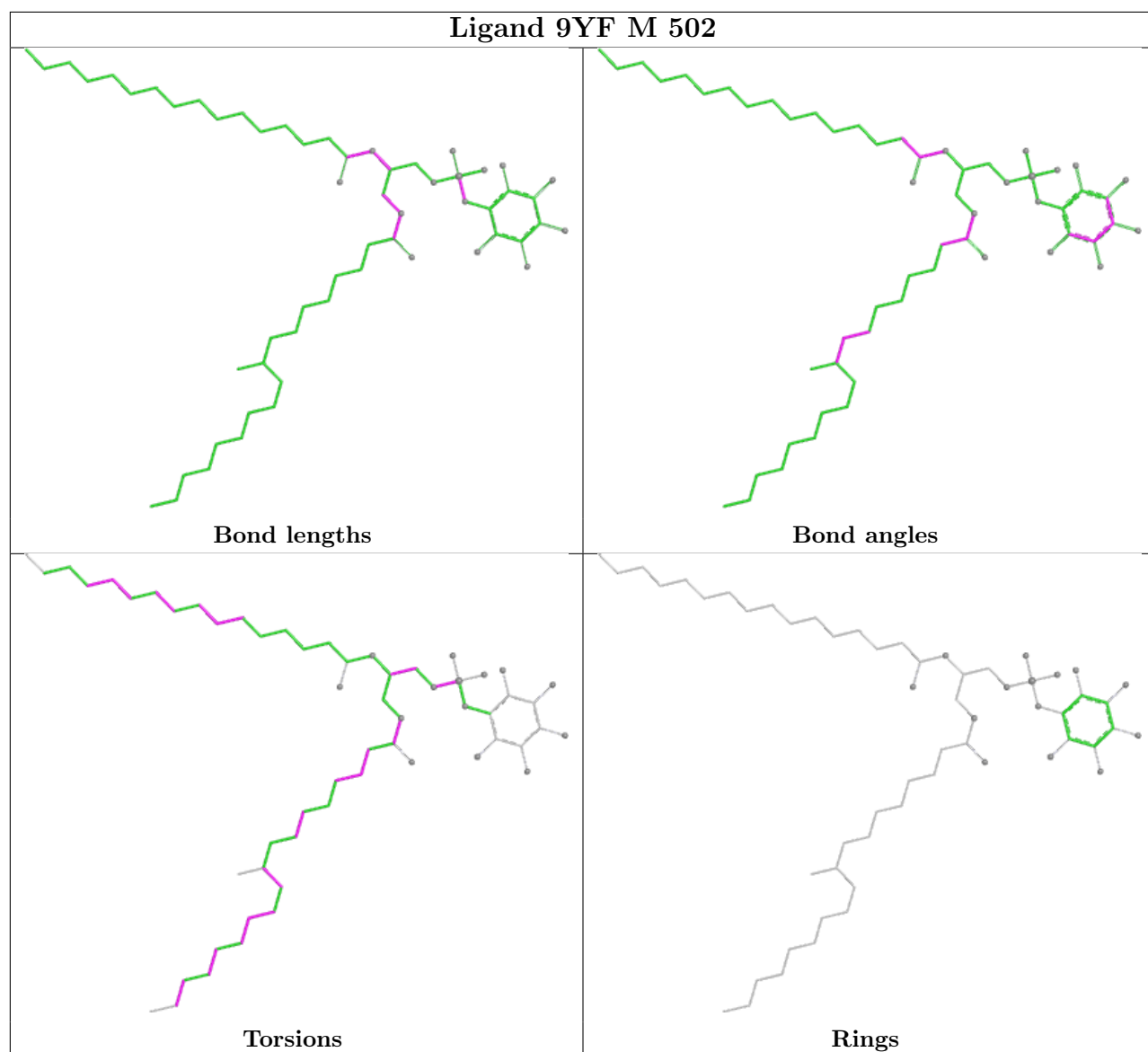
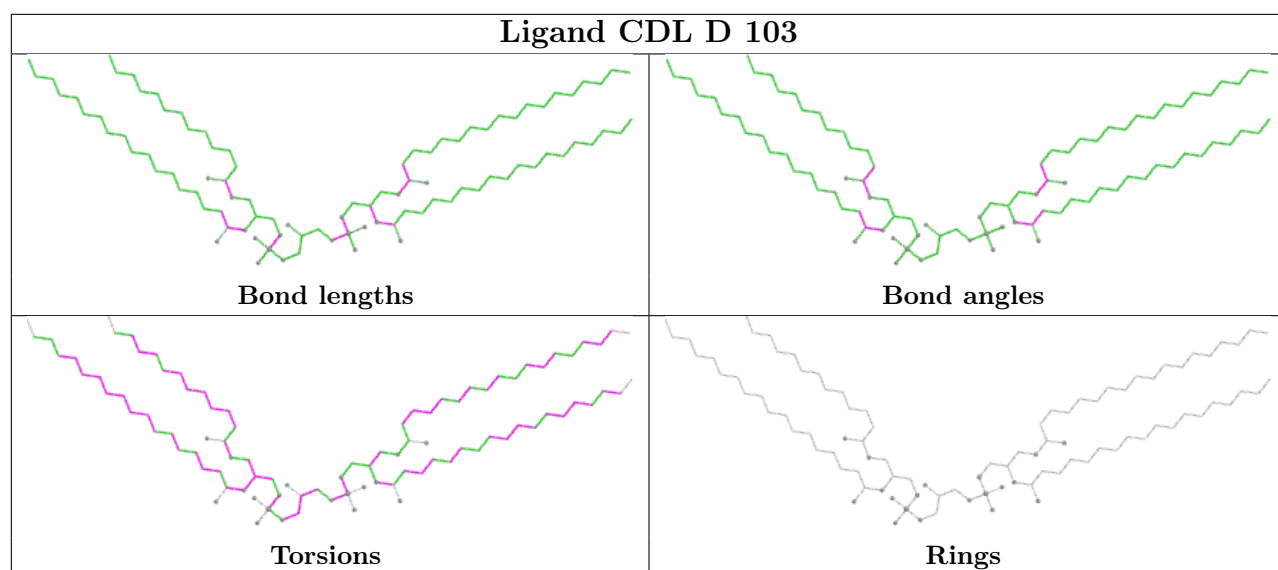
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	N	603	CDL	3	0
24	H	201	MQ7	2	0
16	C	305	CDL	3	0
22	R	602	HEA	6	0
16	R	606	CDL	3	0
14	T	201	PLM	4	0
24	O	301	MQ7	3	0
16	B	604	CDL	4	0
12	A	501	FES	1	0
16	N	604	CDL	2	0
16	F	606	CDL	9	0
20	P	102	9Y0	1	0
16	P	101	CDL	7	0
14	G	302	PLM	1	0
15	N	602	HEM	3	0
15	B	601	HEM	2	0
16	B	603	CDL	5	0

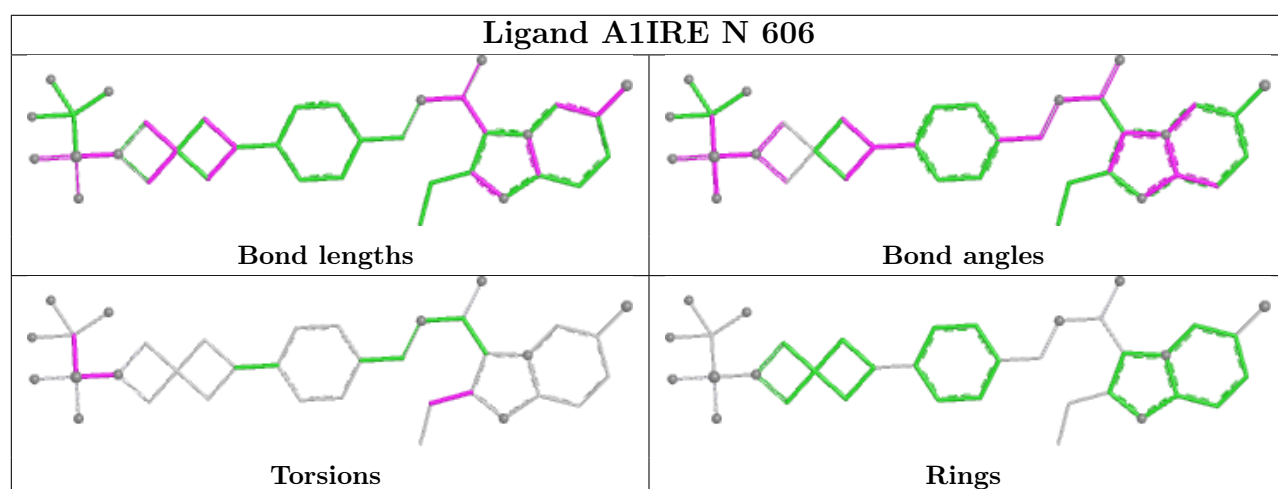
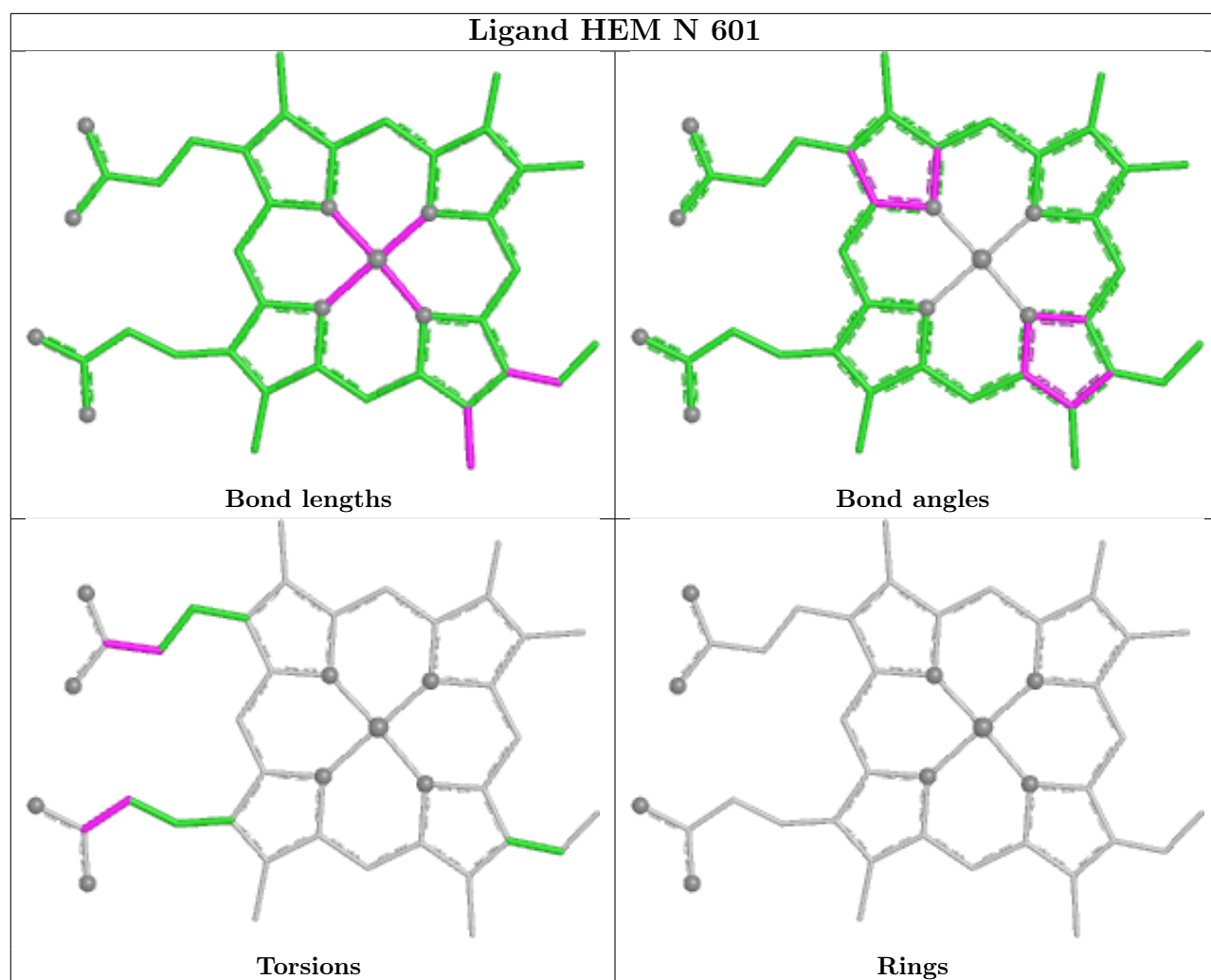
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

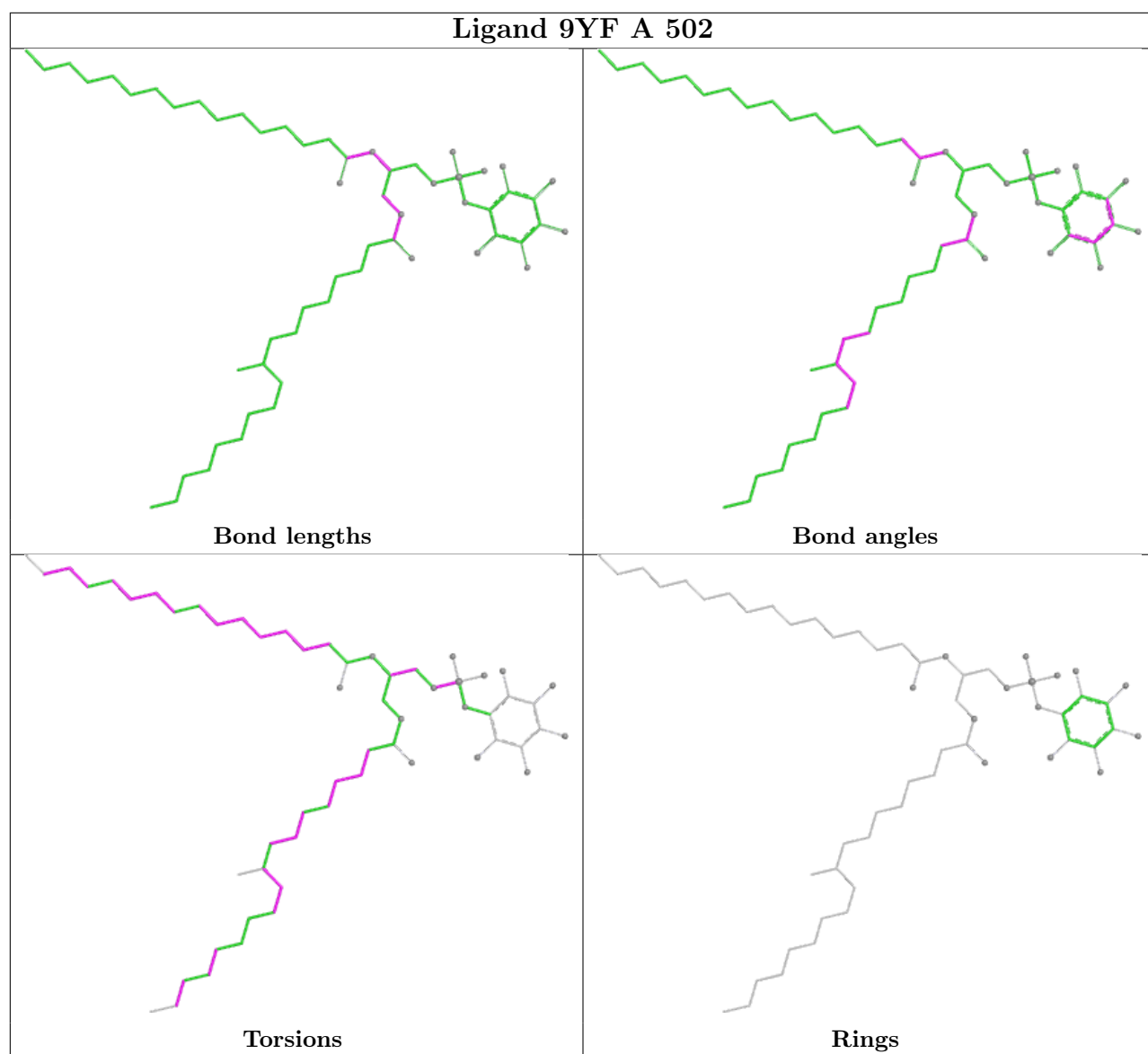
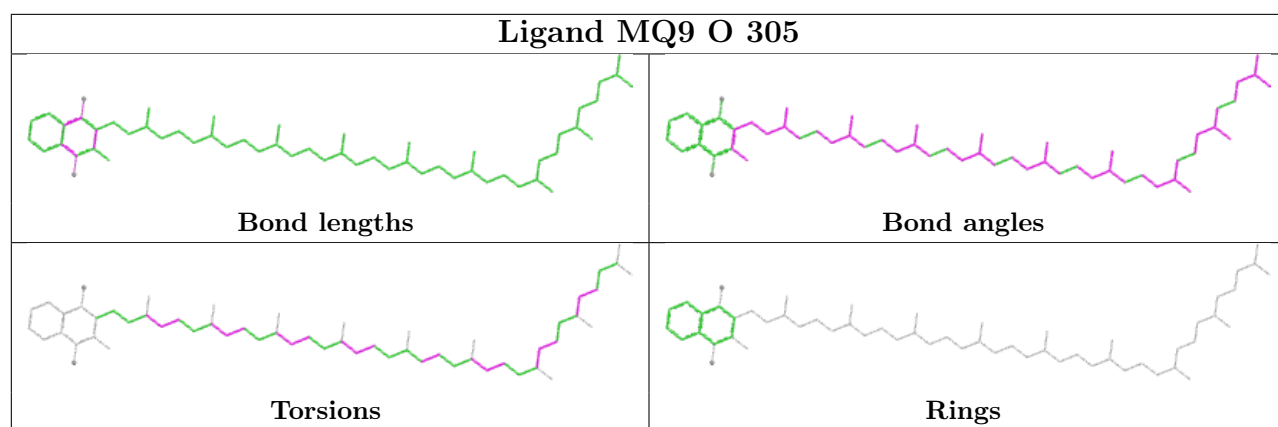


