Full wwPDB EM Validation Report ⓘ

Oct 6, 2024 – 09:53 am BST

PDB ID	:	7O3E
EMDB ID	:	EMD-12705
Title	:	Murine supercomplex CIII2CIV in the intermediate locked conformation
Authors	:	Vercellino, I.; Sazanov, L.A.
Deposited on	:	2021-04-01
Resolution	:	3.60 Å(reported)
Based on initial models	:	5Z62, 5IY5, 1NTZ, 3L75

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:

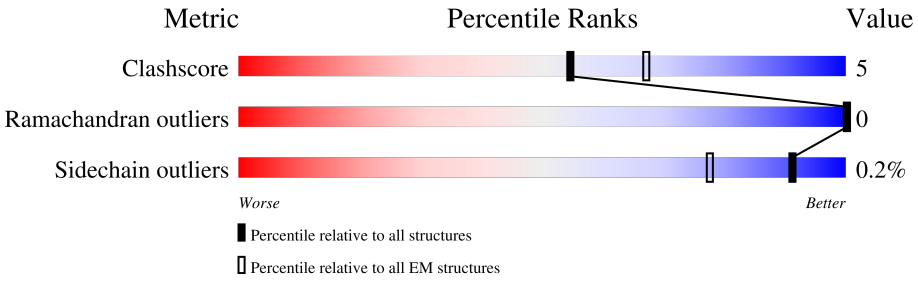
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 <=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	446	87% 13%
1	L	446	85% 15%
2	B	439	80% 15%
2	M	439	84% 12%
3	C	381	91% 9%
3	N	381	84% 15%
4	D	241	6% 87% 13%
4	O	241	6% 88% 11%

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Mol	Chain	Length	Quality of chain
5	F	110	82% 10% 8%
5	Q	110	5% 83% 9% 8%
6	G	81	73% 10% 17%
6	R	81	79% 10% 11%
7	H	76	17% 74% 14% 12%
7	S	76	16% 72% 11% 16%
8	P	196	7% 92%
9	T	78	6% 90% 10%
10	I	113	19% 86% 12%
11	a	514	99%
12	b	227	99%
13	c	261	98%
14	d	147	6% 97%
15	e	109	95% 5%
16	f	99	5% 96%
17	g	85	26% 88% 12%
18	h	85	16% 93% 7%
19	i	75	96%
20	k	56	88% 12%
21	l	47	98%
22	m	46	9% 93% 7%
23	J	63	10% 44% 5% 51%
23	U	63	13% 48% 51%

2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 44039 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cytochrome b-c1 complex subunit 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	446	Total	C	N	O	S	0	0
			3466	2167	611	671	17		
1	L	445	Total	C	N	O	S	0	0
			3460	2163	610	670	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	420	Total	C	N	O	S	0	0
			3154	1980	555	610	9		
2	M	420	Total	C	N	O	S	0	0
			3154	1980	555	610	9		

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	380	Total	C	N	O	S	0	0
			3045	2052	473	499	21		
3	N	380	Total	C	N	O	S	0	0
			3046	2052	473	499	22		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	241	Total	C	N	O	S	0	0
			1919	1224	329	352	14		
4	O	240	Total	C	N	O	S	0	0
			1909	1218	327	350	14		

- Molecule 5 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	101	Total	C	N	O	S	0	0
			894	572	159	160	3		
5	Q	101	Total	C	N	O	S	0	0
			894	572	159	160	3		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
6	G	67	Total	C	N	O	0	0
			565	364	107	94		
6	R	72	Total	C	N	O	0	0
			609	396	112	101		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	67	Total	C	N	O	S	0	0
			554	338	102	109	5		
7	S	64	Total	C	N	O	S	0	0
			530	322	99	104	5		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
8	P	15	Total	C	N	O	0	0
			128	79	24	25		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	T	78	Total	C	N	O	S	0	0
			554	352	103	97	2		

- Molecule 10 is a protein called Cox7a2l protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	111	Total	C	N	O	S	0	0
			834	543	138	148	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	a	514	Total	C	N	O	S	0	0
			4021	2691	623	675	32		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	b	227	Total	C	N	O	S	0	0
			1817	1180	282	336	19		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	c	259	Total	C	N	O	S	0	0
			2111	1414	338	349	10		

- Molecule 14 is a protein called Cytochrome c oxidase subunit 4 isoform 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	d	144	Total	C	N	O	S	0	0
			1195	770	199	219	7		

- Molecule 15 is a protein called Cytochrome c oxidase subunit 5A, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	e	104	Total	C	N	O	S	0	0
			842	538	141	161	2		

- Molecule 16 is a protein called Cytochrome c oxidase subunit 5B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	f	95	Total	C	N	O	S	0	0
			727	452	127	140	8		

- Molecule 17 is a protein called Cytochrome c oxidase subunit 6A2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	g	75	Total	C	N	O	S	0	0
			605	392	114	96	3		

- Molecule 18 is a protein called Cytochrome c oxidase subunit 6B1.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	h	79	Total	C	N	O	S	0	0
			654	416	116	117	5		

- Molecule 19 is a protein called Cytochrome c oxidase subunit 6C.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	i	72	Total	C	N	O	S	0	0
			572	372	103	94	3		

- Molecule 20 is a protein called Cytochrome c oxidase subunit 7B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	k	49	Total	C	N	O	S	0	0
			383	248	65	68	2		

- Molecule 21 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	l	46	Total	C	N	O	S	0	0
			380	253	64	61	2		

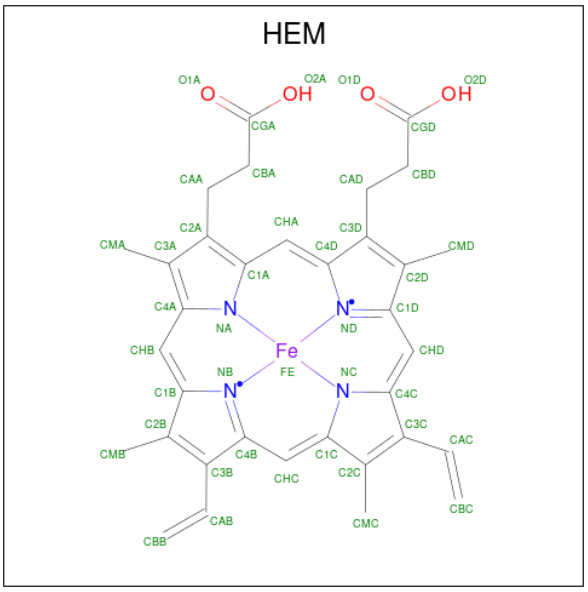
- Molecule 22 is a protein called Cytochrome c oxidase subunit 8B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	m	43	Total	C	N	O	S	0	0
			311	203	51	56	1		

- Molecule 23 is a protein called Cytochrome b-c1 complex subunit 9.

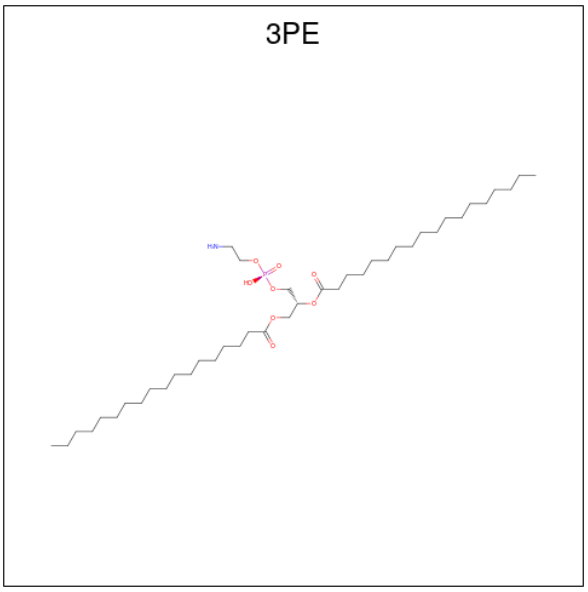
Mol	Chain	Residues	Atoms				AltConf	Trace
23	J	31	Total	C	N	O	0	0
			272	178	47	47		
23	U	31	Total	C	N	O	0	0
			272	178	47	47		

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



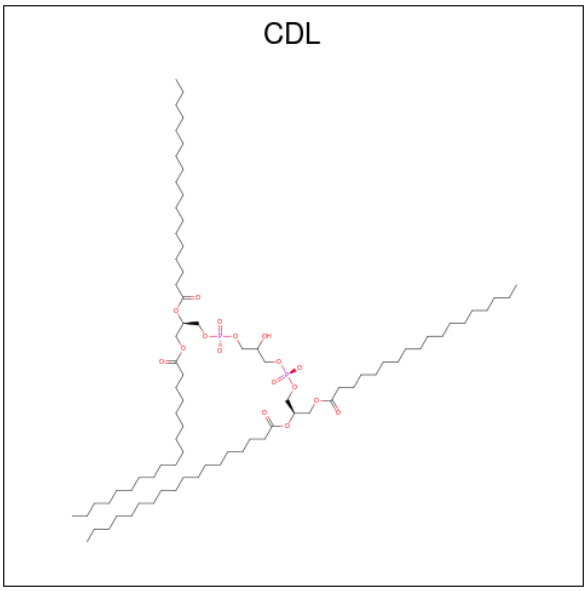
Mol	Chain	Residues	Atoms					AltConf
24	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
24	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
24	N	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
24	N	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

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



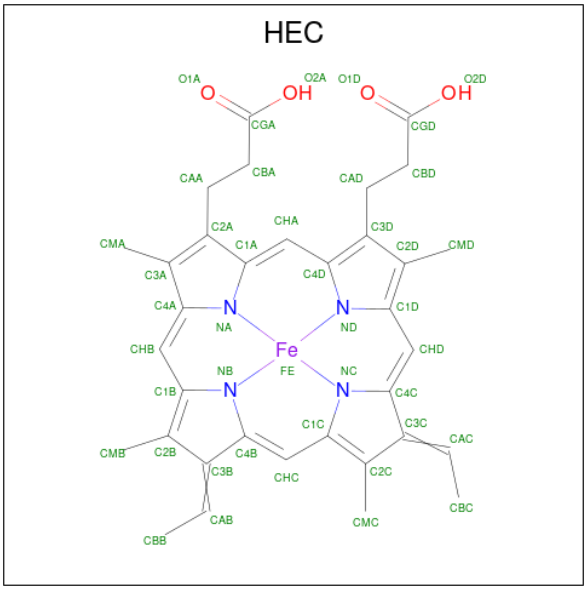
Mol	Chain	Residues	Atoms					AltConf
25	C	1	Total	C	N	O	P	0
			35	25	1	8	1	
25	F	1	Total	C	N	O	P	0
			29	19	1	8	1	
25	F	1	Total	C	N	O	P	0
			34	24	1	8	1	
25	L	1	Total	C	N	O	P	0
			23	13	1	8	1	
25	N	1	Total	C	N	O	P	0
			37	27	1	8	1	
25	N	1	Total	C	N	O	P	0
			51	41	1	8	1	
25	a	1	Total	C	N	O	P	0
			28	18	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
			28	18	1	8	1	
25	c	1	Total	C	N	O	P	0
			45	35	1	8	1	
25	d	1	Total	C	N	O	P	0
			34	24	1	8	1	
25	g	1	Total	C	N	O	P	0
			25	15	1	8	1	
25	k	1	Total	C	N	O	P	0
			27	17	1	8	1	

- Molecule 26 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



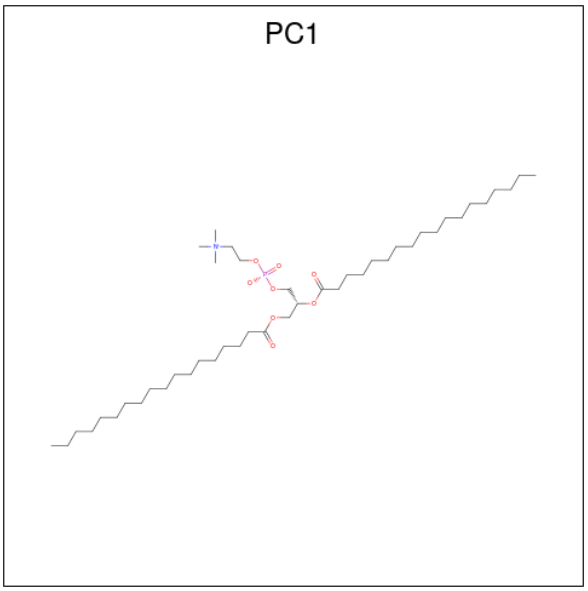
Mol	Chain	Residues	Atoms				AltConf
26	C	1	Total	C	O	P	0
			42	23	17	2	
26	D	1	Total	C	O	P	0
			56	37	17	2	
26	L	1	Total	C	O	P	0
			46	27	17	2	
26	N	1	Total	C	O	P	0
			41	22	17	2	
26	O	1	Total	C	O	P	0
			57	38	17	2	

- Molecule 27 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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

- Molecule 28 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
28	L	1	Total 24	C 14	N 1	O 8	P 1	0
28	a	1	Total 43	C 33	N 1	O 8	P 1	0

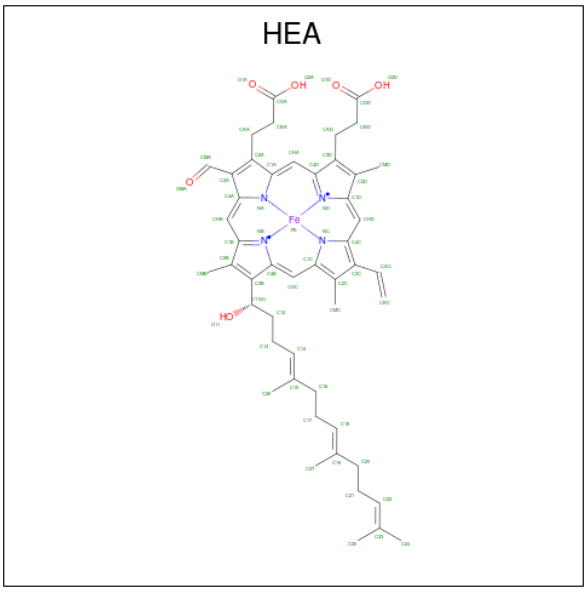
- Molecule 29 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

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

- Molecule 30 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
30	a	1	Total 1	Na 1	0

- Molecule 31 is HEME-A (three-letter code: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).

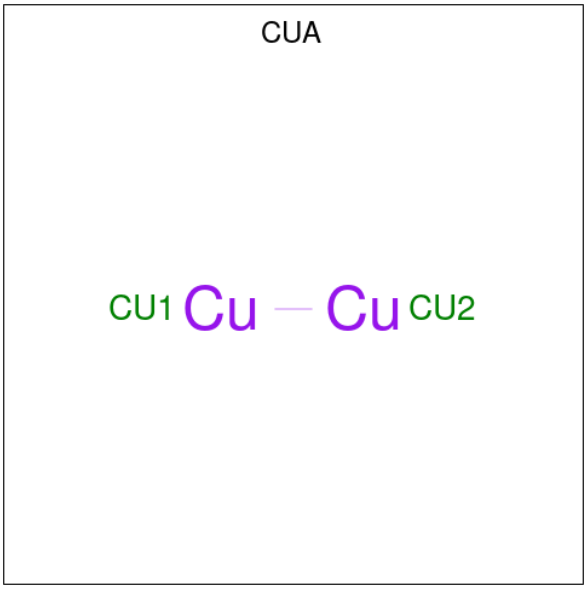


Mol	Chain	Residues	Atoms					AltConf
31	a	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
31	a	1	Total	C	Fe	N	O	0
			60	49	1	4	6	

- Molecule 32 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
32	b	1	Total	Mg	0
			1	1	

- Molecule 33 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu_2).

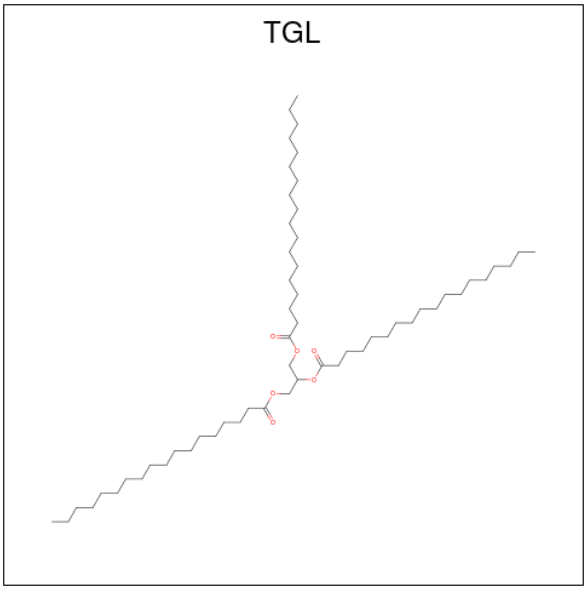


Mol	Chain	Residues	Atoms		AltConf
33	b	1	Total	Cu	0
			2	2	

- Molecule 34 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
34	f	1	Total	Zn	0
			1	1	

- Molecule 35 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: $C_{57}H_{110}O_6$).



Mol	Chain	Residues	Atoms			AltConf
35	l	1	Total	C	O	0
			44	38	6	

3 Residue-property plots (i)

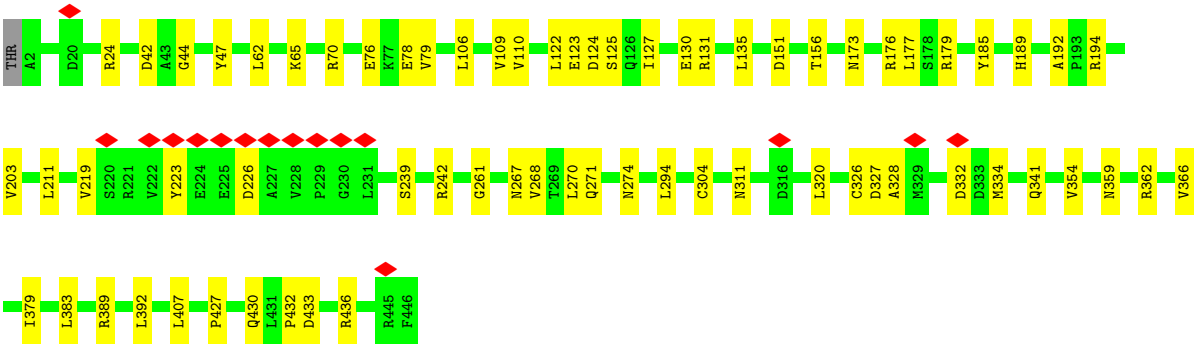
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

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

Chain A:

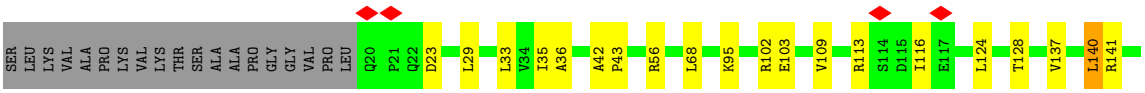
• Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial

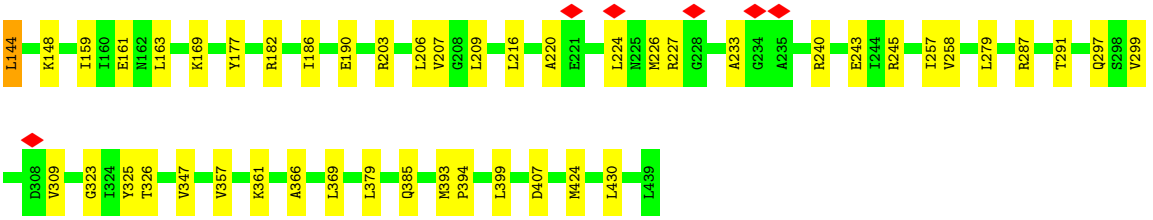
Chain L:



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

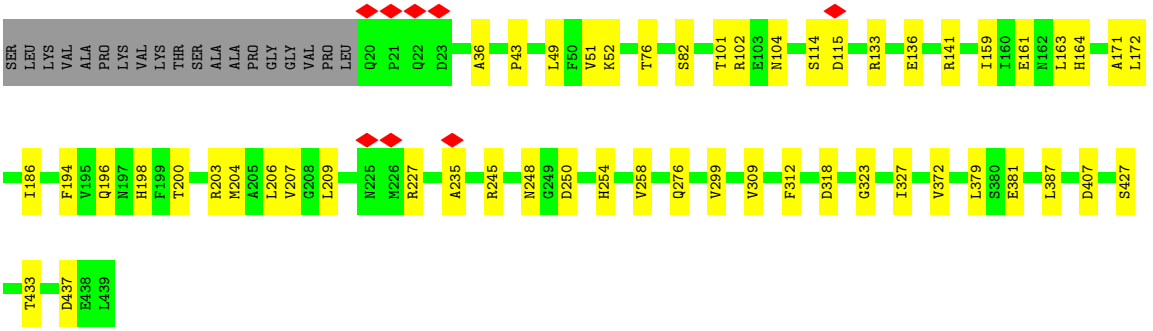
Chain B:





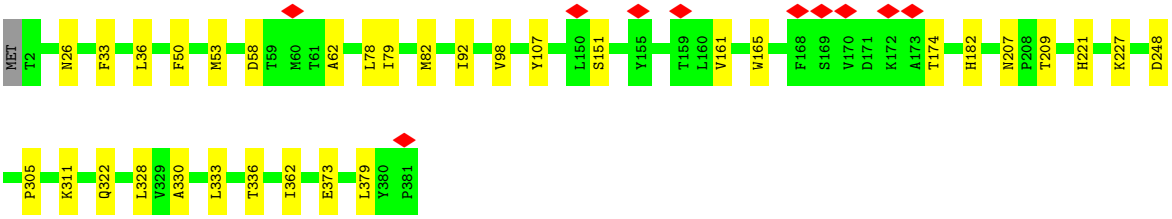
• Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain M:



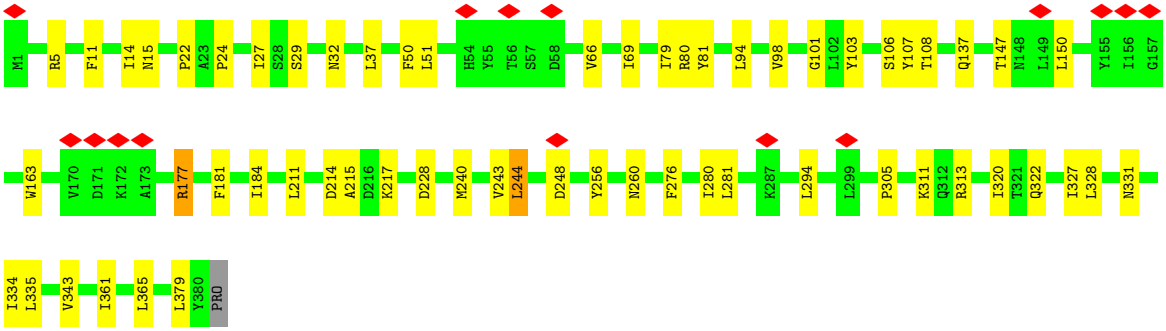
• Molecule 3: Cytochrome b

Chain C:



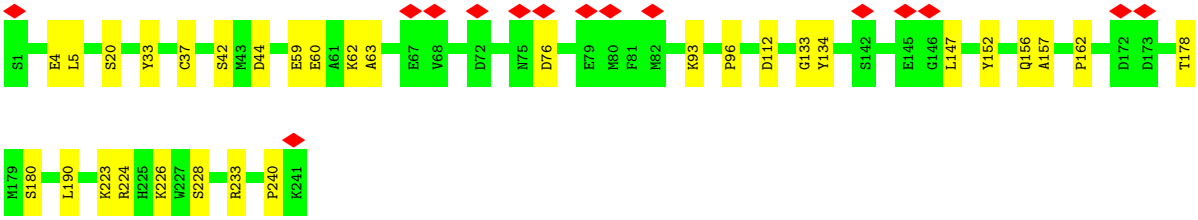
• Molecule 3: Cytochrome b

Chain N:

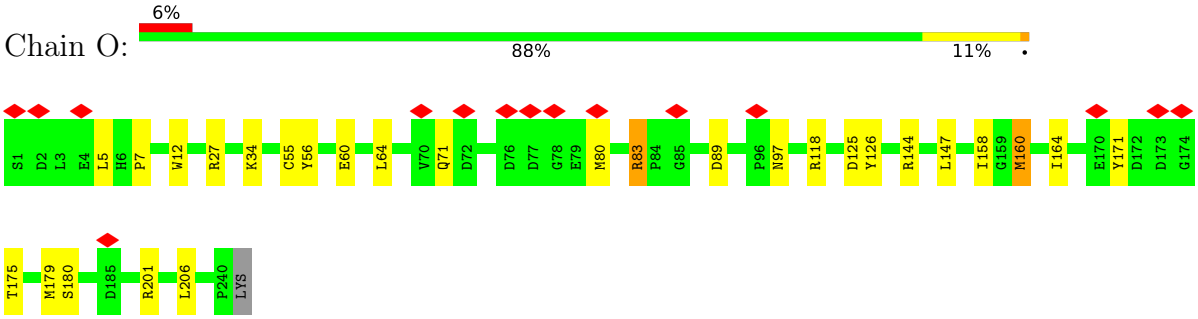


• Molecule 4: Cytochrome c1, heme protein, mitochondrial

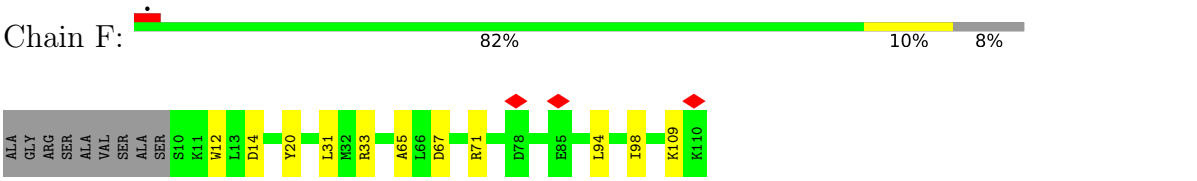
Chain D:



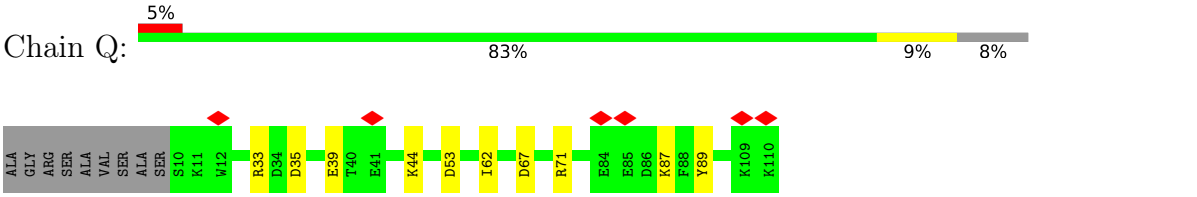
• Molecule 4: Cytochrome c1, heme protein, mitochondrial



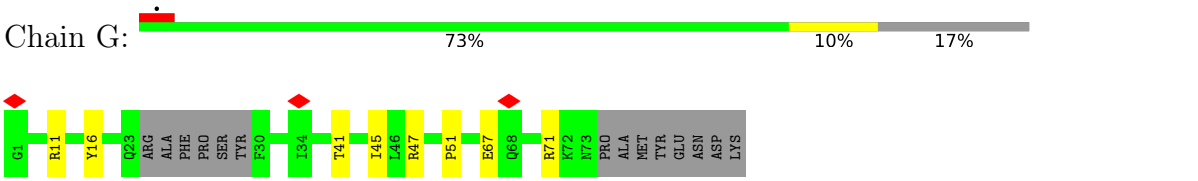
• Molecule 5: Cytochrome b-c1 complex subunit 7



