



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 02:51 PM UTC

PDB ID : 6T0B / pdb_00006t0b
EMDB ID : EMD-10340
Title : The III2-IV(5B)2 respiratory supercomplex from *S. cerevisiae*
Authors : Marechal, A.; Pinotsis, N.; Hartley, A.
Deposited on : 2019-10-02
Resolution : 2.80 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

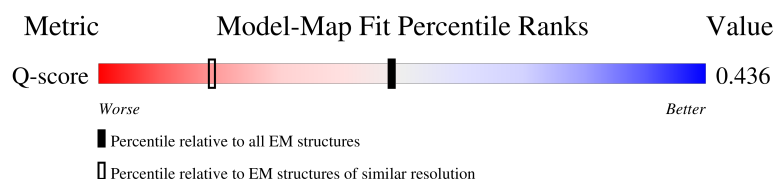
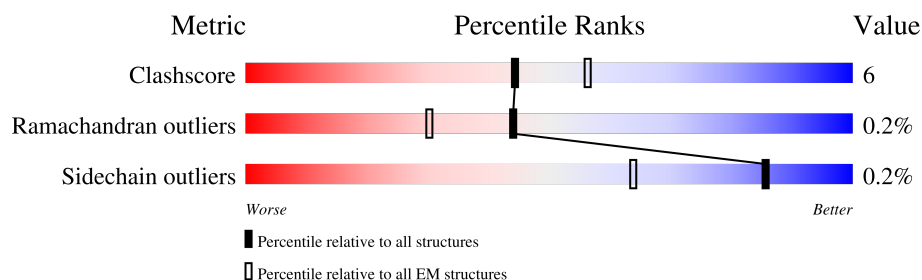
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.80 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	11806 (2.30 - 3.30)

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	431	 88% 12%
1	L	431	 86% 14%
2	B	352	 89% 11%
2	M	352	 86% 14%

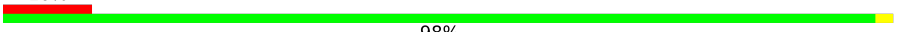
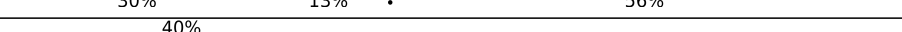
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Mol	Chain	Length	Quality of chain
3	C	385	
3	N	385	
4	D	248	
4	O	248	
5	E	185	
5	P	185	
6	F	147	
6	Q	147	
7	G	127	
7	R	127	
8	H	94	
8	S	94	
9	I	66	
9	T	66	
10	J	77	
10	U	77	
11	a	534	
11	n	534	
12	b	236	
12	o	236	
13	c	269	
13	p	269	
14	d	130	
14	q	130	
15	e	134	

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Mol	Chain	Length	Quality of chain
15	r	134	
16	f	108	
16	s	108	
17	g	59	
17	t	59	
18	h	51	
18	u	51	
19	i	55	
19	v	55	
20	j	82	
20	w	82	
21	k	131	
21	x	131	
22	l	66	
22	y	66	
23	m	224	
23	z	224	

2 Entry composition [i](#)

There are 35 unique types of molecules in this entry. The entry contains 64478 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 b-c1 complex subunit 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	431	Total	C	N	O	S	0	0
			3345	2110	576	653	6		
1	L	431	Total	C	N	O	S	0	0
			3345	2110	576	653	6		

- Molecule 2 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	352	Total	C	N	O	S	0	0
			2735	1747	453	534	1		
2	M	352	Total	C	N	O	S	0	0
			2735	1747	453	534	1		

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	385	Total	C	N	O	S	0	0
			3090	2082	484	503	21		
3	N	385	Total	C	N	O	S	0	0
			3090	2082	484	503	21		

- Molecule 4 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	247	Total	C	N	O	S	0	0
			1951	1243	338	361	9		
4	O	247	Total	C	N	O	S	0	0
			1951	1243	338	361	9		

- Molecule 5 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	185	Total	C	N	O	S	0	0
			1411	893	242	266	10		
5	P	185	Total	C	N	O	S	0	0
			1411	893	242	266	10		

- Molecule 6 is a protein called Cytochrome b-c1 complex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	75	Total	C	N	O	S	0	0
			633	396	109	126	2		
6	Q	75	Total	C	N	O	S	0	0
			633	396	109	126	2		

- Molecule 7 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	126	Total	C	N	O	S	0	0
			1019	653	173	191	2		
7	R	126	Total	C	N	O	S	0	0
			1019	653	173	191	2		

- Molecule 8 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	93	Total	C	N	O	S	0	0
			773	510	131	130	2		
8	S	93	Total	C	N	O	S	0	0
			773	510	131	130	2		

- Molecule 9 is a protein called Cytochrome b-c1 complex subunit 9.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	I	57	Total	C	N	O	0	0
			465	310	77	78		
9	T	57	Total	C	N	O	0	0
			465	310	77	78		

- Molecule 10 is a protein called Cytochrome b-c1 complex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	76	Total	C	N	O	S	0	0
			599	391	98	108	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	U	76	Total	C	N	O	S	0	0
			599	391	98	108	2		

- Molecule 11 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	a	534	Total	C	N	O	S	0	0
			4162	2778	649	713	22		
11	n	534	Total	C	N	O	S	0	0
			4162	2778	649	713	22		

- Molecule 12 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	b	236	Total	C	N	O	S	0	0
			1889	1242	286	351	10		
12	o	236	Total	C	N	O	S	0	0
			1889	1242	286	351	10		

- Molecule 13 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	c	269	Total	C	N	O	S	0	0
			2146	1430	344	357	15		
13	p	269	Total	C	N	O	S	0	0
			2146	1430	344	357	15		

- Molecule 14 is a protein called Cytochrome c oxidase subunit 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	d	120	Total	C	N	O	S	0	0
			906	571	150	180	5		
14	q	121	Total	C	N	O	S	0	0
			913	576	151	181	5		

- Molecule 15 is a protein called Cytochrome c oxidase polypeptide 5B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	e	133	Total	C	N	O	S	0	0
			1075	689	187	197	2		
15	r	133	Total	C	N	O	S	0	0
			1075	689	187	197	2		

- Molecule 16 is a protein called Cytochrome c oxidase subunit 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	f	102	Total	C	N	O	S	0	0
			851	545	137	168	1		
16	s	102	Total	C	N	O	S	0	0
			851	545	137	168	1		

- Molecule 17 is a protein called Cytochrome c oxidase subunit 7.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	g	59	Total	C	N	O	0	0
			484	328	83	73		
17	t	59	Total	C	N	O	0	0
			484	328	83	73		

- Molecule 18 is a protein called Cytochrome c oxidase polypeptide VIII, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	h	51	Total	C	N	O	S	0	0
			409	278	66	64	1		
18	u	51	Total	C	N	O	S	0	0
			409	278	66	64	1		

- Molecule 19 is a protein called Cytochrome c oxidase subunit 7A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	i	55	Total	C	N	O	S	0	0
			456	300	79	74	3		
19	v	55	Total	C	N	O	S	0	0
			456	300	79	74	3		

- Molecule 20 is a protein called Cytochrome c oxidase subunit 6B.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	j	75	Total	C	N	O	S	0	0
			627	403	107	112	5		
20	w	75	Total	C	N	O	S	0	0
			627	403	107	112	5		

- Molecule 21 is a protein called Cytochrome c oxidase subunit 6A, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	k	113	Total	C	N	O	S	0	0
			928	605	160	160	3		
21	x	113	Total	C	N	O	S	0	0
			928	605	160	160	3		

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
k	130	GLY	-	expression tag	UNP P32799
k	131	ALA	-	expression tag	UNP P32799
k	132	ARG	-	expression tag	UNP P32799
k	133	GLY	-	expression tag	UNP P32799
k	134	SER	-	expression tag	UNP P32799
k	135	HIS	-	expression tag	UNP P32799
k	136	HIS	-	expression tag	UNP P32799
k	137	HIS	-	expression tag	UNP P32799
k	138	HIS	-	expression tag	UNP P32799
k	139	HIS	-	expression tag	UNP P32799
k	140	HIS	-	expression tag	UNP P32799
x	130	GLY	-	expression tag	UNP P32799
x	131	ALA	-	expression tag	UNP P32799
x	132	ARG	-	expression tag	UNP P32799
x	133	GLY	-	expression tag	UNP P32799
x	134	SER	-	expression tag	UNP P32799
x	135	HIS	-	expression tag	UNP P32799
x	136	HIS	-	expression tag	UNP P32799
x	137	HIS	-	expression tag	UNP P32799
x	138	HIS	-	expression tag	UNP P32799
x	139	HIS	-	expression tag	UNP P32799
x	140	HIS	-	expression tag	UNP P32799

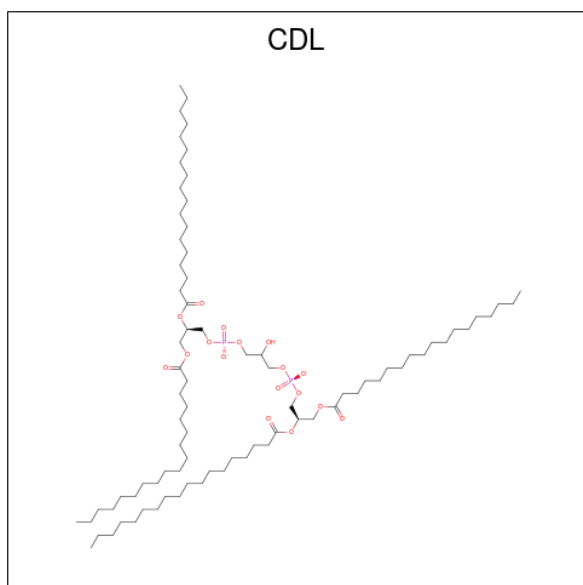
- Molecule 22 is a protein called Cox26.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	l	45	Total	C	N	O	S	0	0
			361	238	63	59	1		
22	y	45	Total	C	N	O	S	0	0
			361	238	63	59	1		

- Molecule 23 is a protein called Respiratory supercomplex factor 2, mitochondrial.

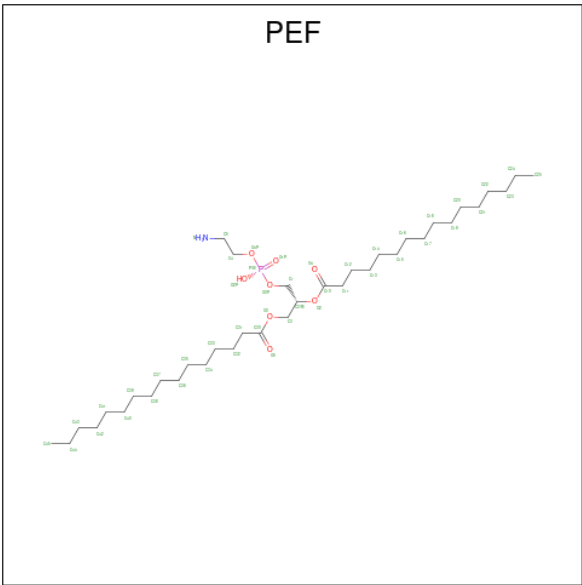
Mol	Chain	Residues	Atoms					AltConf	Trace
23	m	99	Total	C	N	O	S	0	0
			799	511	140	144	4		
23	z	99	Total	C	N	O	S	0	0
			799	511	140	144	4		

- Molecule 24 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
24	A	1	Total	C	O	P	0
			58	39	17	2	
24	C	1	Total	C	O	P	0
			66	47	17	2	
24	D	1	Total	C	O	P	0
			71	52	17	2	
24	H	1	Total	C	O	P	0
			53	34	17	2	
24	L	1	Total	C	O	P	0
			55	36	17	2	
24	N	1	Total	C	O	P	0
			53	34	17	2	
24	N	1	Total	C	O	P	0
			75	56	17	2	
24	S	1	Total	C	O	P	0
			48	29	17	2	

- Molecule 25 is DI-PALMITOYL-3-SN-PHOSPHATIDYLETHANOLAMINE (CCD ID: PEF) (formula: $C_{37}H_{74}NO_8P$).



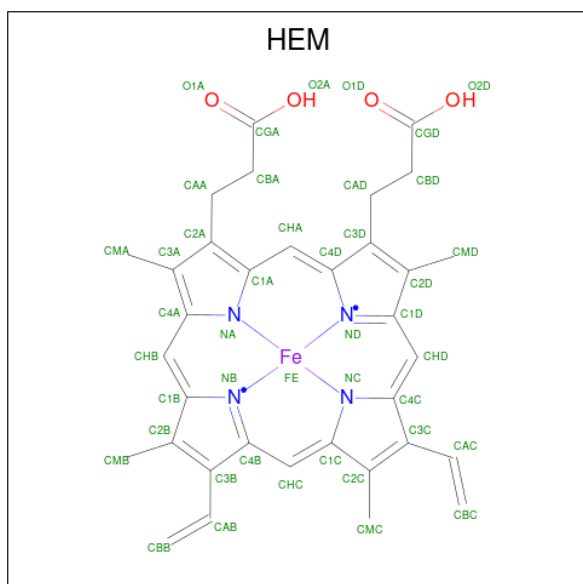
Mol	Chain	Residues	Atoms					AltConf
25	A	1	Total	C	N	O	P	0
			36	26	1	8	1	
25	C	1	Total	C	N	O	P	0
			44	34	1	8	1	
25	C	1	Total	C	N	O	P	0
			39	29	1	8	1	
25	E	1	Total	C	N	O	P	0
			42	32	1	8	1	
25	E	1	Total	C	N	O	P	0
			40	30	1	8	1	
25	E	1	Total	C	N	O	P	0
			34	24	1	8	1	
25	H	1	Total	C	N	O	P	0
			32	22	1	8	1	
25	J	1	Total	C	N	O	P	0
			29	19	1	8	1	
25	L	1	Total	C	N	O	P	0
			31	21	1	8	1	
25	N	1	Total	C	N	O	P	0
			40	30	1	8	1	
25	N	1	Total	C	N	O	P	0
			43	33	1	8	1	
25	O	1	Total	C	N	O	P	0
			43	33	1	8	1	
25	S	1	Total	C	N	O	P	0
			36	26	1	8	1	
25	a	1	Total	C	N	O	P	0
			33	23	1	8	1	

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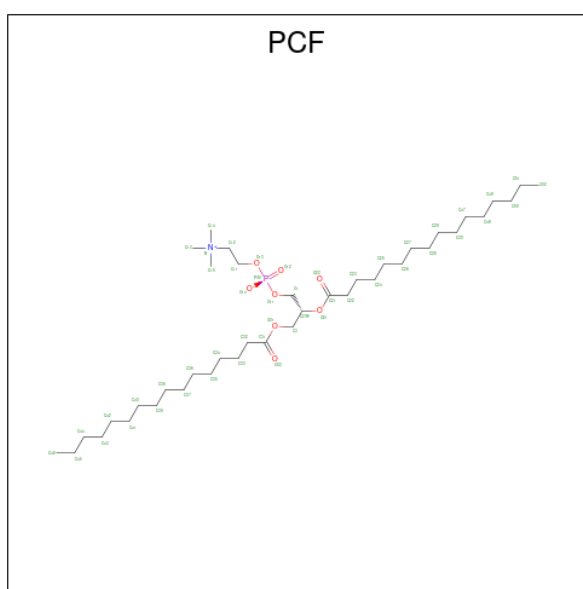
Mol	Chain	Residues	Atoms					AltConf
25	b	1	Total	C	N	O	P	0
			40	30	1	8	1	
25	b	1	Total	C	N	O	P	0
			40	30	1	8	1	
25	c	1	Total	C	N	O	P	0
			36	26	1	8	1	
25	c	1	Total	C	N	O	P	0
			34	24	1	8	1	
25	e	1	Total	C	N	O	P	0
			41	31	1	8	1	
25	l	1	Total	C	N	O	P	0
			33	23	1	8	1	
25	n	1	Total	C	N	O	P	0
			47	37	1	8	1	
25	n	1	Total	C	N	O	P	0
			33	23	1	8	1	
25	n	1	Total	C	N	O	P	0
			33	23	1	8	1	
25	o	1	Total	C	N	O	P	0
			40	30	1	8	1	
25	p	1	Total	C	N	O	P	0
			36	26	1	8	1	
25	r	1	Total	C	N	O	P	0
			41	31	1	8	1	

- Molecule 26 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



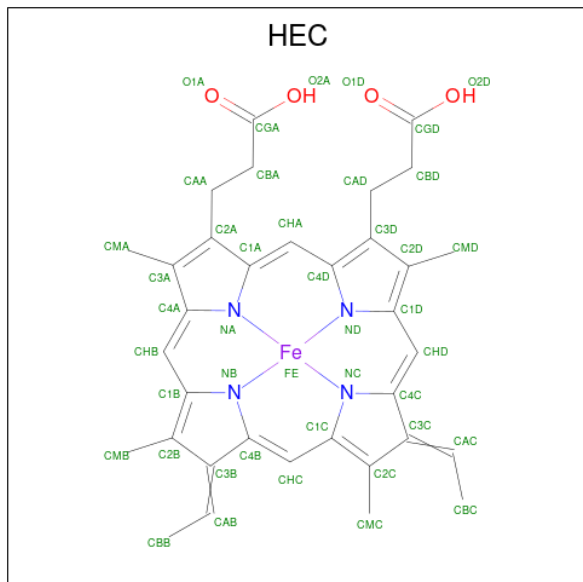
Mol	Chain	Residues	Atoms					AltConf
26	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
26	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
26	N	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
26	N	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 27 is 1,2-DIACYL-SN-GLYCERO-3-PHOSHOCHOLINE (CCD ID: PCF) (formula: $C_{40}H_{80}NO_8P$).



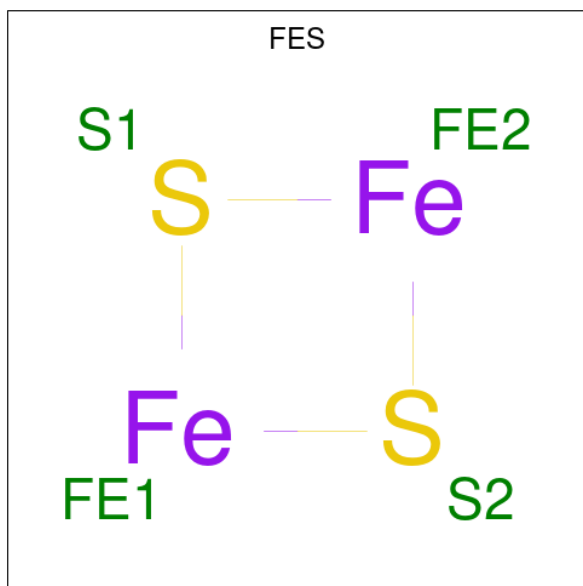
Mol	Chain	Residues	Atoms					AltConf
27	C	1	Total	C	N	O	P	0
			39	29	1	8	1	
27	H	1	Total	C	N	O	P	0
			32	22	1	8	1	
27	I	1	Total	C	N	O	P	0
			30	20	1	8	1	
27	N	1	Total	C	N	O	P	0
			50	40	1	8	1	
27	T	1	Total	C	N	O	P	0
			47	37	1	8	1	
27	e	1	Total	C	N	O	P	0
			36	26	1	8	1	
27	r	1	Total	C	N	O	P	0
			36	26	1	8	1	

- Molecule 28 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 29 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).

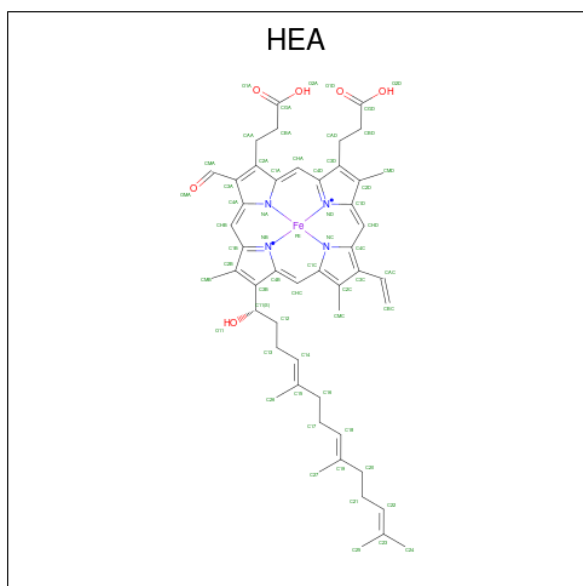


Mol	Chain	Residues	Atoms			AltConf
29	E	1	Total	Fe	S	0
			4	2	2	
29	P	1	Total	Fe	S	0
			4	2	2	

- Molecule 30 is COPPER (II) ION (CCD ID: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
30	a	1	Total	Cu	0
			1	1	
30	n	1	Total	Cu	0
			1	1	

- Molecule 31 is HEME-A (CCD ID: HEA) (formula: C₄₉H₅₆FeN₄O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
31	a	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
31	a	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
31	n	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
31	n	1	Total	C	Fe	N	O	0
			60	49	1	4	6	

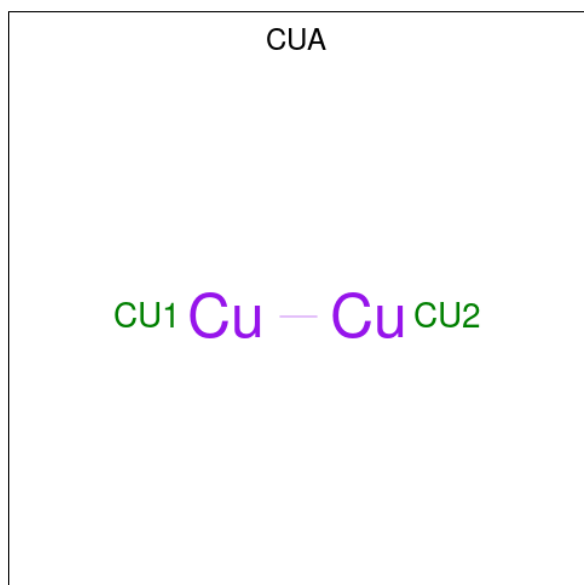
- Molecule 32 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
32	a	1	Total 1	Ca 1	0
32	n	1	Total 1	Ca 1	0

- Molecule 33 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
33	a	1	Total 1	Mg 1	0
33	n	1	Total 1	Mg 1	0

- Molecule 34 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu₂).



Mol	Chain	Residues	Atoms		AltConf
34	b	1	Total 2	Cu 2	0
34	o	1	Total 2	Cu 2	0

- Molecule 35 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

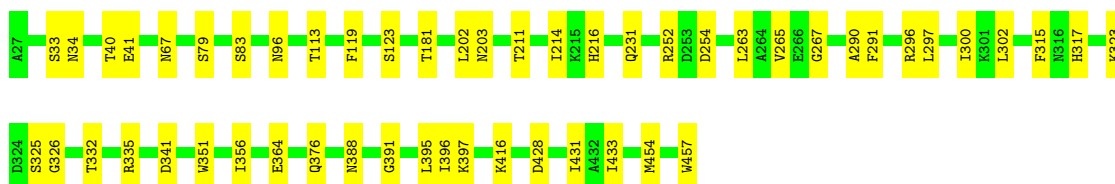
Mol	Chain	Residues	Atoms		AltConf
35	d	1	Total 1	Zn 1	0
35	q	1	Total 1	Zn 1	0

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.

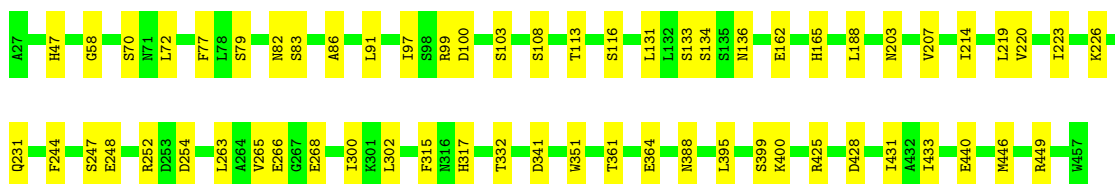
- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial

Chain A: 



- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial

Chain L: 



- Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain B: 



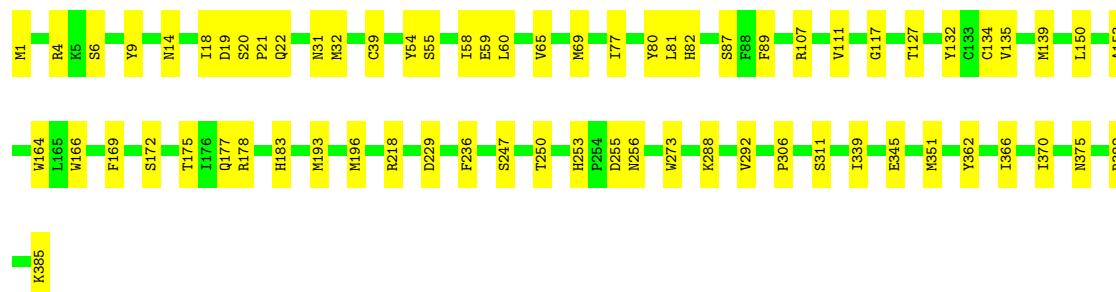
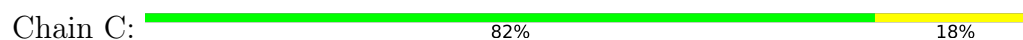
- Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain M: 

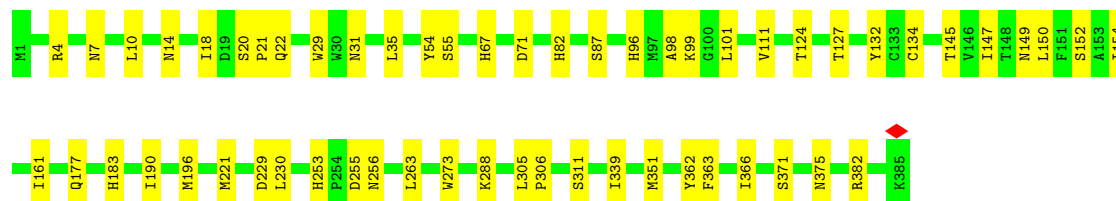
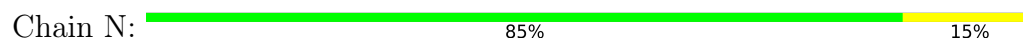




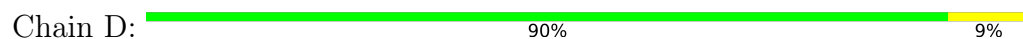
• Molecule 3: Cytochrome b



• Molecule 3: Cytochrome b



• Molecule 4: Cytochrome c1, heme protein, mitochondrial



• Molecule 4: Cytochrome c1, heme protein, mitochondrial

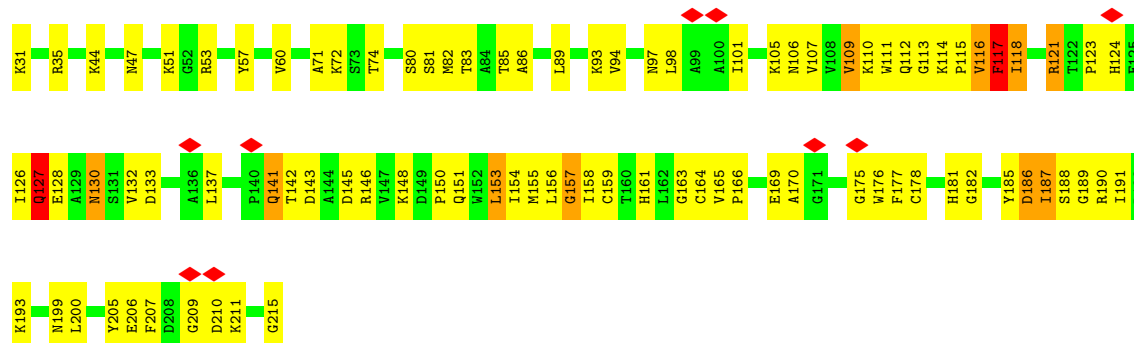


• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

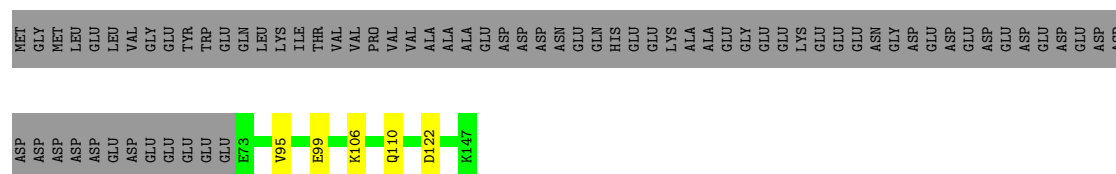




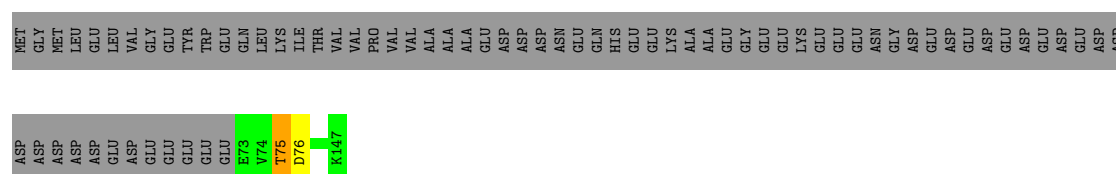
- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial



- Molecule 6: Cytochrome b-c1 complex subunit 6



- Molecule 6: Cytochrome b-c1 complex subunit 6



- Molecule 7: Cytochrome b-c1 complex subunit 7



- Molecule 7: Cytochrome b-c1 complex subunit 7





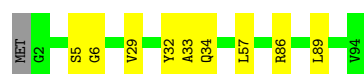
- Molecule 8: Cytochrome b-c1 complex subunit 8

Chain H: 87% 12%



- Molecule 8: Cytochrome b-c1 complex subunit 8

Chain S: 89% 10%



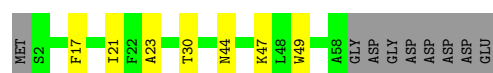
- Molecule 9: Cytochrome b-c1 complex subunit 9

Chain I: 76% 11% 14%



- Molecule 9: Cytochrome b-c1 complex subunit 9

Chain T: 76% 11% 14%



- Molecule 10: Cytochrome b-c1 complex subunit 10

Chain J: 5% 90% 9%



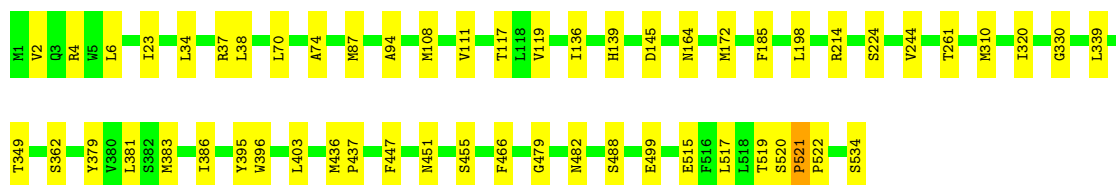
- Molecule 10: Cytochrome b-c1 complex subunit 10

Chain U: 5% 84% 14%

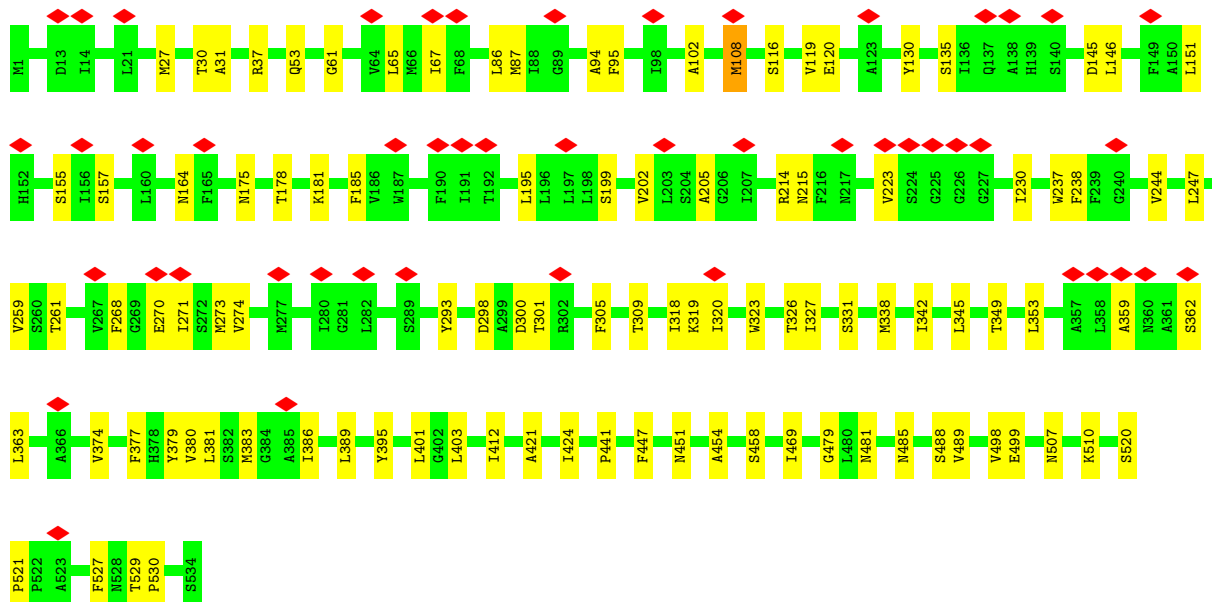
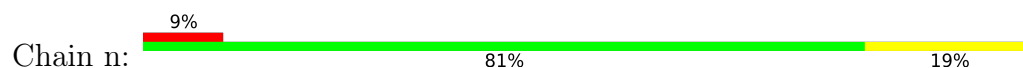


- Molecule 11: Cytochrome c oxidase subunit 1

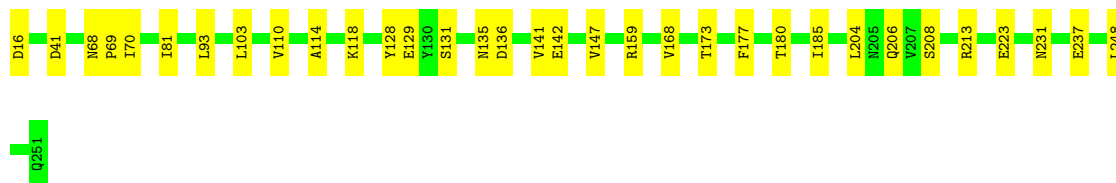
Chain a: 90% 10%



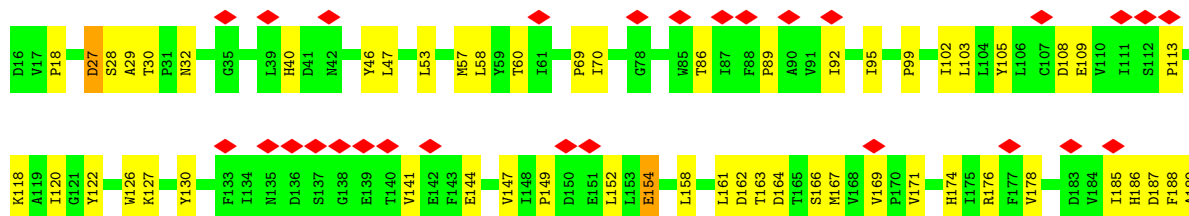
• Molecule 11: Cytochrome c oxidase subunit 1



• Molecule 12: Cytochrome c oxidase subunit 2

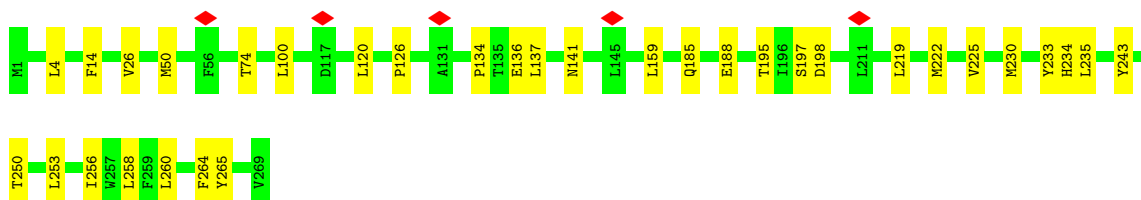
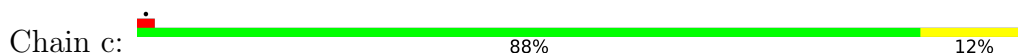


• Molecule 12: Cytochrome c oxidase subunit 2

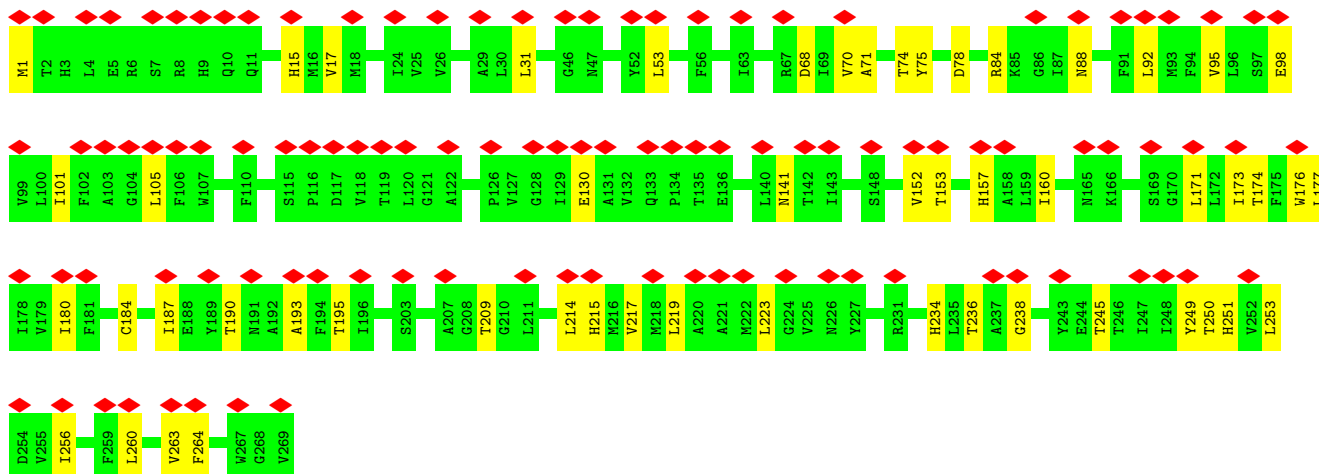
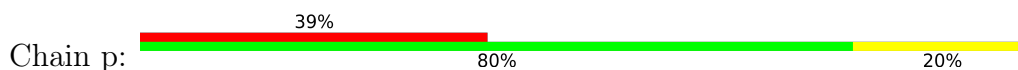




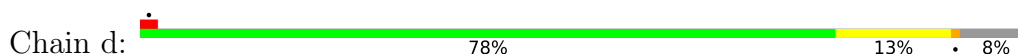
• Molecule 13: Cytochrome c oxidase subunit 3



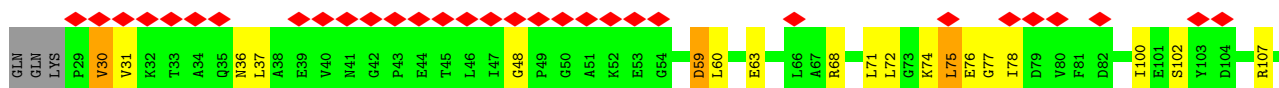
• Molecule 13: Cytochrome c oxidase subunit 3



• Molecule 14: Cytochrome c oxidase subunit 4, mitochondrial



• Molecule 14: Cytochrome c oxidase subunit 4, mitochondrial





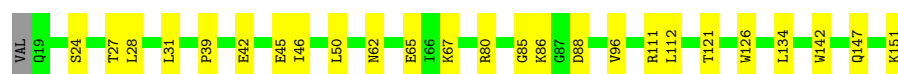
- Molecule 15: Cytochrome c oxidase polypeptide 5B, mitochondrial

Chain e: 91% 8% .



- Molecule 15: Cytochrome c oxidase polypeptide 5B, mitochondrial

Chain r: 81% 19% .



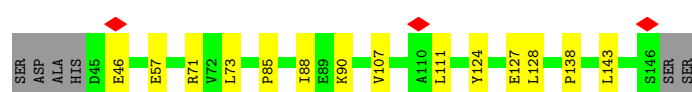
- Molecule 16: Cytochrome c oxidase subunit 6, mitochondrial

Chain f: 85% 9% 6% .



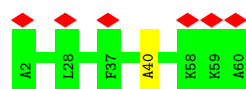
- Molecule 16: Cytochrome c oxidase subunit 6, mitochondrial

Chain s: 81% 13% 6% .



- Molecule 17: Cytochrome c oxidase subunit 7

Chain g: 10% 98% .



- Molecule 17: Cytochrome c oxidase subunit 7

Chain t: 42% 86% 14% .



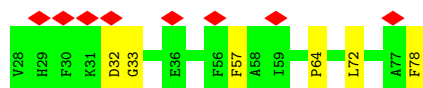
- Molecule 18: Cytochrome c oxidase polypeptide VIII, mitochondrial

Chain h:  88% 12%



- Molecule 18: Cytochrome c oxidase polypeptide VIII, mitochondrial

Chain u:  16% 88% 12%



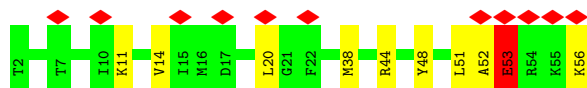
- Molecule 19: Cytochrome c oxidase subunit 7A

Chain i:  84% 16%



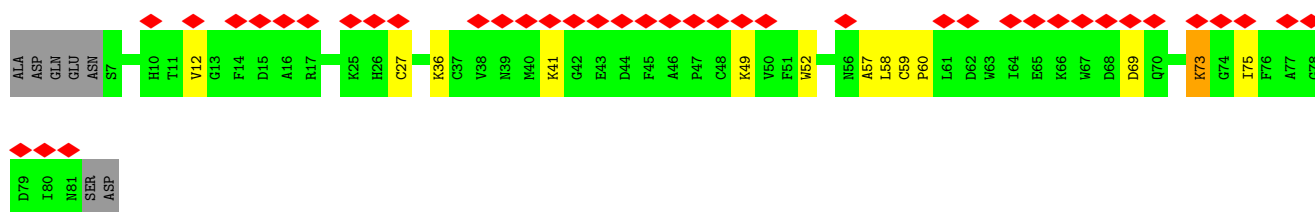
- Molecule 19: Cytochrome c oxidase subunit 7A

Chain v:  20% 82% 16%

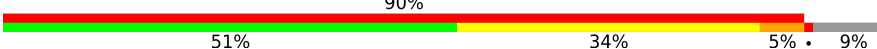


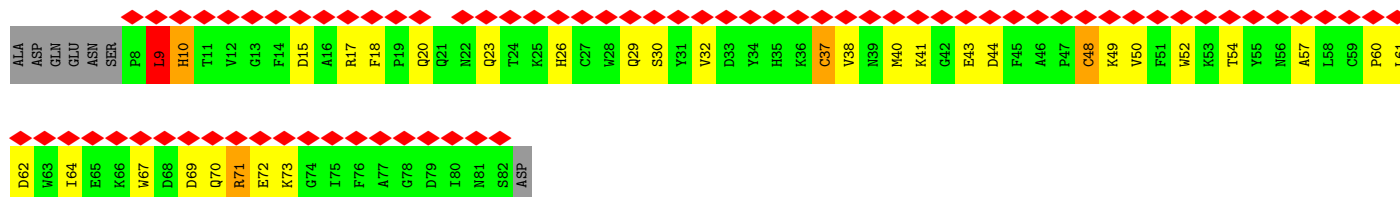
- Molecule 20: Cytochrome c oxidase subunit 6B

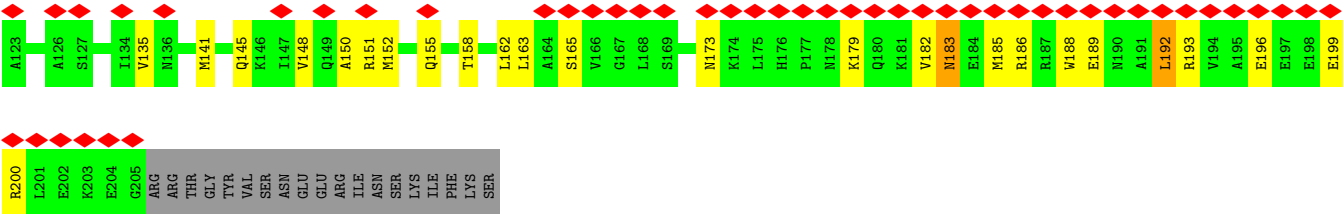
Chain j:  49% 76% 15% 9%



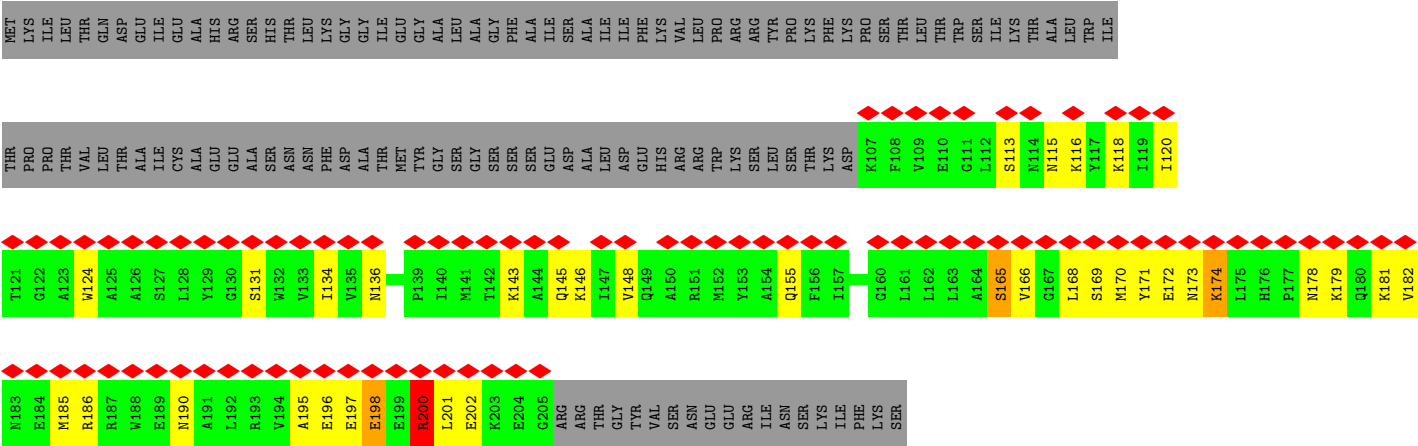
- Molecule 20: Cytochrome c oxidase subunit 6B

Chain w:  90% 51% 34% 5% 9%





• Molecule 23: Respiratory supercomplex factor 2, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	65999	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 ($e^-/\text{\AA}^2$)	56.4	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	3.028	Depositor
Minimum map value	-1.743	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.072	Depositor
Recommended contour level	0.24	Depositor
Map size ($\text{\AA}$)	486.08002, 486.08002, 486.08002	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.085, 1.085, 1.085	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FES, ZN, PCF, CA, MG, HEA, PEF, CDL, HEC, CUA, HEM, CU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.57	1/3406 (0.0%)	0.59	0/4615
1	L	0.54	0/3406	0.59	0/4615
2	B	0.53	0/2781	0.59	3/3764 (0.1%)
2	M	0.52	0/2781	0.60	0/3764
3	C	0.61	0/3192	0.62	0/4354
3	N	0.57	0/3192	0.62	0/4354
4	D	0.56	0/2012	0.55	0/2740
4	O	0.54	0/2012	0.51	0/2740
5	E	0.49	0/1444	0.93	4/1957 (0.2%)
5	P	0.64	2/1444 (0.1%)	1.10	9/1957 (0.5%)
6	F	0.37	0/647	0.56	0/870
6	Q	0.39	0/647	0.57	0/870
7	G	0.49	0/1040	0.54	0/1408
7	R	0.50	0/1040	0.52	0/1408
8	H	0.50	0/804	0.54	0/1088
8	S	0.50	0/804	0.53	0/1088
9	I	0.47	0/479	0.51	0/646
9	T	0.49	0/479	0.49	0/646
10	J	0.29	0/619	0.53	0/841
10	U	0.26	0/619	0.53	0/841
11	a	0.58	0/4290	0.63	0/5857
11	n	0.49	1/4290 (0.0%)	0.70	0/5857
12	b	0.53	0/1941	0.64	0/2653
12	o	0.51	0/1941	0.85	2/2653 (0.1%)
13	c	0.46	0/2218	0.56	0/3036
13	p	0.35	0/2218	0.71	0/3036
14	d	0.55	0/924	0.69	0/1258
14	q	0.44	0/932	0.86	2/1269 (0.2%)
15	e	0.51	0/1103	0.58	0/1493
15	r	0.44	1/1103 (0.1%)	0.64	0/1493
16	f	0.51	0/868	0.61	0/1174
16	s	0.46	0/868	0.68	0/1174

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	g	0.51	0/500	0.64	0/681
17	t	0.35	0/500	0.66	0/681
18	h	0.51	0/424	0.59	0/569
18	u	0.36	0/424	0.64	0/569
19	i	0.44	0/468	0.57	0/626
19	v	0.53	1/468 (0.2%)	0.87	1/626 (0.2%)
20	j	0.46	1/649 (0.2%)	0.87	2/880 (0.2%)
20	w	0.52	0/649	1.16	4/879 (0.5%)
21	k	0.29	0/962	0.54	0/1310
21	x	0.46	0/962	1.20	13/1310 (1.0%)
22	l	0.42	0/372	0.62	0/502
22	y	0.39	0/372	0.94	2/502 (0.4%)
23	m	0.49	0/813	1.02	1/1093 (0.1%)
23	z	0.54	0/813	1.24	6/1093 (0.5%)
All	All	0.51	7/63920 (0.0%)	0.69	49/86840 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
2	M	0	1
3	C	0	1
5	E	0	4
5	P	0	12
11	a	0	2
11	n	0	2
12	o	0	3
14	d	0	1
14	q	0	2
16	s	0	1
19	v	0	3
20	w	0	8
21	x	0	3
23	m	0	2
23	z	0	5
All	All	0	51

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	P	127	GLN	CB-CG	8.38	1.77	1.52
5	P	130	ASN	CG-OD1	6.14	1.35	1.23
11	n	108	MET	SD-CE	-5.92	1.64	1.79
20	j	41	LYS	CD-CE	-5.62	1.35	1.52
15	r	31	LEU	C-N	5.41	1.39	1.34
19	v	53	GLU	CG-CD	-5.20	1.39	1.52
1	A	267	GLY	C-N	-5.10	1.23	1.33

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	x	85	LYS	CA-C-N	-8.06	110.47	122.24
21	x	85	LYS	C-N-CA	-8.06	110.47	122.24
21	x	26	ASP	CA-C-N	7.18	133.78	121.29
21	x	26	ASP	C-N-CA	7.18	133.78	121.29
12	o	154	GLU	CA-C-N	-6.94	113.20	122.85
12	o	154	GLU	C-N-CA	-6.94	113.20	122.85
21	x	100	ASN	CA-C-N	-6.81	112.46	122.68
21	x	100	ASN	C-N-CA	-6.81	112.46	122.68
21	x	34	LYS	CA-C-N	-6.73	111.88	122.65
21	x	34	LYS	C-N-CA	-6.73	111.88	122.65
2	B	203	GLU	CA-CB-CG	6.48	127.05	114.10
23	m	192	LEU	CA-CB-CG	6.39	138.67	116.30
23	z	200	ARG	CA-CB-CG	6.36	126.83	114.10
5	P	153	LEU	CA-CB-CG	6.33	138.46	116.30
14	q	78	ILE	CA-C-N	-6.27	113.96	122.86
14	q	78	ILE	C-N-CA	-6.27	113.96	122.86
19	v	53	GLU	CA-CB-CG	6.19	126.48	114.10
5	P	121	ARG	CA-C-N	6.16	138.87	120.69
5	P	121	ARG	C-N-CA	6.16	138.87	120.69
22	y	28	TRP	CA-C-N	-6.12	112.89	122.56
22	y	28	TRP	C-N-CA	-6.12	112.89	122.56
5	P	123	PRO	CA-C-N	-6.04	113.52	122.83
5	P	123	PRO	C-N-CA	-6.04	113.52	122.83
5	P	126	ILE	CA-CB-CG1	6.04	120.67	110.40
5	E	159	CYS	CA-C-N	5.94	129.74	120.82
5	E	159	CYS	C-N-CA	5.94	129.74	120.82
5	P	117	PHE	CA-CB-CG	5.91	119.71	113.80
21	x	45	LYS	CA-C-N	-5.88	111.75	122.38
21	x	45	LYS	C-N-CA	-5.88	111.75	122.38
23	z	196	GLU	CA-CB-CG	5.87	125.84	114.10
21	x	85	LYS	CA-CB-CG	5.68	125.45	114.10
20	j	73	LYS	CA-CB-CG	5.62	125.33	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	w	71	ARG	CA-C-N	-5.58	114.47	122.67
20	w	71	ARG	C-N-CA	-5.58	114.47	122.67
5	P	118	ILE	CG1-CB-CG2	-5.46	94.31	110.70
5	P	117	PHE	CB-CA-C	-5.39	100.77	109.72
23	z	174	LYS	N-CA-C	-5.34	104.76	113.19
23	z	195	ALA	CA-C-N	-5.33	113.04	122.26
23	z	195	ALA	C-N-CA	-5.33	113.04	122.26
21	x	65	LEU	CA-C-N	-5.21	113.60	122.56
21	x	65	LEU	C-N-CA	-5.21	113.60	122.56
20	w	9	LEU	CA-C-N	5.17	131.41	121.54
20	w	9	LEU	C-N-CA	5.17	131.41	121.54
5	E	126	ILE	CA-C-N	-5.15	114.56	122.60
5	E	126	ILE	C-N-CA	-5.15	114.56	122.60
23	z	200	ARG	N-CA-CB	-5.13	101.81	110.49
2	B	151	PHE	CA-C-N	-5.13	114.47	122.42
2	B	151	PHE	C-N-CA	-5.13	114.47	122.42
20	j	73	LYS	CB-CG-CD	5.02	122.86	111.30

There are no chirality outliers.