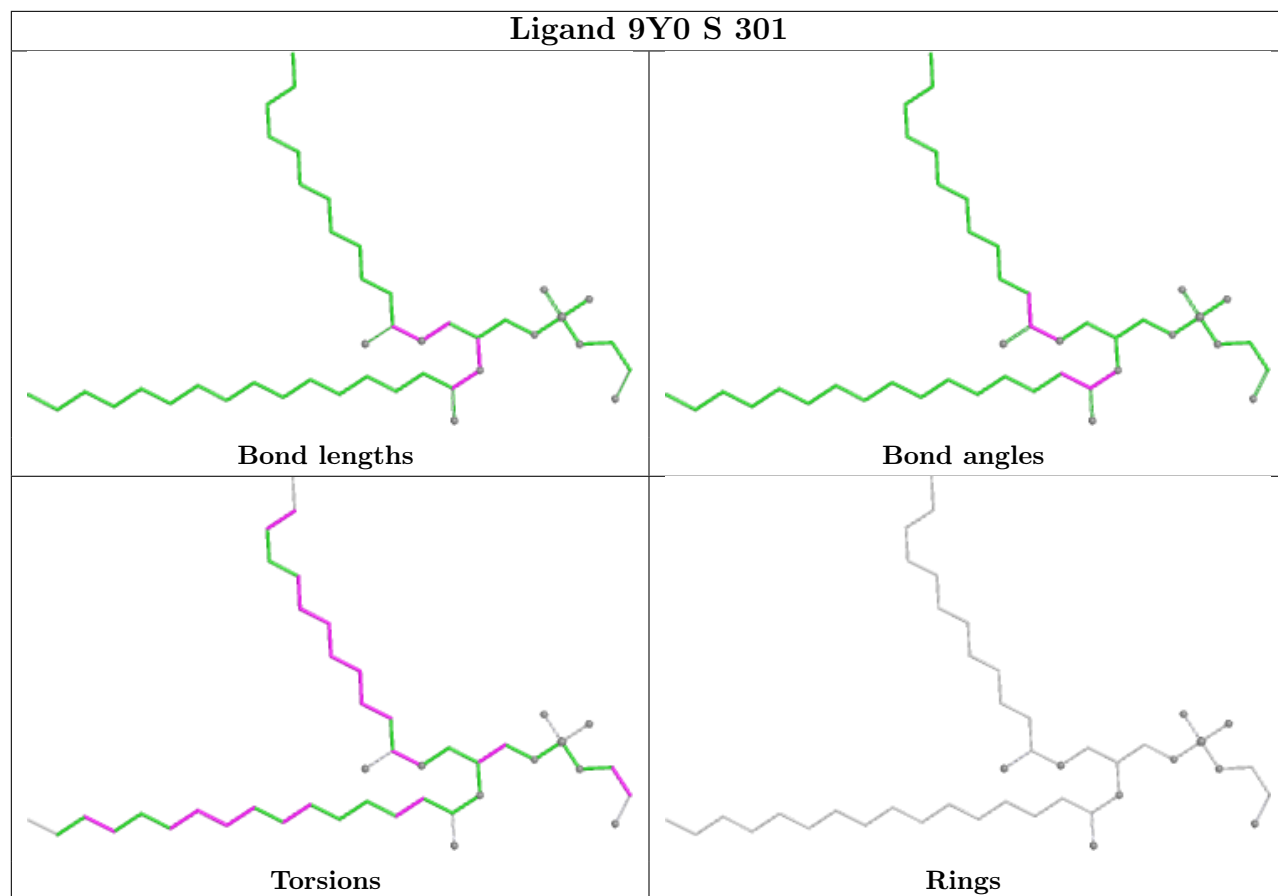


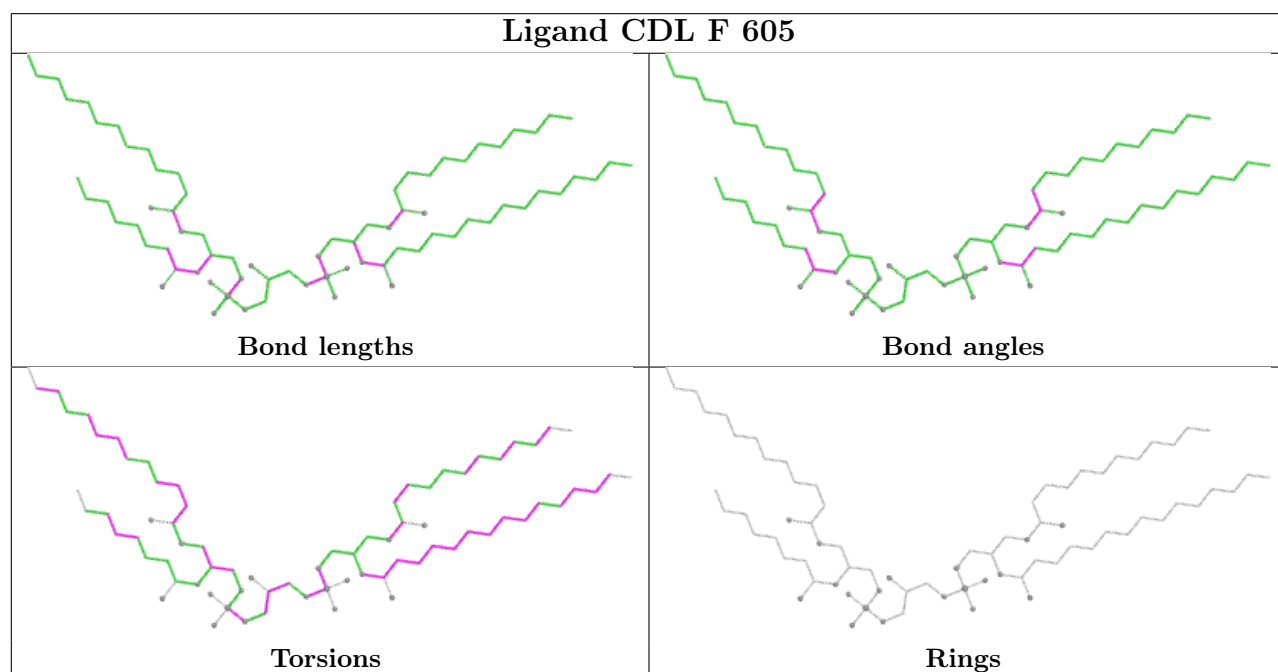
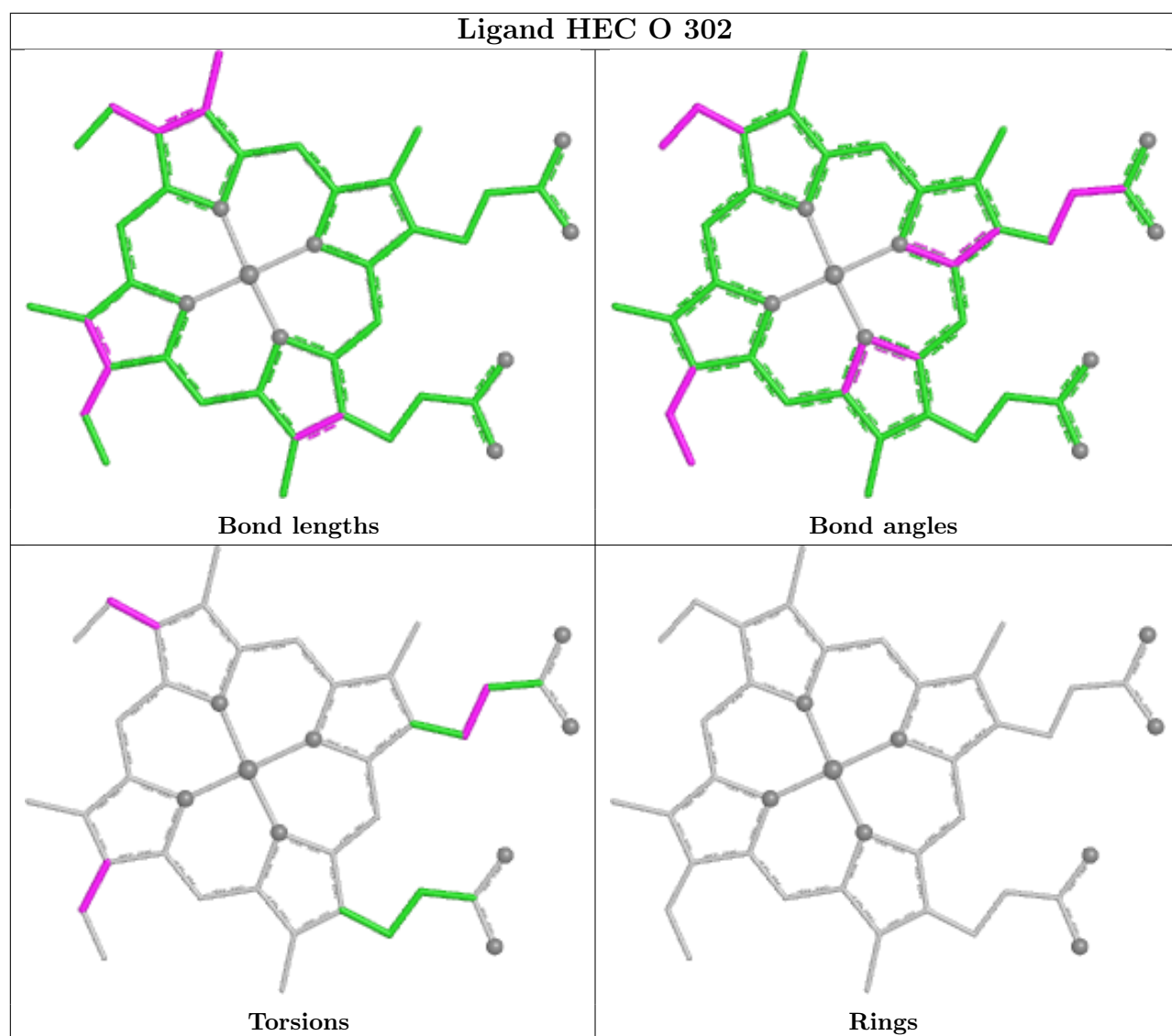


