Full wwPDB EM Validation Report ⓘ

Aug 26, 2026 – 02:29 pm BST

PDB ID	:	7O3C / pdb_00007o3c
EMDB ID	:	EMD-12703
Title	:	Murine supercomplex CIII2CIV in the mature unlocked conformation
Authors	:	Vercellino, I.; Sazanov, L.A.
Deposited on	:	2021-04-01
Resolution	:	3.30 Å(reported)
Based on initial models	:	5Z62, 3L75, 1NTZ, 5IY5

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

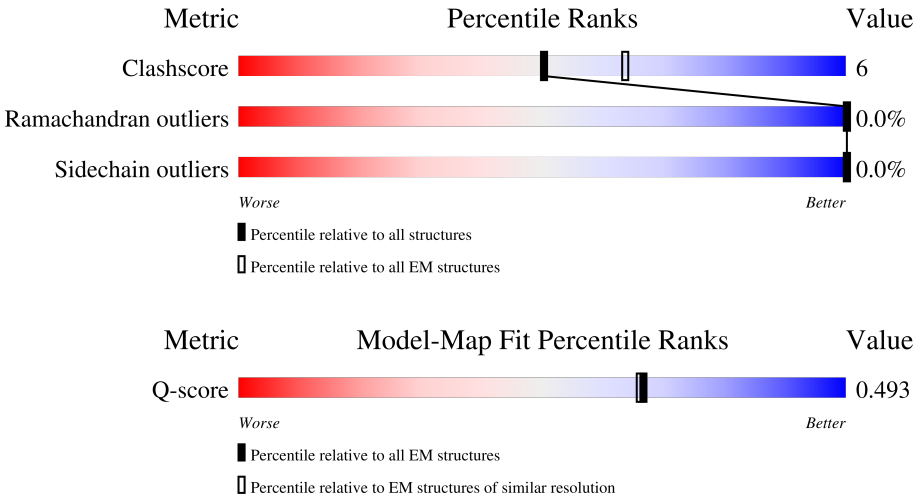
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.30 Å.

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



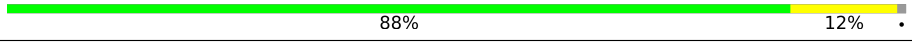
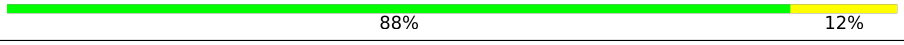
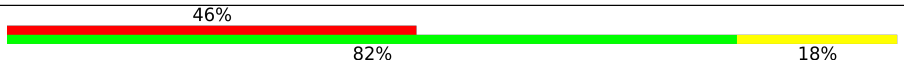
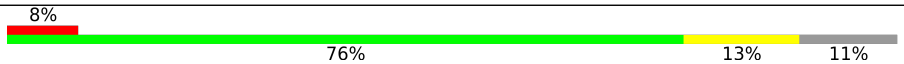
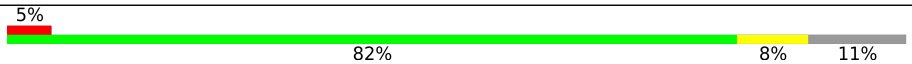
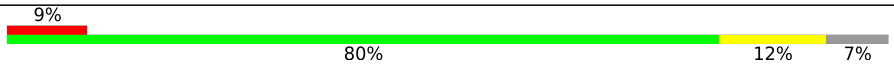
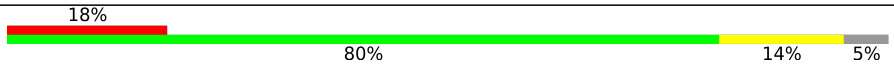
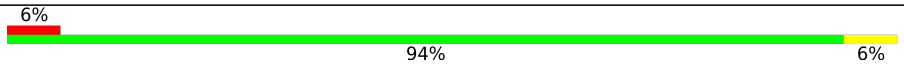
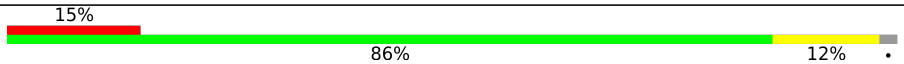
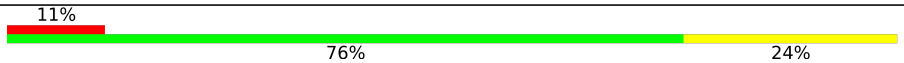
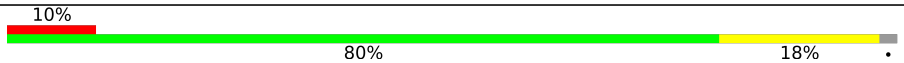
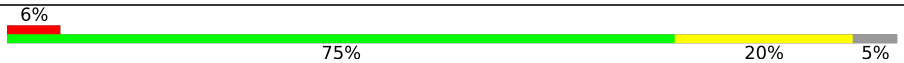
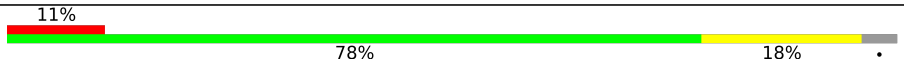
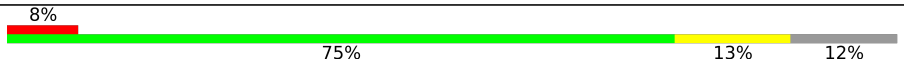
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 (2.80 - 3.80)

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	86% 14%
1	L	446	90% 10%
2	B	439	85% 11%
2	M	439	81% 14%

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Mol	Chain	Length	Quality of chain
3	C	381	
3	N	381	
4	D	241	
4	O	241	
5	E	196	
5	P	196	
6	F	110	
6	Q	110	
7	G	81	
7	R	81	
8	H	76	
8	S	76	
9	J	63	
9	U	63	
10	K	56	
10	V	56	
11	T	78	
12	I	113	
13	a	514	
14	b	227	
15	c	261	
16	d	147	
17	e	109	
18	f	99	
19	g	85	

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Mol	Chain	Length	Quality of chain
20	h	85	12% 78% 14% 7%
21	i	75	11% 76% 20%
22	k	56	70% 18% 12%
23	l	47	77% 21%
24	m	46	9% 70% 24% 7%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
28	HEC	D	302	X	-	-	-
28	HEC	O	303	X	-	-	-

2 Entry composition (i)

There are 37 unique types of molecules in this entry. The entry contains 48532 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	379	Total	C	N	O	S	0	0
			3038	2047	472	498	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 Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	196	Total	C	N	O	S	0	0
			1512	952	263	290	7		
5	P	196	Total	C	N	O	S	0	0
			1512	952	263	290	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	102	Total	C	N	O	S	0	0
			900	575	160	162	3		
6	Q	101	Total	C	N	O	S	0	0
			894	572	159	160	3		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	74	Total	C	N	O	0	0
			624	404	117	103		
7	R	72	Total	C	N	O	0	0
			609	396	112	101		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	68	Total	C	N	O	S	0	0
			563	343	103	112	5		
8	S	68	Total	C	N	O	S	0	0
			563	343	103	112	5		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
9	J	58	Total	C	N	O	0	0
			481	316	83	82		
9	U	60	Total	C	N	O	0	0
			495	323	86	86		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	52	Total	C	N	O	S	0	0
			429	286	75	66	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	V	53	Total	C	N	O	S	0	0
			438	292	77	67	2		

- Molecule 11 is a protein called Cytochrome b-c1 complex subunit 9.

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

- Molecule 12 is a protein called Cox7a2l protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	I	111	Total	C	N	O	S	0	0
			838	546	139	148	5		

- Molecule 13 is a protein called Cytochrome c oxidase subunit 1.

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

- Molecule 14 is a protein called Cytochrome c oxidase subunit 2.

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

- Molecule 15 is a protein called Cytochrome c oxidase subunit 3.

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

- Molecule 16 is a protein called Cytochrome c oxidase subunit 4 isoform 1, mitochondrial.

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

- Molecule 17 is a protein called Cytochrome c oxidase subunit 5A, mitochondrial.

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

- Molecule 18 is a protein called Cytochrome c oxidase subunit 5B, mitochondrial.

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

- Molecule 19 is a protein called Cytochrome c oxidase subunit 6A2, mitochondrial.

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

- Molecule 20 is a protein called Cytochrome c oxidase subunit 6B1.

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

- Molecule 21 is a protein called Cytochrome c oxidase subunit 6C.

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

- Molecule 22 is a protein called Cytochrome c oxidase subunit 7B, mitochondrial.

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

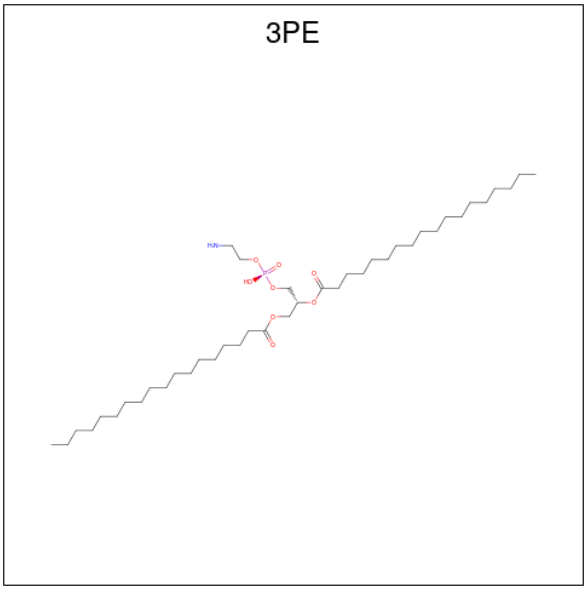
- Molecule 23 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

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

- Molecule 24 is a protein called Cytochrome c oxidase subunit 8B, mitochondrial.

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

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



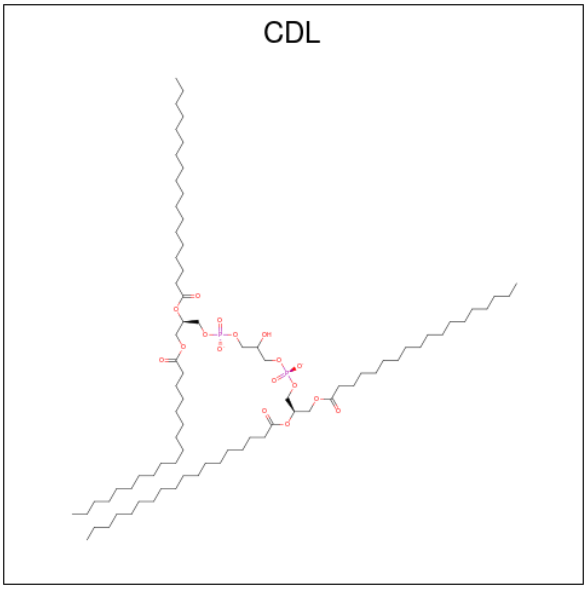
Mol	Chain	Residues	Atoms					AltConf
25	A	1	Total	C	N	O	P	0
			23	13	1	8	1	
25	C	1	Total	C	N	O	P	0
			35	25	1	8	1	
25	E	1	Total	C	N	O	P	0
			32	22	1	8	1	
25	G	1	Total	C	N	O	P	0
			51	41	1	8	1	
25	L	1	Total	C	N	O	P	0
			23	13	1	8	1	
25	N	1	Total	C	N	O	P	0
			37	27	1	8	1	
25	O	1	Total	C	N	O	P	0
			23	13	1	8	1	
25	R	1	Total	C	N	O	P	0
			51	41	1	8	1	
25	a	1	Total	C	N	O	P	0
			34	24	1	8	1	
25	a	1	Total	C	N	O	P	0
			28	18	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
25	a	1	Total	C	N	O	P	0
			27	17	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	g	1	Total	C	N	O	P	0
			25	15	1	8	1	

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



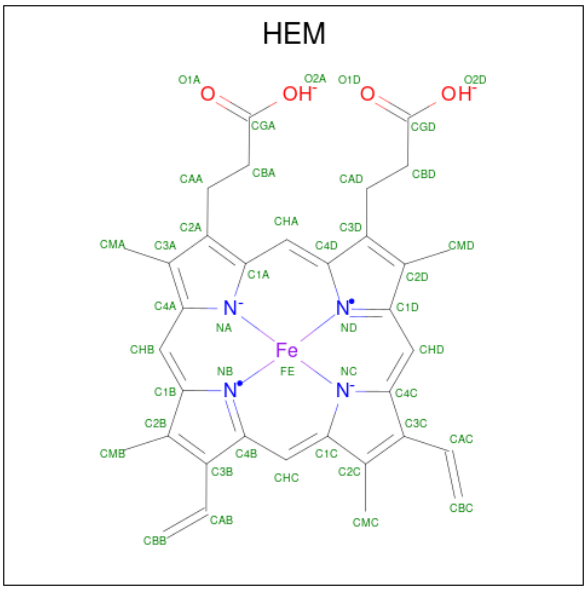
Mol	Chain	Residues	Atoms				AltConf
26	A	1	Total	C	O	P	0
			46	27	17	2	
26	C	1	Total	C	O	P	0
			42	23	17	2	
26	D	1	Total	C	O	P	0
			56	37	17	2	
26	L	1	Total	C	O	P	0
			46	27	17	2	
26	N	1	Total	C	O	P	0
			41	22	17	2	
26	O	1	Total	C	O	P	0
			57	38	17	2	

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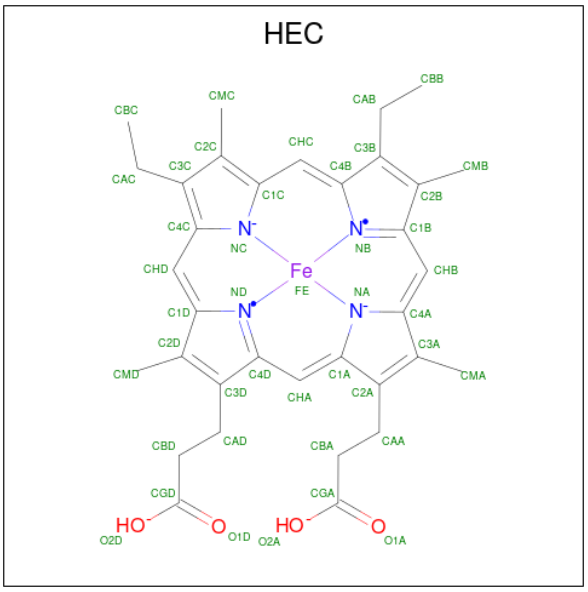
Mol	Chain	Residues	Atoms				AltConf
26	g	1	Total	C	O	P	0
			39	20	17	2	

- Molecule 27 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



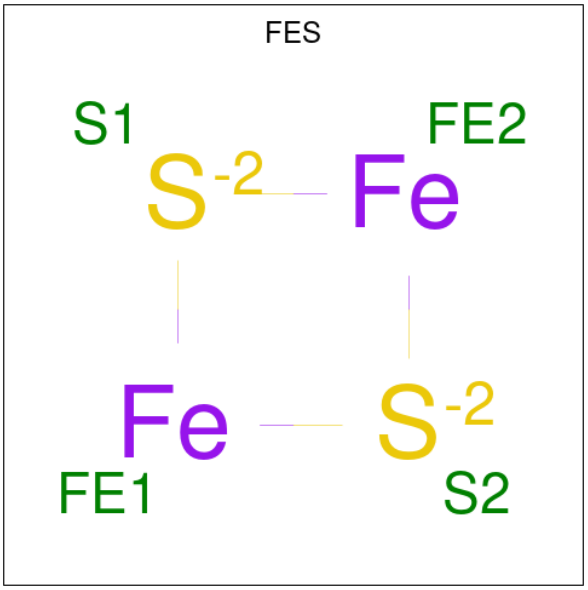
Mol	Chain	Residues	Atoms					AltConf
27	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
27	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
27	N	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
27	N	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 28 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



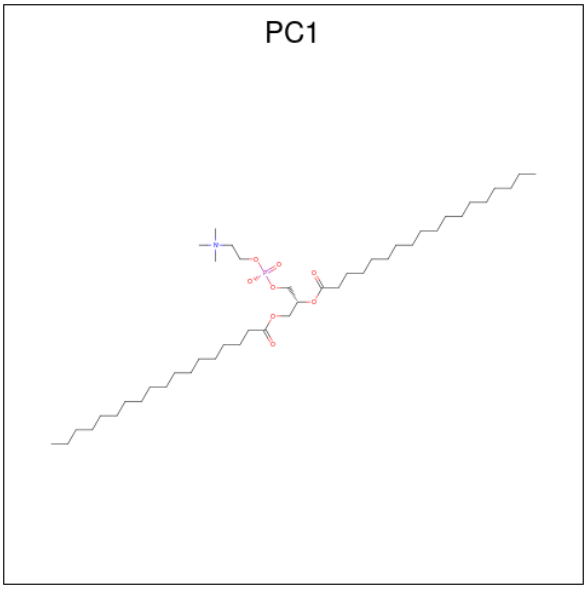
Mol	Chain	Residues	Atoms					AltConf
28	D	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
28	O	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 29 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



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

- Molecule 30 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
30	J	1	Total	C	N	O	P	0
			35	25	1	8	1	
30	P	1	Total	C	N	O	P	0
			24	14	1	8	1	
30	g	1	Total	C	N	O	P	0
			50	40	1	8	1	

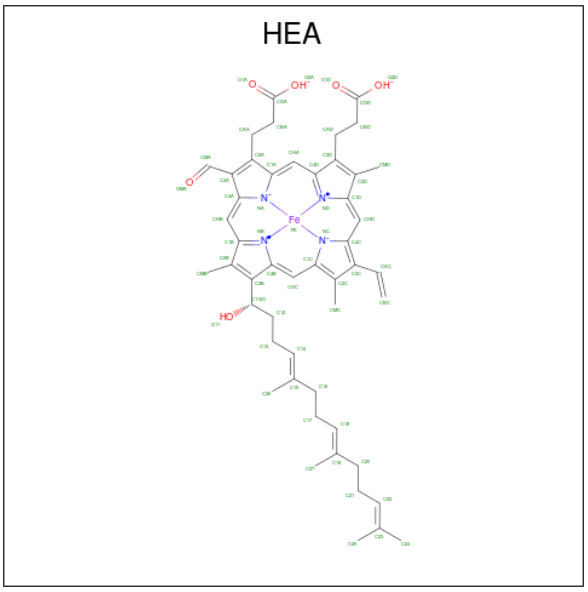
- Molecule 31 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

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

- Molecule 32 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 33 is HEME-A (CCD ID: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).

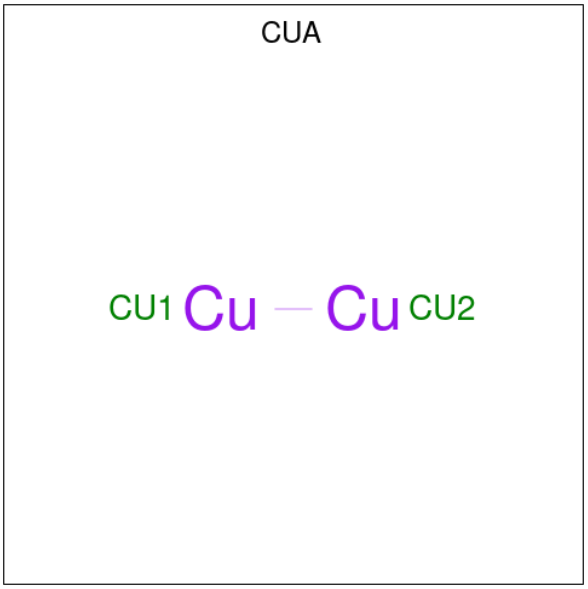


Mol	Chain	Residues	Atoms					AltConf
33	a	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
33	a	1	Total	C	Fe	N	O	0
			60	49	1	4	6	

- Molecule 34 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 35 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu_2).

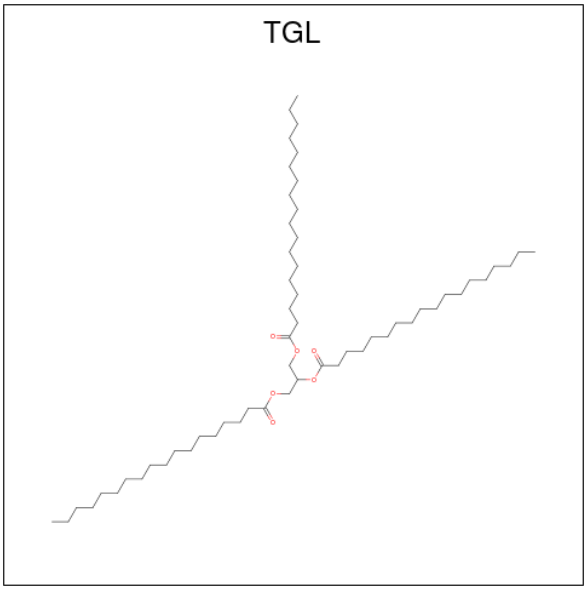


Mol	Chain	Residues	Atoms	AltConf
35	b	1	Total Cu 2 2	0

- Molecule 36 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 37 is TRISTEAROYLGLYCEROL (CCD ID: TGL) (formula: $C_{57}H_{110}O_6$).



