



Full wwPDB EM Validation Report ⓘ

Aug 4, 2026 – 03:28 PM EDT

PDB ID : 7JRP / pdb_00007jrp
EMDB ID : EMD-22448
Title : Plant Mitochondrial complex SC III2+IV from Vigna radiata
Authors : Maldonado, M.; Letts, J.A.
Deposited on : 2020-08-12
Resolution : 3.80 Å(reported)
Based on initial models : 6Q9E, 6HU9

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.dev133
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) : 2.50

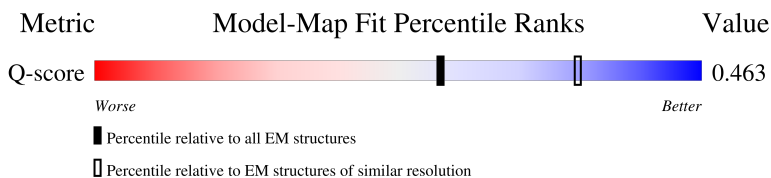
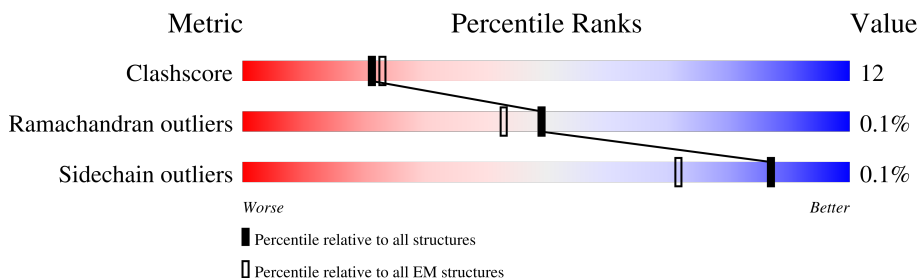
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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.



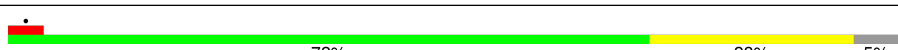
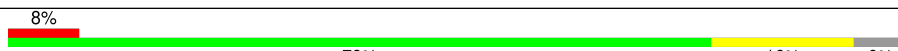
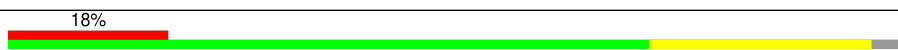
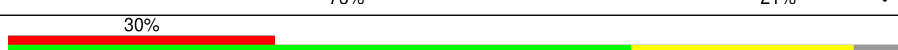
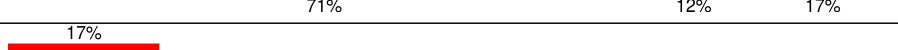
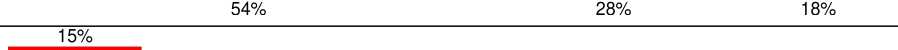
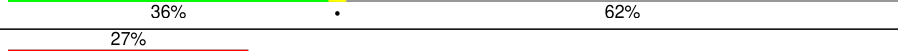
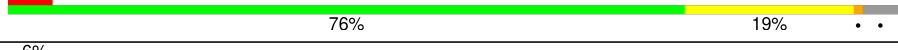
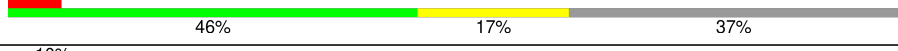
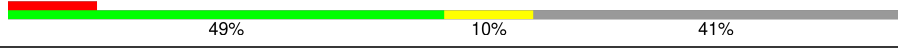
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10198 (3.30 - 4.30)

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	527	
1	M	527	
2	B	506	
2	N	506	

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Mol	Chain	Length	Quality of chain
3	C	393	
3	O	393	
4	D	306	
4	P	306	
5	E	271	
5	Q	271	
6	F	122	
6	R	122	
7	G	72	
7	S	72	
8	H	69	
8	T	69	
9	J	72	
9	V	72	
10	K	81	
10	W	81	
11	a	527	
12	b	251	
13	c	265	
14	d	79	
15	e	150	
16	f	100	
17	g	181	
18	h	64	
19	i	67	

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Mol	Chain	Length	Quality of chain
20	j	96	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	HEC	D	501	X	-	-	-
26	HEC	P	402	X	-	-	-

2 Entry composition

There are 31 unique types of molecules in this entry. The entry contains 45166 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 Mitochondrial-processing peptidase subunit beta, mitochondrial isoform X1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	487	Total	C	N	O	S	0	0
			3838	2409	678	736	15		
1	M	487	Total	C	N	O	S	0	0
			3838	2409	678	736	15		

- Molecule 2 is a protein called Alpha-MPP.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	457	Total	C	N	O	S	0	0
			3471	2196	588	675	12		
2	N	455	Total	C	N	O	S	0	0
			3456	2187	585	672	12		

- Molecule 3 is a protein called COB.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	388	Total	C	N	O	S	0	0
			3104	2088	487	515	14		
3	O	388	Total	C	N	O	S	0	0
			3104	2088	487	515	14		

- Molecule 4 is a protein called cytochrome c1-2, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	244	Total	C	N	O	S	0	0
			1910	1214	327	358	11		
4	P	244	Total	C	N	O	S	0	0
			1910	1214	327	358	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	74	Total	C	N	O	S	0	0
			574	375	97	101	1		
5	Q	74	Total	C	N	O	S	0	0
			574	375	97	101	1		

- Molecule 6 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	116	Total	C	N	O	S	0	0
			965	616	173	172	4		
6	R	115	Total	C	N	O	S	0	0
			959	613	172	170	4		

- Molecule 7 is a protein called cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	70	Total	C	N	O	S	0	0
			578	382	97	98	1		
7	S	70	Total	C	N	O	S	0	0
			578	382	97	98	1		

- Molecule 8 is a protein called Cytochrome b-c1 complex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	65	Total	C	N	O	S	0	0
			536	344	90	96	6		
8	T	64	Total	C	N	O	S	0	0
			527	339	89	93	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	60	Total	C	N	O	S	0	0
			480	313	83	83	1		
9	V	59	Total	C	N	O	S	0	0
			476	311	82	82	1		

- Molecule 10 is a protein called QCR10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	31	Total	C	N	O	S	0	0
			218	144	35	38	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	W	32	Total	C	N	O	S	0	0
			226	150	36	39	1		

- Molecule 11 is a protein called COX1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	a	524	Total	C	N	O	S	0	0
			4074	2726	640	684	24		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	b	239	Total	C	N	O	S	0	0
			1915	1249	308	348	10		

- Molecule 13 is a protein called COX3.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	c	265	Total	C	N	O	S	0	0
			2134	1445	335	347	7		

- Molecule 14 is a protein called COX4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	d	76	Total	C	N	O	S	0	0
			595	387	97	109	2		

- Molecule 15 is a protein called cytochrome c oxidase subunit 5b-2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	e	94	Total	C	N	O	S	0	0
			733	464	124	142	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	f	59	Total	C	N	O	S	0	0
			480	315	76	88	1		

- Molecule 17 is a protein called cytochrome c oxidase subunit 6b-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	g	74	Total	C	N	O	S	0	0
			612	385	110	113	4		

- Molecule 18 is a protein called Cytochrome c oxidase subunit 5C.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	h	49	Total	C	N	O	S	0	0
			391	255	67	68	1		

- Molecule 19 is a protein called COX7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	i	64	Total	C	N	O	S	0	0
			510	331	91	87	1		

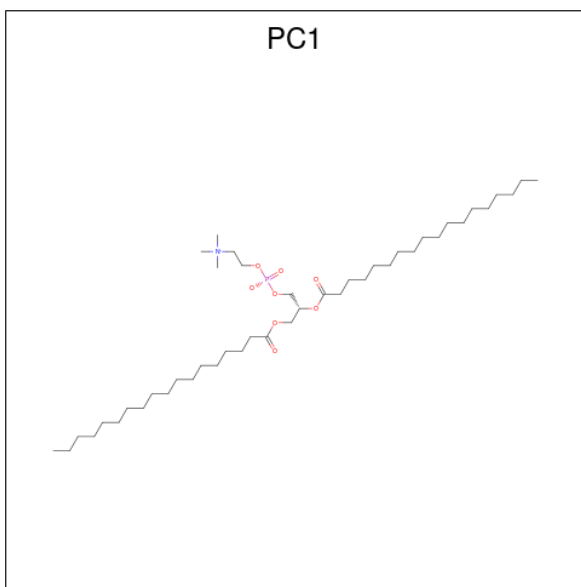
- Molecule 20 is a protein called COX7c.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	j	47	Total	C	N	O	S	0	0
			384	254	67	60	3		

- Molecule 21 is ZINC ION (CCD ID: ZN) (formula: Zn).

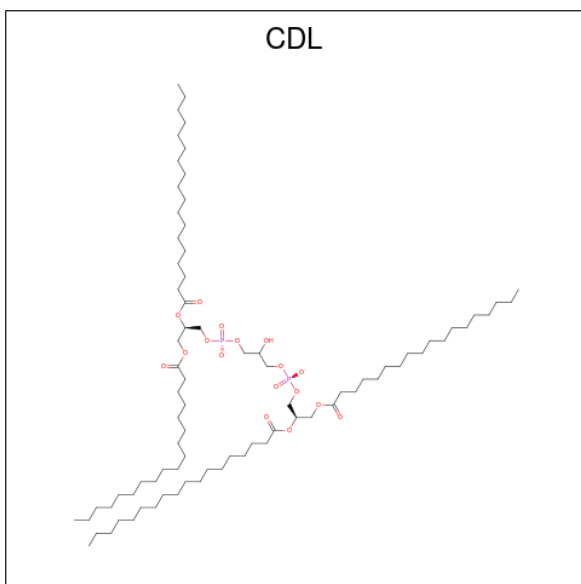
Mol	Chain	Residues	Atoms		AltConf
21	A	1	Total	Zn	0
			1	1	
21	M	1	Total	Zn	0
			1	1	
21	e	1	Total	Zn	0
			1	1	

- Molecule 22 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: C₄₄H₈₈NO₈P).



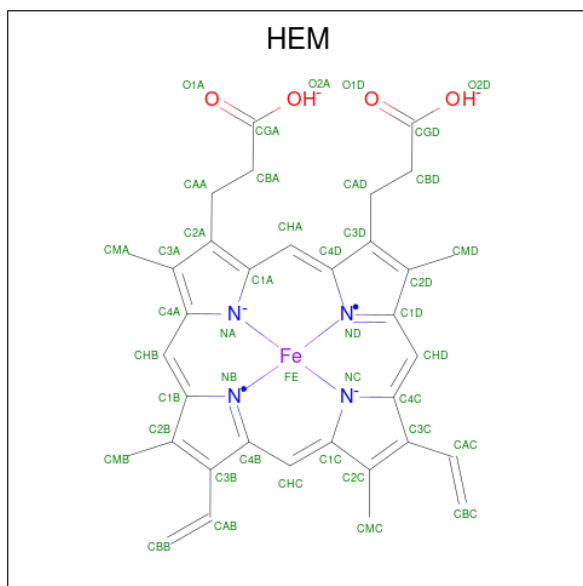
Mol	Chain	Residues	Atoms					AltConf
22	A	1	Total	C	N	O	P	0
			29	19	1	8	1	
22	M	1	Total	C	N	O	P	0
			27	17	1	8	1	
22	S	1	Total	C	N	O	P	0
			28	18	1	8	1	
22	a	1	Total	C	N	O	P	0
			39	29	1	8	1	
22	i	1	Total	C	N	O	P	0
			36	26	1	8	1	

- Molecule 23 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
23	A	1	Total	C	O	P	0
			51	32	17	2	
23	C	1	Total	C	O	P	0
			54	35	17	2	
23	C	1	Total	C	O	P	0
			55	36	17	2	
23	D	1	Total	C	O	P	0
			41	22	17	2	
23	M	1	Total	C	O	P	0
			53	34	17	2	
23	O	1	Total	C	O	P	0
			54	35	17	2	
23	P	1	Total	C	O	P	0
			48	29	17	2	
23	S	1	Total	C	O	P	0
			50	31	17	2	
23	a	1	Total	C	O	P	0
			67	48	17	2	

- Molecule 24 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



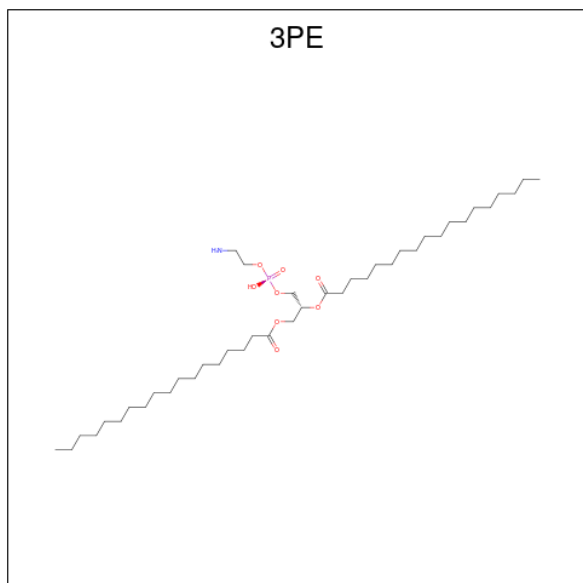
Mol	Chain	Residues	Atoms					AltConf
24	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
24	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

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

- Molecule 25 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



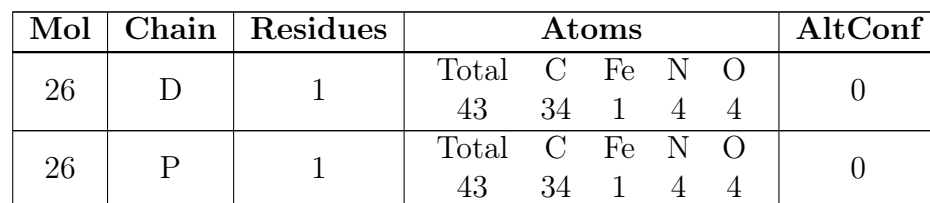
Mol	Chain	Residues	Atoms					AltConf
25	C	1	Total	C	N	O	P	0
			38	28	1	8	1	
25	C	1	Total	C	N	O	P	0
			28	18	1	8	1	
25	C	1	Total	C	N	O	P	0
			29	19	1	8	1	
25	C	1	Total	C	N	O	P	0
			35	25	1	8	1	
25	C	1	Total	C	N	O	P	0
			28	18	1	8	1	
25	F	1	Total	C	N	O	P	0
			32	22	1	8	1	
25	G	1	Total	C	N	O	P	0
			20	10	1	8	1	
25	O	1	Total	C	N	O	P	0
			24	14	1	8	1	
25	O	1	Total	C	N	O	P	0
			26	16	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
25	O	1	Total	C	N	O	P	0
			33	23	1	8	1	
25	O	1	Total	C	N	O	P	0
			26	16	1	8	1	
25	P	1	Total	C	N	O	P	0
			28	18	1	8	1	
25	a	1	Total	C	N	O	P	0
			32	22	1	8	1	
25	a	1	Total	C	N	O	P	0
			40	30	1	8	1	
25	a	1	Total	C	N	O	P	0
			38	28	1	8	1	
25	a	1	Total	C	N	O	P	0
			40	30	1	8	1	
25	a	1	Total	C	N	O	P	0
			38	28	1	8	1	
25	a	1	Total	C	N	O	P	0
			39	29	1	8	1	
25	b	1	Total	C	N	O	P	0
			36	26	1	8	1	
25	b	1	Total	C	N	O	P	0
			29	19	1	8	1	
25	b	1	Total	C	N	O	P	0
			43	33	1	8	1	
25	c	1	Total	C	N	O	P	0
			40	30	1	8	1	
25	c	1	Total	C	N	O	P	0
			40	30	1	8	1	
25	c	1	Total	C	N	O	P	0
			37	27	1	8	1	
25	c	1	Total	C	N	O	P	0
			43	33	1	8	1	
25	c	1	Total	C	N	O	P	0
			40	30	1	8	1	
25	d	1	Total	C	N	O	P	0
			35	25	1	8	1	
25	h	1	Total	C	N	O	P	0
			38	28	1	8	1	
25	i	1	Total	C	N	O	P	0
			35	25	1	8	1	

- Molecule 26 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



- # HEA

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

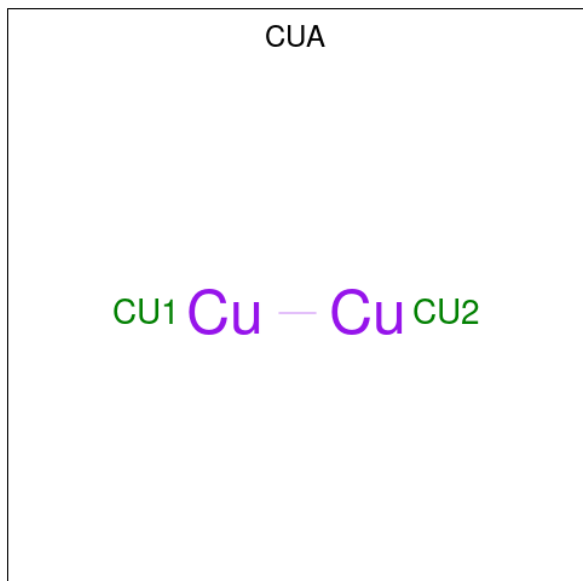
- Molecule 28 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		AltConf
28	a	1	Total	Cu	0
			1	1	

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

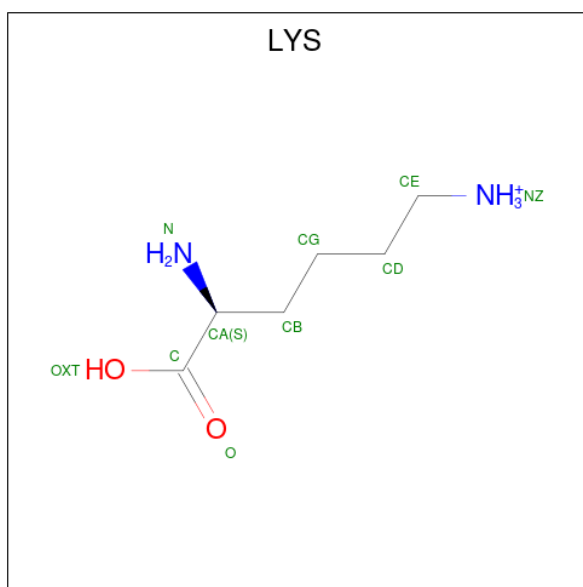
Mol	Chain	Residues	Atoms		AltConf
29	a	1	Total	Mg	0
			1	1	

- Molecule 30 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu₂).



Mol	Chain	Residues	Atoms		AltConf
30	b	1	Total	Cu	0
			2	2	

- Molecule 31 is LYSINE (CCD ID: LYS) (formula: C₆H₁₅N₂O₂).

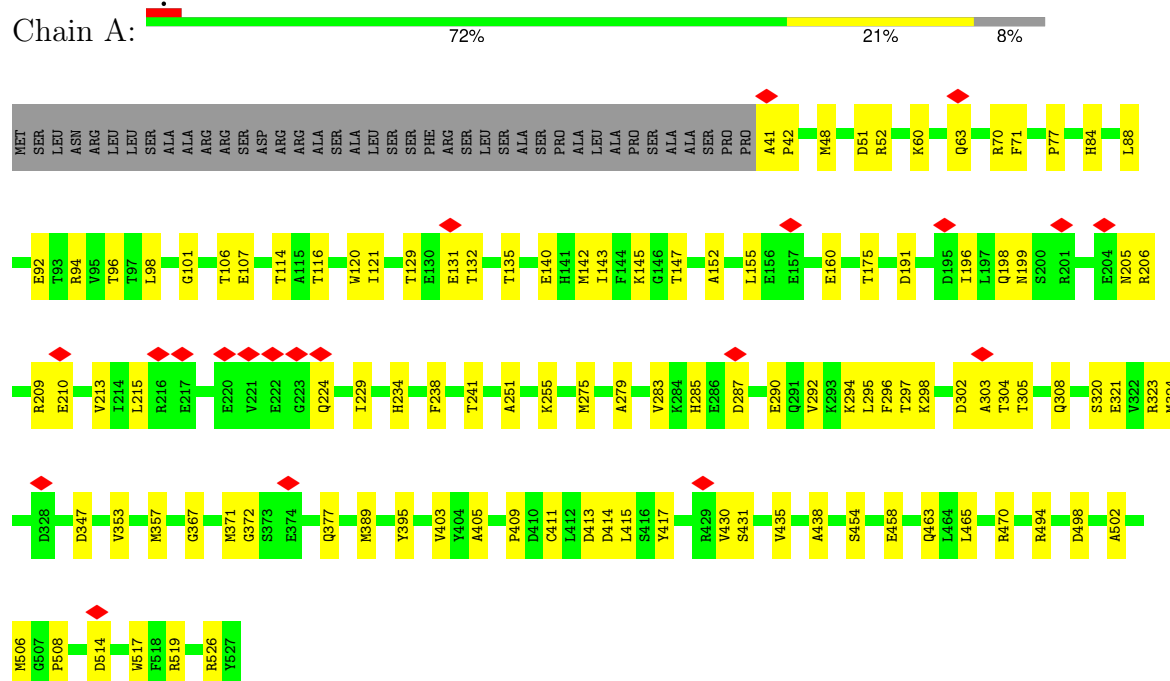


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
31	i	1	9	6	2	1	0

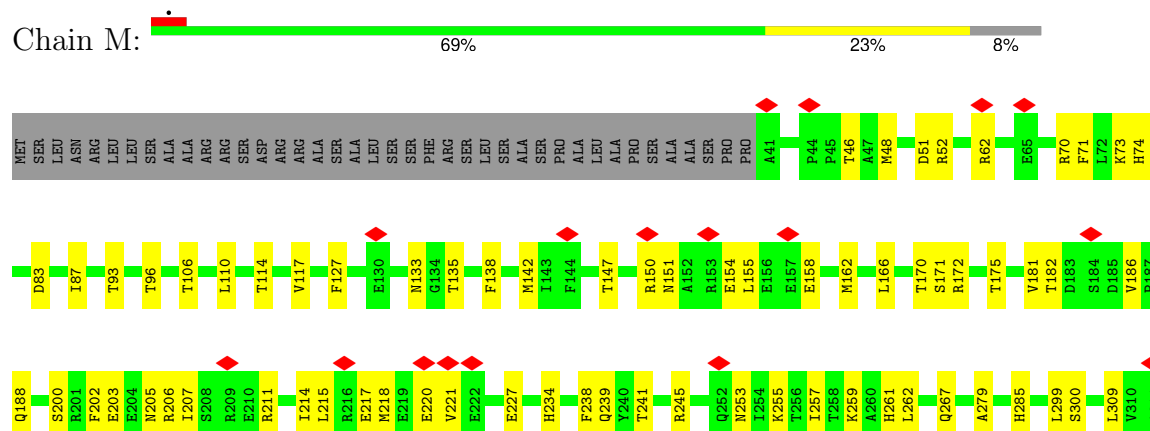
3 Residue-property plots

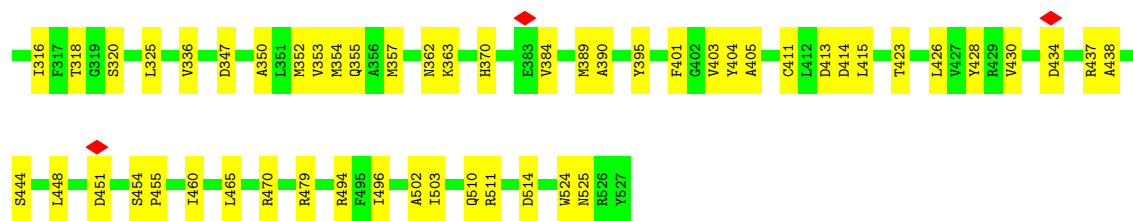
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Mitochondrial-processing peptidase subunit beta, mitochondrial isoform X1

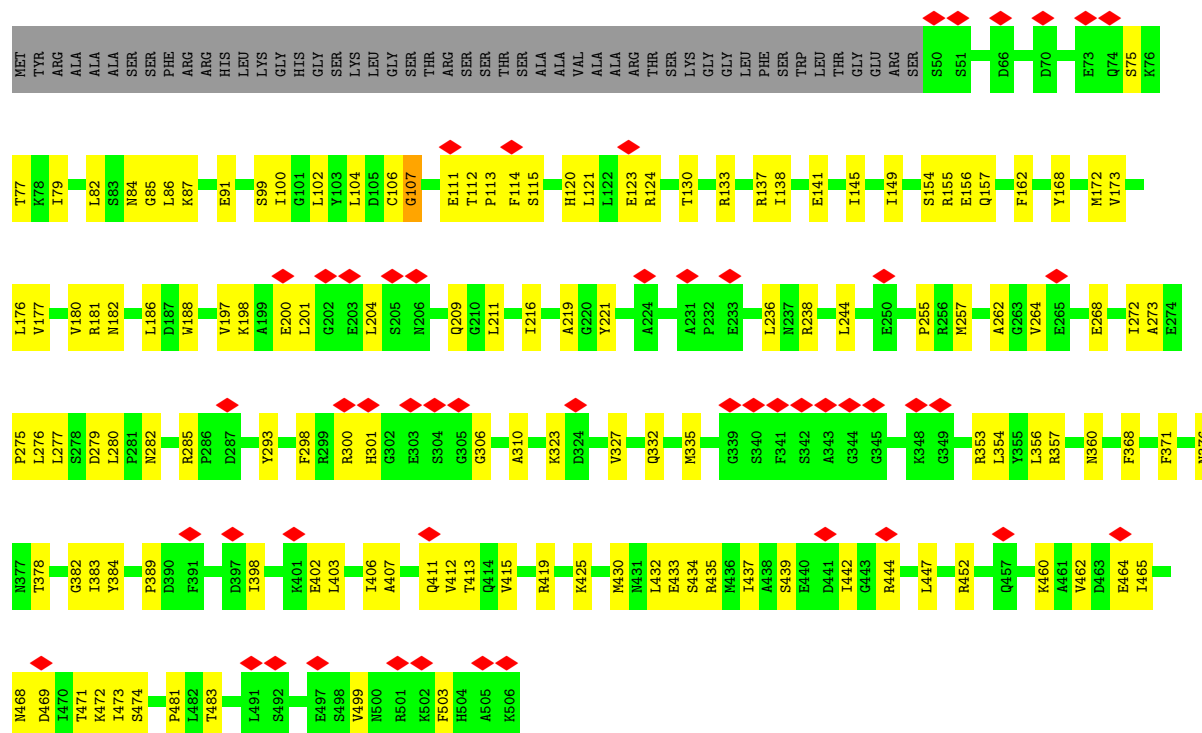


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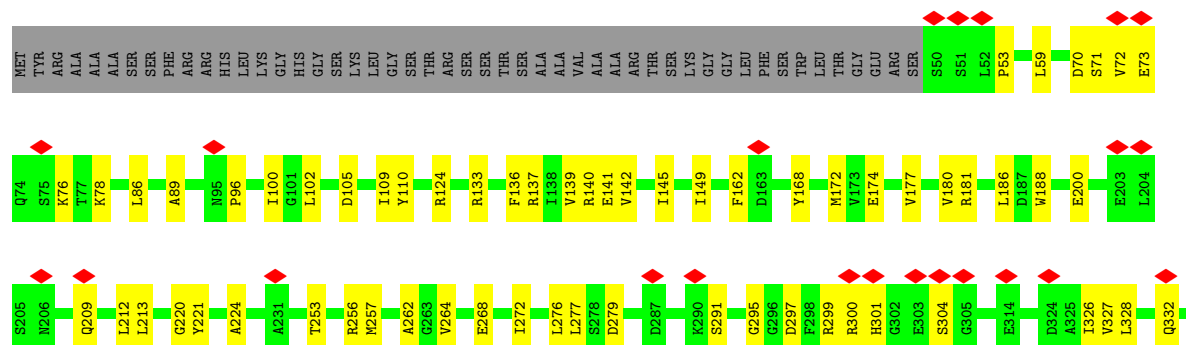


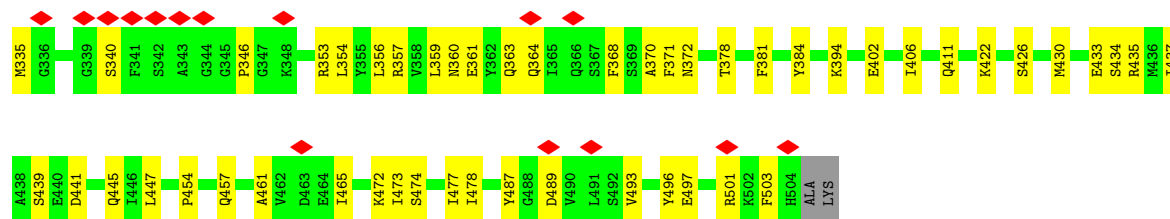


• Molecule 2: Alpha-MPP

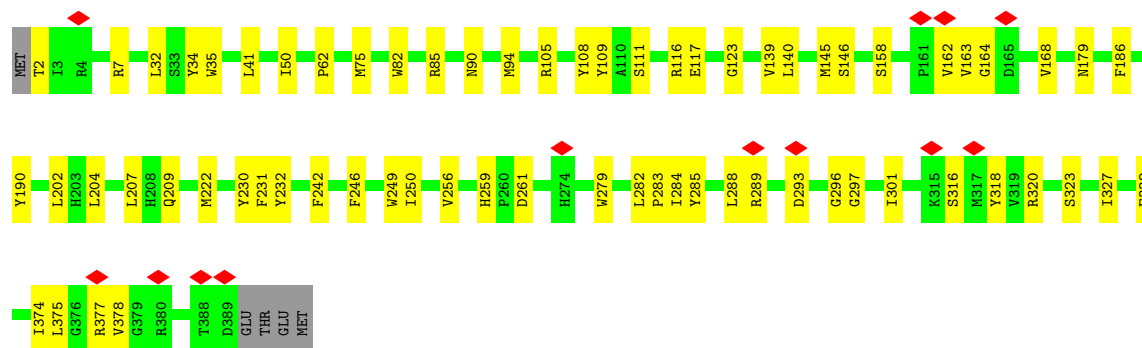
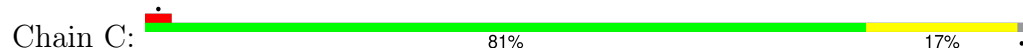


• Molecule 2: Alpha-MPP

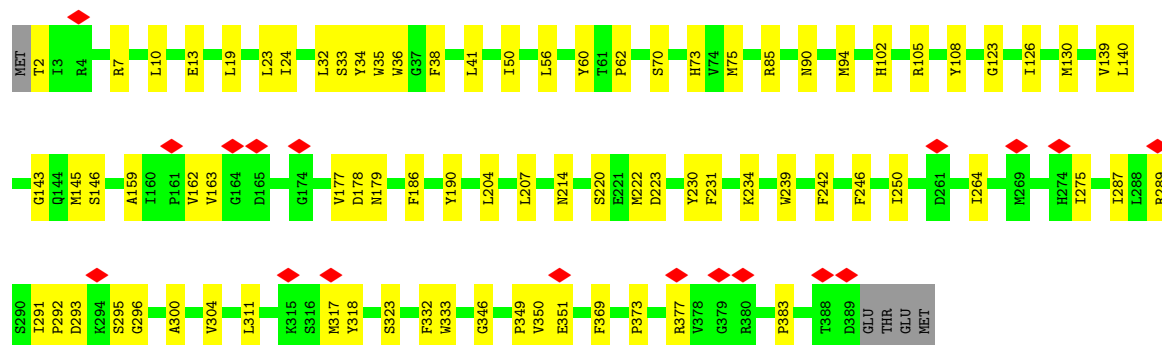
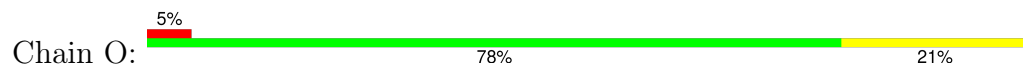




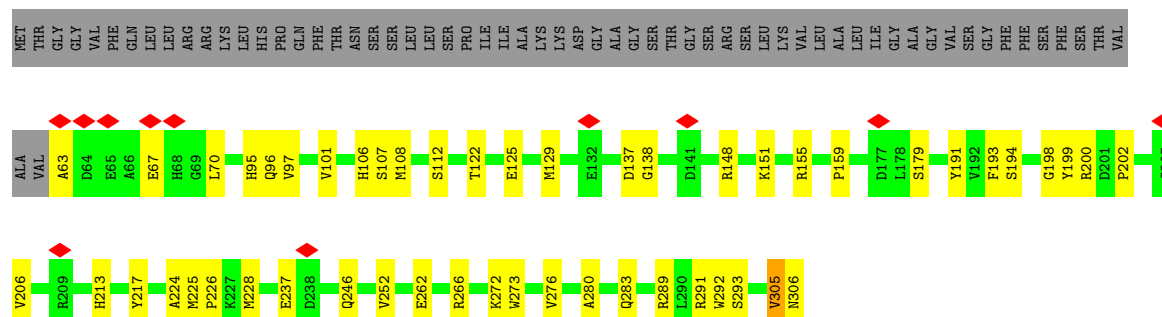
• Molecule 3: COB



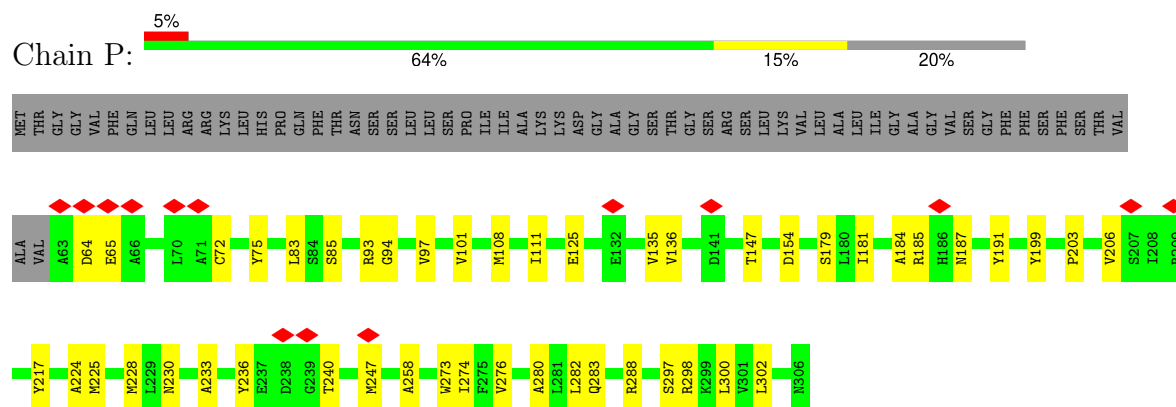
• Molecule 3: COB



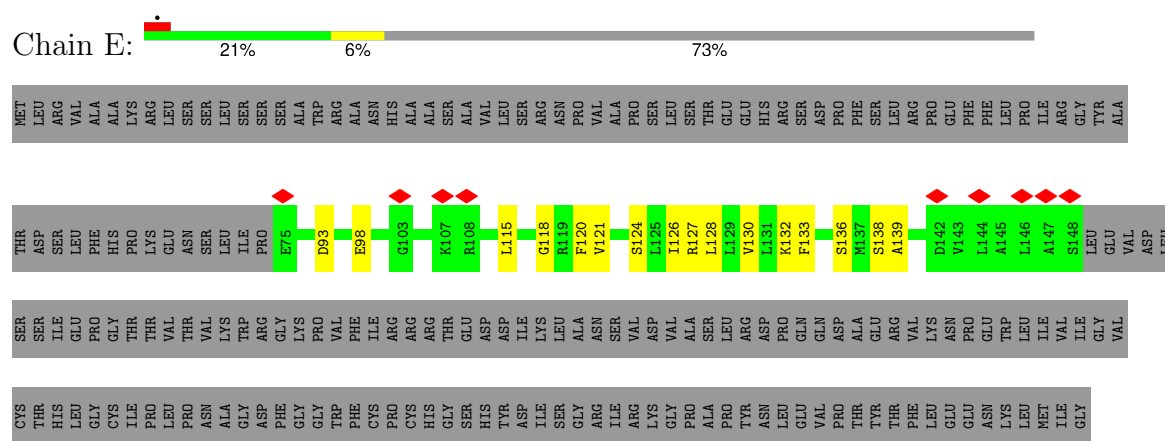
• Molecule 4: cytochrome c1-2, heme protein, mitochondrial



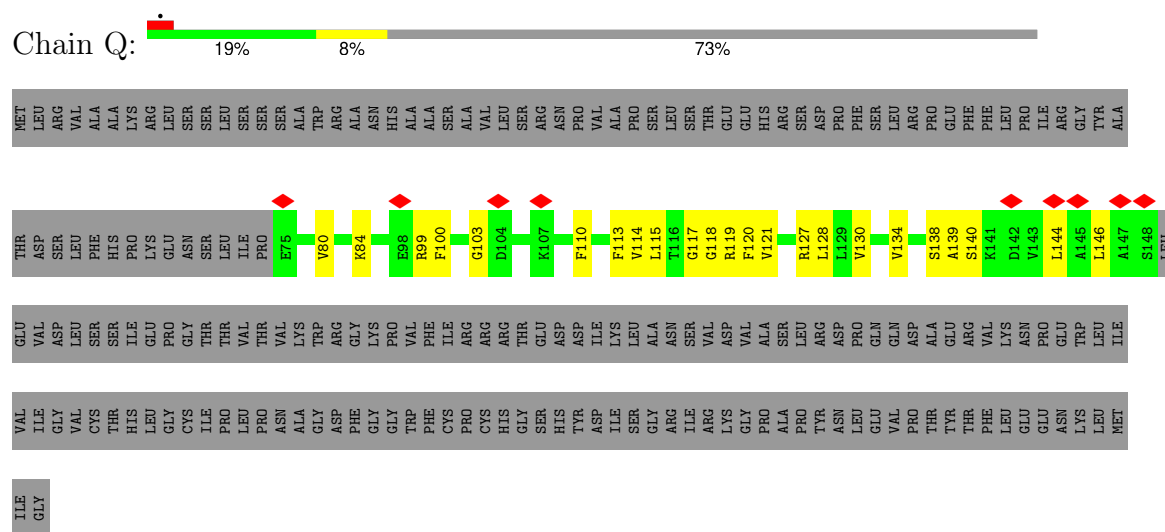
- Molecule 4: cytochrome c1-2, heme protein, mitochondrial



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



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

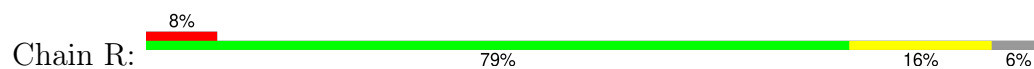


- Molecule 6: Cytochrome b-c1 complex subunit 7

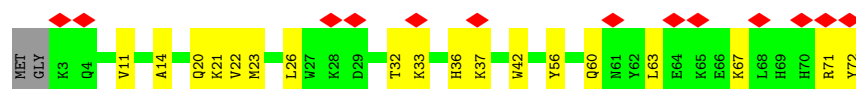




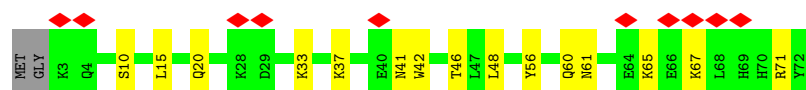
- Molecule 6: Cytochrome b-c1 complex subunit 7



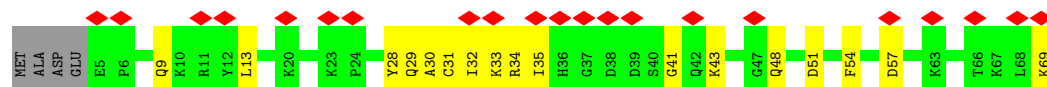
- Molecule 7: cytochrome b-c1 complex subunit 8



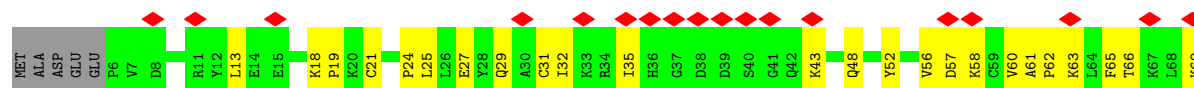
- Molecule 7: cytochrome b-c1 complex subunit 8



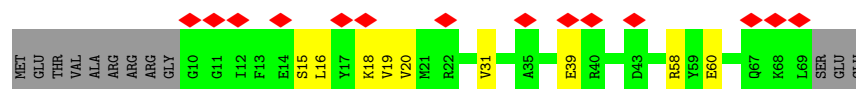
- Molecule 8: Cytochrome b-c1 complex subunit 6



- Molecule 8: Cytochrome b-c1 complex subunit 6



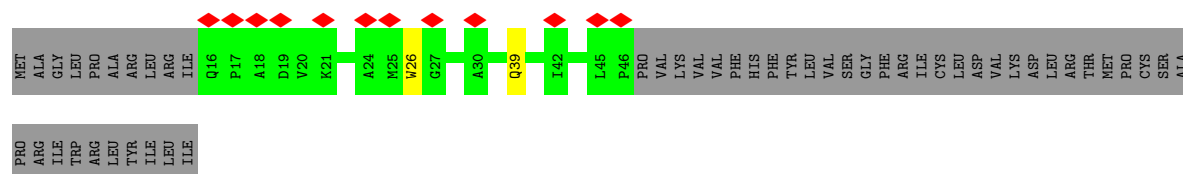
- Molecule 9: cytochrome b-c1 complex subunit 9



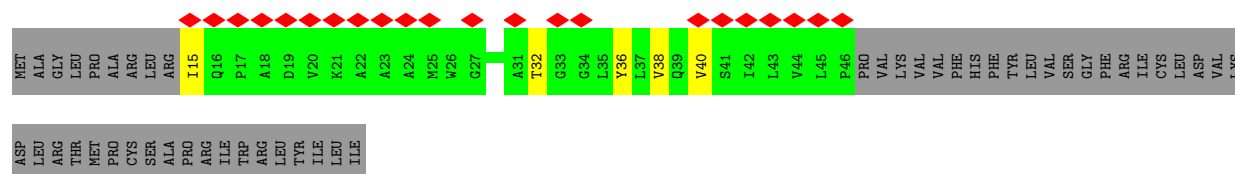
- Molecule 9: cytochrome b-c1 complex subunit 9



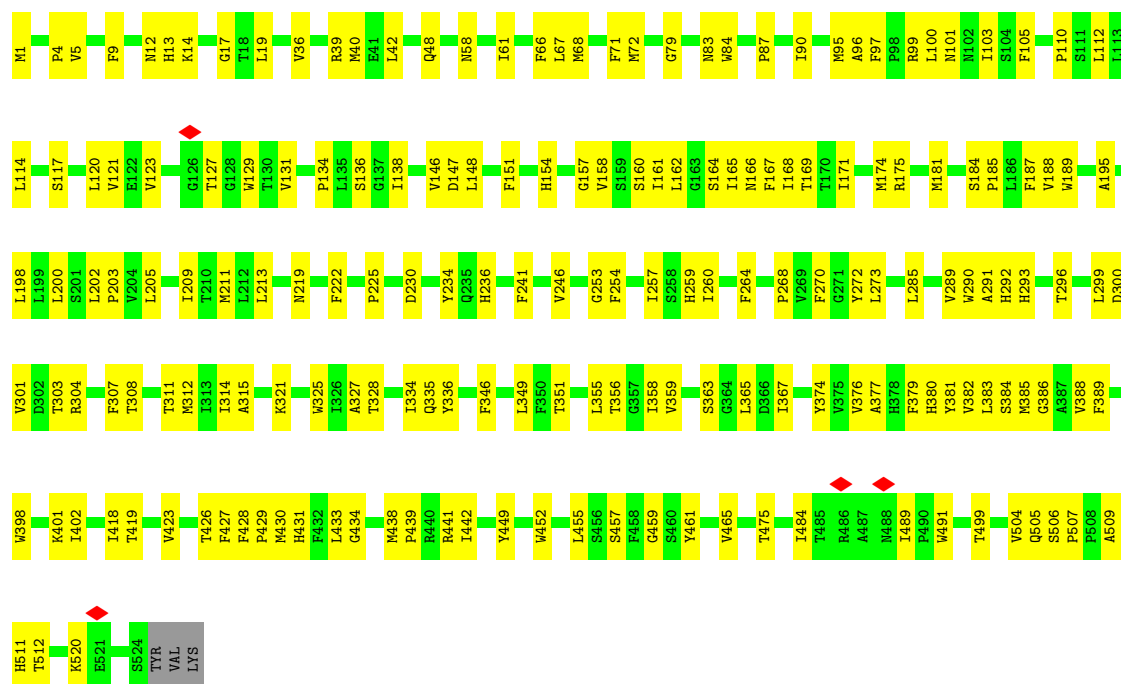
Chain K: 15% 36% 62%



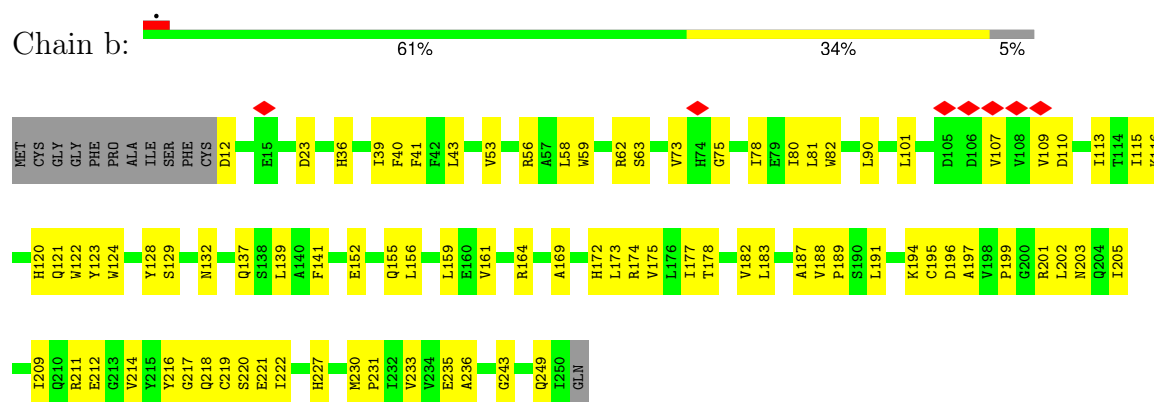
Chain W:



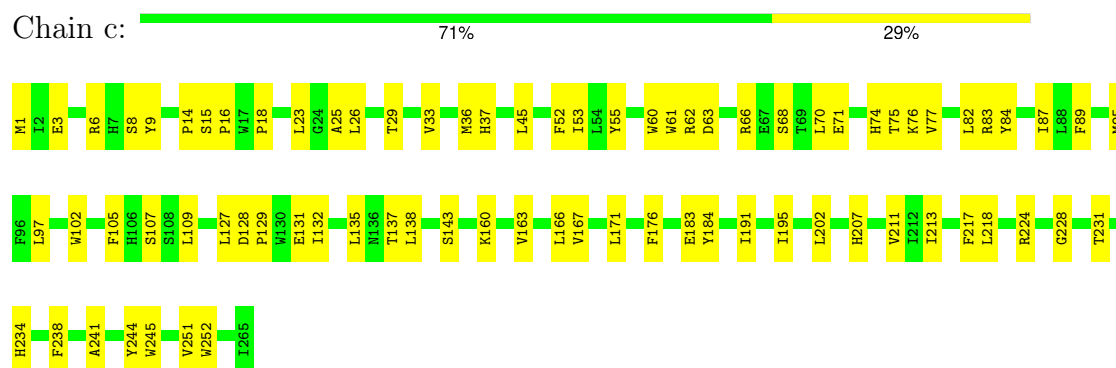
Chain a: 64% 35%



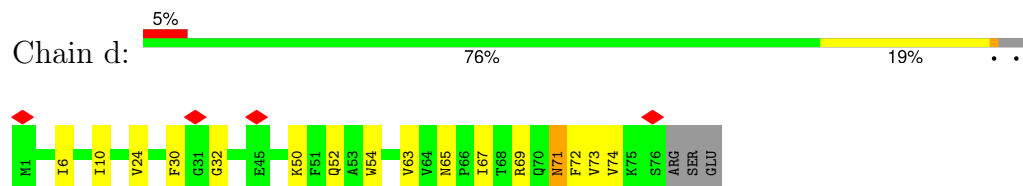
- Molecule 12: Cytochrome c oxidase subunit 2



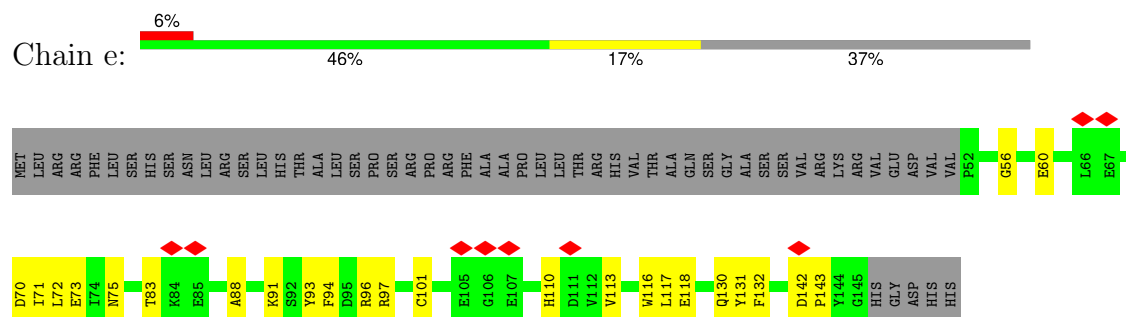
- Molecule 13: COX3



- Molecule 14: COX4

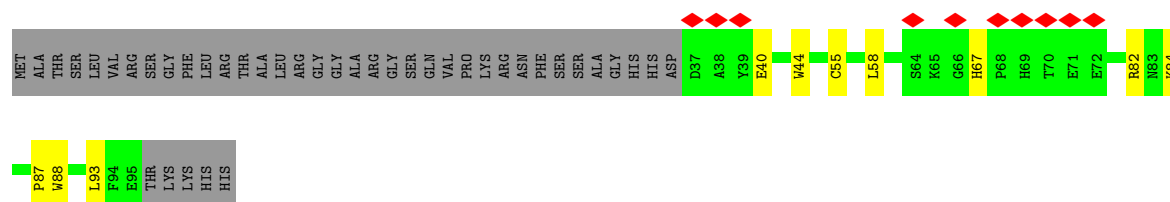


- Molecule 15: cytochrome c oxidase subunit 5b-2, mitochondrial

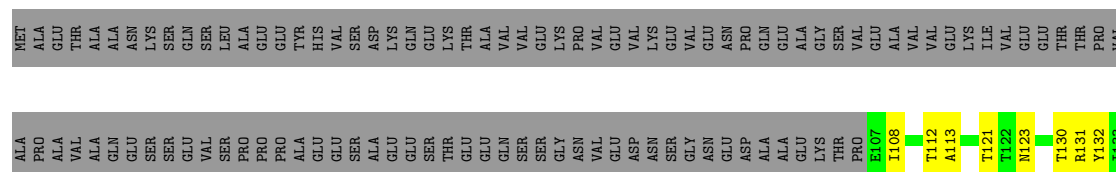


- Molecule 16: cytochrome c oxidase subunit 6a, mitochondrial





• Molecule 17: cytochrome c oxidase subunit 6b-1



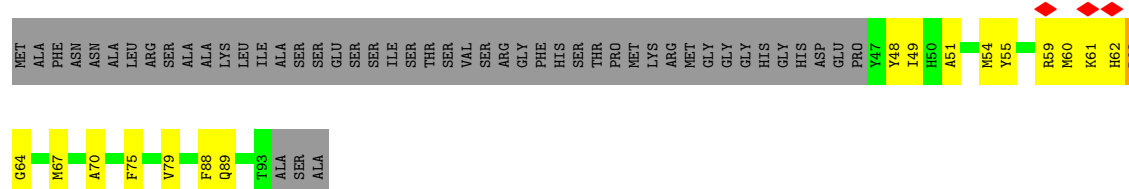
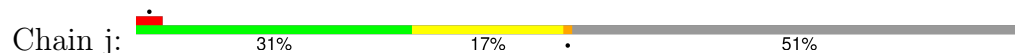
• Molecule 18: Cytochrome c oxidase subunit 5C



• Molecule 19: COX7a



• Molecule 20: COX7c



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	29348	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 ($e^-/\text{\AA}^2$)	86.4	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	60010	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	45.662	Depositor
Minimum map value	-36.912	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.159	Depositor
Recommended contour level	6	Depositor
Map size (Å)	426.5984, 426.5984, 426.5984	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8332, 0.8332, 0.8332	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, CUA, HEC, HEA, ZN, HEM, CDL, 3PE, CU, PC1

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	0.24	0/3914	0.41	0/5309
1	M	0.24	0/3914	0.41	0/5309
2	B	0.22	0/3541	0.41	1/4803 (0.0%)
2	N	0.22	0/3526	0.41	0/4785
3	C	0.28	0/3220	0.40	0/4413
3	O	0.29	0/3220	0.42	0/4413
4	D	0.23	0/1962	0.36	0/2663
4	P	0.24	0/1962	0.37	0/2663
5	E	0.22	0/588	0.37	0/797
5	Q	0.23	0/588	0.42	0/797
6	F	0.25	0/986	0.37	0/1326
6	R	0.25	0/980	0.38	0/1318
7	G	0.20	0/595	0.36	0/807
7	S	0.19	0/595	0.34	0/807
8	H	0.18	0/550	0.35	0/737
8	T	0.19	0/541	0.45	0/724
9	J	0.19	0/490	0.38	0/660
9	V	0.21	0/486	0.43	0/655
10	K	0.16	0/222	0.33	0/305
10	W	0.18	0/230	0.31	0/316
11	a	0.30	0/4214	0.50	0/5758
12	b	0.26	0/1971	0.46	0/2697
13	c	0.27	0/2217	0.39	0/3030
14	d	0.23	0/612	0.44	0/832
15	e	0.22	0/756	0.40	0/1026
16	f	0.17	0/499	0.42	0/682
17	g	0.28	0/631	0.62	0/853
18	h	0.25	0/399	0.44	0/538
19	i	0.24	0/524	0.50	0/705
20	j	0.23	0/394	0.51	0/528
All	All	0.25	0/44327	0.42	1/60256 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	B	107	GLY	N-CA-C	5.73	117.62	110.29

There are no chirality outliers.

There are no planarity outliers.

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	3838	0	3797	78	0
1	M	3838	0	3797	94	0
2	B	3471	0	3471	98	0
2	N	3456	0	3453	85	0
3	C	3104	0	3070	70	0
3	O	3104	0	3070	71	0
4	D	1910	0	1843	48	0
4	P	1910	0	1843	49	0
5	E	574	0	591	16	0
5	Q	574	0	591	30	0
6	F	965	0	982	28	0
6	R	959	0	977	15	0
7	G	578	0	599	17	0
7	S	578	0	599	13	0
8	H	536	0	528	15	0
8	T	527	0	521	26	0
9	J	480	0	486	7	0
9	V	476	0	483	17	0
10	K	218	0	230	2	0
10	W	226	0	241	7	0
11	a	4074	0	4063	187	0
12	b	1915	0	1876	73	0
13	c	2134	0	2098	74	0
14	d	595	0	596	23	0
15	e	733	0	677	16	0
16	f	480	0	452	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	g	612	0	563	12	0
18	h	391	0	405	8	0
19	i	510	0	528	19	0
20	j	384	0	398	16	0
21	A	1	0	0	0	0
21	M	1	0	0	0	0
21	e	1	0	0	0	0
22	A	29	0	32	1	0
22	M	27	0	28	1	0
22	S	28	0	30	2	0
22	a	39	0	52	1	0
22	i	36	0	46	4	0
23	A	51	0	46	1	0
23	C	109	0	106	5	0
23	D	41	0	26	1	0
23	M	53	0	50	4	0
23	O	54	0	55	2	0
23	P	48	0	40	2	0
23	S	50	0	44	2	0
23	a	67	0	78	1	0
24	C	86	0	60	7	0
24	O	86	0	60	9	0
25	C	158	0	189	10	0
25	F	32	0	38	2	0
25	G	20	0	14	0	0
25	O	109	0	114	7	0
25	P	28	0	30	2	0
25	a	227	0	301	7	0
25	b	108	0	141	4	0
25	c	200	0	270	13	0
25	d	35	0	44	1	0
25	h	38	0	50	2	0
25	i	35	0	44	2	0
26	D	43	0	30	8	0
26	P	43	0	30	3	0
27	a	120	0	108	11	0
28	a	1	0	0	0	0
29	a	1	0	0	0	0
30	b	2	0	0	0	0
31	i	9	0	12	0	0
All	All	45166	0	44996	1062	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 12.