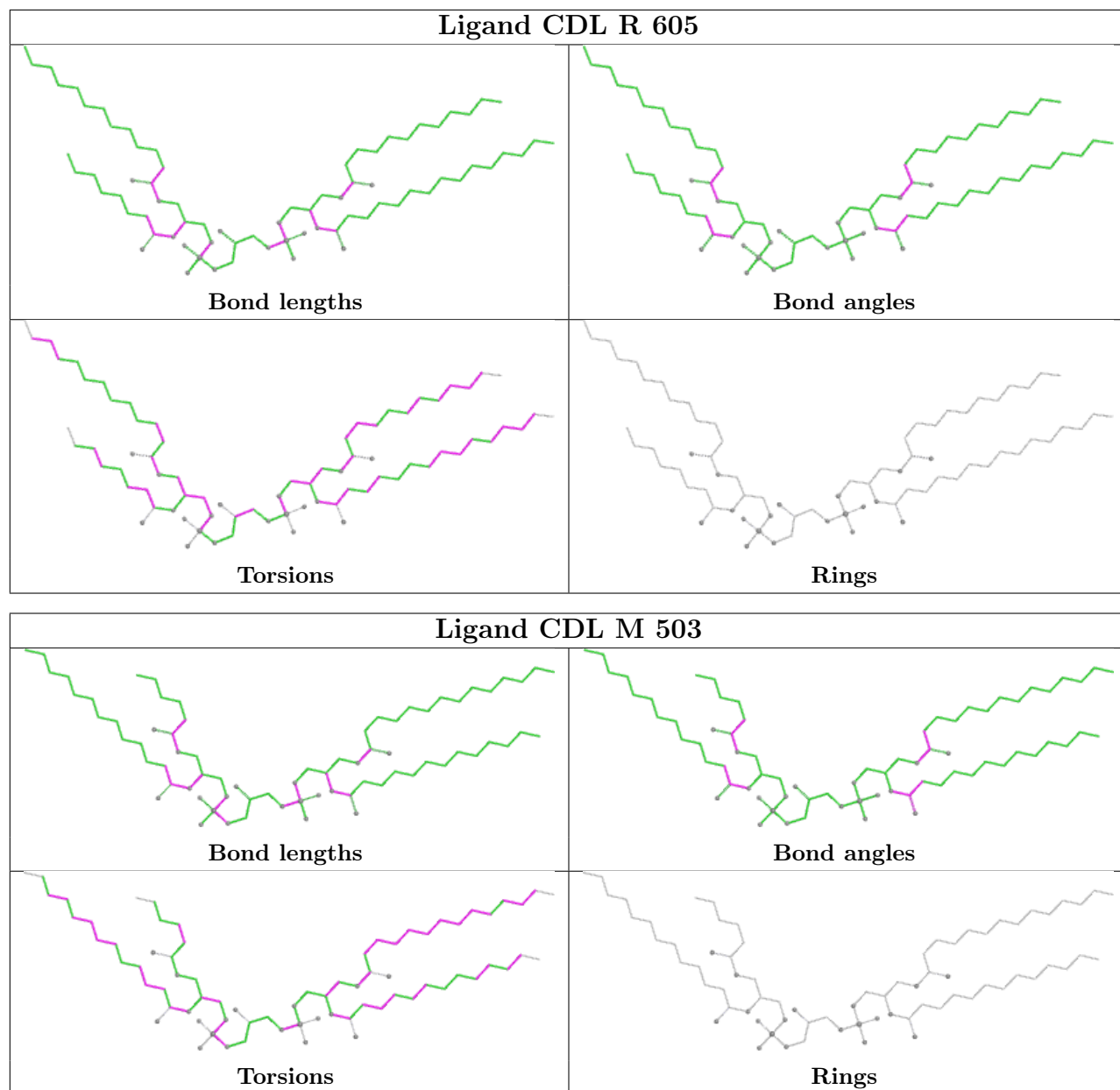


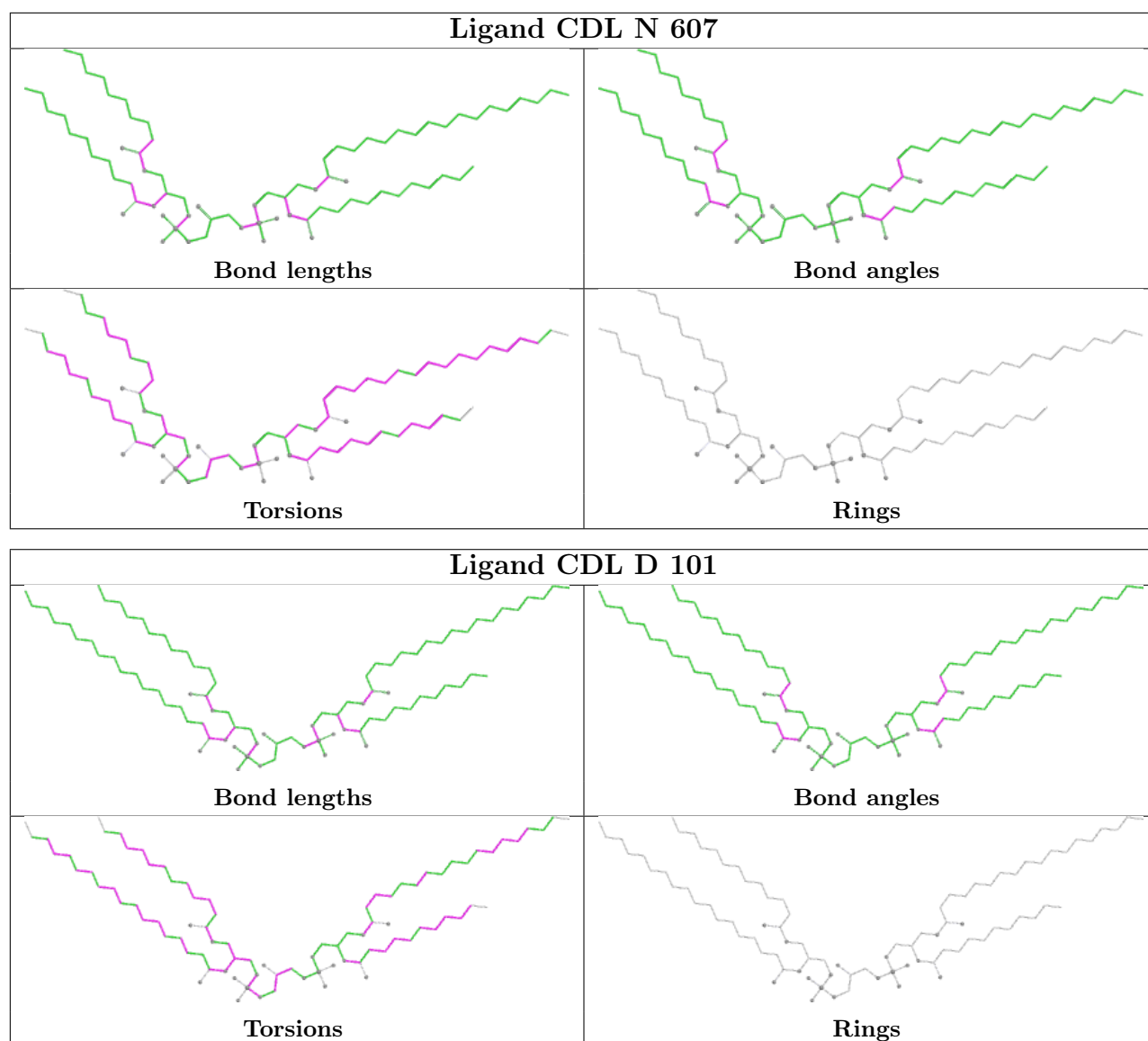




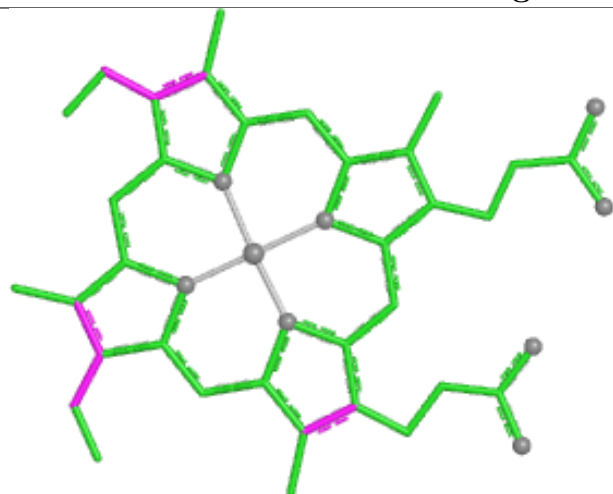




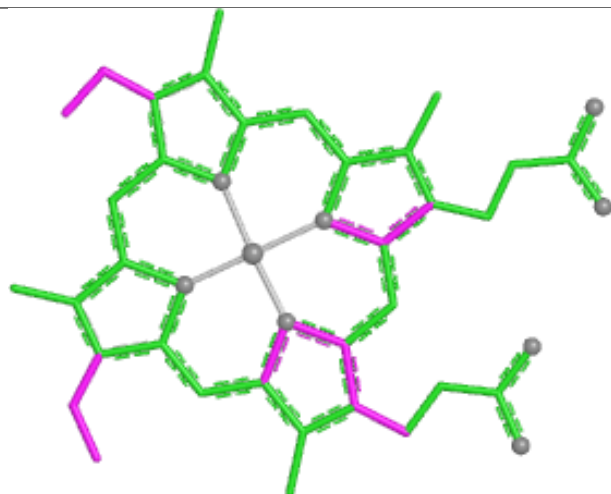




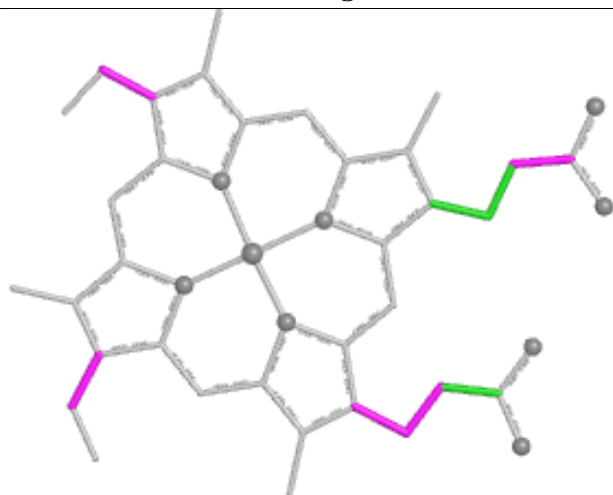
Ligand HEC C 302



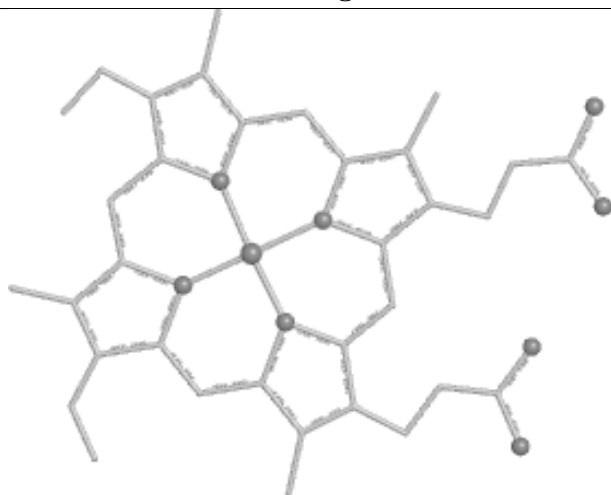
Bond lengths



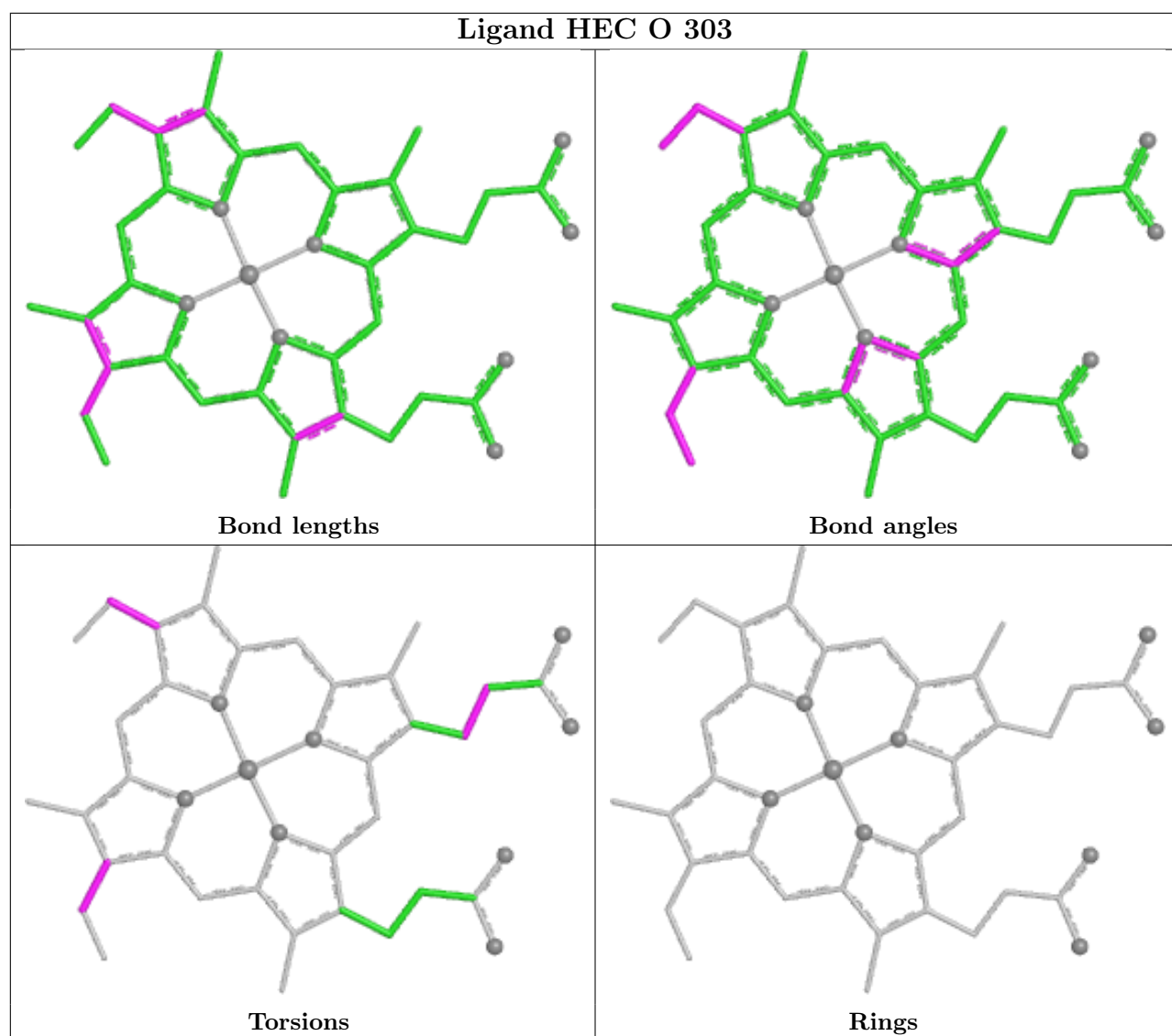
Bond angles

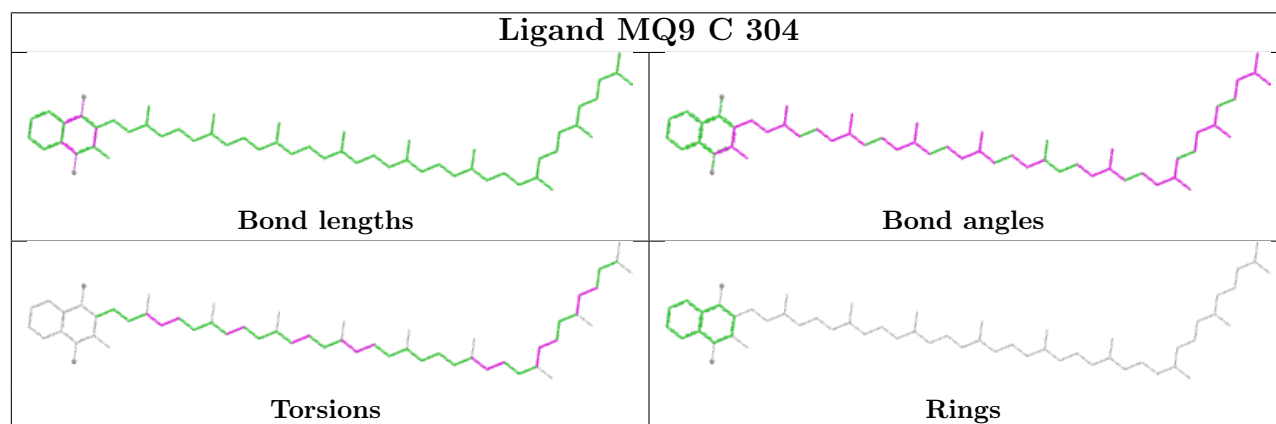
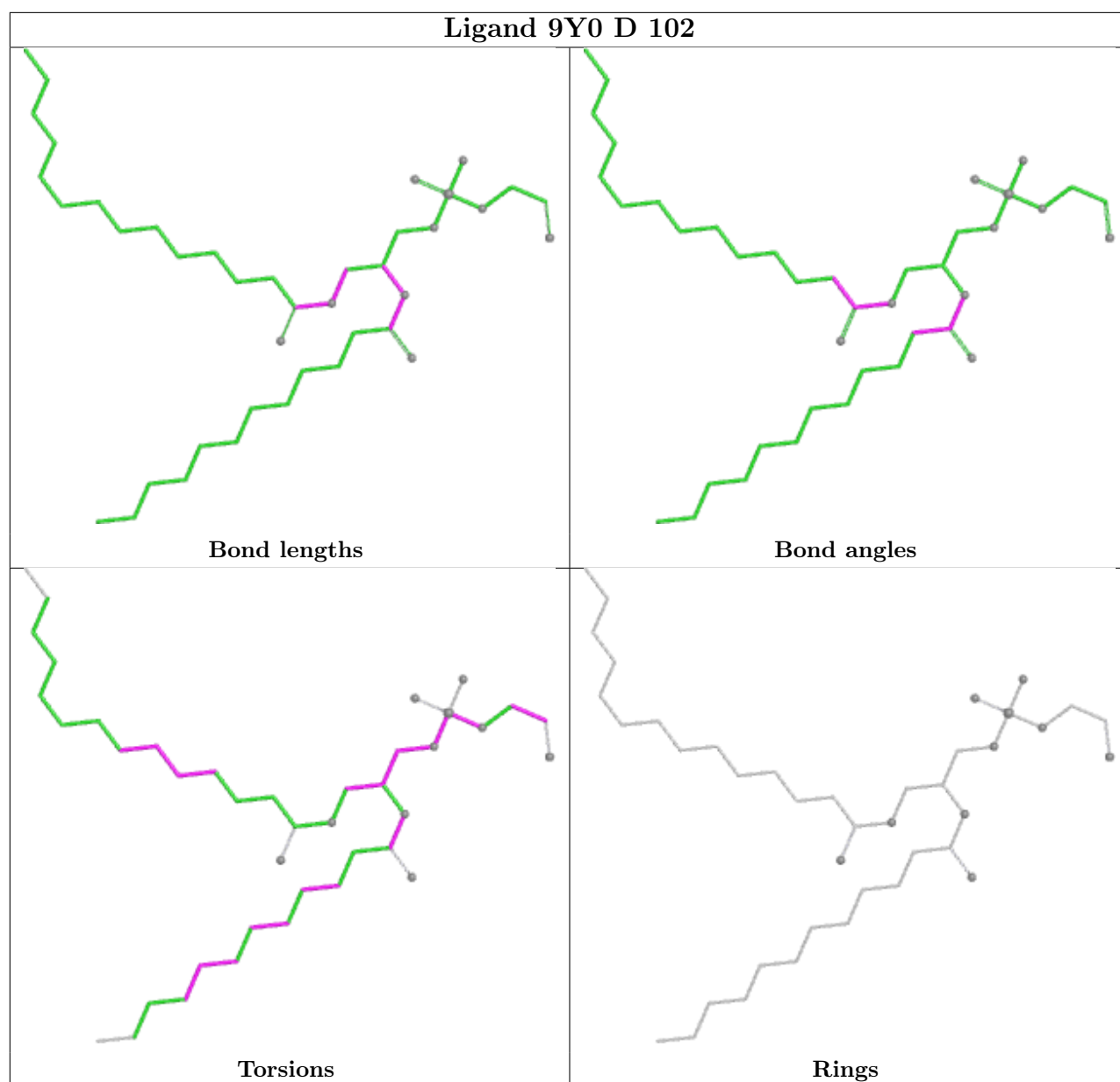


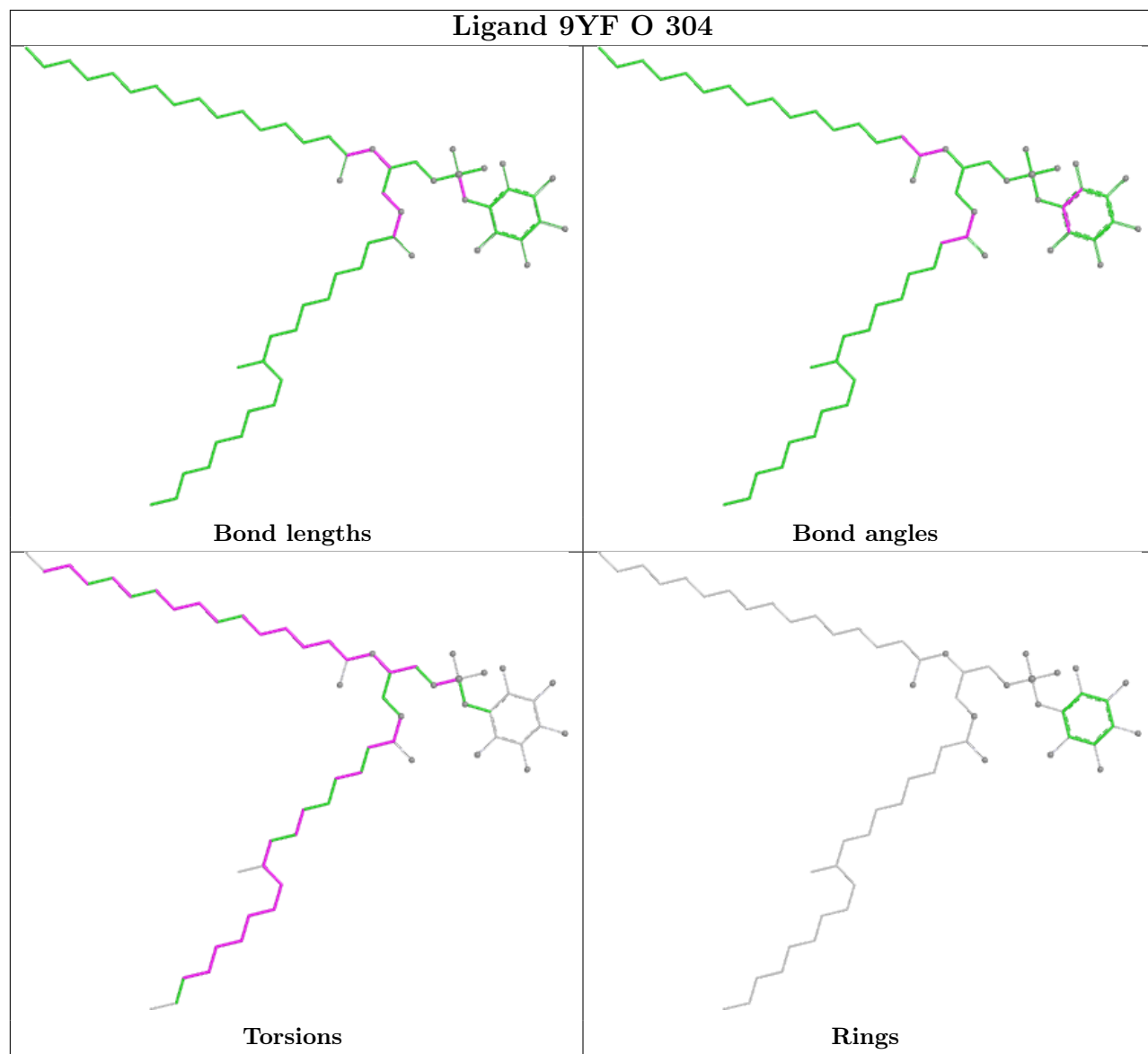
Torsions

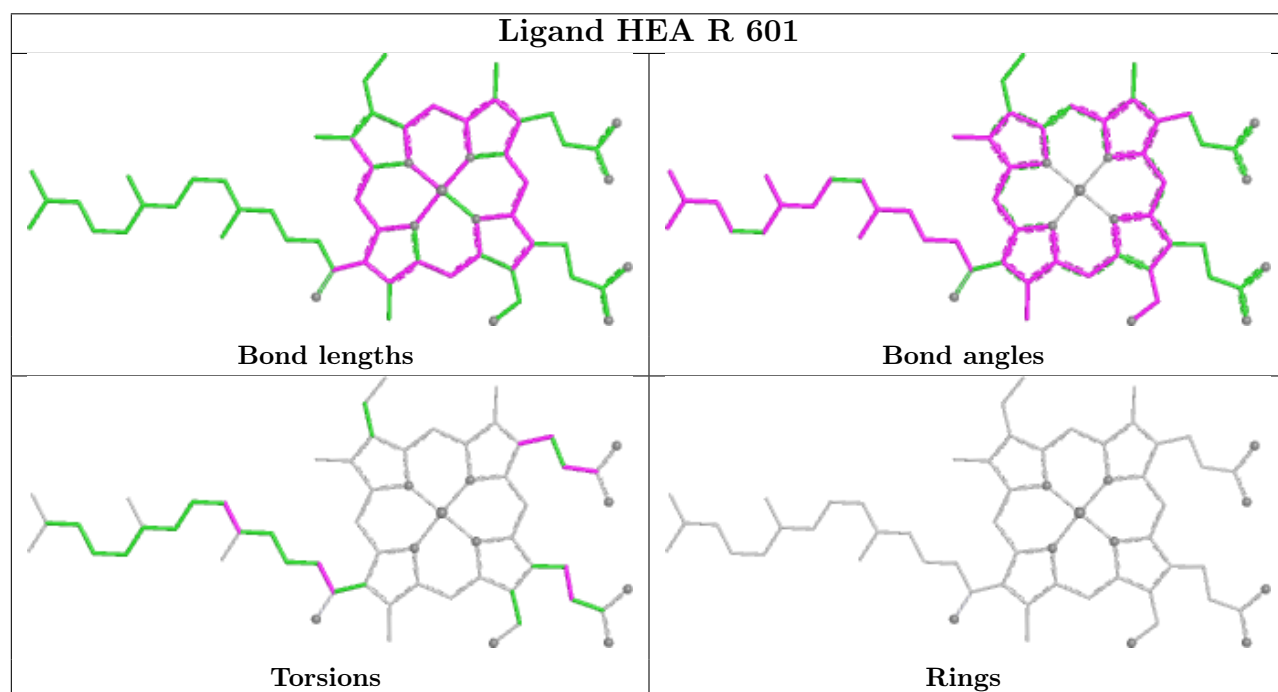
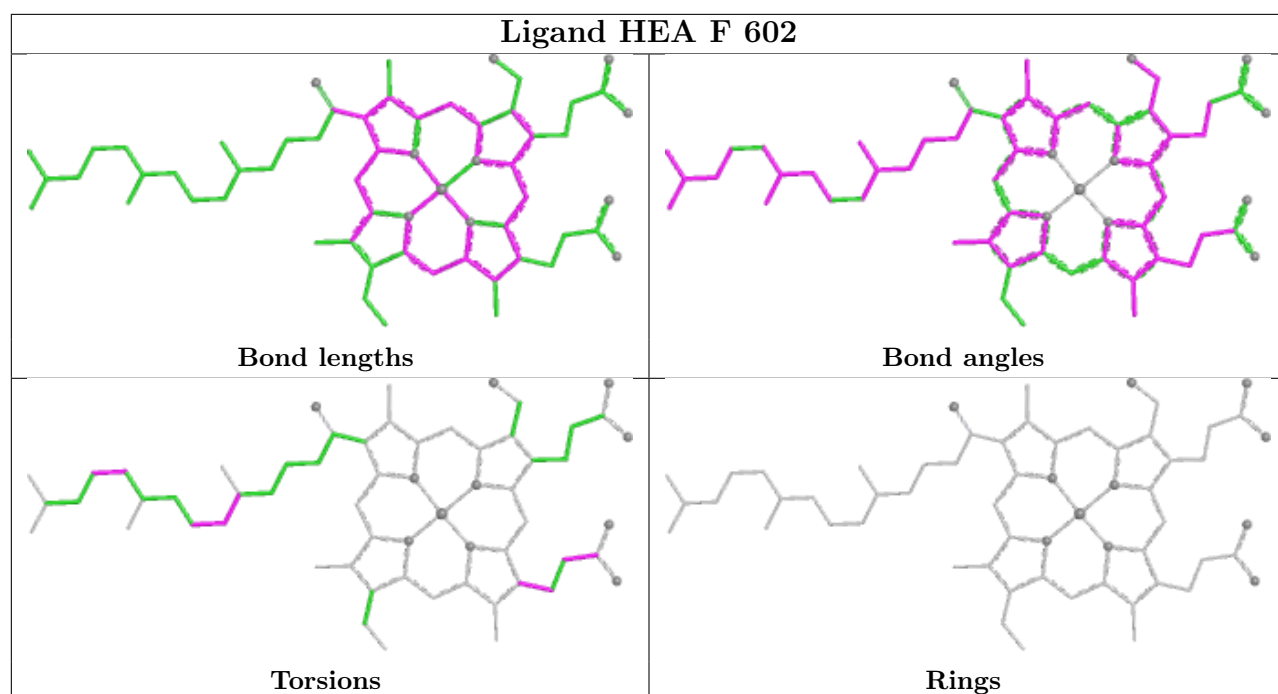