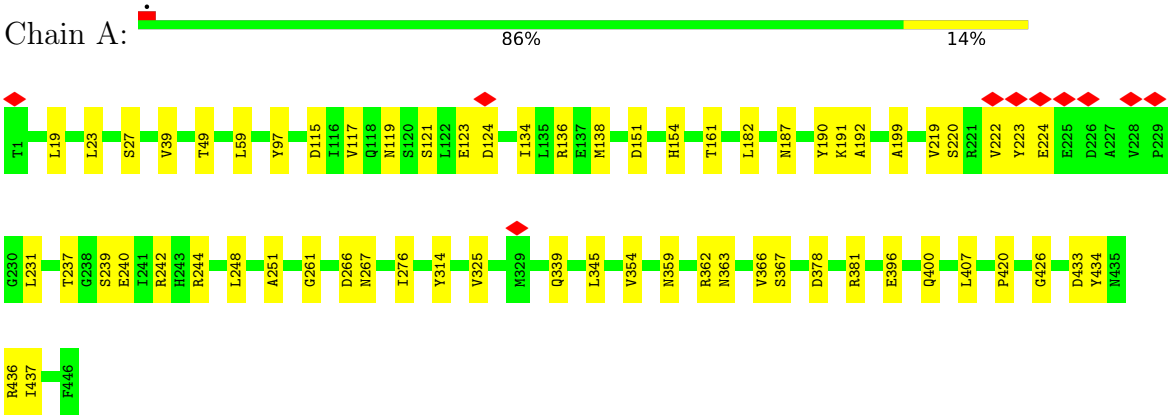
Mol	Chain	Residues	Atoms	AltConf
37	l	1	Total C O 37 31 6	0

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.

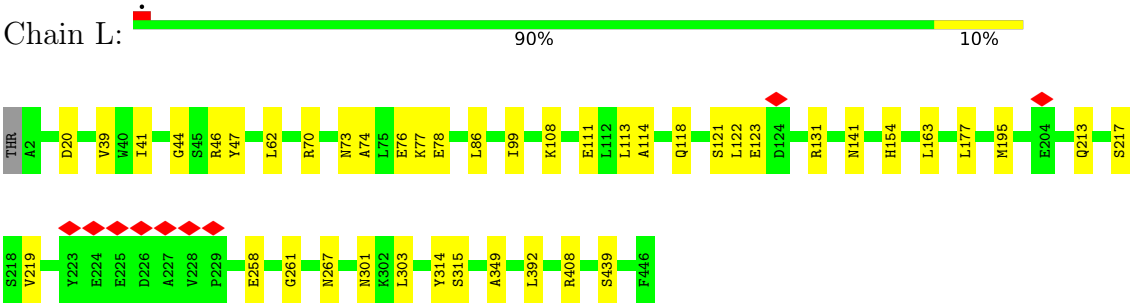
• Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial

Chain A:



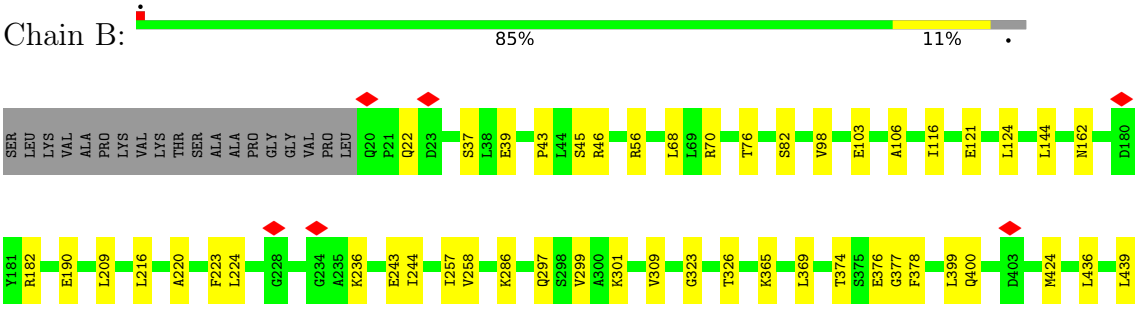
• Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial

Chain L:



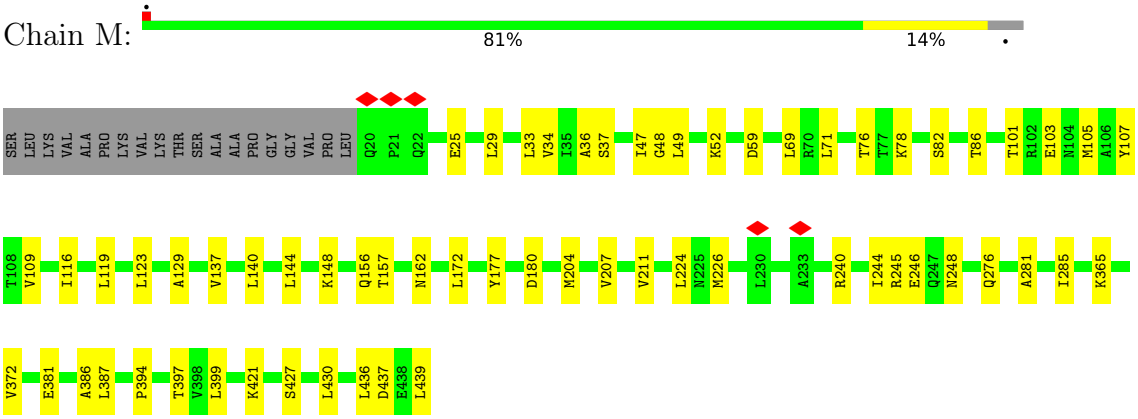
• Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain B:



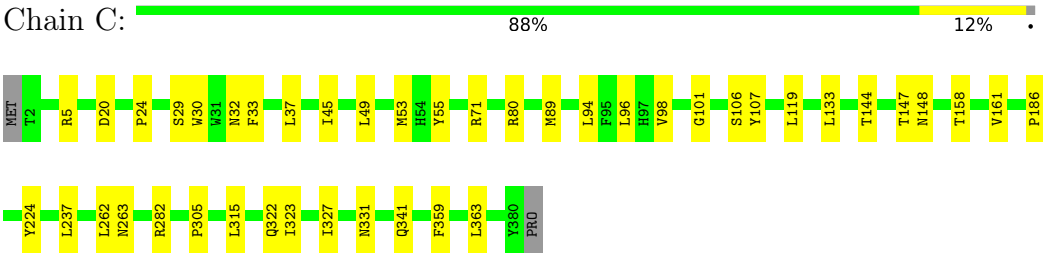
• Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain M:



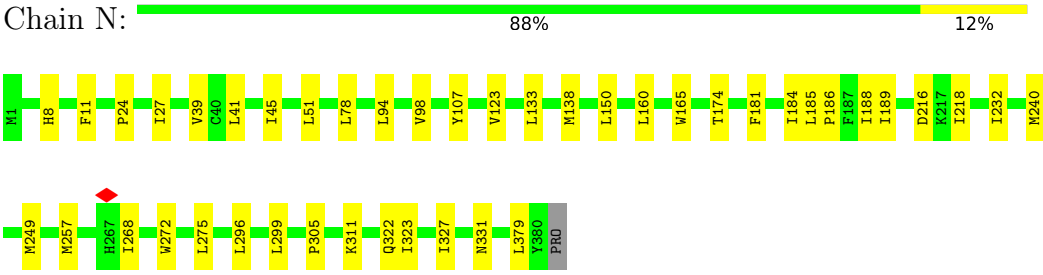
• Molecule 3: Cytochrome b

Chain C:



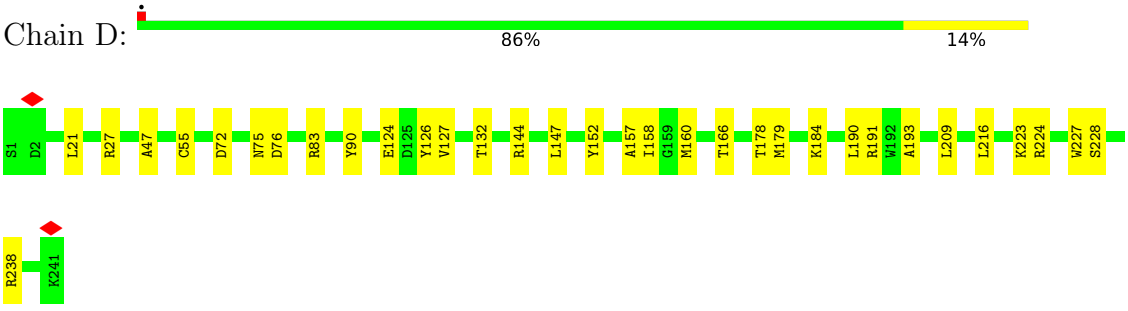
• Molecule 3: Cytochrome b

Chain N:



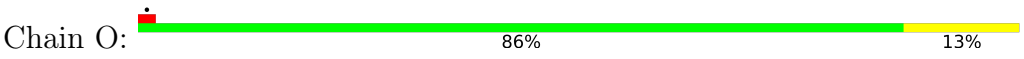
• Molecule 4: Cytochrome c1, heme protein, mitochondrial

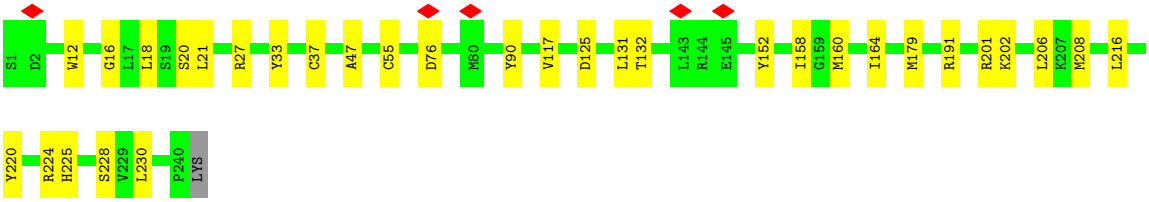
Chain D:



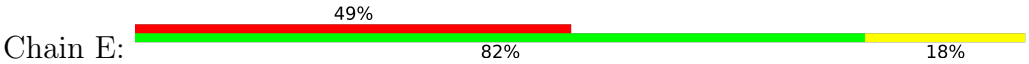
• Molecule 4: Cytochrome c1, heme protein, mitochondrial

Chain O:



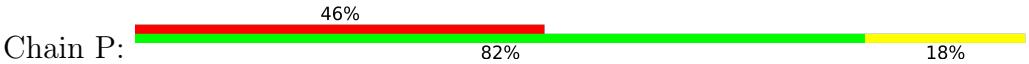


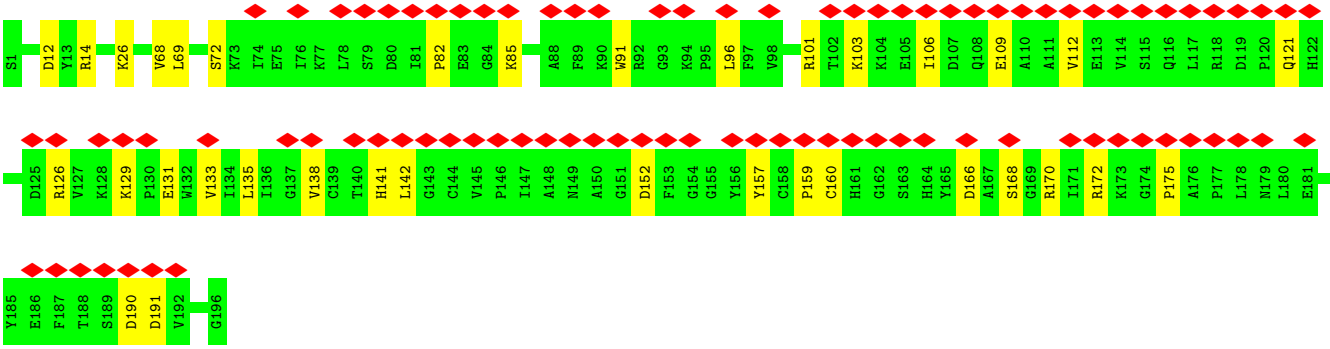
• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial



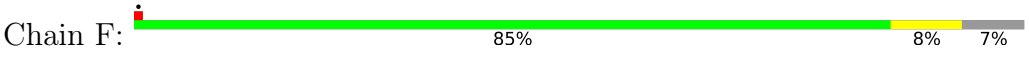


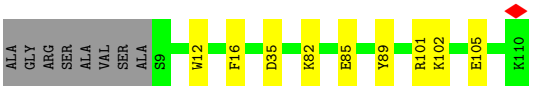
• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial



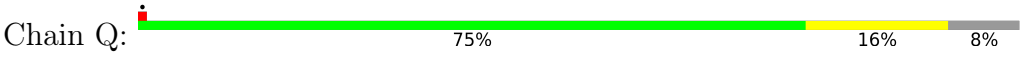


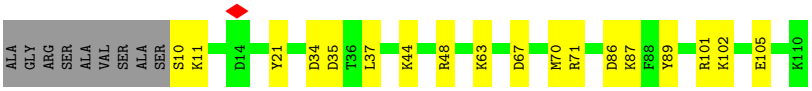
• Molecule 6: Cytochrome b-c1 complex subunit 7



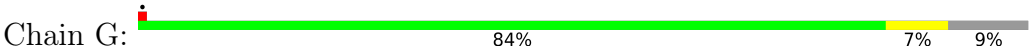


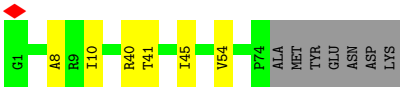
• Molecule 6: Cytochrome b-c1 complex subunit 7



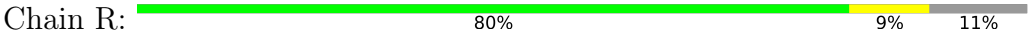


• Molecule 7: Cytochrome b-c1 complex subunit 8





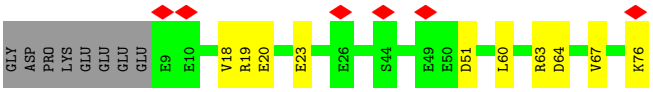
• Molecule 7: Cytochrome b-c1 complex subunit 8



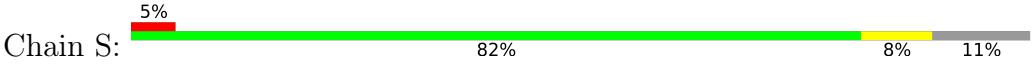


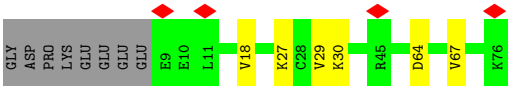
• Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial



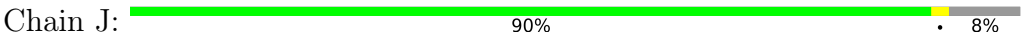


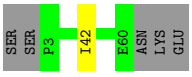
• Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial



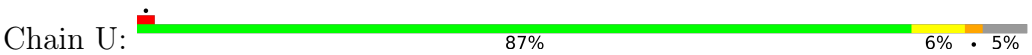


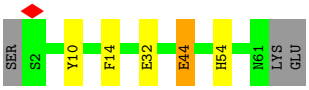
• Molecule 9: Cytochrome b-c1 complex subunit 9





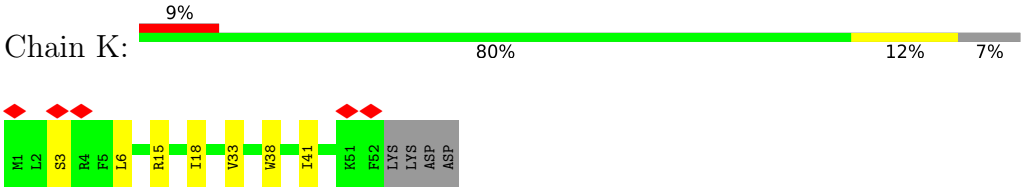
• Molecule 9: Cytochrome b-c1 complex subunit 9





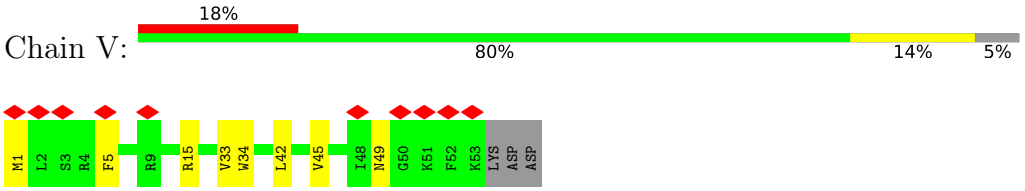
• Molecule 10: Cytochrome b-c1 complex subunit 10

Chain K:



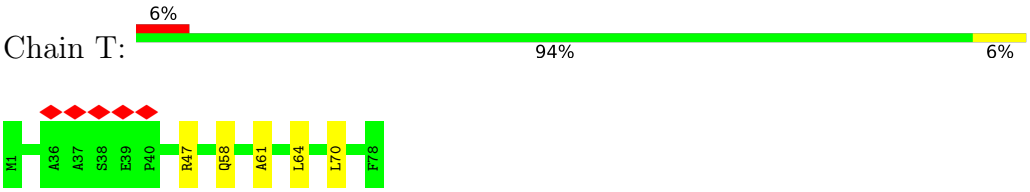
• Molecule 10: Cytochrome b-c1 complex subunit 10

Chain V:



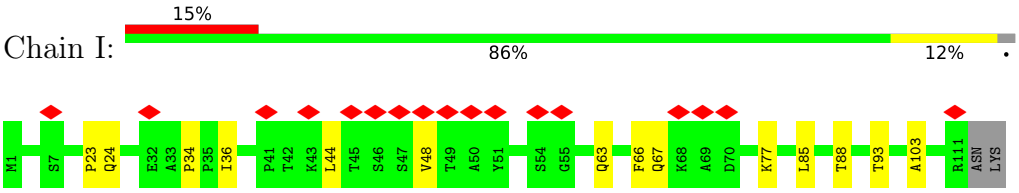
• Molecule 11: Cytochrome b-c1 complex subunit 9

Chain T:



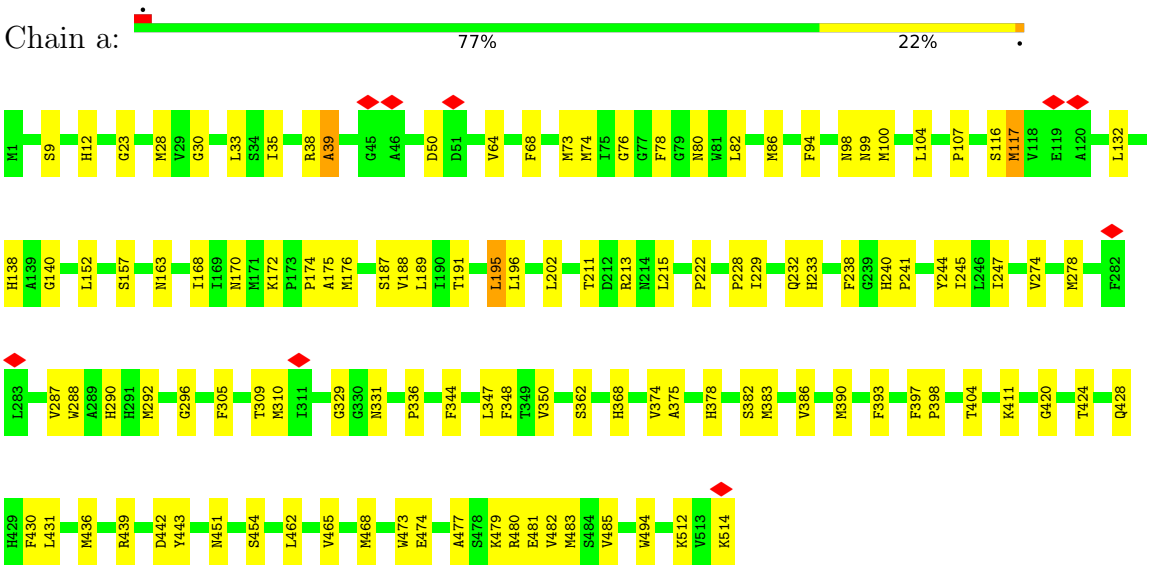
• Molecule 12: Cox7a2l protein

Chain I:



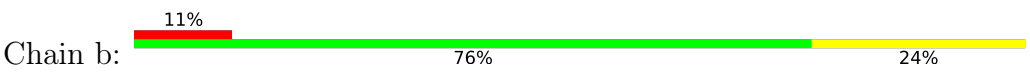
• Molecule 13: Cytochrome c oxidase subunit 1

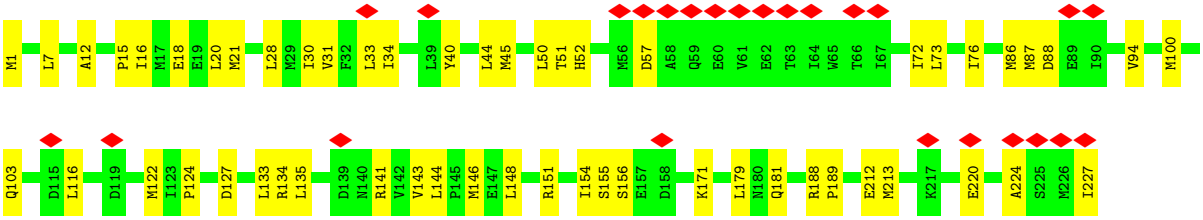
Chain a:



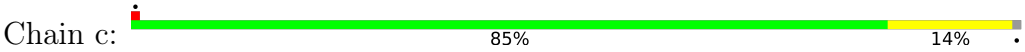
• Molecule 14: Cytochrome c oxidase subunit 2

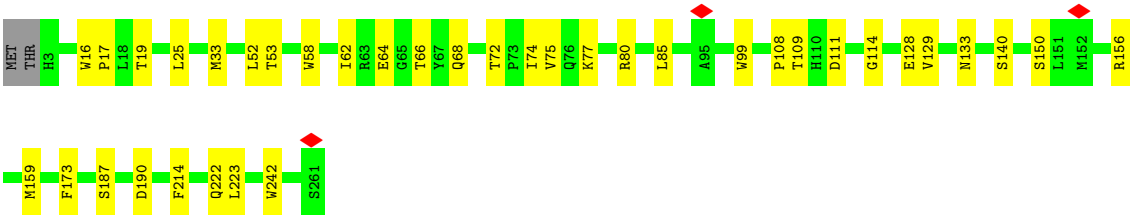
Chain b:



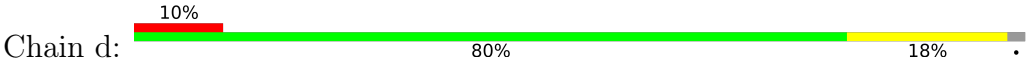


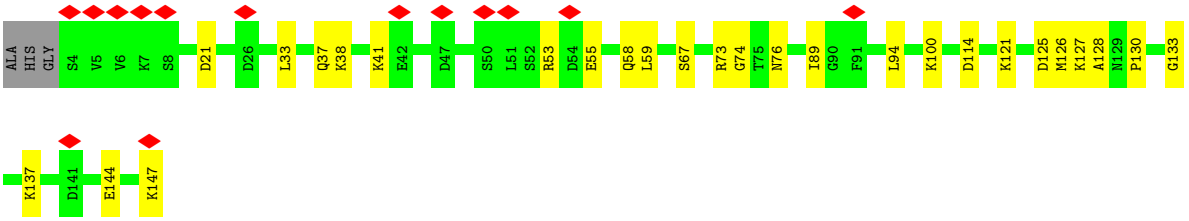
• Molecule 15: Cytochrome c oxidase subunit 3





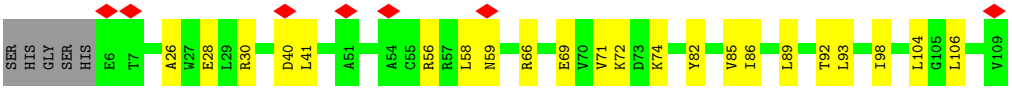
• Molecule 16: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



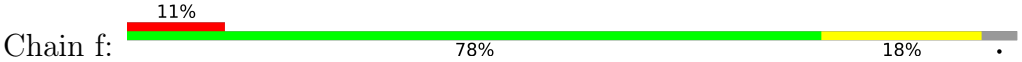


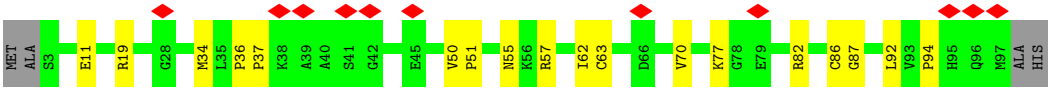
• Molecule 17: Cytochrome c oxidase subunit 5A, mitochondrial





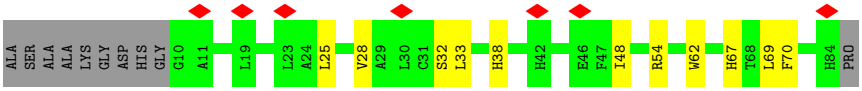
• Molecule 18: Cytochrome c oxidase subunit 5B, mitochondrial



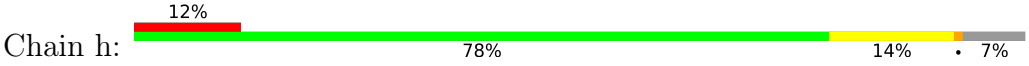


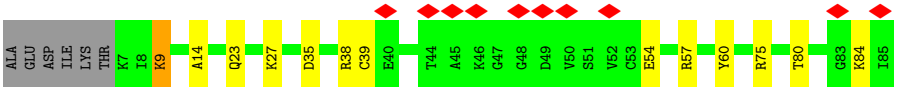
• Molecule 19: Cytochrome c oxidase subunit 6A2, mitochondrial



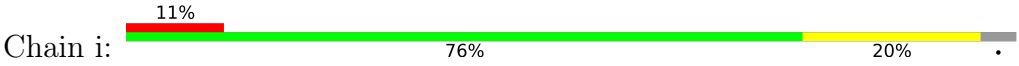


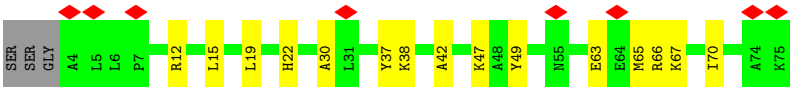
• Molecule 20: Cytochrome c oxidase subunit 6B1





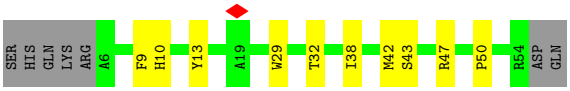
• Molecule 21: Cytochrome c oxidase subunit 6C



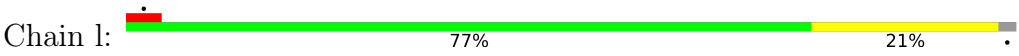


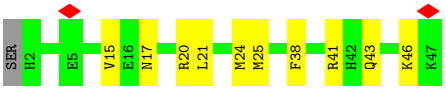
• Molecule 22: Cytochrome c oxidase subunit 7B, mitochondrial





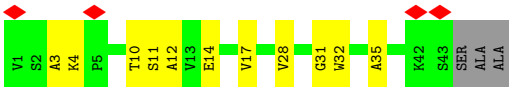
• Molecule 23: Cytochrome c oxidase subunit 7C, mitochondrial





• Molecule 24: Cytochrome c oxidase subunit 8B, mitochondrial





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	16228	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	0.271	Depositor
Minimum map value	-0.021	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	129.808, 230.888, 219.184	wwPDB
Map dimensions	206, 217, 122	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: CU, HEA, ZN, NA, 3PE, HEM, MG, CUA, TGL, FES, PC1, HEC, CDL

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	0.28	0/3536	0.57	2/4803 (0.0%)
1	L	0.26	0/3530	0.55	2/4793 (0.0%)
2	B	0.23	0/3205	0.48	0/4332
2	M	0.23	0/3205	0.50	1/4332 (0.0%)
3	C	0.28	0/3139	0.54	0/4287
3	N	0.28	0/3147	0.56	0/4297
4	D	0.24	0/1978	0.46	0/2685
4	O	0.23	0/1968	0.46	0/2674
5	E	0.21	0/1545	0.50	0/2091
5	P	0.19	0/1545	0.42	0/2091
6	F	0.21	0/922	0.42	0/1234
6	Q	0.24	0/916	0.44	0/1226
7	G	0.30	0/642	0.54	0/867
7	R	0.28	0/627	0.53	0/848
8	H	0.23	0/570	0.50	0/763
8	S	0.27	0/570	0.65	0/763
9	J	0.27	0/495	0.60	0/667
9	U	0.28	0/509	0.62	1/687 (0.1%)
10	K	0.22	0/445	0.49	0/608
10	V	0.23	0/454	0.50	0/619
11	T	0.27	0/565	0.60	0/772
12	I	0.24	0/860	0.65	0/1168
13	a	0.31	0/4162	0.64	4/5686 (0.1%)
14	b	0.29	0/1863	0.68	3/2542 (0.1%)
15	c	0.26	0/2195	0.63	1/3000 (0.0%)
16	d	0.23	0/1229	0.55	2/1659 (0.1%)
17	e	0.27	0/860	0.71	0/1167
18	f	0.24	0/744	0.60	0/1009
19	g	0.21	0/632	0.53	0/866
20	h	0.34	0/674	0.89	4/910 (0.4%)
21	i	0.23	0/584	0.58	0/778
22	k	0.30	0/396	0.69	0/541

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
23	l	0.24	0/393	0.61	0/527
24	m	0.27	0/318	0.63	0/433
All	All	0.26	0/48423	0.56	20/65725 (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	L	0	1
5	E	0	1
20	h	0	1
All	All	0	3

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	a	39	ALA	CA-C-N	-6.56	111.72	122.54
13	a	39	ALA	C-N-CA	-6.56	111.72	122.54
1	L	315	SER	CA-C-N	6.51	133.98	121.54
1	L	315	SER	C-N-CA	6.51	133.98	121.54
20	h	39	CYS	CA-CB-SG	6.26	128.81	114.40
16	d	128	ALA	CA-C-N	5.93	131.38	124.21
16	d	128	ALA	C-N-CA	5.93	131.38	124.21
13	a	195	LEU	CA-CB-CG	5.67	136.16	116.30
15	c	52	LEU	CA-CB-CG	5.60	135.90	116.30
14	b	86	MET	CB-CG-SD	5.57	129.42	112.70
9	U	44	GLU	N-CA-CB	5.48	119.33	110.40
20	h	27	LYS	CB-CG-CD	5.39	123.71	111.30
14	b	103	GLN	CA-C-N	5.28	130.35	122.74
14	b	103	GLN	C-N-CA	5.28	130.35	122.74
20	h	9	LYS	CA-C-N	5.19	131.46	121.54
20	h	9	LYS	C-N-CA	5.19	131.46	121.54
2	M	226	MET	CA-CB-CG	5.18	124.45	114.10
1	A	49	THR	CA-C-N	5.03	131.15	121.54
1	A	49	THR	C-N-CA	5.03	131.15	121.54
13	a	117	MET	CB-CG-SD	5.03	127.78	112.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	E	160	CYS	Peptide
1	L	219	VAL	Peptide
20	h	9	LYS	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	26	0
2	B	3154	0	3158	28	0
2	M	3154	0	3158	40	0
3	C	3038	0	3100	32	0
3	N	3046	0	3112	30	0
4	D	1919	0	1867	25	0
4	O	1909	0	1854	20	0
5	E	1512	0	1495	25	0
5	P	1512	0	1495	26	0
6	F	900	0	887	5	0
6	Q	894	0	882	11	0
7	G	624	0	633	5	0
7	R	609	0	614	5	0
8	H	563	0	541	9	0
8	S	563	0	541	5	0
9	J	481	0	479	1	0
9	U	495	0	489	3	0
10	K	429	0	430	4	0
10	V	438	0	443	5	0
11	T	554	0	590	5	0
12	I	838	0	834	11	0
13	a	4021	0	3997	89	0
14	b	1817	0	1822	40	0
15	c	2111	0	2047	25	0
16	d	1195	0	1161	20	0
17	e	842	0	838	16	0
18	f	727	0	703	16	0
19	g	605	0	570	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	h	654	0	622	8	0
21	i	572	0	596	13	0
22	k	383	0	367	9	0
23	l	380	0	378	8	0
24	m	311	0	329	8	0
25	A	23	0	20	0	0
25	C	35	0	44	0	0
25	E	32	0	38	0	0
25	G	51	0	82	4	0
25	L	23	0	20	1	0
25	N	37	0	48	0	0
25	O	23	0	20	0	0
25	R	51	0	82	2	0
25	a	89	0	100	0	0
25	b	57	0	62	0	0
25	c	45	0	67	3	0
25	g	25	0	24	3	0
26	A	46	0	36	0	0
26	C	42	0	28	2	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	1	0
26	g	39	0	22	1	0
27	C	86	0	60	4	0
27	N	86	0	60	3	0
28	D	43	0	30	1	0
28	O	43	0	30	0	0
29	E	4	0	0	0	0
29	P	4	0	0	1	0
30	J	35	0	44	0	0
30	P	24	0	22	0	0
30	g	50	0	77	0	0
31	a	1	0	0	0	0
32	a	1	0	0	0	0
33	a	120	0	108	7	0
34	b	1	0	0	0	0
35	b	2	0	0	0	0
36	f	1	0	0	0	0
37	l	37	0	49	2	0
All	All	48532	0	48125	536	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 6.