All (51) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	201	VAL	Peptide
3	C	107	ARG	Peptide
5	E	127	GLN	Peptide
5	E	135	SER	Peptide
5	E	173	PHE	Peptide
5	E	97	ASN	Peptide
2	M	94	LEU	Peptide
5	P	117	PHE	Peptide
5	P	127	GLN	Sidechain
5	P	137	LEU	Peptide
5	P	141	GLN	Peptide
5	P	155	MET	Peptide
5	P	157	GLY	Peptide
5	P	186	ASP	Peptide
5	P	187	ILE	Peptide
5	P	193	LYS	Peptide
5	P	206	GLU	Peptide
5	P	209	GLY	Peptide
5	P	97	ASN	Peptide
11	a	119	VAL	Peptide

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Mol	Chain	Res	Type	Group
11	a	520	SER	Peptide
14	d	32	LYS	Peptide
23	m	173	ASN	Peptide
23	m	183	ASN	Peptide
11	n	119	VAL	Peptide
11	n	520	SER	Peptide
12	o	245	LEU	Peptide
12	o	246	GLU	Peptide
12	o	27	ASP	Peptide
14	q	59	ASP	Peptide
14	q	75	LEU	Peptide
16	s	46	GLU	Peptide
19	v	38	MET	Peptide
19	v	52	ALA	Peptide
19	v	53	GLU	Peptide
20	w	10	HIS	Peptide
20	w	29	GLN	Peptide
20	w	43	GLU	Peptide
20	w	48	CYS	Peptide
20	w	50	VAL	Peptide
20	w	70	GLN	Peptide
20	w	72	GLU	Peptide
20	w	9	LEU	Peptide
21	x	35	GLU	Peptide
21	x	85	LYS	Peptide
21	x	91	GLU	Peptide
23	z	165	SER	Peptide
23	z	170	MET	Peptide
23	z	174	LYS	Peptide
23	z	197	GLU	Peptide
23	z	198	GLU	Peptide

5.2 Too-close contacts [i](#)

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	3345	0	3323	34	0
1	L	3345	0	3323	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2735	0	2774	23	0
2	M	2735	0	2774	31	0
3	C	3090	0	3129	46	0
3	N	3090	0	3129	40	0
4	D	1951	0	1875	18	0
4	O	1951	0	1875	14	0
5	E	1411	0	1387	45	0
5	P	1411	0	1386	71	0
6	F	633	0	587	3	0
6	Q	633	0	587	1	0
7	G	1019	0	1034	9	0
7	R	1019	0	1034	7	0
8	H	773	0	736	8	0
8	S	773	0	736	7	0
9	I	465	0	459	7	0
9	T	465	0	459	7	0
10	J	599	0	594	7	0
10	U	599	0	594	9	0
11	a	4162	0	4191	41	0
11	n	4162	0	4191	75	0
12	b	1889	0	1866	22	0
12	o	1889	0	1866	64	0
13	c	2146	0	2137	24	0
13	p	2146	0	2137	35	0
14	d	906	0	901	15	0
14	q	913	0	909	20	0
15	e	1075	0	1072	9	0
15	r	1075	0	1072	19	0
16	f	851	0	822	7	0
16	s	851	0	822	10	0
17	g	484	0	517	1	0
17	t	484	0	517	5	0
18	h	409	0	408	5	0
18	u	409	0	408	4	0
19	i	456	0	469	7	0
19	v	456	0	469	5	0
20	j	627	0	577	8	0
20	w	627	0	578	17	0
21	k	928	0	906	19	0
21	x	928	0	906	30	0
22	l	361	0	363	3	0
22	y	361	0	363	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	m	799	0	819	19	0
23	z	799	0	819	19	0
24	A	58	0	60	3	0
24	C	66	0	76	3	0
24	D	71	0	89	0	0
24	H	53	0	50	2	0
24	L	55	0	54	1	0
24	N	128	0	147	1	0
24	S	48	0	40	2	0
25	A	36	0	45	1	0
25	C	83	0	118	3	0
25	E	116	0	157	7	0
25	H	32	0	37	0	0
25	J	29	0	31	0	0
25	L	31	0	35	0	0
25	N	83	0	115	5	0
25	O	43	0	62	0	0
25	S	36	0	48	1	0
25	a	33	0	39	1	0
25	b	80	0	112	3	0
25	c	70	0	86	3	0
25	e	41	0	58	4	0
25	l	33	0	39	0	0
25	n	113	0	151	5	0
25	o	40	0	56	0	0
25	p	36	0	45	2	0
25	r	41	0	58	3	0
26	C	86	0	60	4	0
26	N	86	0	60	5	0
27	C	39	0	55	0	0
27	H	32	0	38	1	0
27	I	30	0	34	3	0
27	N	50	0	80	2	0
27	T	47	0	71	2	0
27	e	36	0	46	0	0
27	r	36	0	46	1	0
28	D	43	0	31	2	0
28	O	43	0	31	0	0
29	E	4	0	0	0	0
29	P	4	0	0	0	0
30	a	1	0	0	0	0
30	n	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	a	120	0	108	6	0
31	n	120	0	108	5	0
32	a	1	0	0	0	0
32	n	1	0	0	0	0
33	a	1	0	0	0	0
33	n	1	0	0	0	0
34	b	2	0	0	0	0
34	o	2	0	0	0	0
35	d	1	0	0	0	0
35	q	1	0	0	0	0
All	All	64478	0	64476	824	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 6.

All (824) 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)
5:P:127:GLN:CB	5:P:127:GLN:CG	1.77	1.61
5:E:111:TRP:O	5:E:114:LYS:HB2	1.56	1.05
5:P:118:ILE:HA	5:P:153:LEU:O	1.55	1.05
5:P:117:PHE:O	5:P:154:ILE:HA	1.64	0.97
5:E:110:LYS:HA	5:E:114:LYS:O	1.69	0.92
20:w:67:TRP:O	20:w:71:ARG:HB2	1.75	0.86
5:P:176:TRP:HB2	5:P:185:TYR:O	1.75	0.85
20:w:15:ASP:HB3	20:w:17:ARG:HB3	1.58	0.84
21:x:52:VAL:HA	21:x:55:SER:HB3	1.62	0.79
12:o:186:HIS:O	12:o:199:ALA:HB3	1.84	0.76
20:w:49:LYS:HB2	20:w:52:TRP:HB2	1.69	0.74
5:P:106:ASN:HD21	5:P:176:TRP:HE1	1.34	0.74
5:P:107:VAL:HB	5:P:118:ILE:HG22	1.70	0.74
11:n:259:VAL:HB	11:n:327:ILE:HD11	1.70	0.73
5:P:161:HIS:ND1	5:P:181:HIS:CE1	2.56	0.73
5:E:103:LEU:HD22	5:E:120:HIS:HB3	1.72	0.72
5:P:109:VAL:O	5:P:115:PRO:HA	1.89	0.72
11:n:498:VAL:HG11	16:s:73:LEU:HD22	1.72	0.71
11:a:381:LEU:HD13	31:a:602:HEA:HAC	1.73	0.70
12:b:135:ASN:HD21	12:b:248:LEU:HG	1.57	0.69
11:n:273:MET:HE2	11:n:319:LYS:HZ2	1.56	0.69
11:n:529:THR:HG21	14:q:102:SER:HB2	1.75	0.68
2:M:115:LYS:HB2	2:M:118:GLU:HG3	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:116:VAL:HB	5:P:156:LEU:HA	1.76	0.68
13:p:141:ASN:ND2	13:p:184:CYS:SG	2.65	0.67
14:d:41:ASN:H	14:d:45:THR:HG21	1.58	0.67
21:x:66:THR:HA	21:x:69:ASN:HB3	1.77	0.67
2:B:115:LYS:HB2	2:B:118:GLU:HG3	1.77	0.66
12:o:223:GLU:O	12:o:229:HIS:CE1	2.49	0.66
21:x:27:LYS:HD3	21:x:29:ALA:HB3	1.77	0.66
3:C:169:PHE:HB3	5:P:112:GLN:HE21	1.61	0.66
23:m:112:LEU:HG	23:m:115:ASN:HB2	1.77	0.65
11:a:139:HIS:O	11:a:214:ARG:NH2	2.30	0.65
11:n:403:LEU:HB3	11:n:479:GLY:HA3	1.77	0.65
5:E:188:SER:OG	5:E:190:ARG:NH2	2.30	0.65
13:c:74:THR:HG21	13:c:234:HIS:HD2	1.60	0.65
11:a:244:VAL:HB	31:a:603:HEA:HAC	1.80	0.64
15:r:42:GLU:HA	15:r:45:GLU:HG2	1.78	0.64
5:E:116:VAL:HA	5:E:157:GLY:H	1.62	0.64
10:J:48:TRP:HD1	10:J:51:PHE:H	1.45	0.64
5:E:176:TRP:HB2	5:E:185:TYR:HB2	1.80	0.64
1:A:317:HIS:HE1	1:A:351:TRP:HE1	1.45	0.64
5:E:138:LYS:NZ	5:E:191:ILE:O	2.30	0.64
13:p:1:MET:HE2	14:q:37:LEU:HD21	1.78	0.64
23:m:196:GLU:HA	23:m:199:GLU:HG2	1.81	0.63
2:M:255:VAL:HG22	2:M:321:THR:HG21	1.79	0.63
2:M:84:ARG:NH1	2:M:144:ASP:OD1	2.27	0.63
5:P:185:TYR:HE1	5:P:191:ILE:HG12	1.64	0.63
11:a:94:ALA:O	11:a:164:ASN:ND2	2.31	0.63
3:C:31:ASN:ND2	3:C:229:ASP:OD1	2.32	0.63
11:a:499:GLU:O	15:e:80:ARG:NH1	2.32	0.63
11:n:510:LYS:HA	14:q:122:MET:HE1	1.81	0.63
23:z:165:SER:O	23:z:169:SER:OG	2.10	0.63
5:E:191:ILE:HG22	5:E:193:LYS:H	1.64	0.62
13:c:136:GLU:HB3	21:k:73:VAL:HG21	1.79	0.62
13:p:74:THR:HG21	13:p:234:HIS:HD2	1.64	0.62
5:P:109:VAL:HG22	5:P:116:VAL:HG13	1.80	0.62
4:D:268:ARG:HE	9:I:37:THR:HG22	1.65	0.62
11:n:94:ALA:O	11:n:164:ASN:ND2	2.33	0.62
5:E:159:CYS:SG	5:E:185:TYR:OH	2.55	0.62
5:P:121:ARG:HD3	5:P:153:LEU:HD12	1.81	0.62
3:C:127:THR:HG21	26:C:601:HEM:HBB2	1.80	0.61
15:r:67:LYS:NZ	16:s:143:LEU:O	2.32	0.61
20:j:75:ILE:HG23	21:k:96:TYR:HA	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:q:36:ASN:ND2	14:q:76:GLU:OE2	2.33	0.61
23:m:151:ARG:NH1	23:m:155:GLN:OE1	2.33	0.61
2:M:26:THR:OG1	2:M:191:ASN:ND2	2.34	0.61
3:N:253:HIS:HD2	3:N:255:ASP:H	1.47	0.61
5:P:127:GLN:CG	5:P:127:GLN:CA	2.75	0.61
20:w:69:ASP:O	20:w:73:LYS:HB2	2.00	0.61
12:b:81:ILE:HD12	25:b:302:PEF:H132	1.83	0.61
16:s:57:GLU:HG3	16:s:90:LYS:HG3	1.82	0.61
2:B:204:SER:OG	2:B:205:LEU:N	2.33	0.60
5:P:159:CYS:SG	5:P:178:CYS:HB2	2.41	0.60
4:D:265:GLU:OE2	4:D:268:ARG:NH2	2.34	0.60
11:n:87:MET:HE1	11:n:185:PHE:HB3	1.83	0.60
5:P:44:LYS:HE2	24:S:101:CDL:HA21	1.84	0.59
5:P:124:HIS:O	5:P:128:GLU:HB2	2.02	0.59
5:P:93:LYS:HE3	5:P:215:GLY:HA3	1.83	0.59
2:M:102:VAL:HG21	2:M:200:PHE:HB3	1.84	0.59
5:P:127:GLN:CB	5:P:127:GLN:CD	2.72	0.59
10:J:48:TRP:CD1	10:J:51:PHE:H	2.21	0.59
11:a:87:MET:HE1	11:a:185:PHE:HB3	1.84	0.59
9:I:13:ARG:HD3	10:J:29:ASN:HD21	1.68	0.59
1:L:203:ASN:ND2	1:L:231:GLN:O	2.35	0.59
23:m:185:MET:O	23:m:189:GLU:HB2	2.02	0.59
5:P:158:ILE:HG23	5:P:163:GLY:HA2	1.86	0.58
3:N:127:THR:HG21	26:N:601:HEM:HBB2	1.84	0.58
3:N:22:GLN:NE2	3:N:221:MET:SD	2.76	0.58
15:e:25:LYS:O	15:e:29:THR:OG1	2.22	0.58
21:x:60:LEU:O	21:x:64:ALA:HB3	2.04	0.58
5:P:116:VAL:HA	5:P:157:GLY:H	1.68	0.58
5:E:207:PHE:HA	5:E:211:LYS:O	2.04	0.58
1:L:317:HIS:HE1	1:L:351:TRP:HE1	1.51	0.58
11:n:499:GLU:O	15:r:80:ARG:NH2	2.37	0.58
11:n:362:SER:HB3	12:o:103:LEU:HD22	1.86	0.58
2:B:232:ARG:NH1	2:M:45:ASP:OD2	2.36	0.57
5:E:172:ASP:HB2	5:E:184:HIS:HB3	1.86	0.57
5:E:172:ASP:OD1	5:E:193:LYS:NZ	2.37	0.57
13:c:233:TYR:OH	14:d:53:GLU:O	2.21	0.57
12:o:28:SER:OG	12:o:29:ALA:N	2.35	0.57
3:C:58:ILE:HD12	3:C:172:SER:HA	1.87	0.57
5:P:142:THR:O	5:P:146:ARG:CB	2.52	0.57
14:q:132:ALA:O	14:q:140:VAL:HA	2.03	0.57
12:b:110:VAL:HG12	12:b:208:SER:HB2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:98:LEU:HD13	5:E:211:LYS:HA	1.87	0.57
9:I:18:VAL:HG12	27:I:101:PCF:H32	1.87	0.57
12:o:99:PRO:HA	12:o:102:ILE:HG12	1.84	0.57
5:P:146:ARG:HH12	5:P:200:LEU:HB2	1.69	0.57
17:t:29:TYR:HB2	17:t:30:LEU:HD12	1.86	0.57
23:z:182:VAL:HA	23:z:185:MET:HG2	1.85	0.57
23:m:151:ARG:HH22	23:m:152:MET:HE2	1.69	0.57
15:r:28:LEU:HD21	15:r:46:ILE:HD11	1.85	0.57
21:x:123:ARG:NH2	21:x:124:HIS:O	2.38	0.57
15:e:89:VAL:HG22	25:e:201:PEF:H32	1.87	0.57
2:B:58:ASN:ND2	2:B:118:GLU:OE2	2.38	0.57
10:U:30:LEU:HA	10:U:33:TRP:HB2	1.87	0.57
12:o:164:ASP:OD1	12:o:164:ASP:N	2.37	0.57
3:C:9:TYR:HB3	25:C:605:PEF:H192	1.85	0.57
3:N:31:ASN:ND2	3:N:229:ASP:OD1	2.38	0.57
13:c:258:LEU:HD13	23:m:155:GLN:HG2	1.86	0.57
11:a:517:LEU:HD11	14:d:123:TRP:HB3	1.85	0.56
11:n:353:LEU:HD22	12:o:47:LEU:HD22	1.86	0.56
5:P:175:GLY:HA3	5:P:186:ASP:HB3	1.85	0.56
25:E:304:PEF:H151	24:H:101:CDL:H112	1.87	0.56
13:c:134:PRO:HB3	13:c:265:TYR:HB3	1.87	0.56
11:n:424:ILE:HG13	11:n:454:ALA:HB1	1.87	0.56
11:n:488:SER:OG	11:n:489:VAL:N	2.38	0.56
11:n:507:ASN:O	11:n:510:LYS:NZ	2.38	0.56
2:B:255:VAL:HG21	2:B:343:VAL:HG11	1.87	0.56
3:N:183:HIS:HE1	26:N:601:HEM:NB	2.04	0.56
11:a:521:PRO:HG2	18:h:34:VAL:HA	1.86	0.56
11:n:27:MET:HA	11:n:30:THR:HG22	1.87	0.56
11:n:481:ASN:O	11:n:485:ASN:ND2	2.39	0.56
16:f:120:GLN:HG2	22:l:24:ILE:HG23	1.88	0.56
12:o:118:LYS:HZ1	20:w:60:PRO:HA	1.71	0.56
14:q:100:ILE:HD12	14:q:107:ARG:HD3	1.88	0.56
14:d:148:VAL:HG12	21:k:14:PRO:HG2	1.87	0.56
12:b:118:LYS:HE3	20:j:60:PRO:HA	1.87	0.56
1:A:252:ARG:NH1	1:A:254:ASP:OD1	2.39	0.56
4:D:91:ARG:NH1	4:D:124:GLU:OE2	2.38	0.56
1:L:341:ASP:OD1	1:L:341:ASP:N	2.37	0.56
13:p:173:ILE:O	13:p:177:LEU:HB2	2.06	0.56
5:E:110:LYS:HE2	3:N:263:LEU:HD11	1.87	0.55
7:G:121:ASP:OD2	2:M:69:ARG:NH2	2.39	0.55
11:a:320:ILE:HD13	11:a:349:THR:HG22	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:c:137:LEU:HD23	13:c:188:GLU:HG2	1.88	0.55
2:M:196:ASP:OD1	2:M:199:ARG:NH2	2.38	0.55
3:N:382:ARG:NH1	7:R:46:ASP:OD1	2.39	0.55
5:P:114:LYS:HB3	5:P:158:ILE:HD11	1.89	0.55
3:C:65:VAL:HG21	3:C:135:VAL:HG23	1.88	0.55
2:M:204:SER:OG	2:M:205:LEU:N	2.38	0.55
12:o:113:PRO:HG2	12:o:176:ARG:HB3	1.88	0.55
2:B:95:LYS:NZ	2:B:191:ASN:OD1	2.40	0.55
24:C:603:CDL:OA4	8:H:51:ARG:NH2	2.39	0.55
16:f:124:TYR:O	16:f:128:LEU:HB2	2.06	0.55
11:a:339:LEU:HD22	25:e:201:PEF:H152	1.89	0.55
16:f:48:THR:HG23	16:f:51:GLU:H	1.71	0.55
19:v:20:LEU:HD21	22:y:40:ILE:HD11	1.89	0.55
3:N:311:SER:HA	3:N:375:ASN:HD21	1.71	0.55
13:c:195:THR:HA	25:c:302:PEF:H42	1.89	0.55
7:G:123:ILE:HG23	1:L:361:THR:HG21	1.89	0.55
14:q:48:GLY:HA2	14:q:68:ARG:HH22	1.71	0.55
2:B:305:VAL:HG21	2:B:368:LEU:HB3	1.89	0.55
5:P:118:ILE:HD12	5:P:154:ILE:HG23	1.89	0.55
3:C:311:SER:HA	3:C:375:ASN:HD21	1.71	0.54
11:n:61:GLY:O	11:n:65:LEU:HB2	2.07	0.54
3:C:87:SER:OG	3:C:273:TRP:NE1	2.35	0.54
25:C:604:PEF:N	27:I:101:PCF:O12	2.40	0.54
2:M:238:VAL:HG22	2:M:290:ARG:HB2	1.89	0.54
4:O:85:PHE:HB3	4:O:90:ILE:HD11	1.88	0.54
12:o:89:PRO:HA	12:o:92:ILE:HG22	1.89	0.54
3:C:54:TYR:OH	3:C:134:CYS:O	2.23	0.54
1:L:263:LEU:HD13	1:L:433:ILE:HG12	1.89	0.54
1:L:113:THR:HG21	1:L:214:ILE:HD13	1.88	0.54
1:L:252:ARG:NH1	1:L:254:ASP:OD1	2.41	0.54
3:N:82:HIS:HE1	26:N:601:HEM:NC	2.04	0.54
11:a:145:ASP:OD1	11:a:214:ARG:NH1	2.40	0.54
16:f:57:GLU:HG2	16:f:90:LYS:HG3	1.89	0.54
11:n:381:LEU:HD13	31:n:602:HEA:HAC	1.90	0.54
23:z:136:ASN:ND2	23:z:146:LYS:HD3	2.22	0.54
10:J:48:TRP:HE1	10:J:50:LYS:HB3	1.72	0.54
12:b:114:ALA:HB3	12:b:173:THR:HG23	1.88	0.54
5:E:127:GLN:HG3	5:E:130:ASN:HB2	1.90	0.54
5:P:186:ASP:O	5:P:188:SER:N	2.40	0.54
25:n:607:PEF:H121	25:n:607:PEF:H322	1.90	0.54
13:p:171:LEU:HD11	13:p:223:LEU:HD22	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:14:ASN:HA	3:N:18:ILE:HB	1.90	0.54
21:k:73:VAL:HA	21:k:76:GLU:HG3	1.90	0.54
12:o:147:VAL:HA	12:o:163:THR:HG22	1.89	0.54
5:E:122:THR:O	5:E:126:ILE:HB	2.08	0.53
24:L:501:CDL:OB4	3:N:4:ARG:NH2	2.38	0.53
3:N:132:TYR:OH	3:N:256:ASN:ND2	2.38	0.53
5:P:142:THR:O	5:P:146:ARG:HB2	2.08	0.53
12:o:69:PRO:HG2	12:o:70:ILE:HD12	1.89	0.53
21:x:49:ASN:HA	21:x:52:VAL:HG12	1.90	0.53
25:C:605:PEF:H362	3:N:196:MET:HE1	1.90	0.53
25:E:303:PEF:H191	11:a:466:PHE:HB3	1.90	0.53
15:r:24:SER:HB3	15:r:27:THR:HG22	1.88	0.53
5:P:121:ARG:HH11	5:P:150:PRO:HA	1.72	0.53
13:c:141:ASN:ND2	13:c:185:GLN:OE1	2.41	0.53
14:d:134:CYS:HB3	14:d:138:GLY:H	1.72	0.53
11:n:441:PRO:HD2	12:o:230:ALA:HB2	1.91	0.53
1:A:263:LEU:HD13	1:A:433:ILE:HG12	1.89	0.53
3:N:147:ILE:HA	3:N:150:LEU:HD12	1.90	0.53
5:P:51:LYS:HE2	24:S:101:CDL:HA32	1.89	0.53
12:o:185:ILE:HA	12:o:199:ALA:O	2.09	0.53
2:M:339:ASN:OD1	2:M:340:PHE:N	2.40	0.53
13:p:219:LEU:HD13	13:p:249:TYR:HD2	1.74	0.53
2:M:150:THR:OG1	2:M:352:ASN:ND2	2.42	0.53
15:e:35:TRP:O	15:e:43:GLN:NE2	2.40	0.53
20:w:54:THR:HA	20:w:57:ALA:HB3	1.90	0.53
11:a:534:SER:O	14:d:112:THR:OG1	2.26	0.53
16:f:82:VAL:HG12	19:i:6:ILE:HB	1.91	0.53
3:C:382:ARG:NH1	7:G:46:ASP:OD1	2.41	0.53
1:L:315:PHE:HB3	1:L:332:THR:HG22	1.91	0.53
12:b:41:ASP:OD2	19:i:37:HIS:ND1	2.41	0.53
5:P:185:TYR:HB3	5:P:189:GLY:HA2	1.91	0.53
5:E:175:GLY:HA3	5:E:185:TYR:O	2.08	0.52
12:o:27:ASP:OD1	12:o:27:ASP:N	2.41	0.52
4:O:77:SER:O	9:T:47:LYS:NZ	2.42	0.52
13:p:84:ARG:O	13:p:88:ASN:ND2	2.42	0.52
13:p:209:THR:HG22	13:p:260:LEU:HD21	1.90	0.52
25:E:304:PEF:N	25:E:304:PEF:O4	2.41	0.52
1:A:263:LEU:HD11	1:A:431:ILE:HD12	1.91	0.52
11:a:447:PHE:O	11:a:451:ASN:ND2	2.35	0.52
3:C:345:GLU:OE2	4:D:62:MET:N	2.43	0.52
5:E:118:ILE:HD12	5:E:154:ILE:HD12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:a:136:ILE:HG12	21:k:104:LYS:HD2	1.92	0.52
11:n:215:ASN:HA	21:x:104:LYS:HE3	1.92	0.52
25:E:303:PEF:H311	25:E:304:PEF:H131	1.91	0.52
5:P:169:GLU:H	5:P:176:TRP:CD1	2.27	0.52
5:P:177:PHE:HE1	5:P:182:GLY:HA2	1.74	0.52
14:d:51:ALA:H	14:d:62:GLN:HE21	1.57	0.52
23:z:178:ASN:OD1	23:z:181:LYS:NZ	2.42	0.52
4:O:95:GLN:NE2	4:O:235:GLU:O	2.43	0.52
11:a:330:GLY:O	12:b:68:ASN:ND2	2.39	0.52
12:b:16:ASP:N	15:e:140:ASN:OD1	2.43	0.52
1:A:457:TRP:HB2	24:A:501:CDL:HA32	1.92	0.52
4:D:85:PHE:HB3	4:D:90:ILE:HD11	1.91	0.52
1:L:300:ILE:HG22	1:L:302:LEU:H	1.75	0.52
11:a:117:THR:O	18:h:71:GLN:NE2	2.41	0.52
1:L:103:SER:OG	1:L:388:ASN:ND2	2.42	0.52
17:t:12:PHE:O	17:t:22:ARG:NH1	2.43	0.52
4:D:125:VAL:HA	4:D:128:MET:HE2	1.92	0.52
4:O:296:LYS:HE3	7:R:84:THR:HA	1.91	0.52
12:o:130:TYR:HB2	12:o:141:VAL:HG13	1.92	0.52
7:G:125:VAL:HG21	1:L:364:GLU:HG3	1.91	0.51
1:L:247:SER:OG	1:L:248:GLU:N	2.43	0.51
5:P:164:CYS:SG	5:P:165:VAL:N	2.77	0.51
11:n:345:LEU:HD11	12:o:58:LEU:HD21	1.92	0.51
11:n:421:ALA:HA	11:n:424:ILE:HG22	1.92	0.51
20:w:67:TRP:O	20:w:71:ARG:CB	2.55	0.51
11:n:223:VAL:HG21	12:o:202:GLY:HA3	1.92	0.51
7:G:85:HIS:O	8:H:50:ARG:NH2	2.44	0.51
14:d:32:LYS:HD2	14:d:33:THR:H	1.75	0.51
11:n:95:PHE:O	11:n:164:ASN:ND2	2.43	0.51
12:o:166:SER:OG	12:o:167:MET:N	2.42	0.51
5:P:148:LYS:H	5:P:205:TYR:HH	1.59	0.51
20:w:20:GLN:O	20:w:23:GLN:NE2	2.43	0.51
1:L:91:LEU:HD23	1:L:108:SER:HB3	1.91	0.51
5:P:101:ILE:HD13	5:P:107:VAL:HG21	1.91	0.51
11:n:244:VAL:HB	31:n:603:HEA:HAC	1.92	0.51
13:p:130:GLU:HG2	13:p:193:ALA:HB3	1.93	0.51
21:x:108:TRP:NE1	21:x:113:LYS:O	2.44	0.51
1:A:428:ASP:O	5:E:53:ARG:NH2	2.39	0.51
3:C:339:ILE:HD11	3:C:351:MET:HE2	1.91	0.51
5:P:146:ARG:NE	5:P:188:SER:O	2.43	0.51
21:k:89:ASP:OD1	21:k:89:ASP:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:p:236:THR:HG21	14:q:59:ASP:HB3	1.93	0.51
1:L:72:LEU:HD12	1:L:188:LEU:HD23	1.93	0.51
8:S:29:VAL:HB	8:S:34:GLN:HE21	1.75	0.51
14:q:131:VAL:HG12	14:q:142:LYS:HD3	1.92	0.51
16:s:73:LEU:HD11	16:s:107:VAL:HG12	1.93	0.51
1:A:323:LYS:HG3	1:A:396:ILE:HD11	1.92	0.50
2:B:249:SER:O	2:B:249:SER:OG	2.27	0.50
11:n:145:ASP:OD1	11:n:215:ASN:ND2	2.40	0.50
5:E:106:ASN:HD21	5:E:169:GLU:HG2	1.75	0.50
5:P:98:LEU:HD22	5:P:211:LYS:HE3	1.93	0.50
14:d:104:ASP:OD1	14:d:104:ASP:N	2.43	0.50
3:C:247:SER:HG	3:C:250:THR:HG1	1.56	0.50
4:D:188:CYS:SG	4:D:256:ASN:ND2	2.84	0.50
3:N:145:THR:O	3:N:149:ASN:HB2	2.12	0.50
2:B:260:LEU:O	2:B:268:SER:OG	2.26	0.50
3:C:385:LYS:HD3	7:G:17:LYS:HE3	1.91	0.50
13:p:92:LEU:HA	13:p:95:VAL:HG22	1.93	0.50
21:x:44:ALA:O	21:x:47:THR:OG1	2.25	0.50
23:z:131:SER:HA	23:z:134:ILE:HB	1.94	0.50
8:H:41:PHE:HB2	27:H:103:PCF:H11	1.92	0.50
14:q:60:LEU:HD11	14:q:75:LEU:HD21	1.94	0.50
10:U:54:THR:O	10:U:58:LYS:NZ	2.40	0.50
6:F:106:LYS:O	6:F:110:GLN:NE2	2.45	0.50
3:N:7:ASN:HB3	3:N:10:LEU:HB2	1.94	0.50
11:a:534:SER:OG	14:d:112:THR:OG1	2.28	0.50
11:n:27:MET:HE1	11:n:469:ILE:HD12	1.94	0.50
14:q:36:ASN:HA	14:q:72:LEU:HD22	1.94	0.50
3:C:178:ARG:NH1	5:P:82:MET:O	2.45	0.50
1:L:133:SER:OG	1:L:134:SER:O	2.28	0.50
5:P:81:SER:O	5:P:81:SER:OG	2.27	0.50
21:k:43:HIS:HE1	23:m:141:MET:HE2	1.77	0.50
11:n:469:ILE:HD11	18:u:57:PHE:CG	2.47	0.50
2:M:251:ALA:HB2	2:M:338:LEU:HB3	1.93	0.50
1:A:119:PHE:O	1:A:123:SER:OG	2.28	0.49
2:M:305:VAL:HG21	2:M:368:LEU:HB3	1.94	0.49
5:P:143:ASP:HB2	5:P:190:ARG:HH12	1.77	0.49
11:a:396:TRP:NE1	11:a:515:GLU:OE1	2.45	0.49
11:n:271:ILE:HA	11:n:274:VAL:HG12	1.94	0.49
11:n:342:ILE:HD11	12:o:58:LEU:HD22	1.93	0.49
3:C:4:ARG:NH1	3:C:19:ASP:OD2	2.43	0.49
23:m:155:GLN:HA	23:m:158:THR:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:131:LEU:O	1:L:136:ASN:ND2	2.44	0.49
12:o:57:MET:HA	12:o:60:THR:HG22	1.94	0.49
23:z:186:ARG:O	23:z:190:ASN:HB3	2.12	0.49
7:R:118:ASP:O	7:R:122:ASN:ND2	2.45	0.49
12:b:147:VAL:HG11	12:b:231:ASN:HB3	1.94	0.49
11:n:386:ILE:HD13	11:n:389:LEU:HD12	1.94	0.49
13:p:236:THR:HG22	13:p:238:GLY:H	1.77	0.49
19:v:48:TYR:HD1	19:v:51:LEU:HD21	1.76	0.49
3:C:77:ILE:O	3:C:81:LEU:HB2	2.12	0.49
3:C:193:MET:HE1	25:N:606:PEF:H371	1.94	0.49
13:c:222:MET:HA	13:c:225:VAL:HG12	1.95	0.49
15:r:151:LYS:HE3	22:y:62:LYS:HZ3	1.77	0.49
2:B:49:HIS:HD2	2:B:161:TYR:H	1.61	0.49
4:D:83:GLU:HA	9:I:44:ASN:HD21	1.77	0.49
21:x:39:ALA:HA	21:x:42:LYS:HG2	1.95	0.49
5:E:168:GLY:HA2	5:E:176:TRP:CD1	2.48	0.49
5:E:184:HIS:HB2	5:E:193:LYS:HD3	1.94	0.49
25:n:606:PEF:H453	12:o:53:LEU:HD11	1.94	0.49
1:A:391:GLY:O	1:A:395:LEU:HB2	2.13	0.49
3:C:132:TYR:OH	3:C:256:ASN:ND2	2.45	0.49
11:a:519:THR:HG23	11:a:522:PRO:HA	1.93	0.49
12:b:129:GLU:HA	12:b:141:VAL:O	2.13	0.49
23:m:179:LYS:HA	23:m:182:VAL:HG22	1.93	0.48
1:L:399:SER:OG	1:L:400:LYS:N	2.46	0.48
3:N:305:LEU:HD13	3:N:363:PHE:HD1	1.78	0.48
21:x:43:HIS:O	21:x:47:THR:HG23	2.13	0.48
21:x:92:TRP:CE3	21:x:93:PRO:HD2	2.49	0.48
1:L:207:VAL:HG23	1:L:395:LEU:HD12	1.94	0.48
11:a:310:MET:HG2	12:b:93:LEU:HD13	1.93	0.48
8:H:29:VAL:HB	8:H:34:GLN:HE21	1.76	0.48
11:a:534:SER:HB3	14:d:86:LEU:HD23	1.95	0.48
1:A:325:SER:OG	1:A:326:GLY:N	2.46	0.48
13:p:253:LEU:HD23	13:p:256:ILE:HD11	1.95	0.48
1:A:341:ASP:N	1:A:341:ASP:OD1	2.45	0.48
5:E:57:TYR:HA	5:E:60:VAL:HG22	1.96	0.48
1:L:446:MET:HE1	8:S:32:TYR:HE1	1.79	0.48
3:N:98:ALA:HB2	27:N:607:PCF:H421	1.95	0.48
23:m:183:ASN:HA	23:m:186:ARG:H	1.78	0.48
1:L:99:ARG:HH22	1:L:165:HIS:HB3	1.79	0.48
12:b:168:VAL:HG22	12:b:237:GLU:HB2	1.95	0.48
25:n:607:PEF:H12	22:y:61:SER:HA	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:p:251:HIS:CE1	23:z:148:VAL:HG13	2.48	0.48
19:v:11:LYS:HA	19:v:14:VAL:HG22	1.95	0.48
21:x:120:VAL:HG13	21:x:121:VAL:HG13	1.96	0.48
23:z:124:TRP:HE1	23:z:155:GLN:NE2	2.12	0.48
3:C:32:MET:HE1	24:C:603:CDL:H322	1.96	0.48
12:b:177:PHE:O	12:b:206:GLN:HA	2.14	0.48
13:p:152:VAL:HG13	13:p:174:THR:HG21	1.96	0.48
5:E:185:TYR:CE1	5:E:200:LEU:HD11	2.49	0.48
11:n:37:ARG:NH2	11:n:451:ASN:O	2.47	0.48
13:p:71:ALA:O	13:p:75:TYR:HB2	2.12	0.48
5:E:139:ASP:OD1	5:E:141:GLN:NE2	2.46	0.48
3:N:54:TYR:OH	3:N:134:CYS:O	2.27	0.48
3:N:71:ASP:HB2	5:P:86:ALA:HB3	1.94	0.48
5:P:170:ALA:N	5:P:175:GLY:O	2.44	0.47
13:c:219:LEU:HD21	13:c:250:THR:HG22	1.96	0.47
21:k:102:ARG:NH2	21:k:112:ASP:O	2.46	0.47
11:n:205:ALA:HB2	13:p:101:ILE:HG13	1.96	0.47
11:n:353:LEU:HB3	12:o:47:LEU:HD13	1.95	0.47
5:P:89:LEU:O	10:U:77:ASN:ND2	2.47	0.47
11:a:4:ARG:NH2	18:h:36:GLU:O	2.45	0.47
12:b:136:ASP:OD1	12:b:136:ASP:N	2.47	0.47
12:o:92:ILE:HA	12:o:95:ILE:HG22	1.96	0.47
12:o:122:TYR:OH	20:w:62:ASP:OD2	2.32	0.47
1:A:315:PHE:HB3	1:A:332:THR:HG22	1.95	0.47
5:E:125:GLU:HA	5:E:128:GLU:H	1.79	0.47
5:E:158:ILE:HG23	5:E:163:GLY:HA2	1.96	0.47
3:N:29:TRP:HB3	3:N:99:LYS:HG3	1.96	0.47
1:A:113:THR:HG21	1:A:214:ILE:HD13	1.95	0.47
3:C:21:PRO:O	3:C:218:ARG:NH2	2.46	0.47
15:r:50:LEU:HD11	15:r:65:GLU:HB3	1.95	0.47
3:C:196:MET:HE1	25:N:606:PEF:H351	1.96	0.47
23:m:135:VAL:HG11	23:m:150:ALA:HB2	1.96	0.47
23:z:166:VAL:HA	23:z:169:SER:HB2	1.96	0.47
4:D:224:ALA:HB3	28:D:401:HEC:HBD2	1.96	0.47
1:L:99:ARG:NH1	1:L:162:GLU:OE1	2.48	0.47
2:M:99:PRO:HA	2:M:102:VAL:HG22	1.97	0.47
5:P:186:ASP:O	5:P:189:GLY:N	2.31	0.47
11:n:145:ASP:CG	11:n:214:ARG:HH12	2.22	0.47
13:p:263:VAL:HG23	13:p:264:PHE:HD1	1.80	0.47
1:L:79:SER:O	1:L:83:SER:OG	2.25	0.47
1:L:86:ALA:HB1	1:L:91:LEU:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:67:HIS:CE1	5:P:85:THR:HG21	2.50	0.47
5:P:71:ALA:HB1	27:T:101:PCF:H421	1.96	0.47
7:R:66:ASP:OD1	7:R:66:ASP:N	2.39	0.47
11:n:202:VAL:HG21	11:n:238:PHE:HD2	1.78	0.47
11:n:424:ILE:HD12	11:n:458:SER:HB3	1.97	0.47
12:o:120:ILE:HD13	12:o:127:LYS:HD2	1.96	0.47
12:o:127:LYS:HA	12:o:144:GLU:HG3	1.97	0.47
12:o:174:HIS:CD2	12:o:210:LEU:HB2	2.50	0.47
12:o:178:VAL:HA	12:o:205:ASN:O	2.14	0.47
1:L:58:GLY:N	1:L:100:ASP:O	2.48	0.47
12:b:16:ASP:OD1	12:b:213:ARG:NH2	2.40	0.47
12:o:147:VAL:HG21	12:o:231:ASN:HB2	1.96	0.47
12:o:161:LEU:HD11	12:o:218:TYR:HB3	1.96	0.47
12:o:171:VAL:HG22	12:o:240:SER:HA	1.97	0.47
23:z:168:LEU:HD12	23:z:171:TYR:HB2	1.97	0.47
13:p:68:ASP:HB2	17:t:19:LEU:HD22	1.96	0.47
21:x:63:ILE:O	21:x:67:ALA:HB2	2.14	0.47
23:z:143:LYS:HA	23:z:146:LYS:HD2	1.95	0.47
12:o:196:LYS:HE3	12:o:196:LYS:HB2	1.79	0.47
5:P:80:SER:HA	5:P:83:THR:HG23	1.97	0.46
15:r:85:GLY:N	15:r:88:ASP:OD2	2.48	0.46
1:A:119:PHE:O	1:A:123:SER:CB	2.62	0.46
25:E:303:PEF:H141	25:E:303:PEF:H341	1.98	0.46
11:a:23:ILE:HD12	31:a:602:HEA:H252	1.97	0.46
23:z:178:ASN:HB3	23:z:181:LYS:HB2	1.97	0.46
2:B:332:VAL:HG22	2:B:334:SER:H	1.80	0.46
3:C:82:HIS:HE1	26:C:601:HEM:NC	2.10	0.46
3:C:139:MET:HB2	3:C:256:ASN:ND2	2.31	0.46
5:E:89:LEU:O	10:J:77:ASN:ND2	2.48	0.46
5:E:98:LEU:HB3	5:E:211:LYS:HD2	1.95	0.46
5:E:177:PHE:HE1	5:E:182:GLY:HA2	1.80	0.46
5:P:31:LYS:HE2	5:P:35:ARG:HD2	1.98	0.46
23:m:162:LEU:O	23:m:165:SER:HB3	2.16	0.46
14:q:75:LEU:HB2	21:x:34:LYS:HD2	1.97	0.46
1:A:96:ASN:HD22	1:A:388:ASN:HD22	1.63	0.46
3:C:153:ALA:HB2	3:C:288:LYS:HD2	1.96	0.46
5:E:44:LYS:HE2	24:H:101:CDL:HA21	1.96	0.46
4:O:166:ARG:NH2	4:O:171:GLY:O	2.49	0.46
5:P:94:VAL:HG22	5:P:111:TRP:HD1	1.80	0.46
25:S:102:PEF:H382	25:S:102:PEF:H411	1.76	0.46
12:o:190:ILE:HD11	12:o:234:ILE:HG21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:q:124:LEU:HD11	14:q:134:CYS:HA	1.97	0.46
3:C:111:VAL:HG13	3:C:306:PRO:HG2	1.97	0.46
11:a:403:LEU:HB3	11:a:479:GLY:HA3	1.96	0.46
11:n:130:TYR:OH	11:n:237:TRP:NE1	2.39	0.46
11:n:389:LEU:HB3	31:n:602:HEA:H242	1.98	0.46
23:z:115:ASN:ND2	23:z:118:LYS:HD3	2.31	0.46
1:A:254:ASP:HB3	8:H:20:LYS:HD2	1.96	0.46
4:O:165:ALA:O	4:O:169:ASN:ND2	2.48	0.46
12:b:185:ILE:HG22	12:b:223:GLU:HG2	1.98	0.46
22:y:29:VAL:HA	22:y:32:GLU:HB2	1.97	0.46
1:L:265:VAL:HG12	1:L:431:ILE:HG22	1.97	0.46
21:x:15:PRO:O	21:x:19:LYS:NZ	2.48	0.46
23:z:116:LYS:HE3	23:z:120:ILE:HD11	1.98	0.46
16:f:116:GLU:OE2	19:i:12:ARG:NH2	2.42	0.46
15:r:27:THR:HG23	15:r:28:LEU:HD22	1.98	0.46
23:z:186:ARG:O	23:z:190:ASN:CB	2.64	0.46
3:C:164:TRP:O	3:C:178:ARG:NH2	2.48	0.46
3:C:253:HIS:HD2	3:C:255:ASP:HB2	1.80	0.46
5:E:72:LYS:HG3	10:J:44:PHE:HA	1.97	0.46
23:m:117:TYR:HA	23:m:120:ILE:HG12	1.96	0.46
2:B:164:VAL:HG21	2:M:232:ARG:HE	1.80	0.46
3:N:154:ILE:HD12	3:N:161:ILE:HD11	1.98	0.46
3:N:339:ILE:HD11	3:N:351:MET:HE2	1.98	0.46
25:c:302:PEF:O2P	21:k:114:THR:OG1	2.33	0.46
19:i:20:LEU:HD21	22:l:40:ILE:HD11	1.98	0.46
20:j:12:VAL:HG11	20:j:58:LEU:HD23	1.98	0.46
11:n:53:GLN:HB2	12:o:227:THR:HG22	1.98	0.46
11:n:447:PHE:O	11:n:451:ASN:ND2	2.41	0.46
12:o:30:THR:HG22	12:o:32:ASN:H	1.80	0.46
14:q:71:LEU:HA	14:q:74:LYS:HE3	1.98	0.46
1:A:33:SER:O	1:A:34:ASN:ND2	2.49	0.45
8:H:80:LEU:HD23	8:H:80:LEU:HA	1.84	0.45
2:M:80:SER:HA	2:M:88:THR:O	2.15	0.45
1:L:226:LYS:HE2	1:L:226:LYS:HB2	1.72	0.45
23:m:145:GLN:HA	23:m:148:VAL:HG22	1.98	0.45
11:n:67:ILE:HG23	11:n:247:LEU:HD21	1.99	0.45
11:n:116:SER:HB2	11:n:146:LEU:HB2	1.99	0.45
12:o:169:VAL:O	12:o:238:ALA:HA	2.16	0.45
2:B:233:PHE:HB3	2:B:357:GLY:HA2	1.98	0.45
5:E:98:LEU:HD12	5:E:212:VAL:HG23	1.98	0.45
1:L:113:THR:O	1:L:116:SER:OG	2.28	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:101:LEU:HD13	3:N:305:LEU:HD21	1.97	0.45
21:k:70:THR:HA	21:k:73:VAL:HG22	1.98	0.45
13:p:215:HIS:HB3	13:p:253:LEU:HD11	1.98	0.45
15:r:112:LEU:HD21	27:r:202:PCF:H32	1.97	0.45
11:n:293:TYR:OH	11:n:305:PHE:O	2.33	0.45
11:n:318:ILE:HG21	12:o:86:THR:HG22	1.99	0.45
17:t:49:PRO:HA	17:t:52:ILE:HG22	1.97	0.45
21:x:29:ALA:HA	21:x:32:LYS:HG3	1.99	0.45
12:b:128:TYR:O	12:b:142:GLU:HA	2.17	0.45
11:n:135:SER:HA	11:n:214:ARG:HG2	1.98	0.45
12:o:241:LEU:HA	12:o:244:PHE:HB2	1.98	0.45
1:A:79:SER:O	1:A:83:SER:OG	2.25	0.45
1:A:317:HIS:CE1	1:A:351:TRP:HE1	2.30	0.45
3:C:117:GLY:C	26:C:602:HEM:HBC2	2.42	0.45
7:R:47:ASP:OD1	7:R:102:TYR:OH	2.31	0.45
11:a:172:MET:HE2	11:a:172:MET:HB3	1.85	0.45
15:e:84:HIS:CD2	25:e:201:PEF:H11	2.51	0.45
22:y:28:TRP:CD1	22:y:29:VAL:HG13	2.51	0.45
5:E:117:PHE:O	5:E:154:ILE:HA	2.17	0.45
12:b:180:THR:HB	12:b:204:LEU:HD23	1.98	0.45
20:j:36:LYS:HG3	23:m:188:TRP:CZ2	2.51	0.45
13:p:214:LEU:HA	13:p:217:VAL:HG12	1.99	0.45
21:x:80:HIS:O	21:x:84:LEU:HB2	2.17	0.45
1:A:203:ASN:ND2	1:A:231:GLN:O	2.50	0.45
13:c:120:LEU:HD13	13:c:126:PRO:HG3	1.99	0.45
4:D:271:LEU:HD23	9:I:36:ILE:HG23	1.99	0.45
16:s:85:PRO:HG3	16:s:127:GLU:OE2	2.17	0.45
21:x:100:ASN:HB2	21:x:125:ILE:HD12	1.99	0.45
2:B:303:LYS:HE3	2:B:303:LYS:HB2	1.81	0.45
5:P:142:THR:O	5:P:146:ARG:HB3	2.17	0.45
12:b:69:PRO:HG2	12:b:70:ILE:HD12	1.97	0.45
23:m:192:LEU:HD22	23:m:193:ARG:HG3	1.98	0.45
11:n:377:PHE:HA	11:n:380:VAL:HG22	1.97	0.45
16:s:138:PRO:HB2	16:s:143:LEU:HD23	1.99	0.45
5:E:137:LEU:HD11	5:E:191:ILE:O	2.17	0.44
1:L:77:PHE:O	1:L:82:ASN:ND2	2.39	0.44
2:M:233:PHE:HB3	2:M:357:GLY:HA2	1.98	0.44
21:k:80:HIS:HA	21:k:83:HIS:CD2	2.52	0.44
11:n:363:LEU:HD21	12:o:40:HIS:HD2	1.82	0.44
18:u:72:LEU:HD23	18:u:78:PHE:HB2	1.99	0.44
21:x:102:ARG:HE	21:x:112:ASP:HB2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:y:26:GLU:OE2	22:y:30:ILE:HG23	2.17	0.44
22:y:27:SER:HB2	22:y:30:ILE:HG22	1.98	0.44
4:D:184:ARG:NH1	28:D:401:HEC:O1A	2.50	0.44
1:L:317:HIS:CE1	1:L:351:TRP:HE1	2.32	0.44
13:c:120:LEU:HB3	13:c:126:PRO:HB3	1.98	0.44
13:c:195:THR:HG23	13:c:197:SER:H	1.82	0.44
11:n:268:PHE:H	11:n:326:THR:HB	1.81	0.44
11:a:386:ILE:HG21	31:a:602:HEA:H162	1.99	0.44
3:C:1:MET:HG3	3:C:6:SER:HB3	1.99	0.44
21:k:53:LYS:HG2	21:k:57:TRP:HD1	1.82	0.44
11:n:108:MET:HG3	13:p:31:LEU:HD22	2.00	0.44
20:w:26:HIS:O	20:w:30:SER:HB3	2.18	0.44
2:B:83:ASP:OD1	2:B:83:ASP:N	2.50	0.44
2:B:154:GLY:O	2:B:157:ASN:ND2	2.51	0.44
5:E:127:GLN:O	5:E:131:SER:HB3	2.17	0.44
3:N:362:TYR:HA	3:N:366:ILE:HB	2.00	0.44
11:a:224:SER:O	11:a:224:SER:OG	2.33	0.44
31:a:602:HEA:H202	31:a:602:HEA:H171	1.76	0.44
1:L:244:PHE:CG	1:L:266:GLU:HB2	2.53	0.44
21:k:50:MET:HE3	21:k:50:MET:HB2	1.82	0.44
11:n:230:ILE:HD11	12:o:200:THR:HG21	1.99	0.44
13:p:260:LEU:O	13:p:264:PHE:HB2	2.17	0.44
16:s:88:ILE:HD12	16:s:111:LEU:HD11	1.99	0.44
20:w:26:HIS:O	20:w:30:SER:CB	2.65	0.44
22:y:43:TRP:HA	22:y:46:VAL:HG12	1.99	0.44
24:A:501:CDL:HA4	24:A:501:CDL:H512	2.00	0.44
2:B:355:ALA:HB1	2:B:362:LEU:HD12	1.99	0.44
5:P:118:ILE:HG13	5:P:153:LEU:C	2.43	0.44
20:j:69:ASP:O	20:j:73:LYS:HG2	2.18	0.44
11:n:270:GLU:HG2	11:n:271:ILE:HG23	1.99	0.44
31:n:602:HEA:H261	31:n:602:HEA:H172	1.67	0.44
12:o:18:PRO:O	15:r:147:GLN:NE2	2.49	0.44
12:o:187:ASP:HB2	12:o:222:SER:HB2	2.00	0.44
22:y:28:TRP:HD1	22:y:29:VAL:HG13	1.82	0.44
1:A:364:GLU:OE1	7:R:127:LYS:NZ	2.39	0.44
4:D:269:LEU:O	4:D:273:THR:HG23	2.18	0.44
3:N:96:HIS:HD2	26:N:602:HEM:C1C	2.36	0.44
5:P:94:VAL:HG22	5:P:111:TRP:CD1	2.52	0.44
31:a:602:HEA:H172	31:a:602:HEA:H261	1.86	0.44
25:n:608:PEF:H41	13:p:17:VAL:HG11	2.00	0.44
14:q:136:GLU:O	16:s:71:ARG:NH2	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:59:GLU:HG2	3:C:60:LEU:HG	2.00	0.44
5:P:146:ARG:NH2	5:P:200:LEU:O	2.50	0.44
8:S:5:SER:OG	8:S:6:GLY:N	2.51	0.44
11:a:172:MET:HE3	13:c:14:PHE:CG	2.53	0.44
15:e:111:ARG:HD2	15:e:111:ARG:HA	1.85	0.44
25:e:201:PEF:H382	25:e:201:PEF:H351	1.84	0.44
5:P:72:LYS:HG3	10:U:44:PHE:HA	2.00	0.43
11:a:70:LEU:O	11:a:74:ALA:CB	2.66	0.43
13:p:245:THR:HG21	25:p:301:PEF:H142	2.00	0.43
14:q:71:LEU:HA	14:q:74:LYS:HG2	2.00	0.43
4:D:178:SER:O	4:D:178:SER:OG	2.34	0.43
5:E:199:ASN:HB3	5:E:200:LEU:H	1.64	0.43
2:M:228:GLU:HG3	2:M:353:TYR:HD2	1.83	0.43
3:N:35:LEU:HD12	3:N:35:LEU:HA	1.82	0.43
5:P:141:GLN:HE21	5:P:199:ASN:HD21	1.65	0.43
11:n:424:ILE:HA	11:n:454:ALA:HA	2.01	0.43
21:x:72:PHE:O	21:x:76:GLU:HG2	2.17	0.43
3:C:39:CYS:HB3	3:C:89:PHE:HD2	1.83	0.43
5:P:207:PHE:CG	5:P:210:ASP:HA	2.54	0.43
11:a:4:ARG:HD2	18:h:30:PHE:CG	2.53	0.43
11:a:482:ASN:O	11:a:488:SER:OG	2.34	0.43
8:S:86:ARG:O	8:S:89:LEU:N	2.52	0.43
25:b:303:PEF:H161	19:i:32:TRP:HZ3	1.83	0.43
11:n:377:PHE:HD1	11:n:381:LEU:HD12	1.84	0.43
12:o:158:LEU:HB2	12:o:162:ASP:OD2	2.18	0.43
12:o:189:ALA:HB1	12:o:196:LYS:HE2	2.01	0.43
23:z:200:ARG:HG3	23:z:201:LEU:HD22	2.00	0.43
5:E:166:PRO:HB3	5:E:178:CYS:HB2	2.00	0.43
3:N:230:LEU:HD13	25:N:605:PEF:H352	2.00	0.43
5:P:132:VAL:HG12	5:P:133:ASP:O	2.19	0.43
16:s:124:TYR:O	16:s:128:LEU:HG	2.18	0.43
3:C:21:PRO:HB2	3:C:218:ARG:HD3	2.01	0.43
3:N:230:LEU:HD11	25:N:605:PEF:H182	1.99	0.43
6:Q:75:THR:OG1	6:Q:76:ASP:N	2.52	0.43
9:T:49:TRP:NE1	10:U:74:ASP:OD2	2.44	0.43
11:a:34:LEU:O	11:a:38:LEU:HB2	2.18	0.43
11:a:379:TYR:O	11:a:383:MET:HB2	2.18	0.43
18:h:41:LYS:O	18:h:45:ARG:NH2	2.52	0.43
20:w:61:LEU:HA	20:w:64:ILE:HG12	2.01	0.43
1:A:290:ALA:O	1:A:296:ARG:NE	2.45	0.43
2:M:153:LYS:HA	2:M:153:LYS:HD2	1.89	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:o:27:ASP:HB2	15:r:142:TRP:HE3	1.83	0.43
12:o:149:PRO:HD2	12:o:152:LEU:HD21	2.01	0.43
12:o:187:ASP:HB2	12:o:222:SER:H	1.84	0.43
13:p:187:ILE:HA	13:p:190:THR:HG22	2.01	0.43
15:r:142:TRP:NE1	19:v:44:ARG:HA	2.33	0.43
11:n:151:LEU:O	11:n:155:SER:OG	2.33	0.43
13:p:15:HIS:NE2	13:p:78:ASP:OD2	2.51	0.43
14:q:30:VAL:HB	14:q:31:VAL:H	1.57	0.43
3:C:20:SER:OG	3:C:22:GLN:NE2	2.52	0.43
2:M:228:GLU:HA	2:M:353:TYR:O	2.19	0.43
2:M:262:SER:O	2:M:268:SER:OG	2.33	0.43
4:O:63:THR:HG22	4:O:65:ALA:H	1.84	0.43
4:O:83:GLU:HA	9:T:44:ASN:HD21	1.84	0.43
21:k:53:LYS:HG2	21:k:57:TRP:CD1	2.54	0.43
13:p:105:LEU:HD23	13:p:105:LEU:HA	1.83	0.43
21:x:63:ILE:O	21:x:67:ALA:CB	2.67	0.43
3:C:177:GLN:NE2	3:N:55:SER:OG	2.51	0.43
1:L:220:VAL:HA	1:L:223:ILE:HG22	2.00	0.43
11:n:412:ILE:HG22	15:r:96:VAL:HG23	2.00	0.43
12:o:190:ILE:HG21	12:o:193:LEU:HD23	2.01	0.43
2:B:19:VAL:HG21	2:B:201:VAL:HG21	2.01	0.42
5:P:105:LYS:NZ	5:P:169:GLU:HB2	2.33	0.42
5:P:106:ASN:HD21	5:P:176:TRP:NE1	2.10	0.42
16:f:57:GLU:HG3	16:f:87:VAL:HG12	2.01	0.42
11:n:300:ASP:OD1	12:o:105:TYR:OH	2.22	0.42
11:n:331:SER:O	11:n:331:SER:OG	2.31	0.42
12:o:204:LEU:HD21	20:w:60:PRO:HD3	2.00	0.42
4:D:181:VAL:HG12	4:D:191:ILE:HG13	2.01	0.42
7:R:56:MET:HE3	7:R:56:MET:HB3	1.93	0.42
11:a:108:MET:HA	11:a:111:VAL:HG12	2.02	0.42
12:b:159:ARG:HB2	15:e:121:THR:HG21	2.01	0.42
12:o:46:TYR:HB3	12:o:92:ILE:HD11	2.01	0.42
15:r:86:LYS:HE3	25:r:201:PEF:HN2	1.84	0.42
3:C:362:TYR:HA	3:C:366:ILE:HB	2.01	0.42
5:E:116:VAL:HB	5:E:156:LEU:HD13	2.02	0.42
5:P:127:GLN:HA	5:P:130:ASN:HD22	1.84	0.42
13:p:15:HIS:CE1	13:p:17:VAL:HG12	2.53	0.42
16:s:90:LYS:HA	16:s:90:LYS:HD3	1.79	0.42
21:x:14:PRO:HG2	21:x:16:ASN:H	1.84	0.42
3:C:55:SER:OG	3:N:177:GLN:NE2	2.51	0.42
8:H:5:SER:OG	8:H:6:GLY:N	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:n:175:ASN:HD21	11:n:530:PRO:HB2	1.84	0.42
12:o:197:VAL:HG21	12:o:207:VAL:HB	2.00	0.42
3:C:150:LEU:HB3	3:C:292:VAL:HG11	2.02	0.42
3:N:29:TRP:NE1	27:N:607:PCF:O32	2.52	0.42
4:O:97:TYR:HA	4:O:101:CYS:HB2	2.00	0.42
22:l:23:ARG:HD2	22:l:23:ARG:HA	1.71	0.42
21:x:27:LYS:H	21:x:27:LYS:HG2	1.58	0.42
5:E:169:GLU:H	5:E:176:TRP:CD1	2.36	0.42
2:M:96:ASP:OD1	2:M:96:ASP:N	2.47	0.42
12:b:131:SER:OG	20:j:57:ALA:O	2.30	0.42
23:m:163:LEU:HD13	23:m:163:LEU:HA	1.94	0.42
11:n:309:THR:HG23	11:n:359:ALA:HB1	2.02	0.42
25:r:201:PEF:H351	25:r:201:PEF:H322	1.79	0.42
1:A:356:ILE:HD13	1:A:454:MET:HE2	2.01	0.42
1:L:47:HIS:ND1	2:M:330:GLU:OE2	2.34	0.42
5:P:176:TRP:CE3	5:P:186:ASP:HA	2.55	0.42
27:T:101:PCF:H132	27:T:101:PCF:H111	1.83	0.42
25:c:302:PEF:H11	21:k:115:LEU:HB3	2.01	0.42
12:o:152:LEU:H	12:o:152:LEU:HD23	1.85	0.42
13:p:219:LEU:HD21	13:p:250:THR:HG22	2.02	0.42
15:r:62:ASN:OD1	15:r:62:ASN:N	2.52	0.42
4:D:77:SER:O	9:I:47:LYS:NZ	2.53	0.42
5:P:47:ASN:HD21	8:S:33:ALA:HB1	1.85	0.42
13:c:219:LEU:HD22	13:c:253:LEU:HD12	2.01	0.42
25:n:606:PEF:H371	12:o:57:MET:HE1	2.02	0.42
21:x:60:LEU:O	21:x:64:ALA:CB	2.66	0.42
8:H:89:LEU:HA	8:H:92:VAL:HG12	2.01	0.42
3:N:87:SER:OG	3:N:273:TRP:NE1	2.41	0.42
4:O:181:VAL:HG12	4:O:191:ILE:HG13	2.01	0.42
5:P:121:ARG:HB2	5:P:151:GLN:HA	2.01	0.42
11:a:362:SER:HB3	12:b:103:LEU:HD22	2.02	0.42
15:e:106:LEU:HD23	15:e:106:LEU:HA	1.91	0.42
15:r:121:THR:HG23	15:r:126:TRP:CD1	2.54	0.42
19:v:53:GLU:HB2	19:v:56:LYS:C	2.45	0.42
21:x:50:MET:O	21:x:53:LYS:HB2	2.20	0.42
21:x:77:HIS:O	21:x:81:ARG:HB2	2.20	0.42
25:A:502:PEF:H201	25:A:502:PEF:H172	1.86	0.42
1:L:428:ASP:O	5:P:53:ARG:NH2	2.47	0.42
2:M:43:THR:OG1	2:M:44:LYS:N	2.52	0.42
3:N:20:SER:HA	3:N:21:PRO:HD3	1.89	0.42
5:P:57:TYR:HA	5:P:60:VAL:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:a:198:LEU:HA	13:c:100:LEU:HD13	2.02	0.42
11:n:499:GLU:HB3	14:q:135:TRP:CH2	2.54	0.42
9:I:26:PHE:HB2	10:J:43:VAL:HG22	2.01	0.41
1:L:72:LEU:HD23	1:L:72:LEU:HA	1.78	0.41
3:N:152:SER:OG	3:N:288:LYS:NZ	2.43	0.41
13:c:235:LEU:HD21	13:c:243:TYR:HB2	2.01	0.41
14:d:33:THR:HG21	14:d:49:PRO:HD3	2.02	0.41
12:o:154:GLU:H	12:o:154:GLU:CD	2.26	0.41
14:q:63:GLU:HG2	14:q:68:ARG:HB2	2.02	0.41
18:u:32:ASP:OD1	18:u:33:GLY:N	2.53	0.41
1:A:291:PHE:HZ	1:A:335:ARG:HH12	1.68	0.41
1:A:376:GLN:HE21	2:B:92:THR:HG21	1.84	0.41
3:C:247:SER:OG	3:C:250:THR:OG1	2.21	0.41
6:F:95:VAL:O	6:F:99:GLU:HG2	2.20	0.41
1:L:252:ARG:NH1	1:L:440:GLU:HB2	2.35	0.41
1:L:268:GLU:OE2	1:L:425:ARG:NE	2.44	0.41
4:O:62:MET:HB2	4:O:66:GLU:OE2	2.20	0.41
13:p:176:TRP:O	13:p:180:ILE:HG12	2.20	0.41
20:w:9:LEU:HD23	20:w:9:LEU:HA	1.89	0.41
1:A:297:LEU:HB3	2:B:65:LEU:HD12	2.02	0.41
3:C:183:HIS:HE1	26:C:601:HEM:NB	2.17	0.41
5:P:110:LYS:HE2	5:P:113:GLY:HA2	2.01	0.41
12:o:126:TRP:CD1	12:o:232:MET:HG2	2.55	0.41
25:r:201:PEF:H181	25:r:201:PEF:H151	1.88	0.41
1:A:67:ASN:HD22	1:A:181:THR:HG23	1.84	0.41
1:A:416:LYS:HE2	1:A:416:LYS:HB3	1.76	0.41
5:P:142:THR:HB	5:P:145:ASP:HB3	2.01	0.41
11:a:261:THR:HG21	11:a:395:TYR:CE1	2.56	0.41
11:n:381:LEU:HA	11:n:381:LEU:HD23	1.84	0.41
11:n:401:LEU:HD12	11:n:403:LEU:H	1.84	0.41
13:p:70:VAL:HG12	25:p:301:PEF:H31	2.02	0.41
13:p:153:THR:O	13:p:157:HIS:HB2	2.20	0.41
1:A:202:LEU:HD23	1:A:231:GLN:HB3	2.01	0.41
24:A:501:CDL:H551	27:I:101:PCF:H241	2.02	0.41
3:C:14:ASN:HA	3:C:18:ILE:HB	2.03	0.41
4:D:273:THR:HG22	25:E:302:PEF:O2	2.20	0.41
3:N:311:SER:HB2	3:N:371:SER:HB2	2.03	0.41
11:a:37:ARG:HE	11:a:455:SER:HB3	1.85	0.41
14:d:96:ASP:OD1	14:d:96:ASP:N	2.54	0.41
19:i:9:THR:O	19:i:13:ARG:HB2	2.20	0.41
20:j:27:CYS:HB2	20:j:59:CYS:HB2	1.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:m:199:GLU:HG3	23:m:200:ARG:N	2.35	0.41
20:w:37:CYS:HB3	20:w:41:LYS:HD2	2.01	0.41
3:C:166:TRP:O	3:C:175:THR:OG1	2.33	0.41
5:E:87:ASP:N	5:E:87:ASP:OD1	2.50	0.41
3:N:183:HIS:HE1	26:N:601:HEM:C1B	2.38	0.41
24:N:604:CDL:H331	24:N:604:CDL:H361	1.77	0.41
9:T:49:TRP:HE1	10:U:74:ASP:CG	2.28	0.41
12:o:147:VAL:HG11	12:o:231:ASN:HB2	2.02	0.41
12:o:167:MET:HE1	12:o:188:PHE:HZ	1.85	0.41
12:o:243:LYS:HG2	12:o:246:GLU:OE2	2.20	0.41
5:E:116:VAL:HG23	5:E:155:MET:C	2.46	0.41
3:N:111:VAL:HG13	3:N:306:PRO:HG2	2.03	0.41
8:S:57:LEU:HD23	8:S:57:LEU:HA	1.93	0.41
25:b:303:PEF:H112	25:b:303:PEF:H141	1.82	0.41
13:c:4:LEU:HB2	21:k:17:ALA:HB1	2.02	0.41
11:n:195:LEU:O	11:n:199:SER:OG	2.24	0.41
23:z:198:GLU:O	23:z:202:GLU:HB2	2.20	0.41
3:C:236:PHE:HD1	24:C:603:CDL:H382	1.86	0.41
5:E:121:ARG:HH11	5:E:150:PRO:HA	1.84	0.41
11:a:2:VAL:O	11:a:6:LEU:HB2	2.21	0.41
25:a:606:PEF:H152	13:c:26:VAL:HG11	2.02	0.41
21:k:110:ASP:OD1	21:k:113:LYS:NZ	2.54	0.41
11:n:327:ILE:HD12	11:n:338:MET:HE1	2.02	0.41
31:n:602:HEA:H202	31:n:602:HEA:H171	1.68	0.41
12:o:244:PHE:HB3	12:o:245:LEU:HD12	2.03	0.41
13:p:53:LEU:HD11	17:t:36:ILE:HG23	2.03	0.41
23:z:145:GLN:O	23:z:148:VAL:HB	2.21	0.41
1:A:265:VAL:HG12	1:A:431:ILE:HG22	2.02	0.41
2:B:193:VAL:HG12	2:B:196:ASP:H	1.85	0.41
25:E:304:PEF:H142	25:E:304:PEF:H171	1.98	0.41
5:P:166:PRO:HA	5:P:178:CYS:HA	2.03	0.41
5:P:207:PHE:HA	5:P:211:LYS:O	2.21	0.41
9:T:17:PHE:O	9:T:21:ILE:HG12	2.20	0.41
9:T:23:ALA:HB2	10:U:39:LEU:HD23	2.01	0.41
20:j:49:LYS:HA	20:j:52:TRP:HB3	2.02	0.41
11:n:102:ALA:O	11:n:157:SER:OG	2.36	0.41
11:n:298:ASP:HB2	11:n:301:THR:H	1.86	0.41
14:q:102:SER:HB3	14:q:107:ARG:HD2	2.02	0.41
15:r:111:ARG:HD2	15:r:111:ARG:HA	1.86	0.41
15:r:134:LEU:HD23	15:r:134:LEU:HA	1.88	0.41
20:w:17:ARG:HG3	20:w:18:PHE:CD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:GLU:HB3	1:A:211:THR:HG22	2.02	0.41
1:A:300:ILE:HG22	1:A:302:LEU:H	1.86	0.41
2:B:49:HIS:CD2	2:B:161:TYR:H	2.38	0.41
2:M:54:PHE:CZ	2:M:114:PHE:HA	2.56	0.41
4:O:304:PRO:HA	4:O:305:PRO:HD3	1.85	0.41
9:T:30:THR:OG1	10:U:46:GLU:OE2	2.39	0.41
13:c:159:LEU:HD13	13:c:230:MET:HE2	2.02	0.41
21:x:85:LYS:HD3	21:x:92:TRP:CE3	2.56	0.41
22:y:47:LEU:HD12	22:y:47:LEU:HA	1.91	0.41
1:A:40:THR:OG1	1:A:216:HIS:ND1	2.39	0.40
4:D:70:HIS:HE1	4:D:185:HIS:HE1	1.68	0.40
4:D:181:VAL:HG21	4:D:256:ASN:HA	2.03	0.40
2:M:250:LEU:HD11	2:M:278:LYS:HG2	2.03	0.40
4:O:306:LYS:HA	4:O:307:PRO:HD3	1.89	0.40
13:c:50:MET:HE1	17:g:40:ALA:HA	2.01	0.40
13:c:198:ASP:HA	21:k:100:ASN:H	1.86	0.40
13:c:260:LEU:O	13:c:264:PHE:HB2	2.21	0.40
19:i:2:THR:OG1	19:i:3:ILE:N	2.55	0.40
11:n:320:ILE:HD13	11:n:349:THR:HG22	2.03	0.40
11:n:374:VAL:HA	11:n:377:PHE:CE2	2.56	0.40
12:o:108:ASP:OD1	12:o:109:GLU:N	2.55	0.40
12:o:214:GLU:H	12:o:214:GLU:HG3	1.68	0.40
3:C:370:ILE:HD13	3:C:370:ILE:HA	1.92	0.40
1:L:70:SER:HB3	1:L:97:ILE:HD12	2.03	0.40
2:M:83:ASP:N	2:M:83:ASP:OD1	2.54	0.40
3:N:124:THR:HG22	3:N:190:ILE:HD13	2.03	0.40
10:U:68:ASP:HB3	10:U:70:THR:HG23	2.03	0.40
14:d:60:LEU:HD23	14:d:60:LEU:HA	1.88	0.40
11:n:178:THR:OG1	11:n:181:LYS:NZ	2.40	0.40
11:n:379:TYR:O	11:n:383:MET:HB2	2.22	0.40
12:o:208:SER:OG	12:o:209:ALA:N	2.54	0.40
23:z:168:LEU:O	23:z:172:GLU:HG3	2.21	0.40
2:B:289:VAL:HG12	2:B:297:VAL:HG23	2.03	0.40
3:C:247:SER:OG	3:C:247:SER:O	2.36	0.40
7:G:55:ILE:HD13	7:G:55:ILE:HA	1.93	0.40
1:L:428:ASP:OD1	1:L:449:ARG:NH2	2.55	0.40
2:M:140:LYS:HB3	2:M:140:LYS:HE3	1.84	0.40
25:N:606:PEF:H251	25:N:606:PEF:H221	1.93	0.40
21:k:89:ASP:HB2	21:k:125:ILE:HG12	2.02	0.40
23:m:110:GLU:HA	23:m:113:SER:HB3	2.02	0.40
11:n:323:TRP:O	11:n:327:ILE:HG12	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:ILE:HG23	1:A:397:LYS:HG3	2.03	0.40
3:C:69:MET:HE1	3:C:80:TYR:CZ	2.57	0.40
6:F:122:ASP:OD1	6:F:122:ASP:N	2.54	0.40
7:G:66:ASP:OD1	7:G:66:ASP:N	2.54	0.40
1:L:219:LEU:HD12	1:L:219:LEU:HA	1.95	0.40
2:M:117:HIS:HA	2:M:120:THR:HG22	2.03	0.40
4:O:297:THR:OG1	8:S:34:GLN:NE2	2.48	0.40
5:P:71:ALA:HA	5:P:74:THR:HG22	2.04	0.40
11:a:436:MET:HA	11:a:437:PRO:HD3	1.93	0.40
14:d:72:LEU:HD23	14:d:72:LEU:HA	1.95	0.40
11:n:86:LEU:HA	11:n:527:PHE:HE2	1.87	0.40
11:n:261:THR:HG21	11:n:395:TYR:CE1	2.56	0.40
13:p:157:HIS:HA	13:p:160:ILE:HG22	2.03	0.40
20:w:37:CYS:O	20:w:40:MET:N	2.42	0.40
21:x:42:LYS:HE2	21:x:42:LYS:HB2	1.92	0.40
5:E:107:VAL:HB	5:E:118:ILE:HG23	2.03	0.40
5:E:141:GLN:OE1	5:E:199:ASN:ND2	2.54	0.40
7:G:18:SER:HB3	7:G:21:LEU:HB2	2.03	0.40
2:M:105:LEU:HD23	2:M:105:LEU:HA	1.88	0.40
13:c:253:LEU:HD23	13:c:256:ILE:HD11	2.04	0.40
11:n:31:ALA:HB3	18:u:64:PRO:HG2	2.04	0.40
21:x:112:ASP:OD1	21:x:112:ASP:N	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	429/431 (100%)	401 (94%)	28 (6%)	0	100	100
1	L	429/431 (100%)	409 (95%)	20 (5%)	0	100	100
2	B	350/352 (99%)	329 (94%)	21 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	M	350/352 (99%)	328 (94%)	22 (6%)	0	100	100
3	C	383/385 (100%)	370 (97%)	13 (3%)	0	100	100
3	N	383/385 (100%)	373 (97%)	10 (3%)	0	100	100
4	D	245/248 (99%)	238 (97%)	7 (3%)	0	100	100
4	O	245/248 (99%)	240 (98%)	5 (2%)	0	100	100
5	E	183/185 (99%)	157 (86%)	26 (14%)	0	100	100
5	P	183/185 (99%)	149 (81%)	33 (18%)	1 (0%)	24	55
6	F	73/147 (50%)	67 (92%)	6 (8%)	0	100	100
6	Q	73/147 (50%)	71 (97%)	2 (3%)	0	100	100
7	G	124/127 (98%)	120 (97%)	4 (3%)	0	100	100
7	R	124/127 (98%)	121 (98%)	3 (2%)	0	100	100
8	H	91/94 (97%)	84 (92%)	7 (8%)	0	100	100
8	S	91/94 (97%)	88 (97%)	3 (3%)	0	100	100
9	I	55/66 (83%)	55 (100%)	0	0	100	100
9	T	55/66 (83%)	54 (98%)	1 (2%)	0	100	100
10	J	74/77 (96%)	70 (95%)	4 (5%)	0	100	100
10	U	74/77 (96%)	72 (97%)	2 (3%)	0	100	100
11	a	532/534 (100%)	504 (95%)	27 (5%)	1 (0%)	43	72
11	n	532/534 (100%)	502 (94%)	28 (5%)	2 (0%)	30	60
12	b	234/236 (99%)	215 (92%)	19 (8%)	0	100	100
12	o	234/236 (99%)	206 (88%)	28 (12%)	0	100	100
13	c	267/269 (99%)	260 (97%)	7 (3%)	0	100	100
13	p	267/269 (99%)	263 (98%)	4 (2%)	0	100	100
14	d	118/130 (91%)	98 (83%)	20 (17%)	0	100	100
14	q	119/130 (92%)	101 (85%)	16 (13%)	2 (2%)	7	25
15	e	131/134 (98%)	122 (93%)	9 (7%)	0	100	100
15	r	131/134 (98%)	115 (88%)	15 (12%)	1 (1%)	16	44
16	f	100/108 (93%)	94 (94%)	6 (6%)	0	100	100
16	s	100/108 (93%)	94 (94%)	6 (6%)	0	100	100
17	g	57/59 (97%)	55 (96%)	2 (4%)	0	100	100
17	t	57/59 (97%)	53 (93%)	4 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	h	49/51 (96%)	47 (96%)	2 (4%)	0	100	100
18	u	49/51 (96%)	44 (90%)	5 (10%)	0	100	100
19	i	53/55 (96%)	51 (96%)	2 (4%)	0	100	100
19	v	53/55 (96%)	47 (89%)	6 (11%)	0	100	100
20	j	73/82 (89%)	68 (93%)	5 (7%)	0	100	100
20	w	73/82 (89%)	62 (85%)	9 (12%)	2 (3%)	4	15
21	k	111/131 (85%)	104 (94%)	7 (6%)	0	100	100
21	x	111/131 (85%)	95 (86%)	16 (14%)	0	100	100
22	l	43/66 (65%)	41 (95%)	2 (5%)	0	100	100
22	y	43/66 (65%)	38 (88%)	5 (12%)	0	100	100
23	m	97/224 (43%)	90 (93%)	7 (7%)	0	100	100
23	z	97/224 (43%)	87 (90%)	7 (7%)	3 (3%)	3	12
All	All	7745/8382 (92%)	7252 (94%)	481 (6%)	12 (0%)	44	72