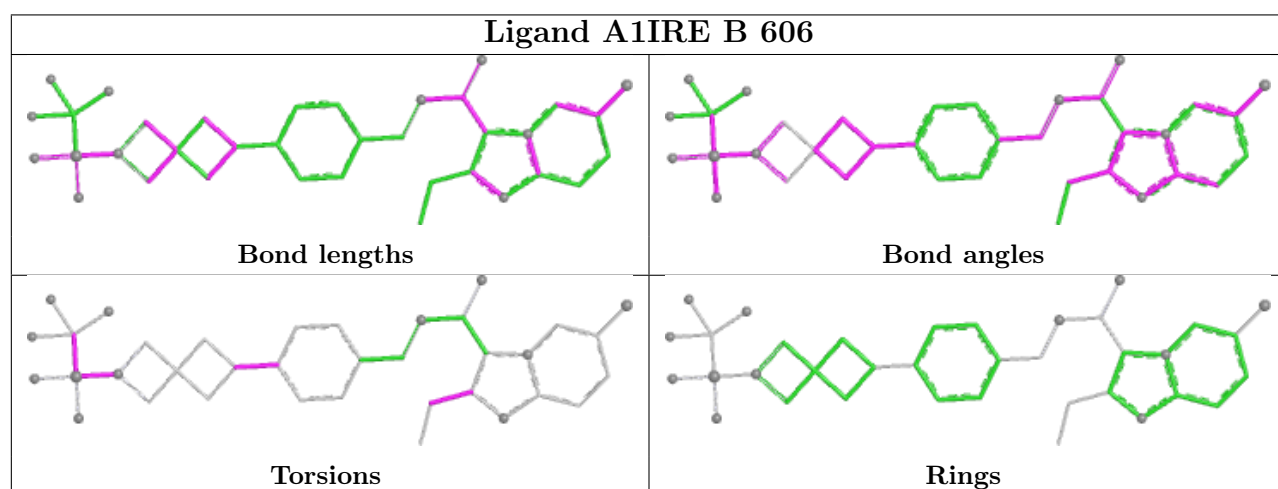
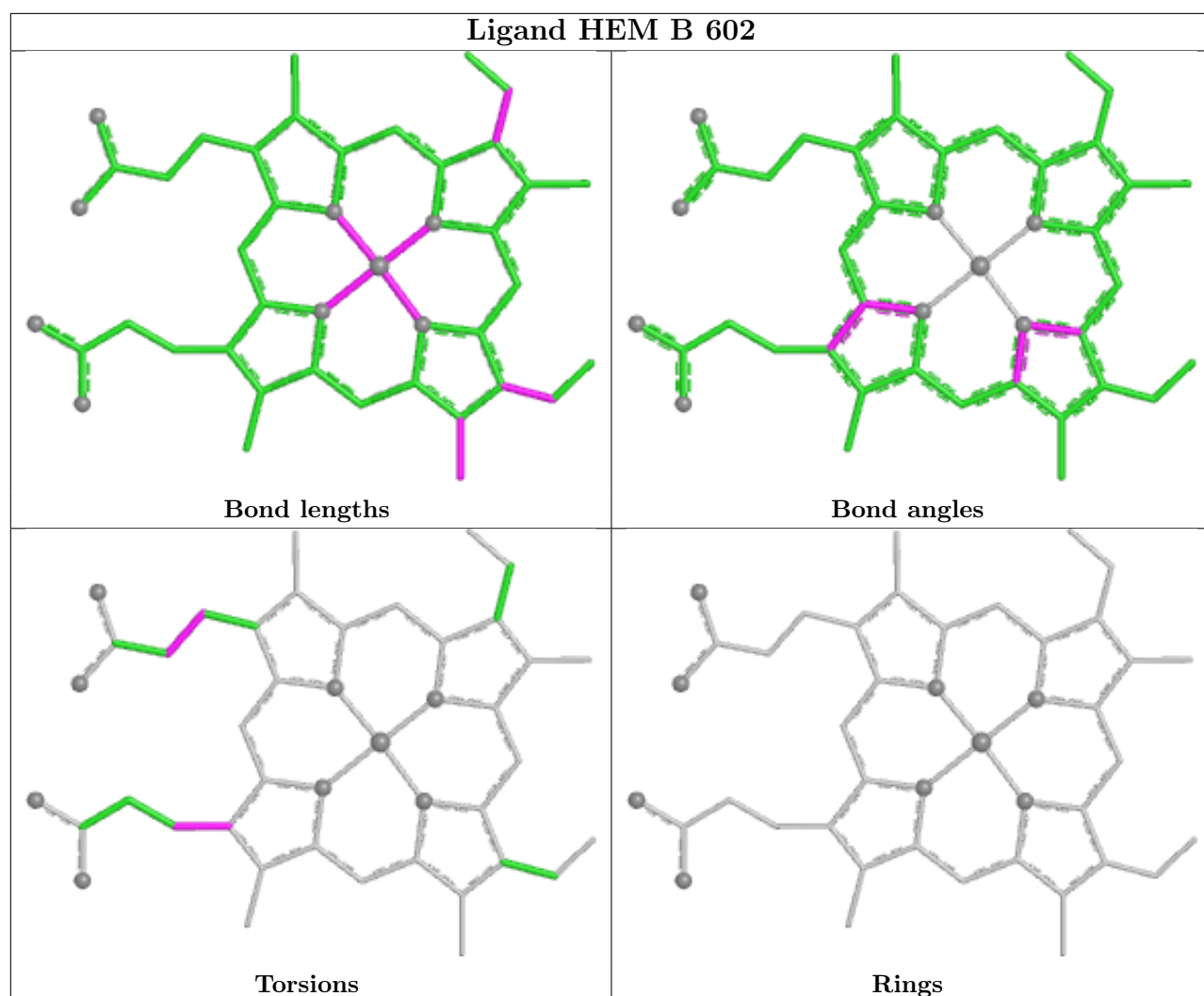
Rings

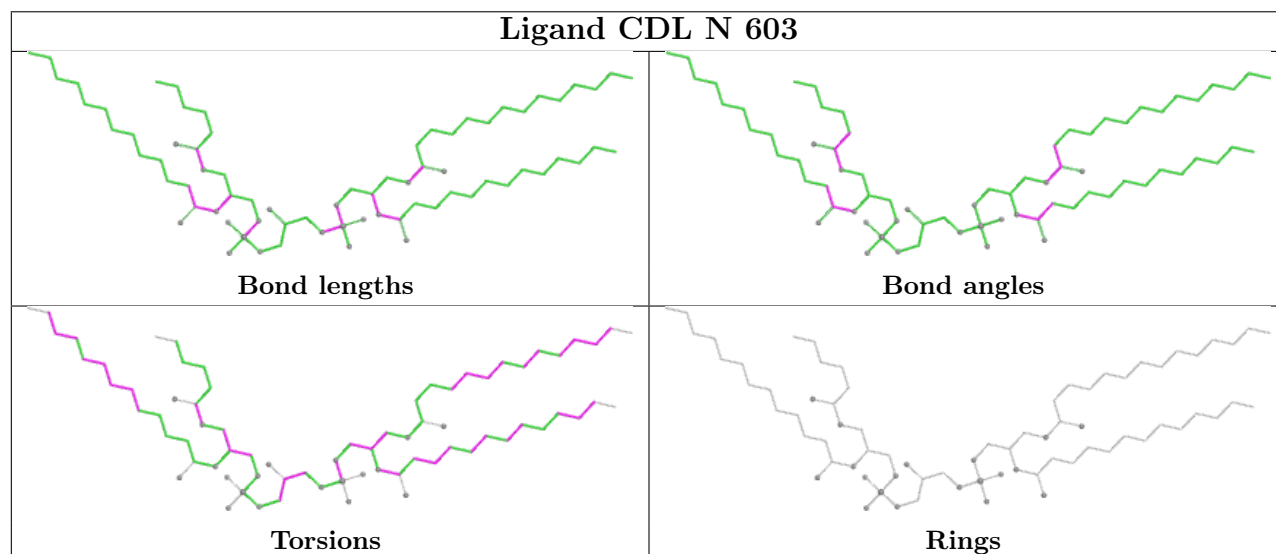
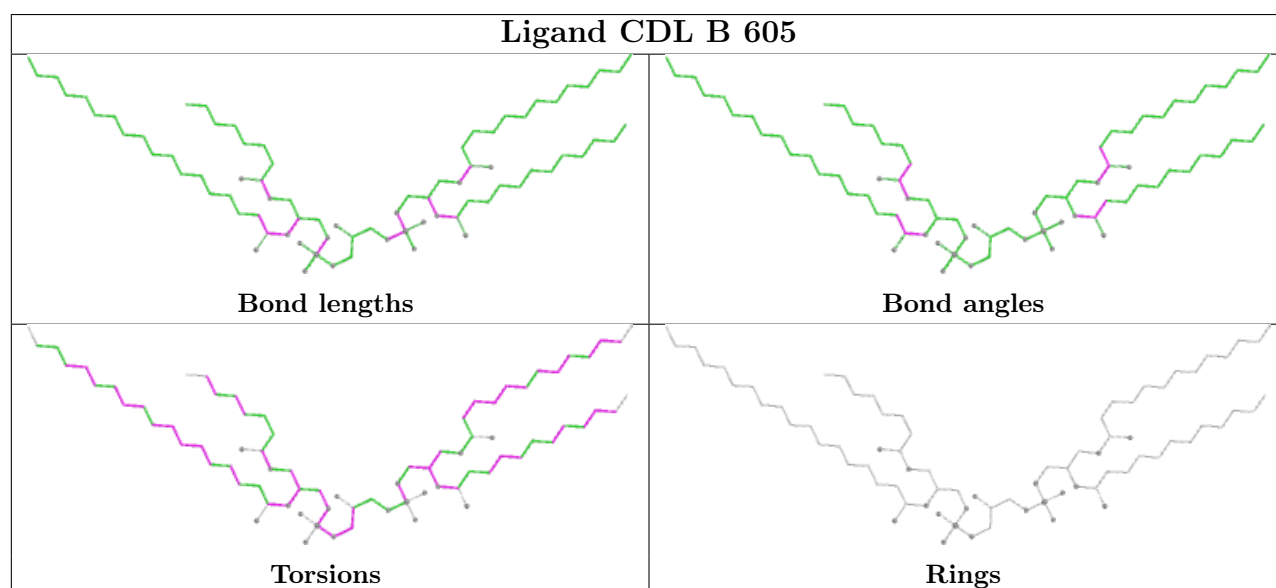
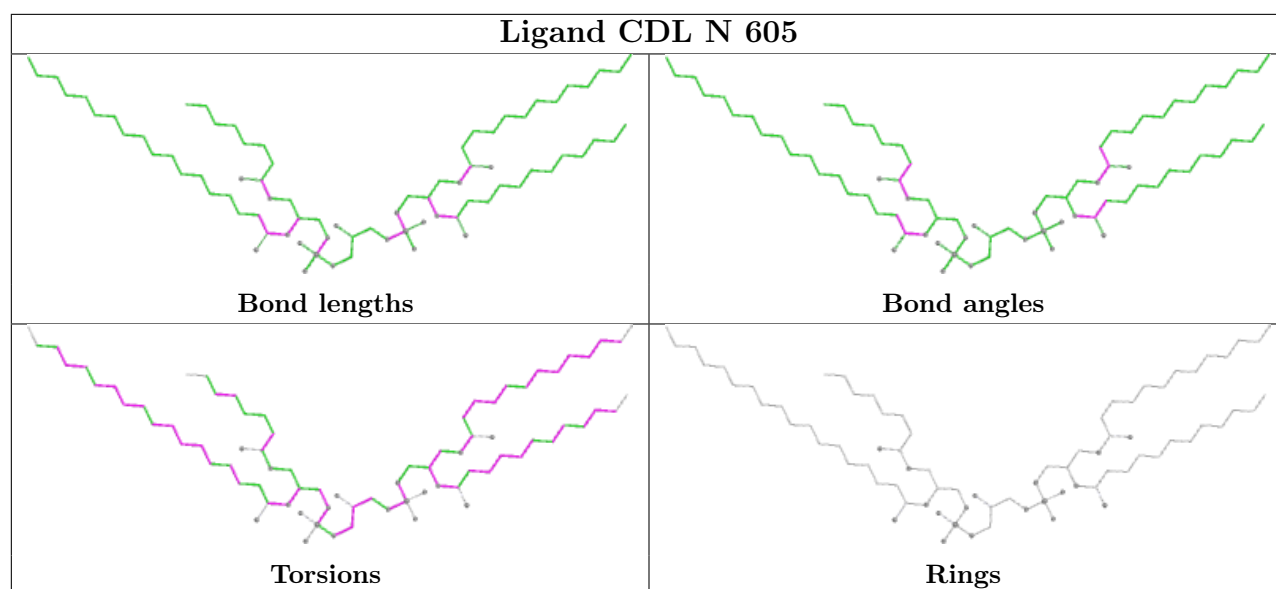