All (1062) 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)
4:P:283:GLN:NE2	5:Q:115:LEU:CA	1.87	1.37
4:P:283:GLN:NE2	5:Q:115:LEU:HA	0.94	1.26
4:P:283:GLN:HE21	5:Q:115:LEU:CA	1.43	1.23
9:V:32:ILE:HG21	10:W:32:THR:HG22	1.25	1.10
11:a:90:ILE:HD11	11:a:175:ARG:HG2	1.21	1.08
3:C:374:ILE:HG12	3:C:377:ARG:NH2	1.72	1.05
11:a:219:ASN:HD21	16:f:82:ARG:HA	1.32	0.93
8:T:19:PRO:CB	14:d:72:PHE:O	2.23	0.86
11:a:90:ILE:CD1	11:a:175:ARG:HG2	2.04	0.85
9:V:32:ILE:HG21	10:W:32:THR:CG2	2.09	0.82
8:T:19:PRO:O	14:d:72:PHE:CE1	2.32	0.82
8:T:19:PRO:HB3	14:d:72:PHE:O	1.81	0.80
11:a:356:THR:HG21	11:a:431:HIS:HE1	1.47	0.79
12:b:219:CYS:SG	12:b:230:MET:CE	2.70	0.79
6:F:16:LEU:HD12	25:F:201:3PE:H352	1.64	0.79
3:O:162:VAL:HG13	3:O:163:VAL:HG13	1.64	0.79
4:P:283:GLN:HE22	5:Q:115:LEU:HA	0.99	0.79
4:D:95:HIS:HE1	4:D:129:MET:HE1	1.45	0.78
11:a:90:ILE:HD11	11:a:175:ARG:CG	2.10	0.78
1:M:106:THR:HG22	1:M:279:ALA:HB3	1.67	0.77
11:a:433:LEU:HD11	11:a:452:TRP:HB2	1.65	0.77
4:D:280:ALA:HB2	5:E:121:VAL:HG11	1.67	0.77
20:j:48:TYR:OH	20:j:59:ARG:NH1	2.19	0.76
7:G:71:ARG:NH1	8:H:51:ASP:OD2	2.19	0.75
11:a:187:PHE:H	11:a:259:HIS:HE1	1.32	0.75
20:j:60:MET:HE1	20:j:67:MET:HE3	1.67	0.75
12:b:174:ARG:HH22	17:g:113:ALA:HB3	1.52	0.75
11:a:99:ARG:NH1	13:c:63:ASP:OD2	2.20	0.75
3:C:374:ILE:HG12	3:C:377:ARG:HH22	1.52	0.74
13:c:163:VAL:HG21	19:i:6:PHE:HE2	1.51	0.74
11:a:299:LEU:O	11:a:304:ARG:NH2	2.20	0.74
11:a:301:VAL:HG12	11:a:304:ARG:NH1	2.03	0.73
13:c:71:GLU:OE2	19:i:29:LYS:NZ	2.21	0.73
3:O:35:TRP:HA	3:O:38:PHE:HD2	1.53	0.73
2:N:212:LEU:HD12	2:N:384:TYR:HE1	1.53	0.73
2:B:84:ASN:HD21	2:B:280:LEU:HB2	1.52	0.72
11:a:264:PHE:CZ	11:a:491:TRP:HZ2	2.07	0.72
4:P:280:ALA:HB2	5:Q:121:VAL:HG11	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:306:ASN:O	6:F:65:ARG:HD3	1.90	0.72
11:a:40:MET:HE3	14:d:24:VAL:HG21	1.72	0.71
11:a:385:MET:HE1	11:a:423:VAL:HG13	1.73	0.71
1:A:107:GLU:OE1	1:A:470:ARG:NH1	2.23	0.71
2:N:357:ARG:O	2:N:361:GLU:HB2	1.91	0.71
8:T:19:PRO:CG	14:d:72:PHE:O	2.39	0.70
19:i:34:LYS:O	19:i:38:VAL:HG22	1.91	0.70
2:N:326:ILE:HG22	2:N:465:ILE:HD11	1.73	0.70
11:a:296:THR:HG22	11:a:367:ILE:HD13	1.72	0.70
2:B:204:LEU:HD13	2:B:211:LEU:HD21	1.73	0.70
17:g:153:ALA:HA	17:g:156:TYR:CE1	2.26	0.69
3:C:62:PRO:HD2	3:O:62:PRO:HD2	1.73	0.69
1:A:526:ARG:O	10:K:26:TRP:NE1	2.22	0.69
3:O:293:ASP:O	3:O:296:GLY:N	2.26	0.69
14:d:71:ASN:HD22	14:d:71:ASN:C	2.01	0.69
11:a:39:ARG:NH2	27:a:602:HEA:OMA	2.26	0.68
6:F:119:ARG:NH1	6:F:122:PRO:OXT	2.26	0.68
2:N:162:PHE:CE2	2:N:172:MET:HG2	2.29	0.68
2:B:468:ASN:HB2	2:B:472:LYS:NZ	2.09	0.68
2:N:335:MET:HE1	2:N:406:ILE:HG21	1.75	0.68
6:F:118:GLN:HE21	25:O:401:3PE:C11	2.06	0.67
3:O:7:ARG:NH2	25:O:401:3PE:O13	2.26	0.67
11:a:363:SER:HB3	12:b:101:LEU:HD11	1.77	0.67
3:C:293:ASP:O	3:C:296:GLY:N	2.28	0.67
4:P:283:GLN:HE21	5:Q:115:LEU:N	1.93	0.67
1:M:46:THR:O	1:M:52:ARG:NH1	2.27	0.67
3:O:105:ARG:HH12	24:O:404:HEM:HBD2	1.60	0.67
12:b:116:LYS:NZ	12:b:129:SER:OG	2.24	0.67
17:g:130:THR:O	17:g:134:GLU:HG2	1.94	0.67
3:C:285:TYR:CE2	3:C:289:ARG:NH1	2.63	0.67
2:N:354:LEU:HD22	2:N:368:PHE:HE2	1.60	0.66
11:a:489:ILE:HB	11:a:491:TRP:CE3	2.30	0.66
4:P:83:LEU:O	9:V:53:ASN:ND2	2.28	0.66
6:R:119:ARG:NH1	6:R:120:SER:O	2.28	0.66
11:a:114:LEU:HD11	13:c:29:THR:HG21	1.77	0.66
3:C:202:LEU:HD22	25:C:405:3PE:H251	1.78	0.66
1:A:121:ILE:HG12	1:A:275:MET:HG2	1.76	0.66
2:B:301:HIS:H	2:N:300:ARG:HH12	1.41	0.66
2:N:137:ARG:NH2	2:N:141:GLU:OE2	2.28	0.66
3:O:36:TRP:NE1	24:O:404:HEM:O2D	2.29	0.66
2:B:84:ASN:O	2:B:282:ASN:ND2	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:274:ILE:HG21	25:P:401:3PE:H271	1.76	0.66
5:E:124:SER:OG	9:J:39:GLU:OE1	2.13	0.65
1:M:70:ARG:HA	1:M:73:LYS:HE3	1.77	0.65
3:O:94:MET:HG3	3:O:246:PHE:HD1	1.60	0.65
1:M:110:LEU:HB2	2:N:71:SER:HB2	1.79	0.65
1:M:162:MET:SD	1:M:188:GLN:NE2	2.70	0.65
11:a:187:PHE:H	11:a:259:HIS:CE1	2.14	0.65
8:T:35:ILE:HG23	8:T:43:LYS:HB2	1.78	0.64
11:a:68:MET:HB3	27:a:602:HEA:HBC1	1.79	0.64
11:a:504:VAL:HG13	11:a:505:GLN:H	1.62	0.64
13:c:231:THR:HG23	13:c:234:HIS:H	1.62	0.64
3:O:291:ILE:HD12	3:O:292:PRO:HD2	1.78	0.64
3:C:327:ILE:HD11	25:F:201:3PE:H341	1.79	0.64
1:M:411:CYS:SG	3:O:2:THR:OG1	2.52	0.64
12:b:177:ILE:HG22	12:b:197:ALA:HB2	1.79	0.64
13:c:66:ARG:NH1	19:i:33:ASP:OD2	2.31	0.64
3:C:117:GLU:OE1	6:F:119:ARG:NH2	2.31	0.64
3:C:7:ARG:NH1	6:R:119:ARG:O	2.31	0.64
6:F:80:PRO:HG2	6:F:83:LEU:HD13	1.80	0.64
2:N:363:GLN:HG2	2:N:364:GLN:OE1	1.98	0.64
4:P:283:GLN:HE21	5:Q:115:LEU:HA	0.83	0.64
6:F:119:ARG:O	3:O:7:ARG:NH1	2.30	0.63
4:P:224:ALA:HB3	26:P:402:HEC:HBD2	1.79	0.63
1:A:71:PHE:O	2:B:133:ARG:NH2	2.31	0.63
4:P:283:GLN:NE2	5:Q:115:LEU:C	2.56	0.63
3:C:323:SER:O	6:F:27:ARG:NH1	2.31	0.63
13:c:184:TYR:O	25:c:302:3PE:N	2.32	0.63
4:D:289:ARG:HH12	7:G:26:LEU:HG	1.63	0.63
12:b:219:CYS:SG	12:b:230:MET:HE2	2.38	0.63
17:g:132:TYR:OH	17:g:169:ASN:OD1	2.17	0.63
1:A:92:GLU:OE2	1:A:94:ARG:NH1	2.32	0.63
2:N:381:PHE:HB3	2:N:477:ILE:HD11	1.79	0.63
7:S:71:ARG:HD3	8:T:48:GLN:HE22	1.64	0.63
8:T:21:CYS:O	8:T:24:PRO:HD2	1.99	0.62
9:V:24:ASN:O	9:V:28:VAL:HG23	1.98	0.62
13:c:75:THR:HG22	13:c:76:LYS:H	1.64	0.62
2:B:353:ARG:NH2	2:B:411:GLN:O	2.32	0.62
1:A:70:ARG:NH1	2:B:275:PRO:O	2.28	0.62
10:W:38:VAL:HG12	10:W:40:VAL:HG13	1.80	0.62
11:a:161:ILE:HD11	11:a:202:LEU:HB3	1.81	0.62
11:a:213:LEU:HD21	13:c:36:MET:HE1	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:320:ARG:NH1	6:F:40:ASP:OD2	2.32	0.62
4:P:233:ALA:HB3	4:P:247:MET:HE1	1.79	0.62
1:M:525:ASN:N	23:M:602:CDL:OB3	2.27	0.62
2:N:297:ASP:OD2	2:N:299:ARG:NH1	2.33	0.62
3:O:222:MET:HE3	6:R:66:LEU:HB3	1.82	0.62
2:B:357:ARG:NH2	2:B:402:GLU:OE1	2.31	0.62
1:M:257:ILE:HG22	1:M:259:LYS:H	1.65	0.62
2:N:262:ALA:HB2	2:N:439:SER:HB3	1.82	0.62
3:C:163:VAL:HG23	3:C:164:GLY:H	1.65	0.62
1:M:170:THR:HG22	1:M:175:THR:HG23	1.81	0.62
1:M:257:ILE:O	1:M:261:HIS:ND1	2.32	0.62
11:a:356:THR:HG21	11:a:431:HIS:CE1	2.33	0.62
2:N:332:GLN:NE2	2:N:370:ALA:O	2.33	0.62
11:a:99:ARG:HB3	13:c:60:TRP:HZ2	1.64	0.62
4:P:125:GLU:HG2	9:V:68:LYS:HB3	1.81	0.62
6:F:118:GLN:HE21	25:O:401:3PE:H112	1.64	0.61
11:a:171:ILE:O	11:a:175:ARG:NH2	2.33	0.61
11:a:505:GLN:HE22	11:a:509:ALA:HB2	1.65	0.61
3:C:209:GLN:OE1	25:C:405:3PE:O22	2.18	0.61
11:a:14:LYS:HE2	20:j:54:MET:SD	2.40	0.61
1:A:70:ARG:NH2	2:B:279:ASP:OD2	2.31	0.61
1:A:302:ASP:OD1	1:A:303:ALA:N	2.32	0.61
9:V:32:ILE:CG2	10:W:32:THR:HG22	2.15	0.61
11:a:398:TRP:O	11:a:402:ILE:HG13	2.00	0.61
2:B:221:TYR:HH	2:B:378:THR:HG1	1.48	0.61
3:O:323:SER:O	6:R:27:ARG:NH1	2.34	0.61
2:B:137:ARG:NH2	2:B:141:GLU:OE2	2.33	0.61
2:B:293:TYR:OH	2:B:483:THR:OG1	2.17	0.61
1:M:267:GLN:O	1:M:300:SER:OG	2.18	0.61
3:O:126:ILE:O	3:O:130:MET:HG3	2.01	0.61
11:a:211:MET:HG3	11:a:222:PHE:CD2	2.36	0.61
2:B:468:ASN:HB2	2:B:472:LYS:HZ3	1.64	0.61
7:S:56:TYR:O	7:S:60:GLN:HG2	2.01	0.61
8:T:29:GLN:HA	8:T:32:ILE:HD12	1.83	0.60
2:B:434:SER:O	2:B:437:ILE:N	2.33	0.60
13:c:224:ARG:NH1	25:c:303:3PE:O13	2.35	0.60
13:c:8:SER:HB2	13:c:75:THR:HG21	1.84	0.60
3:O:33:SER:HG	3:O:35:TRP:CD1	2.19	0.60
1:A:321:GLU:HG2	7:G:14:ALA:HB3	1.84	0.60
3:C:249:TRP:HZ3	3:C:256:VAL:HB	1.65	0.60
3:O:41:LEU:HD21	3:O:242:PHE:HB2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:405:ALA:HB1	1:M:415:LEU:HD21	1.82	0.60
3:O:33:SER:O	3:O:234:LYS:HE2	2.02	0.60
2:B:162:PHE:CE2	2:B:172:MET:HG2	2.36	0.60
20:j:62:HIS:O	20:j:64:GLY:N	2.35	0.60
3:O:223:ASP:OD2	4:P:298:ARG:NH1	2.35	0.60
25:C:407:3PE:H3H2	25:C:407:3PE:H3C2	1.83	0.59
11:a:355:LEU:HD12	12:b:43:LEU:HB3	1.84	0.59
12:b:195:CYS:HB3	12:b:205:ILE:HD11	1.83	0.59
1:A:405:ALA:HB1	1:A:415:LEU:HD21	1.84	0.59
11:a:83:ASN:ND2	11:a:101:ASN:OD1	2.33	0.59
11:a:365:LEU:HD21	12:b:36:HIS:HB2	1.84	0.59
13:c:97:LEU:HD13	13:c:251:VAL:HG11	1.84	0.59
1:A:106:THR:HG22	1:A:279:ALA:HB3	1.84	0.59
5:E:138:SER:OG	5:E:139:ALA:N	2.35	0.59
4:P:72:CYS:SG	4:P:187:ASN:ND2	2.71	0.59
2:B:177:VAL:HG11	2:B:276:LEU:HB3	1.84	0.59
13:c:1:MET:HE2	13:c:3:GLU:HB3	1.84	0.59
4:D:224:ALA:HB3	26:D:501:HEC:HBD2	1.85	0.59
1:M:347:ASP:OD2	1:M:494:ARG:NH1	2.33	0.59
2:B:332:GLN:HE21	2:B:371:PHE:HA	1.68	0.59
3:C:75:MET:HE3	3:C:85:ARG:HD3	1.84	0.59
2:N:162:PHE:CD2	2:N:172:MET:HG2	2.37	0.59
11:a:96:ALA:HB2	11:a:174:MET:HE3	1.85	0.59
2:B:293:TYR:OH	2:B:481:PRO:O	2.20	0.58
25:C:406:3PE:H111	6:F:24:LEU:HD11	1.85	0.58
11:a:268:PRO:HG2	12:b:73:VAL:HG21	1.85	0.58
11:a:377:ALA:HB2	11:a:430:MET:HB2	1.85	0.58
4:D:225:MET:CE	26:D:501:HEC:NC	2.66	0.58
1:M:211:ARG:HH21	1:M:257:ILE:H	1.51	0.58
3:O:90:ASN:O	3:O:94:MET:HG2	2.02	0.58
11:a:157:GLY:HA2	11:a:202:LEU:HD21	1.84	0.58
1:M:93:THR:HG21	1:M:470:ARG:HD3	1.86	0.58
12:b:132:ASN:HD22	12:b:137:GLN:HA	1.68	0.58
12:b:196:ASP:O	12:b:203:ASN:ND2	2.35	0.58
2:B:121:LEU:HD23	2:B:244:LEU:HD11	1.85	0.58
2:B:156:GLU:OE1	2:B:376:ASN:ND2	2.37	0.58
2:B:468:ASN:OD1	2:B:469:ASP:N	2.36	0.58
7:G:67:LYS:O	7:G:71:ARG:HB2	2.02	0.58
15:e:94:PHE:CD2	15:e:143:PRO:HA	2.38	0.58
1:A:48:MET:O	1:A:52:ARG:NE	2.32	0.58
23:A:603:CDL:H131	23:C:401:CDL:HB4	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:288:LEU:HD12	3:C:301:ILE:HG13	1.86	0.58
1:M:205:ASN:OD1	1:M:206:ARG:N	2.36	0.58
3:O:123:GLY:C	24:O:404:HEM:HBC2	2.29	0.58
9:V:20:VAL:HG23	9:V:26:VAL:HG12	1.84	0.58
11:a:433:LEU:HD23	11:a:438:MET:HE2	1.85	0.58
1:A:198:GLN:HE22	1:A:296:PHE:HA	1.68	0.58
23:C:401:CDL:HA22	23:C:401:CDL:HB32	1.85	0.58
23:M:602:CDL:H142	23:O:402:CDL:HA4	1.86	0.58
3:O:289:ARG:HD3	3:O:350:VAL:HG12	1.85	0.57
3:O:34:TYR:HA	3:O:234:LYS:HE3	1.86	0.57
11:a:72:MET:HE1	11:a:388:VAL:HG22	1.86	0.57
13:c:127:LEU:HD11	13:c:183:GLU:OE2	2.04	0.57
7:S:41:ASN:HB2	23:S:102:CDL:H712	1.86	0.57
2:B:168:TYR:O	2:B:172:MET:HG3	2.04	0.57
3:C:316:SER:O	6:F:43:TYR:OH	2.11	0.57
3:O:317:MET:HE3	3:O:317:MET:HA	1.86	0.57
11:a:303:THR:HG22	25:a:607:3PE:H32	1.86	0.57
2:B:77:THR:HG21	2:B:452:ARG:HD2	1.87	0.57
8:T:35:ILE:HD12	8:T:43:LYS:HB2	1.87	0.57
11:a:376:VAL:HA	11:a:379:PHE:CE1	2.39	0.57
3:C:285:TYR:HE2	3:C:289:ARG:NH1	2.00	0.57
1:M:514:ASP:OD1	1:M:514:ASP:N	2.37	0.57
4:D:276:VAL:HG12	5:E:121:VAL:HG13	1.85	0.57
12:b:78:ILE:HG12	12:b:82:TRP:CZ3	2.40	0.57
7:S:15:LEU:HB3	7:S:20:GLN:HE21	1.69	0.57
11:a:9:PHE:CE1	13:c:16:PRO:HB3	2.39	0.57
2:B:100:ILE:HD11	2:B:264:VAL:HG21	1.85	0.57
13:c:131:GLU:HG3	13:c:132:ILE:H	1.70	0.57
11:a:99:ARG:HB3	13:c:60:TRP:CZ2	2.39	0.57
11:a:148:LEU:HD23	13:c:33:VAL:HG21	1.86	0.57
11:a:171:ILE:HD12	11:a:188:VAL:HG13	1.86	0.57
2:N:224:ALA:HB3	2:N:291:SER:HB3	1.87	0.56
12:b:182:VAL:HG22	12:b:183:LEU:H	1.70	0.56
2:B:79:ILE:HD11	2:B:87:LYS:HD2	1.86	0.56
5:Q:110:PHE:HE2	22:S:101:PC1:O22	1.88	0.56
11:a:385:MET:O	11:a:389:PHE:HB2	2.04	0.56
3:C:374:ILE:HG12	3:C:377:ARG:HH21	1.67	0.56
4:D:225:MET:HE1	26:D:501:HEC:C1C	2.34	0.56
1:M:106:THR:OG1	1:M:285:HIS:ND1	2.31	0.56
1:M:138:PHE:HZ	1:M:207:ILE:HG23	1.70	0.56
3:O:318:TYR:OH	6:R:44:ASP:OD2	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:a:489:ILE:HB	11:a:491:TRP:HE3	1.69	0.56
1:M:48:MET:O	1:M:51:ASP:N	2.38	0.56
2:N:327:VAL:HG11	2:N:473:ILE:HG13	1.87	0.56
15:e:101:CYS:SG	15:e:130:GLN:NE2	2.76	0.56
1:A:199:ASN:OD1	1:A:298:LYS:NZ	2.39	0.56
3:C:116:ARG:HH22	3:C:320:ARG:HH22	1.53	0.56
5:E:126:ILE:O	5:E:130:VAL:HG23	2.05	0.56
6:F:46:ASP:OD1	6:F:117:TYR:OH	2.24	0.56
1:M:166:LEU:HB3	2:N:346:PRO:HG2	1.87	0.56
1:M:413:ASP:OD1	1:M:414:ASP:N	2.39	0.56
11:a:97:PHE:HB2	11:a:166:ASN:OD1	2.06	0.56
2:N:124:ARG:NH2	2:N:200:GLU:OE2	2.34	0.56
11:a:334:ILE:O	12:b:63:SER:HB2	2.05	0.56
11:a:505:GLN:NE2	11:a:509:ALA:HB2	2.21	0.56
8:T:19:PRO:O	14:d:72:PHE:CZ	2.59	0.56
11:a:127:THR:HG21	11:a:131:VAL:HG12	1.88	0.56
27:a:602:HEA:H132	27:a:602:HEA:HHC	1.87	0.56
1:M:96:THR:OG1	1:M:285:HIS:NE2	2.39	0.55
12:b:212:GLU:N	12:b:212:GLU:OE2	2.39	0.55
1:A:347:ASP:OD2	1:A:494:ARG:NH1	2.39	0.55
3:C:145:MET:HE2	3:C:261:ASP:HB2	1.87	0.55
1:M:350:ALA:O	1:M:354:MET:HG3	2.06	0.55
13:c:217:PHE:HE1	25:c:303:3PE:H342	1.70	0.55
11:a:427:PHE:HA	11:a:430:MET:HG3	1.88	0.55
1:M:234:HIS:NE2	1:M:395:TYR:OH	2.27	0.55
11:a:419:THR:O	11:a:423:VAL:HG12	2.07	0.55
7:G:22:VAL:HG12	7:G:23:MET:HG2	1.89	0.55
11:a:147:ASP:OD2	13:c:37:HIS:NE2	2.34	0.55
11:a:160:SER:HB3	11:a:198:LEU:HD21	1.87	0.55
12:b:214:VAL:HG12	12:b:235:GLU:HG2	1.88	0.55
4:D:137:ASP:OD1	4:D:138:GLY:N	2.39	0.55
4:P:283:GLN:HE21	5:Q:114:VAL:C	2.13	0.55
11:a:167:PHE:O	11:a:171:ILE:HG12	2.06	0.55
2:B:86:LEU:HG	2:B:257:MET:HB2	1.89	0.55
2:N:53:PRO:HG3	2:N:59:LEU:HA	1.89	0.55
2:N:353:ARG:NH2	2:N:411:GLN:O	2.34	0.55
4:P:217:TYR:OH	8:T:57:ASP:OD2	2.19	0.55
11:a:1:MET:C	11:a:4:PRO:HD2	2.32	0.55
1:A:198:GLN:NE2	1:A:297:THR:O	2.40	0.54
2:B:86:LEU:HD13	2:B:277:LEU:HB3	1.90	0.54
1:M:71:PHE:O	2:N:133:ARG:NH2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:c:70:LEU:HA	19:i:16:GLN:HG2	1.89	0.54
2:B:99:SER:H	2:B:262:ALA:HB3	1.72	0.54
2:N:142:VAL:HG13	2:N:162:PHE:HE1	1.72	0.54
11:a:117:SER:O	11:a:121:VAL:HG13	2.07	0.54
11:a:291:ALA:HB3	11:a:307:PHE:CE1	2.42	0.54
2:N:441:ASP:OD1	2:N:445:GLN:NE2	2.40	0.54
3:O:159:ALA:HB1	3:O:295:SER:HA	1.88	0.54
18:h:52:LEU:HA	18:h:57:ILE:HG23	1.88	0.54
27:a:601:HEA:HHC	27:a:601:HEA:H122	1.90	0.54
3:C:230:TYR:O	4:D:292:TRP:NE1	2.34	0.54
4:D:191:TYR:OH	26:D:501:HEC:O2A	2.21	0.54
4:D:305:VAL:CG1	1:M:48:MET:SD	2.96	0.54
4:P:184:ALA:O	4:P:185:ARG:NH2	2.33	0.54
1:A:229:ILE:HD11	1:A:506:MET:HG2	1.90	0.54
11:a:300:ASP:HB2	25:a:607:3PE:H121	1.89	0.54
6:F:118:GLN:NE2	25:O:401:3PE:C11	2.71	0.54
3:O:50:ILE:HA	24:O:403:HEM:HAB	1.89	0.54
4:D:273:TRP:CE2	5:E:128:LEU:HD22	2.43	0.54
11:a:17:GLY:HA3	11:a:84:TRP:HD1	1.73	0.54
11:a:254:PHE:CD2	11:a:321:LYS:HE2	2.43	0.54
2:B:114:PHE:O	2:B:238:ARG:NH1	2.41	0.54
1:M:147:THR:HG22	1:M:200:SER:HA	1.89	0.54
3:O:60:TYR:OH	3:O:140:LEU:O	2.24	0.54
6:R:47:VAL:HG13	6:R:94:LEU:HD21	1.89	0.54
4:D:96:GLN:HE22	4:D:237:GLU:HG2	1.72	0.53
6:F:118:GLN:NE2	25:O:401:3PE:H111	2.23	0.53
2:N:168:TYR:O	2:N:172:MET:HG3	2.08	0.53
11:a:259:HIS:HD2	11:a:499:THR:HG21	1.73	0.53
5:Q:99:ARG:NH1	5:Q:100:PHE:O	2.40	0.53
7:S:33:LYS:O	7:S:37:LYS:HG2	2.09	0.53
8:T:31:CYS:O	8:T:35:ILE:HG12	2.07	0.53
1:M:181:VAL:HG22	1:M:182:THR:H	1.74	0.53
2:N:221:TYR:HH	2:N:378:THR:HG1	1.57	0.53
3:O:246:PHE:CE2	3:O:250:ILE:HD11	2.43	0.53
4:P:228:MET:HE3	4:P:228:MET:HA	1.91	0.53
12:b:220:SER:O	12:b:221:GLU:HG2	2.09	0.53
13:c:62:ARG:NH2	19:i:33:ASP:OD2	2.42	0.53
4:D:289:ARG:NH1	7:G:26:LEU:HG	2.22	0.53
2:N:133:ARG:NH1	2:N:141:GLU:OE2	2.42	0.53
11:a:383:LEU:CD2	27:a:602:HEA:HAC	2.39	0.53
2:N:212:LEU:HD12	2:N:384:TYR:CE1	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:b:109:VAL:HG21	12:b:172:HIS:NE2	2.24	0.53
2:B:354:LEU:HD13	2:B:368:PHE:CE2	2.43	0.52
3:C:75:MET:HE3	3:C:85:ARG:CD	2.40	0.52
4:P:274:ILE:CG2	25:P:401:3PE:H271	2.39	0.52
2:B:186:LEU:HD13	2:B:188:TRP:CZ2	2.43	0.52
2:B:216:ILE:HD11	2:B:310:ALA:HB1	1.91	0.52
3:C:94:MET:HE1	3:C:249:TRP:CD1	2.45	0.52
4:P:108:MET:O	4:P:179:SER:OG	2.25	0.52
4:P:135:VAL:HG21	4:P:154:ASP:OD2	2.09	0.52
12:b:128:TYR:HE2	12:b:141:PHE:HE1	1.56	0.52
1:A:305:THR:HB	1:A:308:GLN:HG2	1.91	0.52
2:B:162:PHE:CD2	2:B:172:MET:HG2	2.44	0.52
4:D:95:HIS:CE1	4:D:129:MET:HE1	2.35	0.52
8:H:35:ILE:HD12	8:H:43:LYS:HG3	1.91	0.52
1:M:413:ASP:OD2	1:M:511:ARG:NH2	2.42	0.52
13:c:70:LEU:HD22	19:i:19:PHE:CD2	2.45	0.52
4:P:228:MET:O	4:P:230:ASN:ND2	2.41	0.52
9:V:20:VAL:HG21	9:V:30:PHE:HB2	1.90	0.52
11:a:270:PHE:H	11:a:328:THR:HB	1.73	0.52
13:c:207:HIS:NE2	13:c:252:TRP:HB2	2.25	0.52
1:A:413:ASP:OD1	1:A:414:ASP:N	2.41	0.52
3:C:111:SER:OG	24:C:403:HEM:O1D	2.23	0.52
1:M:142:MET:HE3	1:M:142:MET:HA	1.91	0.52
11:a:17:GLY:HA3	11:a:84:TRP:CD1	2.44	0.52
11:a:127:THR:CG2	11:a:131:VAL:HG12	2.40	0.52
11:a:164:SER:OG	11:a:195:ALA:O	2.28	0.52
11:a:418:ILE:HD11	14:d:10:ILE:HA	1.91	0.52
2:B:323:LYS:O	2:B:327:VAL:HG23	2.10	0.52
3:C:123:GLY:C	24:C:403:HEM:HBC2	2.34	0.52
9:V:50:TRP:O	9:V:54:ASN:ND2	2.40	0.52
11:a:289:VAL:HG22	11:a:292:HIS:HD2	1.74	0.52
1:A:77:PRO:HG3	2:B:137:ARG:HG3	1.91	0.52
2:B:262:ALA:HB2	2:B:439:SER:HB3	1.91	0.52
4:P:283:GLN:HE22	5:Q:115:LEU:CA	1.81	0.52
8:T:25:LEU:HD12	8:T:52:TYR:CZ	2.45	0.52
9:V:47:HIS:NE2	9:V:51:GLU:OE2	2.43	0.52
11:a:381:TYR:O	11:a:385:MET:HB2	2.10	0.52
2:B:154:SER:OG	2:B:155:ARG:N	2.41	0.52
1:M:138:PHE:HD1	1:M:214:ILE:HD12	1.73	0.52
3:O:7:ARG:NH2	25:O:401:3PE:C11	2.72	0.52
11:a:219:ASN:ND2	16:f:82:ARG:HD2	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:b:152:GLU:HB2	12:b:155:GLN:NE2	2.25	0.52
2:N:105:ASP:O	2:N:256:ARG:NH2	2.43	0.52
14:d:71:ASN:O	14:d:71:ASN:ND2	2.22	0.52
20:j:62:HIS:O	20:j:63:ARG:HG2	2.10	0.52
11:a:380:HIS:O	11:a:384:SER:HB3	2.11	0.51
12:b:201:ARG:NH1	17:g:123:ASN:OD1	2.42	0.51
2:B:75:SER:OG	2:B:91:GLU:HB2	2.09	0.51
23:P:403:CDL:O1	23:S:102:CDL:OA4	2.20	0.51
5:Q:120:PHE:HB2	9:V:35:ALA:HB2	1.92	0.51
11:a:13:HIS:CE1	11:a:87:PRO:HG2	2.45	0.51
1:A:292:VAL:HG13	1:A:296:PHE:CD2	2.45	0.51
2:B:112:THR:O	2:B:114:PHE:N	2.43	0.51
11:a:205:LEU:HD22	11:a:241:PHE:CE2	2.44	0.51
12:b:110:ASP:OD1	12:b:110:ASP:N	2.41	0.51
13:c:55:TYR:OH	19:i:36:THR:HG23	2.10	0.51
1:A:143:ILE:HG12	1:A:196:ILE:HG23	1.93	0.51
1:A:389:MET:O	1:A:403:VAL:O	2.28	0.51
2:N:78:LYS:O	2:N:89:ALA:HA	2.11	0.51
4:P:273:TRP:CE2	5:Q:128:LEU:HD22	2.46	0.51
13:c:135:LEU:HD12	16:f:58:LEU:HG	1.92	0.51
1:A:210:GLU:HA	1:A:213:VAL:HG12	1.91	0.51
2:B:106:CYS:SG	2:B:107:GLY:N	2.84	0.51
1:M:181:VAL:HG11	1:M:186:VAL:HA	1.93	0.51
5:Q:127:ARG:HD3	10:W:36:TYR:CZ	2.45	0.51
11:a:475:THR:HG21	25:a:610:3PE:H242	1.92	0.51
13:c:75:THR:HG22	13:c:76:LYS:N	2.24	0.51
4:D:283:GLN:HE21	5:E:115:LEU:HA	1.75	0.51
1:M:336:VAL:HG12	1:M:503:ILE:HG12	1.92	0.51
2:N:162:PHE:HE2	2:N:172:MET:HG2	1.74	0.51
4:P:302:LEU:HD23	7:S:10:SER:HB3	1.91	0.51
11:a:520:LYS:HD3	15:e:132:PHE:CE1	2.46	0.51
12:b:132:ASN:ND2	12:b:137:GLN:HA	2.25	0.51
4:D:108:MET:O	4:D:179:SER:OG	2.29	0.51
4:P:93:ARG:HG2	4:P:236:TYR:CE1	2.46	0.51
9:V:32:ILE:CG2	10:W:32:THR:CG2	2.84	0.51
8:H:29:GLN:HA	8:H:32:ILE:HD12	1.93	0.51
1:M:171:SER:OG	1:M:172:ARG:N	2.44	0.51
2:N:268:GLU:O	2:N:272:ILE:HG12	2.11	0.51
6:R:34:ARG:NH1	6:R:91:ARG:O	2.44	0.51
11:a:401:LYS:NZ	11:a:505:GLN:O	2.37	0.51
3:C:158:SER:HB3	3:C:168:VAL:HG21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:a:382:VAL:HG11	27:a:601:HEA:C2C	2.41	0.51
1:M:434:ASP:OD1	1:M:437:ARG:NH2	2.44	0.51
1:A:411:CYS:SG	3:C:2:THR:OG1	2.69	0.50
4:D:262:GLU:O	4:D:266:ARG:HB2	2.11	0.50
5:E:120:PHE:HE1	9:J:31:VAL:HA	1.76	0.50
8:H:41:GLY:H	8:H:43:LYS:NZ	2.08	0.50
8:T:27:GLU:HG3	8:T:48:GLN:HG3	1.92	0.50
14:d:52:GLN:O	14:d:63:VAL:HG12	2.11	0.50
20:j:75:PHE:O	20:j:79:VAL:HG12	2.10	0.50
23:M:602:CDL:H132	3:O:24:ILE:HG12	1.93	0.50
11:a:272:TYR:HD2	11:a:273:LEU:HD22	1.76	0.50
1:M:316:ILE:HD13	5:Q:103:GLY:HA2	1.93	0.50
11:a:426:THR:HB	11:a:459:GLY:HA3	1.93	0.50
1:M:514:ASP:OD2	3:O:230:TYR:OH	2.23	0.50
17:g:112:THR:OG1	17:g:113:ALA:N	2.44	0.50
4:P:288:ARG:NH1	23:P:403:CDL:OA4	2.45	0.50
11:a:230:ASP:OD1	11:a:230:ASP:N	2.43	0.50
20:j:48:TYR:CD1	20:j:51:ALA:HB2	2.46	0.50
1:M:127:PHE:HD2	1:M:309:LEU:HD22	1.77	0.50
1:M:389:MET:O	1:M:403:VAL:C	2.55	0.50
2:N:426:SER:O	2:N:430:MET:HG3	2.12	0.50
3:O:33:SER:HG	3:O:35:TRP:HD1	1.59	0.50
11:a:134:PRO:HB2	12:b:182:VAL:HG23	1.94	0.50
11:a:138:ILE:HG12	16:f:84:LYS:HB2	1.94	0.50
19:i:11:LYS:O	19:i:15:LYS:HG2	2.11	0.50
1:A:234:HIS:NE2	1:A:395:TYR:OH	2.31	0.50
1:M:389:MET:O	1:M:403:VAL:O	2.28	0.50
11:a:205:LEU:HB2	11:a:241:PHE:CG	2.47	0.50
11:a:433:LEU:HD23	11:a:438:MET:CE	2.42	0.50
22:a:605:PC1:H392	13:c:23:LEU:HD22	1.93	0.50
13:c:25:ALA:HA	13:c:53:ILE:HD11	1.93	0.50
2:B:82:LEU:O	2:B:85:GLY:N	2.33	0.49
11:a:504:VAL:HG13	11:a:505:GLN:N	2.27	0.49
12:b:115:ILE:HB	12:b:175:VAL:HG12	1.94	0.49
15:e:96:ARG:CD	15:e:116:TRP:HE1	2.25	0.49
20:j:54:MET:HE3	20:j:55:TYR:CE2	2.47	0.49
1:A:357:MET:HB3	1:A:438:ALA:HB2	1.94	0.49
2:B:327:VAL:HG22	2:B:465:ILE:HD12	1.94	0.49
4:D:70:LEU:HD11	8:H:54:PHE:HB2	1.94	0.49
2:N:70:ASP:O	2:N:71:SER:HB3	2.13	0.49
1:A:48:MET:HB2	1:A:51:ASP:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:151:ASN:HB3	1:M:154:GLU:HG2	1.93	0.49
8:T:13:LEU:HD13	8:T:63:LYS:HB2	1.94	0.49
11:a:134:PRO:HG2	12:b:183:LEU:HG	1.94	0.49
15:e:75:ASN:HA	15:e:97:ARG:HH22	1.77	0.49
3:C:34:TYR:HB2	23:C:409:CDL:HB32	1.94	0.49
3:C:116:ARG:HH22	3:C:320:ARG:NH2	2.10	0.49
1:M:203:GLU:N	1:M:203:GLU:OE1	2.45	0.49
3:O:75:MET:SD	3:O:85:ARG:HD3	2.52	0.49
4:D:272:LYS:NZ	9:J:39:GLU:OE2	2.34	0.49
6:F:111:LEU:HD12	6:F:111:LEU:O	2.13	0.49
11:a:504:VAL:O	11:a:505:GLN:HG2	2.12	0.49
12:b:121:GLN:OE1	12:b:122:TRP:NE1	2.45	0.49
12:b:219:CYS:SG	12:b:230:MET:HE1	2.52	0.49
19:i:8:PRO:O	19:i:9:ARG:HB2	2.12	0.49
2:B:301:HIS:H	2:N:300:ARG:NH1	2.10	0.49
2:B:407:ALA:HA	2:B:474:SER:OG	2.12	0.49
2:N:461:ALA:O	2:N:465:ILE:HG13	2.12	0.49
11:a:222:PHE:HE2	13:c:202:LEU:HD22	1.78	0.49
17:g:148:GLU:O	17:g:151:LYS:HB3	2.13	0.49
1:M:218:MET:O	1:M:221:VAL:HG12	2.13	0.49
2:N:328:LEU:HD11	2:N:381:PHE:HB2	1.93	0.49
2:N:497:GLU:HB3	2:N:501:ARG:HH12	1.77	0.49
3:O:145:MET:HE1	3:O:275:ILE:HA	1.93	0.49
14:d:73:VAL:HG22	14:d:74:VAL:H	1.77	0.49
1:A:215:LEU:HD11	1:A:255:LYS:HE2	1.95	0.49
6:F:40:ASP:HB3	6:F:43:TYR:HB2	1.94	0.49
12:b:221:GLU:O	12:b:227:HIS:CE1	2.66	0.49
2:B:111:GLU:O	2:B:115:SER:HB2	2.13	0.49
2:B:306:GLY:HA2	2:B:389:PRO:HD3	1.94	0.49
3:C:316:SER:HB2	3:C:318:TYR:CE2	2.48	0.49
3:O:94:MET:HG3	3:O:246:PHE:CD1	2.43	0.49
3:O:143:GLY:H	3:O:146:SER:HB3	1.78	0.49
12:b:12:ASP:OD1	12:b:211:ARG:NH2	2.41	0.49
1:A:238:PHE:O	1:A:241:THR:OG1	2.30	0.49
1:M:74:HIS:HB2	2:N:174:GLU:OE1	2.13	0.49
1:M:454:SER:OG	1:M:455:PRO:HD3	2.12	0.49
2:N:145:ILE:HD11	2:N:162:PHE:CZ	2.48	0.49
6:R:111:LEU:HD12	6:R:111:LEU:O	2.13	0.49
11:a:520:LYS:NZ	15:e:88:ALA:HB1	2.27	0.49
25:b:304:3PE:H3E1	25:b:304:3PE:H291	1.94	0.49
13:c:218:LEU:HD12	13:c:241:ALA:HB1	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:j:62:HIS:C	20:j:64:GLY:H	2.21	0.49
2:B:145:ILE:HD11	2:B:162:PHE:CZ	2.48	0.48
4:P:111:ILE:HD11	4:P:258:ALA:HB1	1.95	0.48
12:b:178:THR:HB	12:b:202:LEU:HD12	1.94	0.48
15:e:117:LEU:HD12	15:e:118:GLU:H	1.78	0.48
1:A:320:SER:O	1:A:502:ALA:HA	2.12	0.48
1:M:390:ALA:HA	1:M:403:VAL:HA	1.95	0.48
7:S:61:ASN:O	7:S:65:LYS:HG3	2.13	0.48
11:a:264:PHE:CZ	11:a:491:TRP:CZ2	2.97	0.48
11:a:423:VAL:HA	11:a:426:THR:HG22	1.94	0.48
14:d:72:PHE:CD2	18:h:57:ILE:HG13	2.48	0.48
19:i:3:GLU:OE1	19:i:4:PRO:HD2	2.13	0.48
1:A:116:THR:HG21	1:A:454:SER:HA	1.94	0.48
4:D:107:SER:HB3	4:D:159:PRO:HD2	1.94	0.48
4:P:297:SER:OG	7:S:20:GLN:NE2	2.46	0.48
11:a:99:ARG:HD3	13:c:60:TRP:NE1	2.28	0.48
11:a:157:GLY:O	11:a:161:ILE:HG12	2.14	0.48
2:B:335:MET:SD	2:B:406:ILE:HG21	2.52	0.48
4:P:191:TYR:OH	26:P:402:HEC:O2A	2.20	0.48
11:a:315:ALA:HB2	11:a:358:ILE:HD11	1.95	0.48
12:b:152:GLU:N	12:b:155:GLN:OE1	2.46	0.48
1:A:224:GLN:N	1:A:224:GLN:OE1	2.46	0.48
1:A:389:MET:O	1:A:403:VAL:C	2.56	0.48
2:B:353:ARG:NH2	2:B:412:VAL:HA	2.29	0.48
3:C:109:TYR:OH	25:C:408:3PE:O12	2.24	0.48
4:D:226:PRO:HG2	4:D:228:MET:HE3	1.96	0.48
25:c:305:3PE:H231	25:c:305:3PE:H362	1.96	0.48
1:A:191:ASP:HA	1:A:295:LEU:HD21	1.96	0.48
11:a:311:THR:O	11:a:314:ILE:HG22	2.13	0.48
2:B:327:VAL:HG11	2:B:473:ILE:HG13	1.96	0.48
3:O:7:ARG:HH22	25:O:401:3PE:P	2.37	0.48
11:a:19:LEU:HB3	11:a:105:PHE:CZ	2.49	0.48
11:a:200:LEU:HD22	13:c:95:MET:HE3	1.95	0.48
3:C:94:MET:HG3	3:C:246:PHE:CD1	2.48	0.48
23:C:409:CDL:H352	7:G:42:TRP:HA	1.96	0.48
4:D:213:HIS:NE2	4:D:226:PRO:HB3	2.29	0.48
2:N:72:VAL:HG13	2:N:73:GLU:N	2.29	0.48
3:O:177:VAL:HG12	3:O:177:VAL:O	2.13	0.48
11:a:158:VAL:HG11	25:c:301:3PE:H2A1	1.95	0.48
19:i:40:ILE:HB	19:i:41:PRO:HD3	1.96	0.48
3:C:282:LEU:HD12	25:C:407:3PE:H321	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:434:SER:O	2:N:437:ILE:N	2.40	0.48
4:P:75:TYR:HB3	8:T:65:PHE:CE2	2.48	0.48
1:A:147:THR:OG1	1:A:196:ILE:HD13	2.13	0.48
1:A:160:GLU:HB3	2:B:419:ARG:HD2	1.94	0.48
8:H:9:GLN:OE1	8:H:9:GLN:N	2.46	0.48
2:N:220:GLY:HA2	2:N:295:GLY:HA3	1.95	0.48
3:O:311:LEU:HD11	3:O:369:PHE:HE1	1.79	0.48
11:a:441:ARG:CB	12:b:222:ILE:HD11	2.44	0.48
1:M:114:THR:OG1	2:N:433:GLU:OE2	2.31	0.47
2:N:100:ILE:HD11	2:N:264:VAL:HG21	1.96	0.47
11:a:100:LEU:HA	11:a:103:ILE:HG22	1.96	0.47
11:a:110:PRO:HB3	13:c:26:LEU:HB2	1.95	0.47
11:a:290:TRP:HZ2	25:a:607:3PE:H232	1.78	0.47
12:b:113:ILE:HD11	12:b:173:LEU:HG	1.95	0.47
13:c:66:ARG:NH1	19:i:29:LYS:O	2.38	0.47
18:h:41:GLU:OE2	25:h:101:3PE:N	2.31	0.47
3:C:35:TRP:HB3	3:C:105:ARG:HD3	1.95	0.47
5:E:127:ARG:NH2	10:K:39:GLN:HG3	2.29	0.47
1:M:117:VAL:HG21	1:M:186:VAL:HG13	1.97	0.47
2:N:76:LYS:HE3	2:N:78:LYS:HE3	1.96	0.47
11:a:270:PHE:CZ	12:b:75:GLY:HA3	2.49	0.47
1:A:292:VAL:HG13	1:A:296:PHE:HD2	1.78	0.47
2:N:177:VAL:HG11	2:N:276:LEU:HB3	1.95	0.47
2:N:454:PRO:HG2	2:N:457:GLN:HG2	1.96	0.47
8:T:63:LYS:HA	8:T:66:THR:HG22	1.96	0.47
11:a:219:ASN:HD21	16:f:82:ARG:HD2	1.79	0.47
3:C:32:LEU:HB2	3:C:231:PHE:HE1	1.79	0.47
3:C:139:VAL:HA	3:C:146:SER:HB2	1.96	0.47
4:D:198:GLY:HA3	4:D:217:TYR:HE2	1.78	0.47
1:M:238:PHE:O	1:M:241:THR:OG1	2.32	0.47
3:O:207:LEU:CD2	24:O:404:HEM:HAA1	2.44	0.47
25:c:302:3PE:H32	16:f:93:LEU:HD23	1.95	0.47
2:B:84:ASN:ND2	2:B:277:LEU:O	2.47	0.47
1:M:355:GLN:HB3	1:M:401:PHE:HE2	1.79	0.47
1:M:444:SER:O	1:M:448:LEU:HG	2.14	0.47
3:O:56:LEU:HD13	24:O:403:HEM:HBA1	1.97	0.47
25:a:612:3PE:H222	13:c:84:TYR:CE2	2.49	0.47
1:A:302:ASP:OD1	1:A:304:THR:HG23	2.15	0.47
3:C:378:VAL:HB	25:C:406:3PE:H32	1.96	0.47
1:A:142:MET:HE1	1:A:206:ARG:HB3	1.96	0.47
2:B:149:ILE:HG22	2:B:162:PHE:CD1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:c:9:TYR:HE2	13:c:77:VAL:HG21	1.80	0.47
1:A:140:GLU:O	1:A:143:ILE:HG22	2.14	0.47
2:B:124:ARG:HA	2:B:124:ARG:HD3	1.69	0.47
3:C:75:MET:HE2	3:C:82:TRP:HA	1.96	0.47
4:D:148:ARG:NH2	4:D:151:LYS:HG3	2.30	0.47
5:E:98:GLU:HB3	7:G:21:LYS:HD2	1.97	0.47
2:N:357:ARG:NH1	2:N:402:GLU:OE1	2.48	0.47
4:P:64:ASP:OD1	4:P:65:GLU:N	2.48	0.47
4:P:283:GLN:CG	5:Q:114:VAL:O	2.63	0.47
5:Q:130:VAL:O	5:Q:134:VAL:HG23	2.15	0.47
22:S:101:PC1:H153	22:S:101:PC1:H112	1.66	0.47
3:C:190:TYR:CD2	3:O:190:TYR:CD2	3.03	0.46
5:E:133:PHE:O	5:E:136:SER:OG	2.22	0.46
2:N:72:VAL:HG13	2:N:73:GLU:H	1.79	0.46
4:P:94:GLY:HA2	4:P:97:VAL:HG12	1.97	0.46
8:T:19:PRO:HG2	14:d:72:PHE:O	2.15	0.46
8:T:60:VAL:HG12	8:T:60:VAL:O	2.16	0.46
11:a:58:ASN:O	11:a:61:ILE:HG12	2.15	0.46
11:a:87:PRO:HA	11:a:90:ILE:HG22	1.98	0.46
13:c:191:ILE:N	25:c:302:3PE:O12	2.49	0.46
1:A:96:THR:OG1	1:A:285:HIS:NE2	2.32	0.46
2:B:468:ASN:HA	2:B:471:THR:HG22	1.97	0.46
1:M:460:ILE:HG12	1:M:470:ARG:HD2	1.97	0.46
2:N:497:GLU:O	2:N:501:ARG:HG2	2.15	0.46
11:a:131:VAL:HG23	11:a:234:TYR:OH	2.16	0.46
27:a:601:HEA:H251	12:b:90:LEU:HD21	1.96	0.46
12:b:164:ARG:HD3	12:b:233:VAL:HG11	1.97	0.46
12:b:182:VAL:HG22	12:b:183:LEU:N	2.29	0.46
14:d:6:ILE:O	14:d:10:ILE:HG13	2.15	0.46
1:A:229:ILE:HD13	1:A:506:MET:HE3	1.98	0.46
2:B:432:LEU:HD23	2:B:432:LEU:HA	1.74	0.46
3:C:105:ARG:HH22	24:C:403:HEM:HBD2	1.81	0.46
4:D:97:VAL:O	4:D:101:VAL:HG22	2.15	0.46
7:G:71:ARG:HD2	8:H:48:GLN:HE22	1.81	0.46
11:a:253:GLY:O	11:a:257:ILE:HG12	2.16	0.46
2:B:300:ARG:HH12	2:N:301:HIS:H	1.63	0.46
2:N:149:ILE:HG22	2:N:162:PHE:HD1	1.80	0.46
3:O:349:PRO:HB2	3:O:351:GLU:HG2	1.96	0.46
16:f:67:HIS:O	16:f:67:HIS:ND1	2.48	0.46
20:j:61:LYS:HD3	20:j:61:LYS:HA	1.72	0.46
11:a:36:VAL:O	11:a:40:MET:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:c:14:PRO:HD2	19:i:25:HIS:CE1	2.51	0.46
13:c:143:SER:OG	13:c:245:TRP:NE1	2.48	0.46
13:c:160:LYS:O	13:c:163:VAL:HG22	2.15	0.46
11:a:200:LEU:O	13:c:95:MET:HG2	2.15	0.46
11:a:5:VAL:HG13	11:a:9:PHE:HD2	1.80	0.46
12:b:152:GLU:HB2	12:b:155:GLN:HE22	1.81	0.46
13:c:213:ILE:HD11	13:c:244:TYR:OH	2.15	0.46
14:d:30:PHE:CE1	25:d:101:3PE:H251	2.51	0.46
1:A:145:LYS:NZ	1:A:210:GLU:OE2	2.40	0.46
6:F:15:TRP:HE3	6:F:16:LEU:HD22	1.81	0.46
11:a:351:THR:O	11:a:355:LEU:HD23	2.16	0.46
12:b:214:VAL:HG21	14:d:54:TRP:CD1	2.51	0.46
13:c:137:THR:OG1	13:c:252:TRP:NE1	2.40	0.46
2:B:173:VAL:HG11	2:B:273:ALA:HB2	1.98	0.46
2:B:383:ILE:CD1	2:B:403:LEU:HD11	2.46	0.46
3:C:283:PRO:HG2	25:C:407:3PE:H3B2	1.96	0.46
1:M:354:MET:HE3	1:M:426:LEU:HD23	1.99	0.46
1:M:430:VAL:O	10:W:15:ILE:HD11	2.16	0.46
2:N:181:ARG:NH2	2:N:279:ASP:OD1	2.48	0.46
11:a:308:THR:O	11:a:312:MET:HG2	2.16	0.46
13:c:176:PHE:HE1	13:c:211:VAL:HG21	1.80	0.46
14:d:50:LYS:HB3	14:d:54:TRP:CE3	2.51	0.46
3:C:94:MET:HE1	3:C:249:TRP:HD1	1.80	0.45
3:C:105:ARG:HH12	24:C:403:HEM:HBD2	1.82	0.45
1:M:362:ASN:OD1	1:M:363:LYS:N	2.48	0.45
2:N:209:GLN:O	2:N:213:LEU:HD23	2.16	0.45
3:O:179:ASN:C	3:O:179:ASN:HD22	2.23	0.45
3:O:289:ARG:NH1	3:O:346:GLY:O	2.49	0.45
11:a:285:LEU:HB2	11:a:314:ILE:HD13	1.98	0.45
11:a:384:SER:O	11:a:388:VAL:HB	2.15	0.45
4:D:217:TYR:OH	8:H:57:ASP:OD2	2.25	0.45
7:G:33:LYS:O	7:G:37:LYS:HG2	2.17	0.45
3:O:222:MET:SD	3:O:222:MET:N	2.89	0.45
12:b:195:CYS:SG	12:b:196:ASP:N	2.90	0.45
1:A:279:ALA:HB1	1:A:283:VAL:HG21	1.99	0.45
1:M:135:THR:HG23	1:M:262:LEU:HD23	1.97	0.45
2:N:124:ARG:HH21	2:N:200:GLU:CD	2.24	0.45
3:O:178:ASP:CG	3:O:179:ASN:H	2.24	0.45
5:Q:117:GLY:HA2	5:Q:120:PHE:CE1	2.52	0.45
14:d:52:GLN:HA	14:d:52:GLN:OE1	2.15	0.45
17:g:153:ALA:HA	17:g:156:TYR:CD1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:i:57:TYR:HE1	22:i:101:PC1:H121	1.81	0.45
1:A:114:THR:HG21	2:B:430:MET:HG3	1.98	0.45
1:A:367:GLY:HA3	1:A:371:MET:HE2	1.97	0.45
2:B:268:GLU:O	2:B:272:ILE:HG12	2.16	0.45
8:H:30:ALA:O	8:H:34:ARG:HG3	2.16	0.45
8:H:33:LYS:HE2	8:H:33:LYS:HB2	1.62	0.45
1:M:87:ILE:HG22	2:N:96:PRO:HB3	1.99	0.45
2:N:478:ILE:HD11	2:N:503:PHE:HD1	1.81	0.45
11:a:225:PRO:HG3	12:b:199:PRO:HB2	1.98	0.45
13:c:6:ARG:HD3	15:e:93:TYR:CD2	2.50	0.45
17:g:121:THR:HG23	17:g:123:ASN:H	1.82	0.45
1:A:251:ALA:O	1:A:255:LYS:HG2	2.17	0.45
4:D:225:MET:HE1	26:D:501:HEC:NC	2.32	0.45
2:N:212:LEU:HD23	2:N:212:LEU:HA	1.75	0.45
11:a:84:TRP:CZ2	11:a:402:ILE:HG23	2.52	0.45
12:b:175:VAL:HG23	12:b:205:ILE:HB	1.98	0.45
13:c:45:LEU:HD13	19:i:51:LEU:HB3	1.99	0.45
1:A:514:ASP:OD1	1:A:514:ASP:N	2.50	0.45
3:C:162:VAL:HG23	3:C:163:VAL:HG13	1.97	0.45
2:N:86:LEU:HD11	2:N:277:LEU:HD13	1.98	0.45
2:N:140:ARG:HA	2:N:140:ARG:HD3	1.67	0.45
4:P:276:VAL:CG1	5:Q:121:VAL:HG13	2.47	0.45
15:e:70:ASP:HB3	15:e:73:GLU:HB3	1.98	0.45
15:e:71:ILE:HD12	15:e:71:ILE:H	1.81	0.45
1:A:498:ASP:OD1	1:A:519:ARG:NH2	2.43	0.45
2:B:468:ASN:O	2:B:472:LYS:HE2	2.16	0.45
3:C:279:TRP:HA	3:C:282:LEU:HG	1.99	0.45
4:D:276:VAL:CG1	5:E:121:VAL:HG13	2.47	0.45
6:F:28:LEU:O	6:F:32:GLY:N	2.50	0.45
23:M:602:CDL:H122	23:O:402:CDL:HA32	1.98	0.45
3:O:35:TRP:CB	3:O:105:ARG:HG3	2.46	0.45
13:c:138:LEU:HB3	16:f:55:CYS:SG	2.57	0.45
1:A:205:ASN:HB2	1:A:209:ARG:HH21	1.82	0.45
1:M:127:PHE:CD2	1:M:309:LEU:HD22	2.52	0.45
3:C:179:ASN:C	3:C:179:ASN:HD22	2.25	0.45
8:T:18:LYS:HE3	8:T:25:LEU:HD11	1.99	0.45
11:a:349:LEU:HD13	11:a:385:MET:SD	2.57	0.45
13:c:107:SER:HB2	13:c:195:ILE:HG12	1.98	0.45
3:C:50:ILE:HA	24:C:402:HEM:HAB	1.99	0.45
4:D:63:ALA:O	4:D:67:GLU:HG2	2.17	0.45
4:D:112:SER:HA	4:D:155:ARG:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:293:SER:OG	7:G:20:GLN:OE1	2.33	0.45
1:M:150:ARG:HA	1:M:150:ARG:HD3	1.66	0.45
1:M:217:GLU:O	1:M:220:GLU:HG3	2.16	0.45
1:M:239:GLN:HE21	1:M:318:THR:HG21	1.82	0.45
1:M:448:LEU:HD22	2:N:435:ARG:NH2	2.31	0.45
2:N:186:LEU:HD13	2:N:188:TRP:CZ2	2.51	0.45
5:Q:117:GLY:HA2	5:Q:120:PHE:CZ	2.51	0.45
11:a:246:VAL:O	27:a:601:HEA:HAC	2.17	0.45
11:a:268:PRO:HG2	12:b:73:VAL:CG2	2.45	0.45
11:a:359:VAL:HG23	12:b:43:LEU:HD12	1.99	0.45
16:f:40:GLU:O	16:f:44:TRP:HE3	1.99	0.45
1:A:121:ILE:HB	1:A:175:THR:OG1	2.17	0.44
2:B:425:LYS:HG3	2:B:462:VAL:HG11	1.99	0.44
3:C:207:LEU:CD2	24:C:403:HEM:HAA1	2.46	0.44
4:D:225:MET:HE3	26:D:501:HEC:NC	2.32	0.44
13:c:60:TRP:CZ3	25:c:301:3PE:H232	2.52	0.44
13:c:102:TRP:O	13:c:102:TRP:HD1	2.00	0.44
25:c:304:3PE:O22	25:c:304:3PE:H31	2.16	0.44
18:h:51:LEU:O	18:h:55:GLY:N	2.50	0.44
22:i:101:PC1:H222	25:i:103:3PE:H282	1.98	0.44
3:C:284:ILE:HG23	3:C:301:ILE:HD12	1.99	0.44
1:M:138:PHE:CE2	1:M:257:ILE:HG21	2.53	0.44
7:S:42:TRP:O	7:S:46:THR:HG23	2.18	0.44
15:e:110:HIS:HE1	15:e:113:VAL:HG12	1.82	0.44
2:B:442:ILE:HG12	2:B:452:ARG:HE	1.83	0.44
4:D:280:ALA:HB2	5:E:121:VAL:CG1	2.44	0.44
1:M:357:MET:HB3	1:M:438:ALA:HB2	1.99	0.44
2:N:299:ARG:HH21	2:N:493:VAL:HG23	1.83	0.44
7:S:15:LEU:HB3	7:S:20:GLN:NE2	2.31	0.44
11:a:455:LEU:HD21	25:b:302:3PE:H331	1.98	0.44
12:b:23:ASP:OD1	14:d:67:ILE:HB	2.18	0.44
1:A:321:GLU:OE1	1:A:323:ARG:NE	2.50	0.44
6:F:83:LEU:HD12	6:F:83:LEU:H	1.80	0.44
4:D:202:PRO:HB2	4:D:206:VAL:HG23	1.98	0.44
22:M:603:PC1:O14	5:Q:119:ARG:NH2	2.50	0.44
2:N:102:LEU:HD23	2:N:180:VAL:HG21	1.98	0.44
3:O:264:ILE:HD11	4:P:185:ARG:HH22	1.83	0.44
11:a:438:MET:HB2	11:a:449:TYR:CE1	2.53	0.44
14:d:71:ASN:C	14:d:71:ASN:ND2	2.74	0.44
2:B:198:LYS:HB2	2:B:236:LEU:HD21	1.99	0.44
2:B:335:MET:HE3	2:B:354:LEU:HG	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:354:LEU:HB3	2:B:368:PHE:HE2	1.83	0.44
3:C:232:TYR:OH	23:C:401:CDL:HA32	2.18	0.44
2:N:335:MET:CE	2:N:406:ILE:HG21	2.45	0.44
2:N:447:LEU:HD23	2:N:447:LEU:HA	1.85	0.44
3:O:35:TRP:HB2	3:O:105:ARG:HG3	2.00	0.44
6:R:22:LYS:HB2	6:R:22:LYS:HE3	1.62	0.44
11:a:428:PHE:HB3	11:a:429:PRO:HD3	2.00	0.44
11:a:429:PRO:O	11:a:433:LEU:HD13	2.18	0.44
11:a:438:MET:SD	11:a:442:ILE:HD11	2.58	0.44
12:b:39:ILE:O	12:b:43:LEU:HG	2.18	0.44
2:B:157:GLN:HG3	2:B:444:ARG:NH1	2.33	0.44
25:C:406:3PE:H251	6:F:16:LEU:HB3	2.00	0.44
7:G:56:TYR:O	7:G:60:GLN:HG2	2.16	0.44
7:G:72:TYR:HE2	8:H:43:LYS:HA	1.83	0.44
2:B:382:GLY:C	2:B:383:ILE:HD12	2.43	0.44
6:F:44:ASP:O	6:F:45:LEU:HB2	2.17	0.44
3:O:105:ARG:NH1	24:O:404:HEM:HBD2	2.31	0.44
11:a:79:GLY:O	11:a:83:ASN:HB2	2.18	0.44
12:b:107:VAL:HG13	12:b:107:VAL:O	2.18	0.44
17:g:131:ARG:HA	17:g:131:ARG:HD3	1.82	0.44
1:A:417:TYR:HA	1:A:517:TRP:HH2	1.81	0.44
2:B:447:LEU:HD23	2:B:447:LEU:HA	1.85	0.44
8:T:58:LYS:HB3	8:T:58:LYS:HE2	1.61	0.44
11:a:19:LEU:HB3	11:a:105:PHE:CE2	2.53	0.44
11:a:374:TYR:N	11:a:434:GLY:HA3	2.33	0.44
13:c:52:PHE:HD1	19:i:44:LEU:HG	1.83	0.44
1:A:287:ASP:O	1:A:290:GLU:HG3	2.18	0.43
1:M:423:THR:HG22	1:M:496:ILE:HD13	2.00	0.43
3:O:75:MET:HB3	3:O:75:MET:HE3	1.66	0.43
11:a:100:LEU:HA	11:a:100:LEU:HD23	1.84	0.43
11:a:175:ARG:NH2	11:a:181:MET:SD	2.91	0.43
16:f:87:PRO:HD2	16:f:88:TRP:CZ3	2.53	0.43
2:B:176:LEU:HD23	2:B:176:LEU:HA	1.84	0.43
2:B:201:LEU:HA	2:B:204:LEU:HD23	2.00	0.43
2:B:383:ILE:HD13	2:B:403:LEU:HD11	1.99	0.43
6:F:53:ARG:NH2	6:F:101:VAL:HG22	2.33	0.43
1:M:479:ARG:HH22	2:N:53:PRO:HG2	1.83	0.43
3:O:41:LEU:HD13	3:O:239:TRP:HD1	1.82	0.43
4:P:300:LEU:HD13	4:P:302:LEU:HG	1.99	0.43
5:Q:113:PHE:CZ	9:V:16:LEU:HB3	2.53	0.43
11:a:99:ARG:HD3	13:c:60:TRP:HE1	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:a:433:LEU:HD11	11:a:452:TRP:CB	2.42	0.43
13:c:166:LEU:HD21	13:c:238:PHE:HE1	1.83	0.43
15:e:91:LYS:O	15:e:97:ARG:NH1	2.51	0.43
1:A:60:LYS:O	1:A:63:GLN:HG3	2.17	0.43
2:B:102:LEU:HD23	2:B:180:VAL:HG21	1.99	0.43
2:B:145:ILE:HD11	2:B:162:PHE:HZ	1.84	0.43
11:a:165:ILE:O	11:a:169:THR:HG22	2.18	0.43
11:a:315:ALA:CB	11:a:358:ILE:HD11	2.49	0.43
13:c:61:TRP:CD1	25:c:303:3PE:H262	2.54	0.43
4:D:106:HIS:CD2	26:D:501:HEC:NC	2.84	0.43
11:a:312:MET:HB3	12:b:90:LEU:HD13	2.01	0.43
12:b:40:PHE:HE1	25:h:101:3PE:H352	1.82	0.43
13:c:228:GLY:HA2	19:i:5:PRO:HG2	2.00	0.43
17:g:160:CYS:HB2	17:g:165:ILE:HD11	2.00	0.43
3:C:94:MET:HE3	3:C:246:PHE:HA	2.00	0.43
4:D:246:GLN:NE2	8:H:69:LYS:OXT	2.44	0.43
1:M:370:HIS:HB3	2:N:136:PHE:HD1	1.82	0.43
2:N:394:LYS:HA	2:N:394:LYS:HD2	1.66	0.43
4:P:240:THR:HG23	8:T:69:LYS:HD3	1.99	0.43
15:e:71:ILE:HG22	15:e:72:LEU:HD23	2.00	0.43
1:A:114:THR:OG1	2:B:433:GLU:OE2	2.36	0.43
3:O:190:TYR:CD1	24:O:403:HEM:HMB3	2.53	0.43
3:O:300:ALA:O	3:O:304:VAL:HG23	2.18	0.43
11:a:401:LYS:HD2	11:a:506:SER:O	2.19	0.43
13:c:9:TYR:CE2	13:c:77:VAL:HG21	2.54	0.43
2:B:255:PRO:O	2:B:285:ARG:NH1	2.52	0.43
3:C:374:ILE:CG1	3:C:377:ARG:NH2	2.62	0.43
1:M:133:ASN:HD21	1:M:245:ARG:HB2	1.84	0.43
2:N:372:ASN:HB3	2:N:381:PHE:HD1	1.84	0.43
11:a:365:LEU:HA	11:a:365:LEU:HD23	1.76	0.43
12:b:178:THR:C	12:b:197:ALA:HB1	2.43	0.43
1:A:132:THR:HB	1:A:135:THR:OG1	2.18	0.43
1:A:298:LYS:O	1:A:298:LYS:HG2	2.18	0.43
1:A:353:VAL:O	1:A:357:MET:HG2	2.18	0.43
2:B:149:ILE:HG22	2:B:162:PHE:HD1	1.84	0.43
3:C:75:MET:CE	3:C:82:TRP:HA	2.49	0.43
2:N:297:ASP:HB2	2:N:496:TYR:HB2	2.00	0.43
3:O:102:HIS:HD2	24:O:404:HEM:C1C	2.36	0.43
11:a:181:MET:O	11:a:189:TRP:HZ3	2.02	0.43
11:a:484:ILE:CD1	11:a:489:ILE:HD11	2.48	0.43
12:b:188:VAL:HG13	12:b:191:LEU:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:398:ILE:O	2:B:402:GLU:HG2	2.18	0.43
2:N:332:GLN:HE21	2:N:371:PHE:HA	1.84	0.43
3:O:70:SER:O	3:O:73:HIS:HB3	2.19	0.43
11:a:151:PHE:HB3	13:c:29:THR:OG1	2.19	0.43
11:a:161:ILE:HD11	11:a:203:PRO:HD3	2.01	0.43
12:b:156:LEU:HD22	12:b:159:LEU:HD23	2.01	0.43
12:b:195:CYS:CB	12:b:205:ILE:HD11	2.47	0.43
2:B:300:ARG:HD3	2:N:300:ARG:HH11	1.84	0.43
6:F:11:PRO:HB3	6:F:18:ALA:HA	2.00	0.43
1:M:299:LEU:HD23	1:M:299:LEU:HA	1.84	0.43
3:O:383:PRO:HG3	6:R:35:TYR:CE2	2.54	0.43
18:h:28:LEU:HD23	18:h:28:LEU:HA	1.88	0.43
20:j:54:MET:HE3	20:j:55:TYR:HE2	1.83	0.43
3:C:374:ILE:CG1	3:C:377:ARG:HH22	2.27	0.42
4:D:198:GLY:HA3	4:D:217:TYR:CE2	2.54	0.42
4:D:199:TYR:OH	4:D:225:MET:HG3	2.19	0.42
1:M:62:ARG:NH1	1:M:62:ARG:HB2	2.34	0.42
11:a:325:TRP:HA	11:a:328:THR:HG22	2.01	0.42
1:A:389:MET:HE2	1:A:389:MET:HB3	1.98	0.42
2:B:130:THR:HG23	2:B:138:ILE:HD11	2.00	0.42
2:B:468:ASN:HB2	2:B:472:LYS:HZ1	1.84	0.42
3:C:140:LEU:HD23	3:C:140:LEU:HA	1.83	0.42
6:R:37:ASP:OD1	6:R:93:TYR:OH	2.26	0.42
9:V:64:VAL:HG13	9:V:67:GLN:HB2	2.01	0.42
11:a:381:TYR:O	11:a:382:VAL:C	2.63	0.42
11:a:439:PRO:HG2	11:a:442:ILE:HG21	2.02	0.42
13:c:202:LEU:HA	13:c:202:LEU:HD12	1.78	0.42
3:C:108:TYR:HD2	3:C:332:PHE:CD2	2.38	0.42
1:M:255:LYS:HB2	1:M:255:LYS:HE2	1.85	0.42
1:M:320:SER:O	1:M:502:ALA:HA	2.19	0.42
11:a:39:ARG:HD2	11:a:457:SER:HA	2.01	0.42
1:A:84:HIS:O	1:A:88:LEU:HG	2.19	0.42
2:B:104:LEU:HD21	2:B:257:MET:HE1	2.00	0.42
3:C:375:LEU:HD23	25:C:406:3PE:O32	2.19	0.42
5:E:132:LYS:HA	5:E:132:LYS:HD3	1.85	0.42
1:M:215:LEU:HD23	1:M:215:LEU:HA	1.90	0.42
1:M:353:VAL:O	1:M:357:MET:HG2	2.19	0.42
11:a:123:VAL:O	20:j:89:GLN:NE2	2.52	0.42
13:c:89:PHE:CE1	25:c:301:3PE:H362	2.54	0.42
22:A:602:PC1:H111	22:A:602:PC1:H152	1.50	0.42
4:D:122:THR:OG1	4:D:125:GLU:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:199:TYR:OH	4:P:225:MET:O	2.33	0.42
4:P:283:GLN:HG3	5:Q:118:GLY:H	1.84	0.42
11:a:506:SER:HB3	11:a:507:PRO:HD3	2.01	0.42
13:c:68:SER:OG	13:c:74:HIS:CE1	2.73	0.42
1:A:205:ASN:OD1	1:A:206:ARG:N	2.52	0.42
3:C:186:PHE:HE2	3:O:186:PHE:HE2	1.67	0.42
23:D:502:CDL:HA62	7:G:26:LEU:O	2.19	0.42
5:E:93:ASP:OD2	6:F:75:LYS:HD3	2.18	0.42
8:H:28:TYR:CE2	8:H:32:ILE:HD11	2.55	0.42
1:M:83:ASP:OD1	1:M:83:ASP:N	2.45	0.42
1:M:465:LEU:HD23	1:M:465:LEU:HA	1.85	0.42
4:P:85:SER:HB2	9:V:50:TRP:CZ2	2.55	0.42
6:R:9:LEU:O	6:R:14:ASN:HB2	2.20	0.42
11:a:441:ARG:HE	27:a:602:HEA:CGD	2.33	0.42
23:a:608:CDL:H552	20:j:70:ALA:HB1	2.01	0.42
13:c:26:LEU:HA	13:c:29:THR:HG22	2.01	0.42
7:G:32:THR:O	7:G:36:HIS:ND1	2.40	0.42
2:N:340:SER:HB2	2:N:359:LEU:HD13	2.02	0.42
12:b:124:TRP:NE1	12:b:230:MET:HG2	2.34	0.42
1:A:357:MET:HE1	1:A:430:VAL:HG23	2.02	0.42
1:A:431:SER:O	1:A:435:VAL:HG23	2.20	0.42
2:B:413:THR:HG22	2:B:415:VAL:H	1.85	0.42
3:C:246:PHE:CZ	3:C:250:ILE:HD11	2.55	0.42
1:M:451:ASP:O	1:M:455:PRO:HG2	2.19	0.42
2:N:253:THR:O	2:N:257:MET:HG3	2.19	0.42
3:O:214:ASN:ND2	3:O:220:SER:HB3	2.34	0.42
11:a:39:ARG:HD3	11:a:39:ARG:HA	1.82	0.42
13:c:105:PHE:O	13:c:109:LEU:HD23	2.19	0.42
13:c:207:HIS:O	13:c:211:VAL:HG23	2.19	0.42
3:C:297:GLY:O	3:C:301:ILE:HG12	2.19	0.42
4:D:305:VAL:HG13	1:M:48:MET:SD	2.60	0.42
8:H:13:LEU:HD23	8:H:13:LEU:HA	1.82	0.42
1:M:133:ASN:ND2	1:M:245:ARG:HB2	2.35	0.42
2:N:109:ILE:HG13	2:N:110:TYR:N	2.34	0.42
3:O:32:LEU:HB2	3:O:231:PHE:HE1	1.84	0.42
6:R:44:ASP:HB3	6:R:47:VAL:HG23	2.01	0.42
8:T:13:LEU:HD23	8:T:13:LEU:HA	1.85	0.42
12:b:41:PHE:HB2	18:h:34:TRP:HD1	1.85	0.42
12:b:56:ARG:HG2	18:h:19:GLU:CD	2.45	0.42
12:b:161:VAL:HG22	12:b:231:PRO:HG2	2.01	0.42
15:e:142:ASP:OD1	15:e:143:PRO:HD2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:j:79:VAL:HG22	20:j:79:VAL:O	2.20	0.42
1:A:41:ALA:N	1:A:42:PRO:HD2	2.35	0.42
4:D:194:SER:O	4:D:198:GLY:N	2.43	0.42
2:N:472:LYS:HB2	2:N:472:LYS:HE3	1.83	0.42
3:O:204:LEU:HD12	3:O:204:LEU:HA	1.87	0.42
4:P:225:MET:HB3	26:P:402:HEC:C1D	2.50	0.42
6:R:105:ARG:O	6:R:109:GLU:HG2	2.19	0.42
7:S:67:LYS:HB3	7:S:67:LYS:HE2	1.75	0.42
9:V:15:SER:O	9:V:19:VAL:HG23	2.20	0.42
11:a:42:LEU:HD23	11:a:42:LEU:HA	1.86	0.42
11:a:162:LEU:HD21	25:c:301:3PE:H361	2.01	0.42
22:i:101:PC1:H242	25:i:103:3PE:H2A1	2.02	0.42
1:A:463:GLN:OE1	1:A:470:ARG:HG3	2.20	0.41
3:C:32:LEU:HB2	3:C:231:PHE:CE1	2.55	0.41
6:F:121:ILE:HA	6:F:122:PRO:HA	1.85	0.41
11:a:71:PHE:CE2	11:a:112:LEU:HA	2.55	0.41
11:a:303:THR:HG21	25:a:607:3PE:O12	2.20	0.41
11:a:441:ARG:HB2	12:b:222:ILE:HD11	2.02	0.41
11:a:510:PHE:CD2	20:j:49:ILE:HA	2.55	0.41
13:c:15:SER:O	13:c:18:PRO:HD2	2.20	0.41
1:A:465:LEU:HD23	1:A:465:LEU:HA	1.87	0.41
11:a:254:PHE:CD1	11:a:325:TRP:HH2	2.37	0.41
11:a:260:ILE:O	11:a:264:PHE:HD2	2.03	0.41
12:b:187:ALA:HB3	12:b:218:GLN:O	2.20	0.41
12:b:189:PRO:HD2	12:b:216:TYR:O	2.20	0.41
14:d:73:VAL:HG22	14:d:74:VAL:N	2.34	0.41
4:D:283:GLN:CD	5:E:118:GLY:HA3	2.45	0.41
6:F:83:LEU:O	6:F:87:GLN:HG2	2.20	0.41
1:M:253:ASN:HD22	1:M:253:ASN:C	2.26	0.41
2:N:149:ILE:HG22	2:N:162:PHE:CD1	2.55	0.41
3:O:108:TYR:HD2	3:O:332:PHE:CD2	2.38	0.41
9:V:48:LYS:HD3	9:V:48:LYS:HA	1.60	0.41
11:a:12:ASN:ND2	11:a:510:PHE:CZ	2.88	0.41
11:a:97:PHE:CE1	13:c:82:LEU:HD23	2.55	0.41
11:a:293:HIS:HA	27:a:601:HEA:HBA1	2.00	0.41
1:A:324:MET:HG2	7:G:11:VAL:HG22	2.01	0.41
4:D:225:MET:HE1	26:D:501:HEC:CHC	2.50	0.41
1:M:253:ASN:O	1:M:253:ASN:ND2	2.50	0.41
2:N:300:ARG:O	2:N:487:TYR:HA	2.21	0.41
3:O:333:TRP:CE3	7:S:48:LEU:HD12	2.55	0.41
11:a:103:ILE:HD12	13:c:60:TRP:HZ3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:GLY:O	1:A:377:GLN:NE2	2.43	0.41
9:J:16:LEU:O	9:J:20:VAL:HG12	2.20	0.41
1:M:138:PHE:HD2	1:M:262:LEU:HD21	1.85	0.41
5:Q:138:SER:OG	5:Q:139:ALA:N	2.52	0.41
11:a:259:HIS:CD2	11:a:499:THR:HG21	2.54	0.41
11:a:327:ALA:HA	25:b:303:3PE:H352	2.02	0.41
18:h:50:ASP:O	18:h:54:LYS:HG2	2.21	0.41
4:D:200:ARG:NH1	4:D:217:TYR:OH	2.34	0.41
9:J:15:SER:O	9:J:19:VAL:HG23	2.21	0.41
9:J:18:LYS:HB3	9:J:18:LYS:HE2	1.82	0.41
1:M:138:PHE:CE2	1:M:262:LEU:HD11	2.55	0.41
7:S:56:TYR:CE1	7:S:60:GLN:NE2	2.88	0.41
11:a:66:PHE:CE1	11:a:129:TRP:HD1	2.38	0.41
11:a:120:LEU:HD11	20:j:88:PHE:CD2	2.56	0.41
11:a:504:VAL:HG22	11:a:505:GLN:HG3	2.02	0.41
12:b:169:ALA:HB2	12:b:236:ALA:HB1	2.03	0.41
12:b:243:GLY:HA2	17:g:108:ILE:HD13	2.03	0.41
2:B:293:TYR:HH	2:B:483:THR:HG1	1.60	0.41
3:C:85:ARG:NH1	24:C:402:HEM:O2D	2.53	0.41
9:J:58:ARG:HH12	9:J:60:GLU:HG2	1.85	0.41
1:M:370:HIS:O	2:N:139:VAL:HG11	2.20	0.41
2:N:304:SER:HA	2:N:489:ASP:OD1	2.21	0.41
4:P:136:VAL:HG12	4:P:147:THR:HG22	2.02	0.41
27:a:602:HEA:HHC	27:a:602:HEA:C13	2.50	0.41
12:b:120:HIS:HB2	12:b:123:TYR:O	2.20	0.41
13:c:143:SER:HG	13:c:245:TRP:NE1	2.19	0.41
1:A:120:TRP:CZ2	1:A:458:GLU:HA	2.55	0.41
1:A:409:PRO:HB3	1:A:508:PRO:HB2	2.03	0.41
2:B:177:VAL:O	2:B:181:ARG:HG2	2.21	0.41
1:M:202:PHE:HB2	1:M:259:LYS:HG3	2.03	0.41
1:M:428:TYR:CE1	1:M:524:TRP:HB2	2.56	0.41
11:a:461:TYR:O	11:a:465:VAL:HG23	2.21	0.41
15:e:83:THR:OG1	15:e:131:TYR:HB2	2.21	0.41
1:A:290:GLU:OE1	1:A:294:LYS:NZ	2.54	0.41
2:B:120:HIS:O	2:B:123:GLU:HG2	2.21	0.41
2:B:460:LYS:O	2:B:464:GLU:HG2	2.20	0.41
2:B:473:ILE:HD13	2:B:473:ILE:HA	1.90	0.41
3:C:41:LEU:HD21	3:C:242:PHE:HB2	2.03	0.41
3:C:204:LEU:HD12	3:C:204:LEU:HA	1.85	0.41
3:C:222:MET:HE2	3:C:222:MET:HB2	1.72	0.41
3:C:288:LEU:HB2	3:C:301:ILE:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:193:PHE:HB2	4:D:252:VAL:HG21	2.03	0.41
4:D:291:ARG:HA	4:D:291:ARG:HD3	1.82	0.41
7:G:63:LEU:HD23	7:G:63:LEU:HA	1.94	0.41
1:M:352:MET:O	1:M:355:GLN:HG3	2.20	0.41
1:M:389:MET:O	1:M:404:TYR:HB3	2.21	0.41
3:O:19:LEU:HG	3:O:23:LEU:HD12	2.03	0.41
3:O:139:VAL:HA	3:O:146:SER:OG	2.20	0.41
3:O:179:ASN:O	3:O:179:ASN:ND2	2.54	0.41
3:O:373:PRO:O	3:O:377:ARG:HG3	2.21	0.41
4:P:280:ALA:HB2	5:Q:121:VAL:CG1	2.48	0.41
11:a:71:PHE:HE2	11:a:112:LEU:HA	1.86	0.41
11:a:184:SER:HA	11:a:185:PRO:HD3	1.94	0.41
11:a:236:HIS:HD2	11:a:290:TRP:HE1	1.67	0.41
12:b:188:VAL:HA	12:b:217:GLY:HA3	2.03	0.41
12:b:194:LYS:HE2	12:b:194:LYS:HB2	1.72	0.41
13:c:128:ASP:HA	13:c:129:PRO:HD3	1.92	0.41
13:c:167:VAL:O	13:c:171:LEU:HD23	2.21	0.41
1:A:152:ALA:HB3	1:A:206:ARG:HH21	1.86	0.41
1:A:371:MET:HE3	1:A:371:MET:HB2	1.86	0.41
2:B:100:ILE:HG22	2:B:176:LEU:HD12	2.03	0.41
2:B:356:LEU:O	2:B:360:ASN:HB2	2.20	0.41
1:M:150:ARG:NH1	1:M:158:GLU:OE2	2.54	0.41
2:N:422:LYS:HA	2:N:422:LYS:HD2	1.89	0.41
4:P:97:VAL:O	4:P:101:VAL:HG12	2.20	0.41
11:a:48:GLN:O	14:d:32:GLY:HA3	2.21	0.41
11:a:346:PHE:CD1	11:a:386:GLY:HA2	2.56	0.41
12:b:59:TRP:O	12:b:62:ARG:HG2	2.21	0.41
12:b:80:ILE:HG23	12:b:81:LEU:HD12	2.03	0.41
13:c:83:ARG:O	13:c:87:ILE:HG12	2.21	0.41
14:d:65:ASN:HB3	14:d:69:ARG:HG3	2.03	0.41
3:C:282:LEU:HD23	3:C:282:LEU:HA	1.86	0.40
1:M:150:ARG:HB3	1:M:155:LEU:HB2	2.03	0.40
2:N:474:SER:HA	2:N:477:ILE:HG22	2.03	0.40
6:R:45:LEU:HD23	6:R:45:LEU:HA	1.93	0.40
11:a:67:LEU:HD23	11:a:67:LEU:HA	1.94	0.40
11:a:136:SER:HB3	11:a:146:VAL:HG11	2.03	0.40
11:a:164:SER:O	11:a:168:ILE:HG12	2.20	0.40
11:a:511:HIS:O	11:a:512:THR:OG1	2.29	0.40
2:B:209:GLN:HG3	2:B:384:TYR:CZ	2.56	0.40
2:B:335:MET:HE3	2:B:335:MET:HB3	1.90	0.40
8:H:31:CYS:O	8:H:35:ILE:HG12	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:227:GLU:OE1	1:M:227:GLU:HA	2.20	0.40
1:M:384:VAL:HG12	3:O:2:THR:HG23	2.04	0.40
2:N:356:LEU:O	2:N:360:ASN:HB2	2.21	0.40
3:O:10:LEU:HA	3:O:13:GLU:HG2	2.04	0.40
3:O:287:ILE:O	3:O:291:ILE:HG22	2.22	0.40
5:Q:80:VAL:O	5:Q:84:LYS:HG3	2.20	0.40
11:a:87:PRO:HG3	11:a:95:MET:HG3	2.02	0.40
11:a:290:TRP:CZ2	25:a:607:3PE:H232	2.56	0.40
11:a:356:THR:HG23	11:a:374:TYR:CZ	2.56	0.40
12:b:53:VAL:HG11	25:b:303:3PE:H372	2.03	0.40
19:i:57:TYR:CE1	22:i:101:PC1:H121	2.56	0.40
1:A:98:LEU:O	1:A:101:GLY:N	2.54	0.40
2:B:130:THR:HB	2:B:182:ASN:O	2.21	0.40
2:B:219:ALA:HB2	2:B:298:PHE:HB2	2.03	0.40
6:F:14:ASN:HB3	6:F:17:ALA:HB3	2.02	0.40
1:M:325:LEU:HD11	1:M:510:GLN:NE2	2.35	0.40
4:P:203:PRO:HG2	4:P:206:VAL:HG11	2.03	0.40
4:P:283:GLN:HG3	5:Q:114:VAL:O	2.21	0.40
8:T:18:LYS:HB3	8:T:19:PRO:HD3	2.02	0.40
11:a:334:ILE:HG22	11:a:335:GLN:N	2.36	0.40
12:b:139:LEU:HD13	12:b:249:GLN:HG2	2.03	0.40
13:c:224:ARG:NH2	25:c:303:3PE:O22	2.54	0.40
3:C:90:ASN:O	3:C:94:MET:HG2	2.22	0.40
5:Q:140:SER:O	5:Q:144:LEU:HG	2.21	0.40
8:T:61:ALA:HB3	8:T:62:PRO:HD3	2.02	0.40
11:a:291:ALA:C	11:a:293:HIS:H	2.29	0.40
11:a:428:PHE:O	11:a:431:HIS:HB2	2.21	0.40
1:A:129:THR:C	1:A:131:GLU:H	2.29	0.40
1:A:155:LEU:HD22	1:A:196:ILE:HD11	2.03	0.40
2:B:197:VAL:HA	2:B:200:GLU:HG2	2.02	0.40
2:B:499:VAL:O	2:B:503:PHE:HD1	2.05	0.40
3:C:75:MET:HE2	3:C:75:MET:HA	2.03	0.40
4:P:181:ILE:HD12	4:P:181:ILE:HA	1.90	0.40
5:Q:146:LEU:HD23	5:Q:146:LEU:HA	1.93	0.40
8:T:52:TYR:O	8:T:56:VAL:HG23	2.21	0.40
11:a:154:HIS:HD2	11:a:209:ILE:HD11	1.85	0.40
11:a:336:TYR:OH	12:b:58:LEU:O	2.39	0.40
12:b:209:ILE:H	12:b:209:ILE:HD12	1.87	0.40
13:c:176:PHE:CE1	13:c:211:VAL:HG21	2.56	0.40
15:e:56:GLY:O	15:e:60:GLU:HG3	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	485/527 (92%)	450 (93%)	35 (7%)	0	100	100
1	M	485/527 (92%)	451 (93%)	34 (7%)	0	100	100
2	B	455/506 (90%)	411 (90%)	42 (9%)	2 (0%)	30	62
2	N	453/506 (90%)	406 (90%)	47 (10%)	0	100	100
3	C	386/393 (98%)	365 (95%)	21 (5%)	0	100	100
3	O	386/393 (98%)	363 (94%)	23 (6%)	0	100	100
4	D	242/306 (79%)	234 (97%)	8 (3%)	0	100	100
4	P	242/306 (79%)	229 (95%)	13 (5%)	0	100	100
5	E	72/271 (27%)	68 (94%)	4 (6%)	0	100	100
5	Q	72/271 (27%)	66 (92%)	6 (8%)	0	100	100
6	F	114/122 (93%)	111 (97%)	3 (3%)	0	100	100
6	R	113/122 (93%)	109 (96%)	4 (4%)	0	100	100
7	G	68/72 (94%)	66 (97%)	2 (3%)	0	100	100
7	S	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
8	H	63/69 (91%)	59 (94%)	4 (6%)	0	100	100
8	T	62/69 (90%)	55 (89%)	7 (11%)	0	100	100
9	J	58/72 (81%)	54 (93%)	4 (7%)	0	100	100
9	V	57/72 (79%)	55 (96%)	2 (4%)	0	100	100
10	K	29/81 (36%)	25 (86%)	4 (14%)	0	100	100
10	W	30/81 (37%)	28 (93%)	2 (7%)	0	100	100
11	a	522/527 (99%)	471 (90%)	51 (10%)	0	100	100
12	b	237/251 (94%)	206 (87%)	31 (13%)	0	100	100
13	c	263/265 (99%)	249 (95%)	14 (5%)	0	100	100
14	d	74/79 (94%)	67 (90%)	7 (10%)	0	100	100
15	e	92/150 (61%)	83 (90%)	9 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	f	57/100 (57%)	54 (95%)	3 (5%)	0	100	100
17	g	72/181 (40%)	63 (88%)	9 (12%)	0	100	100
18	h	47/64 (73%)	46 (98%)	1 (2%)	0	100	100
19	i	62/67 (92%)	57 (92%)	5 (8%)	0	100	100
20	j	45/96 (47%)	39 (87%)	5 (11%)	1 (2%)	5	30
All	All	5411/6618 (82%)	5007 (92%)	401 (7%)	3 (0%)	49	79