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	P	187	ILE
11	n	120	GLU
11	n	521	PRO
20	w	10	HIS
23	z	173	ASN
11	a	521	PRO
20	w	44	ASP
23	z	179	LYS
14	q	30	VAL
23	z	200	ARG
15	r	39	PRO
14	q	77	GLY

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	370/370 (100%)	370 (100%)	0	100	100
1	L	370/370 (100%)	370 (100%)	0	100	100
2	B	301/301 (100%)	301 (100%)	0	100	100
2	M	301/301 (100%)	301 (100%)	0	100	100
3	C	338/338 (100%)	338 (100%)	0	100	100
3	N	338/338 (100%)	338 (100%)	0	100	100
4	D	205/206 (100%)	205 (100%)	0	100	100
4	O	205/206 (100%)	205 (100%)	0	100	100
5	E	151/151 (100%)	148 (98%)	3 (2%)	48	80
5	P	151/151 (100%)	149 (99%)	2 (1%)	61	86
6	F	68/131 (52%)	68 (100%)	0	100	100
6	Q	68/131 (52%)	67 (98%)	1 (2%)	57	84
7	G	110/111 (99%)	110 (100%)	0	100	100
7	R	110/111 (99%)	110 (100%)	0	100	100
8	H	77/78 (99%)	77 (100%)	0	100	100
8	S	77/78 (99%)	77 (100%)	0	100	100
9	I	47/54 (87%)	47 (100%)	0	100	100
9	T	47/54 (87%)	47 (100%)	0	100	100
10	J	65/66 (98%)	65 (100%)	0	100	100
10	U	65/66 (98%)	65 (100%)	0	100	100
11	a	447/447 (100%)	447 (100%)	0	100	100
11	n	447/447 (100%)	447 (100%)	0	100	100
12	b	209/209 (100%)	209 (100%)	0	100	100
12	o	209/209 (100%)	209 (100%)	0	100	100
13	c	228/228 (100%)	228 (100%)	0	100	100
13	p	228/228 (100%)	226 (99%)	2 (1%)	70	89
14	d	101/111 (91%)	101 (100%)	0	100	100
14	q	102/111 (92%)	102 (100%)	0	100	100
15	e	114/115 (99%)	114 (100%)	0	100	100
15	r	114/115 (99%)	114 (100%)	0	100	100
16	f	91/96 (95%)	91 (100%)	0	100	100
16	s	91/96 (95%)	91 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	g	50/50 (100%)	50 (100%)	0	100	100
17	t	50/50 (100%)	50 (100%)	0	100	100
18	h	41/41 (100%)	41 (100%)	0	100	100
18	u	41/41 (100%)	41 (100%)	0	100	100
19	i	46/46 (100%)	46 (100%)	0	100	100
19	v	46/46 (100%)	46 (100%)	0	100	100
20	j	67/73 (92%)	67 (100%)	0	100	100
20	w	67/73 (92%)	63 (94%)	4 (6%)	17	47
21	k	99/113 (88%)	99 (100%)	0	100	100
21	x	99/113 (88%)	98 (99%)	1 (1%)	68	88
22	l	36/53 (68%)	36 (100%)	0	100	100
22	y	36/53 (68%)	36 (100%)	0	100	100
23	m	84/191 (44%)	84 (100%)	0	100	100
23	z	84/191 (44%)	83 (99%)	1 (1%)	63	87
All	All	6691/7158 (94%)	6677 (100%)	14 (0%)	85	96

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	E	116	VAL
5	E	180	CYS
5	E	214	VAL
5	P	109	VAL
5	P	116	VAL
6	Q	75	THR
13	p	98	GLU
13	p	195	THR
20	w	32	VAL
20	w	37	CYS
20	w	38	VAL
20	w	48	CYS
21	x	73	VAL
23	z	113	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (142) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	63	ASN
1	A	67	ASN
1	A	171	ASN
1	A	187	ASN
1	A	231	GLN
1	A	274	ASN
1	A	283	GLN
1	A	298	GLN
1	A	317	HIS
1	A	352	ASN
1	A	385	ASN
1	A	388	ASN
2	B	58	ASN
2	B	103	ASN
2	B	136	GLN
2	B	157	ASN
2	B	329	ASN
2	B	352	ASN
2	B	361	ASN
3	C	22	GLN
3	C	138	GLN
3	C	173	ASN
3	C	177	GLN
3	C	208	ASN
3	C	215	ASN
3	C	253	HIS
3	C	256	ASN
3	C	343	HIS
3	C	375	ASN
4	D	79	ASN
4	D	127	ASN
4	D	185	HIS
4	D	213	ASN
4	D	256	ASN
5	E	97	ASN
5	E	141	GLN
5	E	184	HIS
5	E	199	ASN
6	F	87	ASN
6	F	110	GLN
7	G	30	ASN
8	H	34	GLN

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Mol	Chain	Res	Type
8	H	77	ASN
9	I	42	ASN
9	I	44	ASN
10	J	29	ASN
1	L	75	ASN
1	L	156	HIS
1	L	171	ASN
1	L	199	ASN
1	L	274	ASN
1	L	283	GLN
1	L	298	GLN
1	L	317	HIS
1	L	388	ASN
2	M	49	HIS
2	M	52	ASN
2	M	58	ASN
2	M	103	ASN
2	M	191	ASN
2	M	325	ASN
2	M	361	ASN
3	N	173	ASN
3	N	177	GLN
3	N	253	HIS
3	N	256	ASN
3	N	332	ASN
3	N	384	ASN
4	O	78	HIS
4	O	79	ASN
4	O	127	ASN
4	O	169	ASN
5	P	47	ASN
5	P	106	ASN
5	P	112	GLN
5	P	130	ASN
5	P	199	ASN
6	Q	87	ASN
6	Q	96	HIS
7	R	30	ASN
8	S	34	GLN
8	S	77	ASN
9	T	44	ASN
10	U	6	HIS

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Mol	Chain	Res	Type
11	a	215	ASN
11	a	257	HIS
11	a	406	ASN
11	a	478	ASN
11	a	482	ASN
11	a	486	ASN
11	a	528	ASN
12	b	135	ASN
12	b	157	GLN
12	b	205	ASN
12	b	212	GLN
12	b	249	ASN
13	c	11	GLN
13	c	141	ASN
13	c	165	ASN
13	c	185	GLN
14	d	41	ASN
14	d	119	HIS
15	e	84	HIS
18	h	29	HIS
18	h	37	ASN
18	h	53	HIS
19	i	42	ASN
21	k	43	HIS
21	k	83	HIS
22	l	42	GLN
23	m	115	ASN
23	m	173	ASN
11	n	51	ASN
11	n	164	ASN
11	n	399	GLN
11	n	482	ASN
12	o	33	GLN
12	o	40	HIS
12	o	123	GLN
12	o	251	GLN
13	p	141	ASN
13	p	226	ASN
13	p	232	ASN
13	p	234	HIS
14	q	129	ASN
15	r	19	GLN

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Mol	Chain	Res	Type
15	r	127	GLN
15	r	149	GLN
16	s	133	GLN
18	u	37	ASN
20	w	23	GLN
20	w	70	GLN
21	x	16	ASN
21	x	43	HIS
21	x	49	ASN
21	x	124	HIS
22	y	42	GLN
23	z	115	ASN
23	z	136	ASN
23	z	155	GLN
23	z	190	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 63 ligands modelled in this entry, 8 are monoatomic - leaving 55 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	PEF	E	303	-	39,39,46	1.01	2 (5%)	42,44,51	1.25	3 (7%)
25	PEF	r	201	-	40,40,46	0.99	2 (5%)	43,45,51	1.14	3 (6%)
24	CDL	H	101	-	52,52,99	1.22	4 (7%)	58,64,111	1.34	9 (15%)
25	PEF	n	606	-	46,46,46	0.95	2 (4%)	49,51,51	1.16	4 (8%)
25	PEF	S	102	-	35,35,46	1.06	2 (5%)	38,40,51	1.23	3 (7%)
25	PEF	H	102	-	31,31,46	1.11	2 (6%)	34,36,51	1.35	4 (11%)
24	CDL	L	501	-	54,54,99	1.13	4 (7%)	60,66,111	1.29	5 (8%)
25	PEF	N	606	-	42,42,46	0.94	2 (4%)	45,47,51	1.20	4 (8%)
27	PCF	I	101	-	29,29,49	1.28	2 (6%)	35,37,57	1.31	4 (11%)
24	CDL	C	603	-	65,65,99	1.12	4 (6%)	71,77,111	1.39	8 (11%)
31	HEA	n	602	11	67,67,67	2.25	24 (35%)	81,103,103	2.59	39 (48%)
25	PEF	n	607	-	32,32,46	1.14	2 (6%)	35,37,51	1.21	4 (11%)
34	CUA	o	301	12	0,1,1	-	-	-	-	-
27	PCF	H	103	-	31,31,49	1.18	2 (6%)	37,39,57	1.20	4 (10%)
26	HEM	C	602	3	50,50,50	1.80	11 (22%)	67,82,82	1.73	17 (25%)
25	PEF	C	604	-	43,43,46	0.98	2 (4%)	46,48,51	1.11	3 (6%)
27	PCF	T	101	-	46,46,49	1.00	2 (4%)	52,54,57	1.15	4 (7%)
25	PEF	L	502	-	30,30,46	1.16	2 (6%)	33,35,51	1.22	4 (12%)
31	HEA	a	603	11	67,67,67	2.24	23 (34%)	81,103,103	2.53	35 (43%)
25	PEF	C	605	-	38,38,46	1.02	2 (5%)	41,43,51	1.10	2 (4%)
25	PEF	J	101	-	28,28,46	1.23	2 (7%)	31,33,51	1.28	3 (9%)
27	PCF	e	202	-	35,35,49	1.16	2 (5%)	41,43,57	1.18	3 (7%)
25	PEF	l	101	-	32,32,46	1.11	2 (6%)	35,37,51	1.30	5 (14%)
26	HEM	N	601	3	50,50,50	1.75	12 (24%)	67,82,82	1.94	12 (17%)
27	PCF	C	606	-	38,38,49	1.06	2 (5%)	44,46,57	1.32	6 (13%)
25	PEF	O	402	-	42,42,46	1.00	2 (4%)	45,47,51	1.10	3 (6%)
27	PCF	N	607	-	49,49,49	0.93	3 (6%)	55,57,57	1.17	4 (7%)
25	PEF	c	301	-	35,35,46	1.06	2 (5%)	38,40,51	1.14	3 (7%)
25	PEF	o	302	-	39,39,46	1.05	2 (5%)	42,44,51	1.10	4 (9%)
24	CDL	N	604	-	74,74,99	1.05	5 (6%)	80,86,111	1.20	6 (7%)
25	PEF	c	302	-	33,33,46	1.12	2 (6%)	36,38,51	1.07	2 (5%)
28	HEC	O	401	4	46,50,50	2.51	23 (50%)	58,82,82	2.17	19 (32%)
24	CDL	D	402	-	70,70,99	1.03	5 (7%)	76,82,111	1.26	7 (9%)
25	PEF	b	302	-	39,39,46	1.01	2 (5%)	42,44,51	1.13	3 (7%)
25	PEF	a	606	-	32,32,46	1.15	2 (6%)	35,37,51	1.09	3 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	PEF	b	303	-	39,39,46	1.04	2 (5%)	42,44,51	1.10	3 (7%)
26	HEM	N	602	3	50,50,50	1.80	12 (24%)	67,82,82	1.73	14 (20%)
29	FES	P	301	5	0,4,4	-	-	-	-	-
25	PEF	E	304	-	33,33,46	1.09	2 (6%)	36,38,51	1.27	5 (13%)
25	PEF	p	301	-	35,35,46	1.10	3 (8%)	38,40,51	1.13	3 (7%)
31	HEA	n	603	11	67,67,67	2.30	24 (35%)	81,103,103	2.57	32 (39%)
28	HEC	D	401	4	46,50,50	2.52	23 (50%)	58,82,82	2.13	18 (31%)
25	PEF	e	201	-	40,40,46	0.97	3 (7%)	43,45,51	1.37	5 (11%)
34	CUA	b	301	12	0,1,1	-	-	-	-	-
26	HEM	C	601	3	50,50,50	1.81	11 (22%)	67,82,82	1.86	15 (22%)
25	PEF	A	502	-	35,35,46	1.07	2 (5%)	38,40,51	1.16	3 (7%)
25	PEF	n	608	-	32,32,46	1.14	2 (6%)	35,37,51	1.13	2 (5%)
31	HEA	a	602	11	67,67,67	2.23	24 (35%)	81,103,103	2.80	40 (49%)
24	CDL	N	603	-	52,52,99	1.23	5 (9%)	58,64,111	1.45	8 (13%)
24	CDL	S	101	-	47,47,99	1.31	4 (8%)	53,59,111	1.44	9 (16%)
25	PEF	E	302	-	41,41,46	1.01	2 (4%)	44,46,51	1.10	3 (6%)
29	FES	E	301	5	0,4,4	-	-	-	-	-
27	PCF	r	202	-	35,35,49	1.15	2 (5%)	41,43,57	1.04	3 (7%)
25	PEF	N	605	-	39,39,46	1.01	2 (5%)	42,44,51	1.17	3 (7%)
24	CDL	A	501	-	57,57,99	1.18	4 (7%)	63,69,111	1.42	8 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	PEF	E	303	-	-	19/43/43/50	-
25	PEF	r	201	-	-	15/44/44/50	-
24	CDL	H	101	-	-	28/63/63/110	-
25	PEF	n	606	-	-	18/50/50/50	-
25	PEF	S	102	-	-	11/39/39/50	-
25	PEF	H	102	-	-	9/35/35/50	-
24	CDL	L	501	-	-	31/64/64/110	-
25	PEF	N	606	-	-	11/46/46/50	-
27	PCF	I	101	-	-	5/33/33/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CDL	C	603	-	-	26/76/76/110	-
31	HEA	n	602	11	-	9/36/76/76	-
25	PEF	n	607	-	-	16/36/36/50	-
27	PCF	H	103	-	-	16/35/35/53	-
26	HEM	C	602	3	-	6/14/54/54	-
25	PEF	C	604	-	-	15/47/47/50	-
27	PCF	T	101	-	-	4/50/50/53	-
25	PEF	L	502	-	-	17/34/34/50	-
31	HEA	a	603	11	-	7/36/76/76	-
25	PEF	C	605	-	-	9/42/42/50	-
25	PEF	J	101	-	-	12/32/32/50	-
27	PCF	e	202	-	-	11/39/39/53	-
25	PEF	l	101	-	-	6/36/36/50	-
26	HEM	N	601	3	-	8/14/54/54	-
27	PCF	C	606	-	-	19/42/42/53	-
25	PEF	O	402	-	-	20/46/46/50	-
27	PCF	N	607	-	-	21/53/53/53	-
25	PEF	c	301	-	-	9/39/39/50	-
25	PEF	o	302	-	-	14/43/43/50	-
24	CDL	N	604	-	-	33/85/85/110	-
25	PEF	c	302	-	-	14/37/37/50	-
28	HEC	O	401	4	-	3/14/54/54	-
24	CDL	D	402	-	-	22/81/81/110	-
25	PEF	b	302	-	-	15/43/43/50	-
25	PEF	a	606	-	-	12/36/36/50	-
25	PEF	b	303	-	-	16/43/43/50	-
26	HEM	N	602	3	-	6/14/54/54	-
29	FES	P	301	5	-	-	0/1/1/1
25	PEF	E	304	-	-	16/37/37/50	-
25	PEF	p	301	-	-	11/39/39/50	-
31	HEA	n	603	11	-	6/36/76/76	-
28	HEC	D	401	4	-	1/14/54/54	-
25	PEF	e	201	-	-	17/44/44/50	-
26	HEM	C	601	3	-	10/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	PEF	A	502	-	-	10/39/39/50	-
25	PEF	n	608	-	-	7/36/36/50	-
31	HEA	a	602	11	-	10/36/76/76	-
24	CDL	N	603	-	-	22/63/63/110	-
24	CDL	S	101	-	-	16/58/58/110	-
25	PEF	E	302	-	-	19/45/45/50	-
29	FES	E	301	5	-	-	0/1/1/1
27	PCF	r	202	-	-	11/39/39/53	-
25	PEF	N	605	-	-	19/43/43/50	-
24	CDL	A	501	-	-	25/68/68/110	-