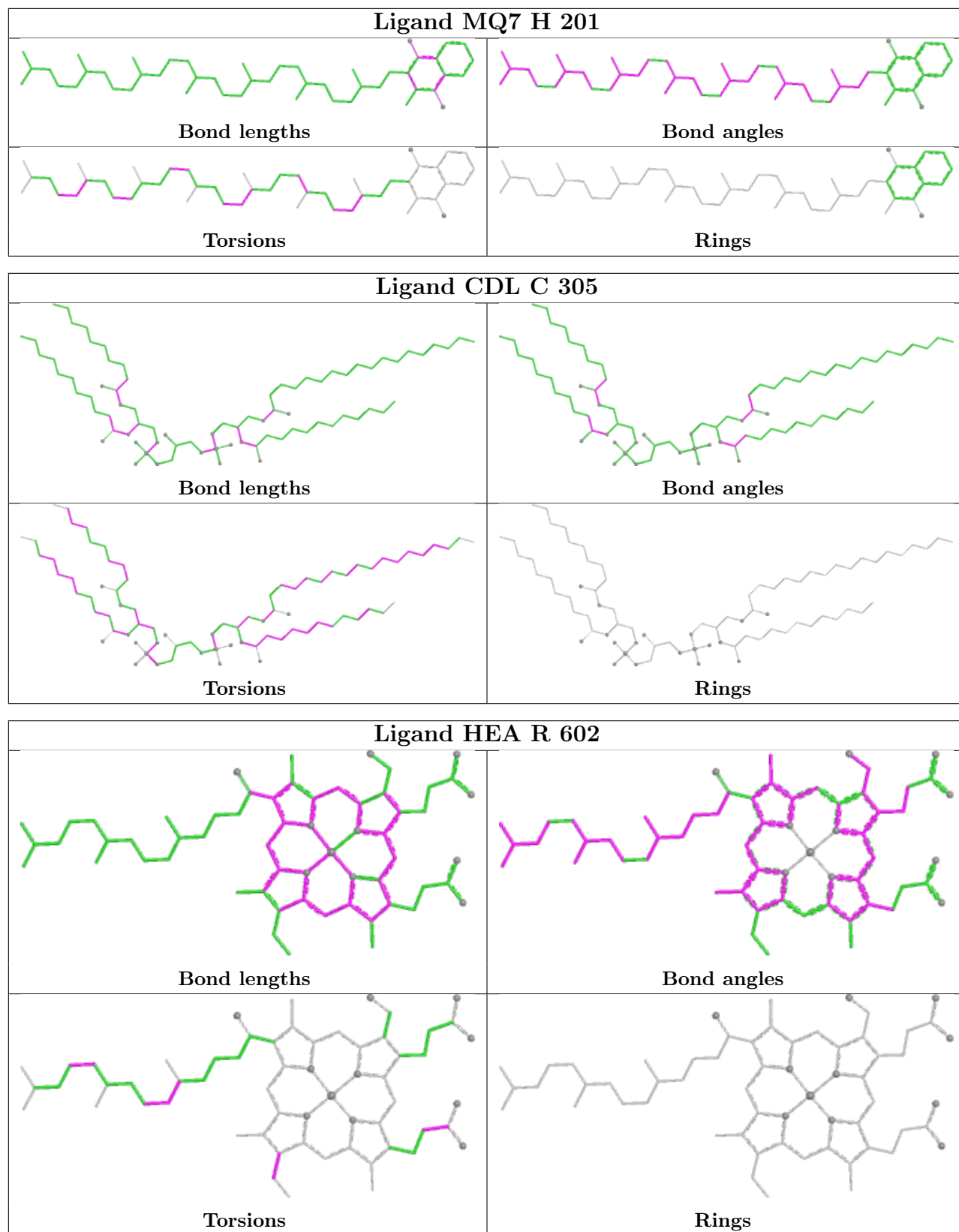


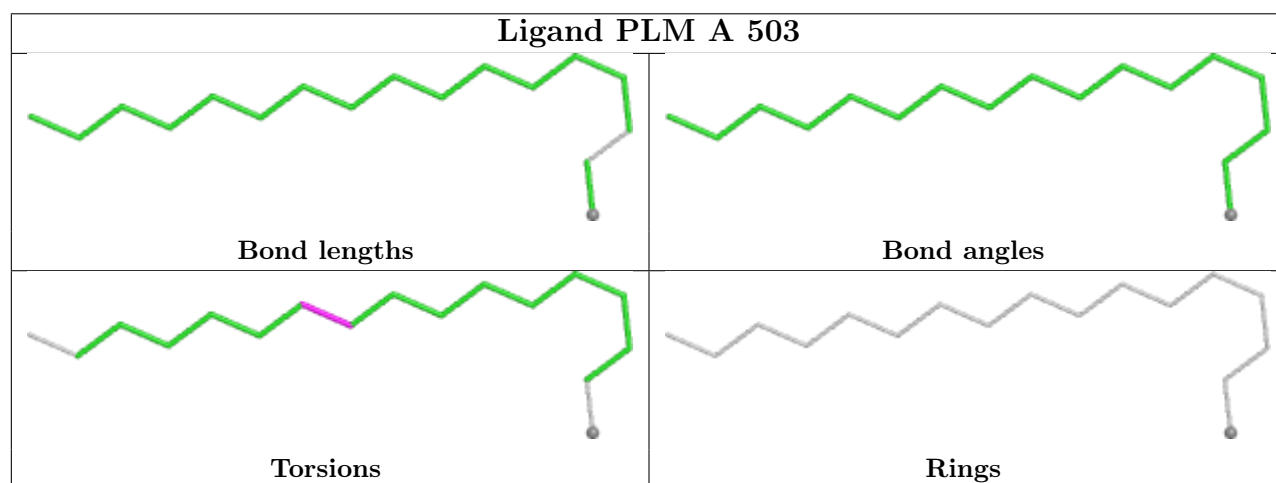
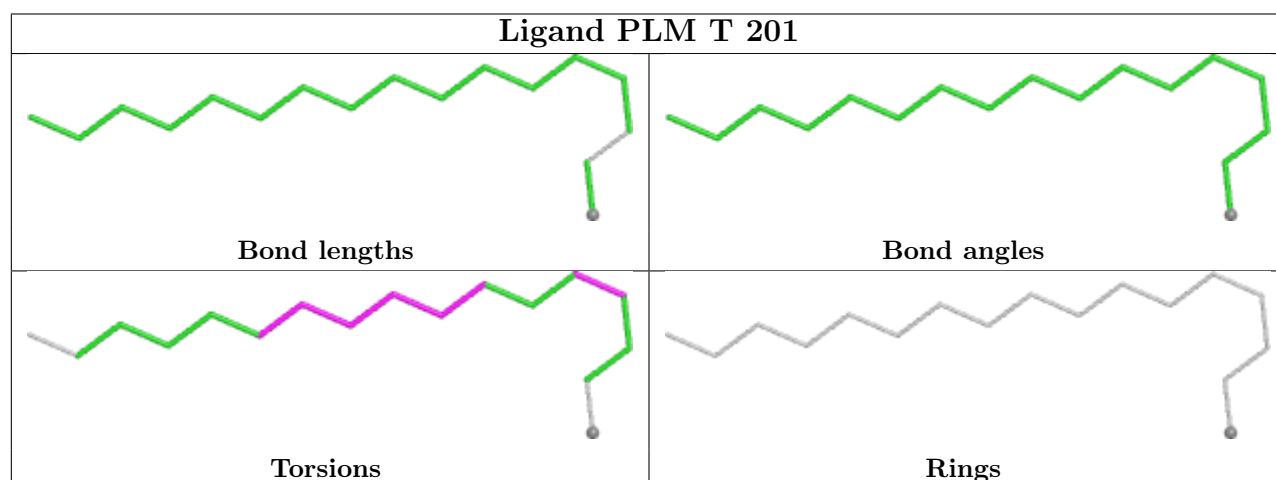
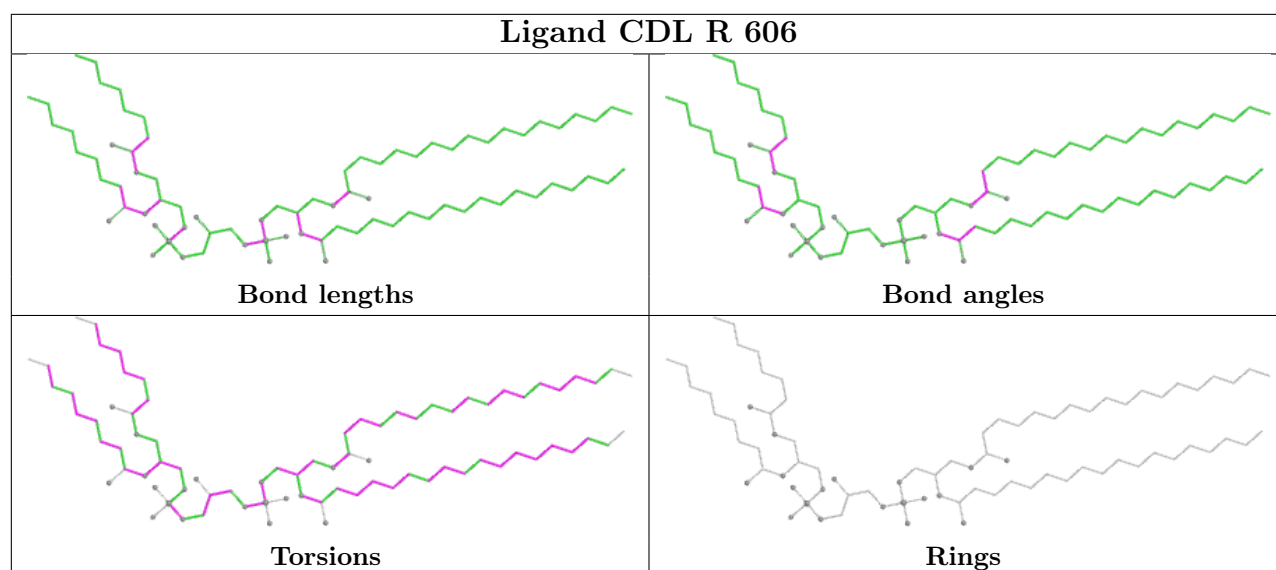


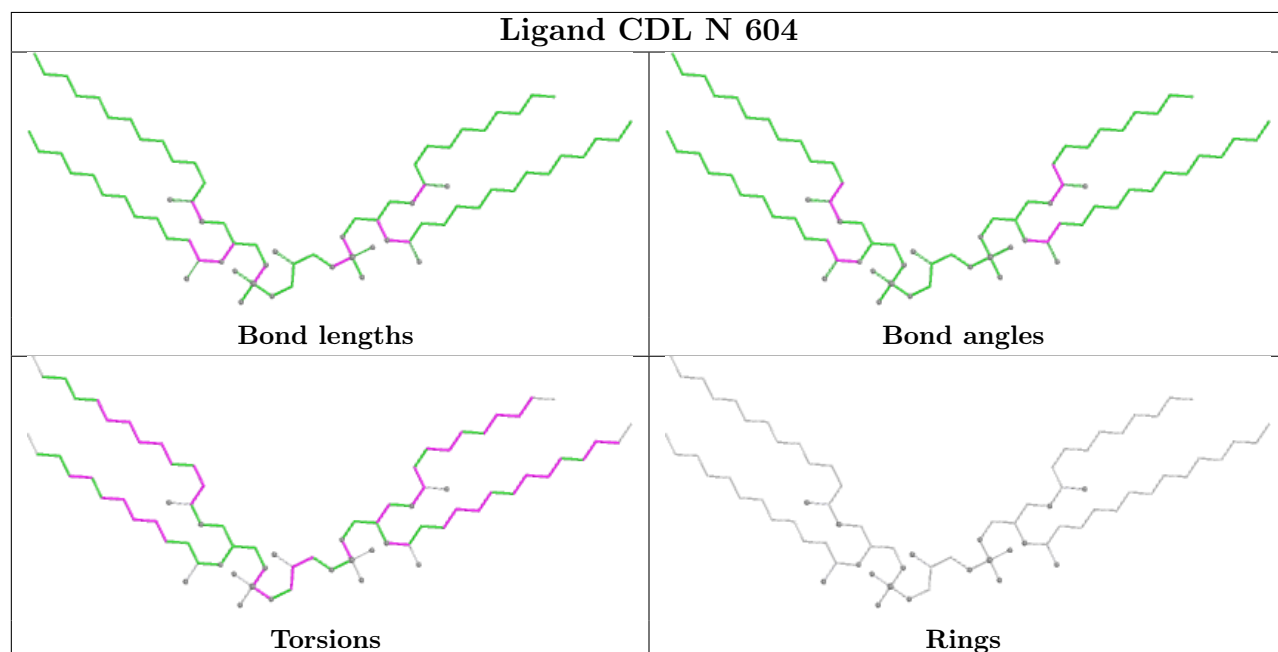
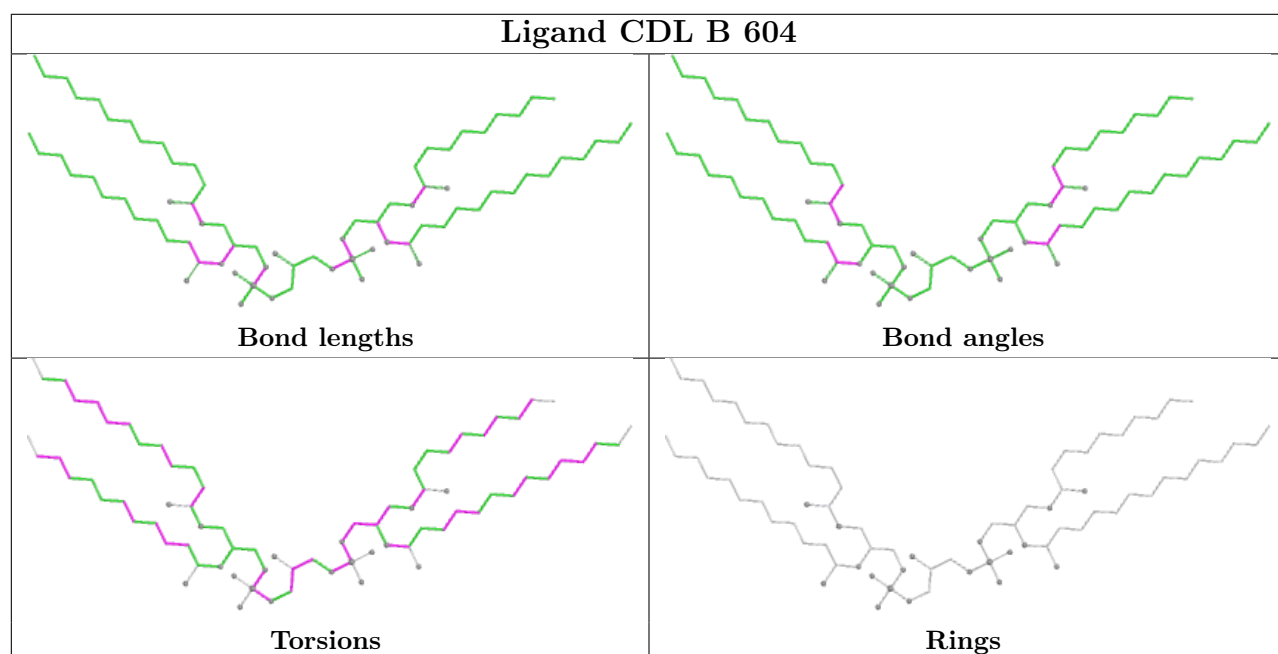
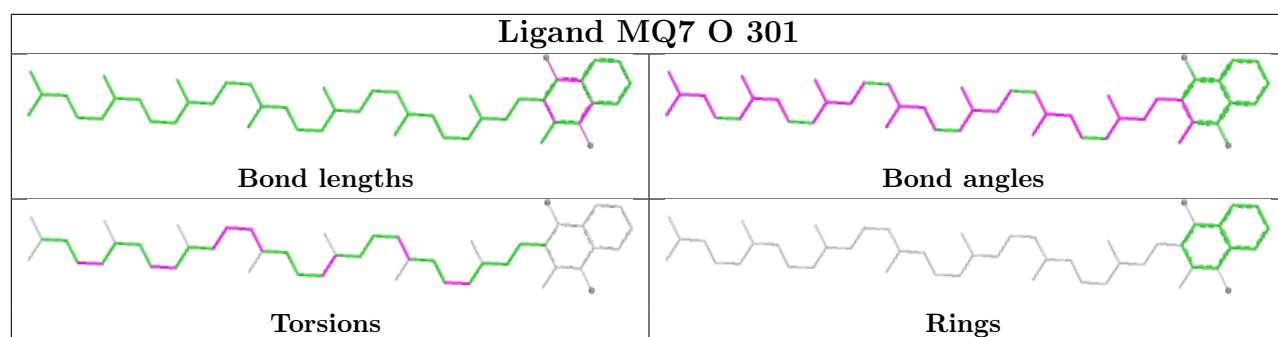


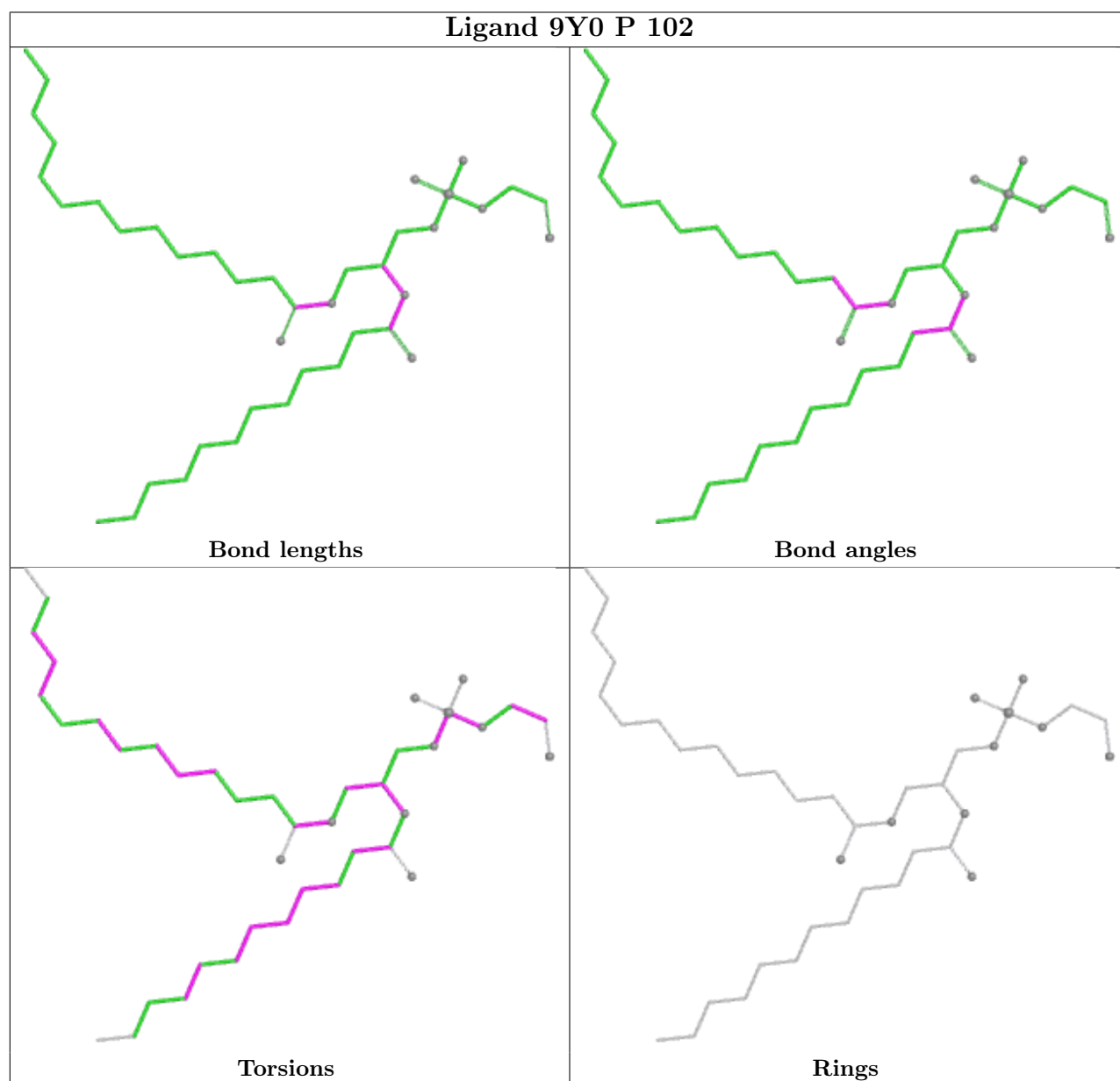
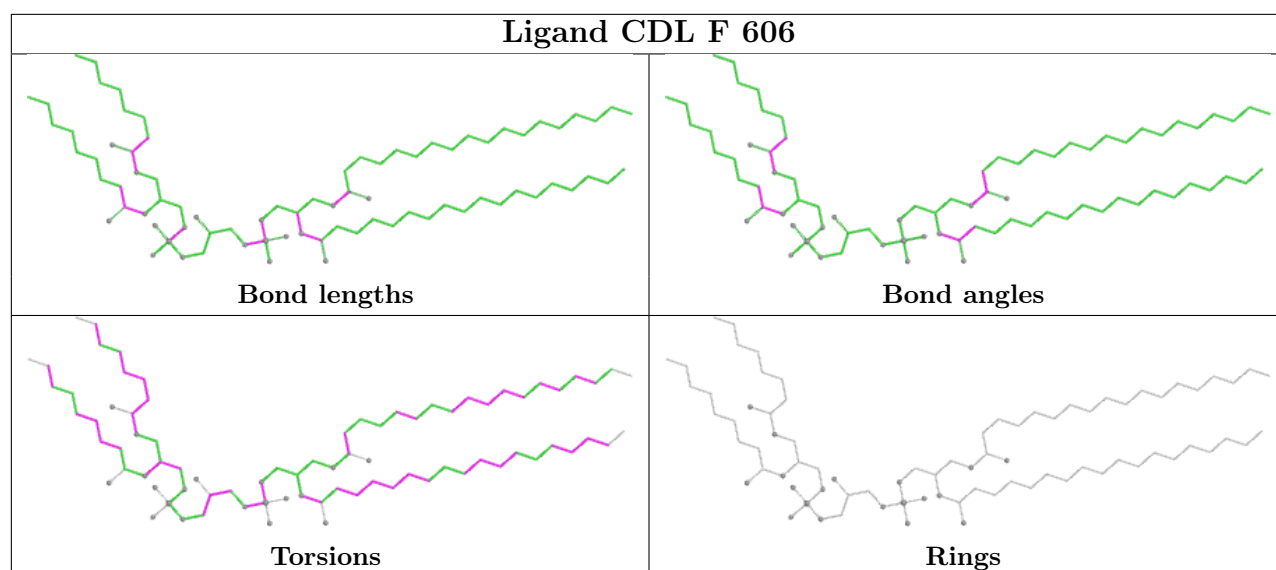