• Molecule 5: Cytochrome b-c1 complex subunit 7



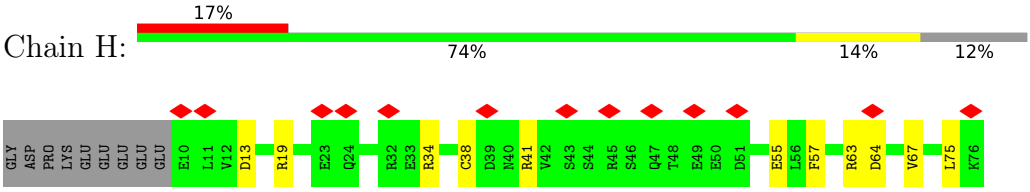
• Molecule 6: Cytochrome b-c1 complex subunit 8



• Molecule 6: Cytochrome b-c1 complex subunit 8

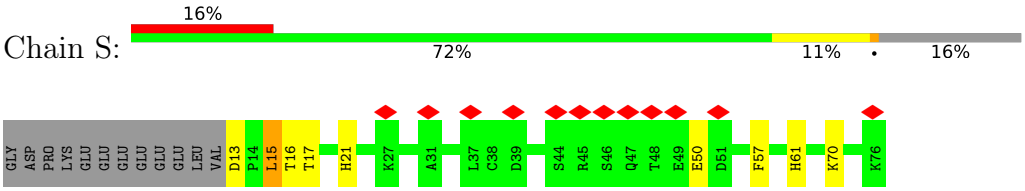
• Molecule 7: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain H:



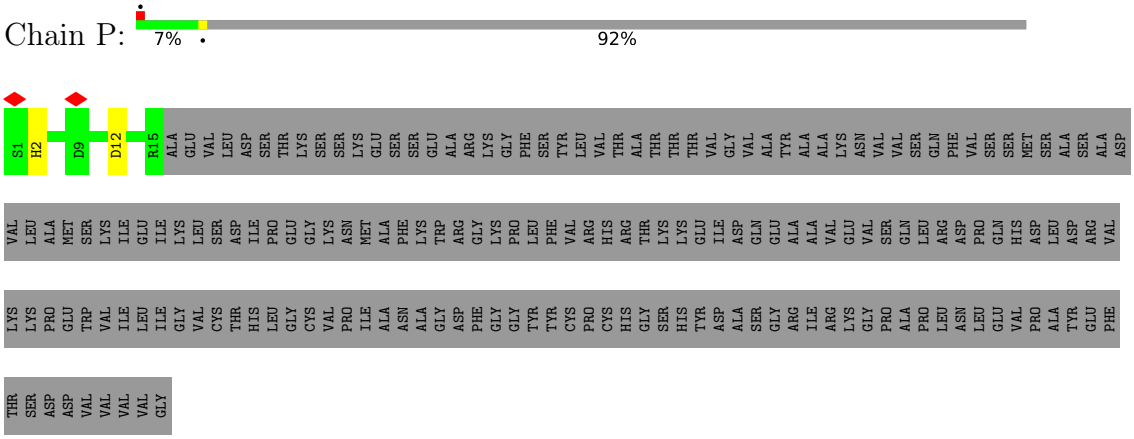
• Molecule 7: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain S:



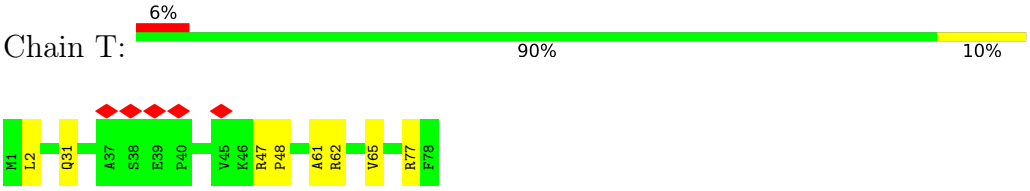
• Molecule 8: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain P:



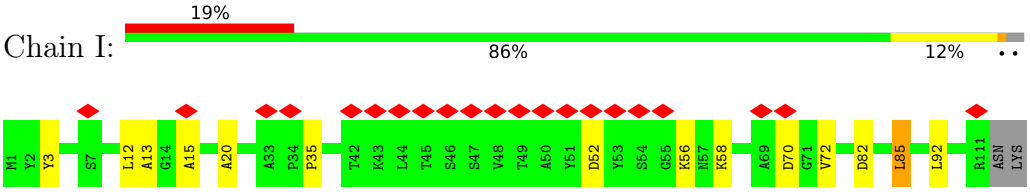
• Molecule 9: Cytochrome b-c1 complex subunit 9

Chain T:



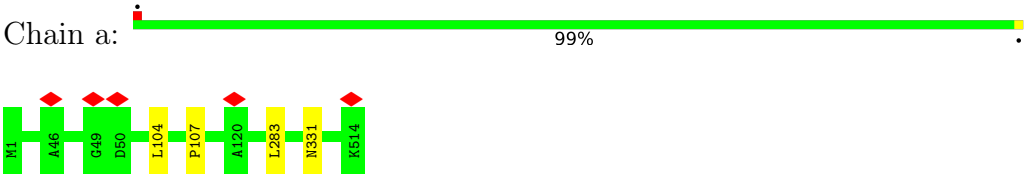
• Molecule 10: Cox7a2l protein

Chain I:



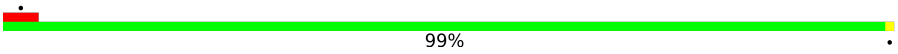
• Molecule 11: Cytochrome c oxidase subunit 1

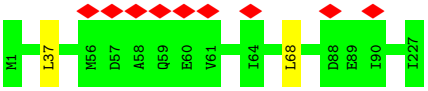
Chain a:



• Molecule 12: Cytochrome c oxidase subunit 2

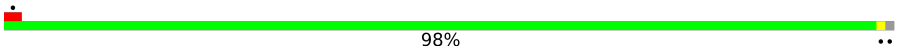
Chain b:

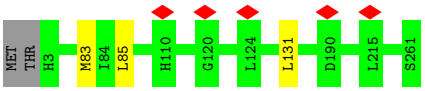




• Molecule 13: Cytochrome c oxidase subunit 3

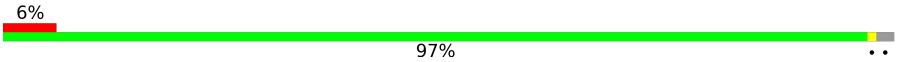
Chain c:

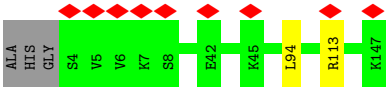




• Molecule 14: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

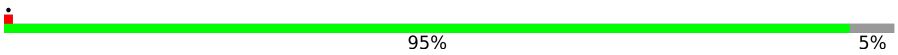
Chain d:

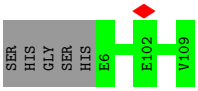




• Molecule 15: Cytochrome c oxidase subunit 5A, mitochondrial

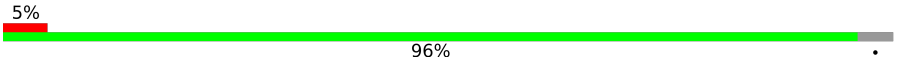
Chain e:

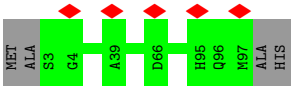




• Molecule 16: Cytochrome c oxidase subunit 5B, mitochondrial

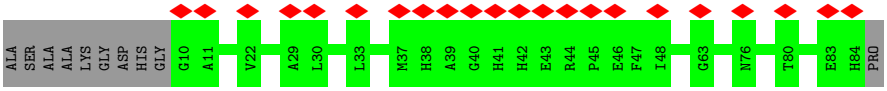
Chain f:





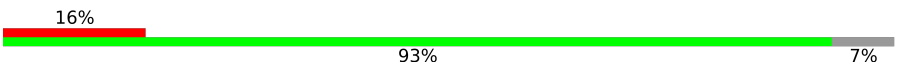
• Molecule 17: Cytochrome c oxidase subunit 6A2, mitochondrial

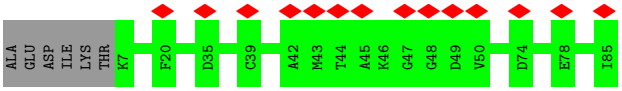
Chain g:



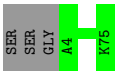
• Molecule 18: Cytochrome c oxidase subunit 6B1

Chain h:

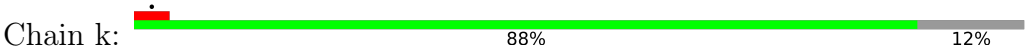


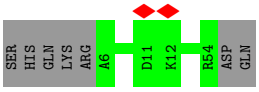


• Molecule 19: Cytochrome c oxidase subunit 6C



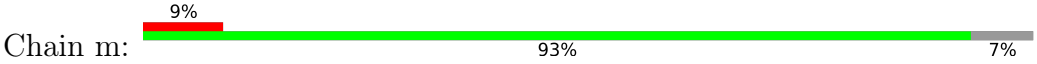
• Molecule 20: Cytochrome c oxidase subunit 7B, mitochondrial

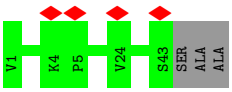




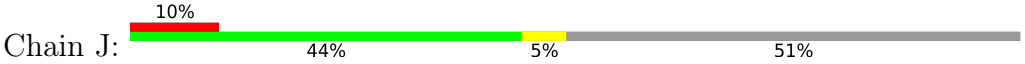
• Molecule 21: Cytochrome c oxidase subunit 7C, mitochondrial

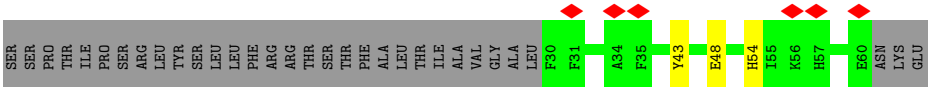
• Molecule 22: Cytochrome c oxidase subunit 8B, mitochondrial



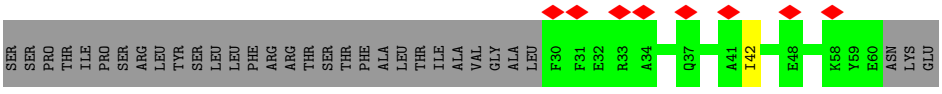


• Molecule 23: Cytochrome b-c1 complex subunit 9





• Molecule 23: Cytochrome b-c1 complex subunit 9



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	8426	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 ($e^-/Å^2$)	90.66	Depositor
Minimum defocus (nm)	200	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.330	Depositor
Minimum map value	-0.026	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	161.728, 214.92801, 180.88	wwPDB
Map dimensions	170, 202, 152	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.064, 1.064, 1.064	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.29	0/3536	0.59	0/4803
1	L	0.28	0/3530	0.58	0/4793
2	B	0.29	0/3205	0.59	3/4332 (0.1%)
2	M	0.28	0/3205	0.54	0/4332
3	C	0.29	0/3147	0.58	0/4299
3	N	0.31	0/3147	0.62	2/4297 (0.0%)
4	D	0.29	0/1978	0.61	1/2685 (0.0%)
4	O	0.28	0/1968	0.58	0/2674
5	F	0.29	0/916	0.63	1/1226 (0.1%)
5	Q	0.29	0/916	0.59	1/1226 (0.1%)
6	G	0.32	0/578	0.62	0/777
6	R	0.34	0/627	0.70	0/848
7	H	0.32	0/561	0.64	0/751
7	S	0.35	0/537	0.77	1/718 (0.1%)
8	P	0.25	0/131	0.60	0/176
9	T	0.31	0/565	0.67	0/772
10	I	0.32	0/856	0.71	2/1164 (0.2%)
11	a	0.36	0/4162	0.59	3/5686 (0.1%)
12	b	0.34	0/1863	0.70	2/2542 (0.1%)
13	c	0.35	0/2195	0.63	3/3000 (0.1%)
14	d	0.33	0/1229	0.62	1/1659 (0.1%)
15	e	0.32	0/860	0.69	0/1167
16	f	0.32	0/744	0.66	0/1009
17	g	0.28	0/632	0.53	0/866
18	h	0.32	0/674	0.65	0/910
19	i	0.36	0/584	0.70	0/778
20	k	0.30	0/396	0.55	0/541
21	l	0.36	0/393	0.64	0/527
22	m	0.36	0/318	0.56	0/433
23	J	0.30	0/281	0.61	0/375
23	U	0.33	0/281	0.52	0/375
All	All	0.31	0/44015	0.61	20/59741 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
4	O	0	1
All	All	0	2

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	b	68	LEU	CA-CB-CG	8.15	134.06	115.30
10	I	85	LEU	CA-CB-CG	7.64	132.86	115.30
12	b	37	LEU	CA-CB-CG	7.32	132.14	115.30
5	Q	53	ASP	CB-CG-OD1	7.24	124.82	118.30
2	B	140	LEU	CA-CB-CG	7.16	131.76	115.30
2	B	144	LEU	CA-CB-CG	6.91	131.19	115.30
5	F	14	ASP	CB-CG-OD2	6.91	124.52	118.30
4	D	190	LEU	CA-CB-CG	6.31	129.82	115.30
3	N	244	LEU	CA-CB-CG	6.00	129.10	115.30
11	a	104	LEU	CA-CB-CG	5.83	128.71	115.30
10	I	92	LEU	CA-CB-CG	5.40	127.71	115.30
2	B	216	LEU	CA-CB-CG	5.39	127.69	115.30
11	a	107	PRO	CA-N-CD	-5.26	104.14	111.50
11	a	283	LEU	CA-CB-CG	5.26	127.39	115.30
14	d	94	LEU	CA-CB-CG	5.18	127.21	115.30
13	c	85	LEU	CB-CG-CD2	-5.15	102.24	111.00
13	c	131	LEU	CB-CG-CD2	5.14	119.75	111.00
13	c	83	MET	CG-SD-CE	-5.14	91.98	100.20
7	S	15	LEU	CA-CB-CG	5.10	127.03	115.30
3	N	343	VAL	CA-CB-CG1	5.03	118.44	110.90

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	330	SER	Peptide
4	O	160	MET	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3466	0	3377	37	0
1	L	3460	0	3367	41	0
2	B	3154	0	3158	39	0
2	M	3154	0	3158	34	0
3	C	3045	0	3107	23	0
3	N	3046	0	3112	39	0
4	D	1919	0	1867	22	0
4	O	1909	0	1854	22	0
5	F	894	0	882	8	0
5	Q	894	0	882	6	0
6	G	565	0	577	6	0
6	R	609	0	614	7	0
7	H	554	0	535	7	0
7	S	530	0	509	6	0
8	P	128	0	120	2	0
9	T	554	0	590	7	0
10	I	834	0	823	7	0
11	a	4021	0	3998	0	0
12	b	1817	0	1822	0	0
13	c	2111	0	2047	0	0
14	d	1195	0	1161	0	0
15	e	842	0	838	0	0
16	f	727	0	703	0	0
17	g	605	0	570	0	0
18	h	654	0	622	0	0
19	i	572	0	596	0	0
20	k	383	0	367	0	0
21	l	380	0	378	0	0
22	m	311	0	329	0	0
23	J	272	0	251	2	0
23	U	272	0	251	1	0
24	C	86	0	60	2	0
24	N	86	0	60	2	0
25	C	35	0	44	0	0
25	F	63	0	74	1	0
25	L	23	0	20	0	0
25	N	88	0	130	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	a	28	0	30	0	0
25	b	57	0	62	0	0
25	c	45	0	67	0	0
25	d	34	0	42	0	0
25	g	25	0	24	0	0
25	k	27	0	28	0	0
26	C	42	0	28	0	0
26	D	56	0	56	2	0
26	L	46	0	36	0	0
26	N	41	0	26	0	0
26	O	57	0	58	2	0
27	D	43	0	30	0	0
27	O	43	0	30	0	0
28	L	24	0	22	0	0
28	a	43	0	60	0	0
29	a	1	0	0	0	0
30	a	1	0	0	0	0
31	a	120	0	108	0	0
32	b	1	0	0	0	0
33	b	2	0	0	0	0
34	f	1	0	0	0	0
35	l	44	0	63	0	0
All	All	44039	0	43623	278	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 5.