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
20	j	63	ARG
2	B	435	ARG
2	B	113	PRO

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	407/438 (93%)	407 (100%)	0	100	100
1	M	407/438 (93%)	407 (100%)	0	100	100
2	B	378/414 (91%)	378 (100%)	0	100	100
2	N	377/414 (91%)	377 (100%)	0	100	100
3	C	333/338 (98%)	332 (100%)	1 (0%)	86	84
3	O	333/338 (98%)	333 (100%)	0	100	100
4	D	198/247 (80%)	197 (100%)	1 (0%)	81	81
4	P	198/247 (80%)	197 (100%)	1 (0%)	81	81
5	E	62/233 (27%)	62 (100%)	0	100	100
5	Q	62/233 (27%)	62 (100%)	0	100	100
6	F	102/107 (95%)	102 (100%)	0	100	100
6	R	101/107 (94%)	101 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	G	64/65 (98%)	64 (100%)	0	100	100
7	S	64/65 (98%)	64 (100%)	0	100	100
8	H	60/63 (95%)	60 (100%)	0	100	100
8	T	59/63 (94%)	59 (100%)	0	100	100
9	J	49/59 (83%)	49 (100%)	0	100	100
9	V	49/59 (83%)	48 (98%)	1 (2%)	48	65
10	K	21/66 (32%)	21 (100%)	0	100	100
10	W	22/66 (33%)	22 (100%)	0	100	100
11	a	433/436 (99%)	433 (100%)	0	100	100
12	b	213/222 (96%)	213 (100%)	0	100	100
13	c	219/219 (100%)	219 (100%)	0	100	100
14	d	65/68 (96%)	64 (98%)	1 (2%)	57	69
15	e	77/126 (61%)	77 (100%)	0	100	100
16	f	50/82 (61%)	50 (100%)	0	100	100
17	g	63/153 (41%)	63 (100%)	0	100	100
18	h	42/52 (81%)	42 (100%)	0	100	100
19	i	55/58 (95%)	55 (100%)	0	100	100
20	j	40/77 (52%)	40 (100%)	0	100	100
All	All	4603/5553 (83%)	4598 (100%)	5 (0%)	87	89

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	259	HIS
4	D	305	VAL
4	P	282	LEU
9	V	31	VAL
14	d	71	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	133	ASN
1	A	165	HIS
1	A	198	GLN

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Mol	Chain	Res	Type
1	A	263	GLN
2	B	84	ASN
2	B	135	HIS
2	B	332	GLN
2	B	351	HIS
3	C	59	HIS
3	C	73	HIS
3	C	90	ASN
3	C	329	GLN
4	D	95	HIS
4	D	96	GLN
6	F	118	GLN
1	M	66	ASN
1	M	133	ASN
2	N	74	GLN
2	N	414	GLN
3	O	6	GLN
3	O	267	ASN
4	P	283	GLN
4	P	306	ASN
5	Q	95	HIS
7	S	20	GLN
8	T	48	GLN
11	a	12	ASN
11	a	219	ASN
11	a	259	HIS
11	a	370	HIS
11	a	431	HIS
11	a	505	GLN
12	b	18	GLN
15	e	76	HIS
17	g	124	GLN
17	g	171	GLN
20	j	62	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 58 ligands modelled in this entry, 5 are monoatomic - leaving 53 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	$\# Z > 2$
22	PC1	M	603	-	26,26,53	0.38	0	32,34,61	0.41	0
25	3PE	i	103	-	34,34,50	0.36	0	37,39,55	0.30	0
23	CDL	M	602	-	52,52,99	0.39	0	58,64,111	0.43	0
26	HEC	D	501	4	50,50,50	1.34	6 (12%)	68,82,82	1.24	5 (7%)
26	HEC	P	402	4	50,50,50	1.35	6 (12%)	68,82,82	1.18	4 (5%)
25	3PE	a	609	-	37,37,50	0.35	0	40,42,55	0.41	0
31	LYS	i	102	-	7,8,9	0.48	0	3,8,10	0.39	0
25	3PE	a	610	-	39,39,50	0.34	0	42,44,55	0.32	0
25	3PE	C	404	-	37,37,50	0.35	0	40,42,55	0.37	0
23	CDL	P	403	-	47,47,99	0.40	0	53,59,111	0.50	0
23	CDL	C	401	-	53,53,99	0.40	0	59,65,111	0.36	0
23	CDL	O	402	-	53,53,99	0.38	0	59,65,111	0.47	0
23	CDL	S	102	-	49,49,99	0.41	0	55,61,111	0.40	0
25	3PE	a	606	-	31,31,50	0.37	0	34,36,55	0.39	0
23	CDL	a	608	-	66,66,99	0.36	0	72,78,111	0.37	0
22	PC1	S	101	-	27,27,53	1.13	2 (7%)	33,35,61	1.16	3 (9%)
24	HEM	C	402	3	50,50,50	1.36	7 (14%)	67,82,82	1.69	15 (22%)
25	3PE	O	401	-	23,23,50	1.17	2 (8%)	26,28,55	1.18	2 (7%)
23	CDL	A	603	-	50,50,99	0.38	0	56,62,111	0.36	0
23	CDL	D	502	-	40,40,99	0.43	0	46,52,111	0.44	0
25	3PE	b	304	-	42,42,50	0.32	0	45,47,55	0.33	0
30	CUA	b	301	12	0,1,1	-	-	-	-	-
22	PC1	A	602	-	28,28,53	1.39	2 (7%)	34,36,61	1.31	3 (8%)
25	3PE	b	303	-	28,28,50	0.40	0	31,33,55	0.44	0
22	PC1	i	101	-	35,35,53	0.35	0	41,43,61	0.42	0
25	3PE	F	201	-	31,31,50	0.39	0	34,36,55	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	3PE	O	405	-	25,25,50	1.30	2 (8%)	28,30,55	1.30	3 (10%)
25	3PE	P	401	-	27,27,50	1.08	2 (7%)	30,32,55	1.15	2 (6%)
23	CDL	C	409	-	54,54,99	0.38	0	60,66,111	0.35	0
27	HEA	a	602	11	67,67,67	1.25	9 (13%)	81,103,103	1.41	14 (17%)
25	3PE	C	408	-	27,27,50	0.40	0	30,32,55	0.37	0
25	3PE	a	611	-	37,37,50	0.35	0	40,42,55	0.31	0
24	HEM	O	404	3	50,50,50	1.39	7 (14%)	67,82,82	1.63	14 (20%)
25	3PE	C	407	-	34,34,50	0.34	0	37,39,55	0.47	0
25	3PE	a	607	-	39,39,50	0.34	0	42,44,55	0.33	0
25	3PE	c	305	-	39,39,50	0.34	0	42,44,55	0.33	0
25	3PE	c	304	-	42,42,50	0.35	0	45,47,55	0.46	0
25	3PE	c	301	-	39,39,50	0.35	0	42,44,55	0.38	0
25	3PE	G	101	-	19,19,50	1.27	2 (10%)	22,24,55	1.08	2 (9%)
22	PC1	a	605	-	38,38,53	0.35	0	44,46,61	0.38	0
25	3PE	b	302	-	35,35,50	0.36	0	38,40,55	0.34	0
25	3PE	c	302	-	39,39,50	0.35	0	42,44,55	0.50	0
25	3PE	O	407	-	25,25,50	0.41	0	28,30,55	0.43	0
25	3PE	h	101	-	37,37,50	0.35	0	40,42,55	0.33	0
25	3PE	c	303	-	36,36,50	0.35	0	39,41,55	0.35	0
24	HEM	O	403	3	50,50,50	1.37	6 (12%)	67,82,82	1.68	15 (22%)
27	HEA	a	601	11	67,67,67	1.24	8 (11%)	81,103,103	1.79	20 (24%)
25	3PE	C	406	-	28,28,50	0.40	0	31,33,55	0.41	0
25	3PE	a	612	-	38,38,50	0.34	0	41,43,55	0.32	0
25	3PE	C	405	-	27,27,50	1.26	2 (7%)	30,32,55	1.26	3 (10%)
25	3PE	O	406	-	32,32,50	0.37	0	35,37,55	0.35	0
25	3PE	d	101	-	34,34,50	0.36	0	37,39,55	0.33	0
24	HEM	C	403	3	50,50,50	1.36	7 (14%)	67,82,82	1.64	13 (19%)

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
26	HEC	P	402	4	1/1/3/7	2/14/54/54	-
22	PC1	M	603	-	-	1/29/29/57	-
23	CDL	M	602	-	-	7/62/62/110	-
26	HEC	D	501	4	1/1/3/7	4/14/54/54	-
25	3PE	i	103	-	-	9/38/38/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	3PE	a	609	-	-	14/41/41/54	-
31	LYS	i	102	-	-	1/6/7/9	-
25	3PE	a	610	-	-	10/43/43/54	-
25	3PE	C	404	-	-	9/41/41/54	-
23	CDL	P	403	-	-	14/56/56/110	-
23	CDL	C	401	-	-	11/64/64/110	-
23	CDL	O	402	-	-	14/62/62/110	-
23	CDL	S	102	-	-	13/60/60/110	-
25	3PE	a	606	-	-	10/35/35/54	-
23	CDL	a	608	-	-	14/77/77/110	-
22	PC1	S	101	-	-	12/30/30/57	-
24	HEM	C	402	3	-	5/14/54/54	-
25	3PE	O	401	-	-	1/26/26/54	-
23	CDL	A	603	-	-	13/59/59/110	-
23	CDL	D	502	-	-	14/49/49/110	-
25	3PE	b	304	-	-	6/46/46/54	-
22	PC1	A	602	-	-	5/31/31/57	-
25	3PE	b	303	-	-	9/32/32/54	-
22	PC1	i	101	-	-	5/39/39/57	-
25	3PE	F	201	-	-	9/35/35/54	-
25	3PE	O	405	-	-	9/29/29/54	-
25	3PE	P	401	-	-	9/30/30/54	-
23	CDL	C	409	-	-	7/64/64/110	-
27	HEA	a	602	11	-	8/36/76/76	-
25	3PE	C	408	-	-	5/31/31/54	-
25	3PE	a	611	-	-	5/41/41/54	-
24	HEM	O	404	3	-	9/14/54/54	-
25	3PE	C	407	-	-	12/37/37/54	-
25	3PE	a	607	-	-	4/43/43/54	-
25	3PE	c	305	-	-	7/43/43/54	-
25	3PE	c	304	-	-	12/46/46/54	-
25	3PE	c	301	-	-	11/43/43/54	-
25	3PE	G	101	-	-	6/22/22/54	-
22	PC1	a	605	-	-	14/42/42/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	3PE	b	302	-	-	8/39/39/54	-
25	3PE	c	302	-	-	8/43/43/54	-
25	3PE	O	407	-	-	2/29/29/54	-
25	3PE	h	101	-	-	2/41/41/54	-
25	3PE	c	303	-	-	8/40/40/54	-
24	HEM	O	403	3	-	10/14/54/54	-
27	HEA	a	601	11	-	12/36/76/76	-
25	3PE	C	406	-	-	6/32/32/54	-
25	3PE	a	612	-	-	5/42/42/54	-
25	3PE	C	405	-	-	14/31/31/54	-
25	3PE	O	406	-	-	7/36/36/54	-
25	3PE	d	101	-	-	15/38/38/54	-
24	HEM	C	403	3	-	8/14/54/54	-

All (70) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	602	PC1	O21-C21	4.96	1.46	1.35
25	C	405	3PE	O31-C31	4.30	1.45	1.33
22	A	602	PC1	O31-C31	4.28	1.45	1.33
25	O	405	3PE	O31-C31	4.26	1.45	1.33
25	O	401	3PE	O21-C21	4.18	1.46	1.34
25	G	101	3PE	O21-C21	4.17	1.46	1.34
25	P	401	3PE	O21-C21	4.13	1.46	1.34
25	C	405	3PE	O21-C21	4.11	1.45	1.34
22	S	101	PC1	O21-C21	4.11	1.45	1.34
25	O	405	3PE	O21-C21	4.10	1.45	1.34
24	O	403	HEM	C4D-ND	-3.88	1.33	1.40
24	C	402	HEM	C4D-ND	-3.86	1.33	1.40
24	O	404	HEM	C4D-ND	-3.68	1.33	1.40
24	C	403	HEM	C4D-ND	-3.67	1.33	1.40
27	a	601	HEA	C3A-C4A	-3.54	1.39	1.46
26	P	402	HEC	CBC-CAC	-3.53	1.36	1.51
26	D	501	HEC	CBC-CAC	-3.49	1.36	1.51
24	C	402	HEM	C1B-NB	-3.48	1.34	1.40
24	O	403	HEM	C1B-NB	-3.48	1.34	1.40
24	O	404	HEM	C1B-NB	-3.42	1.34	1.40
24	C	403	HEM	C1B-NB	-3.38	1.34	1.40
27	a	601	HEA	C1D-ND	-3.33	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	a	602	HEA	C1D-ND	-3.27	1.34	1.40
27	a	601	HEA	C4D-C3D	3.08	1.50	1.45
27	a	602	HEA	C3A-C4A	-2.99	1.40	1.46
24	O	403	HEM	C1D-ND	-2.93	1.33	1.38
24	O	403	HEM	C1C-C2C	-2.93	1.39	1.45
24	C	403	HEM	C1C-C2C	-2.93	1.39	1.45
27	a	602	HEA	FE-NB	2.93	2.03	1.94
24	O	404	HEM	C1D-ND	-2.91	1.33	1.38
27	a	602	HEA	FE-ND	2.86	2.03	1.94
24	O	404	HEM	C1C-C2C	-2.86	1.39	1.45
27	a	602	HEA	C1A-C2A	-2.81	1.40	1.45
24	C	402	HEM	C1C-C2C	-2.80	1.39	1.45
27	a	601	HEA	C4B-NB	-2.80	1.35	1.40
24	C	403	HEM	C1D-ND	-2.78	1.33	1.38
24	C	402	HEM	C1D-ND	-2.75	1.33	1.38
26	P	402	HEC	CAC-C3C	2.75	1.58	1.51
27	a	602	HEA	C4D-C3D	2.73	1.49	1.45
26	D	501	HEC	CAC-C3C	2.72	1.58	1.51
27	a	602	HEA	C4B-NB	-2.70	1.35	1.40
27	a	601	HEA	FE-NB	2.67	2.03	1.94
25	O	401	3PE	O31-C31	2.60	1.45	1.33
25	P	401	3PE	O31-C31	2.60	1.45	1.33
22	S	101	PC1	O31-C31	2.59	1.45	1.33
25	G	101	3PE	O31-C31	2.58	1.45	1.33
26	D	501	HEC	CBB-CAB	-2.57	1.40	1.51
26	P	402	HEC	CBB-CAB	-2.53	1.40	1.51
27	a	601	HEA	FE-ND	2.43	2.02	1.94
24	O	404	HEM	FE-NB	2.41	2.02	1.94
24	C	403	HEM	FE-NB	2.40	2.02	1.94
27	a	601	HEA	C1A-C2A	-2.39	1.41	1.45
24	O	403	HEM	C4B-NB	-2.38	1.34	1.38
24	C	402	HEM	C4B-NB	-2.25	1.34	1.38
24	O	404	HEM	C4B-NB	-2.25	1.34	1.38
27	a	601	HEA	CMA-C3A	2.22	1.50	1.45
27	a	602	HEA	FE-NC	2.20	2.02	1.95
24	C	402	HEM	FE-NB	2.19	2.01	1.94
24	C	403	HEM	C4B-NB	-2.19	1.34	1.38
27	a	602	HEA	CMA-C3A	2.15	1.50	1.45
26	D	501	HEC	CMD-C2D	2.15	1.55	1.50
24	C	402	HEM	C3C-C4C	-2.10	1.42	1.46
24	O	404	HEM	C3C-C4C	-2.10	1.42	1.46
26	D	501	HEC	C3C-C2C	-2.07	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	O	403	HEM	FE-NB	2.06	2.01	1.94
24	C	403	HEM	C3C-C4C	-2.06	1.42	1.46
26	P	402	HEC	CAB-C3B	2.06	1.56	1.51
26	P	402	HEC	CMD-C2D	2.03	1.54	1.50
26	D	501	HEC	CMA-C3A	2.01	1.54	1.50
26	P	402	HEC	C3C-C2C	-2.01	1.33	1.38

All (118) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	O	403	HEM	CHC-C4B-NB	4.91	129.71	124.42
22	A	602	PC1	O21-C21-C22	4.85	119.74	111.09
24	C	402	HEM	CHC-C4B-NB	4.81	129.59	124.42
27	a	601	HEA	C3C-C4C-NC	-4.63	105.90	109.80
24	C	402	HEM	CHD-C4C-NC	4.53	129.38	124.45
27	a	601	HEA	C13-C12-C11	-4.43	107.32	114.39
24	C	402	HEM	CHB-C1B-NB	4.40	129.81	124.37
24	O	404	HEM	CHB-C1B-NB	4.34	129.73	124.37
24	O	403	HEM	CHB-C1B-NB	4.31	129.69	124.37
24	O	404	HEM	CHC-C4B-NB	4.24	128.98	124.42
24	C	403	HEM	CHB-C1B-NB	4.22	129.59	124.37
24	C	403	HEM	CHC-C4B-NB	4.18	128.92	124.42
24	C	403	HEM	CHD-C4C-NC	4.14	128.97	124.45
24	O	404	HEM	CHD-C4C-NC	4.11	128.93	124.45
25	C	405	3PE	O21-C21-C22	4.02	120.18	111.48
25	O	405	3PE	O21-C21-C22	4.02	120.17	111.48
22	S	101	PC1	O21-C21-C22	4.01	120.16	111.48
24	O	403	HEM	CHD-C4C-NC	3.99	128.80	124.45
25	P	401	3PE	O21-C21-C22	3.95	120.02	111.48
27	a	601	HEA	C1D-ND-C4D	3.92	109.84	105.21
25	O	401	3PE	O21-C21-C22	3.89	119.90	111.48
27	a	601	HEA	CAA-CBA-CGA	-3.48	104.43	113.67
24	C	403	HEM	C4D-ND-C1D	3.44	109.28	105.21
27	a	601	HEA	C3D-C4D-ND	-3.34	107.13	110.35
24	O	404	HEM	C4D-ND-C1D	3.32	109.14	105.21
27	a	601	HEA	C13-C14-C15	-3.26	120.16	127.62
27	a	601	HEA	C4B-NB-C1B	3.24	109.04	105.21
24	O	403	HEM	CHA-C4D-ND	3.16	128.27	124.37
24	C	402	HEM	CHA-C4D-ND	3.15	128.26	124.37
27	a	602	HEA	C17-C18-C19	-3.14	120.44	127.62
27	a	601	HEA	C2A-C1A-NA	-3.13	107.31	110.32
27	a	601	HEA	OMA-CMA-C3A	-3.07	118.69	125.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	a	601	HEA	CHB-C4A-NA	3.05	127.78	124.45
24	O	403	HEM	C4D-ND-C1D	3.05	108.82	105.21
27	a	602	HEA	CAA-CBA-CGA	-3.00	105.70	113.67
24	C	403	HEM	CHD-C1D-ND	2.98	127.63	124.42
24	C	402	HEM	C4D-ND-C1D	2.95	108.69	105.21
27	a	602	HEA	C13-C12-C11	-2.94	109.70	114.39
24	C	402	HEM	CHD-C1D-ND	2.91	127.55	124.42
27	a	602	HEA	CHB-C4A-NA	2.90	127.61	124.45
26	P	402	HEC	O1D-CGD-CBD	-2.90	113.88	123.09
27	a	602	HEA	C13-C14-C15	-2.90	120.98	127.62
26	D	501	HEC	O1D-CGD-CBD	-2.88	113.96	123.09
24	O	404	HEM	CHD-C1D-ND	2.87	127.51	124.42
27	a	602	HEA	C3C-C4C-NC	-2.86	107.39	109.80
24	O	404	HEM	CHB-C1B-C2B	-2.84	118.89	126.95
24	C	403	HEM	CHB-C1B-C2B	-2.76	119.10	126.95
25	O	405	3PE	O31-C31-C32	2.75	120.23	111.83
22	A	602	PC1	C2-O21-C21	-2.73	113.02	117.85
25	C	405	3PE	O31-C31-C32	2.73	120.17	111.83
22	A	602	PC1	O31-C31-C32	2.73	120.16	111.83
24	O	403	HEM	C1B-NB-C4B	2.73	108.44	105.21
27	a	601	HEA	C17-C18-C19	-2.68	121.49	127.62
24	C	402	HEM	CHA-C1A-NA	2.68	128.72	123.86
24	C	403	HEM	CHA-C4D-ND	2.67	127.67	124.37
27	a	601	HEA	C4C-NC-C1C	2.67	110.17	105.82
27	a	601	HEA	C21-C22-C23	-2.64	118.83	127.64
24	O	403	HEM	CHA-C1A-NA	2.64	128.65	123.86
26	D	501	HEC	CHC-C4B-NB	2.63	127.61	124.37
24	C	402	HEM	C1B-NB-C4B	2.62	108.30	105.21
24	O	403	HEM	CHD-C1D-ND	2.61	127.23	124.42
24	C	403	HEM	C2A-C1A-NA	-2.53	107.34	110.15
25	C	405	3PE	C2-O21-C21	-2.52	111.76	117.80
22	S	101	PC1	C2-O21-C21	-2.52	111.76	117.80
25	O	405	3PE	C2-O21-C21	-2.51	111.78	117.80
27	a	601	HEA	CHA-C4D-C3D	2.47	128.38	124.77
24	O	404	HEM	CAD-C3D-C4D	2.47	129.00	124.70
27	a	601	HEA	CMB-C2B-C3B	-2.46	125.51	130.28
24	C	403	HEM	C4A-CHB-C1B	-2.45	120.49	126.25
24	C	402	HEM	CHB-C1B-C2B	-2.45	120.00	126.95
25	G	101	3PE	O21-C21-C22	2.44	119.91	110.93
24	O	403	HEM	C4B-C3B-C2B	-2.44	105.03	107.28
24	O	403	HEM	C1C-CHC-C4B	-2.40	120.92	126.02
24	O	404	HEM	C4A-CHB-C1B	-2.37	120.69	126.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	402	HEM	C4B-C3B-C2B	-2.36	105.11	107.28
24	O	403	HEM	CAA-CBA-CGA	-2.34	107.45	113.67
27	a	601	HEA	CHA-C1A-C2A	2.34	128.55	124.86
24	O	404	HEM	C2A-C1A-NA	-2.33	107.57	110.15
24	C	403	HEM	CHA-C1A-NA	2.32	128.07	123.86
24	O	403	HEM	CHB-C1B-C2B	-2.32	120.35	126.95
24	O	404	HEM	CHA-C1A-NA	2.32	128.06	123.86
25	P	401	3PE	C2-O21-C21	-2.31	112.27	117.80
24	C	402	HEM	CAA-CBA-CGA	-2.31	107.55	113.67
26	D	501	HEC	O1A-CGA-CBA	-2.29	115.82	123.09
24	O	404	HEM	CHA-C4D-ND	2.28	127.18	124.37
27	a	601	HEA	C26-C15-C14	-2.26	117.82	123.63
26	P	402	HEC	O1A-CGA-CBA	-2.25	115.97	123.09
24	C	402	HEM	C1C-CHC-C4B	-2.24	121.25	126.02
24	O	404	HEM	C1C-CHC-C4B	-2.24	121.26	126.02
27	a	601	HEA	C27-C19-C20	2.23	119.10	115.23
27	a	602	HEA	OMA-CMA-C3A	-2.23	120.59	125.62
24	C	403	HEM	C1C-CHC-C4B	-2.22	121.30	126.02
27	a	602	HEA	C4B-NB-C1B	2.21	107.83	105.21
27	a	602	HEA	CAD-CBD-CGD	-2.21	107.80	113.67
24	O	403	HEM	C4A-CHB-C1B	-2.21	121.05	126.25
27	a	602	HEA	C1D-ND-C4D	2.20	107.81	105.21
26	P	402	HEC	CHC-C4B-NB	2.19	127.08	124.37
27	a	602	HEA	C26-C15-C16	2.16	118.97	115.23
27	a	601	HEA	C2C-C1C-NC	-2.15	106.69	110.14
25	G	101	3PE	C2-O21-C21	-2.14	112.68	117.80
24	C	402	HEM	C4A-CHB-C1B	-2.13	121.25	126.25
26	D	501	HEC	CMD-C2D-C1D	-2.13	121.71	125.03
27	a	602	HEA	C25-C23-C24	2.11	119.44	114.59
24	C	403	HEM	O2A-CGA-CBA	2.11	120.66	114.00
24	C	402	HEM	O2A-CGA-CBA	2.11	120.65	114.00
27	a	602	HEA	CMB-C2B-C3B	-2.09	126.23	130.28
24	O	404	HEM	C1B-NB-C4B	2.09	107.68	105.21
24	O	403	HEM	C2A-C1A-NA	-2.08	107.84	110.15
26	P	402	HEC	CMD-C2D-C1D	-2.08	121.78	125.03
26	D	501	HEC	C3D-C4D-ND	-2.08	108.34	110.35
25	O	401	3PE	C2-O21-C21	-2.08	112.83	117.80
24	C	403	HEM	C1B-NB-C4B	2.08	107.67	105.21
24	O	403	HEM	C3B-C2B-C1B	2.07	107.97	106.41
27	a	602	HEA	C21-C22-C23	-2.07	120.75	127.64
27	a	601	HEA	C25-C23-C24	2.05	119.31	114.59
24	O	404	HEM	O2A-CGA-CBA	2.04	120.44	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	402	HEM	C3B-C2B-C1B	2.03	107.93	106.41
22	S	101	PC1	C11-C12-N	-2.00	109.40	115.82

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
26	D	501	HEC	NA
26	P	402	HEC	NA

All (435) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	A	602	PC1	C11-O13-P-O12
22	A	602	PC1	C11-O13-P-O14
22	A	602	PC1	C11-O13-P-O11
22	S	101	PC1	C1-O11-P-O12
22	S	101	PC1	C1-O11-P-O14
22	S	101	PC1	C1-O11-P-O13
22	S	101	PC1	O13-C11-C12-N
22	a	605	PC1	C1-O11-P-O12
22	i	101	PC1	C11-O13-P-O12
22	i	101	PC1	C11-O13-P-O14
22	i	101	PC1	C11-O13-P-O11
23	A	603	CDL	CB2-OB2-PB2-OB3
23	A	603	CDL	CB2-OB2-PB2-OB4
23	A	603	CDL	CB2-OB2-PB2-OB5
23	A	603	CDL	CB3-OB5-PB2-OB2
23	A	603	CDL	CB3-OB5-PB2-OB3
23	A	603	CDL	CB3-OB5-PB2-OB4
23	C	401	CDL	CA3-OA5-PA1-OA2
23	C	401	CDL	CA3-OA5-PA1-OA3
23	C	401	CDL	CB2-OB2-PB2-OB4
23	C	401	CDL	CB2-OB2-PB2-OB5
23	C	401	CDL	CB3-OB5-PB2-OB2
23	C	401	CDL	CB3-OB5-PB2-OB3
23	C	401	CDL	CB3-OB5-PB2-OB4
23	C	409	CDL	CA3-OA5-PA1-OA2
23	C	409	CDL	CA3-OA5-PA1-OA3
23	C	409	CDL	CB3-OB5-PB2-OB2
23	C	409	CDL	CB3-OB5-PB2-OB3
23	C	409	CDL	CB3-OB5-PB2-OB4
23	D	502	CDL	CA2-OA2-PA1-OA3

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Mol	Chain	Res	Type	Atoms
23	D	502	CDL	CA2-OA2-PA1-OA5
23	D	502	CDL	CB2-OB2-PB2-OB4
23	D	502	CDL	CB2-OB2-PB2-OB5
23	D	502	CDL	CB3-OB5-PB2-OB2
23	D	502	CDL	CB3-OB5-PB2-OB3
23	D	502	CDL	CB3-OB5-PB2-OB4
23	M	602	CDL	CB2-OB2-PB2-OB5
23	O	402	CDL	CA3-OA5-PA1-OA3
23	O	402	CDL	CB2-OB2-PB2-OB3
23	O	402	CDL	CB3-OB5-PB2-OB2
23	O	402	CDL	CB3-OB5-PB2-OB4
23	P	403	CDL	CA2-OA2-PA1-OA4
23	P	403	CDL	CA2-OA2-PA1-OA5
23	P	403	CDL	CA3-OA5-PA1-OA2
23	P	403	CDL	CA3-OA5-PA1-OA4
23	P	403	CDL	CB2-OB2-PB2-OB3
23	P	403	CDL	CB2-OB2-PB2-OB4
23	P	403	CDL	CB2-OB2-PB2-OB5
23	S	102	CDL	CA2-OA2-PA1-OA4
23	S	102	CDL	CA3-OA5-PA1-OA2
23	S	102	CDL	CA3-OA5-PA1-OA4
23	a	608	CDL	CA2-OA2-PA1-OA3
23	a	608	CDL	CA2-OA2-PA1-OA4
23	a	608	CDL	CA2-OA2-PA1-OA5
23	a	608	CDL	CA3-OA5-PA1-OA2
23	a	608	CDL	CB3-OB5-PB2-OB3
24	O	403	HEM	C2C-C3C-CAC-CBC
24	O	403	HEM	C4C-C3C-CAC-CBC
25	C	404	3PE	C11-O13-P-O11
25	C	404	3PE	C11-O13-P-O14
25	C	404	3PE	O13-C11-C12-N
25	C	405	3PE	C1-O11-P-O12
25	C	405	3PE	C1-O11-P-O13
25	C	405	3PE	C12-C11-O13-P
25	C	405	3PE	O13-C11-C12-N
25	C	405	3PE	C22-C21-O21-C2
25	C	406	3PE	O13-C11-C12-N
25	C	406	3PE	O21-C2-C3-O31
25	C	407	3PE	C1-O11-P-O13
25	C	407	3PE	C1-O11-P-O14
25	C	407	3PE	C11-O13-P-O11
25	C	408	3PE	C1-O11-P-O12

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Mol	Chain	Res	Type	Atoms
25	C	408	3PE	C1-O11-P-O13
25	C	408	3PE	C1-O11-P-O14
25	F	201	3PE	C1-O11-P-O14
25	F	201	3PE	C11-O13-P-O11
25	F	201	3PE	C12-C11-O13-P
25	G	101	3PE	C1-O11-P-O12
25	G	101	3PE	C1-O11-P-O13
25	G	101	3PE	C1-O11-P-O14
25	G	101	3PE	C11-O13-P-O11
25	G	101	3PE	C11-O13-P-O12
25	G	101	3PE	C11-O13-P-O14
25	O	401	3PE	O13-C11-C12-N
25	O	405	3PE	C1-O11-P-O13
25	O	405	3PE	C1-O11-P-O14
25	O	405	3PE	C11-O13-P-O12
25	O	406	3PE	O13-C11-C12-N
25	P	401	3PE	C11-O13-P-O11
25	P	401	3PE	C11-O13-P-O12
25	P	401	3PE	C11-O13-P-O14
25	P	401	3PE	O13-C11-C12-N
25	a	606	3PE	C11-O13-P-O11
25	a	606	3PE	C11-O13-P-O12
25	a	606	3PE	O13-C11-C12-N
25	a	607	3PE	C11-O13-P-O14
25	a	607	3PE	O13-C11-C12-N
25	a	609	3PE	C11-O13-P-O11
25	a	609	3PE	C11-O13-P-O14
25	a	609	3PE	O13-C11-C12-N
25	a	610	3PE	C11-O13-P-O11
25	a	610	3PE	C11-O13-P-O14
25	a	610	3PE	O13-C11-C12-N
25	a	611	3PE	C1-O11-P-O13
25	a	611	3PE	C11-O13-P-O11
25	a	611	3PE	C11-O13-P-O12
25	a	611	3PE	O13-C11-C12-N
25	a	612	3PE	C1-O11-P-O12
25	b	302	3PE	O13-C11-C12-N
25	b	303	3PE	C1-O11-P-O12
25	b	303	3PE	C1-O11-P-O13
25	b	303	3PE	O13-C11-C12-N
25	b	304	3PE	C1-O11-P-O12
25	b	304	3PE	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
25	b	304	3PE	C11-O13-P-O11
25	b	304	3PE	C11-O13-P-O12
25	b	304	3PE	O13-C11-C12-N
25	c	301	3PE	C11-O13-P-O11
25	c	301	3PE	C11-O13-P-O12
25	c	301	3PE	C11-O13-P-O14
25	c	301	3PE	O13-C11-C12-N
25	c	302	3PE	C11-O13-P-O11
25	c	302	3PE	O13-C11-C12-N
25	c	303	3PE	C1-O11-P-O12
25	c	303	3PE	C1-O11-P-O13
25	c	303	3PE	C11-O13-P-O12
25	c	304	3PE	C11-O13-P-O11
25	c	304	3PE	C11-O13-P-O12
25	c	305	3PE	C11-O13-P-O11
25	c	305	3PE	C11-O13-P-O12
25	c	305	3PE	O13-C11-C12-N
25	d	101	3PE	C1-O11-P-O12
25	d	101	3PE	C1-O11-P-O13
25	d	101	3PE	C11-O13-P-O11
25	d	101	3PE	C11-O13-P-O12
25	d	101	3PE	C11-O13-P-O14
25	d	101	3PE	O13-C11-C12-N
25	i	103	3PE	C1-O11-P-O12
25	i	103	3PE	C1-O11-P-O13
25	i	103	3PE	C11-O13-P-O11
25	i	103	3PE	C11-O13-P-O12
25	i	103	3PE	C11-O13-P-O14
25	i	103	3PE	O13-C11-C12-N
27	a	601	HEA	C2A-C3A-CMA-OMA
27	a	601	HEA	C4A-C3A-CMA-OMA
27	a	602	HEA	C3B-C11-C12-C13
31	i	102	LYS	O-C-CA-CB
25	C	405	3PE	O32-C31-O31-C3
27	a	601	HEA	C21-C22-C23-C25
25	C	405	3PE	C32-C31-O31-C3
22	S	101	PC1	C32-C31-O31-C3
25	C	405	3PE	O22-C21-O21-C2
27	a	601	HEA	C13-C14-C15-C26
27	a	601	HEA	C21-C22-C23-C24
23	C	401	CDL	O1-C1-CA2-OA2
27	a	602	HEA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
24	O	403	HEM	C2A-CAA-CBA-CGA
22	S	101	PC1	O32-C31-O31-C3
27	a	602	HEA	C13-C14-C15-C26
22	a	605	PC1	C11-C12-N-C15
27	a	602	HEA	C21-C22-C23-C25
22	a	605	PC1	C11-C12-N-C13
22	a	605	PC1	C21-C22-C23-C24
25	a	610	3PE	C21-C22-C23-C24
25	c	301	3PE	C31-C32-C33-C34
27	a	602	HEA	O11-C11-C12-C13
22	a	605	PC1	C33-C34-C35-C36
25	c	304	3PE	C32-C33-C34-C35
25	b	302	3PE	C29-C2A-C2B-C2C
23	D	502	CDL	CB7-C71-C72-C73
25	P	401	3PE	C27-C28-C29-C2A
25	i	103	3PE	C22-C23-C24-C25
25	C	406	3PE	C23-C24-C25-C26
22	a	605	PC1	C11-C12-N-C14
25	O	405	3PE	C22-C21-O21-C2
25	C	405	3PE	C22-C23-C24-C25
25	c	305	3PE	C23-C24-C25-C26
23	A	603	CDL	C16-C17-C18-C19
25	P	401	3PE	C25-C26-C27-C28
22	S	101	PC1	C22-C21-O21-C2
25	C	407	3PE	C3E-C3F-C3G-C3H
22	S	101	PC1	O22-C21-O21-C2
23	S	102	CDL	OB5-CB3-CB4-OB6
25	C	406	3PE	C21-C22-C23-C24
25	a	606	3PE	O21-C2-C3-O31
24	C	402	HEM	C2A-CAA-CBA-CGA
23	C	401	CDL	CB2-C1-CA2-OA2
23	O	402	CDL	C53-C54-C55-C56
27	a	602	HEA	C21-C22-C23-C24
23	S	102	CDL	OB5-CB3-CB4-CB6
25	C	407	3PE	O11-C1-C2-C3
25	a	610	3PE	O11-C1-C2-C3
25	O	405	3PE	O22-C21-O21-C2
23	O	402	CDL	C57-C58-C59-C60
25	c	304	3PE	C22-C23-C24-C25
25	a	609	3PE	C36-C37-C38-C39
23	O	402	CDL	C62-C63-C64-C65
25	c	305	3PE	C37-C38-C39-C3A