All (536) 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)
13:a:240:HIS:NE2	13:a:244:TYR:CE2	1.71	1.57
13:a:240:HIS:NE2	13:a:244:TYR:HE2	0.96	1.40
13:a:240:HIS:CD2	13:a:244:TYR:HE2	1.50	1.29
13:a:240:HIS:CD2	13:a:244:TYR:CE2	2.26	1.20
17:e:26:ALA:O	17:e:30:ARG:HB2	1.75	0.86
13:a:378:HIS:O	13:a:382:SER:HB2	1.76	0.83
1:L:108:LYS:O	1:L:111:GLU:HB3	1.83	0.78
22:k:9:PHE:O	22:k:13:TYR:HB2	1.85	0.77
13:a:240:HIS:CD2	13:a:244:TYR:CD2	2.74	0.75
13:a:240:HIS:NE2	13:a:244:TYR:CZ	2.51	0.74
14:b:154:ILE:O	14:b:179:LEU:HA	1.86	0.74
8:H:60:LEU:HD22	8:H:63:ARG:HH21	1.55	0.70
13:a:64:VAL:O	13:a:68:PHE:HB2	1.91	0.69
5:E:84:GLY:H	5:E:100:HIS:HB3	1.56	0.69
3:N:98:VAL:HG22	27:N:402:HEM:HBC2	1.73	0.69
5:P:68:VAL:O	5:P:72:SER:HB3	1.93	0.68
4:D:224:ARG:O	4:D:228:SER:HB3	1.95	0.67
13:a:344:PHE:O	13:a:348:PHE:HB3	1.94	0.67
5:E:117:LEU:HD13	5:E:121:GLN:H	1.62	0.64
14:b:143:VAL:HA	14:b:212:GLU:O	1.98	0.64
3:C:98:VAL:HG22	27:C:402:HEM:HBC2	1.79	0.64
13:a:195:LEU:HD22	13:a:245:ILE:HD12	1.78	0.64
18:f:82:ARG:HH11	18:f:87:GLY:HA2	1.62	0.64
12:I:103:ALA:HB1	15:c:33:MET:HE2	1.80	0.63
14:b:94:VAL:HG21	14:b:148:LEU:HD22	1.80	0.63
3:N:39:VAL:HG11	3:N:232:ILE:HG12	1.79	0.63
14:b:181:GLN:O	20:h:23:GLN:NE2	2.32	0.62
8:H:64:ASP:HA	8:H:67:VAL:HG22	1.81	0.62
3:N:323:ILE:HD11	25:R:101:3PE:H12	1.82	0.62
4:D:144:ARG:HH12	5:P:159:PRO:HA	1.65	0.61
2:B:45:SER:HB2	2:B:116:ILE:HG21	1.81	0.61
1:L:76:GLU:HG3	2:M:285:ILE:HD12	1.81	0.61
5:E:35:PHE:HB2	26:g:301:CDL:HA4	1.82	0.61
4:O:117:VAL:HG11	4:O:191:ARG:HA	1.82	0.61
12:I:63:GLN:O	12:I:67:GLN:NE2	2.34	0.61
17:e:71:VAL:HG11	17:e:85:VAL:HG11	1.83	0.60
9:J:42:ILE:HD11	19:g:33:LEU:HD21	1.82	0.60
5:P:14:ARG:HA	7:R:23:GLN:HA	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:46:ARG:NH2	2:B:376:GLU:OE1	2.34	0.60
3:N:296:LEU:HA	3:N:299:LEU:HB2	1.84	0.60
13:a:442:ASP:OD2	14:b:134:ARG:NH1	2.35	0.60
3:N:138:MET:HE1	3:N:268:ILE:HA	1.84	0.59
2:M:76:THR:HG22	2:M:82:SER:H	1.68	0.59
14:b:50:LEU:HB2	21:i:15:LEU:HD12	1.83	0.59
3:C:315:LEU:O	3:C:322:GLN:NE2	2.35	0.59
2:M:365:LYS:HB2	2:M:399:LEU:HD22	1.84	0.59
3:N:218:ILE:HG21	4:O:230:LEU:HD21	1.85	0.59
33:a:604:HEA:H211	14:b:34:ILE:HG12	1.84	0.59
5:E:118:ARG:NH1	5:E:174:GLY:O	2.36	0.58
10:V:1:MET:HA	10:V:5:PHE:HB2	1.85	0.58
13:a:35:ILE:O	13:a:39:ALA:HB2	2.03	0.58
5:E:99:ARG:NH2	5:E:167:ALA:O	2.37	0.58
1:A:244:ARG:HE	7:G:10:ILE:HB	1.68	0.58
9:U:10:TYR:HA	9:U:14:PHE:HB2	1.86	0.57
3:N:51:LEU:HD13	27:N:401:HEM:HBA1	1.85	0.57
18:f:86:CYS:SG	18:f:87:GLY:N	2.77	0.57
3:C:119:LEU:HD22	27:C:402:HEM:HBB2	1.85	0.57
13:a:116:SER:O	23:l:43:GLN:NE2	2.37	0.57
3:C:107:TYR:HB2	3:C:305:PRO:HG3	1.87	0.57
8:S:29:VAL:HG23	8:S:30:LYS:HD2	1.86	0.57
13:a:172:LYS:NZ	13:a:176:MET:O	2.37	0.57
14:b:16:ILE:HD11	14:b:87:MET:HE2	1.85	0.57
17:e:28:GLU:OE1	18:f:82:ARG:NH2	2.38	0.57
4:D:147:LEU:HD13	4:D:157:ALA:HB1	1.86	0.57
17:e:93:LEU:HD13	17:e:98:ILE:HG13	1.87	0.57
13:a:64:VAL:HA	13:a:68:PHE:HD2	1.70	0.57
13:a:287:VAL:O	13:a:290:HIS:ND1	2.33	0.56
13:a:117:MET:O	23:l:46:LYS:NZ	2.38	0.56
13:a:296:GLY:HA2	20:h:23:GLN:HG2	1.87	0.56
14:b:51:THR:O	17:e:74:LYS:NZ	2.38	0.56
13:a:512:LYS:HZ2	13:a:514:LYS:H	1.54	0.56
4:D:158:ILE:HG12	4:D:160:MET:H	1.71	0.56
8:S:64:ASP:HA	8:S:67:VAL:HG22	1.86	0.56
1:L:46:ARG:HD2	1:L:163:LEU:HD13	1.86	0.56
13:a:336:PRO:HG3	13:a:411:LYS:HG3	1.88	0.56
13:a:483:MET:HE2	24:m:4:LYS:HA	1.87	0.56
1:A:191:LYS:HE3	1:A:223:TYR:HA	1.87	0.56
3:N:327:ILE:HG23	25:R:101:3PE:H2C2	1.87	0.56
16:d:126:MET:HA	21:i:65:MET:HG2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:k:43:SER:O	22:k:47:ARG:NH1	2.39	0.56
13:a:107:PRO:HB3	15:c:25:LEU:HB2	1.88	0.56
13:a:38:ARG:NH2	13:a:454:SER:OG	2.39	0.55
5:E:114:VAL:HA	5:E:117:LEU:HD12	1.88	0.55
5:E:161:HIS:HD1	5:E:163:SER:HG	1.53	0.55
2:M:372:VAL:HG12	2:M:381:GLU:HG3	1.89	0.55
18:f:11:GLU:O	18:f:19:ARG:NH1	2.40	0.55
15:c:62:ILE:HG13	25:c:301:3PE:H221	1.88	0.55
5:P:126:ARG:NH1	5:P:168:SER:O	2.39	0.55
13:a:38:ARG:NH2	13:a:451:ASN:O	2.39	0.55
14:b:1:MET:HE1	14:b:133:LEU:HD21	1.89	0.55
1:A:354:VAL:HG22	1:A:407:LEU:HD13	1.89	0.55
12:I:63:GLN:NE2	15:c:66:THR:O	2.35	0.55
20:h:75:ARG:HG3	20:h:80:THR:HG23	1.88	0.55
6:Q:87:LYS:HE2	6:Q:89:TYR:HB3	1.89	0.54
23:l:17:ASN:HB3	23:l:20:ARG:HG2	1.88	0.54
10:V:45:VAL:O	10:V:49:ASN:ND2	2.41	0.54
24:m:31:GLY:O	24:m:35:ALA:HB2	2.07	0.54
8:H:20:GLU:HA	8:H:23:GLU:HG2	1.89	0.54
4:O:16:GLY:O	4:O:202:LYS:NZ	2.40	0.54
5:P:121:GLN:HB3	5:P:170:ARG:HH12	1.70	0.54
1:L:62:LEU:HD13	1:L:122:LEU:HD22	1.89	0.54
13:a:474:GLU:OE1	13:a:480:ARG:NH2	2.39	0.54
19:g:48:ILE:O	19:g:54:ARG:NH2	2.41	0.54
4:D:47:ALA:HA	4:D:90:TYR:HA	1.89	0.54
4:D:144:ARG:NH1	5:P:157:TYR:OH	2.40	0.54
5:P:141:HIS:HE1	5:P:175:PRO:HG2	1.72	0.54
24:m:28:VAL:O	24:m:32:TRP:HB2	2.08	0.54
16:d:53:ARG:HD3	17:e:104:LEU:HA	1.89	0.54
3:C:101:GLY:HA2	3:C:106:SER:HB2	1.88	0.53
13:a:482:VAL:HA	24:m:3:ALA:HA	1.88	0.53
18:f:51:PRO:O	18:f:57:ARG:NH1	2.37	0.53
1:L:131:ARG:NH2	1:L:177:LEU:O	2.41	0.53
5:P:101:ARG:NH2	5:P:109:GLU:OE1	2.41	0.53
13:a:481:GLU:HB3	24:m:4:LYS:HE2	1.90	0.53
6:Q:34:ASP:HA	6:Q:37:LEU:HD23	1.91	0.53
13:a:98:ASN:HB2	13:a:163:ASN:HD22	1.73	0.53
1:A:115:ASP:HB2	1:A:119:ASN:HB2	1.91	0.53
2:M:109:VAL:HG13	2:M:123:LEU:HD12	1.90	0.53
16:d:133:GLY:O	16:d:137:LYS:NZ	2.40	0.53
13:a:368:HIS:ND1	33:a:604:HEA:O1A	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:m:11:SER:OG	24:m:12:ALA:N	2.42	0.53
2:M:47:ILE:HD11	2:M:211:VAL:HG11	1.90	0.53
4:O:27:ARG:NH1	4:O:55:CYS:O	2.43	0.52
13:a:375:ALA:HB2	13:a:428:GLN:HG3	1.91	0.52
25:G:101:3PE:H121	25:G:101:3PE:H221	1.91	0.52
4:O:12:TRP:NE1	4:O:125:ASP:OD1	2.36	0.52
4:O:220:TYR:OH	4:O:224:ARG:NH2	2.41	0.52
2:M:116:ILE:HD12	2:M:119:LEU:HD12	1.90	0.52
14:b:21:MET:SD	21:i:49:TYR:OH	2.67	0.52
10:K:33:VAL:HG23	10:K:38:TRP:HB3	1.91	0.52
13:a:9:SER:O	13:a:99:ASN:ND2	2.42	0.52
13:a:374:VAL:O	13:a:378:HIS:HB2	2.10	0.52
4:D:238:ARG:HD3	12:I:36:ILE:HG13	1.92	0.52
2:M:246:GLU:OE1	2:M:248:ASN:ND2	2.43	0.52
3:N:185:LEU:HD23	3:N:188:ILE:HD12	1.91	0.52
13:a:211:THR:HG23	13:a:215:LEU:HD12	1.92	0.52
14:b:30:ILE:HG21	14:b:76:ILE:HD11	1.91	0.52
18:f:82:ARG:HD2	18:f:87:GLY:HA2	1.92	0.52
1:A:240:GLU:OE1	1:A:242:ARG:NH1	2.42	0.52
3:C:49:LEU:HG	3:C:53:MET:HE3	1.92	0.52
3:C:282:ARG:NH2	3:C:341:GLN:O	2.41	0.52
2:M:248:ASN:ND2	2:M:427:SER:OG	2.41	0.52
14:b:144:LEU:O	14:b:213:MET:HA	2.10	0.52
19:g:62:TRP:NE1	19:g:67:HIS:O	2.43	0.52
20:h:35:ASP:HA	20:h:38:ARG:HB2	1.92	0.52
1:L:111:GLU:O	1:L:114:ALA:HB3	2.10	0.51
2:M:240:ARG:O	2:M:421:LYS:NZ	2.43	0.51
13:a:23:GLY:HA3	13:a:73:MET:HG2	1.92	0.51
2:B:220:ALA:HA	2:B:224:LEU:HD23	1.92	0.51
10:K:33:VAL:HG21	10:K:41:ILE:HB	1.92	0.51
2:M:162:ASN:HB3	2:M:244:ILE:HG21	1.91	0.51
23:l:25:MET:HG2	37:l:601:TGL:HB51	1.93	0.51
2:B:182:ARG:NH2	2:B:190:GLU:OE1	2.42	0.51
3:C:32:ASN:ND2	26:D:301:CDL:OB9	2.42	0.51
6:F:101:ARG:NH1	6:F:105:GLU:OE2	2.43	0.51
13:a:244:TYR:HA	13:a:247:ILE:HG22	1.92	0.51
15:c:133:ASN:HB3	15:c:173:PHE:HE1	1.76	0.51
22:k:29:TRP:HA	22:k:32:THR:HG22	1.92	0.51
16:d:55:GLU:O	16:d:59:LEU:HB2	2.11	0.51
2:B:121:GLU:O	2:B:124:LEU:HB3	2.11	0.51
1:L:213:GLN:O	1:L:217:SER:HB2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:91:TRP:HE3	5:P:96:LEU:HD21	1.76	0.51
15:c:64:GLU:HA	15:c:68:GLN:HB2	1.92	0.51
1:A:59:LEU:HG	1:A:182:LEU:HD12	1.93	0.51
1:A:339:GLN:NE2	1:A:437:ILE:O	2.41	0.51
5:P:82:PRO:HD2	5:P:85:LYS:HD2	1.92	0.51
16:d:73:ARG:NH2	16:d:74:GLY:O	2.43	0.51
5:E:20:ASP:OD1	5:E:20:ASP:N	2.44	0.50
3:C:323:ILE:HD11	25:G:101:3PE:H12	1.91	0.50
13:a:12:HIS:ND1	13:a:80:ASN:O	2.37	0.50
14:b:57:ASP:OD1	14:b:57:ASP:N	2.43	0.50
16:d:55:GLU:HA	16:d:58:GLN:HG2	1.92	0.50
1:A:396:GLU:OE1	1:A:400:GLN:NE2	2.44	0.50
2:B:56:ARG:HD3	2:B:103:GLU:HG2	1.92	0.50
4:D:124:GLU:OE2	4:D:191:ARG:NH1	2.45	0.50
13:a:196:LEU:HD11	15:c:85:LEU:HB3	1.94	0.50
22:k:42:MET:HB3	22:k:47:ARG:HH22	1.76	0.50
1:A:136:ARG:NH2	12:I:24:GLN:OE1	2.45	0.50
3:N:107:TYR:HB2	3:N:305:PRO:HG3	1.93	0.50
1:A:276:ILE:HG21	1:A:345:LEU:HD21	1.94	0.50
5:P:152:ASP:OD1	5:P:152:ASP:N	2.43	0.50
2:B:374:THR:HG23	2:B:377:GLY:H	1.76	0.50
13:a:382:SER:HA	33:a:603:HEA:HMC2	1.93	0.50
1:A:192:ALA:HB2	1:A:219:VAL:HB	1.92	0.50
10:K:3:SER:HA	10:K:6:LEU:HD23	1.94	0.50
4:O:47:ALA:HA	4:O:90:TYR:HA	1.93	0.50
5:P:103:LYS:HA	5:P:106:ILE:HD12	1.94	0.50
1:A:237:THR:HG22	1:A:239:SER:HB3	1.94	0.49
2:M:78:LYS:HB2	2:M:129:ALA:HB1	1.93	0.49
3:N:150:LEU:HD21	3:N:160:LEU:HD23	1.93	0.49
4:O:76:ASP:N	4:O:76:ASP:OD1	2.45	0.49
6:Q:21:TYR:OH	6:Q:86:ASP:OD2	2.26	0.49
4:D:238:ARG:NE	12:I:34:PRO:O	2.45	0.49
13:a:439:ARG:NE	33:a:603:HEA:O2D	2.45	0.49
2:B:286:LYS:HE2	12:I:23:PRO:HG3	1.94	0.49
1:L:121:SER:OG	1:L:123:GLU:OE2	2.31	0.49
2:M:29:LEU:HD12	2:M:33:LEU:HD23	1.94	0.49
5:P:133:VAL:HG12	5:P:135:LEU:HD22	1.94	0.49
23:l:38:PHE:HA	23:l:41:ARG:HG2	1.94	0.49
1:L:74:ALA:HA	1:L:77:LYS:HD3	1.95	0.49
13:a:229:ILE:HA	13:a:232:GLN:HG3	1.93	0.49
2:B:369:LEU:HD11	2:B:399:LEU:HD11	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:PRO:O	1:A:434:TYR:OH	2.26	0.49
3:C:359:PHE:O	3:C:363:LEU:HB2	2.13	0.49
5:P:166:ASP:OD2	5:P:172:ARG:NH1	2.46	0.49
15:c:109:THR:HG23	15:c:111:ASP:H	1.78	0.49
10:K:15:ARG:HA	10:K:18:ILE:HG12	1.94	0.49
7:R:59:TYR:O	7:R:63:ASN:ND2	2.46	0.49
13:a:104:LEU:HD11	13:a:152:LEU:HD22	1.94	0.49
2:B:309:VAL:HG13	2:B:326:THR:HG22	1.93	0.49
1:L:44:GLY:H	1:L:47:TYR:HD2	1.60	0.49
4:D:21:LEU:HD21	4:D:191:ARG:HG3	1.95	0.48
3:C:147:THR:HG22	3:C:161:VAL:HG23	1.94	0.48
16:d:144:GLU:OE1	16:d:147:LYS:NZ	2.47	0.48
1:A:436:ARG:NH2	3:C:20:ASP:OD1	2.45	0.48
2:M:148:LYS:NZ	2:M:180:ASP:OD1	2.44	0.48
5:P:191:ASP:OD1	5:P:191:ASP:N	2.46	0.48
13:a:174:PRO:HB2	18:f:36:PRO:HG3	1.96	0.48
1:A:151:ASP:OD2	5:E:2:HIS:NE2	2.47	0.48
5:E:148:ALA:HA	5:E:156:TYR:HA	1.93	0.48
6:F:12:TRP:O	6:F:16:PHE:N	2.39	0.48
2:M:69:LEU:HD22	2:M:105:MET:HE1	1.96	0.48
5:P:121:GLN:O	5:P:170:ARG:NH2	2.47	0.48
5:E:67:ASP:OD1	5:E:67:ASP:N	2.46	0.48
12:I:66:PHE:HD1	12:I:77:LYS:HZ3	1.62	0.48
15:c:58:TRP:CG	25:c:301:3PE:H251	2.49	0.48
20:h:38:ARG:HH12	20:h:84:LYS:HG3	1.79	0.48
1:A:187:ASN:O	1:A:191:LYS:NZ	2.46	0.48
2:B:22:GLN:NE2	2:B:39:GLU:OE1	2.46	0.48
13:a:465:VAL:O	13:a:468:MET:HB3	2.14	0.48
5:E:99:ARG:HH12	5:E:167:ALA:HB1	1.78	0.48
1:L:20:ASP:OD1	1:L:20:ASP:N	2.43	0.48
13:a:50:ASP:OD1	13:a:50:ASP:N	2.45	0.48
13:a:222:PRO:HG3	13:a:228:PRO:HD3	1.95	0.48
13:a:477:ALA:O	24:m:10:THR:OG1	2.32	0.48
13:a:479:LYS:NZ	23:l:15:VAL:O	2.47	0.48
14:b:28:LEU:HA	14:b:31:VAL:HG12	1.96	0.48
26:C:404:CDL:OB4	7:G:40:ARG:NE	2.47	0.47
1:L:70:ARG:NE	1:L:78:GLU:OE1	2.47	0.47
16:d:33:LEU:HD12	16:d:37:GLN:HB3	1.95	0.47
16:d:121:LYS:HD3	22:k:50:PRO:HB2	1.96	0.47
1:A:378:ASP:OD1	1:A:381:ARG:NH2	2.46	0.47
2:M:71:LEU:HD12	2:M:144:LEU:HD23	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Q:10:SER:OG	6:Q:11:LYS:N	2.47	0.47
14:b:33:LEU:HG	21:i:30:ALA:HB1	1.96	0.47
3:C:24:PRO:O	3:C:224:TYR:OH	2.26	0.47
1:L:261:GLY:O	1:L:267:ASN:ND2	2.47	0.47
2:M:25:GLU:OE2	2:M:37:SER:OG	2.32	0.47
6:Q:101:ARG:NH1	6:Q:105:GLU:OE2	2.44	0.47
16:d:127:LYS:HB3	16:d:130:PRO:HG3	1.95	0.47
3:C:71:ARG:NH2	4:D:193:ALA:O	2.44	0.47
13:a:30:GLY:HA2	13:a:33:LEU:HD12	1.97	0.47
2:M:437:ASP:OD1	2:M:437:ASP:N	2.46	0.47
6:Q:35:ASP:OD1	6:Q:89:TYR:OH	2.25	0.47
18:f:50:VAL:HG13	18:f:92:LEU:HD12	1.97	0.47
1:A:124:ASP:OD1	1:A:124:ASP:N	2.46	0.47
5:E:103:LYS:HA	5:E:106:ILE:HD12	1.96	0.47
3:N:94:LEU:HD11	3:N:123:VAL:HG11	1.96	0.47
13:a:274:VAL:HG12	13:a:278:MET:HE2	1.95	0.47
13:a:436:MET:HE3	13:a:443:TYR:HB3	1.96	0.47
15:c:156:ARG:HH22	15:c:223:LEU:HD13	1.79	0.47
2:B:257:ILE:HG13	2:B:424:MET:HG3	1.96	0.47
4:D:126:TYR:OH	28:D:302:HEC:O2A	2.29	0.47
5:E:94:LYS:NZ	5:E:181:GLU:OE2	2.47	0.47
2:M:157:THR:HG23	11:T:64:LEU:HD11	1.97	0.47
13:a:100:MET:HG3	15:c:17:PRO:HA	1.96	0.47
1:A:222:VAL:HG12	1:A:224:GLU:H	1.80	0.47
7:G:41:THR:O	7:G:45:ILE:HB	2.15	0.47
3:N:186:PRO:HA	3:N:189:ILE:HD12	1.97	0.47
5:P:129:LYS:HE2	5:P:131:GLU:HB2	1.97	0.47
2:B:124:LEU:HD11	2:B:223:PHE:HB3	1.96	0.47
5:P:12:ASP:O	7:R:24:ARG:NH2	2.48	0.47
6:Q:67:ASP:OD2	6:Q:71:ARG:NH1	2.48	0.47
1:L:86:LEU:HD13	1:L:99:ILE:HD12	1.97	0.46
13:a:386:VAL:O	13:a:390:MET:HG2	2.16	0.46
18:f:77:LYS:HE2	18:f:94:PRO:HG3	1.96	0.46
21:i:38:LYS:HD2	21:i:42:ALA:HB3	1.98	0.46
4:D:144:ARG:NH2	5:P:159:PRO:O	2.38	0.46
3:N:244:LEU:O	4:O:201:ARG:NH1	2.46	0.46
10:V:33:VAL:HG22	10:V:42:LEU:HG	1.98	0.46
13:a:82:LEU:HD12	13:a:86:MET:HE3	1.97	0.46
13:a:310:MET:HG3	14:b:73:LEU:HD22	1.97	0.46
13:a:473:TRP:O	13:a:477:ALA:N	2.49	0.46
2:M:86:THR:HG23	11:T:70:LEU:HD21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:101:THR:HG23	2:M:103:GLU:H	1.80	0.46
14:b:155:SER:OG	14:b:156:SER:N	2.49	0.46
3:C:80:ARG:NH1	27:C:401:HEM:O2D	2.41	0.46
15:c:140:SER:HB3	15:c:242:TRP:HE1	1.80	0.46
1:A:261:GLY:O	1:A:267:ASN:ND2	2.49	0.46
2:M:52:LYS:HG3	2:M:387:LEU:HD13	1.98	0.46
2:M:59:ASP:OD1	2:M:59:ASP:N	2.48	0.46
13:a:347:LEU:HA	13:a:350:VAL:HG12	1.98	0.46
14:b:220:GLU:O	14:b:224:ALA:HB3	2.16	0.46
15:c:16:TRP:HD1	15:c:53:THR:HG23	1.81	0.46
21:i:15:LEU:HD23	21:i:19:LEU:HD23	1.98	0.46
1:A:19:LEU:HD22	1:A:23:LEU:HD23	1.97	0.46
1:A:359:ASN:OD1	1:A:362:ARG:NH1	2.49	0.46
2:B:436:LEU:HA	2:B:439:LEU:HD23	1.96	0.46
4:D:166:THR:HG23	4:D:178:THR:HA	1.97	0.46
8:H:18:VAL:HG12	8:H:67:VAL:HG12	1.97	0.46
2:M:245:ARG:HB3	2:M:430:LEU:HD13	1.97	0.46
4:O:152:TYR:OH	8:S:64:ASP:OD2	2.30	0.46
13:a:175:ALA:HB2	18:f:36:PRO:HB3	1.98	0.46
16:d:121:LYS:O	16:d:125:ASP:HB2	2.16	0.46
13:a:241:PRO:O	13:a:245:ILE:HG12	2.15	0.46
21:i:63:GLU:HA	21:i:66:ARG:HG2	1.98	0.46
24:m:14:GLU:HA	24:m:17:VAL:HG22	1.97	0.46
1:A:121:SER:OG	1:A:123:GLU:OE2	2.34	0.46
3:N:8:HIS:HB3	3:N:11:PHE:HB2	1.98	0.46
15:c:150:SER:HB3	15:c:159:MET:HB3	1.98	0.46
1:L:439:SER:HB3	25:L:501:3PE:H111	1.99	0.45
4:O:131:LEU:HB3	4:O:164:ILE:HD11	1.98	0.45
13:a:176:MET:HE3	18:f:70:VAL:HG21	1.98	0.45
13:a:202:LEU:HB2	13:a:238:PHE:CG	2.51	0.45
3:N:322:GLN:OE1	7:R:47:ARG:NH1	2.49	0.45
9:U:32:GLU:OE1	10:V:34:TRP:NE1	2.49	0.45
16:d:38:LYS:HD3	16:d:41:LYS:HZ3	1.82	0.45
2:B:365:LYS:HB2	2:B:399:LEU:HD22	1.99	0.45
4:D:223:LYS:O	4:D:227:TRP:HB2	2.17	0.45
8:H:51:ASP:OD1	8:H:51:ASP:N	2.50	0.45
3:C:30:TRP:HZ3	3:C:96:LEU:HD22	1.82	0.45
3:C:30:TRP:O	3:C:33:PHE:HB2	2.16	0.45
3:C:263:ASN:HA	5:P:142:LEU:HA	1.99	0.45
13:a:215:LEU:HD13	25:g:303:3PE:H321	1.99	0.45
13:a:331:ASN:HD22	16:d:21:ASP:HB2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:a:420:GLY:O	13:a:424:THR:OG1	2.30	0.45
14:b:100:MET:HA	14:b:155:SER:O	2.16	0.45
1:A:433:ASP:N	1:A:433:ASP:OD1	2.48	0.45
5:E:82:PRO:HD2	5:E:85:LYS:HE3	1.99	0.45
1:L:141:ASN:OD1	11:T:47:ARG:NH2	2.46	0.45
1:L:258:GLU:O	5:P:26:LYS:NZ	2.49	0.45
13:a:94:PHE:O	13:a:163:ASN:ND2	2.50	0.45
13:a:368:HIS:HB3	14:b:171:LYS:HD2	1.98	0.45
13:a:398:PRO:HG3	13:a:404:THR:HG22	1.98	0.45
5:P:129:LYS:NZ	5:P:190:ASP:OD2	2.50	0.45
8:S:27:LYS:HB3	8:S:27:LYS:HE3	1.87	0.45
15:c:128:GLU:HG2	15:c:129:VAL:HG23	1.97	0.45
1:A:154:HIS:NE2	1:A:314:TYR:OH	2.36	0.45
13:a:76:GLY:O	13:a:80:ASN:ND2	2.49	0.45
13:a:187:SER:O	13:a:191:THR:OG1	2.27	0.45
17:e:86:ILE:HD12	17:e:86:ILE:HA	1.88	0.45
18:f:63:CYS:HB2	18:f:86:CYS:SG	2.56	0.45
2:M:36:ALA:O	2:M:207:VAL:HA	2.17	0.45
14:b:151:ARG:NH2	20:h:14:ALA:O	2.43	0.45
16:d:114:ASP:N	16:d:114:ASP:OD1	2.44	0.45
1:A:39:VAL:HG11	1:A:117:VAL:HG11	2.00	0.44
15:c:156:ARG:NH1	15:c:222:GLN:OE1	2.50	0.44
3:C:5:ARG:NH1	3:C:20:ASP:OD2	2.50	0.44
3:C:55:TYR:OH	3:C:133:LEU:O	2.33	0.44
14:b:45:MET:HE3	14:b:45:MET:HB2	1.78	0.44
17:e:82:TYR:HA	17:e:85:VAL:HB	1.99	0.44
18:f:36:PRO:HA	18:f:37:PRO:HD3	1.85	0.44
1:A:366:VAL:HG11	2:B:43:PRO:HB2	1.99	0.44
4:D:27:ARG:HB2	4:D:55:CYS:HB2	1.98	0.44
17:e:66:ARG:HA	17:e:69:GLU:HG2	1.99	0.44
1:A:191:LYS:HA	1:A:220:SER:HB2	1.99	0.44
2:B:68:LEU:HD13	2:B:144:LEU:HD23	1.98	0.44
13:a:74:MET:O	13:a:78:PHE:HB2	2.17	0.44
13:a:168:ILE:HD11	13:a:188:VAL:HG23	2.00	0.44
18:f:55:ASN:HB3	18:f:77:LYS:HE3	2.00	0.44
4:D:184:LYS:NZ	8:H:76:LYS:OXT	2.45	0.44
13:a:170:ASN:ND2	15:c:74:ILE:O	2.47	0.44
14:b:15:PRO:HA	14:b:18:GLU:HG2	2.00	0.44
13:a:157:SER:HB3	13:a:195:LEU:HD12	1.99	0.44
2:B:162:ASN:HB3	2:B:244:ILE:HG21	2.00	0.44
6:F:102:LYS:HD3	6:F:102:LYS:HA	1.79	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:301:ASN:HB2	1:L:303:LEU:HG	1.99	0.44
14:b:12:ALA:O	14:b:188:ARG:NH1	2.37	0.44
2:B:37:SER:HB3	2:B:216:LEU:HD12	2.00	0.44
3:C:237:LEU:HD22	4:D:216:LEU:HD11	2.00	0.44
15:c:77:LYS:HA	15:c:80:ARG:HG2	2.00	0.44
20:h:54:GLU:HG2	20:h:57:ARG:NH1	2.33	0.43
3:N:24:PRO:HB2	3:N:27:ILE:HG23	1.99	0.43
1:L:349:ALA:O	1:L:408:ARG:NH1	2.51	0.43
13:a:428:GLN:HA	13:a:431:LEU:HB2	2.00	0.43
13:a:485:VAL:HG11	13:a:494:TRP:HB3	1.99	0.43
14:b:146:MET:HE2	14:b:146:MET:HB2	1.88	0.43
1:L:154:HIS:NE2	1:L:314:TYR:OH	2.50	0.43
14:b:124:PRO:HD2	14:b:127:ASP:HB2	2.01	0.43
2:B:243:GLU:HA	2:B:424:MET:O	2.18	0.43
6:F:82:LYS:HB2	6:F:85:GLU:HB2	2.00	0.43
3:N:41:LEU:O	3:N:45:ILE:HG12	2.18	0.43
13:a:305:PHE:O	13:a:309:THR:OG1	2.27	0.43
16:d:89:ILE:HG22	22:k:29:TRP:NE1	2.33	0.43
3:C:45:ILE:HA	27:C:401:HEM:HAB	2.00	0.43
4:D:132:THR:HA	4:D:179:MET:HE2	1.99	0.43
4:D:132:THR:O	8:H:19:ARG:NH2	2.52	0.43
2:M:156:GLN:NE2	11:T:58:GLN:O	2.51	0.43
15:c:128:GLU:HB3	19:g:38:HIS:HD1	1.84	0.43
19:g:69:LEU:HD22	25:g:303:3PE:H331	2.00	0.43
23:l:21:LEU:HA	23:l:24:MET:HG2	1.99	0.43
1:A:97:TYR:OH	1:A:190:TYR:OH	2.35	0.43
3:N:181:PHE:HA	3:N:184:ILE:HG22	2.00	0.43
4:O:132:THR:HG22	4:O:179:MET:HE3	2.00	0.43
13:a:233:HIS:HB3	15:c:99:TRP:HH2	1.84	0.43
13:a:247:ILE:HB	33:a:604:HEA:HBC1	2.01	0.43
17:e:89:LEU:O	17:e:92:THR:OG1	2.36	0.43
5:E:128:LYS:HD2	5:E:128:LYS:HA	1.87	0.43
8:H:19:ARG:HG2	8:H:63:ARG:HH11	1.84	0.43
3:N:133:LEU:HD23	3:N:133:LEU:HA	1.84	0.43
3:N:165:TRP:O	3:N:174:THR:OG1	2.34	0.43
4:O:33:TYR:HD1	4:O:37:CYS:HB2	1.83	0.43
13:a:140:GLY:O	13:a:213:ARG:NH2	2.52	0.43
2:M:276:GLN:HG2	2:M:281:ALA:HB2	2.01	0.43
13:a:78:PHE:O	13:a:82:LEU:HB2	2.19	0.43
4:D:209:LEU:HD23	4:D:209:LEU:HA	1.91	0.43
15:c:108:PRO:HB2	15:c:114:GLY:HA2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:94:LYS:HZ2	5:E:136:ILE:HG13	1.83	0.42
2:M:137:VAL:HA	2:M:140:LEU:HD23	2.00	0.42
2:M:276:GLN:HE21	11:T:61:ALA:HB1	1.84	0.42
8:S:18:VAL:HG12	8:S:67:VAL:HG12	2.01	0.42
13:a:383:MET:HA	13:a:386:VAL:HB	2.01	0.42
33:a:604:HEA:H251	14:b:72:ILE:HB	2.01	0.42
14:b:44:LEU:HD21	21:i:22:HIS:HB3	2.01	0.42
14:b:88:ASP:OD1	14:b:88:ASP:N	2.52	0.42
14:b:122:MET:HE3	14:b:135:LEU:HA	2.00	0.42
20:h:57:ARG:HA	20:h:60:TYR:CE1	2.54	0.42
6:Q:70:MET:HE2	6:Q:70:MET:HB3	1.97	0.42
12:I:85:LEU:HA	12:I:88:THR:HG22	2.01	0.42
2:B:76:THR:HG22	2:B:82:SER:H	1.85	0.42
2:B:258:VAL:HA	2:B:323:GLY:HA3	2.01	0.42
4:O:216:LEU:HD13	26:O:301:CDL:H552	2.00	0.42
3:C:144:THR:O	3:C:148:ASN:HB2	2.19	0.42
3:C:186:PRO:HA	3:C:189:ILE:HB	2.02	0.42
19:g:70:PHE:HD2	25:g:303:3PE:H11	1.83	0.42
5:E:188:THR:OG1	5:E:192:VAL:O	2.34	0.42
3:N:257:MET:HE2	3:N:257:MET:HB3	1.95	0.42
13:a:362:SER:HB2	14:b:20:LEU:HD21	2.00	0.42
16:d:67:SER:HB3	17:e:106:LEU:HD22	2.02	0.42
26:D:301:CDL:H121	26:D:301:CDL:H511	2.00	0.42
2:M:49:LEU:HD11	2:M:204:MET:HB3	2.01	0.42
3:N:78:LEU:HD11	3:N:240:MET:HE1	2.00	0.42
2:B:297:GLN:HG2	2:B:301:LYS:HE2	2.02	0.42
1:L:118:GLN:HE21	1:L:118:GLN:HB3	1.71	0.42
2:M:387:LEU:HD23	2:M:387:LEU:HA	1.90	0.42
14:b:40:TYR:O	14:b:44:LEU:HB2	2.20	0.42
16:d:100:LYS:HE3	22:k:38:ILE:HG22	2.01	0.42
23:l:24:MET:HE1	37:l:601:TGL:HC31	2.00	0.42
1:A:134:ILE:O	1:A:138:MET:HG3	2.19	0.42
3:N:311:LYS:HD3	3:N:379:LEU:HD23	2.00	0.42
6:Q:44:LYS:HE3	6:Q:48:ARG:HH22	1.85	0.42
13:a:28:MET:HE3	13:a:28:MET:HB3	1.85	0.42
13:a:393:PHE:O	13:a:397:PHE:HB2	2.19	0.42
13:a:430:PHE:HB3	14:b:7:LEU:HA	2.01	0.42
15:c:214:PHE:HD1	25:c:301:3PE:H281	1.85	0.42
18:f:34:MET:HE3	18:f:34:MET:HB3	1.92	0.42
21:i:47:LYS:HB3	21:i:47:LYS:HE2	1.79	0.42
4:D:127:VAL:HG11	4:D:190:LEU:HD12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:54:VAL:HG11	25:G:101:3PE:H2A1	2.02	0.42
1:L:39:VAL:HG23	1:L:113:LEU:HD13	2.02	0.42
2:B:209:LEU:HD21	2:B:378:PHE:HD2	1.84	0.42
1:A:27:SER:HA	1:A:199:ALA:O	2.20	0.41
1:A:231:LEU:HD23	1:A:231:LEU:HA	1.91	0.41
1:A:266:ASP:OD1	1:A:266:ASP:N	2.51	0.41
6:F:35:ASP:OD1	6:F:89:TYR:OH	2.32	0.41
13:a:329:GLY:O	14:b:52:HIS:N	2.43	0.41
14:b:189:PRO:HA	14:b:213:MET:HG2	2.01	0.41
17:e:26:ALA:HB2	17:e:58:LEU:HD11	2.01	0.41
3:C:29:SER:OG	26:C:404:CDL:OA9	2.33	0.41
4:D:152:TYR:OH	8:H:64:ASP:OD2	2.24	0.41
1:A:251:ALA:O	1:A:325:VAL:HA	2.20	0.41
5:P:112:VAL:HG22	5:P:172:ARG:HH22	1.85	0.41
12:I:93:THR:HG21	15:c:19:THR:HG23	2.02	0.41
15:c:72:THR:HB	15:c:75:VAL:HG23	2.02	0.41
3:N:45:ILE:HA	27:N:401:HEM:HAB	2.00	0.41
10:V:15:ARG:HA	10:V:15:ARG:HD2	1.89	0.41
13:a:168:ILE:HG21	13:a:189:LEU:HD12	2.02	0.41
19:g:25:LEU:HA	19:g:28:VAL:HG12	2.02	0.41
2:M:148:LYS:HG3	2:M:177:TYR:HB3	2.03	0.41
3:N:216:ASP:HB2	6:Q:63:LYS:HG3	2.02	0.41
4:O:208:MET:HE3	4:O:208:MET:HB3	1.94	0.41
4:O:225:HIS:O	4:O:228:SER:OG	2.39	0.41
13:a:132:LEU:O	13:a:138:HIS:ND1	2.47	0.41
14:b:141:ARG:NH2	21:i:70:ILE:O	2.54	0.41
5:E:14:ARG:HG2	5:E:18:VAL:HG23	2.02	0.41
5:E:136:ILE:HD13	5:E:136:ILE:HA	1.93	0.41
4:O:18:LEU:HD22	4:O:206:LEU:HB2	2.03	0.41
5:P:69:LEU:HD23	5:P:69:LEU:HA	1.96	0.41
9:U:44:GLU:HB2	9:U:54:HIS:CE1	2.56	0.41
17:e:56:ARG:NH2	17:e:59:ASN:OD1	2.54	0.41
1:A:161:THR:HG22	5:E:21:SER:HB2	2.02	0.41
1:A:363:ASN:O	1:A:367:SER:OG	2.34	0.41
3:C:37:LEU:HD11	3:C:94:LEU:HA	2.03	0.41
1:L:41:ILE:HG12	1:L:195:MET:HG2	2.03	0.41
2:M:439:LEU:HD23	2:M:439:LEU:HA	1.94	0.41
15:c:187:SER:N	15:c:190:ASP:OD2	2.45	0.41
16:d:94:LEU:HD23	16:d:94:LEU:HA	1.90	0.41
2:B:98:VAL:HA	2:B:106:ALA:O	2.21	0.41
5:E:9:ASP:OD2	5:E:11:SER:OG	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:392:LEU:HD12	1:L:392:LEU:HA	1.94	0.41
13:a:35:ILE:HD11	13:a:462:LEU:HB2	2.02	0.41
2:B:70:ARG:HG3	2:B:98:VAL:HG13	2.02	0.41
4:D:72:ASP:HB2	4:D:83:ARG:HG2	2.03	0.41
5:E:23:LYS:HA	5:E:23:LYS:HD3	1.85	0.41
1:L:86:LEU:HB3	2:M:285:ILE:HG12	2.03	0.41
6:Q:102:LYS:HD3	6:Q:102:LYS:HA	1.85	0.41
19:g:28:VAL:O	19:g:32:SER:OG	2.30	0.41
1:A:248:LEU:HD12	1:A:426:GLY:HA2	2.03	0.41
2:B:299:VAL:HG21	2:B:309:VAL:HG21	2.02	0.41
5:E:8:PRO:HA	12:I:44:LEU:HA	2.03	0.41
2:M:48:GLY:HA2	2:M:107:TYR:O	2.21	0.41
2:M:172:LEU:HD23	2:M:172:LEU:HA	1.90	0.41
2:M:224:LEU:HD23	2:M:224:LEU:HA	1.96	0.41
17:e:72:LYS:HD2	17:e:82:TYR:CD1	2.56	0.41
3:C:158:THR:HA	3:C:161:VAL:HG12	2.03	0.40
3:C:262:LEU:HD22	5:P:138:VAL:HG21	2.01	0.40
2:M:394:PRO:O	2:M:397:THR:OG1	2.33	0.40
2:M:436:LEU:HD23	2:M:436:LEU:HA	1.92	0.40
4:O:20:SER:OG	4:O:21:LEU:N	2.54	0.40
5:P:160:CYS:HB2	29:P:201:FES:S2	2.62	0.40
14:b:28:LEU:HD23	21:i:37:TYR:CZ	2.57	0.40
21:i:63:GLU:O	21:i:67:LYS:HG2	2.21	0.40
3:C:327:ILE:HD11	25:G:101:3PE:H272	2.04	0.40
1:L:73:ASN:O	1:L:76:GLU:HB2	2.20	0.40
3:N:246:PHE:HB3	3:N:249:MET:HE3	2.04	0.40
3:N:272:TRP:HA	3:N:275:LEU:HG	2.03	0.40
14:b:52:HIS:CG	17:e:40:ASP:HB2	2.56	0.40
14:b:116:LEU:HB2	14:b:227:ILE:HD11	2.03	0.40
16:d:89:ILE:HG22	22:k:29:TRP:HE1	1.86	0.40
17:e:41:LEU:HD13	21:i:12:ARG:HG3	2.03	0.40
3:C:89:MET:HE2	3:C:89:MET:HB2	1.86	0.40
3:C:331:ASN:C	3:C:331:ASN:HD22	2.30	0.40
4:D:75:ASN:OD1	4:D:76:ASP:N	2.51	0.40
5:E:90:LYS:HD3	5:E:90:LYS:HA	1.88	0.40
3:N:331:ASN:C	3:N:331:ASN:HD22	2.30	0.40
13:a:288:TRP:CD1	13:a:292:MET:HE1	2.56	0.40
33:a:604:HEA:H261	33:a:604:HEA:H172	1.67	0.40
18:f:62:ILE:HG12	18:f:70:VAL:HG22	2.02	0.40
2:B:236:LYS:HD2	2:B:236:LYS:HA	1.85	0.40
3:C:214:ASP:HB3	7:G:8:ALA:HB2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:34:VAL:HG11	2:M:386:ALA:HB1	2.03	0.40
4:O:179:MET:HE2	4:O:179:MET:HB3	1.95	0.40
16:d:76:ASN:HB3	22:k:10:HIS:HB3	2.03	0.40
3:N:311:LYS:HB3	3:N:311:LYS:HE3	1.85	0.40
4:O:158:ILE:HG23	4:O:160:MET:H	1.87	0.40
7:R:52:PHE:HA	7:R:55:VAL:HG22	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%)	425 (96%)	18 (4%)	0	100	100
2	B	418/439 (95%)	406 (97%)	12 (3%)	0	100	100
2	M	418/439 (95%)	395 (94%)	23 (6%)	0	100	100
3	C	377/381 (99%)	366 (97%)	11 (3%)	0	100	100
3	N	378/381 (99%)	367 (97%)	11 (3%)	0	100	100
4	D	239/241 (99%)	237 (99%)	2 (1%)	0	100	100
4	O	238/241 (99%)	229 (96%)	9 (4%)	0	100	100
5	E	194/196 (99%)	184 (95%)	10 (5%)	0	100	100
5	P	194/196 (99%)	182 (94%)	12 (6%)	0	100	100
6	F	100/110 (91%)	97 (97%)	3 (3%)	0	100	100
6	Q	99/110 (90%)	97 (98%)	2 (2%)	0	100	100
7	G	72/81 (89%)	70 (97%)	2 (3%)	0	100	100
7	R	70/81 (86%)	67 (96%)	3 (4%)	0	100	100
8	H	66/76 (87%)	61 (92%)	5 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	S	66/76 (87%)	64 (97%)	2 (3%)	0	100	100
9	J	56/63 (89%)	54 (96%)	2 (4%)	0	100	100
9	U	58/63 (92%)	56 (97%)	2 (3%)	0	100	100
10	K	50/56 (89%)	47 (94%)	3 (6%)	0	100	100
10	V	51/56 (91%)	47 (92%)	4 (8%)	0	100	100
11	T	76/78 (97%)	68 (90%)	8 (10%)	0	100	100
12	I	109/113 (96%)	99 (91%)	9 (8%)	1 (1%)	14	43
13	a	512/514 (100%)	492 (96%)	20 (4%)	0	100	100
14	b	225/227 (99%)	207 (92%)	18 (8%)	0	100	100
15	c	257/261 (98%)	246 (96%)	11 (4%)	0	100	100
16	d	142/147 (97%)	135 (95%)	7 (5%)	0	100	100
17	e	102/109 (94%)	98 (96%)	4 (4%)	0	100	100
18	f	93/99 (94%)	86 (92%)	7 (8%)	0	100	100
19	g	73/85 (86%)	67 (92%)	6 (8%)	0	100	100
20	h	77/85 (91%)	74 (96%)	3 (4%)	0	100	100
21	i	70/75 (93%)	65 (93%)	5 (7%)	0	100	100
22	k	47/56 (84%)	43 (92%)	4 (8%)	0	100	100
23	l	44/47 (94%)	44 (100%)	0	0	100	100
24	m	41/46 (89%)	39 (95%)	2 (5%)	0	100	100
All	All	5899/6120 (96%)	5637 (96%)	261 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	I	48	VAL