All (278) 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)
7:H:34:ARG:HG3	7:H:55:GLU:HG3	1.73	0.70
4:D:233:ARG:HA	6:G:16:TYR:O	1.91	0.69
2:B:226:MET:HG2	2:B:227:ARG:HG3	1.77	0.66
2:B:220:ALA:HA	2:B:224:LEU:HD23	1.80	0.63
4:O:71:GLN:HE21	4:O:80:MET:HG3	1.64	0.62
3:N:107:TYR:HB2	3:N:305:PRO:HG3	1.80	0.61
3:C:107:TYR:HB2	3:C:305:PRO:HG3	1.82	0.60
3:N:181:PHE:HA	3:N:184:ILE:HG12	1.84	0.60
4:O:34:LYS:HE3	4:O:64:LEU:HD22	1.85	0.58
2:M:141:ARG:NH1	2:M:186:ILE:O	2.37	0.58
3:N:379:LEU:HD13	5:Q:33:ARG:HH12	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:58:ASP:O	3:C:62:ALA:N	2.35	0.58
2:M:36:ALA:HB3	2:M:207:VAL:HG12	1.85	0.57
10:I:3:TYR:HA	10:I:13:ALA:O	2.05	0.56
4:O:12:TRP:NE1	4:O:125:ASP:OD1	2.35	0.56
3:N:147:THR:HA	3:N:150:LEU:HG	1.88	0.56
2:B:257:ILE:HG13	2:B:424:MET:HG3	1.86	0.56
3:C:98:VAL:HG22	24:C:402:HEM:HBC2	1.87	0.56
4:O:71:GLN:O	4:O:83:ARG:NH1	2.38	0.56
9:T:65:VAL:HB	9:T:77:ARG:HB3	1.88	0.56
2:B:42:ALA:O	2:B:113:ARG:NH1	2.38	0.55
10:I:52:ASP:O	10:I:58:LYS:NZ	2.39	0.55
7:S:61:HIS:HB2	4:O:5:LEU:HD11	1.89	0.55
2:B:203:ARG:HH12	2:B:233:ALA:HB2	1.70	0.55
4:D:233:ARG:O	5:F:71:ARG:NH2	2.40	0.55
2:M:52:LYS:O	2:M:203:ARG:NH2	2.40	0.55
4:D:224:ARG:NH1	26:D:301:CDL:O1	2.40	0.54
2:B:243:GLU:HG3	2:B:424:MET:HB3	1.88	0.54
2:B:299:VAL:HG21	2:B:309:VAL:HG21	1.89	0.54
1:L:261:GLY:O	1:L:267:ASN:ND2	2.40	0.54
1:L:173:ASN:HA	1:L:176:ARG:HG2	1.89	0.54
1:A:354:VAL:HG22	1:A:407:LEU:HD13	1.89	0.54
1:A:261:GLY:O	1:A:267:ASN:ND2	2.41	0.54
3:N:103:TYR:OH	3:N:322:GLN:NE2	2.40	0.54
3:N:163:TRP:O	3:N:177:ARG:NH1	2.40	0.54
1:A:21:ASN:HB3	1:A:192:ALA:HB1	1.90	0.53
3:N:98:VAL:HG22	24:N:402:HEM:HBC2	1.90	0.53
3:N:328:LEU:HB2	3:N:361:ILE:HG21	1.91	0.53
1:A:158:PHE:O	1:A:161:THR:OG1	2.27	0.53
3:C:50:PHE:HA	3:C:53:MET:HG2	1.91	0.53
5:F:67:ASP:O	5:F:71:ARG:NH1	2.41	0.53
2:B:113:ARG:HA	2:B:116:ILE:HD11	1.90	0.53
2:B:141:ARG:NH1	2:B:186:ILE:O	2.42	0.53
2:M:104:ASN:HD22	2:M:387:LEU:HD12	1.73	0.53
2:B:169:LYS:HE3	2:B:240:ARG:HB3	1.90	0.53
3:N:5:ARG:O	3:N:15:ASN:ND2	2.42	0.53
3:N:240:MET:HA	3:N:243:VAL:HB	1.90	0.53
1:A:308:GLN:NE2	9:T:31:GLN:OE1	2.42	0.53
2:B:36:ALA:HB3	2:B:207:VAL:HG22	1.91	0.53
3:N:214:ASP:HB3	6:R:8:ALA:HB2	1.91	0.53
4:O:83:ARG:NH2	4:O:89:ASP:OD1	2.42	0.53
4:O:158:ILE:HG13	4:O:160:MET:H	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:ARG:NH2	1:A:429:GLU:OE1	2.42	0.52
1:L:106:LEU:HD11	1:L:203:VAL:HG23	1.90	0.52
23:U:42:ILE:HG23	4:O:206:LEU:HD21	1.91	0.52
2:B:385:GLN:HA	9:T:2:LEU:HD12	1.91	0.52
2:B:407:ASP:N	2:B:407:ASP:OD1	2.42	0.52
4:D:59:GLU:O	4:D:62:LYS:HB3	2.10	0.52
2:M:102:ARG:NH2	2:M:161:GLU:OE1	2.42	0.52
2:M:76:THR:HG22	2:M:82:SER:H	1.75	0.52
1:A:25:VAL:HG22	1:A:197:LEU:HB3	1.92	0.51
3:N:244:LEU:HD12	4:O:201:ARG:HG3	1.92	0.51
1:L:70:ARG:NH1	1:L:78:GLU:OE1	2.43	0.51
1:L:354:VAL:HG22	1:L:407:LEU:HD13	1.93	0.51
3:N:66:VAL:HA	3:N:69:ILE:HD12	1.92	0.51
2:B:68:LEU:HD13	2:B:144:LEU:HD23	1.93	0.51
10:I:15:ALA:HB3	10:I:20:ALA:HB2	1.92	0.51
1:L:62:LEU:HD13	1:L:122:LEU:HD22	1.90	0.51
1:L:106:LEU:HA	1:L:109:VAL:HG12	1.93	0.51
10:I:70:ASP:HB3	10:I:72:VAL:HG12	1.91	0.51
3:N:50:PHE:HB3	3:N:79:ILE:HD12	1.92	0.51
4:D:4:GLU:OE2	4:D:156:GLN:NE2	2.44	0.51
2:M:133:ARG:HB2	2:M:136:GLU:HG3	1.92	0.51
6:R:40:ARG:NH1	26:O:301:CDL:OA3	2.43	0.51
2:M:102:ARG:NH1	2:M:172:LEU:O	2.44	0.51
2:B:309:VAL:HG13	2:B:326:THR:HG22	1.93	0.51
2:M:171:ALA:HB2	2:M:235:ALA:HB3	1.93	0.51
1:A:61:HIS:NE2	1:A:137:GLU:OE1	2.41	0.50
1:A:105:ASP:OD1	1:A:105:ASP:N	2.43	0.50
1:L:24:ARG:HD2	1:L:383:LEU:HD23	1.93	0.50
3:N:215:ALA:HA	6:R:10:ILE:HD11	1.92	0.50
3:N:327:ILE:HG23	25:N:405:3PE:H2C2	1.93	0.50
2:B:369:LEU:HD11	2:B:399:LEU:HD11	1.92	0.50
1:A:245:ASP:OD1	6:G:11:ARG:NH1	2.42	0.50
1:A:131:ARG:NH2	1:A:177:LEU:O	2.45	0.50
2:B:128:THR:HG23	2:B:226:MET:HE2	1.93	0.50
3:N:37:LEU:HD11	3:N:94:LEU:HA	1.92	0.50
4:D:20:SER:OG	23:J:43:TYR:OH	2.29	0.49
1:L:42:ASP:O	1:L:194:ARG:NH1	2.45	0.49
1:A:155:ALA:HA	1:A:164:ALA:HB1	1.95	0.49
1:A:60:GLU:OE2	2:B:287:ARG:NH2	2.44	0.49
3:N:248:ASP:HB2	4:O:118:ARG:HH21	1.77	0.49
3:N:311:LYS:HD2	3:N:379:LEU:HD21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Q:35:ASP:OD1	5:Q:89:TYR:OH	2.28	0.49
2:M:196:GLN:O	2:M:227:ARG:NH2	2.45	0.49
3:C:330:ALA:HB2	6:G:51:PRO:HB3	1.95	0.49
2:M:248:ASN:ND2	2:M:250:ASP:OD2	2.45	0.49
3:N:211:LEU:HD13	5:Q:62:ILE:HD12	1.95	0.48
4:O:144:ARG:HH21	4:O:147:LEU:HD11	1.78	0.48
1:A:366:VAL:HG11	2:B:43:PRO:HB2	1.95	0.48
3:C:207:ASN:ND2	3:C:209:THR:OG1	2.46	0.48
2:M:200:THR:HA	2:M:227:ARG:HE	1.77	0.48
5:Q:67:ASP:OD1	5:Q:71:ARG:NH1	2.46	0.48
3:N:32:ASN:ND2	3:N:228:ASP:OD1	2.44	0.48
4:D:60:GLU:O	4:D:63:ALA:HB3	2.14	0.48
5:F:12:TRP:HE3	25:F:201:3PE:H352	1.77	0.48
3:N:361:ILE:HA	3:N:365:LEU:HB2	1.96	0.48
1:L:110:VAL:HG21	1:L:211:LEU:HB3	1.96	0.48
1:L:366:VAL:HG11	2:M:43:PRO:HB2	1.95	0.48
3:N:108:THR:OG1	3:N:313:ARG:NH2	2.47	0.48
1:A:67:THR:HG23	1:A:70:ARG:H	1.79	0.47
4:D:178:THR:OG1	7:H:13:ASP:OD1	2.30	0.47
3:N:81:TYR:OH	4:O:118:ARG:NH1	2.45	0.47
4:D:180:SER:HB3	7:H:75:LEU:HD11	1.96	0.47
1:L:242:ARG:NH2	1:L:432:PRO:O	2.46	0.47
2:B:23:ASP:OD1	2:B:23:ASP:N	2.46	0.47
4:D:5:LEU:HB2	7:H:57:PHE:HD2	1.79	0.47
1:A:240:GLU:OE2	1:A:242:ARG:NH1	2.42	0.47
2:B:137:VAL:HA	2:B:140:LEU:HD23	1.96	0.47
1:A:436:ARG:NH2	3:C:221:HIS:O	2.47	0.47
3:N:276:PHE:HB2	3:N:335:LEU:HB3	1.96	0.47
1:L:131:ARG:NH2	1:L:177:LEU:O	2.48	0.47
1:L:156:THR:O	1:L:239:SER:OG	2.31	0.47
3:N:320:ILE:HD11	25:N:405:3PE:H122	1.96	0.47
1:L:42:ASP:OD1	1:L:42:ASP:N	2.41	0.47
1:L:366:VAL:HG22	1:L:392:LEU:HD21	1.97	0.47
6:R:67:GLU:O	6:R:71:ARG:NH1	2.46	0.47
3:C:92:ILE:HG21	26:D:301:CDL:H791	1.96	0.47
1:L:122:LEU:O	1:L:179:ARG:NH1	2.48	0.47
2:M:299:VAL:HG21	2:M:309:VAL:HG21	1.97	0.47
4:D:112:ASP:N	4:D:112:ASP:OD1	4.37	0.47
1:A:294:LEU:HB2	1:A:341:GLN:HG3	1.97	0.46
1:L:76:GLU:HA	1:L:79:VAL:HG12	1.98	0.46
2:M:159:ILE:HD11	2:M:427:SER:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:209:LEU:HG	2:M:379:LEU:HD13	1.96	0.46
4:D:147:LEU:HD23	4:D:157:ALA:HB1	1.96	0.46
1:L:328:ALA:HB2	1:L:427:PRO:HB2	1.96	0.46
2:M:258:VAL:HA	2:M:323:GLY:HA3	1.98	0.46
2:M:194:PHE:O	2:M:198:HIS:HB2	2.16	0.46
2:B:279:LEU:HD21	2:B:347:VAL:HG21	1.98	0.46
3:N:101:GLY:HA2	3:N:106:SER:HB2	1.96	0.46
4:O:164:ILE:HG12	4:O:179:MET:HG3	1.98	0.46
7:S:17:THR:O	7:S:21:HIS:ND1	2.42	0.46
1:A:327:ASP:OD1	1:A:327:ASP:N	2.46	0.46
4:D:224:ARG:O	4:D:228:SER:HB3	2.15	0.46
1:A:74:ALA:O	1:A:77:LYS:HB2	2.16	0.45
1:A:328:ALA:HB2	1:A:427:PRO:HB2	1.97	0.45
3:C:379:LEU:HD11	5:F:33:ARG:HD2	1.98	0.45
4:D:240:PRO:HA	10:I:35:PRO:HD3	1.98	0.45
4:D:133:GLY:HA3	4:D:152:TYR:HE2	1.81	0.45
6:G:67:GLU:HG3	6:G:71:ARG:HH21	1.81	0.45
1:L:270:LEU:HD13	1:L:320:LEU:HD22	1.98	0.45
7:S:13:ASP:O	7:S:16:THR:OG1	2.33	0.45
1:A:377:GLU:HG3	10:I:12:LEU:HG	1.98	0.45
2:B:95:LYS:O	2:B:109:VAL:HA	2.16	0.45
2:B:258:VAL:HA	2:B:323:GLY:HA3	1.99	0.45
1:L:433:ASP:OD1	1:L:433:ASP:N	2.47	0.45
1:A:67:THR:HA	1:A:121:SER:H	1.80	0.45
1:A:248:LEU:HD12	1:A:426:GLY:HA2	1.98	0.45
2:B:102:ARG:NH2	2:B:161:GLU:OE1	2.45	0.45
3:C:165:TRP:O	3:C:174:THR:OG1	2.34	0.45
8:P:12:ASP:O	6:R:24:ARG:NH2	2.50	0.45
3:C:50:PHE:HB3	3:C:79:ILE:HG21	1.99	0.45
3:C:182:HIS:CE1	24:C:401:HEM:NC	2.85	0.45
4:D:76:ASP:OD2	4:O:97:ASN:N	2.43	0.45
4:O:171:TYR:HD2	4:O:175:THR:HB	1.82	0.45
4:D:93:LYS:HE3	4:D:96:PRO:HA	1.99	0.44
1:L:359:ASN:OD1	1:L:362:ARG:NH1	2.50	0.44
7:S:57:PHE:HB3	4:O:5:LEU:HD13	1.98	0.44
5:F:94:LEU:O	5:F:98:ILE:HG12	2.18	0.44
1:A:3:THR:OG1	1:A:4:PHE:N	2.51	0.44
3:C:151:SER:HB2	3:C:161:VAL:HG21	1.98	0.44
4:D:33:TYR:HA	4:D:37:CYS:HB3	1.98	0.44
2:M:318:ASP:OD1	2:M:318:ASP:N	2.50	0.44
7:H:19:ARG:HB2	7:H:63:ARG:HD3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:437:ASP:OD1	2:M:437:ASP:N	2.51	0.44
6:R:72:LYS:HE3	7:S:50:GLU:HG2	1.99	0.44
23:J:48:GLU:HA	23:J:54:HIS:HE1	1.83	0.44
5:F:31:LEU:HD11	5:F:65:ALA:HB2	1.99	0.44
4:O:7:PRO:HG3	4:O:126:TYR:HB2	2.00	0.44
4:O:27:ARG:HB2	4:O:55:CYS:HB3	2.00	0.44
1:A:149:VAL:HG21	1:A:252:HIS:HB2	2.00	0.44
1:A:53:ASN:HD21	1:A:165:GLN:HB2	1.82	0.44
1:L:223:TYR:HB3	1:L:226:ASP:HA	2.00	0.44
2:M:372:VAL:HG12	2:M:381:GLU:HG2	2.00	0.44
3:N:24:PRO:HD2	3:N:27:ILE:HD11	1.98	0.44
2:M:51:VAL:HG22	2:M:204:MET:HG2	2.00	0.44
25:N:405:3PE:H282	6:R:54:VAL:HG21	2.00	0.44
3:N:281:LEU:HD11	3:N:294:LEU:HD11	1.99	0.43
9:T:62:ARG:HH21	9:T:77:ARG:HE	1.64	0.43
2:B:56:ARG:NH1	2:B:103:GLU:OE2	2.52	0.43
3:C:26:ASN:HD21	3:C:207:ASN:HB2	1.82	0.43
3:C:322:GLN:OE1	6:G:47:ARG:NH1	2.51	0.43
2:B:245:ARG:HB3	2:B:430:LEU:HD13	2.00	0.43
2:M:101:THR:OG1	2:M:102:ARG:N	2.52	0.43
2:B:29:LEU:HD12	2:B:33:LEU:HD23	1.99	0.43
4:D:226:LYS:HA	4:D:226:LYS:HD2	1.89	0.43
2:M:115:ASP:OD2	2:M:115:ASP:N	2.51	0.43
1:L:294:LEU:HB2	1:L:341:GLN:HG3	2.00	0.43
2:M:36:ALA:O	2:M:207:VAL:HA	2.18	0.43
4:O:71:GLN:NE2	4:O:80:MET:HG3	2.29	0.43
1:L:192:ALA:HB2	1:L:219:VAL:HG11	2.01	0.43
1:A:156:THR:O	1:A:239:SER:OG	2.35	0.43
3:C:227:LYS:HD3	4:D:223:LYS:HE3	2.00	0.43
2:B:124:LEU:HD23	2:B:124:LEU:HA	1.89	0.43
7:H:64:ASP:HA	7:H:67:VAL:HG12	2.01	0.43
1:L:327:ASP:OD1	1:L:327:ASP:N	2.45	0.43
2:B:35:ILE:HD13	2:B:206:LEU:HB3	2.01	0.43
1:L:379:ILE:HG12	1:L:389:ARG:HD3	2.01	0.43
2:M:49:LEU:HD13	2:M:206:LEU:HD13	2.01	0.43
2:M:407:ASP:OD1	2:M:407:ASP:N	2.50	0.43
9:T:47:ARG:HD2	9:T:48:PRO:HD2	2.01	0.43
10:I:82:ASP:HA	10:I:85:LEU:HD23	2.01	0.43
1:A:102:LEU:HD21	2:B:366:ALA:HA	2.01	0.42
3:C:33:PHE:O	3:C:36:LEU:HB2	2.19	0.42
1:A:110:VAL:HG11	1:A:211:LEU:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Q:39:GLU:O	5:Q:44:LYS:NZ	2.52	0.42
3:N:11:PHE:HA	3:N:14:ILE:HG12	2.01	0.42
1:L:274:ASN:HD21	1:L:311:ASN:HB2	1.85	0.42
1:L:65:LYS:HA	1:L:65:LYS:HD3	1.90	0.42
2:M:114:SER:OG	2:M:115:ASP:N	2.53	0.42
2:B:291:THR:O	2:B:297:GLN:NE2	2.52	0.42
2:B:357:VAL:HG12	2:B:361:LYS:HE3	2.02	0.42
1:L:268:VAL:O	1:L:271:GLN:HB2	2.19	0.42
3:C:311:LYS:HE3	3:C:311:LYS:HB3	1.85	0.42
1:L:44:GLY:H	1:L:47:TYR:HD2	1.66	0.42
1:L:124:ASP:HA	1:L:127:ILE:HG22	2.02	0.42
3:N:22:PRO:HB2	3:N:217:LYS:HE3	2.02	0.42
3:N:137:GLN:HE22	3:N:260:ASN:H	1.68	0.42
1:L:436:ARG:HD2	1:L:436:ARG:HA	1.76	0.42
4:D:42:SER:OG	4:D:44:ASP:OD1	2.36	0.42
2:B:159:ILE:HG21	2:B:325:TYR:HE1	1.85	0.41
6:G:41:THR:O	6:G:45:ILE:HB	2.21	0.41
2:M:102:ARG:HH12	2:M:164:HIS:HB3	1.85	0.41
3:N:137:GLN:NE2	3:N:260:ASN:H	2.17	0.41
7:S:15:LEU:HD23	4:O:180:SER:HB3	2.01	0.41
1:A:8:LEU:HD12	1:A:392:LEU:HB3	2.02	0.41
3:N:80:ARG:HH22	3:N:256:TYR:HE1	1.67	0.41
1:A:192:ALA:HB2	1:A:219:VAL:HB	2.02	0.41
1:A:255:ILE:HG12	1:A:422:VAL:HG13	2.03	0.41
3:C:78:LEU:HG	3:C:82:MET:HE2	2.02	0.41
7:H:38:CYS:HA	7:H:41:ARG:HG2	2.02	0.41
2:M:163:LEU:HD11	2:M:258:VAL:HG22	2.02	0.41
1:L:123:GLU:OE1	1:L:125:SER:N	2.53	0.41
1:L:185:TYR:O	1:L:189:HIS:HB2	2.20	0.41
2:M:254:HIS:CE1	2:M:327:ILE:HD12	2.56	0.41
2:B:393:MET:HA	2:B:394:PRO:HD3	1.95	0.41
2:B:182:ARG:NH2	2:B:190:GLU:OE1	2.40	0.41
3:C:328:LEU:HD11	3:C:362:ILE:HD13	2.02	0.41
3:N:29:SER:O	3:N:32:ASN:HB2	2.21	0.41
3:N:334:ILE:HD13	3:N:334:ILE:HA	1.96	0.41
4:O:27:ARG:HH21	4:O:56:TYR:HA	1.86	0.41
1:A:339:GLN:NE2	1:A:437:ILE:O	2.54	0.41
3:C:333:LEU:HA	3:C:336:THR:HG22	2.03	0.41
4:D:134:TYR:CG	4:D:162:PRO:HG3	2.55	0.41
1:L:65:LYS:NZ	1:L:130:GLU:OE2	2.53	0.41
1:L:135:LEU:HD23	1:L:135:LEU:HA	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:304:CYS:HA	1:L:326:CYS:HB3	2.03	0.41
2:M:245:ARG:HH21	2:M:433:THR:HB	1.85	0.41
2:M:312:PHE:HA	9:T:61:ALA:HA	2.02	0.41
3:N:29:SER:HB2	26:O:301:CDL:H721	2.02	0.41
2:B:209:LEU:HD12	2:B:379:LEU:HB2	2.02	0.41
3:C:248:ASP:OD1	3:C:248:ASP:N	2.54	0.41
2:M:276:GLN:HE21	9:T:61:ALA:HB1	1.85	0.41
1:A:113:LEU:HD23	1:A:113:LEU:HA	1.92	0.40
1:A:197:LEU:HD23	1:A:197:LEU:HA	4.50	0.40
1:L:151:ASP:OD2	8:P:2:HIS:NE2	2.51	0.40
1:L:304:CYS:HB3	1:L:334:MET:SD	2.62	0.40
2:B:163:LEU:HD11	2:B:258:VAL:HG22	2.04	0.40
5:F:109:LYS:HE3	5:F:109:LYS:HB3	1.82	0.40
3:N:51:LEU:HD13	24:N:401:HEM:HBA1	2.02	0.40
4:O:56:TYR:HD2	4:O:60:GLU:HB3	1.86	0.40
2:B:148:LYS:HG3	2:B:177:TYR:HB3	2.03	0.40
3:N:280:ILE:H	3:N:280:ILE:HG13	1.76	0.40
5:Q:87:LYS:HB2	5:Q:87:LYS:HE2	1.92	0.40
1:A:59:LEU:HD23	1:A:59:LEU:HA	1.99	0.40
3:C:373:GLU:OE2	5:F:20:TYR:OH	2.37	0.40
1:L:332:ASP:HB2	1:L:430:GLN:HG2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	444/446 (100%)	423 (95%)	21 (5%)	0	100	100
1	L	443/446 (99%)	426 (96%)	17 (4%)	0	100	100
2	B	418/439 (95%)	398 (95%)	20 (5%)	0	100	100
2	M	418/439 (95%)	400 (96%)	18 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	378/381 (99%)	365 (97%)	13 (3%)	0	100	100
3	N	378/381 (99%)	359 (95%)	19 (5%)	0	100	100
4	D	239/241 (99%)	226 (95%)	13 (5%)	0	100	100
4	O	238/241 (99%)	227 (95%)	11 (5%)	0	100	100
5	F	99/110 (90%)	99 (100%)	0	0	100	100
5	Q	99/110 (90%)	99 (100%)	0	0	100	100
6	G	63/81 (78%)	60 (95%)	3 (5%)	0	100	100
6	R	70/81 (86%)	66 (94%)	4 (6%)	0	100	100
7	H	65/76 (86%)	62 (95%)	3 (5%)	0	100	100
7	S	62/76 (82%)	57 (92%)	5 (8%)	0	100	100
8	P	13/196 (7%)	12 (92%)	1 (8%)	0	100	100
9	T	76/78 (97%)	66 (87%)	10 (13%)	0	100	100
10	I	109/113 (96%)	96 (88%)	13 (12%)	0	100	100
11	a	512/514 (100%)	498 (97%)	14 (3%)	0	100	100
12	b	225/227 (99%)	210 (93%)	15 (7%)	0	100	100
13	c	257/261 (98%)	250 (97%)	7 (3%)	0	100	100
14	d	142/147 (97%)	132 (93%)	10 (7%)	0	100	100
15	e	102/109 (94%)	97 (95%)	5 (5%)	0	100	100
16	f	93/99 (94%)	84 (90%)	9 (10%)	0	100	100
17	g	73/85 (86%)	67 (92%)	6 (8%)	0	100	100
18	h	77/85 (91%)	75 (97%)	2 (3%)	0	100	100
19	i	70/75 (93%)	67 (96%)	3 (4%)	0	100	100
20	k	47/56 (84%)	47 (100%)	0	0	100	100
21	l	44/47 (94%)	43 (98%)	1 (2%)	0	100	100
22	m	41/46 (89%)	38 (93%)	3 (7%)	0	100	100
23	J	29/63 (46%)	28 (97%)	1 (3%)	0	100	100
23	U	29/63 (46%)	25 (86%)	4 (14%)	0	100	100
All	All	5353/5812 (92%)	5102 (95%)	251 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	373/373 (100%)	373 (100%)	0	100 100
1	L	372/373 (100%)	372 (100%)	0	100 100
2	B	330/344 (96%)	330 (100%)	0	100 100
2	M	330/344 (96%)	330 (100%)	0	100 100
3	C	332/333 (100%)	332 (100%)	0	100 100
3	N	332/333 (100%)	330 (99%)	2 (1%)	84 92
4	D	206/206 (100%)	206 (100%)	0	100 100
4	O	205/206 (100%)	204 (100%)	1 (0%)	86 93
5	F	93/98 (95%)	93 (100%)	0	100 100
5	Q	93/98 (95%)	93 (100%)	0	100 100
6	G	61/73 (84%)	61 (100%)	0	100 100
6	R	66/73 (90%)	66 (100%)	0	100 100
7	H	64/72 (89%)	64 (100%)	0	100 100
7	S	61/72 (85%)	60 (98%)	1 (2%)	58 76
8	P	15/166 (9%)	15 (100%)	0	100 100
9	T	58/58 (100%)	58 (100%)	0	100 100
10	I	82/95 (86%)	81 (99%)	1 (1%)	67 82
11	a	425/425 (100%)	424 (100%)	1 (0%)	92 96
12	b	210/210 (100%)	210 (100%)	0	100 100
13	c	225/227 (99%)	225 (100%)	0	100 100
14	d	127/128 (99%)	126 (99%)	1 (1%)	79 88
15	e	91/95 (96%)	91 (100%)	0	100 100
16	f	81/83 (98%)	81 (100%)	0	100 100
17	g	62/67 (92%)	62 (100%)	0	100 100
18	h	70/75 (93%)	70 (100%)	0	100 100
19	i	54/56 (96%)	54 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
20	k	39/46 (85%)	39 (100%)	0	100 100
21	l	39/40 (98%)	39 (100%)	0	100 100
22	m	33/34 (97%)	33 (100%)	0	100 100
23	J	26/54 (48%)	26 (100%)	0	100 100
23	U	26/54 (48%)	26 (100%)	0	100 100
All	All	4581/4911 (93%)	4574 (100%)	7 (0%)	91 96

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	N	177	ARG
3	N	331	ASN
7	S	70	LYS
10	I	56	LYS
11	a	331	ASN
14	d	113	ARG
4	O	83	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
11	a	331	ASN
11	a	451	ASN
14	d	76	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 34 ligands modelled in this entry, 4 are monoatomic - leaving 30 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
25	3PE	N	405	-	50,50,50	0.31	0	53,55,55	0.30	0
26	CDL	N	404	-	40,40,99	0.46	0	46,52,111	0.59	1 (2%)
25	3PE	b	302	-	28,28,50	0.39	0	31,33,55	0.35	0
24	HEM	C	401	3	41,50,50	1.24	5 (12%)	45,82,82	1.69	7 (15%)
31	HEA	a	603	11	57,67,67	1.43	8 (14%)	61,103,103	2.36	23 (37%)
27	HEC	D	302	4	32,50,50	2.18	3 (9%)	24,82,82	1.53	2 (8%)
26	CDL	D	301	-	55,55,99	0.38	0	61,67,111	0.32	0
28	PC1	L	501	-	23,23,53	0.45	0	29,31,61	0.67	1 (3%)
25	3PE	N	403	-	36,36,50	0.35	0	39,41,55	0.34	0
25	3PE	a	606	-	27,27,50	0.40	0	30,32,55	0.45	0
25	3PE	L	502	-	22,22,50	0.44	0	25,27,55	0.39	0
33	CUA	b	303	12	0,1,1	-	-	-		
25	3PE	C	403	-	34,34,50	0.36	0	37,39,55	0.37	0
25	3PE	g	101	-	24,24,50	0.44	0	27,29,55	0.68	1 (3%)
24	HEM	N	402	3	41,50,50	1.26	3 (7%)	45,82,82	1.79	8 (17%)
25	3PE	b	304	-	27,27,50	0.40	0	30,32,55	0.39	0
25	3PE	c	301	-	44,44,50	0.32	0	47,49,55	0.37	0
27	HEC	O	302	4	32,50,50	2.19	4 (12%)	24,82,82	1.51	2 (8%)
28	PC1	a	605	-	42,42,53	0.33	0	48,50,61	0.33	0
25	3PE	F	202	-	33,33,50	0.37	0	36,38,55	0.32	0
26	CDL	O	301	-	56,56,99	0.38	0	62,68,111	0.32	0
26	CDL	L	503	-	45,45,99	0.44	0	51,57,111	0.55	1 (1%)
24	HEM	C	402	3	41,50,50	1.26	5 (12%)	45,82,82	1.68	8 (17%)
31	HEA	a	604	11	57,67,67	1.43	8 (14%)	61,103,103	2.28	22 (36%)
25	3PE	F	201	-	28,28,50	0.39	0	31,33,55	0.40	0
35	TGL	l	601	-	43,43,62	0.21	0	46,46,65	0.24	0
25	3PE	d	201	-	33,33,50	0.39	0	36,38,55	0.60	1 (2%)
24	HEM	N	401	3	41,50,50	1.22	4 (9%)	45,82,82	1.73	8 (17%)
25	3PE	k	101	-	26,26,50	0.41	0	29,31,55	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	CDL	C	404	-	41,41,99	0.44	0	47,53,111	0.36	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	3PE	N	405	-	-	13/54/54/54	-
26	CDL	N	404	-	-	12/51/51/110	-
25	3PE	b	302	-	-	8/32/32/54	-
24	HEM	C	401	3	-	4/12/54/54	-
31	HEA	a	603	11	-	10/32/76/76	-
27	HEC	D	302	4	-	0/10/54/54	-
26	CDL	D	301	-	-	18/66/66/110	-
28	PC1	L	501	-	-	8/27/27/57	-
25	3PE	N	403	-	-	6/40/40/54	-
25	3PE	a	606	-	-	12/31/31/54	-
25	3PE	L	502	-	-	9/26/26/54	-
25	3PE	C	403	-	-	10/38/38/54	-
25	3PE	g	101	-	-	10/28/28/54	-
24	HEM	N	402	3	-	8/12/54/54	-
25	3PE	b	304	-	-	7/31/31/54	-
25	3PE	c	301	-	-	7/48/48/54	-
27	HEC	O	302	4	-	0/10/54/54	-
28	PC1	a	605	-	-	8/46/46/57	-
25	3PE	F	202	-	-	9/37/37/54	-
26	CDL	O	301	-	-	20/67/67/110	-
26	CDL	L	503	-	-	16/56/56/110	-
24	HEM	C	402	3	-	6/12/54/54	-
31	HEA	a	604	11	-	5/32/76/76	-
25	3PE	F	201	-	-	6/32/32/54	-
35	TGL	l	601	-	-	4/46/46/65	-
25	3PE	d	201	-	-	9/37/37/54	-
24	HEM	N	401	3	-	5/12/54/54	-
25	3PE	k	101	-	-	6/30/30/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CDL	C	404	-	-	12/52/52/110	-

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	D	302	HEC	C2B-C3B	-6.35	1.34	1.40
27	D	302	HEC	C3C-C2C	-6.25	1.34	1.40
27	O	302	HEC	C3C-C2C	-6.22	1.34	1.40
27	O	302	HEC	C2B-C3B	-6.21	1.34	1.40
27	O	302	HEC	C3D-C2D	5.44	1.53	1.37
27	D	302	HEC	C3D-C2D	5.27	1.53	1.37
31	a	604	HEA	C3B-C2B	4.45	1.44	1.34
31	a	603	HEA	C3B-C2B	4.32	1.44	1.34
31	a	604	HEA	C3D-C2D	3.96	1.45	1.36
24	C	402	HEM	C4D-ND	-3.94	1.33	1.40
31	a	603	HEA	C3D-C2D	3.81	1.44	1.36
24	C	401	HEM	C4D-ND	-3.77	1.33	1.40
24	N	402	HEM	C4D-ND	-3.71	1.33	1.40
31	a	603	HEA	C3A-C2A	3.71	1.45	1.40
24	N	401	HEM	C4D-ND	-3.56	1.34	1.40
31	a	603	HEA	C3C-C2C	3.33	1.45	1.40
31	a	604	HEA	C4B-C3B	3.26	1.50	1.44
24	N	402	HEM	C1B-NB	-3.23	1.34	1.40
31	a	604	HEA	C3A-C2A	3.20	1.44	1.40
24	C	401	HEM	C1B-NB	-3.17	1.34	1.40
24	N	401	HEM	C1B-NB	-3.16	1.34	1.40
31	a	604	HEA	C3C-C2C	3.14	1.44	1.40
31	a	603	HEA	C4B-C3B	3.12	1.49	1.44
24	C	402	HEM	C1B-NB	-3.12	1.34	1.40
24	C	402	HEM	C1D-ND	-2.79	1.33	1.38
31	a	603	HEA	C1D-ND	-2.66	1.35	1.40
24	N	402	HEM	C1D-ND	-2.63	1.33	1.38
24	C	401	HEM	C1D-ND	-2.59	1.33	1.38
24	N	401	HEM	C1D-ND	-2.55	1.33	1.38
31	a	604	HEA	C2A-C1A	2.41	1.48	1.42
31	a	604	HEA	C1D-ND	-2.34	1.36	1.40
31	a	603	HEA	C2A-C1A	2.32	1.47	1.42
27	O	302	HEC	CAD-C3D	2.27	1.55	1.52
24	C	401	HEM	CHB-C1B	2.11	1.40	1.35
31	a	604	HEA	C4D-C3D	2.07	1.48	1.45
31	a	603	HEA	C4D-C3D	2.06	1.48	1.45
24	C	401	HEM	C4B-NB	-2.05	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	N	401	HEM	CHB-C1B	2.04	1.40	1.35
24	C	402	HEM	CHB-C1B	2.01	1.40	1.35
24	C	402	HEM	C4B-NB	-2.01	1.34	1.38

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	a	604	HEA	CMC-C2C-C3C	7.05	137.88	124.68
31	a	603	HEA	CMC-C2C-C3C	6.99	137.75	124.68
31	a	604	HEA	CMC-C2C-C1C	-6.31	118.77	128.46
31	a	603	HEA	CMC-C2C-C1C	-6.15	119.02	128.46
24	N	401	HEM	CHC-C4B-NB	4.88	129.73	124.43
24	C	401	HEM	CHC-C4B-NB	4.80	129.65	124.43
31	a	603	HEA	CMD-C2D-C1D	-4.71	117.87	125.04
31	a	603	HEA	C3D-C4D-ND	4.62	114.83	110.36
31	a	604	HEA	C3D-C4D-ND	4.52	114.73	110.36
24	C	402	HEM	CHC-C4B-NB	4.51	129.33	124.43
24	N	402	HEM	CHC-C4B-NB	4.45	129.26	124.43
31	a	604	HEA	CMB-C2B-C1B	-4.28	118.52	125.04
24	N	402	HEM	CHB-C1B-NB	4.19	129.55	124.38
31	a	603	HEA	CMB-C2B-C1B	-4.17	118.68	125.04
24	C	401	HEM	CHB-C1B-NB	4.17	129.53	124.38
27	D	302	HEC	CMC-C2C-C1C	-4.10	122.16	128.46
24	N	402	HEM	C4D-ND-C1D	4.02	109.22	105.07
24	N	401	HEM	CHB-C1B-NB	4.00	129.32	124.38
31	a	603	HEA	C4D-C3D-C2D	-3.98	101.10	106.90
31	a	604	HEA	CMD-C2D-C1D	-3.90	119.09	125.04
24	C	402	HEM	C4D-ND-C1D	3.90	109.10	105.07
27	O	302	HEC	CMC-C2C-C1C	-3.89	122.48	128.46
24	C	402	HEM	CHB-C1B-NB	3.78	129.05	124.38
31	a	604	HEA	C4D-C3D-C2D	-3.66	101.57	106.90
31	a	603	HEA	C13-C12-C11	-3.64	108.89	114.35
24	C	401	HEM	C1B-NB-C4B	3.57	108.77	105.07
24	N	401	HEM	C1B-NB-C4B	3.42	108.61	105.07
31	a	603	HEA	CHA-C4D-C3D	-3.42	119.81	124.84
24	C	401	HEM	C4D-ND-C1D	3.34	108.52	105.07
31	a	603	HEA	CMD-C2D-C3D	3.33	135.16	126.12
31	a	604	HEA	CHA-C4D-C3D	-3.33	119.95	124.84
24	N	401	HEM	C4D-ND-C1D	3.26	108.44	105.07
24	C	402	HEM	C1B-NB-C4B	3.25	108.43	105.07
31	a	603	HEA	C26-C15-C16	3.19	120.64	115.27
24	N	402	HEM	CHD-C1D-ND	3.10	127.80	124.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	a	604	HEA	CMB-C2B-C3B	3.08	136.21	130.34
31	a	604	HEA	CAD-C3D-C4D	3.05	129.99	124.66
31	a	604	HEA	CMD-C2D-C3D	3.05	134.40	126.12
24	N	402	HEM	CAD-CBD-CGD	-2.99	107.16	113.60
31	a	603	HEA	CAD-C3D-C4D	2.96	129.83	124.66
31	a	603	HEA	CMB-C2B-C3B	2.89	135.85	130.34
24	N	402	HEM	CHA-C4D-ND	2.84	127.89	124.38
24	N	402	HEM	C1B-NB-C4B	2.82	107.98	105.07
31	a	604	HEA	CHB-C1B-C2B	-2.80	120.60	124.98
31	a	603	HEA	CAA-CBA-CGA	-2.79	105.93	113.76
27	D	302	HEC	CMB-C2B-C1B	-2.79	124.18	128.46
24	C	401	HEM	CHA-C4D-ND	2.74	127.77	124.38
31	a	603	HEA	CHB-C1B-C2B	-2.74	120.69	124.98
31	a	604	HEA	CAD-CBD-CGD	-2.72	107.75	113.60
24	N	401	HEM	CHD-C1D-ND	2.71	127.38	124.43
24	N	401	HEM	CHA-C4D-ND	2.68	127.69	124.38
24	N	402	HEM	CHB-C1B-C2B	-2.59	119.56	126.72
31	a	604	HEA	C2B-C1B-NB	2.58	112.97	109.88
24	C	402	HEM	CHD-C1D-ND	2.57	127.23	124.43
31	a	603	HEA	C27-C19-C20	2.56	119.58	115.27
31	a	604	HEA	C26-C15-C16	2.51	119.49	115.27
27	O	302	HEC	CMB-C2B-C1B	-2.50	124.62	128.46
24	C	401	HEM	CHD-C1D-ND	2.49	127.13	124.43
31	a	603	HEA	CAA-C2A-C3A	2.47	132.94	126.86
24	C	402	HEM	CHA-C4D-ND	2.42	127.37	124.38
31	a	603	HEA	C17-C18-C19	-2.41	121.86	127.66
31	a	604	HEA	C4B-C3B-C2B	-2.39	103.33	107.41
26	N	404	CDL	CA4-OA6-CA5	2.38	123.66	117.79
25	g	101	3PE	C2-O21-C21	2.38	123.65	117.79
26	L	503	CDL	CB4-OB6-CB5	2.33	123.52	117.79
31	a	604	HEA	C12-C13-C14	-2.32	106.11	112.23
24	C	401	HEM	CHB-C1B-C2B	-2.29	120.39	126.72
31	a	604	HEA	C3B-C4B-NB	2.28	112.55	109.84
31	a	604	HEA	C27-C19-C20	2.28	119.10	115.27
24	N	401	HEM	CAD-CBD-CGD	-2.26	108.73	113.60
31	a	604	HEA	C26-C15-C14	-2.26	117.88	123.68
31	a	603	HEA	CHB-C1B-NB	2.25	126.87	124.43
28	L	501	PC1	C2-O21-C21	2.23	123.29	117.79
24	N	401	HEM	CHB-C1B-C2B	-2.23	120.55	126.72
31	a	603	HEA	OMA-CMA-C3A	-2.23	120.05	124.91
25	d	201	3PE	C2-O21-C21	2.22	123.25	117.79
24	C	402	HEM	CHB-C1B-C2B	-2.22	120.59	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	a	603	HEA	C25-C23-C24	2.21	119.48	114.60
31	a	604	HEA	CAA-CBA-CGA	-2.20	107.58	113.76
31	a	604	HEA	C25-C23-C24	2.19	119.44	114.60
31	a	603	HEA	C2B-C1B-NB	2.13	112.43	109.88
31	a	603	HEA	C4B-C3B-C2B	-2.13	103.77	107.41
31	a	604	HEA	C21-C22-C23	-2.12	120.49	127.75
31	a	603	HEA	C13-C14-C15	-2.07	122.67	127.66
24	C	402	HEM	CAD-CBD-CGD	-2.03	109.24	113.60

There are no chirality outliers.