All (291) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	n	603	HEA	FE-NB	5.09	2.10	1.94
31	n	602	HEA	FE-NB	5.08	2.10	1.94
31	n	603	HEA	FE-ND	5.06	2.10	1.94
28	O	401	HEC	CHD-C4C	5.06	1.48	1.38
31	a	603	HEA	FE-ND	5.03	2.10	1.94
31	a	603	HEA	FE-NB	4.99	2.10	1.94
31	a	602	HEA	FE-NB	4.99	2.10	1.94
31	a	602	HEA	FE-ND	4.97	2.10	1.94
26	N	601	HEM	FE-NB	4.95	2.10	1.94
31	n	602	HEA	FE-ND	4.95	2.10	1.94
31	a	603	HEA	C3B-C2B	4.95	1.46	1.34
26	C	601	HEM	FE-NB	4.92	2.10	1.94
31	n	603	HEA	C3B-C2B	4.91	1.45	1.34
31	n	602	HEA	C3B-C2B	4.78	1.45	1.34
26	N	602	HEM	FE-NB	4.74	2.09	1.94
28	D	401	HEC	CHD-C4C	4.65	1.47	1.38
26	C	602	HEM	FE-NB	4.65	2.09	1.94
31	n	603	HEA	C3D-C2D	4.63	1.46	1.36
31	a	603	HEA	C3D-C2D	4.61	1.46	1.36
28	D	401	HEC	CAC-C3C	4.58	1.49	1.35
28	D	401	HEC	CHC-C4B	4.54	1.47	1.38
31	n	603	HEA	FE-NC	4.52	2.10	1.95
28	O	401	HEC	CAC-C3C	4.51	1.49	1.35
28	O	401	HEC	CHC-C4B	4.49	1.47	1.38
31	a	603	HEA	FE-NC	4.40	2.09	1.95
28	D	401	HEC	C2A-C3A	4.39	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	a	602	HEA	C3B-C2B	4.37	1.44	1.34
28	D	401	HEC	CHA-C1A	4.36	1.46	1.38
31	n	602	HEA	C3D-C2D	4.35	1.46	1.36
25	b	303	PEF	O2-C10	4.34	1.46	1.34
25	J	101	PEF	O3-C30	4.32	1.45	1.33
25	E	303	PEF	O3-C30	4.31	1.45	1.33
31	n	602	HEA	FE-NC	4.29	2.09	1.95
31	a	602	HEA	FE-NC	4.29	2.09	1.95
31	n	603	HEA	C3A-C2A	4.29	1.47	1.37
31	a	602	HEA	C3D-C2D	4.27	1.46	1.36
24	S	101	CDL	OA6-CA5	4.27	1.46	1.34
27	r	202	PCF	O31-C31	4.27	1.45	1.33
28	O	401	HEC	C2A-C3A	4.27	1.46	1.36
24	N	604	CDL	OB8-CB7	4.26	1.45	1.33
26	C	602	HEM	C1B-NB	-4.25	1.32	1.40
25	E	302	PEF	O2-C10	4.25	1.46	1.34
28	O	401	HEC	CHA-C1A	4.25	1.46	1.38
26	N	602	HEM	C1B-NB	-4.24	1.32	1.40
31	n	602	HEA	CHC-C4B	4.23	1.47	1.38
25	C	605	PEF	O2-C10	4.23	1.46	1.34
24	S	101	CDL	OB8-CB7	4.22	1.45	1.33
24	H	101	CDL	OB8-CB7	4.22	1.45	1.33
24	A	501	CDL	OA8-CA7	4.21	1.45	1.33
25	n	607	PEF	O3-C30	4.19	1.45	1.33
27	e	202	PCF	O31-C31	4.18	1.45	1.33
25	p	301	PEF	O3-C30	4.18	1.45	1.33
26	C	602	HEM	C4D-ND	-4.18	1.33	1.40
25	o	302	PEF	O3-C30	4.18	1.45	1.33
31	a	602	HEA	C11-C3B	-4.18	1.46	1.51
27	H	103	PCF	O31-C31	4.16	1.45	1.33
25	a	606	PEF	O3-C30	4.16	1.45	1.33
25	L	502	PEF	O3-C30	4.15	1.45	1.33
28	O	401	HEC	CAB-C3B	4.15	1.48	1.35
25	o	302	PEF	O2-C10	4.15	1.46	1.34
25	b	302	PEF	O3-C30	4.14	1.45	1.33
25	O	402	PEF	O2-C10	4.14	1.46	1.34
25	c	302	PEF	O2-C10	4.14	1.46	1.34
27	I	101	PCF	O31-C31	4.14	1.45	1.33
31	a	603	HEA	CHD-C1D	4.14	1.46	1.38
31	n	603	HEA	CHD-C1D	4.13	1.46	1.38
25	n	607	PEF	O2-C10	4.13	1.45	1.34
24	C	603	CDL	OA6-CA5	4.13	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	D	401	HEC	CAB-C3B	4.12	1.48	1.35
25	S	102	PEF	O2-C10	4.12	1.45	1.34
24	C	603	CDL	OB6-CB5	4.12	1.45	1.34
25	c	302	PEF	O3-C30	4.12	1.45	1.33
25	r	201	PEF	O3-C30	4.12	1.45	1.33
25	n	606	PEF	O2-C10	4.11	1.45	1.34
25	E	304	PEF	O2-C10	4.10	1.45	1.34
25	n	606	PEF	O3-C30	4.10	1.45	1.33
24	C	603	CDL	OA8-CA7	4.09	1.45	1.33
25	N	605	PEF	O2-C10	4.09	1.45	1.34
24	A	501	CDL	OA6-CA5	4.08	1.45	1.34
24	S	101	CDL	OB6-CB5	4.07	1.45	1.34
25	n	608	PEF	O3-C30	4.06	1.45	1.33
25	b	303	PEF	O3-C30	4.05	1.45	1.33
25	O	402	PEF	O3-C30	4.04	1.45	1.33
25	J	101	PEF	O2-C10	4.04	1.45	1.34
25	C	604	PEF	O2-C10	4.04	1.45	1.34
31	a	602	HEA	C3A-C2A	4.04	1.46	1.37
24	L	501	CDL	OA6-CA5	4.04	1.45	1.34
25	n	608	PEF	O2-C10	4.04	1.45	1.34
25	A	502	PEF	O3-C30	4.03	1.45	1.33
25	C	604	PEF	O3-C30	4.03	1.45	1.33
31	a	602	HEA	CHC-C4B	4.02	1.46	1.38
25	E	302	PEF	O3-C30	4.02	1.45	1.33
24	A	501	CDL	OB8-CB7	4.01	1.45	1.33
28	O	401	HEC	CHB-C4A	4.00	1.46	1.38
27	I	101	PCF	O21-C21	4.00	1.45	1.34
25	A	502	PEF	O2-C10	4.00	1.45	1.34
31	n	603	HEA	CHB-C4A	3.99	1.46	1.38
25	b	302	PEF	O2-C10	3.99	1.45	1.34
24	N	603	CDL	OB6-CB5	3.98	1.45	1.34
27	e	202	PCF	O21-C21	3.98	1.45	1.34
24	L	501	CDL	OB8-CB7	3.97	1.44	1.33
31	n	602	HEA	C3A-C2A	3.96	1.46	1.37
31	a	603	HEA	C3A-C2A	3.96	1.46	1.37
27	H	103	PCF	O21-C21	3.96	1.45	1.34
25	H	102	PEF	O2-C10	3.96	1.45	1.34
31	n	602	HEA	CHD-C1D	3.95	1.46	1.38
26	C	601	HEM	C1B-NB	-3.95	1.33	1.40
24	H	101	CDL	OA6-CA5	3.94	1.45	1.34
28	D	401	HEC	CHB-C4A	3.94	1.46	1.38
27	r	202	PCF	O21-C21	3.94	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	C	606	PCF	O21-C21	3.94	1.45	1.34
25	a	606	PEF	O2-C10	3.94	1.45	1.34
25	c	301	PEF	O3-C30	3.93	1.44	1.33
26	N	602	HEM	C4D-ND	-3.93	1.33	1.40
24	N	603	CDL	OA8-CA7	3.92	1.44	1.33
25	l	101	PEF	O2-C10	3.92	1.45	1.34
25	L	502	PEF	O2-C10	3.91	1.45	1.34
31	a	603	HEA	CHC-C4B	3.90	1.46	1.38
25	c	301	PEF	O2-C10	3.89	1.45	1.34
27	T	101	PCF	O21-C21	3.89	1.45	1.34
31	a	602	HEA	CHD-C1D	3.89	1.46	1.38
24	L	501	CDL	OB6-CB5	3.88	1.45	1.34
27	T	101	PCF	O31-C31	3.88	1.44	1.33
25	H	102	PEF	O3-C30	3.88	1.44	1.33
24	H	101	CDL	OB6-CB5	3.88	1.45	1.34
25	N	605	PEF	O3-C30	3.88	1.44	1.33
24	D	402	CDL	OB8-CB7	3.88	1.44	1.33
24	N	604	CDL	OA6-CA5	3.86	1.45	1.34
24	N	604	CDL	OB6-CB5	3.86	1.45	1.34
25	S	102	PEF	O3-C30	3.86	1.44	1.33
25	C	605	PEF	O3-C30	3.86	1.44	1.33
24	S	101	CDL	OA8-CA7	3.85	1.44	1.33
25	p	301	PEF	O2-C10	3.85	1.45	1.34
25	l	101	PEF	O3-C30	3.84	1.44	1.33
25	r	201	PEF	O2-C10	3.83	1.45	1.34
25	N	606	PEF	O2-C10	3.83	1.45	1.34
25	E	304	PEF	O3-C30	3.82	1.44	1.33
25	e	201	PEF	O3-C30	3.81	1.44	1.33
24	D	402	CDL	OB6-CB5	3.80	1.45	1.34
24	A	501	CDL	OB6-CB5	3.78	1.45	1.34
31	n	602	HEA	CHB-C4A	3.78	1.45	1.38
27	C	606	PCF	O31-C31	3.78	1.44	1.33
24	N	603	CDL	OA6-CA5	3.77	1.44	1.34
26	N	601	HEM	FE-NC	3.76	2.07	1.95
31	n	603	HEA	CHC-C4B	3.76	1.46	1.38
26	N	602	HEM	FE-NC	3.75	2.07	1.95
31	n	603	HEA	C4A-NA	3.75	1.46	1.39
24	N	604	CDL	OA8-CA7	3.74	1.44	1.33
24	D	402	CDL	OA6-CA5	3.73	1.44	1.34
24	N	603	CDL	OB8-CB7	3.73	1.44	1.33
24	H	101	CDL	OA8-CA7	3.72	1.44	1.33
25	N	606	PEF	O3-C30	3.72	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	D	401	HEC	CHC-C1C	3.71	1.47	1.39
25	e	201	PEF	O2-C10	3.69	1.44	1.34
31	n	603	HEA	C1A-NA	3.69	1.46	1.39
26	N	601	HEM	C1B-NB	-3.69	1.33	1.40
25	E	303	PEF	O2-C10	3.67	1.44	1.34
26	C	601	HEM	FE-NC	3.67	2.07	1.95
31	a	603	HEA	CHB-C4A	3.67	1.45	1.38
24	D	402	CDL	OA8-CA7	3.66	1.44	1.33
26	C	602	HEM	FE-NC	3.65	2.07	1.95
31	n	603	HEA	CHA-C1A	3.64	1.45	1.38
27	N	607	PCF	O31-C31	3.64	1.44	1.33
31	n	602	HEA	C1A-NA	3.60	1.46	1.39
31	n	602	HEA	CHA-C1A	3.57	1.45	1.38
24	C	603	CDL	OB8-CB7	3.56	1.43	1.33
31	a	603	HEA	C1A-NA	3.55	1.46	1.39
28	O	401	HEC	CHC-C1C	3.54	1.47	1.39
26	C	601	HEM	C4D-ND	-3.49	1.34	1.40
31	a	602	HEA	CHA-C1A	3.44	1.45	1.38
27	N	607	PCF	O21-C21	3.44	1.44	1.34
28	O	401	HEC	CHA-C4D	3.43	1.47	1.39
31	a	602	HEA	C1D-ND	-3.43	1.34	1.40
28	D	401	HEC	CHA-C4D	3.43	1.47	1.39
31	a	603	HEA	C1D-ND	-3.43	1.34	1.40
28	O	401	HEC	CHD-C1D	3.41	1.47	1.39
31	n	602	HEA	CHC-C1C	3.41	1.47	1.39
26	C	601	HEM	C3C-C4C	-3.39	1.40	1.46
31	n	602	HEA	C1D-ND	-3.36	1.34	1.40
31	a	603	HEA	C4B-NB	-3.34	1.34	1.40
31	a	603	HEA	C4A-NA	3.33	1.45	1.39
28	D	401	HEC	C4A-NA	-3.32	1.33	1.39
28	D	401	HEC	C1D-ND	-3.31	1.33	1.39
31	n	603	HEA	C4B-NB	-3.29	1.34	1.40
31	n	603	HEA	CHD-C4C	3.29	1.46	1.39
31	a	602	HEA	C1A-NA	3.28	1.45	1.39
31	a	602	HEA	C4A-NA	3.27	1.45	1.39
31	a	602	HEA	C4B-NB	-3.25	1.34	1.40
26	N	601	HEM	C4D-ND	-3.24	1.34	1.40
26	C	602	HEM	C3C-C4C	-3.24	1.40	1.46
31	n	602	HEA	C4A-NA	3.24	1.45	1.39
26	C	602	HEM	FE-ND	-3.24	1.84	1.94
31	a	602	HEA	CHC-C1C	3.23	1.46	1.39
31	a	603	HEA	CHD-C4C	3.23	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	a	603	HEA	C11-C3B	-3.21	1.47	1.51
26	N	602	HEM	FE-ND	-3.19	1.85	1.94
28	O	401	HEC	C1D-ND	-3.19	1.33	1.39
31	a	603	HEA	CHA-C1A	3.17	1.44	1.38
31	n	603	HEA	C1D-ND	-3.14	1.34	1.40
31	n	602	HEA	C11-C3B	-3.13	1.47	1.51
26	N	601	HEM	C3C-C4C	-3.13	1.40	1.46
28	D	401	HEC	CHD-C1D	3.13	1.46	1.39
31	a	602	HEA	CHB-C4A	3.10	1.44	1.38
28	D	401	HEC	CHB-C1B	3.10	1.46	1.39
28	O	401	HEC	CHB-C1B	3.07	1.46	1.39
26	N	602	HEM	C1C-C2C	-3.07	1.39	1.45
31	a	602	HEA	CHD-C4C	3.05	1.46	1.39
28	O	401	HEC	C4A-NA	-3.04	1.33	1.39
28	O	401	HEC	C4D-ND	-3.03	1.33	1.39
26	C	602	HEM	C1C-C2C	-3.03	1.39	1.45
31	n	602	HEA	C4B-NB	-3.00	1.35	1.40
26	N	602	HEM	C3C-C4C	-2.98	1.40	1.46
28	D	401	HEC	C4D-ND	-2.98	1.34	1.39
31	n	602	HEA	CHD-C4C	2.98	1.46	1.39
28	O	401	HEC	C1A-NA	-2.97	1.34	1.39
31	n	603	HEA	CHB-C1B	2.96	1.45	1.39
31	n	602	HEA	CHB-C1B	2.95	1.45	1.39
31	a	602	HEA	CHA-C4D	2.95	1.45	1.39
28	D	401	HEC	C1B-NB	-2.95	1.34	1.39
28	D	401	HEC	C3D-C2D	2.92	1.46	1.38
31	a	602	HEA	C4C-NC	-2.90	1.34	1.39
31	n	603	HEA	CHC-C1C	2.88	1.45	1.39
31	n	602	HEA	CHA-C4D	2.87	1.45	1.39
26	C	601	HEM	C1D-ND	-2.86	1.33	1.38
31	a	603	HEA	C4C-NC	-2.86	1.34	1.39
31	n	603	HEA	CHA-C4D	2.85	1.45	1.39
28	O	401	HEC	C3D-C2D	2.85	1.46	1.38
26	N	601	HEM	C1D-ND	-2.85	1.33	1.38
31	a	603	HEA	CHC-C1C	2.82	1.45	1.39
31	n	603	HEA	C11-C3B	-2.82	1.47	1.51
28	D	401	HEC	C1A-NA	-2.81	1.34	1.39
28	O	401	HEC	C1B-NB	-2.80	1.34	1.39
26	C	601	HEM	C1C-C2C	-2.78	1.39	1.45
26	C	602	HEM	C4B-NB	-2.78	1.33	1.38
31	a	603	HEA	CHB-C1B	2.75	1.45	1.39
31	n	603	HEA	C4C-NC	-2.75	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	C	601	HEM	FE-ND	-2.73	1.86	1.94
26	C	602	HEM	C1D-ND	-2.72	1.33	1.38
26	N	602	HEM	C1D-ND	-2.71	1.33	1.38
31	n	602	HEA	C4C-NC	-2.69	1.34	1.39
26	N	602	HEM	C4B-NB	-2.68	1.33	1.38
26	C	601	HEM	C1A-C2A	-2.68	1.39	1.44
26	N	601	HEM	FE-ND	-2.67	1.86	1.94
31	n	602	HEA	C1C-NC	-2.67	1.34	1.39
31	n	603	HEA	C1C-NC	-2.64	1.34	1.39
26	N	601	HEM	C1C-C2C	-2.63	1.40	1.45
31	a	603	HEA	C1B-NB	-2.61	1.33	1.38
28	O	401	HEC	C1C-NC	-2.60	1.34	1.39
31	a	602	HEA	C1B-NB	-2.57	1.33	1.38
26	C	601	HEM	C4B-NB	-2.57	1.33	1.38
24	L	501	CDL	OA8-CA7	2.57	1.45	1.33
28	D	401	HEC	C1C-NC	-2.56	1.34	1.39
31	a	603	HEA	CHA-C4D	2.56	1.45	1.39
27	N	607	PCF	O21-C2	-2.55	1.40	1.46
31	a	603	HEA	C1C-NC	-2.54	1.34	1.39
28	D	401	HEC	C4B-NB	-2.51	1.34	1.39
31	a	602	HEA	C1C-NC	-2.48	1.34	1.39
31	n	603	HEA	C4D-ND	-2.47	1.34	1.38
26	N	601	HEM	C4B-NB	-2.42	1.34	1.38
31	a	603	HEA	C4D-ND	-2.42	1.34	1.38
26	N	601	HEM	C1A-C2A	-2.41	1.39	1.44
28	O	401	HEC	C4B-NB	-2.40	1.35	1.39
31	n	602	HEA	C4B-C3B	2.36	1.48	1.44
31	n	602	HEA	C4D-ND	-2.34	1.34	1.38
31	n	603	HEA	C1B-NB	-2.33	1.34	1.38
28	O	401	HEC	C4C-NC	-2.32	1.35	1.39
31	a	602	HEA	CHB-C1B	2.30	1.44	1.39
28	D	401	HEC	C4C-NC	-2.30	1.35	1.39
31	n	602	HEA	C1B-NB	-2.29	1.34	1.38
31	a	602	HEA	C4B-C3B	2.25	1.48	1.44
26	N	602	HEM	C1A-C2A	-2.24	1.40	1.44
31	a	602	HEA	C4D-ND	-2.20	1.34	1.38
26	C	601	HEM	C1A-NA	-2.18	1.35	1.39
25	p	301	PEF	O2-C2	-2.17	1.41	1.46
28	D	401	HEC	C1C-C2C	2.17	1.48	1.43
28	D	401	HEC	C3C-C4C	2.15	1.49	1.46
28	O	401	HEC	C3C-C4C	2.15	1.49	1.46
24	N	604	CDL	OA6-CA4	-2.15	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	C	602	HEM	C1B-C2B	-2.11	1.40	1.44
31	n	603	HEA	C4B-C3B	2.10	1.48	1.44
26	N	602	HEM	C1B-C2B	-2.10	1.40	1.44
28	D	401	HEC	C3B-C4B	2.10	1.49	1.46
26	N	602	HEM	C4C-NC	-2.09	1.35	1.39
28	O	401	HEC	C3B-C4B	2.08	1.49	1.46
26	N	601	HEM	C4D-C3D	2.08	1.48	1.45
25	e	201	PEF	O2-C2	-2.07	1.41	1.46
26	N	601	HEM	C1C-NC	-2.06	1.35	1.39
24	D	402	CDL	OA6-CA4	-2.05	1.41	1.46
24	N	603	CDL	OA6-CA4	-2.04	1.41	1.46
26	C	602	HEM	C1A-C2A	-2.04	1.40	1.44
28	O	401	HEC	C1C-C2C	2.01	1.47	1.43

All (416) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a	602	HEA	C13-C12-C11	-7.47	102.46	114.39
31	a	603	HEA	C3D-C4D-ND	7.41	117.51	110.35
31	n	603	HEA	C3D-C4D-ND	6.80	116.92	110.35
31	a	602	HEA	C2B-C1B-NB	6.77	117.72	109.90
31	n	602	HEA	C3D-C4D-ND	6.33	116.47	110.35
26	N	601	HEM	CAD-C3D-C4D	6.25	135.59	124.70
31	n	602	HEA	C3C-C4C-NC	6.21	115.03	109.80
31	a	603	HEA	C2B-C1B-NB	6.17	117.04	109.90
31	a	602	HEA	C3D-C4D-ND	6.14	116.28	110.35
31	n	603	HEA	C3C-C2C-C1C	-6.08	100.00	107.17
26	C	601	HEM	CAD-C3D-C4D	6.07	135.27	124.70
31	n	603	HEA	C2B-C1B-NB	5.96	116.79	109.90
31	n	602	HEA	C2B-C1B-NB	5.88	116.70	109.90
31	a	603	HEA	C3C-C2C-C1C	-5.84	100.28	107.17
31	n	603	HEA	C2D-C1D-ND	5.83	116.54	109.84
31	n	603	HEA	C3B-C4B-NB	5.78	116.48	109.84
31	a	602	HEA	C3C-C4C-NC	5.65	114.55	109.80
31	n	602	HEA	C2D-C1D-ND	5.58	116.25	109.84
26	N	601	HEM	CHD-C1D-ND	5.55	130.40	124.42
31	a	603	HEA	C2D-C1D-ND	5.55	116.22	109.84
26	N	601	HEM	CHC-C4B-NB	5.52	130.36	124.42
31	n	602	HEA	C2A-C1A-NA	5.48	115.61	110.32
31	n	603	HEA	C3C-C4C-NC	5.48	114.41	109.80
28	O	401	HEC	C2A-C1A-NA	5.43	115.56	110.32
31	n	603	HEA	C2A-C1A-NA	5.39	115.52	110.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a	602	HEA	C2D-C1D-ND	5.38	116.03	109.84
31	a	602	HEA	C26-C15-C16	5.38	124.56	115.23
31	a	603	HEA	C3B-C4B-NB	5.32	115.96	109.84
26	C	602	HEM	CHC-C4B-NB	5.32	130.15	124.42
31	a	602	HEA	C3C-C2C-C1C	-5.32	100.90	107.17
27	C	606	PCF	O21-C21-C22	5.29	122.93	111.48
26	N	602	HEM	CHC-C4B-NB	5.25	130.07	124.42
31	a	602	HEA	C2A-C1A-NA	5.21	115.35	110.32
28	D	401	HEC	C2A-C1A-NA	5.13	115.27	110.32
31	n	602	HEA	C13-C12-C11	-4.97	106.45	114.39
26	C	601	HEM	CHC-C4B-NB	4.94	129.74	124.42
31	a	603	HEA	C2A-C1A-NA	4.91	115.06	110.32
31	n	602	HEA	C3B-C4B-NB	4.87	115.44	109.84
24	D	402	CDL	OB6-CB5-C51	4.78	121.83	111.48
31	n	602	HEA	C3C-C2C-C1C	-4.77	101.55	107.17
26	N	602	HEM	CHD-C1D-ND	4.76	129.54	124.42
24	A	501	CDL	OA6-CA5-C11	4.73	121.70	111.48
31	n	603	HEA	C2C-C1C-NC	4.72	117.70	110.14
31	n	603	HEA	C1D-C2D-C3D	-4.70	102.04	106.98
26	C	601	HEM	CHD-C1D-ND	4.68	129.46	124.42
28	O	401	HEC	C3D-C4D-ND	4.63	115.29	110.15
31	a	603	HEA	C3C-C4C-NC	4.63	113.70	109.80
25	E	304	PEF	O2-C10-C11	4.59	121.41	111.48
25	e	201	PEF	C2-O2-C10	-4.52	106.99	117.80
26	N	601	HEM	CAD-C3D-C2D	-4.51	119.42	127.87
25	n	607	PEF	O2-C10-C11	4.51	121.23	111.48
25	n	606	PEF	O2-C10-C11	4.43	121.07	111.48
26	C	602	HEM	CHD-C1D-ND	4.41	129.17	124.42
24	L	501	CDL	OA6-CA5-C11	4.39	120.98	111.48
25	L	502	PEF	O2-C10-C11	4.38	120.96	111.48
27	I	101	PCF	O21-C21-C22	4.36	120.91	111.48
31	n	602	HEA	C1D-C2D-C3D	-4.35	102.40	106.98
31	a	603	HEA	C2C-C1C-NC	4.35	117.12	110.14
31	a	603	HEA	C1D-C2D-C3D	-4.34	102.42	106.98
24	C	603	CDL	OB6-CB5-C51	4.33	120.85	111.48
24	N	603	CDL	OA6-CA5-C11	4.30	120.79	111.48
24	S	101	CDL	OB6-CB5-C51	4.29	120.77	111.48
31	a	602	HEA	C1B-C2B-C3B	-4.28	101.84	106.80
24	N	604	CDL	OB6-CB5-C51	4.27	120.71	111.48
31	a	602	HEA	C3B-C4B-NB	4.26	114.74	109.84
25	N	606	PEF	O2-C10-C11	4.26	120.69	111.48
26	C	601	HEM	CAD-C3D-C2D	-4.23	119.94	127.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a	602	HEA	C12-C11-C3B	4.22	118.71	112.12
31	n	603	HEA	C13-C12-C11	-4.20	107.69	114.39
24	C	603	CDL	OA6-CA5-C11	4.17	120.51	111.48
27	e	202	PCF	O21-C21-C22	4.17	120.50	111.48
25	H	102	PEF	O2-C10-C11	4.15	120.45	111.48
28	D	401	HEC	C2B-C1B-NB	4.13	116.76	110.14
31	n	602	HEA	C26-C15-C16	4.13	122.39	115.23
24	A	501	CDL	OB6-CB5-C51	4.12	120.39	111.48
24	H	101	CDL	OA6-CA5-C11	4.12	120.39	111.48
24	N	603	CDL	OB6-CB5-C51	4.12	120.38	111.48
31	n	602	HEA	C3A-C2A-C1A	-4.10	103.16	107.05
28	D	401	HEC	C3D-C4D-ND	4.08	114.68	110.15
28	O	401	HEC	C2B-C1B-NB	4.07	116.67	110.14
25	S	102	PEF	O2-C10-C11	4.06	120.26	111.48
25	l	101	PEF	O2-C10-C11	4.03	120.20	111.48
25	E	303	PEF	C2-O2-C10	-4.02	108.17	117.80
31	a	603	HEA	C1B-C2B-C3B	-3.98	102.19	106.80
31	a	603	HEA	C3A-C2A-C1A	-3.97	103.29	107.05
25	c	301	PEF	O2-C10-C11	3.97	120.07	111.48
26	C	602	HEM	CHA-C4D-ND	3.97	129.27	124.37
25	C	605	PEF	O2-C10-C11	3.96	120.05	111.48
25	O	402	PEF	O2-C10-C11	3.96	120.05	111.48
25	A	502	PEF	O2-C10-C11	3.95	120.03	111.48
24	S	101	CDL	OA6-CA5-C11	3.95	120.02	111.48
25	b	302	PEF	O2-C10-C11	3.93	119.97	111.48
25	b	303	PEF	O2-C10-C11	3.92	119.96	111.48
25	o	302	PEF	O2-C10-C11	3.91	119.94	111.48
31	a	602	HEA	C2C-C1C-NC	3.90	116.39	110.14
28	D	401	HEC	C1A-C2A-C3A	-3.90	101.98	107.11
27	r	202	PCF	O21-C21-C22	3.89	119.90	111.48
24	N	604	CDL	OA6-CA5-C11	3.88	119.87	111.48
31	a	602	HEA	C1D-C2D-C3D	-3.88	102.90	106.98
31	a	603	HEA	C13-C12-C11	-3.86	108.22	114.39
25	J	101	PEF	O2-C10-C11	3.86	119.83	111.48
25	n	608	PEF	O2-C10-C11	3.85	119.81	111.48
26	N	602	HEM	CHA-C4D-ND	3.85	129.13	124.37
25	E	303	PEF	O2-C10-C11	3.85	119.80	111.48
28	D	401	HEC	CHC-C4B-NB	-3.83	120.28	124.45
28	D	401	HEC	C1D-C2D-C3D	-3.80	102.47	106.82
25	E	302	PEF	O2-C10-C11	3.79	119.69	111.48
31	n	603	HEA	C1B-C2B-C3B	-3.78	102.41	106.80
31	n	603	HEA	C3A-C2A-C1A	-3.78	103.47	107.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	302	PEF	O2-C10-C11	3.78	119.66	111.48
24	N	603	CDL	CA4-OA6-CA5	-3.77	108.77	117.80
31	n	602	HEA	C2C-C1C-NC	3.77	116.18	110.14
25	e	201	PEF	O2-C10-C11	3.77	119.63	111.48
26	C	602	HEM	CHB-C1B-NB	3.76	129.02	124.37
25	N	605	PEF	O2-C10-C11	3.73	119.55	111.48
31	a	602	HEA	O11-C11-C3B	-3.72	104.43	111.26
24	L	501	CDL	OB6-CB5-C51	3.72	119.53	111.48
27	N	607	PCF	O21-C21-C22	3.71	119.50	111.48
28	O	401	HEC	CHC-C4B-NB	-3.70	120.42	124.45
24	H	101	CDL	OB6-CB5-C51	3.68	119.43	111.48
28	O	401	HEC	C1A-C2A-C3A	-3.67	102.27	107.11
27	T	101	PCF	O21-C21-C22	3.67	119.42	111.48
31	n	602	HEA	C1B-C2B-C3B	-3.66	102.55	106.80
26	N	601	HEM	CHD-C1D-C2D	-3.66	119.25	125.03
25	C	604	PEF	O2-C10-C11	3.66	119.39	111.48
28	O	401	HEC	C1D-C2D-C3D	-3.64	102.64	106.82
31	a	602	HEA	C4A-NA-C1A	-3.61	99.93	105.82
24	A	501	CDL	OB8-CB7-C71	3.60	122.81	111.83
25	r	201	PEF	O2-C10-C11	3.60	119.26	111.48
28	D	401	HEC	CHD-C4C-NC	-3.59	120.55	124.45
31	a	602	HEA	CHB-C1B-C2B	-3.58	119.38	125.03
26	C	601	HEM	CBD-CAD-C3D	3.56	122.37	112.53
31	a	602	HEA	CAD-C3D-C4D	3.54	130.87	124.70
28	O	401	HEC	CAA-CBA-CGA	-3.54	104.28	113.67
28	O	401	HEC	C2C-C1C-NC	3.53	115.79	110.14
27	N	607	PCF	O31-C31-C32	3.53	122.58	111.83
25	p	301	PEF	O2-C10-C11	3.52	119.10	111.48
31	a	603	HEA	C4D-C3D-C2D	-3.51	101.78	106.89
26	N	601	HEM	CBD-CAD-C3D	3.50	122.22	112.53
26	C	601	HEM	CHB-C1B-NB	3.47	128.66	124.37
28	O	401	HEC	CHD-C4C-NC	-3.46	120.69	124.45
31	n	602	HEA	C4A-NA-C1A	-3.44	100.22	105.82
25	l	101	PEF	C2-O2-C10	-3.44	109.57	117.80
26	N	602	HEM	CHB-C1B-NB	3.43	128.61	124.37
26	C	602	HEM	C1B-NB-C4B	3.42	109.26	105.21
25	H	102	PEF	O3-C30-C31	3.41	122.22	111.83
24	D	402	CDL	OB8-CB7-C71	3.40	121.47	111.15
25	E	302	PEF	O3-C30-C31	3.40	122.20	111.83
28	D	401	HEC	C3A-C4A-NA	3.39	115.91	109.64
28	D	401	HEC	CAA-CBA-CGA	-3.38	104.70	113.67
28	O	401	HEC	C3A-C4A-NA	3.34	115.81	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a	602	HEA	C3A-C2A-C1A	-3.34	103.89	107.05
25	J	101	PEF	O3-C30-C31	3.33	121.98	111.83
31	a	602	HEA	C4D-C3D-C2D	-3.31	102.07	106.89
25	n	606	PEF	O3-C30-C31	3.31	121.91	111.83
31	n	602	HEA	OMA-CMA-C3A	-3.30	118.18	125.62
31	a	602	HEA	CHA-C4D-ND	-3.29	120.88	124.42
27	T	101	PCF	C3-C2-C1	-3.29	104.12	111.78
31	n	603	HEA	C4A-NA-C1A	-3.29	100.46	105.82
31	a	602	HEA	CBA-CAA-C2A	-3.28	103.45	112.53
27	N	607	PCF	C2-O21-C21	-3.28	109.96	117.80
28	D	401	HEC	C2C-C1C-NC	3.27	115.39	110.14
27	C	606	PCF	O31-C31-C32	3.21	121.64	111.83
28	O	401	HEC	C2D-C1D-ND	3.20	115.28	110.14
24	D	402	CDL	OA6-CA5-C11	3.20	118.40	111.48
26	C	601	HEM	CHD-C1D-C2D	-3.19	119.99	125.03
26	N	602	HEM	C1B-NB-C4B	3.19	108.98	105.21
28	D	401	HEC	C2D-C1D-ND	3.18	115.24	110.14
31	n	602	HEA	CAD-CBD-CGD	-3.18	105.23	113.67
24	C	603	CDL	CB4-OB6-CB5	-3.18	110.20	117.80
24	H	101	CDL	OB8-CB7-C71	3.17	121.49	111.83
31	n	603	HEA	C4D-C3D-C2D	-3.17	102.28	106.89
24	C	603	CDL	OA8-CA7-C31	3.16	121.48	111.83
24	A	501	CDL	CB4-OB6-CB5	-3.16	110.23	117.80
25	r	201	PEF	C2-O2-C10	-3.15	110.27	117.80
31	n	603	HEA	C4B-C3B-C2B	-3.12	102.20	107.44
25	a	606	PEF	O2-C10-C11	3.12	118.22	111.48
27	T	101	PCF	O31-C31-C32	3.11	121.32	111.83
26	N	601	HEM	C1B-NB-C4B	3.11	108.89	105.21
31	n	602	HEA	C4D-C3D-C2D	-3.10	102.38	106.89
26	N	601	HEM	CHB-C1B-NB	3.05	128.13	124.37
31	n	603	HEA	CHA-C4D-ND	-3.00	121.19	124.42
31	a	603	HEA	C4A-NA-C1A	-3.00	100.93	105.82
26	C	601	HEM	CHD-C4C-NC	2.99	127.71	124.45
31	a	603	HEA	C4B-C3B-C2B	-2.99	102.42	107.44
25	C	604	PEF	C2-O2-C10	-2.97	110.68	117.80
31	a	602	HEA	C27-C19-C20	2.95	120.35	115.23
28	O	401	HEC	CHB-C1B-C2B	-2.95	118.86	127.43
27	H	103	PCF	O31-C31-C32	2.95	120.82	111.83
26	N	602	HEM	CHD-C1D-C2D	-2.95	120.38	125.03
26	N	601	HEM	CHD-C4C-NC	2.94	127.65	124.45
25	N	605	PEF	O3-C30-C31	2.93	120.78	111.83
25	b	303	PEF	O3-C30-C31	2.92	120.75	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	S	101	CDL	OA8-CA7-C31	2.92	120.73	111.83
24	H	101	CDL	OA8-CA7-C31	2.92	120.73	111.83
25	n	607	PEF	O3-C30-C31	2.90	120.68	111.83
24	N	604	CDL	OB8-CB7-C71	2.89	120.66	111.83
31	n	603	HEA	CMC-C2C-C3C	2.89	133.34	126.55
31	a	602	HEA	C16-C15-C14	-2.88	114.69	121.17
25	A	502	PEF	O3-C30-C31	2.88	120.63	111.83
25	O	402	PEF	O3-C30-C31	2.88	120.62	111.83
25	E	303	PEF	O3-C30-C31	2.88	120.62	111.83
26	N	602	HEM	CHD-C4C-NC	2.88	127.58	124.45
31	a	603	HEA	CAD-CBD-CGD	-2.88	106.04	113.67
31	a	602	HEA	CAD-CBD-CGD	-2.87	106.06	113.67
26	C	601	HEM	C1B-NB-C4B	2.86	108.60	105.21
31	a	603	HEA	C27-C19-C20	2.86	120.18	115.23
25	a	606	PEF	O3-C30-C31	2.85	120.53	111.83
31	n	602	HEA	C17-C18-C19	-2.85	121.10	127.62
27	e	202	PCF	O31-C31-C32	2.85	120.52	111.83
24	D	402	CDL	OA8-CA7-C31	2.85	120.51	111.83
31	n	602	HEA	C4B-C3B-C2B	-2.84	102.67	107.44
25	E	304	PEF	O3-C30-C31	2.83	120.48	111.83
31	n	603	HEA	CHC-C1C-C2C	-2.83	119.21	127.43
31	n	603	HEA	CAD-CBD-CGD	-2.83	106.16	113.67
24	S	101	CDL	OB8-CB7-C71	2.82	120.44	111.83
25	o	302	PEF	O3-C30-C31	2.82	120.42	111.83
26	C	602	HEM	C3B-C4B-NB	-2.82	107.45	109.47
25	l	101	PEF	O3-C30-C31	2.81	120.41	111.83
25	b	302	PEF	O3-C30-C31	2.81	120.39	111.83
27	N	607	PCF	O31-C31-O32	-2.79	116.64	123.63
25	C	604	PEF	O3-C30-C31	2.78	120.31	111.83
31	n	602	HEA	C4C-C3C-C2C	-2.77	103.86	107.30
28	D	401	HEC	CHB-C1B-C2B	-2.77	119.39	127.43
28	D	401	HEC	CHA-C1A-NA	-2.76	121.44	124.45
25	S	102	PEF	C2-O2-C10	-2.76	111.18	117.80
24	C	603	CDL	OB8-CB6-CB4	-2.76	100.44	108.40
25	p	301	PEF	O3-C30-C31	2.76	120.25	111.83
24	N	603	CDL	CB4-OB6-CB5	-2.75	111.22	117.80
24	A	501	CDL	OA8-CA7-C31	2.74	120.20	111.83
28	O	401	HEC	C4A-C3A-C2A	-2.73	102.92	106.97
28	O	401	HEC	C4D-C3D-C2D	-2.72	102.67	106.87
24	N	603	CDL	OB8-CB7-C71	2.71	120.10	111.83
27	I	101	PCF	C3-C2-C1	-2.71	105.47	111.78
25	p	301	PEF	C2-O2-C10	-2.71	111.32	117.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	N	606	PEF	C2-O2-C10	-2.70	111.33	117.80
26	C	602	HEM	CHD-C1D-C2D	-2.70	120.77	125.03
25	N	605	PEF	C2-O2-C10	-2.69	111.36	117.80
31	a	603	HEA	CHA-C4D-ND	-2.68	121.53	124.42
31	a	602	HEA	C13-C14-C15	-2.68	121.48	127.62
31	n	602	HEA	CMC-C2C-C3C	2.68	132.85	126.55
26	N	602	HEM	C3B-C4B-NB	-2.67	107.55	109.47
31	a	603	HEA	CHC-C1C-C2C	-2.67	119.68	127.43
25	N	606	PEF	O3-C30-C31	2.66	119.96	111.83
31	a	602	HEA	C12-C13-C14	-2.65	105.20	112.16
31	a	603	HEA	C13-C14-C15	-2.65	121.56	127.62
31	a	603	HEA	C1D-ND-C4D	-2.65	102.07	105.21
31	a	602	HEA	C17-C18-C19	-2.64	121.58	127.62
24	L	501	CDL	OB8-CB7-C71	2.63	119.86	111.83
28	O	401	HEC	CAD-CBD-CGD	-2.62	106.71	113.67
31	a	603	HEA	CHA-C4D-C3D	-2.62	120.95	124.77
31	n	603	HEA	C4B-NB-C1B	-2.62	102.11	105.21
31	a	603	HEA	CHB-C1B-C2B	-2.62	120.90	125.03
31	n	603	HEA	C13-C14-C15	-2.61	121.64	127.62
31	n	603	HEA	CMB-C2B-C1B	2.60	129.10	125.03
25	H	102	PEF	C2-O2-C10	-2.60	111.58	117.80
25	c	301	PEF	O3-C30-C31	2.59	119.75	111.83
27	I	101	PCF	O31-C31-C32	2.59	119.73	111.83
24	C	603	CDL	CA4-OA6-CA5	-2.59	111.61	117.80
24	L	501	CDL	CB4-OB6-CB5	-2.58	111.61	117.80
31	n	603	HEA	CHB-C1B-NB	-2.58	121.65	124.42
26	C	602	HEM	C4A-CHB-C1B	-2.58	120.19	126.25
28	D	401	HEC	CAD-CBD-CGD	-2.58	106.83	113.67
25	L	502	PEF	O3-C30-C31	2.56	119.63	111.83
31	n	602	HEA	CHC-C1C-C2C	-2.55	120.02	127.43
26	N	601	HEM	C3B-C4B-NB	-2.55	107.64	109.47
27	H	103	PCF	C3-C2-C1	-2.55	105.85	111.78
28	D	401	HEC	C4A-C3A-C2A	-2.55	103.20	106.97
25	r	201	PEF	O3-C30-C31	2.54	119.59	111.83
31	n	603	HEA	C1D-ND-C4D	-2.53	102.21	105.21
26	N	602	HEM	C1A-CHA-C4D	-2.52	120.31	126.25
31	a	603	HEA	CAD-C3D-C2D	2.52	132.59	127.87
24	N	603	CDL	OA8-CA7-C31	2.52	119.52	111.83
31	a	602	HEA	CHC-C1C-C2C	-2.51	120.13	127.43
26	C	602	HEM	CHD-C4C-NC	2.51	127.19	124.45
31	n	602	HEA	CHB-C4A-NA	-2.51	121.72	124.45
24	S	101	CDL	CB4-OB6-CB5	-2.50	111.80	117.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	H	103	PCF	O21-C21-C22	2.50	116.89	111.48
24	L	501	CDL	CA4-OA6-CA5	-2.49	111.83	117.80
24	H	101	CDL	CA4-OA6-CA5	-2.48	111.85	117.80
24	N	604	CDL	OA8-CA7-C31	2.48	119.39	111.83
28	D	401	HEC	C4D-C3D-C2D	-2.48	103.03	106.87
27	e	202	PCF	C2-O21-C21	-2.47	111.88	117.80
31	a	602	HEA	C4B-NB-C1B	-2.47	102.29	105.21
24	D	402	CDL	OB8-CB7-OB9	-2.46	117.48	123.63
31	n	602	HEA	C27-C19-C20	2.45	119.48	115.23
27	T	101	PCF	O31-C31-O32	-2.45	117.51	123.63
31	a	602	HEA	CMD-C2D-C1D	2.45	128.85	125.03
25	H	102	PEF	O3-C30-O5	-2.44	117.53	123.63
31	n	602	HEA	CHA-C4D-ND	-2.43	121.81	124.42
25	n	606	PEF	C32-C31-C30	-2.43	104.79	113.69
31	a	602	HEA	C4B-C3B-C2B	-2.42	103.37	107.44
24	A	501	CDL	OB8-CB7-OB9	-2.42	117.58	123.63
28	D	401	HEC	CAA-C2A-C1A	2.42	129.76	124.85
25	A	502	PEF	O3-C30-O5	-2.41	117.61	123.63
31	a	603	HEA	C4B-NB-C1B	-2.40	102.36	105.21
28	O	401	HEC	CHA-C1A-NA	-2.40	121.84	124.45
25	e	201	PEF	O3-C30-C31	2.40	119.16	111.83
25	E	304	PEF	C2-O2-C10	-2.40	112.05	117.80
31	a	602	HEA	CMB-C2B-C1B	2.39	128.78	125.03
31	n	602	HEA	CHB-C1B-NB	-2.39	121.85	124.42
26	C	602	HEM	CHB-C1B-C2B	-2.39	120.16	126.95
25	n	608	PEF	O3-C30-C31	2.38	119.10	111.83
24	N	604	CDL	CB2-C1-CA2	-2.37	105.81	112.65
25	L	502	PEF	C2-O2-C10	-2.36	112.16	117.80
31	a	603	HEA	C1A-CHA-C4D	-2.35	121.02	126.02
24	S	101	CDL	OA8-CA7-OA9	-2.35	117.74	123.63
24	D	402	CDL	CB4-OB6-CB5	-2.35	112.18	117.80
31	a	602	HEA	C27-C19-C18	-2.35	117.60	123.63
31	a	603	HEA	CHB-C4A-NA	-2.34	121.91	124.45
25	S	102	PEF	O3-C30-C31	2.34	118.96	111.83
31	n	602	HEA	CAD-C3D-C4D	2.34	128.77	124.70
31	n	603	HEA	CHD-C1D-C2D	-2.34	120.31	126.95
27	C	606	PCF	O31-C31-O32	-2.33	117.81	123.63
28	D	401	HEC	CHB-C4A-C3A	-2.32	120.66	125.49
24	H	101	CDL	OA8-CA7-OA9	-2.32	117.83	123.63
24	H	101	CDL	CB4-OB6-CB5	-2.32	112.25	117.80
26	N	602	HEM	CAD-CBD-CGD	-2.32	107.52	113.67
26	N	602	HEM	CHB-C1B-C2B	-2.31	120.38	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	N	602	HEM	C4D-ND-C1D	2.31	107.94	105.21
31	n	603	HEA	C27-C19-C20	2.31	119.23	115.23
31	n	602	HEA	CMB-C2B-C1B	2.31	128.64	125.03
26	C	602	HEM	C1A-CHA-C4D	-2.30	120.83	126.25
31	a	602	HEA	CHB-C4A-NA	-2.30	121.95	124.45
31	n	602	HEA	C1D-ND-C4D	-2.29	102.49	105.21
31	a	603	HEA	CAA-CBA-CGA	-2.29	107.59	113.67
31	n	602	HEA	CHD-C1D-C2D	-2.29	120.45	126.95
26	N	601	HEM	C4C-CHD-C1D	-2.29	121.16	126.02
25	o	302	PEF	C2-O2-C10	-2.28	112.33	117.80
25	C	605	PEF	O3-C30-C31	2.28	118.79	111.83
26	C	601	HEM	C3B-C4B-NB	-2.28	107.83	109.47
25	E	302	PEF	O3-C30-O5	-2.28	117.93	123.63
24	S	101	CDL	OA6-CA4-CA6	2.28	116.51	108.34
31	a	603	HEA	CHB-C1B-NB	-2.27	121.97	124.42
31	n	602	HEA	CHB-C1B-C2B	-2.27	121.44	125.03
27	C	606	PCF	C2-O21-C21	-2.27	112.37	117.80
27	H	103	PCF	O21-C2-C1	2.26	116.46	108.34
25	b	302	PEF	C2-O2-C10	-2.26	112.39	117.80
26	C	602	HEM	C4C-CHD-C1D	-2.24	121.26	126.02
31	a	602	HEA	C21-C22-C23	-2.24	120.18	127.64
26	N	602	HEM	C4A-CHB-C1B	-2.22	121.02	126.25
27	C	606	PCF	O21-C21-O22	-2.22	118.51	123.70
24	S	101	CDL	OB4-PB2-OB3	2.22	122.78	112.44
24	N	603	CDL	OB4-PB2-OB3	2.22	122.77	112.44
25	l	101	PEF	O3-C30-O5	-2.22	118.08	123.63
31	n	603	HEA	CHB-C1B-C2B	-2.21	121.53	125.03
31	a	602	HEA	CHA-C1A-NA	-2.21	122.05	124.45
31	a	602	HEA	CHD-C1D-C2D	-2.21	120.67	126.95
31	n	602	HEA	C4A-CHB-C1B	-2.20	121.34	126.02
28	O	401	HEC	CHC-C1C-C2C	-2.20	121.03	127.43
25	N	606	PEF	O3-C30-O5	-2.20	118.13	123.63
31	n	602	HEA	C25-C23-C24	2.19	119.64	114.59
31	a	602	HEA	C21-C20-C19	-2.19	105.92	113.19
25	c	302	PEF	O3-C30-C31	2.19	118.51	111.83
26	N	602	HEM	C4C-CHD-C1D	-2.19	121.36	126.02
31	n	602	HEA	CAA-CBA-CGA	-2.19	107.86	113.67
26	C	601	HEM	CHB-C1B-C2B	-2.19	120.73	126.95
31	n	603	HEA	CHB-C4A-NA	-2.19	122.07	124.45
24	S	101	CDL	CA6-CA4-CA3	-2.18	106.69	111.78
27	C	606	PCF	O14-P-O12	2.18	122.60	112.44
26	C	602	HEM	O2A-CGA-CBA	2.18	120.89	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	603	CDL	OB8-CB7-C71	2.18	118.48	111.83
25	J	101	PEF	O3-C30-O5	-2.18	118.17	123.63
24	H	101	CDL	OB4-PB2-OB3	2.18	122.57	112.44
31	n	602	HEA	C4B-NB-C1B	-2.17	102.64	105.21
26	C	602	HEM	C4D-ND-C1D	2.17	107.78	105.21
25	a	606	PEF	C3-C2-C1	-2.17	106.73	111.78
25	n	606	PEF	C2-O2-C10	-2.15	112.65	117.80
27	r	202	PCF	O31-C31-C32	2.15	118.38	111.83
24	N	604	CDL	CB4-OB6-CB5	-2.14	112.67	117.80
25	O	402	PEF	C2-O2-C10	-2.14	112.67	117.80
27	I	101	PCF	O21-C21-O22	-2.14	118.71	123.70
31	a	603	HEA	C25-C23-C24	2.14	119.50	114.59
31	a	603	HEA	CHD-C1D-C2D	-2.14	120.88	126.95
25	n	607	PEF	O2-C10-O4	-2.13	118.72	123.70
26	C	601	HEM	C1C-CHC-C4B	-2.13	121.49	126.02
24	D	402	CDL	OB6-CB5-OB7	-2.12	118.75	123.70
31	a	603	HEA	CHA-C1A-C2A	-2.12	121.52	124.86
31	n	603	HEA	C25-C23-C24	2.12	119.46	114.59
31	n	602	HEA	C13-C14-C15	-2.12	122.78	127.62
31	n	603	HEA	CAA-CBA-CGA	-2.11	108.06	113.67
26	C	602	HEM	CHA-C4D-C3D	-2.11	121.33	125.23
24	A	501	CDL	OA6-CA5-OA7	-2.11	118.77	123.70
31	a	602	HEA	C1D-ND-C4D	-2.11	102.71	105.21
31	n	603	HEA	CHA-C1A-NA	-2.10	122.16	124.45
31	n	602	HEA	CHA-C4D-C3D	-2.09	121.72	124.77
25	o	302	PEF	O3-C30-O5	-2.09	118.40	123.63
31	a	602	HEA	C4C-C3C-C2C	-2.09	104.71	107.30
25	L	502	PEF	O2-C10-O4	-2.08	118.84	123.70
31	n	602	HEA	CHA-C1A-C2A	-2.07	121.59	124.86
24	A	501	CDL	OB6-CB5-OB7	-2.07	118.86	123.70
26	C	601	HEM	O2D-CGD-CBD	2.07	120.55	114.00
25	E	304	PEF	O2-C10-O4	-2.07	118.86	123.70
26	C	602	HEM	CMB-C2B-C1B	-2.07	121.80	125.03
25	c	301	PEF	C2-O2-C10	-2.07	112.84	117.80
31	a	603	HEA	CMB-C2B-C1B	2.07	128.26	125.03
26	N	601	HEM	C4A-CHB-C1B	-2.06	121.39	126.25
26	C	601	HEM	CHA-C1A-NA	2.06	127.60	123.86
25	b	303	PEF	O3-C30-O5	-2.06	118.48	123.63
25	l	101	PEF	O2-C10-O4	-2.06	118.90	123.70
31	n	602	HEA	C12-C13-C14	-2.06	106.76	112.16
31	n	603	HEA	C1A-CHA-C4D	-2.06	121.65	126.02
26	C	601	HEM	C4C-CHD-C1D	-2.05	121.65	126.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	r	202	PCF	C2-O21-C21	-2.05	112.90	117.80
25	e	201	PEF	C12-C11-C10	-2.05	106.20	113.69
25	E	304	PEF	O3-C30-O5	-2.04	118.52	123.63
26	C	602	HEM	CAD-CBD-CGD	-2.04	108.25	113.67
25	n	607	PEF	O3-C30-O5	-2.03	118.56	123.63
28	O	401	HEC	CHB-C4A-C3A	-2.02	121.28	125.49
24	N	603	CDL	OA6-CA5-OA7	-2.02	118.99	123.70
28	O	401	HEC	CAA-C2A-C1A	2.02	128.95	124.85
24	C	603	CDL	OB4-PB2-OB3	2.01	121.81	112.44
24	H	101	CDL	OB8-CB7-OB9	-2.01	118.61	123.63
31	a	603	HEA	CMC-C2C-C1C	2.01	128.47	125.42
25	e	201	PEF	O3-C3-C2	-2.01	102.61	108.40
31	a	603	HEA	CHC-C4B-NB	-2.00	121.89	124.37

There are no chirality outliers.