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%)	329 (100%)	1 (0%)	86	86
2	M	330/344 (96%)	330 (100%)	0	100	100
3	C	331/333 (99%)	331 (100%)	0	100	100
3	N	332/333 (100%)	332 (100%)	0	100	100
4	D	206/206 (100%)	206 (100%)	0	100	100
4	O	205/206 (100%)	205 (100%)	0	100	100
5	E	166/166 (100%)	166 (100%)	0	100	100
5	P	166/166 (100%)	166 (100%)	0	100	100
6	F	94/98 (96%)	94 (100%)	0	100	100
6	Q	93/98 (95%)	93 (100%)	0	100	100
7	G	67/73 (92%)	67 (100%)	0	100	100
7	R	66/73 (90%)	66 (100%)	0	100	100
8	H	65/72 (90%)	65 (100%)	0	100	100
8	S	65/72 (90%)	65 (100%)	0	100	100
9	J	49/54 (91%)	49 (100%)	0	100	100
9	U	51/54 (94%)	51 (100%)	0	100	100
10	K	42/46 (91%)	42 (100%)	0	100	100
10	V	43/46 (94%)	43 (100%)	0	100	100
11	T	58/58 (100%)	58 (100%)	0	100	100
12	I	83/95 (87%)	83 (100%)	0	100	100
13	a	425/425 (100%)	425 (100%)	0	100	100
14	b	210/210 (100%)	210 (100%)	0	100	100
15	c	225/227 (99%)	225 (100%)	0	100	100
16	d	127/128 (99%)	127 (100%)	0	100	100
17	e	91/95 (96%)	91 (100%)	0	100	100
18	f	81/83 (98%)	81 (100%)	0	100	100
19	g	62/67 (92%)	62 (100%)	0	100	100
20	h	70/75 (93%)	70 (100%)	0	100	100
21	i	54/56 (96%)	54 (100%)	0	100	100
22	k	39/46 (85%)	39 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	l	39/40 (98%)	39 (100%)	0	100	100
24	m	33/34 (97%)	33 (100%)	0	100	100
All	All	5043/5169 (98%)	5042 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	400	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	213	GLN
1	A	274	ASN
1	A	305	GLN
1	A	323	HIS
2	B	218	GLN
2	B	222	GLN
2	B	304	HIS
2	B	338	ASN
3	C	8	HIS
3	C	68	HIS
1	L	21	ASN
1	L	118	GLN
1	L	119	ASN
1	L	187	ASN
1	L	267	ASN
1	L	405	GLN
2	M	143	GLN
2	M	218	GLN
2	M	222	GLN
2	M	276	GLN
2	M	289	ASN
2	M	329	GLN
2	M	343	GLN
2	M	358	GLN
3	N	8	HIS
3	N	341	GLN
4	O	198	HIS
7	R	73	ASN