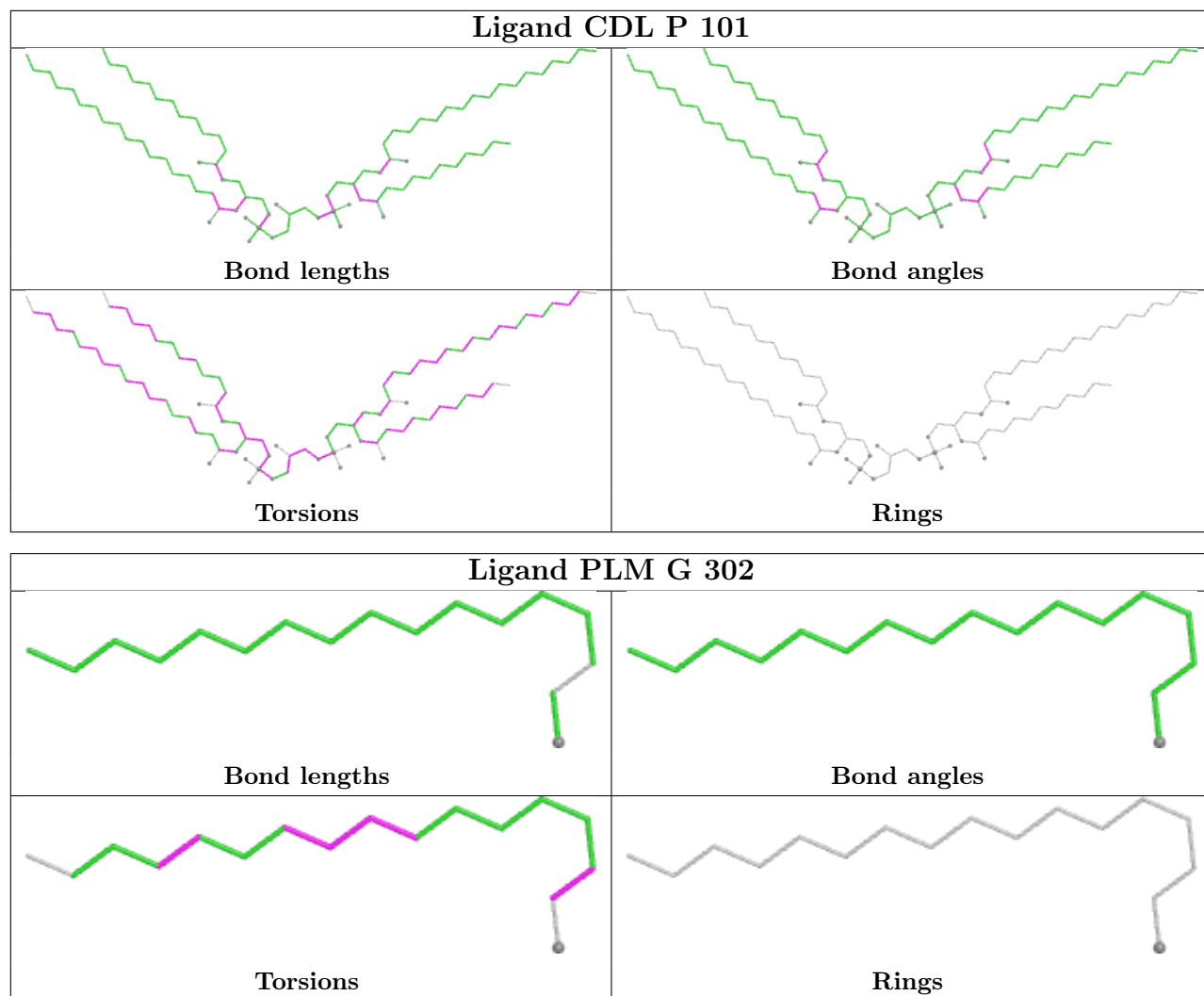


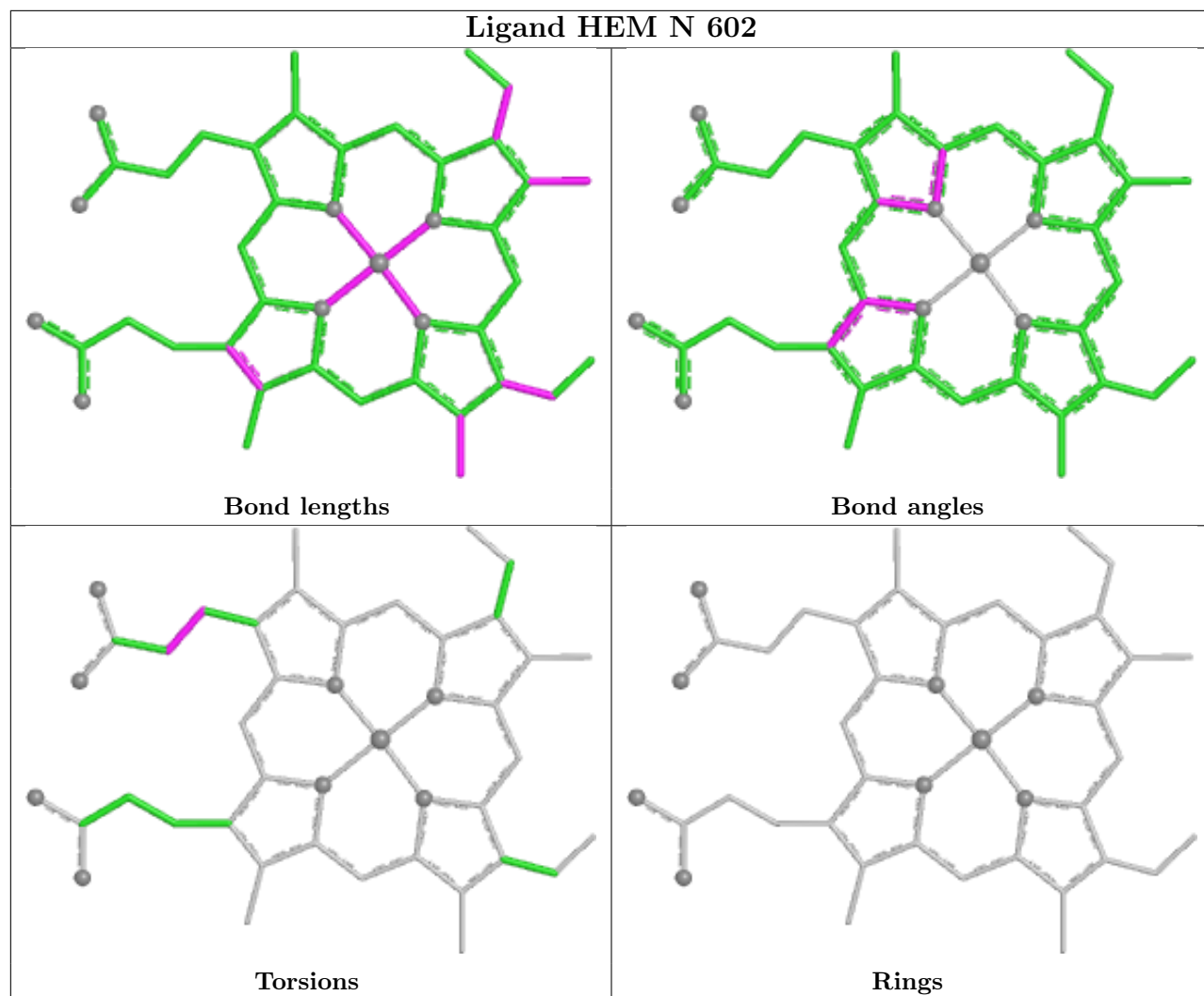


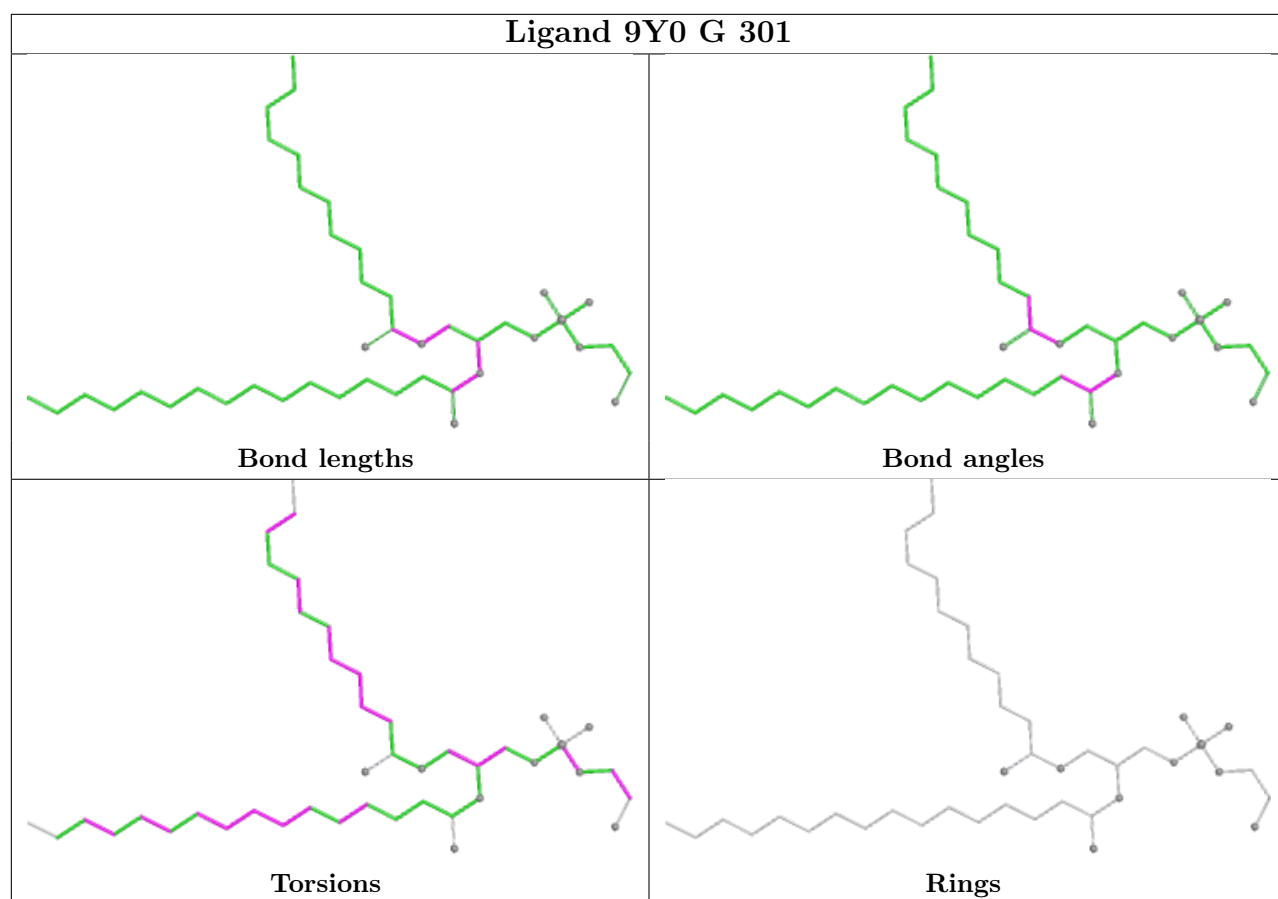




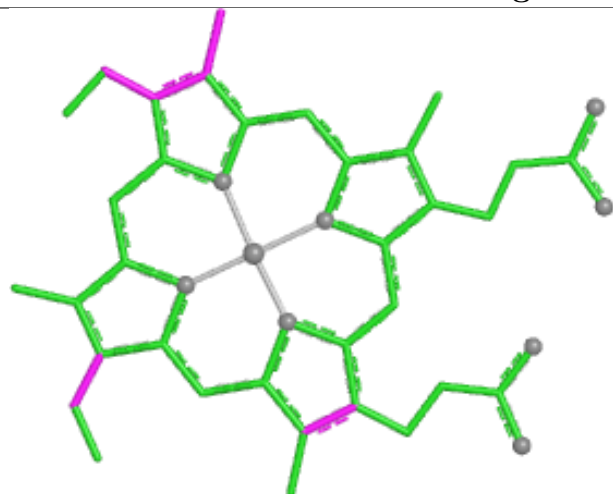




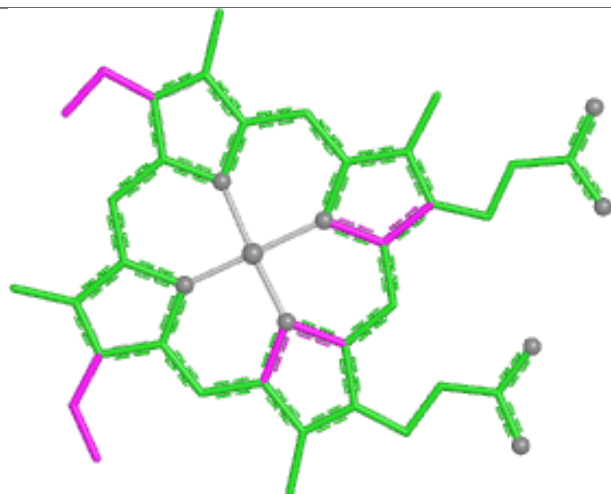




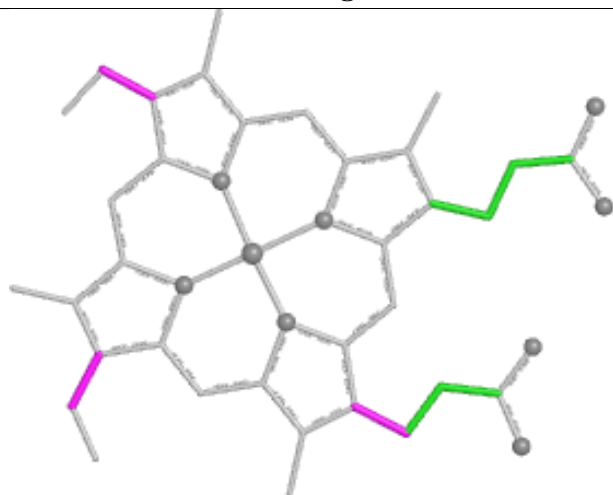
Ligand HEC C 301



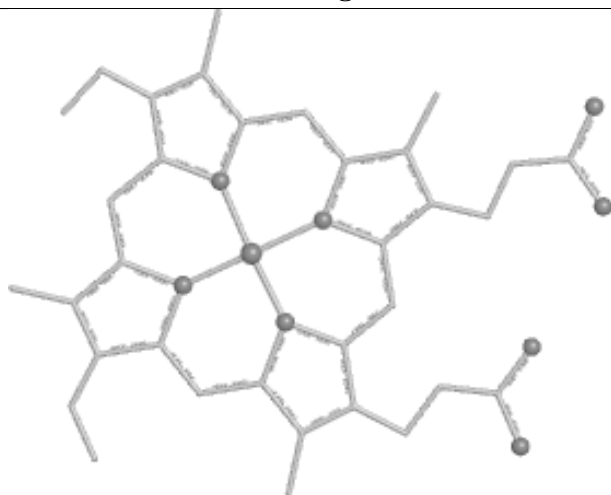
Bond lengths



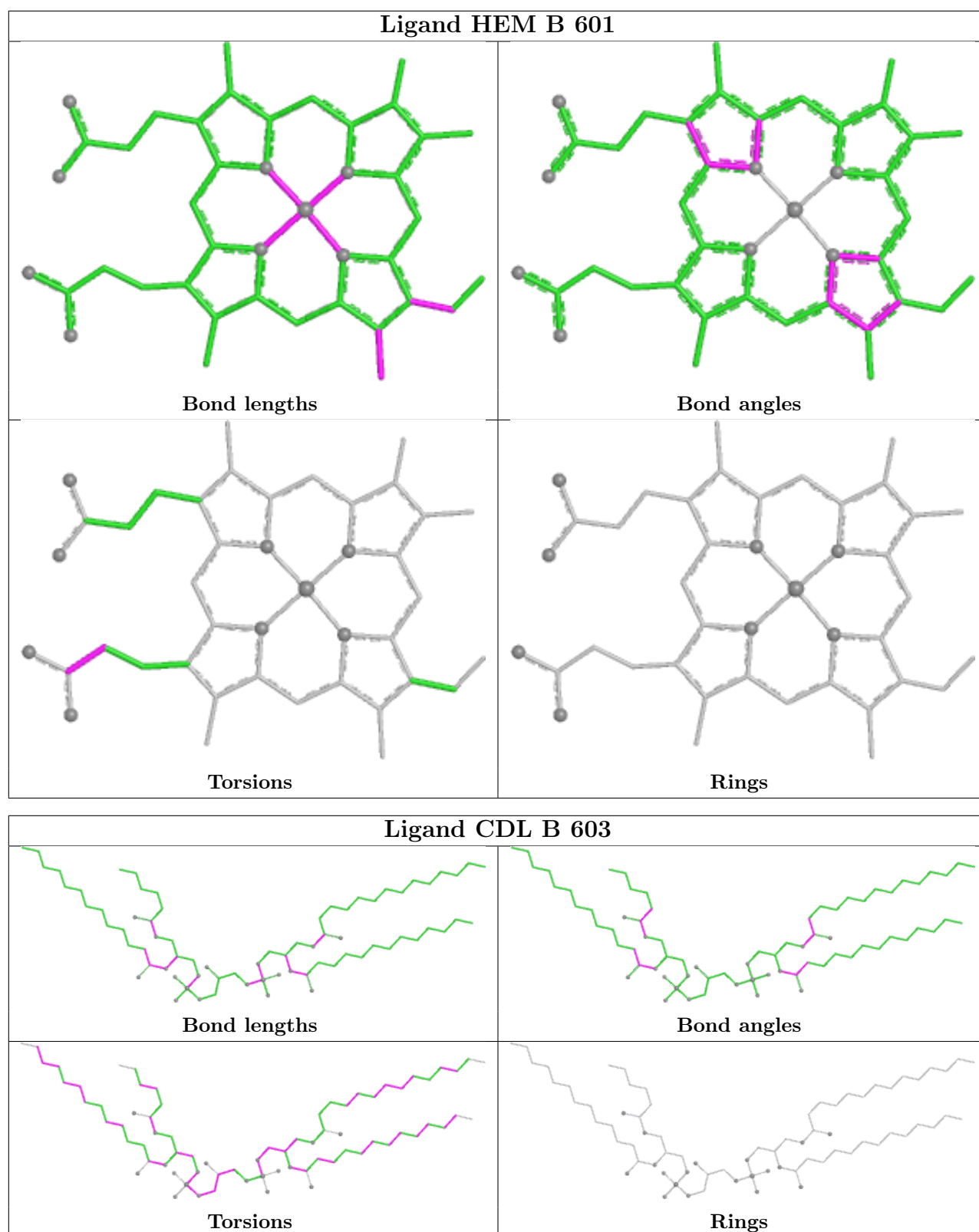
Bond angles



Torsions



Rings



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

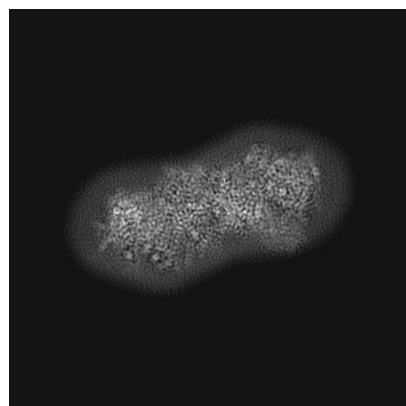
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51689. These allow visual inspection of the internal detail of the map and identification of artifacts.