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Mol	Chain	Res	Type	Atoms
24	O	404	HEM	C4D-C3D-CAD-CBD
23	D	502	CDL	OA6-CA4-CA6-OA8
25	c	304	3PE	O21-C2-C3-O31
22	S	101	PC1	C23-C24-C25-C26
23	M	602	CDL	CA4-CA3-OA5-PA1
25	C	407	3PE	C2-C1-O11-P
23	A	603	CDL	OA5-CA3-CA4-CA6
23	D	502	CDL	OB5-CB3-CB4-CB6
25	C	404	3PE	O11-C1-C2-C3
25	C	405	3PE	O11-C1-C2-C3
25	O	406	3PE	O11-C1-C2-C3
25	c	302	3PE	O11-C1-C2-C3
25	d	101	3PE	O11-C1-C2-C3
22	a	605	PC1	C32-C33-C34-C35
22	A	602	PC1	C33-C34-C35-C36
25	C	405	3PE	C32-C33-C34-C35
25	c	304	3PE	C23-C24-C25-C26
23	D	502	CDL	CA3-CA4-CA6-OA8
23	a	608	CDL	CB3-CB4-CB6-OB8
25	a	606	3PE	C1-C2-C3-O31
25	b	302	3PE	C1-C2-C3-O31
25	b	303	3PE	C1-C2-C3-O31
25	b	302	3PE	C32-C33-C34-C35
23	M	602	CDL	CA7-C31-C32-C33
23	A	603	CDL	OB5-CB3-CB4-OB6
25	C	408	3PE	O11-C1-C2-O21
25	c	302	3PE	O11-C1-C2-O21
23	P	403	CDL	C32-C31-CA7-OA8
23	A	603	CDL	CA4-CA3-OA5-PA1
25	F	201	3PE	C2-C1-O11-P
25	d	101	3PE	C2-C1-O11-P
25	O	406	3PE	O21-C21-C22-C23
25	b	303	3PE	O21-C2-C3-O31
25	d	101	3PE	O21-C2-C3-O31
25	a	609	3PE	C24-C25-C26-C27
25	a	609	3PE	C21-C22-C23-C24
25	O	405	3PE	C32-C31-O31-C3
25	c	303	3PE	O11-C1-C2-C3
24	C	402	HEM	C2C-C3C-CAC-CBC
24	C	403	HEM	C2B-C3B-CAB-CBB
24	O	403	HEM	C2B-C3B-CAB-CBB
24	O	404	HEM	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
24	O	404	HEM	C2C-C3C-CAC-CBC
23	O	402	CDL	OB5-CB3-CB4-OB6
22	S	101	PC1	C1-C2-C3-O31
25	C	406	3PE	C1-C2-C3-O31
25	c	301	3PE	C1-C2-C3-O31
24	O	404	HEM	C2D-C3D-CAD-CBD
23	S	102	CDL	OB6-CB4-CB6-OB8
25	c	301	3PE	O21-C2-C3-O31
22	i	101	PC1	O13-C11-C12-N
25	O	405	3PE	O32-C31-O31-C3
27	a	601	HEA	C4C-C3C-CAC-CBC
23	C	401	CDL	C1-CB2-OB2-PB2
25	a	610	3PE	C2-C1-O11-P
23	A	603	CDL	OA5-CA3-CA4-OA6
23	D	502	CDL	OB5-CB3-CB4-OB6
23	P	403	CDL	OB5-CB3-CB4-OB6
23	a	608	CDL	OB5-CB3-CB4-OB6
25	C	404	3PE	O11-C1-C2-O21
25	C	405	3PE	O11-C1-C2-O21
25	C	407	3PE	O11-C1-C2-O21
25	O	406	3PE	O11-C1-C2-O21
25	c	303	3PE	O11-C1-C2-O21
25	d	101	3PE	O11-C1-C2-O21
25	O	407	3PE	C31-C32-C33-C34
25	C	405	3PE	C24-C25-C26-C27
23	a	608	CDL	OB6-CB4-CB6-OB8
25	b	302	3PE	O21-C2-C3-O31
22	M	603	PC1	C1-O11-P-O14
22	a	605	PC1	C1-O11-P-O14
22	a	605	PC1	C1-O11-P-O13
23	C	409	CDL	CA3-OA5-PA1-OA4
23	D	502	CDL	CA2-OA2-PA1-OA4
23	D	502	CDL	CB2-OB2-PB2-OB3
23	M	602	CDL	CA2-OA2-PA1-OA3
23	M	602	CDL	CB2-OB2-PB2-OB3
23	O	402	CDL	CA2-OA2-PA1-OA3
23	O	402	CDL	CB2-OB2-PB2-OB4
23	O	402	CDL	CB2-OB2-PB2-OB5
23	O	402	CDL	CB3-OB5-PB2-OB3
23	P	403	CDL	CA3-OA5-PA1-OA3
23	S	102	CDL	CA2-OA2-PA1-OA3
23	S	102	CDL	CA2-OA2-PA1-OA5

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Mol	Chain	Res	Type	Atoms
23	S	102	CDL	CA3-OA5-PA1-OA3
23	a	608	CDL	CA3-OA5-PA1-OA3
23	a	608	CDL	CB3-OB5-PB2-OB4
25	C	404	3PE	C11-O13-P-O12
25	C	407	3PE	C1-O11-P-O12
25	C	407	3PE	C11-O13-P-O14
25	F	201	3PE	C1-O11-P-O12
25	F	201	3PE	C1-O11-P-O13
25	F	201	3PE	C11-O13-P-O14
25	O	405	3PE	C1-O11-P-O12
25	O	405	3PE	C11-O13-P-O11
25	O	407	3PE	O13-C11-C12-N
25	a	609	3PE	C1-O11-P-O12
25	a	609	3PE	C1-O11-P-O13
25	a	609	3PE	C1-O11-P-O14
25	a	609	3PE	C11-O13-P-O12
25	a	610	3PE	C11-O13-P-O12
25	a	611	3PE	C1-O11-P-O14
25	a	612	3PE	C1-O11-P-O13
25	a	612	3PE	C1-O11-P-O14
25	b	302	3PE	C1-O11-P-O14
25	b	302	3PE	C11-O13-P-O12
25	b	303	3PE	C11-O13-P-O12
25	c	301	3PE	C1-O11-P-O14
25	c	302	3PE	C11-O13-P-O14
25	c	304	3PE	C1-O11-P-O12
25	c	304	3PE	C1-O11-P-O13
25	c	304	3PE	C1-O11-P-O14
25	c	305	3PE	C11-O13-P-O14
25	d	101	3PE	C1-O11-P-O14
25	h	101	3PE	C11-O13-P-O11
25	i	103	3PE	C1-O11-P-O14
27	a	601	HEA	C2C-C3C-CAC-CBC
23	P	403	CDL	C1-CB2-OB2-PB2
25	C	404	3PE	C2-C1-O11-P
25	a	606	3PE	C2-C1-O11-P
25	O	406	3PE	C24-C25-C26-C27
22	a	605	PC1	C31-C32-C33-C34
25	F	201	3PE	C1-C2-O21-C21
22	S	101	PC1	C22-C23-C24-C25
23	O	402	CDL	OB5-CB3-CB4-CB6
23	P	403	CDL	OB5-CB3-CB4-CB6

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Mol	Chain	Res	Type	Atoms
25	C	408	3PE	O11-C1-C2-C3
25	a	610	3PE	O11-C1-C2-O21
25	P	401	3PE	C21-C22-C23-C24
25	c	302	3PE	C2-C1-O11-P
25	a	606	3PE	C34-C35-C36-C37
25	c	301	3PE	O31-C31-C32-C33
25	c	305	3PE	O31-C31-C32-C33
25	c	304	3PE	C1-C2-C3-O31
25	c	301	3PE	C37-C38-C39-C3A
25	b	304	3PE	O31-C31-C32-C33
27	a	602	HEA	C13-C14-C15-C16
26	D	501	HEC	C3A-C2A-CAA-CBA
24	O	404	HEM	C4B-C3B-CAB-CBB
26	D	501	HEC	C1A-C2A-CAA-CBA
25	C	404	3PE	O21-C2-C3-O31
23	C	401	CDL	C1-CA2-OA2-PA1
25	a	607	3PE	C26-C27-C28-C29
24	O	403	HEM	CAD-CBD-CGD-O1D
23	M	602	CDL	CA6-CA4-OA6-CA5
23	P	403	CDL	CA6-CA4-OA6-CA5
25	c	302	3PE	C1-C2-O21-C21
25	c	304	3PE	C3-C2-O21-C21
25	a	609	3PE	C39-C3A-C3B-C3C
25	b	302	3PE	C33-C34-C35-C36
25	c	303	3PE	C2-C1-O11-P
24	O	403	HEM	CAD-CBD-CGD-O2D
27	a	601	HEA	CAD-CBD-CGD-O1D
23	C	409	CDL	C55-C56-C57-C58
23	a	608	CDL	C54-C55-C56-C57
25	O	406	3PE	C23-C24-C25-C26
25	b	303	3PE	C2-C1-O11-P
25	C	407	3PE	C3C-C3D-C3E-C3F
27	a	601	HEA	CAD-CBD-CGD-O2D
24	O	403	HEM	C3D-CAD-CBD-CGD
25	C	404	3PE	C1-C2-C3-O31
27	a	601	HEA	CAA-CBA-CGA-O2A
25	a	609	3PE	C31-C32-C33-C34
24	C	402	HEM	CAD-CBD-CGD-O2D
26	P	402	HEC	CAD-CBD-CGD-O2D
27	a	601	HEA	CAA-CBA-CGA-O1A
23	A	603	CDL	OB5-CB3-CB4-CB6
22	S	101	PC1	O21-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
24	C	403	HEM	CAA-CBA-CGA-O2A
24	C	403	HEM	CAD-CBD-CGD-O1D
23	P	403	CDL	C12-C13-C14-C15
22	i	101	PC1	C32-C33-C34-C35
24	C	403	HEM	CAD-CBD-CGD-O2D
24	C	403	HEM	C2C-C3C-CAC-CBC
24	O	404	HEM	CAA-CBA-CGA-O2A
22	a	605	PC1	C3-C2-O21-C21
23	S	102	CDL	CA3-CA4-OA6-CA5
25	C	407	3PE	C3-C2-O21-C21
25	a	609	3PE	C1-C2-O21-C21
25	b	303	3PE	C3-C2-O21-C21
24	C	402	HEM	CAD-CBD-CGD-O1D
24	O	403	HEM	CAA-CBA-CGA-O2A
26	P	402	HEC	CAD-CBD-CGD-O1D
25	d	101	3PE	O21-C21-C22-C23
25	d	101	3PE	C1-C2-C3-O31
24	C	402	HEM	C4C-C3C-CAC-CBC
24	C	403	HEM	C4B-C3B-CAB-CBB
24	C	403	HEM	C4C-C3C-CAC-CBC
24	O	403	HEM	C4B-C3B-CAB-CBB
24	O	404	HEM	C4C-C3C-CAC-CBC
27	a	601	HEA	C26-C15-C16-C17
24	O	404	HEM	CAA-CBA-CGA-O1A
24	C	403	HEM	CAA-CBA-CGA-O1A
24	O	403	HEM	CAA-CBA-CGA-O1A
25	a	612	3PE	O21-C2-C3-O31
25	O	406	3PE	O22-C21-C22-C23
25	h	101	3PE	C26-C27-C28-C29
25	a	606	3PE	O31-C31-C32-C33
23	a	608	CDL	C14-C15-C16-C17
23	O	402	CDL	C1-CB2-OB2-PB2
25	c	301	3PE	C27-C28-C29-C2A
25	a	606	3PE	O21-C21-C22-C23
23	S	102	CDL	C32-C31-CA7-OA8
25	c	303	3PE	O21-C21-C22-C23
25	a	607	3PE	C25-C26-C27-C28
22	a	605	PC1	O21-C21-C22-C23
25	d	101	3PE	O31-C31-C32-C33
25	a	612	3PE	C23-C24-C25-C26
25	P	401	3PE	O21-C21-C22-C23
23	a	608	CDL	C52-C51-CB5-OB6

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Mol	Chain	Res	Type	Atoms
25	a	610	3PE	O31-C31-C32-C33
22	a	605	PC1	C1-C2-O21-C21
23	S	102	CDL	CA6-CA4-OA6-CA5
25	C	407	3PE	C1-C2-O21-C21
25	a	609	3PE	C3-C2-O21-C21
25	b	303	3PE	C1-C2-O21-C21
25	c	304	3PE	C1-C2-O21-C21
27	a	602	HEA	CAD-CBD-CGD-O2D
25	c	302	3PE	C33-C34-C35-C36
22	A	602	PC1	C31-C32-C33-C34
24	O	404	HEM	C3D-CAD-CBD-CGD
25	d	101	3PE	O32-C31-C32-C33
25	c	303	3PE	O22-C21-C22-C23
25	a	606	3PE	O32-C31-C32-C33
26	D	501	HEC	CAD-CBD-CGD-O2D
25	C	406	3PE	C22-C23-C24-C25
23	S	102	CDL	C32-C31-CA7-OA9
25	a	610	3PE	O32-C31-C32-C33
23	A	603	CDL	C1-CB2-OB2-PB2
25	P	401	3PE	O22-C21-C22-C23
25	C	405	3PE	O21-C21-C22-C23
22	a	605	PC1	O22-C21-C22-C23
23	a	608	CDL	C52-C51-CB5-OB7
23	M	602	CDL	C12-C11-CA5-OA6
25	i	103	3PE	O31-C31-C32-C33
26	D	501	HEC	CAD-CBD-CGD-O1D
25	F	201	3PE	O31-C31-C32-C33

There are no ring outliers.

43 monomers are involved in 109 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	M	603	PC1	1	0
25	i	103	3PE	2	0
23	M	602	CDL	4	0
26	D	501	HEC	8	0
26	P	402	HEC	3	0
25	a	610	3PE	1	0
23	P	403	CDL	2	0
23	C	401	CDL	3	0
23	O	402	CDL	2	0
23	S	102	CDL	2	0

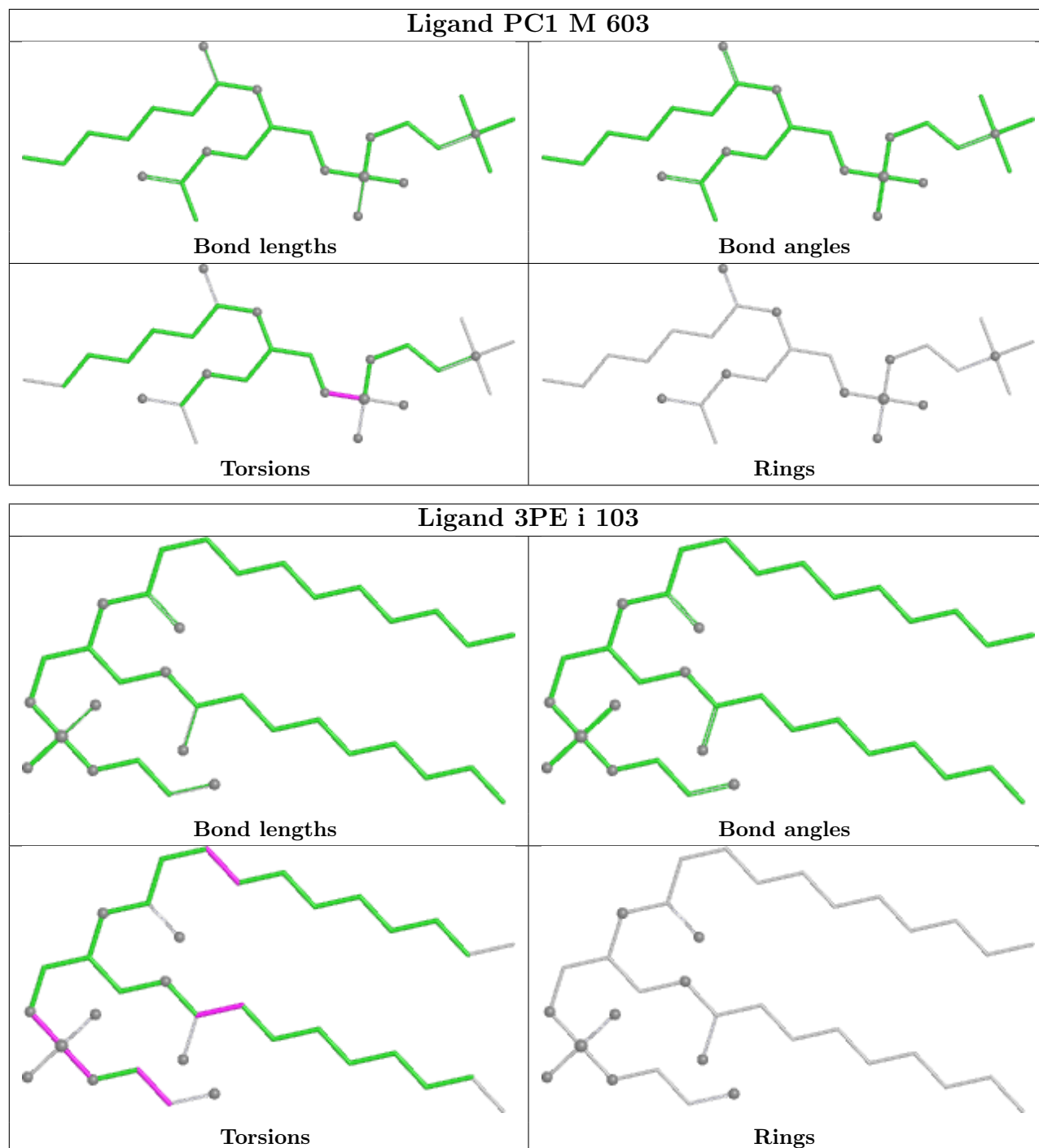
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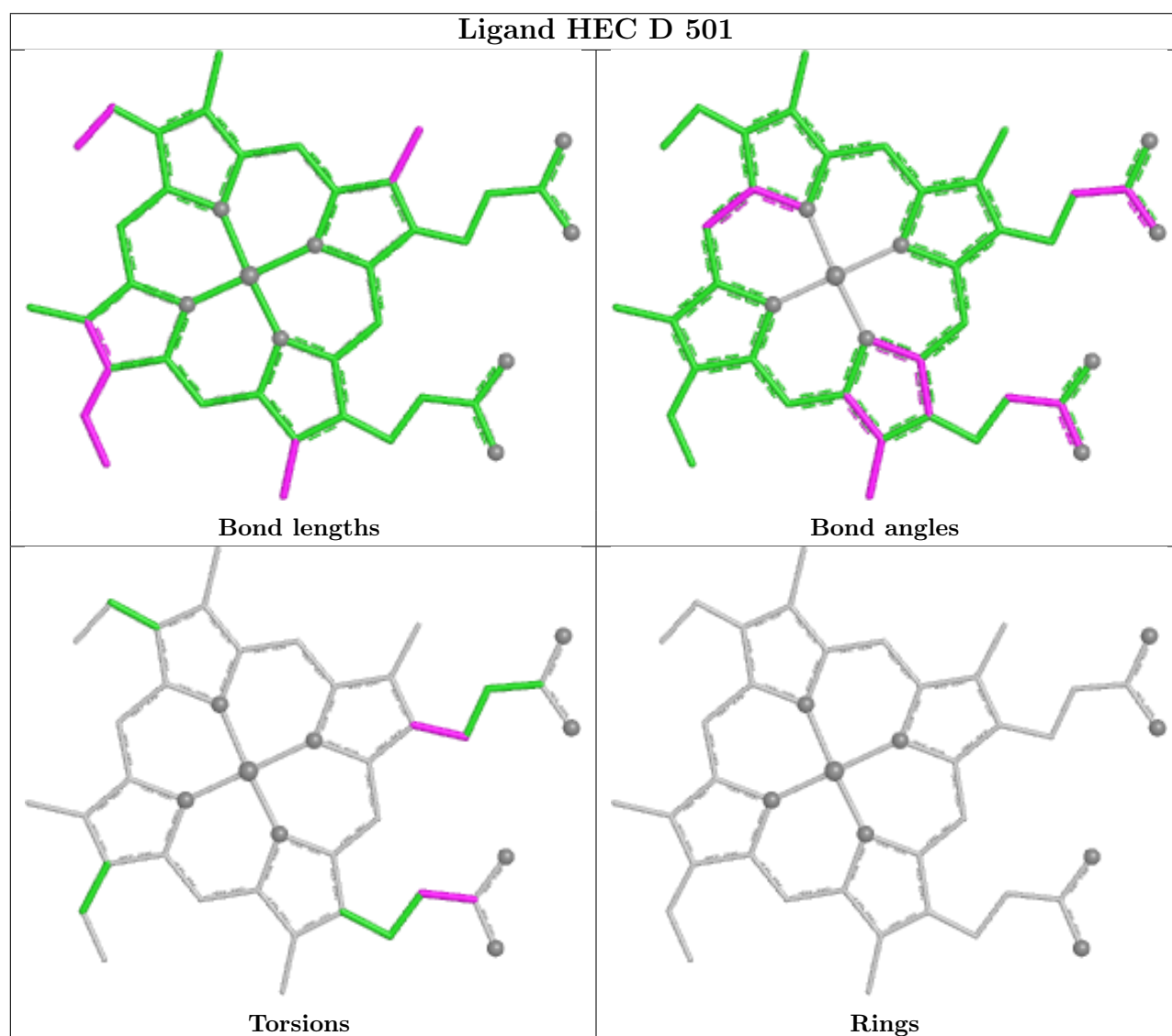
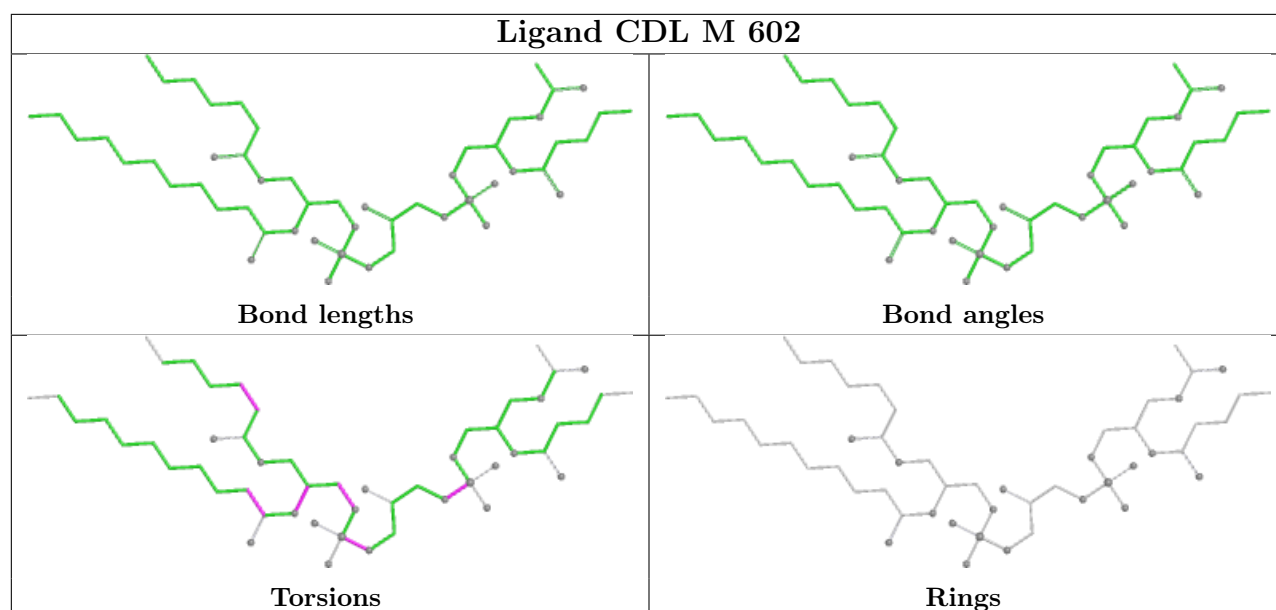
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	a	608	CDL	1	0
22	S	101	PC1	2	0
24	C	402	HEM	2	0
25	O	401	3PE	7	0
23	A	603	CDL	1	0
23	D	502	CDL	1	0
25	b	304	3PE	1	0
22	A	602	PC1	1	0
25	b	303	3PE	2	0
22	i	101	PC1	4	0
25	F	201	3PE	2	0
25	P	401	3PE	2	0
23	C	409	CDL	2	0
27	a	602	HEA	6	0
25	C	408	3PE	1	0
24	O	404	HEM	6	0
25	C	407	3PE	3	0
25	a	607	3PE	5	0
25	c	305	3PE	1	0
25	c	304	3PE	1	0
25	c	301	3PE	4	0
22	a	605	PC1	1	0
25	b	302	3PE	1	0
25	c	302	3PE	3	0
25	h	101	3PE	2	0
25	c	303	3PE	4	0
24	O	403	HEM	3	0
27	a	601	HEA	5	0
25	C	406	3PE	4	0
25	a	612	3PE	1	0
25	C	405	3PE	2	0
25	d	101	3PE	1	0
24	C	403	HEM	5	0

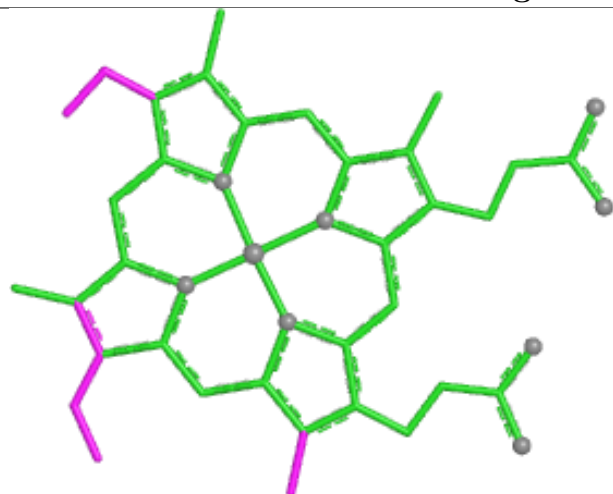
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

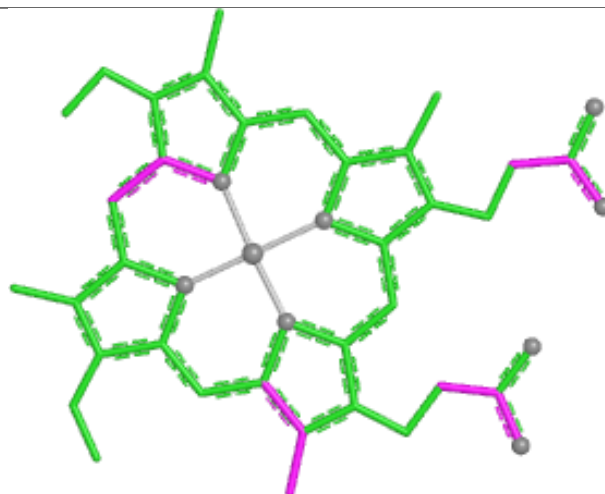




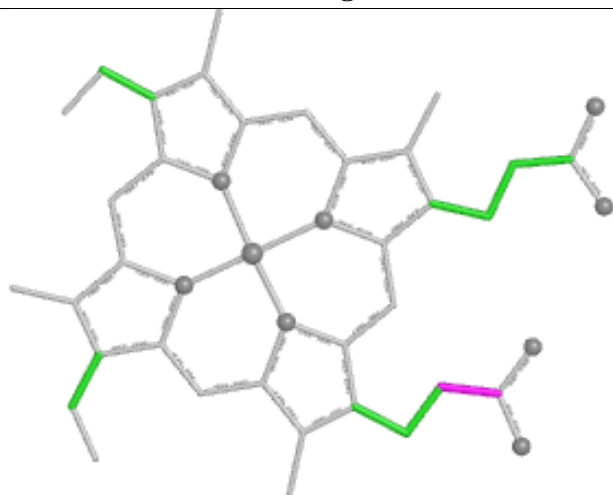
Ligand HEC P 402



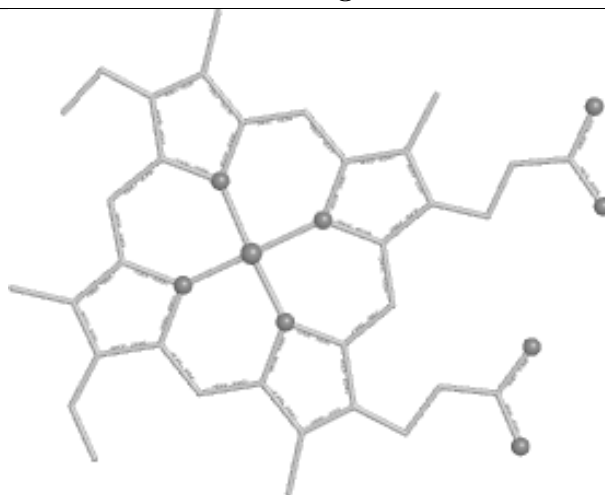
Bond lengths



Bond angles

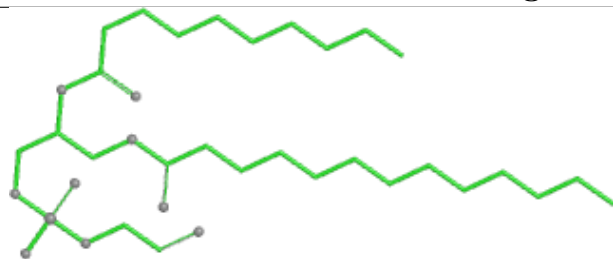


Torsions

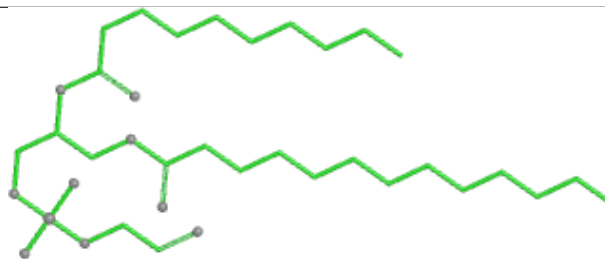


Rings

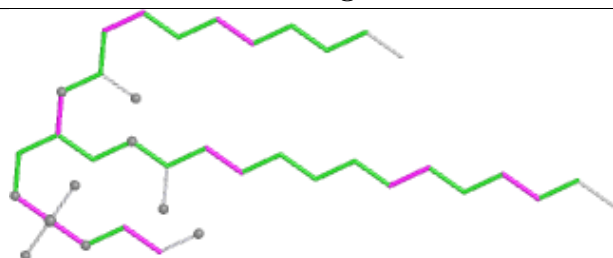
Ligand 3PE a 609



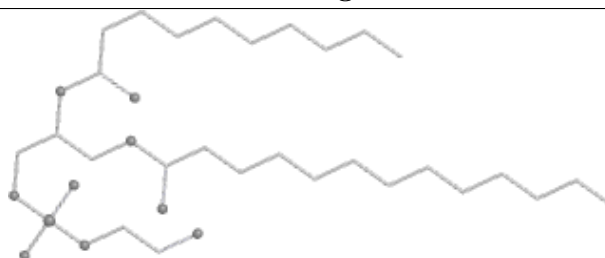
Bond lengths



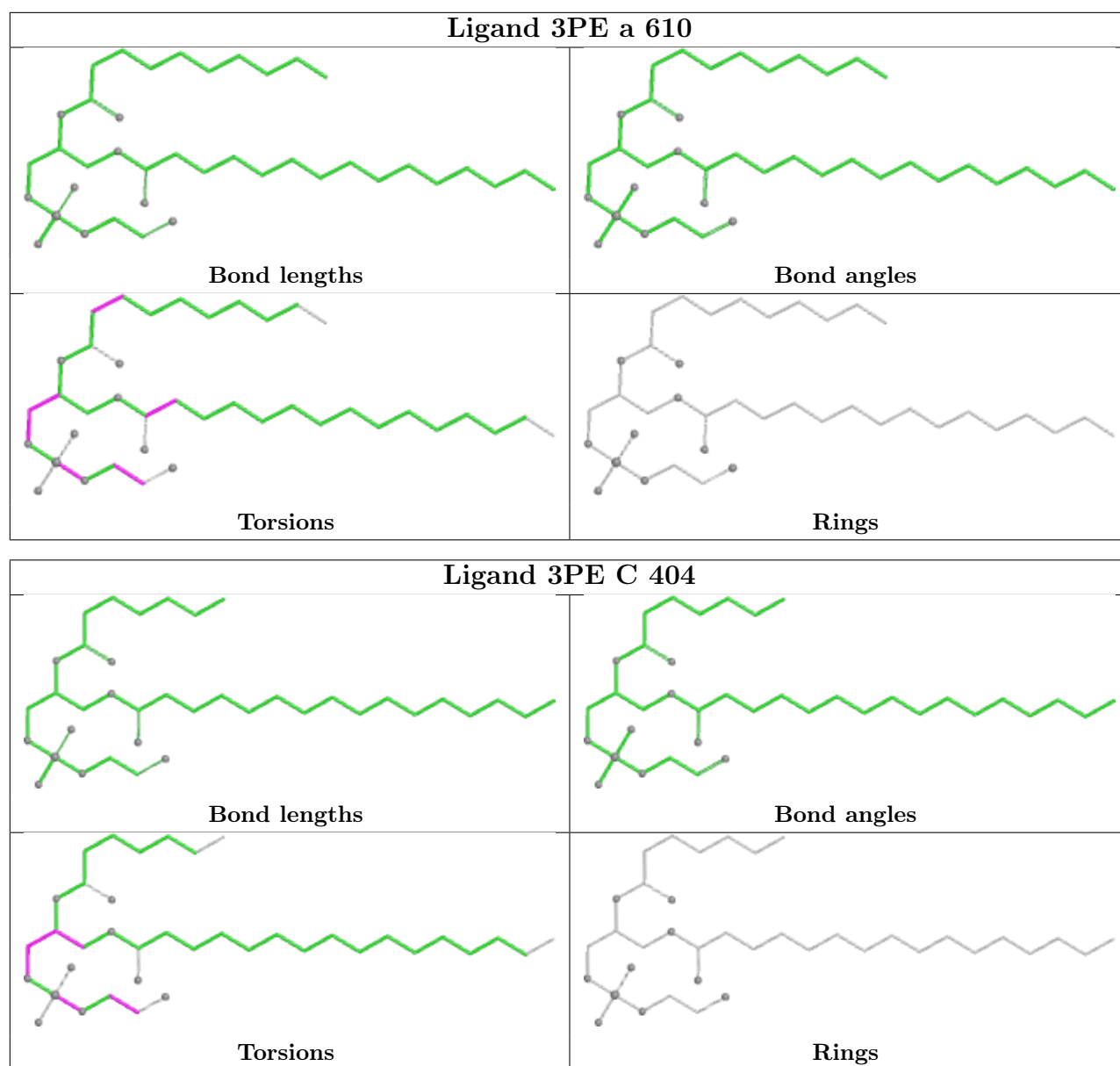
Bond angles

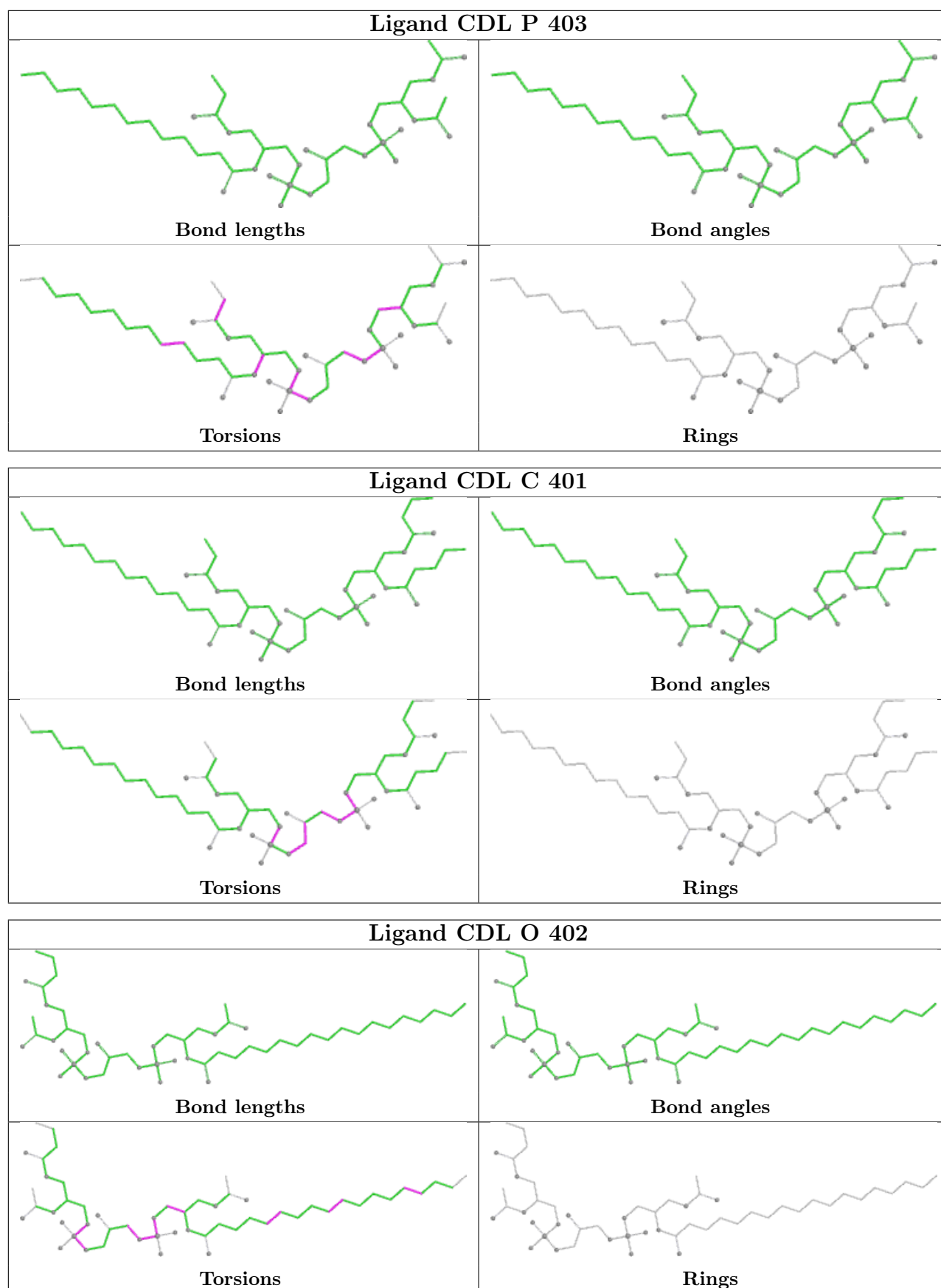


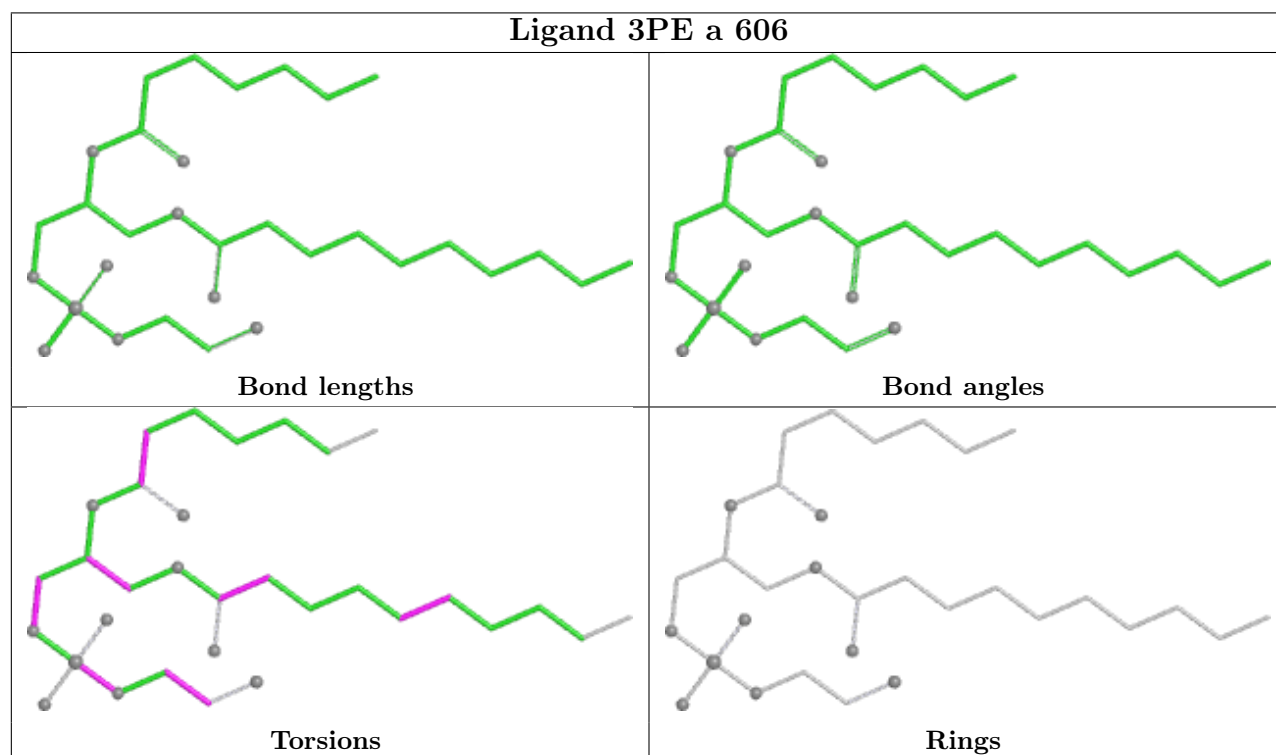
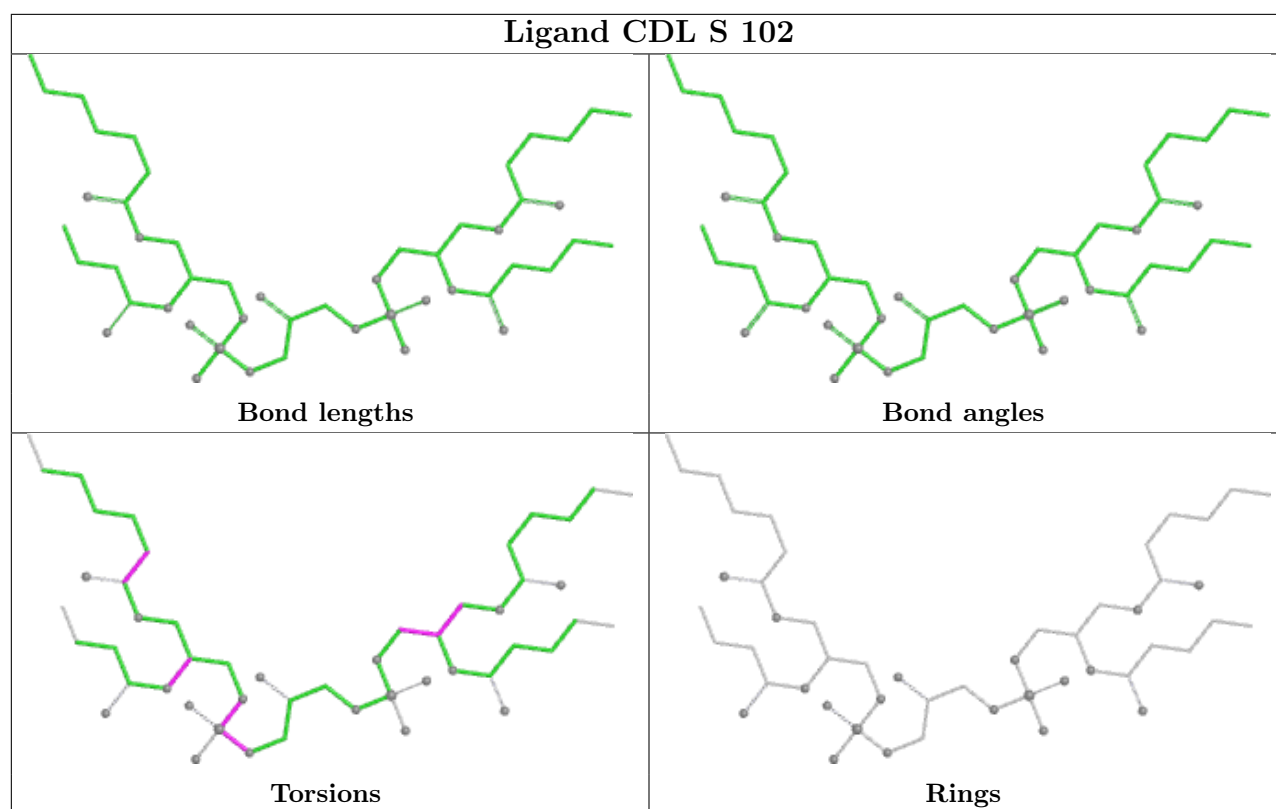
Torsions