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Mol	Chain	Res	Type
8	S	21	HIS
11	T	58	GLN
13	a	98	ASN
13	a	170	ASN
13	a	178	GLN
13	a	360	ASN
13	a	428	GLN
14	b	24	HIS
14	b	102	HIS
14	b	103	GLN
14	b	187	ASN
15	c	204	HIS
16	d	76	ASN
16	d	143	ASN
17	e	20	ASN
18	f	85	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 41 ligands modelled in this entry, 4 are monoatomic - leaving 37 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	$\#\|Z\|>2$
33	HEA	a	603	13	66,67,67	1.41	6 (9%)	78,103,103	2.35	27 (34%)
25	3PE	N	403	-	36,36,50	0.35	0	39,41,55	0.36	0
27	HEM	N	401	3	50,50,50	1.38	5 (10%)	66,82,82	1.81	15 (22%)
29	FES	E	202	5	0,4,4	-	-	-		
25	3PE	L	501	-	22,22,50	0.44	0	25,27,55	0.36	0
26	CDL	A	502	-	45,45,99	0.44	0	51,57,111	0.40	0
28	HEC	O	303	4	50,50,50	1.63	5 (10%)	68,82,82	1.27	3 (4%)
29	FES	P	201	5	0,4,4	-	-	-		
25	3PE	g	303	-	24,24,50	0.44	0	27,29,55	0.69	1 (3%)
25	3PE	E	201	-	31,31,50	0.39	0	34,36,55	0.33	0
25	3PE	C	403	-	34,34,50	0.36	0	37,39,55	0.33	0
26	CDL	L	502	-	45,45,99	0.44	0	51,57,111	0.58	1 (1%)
25	3PE	b	304	-	27,27,50	0.39	0	30,32,55	0.39	0
25	3PE	R	101	-	50,50,50	0.32	0	53,55,55	0.55	1 (1%)
26	CDL	O	301	-	56,56,99	0.38	0	62,68,111	0.35	0
28	HEC	D	302	4	50,50,50	1.65	4 (8%)	68,82,82	1.32	4 (5%)
25	3PE	O	302	-	22,22,50	0.44	0	25,27,55	0.42	0
27	HEM	C	402	3	50,50,50	1.37	6 (12%)	66,82,82	1.74	16 (24%)
25	3PE	a	607	-	26,26,50	0.40	0	29,31,55	0.44	0
27	HEM	N	402	3	50,50,50	1.41	7 (14%)	66,82,82	1.66	16 (24%)
30	PC1	J	101	-	34,34,53	0.36	0	40,42,61	0.34	0
25	3PE	b	302	-	28,28,50	0.39	0	31,33,55	0.35	0
25	3PE	c	301	-	44,44,50	0.31	0	47,49,55	0.39	0
35	CUA	b	303	14	0,1,1	-	-	-		
25	3PE	A	501	-	22,22,50	0.46	0	25,27,55	0.74	1 (4%)
26	CDL	C	404	-	41,41,99	0.45	0	47,53,111	0.34	0
30	PC1	P	202	-	23,23,53	0.45	0	29,31,61	0.69	1 (3%)
30	PC1	g	302	-	49,49,53	0.30	0	55,57,61	0.30	0
37	TGL	l	601	-	36,36,62	0.23	0	39,39,65	0.29	0
26	CDL	D	301	-	55,55,99	0.39	0	61,67,111	0.36	0
26	CDL	g	301	-	38,38,99	0.45	0	44,50,111	0.65	1 (2%)
26	CDL	N	404	-	40,40,99	0.47	0	46,52,111	0.63	1 (2%)
27	HEM	C	401	3	50,50,50	1.35	7 (14%)	66,82,82	1.76	16 (24%)
25	3PE	G	101	-	50,50,50	0.31	0	53,55,55	0.30	0
33	HEA	a	604	13	66,67,67	1.41	7 (10%)	78,103,103	2.39	26 (33%)
25	3PE	a	606	-	27,27,50	0.40	0	30,32,55	0.40	0
25	3PE	a	605	-	33,33,50	0.39	0	36,38,55	0.62	1 (2%)

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
33	HEA	a	603	13	-	14/36/76/76	-
25	3PE	N	403	-	-	8/40/40/54	-
27	HEM	N	401	3	-	7/14/54/54	-
29	FES	E	202	5	-	-	0/1/1/1
28	HEC	O	303	4	1/1/3/7	2/14/54/54	-
26	CDL	A	502	-	-	20/56/56/110	-
25	3PE	L	501	-	-	5/26/26/54	-
29	FES	P	201	5	-	-	0/1/1/1
25	3PE	g	303	-	-	5/28/28/54	-
25	3PE	E	201	-	-	9/35/35/54	-
25	3PE	C	403	-	-	9/38/38/54	-
26	CDL	L	502	-	-	13/56/56/110	-
25	3PE	b	304	-	-	5/31/31/54	-
25	3PE	R	101	-	-	12/54/54/54	-
26	CDL	O	301	-	-	22/67/67/110	-
28	HEC	D	302	4	1/1/3/7	2/14/54/54	-
25	3PE	O	302	-	-	7/26/26/54	-
27	HEM	C	402	3	-	9/14/54/54	-
25	3PE	a	607	-	-	11/30/30/54	-
27	HEM	N	402	3	-	8/14/54/54	-
30	PC1	J	101	-	-	6/38/38/57	-
25	3PE	b	302	-	-	10/32/32/54	-
25	3PE	c	301	-	-	13/48/48/54	-
25	3PE	A	501	-	-	8/26/26/54	-
26	CDL	C	404	-	-	17/52/52/110	-
30	PC1	P	202	-	-	10/27/27/57	-
30	PC1	g	302	-	-	7/53/53/57	-
37	TGL	l	601	-	-	3/39/39/65	-
26	CDL	D	301	-	-	13/66/66/110	-
26	CDL	g	301	-	-	14/47/47/110	-
26	CDL	N	404	-	-	15/51/51/110	-
27	HEM	C	401	3	-	7/14/54/54	-
25	3PE	G	101	-	-	10/54/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	HEA	a	604	13	-	12/36/76/76	-
25	3PE	a	606	-	-	13/31/31/54	-
25	3PE	a	605	-	-	6/37/37/54	-

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	D	302	HEC	C3D-C2D	7.80	1.53	1.36
28	O	303	HEC	C3D-C2D	7.68	1.53	1.36
33	a	603	HEA	C3B-C2B	4.37	1.44	1.34
33	a	604	HEA	C3D-C2D	4.28	1.45	1.36
27	N	402	HEM	C4D-ND	-4.21	1.33	1.40
33	a	603	HEA	C3A-C2A	4.13	1.45	1.36
33	a	604	HEA	C3B-C2B	4.03	1.43	1.34
33	a	603	HEA	C3D-C2D	3.96	1.45	1.36
27	N	401	HEM	C4D-ND	-3.84	1.33	1.40
33	a	604	HEA	C3A-C2A	3.77	1.44	1.36
27	C	401	HEM	C4D-ND	-3.76	1.33	1.40
27	N	401	HEM	C1B-NB	-3.74	1.33	1.40
27	C	402	HEM	C4D-ND	-3.60	1.34	1.40
27	C	401	HEM	C1B-NB	-3.52	1.34	1.40
27	C	402	HEM	C1B-NB	-3.46	1.34	1.40
27	N	402	HEM	C1B-NB	-3.44	1.34	1.40
28	O	303	HEC	FE-ND	3.18	2.04	1.94
27	N	402	HEM	C1C-C2C	-3.16	1.39	1.45
28	D	302	HEC	FE-NA	3.12	2.05	1.95
28	O	303	HEC	FE-NB	3.10	2.04	1.94
33	a	603	HEA	C4B-C3B	3.07	1.49	1.44
27	C	402	HEM	C1C-C2C	-3.06	1.39	1.45
28	D	302	HEC	FE-NB	2.92	2.03	1.94
27	C	402	HEM	C1D-ND	-2.90	1.32	1.38
33	a	604	HEA	C4B-C3B	2.89	1.49	1.44
27	N	401	HEM	C1C-C2C	-2.89	1.39	1.45
27	C	401	HEM	C1C-C2C	-2.85	1.39	1.45
27	N	402	HEM	C1D-ND	-2.83	1.33	1.38
27	C	401	HEM	C1D-ND	-2.77	1.33	1.38
27	N	401	HEM	C1D-ND	-2.71	1.33	1.38
28	D	302	HEC	FE-ND	2.66	2.03	1.94
33	a	603	HEA	C1D-ND	-2.58	1.35	1.40
33	a	604	HEA	C1D-ND	-2.40	1.36	1.40
27	N	402	HEM	FE-NB	2.35	2.02	1.94
28	O	303	HEC	FE-NA	2.35	2.03	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	C	401	HEM	C3C-C4C	-2.30	1.42	1.46
33	a	604	HEA	C3C-C4C	2.25	1.48	1.42
33	a	603	HEA	C4A-NA	-2.24	1.35	1.39
27	N	402	HEM	C3C-C4C	-2.22	1.42	1.46
28	O	303	HEC	FE-NC	2.22	2.02	1.95
27	C	402	HEM	FE-NB	2.22	2.01	1.94
27	C	402	HEM	C4B-NB	-2.17	1.34	1.38
27	N	402	HEM	C4B-NB	-2.17	1.34	1.38
27	C	401	HEM	FE-NB	2.13	2.01	1.94
27	C	401	HEM	C4B-NB	-2.10	1.34	1.38
33	a	604	HEA	C1D-C2D	2.08	1.48	1.44
27	N	401	HEM	C4B-NB	-2.04	1.34	1.38

All (131) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	a	603	HEA	C3A-C2A-C1A	-7.43	99.98	107.08
33	a	604	HEA	C3A-C2A-C1A	-6.53	100.84	107.08
28	D	302	HEC	C1D-ND-C4D	6.03	111.30	105.07
33	a	604	HEA	CMC-C2C-C3C	5.97	141.05	126.59
28	O	303	HEC	C1D-ND-C4D	5.90	111.17	105.07
33	a	604	HEA	CMC-C2C-C1C	-5.79	116.55	125.37
33	a	603	HEA	C2A-C1A-NA	5.53	115.70	110.32
27	N	401	HEM	CHC-C4B-NB	5.12	129.98	124.42
27	C	401	HEM	CHC-C4B-NB	5.08	129.94	124.42
33	a	604	HEA	C3D-C4D-ND	5.06	115.26	110.36
33	a	603	HEA	C3D-C4D-ND	5.02	115.21	110.36
27	N	401	HEM	CHB-C1B-NB	4.91	130.43	124.37
33	a	604	HEA	C2A-C1A-NA	4.78	114.97	110.32
33	a	603	HEA	CMD-C2D-C1D	-4.71	117.87	125.04
33	a	604	HEA	CMD-C2D-C1D	-4.56	118.09	125.04
27	C	402	HEM	C4D-ND-C1D	4.42	109.64	105.07
33	a	603	HEA	CMC-C2C-C3C	4.37	137.18	126.59
27	C	402	HEM	CHC-C4B-NB	4.35	129.15	124.42
27	C	401	HEM	CHD-C4C-NC	4.33	129.12	124.44
27	C	401	HEM	CHB-C1B-NB	4.30	129.68	124.37
33	a	603	HEA	CHA-C1A-C2A	-4.15	118.21	124.94
33	a	603	HEA	CMC-C2C-C1C	-4.12	119.10	125.37
27	N	402	HEM	CHD-C4C-NC	4.11	128.88	124.44
27	C	402	HEM	CHB-C1B-NB	4.10	129.43	124.37
27	N	402	HEM	C4D-ND-C1D	4.07	109.27	105.07
33	a	604	HEA	CHA-C4D-C3D	-4.04	118.90	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	a	604	HEA	CMB-C2B-C1B	-4.03	118.90	125.04
27	N	401	HEM	CHD-C4C-NC	4.00	128.77	124.44
33	a	604	HEA	CAA-CBA-CGA	-4.00	104.99	113.60
33	a	603	HEA	CMB-C2B-C1B	-3.97	119.00	125.04
33	a	604	HEA	C3C-C2C-C1C	-3.95	102.39	107.16
27	N	402	HEM	CHC-C4B-NB	3.95	128.71	124.42
33	a	603	HEA	C4D-C3D-C2D	-3.93	101.17	106.90
27	N	402	HEM	CHB-C1B-NB	3.90	129.19	124.37
27	C	402	HEM	CHD-C4C-NC	3.88	128.64	124.44
33	a	603	HEA	CHA-C4D-C3D	-3.84	119.19	124.84
33	a	604	HEA	C4D-C3D-C2D	-3.74	101.45	106.90
33	a	604	HEA	CAD-CBD-CGD	-3.67	105.71	113.60
33	a	603	HEA	C26-C15-C16	3.61	121.35	115.27
33	a	604	HEA	CMD-C2D-C3D	3.59	135.85	126.12
27	N	401	HEM	C4D-ND-C1D	3.58	108.77	105.07
33	a	603	HEA	C13-C12-C11	-3.56	109.00	114.35
27	C	401	HEM	C4D-ND-C1D	3.50	108.69	105.07
33	a	603	HEA	CMD-C2D-C3D	3.49	135.58	126.12
33	a	604	HEA	CHA-C1A-C2A	-3.46	119.33	124.94
27	N	401	HEM	C1B-NB-C4B	3.37	108.56	105.07
27	C	402	HEM	CHD-C1D-ND	3.32	128.02	124.42
33	a	603	HEA	OMA-CMA-C3A	-3.23	118.39	125.69
27	C	401	HEM	C1B-NB-C4B	3.22	108.40	105.07
27	C	402	HEM	C1B-NB-C4B	3.17	108.34	105.07
27	C	401	HEM	CHD-C1D-ND	3.15	127.84	124.42
27	N	402	HEM	C4C-NC-C1C	3.14	108.43	105.35
33	a	604	HEA	C26-C15-C16	3.14	120.55	115.27
27	N	401	HEM	C3B-C2B-C1B	3.09	108.78	106.49
27	N	401	HEM	C4B-C3B-C2B	-3.05	104.69	107.11
27	N	402	HEM	C1B-NB-C4B	2.99	108.16	105.07
27	N	401	HEM	CHA-C4D-ND	2.95	128.01	124.37
27	N	401	HEM	CHD-C1D-ND	2.93	127.60	124.42
27	C	401	HEM	CHA-C4D-ND	2.91	127.97	124.37
33	a	604	HEA	C4B-C3B-C2B	-2.89	102.47	107.41
33	a	604	HEA	C3B-C4B-NB	2.89	113.26	109.84
27	N	402	HEM	C4A-NA-C1A	2.88	108.17	105.35
33	a	603	HEA	C3C-C2C-C1C	-2.87	103.70	107.16
27	C	402	HEM	C4C-NC-C1C	2.81	108.10	105.35
33	a	604	HEA	C25-C23-C24	2.77	120.72	114.60
33	a	603	HEA	CAA-CBA-CGA	-2.76	107.67	113.60
27	C	402	HEM	CAD-C3D-C4D	2.68	129.34	124.66
33	a	603	HEA	CMB-C2B-C3B	2.68	135.45	130.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	a	604	HEA	CHC-C1C-C2C	-2.67	119.69	127.24
27	N	402	HEM	C4A-CHB-C1B	-2.67	120.01	126.34
27	C	402	HEM	C4A-NA-C1A	2.64	107.93	105.35
27	C	401	HEM	CHA-C1A-NA	2.62	128.66	123.85
27	C	401	HEM	CHB-C1B-C2B	-2.55	119.65	126.73
33	a	603	HEA	CHB-C1B-C2B	-2.55	121.00	124.98
27	C	402	HEM	C4A-CHB-C1B	-2.54	120.31	126.34
27	N	401	HEM	C1C-CHC-C4B	-2.54	120.58	126.06
27	N	402	HEM	CHB-C1B-C2B	-2.53	119.70	126.73
28	D	302	HEC	CAA-CBA-CGA	-2.52	108.17	113.60
27	C	402	HEM	CHB-C1B-C2B	-2.52	119.72	126.73
27	N	402	HEM	CAD-CBD-CGD	-2.52	108.18	113.60
27	N	401	HEM	CAA-CBA-CGA	-2.52	108.19	113.60
27	C	402	HEM	C2A-C1A-NA	-2.51	107.35	110.15
27	C	401	HEM	CAA-CBA-CGA	-2.48	108.27	113.60
27	N	401	HEM	CHA-C1A-NA	2.47	128.40	123.85
33	a	603	HEA	C27-C19-C20	2.46	119.42	115.27
27	C	402	HEM	C1C-CHC-C4B	-2.45	120.78	126.06
33	a	604	HEA	CAD-C3D-C2D	2.44	132.42	127.88
26	g	301	CDL	CB4-OB6-CB5	2.44	123.79	117.79
27	C	401	HEM	C4C-NC-C1C	2.43	107.73	105.35
33	a	604	HEA	C2C-C1C-NC	2.43	113.78	110.08
27	N	402	HEM	CHD-C1D-ND	2.40	127.03	124.42
27	N	401	HEM	CHB-C1B-C2B	-2.39	120.08	126.73
26	L	502	CDL	CB4-OB6-CB5	2.39	123.67	117.79
25	g	303	3PE	C2-O21-C21	2.37	123.62	117.79
27	C	401	HEM	C1C-CHC-C4B	-2.36	120.96	126.06
33	a	603	HEA	CAD-C3D-C4D	2.35	128.77	124.66
28	D	302	HEC	CHA-C4D-ND	2.35	126.97	124.42
27	C	402	HEM	CHA-C1A-NA	2.34	128.15	123.85
28	O	303	HEC	CAA-CBA-CGA	-2.34	108.58	113.60
27	N	402	HEM	CHA-C1A-NA	2.31	128.10	123.85
27	N	402	HEM	C2A-C1A-NA	-2.31	107.56	110.15
33	a	604	HEA	CHB-C1B-C2B	-2.31	121.37	124.98
30	P	202	PC1	C2-O21-C21	2.29	123.43	117.79
27	C	401	HEM	CAD-CBD-CGD	-2.29	108.68	113.60
25	a	605	3PE	C2-O21-C21	2.28	123.40	117.79
27	N	402	HEM	C1C-CHC-C4B	-2.28	121.15	126.06
25	A	501	3PE	C2-O21-C21	2.27	123.39	117.79
27	N	402	HEM	C4C-CHD-C1D	-2.26	121.18	126.06
33	a	604	HEA	CMB-C2B-C3B	2.24	134.62	130.34
27	N	401	HEM	C4C-NC-C1C	2.24	107.54	105.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	a	603	HEA	C25-C23-C24	2.24	119.54	114.60
33	a	603	HEA	CHB-C1B-NB	2.22	126.83	124.42
25	R	101	3PE	C2-O21-C21	2.22	123.25	117.79
33	a	603	HEA	C13-C14-C15	-2.21	122.35	127.66
33	a	604	HEA	OMA-CMA-C3A	-2.21	120.70	125.69
33	a	603	HEA	C17-C18-C19	-2.20	122.37	127.66
27	N	402	HEM	CHA-C4D-ND	2.19	127.08	124.37
33	a	603	HEA	C4B-C3B-C2B	-2.19	103.68	107.41
27	C	401	HEM	C4A-CHB-C1B	-2.16	121.22	126.34
27	C	401	HEM	C4B-C3B-C2B	-2.15	105.41	107.11
33	a	603	HEA	CHC-C1C-C2C	-2.14	121.20	127.24
33	a	604	HEA	C26-C15-C14	-2.13	118.21	123.68
26	N	404	CDL	CA4-OA6-CA5	2.13	123.04	117.79
27	N	401	HEM	C4A-CHB-C1B	-2.10	121.35	126.34
27	C	402	HEM	C4C-CHD-C1D	-2.09	121.55	126.06
27	C	401	HEM	C4A-NA-C1A	2.08	107.39	105.35
27	C	402	HEM	O2A-CGA-CBA	2.06	120.64	114.03
33	a	604	HEA	CHB-C1B-NB	2.05	126.64	124.42
28	D	302	HEC	CMC-C2C-C1C	-2.04	122.26	125.37
28	O	303	HEC	C2A-C1A-NA	-2.02	108.36	110.32
33	a	603	HEA	C3C-C4C-NC	2.02	111.49	110.25