All (248) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	C	401	HEM	C2B-C3B-CAB-CBB
24	C	401	HEM	C4B-C3B-CAB-CBB
24	C	402	HEM	C2B-C3B-CAB-CBB
24	C	402	HEM	C4B-C3B-CAB-CBB
24	N	401	HEM	C2B-C3B-CAB-CBB
24	N	401	HEM	C4B-C3B-CAB-CBB
24	N	402	HEM	C2B-C3B-CAB-CBB
24	N	402	HEM	C4B-C3B-CAB-CBB
25	C	403	3PE	C1-O11-P-O14
25	C	403	3PE	O13-C11-C12-N
25	F	201	3PE	C1-O11-P-O12
25	F	201	3PE	C1-O11-P-O14
25	F	201	3PE	O13-C11-C12-N
25	F	202	3PE	C1-O11-P-O12
25	F	202	3PE	O13-C11-C12-N
25	L	502	3PE	C1-O11-P-O14
25	L	502	3PE	C11-O13-P-O12
25	L	502	3PE	C11-O13-P-O14
25	N	405	3PE	C1-O11-P-O14
25	N	405	3PE	C11-O13-P-O14
25	N	405	3PE	O13-C11-C12-N
25	a	606	3PE	C1-O11-P-O12
25	a	606	3PE	C1-O11-P-O13
25	a	606	3PE	C1-O11-P-O14
25	a	606	3PE	O13-C11-C12-N
25	b	302	3PE	C1-O11-P-O13
25	b	302	3PE	C11-O13-P-O11
25	b	302	3PE	C11-O13-P-O14
25	b	302	3PE	O13-C11-C12-N

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Mol	Chain	Res	Type	Atoms
25	b	304	3PE	C11-O13-P-O12
25	c	301	3PE	O13-C11-C12-N
25	d	201	3PE	C1-O11-P-O12
25	d	201	3PE	C1-O11-P-O13
25	d	201	3PE	C1-O11-P-O14
25	g	101	3PE	C11-O13-P-O12
25	g	101	3PE	O13-C11-C12-N
25	k	101	3PE	C2-C1-O11-P
25	k	101	3PE	O13-C11-C12-N
26	C	404	CDL	CB2-OB2-PB2-OB3
26	C	404	CDL	CB2-OB2-PB2-OB4
26	C	404	CDL	CB2-OB2-PB2-OB5
26	C	404	CDL	CB3-OB5-PB2-OB3
26	D	301	CDL	CB2-OB2-PB2-OB3
26	D	301	CDL	CB3-OB5-PB2-OB2
26	D	301	CDL	CB3-OB5-PB2-OB3
26	D	301	CDL	CB3-OB5-PB2-OB4
26	L	503	CDL	CA2-OA2-PA1-OA3
26	L	503	CDL	CA2-OA2-PA1-OA4
26	L	503	CDL	CB3-OB5-PB2-OB3
26	N	404	CDL	CA2-OA2-PA1-OA4
26	N	404	CDL	CB2-OB2-PB2-OB3
26	O	301	CDL	CA3-OA5-PA1-OA3
26	O	301	CDL	CB2-OB2-PB2-OB3
26	O	301	CDL	OB5-CB3-CB4-OB6
28	L	501	PC1	C11-O13-P-O12
28	L	501	PC1	C1-O11-P-O14
28	a	605	PC1	C11-O13-P-O14
28	a	605	PC1	C11-O13-P-O11
28	a	605	PC1	C1-O11-P-O14
31	a	603	HEA	C1A-C2A-CAA-CBA
31	a	603	HEA	C3A-C2A-CAA-CBA
31	a	603	HEA	C11-C12-C13-C14
31	a	603	HEA	C15-C16-C17-C18
31	a	604	HEA	C15-C16-C17-C18
26	O	301	CDL	C1-CA2-OA2-PA1
24	N	401	HEM	C2A-CAA-CBA-CGA
25	F	201	3PE	C1-O11-P-O13
25	F	202	3PE	C1-O11-P-O13
25	L	502	3PE	C1-O11-P-O13
25	L	502	3PE	C11-O13-P-O11
25	N	405	3PE	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
25	N	405	3PE	C11-O13-P-O11
25	b	304	3PE	C11-O13-P-O11
25	d	201	3PE	C11-O13-P-O11
25	g	101	3PE	C11-O13-P-O11
25	k	101	3PE	C1-O11-P-O13
26	D	301	CDL	CA2-OA2-PA1-OA5
26	D	301	CDL	CA3-OA5-PA1-OA2
26	L	503	CDL	CA2-OA2-PA1-OA5
26	L	503	CDL	CA3-OA5-PA1-OA2
26	L	503	CDL	CB3-OB5-PB2-OB2
26	N	404	CDL	CA2-OA2-PA1-OA5
26	O	301	CDL	CA2-OA2-PA1-OA5
26	O	301	CDL	CB2-OB2-PB2-OB5
28	L	501	PC1	C11-O13-P-O11
35	l	601	TGL	CC3-CC4-CC5-CC6
26	L	503	CDL	C33-C34-C35-C36
25	a	606	3PE	C2-C1-O11-P
25	N	405	3PE	C3B-C3C-C3D-C3E
28	a	605	PC1	C28-C29-C2A-C2B
25	d	201	3PE	C22-C23-C24-C25
31	a	604	HEA	C19-C20-C21-C22
25	F	202	3PE	C36-C37-C38-C39
25	N	405	3PE	C3D-C3E-C3F-C3G
25	N	405	3PE	C33-C34-C35-C36
25	C	403	3PE	C1-O11-P-O13
26	C	404	CDL	CB3-OB5-PB2-OB2
26	D	301	CDL	CB2-OB2-PB2-OB5
28	a	605	PC1	C1-O11-P-O13
25	F	202	3PE	C32-C33-C34-C35
25	a	606	3PE	O11-C1-C2-C3
26	C	404	CDL	OB5-CB3-CB4-CB6
26	O	301	CDL	OB5-CB3-CB4-CB6
26	O	301	CDL	CB2-C1-CA2-OA2
24	N	402	HEM	C2A-CAA-CBA-CGA
25	C	403	3PE	C1-C2-C3-O31
25	C	403	3PE	C23-C24-C25-C26
25	c	301	3PE	C23-C24-C25-C26
25	a	606	3PE	O11-C1-C2-O21
26	C	404	CDL	OB5-CB3-CB4-OB6
25	k	101	3PE	C21-C22-C23-C24
25	L	502	3PE	C32-C33-C34-C35
35	l	601	TGL	OG2-CB1-CB2-CB3

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Mol	Chain	Res	Type	Atoms
25	F	202	3PE	C1-C2-C3-O31
28	L	501	PC1	C1-O11-P-O13
26	N	404	CDL	OB5-CB3-CB4-OB6
25	C	403	3PE	O21-C2-C3-O31
26	L	503	CDL	C1-CA2-OA2-PA1
26	O	301	CDL	C1-CB2-OB2-PB2
26	O	301	CDL	CB4-CB3-OB5-PB2
28	L	501	PC1	C2-C1-O11-P
25	c	301	3PE	C31-C32-C33-C34
26	L	503	CDL	OB5-CB3-CB4-CB6
25	N	405	3PE	C2-C1-O11-P
26	D	301	CDL	C1-CA2-OA2-PA1
26	L	503	CDL	OB5-CB3-CB4-OB6
26	N	404	CDL	OA5-CA3-CA4-OA6
25	b	304	3PE	O21-C2-C3-O31
25	a	606	3PE	C22-C23-C24-C25
26	N	404	CDL	CB2-OB2-PB2-OB5
26	O	301	CDL	CA3-OA5-PA1-OA2
26	D	301	CDL	C73-C74-C75-C76
26	O	301	CDL	O1-C1-CA2-OA2
25	g	101	3PE	C2-C1-O11-P
26	C	404	CDL	C1-CB2-OB2-PB2
26	L	503	CDL	C1-CB2-OB2-PB2
25	L	502	3PE	C1-O11-P-O12
25	N	403	3PE	C1-O11-P-O14
25	N	405	3PE	C1-O11-P-O12
25	N	405	3PE	C11-O13-P-O12
25	b	302	3PE	C1-O11-P-O12
25	b	304	3PE	C11-O13-P-O14
25	d	201	3PE	C11-O13-P-O14
25	g	101	3PE	C11-O13-P-O14
25	k	101	3PE	C1-O11-P-O14
26	D	301	CDL	CA2-OA2-PA1-OA3
26	D	301	CDL	CA3-OA5-PA1-OA3
26	D	301	CDL	CA3-OA5-PA1-OA4
26	D	301	CDL	CB2-OB2-PB2-OB4
26	L	503	CDL	CA3-OA5-PA1-OA3
26	L	503	CDL	CA3-OA5-PA1-OA4
26	O	301	CDL	CA2-OA2-PA1-OA3
26	O	301	CDL	CA2-OA2-PA1-OA4
26	O	301	CDL	CB2-OB2-PB2-OB4
25	g	101	3PE	O11-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
26	N	404	CDL	OB5-CB3-CB4-CB6
25	d	201	3PE	O13-C11-C12-N
31	a	603	HEA	O11-C11-C12-C13
25	b	302	3PE	C1-C2-C3-O31
28	L	501	PC1	O13-C11-C12-N
28	a	605	PC1	O13-C11-C12-N
31	a	604	HEA	C1A-C2A-CAA-CBA
25	F	202	3PE	O21-C2-C3-O31
25	b	302	3PE	O21-C2-C3-O31
26	O	301	CDL	OA6-CA4-CA6-OA8
25	c	301	3PE	C2-C1-O11-P
26	C	404	CDL	C12-C11-CA5-OA7
26	D	301	CDL	C71-C72-C73-C74
26	N	404	CDL	CA4-CA3-OA5-PA1
25	N	403	3PE	C1-O11-P-O13
25	a	606	3PE	C11-O13-P-O11
25	c	301	3PE	C11-O13-P-O11
26	C	404	CDL	CA2-OA2-PA1-OA5
26	L	503	CDL	CB2-OB2-PB2-OB5
25	N	405	3PE	C32-C33-C34-C35
31	a	604	HEA	CAD-CBD-CGD-O2D
24	N	402	HEM	CAD-CBD-CGD-O2D
31	a	604	HEA	CAD-CBD-CGD-O1D
24	N	402	HEM	CAD-CBD-CGD-O1D
24	C	401	HEM	CAD-CBD-CGD-O1D
31	a	603	HEA	CAD-CBD-CGD-O2D
24	N	401	HEM	CAD-CBD-CGD-O1D
31	a	603	HEA	CAD-CBD-CGD-O1D
26	L	503	CDL	C32-C33-C34-C35
26	D	301	CDL	C72-C73-C74-C75
26	C	404	CDL	C12-C11-CA5-OA6
25	g	101	3PE	O31-C31-C32-C33
24	N	401	HEM	CAD-CBD-CGD-O2D
26	D	301	CDL	O1-C1-CA2-OA2
24	C	402	HEM	C3D-CAD-CBD-CGD
24	N	402	HEM	CAA-CBA-CGA-O2A
25	C	403	3PE	C27-C28-C29-C2A
31	a	603	HEA	CAA-CBA-CGA-O1A
24	N	402	HEM	CAA-CBA-CGA-O1A
35	l	601	TGL	OB1-CB1-CB2-CB3
24	N	402	HEM	C3D-CAD-CBD-CGD
25	F	202	3PE	O11-C1-C2-O21

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Mol	Chain	Res	Type	Atoms
24	C	402	HEM	CAA-CBA-CGA-O2A
26	N	404	CDL	OA5-CA3-CA4-CA6
25	d	201	3PE	C31-C32-C33-C34
25	N	403	3PE	C27-C28-C29-C2A
26	N	404	CDL	C52-C51-CB5-OB6
25	k	101	3PE	O21-C2-C3-O31
26	O	301	CDL	C72-C71-CB7-OB8
35	l	601	TGL	OG1-CA1-CA2-CA3
25	N	403	3PE	O31-C31-C32-C33
26	D	301	CDL	C52-C51-CB5-OB6
24	C	401	HEM	CAD-CBD-CGD-O2D
24	C	402	HEM	CAA-CBA-CGA-O1A
25	g	101	3PE	C3-C2-O21-C21
25	C	403	3PE	O31-C31-C32-C33
25	L	502	3PE	O31-C31-C32-C33
25	C	403	3PE	C24-C25-C26-C27
25	F	201	3PE	C1-C2-C3-O31
25	a	606	3PE	C1-C2-C3-O31
25	b	304	3PE	C1-C2-C3-O31
25	g	101	3PE	O11-C1-C2-O21
26	C	404	CDL	C32-C31-CA7-OA8
25	N	405	3PE	C2B-C2C-C2D-C2E
25	a	606	3PE	O21-C2-C3-O31
26	N	404	CDL	C52-C51-CB5-OB7
28	a	605	PC1	C27-C28-C29-C2A
26	O	301	CDL	C52-C51-CB5-OB6
25	b	304	3PE	O31-C31-C32-C33
26	N	404	CDL	C12-C11-CA5-OA6
25	C	403	3PE	O32-C31-C32-C33
31	a	603	HEA	CAA-CBA-CGA-O2A
25	L	502	3PE	O32-C31-C32-C33
25	c	301	3PE	C21-C22-C23-C24
26	O	301	CDL	C72-C71-CB7-OB9
31	a	603	HEA	C27-C19-C20-C21
26	D	301	CDL	C1-CB2-OB2-PB2
25	N	403	3PE	O32-C31-C32-C33
25	F	202	3PE	C11-O13-P-O14
25	a	606	3PE	C11-O13-P-O14
25	b	304	3PE	C1-O11-P-O14
25	c	301	3PE	C11-O13-P-O14
26	L	503	CDL	CB3-OB5-PB2-OB4
28	L	501	PC1	C11-O13-P-O14

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Mol	Chain	Res	Type	Atoms
25	N	403	3PE	O13-C11-C12-N
25	b	302	3PE	C12-C11-O13-P
25	d	201	3PE	C1-C2-O21-C21
25	g	101	3PE	C12-C11-O13-P
28	L	501	PC1	C1-C2-O21-C21
26	O	301	CDL	C52-C51-CB5-OB7
25	F	201	3PE	O31-C31-C32-C33
28	a	605	PC1	C22-C23-C24-C25
24	C	402	HEM	CAD-CBD-CGD-O1D

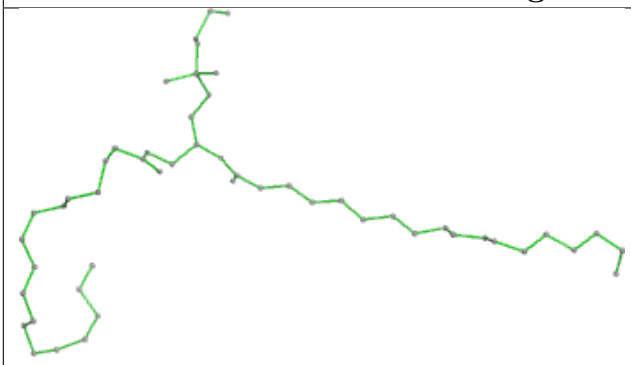
There are no ring outliers.

8 monomers are involved in 12 short contacts:

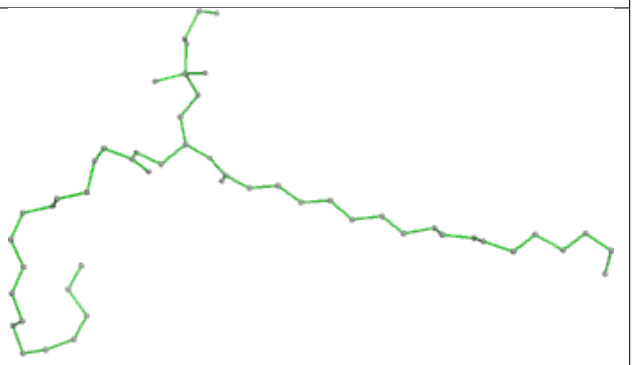
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	N	405	3PE	3	0
24	C	401	HEM	1	0
26	D	301	CDL	2	0
24	N	402	HEM	1	0
26	O	301	CDL	2	0
24	C	402	HEM	1	0
25	F	201	3PE	1	0
24	N	401	HEM	1	0

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

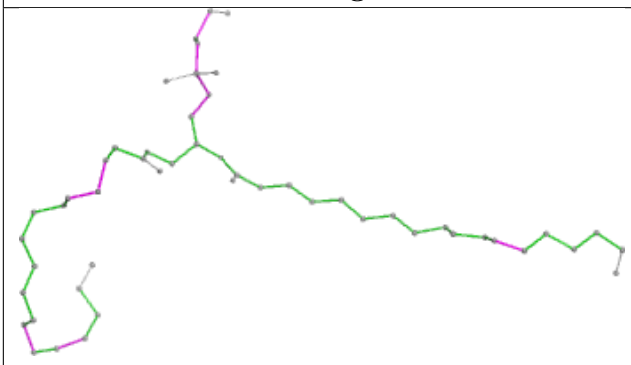
Ligand 3PE N 405



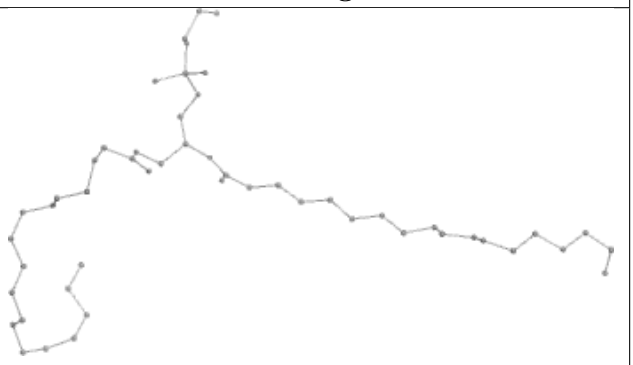
Bond lengths



Bond angles

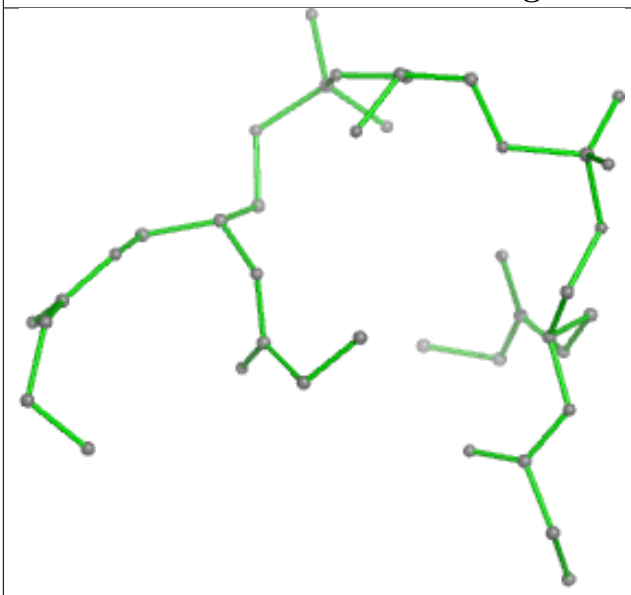


Torsions

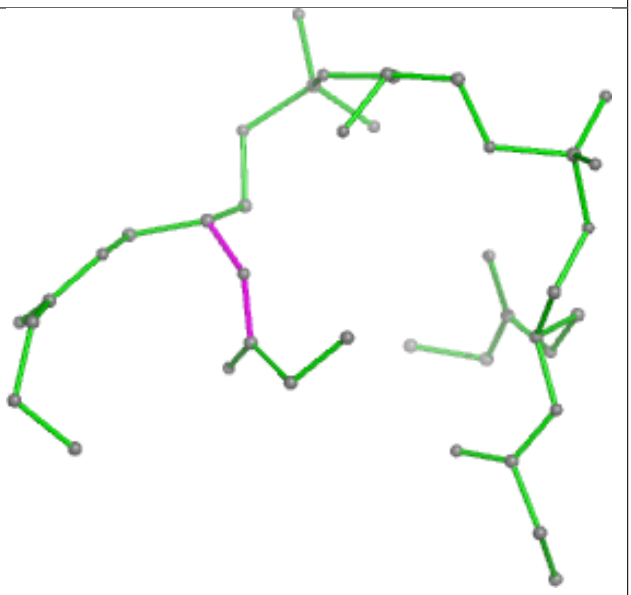


Rings

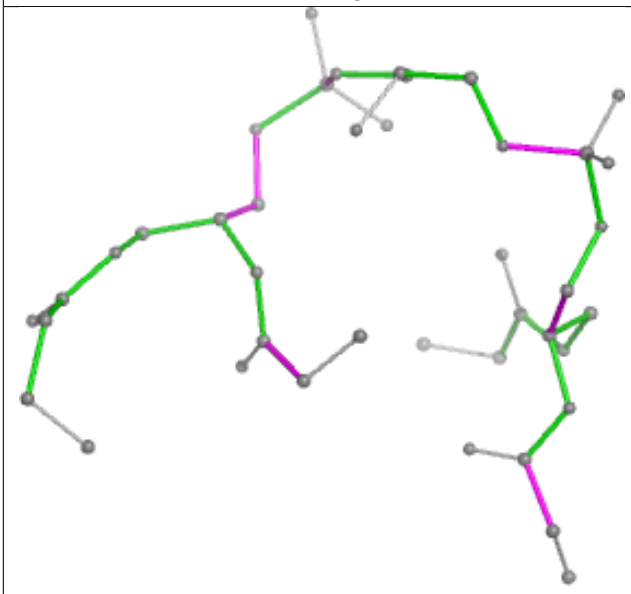
Ligand CDL N 404



Bond lengths



Bond angles



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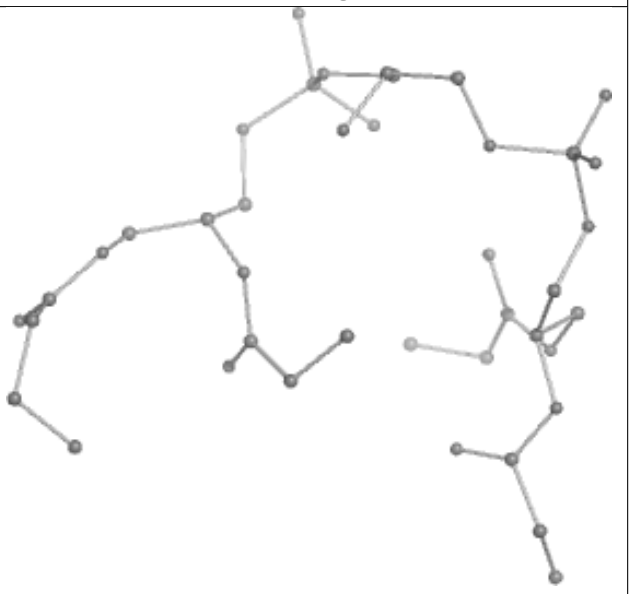
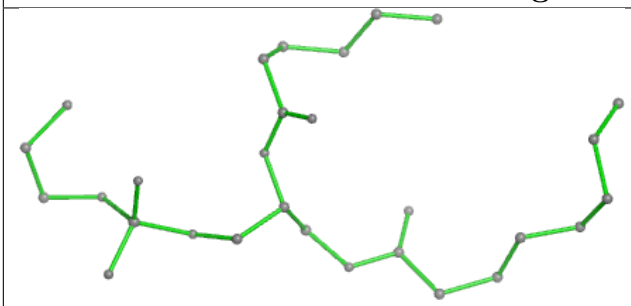
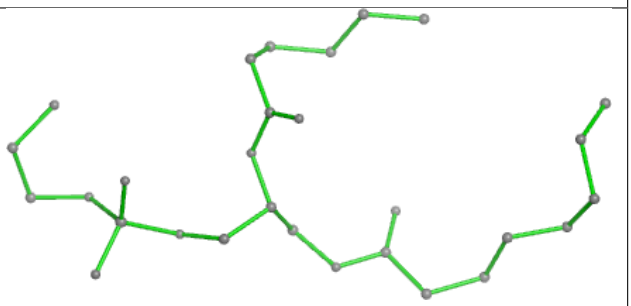