All (713) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	A	501	CDL	CA2-OA2-PA1-OA3
24	A	501	CDL	CA2-OA2-PA1-OA5
24	A	501	CDL	CA3-OA5-PA1-OA2
24	A	501	CDL	CA3-OA5-PA1-OA3
24	A	501	CDL	CB2-OB2-PB2-OB5
24	A	501	CDL	CB3-OB5-PB2-OB2
24	C	603	CDL	CA3-OA5-PA1-OA2
24	C	603	CDL	CA3-OA5-PA1-OA3
24	C	603	CDL	CB2-OB2-PB2-OB4
24	C	603	CDL	CB2-OB2-PB2-OB5
24	D	402	CDL	CA2-OA2-PA1-OA3
24	D	402	CDL	CA2-OA2-PA1-OA5
24	D	402	CDL	CA3-OA5-PA1-OA2
24	D	402	CDL	CA3-OA5-PA1-OA3
24	D	402	CDL	CA3-OA5-PA1-OA4
24	D	402	CDL	CB2-OB2-PB2-OB5
24	D	402	CDL	CB3-OB5-PB2-OB2
24	D	402	CDL	CB3-OB5-PB2-OB3
24	D	402	CDL	CB3-OB5-PB2-OB4
24	H	101	CDL	CA2-OA2-PA1-OA3
24	H	101	CDL	CA2-OA2-PA1-OA4
24	H	101	CDL	CA2-OA2-PA1-OA5
24	H	101	CDL	CB2-OB2-PB2-OB3
24	H	101	CDL	CB2-OB2-PB2-OB4

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Mol	Chain	Res	Type	Atoms
24	H	101	CDL	CB2-OB2-PB2-OB5
24	H	101	CDL	CB3-OB5-PB2-OB2
24	L	501	CDL	CA2-OA2-PA1-OA3
24	L	501	CDL	CA2-OA2-PA1-OA4
24	L	501	CDL	CA2-OA2-PA1-OA5
24	L	501	CDL	CA3-OA5-PA1-OA2
24	L	501	CDL	CA3-OA5-PA1-OA3
24	L	501	CDL	CB2-OB2-PB2-OB3
24	L	501	CDL	CB2-OB2-PB2-OB5
24	L	501	CDL	CB3-OB5-PB2-OB2
24	L	501	CDL	CB3-OB5-PB2-OB3
24	L	501	CDL	CB3-OB5-PB2-OB4
24	N	603	CDL	CA2-OA2-PA1-OA3
24	N	603	CDL	CA2-OA2-PA1-OA4
24	N	603	CDL	CA2-OA2-PA1-OA5
24	N	603	CDL	CA3-OA5-PA1-OA2
24	N	603	CDL	CA3-OA5-PA1-OA3
24	N	603	CDL	CA3-OA5-PA1-OA4
24	N	603	CDL	CB2-OB2-PB2-OB3
24	N	603	CDL	CB2-OB2-PB2-OB4
24	N	603	CDL	CB2-OB2-PB2-OB5
24	N	604	CDL	O1-C1-CB2-OB2
24	N	604	CDL	CA3-OA5-PA1-OA3
24	N	604	CDL	CB3-OB5-PB2-OB2
24	N	604	CDL	CB3-OB5-PB2-OB3
24	N	604	CDL	CB3-OB5-PB2-OB4
24	S	101	CDL	CA2-OA2-PA1-OA5
24	S	101	CDL	CA3-OA5-PA1-OA2
24	S	101	CDL	CA3-OA5-PA1-OA4
24	S	101	CDL	C11-CA5-OA6-CA4
25	A	502	PEF	C4-O4P-P-O3P
25	C	604	PEF	O4P-C4-C5-N
25	C	604	PEF	C1-O3P-P-O2P
25	C	604	PEF	C1-O3P-P-O4P
25	C	604	PEF	C4-O4P-P-O3P
25	E	302	PEF	C1-O3P-P-O1P
25	E	302	PEF	C1-O3P-P-O4P
25	E	302	PEF	C4-O4P-P-O1P
25	E	302	PEF	C4-O4P-P-O2P
25	E	303	PEF	C1-O3P-P-O1P
25	E	303	PEF	C1-O3P-P-O2P
25	E	303	PEF	C1-O3P-P-O4P

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Mol	Chain	Res	Type	Atoms
25	E	303	PEF	C4-O4P-P-O1P
25	E	303	PEF	C4-O4P-P-O2P
25	E	303	PEF	C4-O4P-P-O3P
25	E	304	PEF	C1-O3P-P-O1P
25	E	304	PEF	C1-O3P-P-O4P
25	E	304	PEF	C4-O4P-P-O3P
25	H	102	PEF	C1-O3P-P-O4P
25	H	102	PEF	C4-O4P-P-O3P
25	J	101	PEF	C1-O3P-P-O2P
25	J	101	PEF	C1-O3P-P-O4P
25	J	101	PEF	C4-O4P-P-O1P
25	J	101	PEF	C4-O4P-P-O3P
25	L	502	PEF	C1-O3P-P-O1P
25	L	502	PEF	C1-O3P-P-O2P
25	L	502	PEF	C4-O4P-P-O1P
25	L	502	PEF	C4-O4P-P-O2P
25	L	502	PEF	C4-O4P-P-O3P
25	N	605	PEF	C1-O3P-P-O1P
25	N	605	PEF	C1-O3P-P-O2P
25	N	605	PEF	C1-O3P-P-O4P
25	N	605	PEF	C4-O4P-P-O1P
25	N	606	PEF	C4-O4P-P-O2P
25	N	606	PEF	C4-O4P-P-O3P
25	O	402	PEF	C31-C30-O3-C3
25	O	402	PEF	O5-C30-O3-C3
25	O	402	PEF	C1-O3P-P-O4P
25	S	102	PEF	C4-O4P-P-O1P
25	S	102	PEF	C4-O4P-P-O2P
25	S	102	PEF	C4-O4P-P-O3P
25	a	606	PEF	O4P-C4-C5-N
25	a	606	PEF	C1-O3P-P-O1P
25	a	606	PEF	C4-O4P-P-O1P
25	a	606	PEF	C4-O4P-P-O2P
25	a	606	PEF	C4-O4P-P-O3P
25	b	302	PEF	O2-C2-C3-O3
25	b	302	PEF	O4P-C4-C5-N
25	b	302	PEF	C1-O3P-P-O2P
25	b	302	PEF	C4-O4P-P-O1P
25	b	302	PEF	C4-O4P-P-O2P
25	b	302	PEF	C4-O4P-P-O3P
25	b	303	PEF	C11-C10-O2-C2
25	b	303	PEF	O4-C10-O2-C2

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Mol	Chain	Res	Type	Atoms
25	b	303	PEF	C1-O3P-P-O2P
25	b	303	PEF	C1-O3P-P-O4P
25	b	303	PEF	C4-O4P-P-O3P
25	c	301	PEF	C1-O3P-P-O2P
25	c	301	PEF	C1-O3P-P-O4P
25	c	302	PEF	O4P-C4-C5-N
25	c	302	PEF	C1-O3P-P-O1P
25	c	302	PEF	C1-O3P-P-O4P
25	c	302	PEF	C4-O4P-P-O2P
25	c	302	PEF	C4-O4P-P-O3P
25	e	201	PEF	C11-C10-O2-C2
25	e	201	PEF	C1-O3P-P-O4P
25	e	201	PEF	C4-O4P-P-O3P
25	l	101	PEF	C4-O4P-P-O1P
25	n	606	PEF	C4-O4P-P-O1P
25	n	606	PEF	C4-O4P-P-O2P
25	n	606	PEF	C4-O4P-P-O3P
25	n	607	PEF	C11-C10-O2-C2
25	n	607	PEF	O4-C10-O2-C2
25	n	607	PEF	C1-O3P-P-O1P
25	n	607	PEF	C1-O3P-P-O4P
25	n	607	PEF	C4-O4P-P-O1P
25	n	607	PEF	C4-O4P-P-O3P
25	n	608	PEF	C4-O4P-P-O1P
25	o	302	PEF	C4-O4P-P-O2P
25	o	302	PEF	C4-O4P-P-O3P
25	p	301	PEF	C1-O3P-P-O1P
25	p	301	PEF	C1-O3P-P-O2P
25	p	301	PEF	C1-O3P-P-O4P
25	r	201	PEF	C1-O3P-P-O2P
25	r	201	PEF	C1-O3P-P-O4P
25	r	201	PEF	C4-O4P-P-O3P
26	C	601	HEM	C2B-C3B-CAB-CBB
26	C	601	HEM	C4B-C3B-CAB-CBB
26	C	601	HEM	C2D-C3D-CAD-CBD
26	C	601	HEM	C4D-C3D-CAD-CBD
26	N	601	HEM	C2B-C3B-CAB-CBB
26	N	601	HEM	C4B-C3B-CAB-CBB
26	N	601	HEM	C2D-C3D-CAD-CBD
26	N	601	HEM	C4D-C3D-CAD-CBD
27	C	606	PCF	C1-O11-P-O12
27	C	606	PCF	C11-O13-P-O11

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Mol	Chain	Res	Type	Atoms
27	H	103	PCF	C1-O11-P-O14
27	H	103	PCF	C11-O13-P-O12
27	r	202	PCF	C22-C21-O21-C2
31	a	602	HEA	C2A-C3A-CMA-OMA
31	a	602	HEA	C4A-C3A-CMA-OMA
31	a	602	HEA	C11-C12-C13-C14
31	n	602	HEA	C2A-C3A-CMA-OMA
31	n	602	HEA	C4A-C3A-CMA-OMA
31	n	602	HEA	C11-C12-C13-C14
24	N	604	CDL	OB9-CB7-OB8-CB6
24	S	101	CDL	OA7-CA5-OA6-CA4
25	E	302	PEF	O4-C10-O2-C2
25	e	201	PEF	O4-C10-O2-C2
27	r	202	PCF	O22-C21-O21-C2
31	n	602	HEA	C26-C15-C16-C17
24	L	501	CDL	OA9-CA7-OA8-CA6
24	L	501	CDL	C71-CB7-OB8-CB6
24	N	604	CDL	C71-CB7-OB8-CB6
24	L	501	CDL	C31-CA7-OA8-CA6
24	C	603	CDL	O1-C1-CB2-OB2
24	D	402	CDL	O1-C1-CB2-OB2
25	C	604	PEF	C11-C10-O2-C2
25	E	302	PEF	C11-C10-O2-C2
31	a	602	HEA	C26-C15-C16-C17
31	a	602	HEA	C14-C15-C16-C17
24	L	501	CDL	OB9-CB7-OB8-CB6
31	n	602	HEA	C2A-CAA-CBA-CGA
24	S	101	CDL	C51-CB5-OB6-CB4
25	C	604	PEF	O4-C10-O2-C2
24	N	604	CDL	CA2-C1-CB2-OB2
24	S	101	CDL	C71-CB7-OB8-CB6
31	n	602	HEA	C14-C15-C16-C17
25	a	606	PEF	C30-C31-C32-C33
24	H	101	CDL	O1-C1-CA2-OA2
25	A	502	PEF	O3P-C1-C2-O2
24	H	101	CDL	C11-CA5-OA6-CA4
24	L	501	CDL	CB5-C51-C52-C53
24	S	101	CDL	CB5-C51-C52-C53
25	J	101	PEF	C10-C11-C12-C13
25	p	301	PEF	C10-C11-C12-C13
27	N	607	PCF	C21-C22-C23-C24
24	S	101	CDL	OB9-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
25	C	605	PEF	C30-C31-C32-C33
25	E	303	PEF	C30-C31-C32-C33
25	S	102	PEF	C30-C31-C32-C33
25	n	606	PEF	C30-C31-C32-C33
27	C	606	PCF	C21-C22-C23-C24
25	O	402	PEF	C11-C10-O2-C2
31	n	603	HEA	C2A-CAA-CBA-CGA
25	E	302	PEF	C10-C11-C12-C13
24	A	501	CDL	O1-C1-CB2-OB2
24	H	101	CDL	CA7-C31-C32-C33
27	C	606	PCF	C31-C32-C33-C34
27	N	607	PCF	C31-C32-C33-C34
25	c	302	PEF	C11-C10-O2-C2
27	H	103	PCF	C21-C22-C23-C24
24	H	101	CDL	OA7-CA5-OA6-CA4
24	S	101	CDL	OB7-CB5-OB6-CB4
25	O	402	PEF	O4-C10-O2-C2
25	c	302	PEF	O4-C10-O2-C2
24	A	501	CDL	CA2-C1-CB2-OB2
27	I	101	PCF	C11-C12-N-C14
27	I	101	PCF	C11-C12-N-C15
24	N	604	CDL	C11-CA5-OA6-CA4
25	E	303	PEF	C11-C10-O2-C2
27	H	103	PCF	C22-C21-O21-C2
24	N	604	CDL	OA7-CA5-OA6-CA4
25	E	303	PEF	O4-C10-O2-C2
27	H	103	PCF	O22-C21-O21-C2
24	S	101	CDL	CA6-CA4-OA6-CA5
24	C	603	CDL	C11-CA5-OA6-CA4
24	N	603	CDL	C11-CA5-OA6-CA4
25	J	101	PEF	C11-C10-O2-C2
24	S	101	CDL	CA7-C31-C32-C33
25	N	606	PEF	C13-C14-C15-C16
25	N	606	PEF	C31-C32-C33-C34
25	O	402	PEF	C41-C42-C43-C44
24	C	603	CDL	CB5-C51-C52-C53
25	b	303	PEF	C34-C35-C36-C37
25	E	304	PEF	C32-C33-C34-C35
25	b	302	PEF	C39-C40-C41-C42
25	o	302	PEF	C12-C13-C14-C15
25	o	302	PEF	C34-C35-C36-C37
25	J	101	PEF	O4-C10-O2-C2

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Mol	Chain	Res	Type	Atoms
25	E	304	PEF	C12-C13-C14-C15
25	e	201	PEF	C15-C16-C17-C18
27	T	101	PCF	C39-C40-C41-C42
24	N	604	CDL	C51-CB5-OB6-CB4
25	C	605	PEF	C11-C10-O2-C2
25	r	201	PEF	C11-C10-O2-C2
24	L	501	CDL	O1-C1-CB2-OB2
24	N	604	CDL	C57-C58-C59-C60
24	N	603	CDL	CA5-C11-C12-C13
25	C	604	PEF	C34-C35-C36-C37
25	E	303	PEF	C11-C12-C13-C14
24	D	402	CDL	CA2-C1-CB2-OB2
25	o	302	PEF	C16-C17-C18-C19
27	I	101	PCF	C11-C12-N-C13
25	n	606	PEF	C37-C38-C39-C40
25	o	302	PEF	C10-C11-C12-C13
25	E	302	PEF	C15-C16-C17-C18
24	A	501	CDL	C51-CB5-OB6-CB4
25	L	502	PEF	C11-C10-O2-C2
25	N	605	PEF	C11-C10-O2-C2
24	N	604	CDL	C32-C33-C34-C35
25	o	302	PEF	C15-C16-C17-C18
24	D	402	CDL	C51-C52-C53-C54
24	N	603	CDL	OA7-CA5-OA6-CA4
24	N	604	CDL	OB7-CB5-OB6-CB4
25	r	201	PEF	O4-C10-O2-C2
25	O	402	PEF	C40-C41-C42-C43
25	n	606	PEF	C31-C32-C33-C34
25	n	606	PEF	C40-C41-C42-C43
25	n	606	PEF	C13-C14-C15-C16
27	C	606	PCF	C32-C31-O31-C3
25	O	402	PEF	C33-C34-C35-C36
25	O	402	PEF	C34-C35-C36-C37
25	E	303	PEF	C21-C22-C23-C24
25	n	606	PEF	C35-C36-C37-C38
24	C	603	CDL	C36-C37-C38-C39
27	N	607	PCF	C22-C21-O21-C2
24	D	402	CDL	C61-C62-C63-C64
25	N	605	PEF	C34-C35-C36-C37
24	A	501	CDL	OB7-CB5-OB6-CB4
24	C	603	CDL	OA7-CA5-OA6-CA4
25	C	605	PEF	O4-C10-O2-C2

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Mol	Chain	Res	Type	Atoms
27	N	607	PCF	O22-C21-O21-C2
24	N	603	CDL	C34-C35-C36-C37
25	E	303	PEF	C13-C14-C15-C16
25	O	402	PEF	C14-C15-C16-C17
25	e	201	PEF	C19-C20-C21-C22
25	N	606	PEF	C35-C36-C37-C38
25	r	201	PEF	C12-C13-C14-C15
25	n	606	PEF	C41-C42-C43-C44
25	C	604	PEF	C37-C38-C39-C40
27	e	202	PCF	C21-C22-C23-C24
24	L	501	CDL	OB5-CB3-CB4-OB6
25	L	502	PEF	O3P-C1-C2-O2
24	N	604	CDL	C56-C57-C58-C59
25	b	303	PEF	C16-C17-C18-C19
25	a	606	PEF	C11-C10-O2-C2
25	N	606	PEF	C11-C12-C13-C14
24	A	501	CDL	OB6-CB4-CB6-OB8
27	I	101	PCF	O21-C2-C3-O31
24	N	604	CDL	C31-C32-C33-C34
24	C	603	CDL	C71-C72-C73-C74
25	C	605	PEF	C11-C12-C13-C14
27	N	607	PCF	C30-C47-C48-C49
31	a	602	HEA	C2A-CAA-CBA-CGA
24	A	501	CDL	CA5-C11-C12-C13
25	N	605	PEF	C11-C12-C13-C14
24	D	402	CDL	C11-CA5-OA6-CA4
25	E	302	PEF	C38-C39-C40-C41
25	n	606	PEF	C11-C12-C13-C14
27	e	202	PCF	C11-C12-N-C13
25	E	304	PEF	C34-C35-C36-C37
24	N	603	CDL	OA5-CA3-CA4-CA6
25	o	302	PEF	O3P-C1-C2-C3
25	L	502	PEF	O4-C10-O2-C2
24	N	604	CDL	C71-C72-C73-C74
27	C	606	PCF	O32-C31-O31-C3
24	H	101	CDL	CB5-C51-C52-C53
25	E	304	PEF	C11-C10-O2-C2
24	C	603	CDL	C73-C74-C75-C76
24	A	501	CDL	C52-C53-C54-C55
25	N	605	PEF	O4-C10-O2-C2
24	H	101	CDL	CA3-CA4-CA6-OA8
24	H	101	CDL	CB3-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
24	L	501	CDL	CB3-CB4-CB6-OB8
24	N	604	CDL	CB3-CB4-CB6-OB8
25	A	502	PEF	C1-C2-C3-O3
25	C	604	PEF	C1-C2-C3-O3
25	N	605	PEF	C1-C2-C3-O3
25	O	402	PEF	C1-C2-C3-O3
25	S	102	PEF	C1-C2-C3-O3
25	b	302	PEF	C1-C2-C3-O3
25	n	607	PEF	C1-C2-C3-O3
25	e	201	PEF	C18-C19-C20-C21
25	n	606	PEF	C39-C40-C41-C42
25	N	605	PEF	C33-C34-C35-C36
24	D	402	CDL	C31-CA7-OA8-CA6
27	H	103	PCF	C23-C24-C25-C26
27	e	202	PCF	C32-C33-C34-C35
25	r	201	PEF	C34-C35-C36-C37
25	N	606	PEF	C20-C21-C22-C23
25	b	302	PEF	C30-C31-C32-C33
25	r	201	PEF	C30-C31-C32-C33
25	L	502	PEF	C30-C31-C32-C33
25	e	201	PEF	C31-C30-O3-C3
27	H	103	PCF	C1-C2-O21-C21
25	n	606	PEF	C20-C21-C22-C23
31	n	603	HEA	C2A-C3A-CMA-OMA
27	N	607	PCF	C38-C39-C40-C41
25	n	608	PEF	C31-C30-O3-C3
25	n	606	PEF	C42-C43-C44-C45
24	L	501	CDL	C51-C52-C53-C54
27	N	607	PCF	C35-C36-C37-C38
25	C	605	PEF	C15-C16-C17-C18
25	o	302	PEF	C14-C15-C16-C17
24	N	604	CDL	OB6-CB4-CB6-OB8
25	a	606	PEF	O2-C2-C3-O3
25	p	301	PEF	O2-C2-C3-O3
27	C	606	PCF	C27-C28-C29-C30
24	C	603	CDL	C53-C54-C55-C56
27	e	202	PCF	C11-C12-N-C15
25	a	606	PEF	O4-C10-O2-C2
24	N	604	CDL	C73-C74-C75-C76
25	l	101	PEF	C31-C30-O3-C3
25	o	302	PEF	C33-C34-C35-C36
25	n	607	PEF	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
24	D	402	CDL	OA9-CA7-OA8-CA6
25	N	605	PEF	C37-C38-C39-C40
31	a	603	HEA	C4D-C3D-CAD-CBD
25	C	604	PEF	C35-C36-C37-C38
31	a	603	HEA	C4C-C3C-CAC-CBC
25	E	302	PEF	C37-C38-C39-C40
25	N	605	PEF	C15-C16-C17-C18
25	b	302	PEF	C33-C34-C35-C36
25	c	302	PEF	C36-C37-C38-C39
24	A	501	CDL	OA5-CA3-CA4-CA6
25	A	502	PEF	O3P-C1-C2-C3
25	L	502	PEF	O3P-C1-C2-C3
25	p	301	PEF	O3P-C1-C2-C3
25	r	201	PEF	O3P-C1-C2-C3
27	C	606	PCF	O11-C1-C2-C3
24	S	101	CDL	C71-C72-C73-C74
27	e	202	PCF	C11-C12-N-C14
25	O	402	PEF	C10-C11-C12-C13
25	N	605	PEF	C19-C20-C21-C22
27	N	607	PCF	C22-C23-C24-C25
25	J	101	PEF	C31-C32-C33-C34
25	O	402	PEF	C32-C33-C34-C35
25	e	201	PEF	O5-C30-O3-C3
24	C	603	CDL	C74-C75-C76-C77
24	D	402	CDL	C11-C12-C13-C14
25	S	102	PEF	C10-C11-C12-C13
25	E	303	PEF	C22-C23-C24-C25
24	A	501	CDL	CB3-CB4-CB6-OB8
24	N	604	CDL	CA3-CA4-CA6-OA8
25	O	402	PEF	C31-C32-C33-C34
24	D	402	CDL	CA7-C31-C32-C33
25	c	302	PEF	C32-C33-C34-C35
27	C	606	PCF	C29-C30-C47-C48
24	H	101	CDL	OB5-CB3-CB4-OB6
24	N	604	CDL	OB5-CB3-CB4-OB6
25	n	607	PEF	O3P-C1-C2-O2
27	e	202	PCF	O11-C1-C2-O21
25	b	303	PEF	C19-C20-C21-C22
27	e	202	PCF	C35-C36-C37-C38
24	A	501	CDL	C11-C12-C13-C14
25	C	605	PEF	C12-C13-C14-C15
24	C	603	CDL	OB6-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
24	L	501	CDL	OB6-CB4-CB6-OB8
25	C	604	PEF	O2-C2-C3-O3
25	n	608	PEF	O2-C2-C3-O3
27	H	103	PCF	O21-C2-C3-O31
27	N	607	PCF	O21-C2-C3-O31
24	C	603	CDL	C51-C52-C53-C54
27	N	607	PCF	C36-C37-C38-C39
25	S	102	PEF	C40-C41-C42-C43
25	E	304	PEF	O4-C10-O2-C2
31	n	602	HEA	C15-C16-C17-C18
24	H	101	CDL	C71-CB7-OB8-CB6
24	L	501	CDL	C13-C14-C15-C16
24	L	501	CDL	C52-C53-C54-C55
24	H	101	CDL	CB2-C1-CA2-OA2
25	c	302	PEF	C33-C34-C35-C36
27	C	606	PCF	C25-C26-C27-C28
24	A	501	CDL	OB5-CB3-CB4-CB6
24	C	603	CDL	OB5-CB3-CB4-CB6
24	H	101	CDL	OB5-CB3-CB4-CB6
25	S	102	PEF	O3P-C1-C2-C3
25	n	608	PEF	O3P-C1-C2-C3
27	e	202	PCF	O11-C1-C2-C3
27	r	202	PCF	C21-C22-C23-C24
24	N	604	CDL	C55-C56-C57-C58
25	o	302	PEF	C17-C18-C19-C20
25	N	606	PEF	C12-C13-C14-C15
25	n	608	PEF	O5-C30-O3-C3
24	C	603	CDL	CA5-C11-C12-C13
25	b	303	PEF	C31-C32-C33-C34
24	D	402	CDL	OA7-CA5-OA6-CA4
26	C	601	HEM	C2C-C3C-CAC-CBC
26	C	602	HEM	C2C-C3C-CAC-CBC
26	N	602	HEM	C2C-C3C-CAC-CBC
24	S	101	CDL	CA5-C11-C12-C13
25	n	607	PEF	C3-C2-O2-C10
25	l	101	PEF	O5-C30-O3-C3
25	E	302	PEF	C41-C42-C43-C44
27	r	202	PCF	C32-C31-O31-C3
25	c	302	PEF	C31-C32-C33-C34
25	S	102	PEF	O3P-C1-C2-O2
25	r	201	PEF	O3P-C1-C2-O2
25	E	302	PEF	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
24	C	603	CDL	CB3-CB4-CB6-OB8
24	N	603	CDL	CB3-CB4-CB6-OB8
25	r	201	PEF	C1-C2-C3-O3
27	I	101	PCF	C1-C2-C3-O31
27	N	607	PCF	C1-C2-C3-O31
27	e	202	PCF	C22-C21-O21-C2
31	a	603	HEA	C2D-C3D-CAD-CBD
27	H	103	PCF	C32-C31-O31-C3
24	H	101	CDL	OA6-CA4-CA6-OA8
24	N	604	CDL	OA6-CA4-CA6-OA8
25	A	502	PEF	O2-C2-C3-O3
25	J	101	PEF	O2-C2-C3-O3
25	N	605	PEF	O2-C2-C3-O3
25	S	102	PEF	O2-C2-C3-O3
25	n	606	PEF	O2-C2-C3-O3
25	n	607	PEF	O2-C2-C3-O3
24	N	603	CDL	C35-C36-C37-C38
27	N	607	PCF	C27-C28-C29-C30
27	C	606	PCF	C28-C29-C30-C47
27	H	103	PCF	C32-C33-C34-C35
27	r	202	PCF	O32-C31-O31-C3
24	C	603	CDL	C31-C32-C33-C34
27	T	101	PCF	O13-C11-C12-N
25	E	303	PEF	C14-C15-C16-C17
25	H	102	PEF	C34-C35-C36-C37
27	N	607	PCF	C48-C49-C50-C51
25	E	302	PEF	C35-C36-C37-C38
24	C	603	CDL	C52-C53-C54-C55
25	b	303	PEF	C13-C14-C15-C16
24	N	604	CDL	C58-C59-C60-C61
27	N	607	PCF	C39-C40-C41-C42
24	L	501	CDL	C12-C13-C14-C15
25	b	303	PEF	C17-C18-C19-C20
24	L	501	CDL	OA5-CA3-CA4-CA6
24	L	501	CDL	OB5-CB3-CB4-CB6
24	N	604	CDL	OB5-CB3-CB4-CB6
27	r	202	PCF	O11-C1-C2-C3
25	p	301	PEF	O4-C10-O2-C2
27	H	103	PCF	O32-C31-O31-C3
24	H	101	CDL	C1-CA2-OA2-PA1
24	N	604	CDL	CA4-CA3-OA5-PA1
27	e	202	PCF	O22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
24	A	501	CDL	OA5-CA3-CA4-OA6
24	A	501	CDL	OB5-CB3-CB4-OB6
24	C	603	CDL	OB5-CB3-CB4-OB6
24	D	402	CDL	OB5-CB3-CB4-OB6
24	L	501	CDL	OA5-CA3-CA4-OA6
24	N	603	CDL	OA5-CA3-CA4-OA6
25	b	302	PEF	O3P-C1-C2-O2
25	n	608	PEF	O3P-C1-C2-O2
25	o	302	PEF	O3P-C1-C2-O2
25	p	301	PEF	O3P-C1-C2-O2
27	C	606	PCF	O11-C1-C2-O21
25	l	101	PEF	C11-C10-O2-C2
24	N	604	CDL	C75-C76-C77-C78
31	n	603	HEA	C4A-C3A-CMA-OMA
25	e	201	PEF	C34-C35-C36-C37
24	H	101	CDL	OB6-CB4-CB6-OB8
27	C	606	PCF	C23-C24-C25-C26
25	c	301	PEF	C35-C36-C37-C38
27	C	606	PCF	C1-C2-C3-O31
25	e	201	PEF	C22-C23-C24-C25
25	p	301	PEF	C11-C10-O2-C2
24	N	603	CDL	C71-C72-C73-C74
27	e	202	PCF	C23-C24-C25-C26
24	H	101	CDL	OB9-CB7-OB8-CB6
24	A	501	CDL	CA2-OA2-PA1-OA4
24	A	501	CDL	CA3-OA5-PA1-OA4
24	A	501	CDL	CB2-OB2-PB2-OB3
24	A	501	CDL	CB3-OB5-PB2-OB3
24	D	402	CDL	CB2-OB2-PB2-OB3
24	H	101	CDL	CA3-OA5-PA1-OA3
24	H	101	CDL	CB3-OB5-PB2-OB3
24	L	501	CDL	CA3-OA5-PA1-OA4
24	L	501	CDL	CB2-OB2-PB2-OB4
24	N	603	CDL	CB3-OB5-PB2-OB3
24	S	101	CDL	CA2-OA2-PA1-OA3
25	A	502	PEF	C4-O4P-P-O1P
25	C	604	PEF	C4-O4P-P-O1P
25	E	302	PEF	C4-O4P-P-O3P
25	E	303	PEF	O4P-C4-C5-N
25	E	304	PEF	C4-O4P-P-O1P
25	H	102	PEF	C1-O3P-P-O1P
25	H	102	PEF	C4-O4P-P-O1P

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Mol	Chain	Res	Type	Atoms
25	J	101	PEF	C1-O3P-P-O1P
25	J	101	PEF	C4-O4P-P-O2P
25	L	502	PEF	C1-O3P-P-O4P
25	N	605	PEF	O4P-C4-C5-N
25	N	605	PEF	C4-O4P-P-O2P
25	N	605	PEF	C4-O4P-P-O3P
25	N	606	PEF	C4-O4P-P-O1P
25	O	402	PEF	C1-O3P-P-O1P
25	O	402	PEF	C4-O4P-P-O1P
25	O	402	PEF	C4-O4P-P-O2P
25	O	402	PEF	C4-O4P-P-O3P
25	b	302	PEF	C1-O3P-P-O1P
25	b	302	PEF	C1-O3P-P-O4P
25	b	303	PEF	C4-O4P-P-O1P
25	e	201	PEF	C1-O3P-P-O1P
25	e	201	PEF	C4-O4P-P-O1P
25	o	302	PEF	C4-O4P-P-O1P
25	r	201	PEF	C1-O3P-P-O1P
25	r	201	PEF	C4-O4P-P-O1P
27	C	606	PCF	C11-O13-P-O12
27	H	103	PCF	C1-O11-P-O13
27	H	103	PCF	C11-O13-P-O11
27	N	607	PCF	C11-C12-N-C14
31	a	603	HEA	C2C-C3C-CAC-CBC
25	L	502	PEF	C13-C14-C15-C16
25	E	302	PEF	C30-C31-C32-C33
27	H	103	PCF	C33-C34-C35-C36
25	c	301	PEF	C30-C31-C32-C33
25	C	605	PEF	C3-C2-O2-C10
25	E	303	PEF	C10-C11-C12-C13
27	N	607	PCF	C11-C12-N-C15
24	D	402	CDL	OB5-CB3-CB4-CB6
25	N	606	PEF	O3P-C1-C2-C3
25	c	301	PEF	O3P-C1-C2-C3
25	n	607	PEF	O3P-C1-C2-C3
25	b	303	PEF	C20-C21-C22-C23
25	c	302	PEF	C31-C30-O3-C3
24	L	501	CDL	CA2-C1-CB2-OB2
25	c	301	PEF	O3P-C1-C2-O2
27	r	202	PCF	O11-C1-C2-O21
25	E	304	PEF	O2-C10-C11-C12
25	c	302	PEF	O5-C30-O3-C3

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Mol	Chain	Res	Type	Atoms
25	l	101	PEF	O4-C10-O2-C2
25	E	304	PEF	C35-C36-C37-C38
25	O	402	PEF	O2-C2-C3-O3
25	r	201	PEF	O2-C2-C3-O3
24	N	603	CDL	C31-C32-C33-C34
25	C	605	PEF	C13-C14-C15-C16
25	S	102	PEF	C37-C38-C39-C40
27	N	607	PCF	C34-C35-C36-C37
25	E	302	PEF	O3-C30-C31-C32
25	p	301	PEF	C1-C2-C3-O3
31	a	602	HEA	C15-C16-C17-C18
27	r	202	PCF	C34-C35-C36-C37
25	H	102	PEF	C31-C30-O3-C3
25	b	303	PEF	O3P-C1-C2-O2
25	H	102	PEF	O5-C30-O3-C3
25	E	304	PEF	C36-C37-C38-C39
25	L	502	PEF	C11-C12-C13-C14
25	b	303	PEF	C11-C12-C13-C14
25	E	304	PEF	C15-C16-C17-C18
25	E	303	PEF	C19-C20-C21-C22
24	S	101	CDL	CB4-CB3-OB5-PB2
25	C	604	PEF	C11-C12-C13-C14
24	N	604	CDL	C61-C62-C63-C64
26	C	602	HEM	CAD-CBD-CGD-O2D
26	N	602	HEM	CAD-CBD-CGD-O2D
27	N	607	PCF	C11-C12-N-C13
26	N	602	HEM	CAD-CBD-CGD-O1D
25	e	201	PEF	C1-C2-C3-O3
25	n	606	PEF	C1-C2-C3-O3
26	C	602	HEM	CAD-CBD-CGD-O1D
25	E	302	PEF	O5-C30-O3-C3
25	e	201	PEF	C12-C13-C14-C15
24	N	604	CDL	CA6-CA4-OA6-CA5
25	b	302	PEF	C32-C33-C34-C35
25	E	304	PEF	C10-C11-C12-C13
25	N	605	PEF	C35-C36-C37-C38
25	E	303	PEF	O3P-C1-C2-O2
31	a	603	HEA	CAD-CBD-CGD-O2D
25	b	302	PEF	O3P-C1-C2-C3
31	a	602	HEA	CAD-CBD-CGD-O1D
24	A	501	CDL	C51-C52-C53-C54
24	C	603	CDL	CA2-C1-CB2-OB2

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Mol	Chain	Res	Type	Atoms
25	c	301	PEF	C32-C33-C34-C35
25	L	502	PEF	C31-C32-C33-C34
25	E	302	PEF	C31-C30-O3-C3
24	H	101	CDL	CA5-C11-C12-C13
24	N	604	CDL	C63-C64-C65-C66
26	C	601	HEM	CAA-CBA-CGA-O2A
26	N	602	HEM	CAA-CBA-CGA-O2A
24	N	603	CDL	CB4-CB3-OB5-PB2
31	a	602	HEA	CAD-CBD-CGD-O2D
31	a	603	HEA	CAD-CBD-CGD-O1D
25	J	101	PEF	C1-C2-C3-O3
25	c	302	PEF	C1-C2-C3-O3
24	A	501	CDL	C15-C16-C17-C18
26	N	601	HEM	CAD-CBD-CGD-O2D
27	N	607	PCF	C33-C34-C35-C36
24	C	603	CDL	CA7-C31-C32-C33
31	n	603	HEA	CAD-CBD-CGD-O2D
25	A	502	PEF	O4-C10-O2-C2
24	N	603	CDL	OB6-CB4-CB6-OB8
26	C	601	HEM	CAA-CBA-CGA-O1A
25	E	304	PEF	C33-C34-C35-C36
24	N	604	CDL	C35-C36-C37-C38
25	C	605	PEF	O3-C30-C31-C32
26	N	601	HEM	CAA-CBA-CGA-O2A
28	O	401	HEC	CAD-CBD-CGD-O2D
25	b	303	PEF	O2-C10-C11-C12
25	n	606	PEF	C19-C20-C21-C22
25	a	606	PEF	C3-C2-O2-C10
26	C	602	HEM	CAA-CBA-CGA-O2A
26	N	602	HEM	CAA-CBA-CGA-O1A
31	n	603	HEA	CAD-CBD-CGD-O1D
27	N	607	PCF	C40-C41-C42-C43
27	T	101	PCF	C37-C38-C39-C40
26	C	601	HEM	CAD-CBD-CGD-O2D
26	N	601	HEM	CAD-CBD-CGD-O1D
25	e	201	PEF	O3P-C1-C2-O2
27	H	103	PCF	C1-C2-C3-O31
26	C	601	HEM	C4C-C3C-CAC-CBC
26	C	602	HEM	C4C-C3C-CAC-CBC
26	N	602	HEM	C4C-C3C-CAC-CBC
28	O	401	HEC	CAD-CBD-CGD-O1D
26	C	602	HEM	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
26	N	601	HEM	CAA-CBA-CGA-O1A
25	e	201	PEF	O3P-C1-C2-C3
27	N	607	PCF	O11-C1-C2-C3
26	C	601	HEM	CAD-CBD-CGD-O1D
25	O	402	PEF	C17-C18-C19-C20
25	E	304	PEF	C2-C1-O3P-P
25	n	606	PEF	C12-C13-C14-C15
27	C	606	PCF	C30-C47-C48-C49
25	a	606	PEF	C13-C14-C15-C16
27	H	103	PCF	O13-C11-C12-N
27	r	202	PCF	O13-C11-C12-N
24	C	603	CDL	C13-C14-C15-C16
25	o	302	PEF	C11-C12-C13-C14
27	C	606	PCF	C22-C21-O21-C2
24	H	101	CDL	C54-C55-C56-C57
31	a	603	HEA	C26-C15-C16-C17
31	n	603	HEA	C26-C15-C16-C17
25	L	502	PEF	C10-C11-C12-C13
25	A	502	PEF	O3-C30-C31-C32
25	L	502	PEF	O2-C10-C11-C12
25	l	101	PEF	C33-C34-C35-C36
25	C	604	PEF	C32-C33-C34-C35
31	n	602	HEA	CAD-CBD-CGD-O1D
27	r	202	PCF	C23-C24-C25-C26
25	a	606	PEF	C1-C2-C3-O3
25	n	608	PEF	C1-C2-C3-O3
24	C	603	CDL	C72-C71-CB7-OB8
24	H	101	CDL	C12-C11-CA5-OA6
25	n	607	PEF	C11-C12-C13-C14
31	n	602	HEA	CAD-CBD-CGD-O2D
24	N	604	CDL	C33-C34-C35-C36
25	n	607	PEF	O3-C30-C31-C32
28	O	401	HEC	CAA-CBA-CGA-O2A
25	E	303	PEF	C33-C34-C35-C36
25	A	502	PEF	O5-C30-C31-C32
25	c	301	PEF	O5-C30-O3-C3
25	L	502	PEF	O4-C10-C11-C12
25	c	301	PEF	C11-C12-C13-C14
25	N	606	PEF	O3-C30-C31-C32
28	D	401	HEC	CAA-CBA-CGA-O2A
27	C	606	PCF	O22-C21-O21-C2
25	A	502	PEF	O2-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
27	T	101	PCF	C36-C37-C38-C39
24	L	501	CDL	OB7-CB5-OB6-CB4
25	N	605	PEF	C13-C14-C15-C16
25	p	301	PEF	O2-C10-C11-C12
27	C	606	PCF	O21-C21-C22-C23
25	E	302	PEF	O3P-C1-C2-C3
27	r	202	PCF	O31-C31-C32-C33
25	r	201	PEF	C31-C32-C33-C34
31	a	602	HEA	CAA-CBA-CGA-O2A
25	H	102	PEF	O2-C10-C11-C12
24	L	501	CDL	C55-C56-C57-C58
24	C	603	CDL	C72-C71-CB7-OB9
25	n	607	PEF	O5-C30-C31-C32
25	H	102	PEF	C35-C36-C37-C38
25	n	607	PEF	C30-C31-C32-C33
24	H	101	CDL	C12-C11-CA5-OA7
25	C	604	PEF	C38-C39-C40-C41

There are no ring outliers.

39 monomers are involved in 78 short contacts:

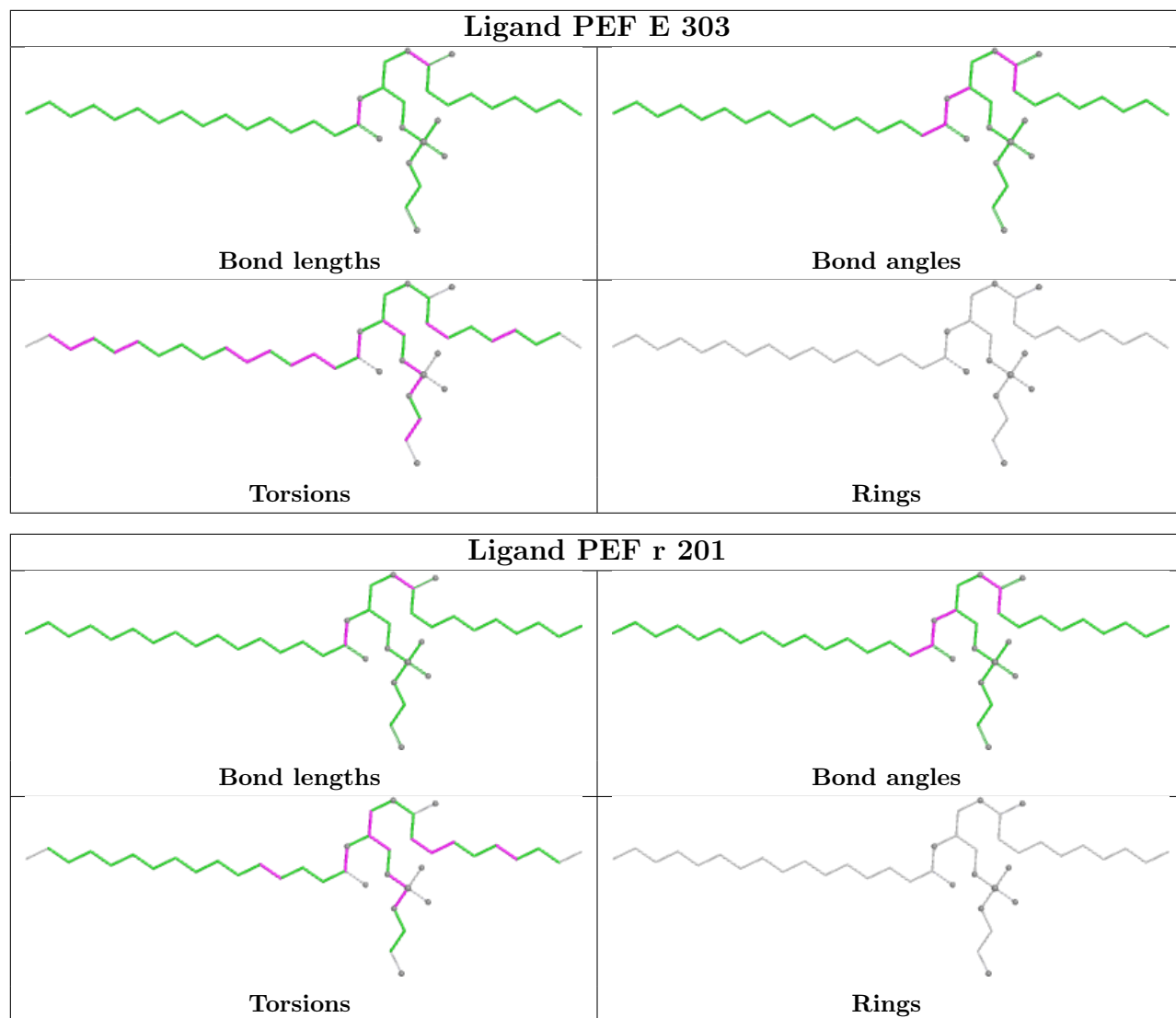
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	E	303	PEF	3	0
25	r	201	PEF	3	0
24	H	101	CDL	2	0
25	n	606	PEF	2	0
25	S	102	PEF	1	0
24	L	501	CDL	1	0
25	N	606	PEF	3	0
27	I	101	PCF	3	0
24	C	603	CDL	3	0
31	n	602	HEA	4	0
25	n	607	PEF	2	0
27	H	103	PCF	1	0
26	C	602	HEM	1	0
25	C	604	PEF	1	0
27	T	101	PCF	2	0
31	a	603	HEA	1	0
25	C	605	PEF	2	0
26	N	601	HEM	4	0
27	N	607	PCF	2	0
24	N	604	CDL	1	0

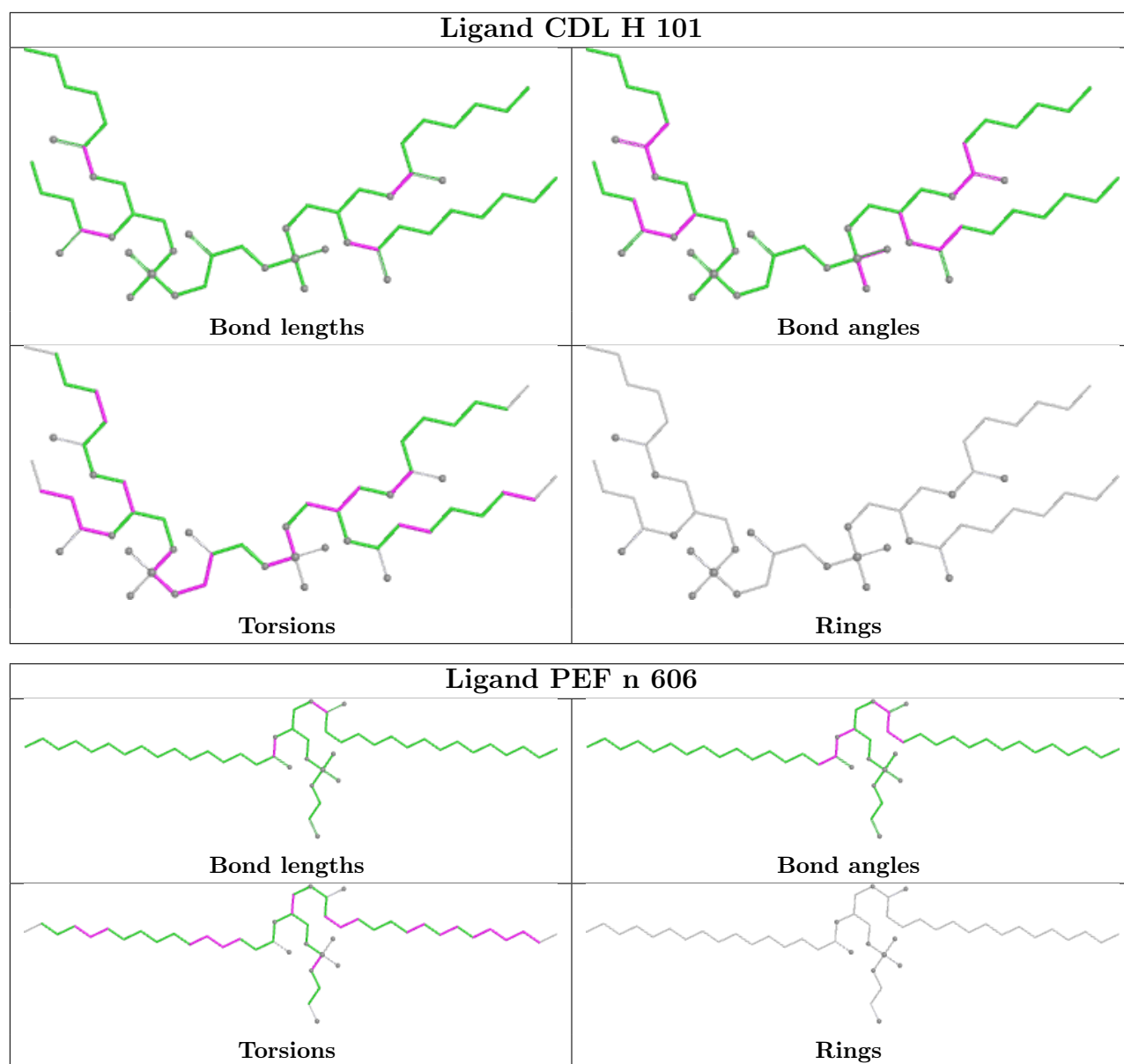
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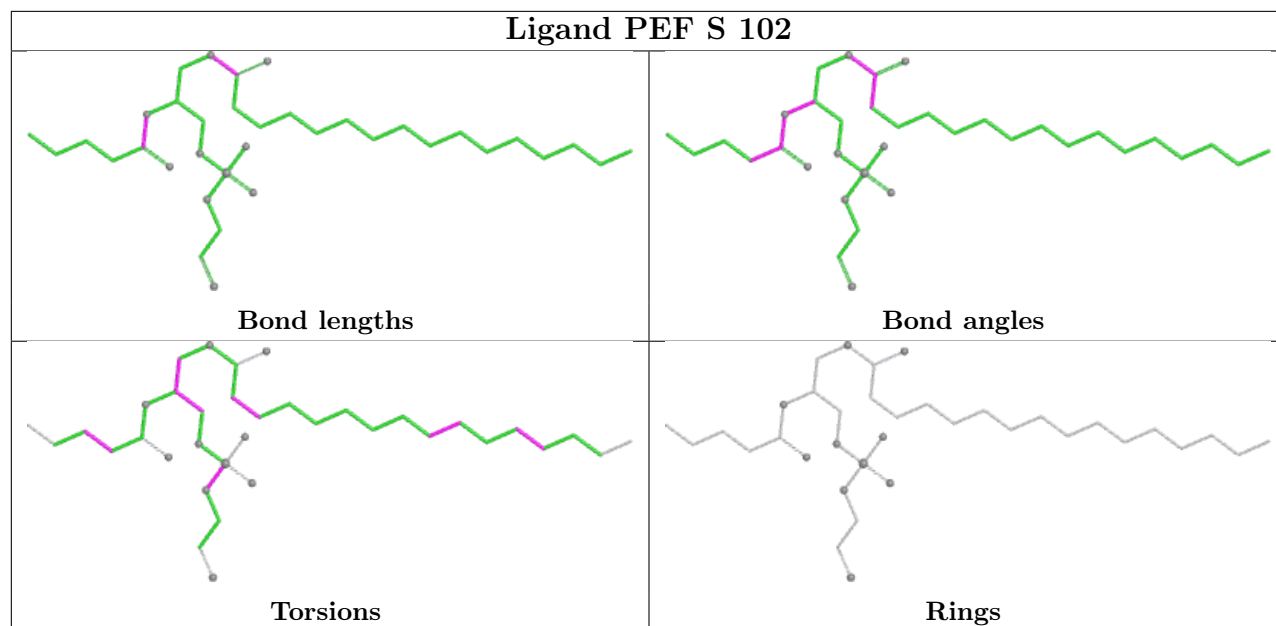
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	c	302	PEF	3	0
25	b	302	PEF	1	0
25	a	606	PEF	1	0
25	b	303	PEF	2	0
26	N	602	HEM	1	0
25	E	304	PEF	4	0
25	p	301	PEF	2	0
31	n	603	HEA	1	0
28	D	401	HEC	2	0
25	e	201	PEF	4	0
26	C	601	HEM	3	0
25	A	502	PEF	1	0
25	n	608	PEF	1	0
31	a	602	HEA	5	0
24	S	101	CDL	2	0
25	E	302	PEF	1	0
27	r	202	PCF	1	0
25	N	605	PEF	2	0
24	A	501	CDL	3	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.