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
28	D	302	HEC	NA
28	O	303	HEC	NA

All (332) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	A	501	3PE	C11-O13-P-O11
25	A	501	3PE	C11-O13-P-O12
25	A	501	3PE	C11-O13-P-O14
25	A	501	3PE	O13-C11-C12-N
25	C	403	3PE	C1-O11-P-O14
25	C	403	3PE	O21-C2-C3-O31
25	E	201	3PE	C1-O11-P-O12
25	E	201	3PE	C1-O11-P-O14
25	E	201	3PE	O13-C11-C12-N
25	G	101	3PE	O13-C11-C12-N
25	N	403	3PE	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
25	N	403	3PE	C11-O13-P-O14
25	N	403	3PE	O13-C11-C12-N
25	O	302	3PE	C11-O13-P-O12
25	R	101	3PE	C1-O11-P-O12
25	R	101	3PE	C1-O11-P-O13
25	R	101	3PE	C1-O11-P-O14
25	a	605	3PE	C11-O13-P-O12
25	a	605	3PE	C11-O13-P-O14
25	a	605	3PE	O13-C11-C12-N
25	a	606	3PE	C1-O11-P-O12
25	a	606	3PE	C1-O11-P-O14
25	a	606	3PE	C11-O13-P-O14
25	a	607	3PE	C11-O13-P-O14
25	a	607	3PE	O13-C11-C12-N
25	b	302	3PE	C1-O11-P-O14
25	b	304	3PE	O13-C11-C12-N
25	c	301	3PE	C1-O11-P-O14
25	c	301	3PE	C11-O13-P-O14
25	g	303	3PE	O13-C11-C12-N
26	A	502	CDL	CA2-OA2-PA1-OA3
26	A	502	CDL	CB2-OB2-PB2-OB3
26	A	502	CDL	CB2-OB2-PB2-OB4
26	A	502	CDL	CB3-OB5-PB2-OB4
26	C	404	CDL	CA3-OA5-PA1-OA3
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	CA2-OA2-PA1-OA3
26	D	301	CDL	CB2-OB2-PB2-OB4
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	502	CDL	CB2-OB2-PB2-OB4
26	N	404	CDL	CA2-OA2-PA1-OA5
26	N	404	CDL	CB2-OB2-PB2-OB4
26	N	404	CDL	CB3-OB5-PB2-OB3
26	N	404	CDL	CB3-OB5-PB2-OB4
26	O	301	CDL	CA2-OA2-PA1-OA3
26	O	301	CDL	CA2-OA2-PA1-OA4
26	O	301	CDL	CA2-OA2-PA1-OA5
26	O	301	CDL	CB2-OB2-PB2-OB3

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Mol	Chain	Res	Type	Atoms
26	O	301	CDL	OB5-CB3-CB4-OB6
26	g	301	CDL	CA2-OA2-PA1-OA4
26	g	301	CDL	CB3-OB5-PB2-OB2
26	g	301	CDL	CB3-OB5-PB2-OB3
26	g	301	CDL	CB3-OB5-PB2-OB4
27	C	401	HEM	C2C-C3C-CAC-CBC
27	C	401	HEM	C4C-C3C-CAC-CBC
27	C	402	HEM	C2B-C3B-CAB-CBB
27	C	402	HEM	C4B-C3B-CAB-CBB
27	C	402	HEM	C2C-C3C-CAC-CBC
27	N	401	HEM	C2B-C3B-CAB-CBB
27	N	401	HEM	C2C-C3C-CAC-CBC
27	N	402	HEM	C2B-C3B-CAB-CBB
27	N	402	HEM	C4B-C3B-CAB-CBB
27	N	402	HEM	C2C-C3C-CAC-CBC
30	J	101	PC1	C1-O11-P-O14
30	J	101	PC1	O13-C11-C12-N
30	P	202	PC1	C11-O13-P-O14
30	P	202	PC1	C1-O11-P-O12
30	P	202	PC1	C1-O11-P-O14
30	P	202	PC1	C1-O11-P-O13
30	g	302	PC1	C1-O11-P-O14
33	a	603	HEA	C1A-C2A-CAA-CBA
33	a	603	HEA	C3A-C2A-CAA-CBA
33	a	603	HEA	C2A-C3A-CMA-OMA
33	a	603	HEA	C4A-C3A-CMA-OMA
33	a	603	HEA	C11-C12-C13-C14
33	a	603	HEA	C14-C15-C16-C17
33	a	603	HEA	C26-C15-C16-C17
33	a	603	HEA	C15-C16-C17-C18
33	a	604	HEA	C2A-C3A-CMA-OMA
33	a	604	HEA	C4A-C3A-CMA-OMA
33	a	604	HEA	C14-C15-C16-C17
33	a	604	HEA	C26-C15-C16-C17
33	a	604	HEA	C4D-C3D-CAD-CBD
27	N	401	HEM	C2A-CAA-CBA-CGA
33	a	603	HEA	C19-C20-C21-C22
33	a	604	HEA	C15-C16-C17-C18
33	a	604	HEA	C2D-C3D-CAD-CBD
25	R	101	3PE	C32-C33-C34-C35
25	E	201	3PE	C1-O11-P-O13
25	N	403	3PE	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
25	N	403	3PE	C11-O13-P-O11
25	R	101	3PE	C11-O13-P-O11
25	a	605	3PE	C11-O13-P-O11
25	a	606	3PE	C1-O11-P-O13
25	a	606	3PE	C11-O13-P-O11
25	a	607	3PE	C1-O11-P-O13
25	b	302	3PE	C11-O13-P-O11
25	c	301	3PE	C1-O11-P-O13
25	c	301	3PE	C11-O13-P-O11
26	A	502	CDL	CB2-OB2-PB2-OB5
26	A	502	CDL	CB3-OB5-PB2-OB2
26	C	404	CDL	CB3-OB5-PB2-OB2
26	D	301	CDL	CA2-OA2-PA1-OA5
26	D	301	CDL	CB2-OB2-PB2-OB5
26	N	404	CDL	CB2-OB2-PB2-OB5
26	N	404	CDL	CB3-OB5-PB2-OB2
26	O	301	CDL	CA3-OA5-PA1-OA2
26	O	301	CDL	CB2-OB2-PB2-OB5
30	P	202	PC1	C11-O13-P-O11
25	G	101	3PE	C37-C38-C39-C3A
25	R	101	3PE	C37-C38-C39-C3A
25	R	101	3PE	C3C-C3D-C3E-C3F
25	C	403	3PE	C23-C24-C25-C26
25	a	606	3PE	O13-C11-C12-N
25	c	301	3PE	O13-C11-C12-N
25	N	403	3PE	C25-C26-C27-C28
37	l	601	TGL	OG1-CG1-CG2-CG3
27	C	401	HEM	C2A-CAA-CBA-CGA
25	c	301	3PE	C22-C23-C24-C25
25	a	606	3PE	O11-C1-C2-O21
27	C	402	HEM	C4C-C3C-CAC-CBC
27	N	401	HEM	C4B-C3B-CAB-CBB
27	N	401	HEM	C4C-C3C-CAC-CBC
27	N	402	HEM	C4C-C3C-CAC-CBC
25	O	302	3PE	O21-C2-C3-O31
25	a	607	3PE	C11-O13-P-O11
26	L	502	CDL	CB2-OB2-PB2-OB5
30	J	101	PC1	C1-O11-P-O13
26	C	404	CDL	OB5-CB3-CB4-CB6
26	O	301	CDL	OB5-CB3-CB4-CB6
30	J	101	PC1	C21-C22-C23-C24
25	O	302	3PE	C1-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
26	L	502	CDL	CA3-CA4-CA6-OA8
26	g	301	CDL	CA3-CA4-CA6-OA8
37	l	601	TGL	CC1-CC2-CC3-CC4
25	L	501	3PE	C32-C33-C34-C35
26	N	404	CDL	OB5-CB3-CB4-OB6
26	L	502	CDL	OB5-CB3-CB4-CB6
30	P	202	PC1	O11-C1-C2-C3
25	O	302	3PE	O13-C11-C12-N
25	a	607	3PE	C2-C1-O11-P
26	C	404	CDL	C1-CB2-OB2-PB2
26	D	301	CDL	CB4-CB3-OB5-PB2
26	C	404	CDL	CA2-OA2-PA1-OA5
26	C	404	CDL	CA3-OA5-PA1-OA2
26	g	301	CDL	CA3-OA5-PA1-OA2
30	g	302	PC1	C3B-C3C-C3D-C3E
26	C	404	CDL	OB5-CB3-CB4-OB6
25	b	302	3PE	O21-C2-C3-O31
26	L	502	CDL	OA6-CA4-CA6-OA8
25	G	101	3PE	C34-C35-C36-C37
26	A	502	CDL	CB4-CB3-OB5-PB2
26	L	502	CDL	CB4-CB3-OB5-PB2
26	g	301	CDL	C1-CB2-OB2-PB2
26	N	404	CDL	OB5-CB3-CB4-CB6
26	L	502	CDL	C72-C71-CB7-OB8
27	C	401	HEM	C2B-C3B-CAB-CBB
25	C	403	3PE	C1-C2-C3-O31
25	b	302	3PE	C1-C2-C3-O31
26	A	502	CDL	CA3-CA4-CA6-OA8
26	N	404	CDL	CA4-CA3-OA5-PA1
25	L	501	3PE	O11-C1-C2-O21
30	g	302	PC1	C35-C36-C37-C38
30	g	302	PC1	C34-C35-C36-C37
25	a	607	3PE	O21-C2-C3-O31
26	A	502	CDL	OA6-CA4-CA6-OA8
25	c	301	3PE	C25-C26-C27-C28
25	O	302	3PE	C21-C22-C23-C24
25	C	403	3PE	C1-O11-P-O13
25	b	302	3PE	C1-O11-P-O13
26	A	502	CDL	CA2-OA2-PA1-OA5
25	L	501	3PE	C2-C1-O11-P
25	c	301	3PE	C2-C1-O11-P
25	g	303	3PE	C2-C1-O11-P

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Mol	Chain	Res	Type	Atoms
26	O	301	CDL	CB4-CB3-OB5-PB2
25	N	403	3PE	C1-O11-P-O12
25	N	403	3PE	C11-O13-P-O12
25	O	302	3PE	C11-O13-P-O14
25	R	101	3PE	C11-O13-P-O14
25	a	607	3PE	C1-O11-P-O14
25	a	607	3PE	C11-O13-P-O12
25	b	302	3PE	C11-O13-P-O14
25	c	301	3PE	C1-O11-P-O12
25	c	301	3PE	C11-O13-P-O12
26	A	502	CDL	CB3-OB5-PB2-OB3
26	C	404	CDL	CB3-OB5-PB2-OB4
26	D	301	CDL	CA2-OA2-PA1-OA4
26	L	502	CDL	CB2-OB2-PB2-OB3
26	N	404	CDL	CA2-OA2-PA1-OA4
26	O	301	CDL	CA3-OA5-PA1-OA3
26	O	301	CDL	CB2-OB2-PB2-OB4
26	g	301	CDL	CA3-OA5-PA1-OA4
30	P	202	PC1	C11-O13-P-O12
25	L	501	3PE	O11-C1-C2-C3
25	a	606	3PE	C12-C11-O13-P
25	b	302	3PE	C12-C11-O13-P
26	L	502	CDL	CA2-C1-CB2-OB2
25	b	304	3PE	O11-C1-C2-O21
26	A	502	CDL	OB5-CB3-CB4-OB6
30	P	202	PC1	O11-C1-C2-O21
25	C	403	3PE	C2B-C2C-C2D-C2E
26	N	404	CDL	C72-C71-CB7-OB8
26	C	404	CDL	C32-C31-CA7-OA8
30	P	202	PC1	O13-C11-C12-N
30	g	302	PC1	O13-C11-C12-N
37	l	601	TGL	OG1-CG1-CG2-OG2
26	O	301	CDL	CA4-CA3-OA5-PA1
25	a	606	3PE	C22-C23-C24-C25
25	R	101	3PE	C35-C36-C37-C38
26	N	404	CDL	C72-C71-CB7-OB9
25	a	606	3PE	O11-C1-C2-C3
26	A	502	CDL	OB5-CB3-CB4-CB6
33	a	604	HEA	C11-C12-C13-C14
26	L	502	CDL	C1-CA2-OA2-PA1
25	R	101	3PE	O11-C1-C2-O21
26	L	502	CDL	OB5-CB3-CB4-OB6

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Mol	Chain	Res	Type	Atoms
26	O	301	CDL	OA5-CA3-CA4-OA6
26	D	301	CDL	C52-C51-CB5-OB6
33	a	603	HEA	C2A-CAA-CBA-CGA
25	G	101	3PE	C32-C33-C34-C35
25	G	101	3PE	C11-O13-P-O11
25	L	501	3PE	C11-O13-P-O11
25	O	302	3PE	C11-O13-P-O11
26	g	301	CDL	CB2-OB2-PB2-OB5
30	g	302	PC1	C11-O13-P-O11
25	A	501	3PE	O21-C21-C22-C23
26	N	404	CDL	C52-C51-CB5-OB6
25	b	304	3PE	C2-C1-O11-P
26	C	404	CDL	CA4-CA3-OA5-PA1
26	D	301	CDL	C1-CA2-OA2-PA1
26	O	301	CDL	OA5-CA3-CA4-CA6
33	a	604	HEA	CAD-CBD-CGD-O1D
26	C	404	CDL	C12-C11-CA5-OA7
25	b	302	3PE	C34-C35-C36-C37
25	a	606	3PE	C2-C1-O11-P
27	C	402	HEM	CAD-CBD-CGD-O1D
33	a	603	HEA	CAD-CBD-CGD-O2D
33	a	604	HEA	CAD-CBD-CGD-O2D
33	a	604	HEA	CAA-CBA-CGA-O1A
26	D	301	CDL	CB2-C1-CA2-OA2
33	a	603	HEA	CAD-CBD-CGD-O1D
26	C	404	CDL	C12-C11-CA5-OA6
28	O	303	HEC	CAD-CBD-CGD-O2D
33	a	604	HEA	CAA-CBA-CGA-O2A
27	C	401	HEM	CAD-CBD-CGD-O2D
26	g	301	CDL	OA6-CA4-CA6-OA8
27	C	401	HEM	CAD-CBD-CGD-O1D
25	E	201	3PE	C33-C34-C35-C36
25	G	101	3PE	C3B-C3C-C3D-C3E
26	A	502	CDL	C31-C32-C33-C34
27	C	402	HEM	CAD-CBD-CGD-O2D
28	O	303	HEC	CAD-CBD-CGD-O1D
25	A	501	3PE	O22-C21-C22-C23
25	a	606	3PE	C23-C24-C25-C26
27	C	402	HEM	C3D-CAD-CBD-CGD
25	C	403	3PE	C24-C25-C26-C27
27	N	402	HEM	CAA-CBA-CGA-O2A
26	D	301	CDL	CA5-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
33	a	603	HEA	CAA-CBA-CGA-O2A
25	G	101	3PE	O31-C31-C32-C33
26	O	301	CDL	C75-C76-C77-C78
26	O	301	CDL	C32-C31-CA7-OA8
27	C	402	HEM	CAA-CBA-CGA-O2A
25	E	201	3PE	O21-C21-C22-C23
27	N	401	HEM	CAD-CBD-CGD-O2D
25	g	303	3PE	C3-C2-O21-C21
25	R	101	3PE	O21-C21-C22-C23
25	b	302	3PE	O21-C21-C22-C23
26	A	502	CDL	C12-C11-CA5-OA6
26	O	301	CDL	C72-C71-CB7-OB8
25	a	606	3PE	C21-C22-C23-C24
26	g	301	CDL	C12-C11-CA5-OA6
27	N	402	HEM	CAA-CBA-CGA-O1A
27	C	401	HEM	C4B-C3B-CAB-CBB
27	C	402	HEM	CAA-CBA-CGA-O1A
27	N	402	HEM	CAD-CBD-CGD-O2D
25	C	403	3PE	O11-C1-C2-C3
27	N	401	HEM	CAD-CBD-CGD-O1D
26	N	404	CDL	C52-C51-CB5-OB7
25	a	607	3PE	O21-C21-C22-C23
25	c	301	3PE	O31-C31-C32-C33
25	G	101	3PE	O21-C21-C22-C23
26	A	502	CDL	C32-C31-CA7-OA8
26	A	502	CDL	C72-C71-CB7-OB8
26	L	502	CDL	C52-C51-CB5-OB6
33	a	603	HEA	CAA-CBA-CGA-O1A
26	O	301	CDL	C72-C71-CB7-OB9
26	O	301	CDL	C32-C31-CA7-OA9
25	E	201	3PE	O22-C21-C22-C23
25	G	101	3PE	O32-C31-C32-C33
26	g	301	CDL	C12-C11-CA5-OA7
25	g	303	3PE	O31-C31-C32-C33
30	J	101	PC1	C22-C23-C24-C25
25	A	501	3PE	C1-O11-P-O14
25	g	303	3PE	C11-O13-P-O14
26	A	502	CDL	CA3-OA5-PA1-OA3
26	C	404	CDL	CA2-OA2-PA1-OA4
26	g	301	CDL	CA2-OA2-PA1-OA3
30	J	101	PC1	C1-O11-P-O12
30	g	302	PC1	C11-O13-P-O14

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Mol	Chain	Res	Type	Atoms
25	R	101	3PE	O22-C21-C22-C23
25	a	607	3PE	O22-C21-C22-C23
25	c	301	3PE	O32-C31-C32-C33
26	A	502	CDL	C12-C11-CA5-OA7
27	N	402	HEM	CAD-CBD-CGD-O1D
25	C	403	3PE	O13-C11-C12-N
25	b	302	3PE	O22-C21-C22-C23
25	A	501	3PE	C1-C2-O21-C21
25	c	301	3PE	C12-C11-O13-P
26	g	301	CDL	CB6-CB4-OB6-CB5
30	P	202	PC1	C1-C2-O21-C21
26	N	404	CDL	O1-C1-CA2-OA2
25	E	201	3PE	O31-C31-C32-C33
26	L	502	CDL	C12-C11-CA5-OA6
26	O	301	CDL	C12-C11-CA5-OA6
25	G	101	3PE	O22-C21-C22-C23
25	a	605	3PE	O21-C21-C22-C23
26	O	301	CDL	C52-C51-CB5-OB6
28	D	302	HEC	CAD-CBD-CGD-O2D
25	E	201	3PE	O32-C31-C32-C33
26	A	502	CDL	C32-C31-CA7-OA9
28	D	302	HEC	CAD-CBD-CGD-O1D
25	b	304	3PE	O21-C21-C22-C23
25	b	304	3PE	O22-C21-C22-C23
25	a	607	3PE	O31-C31-C32-C33
25	a	605	3PE	O22-C21-C22-C23
26	O	301	CDL	C52-C51-CB5-OB7

There are no ring outliers.