Rings

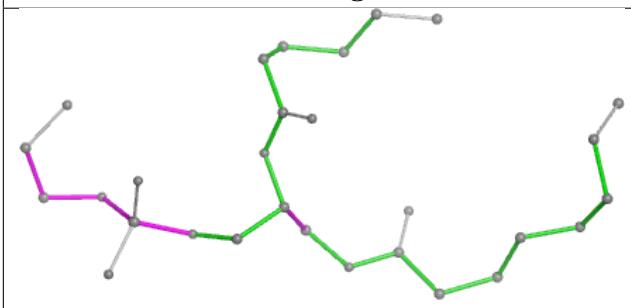
Ligand 3PE b 302



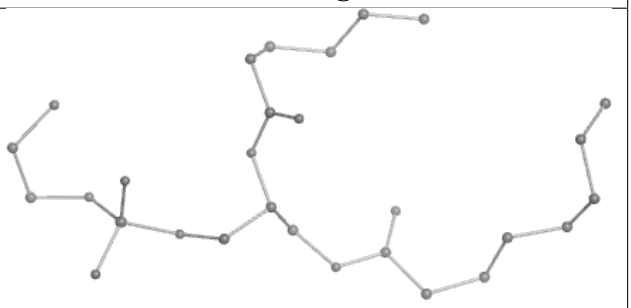
Bond lengths



Bond angles

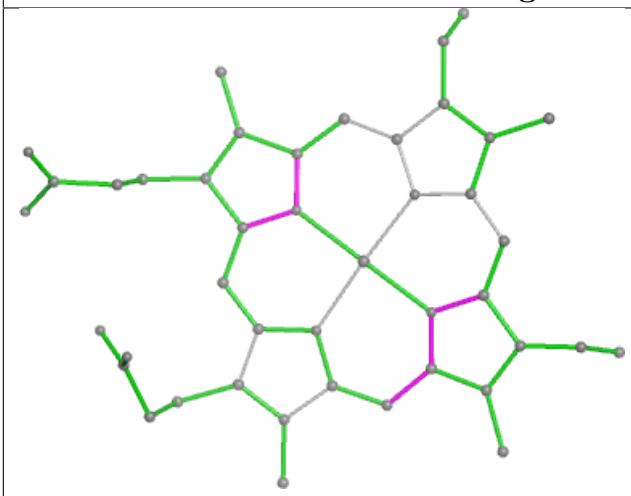


Torsions

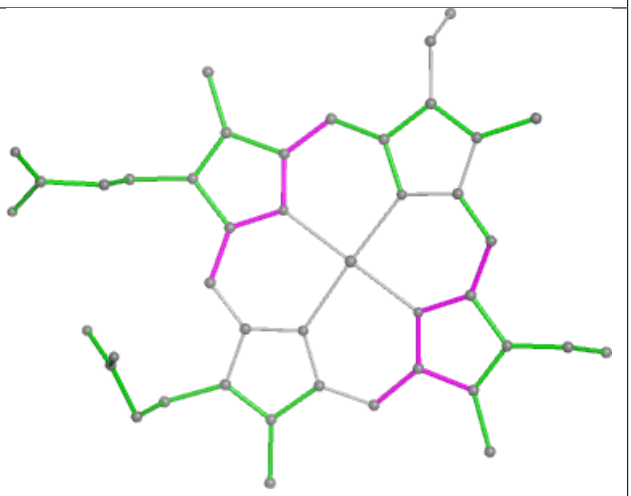


Rings

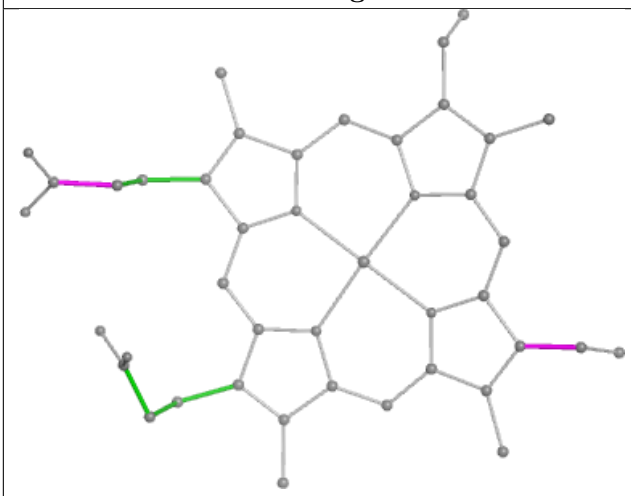
Ligand HEM C 401



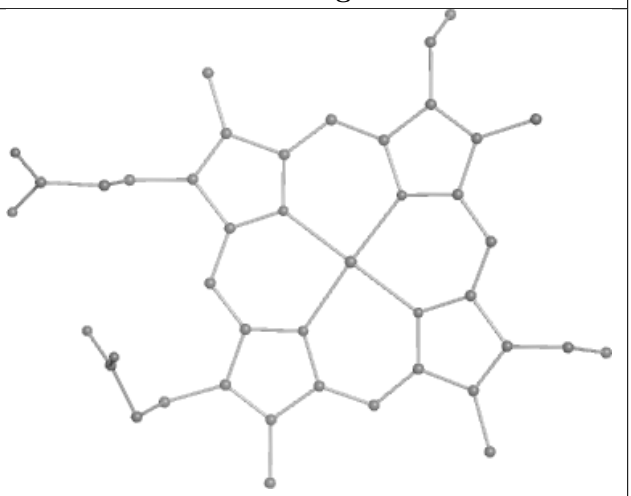
Bond lengths



Bond angles

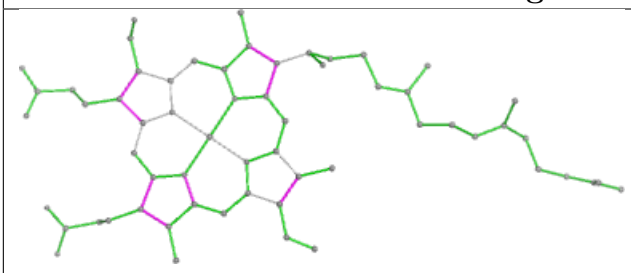


Torsions

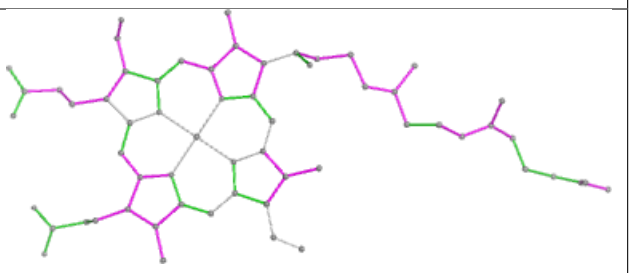


Rings

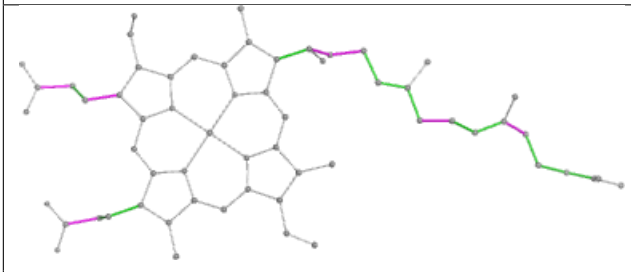
Ligand HEA a 603



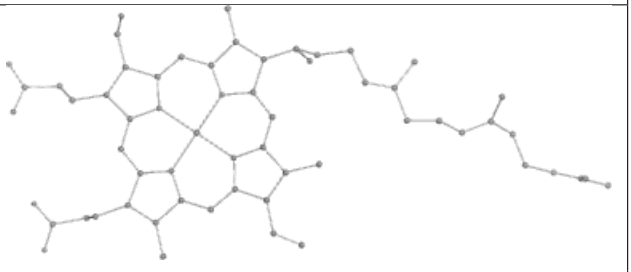
Bond lengths



Bond angles

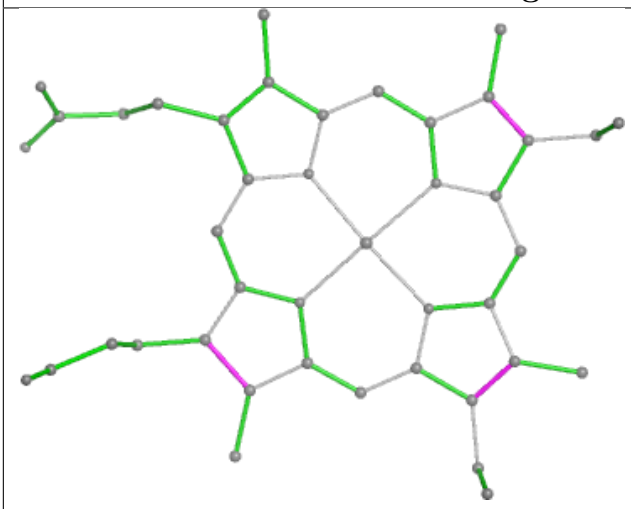


Torsions

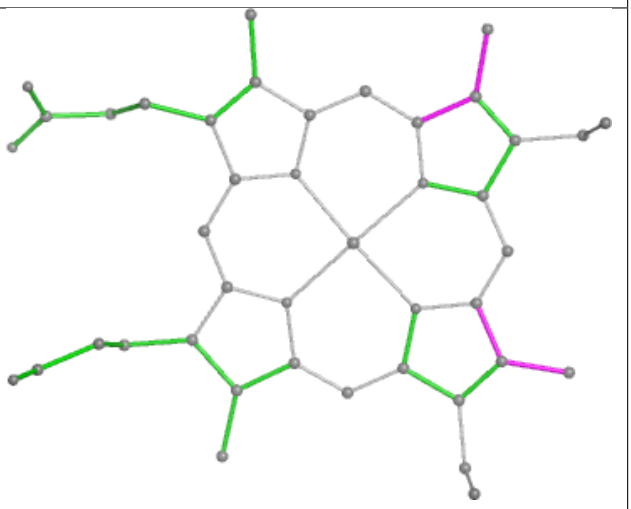


Rings

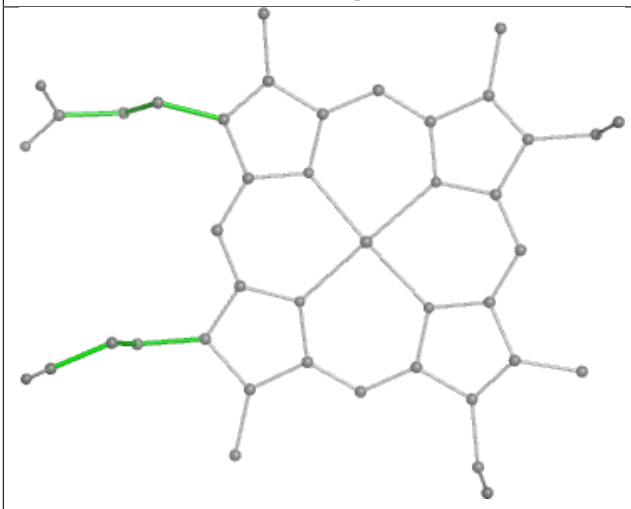
Ligand HEC D 302



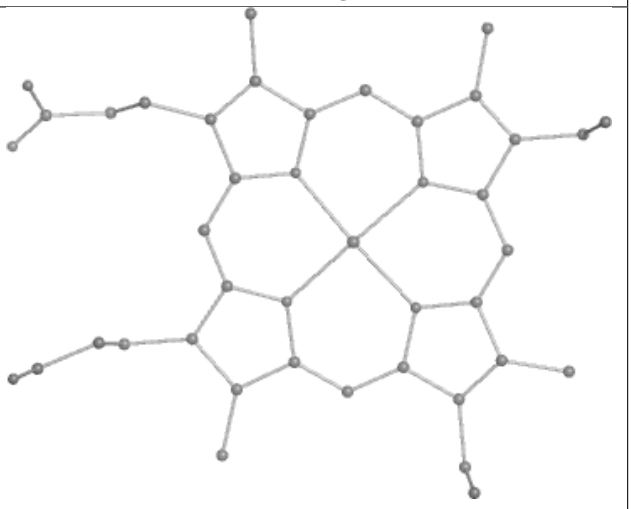
Bond lengths



Bond angles

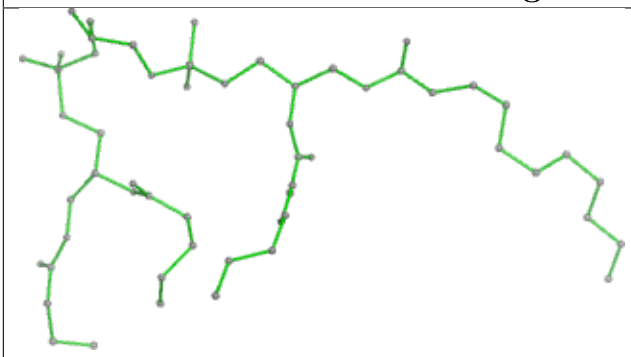


Torsions

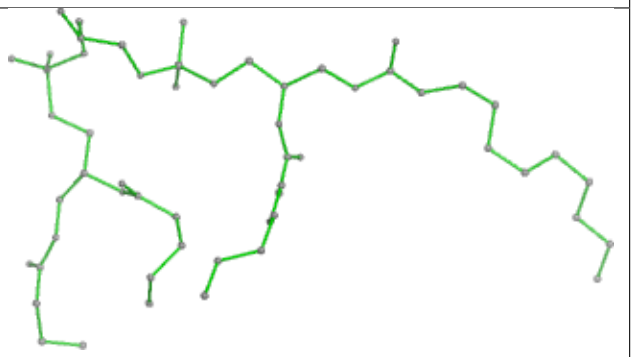


Rings

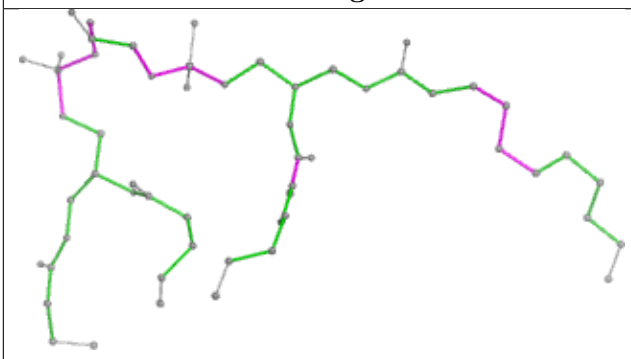
Ligand CDL D 301



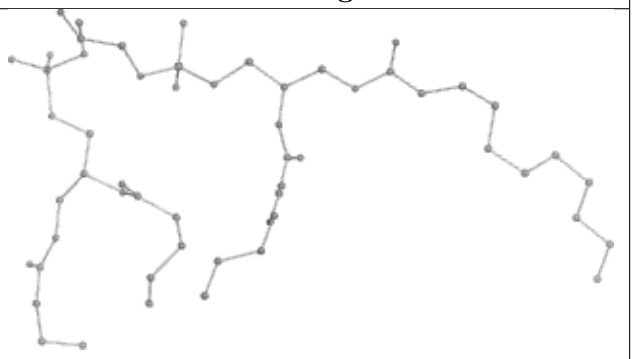
Bond lengths



Bond angles

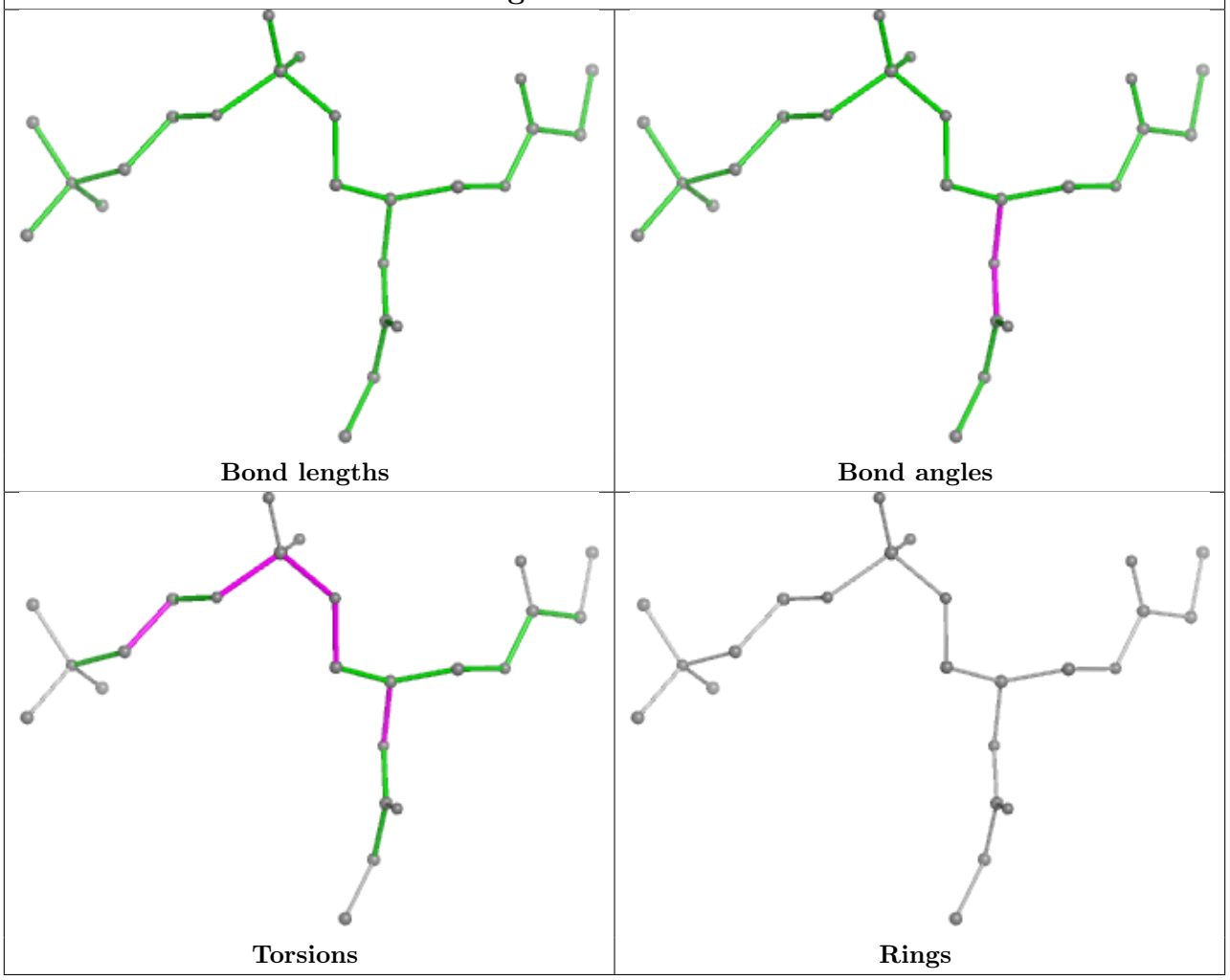


Torsions

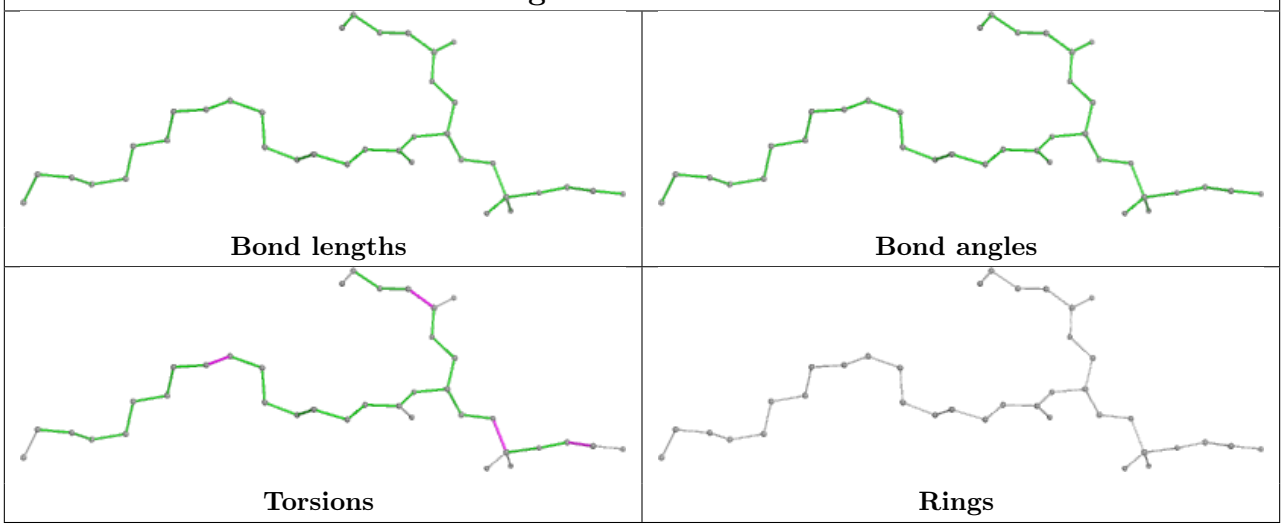


Rings

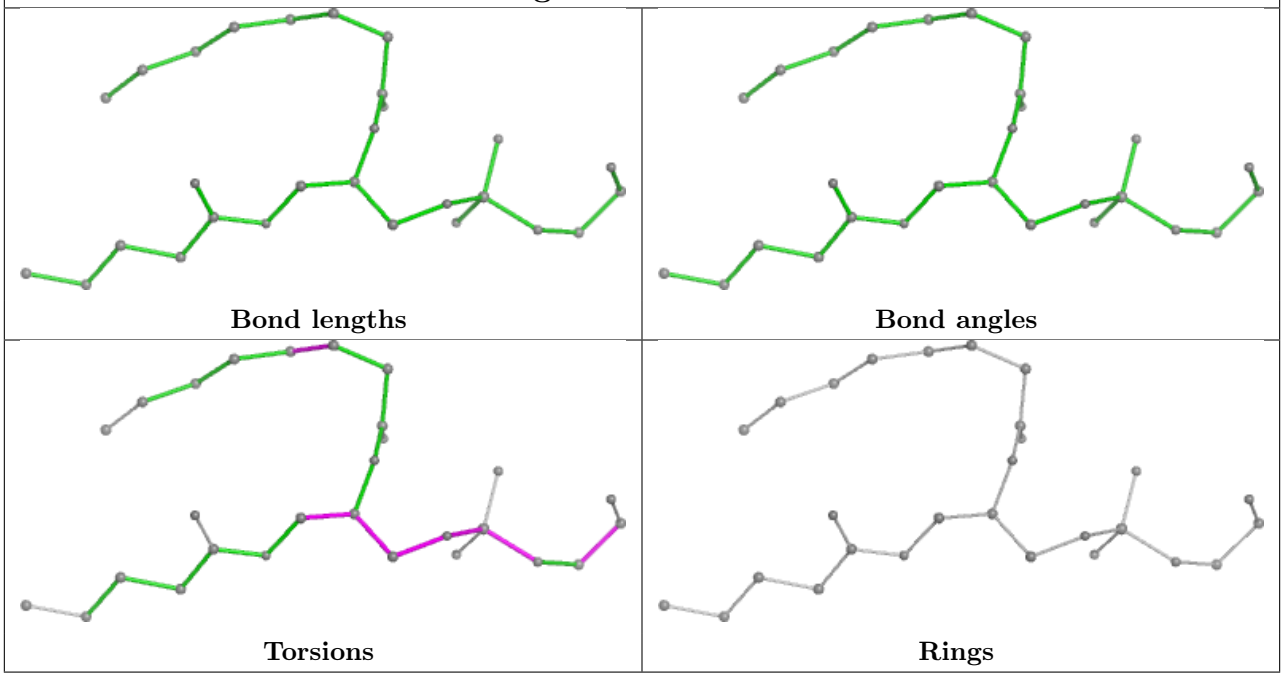
Ligand PC1 L 501



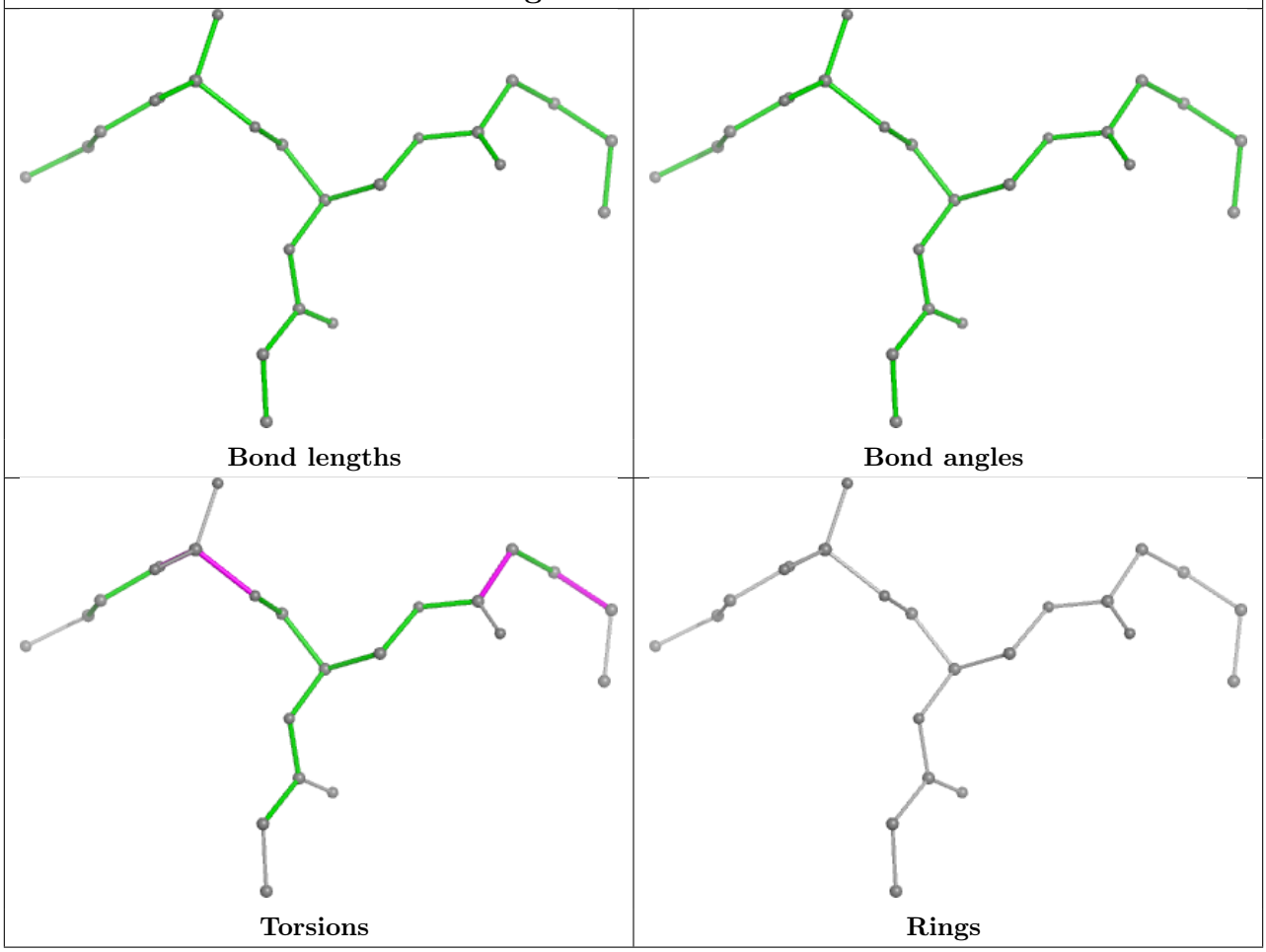
Ligand 3PE N 403



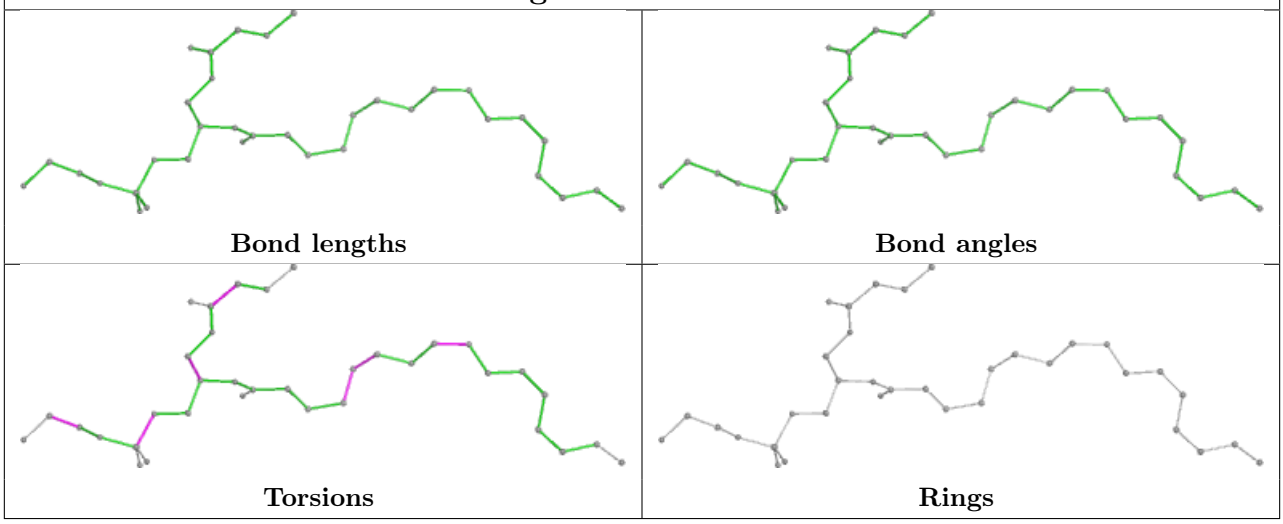
Ligand 3PE a 606



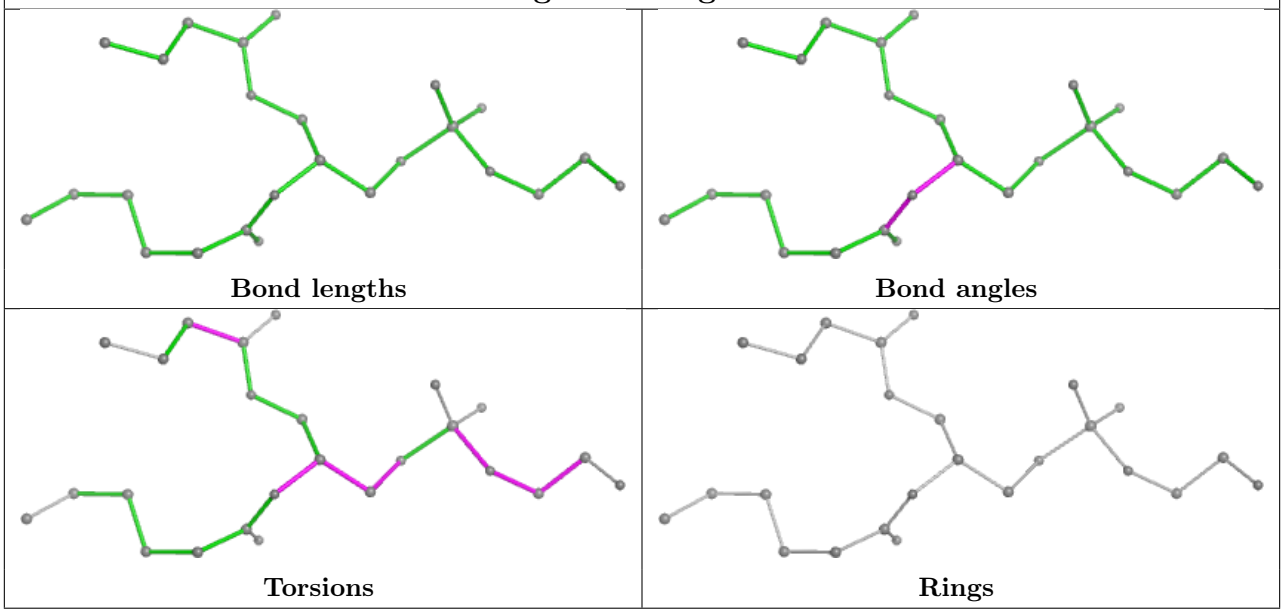
Ligand 3PE L 502



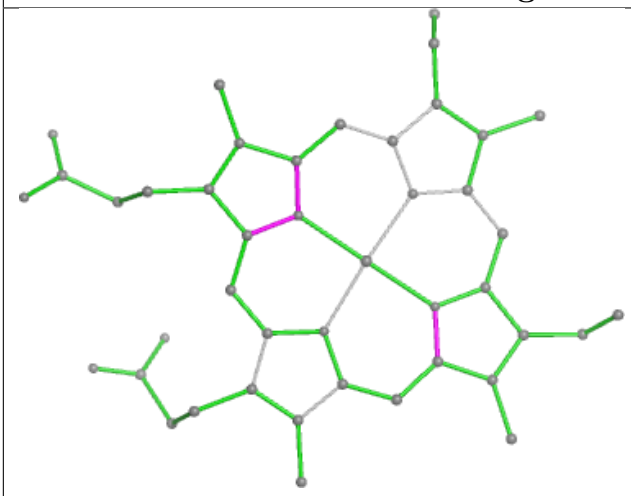
Ligand 3PE C 403



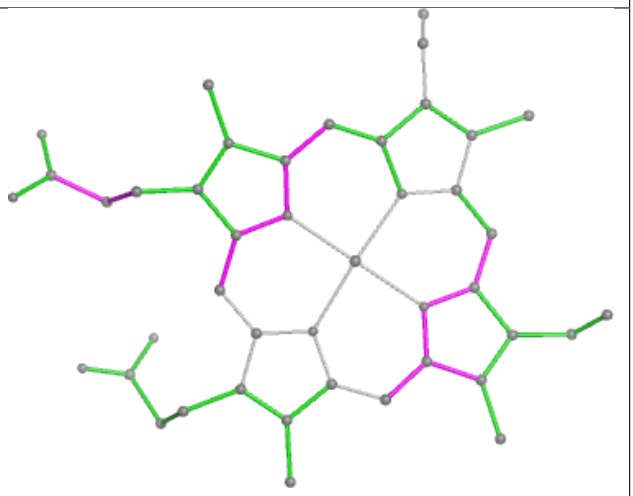
Ligand 3PE g 101



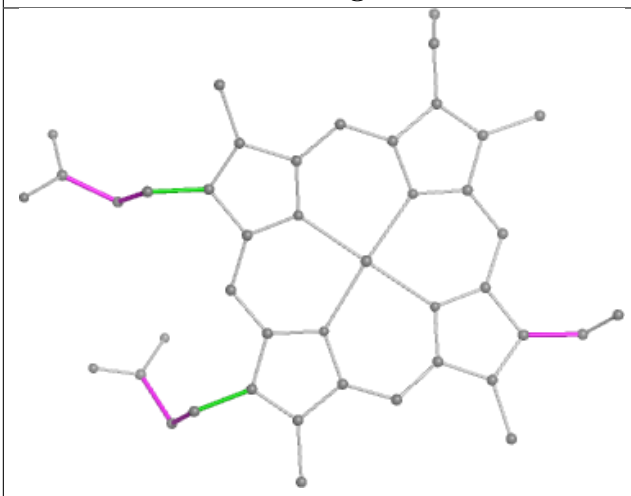
Ligand HEM N 402



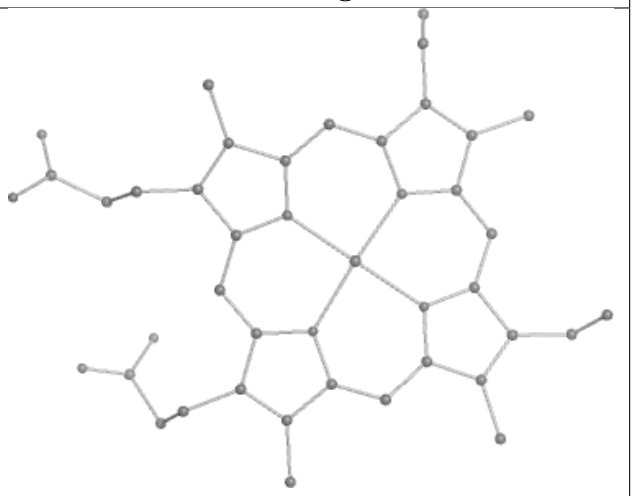
Bond lengths



Bond angles

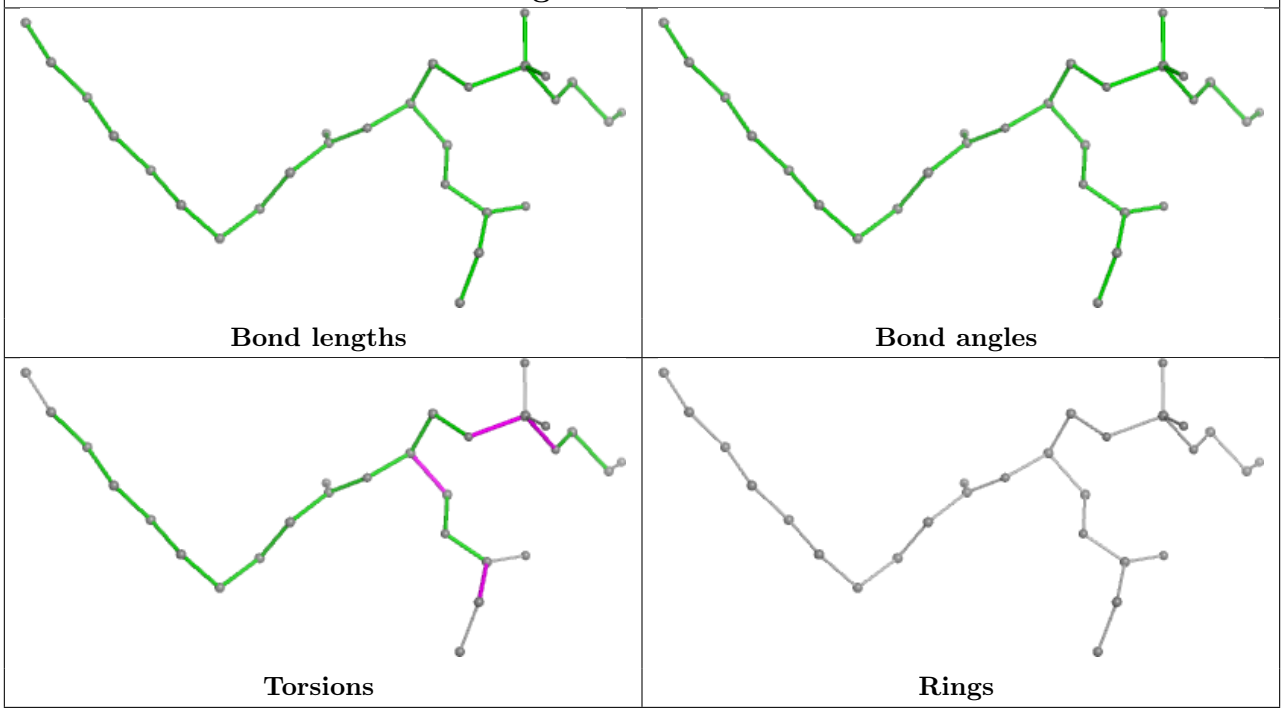


Torsions

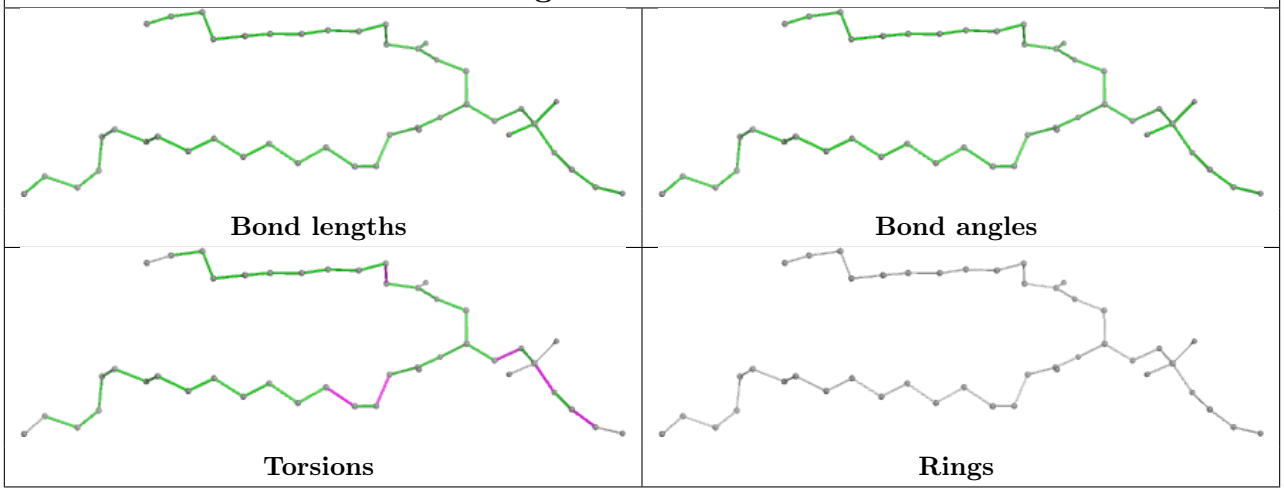


Rings

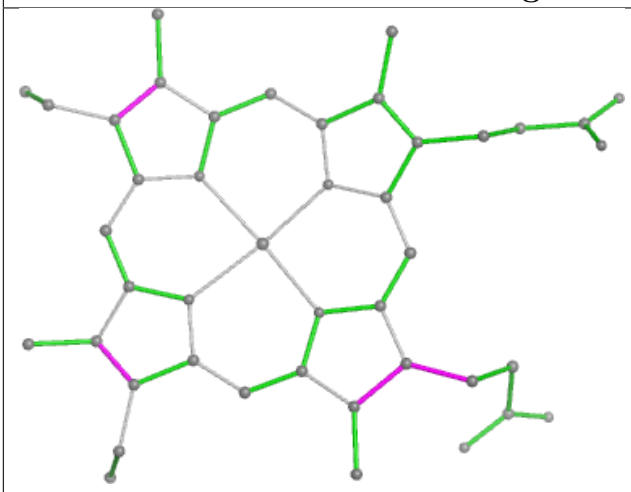
Ligand 3PE b 304