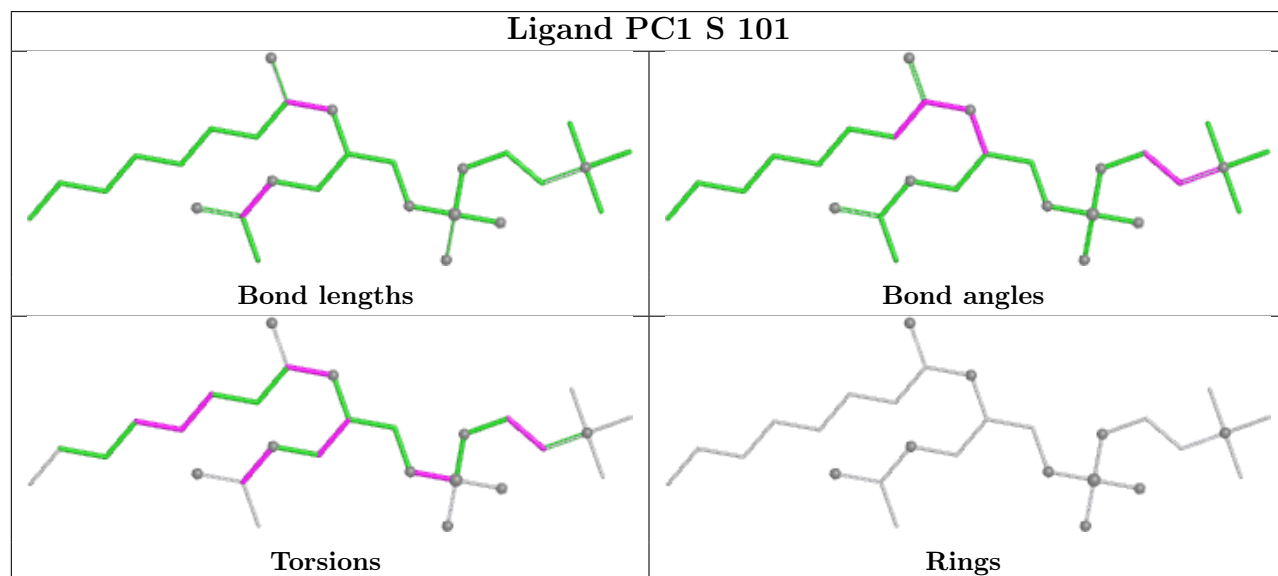
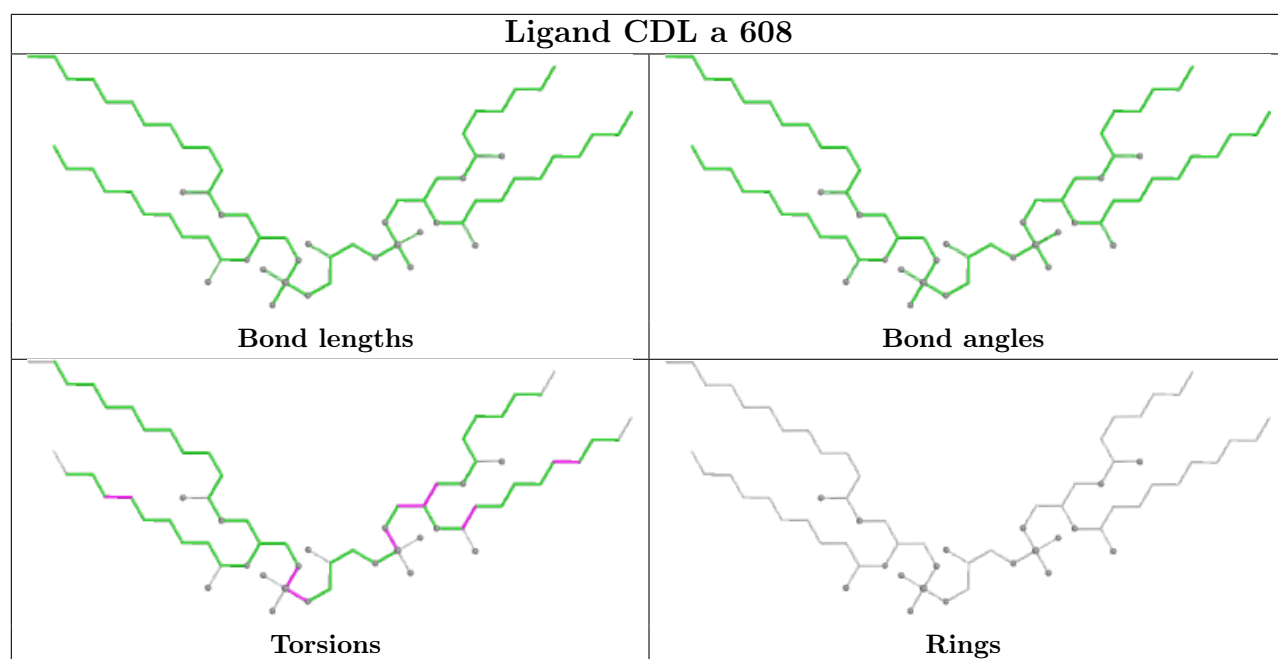


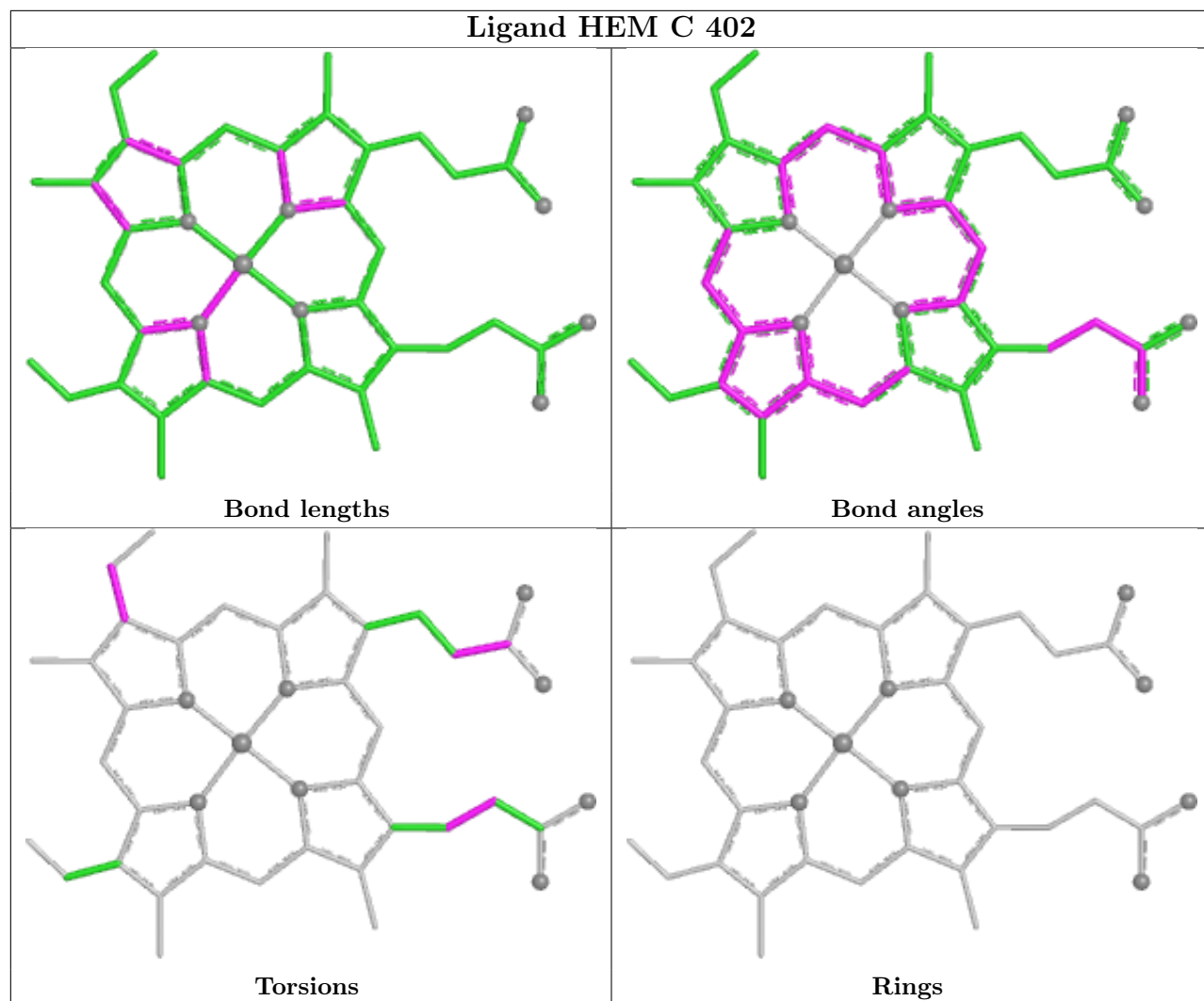
Rings

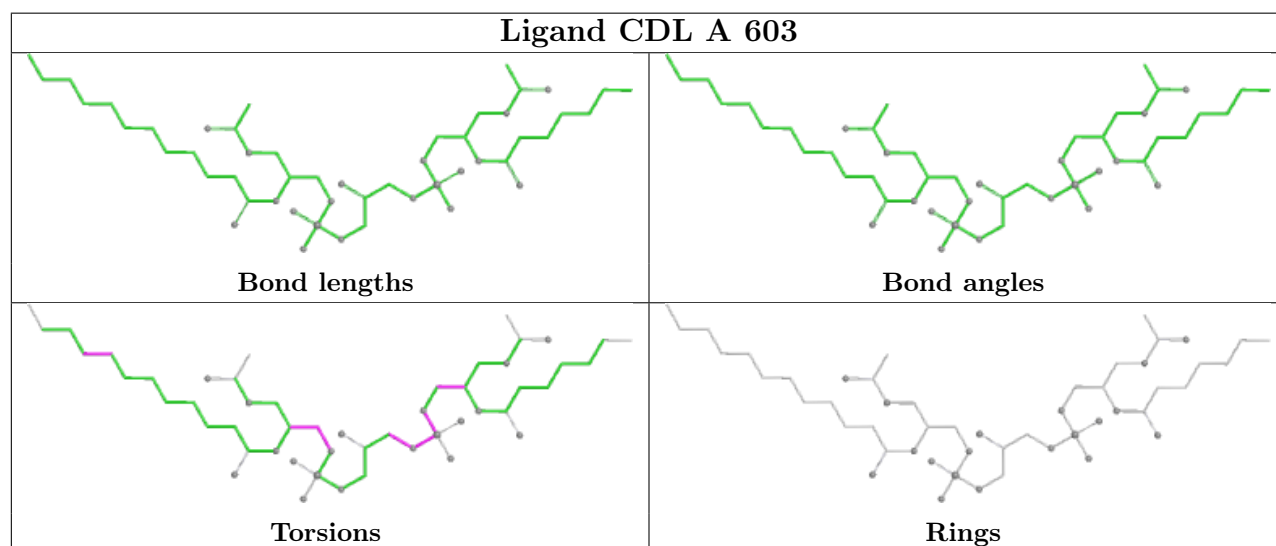
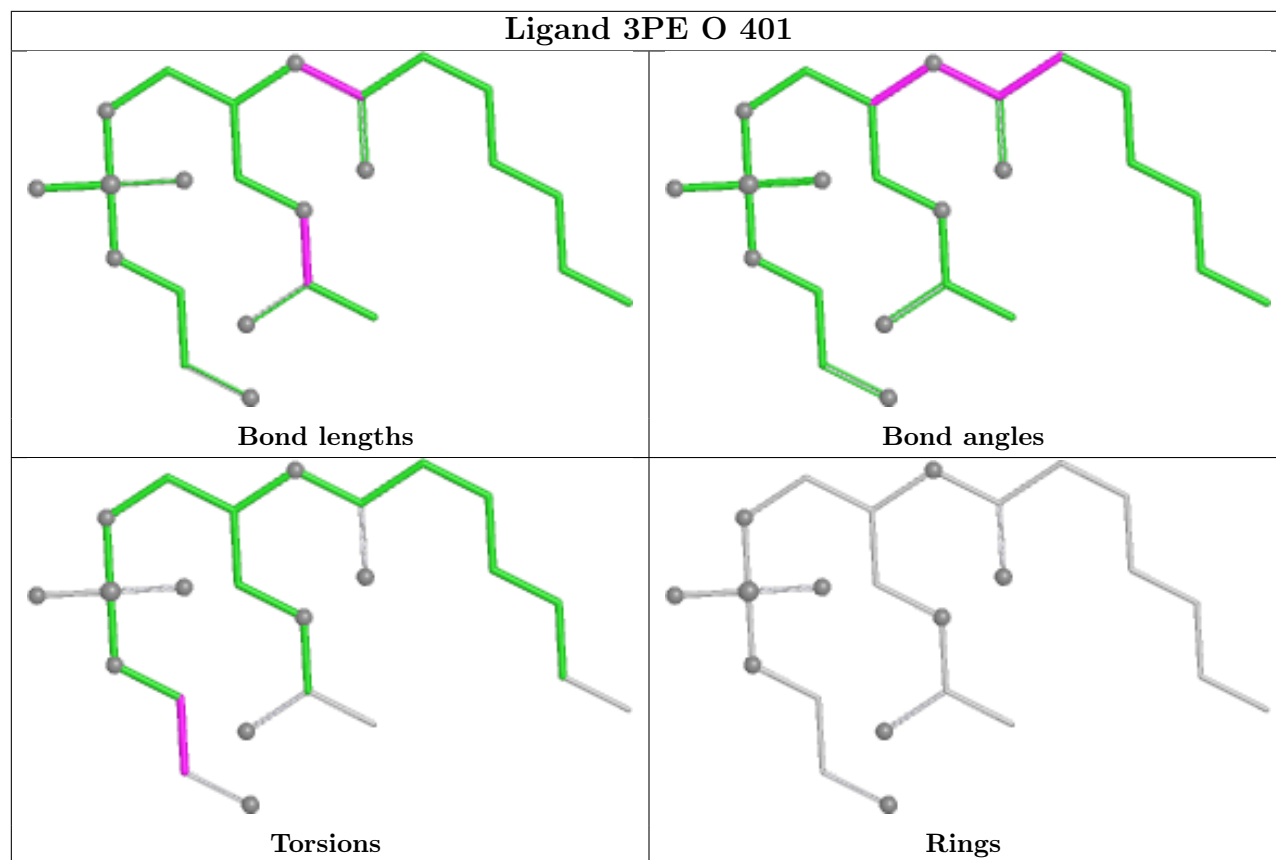


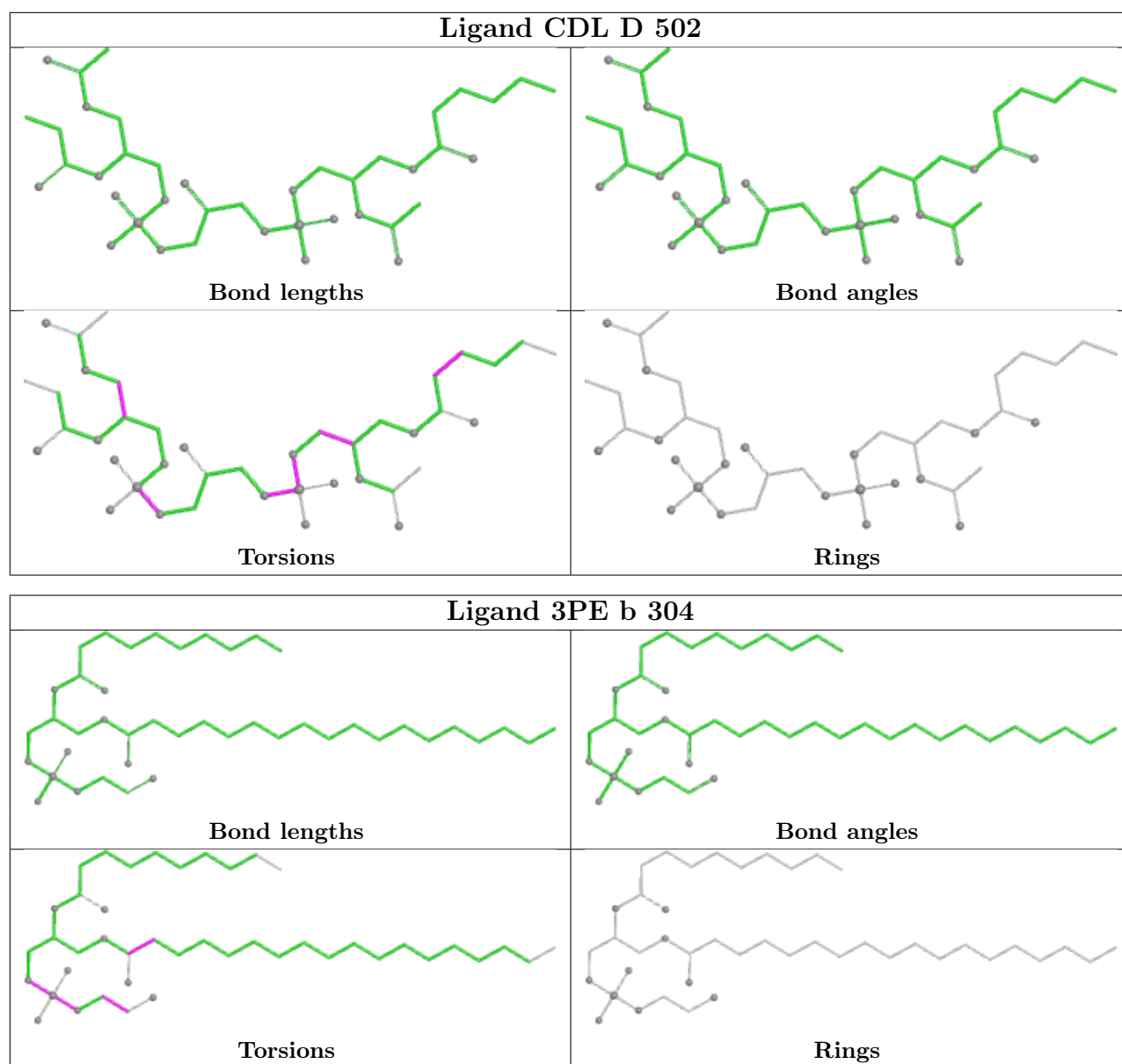


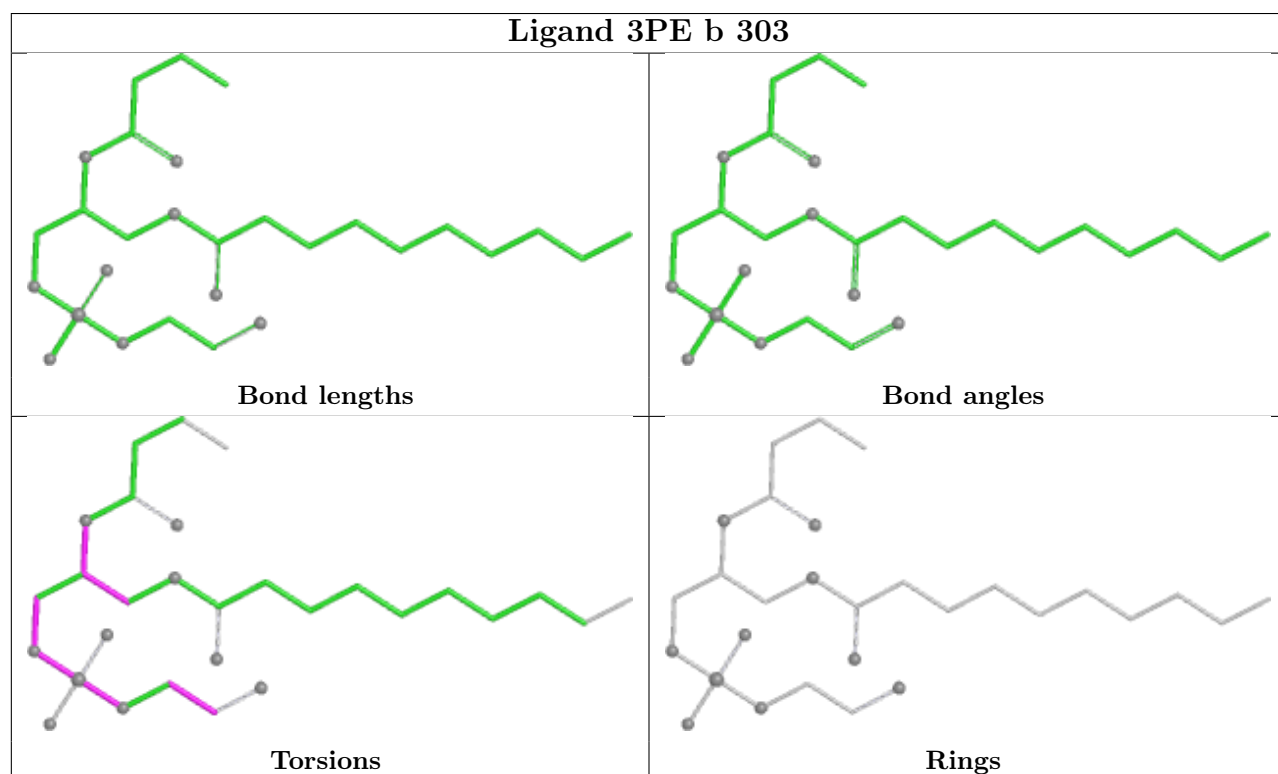
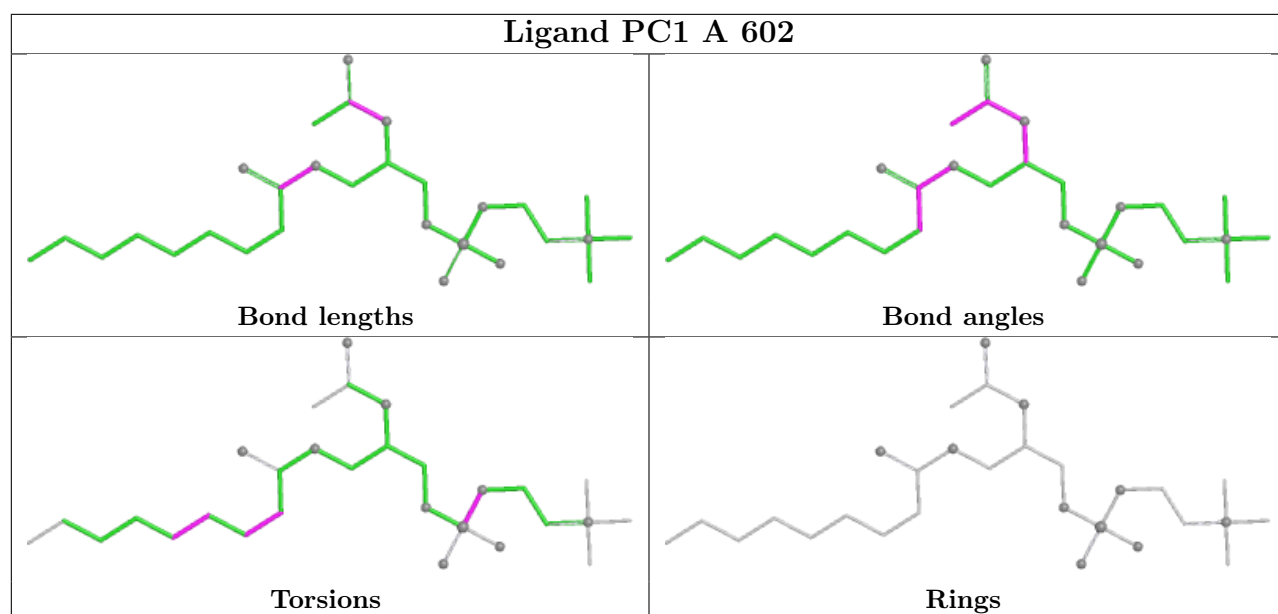


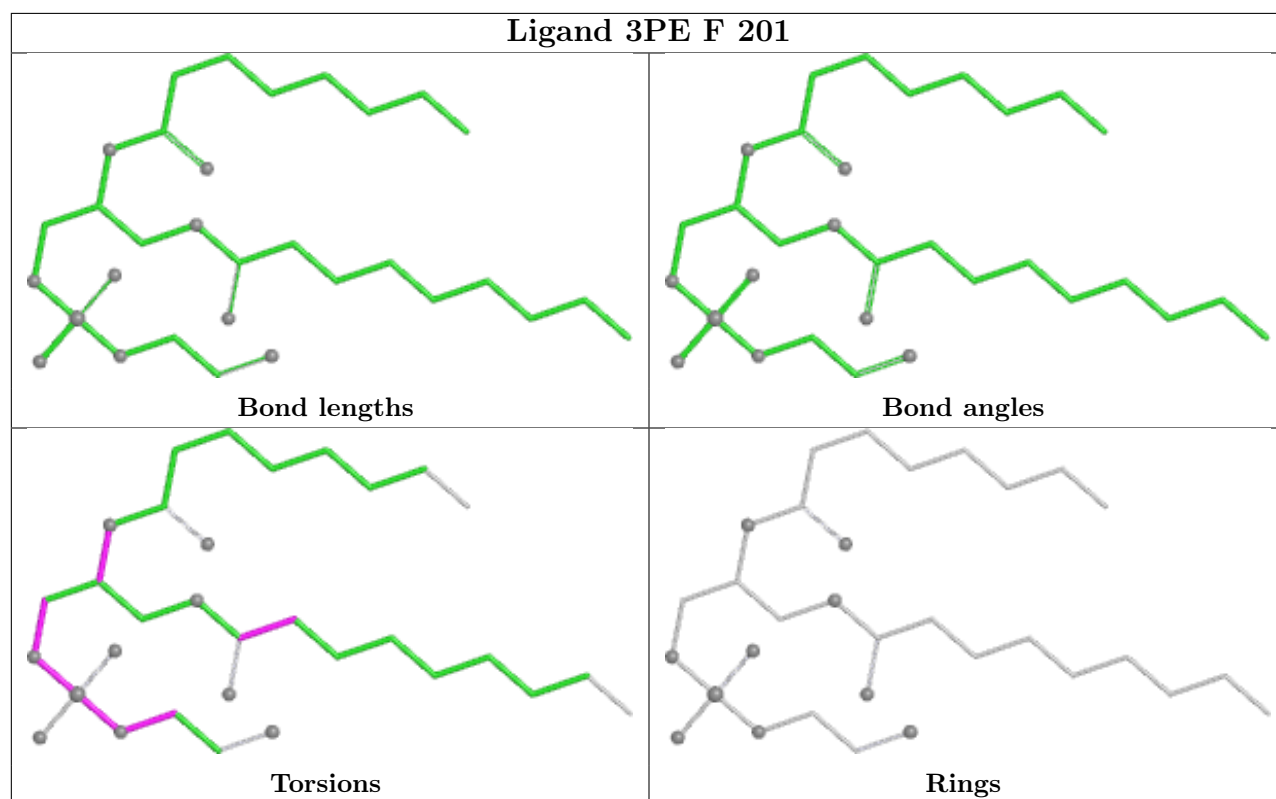
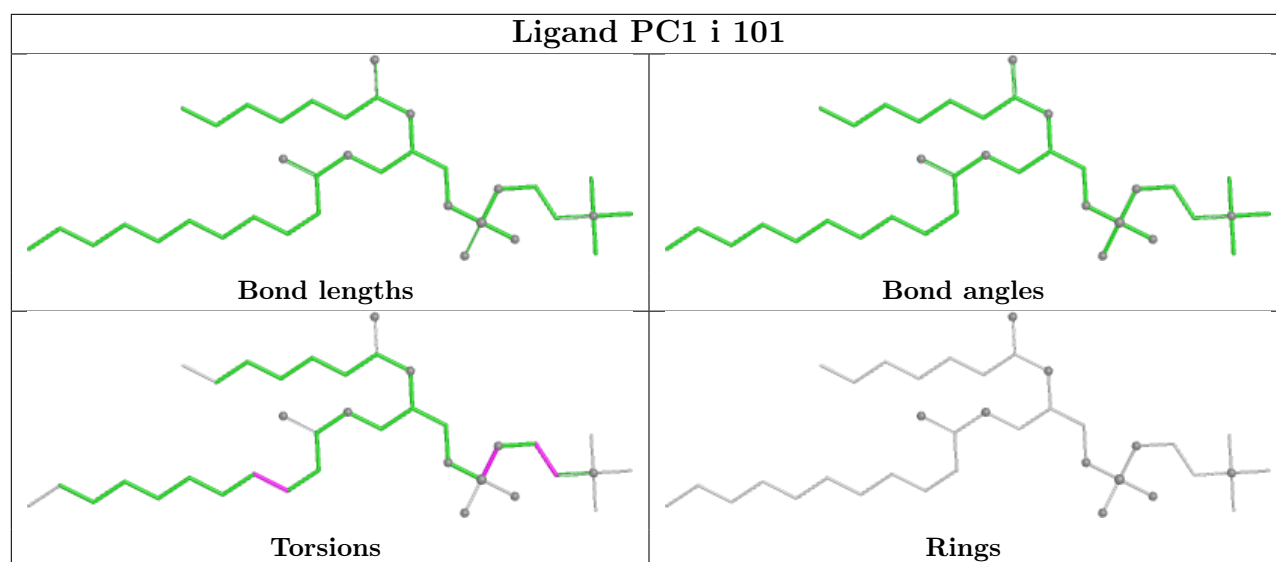




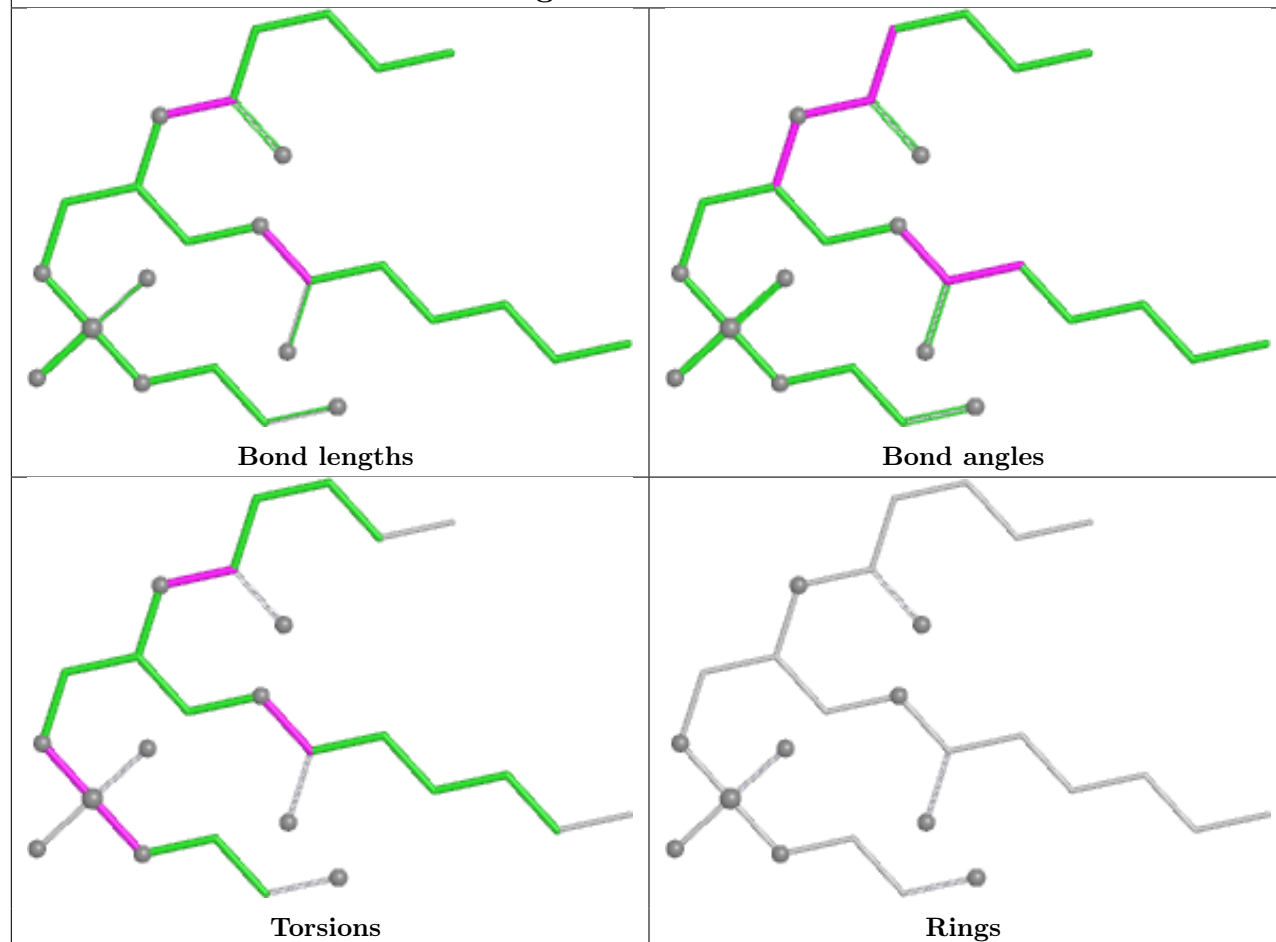




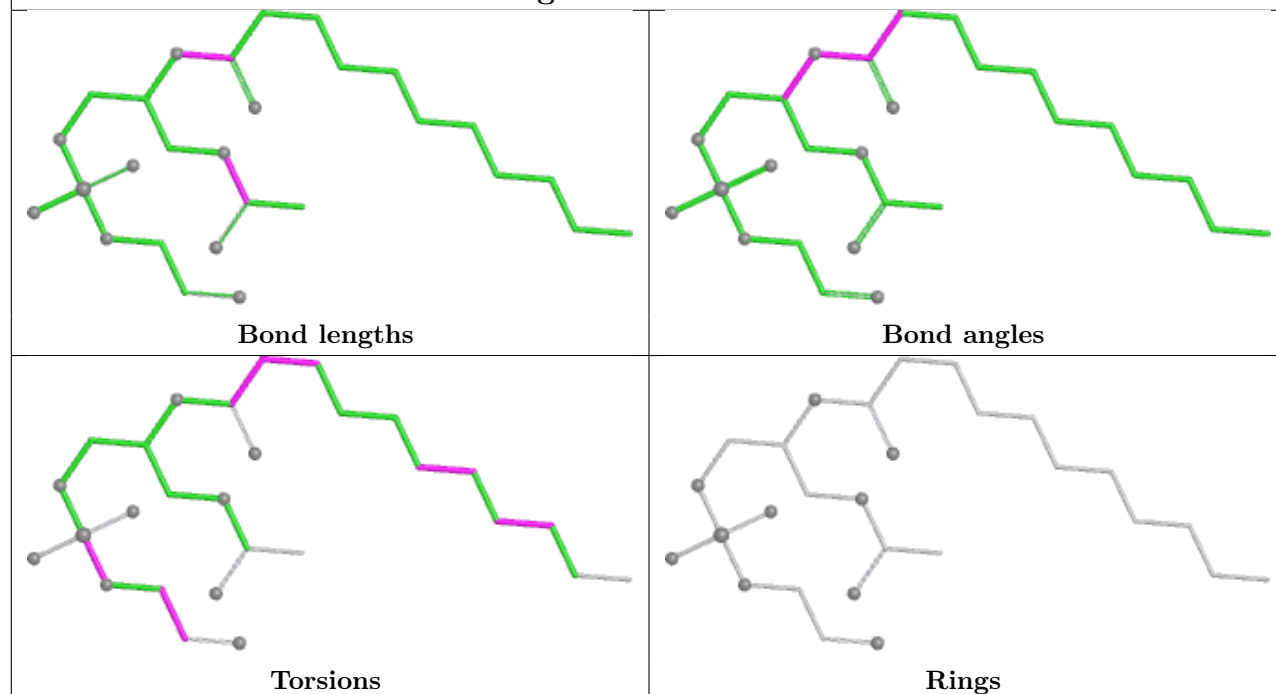


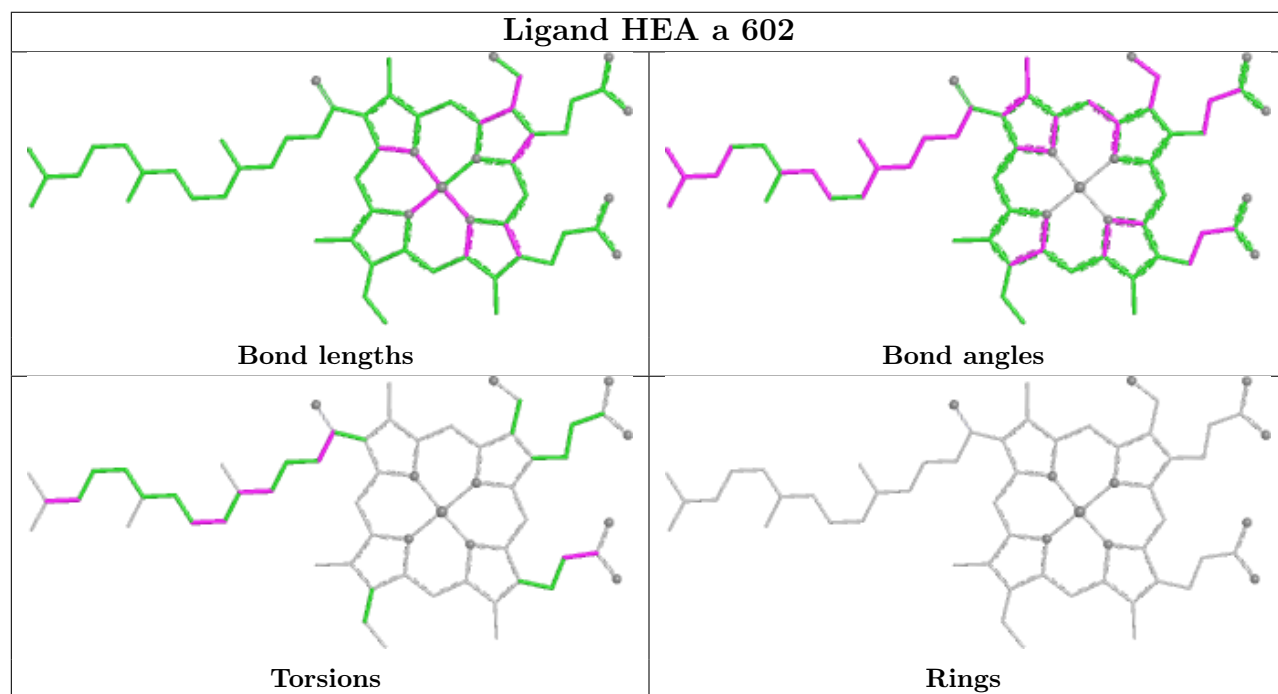
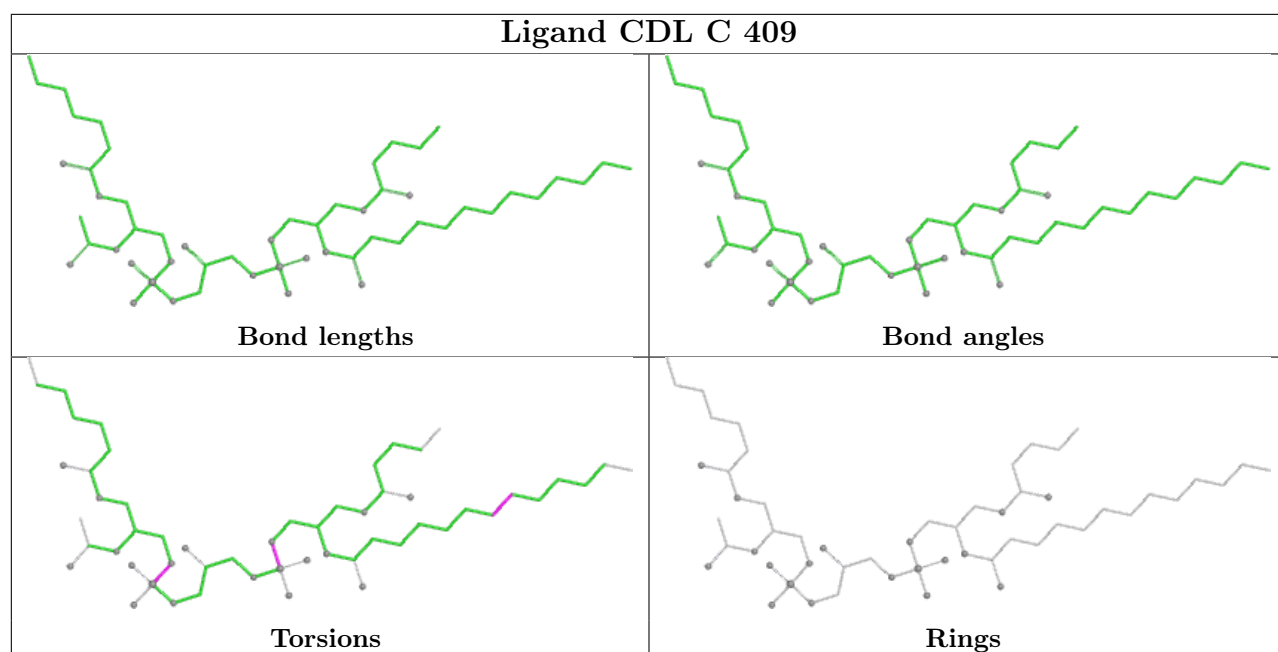


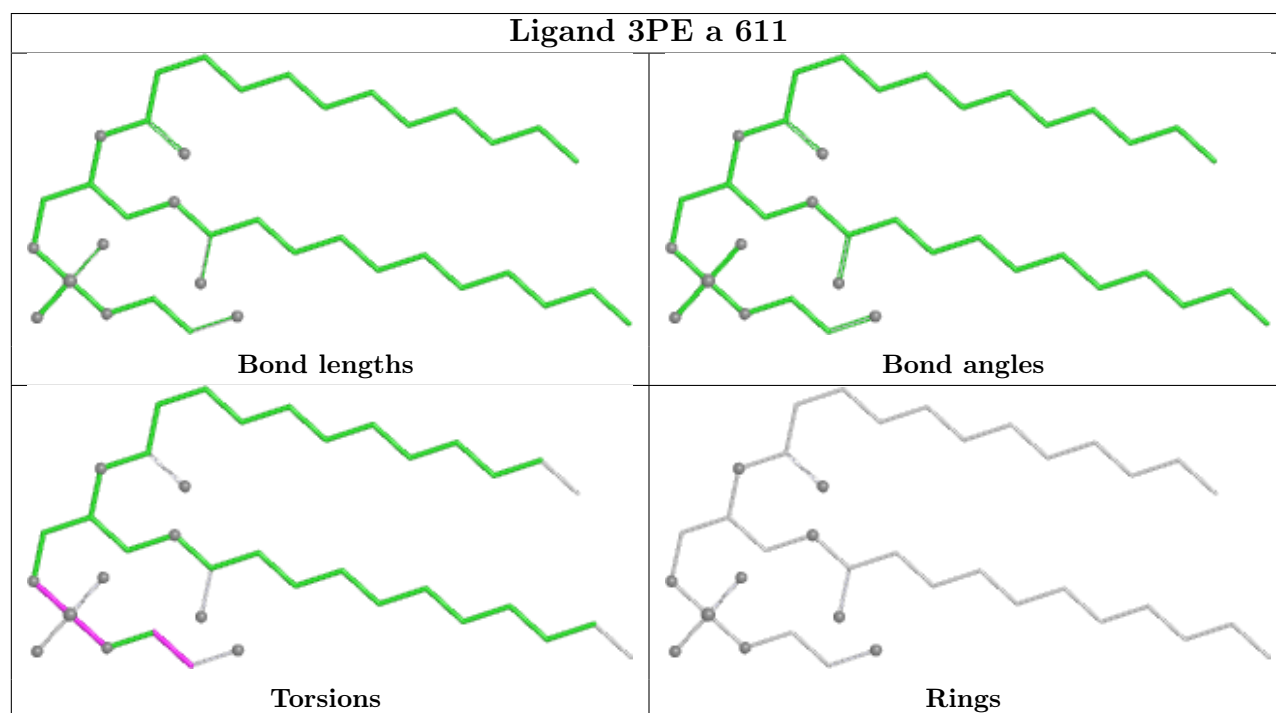
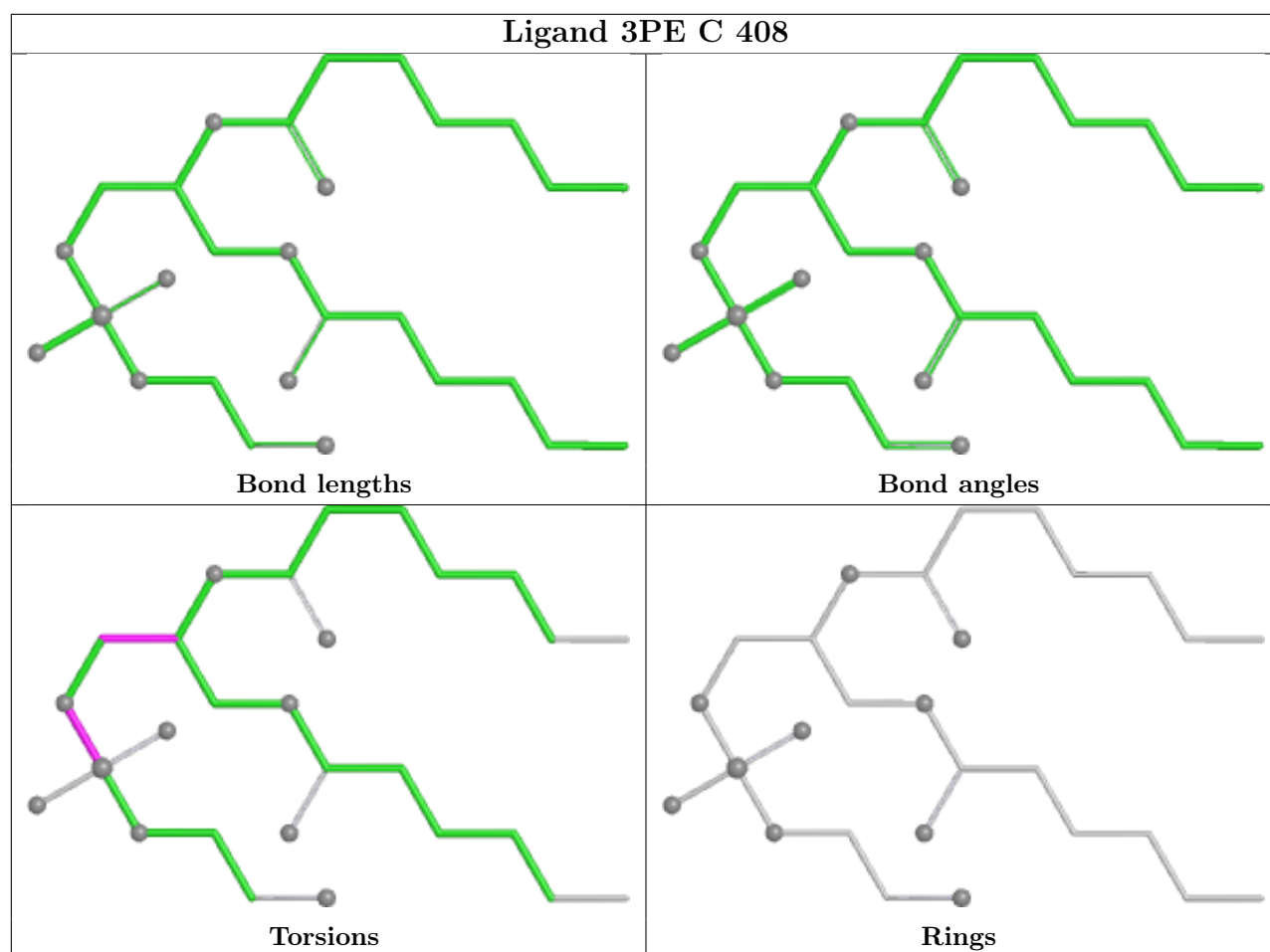
Ligand 3PE O 405