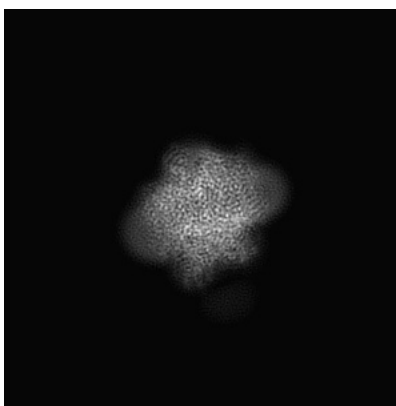
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

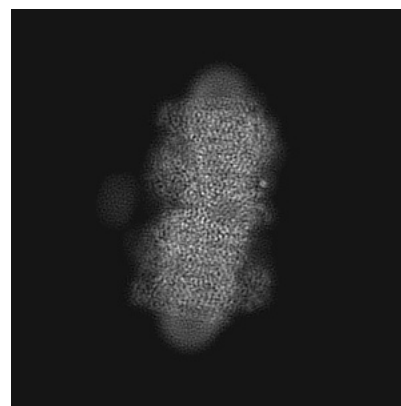
6.1.1 Primary map



X

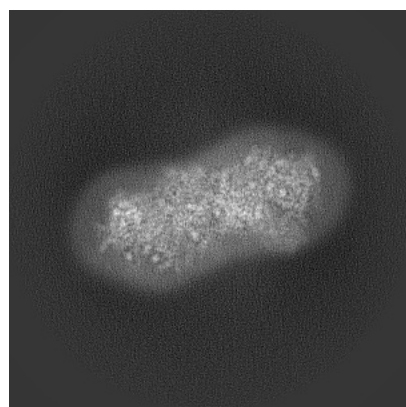


Y

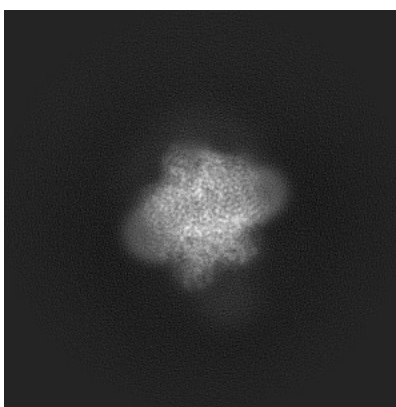


Z

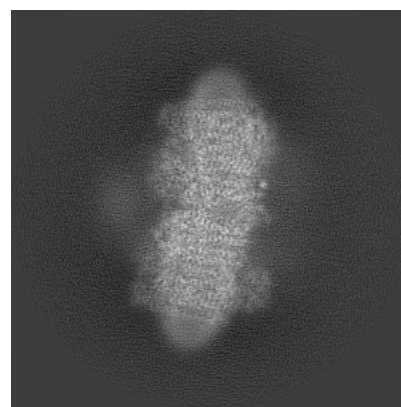
6.1.2 Raw map



X



Y

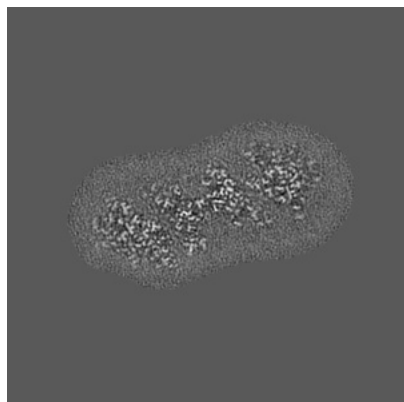


Z

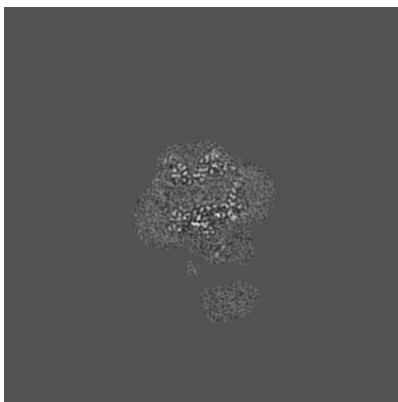
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

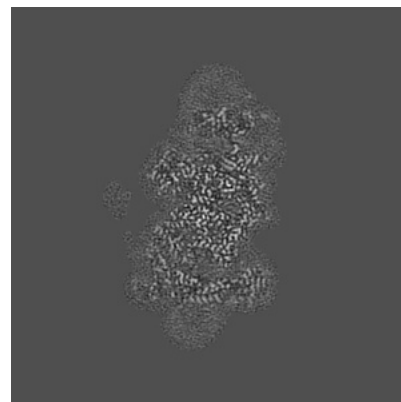
6.2.1 Primary map



X Index: 210

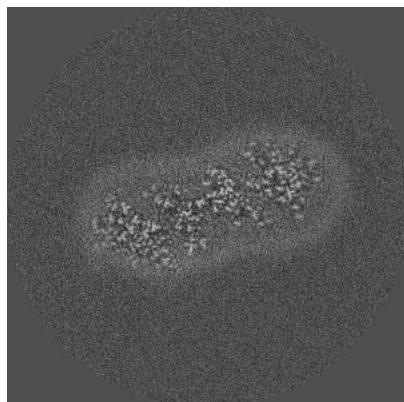


Y Index: 210

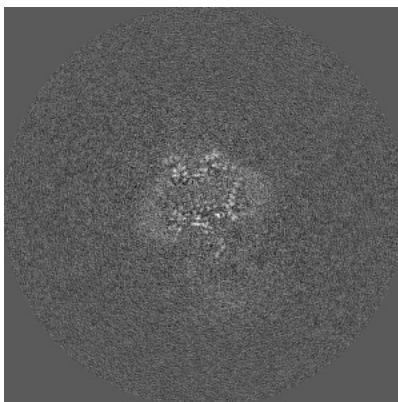


Z Index: 210

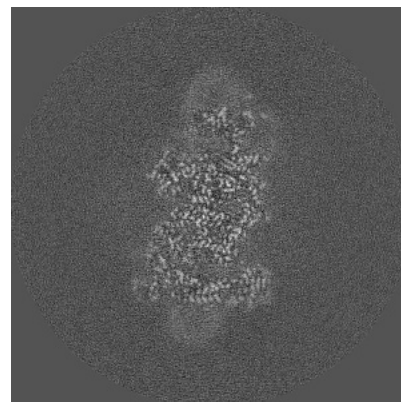
6.2.2 Raw map



X Index: 210



Y Index: 210

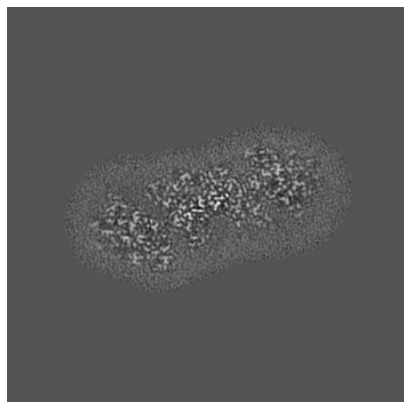


Z Index: 210

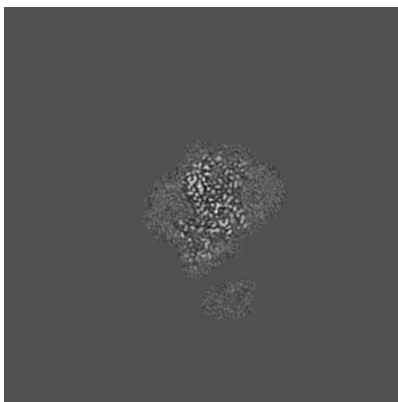
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

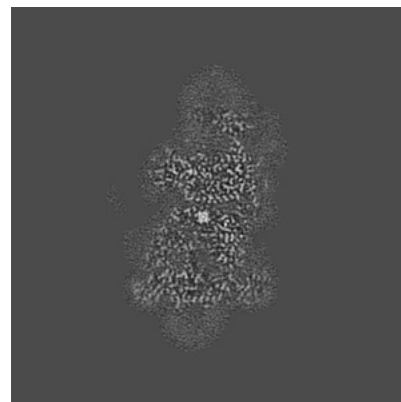
6.3.1 Primary map



X Index: 204

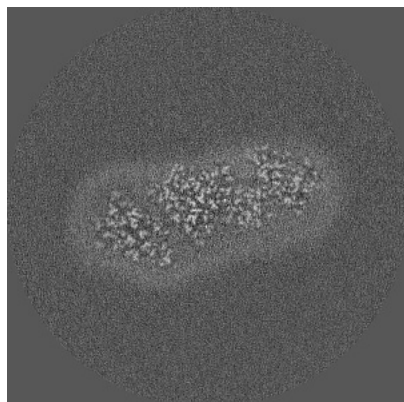


Y Index: 230

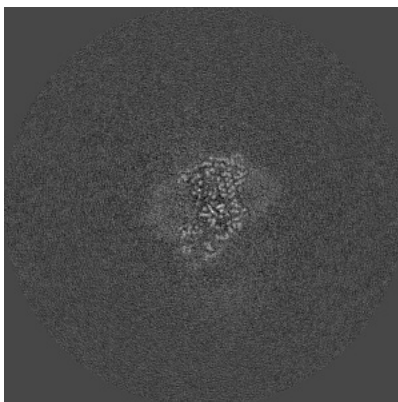


Z Index: 206

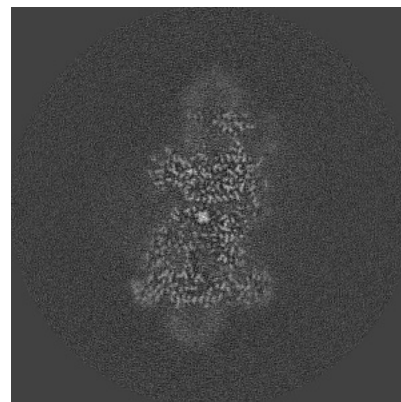
6.3.2 Raw map



X Index: 199



Y Index: 225

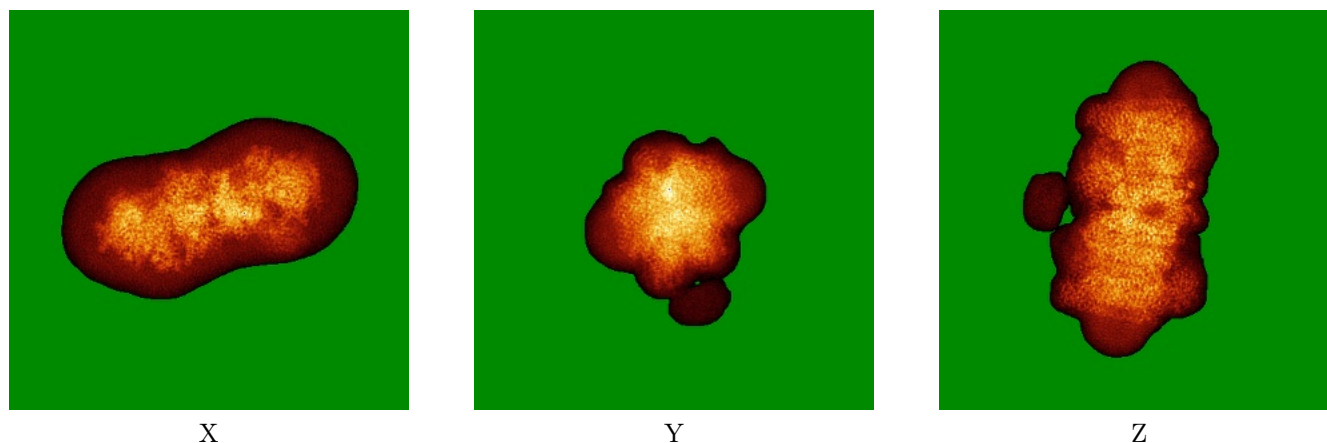


Z Index: 206

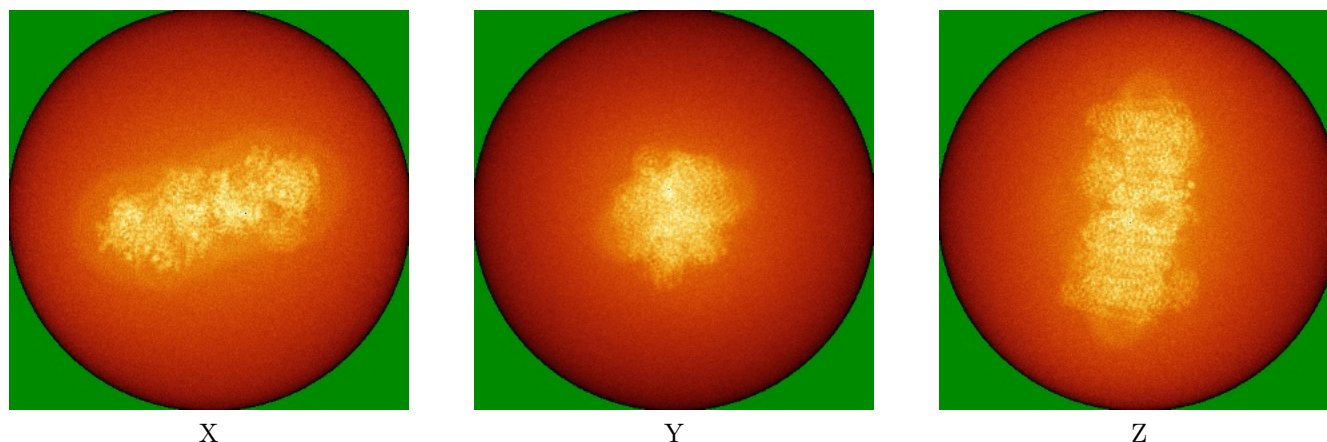
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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

6.5 Orthogonal surface views [i](#)

This section was not generated.

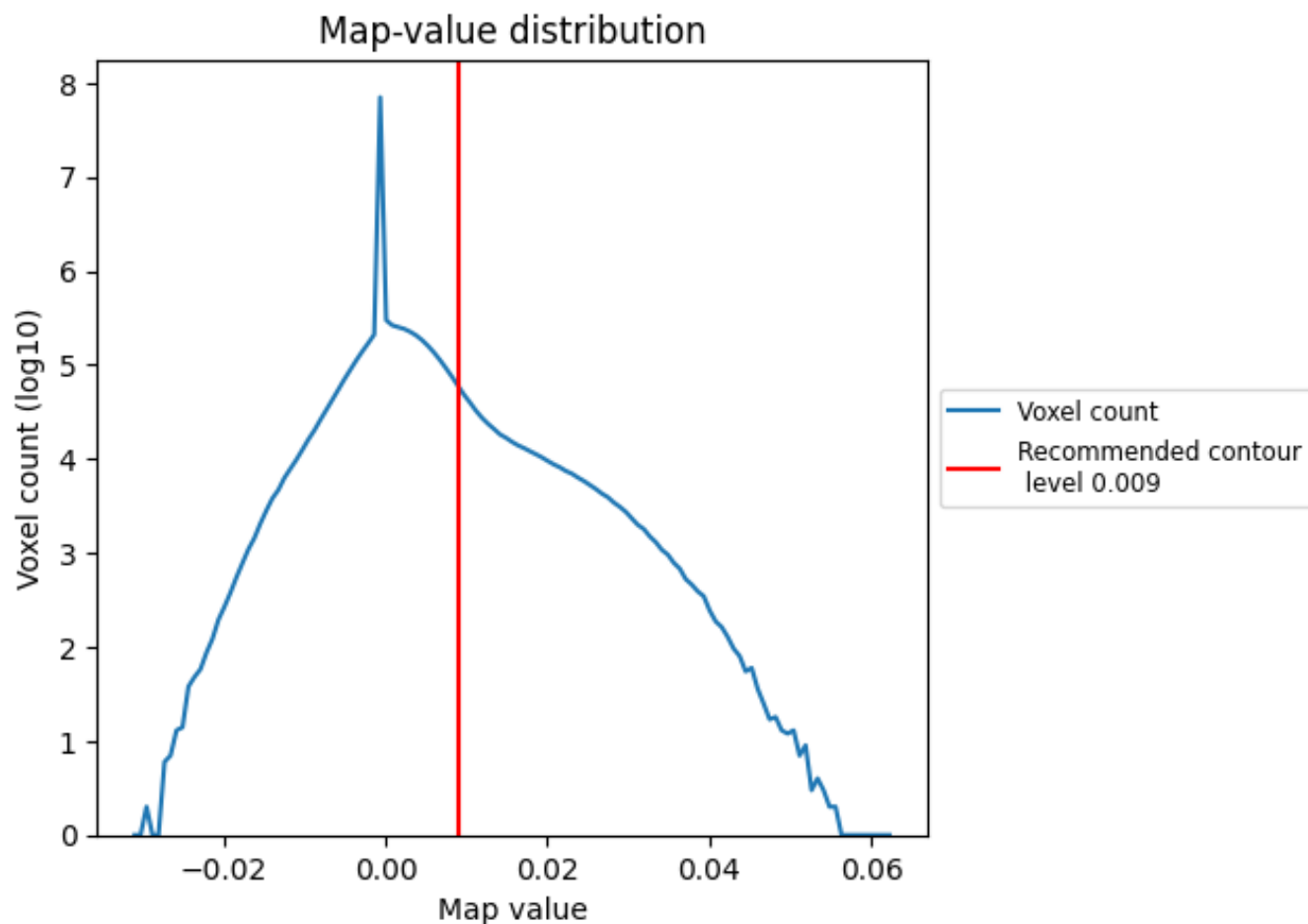
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