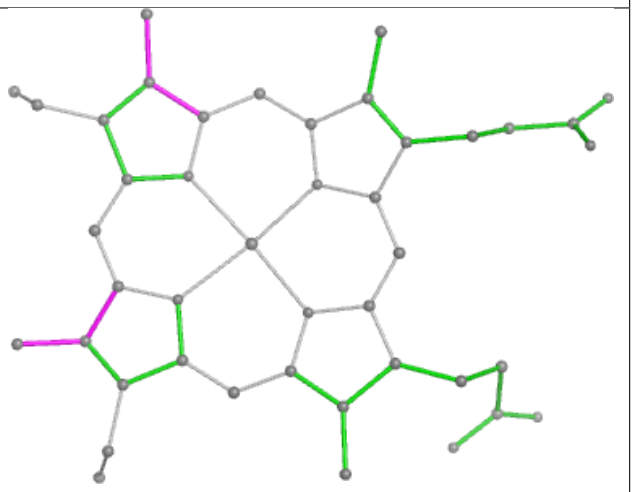
Ligand 3PE c 301



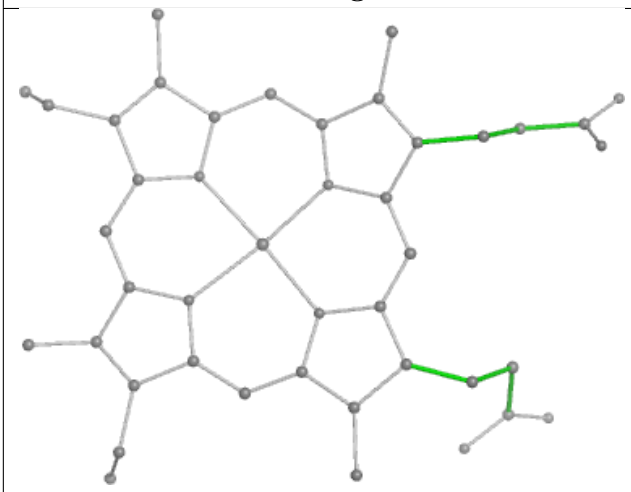
Ligand HEC O 302



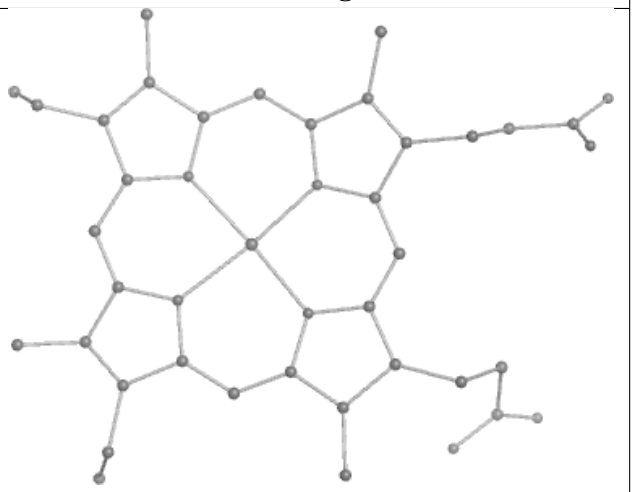
Bond lengths



Bond angles

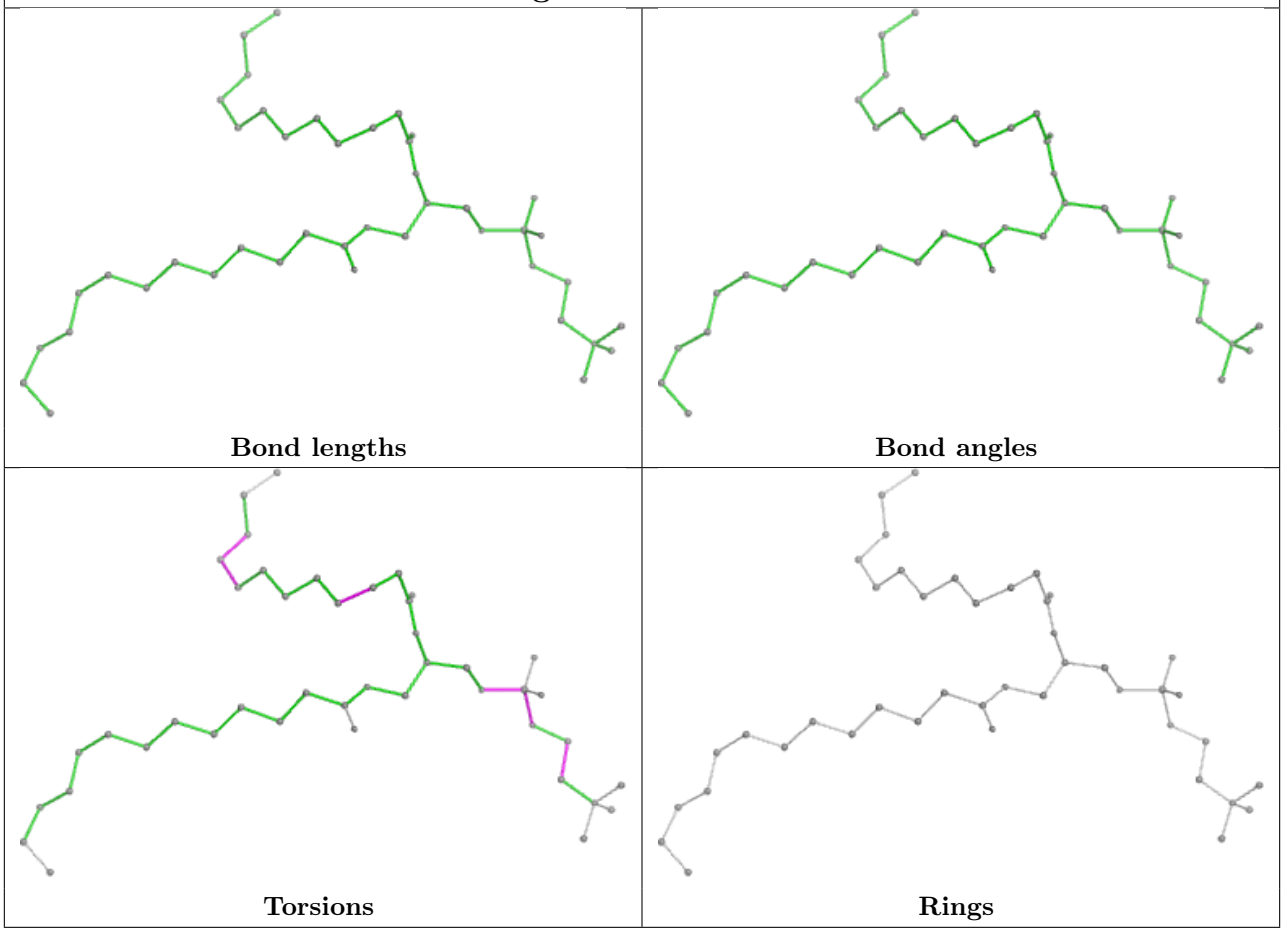


Torsions

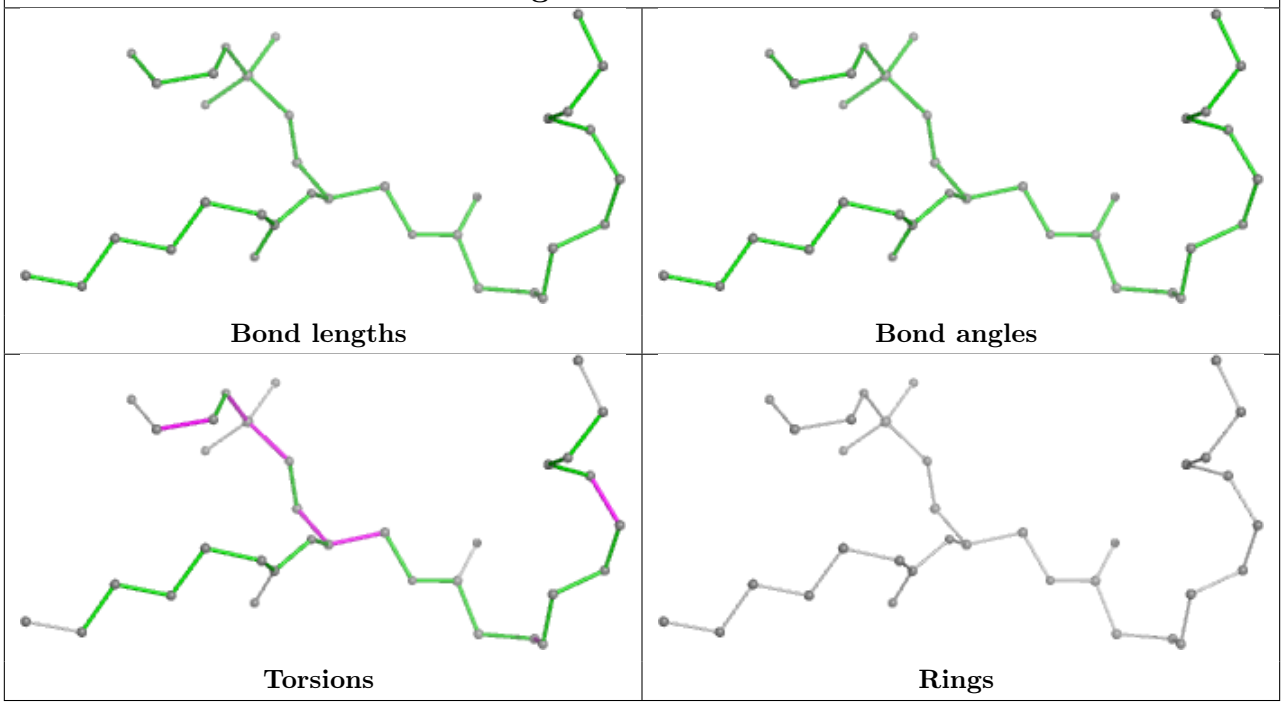


Rings

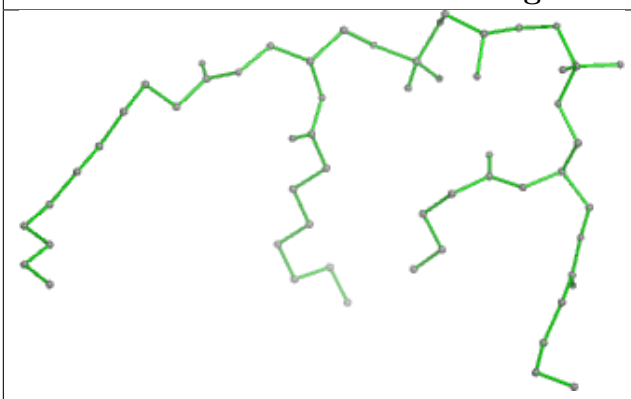
Ligand PC1 a 605



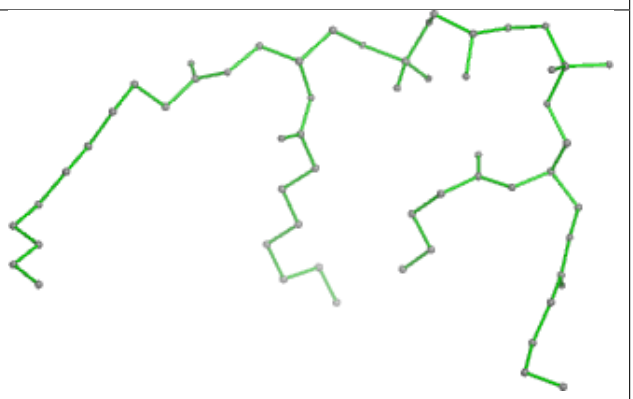
Ligand 3PE F 202



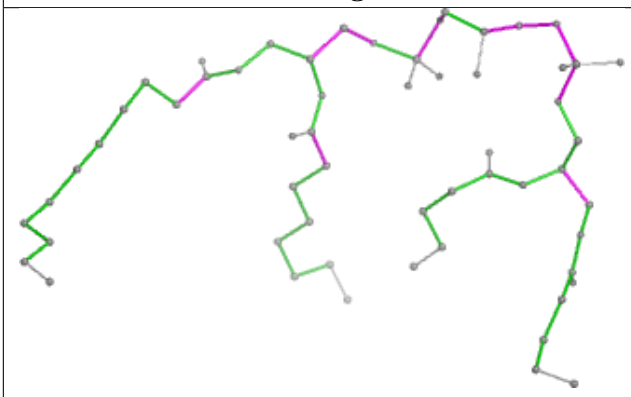
Ligand CDL O 301



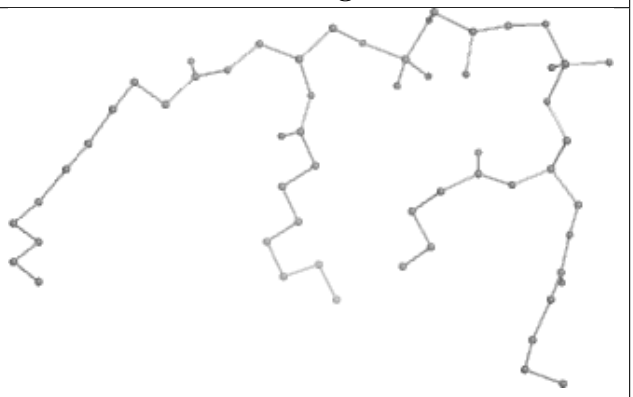
Bond lengths



Bond angles

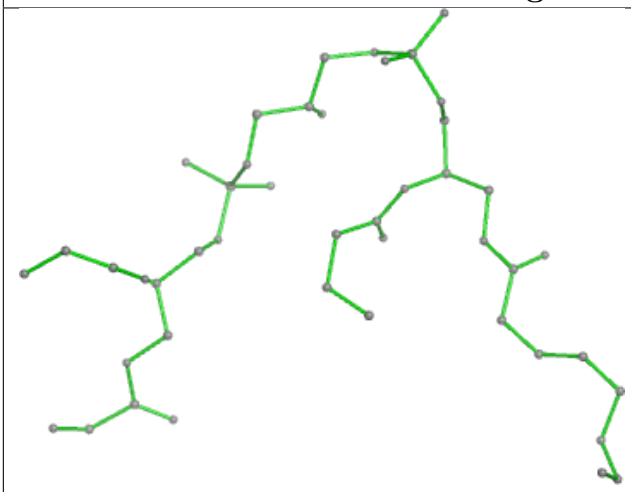


Torsions

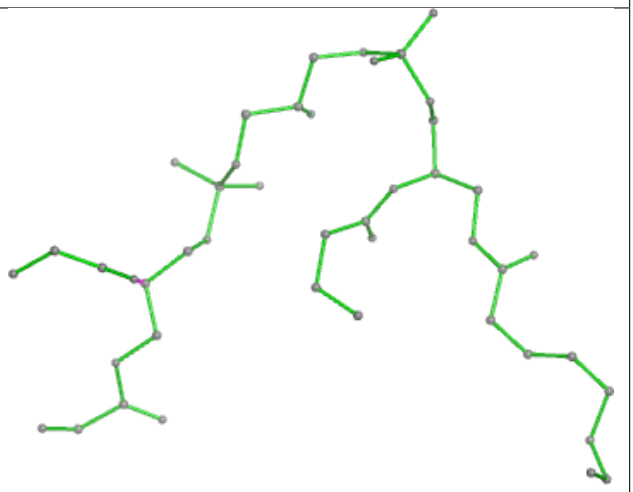


Rings

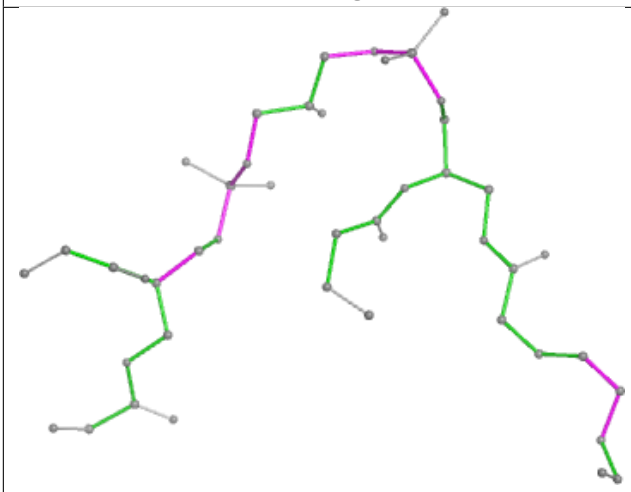
Ligand CDL L 503



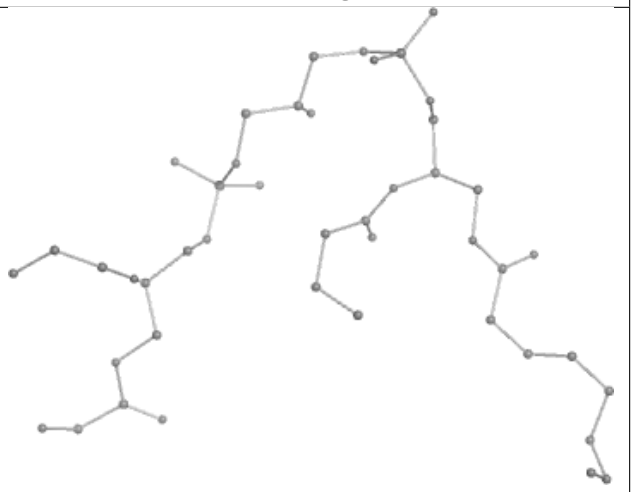
Bond lengths



Bond angles

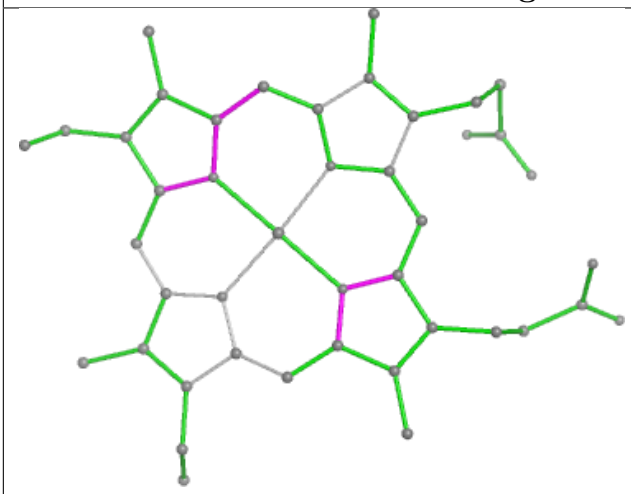


Torsions

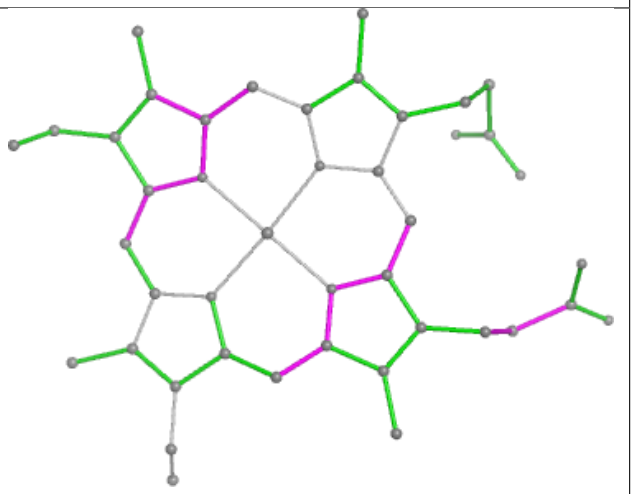


Rings

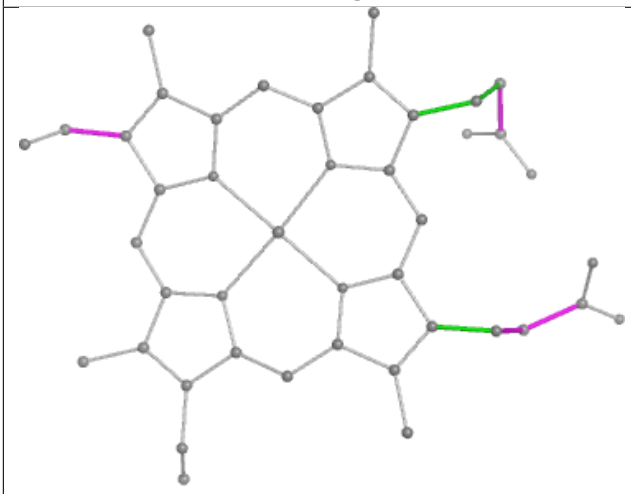
Ligand HEM C 402



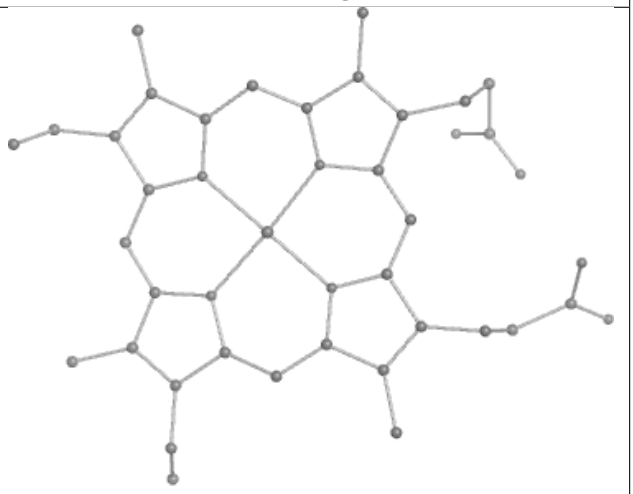
Bond lengths



Bond angles

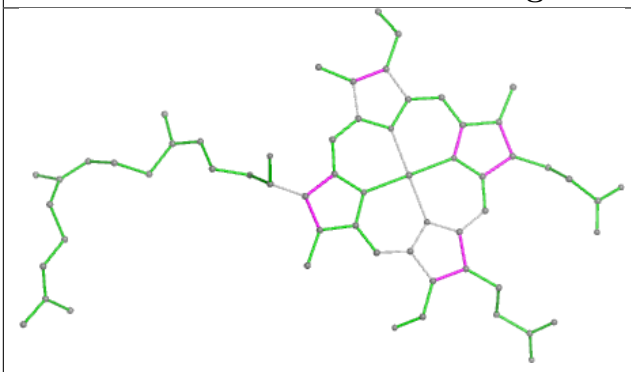


Torsions

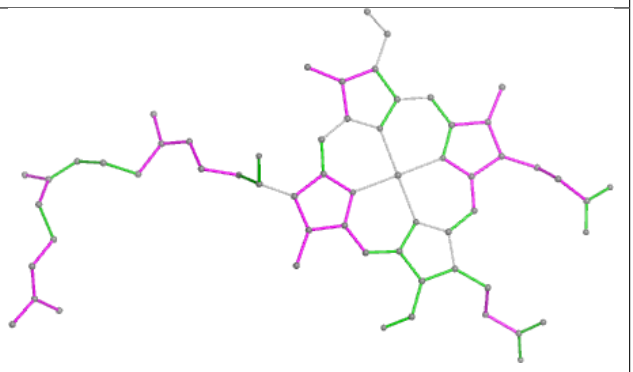


Rings

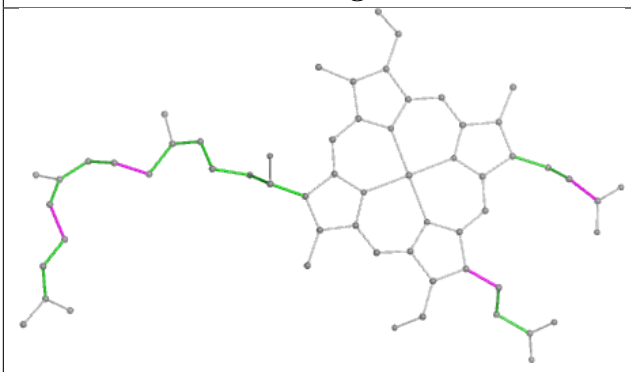
Ligand HEA a 604



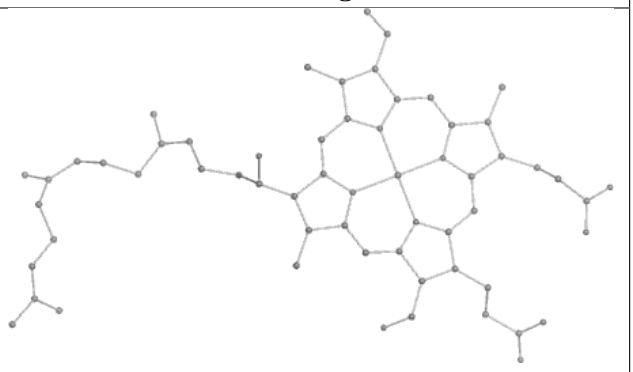
Bond lengths



Bond angles

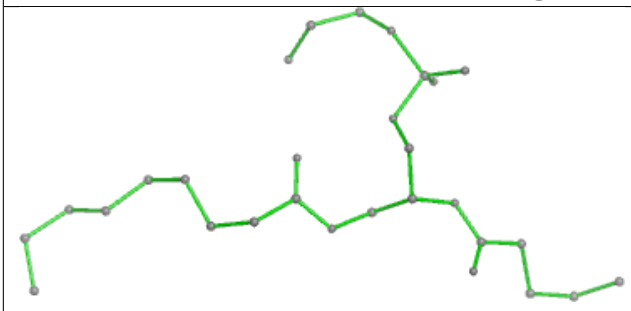


Torsions

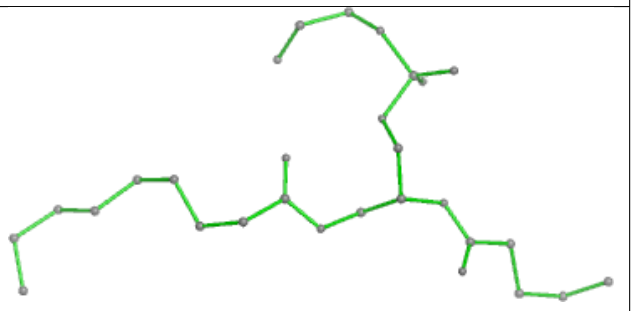


Rings

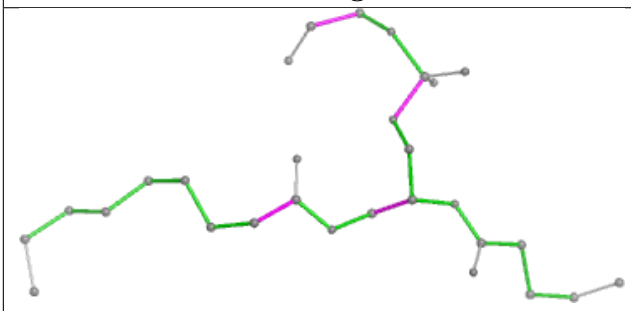
Ligand 3PE F 201



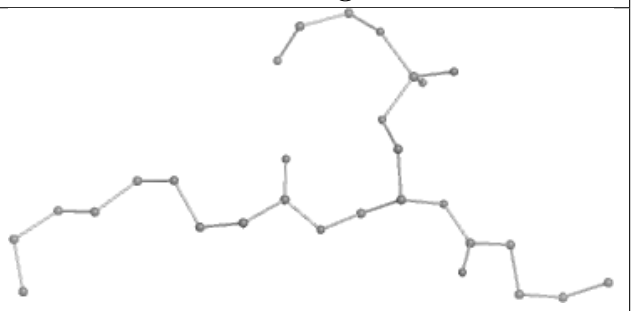
Bond lengths



Bond angles

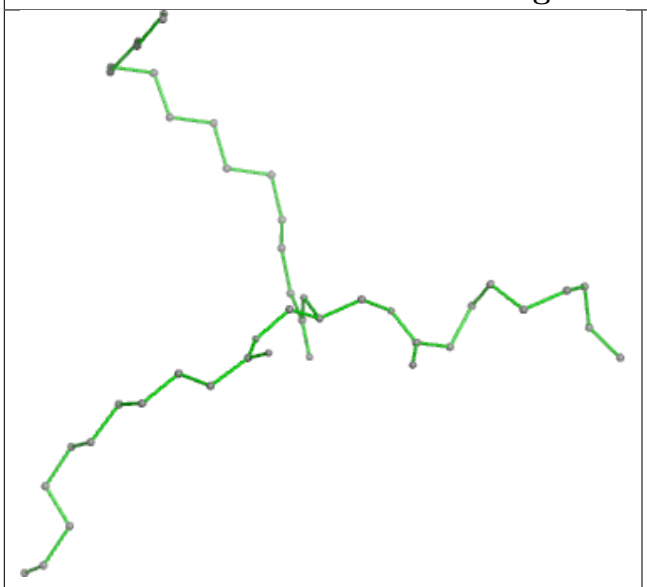


Torsions

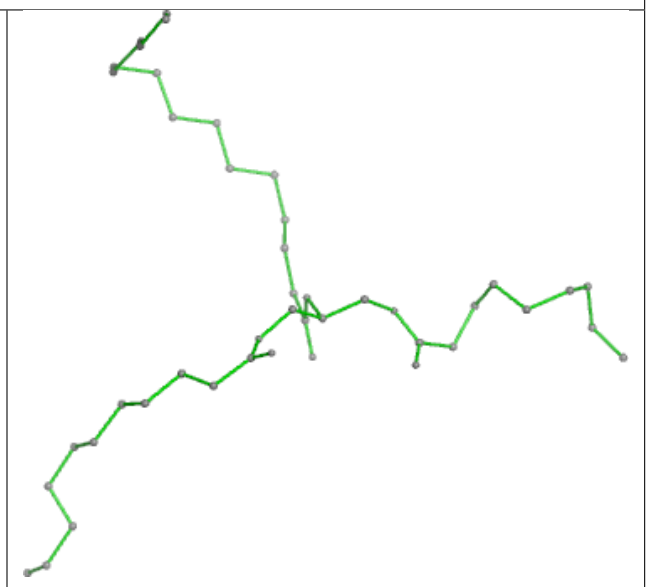


Rings

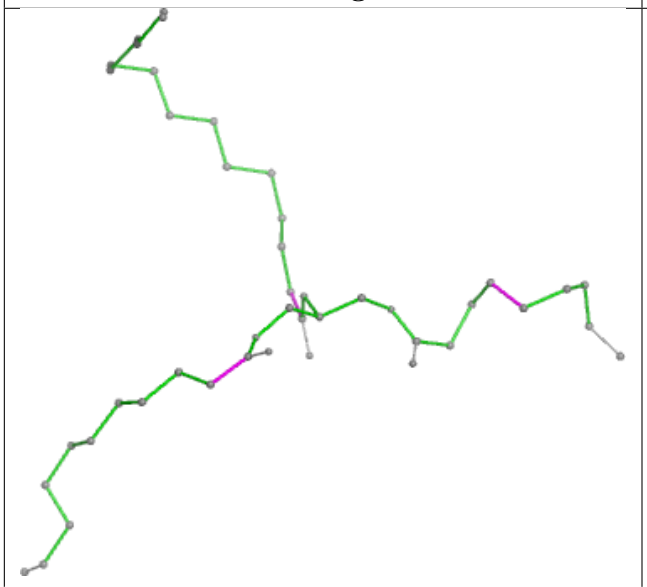
Ligand TGL l 601



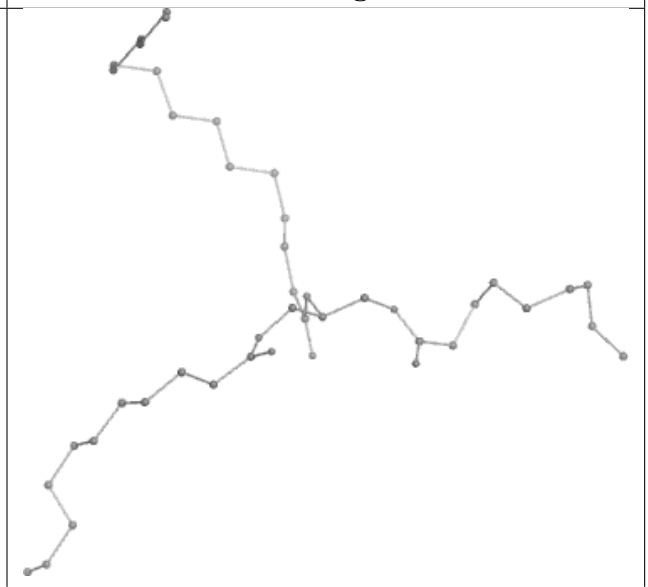
Bond lengths



Bond angles

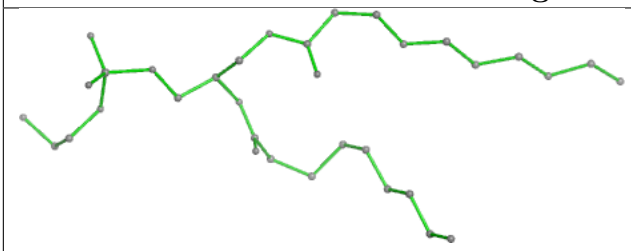


Torsions

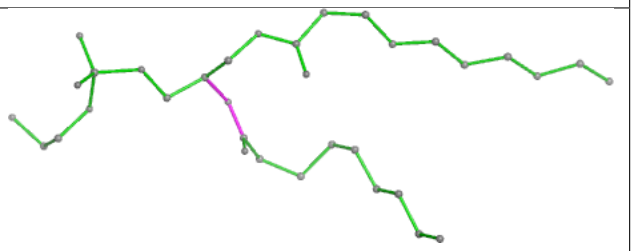


Rings

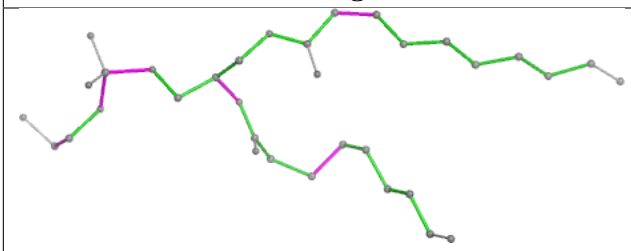