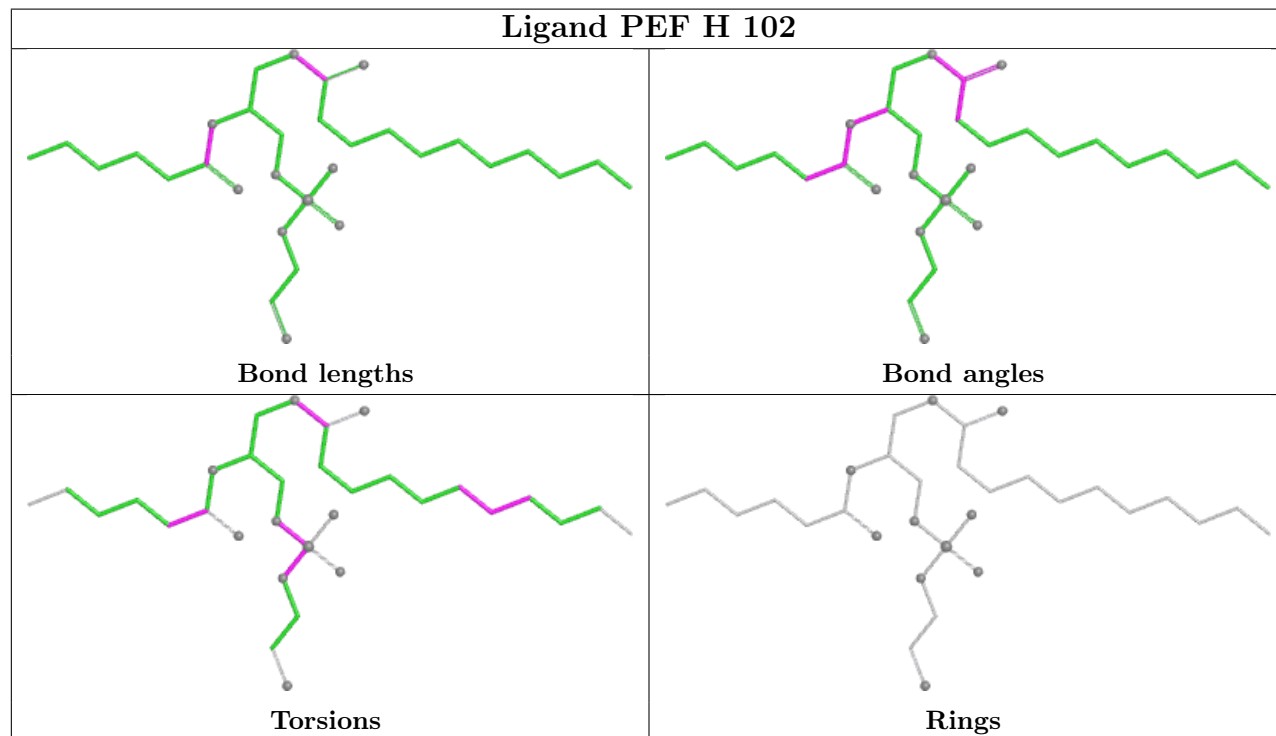


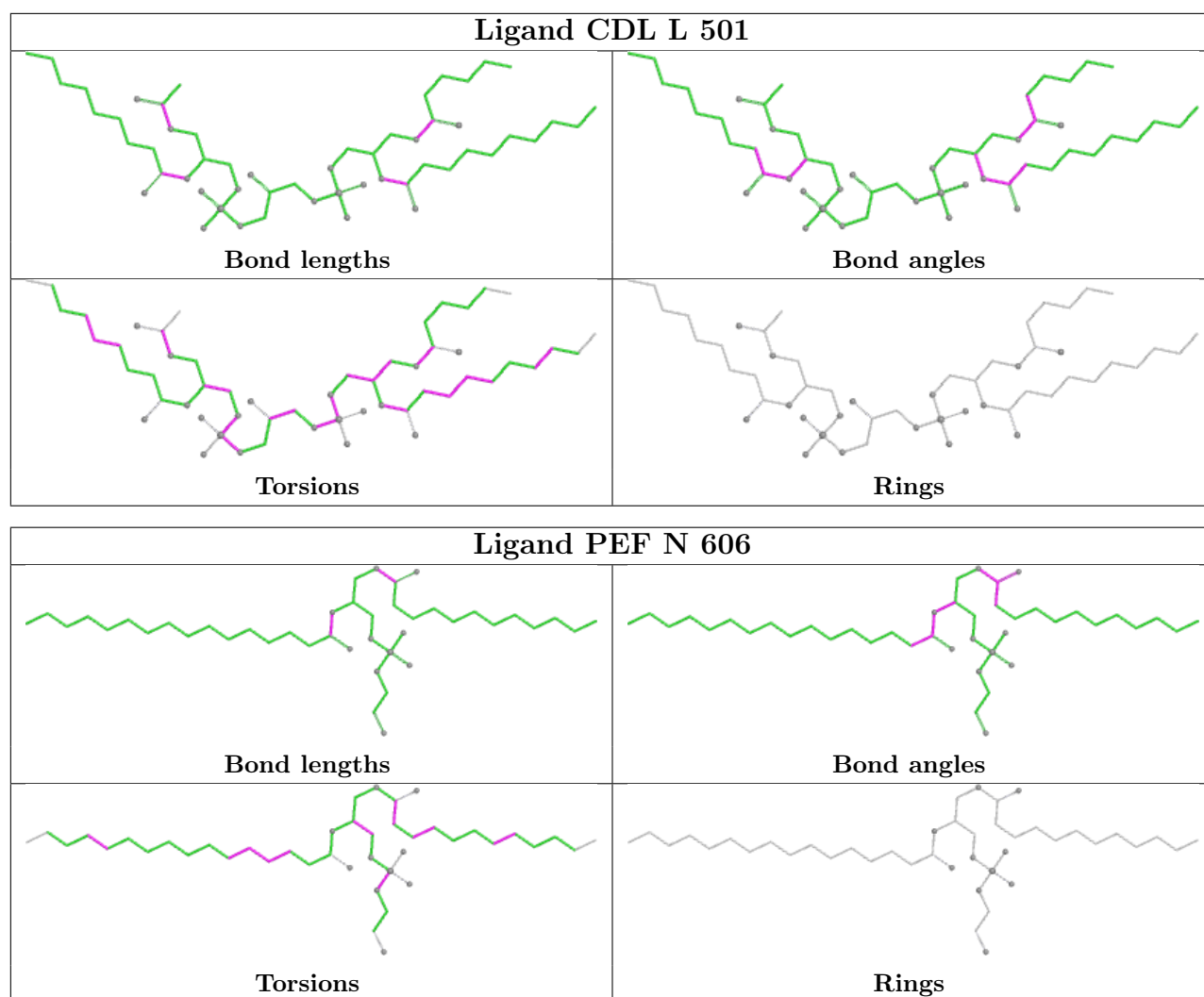


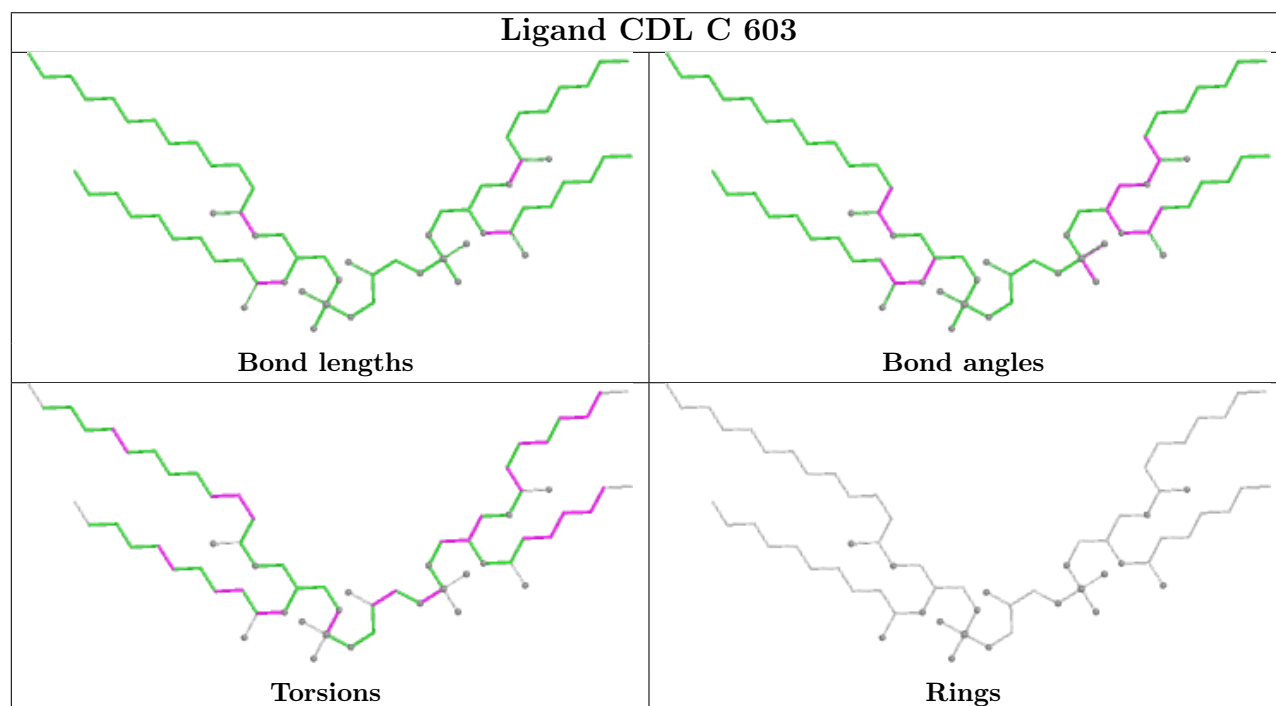
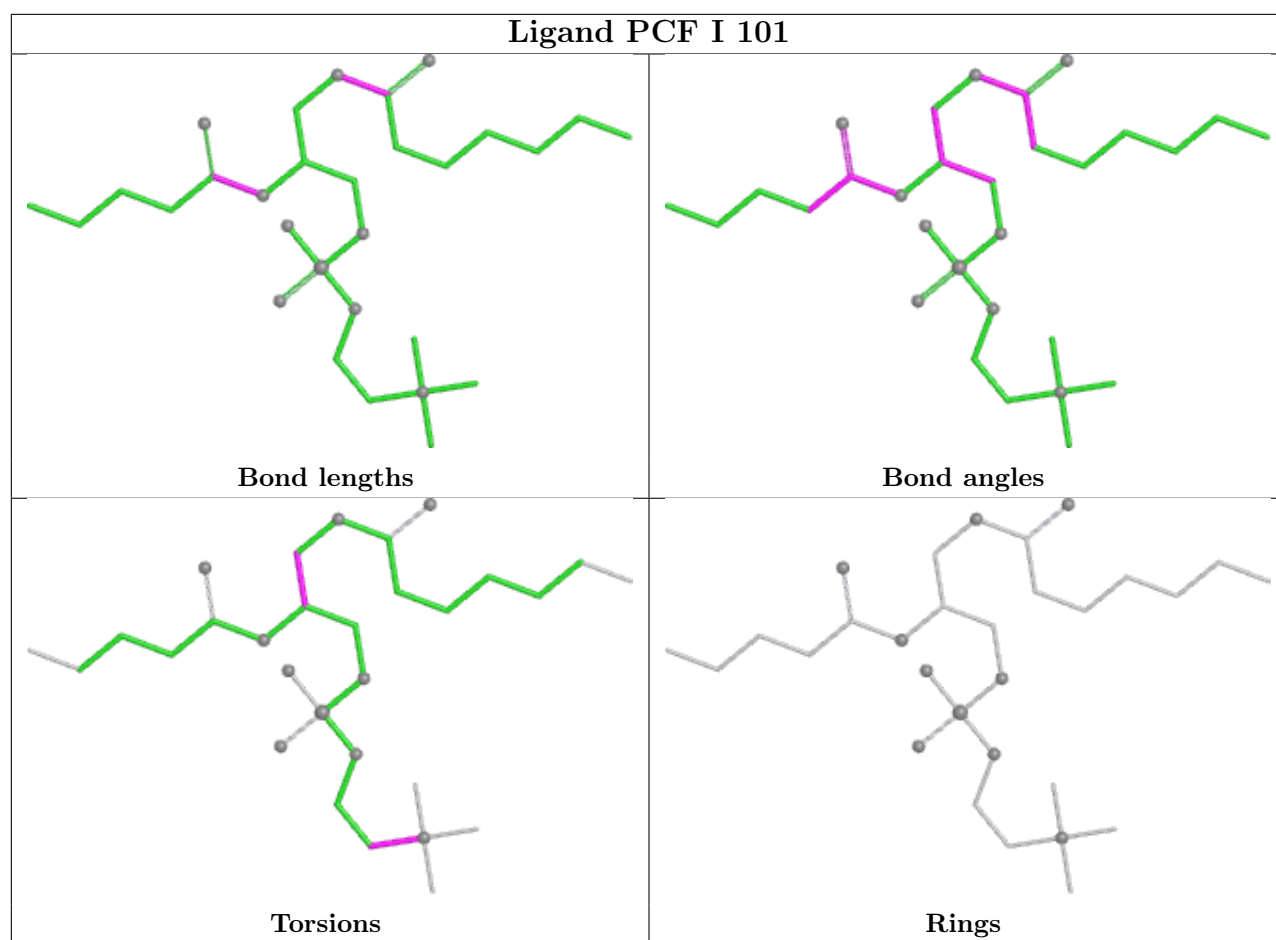
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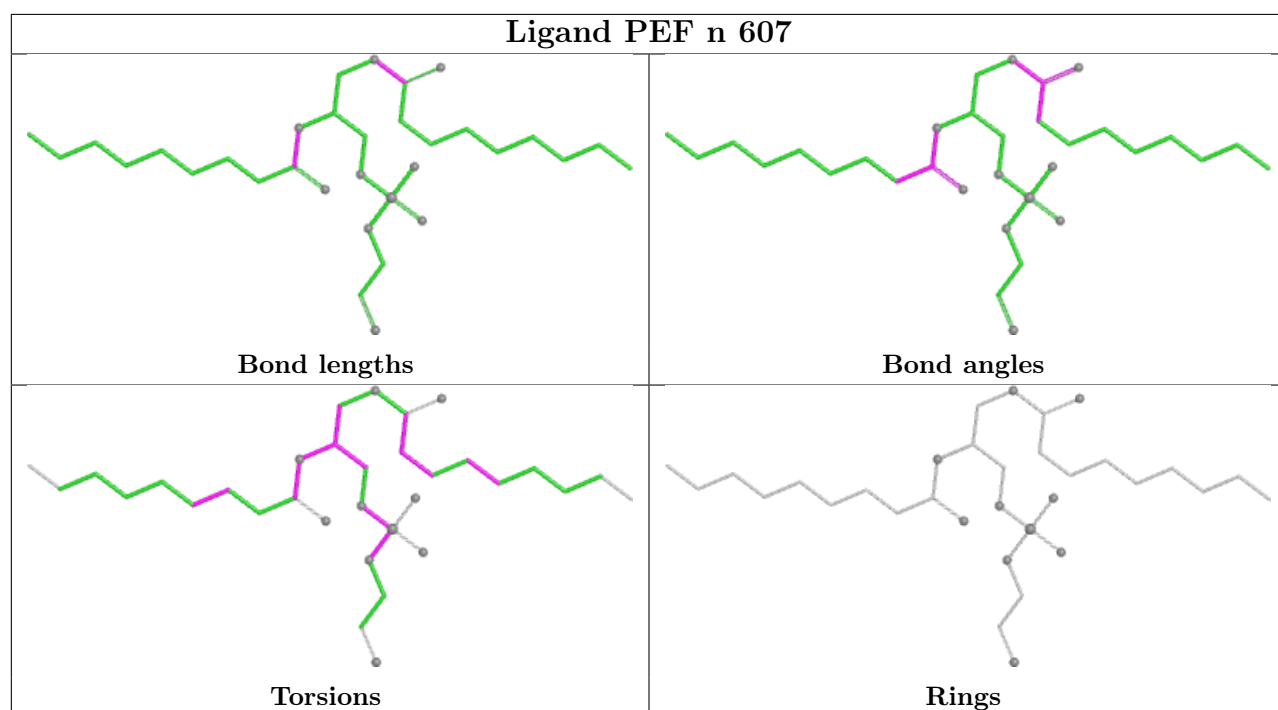
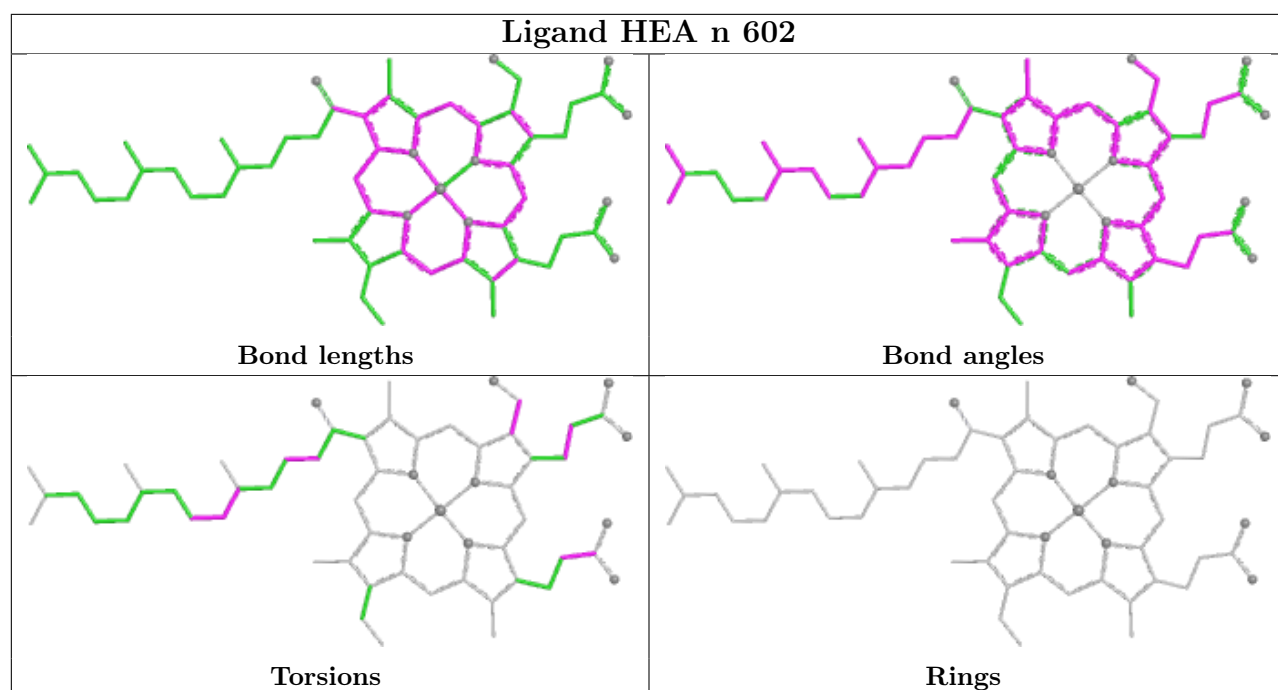


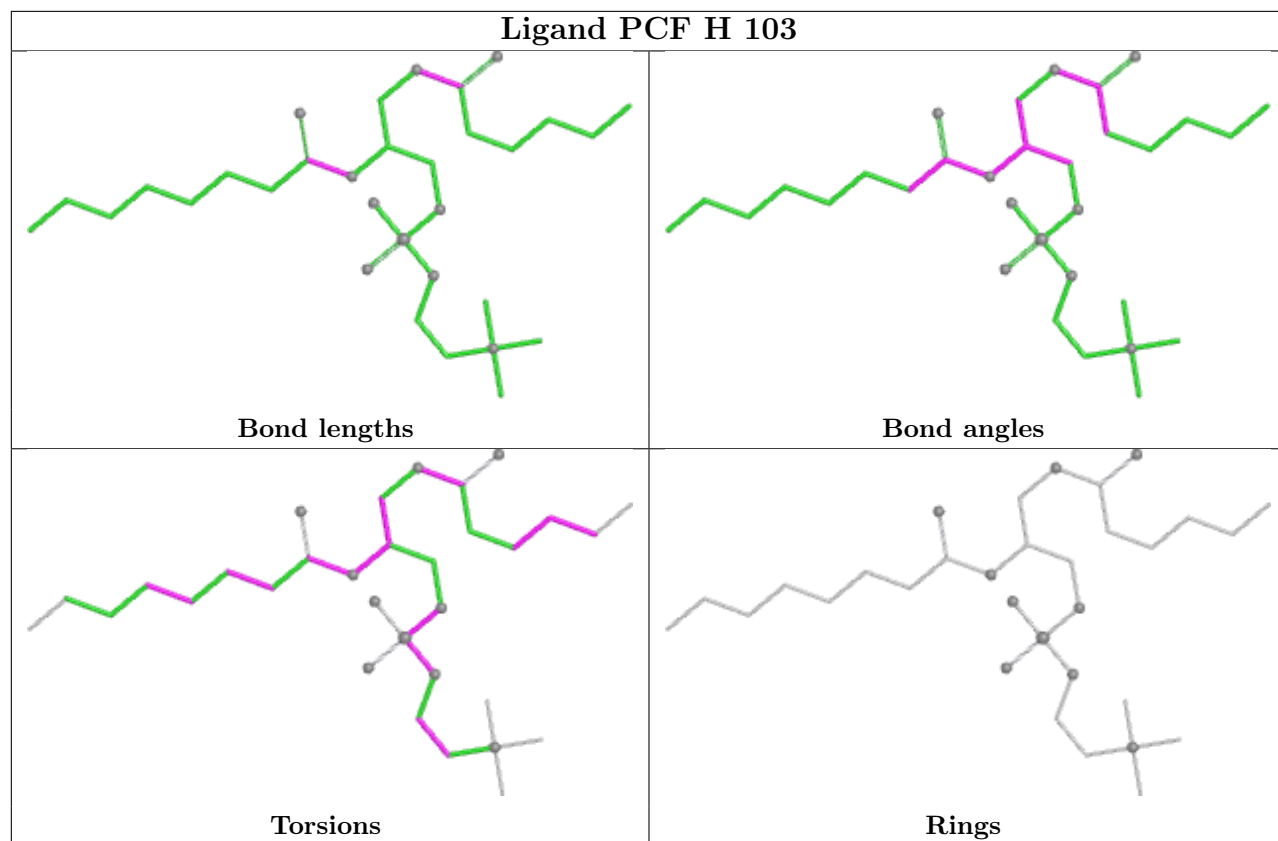
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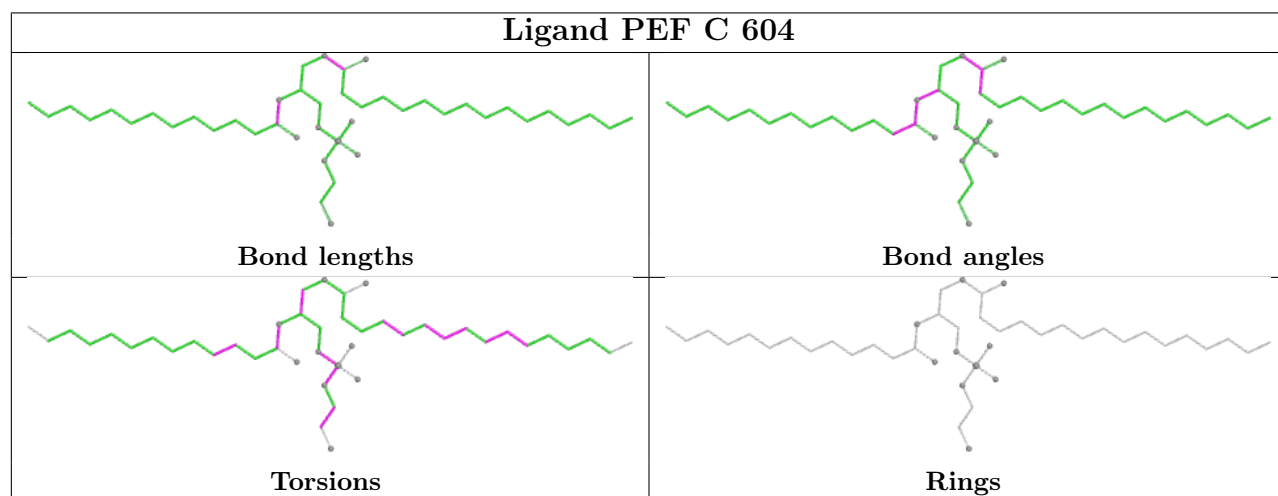
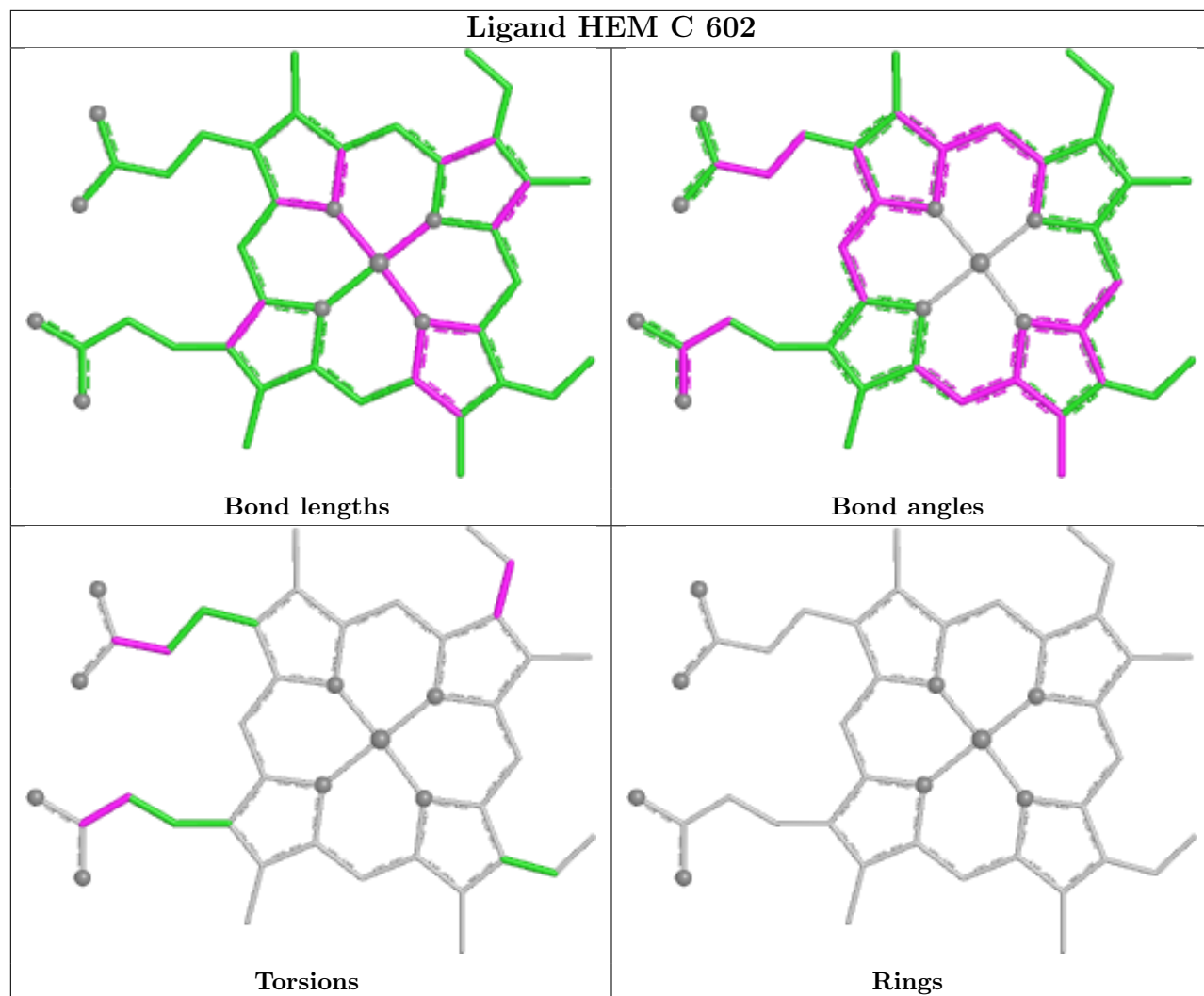


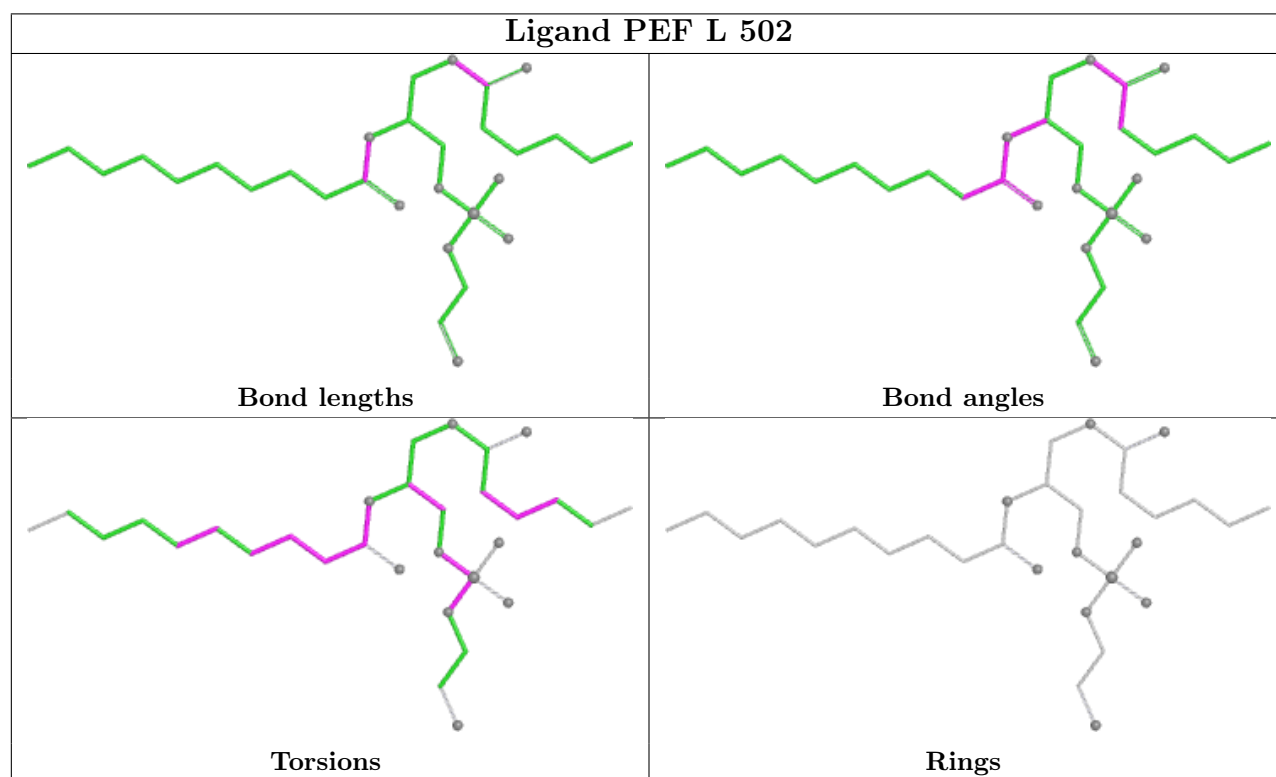
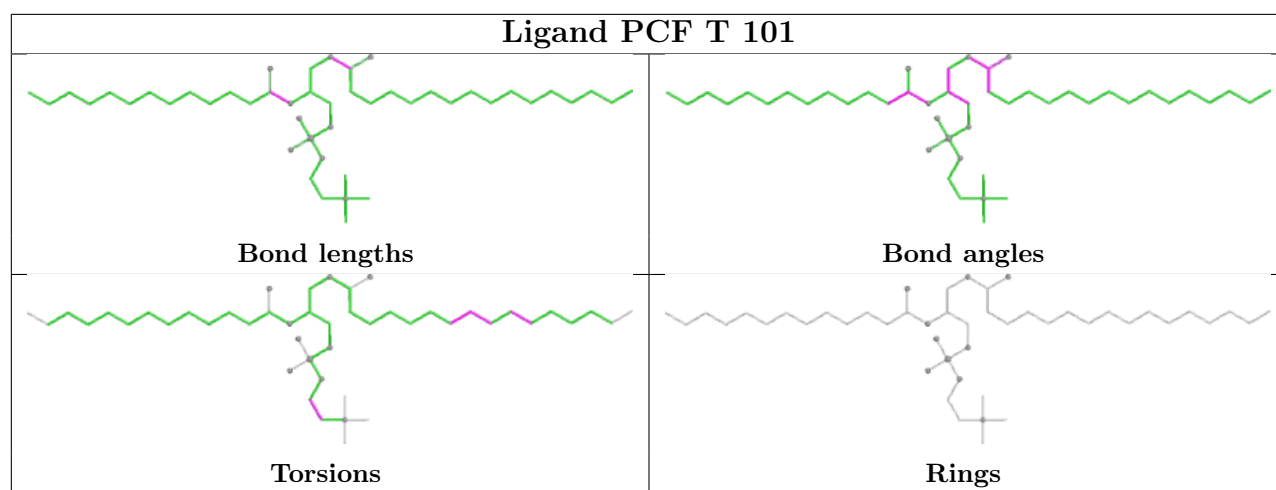


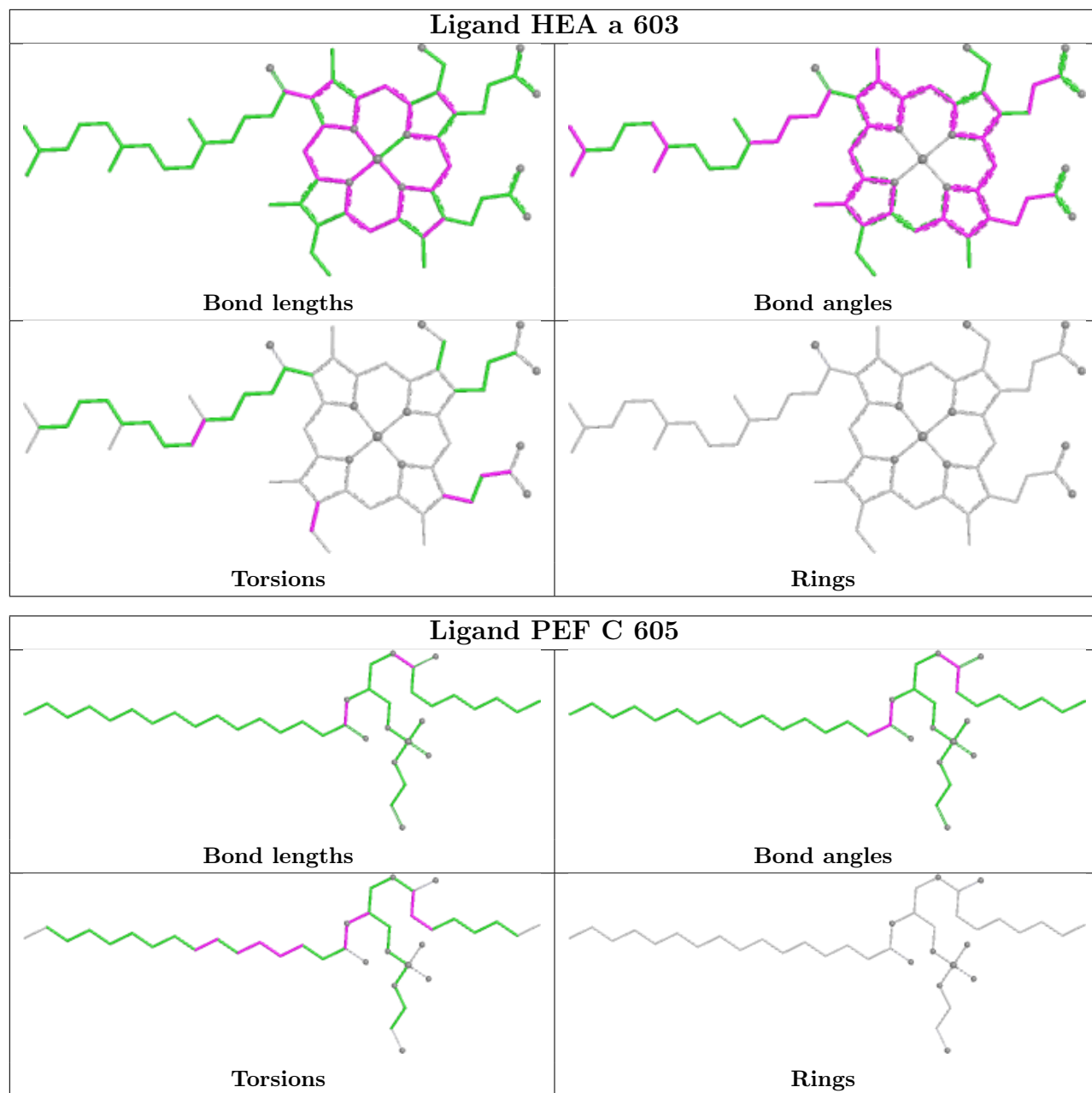


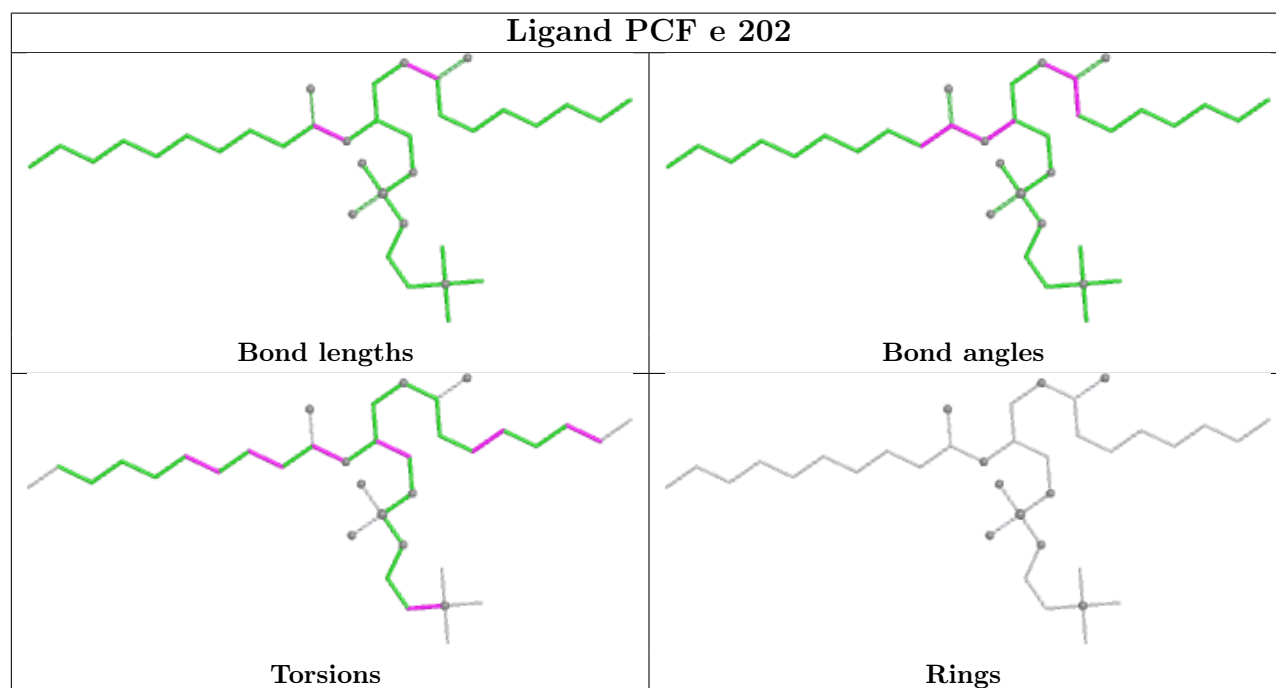
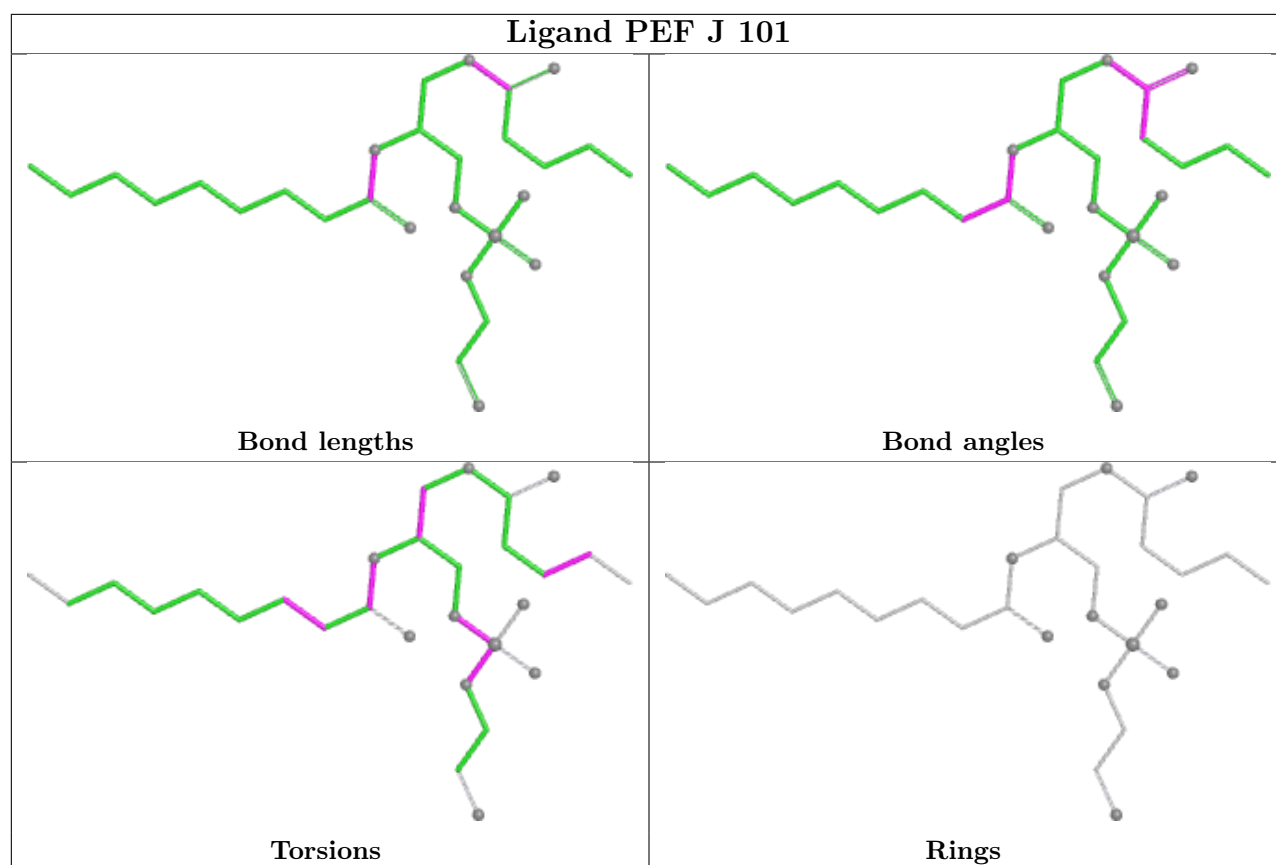




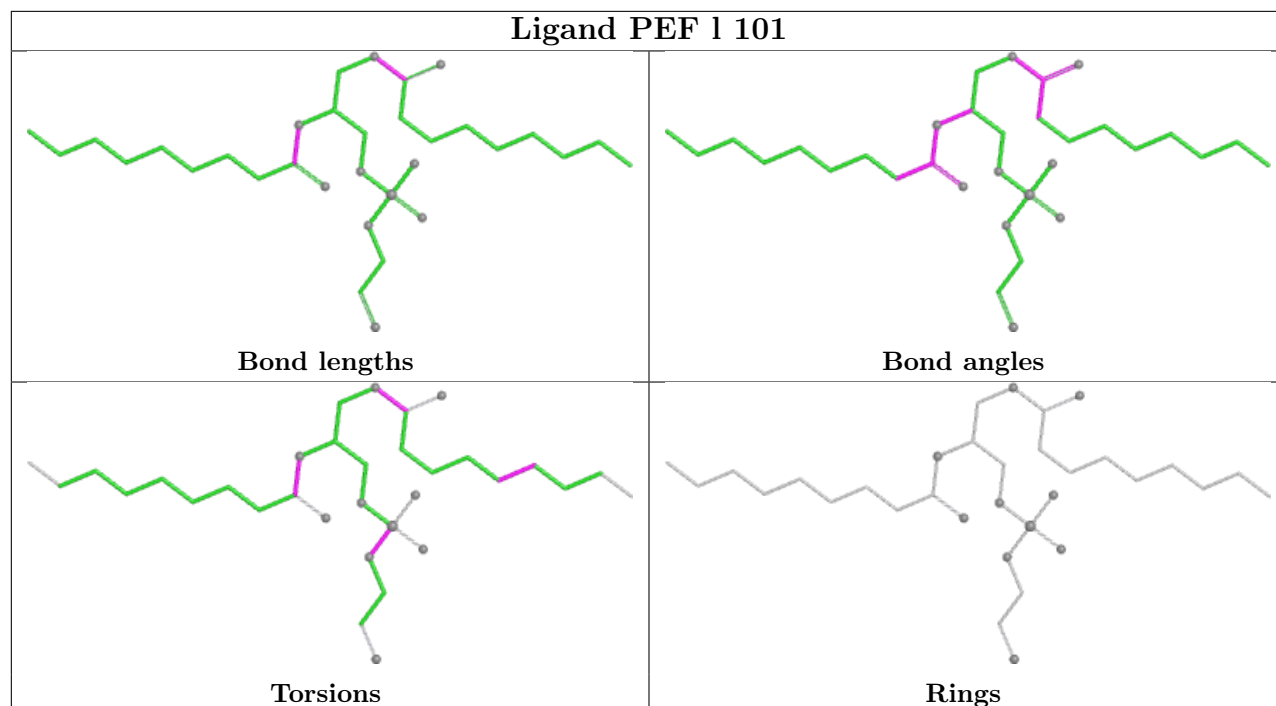




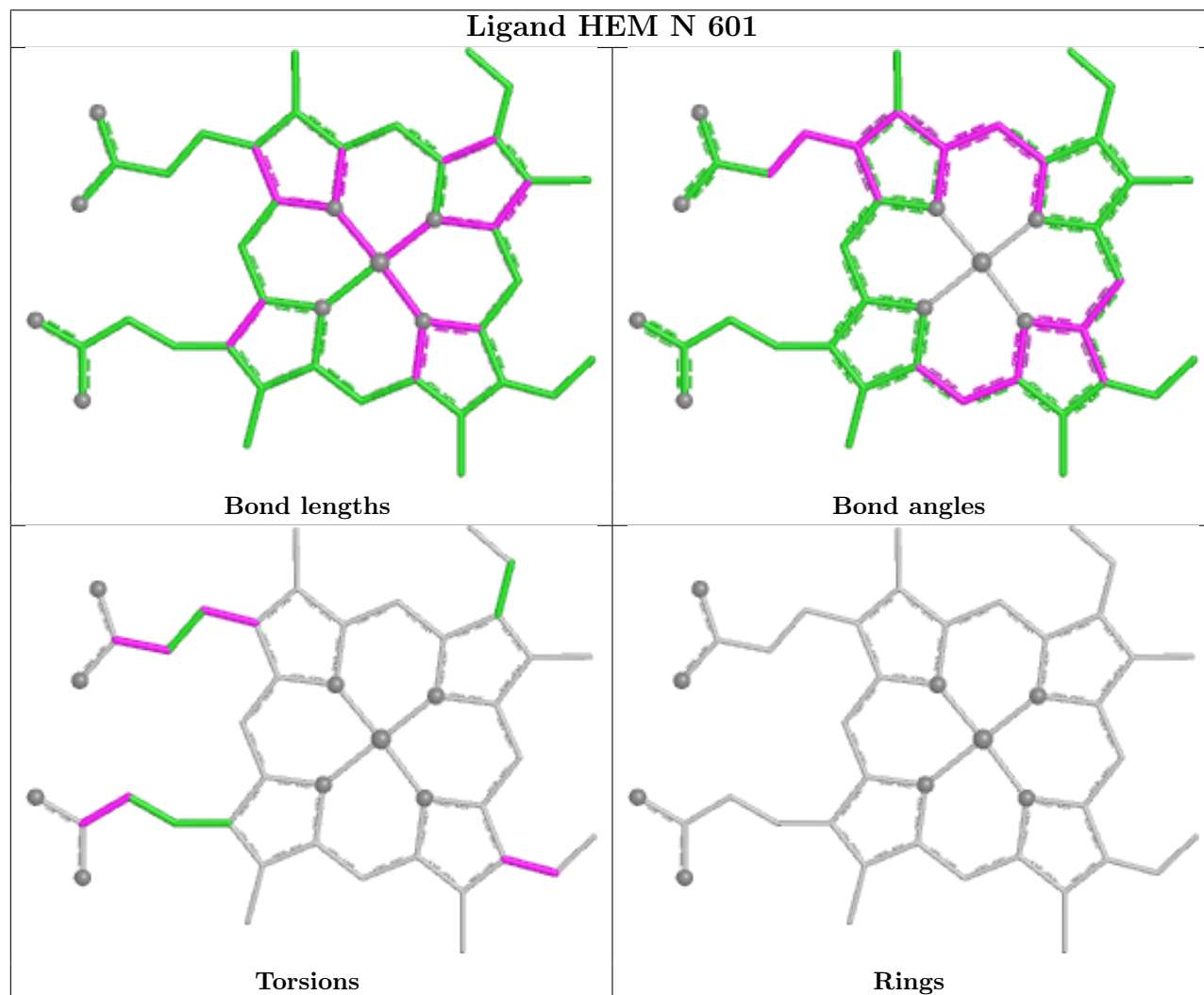


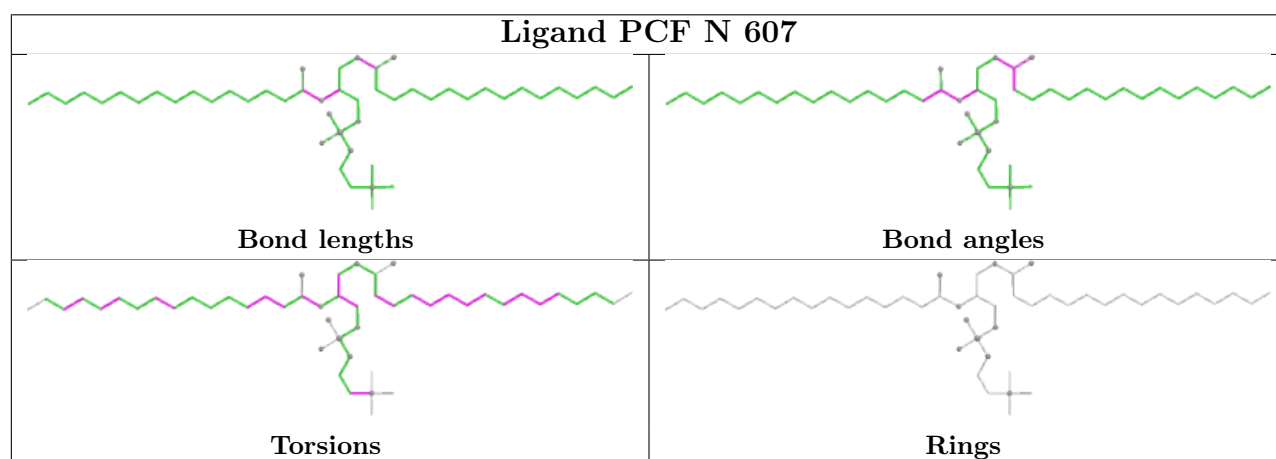
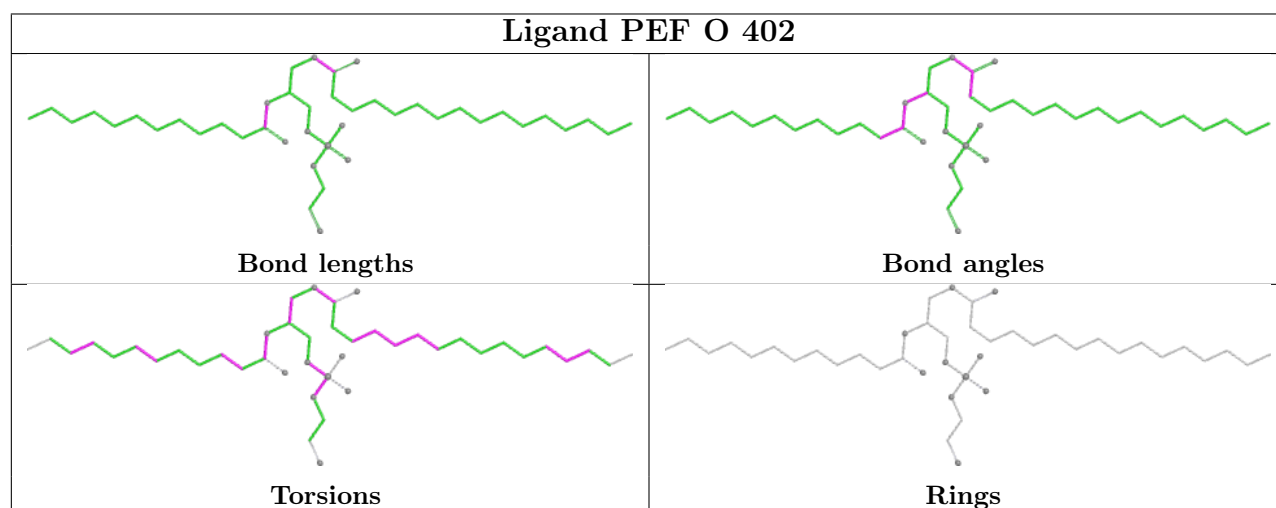
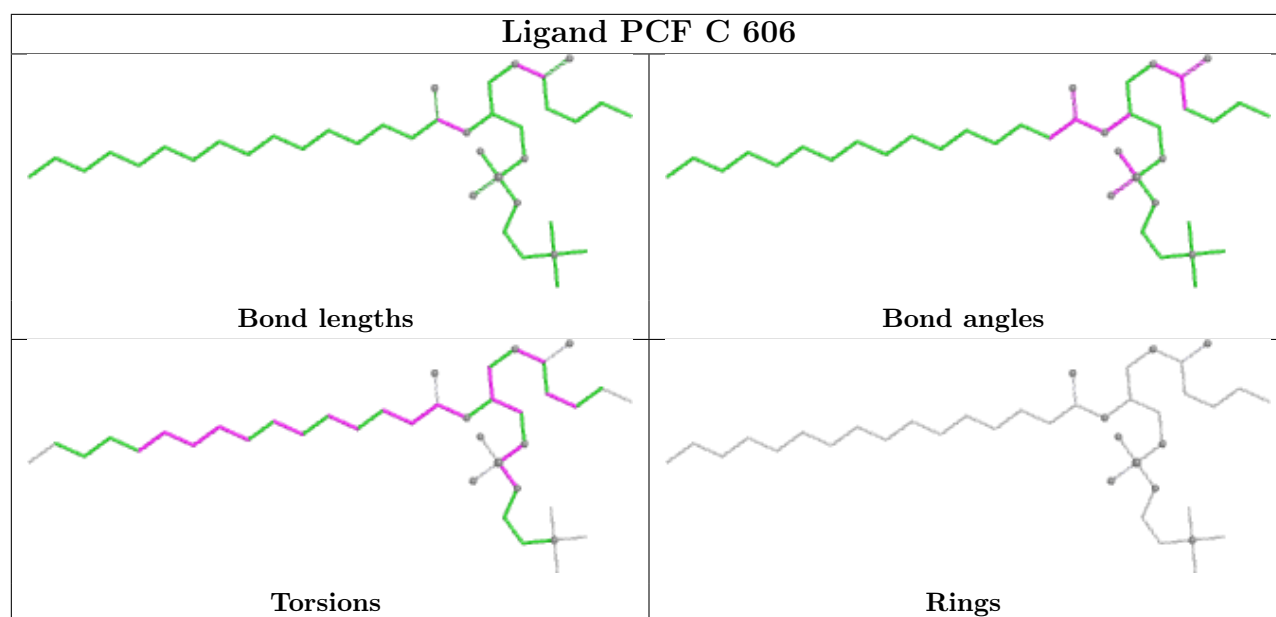