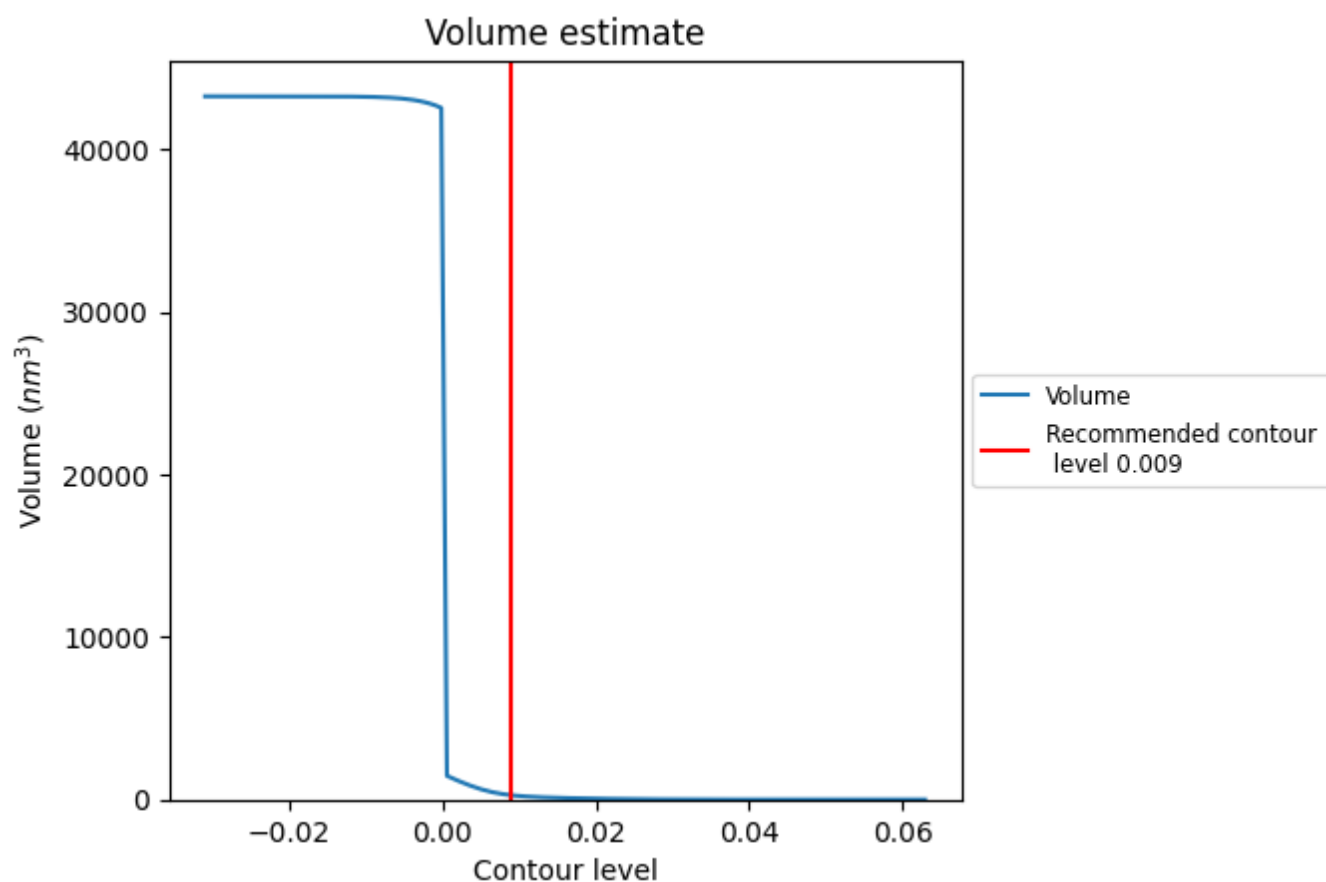
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

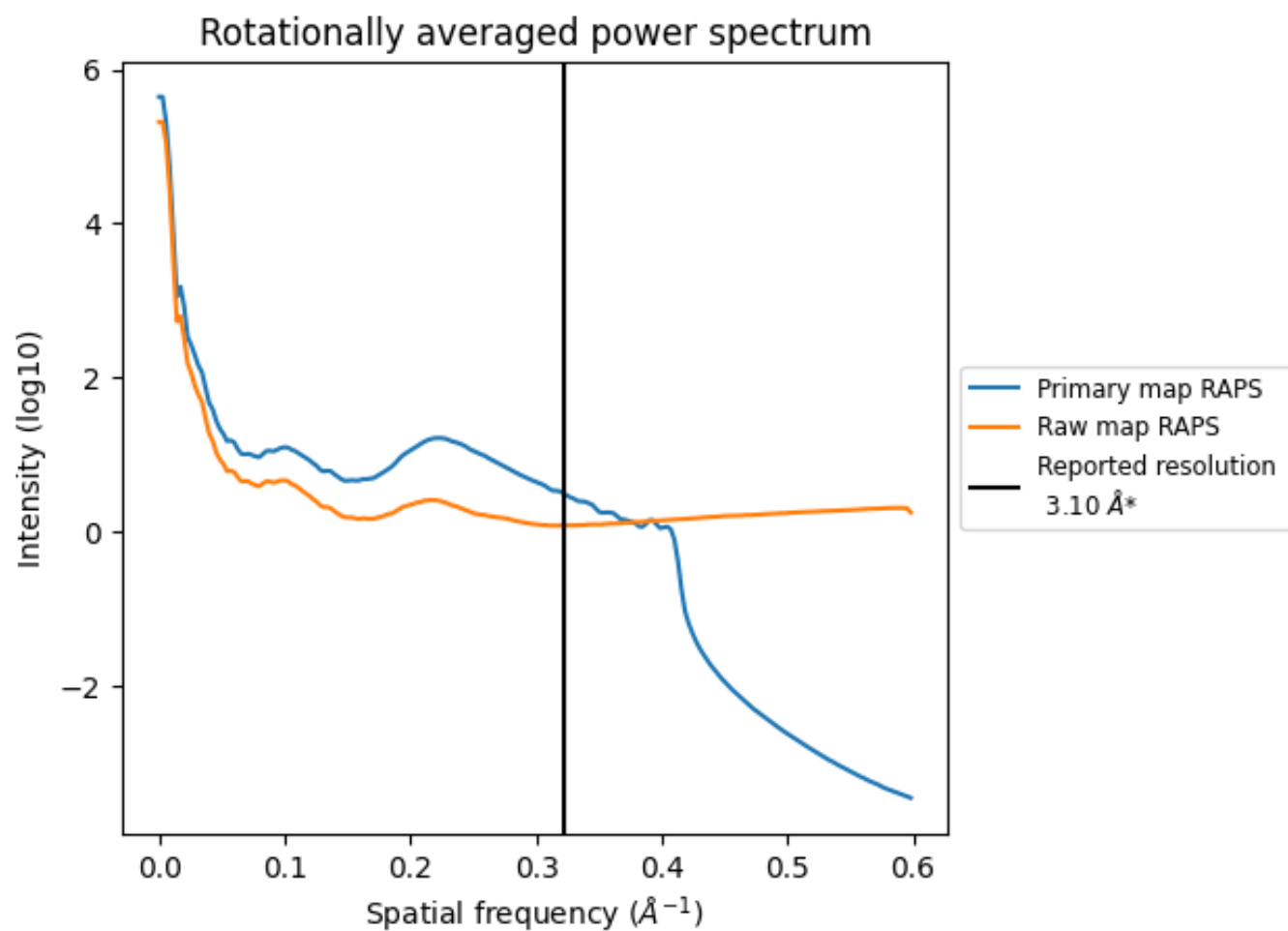
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 268 nm³; this corresponds to an approximate mass of 242 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 ⓘ

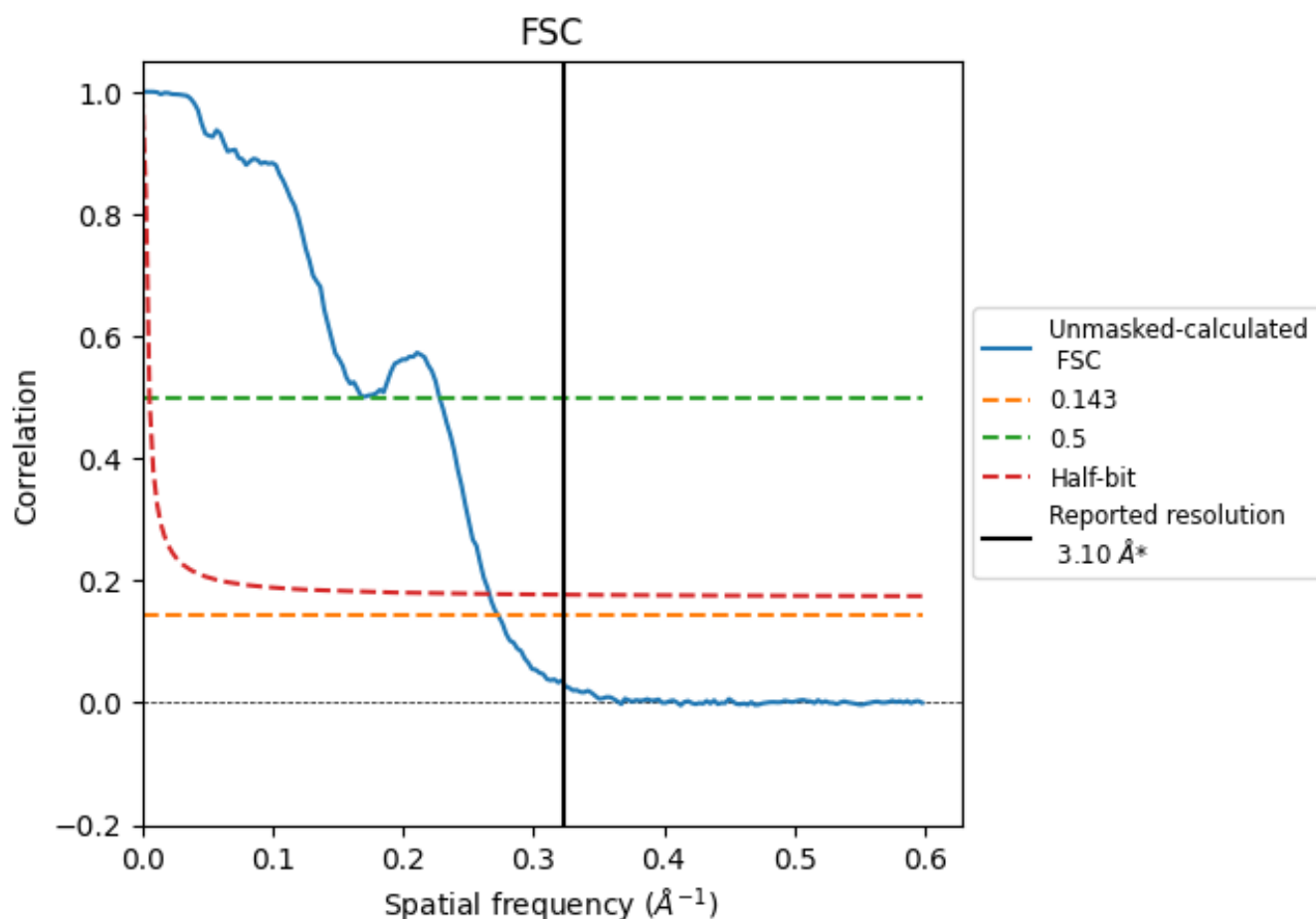


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

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 0.323 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.66	4.39	3.76

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.66 differs from the reported value 3.1 by more than 10 %

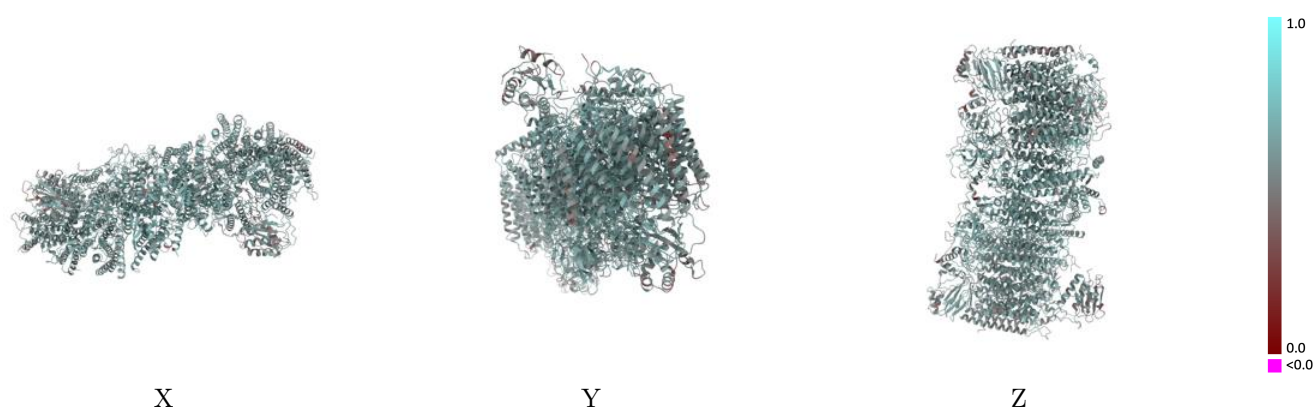
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-51689 and PDB model 9GY6. Per-residue inclusion information can be found in section 3 on page 18.

9.1 Map-model overlay [i](#)

This section was not generated.

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



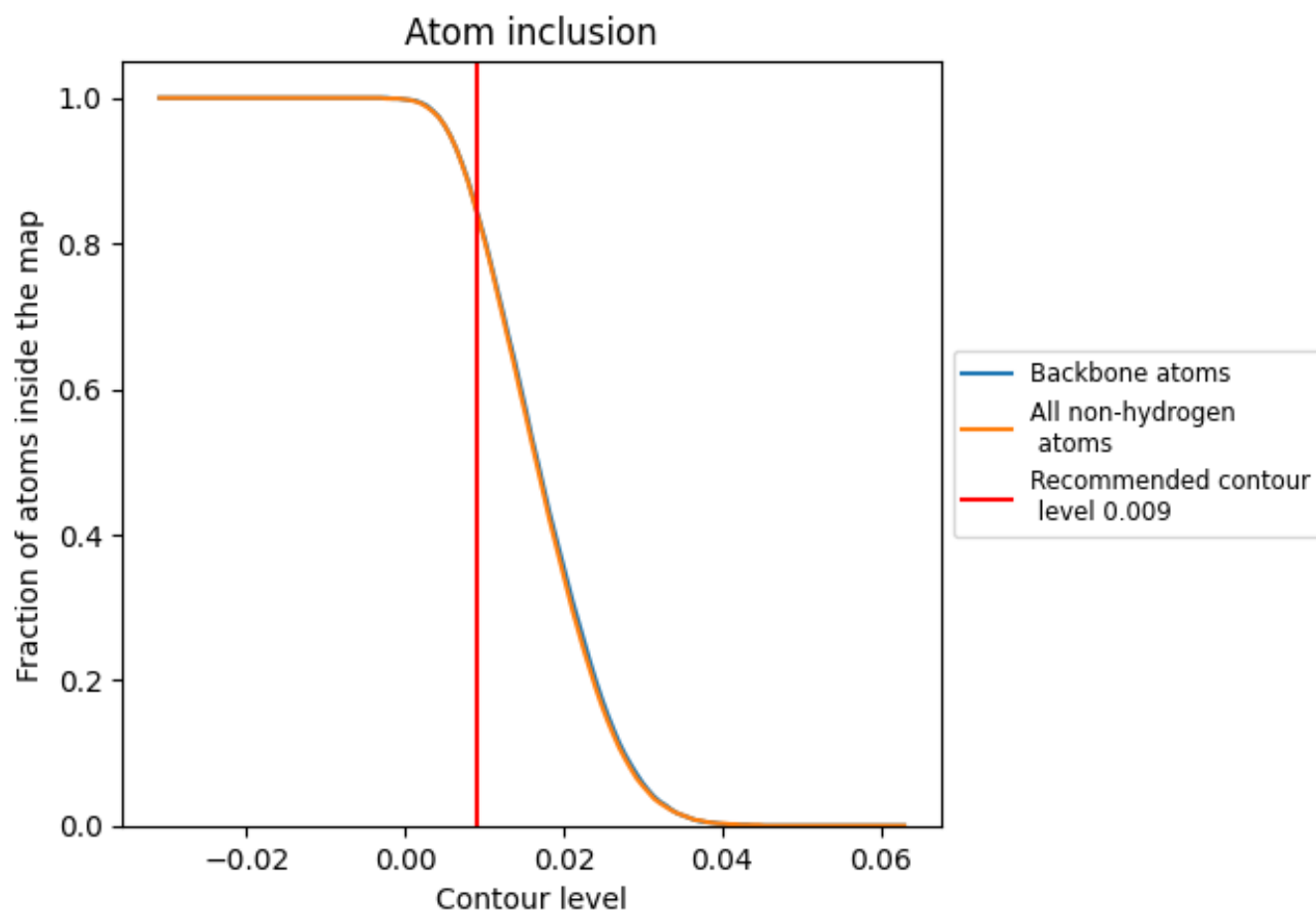
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.009).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 84% 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 (0.009) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8440	 0.5920
A	 0.8950	 0.6120
B	 0.9240	 0.6310
C	 0.8130	 0.5800
D	 0.7510	 0.5750
E	 0.7310	 0.5460
F	 0.8890	 0.6030
G	 0.8380	 0.5810
H	 0.8240	 0.5900
I	 0.7140	 0.5200
J	 0.7010	 0.5140
L	 0.7660	 0.5490
M	 0.8730	 0.6080
N	 0.9180	 0.6270
O	 0.7950	 0.5790
P	 0.7360	 0.5710
Q	 0.7310	 0.5410
R	 0.8980	 0.6040
S	 0.8580	 0.5840
T	 0.8450	 0.5870
U	 0.7000	 0.5330
V	 0.7110	 0.5240
X	 0.7010	 0.5420