Ligand 3PE d 201



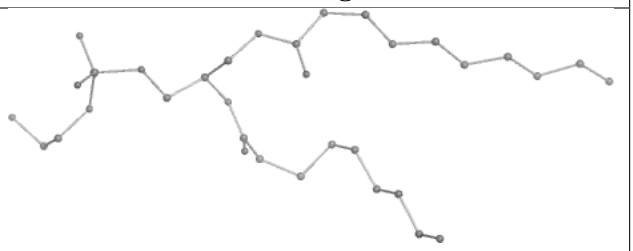
Bond lengths



Bond angles

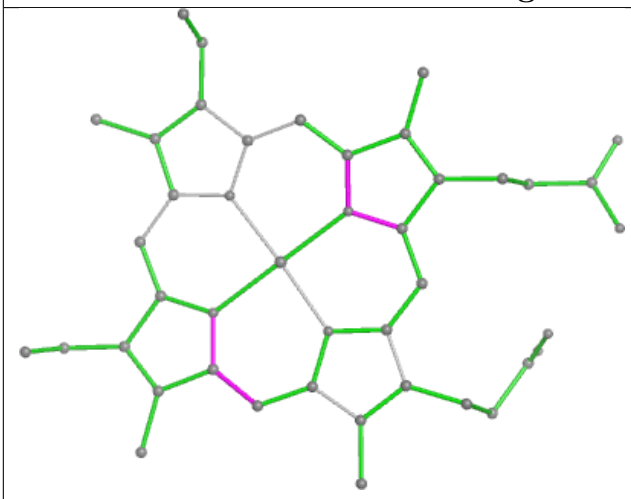


Torsions

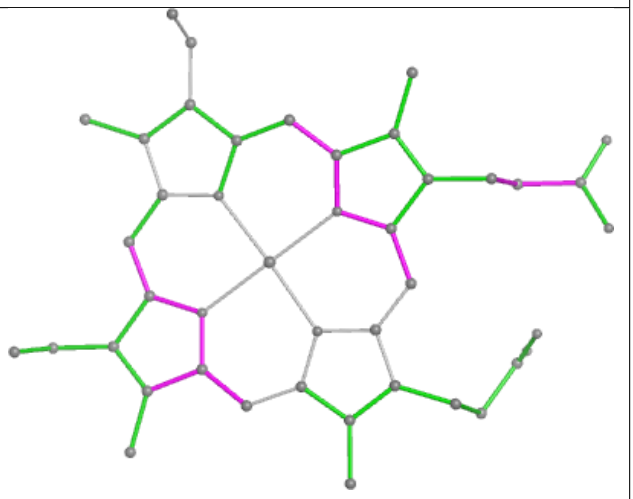


Rings

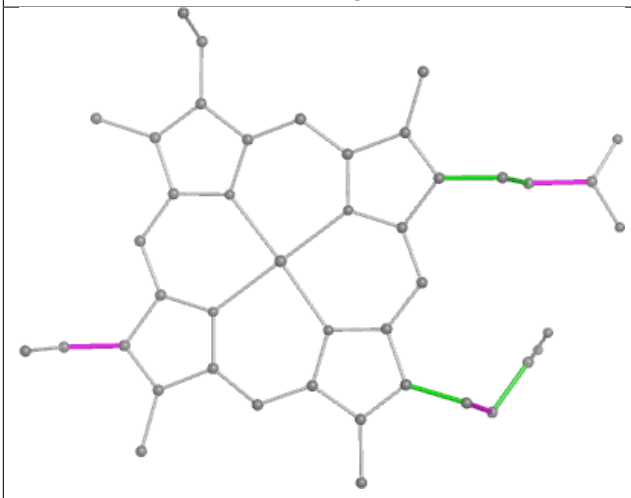
Ligand HEM N 401



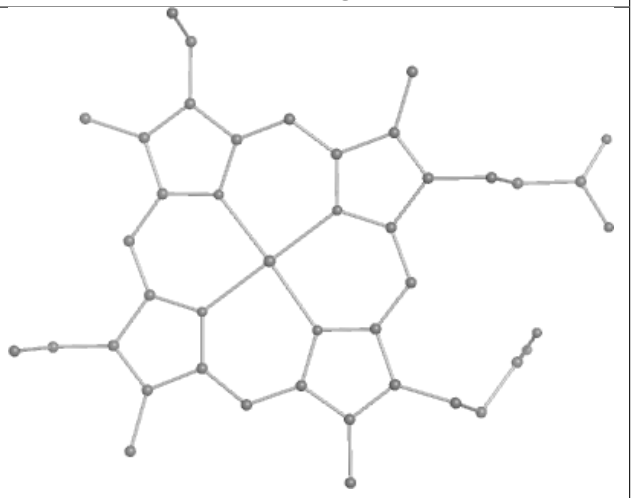
Bond lengths



Bond angles

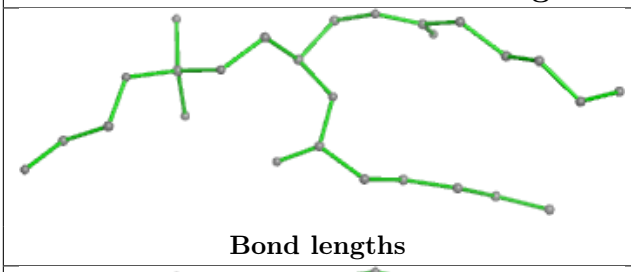


Torsions

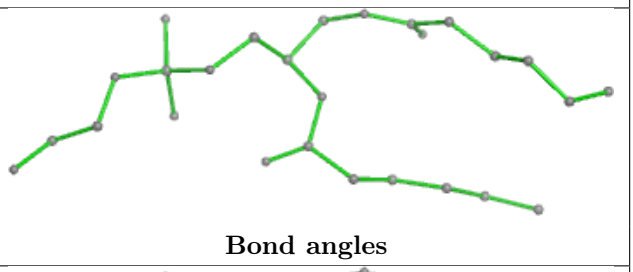


Rings

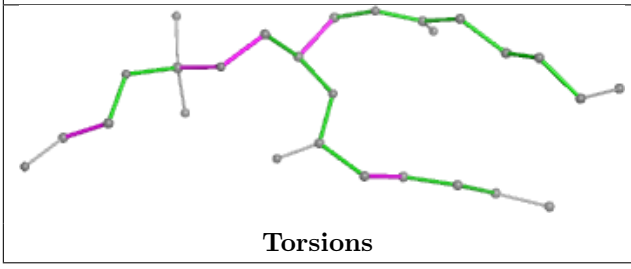
Ligand 3PE k 101



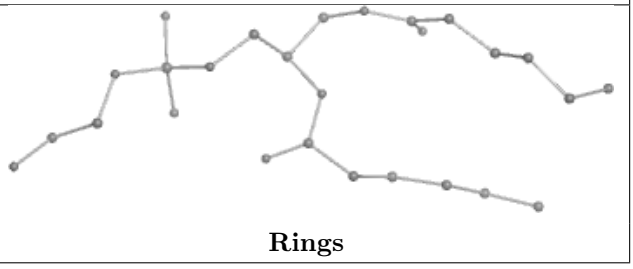
Bond lengths



Bond angles

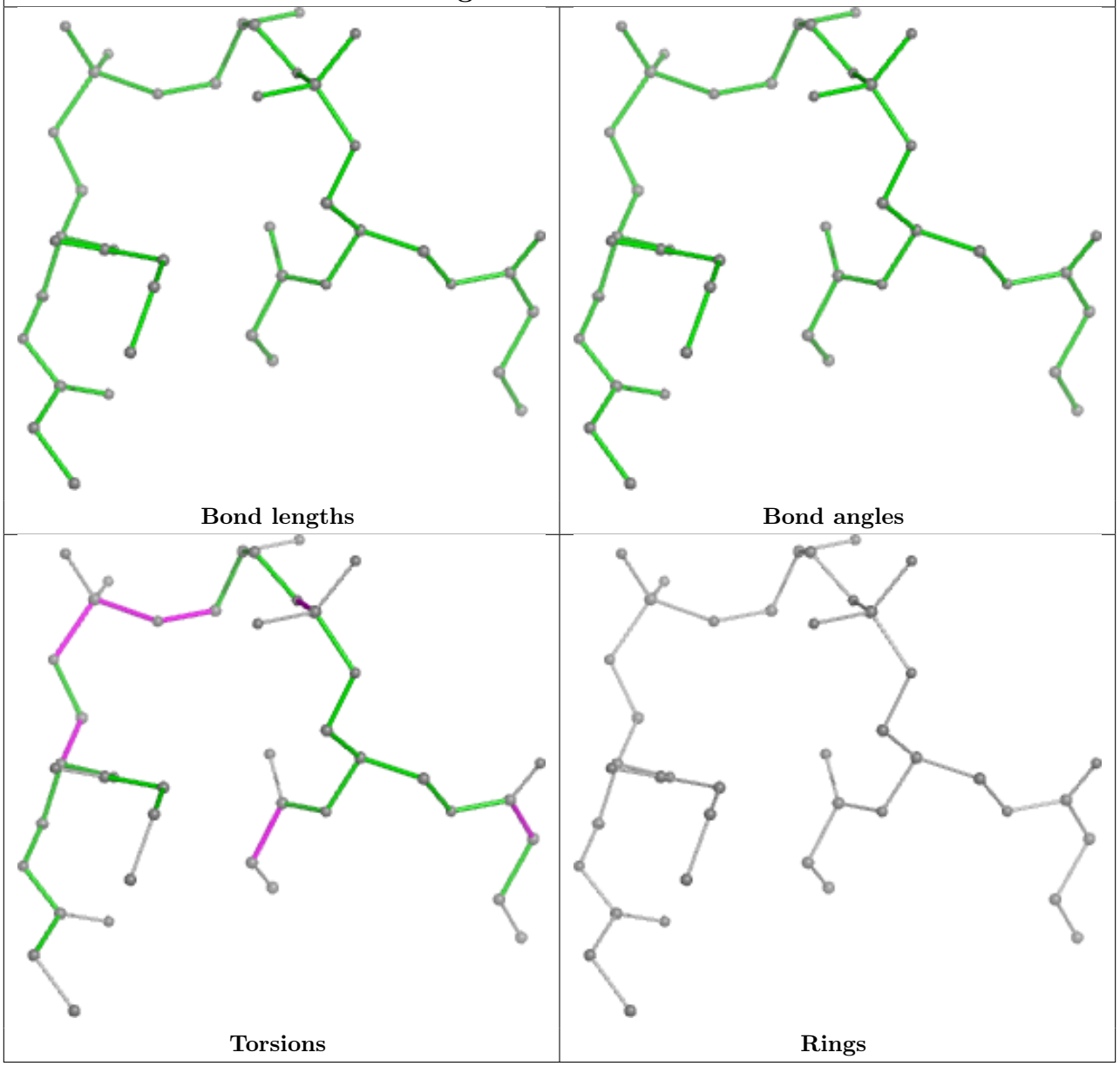


Torsions



Rings

Ligand CDL C 404



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.

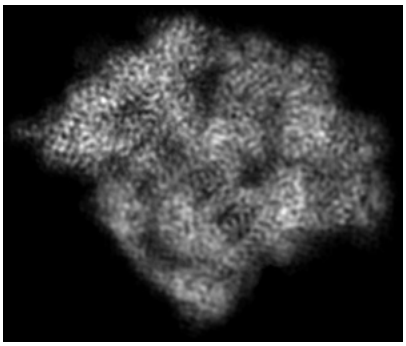
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-12705. These allow visual inspection of the internal detail of the map and identification of artifacts.

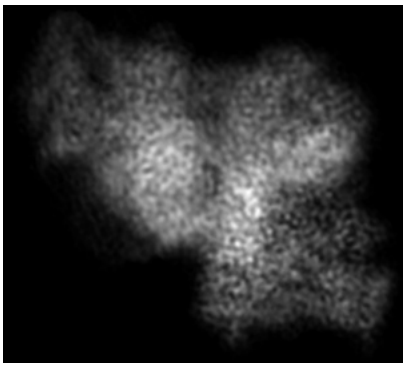
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

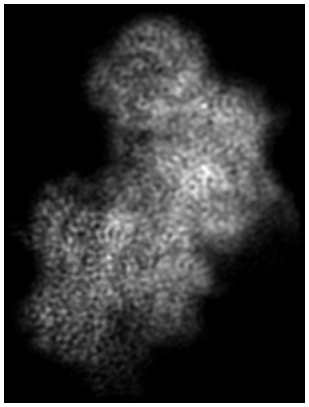
6.1.1 Primary map



X



Y

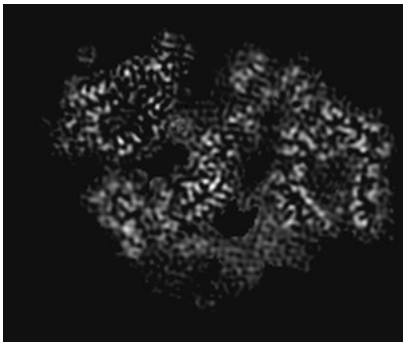


Z

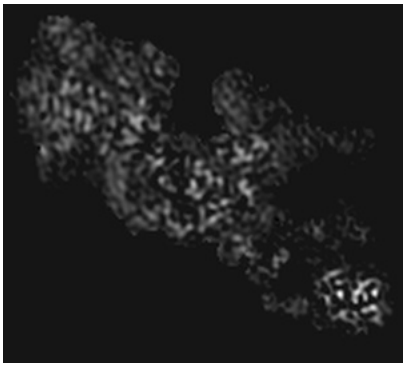
The images above show the map projected in three orthogonal directions.

6.2 Central slices

6.2.1 Primary map



X Index: 76



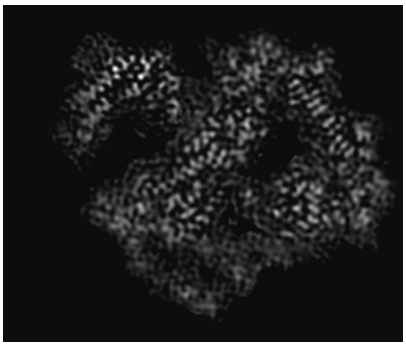
Y Index: 101

Z Index: 85

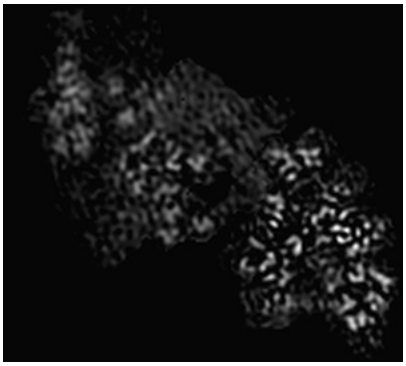
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

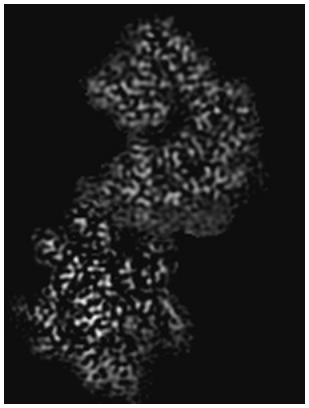
6.3.1 Primary map



X Index: 87



Y Index: 87

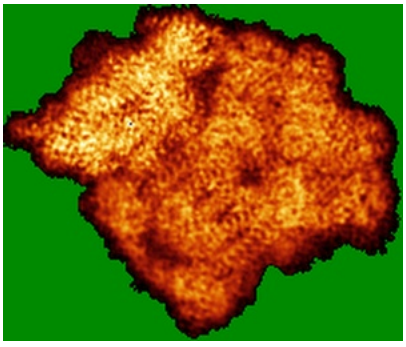


Z Index: 104

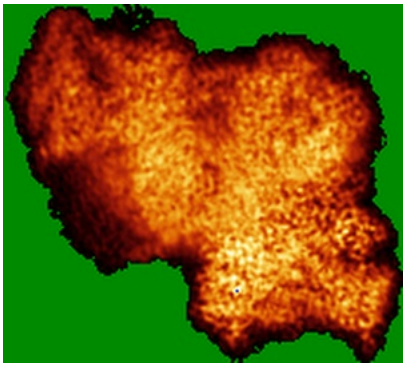
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

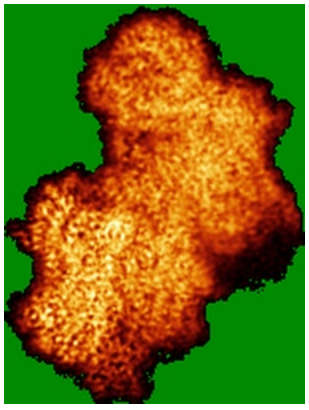
6.4.1 Primary map



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 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