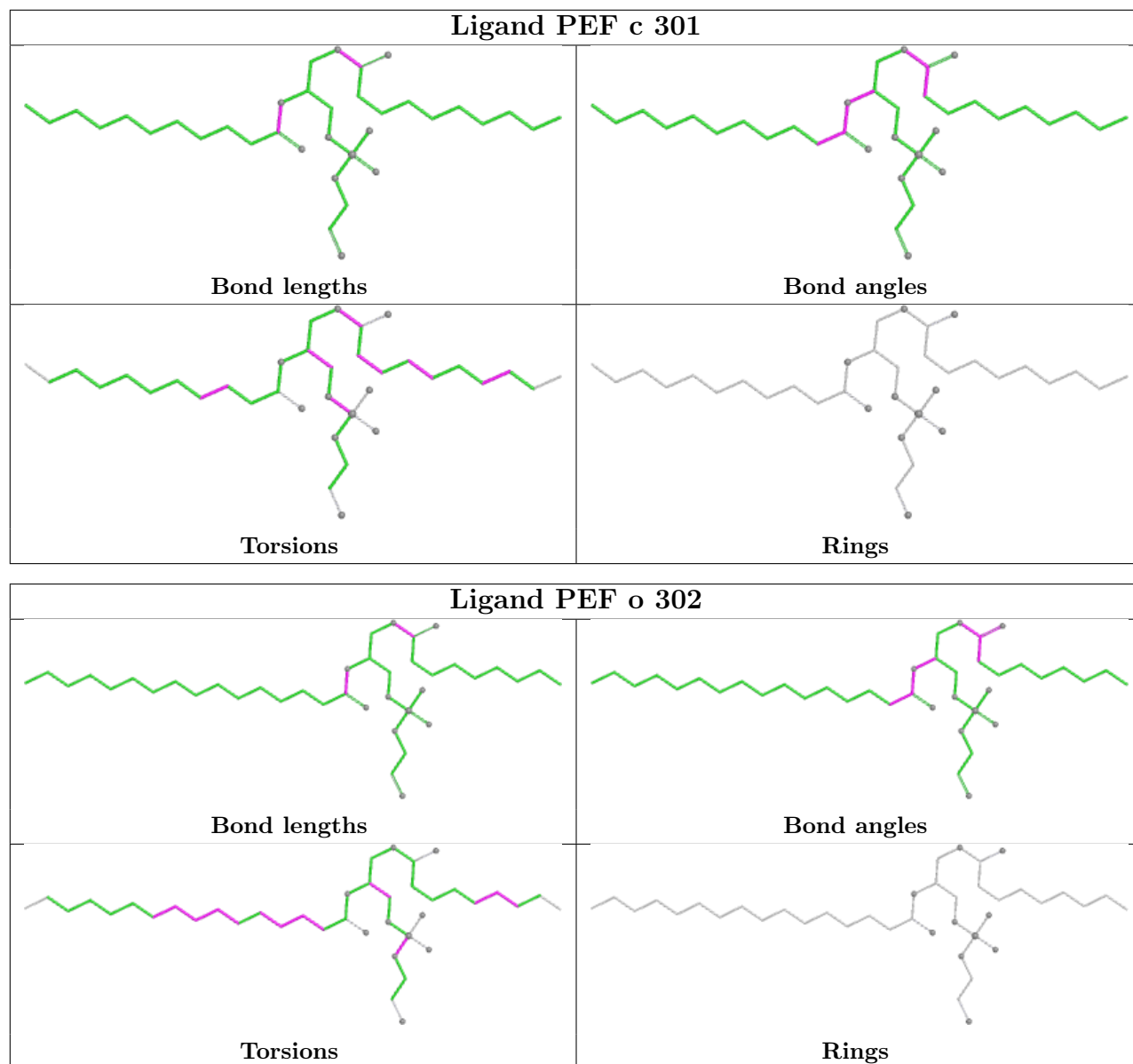
Ligand PEF 1 101

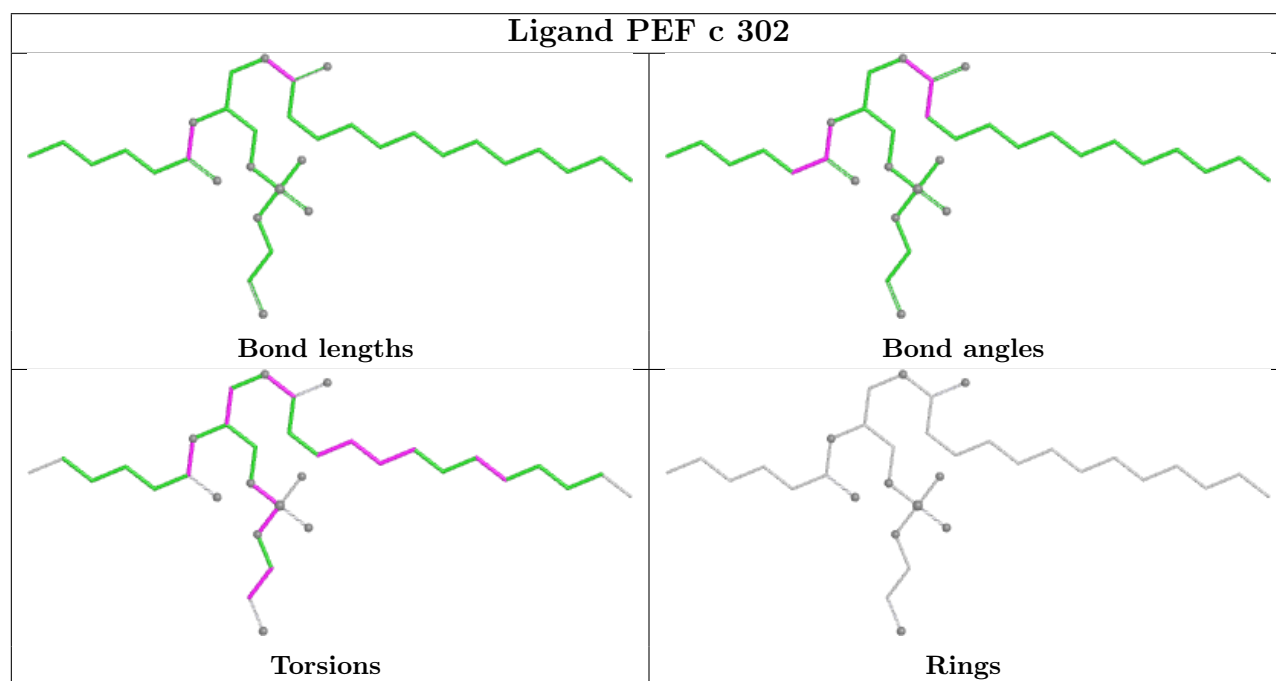
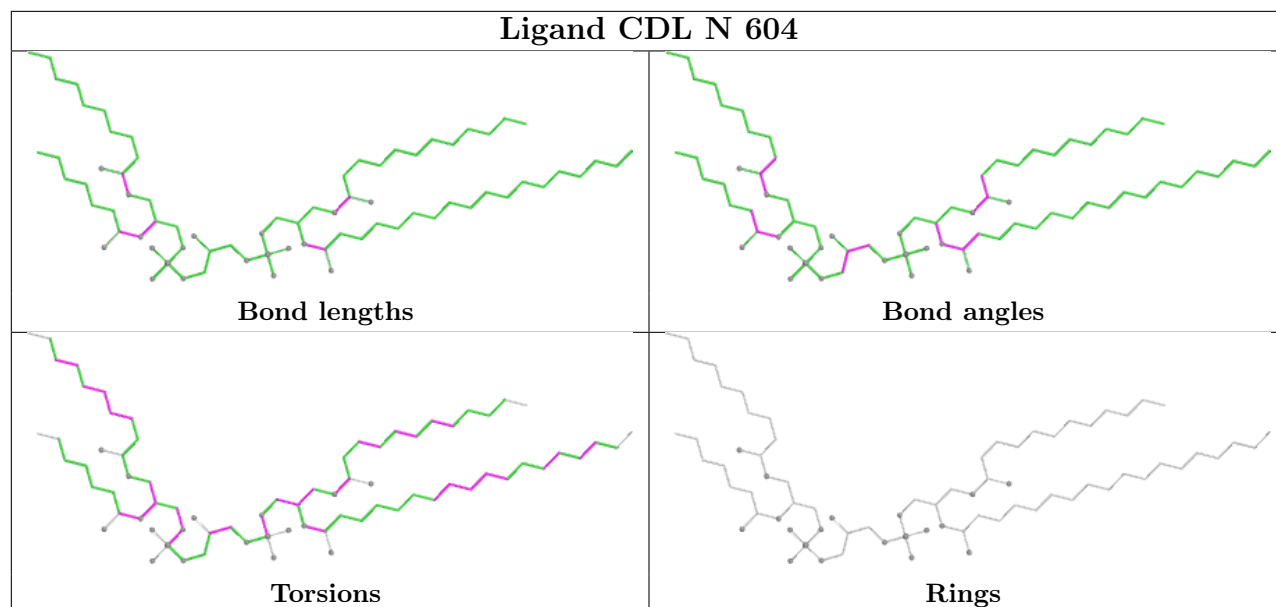


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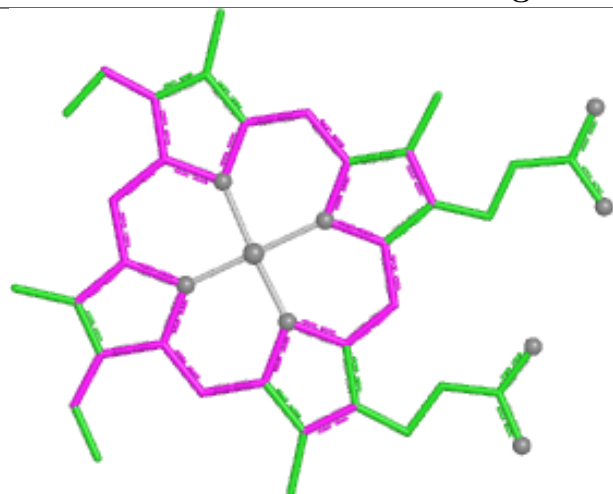




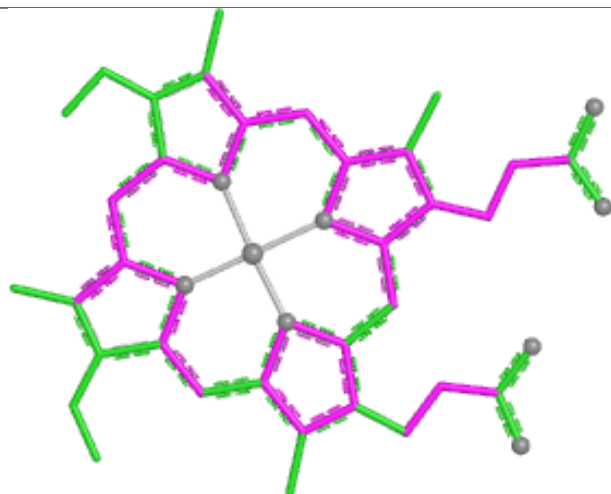




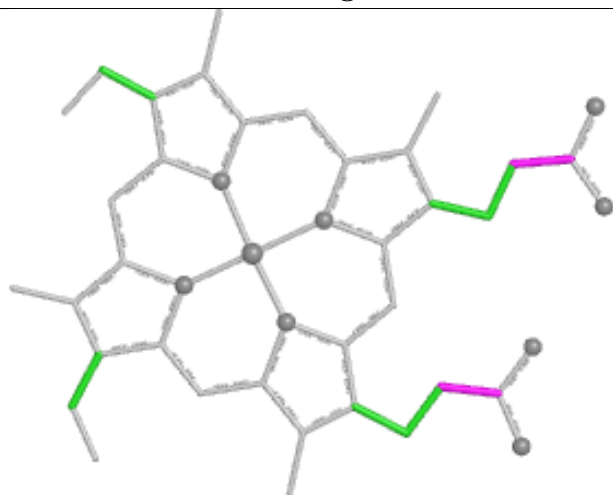
Ligand HEC O 401



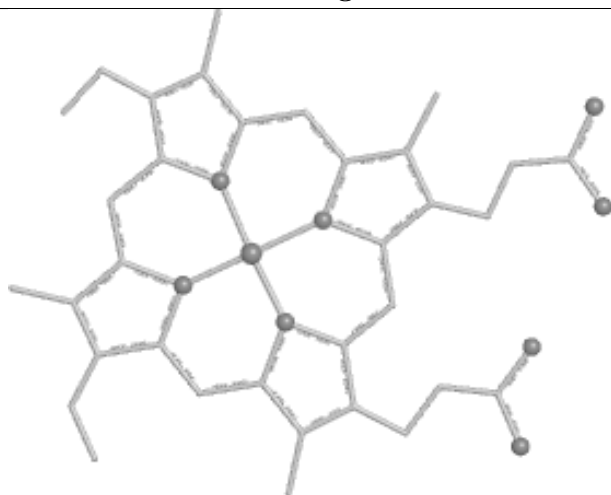
Bond lengths



Bond angles

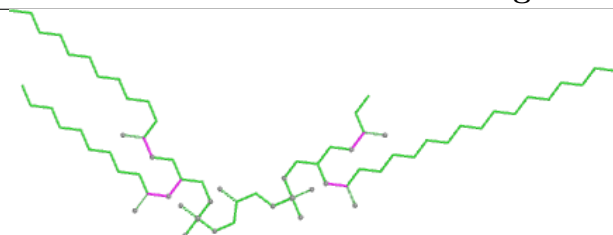


Torsions

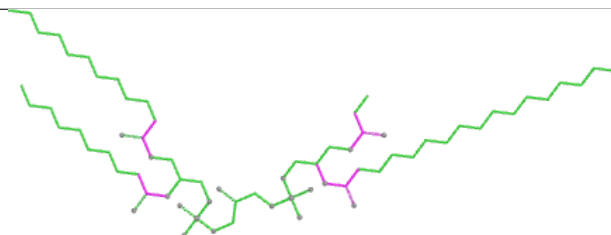


Rings

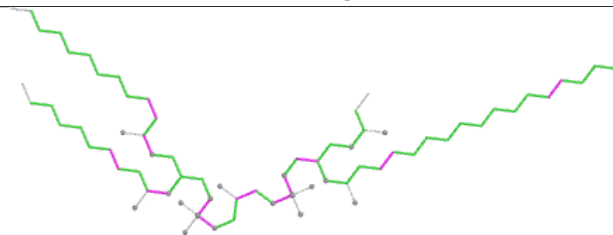
Ligand CDL D 402



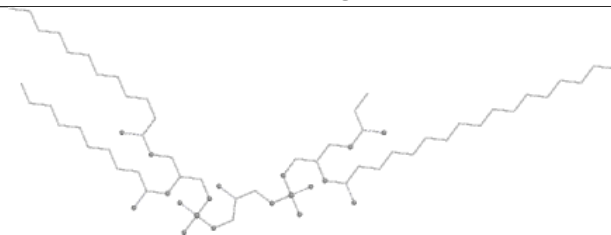
Bond lengths



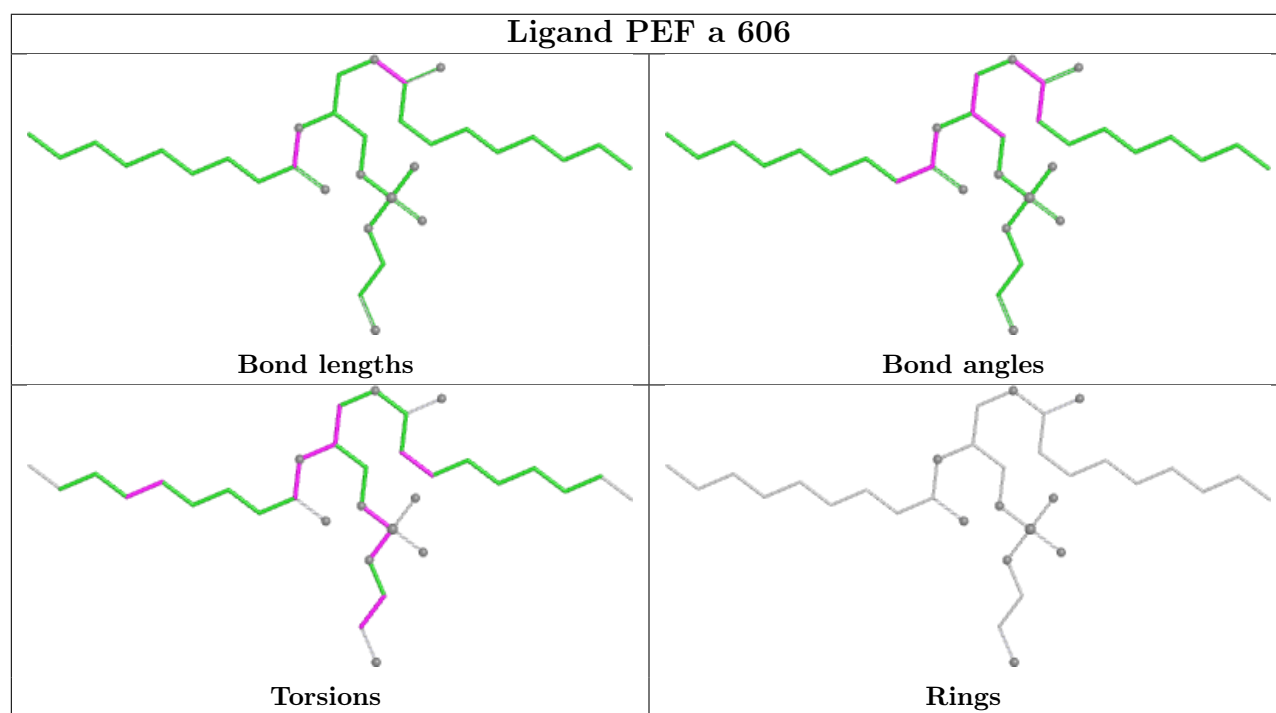
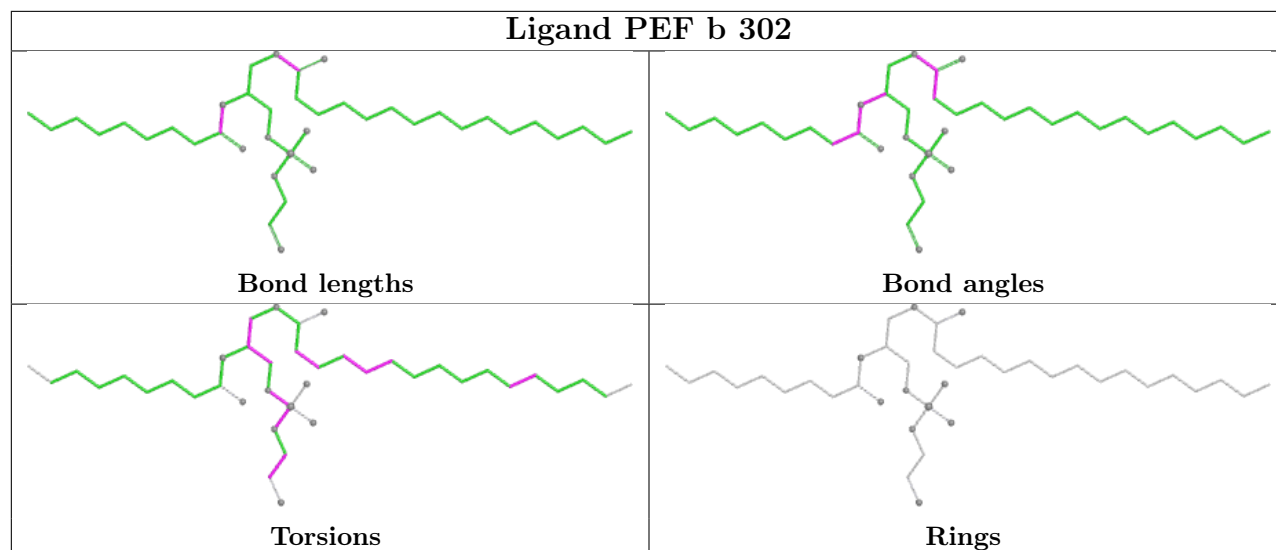
Bond angles

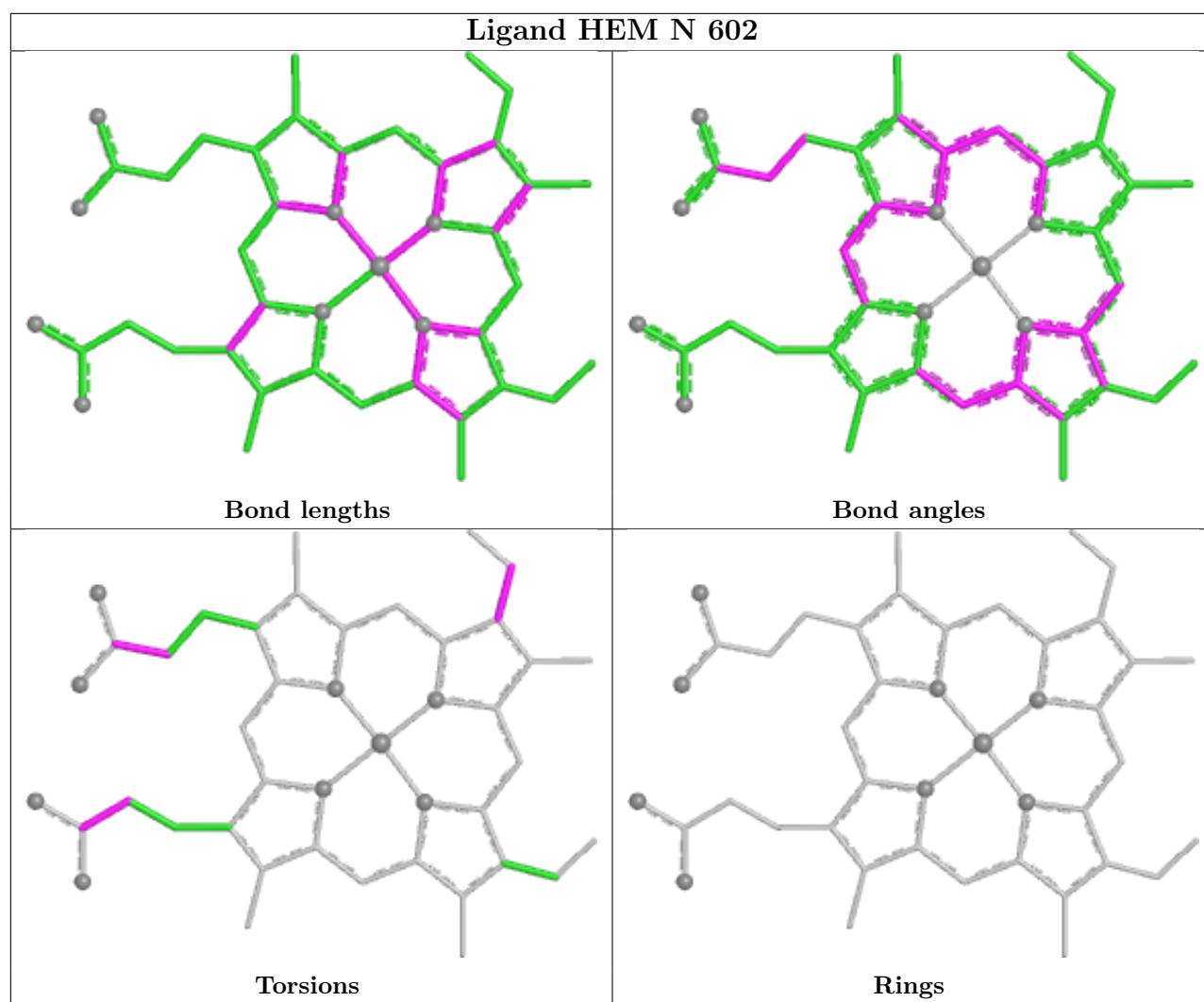
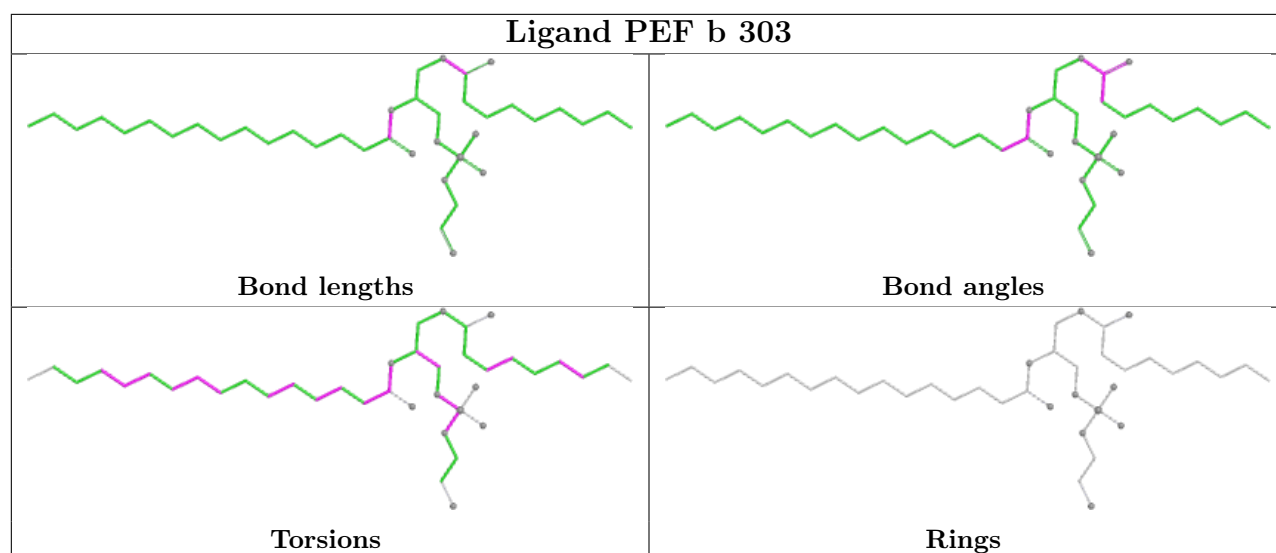


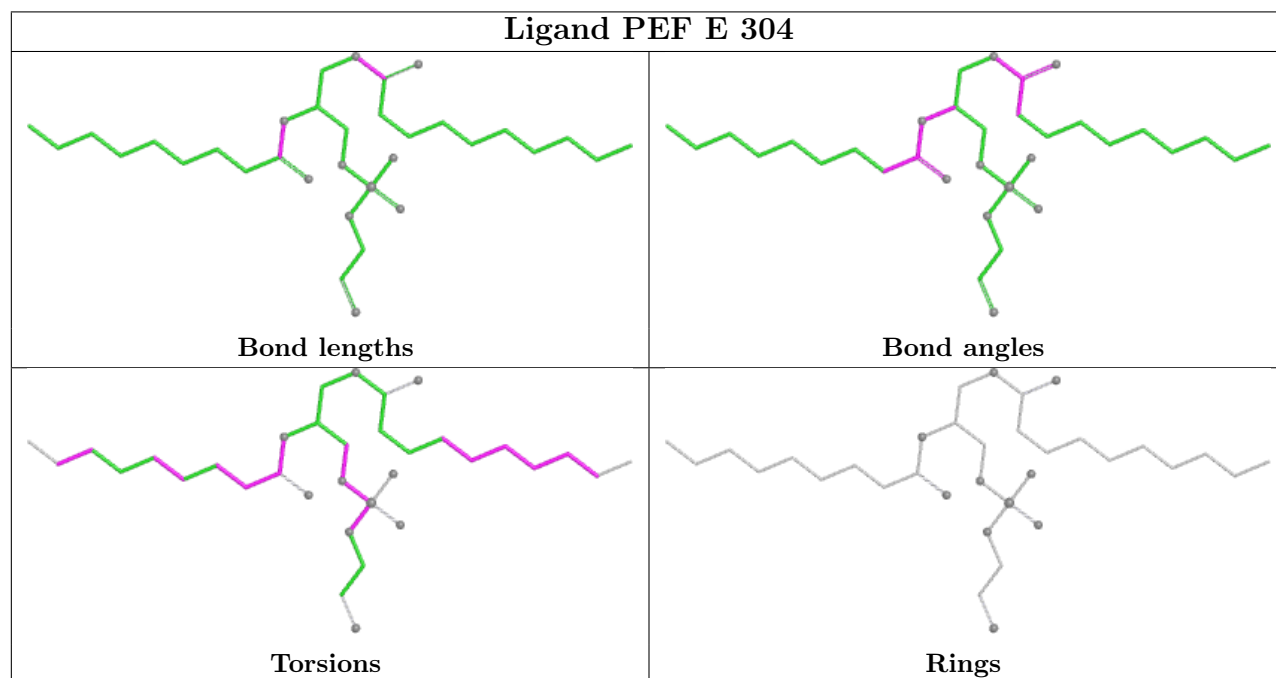
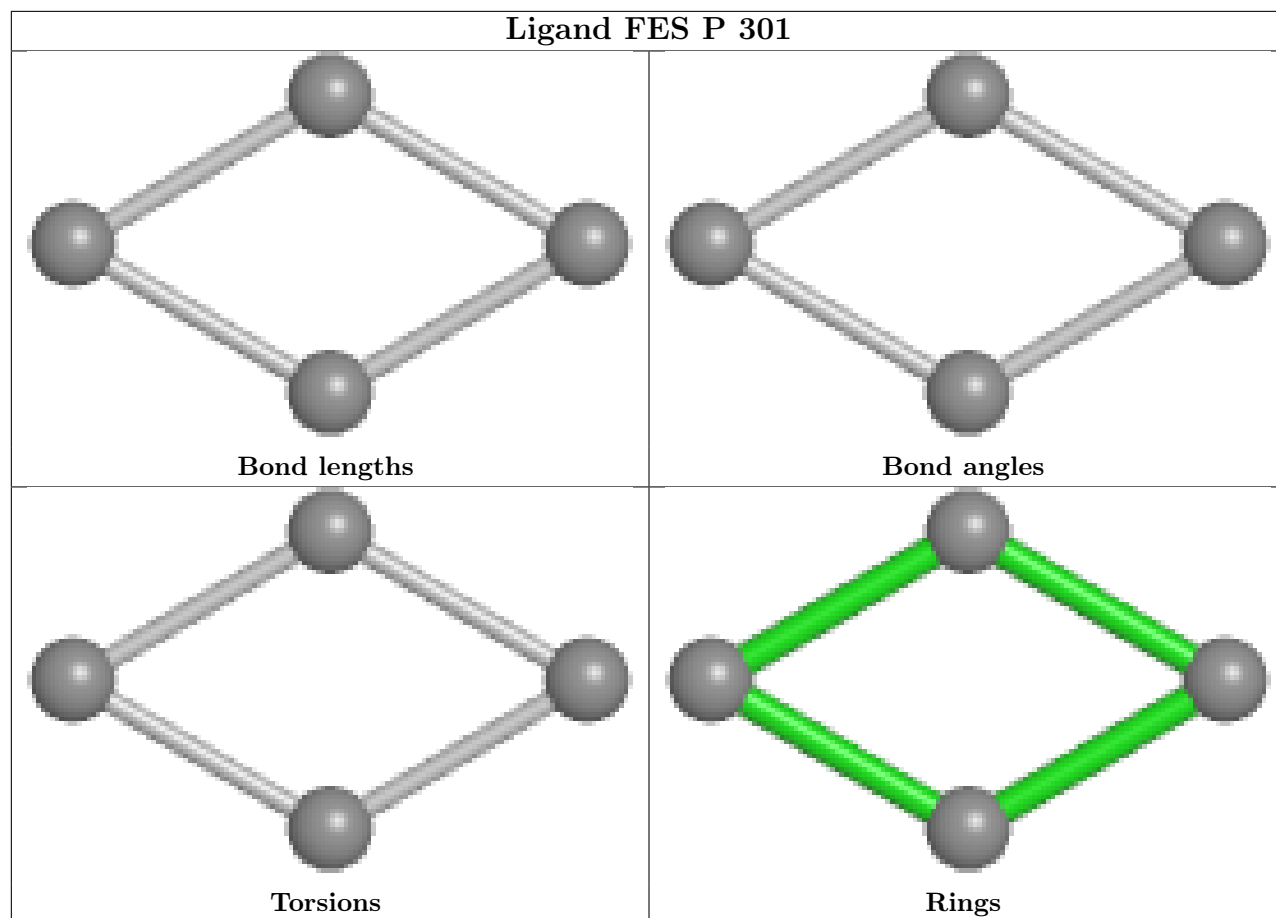
Torsions

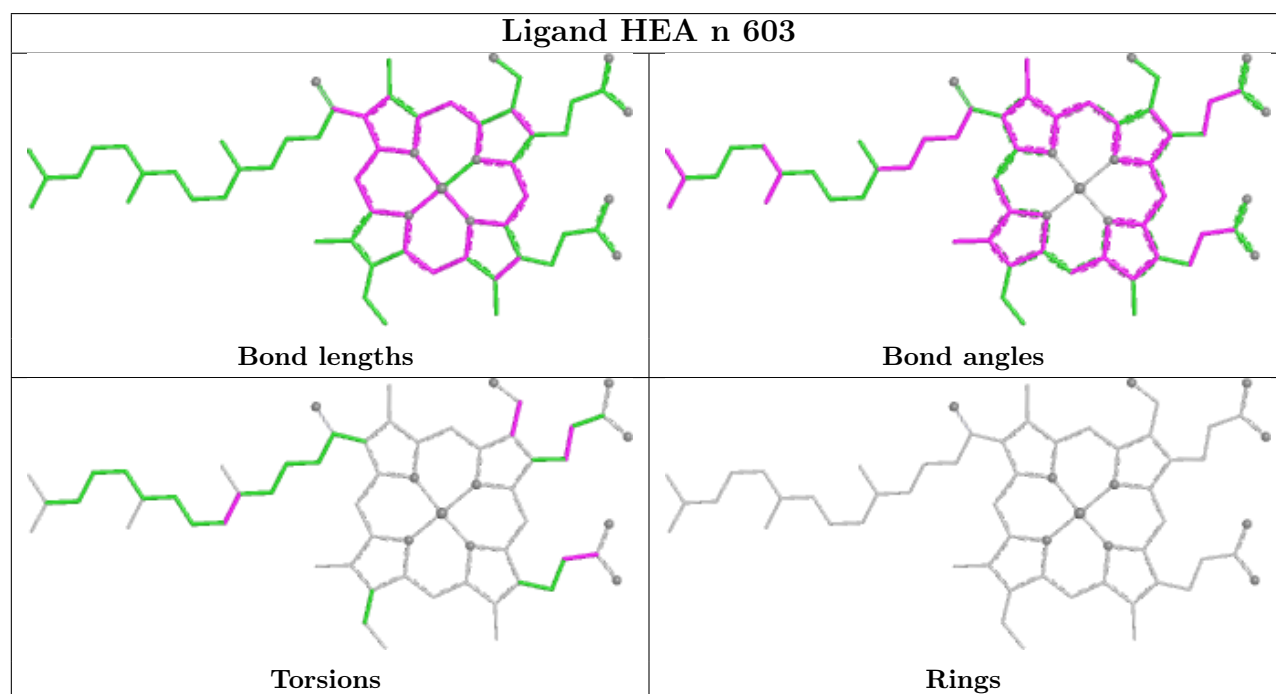
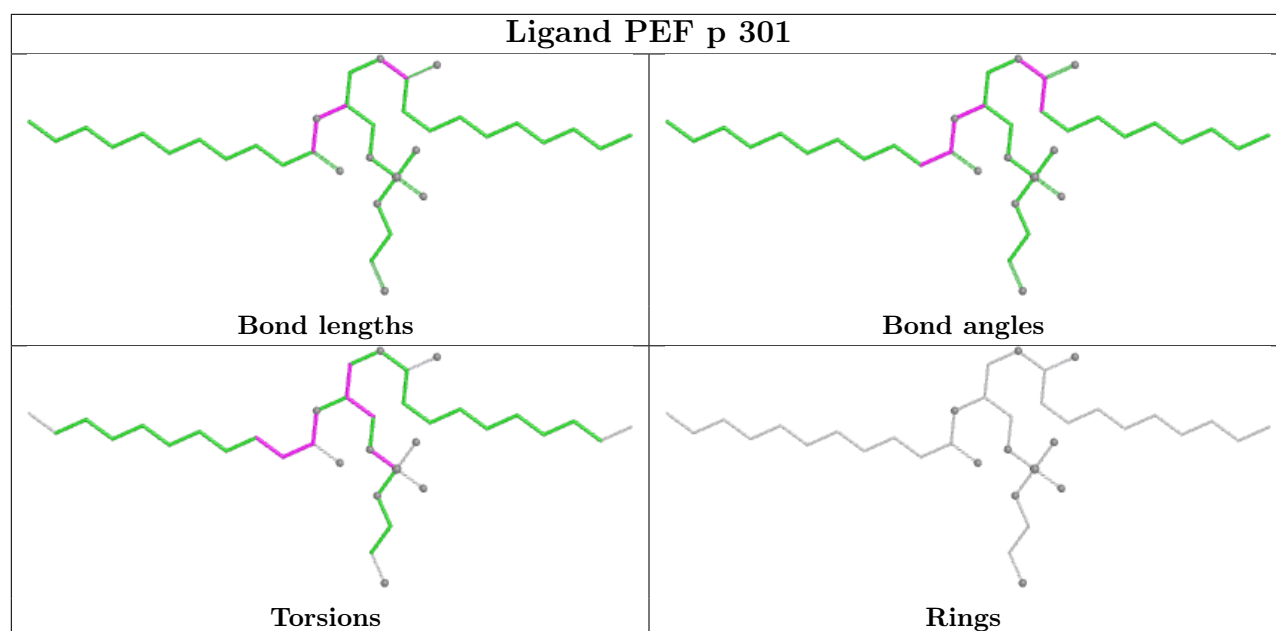


Rings

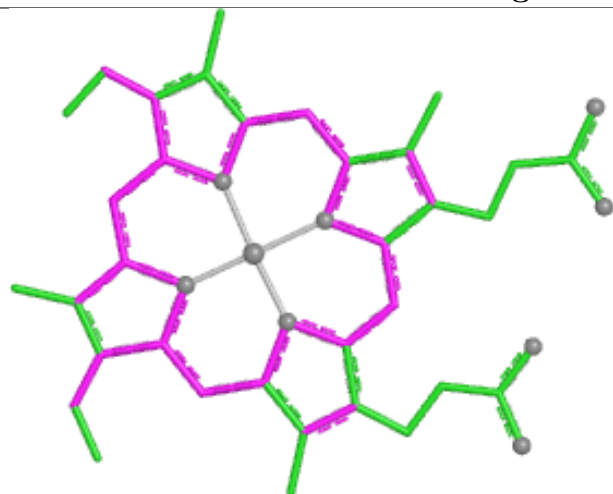




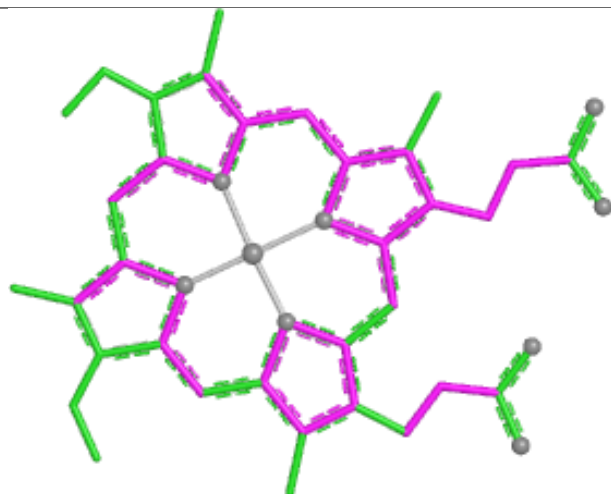




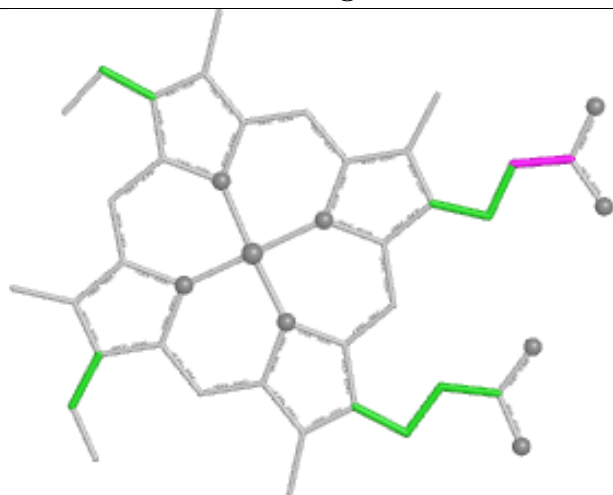
Ligand HEC D 401



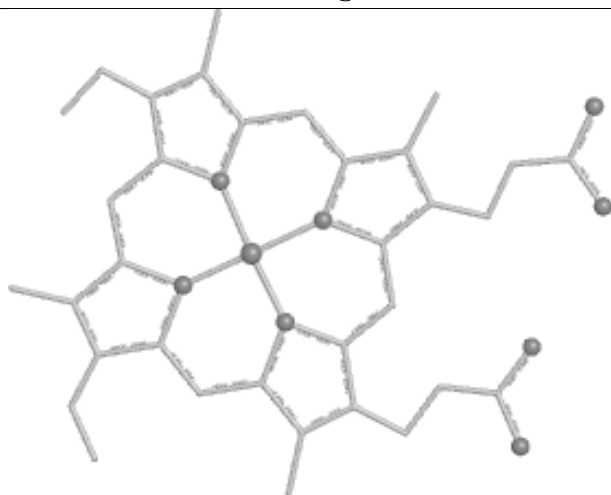
Bond lengths



Bond angles

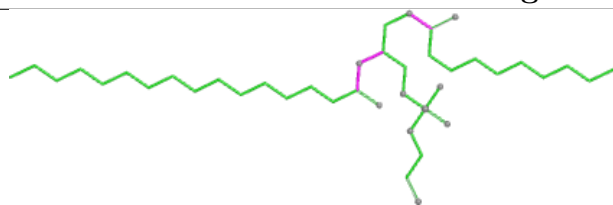


Torsions

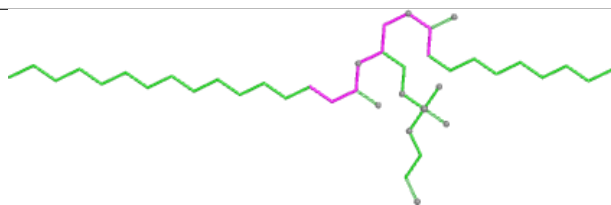


Rings

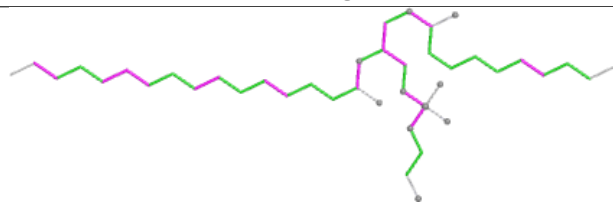
Ligand PEF e 201



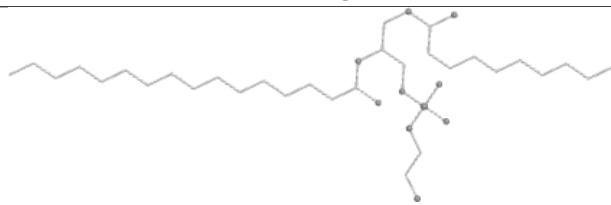
Bond lengths



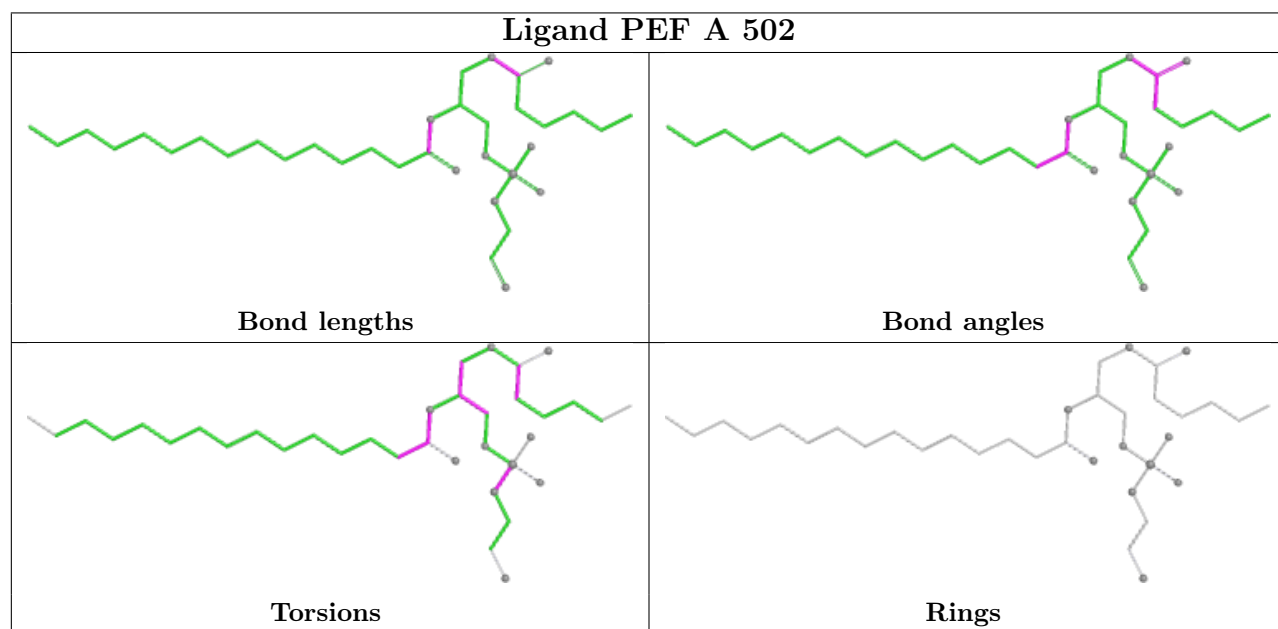
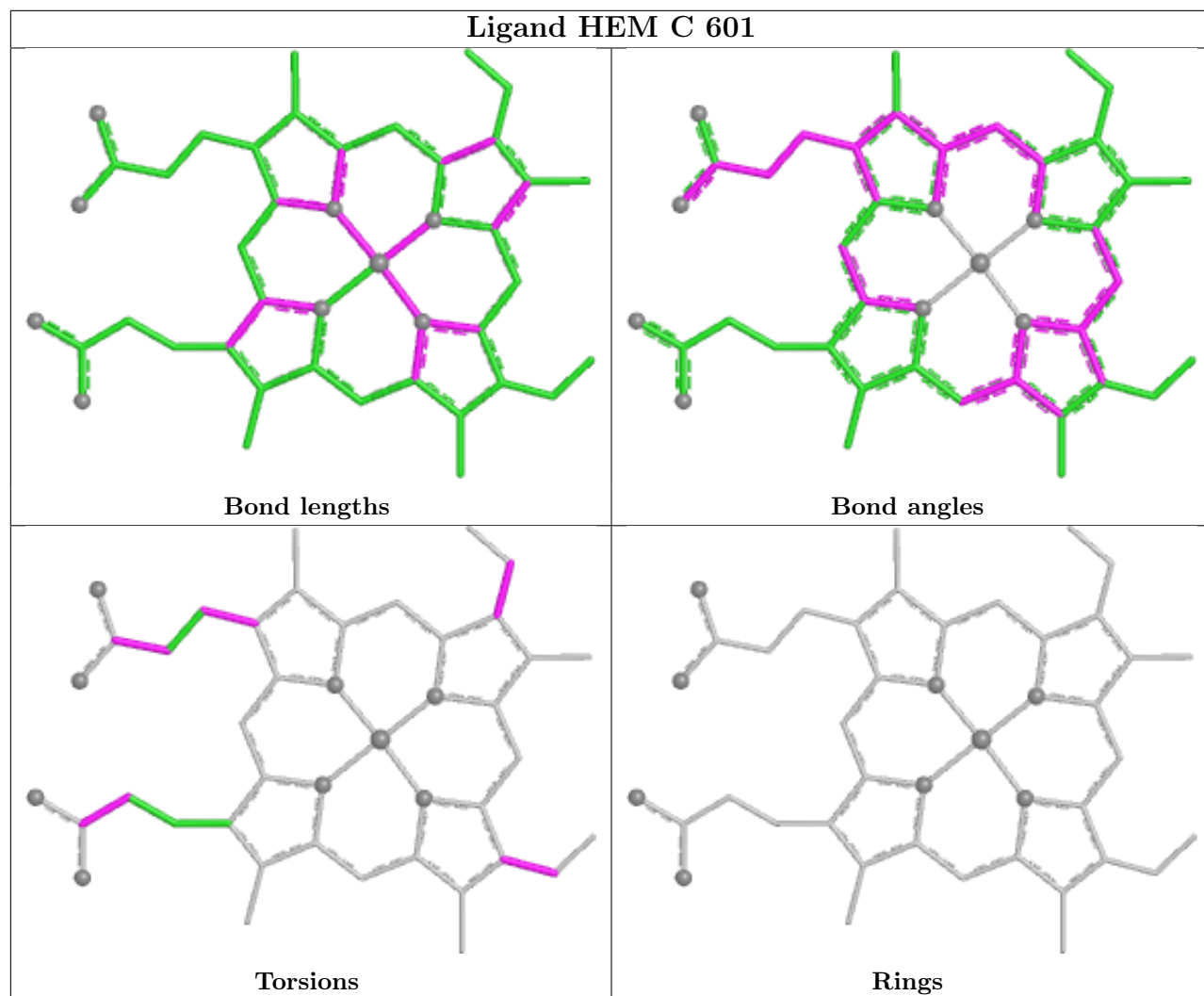
Bond angles

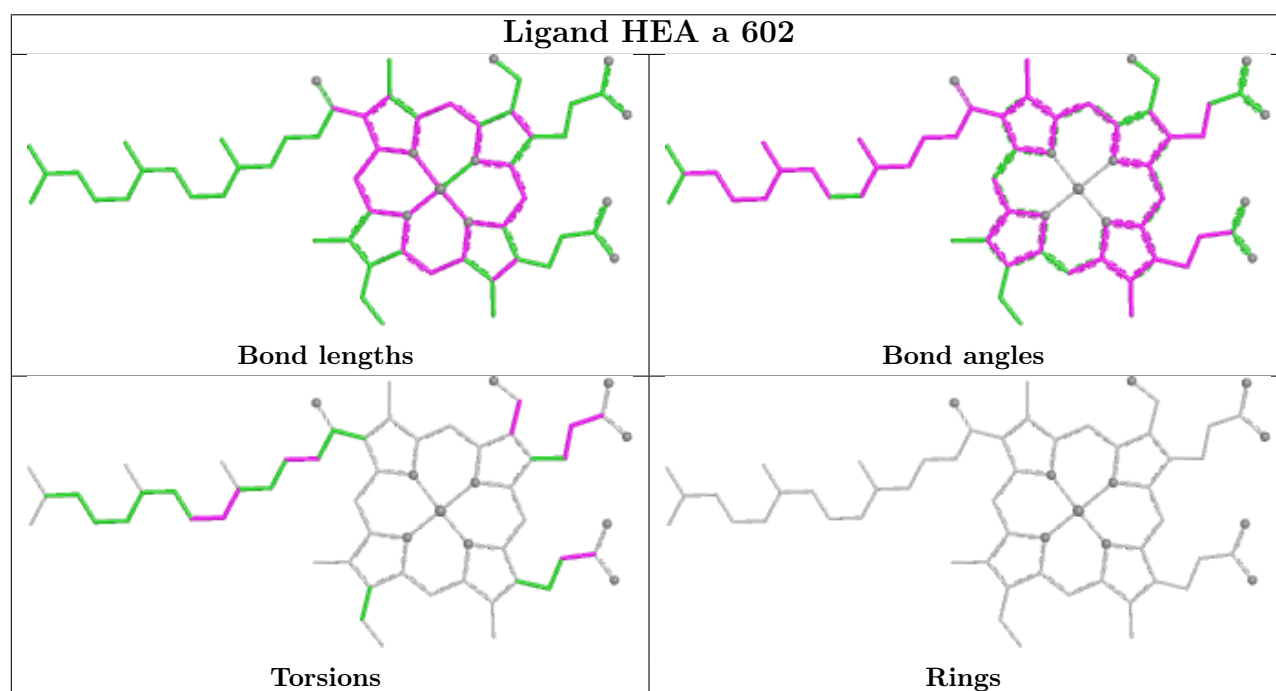
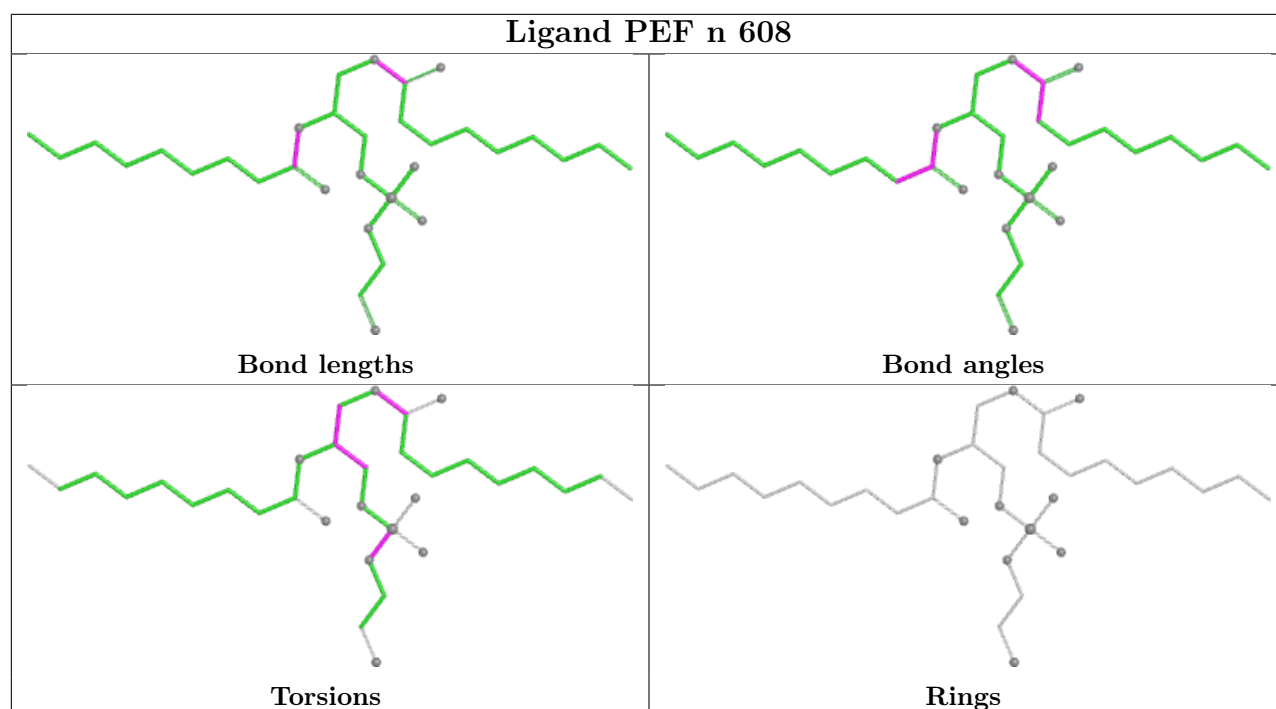