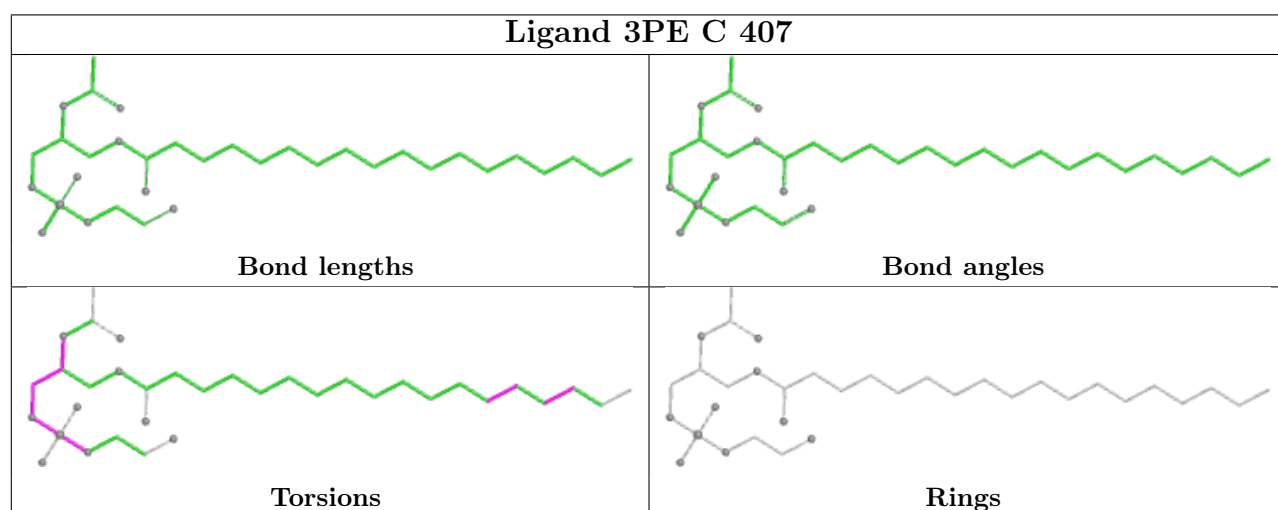
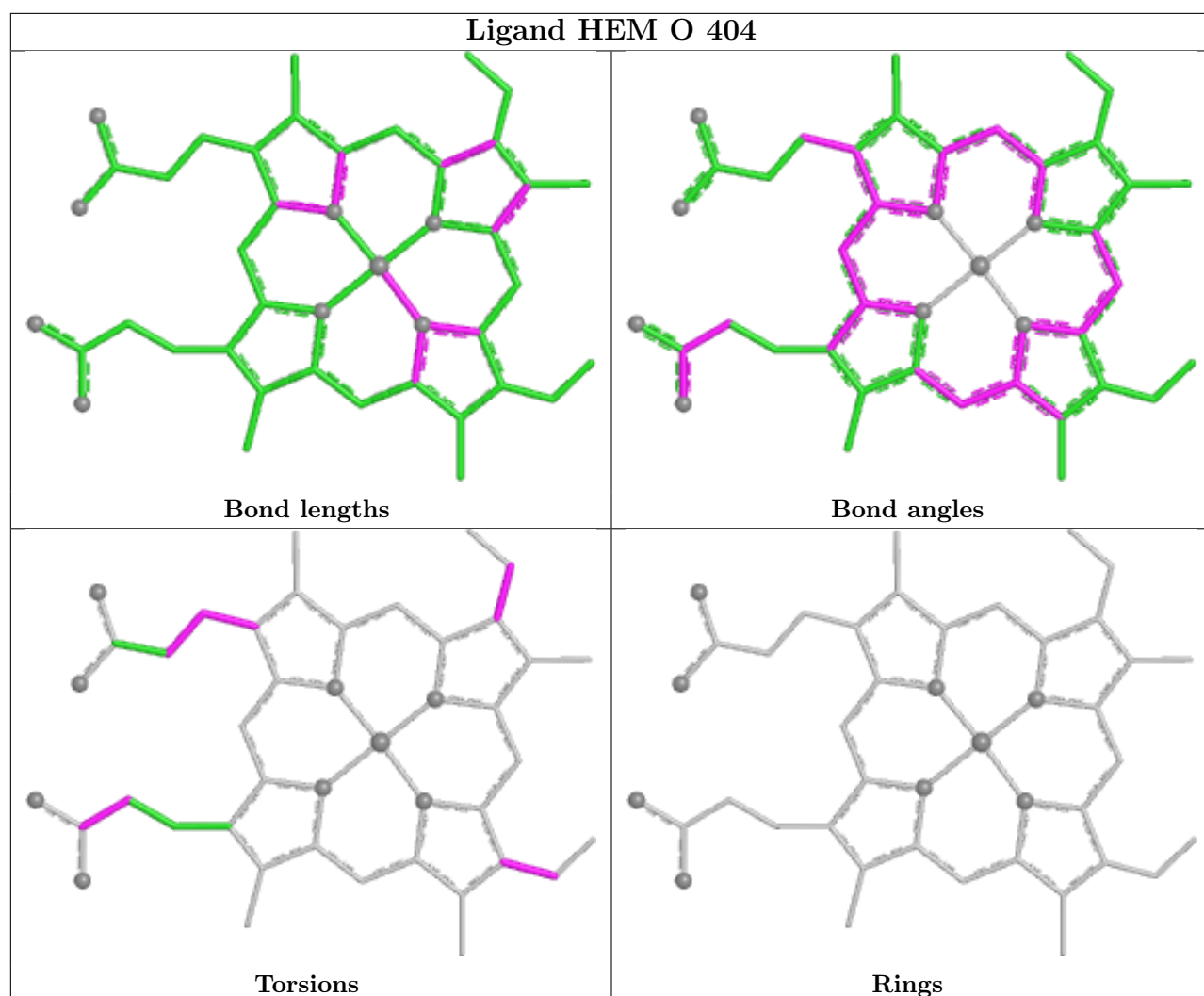


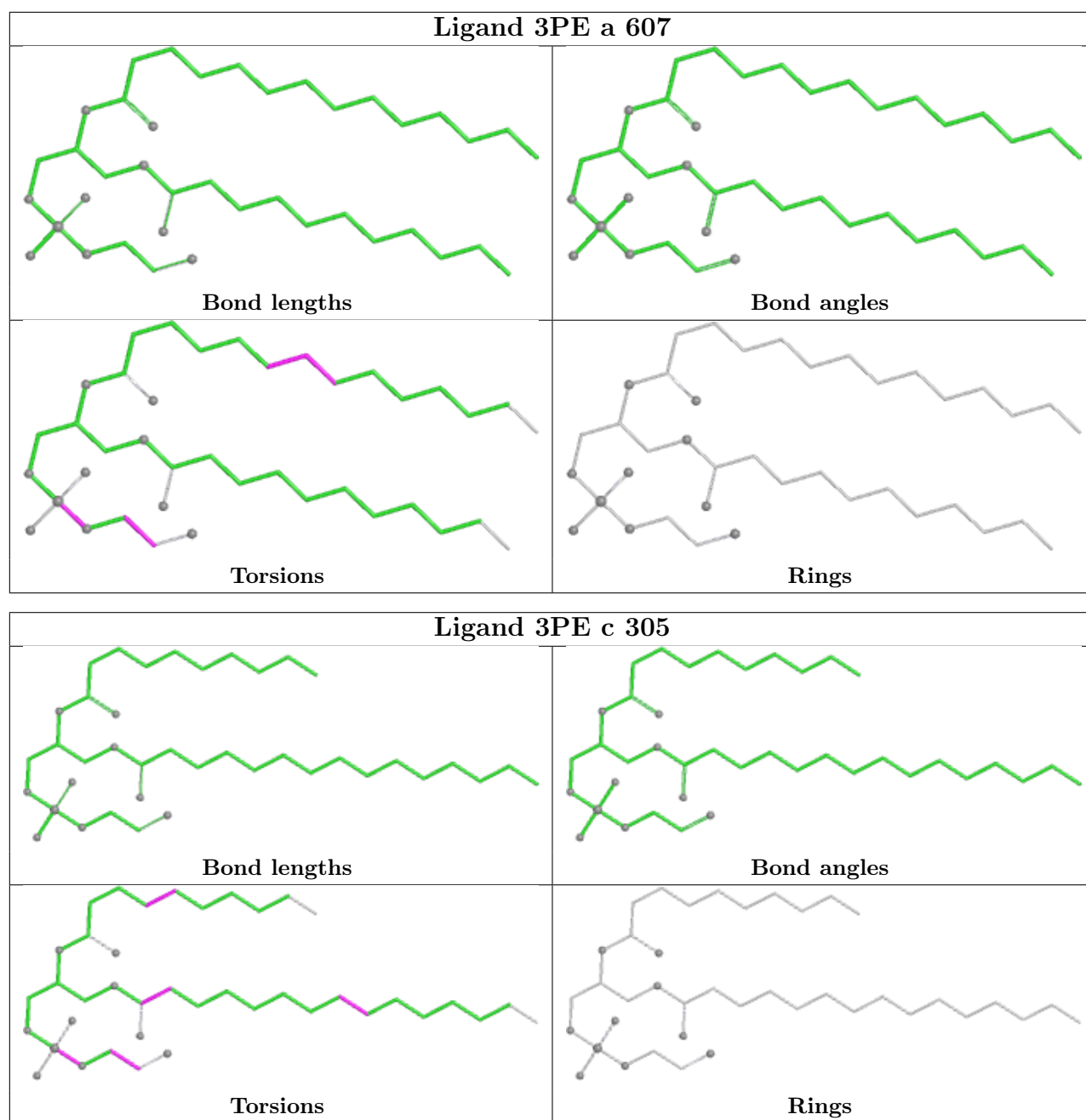
Ligand 3PE P 401

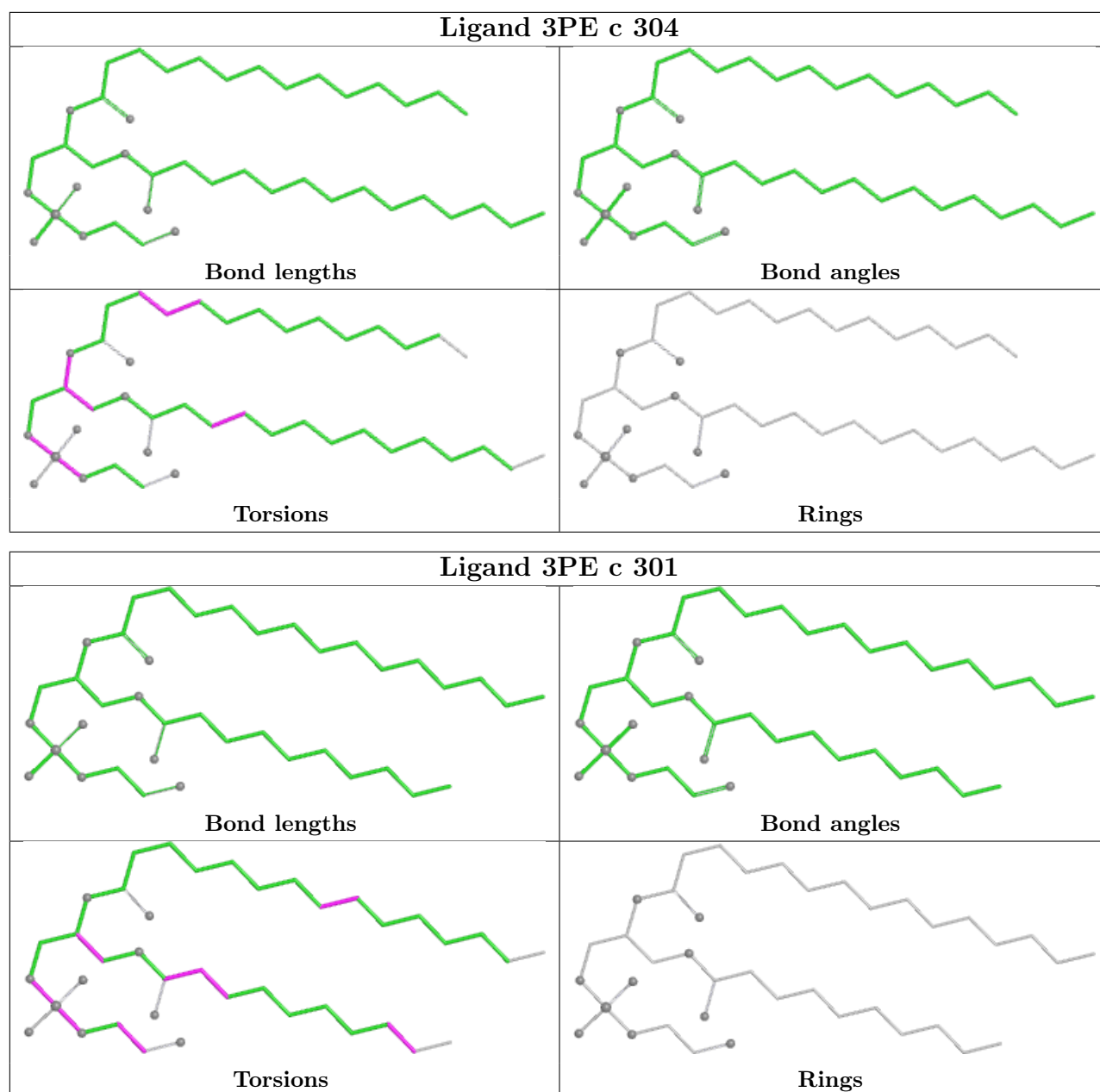




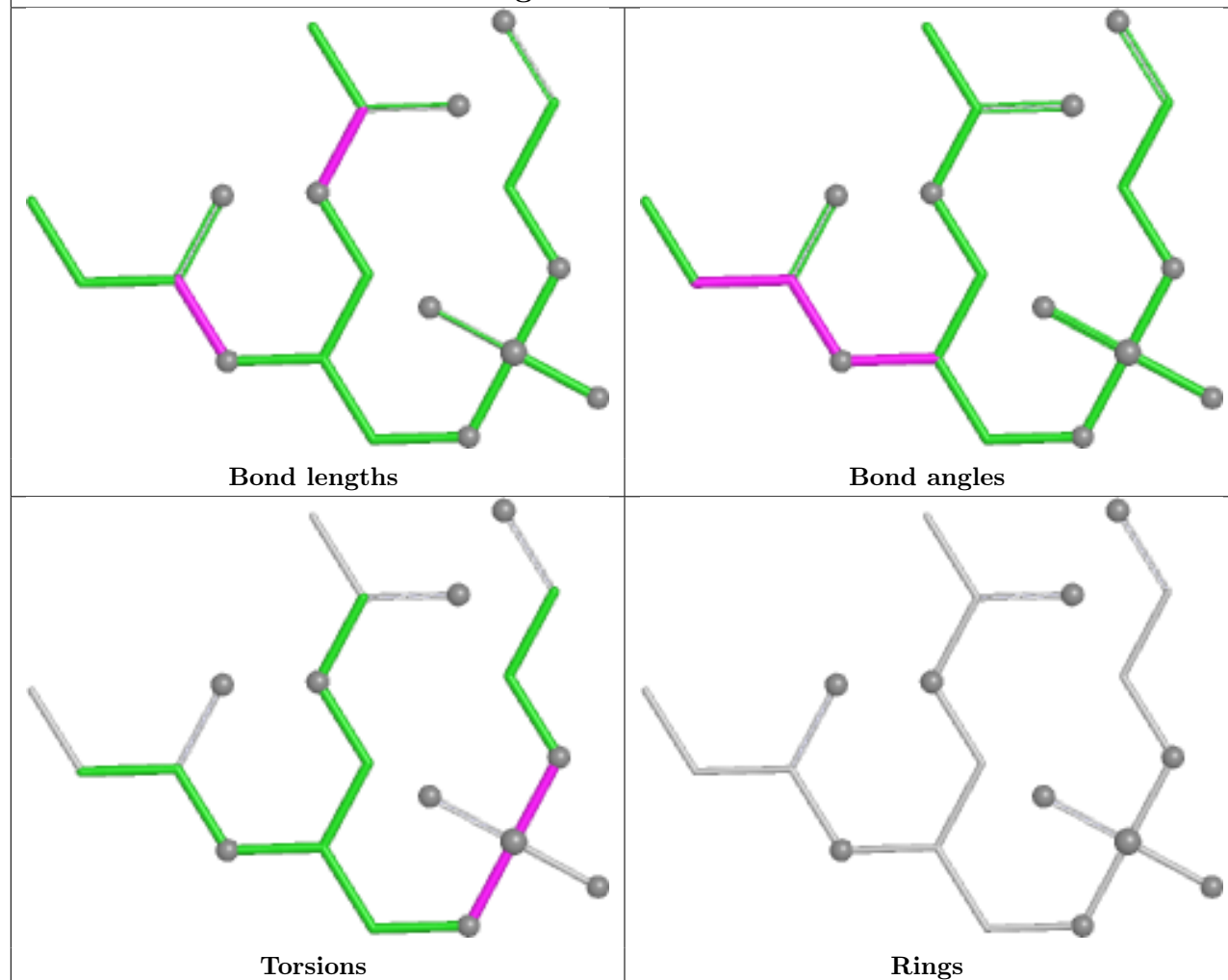




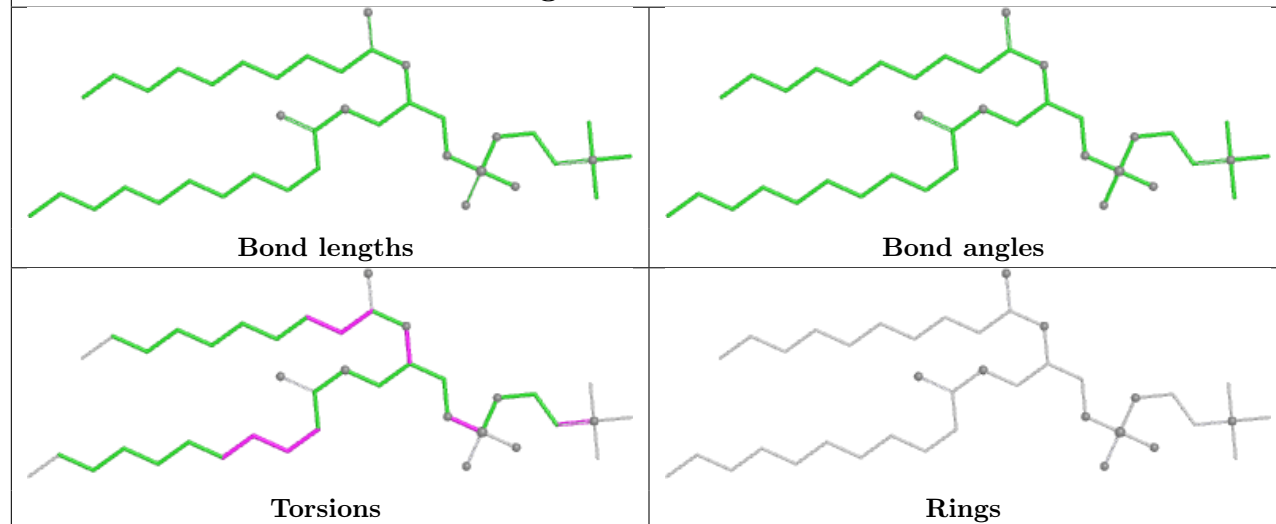


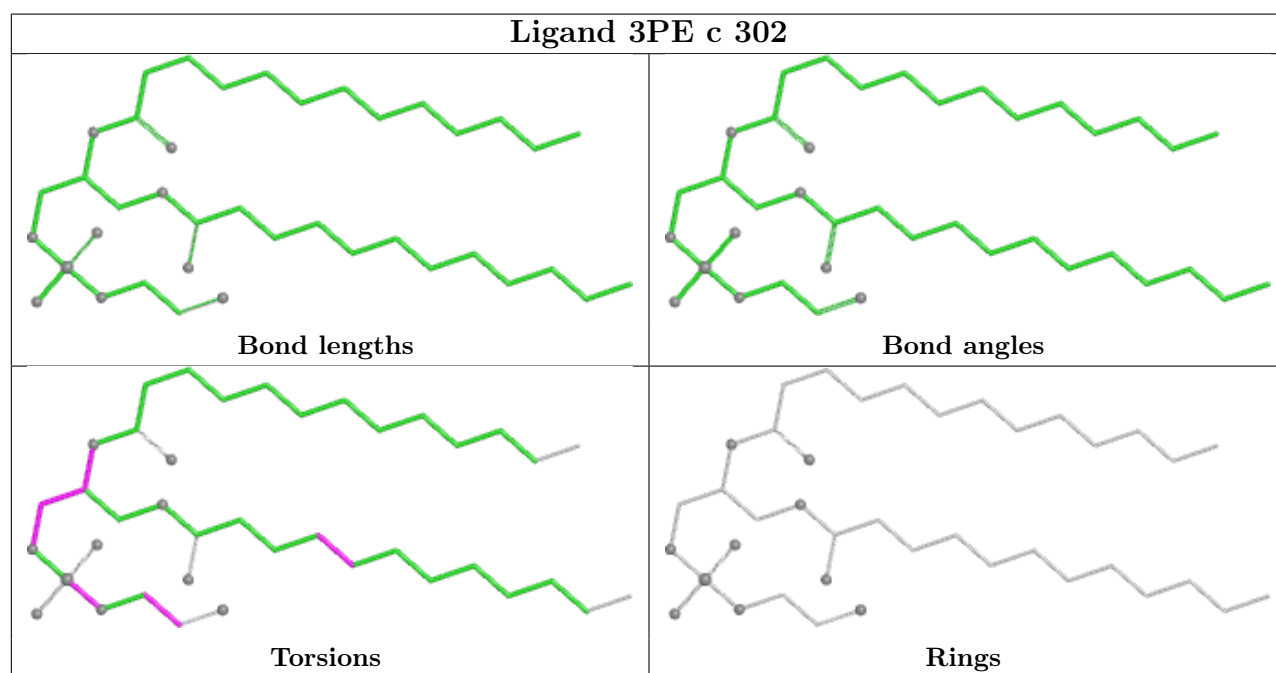
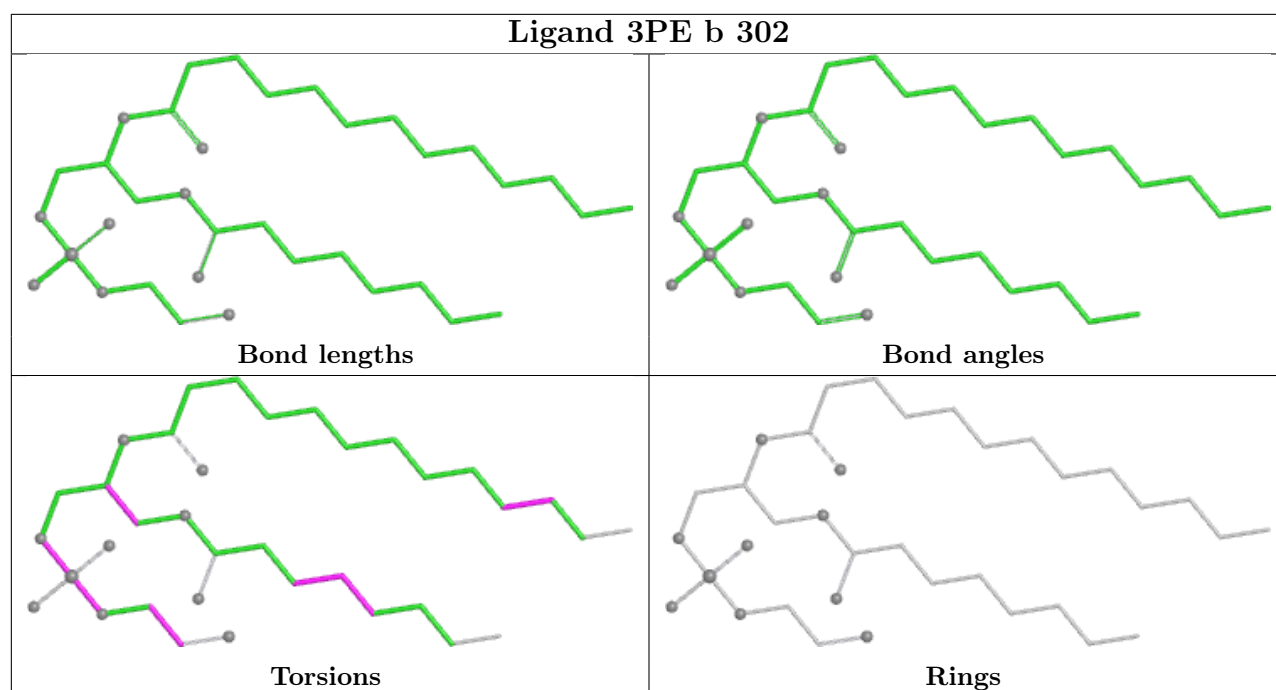


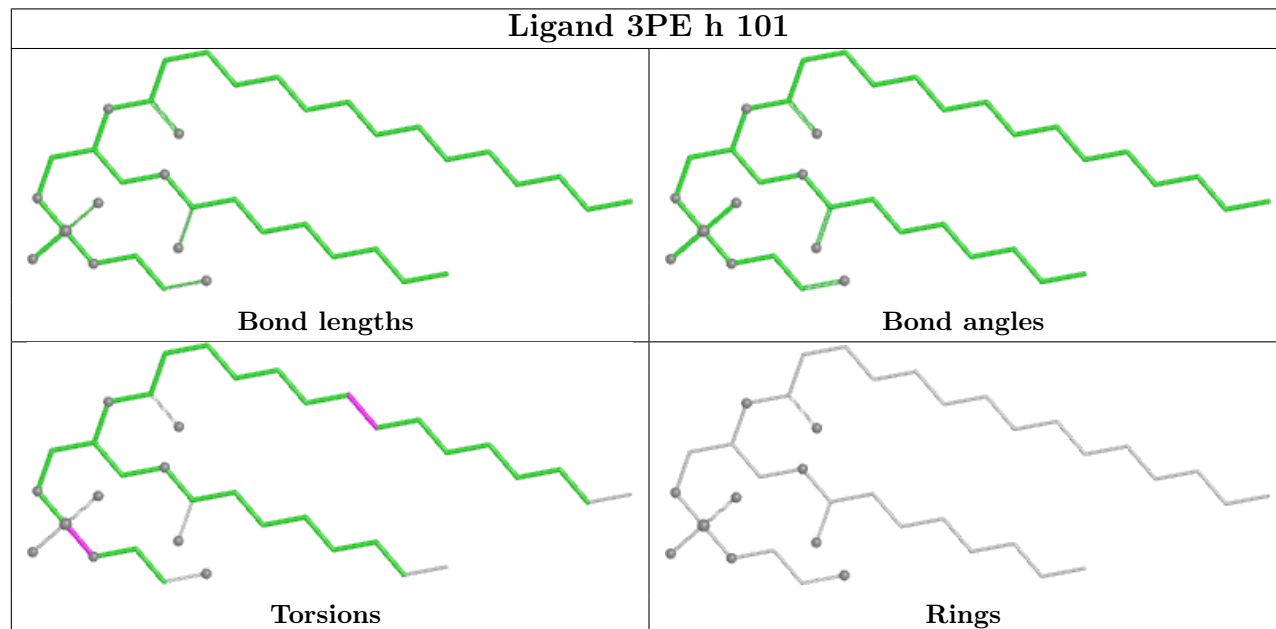
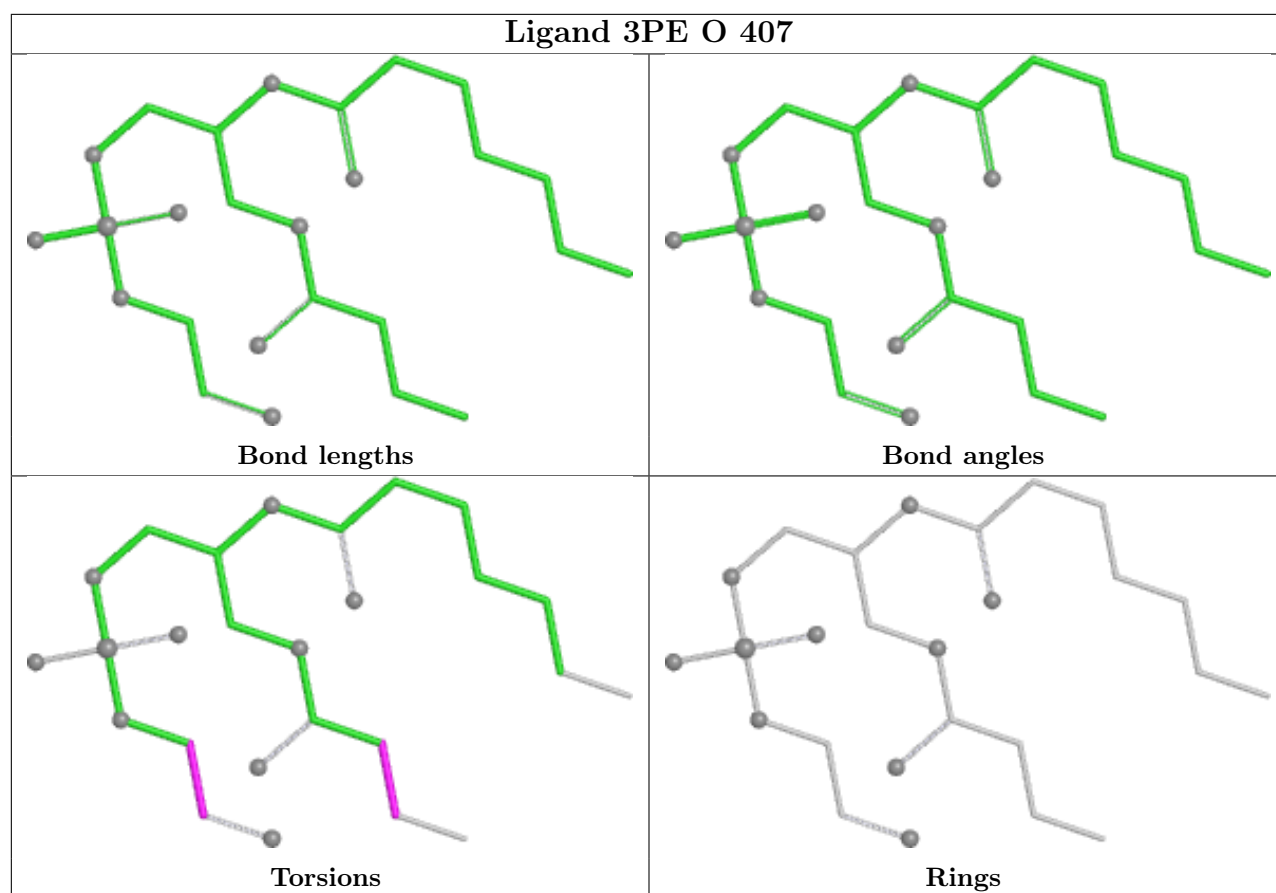
Ligand 3PE G 101

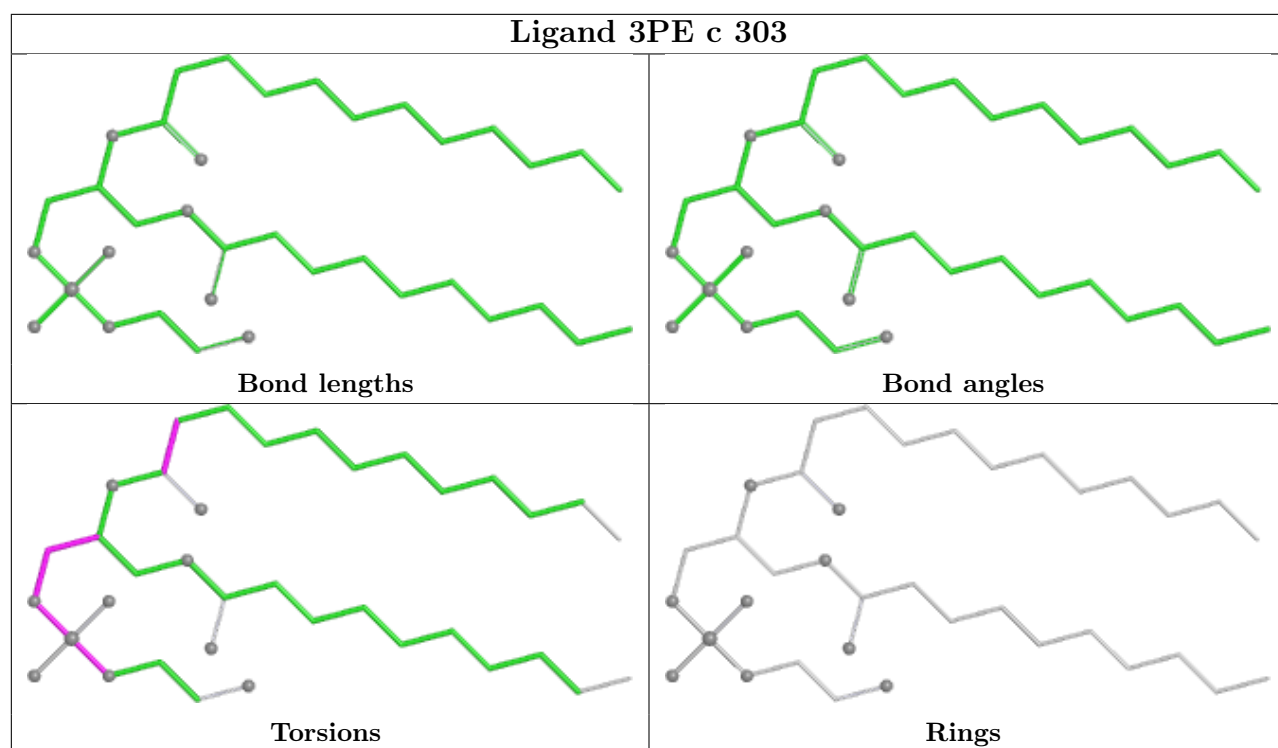


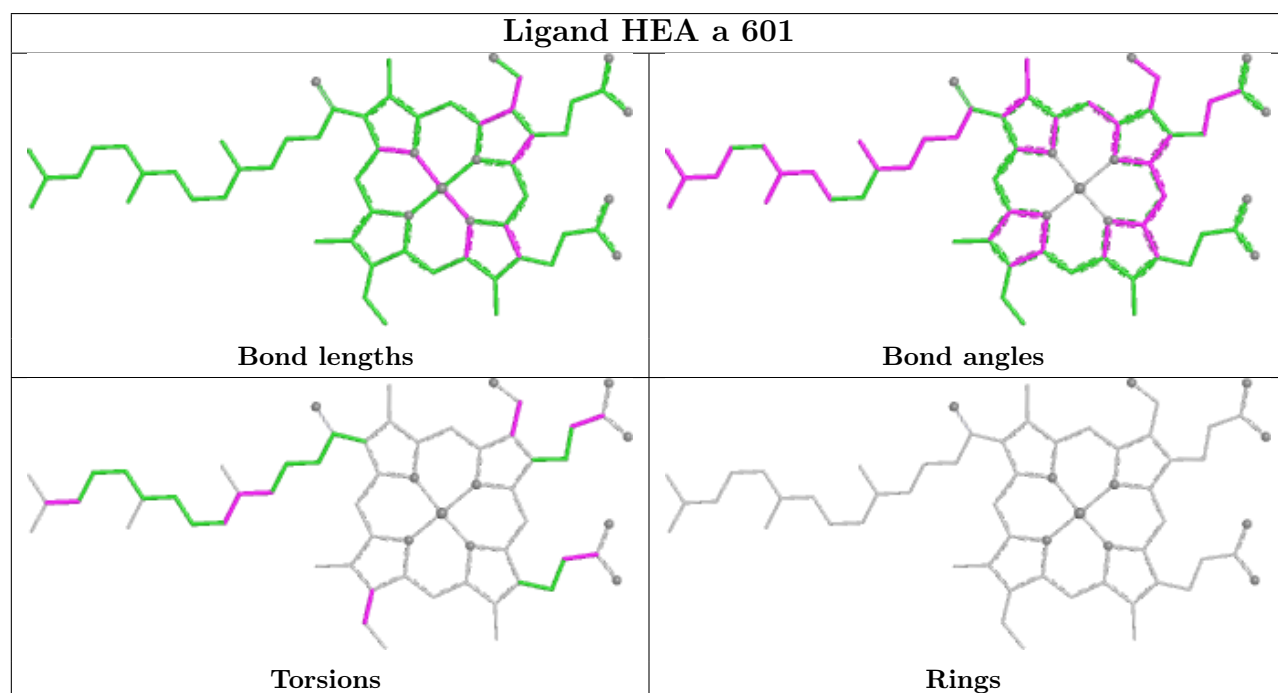
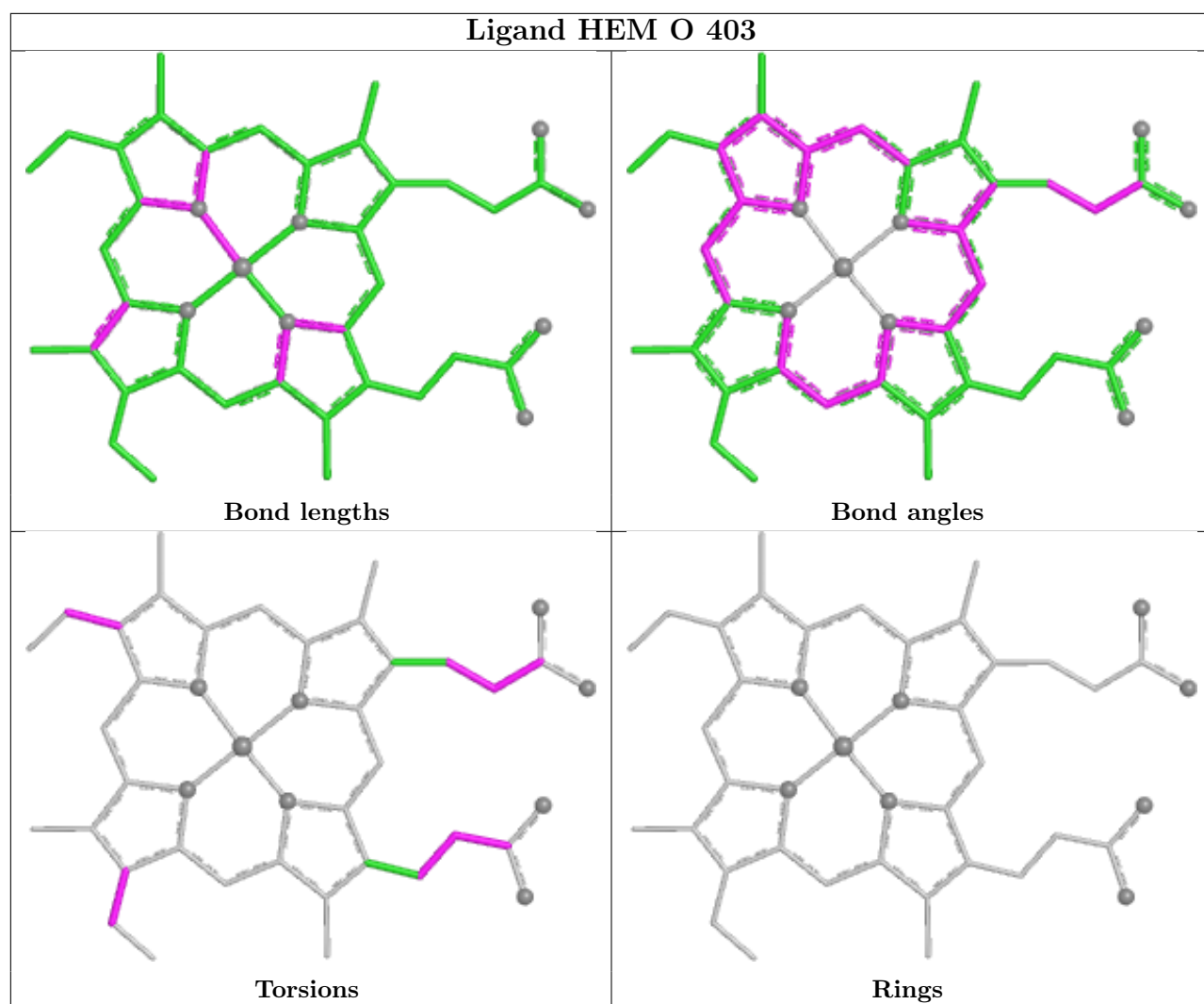
Ligand PC1 a 605