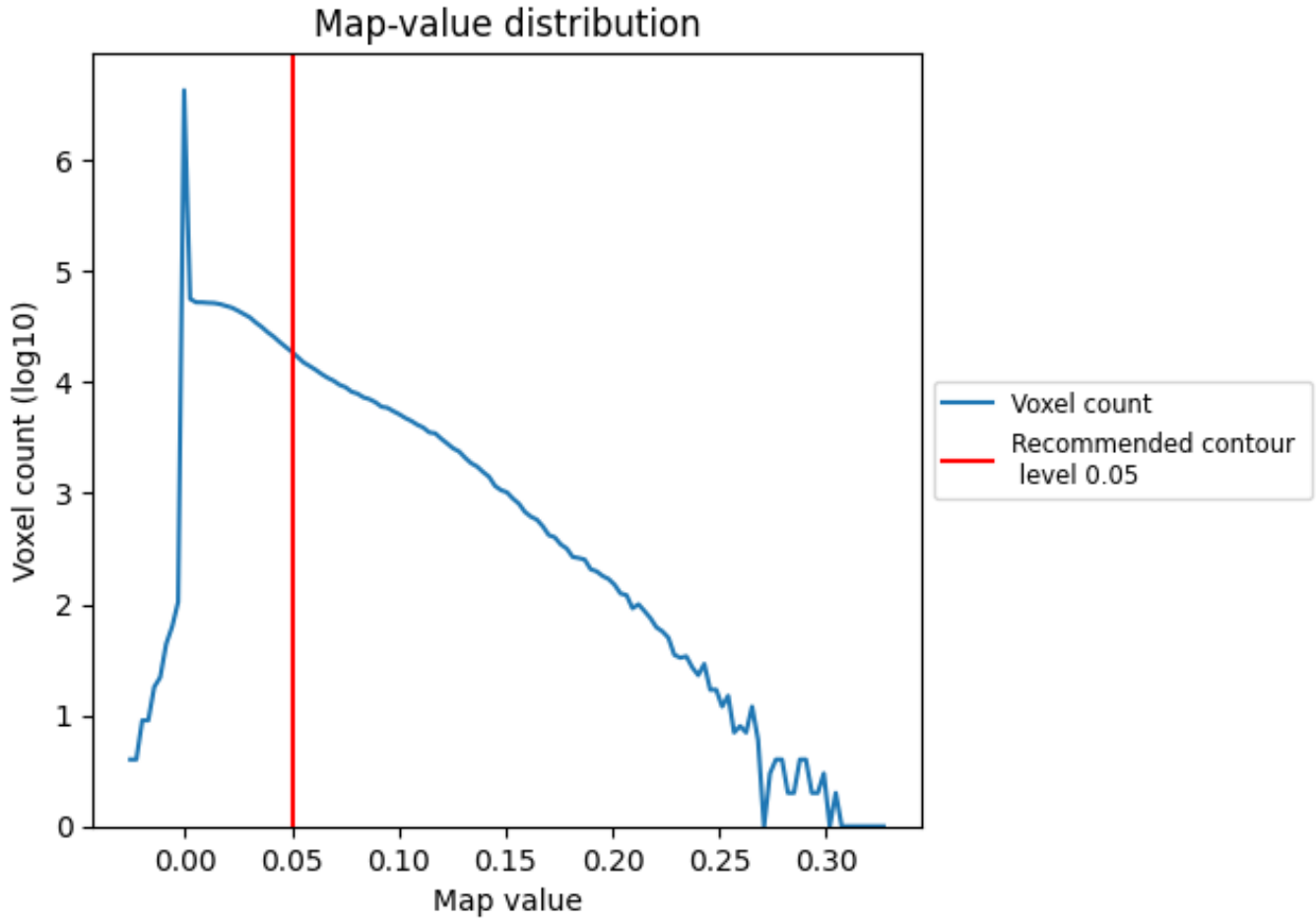
6.6 Mask visualisation (i)

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

7 Map analysis

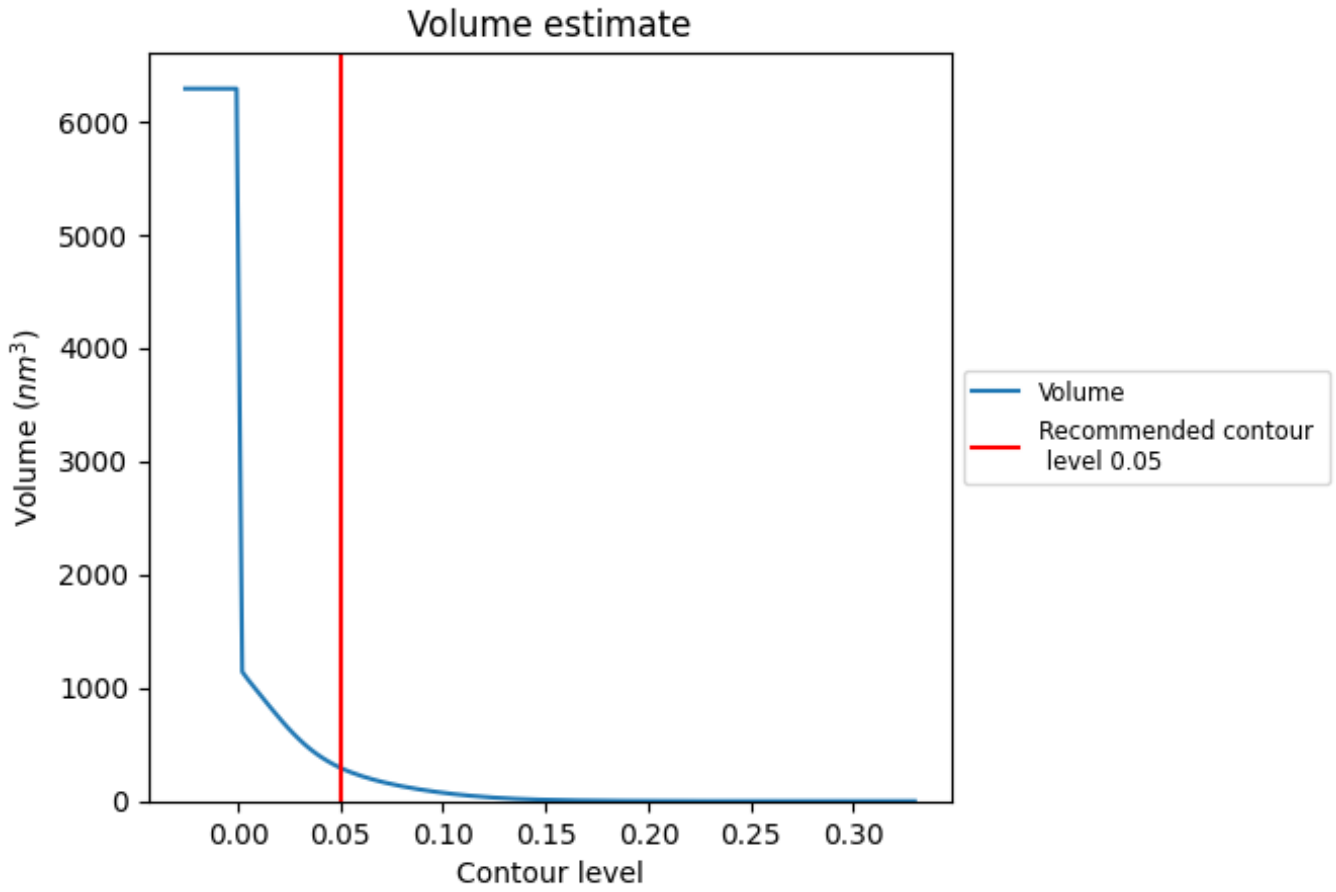
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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 294 nm^3; this corresponds to an approximate mass of 266 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 (i)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

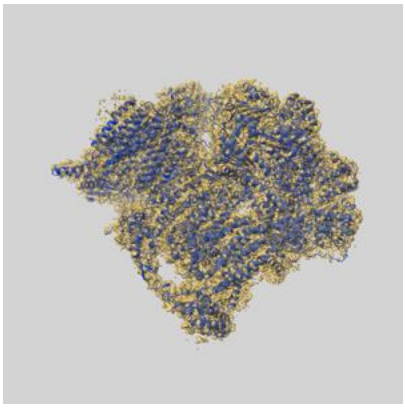
8 Fourier-Shell correlation

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

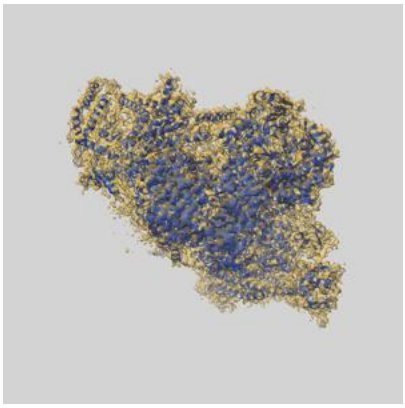
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-12705 and PDB model 7O3E. Per-residue inclusion information can be found in section 3 on page 14.

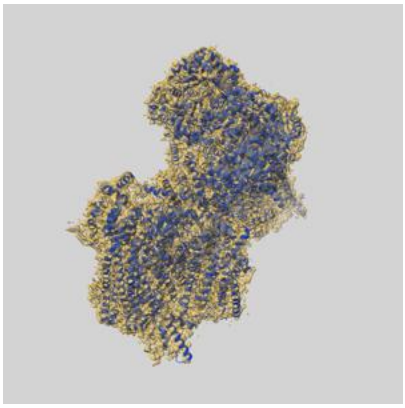
9.1 Map-model overlay



X



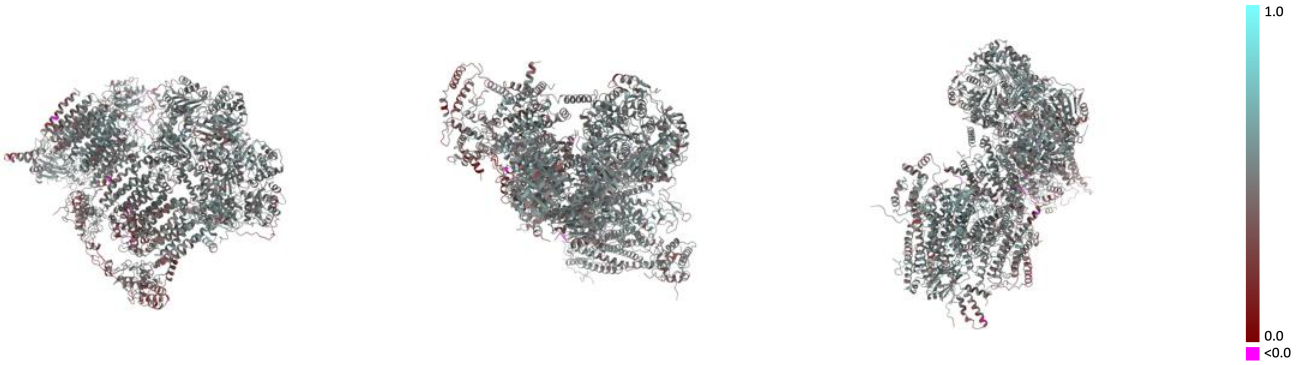
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05 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.

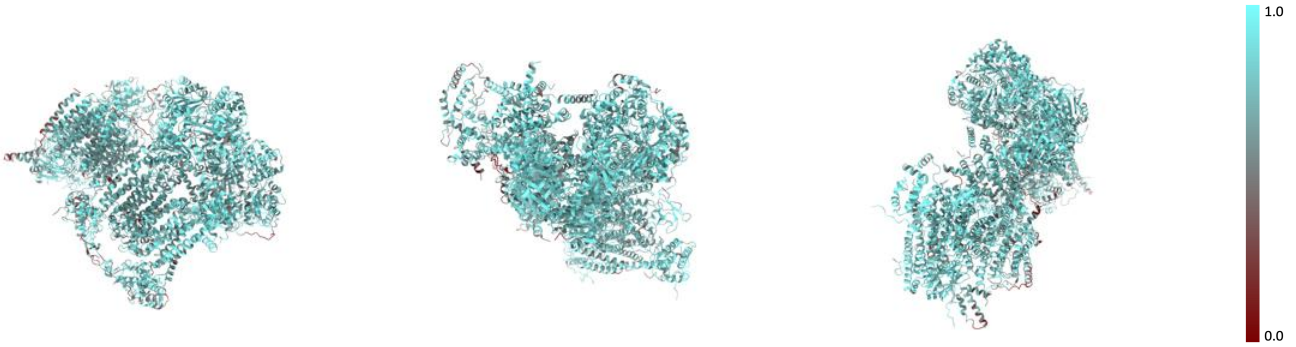
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

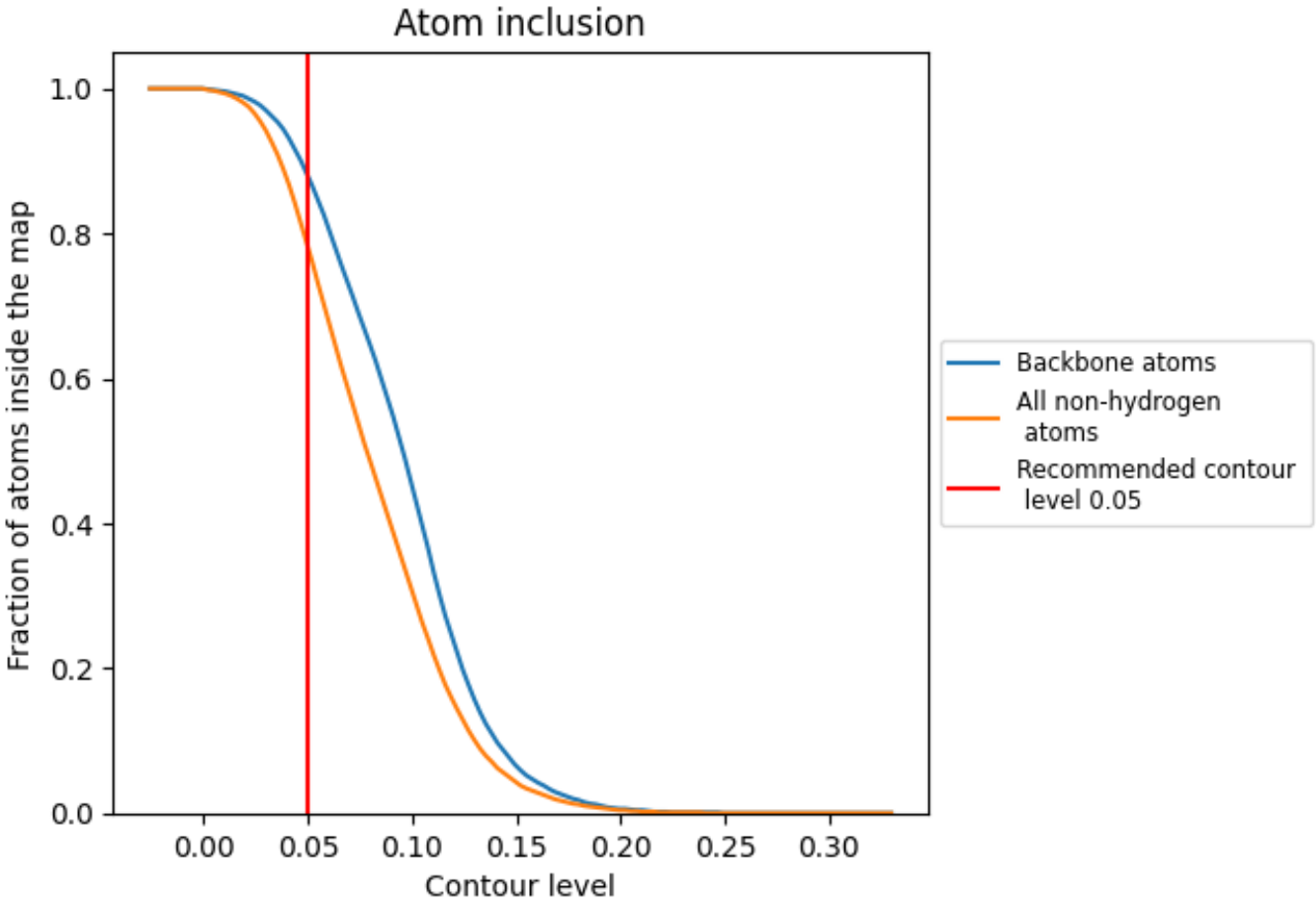
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.05).

9.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 78% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7820	0.4800
A	0.8050	0.4950
B	0.8170	0.5000
C	0.7750	0.4670
D	0.7710	0.4430
F	0.8000	0.5140
G	0.7880	0.4790
H	0.6530	0.3540
I	0.6590	0.4410
J	0.6440	0.3610
L	0.7820	0.4840
M	0.8110	0.4950
N	0.7580	0.4620
O	0.7760	0.4420
P	0.7970	0.4970
Q	0.8120	0.4900
R	0.8070	0.4860
S	0.6350	0.3400
T	0.7650	0.4710
U	0.6630	0.3520
a	0.8280	0.5380
b	0.8190	0.5060
c	0.7800	0.4830
d	0.7790	0.4760
e	0.8540	0.4710
f	0.7920	0.5030
g	0.5490	0.4340
h	0.6630	0.4290
i	0.8290	0.4730
k	0.7710	0.4920
l	0.7770	0.5350
m	0.7150	0.4380