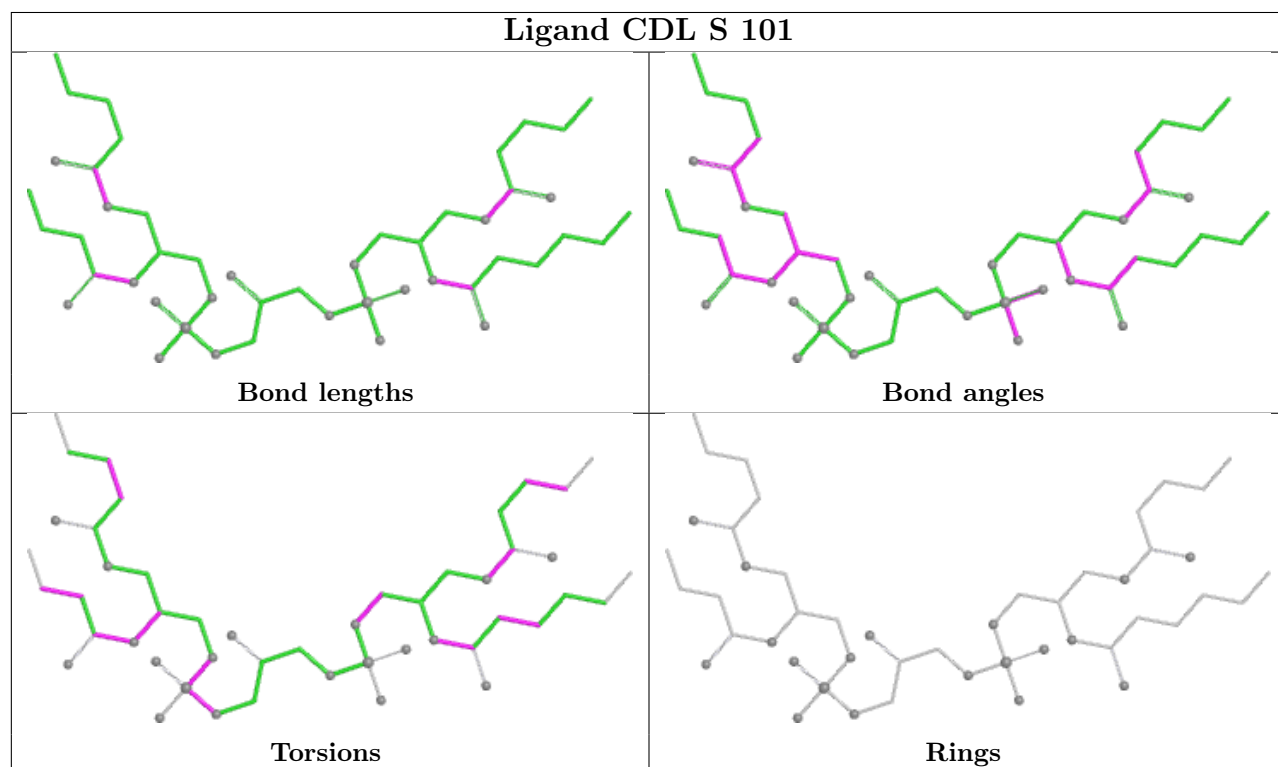
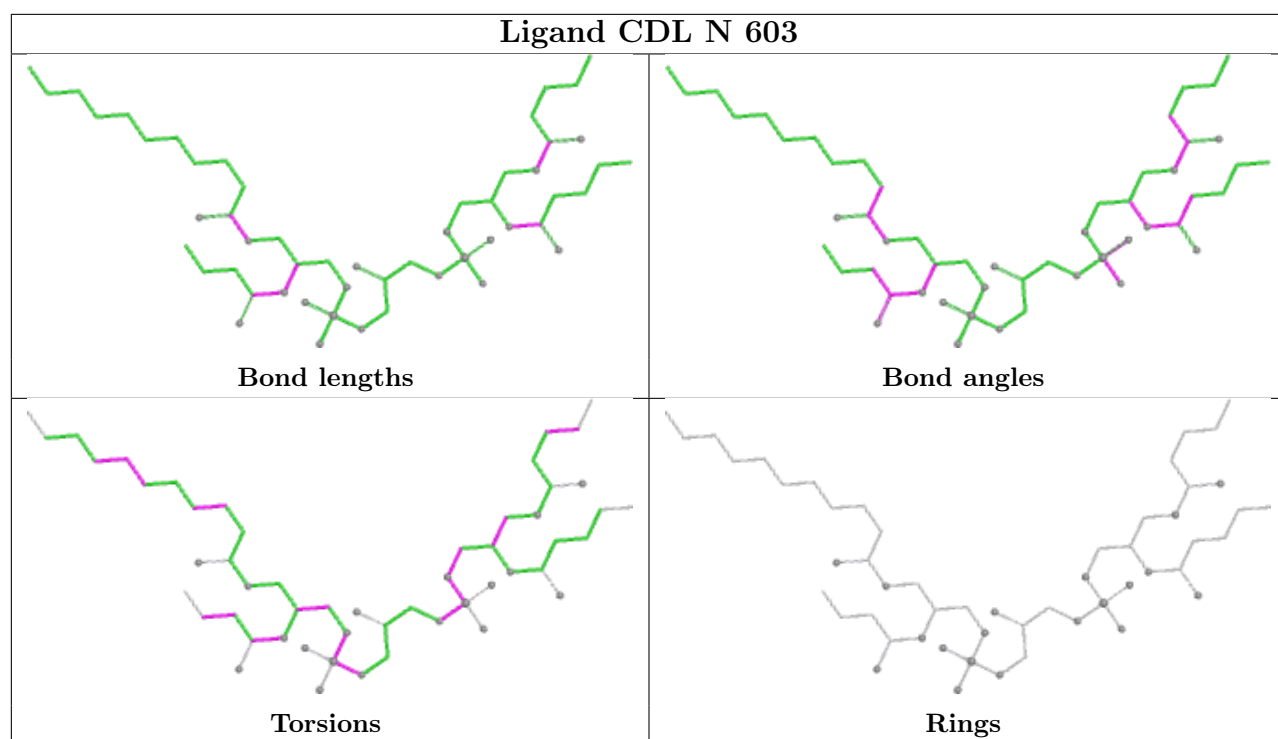
Torsions

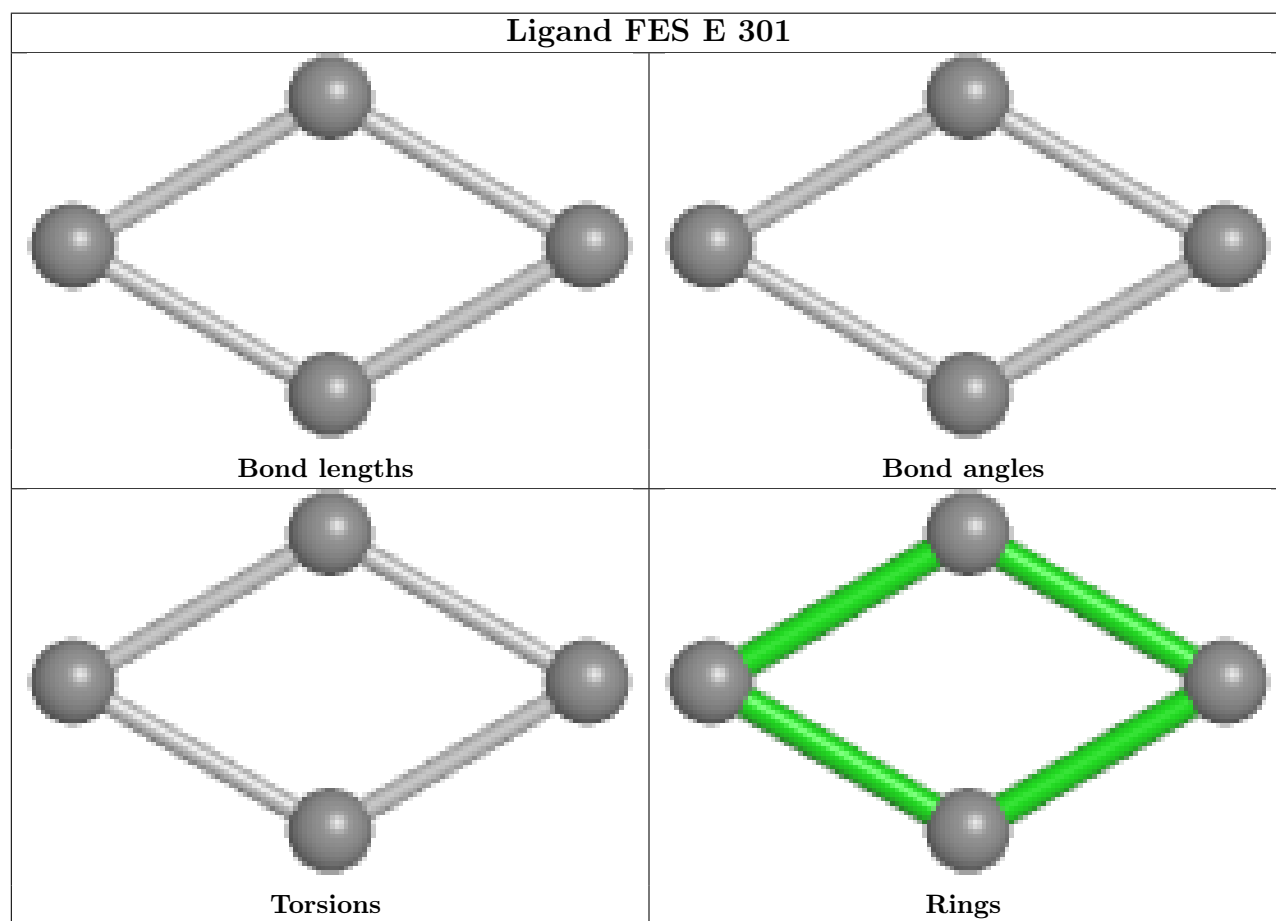
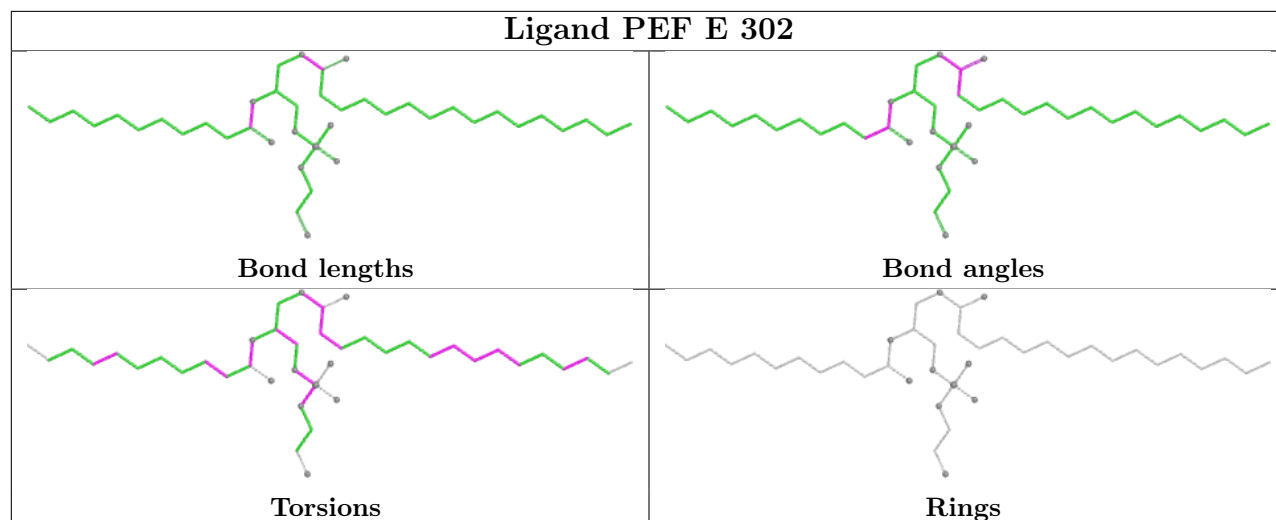


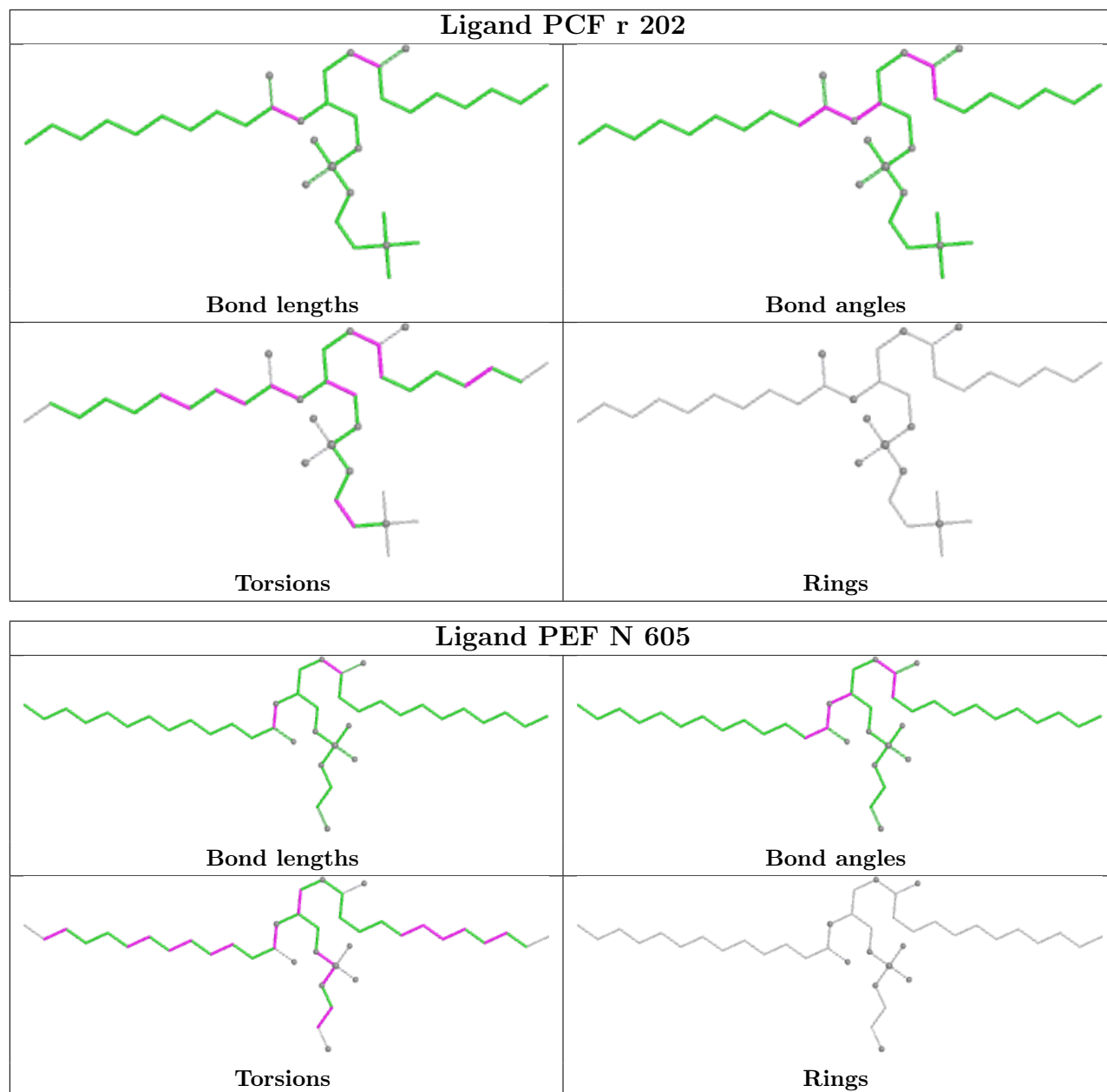
Rings

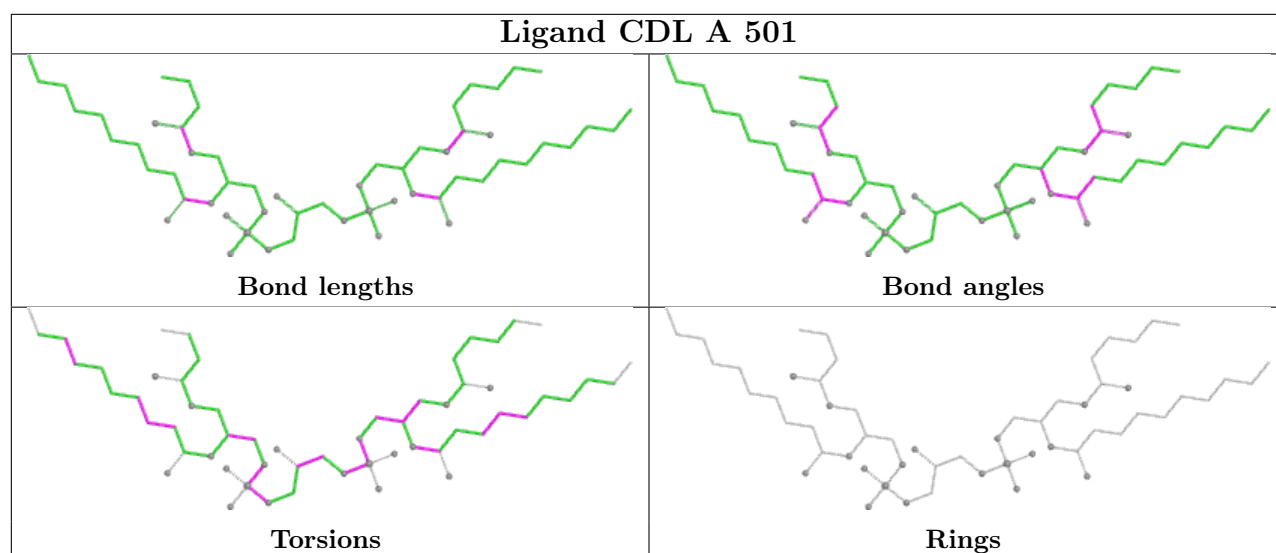












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

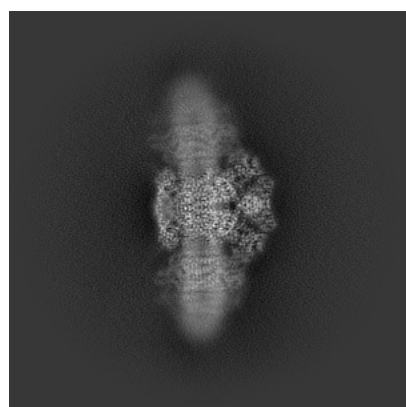
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10340. These allow visual inspection of the internal detail of the map and identification of artifacts.

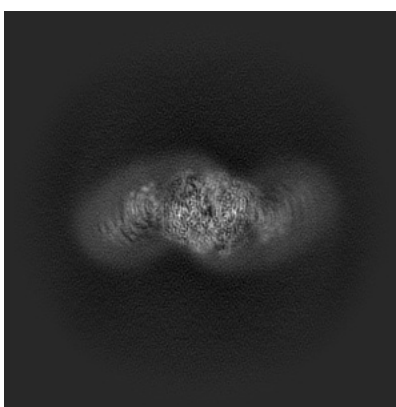
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

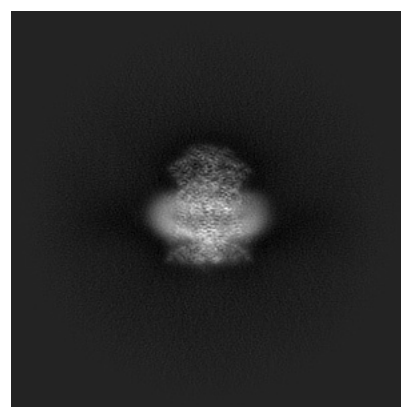
6.1.1 Primary map



X



Y

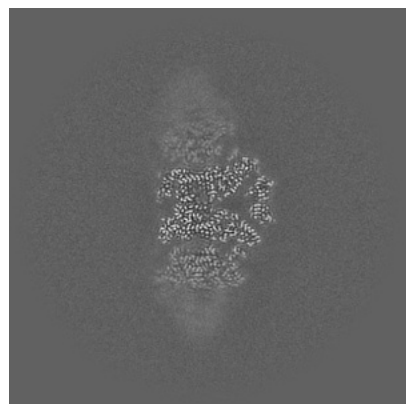


Z

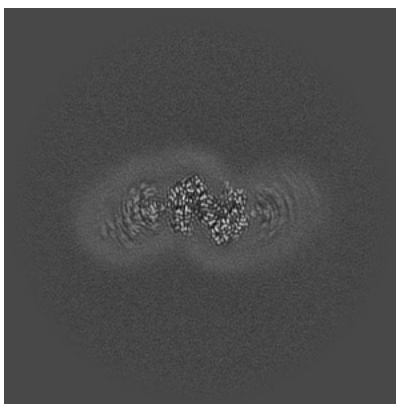
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

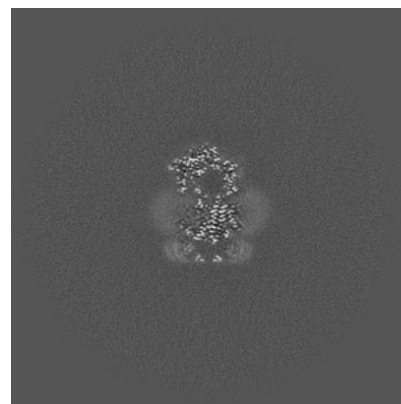
6.2.1 Primary map



X Index: 224



Y Index: 224

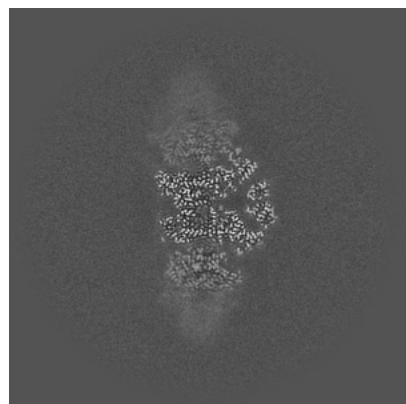


Z Index: 224

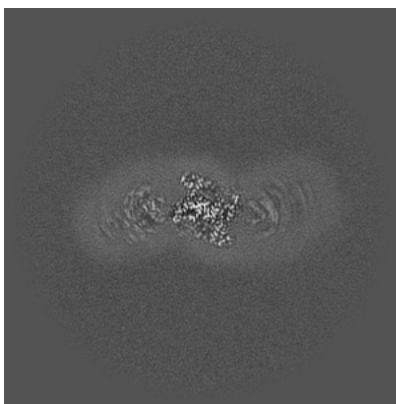
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

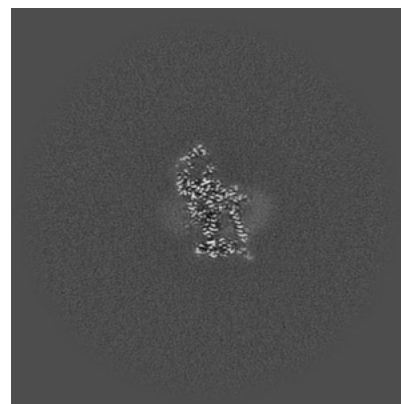
6.3.1 Primary map



X Index: 218



Y Index: 202

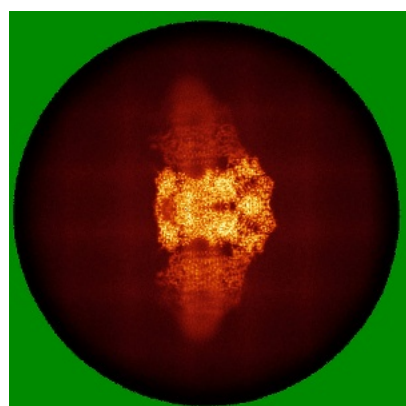


Z Index: 200

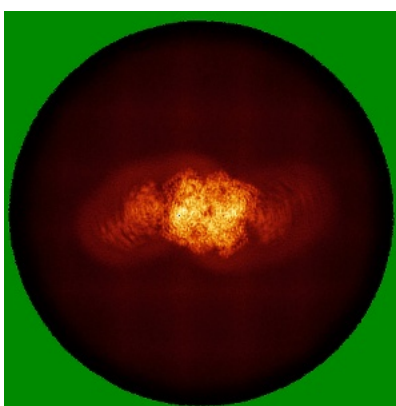
The images above show the largest variance slices of the map in three orthogonal directions.

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

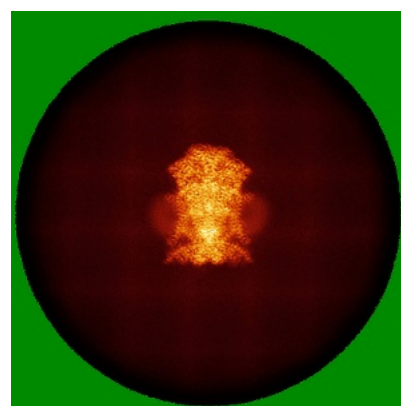
6.4.1 Primary map



X



Y

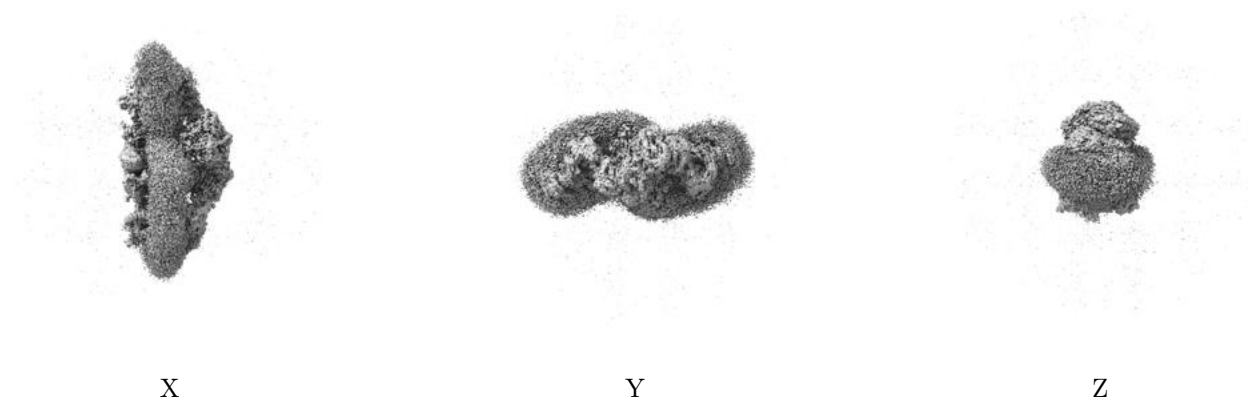


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.24. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

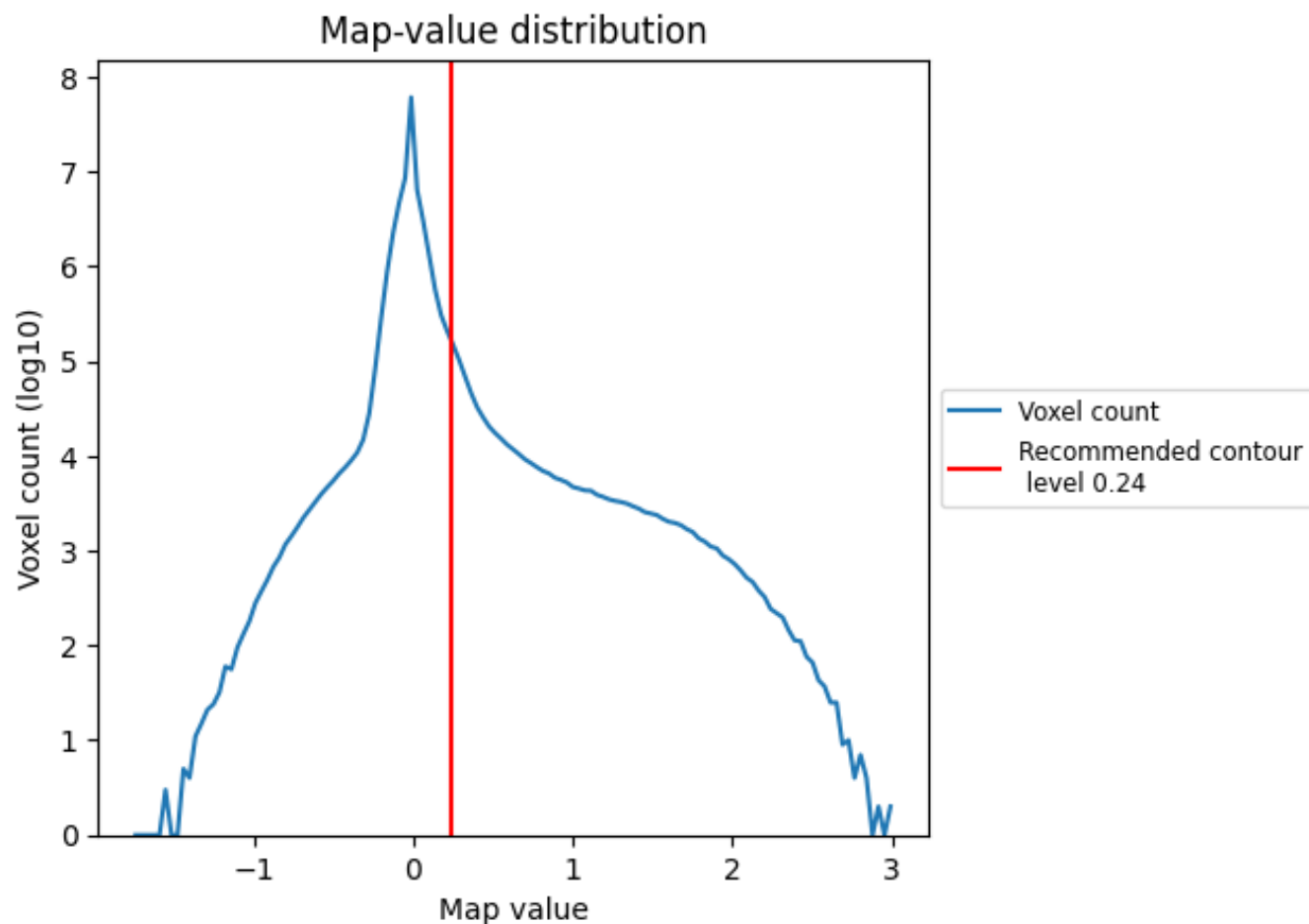
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

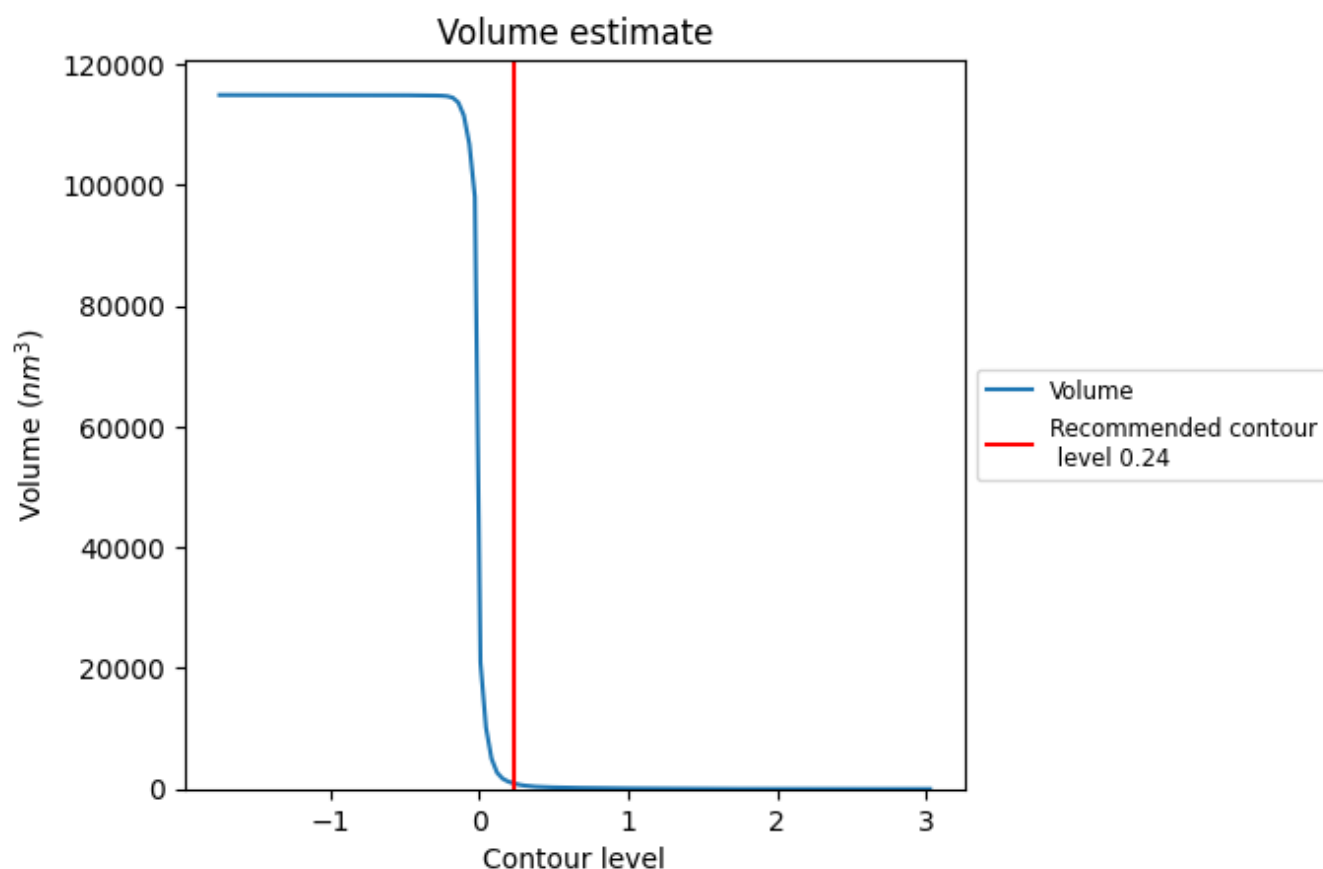
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

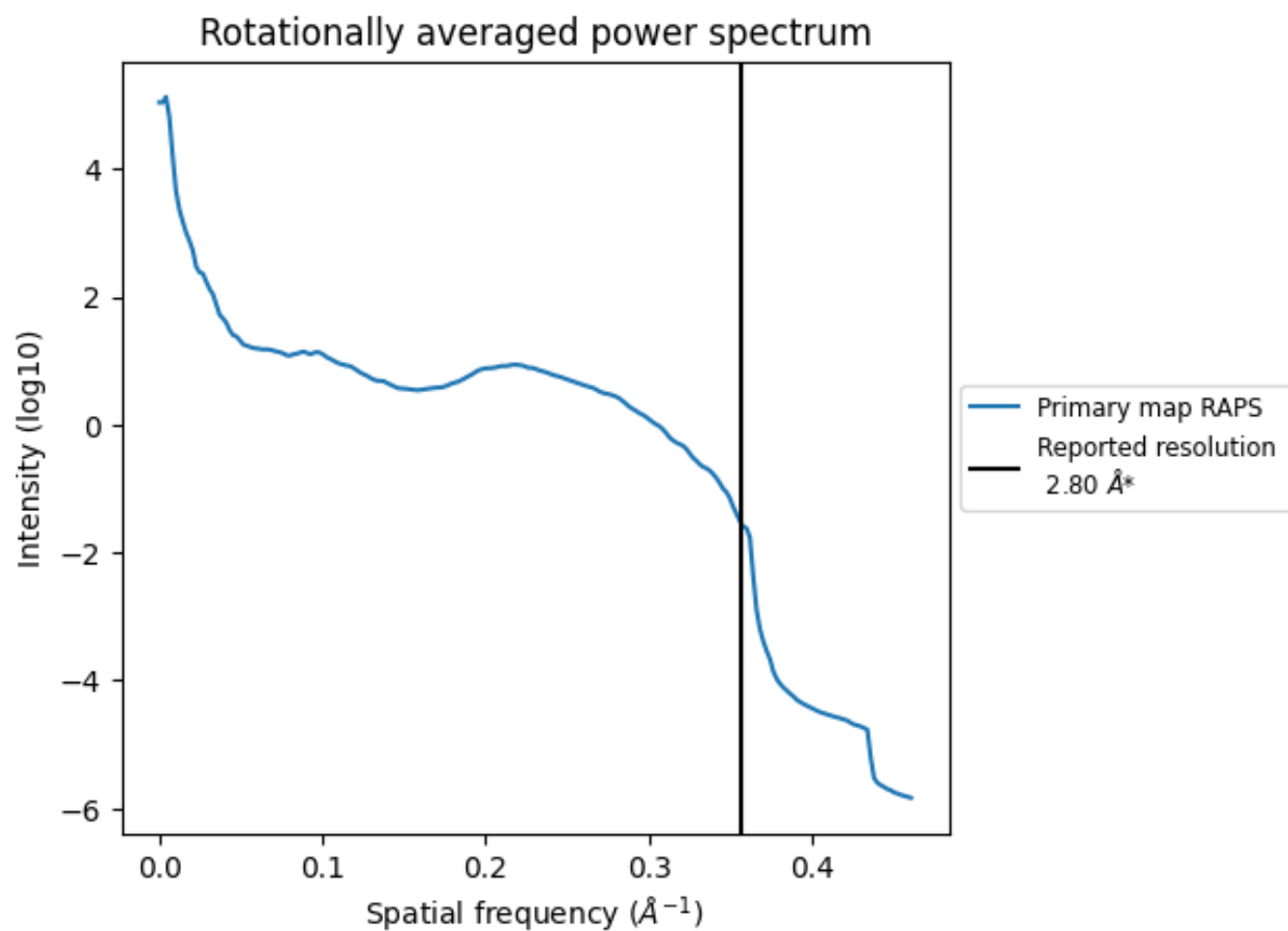
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 878 nm³; this corresponds to an approximate mass of 793 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 ⓘ

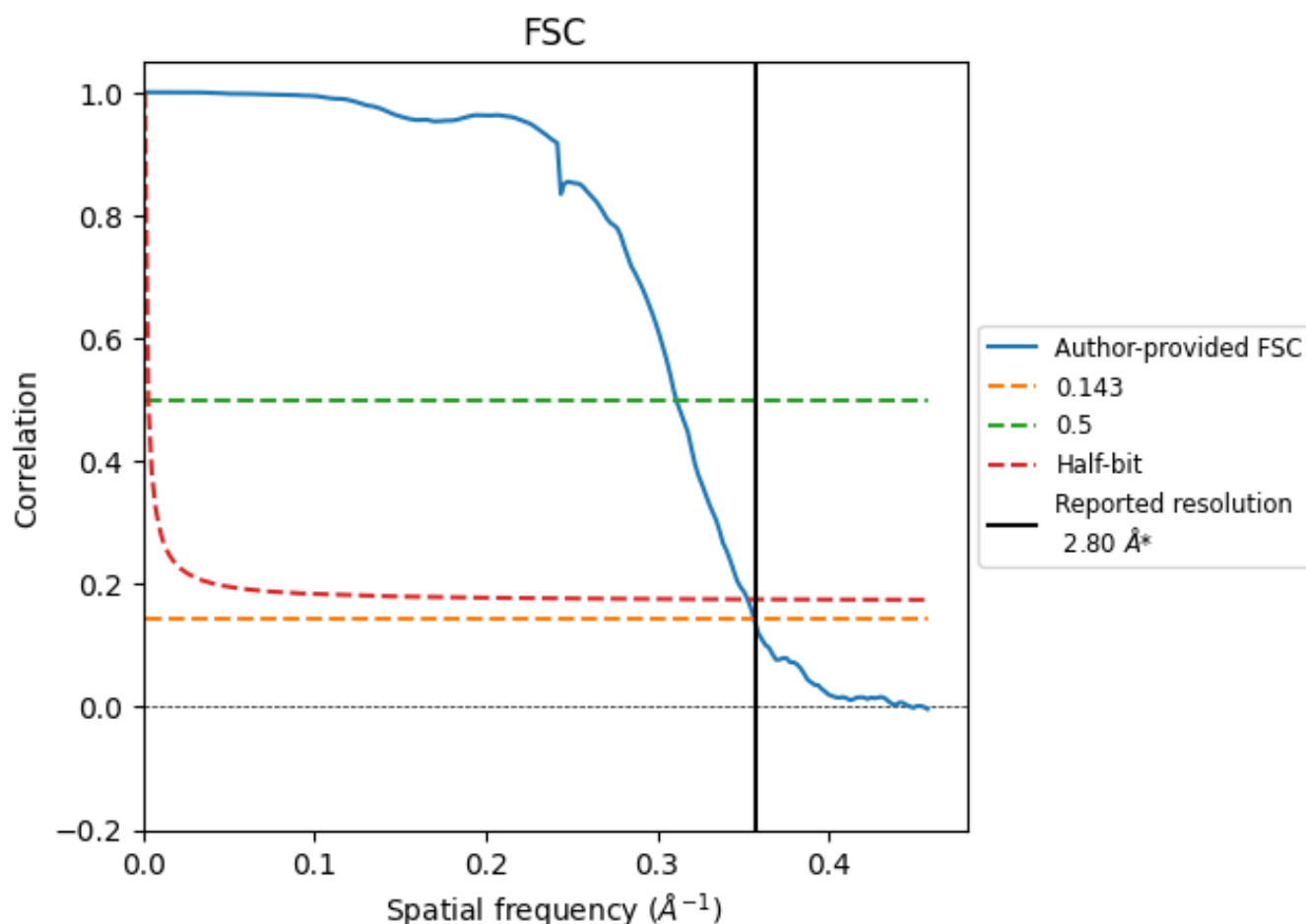


*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

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 0.357 Å⁻¹

8.2 Resolution estimates [i](#)

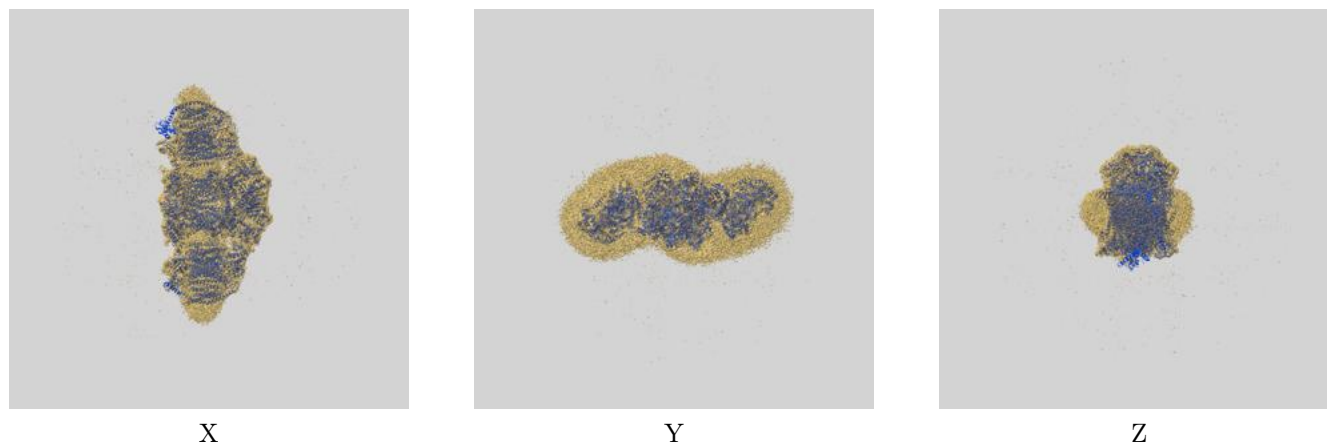
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.80	3.21	2.83
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

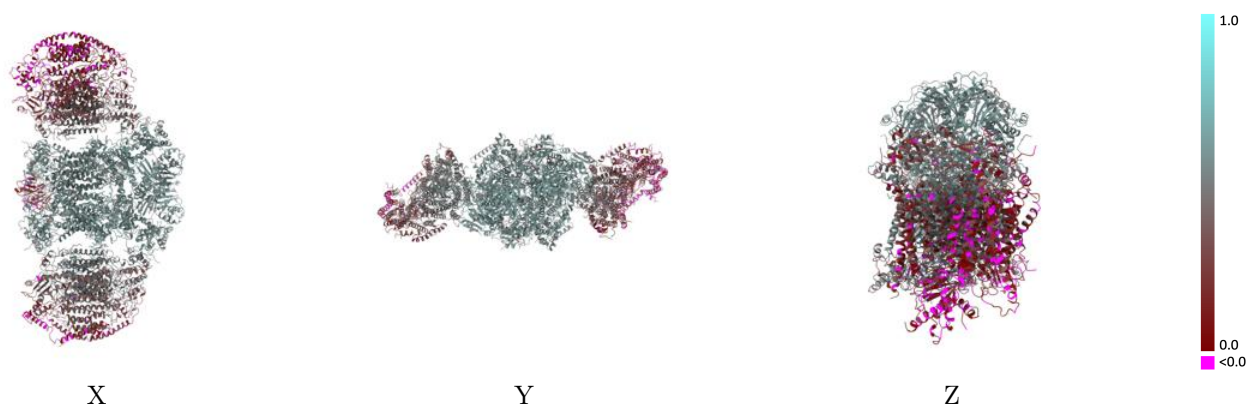
This section contains information regarding the fit between EMDB map EMD-10340 and PDB model 6T0B. Per-residue inclusion information can be found in [section 3](#) on [page 18](#).

9.1 Map-model overlay [i](#)



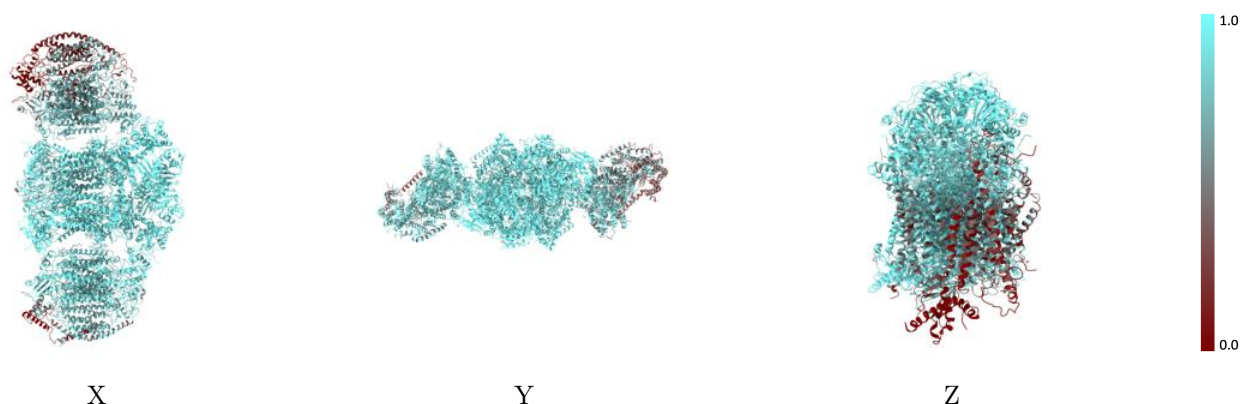
The images above show the 3D surface view of the map at the recommended contour level 0.24 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



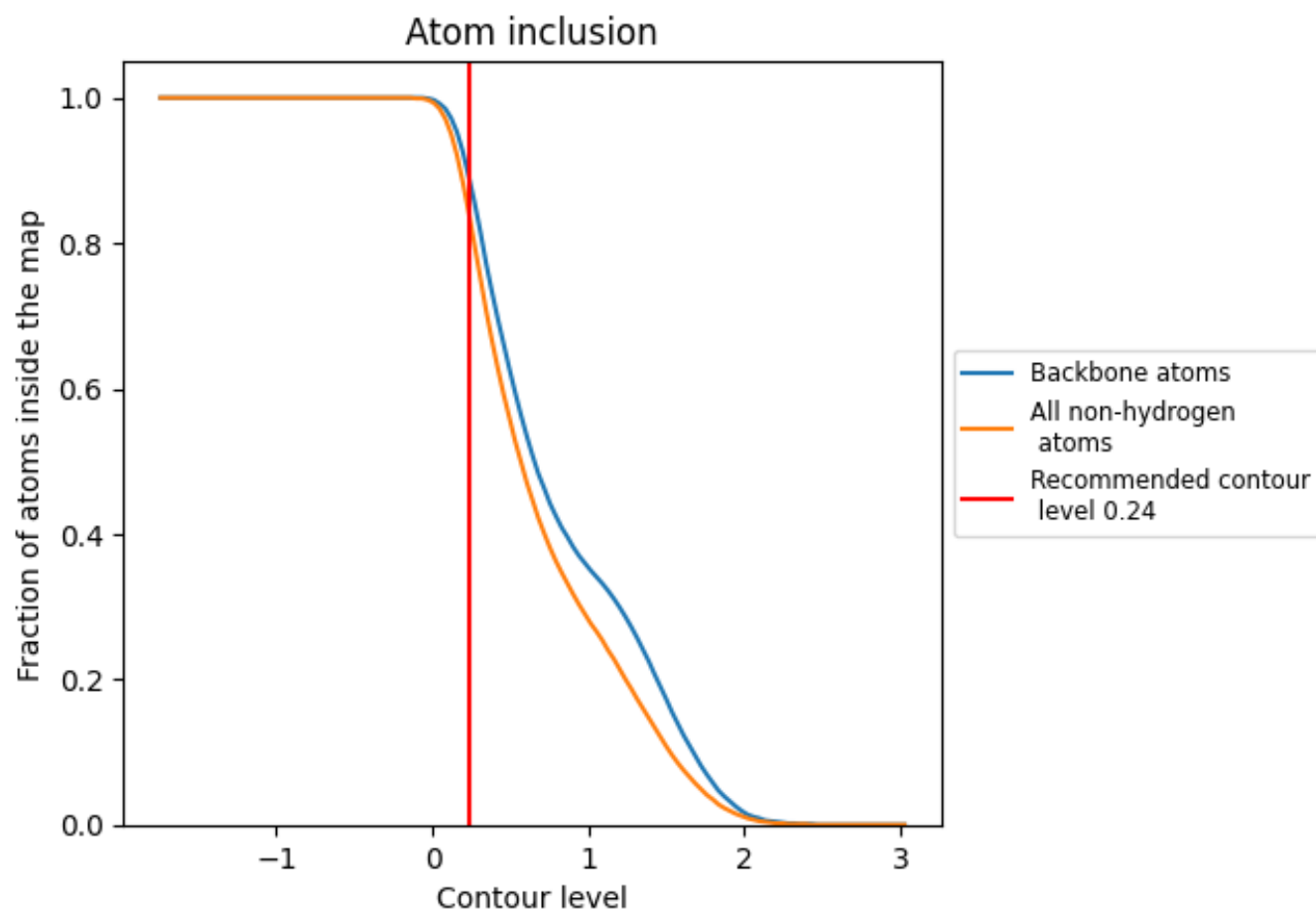
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.24).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% 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 (0.24) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8350	 0.4360
A	 0.9740	 0.5720
B	 0.9830	 0.5720
C	 0.9750	 0.5820
D	 0.9800	 0.5780
E	 0.8540	 0.3440
F	 0.9420	 0.5070
G	 0.9690	 0.5670
H	 0.9710	 0.5690
I	 0.9770	 0.5700
J	 0.8420	 0.4960
L	 0.9780	 0.5700
M	 0.9780	 0.5630
N	 0.9800	 0.5850
O	 0.9790	 0.5750
P	 0.8660	 0.3400
Q	 0.9540	 0.5130
R	 0.9660	 0.5680
S	 0.9730	 0.5690
T	 0.9560	 0.5650
U	 0.8290	 0.4880
a	 0.9050	 0.4820
b	 0.8750	 0.4200
c	 0.8110	 0.3190
d	 0.8780	 0.3740
e	 0.9170	 0.5060
f	 0.9180	 0.4260
g	 0.7800	 0.2750
h	 0.8910	 0.4360
i	 0.8780	 0.3990
j	 0.4270	 0.2400
k	 0.5260	 0.1690
l	 0.8820	 0.4460
m	 0.3860	 0.0990
n	 0.7250	 0.3360



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Chain	Atom inclusion	Q-score
o	 0.6550	 0.2310
p	 0.4860	 0.1790
q	 0.5760	 0.2320
r	 0.8550	 0.4200
s	 0.8260	 0.3080
t	 0.4870	 0.1540
u	 0.6780	 0.2870
v	 0.6050	 0.2010
w	 0.0340	 0.0850
x	 0.1430	 0.0690
y	 0.7540	 0.3060
z	 0.1420	 0.0450