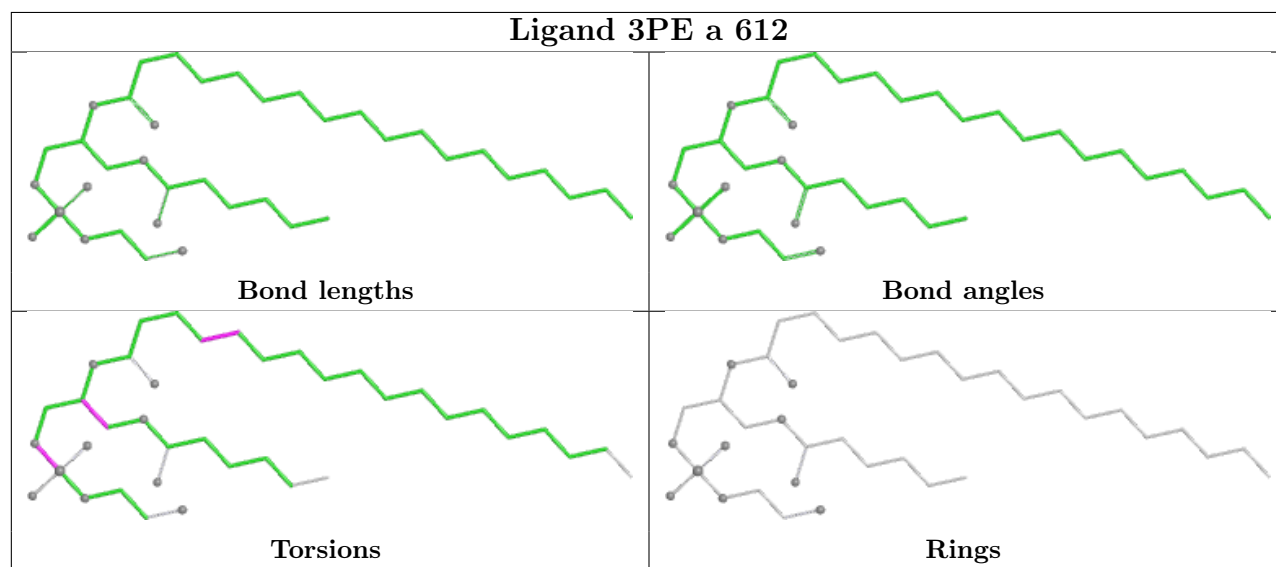
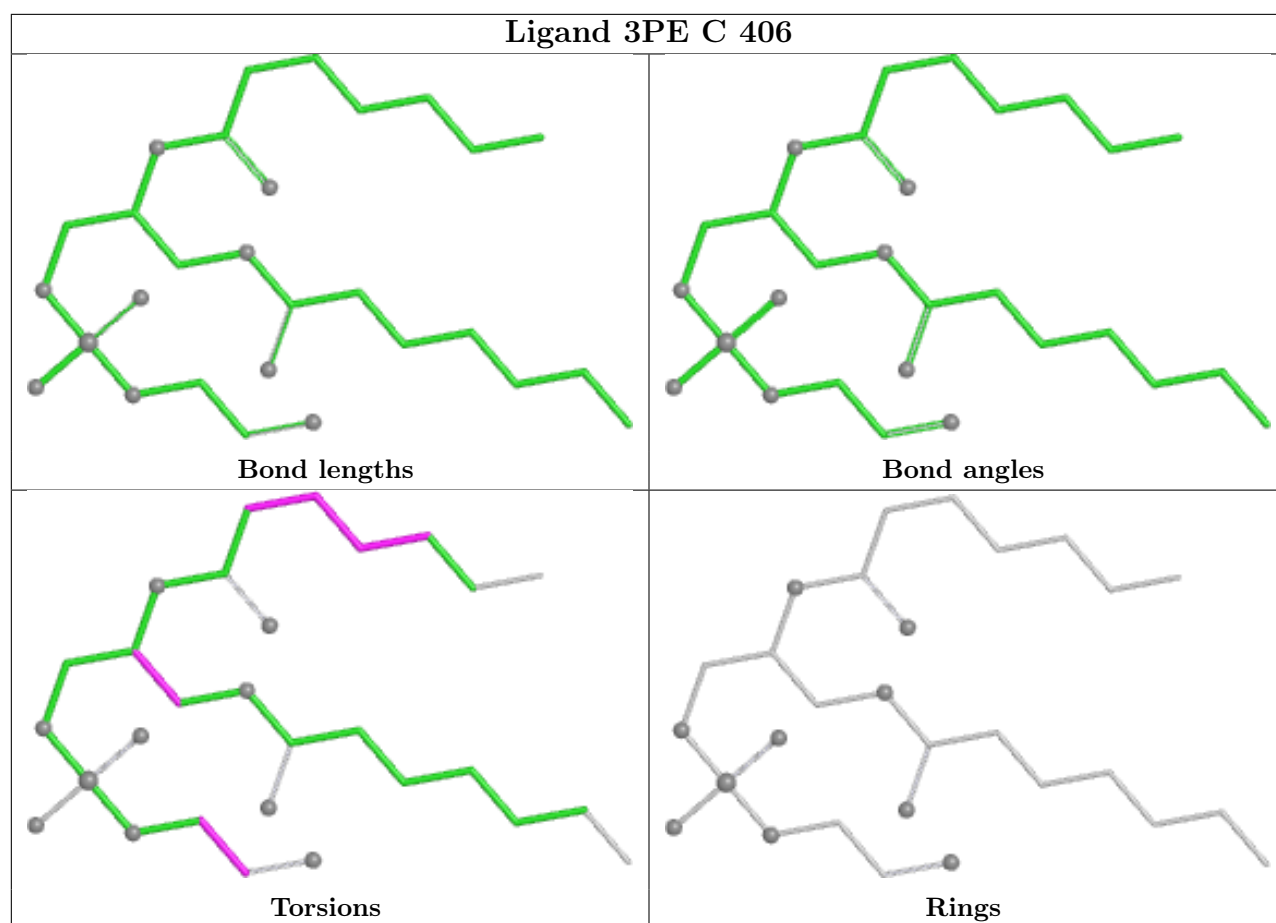


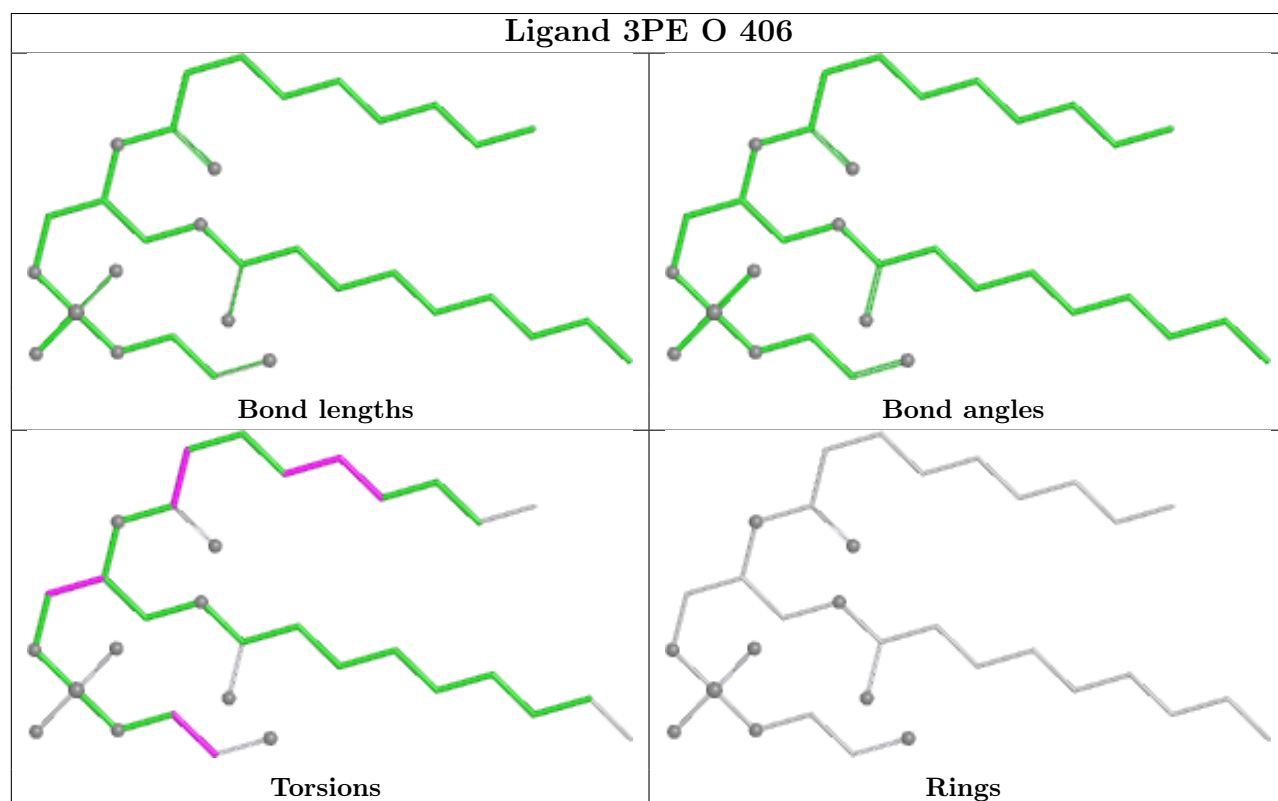
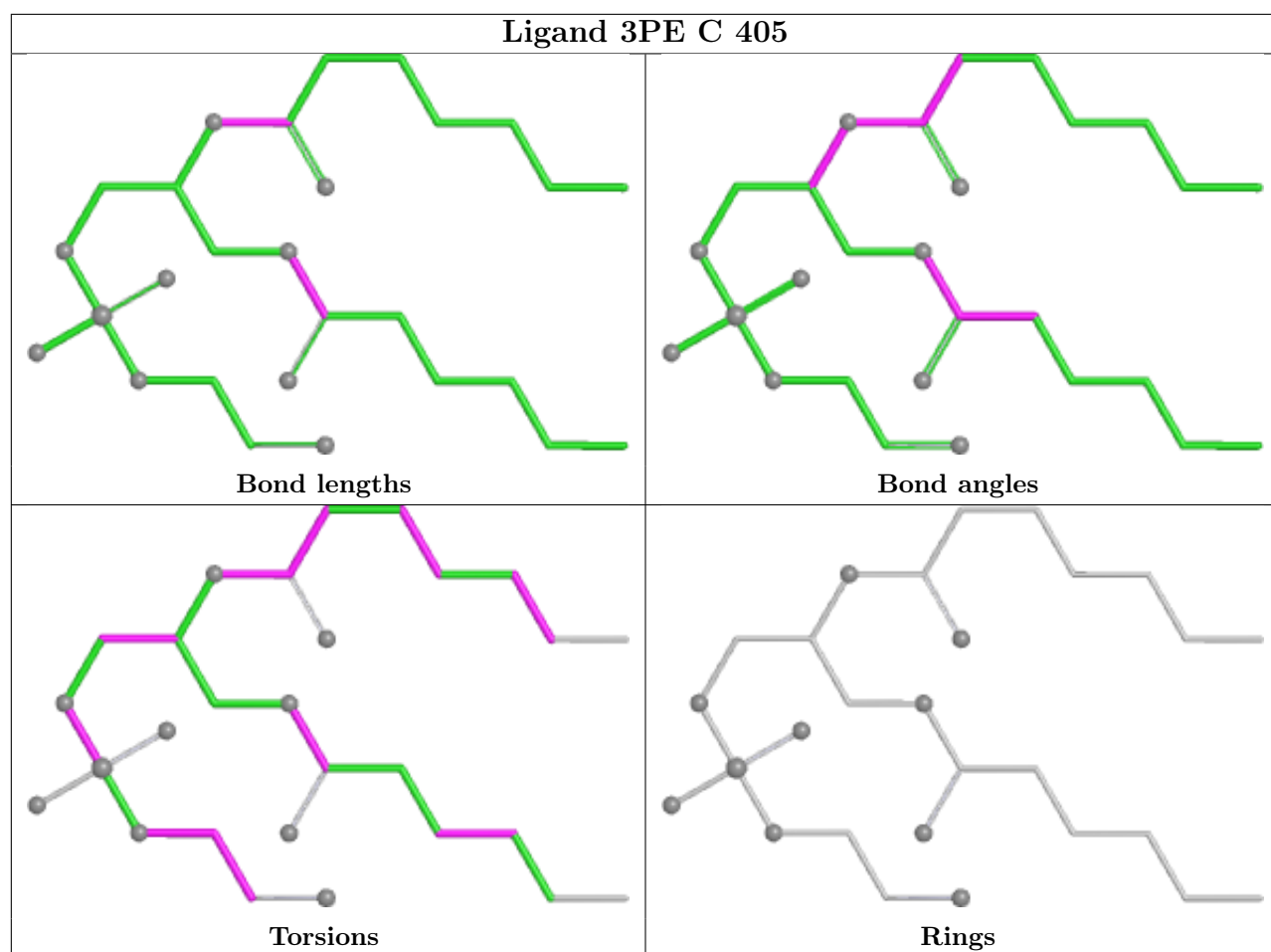


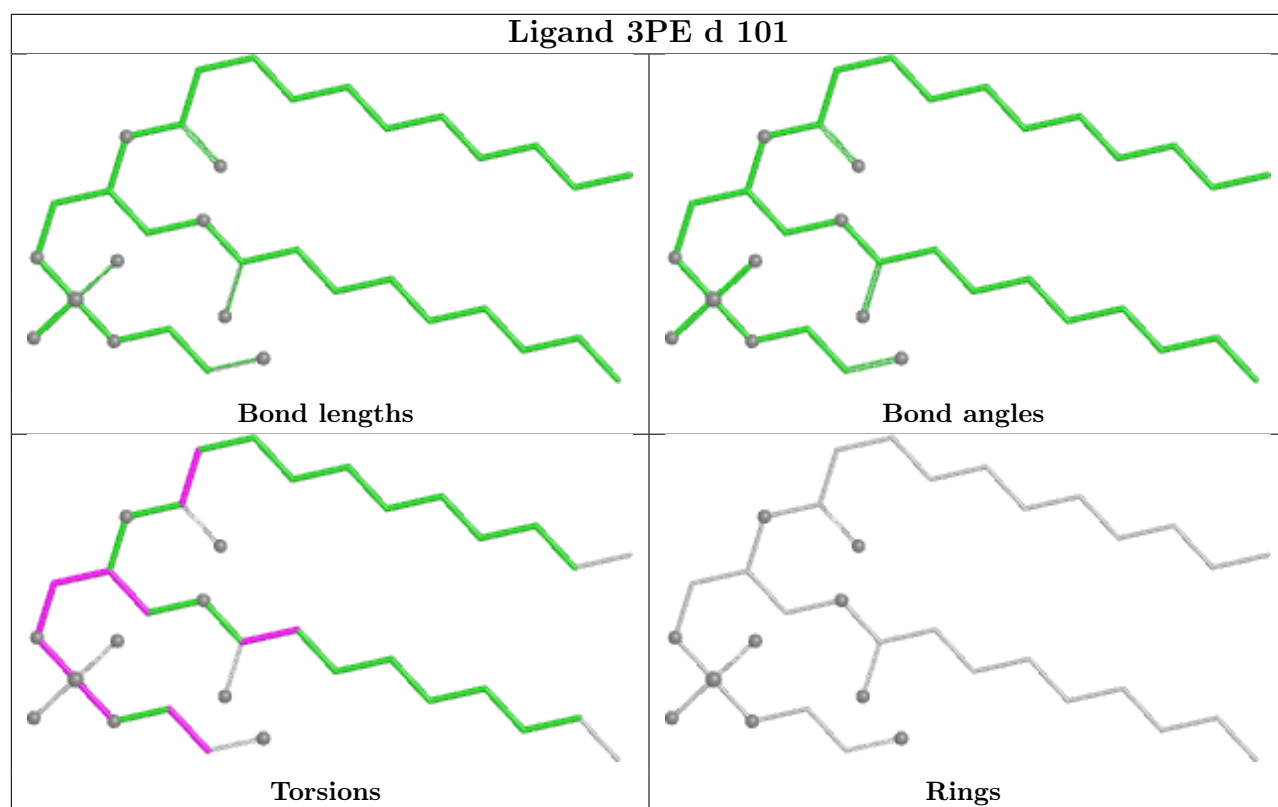


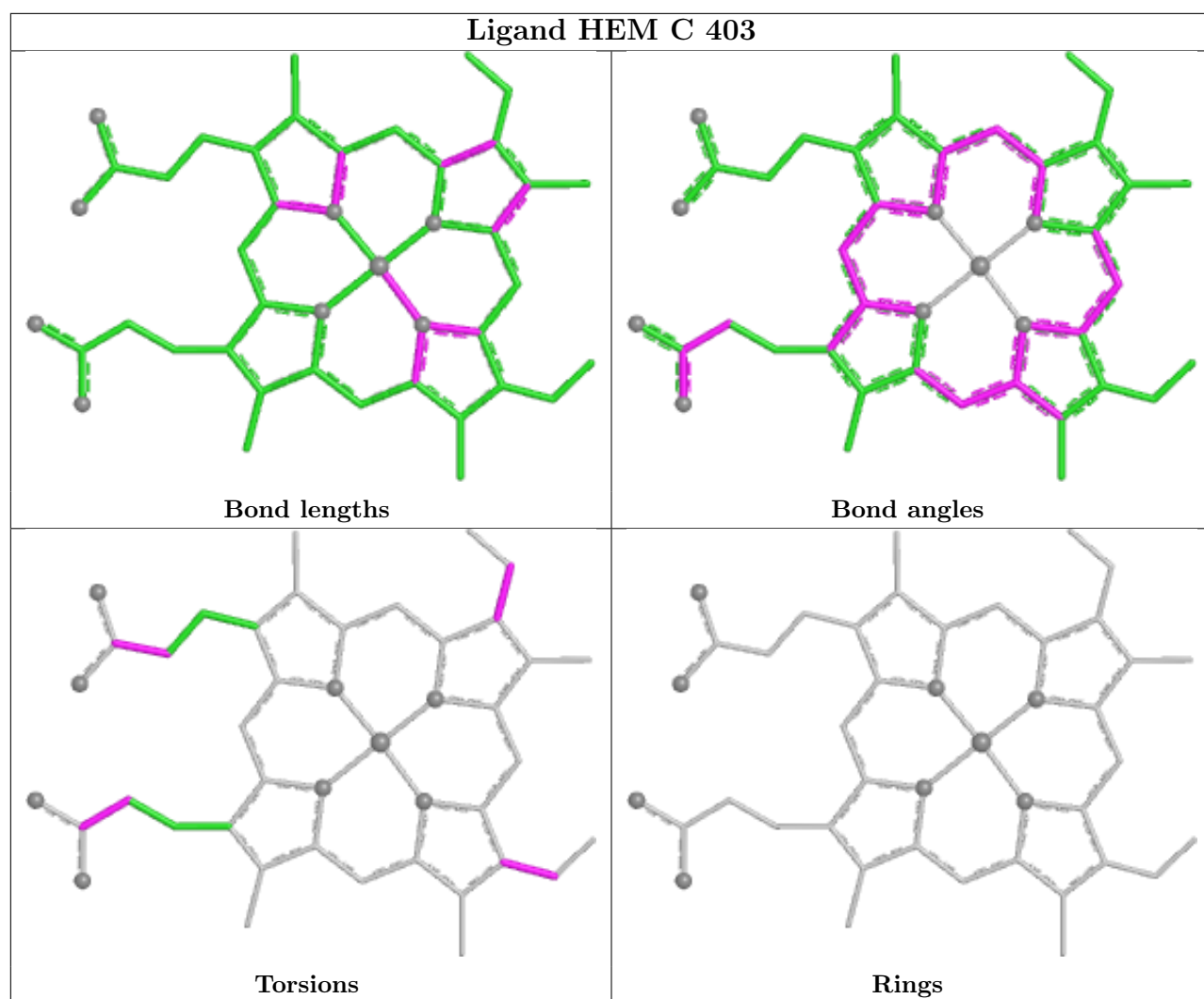












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

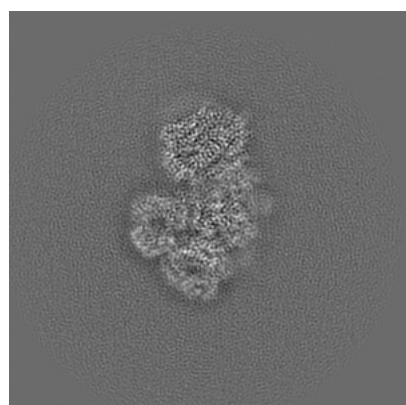
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22448. These allow visual inspection of the internal detail of the map and identification of artifacts.

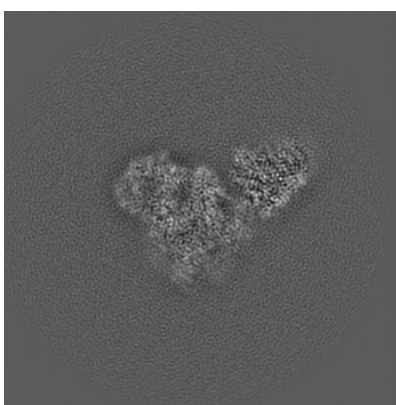
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

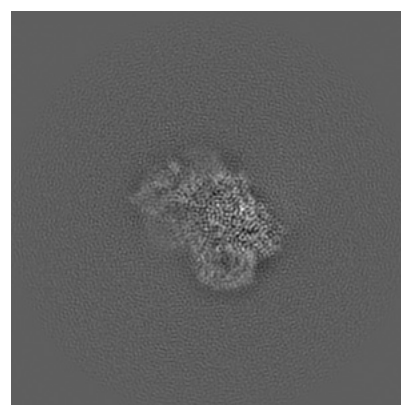
6.1.1 Primary map



X



Y

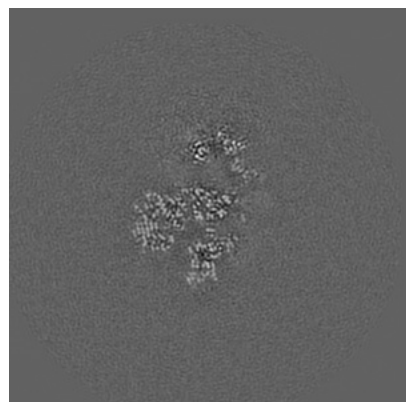


Z

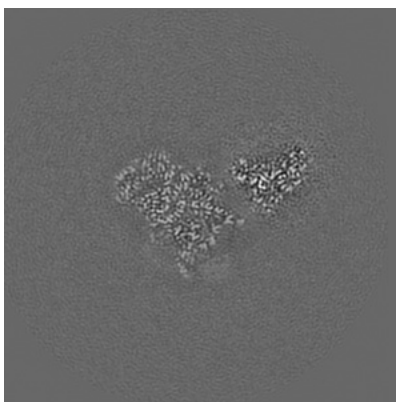
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

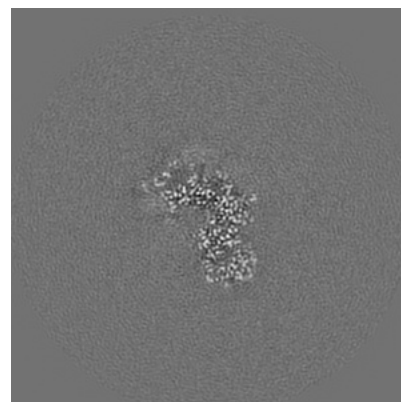
6.2.1 Primary map



X Index: 256



Y Index: 256

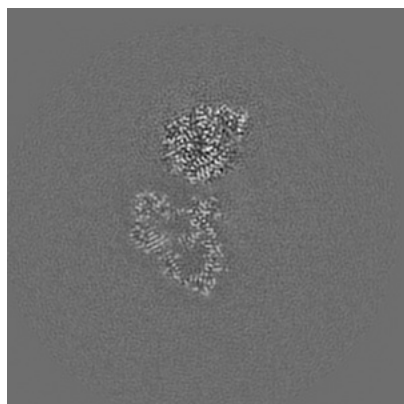


Z Index: 256

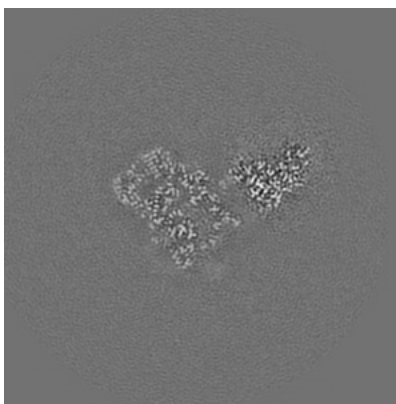
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

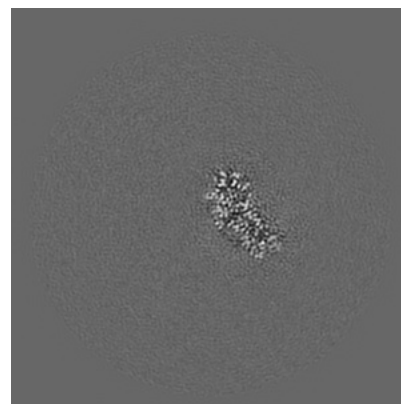
6.3.1 Primary map



X Index: 294



Y Index: 251

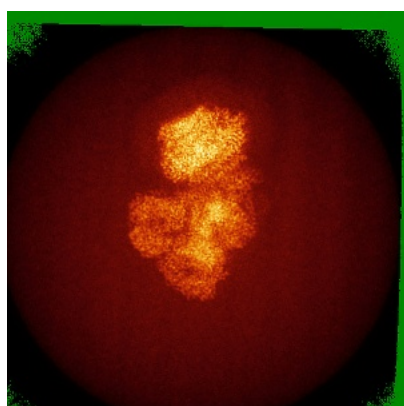


Z Index: 349

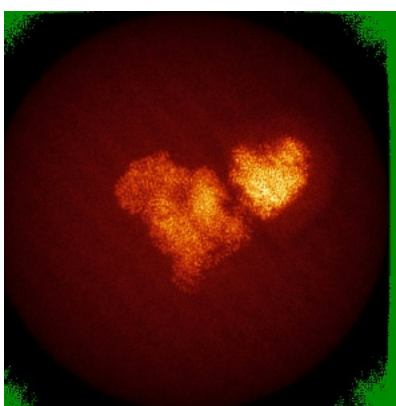
The images above show the largest variance slices of the map in three orthogonal directions.

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

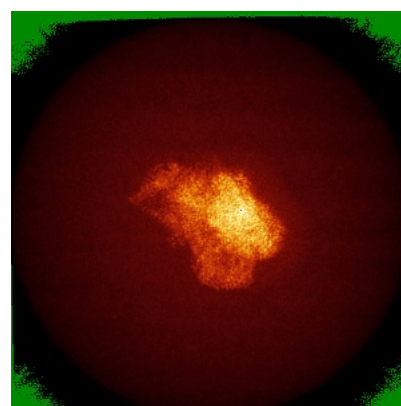
6.4.1 Primary map



X



Y

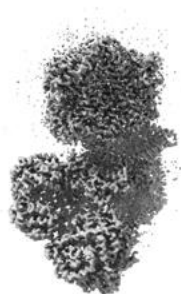


Z

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



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 6.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

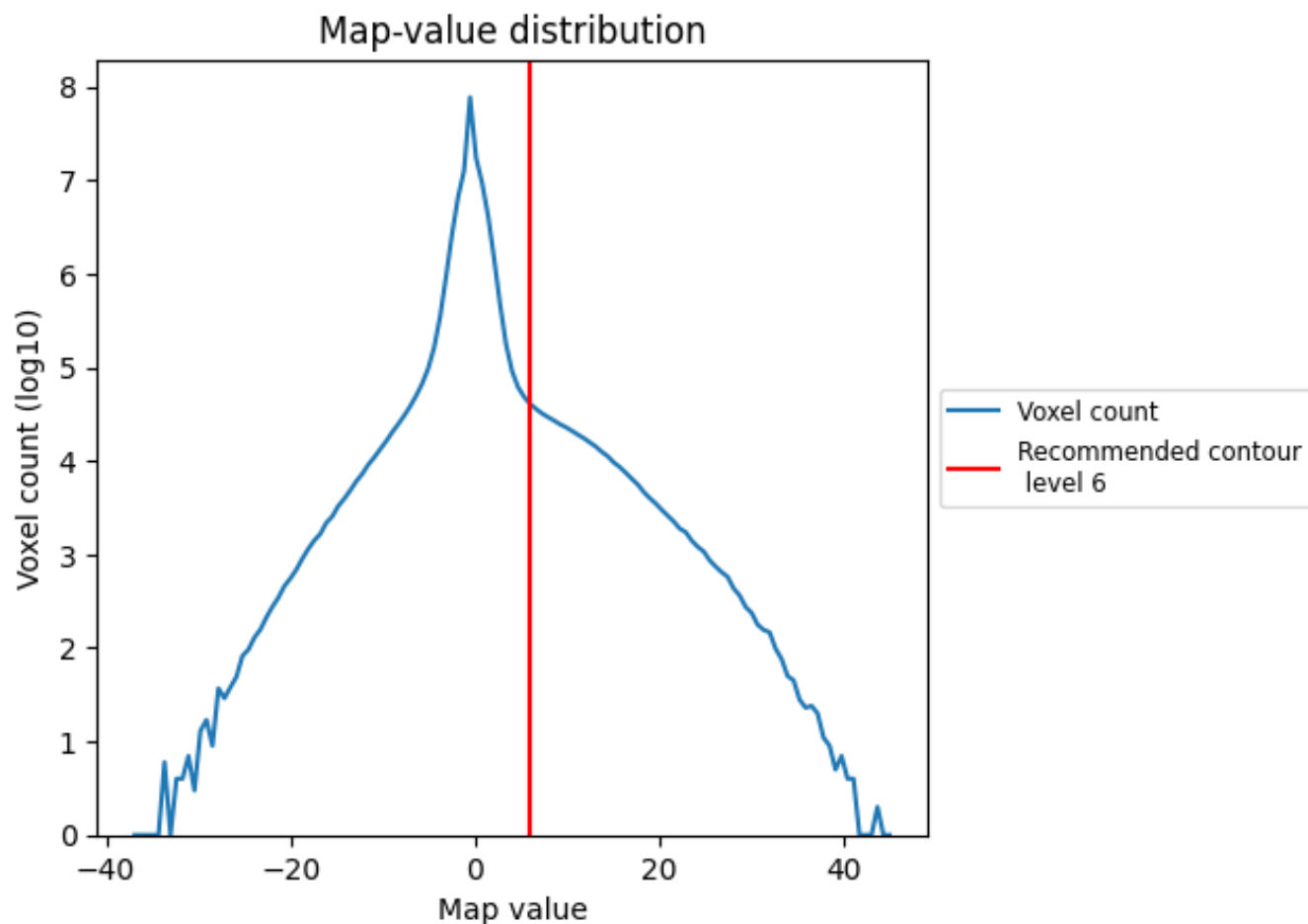
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

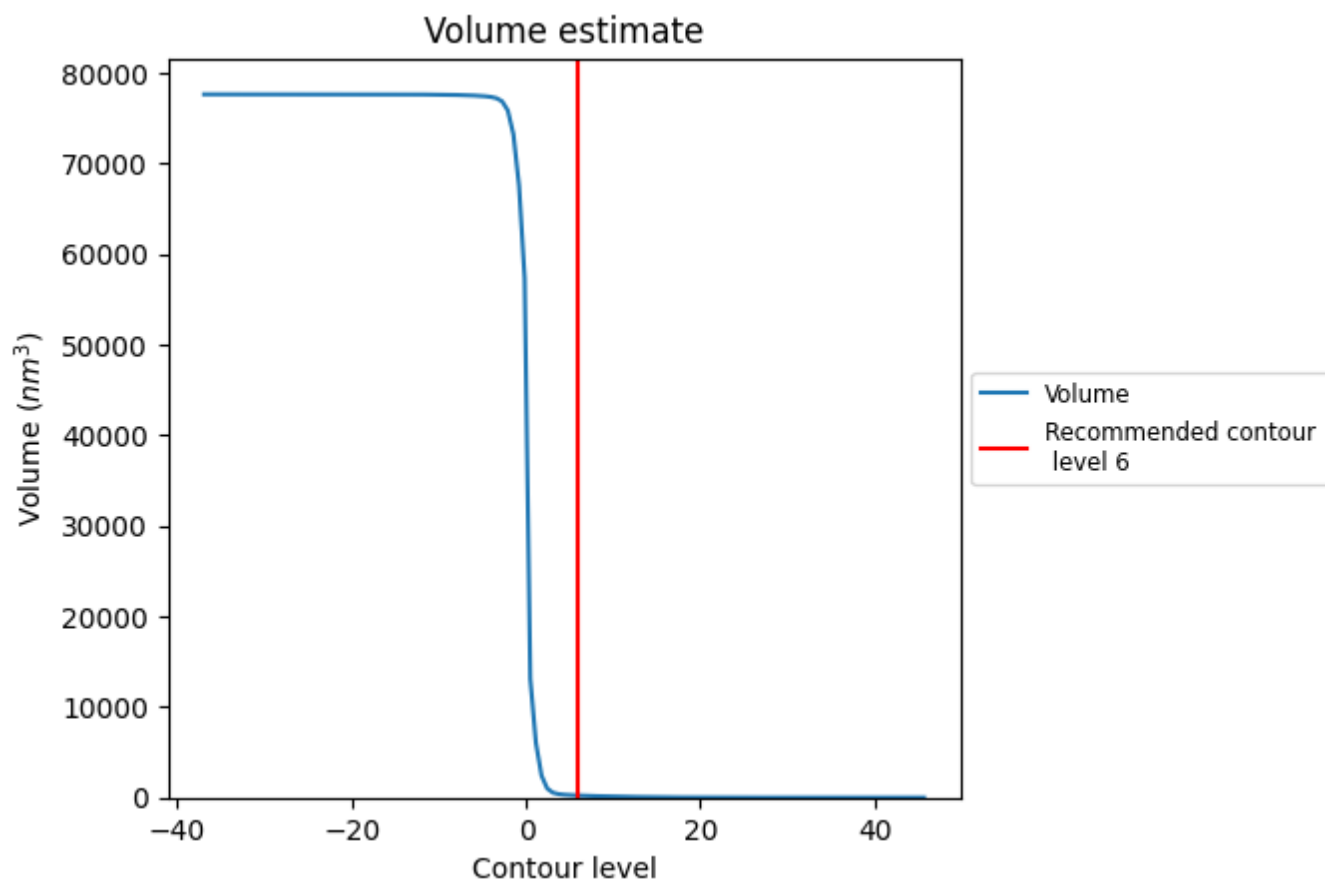
This section contains the results of statistical analysis of the map.

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.

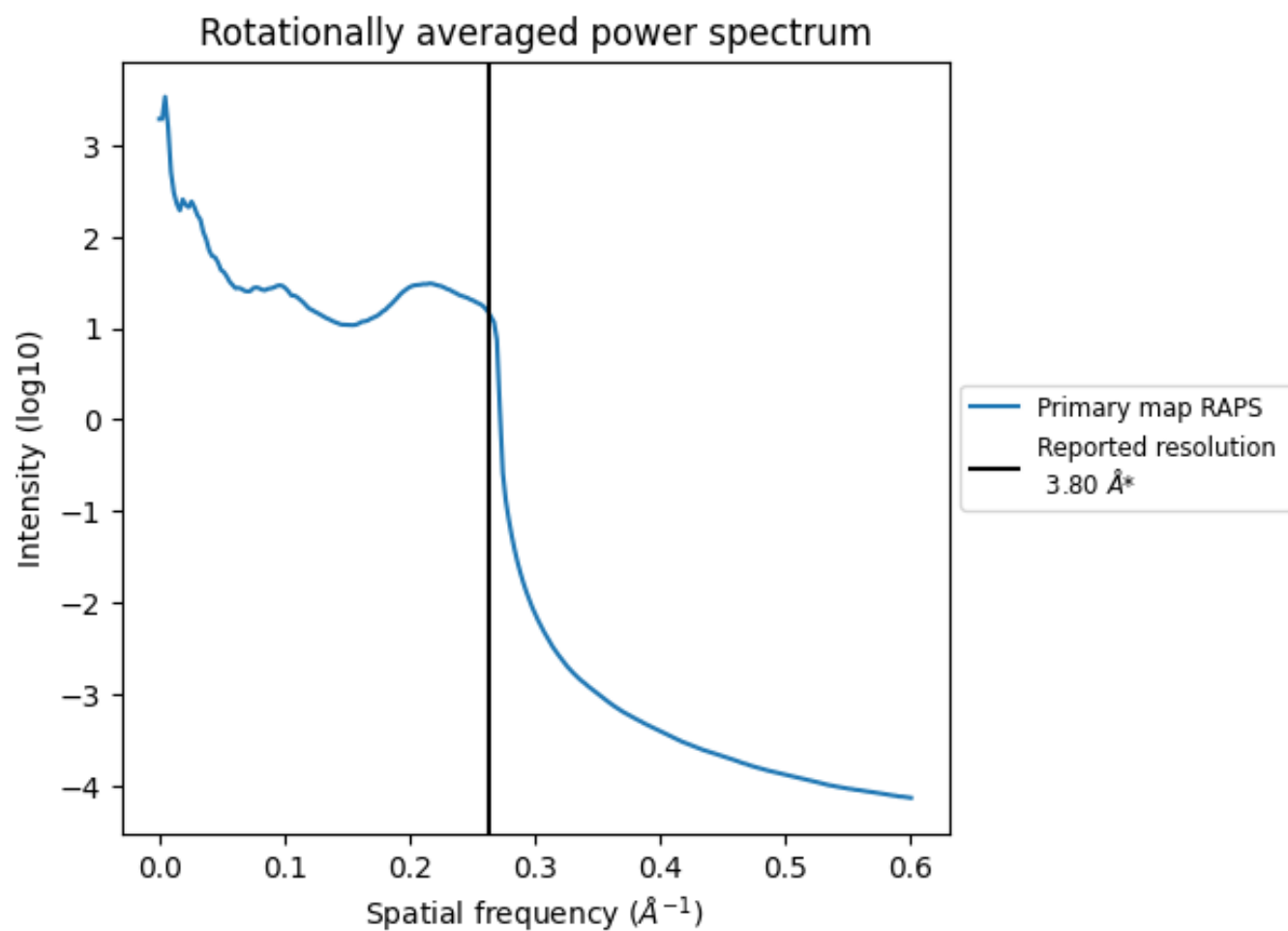
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 228 nm³; this corresponds to an approximate mass of 206 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 0.263 Å⁻¹

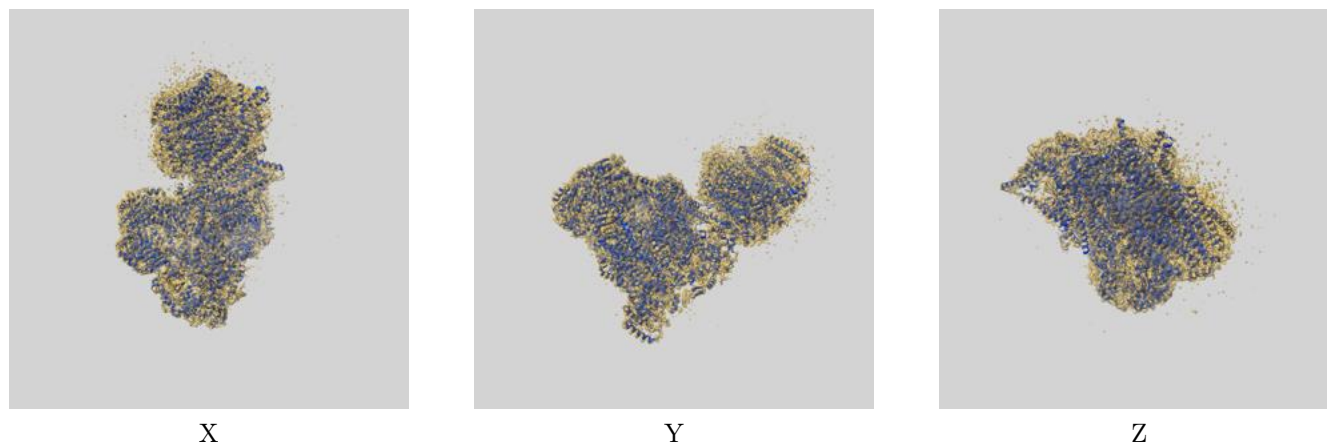
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

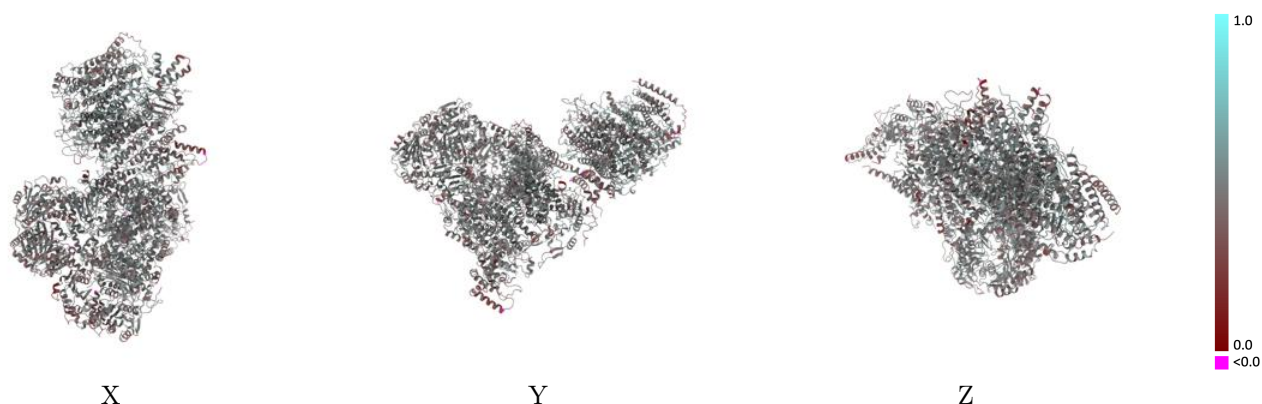
This section contains information regarding the fit between EMDB map EMD-22448 and PDB model 7JRP. Per-residue inclusion information can be found in section [3](#) on page [16](#).

9.1 Map-model overlay [i](#)



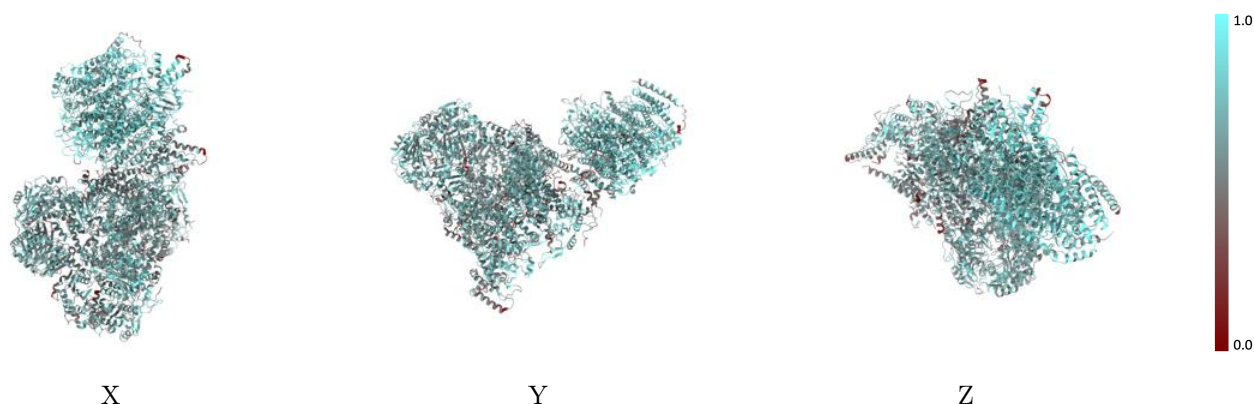
The images above show the 3D surface view of the map at the recommended contour level 6.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



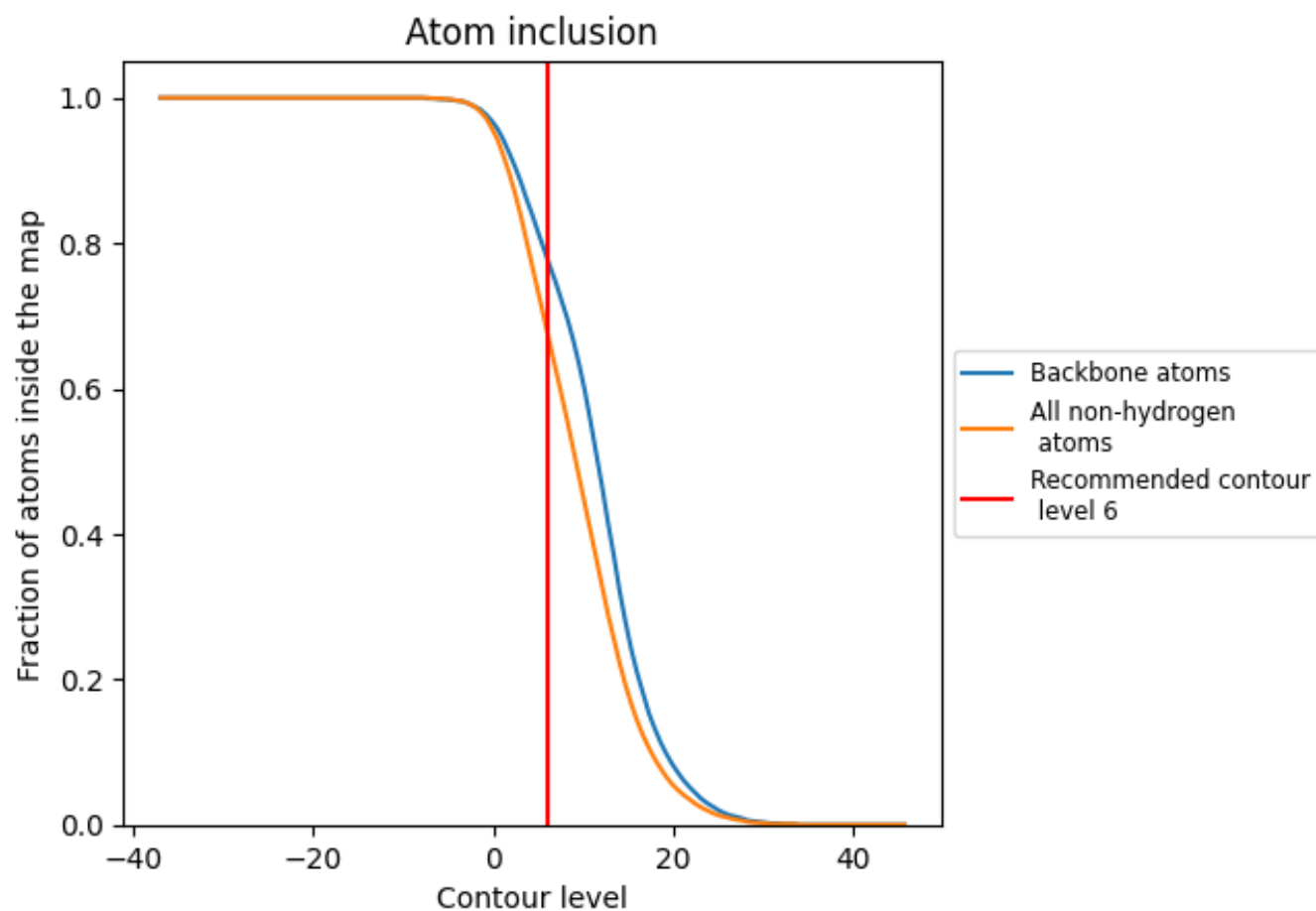
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (6).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 68% 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 (6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6790	 0.4630
A	 0.6750	 0.4630
B	 0.6150	 0.4340
C	 0.6710	 0.4840
D	 0.6920	 0.4650
E	 0.6020	 0.4600
F	 0.6670	 0.4810
G	 0.5470	 0.4320
H	 0.4820	 0.3410
J	 0.5520	 0.4310
K	 0.4720	 0.3930
M	 0.6630	 0.4590
N	 0.6200	 0.4380
O	 0.6980	 0.4870
P	 0.6670	 0.4690
Q	 0.6000	 0.4640
R	 0.6690	 0.4740
S	 0.5660	 0.4600
T	 0.5000	 0.3520
V	 0.5510	 0.4110
W	 0.3480	 0.3550
a	 0.7970	 0.4960
b	 0.7670	 0.4900
c	 0.7920	 0.4890
d	 0.7210	 0.4550
e	 0.7490	 0.4440
f	 0.6790	 0.4400
g	 0.7650	 0.4530
h	 0.6820	 0.4370
i	 0.7530	 0.4730
j	 0.7500	 0.4690