18 monomers are involved in 37 short contacts:

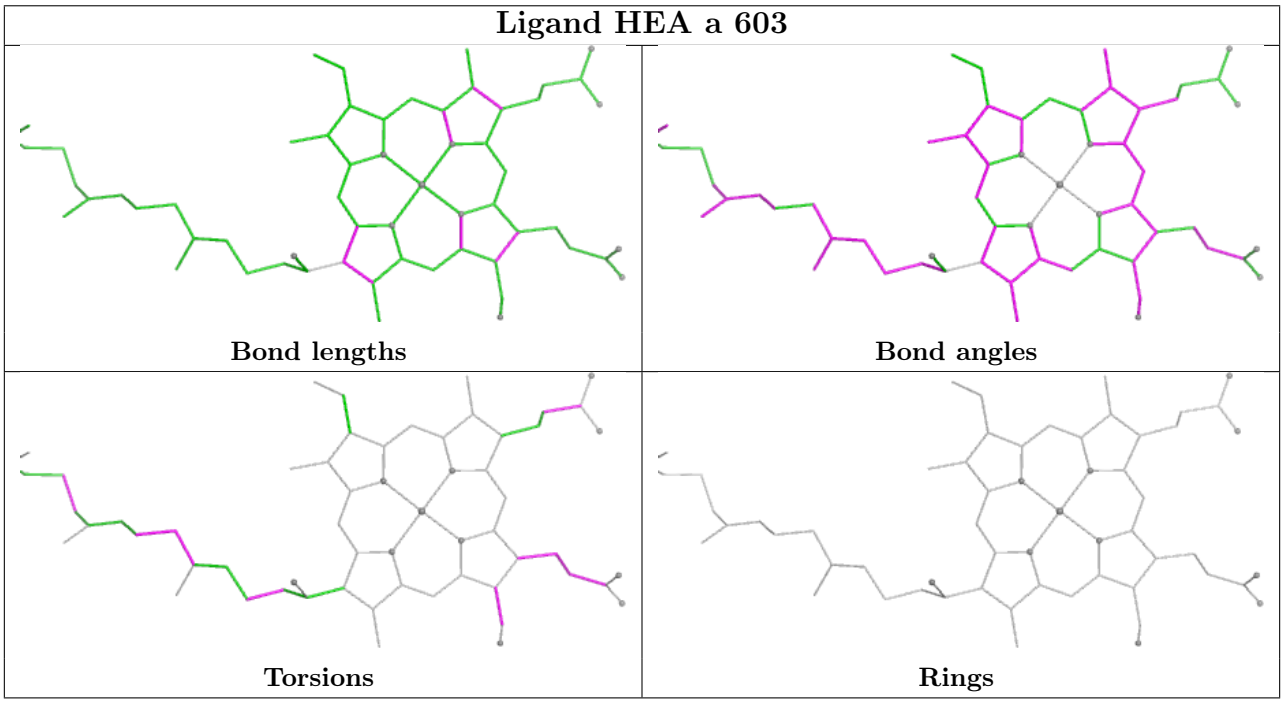
Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	a	603	HEA	2	0
27	N	401	HEM	2	0
25	L	501	3PE	1	0
29	P	201	FES	1	0
25	g	303	3PE	3	0
25	R	101	3PE	2	0
26	O	301	CDL	1	0
28	D	302	HEC	1	0
27	C	402	HEM	2	0
27	N	402	HEM	1	0

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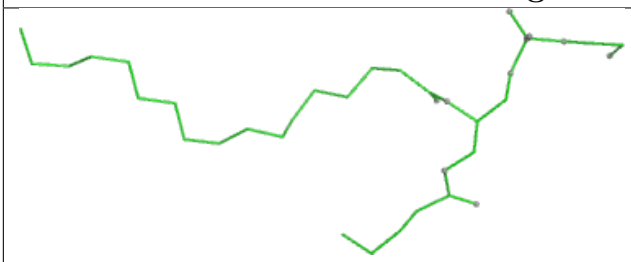
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	c	301	3PE	3	0
26	C	404	CDL	2	0
37	l	601	TGL	2	0
26	D	301	CDL	2	0
26	g	301	CDL	1	0
27	C	401	HEM	2	0
25	G	101	3PE	4	0
33	a	604	HEA	5	0

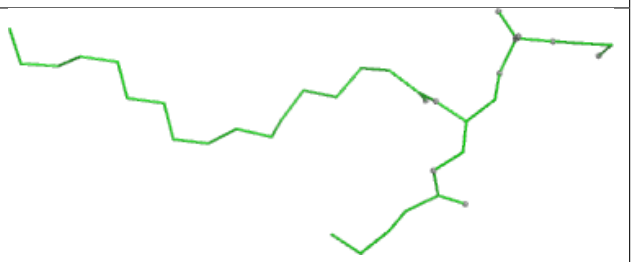
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



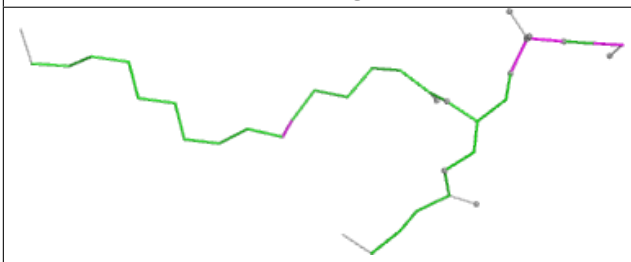
Ligand 3PE N 403



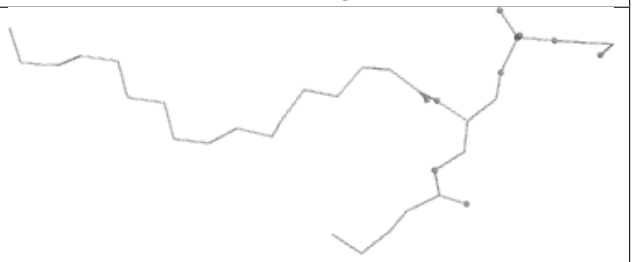
Bond lengths



Bond angles

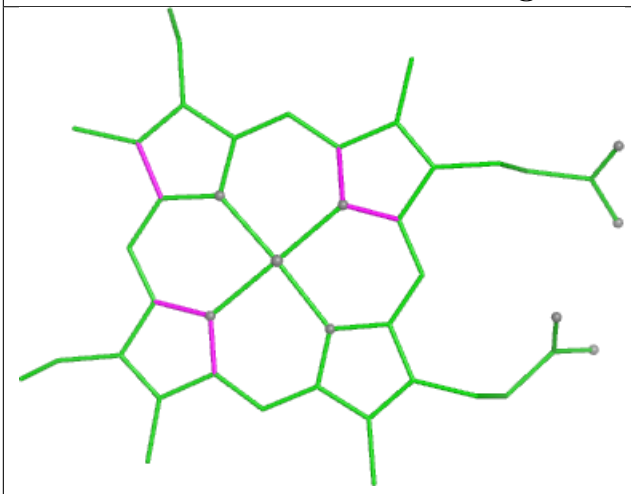


Torsions

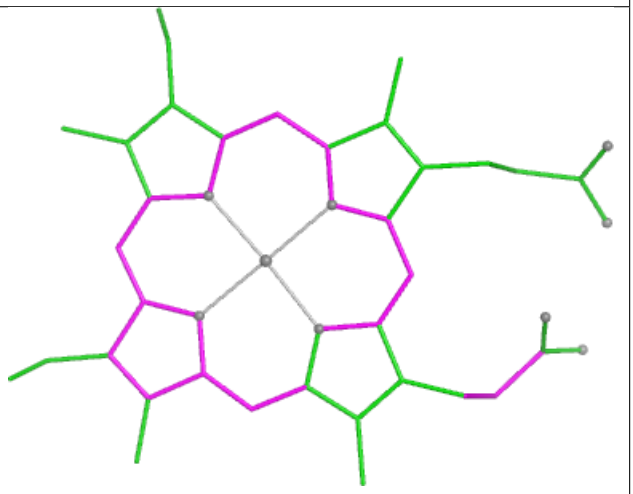


Rings

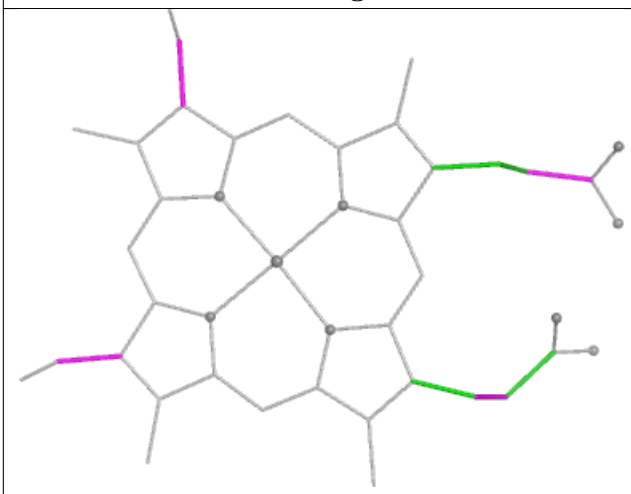
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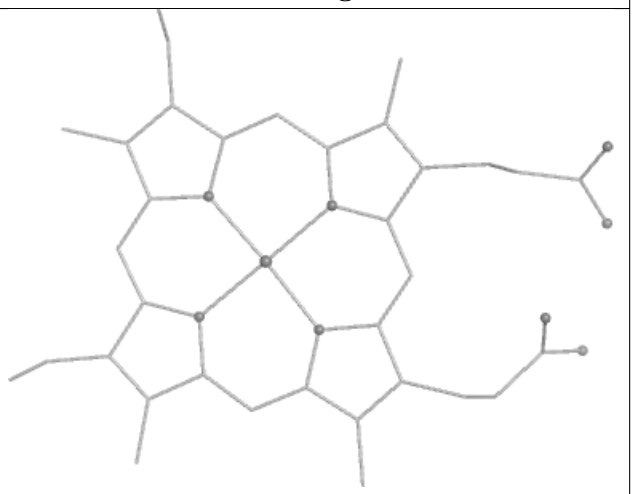
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Bond angles

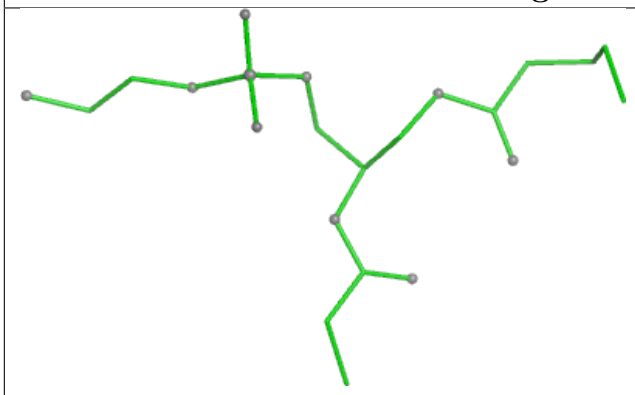


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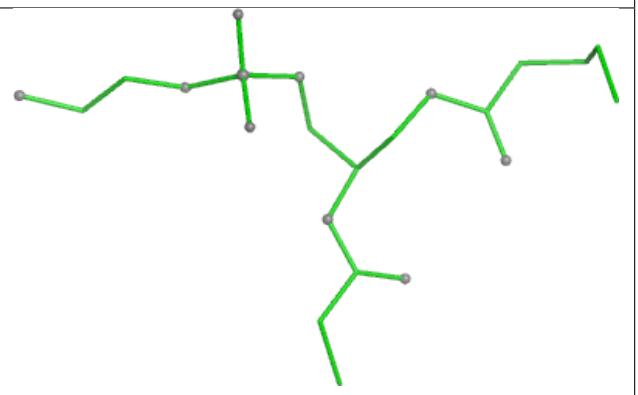


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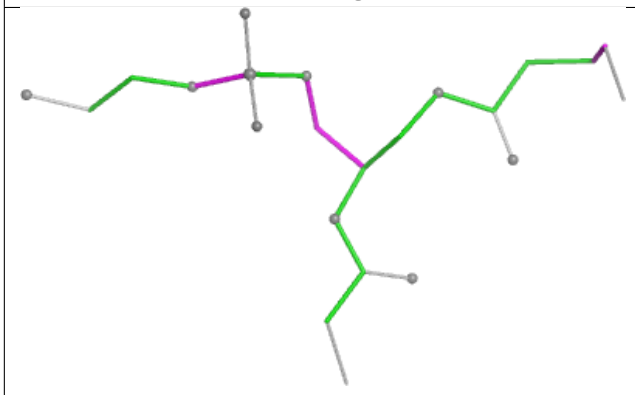
Ligand 3PE L 501



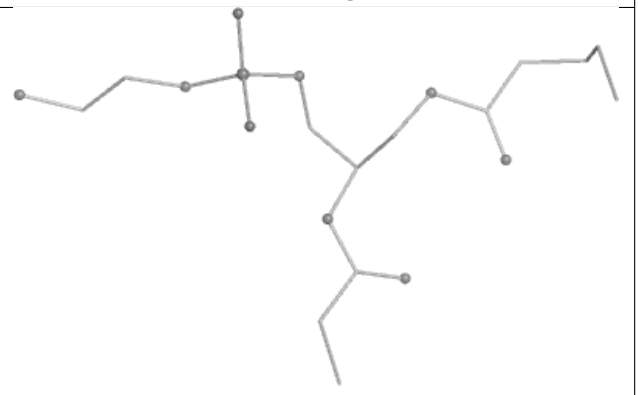
Bond lengths



Bond angles

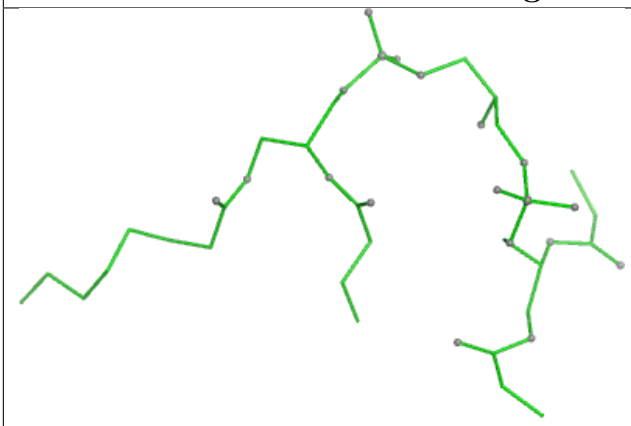


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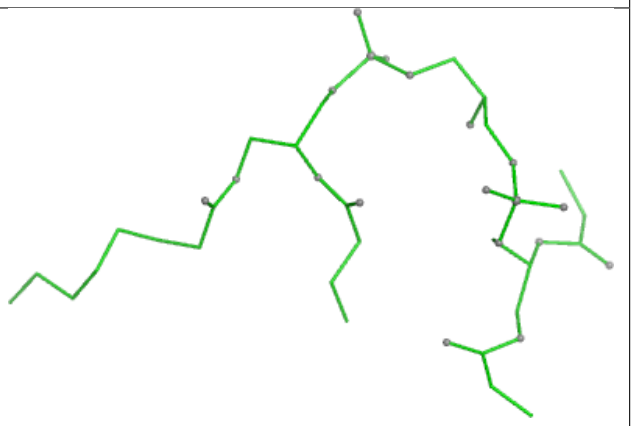


Rings

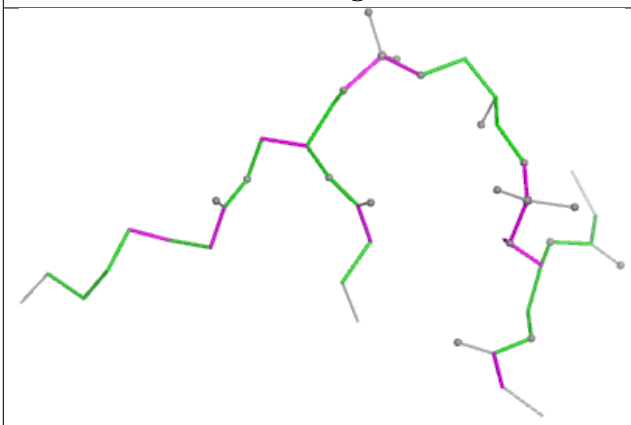
Ligand CDL A 502



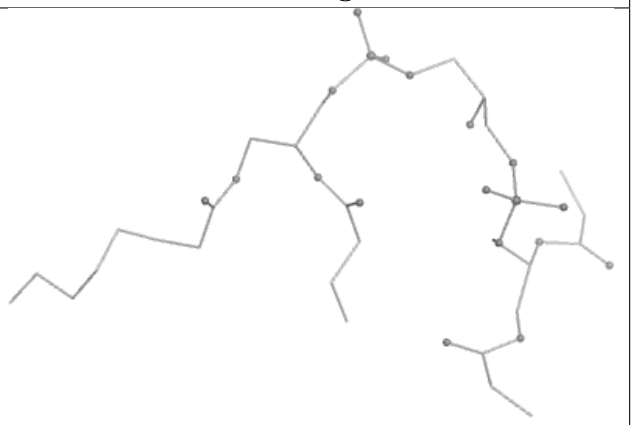
Bond lengths



Bond angles

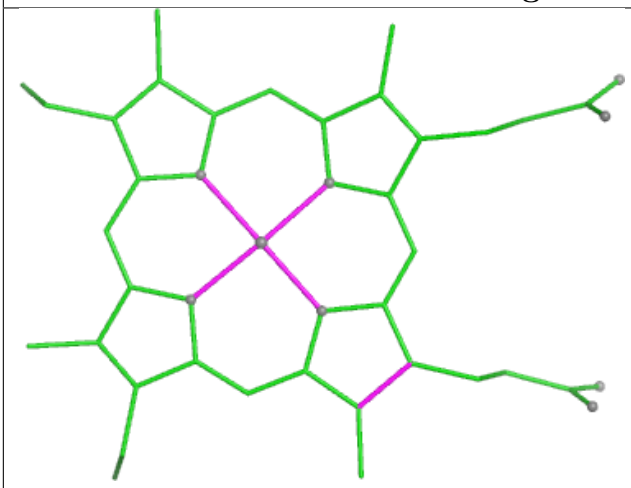


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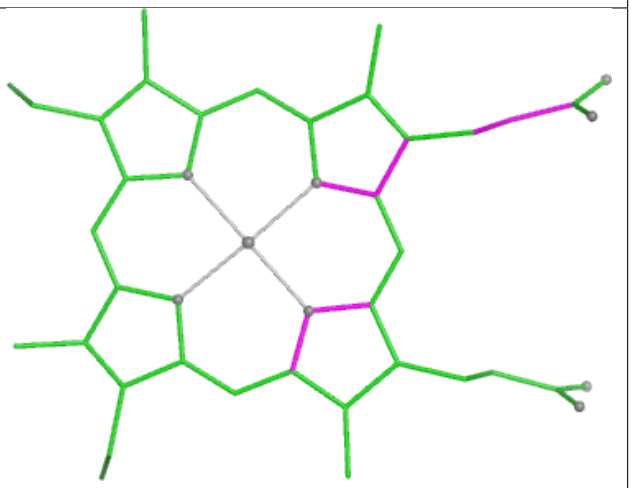


Rings

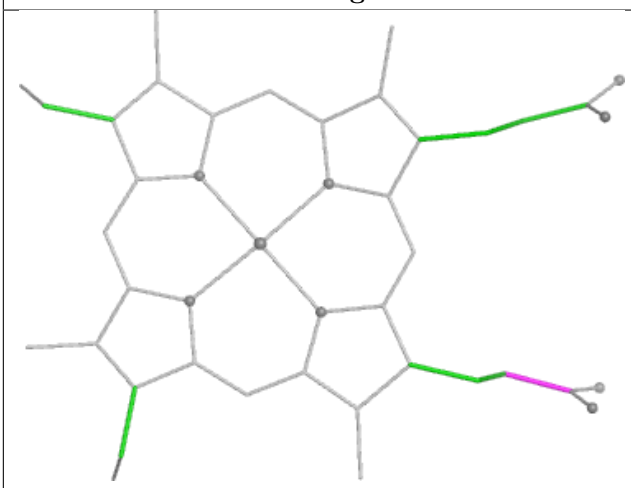
Ligand HEC O 303



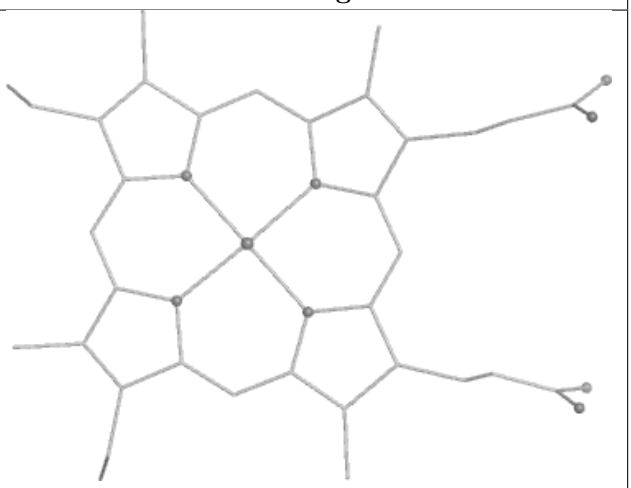
Bond lengths



Bond angles

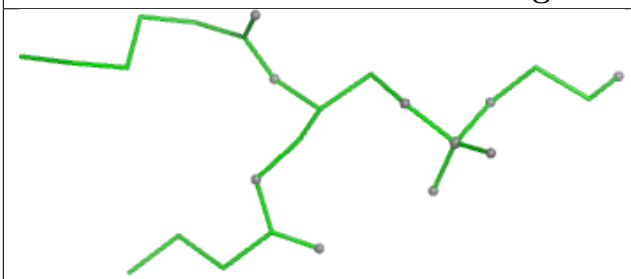


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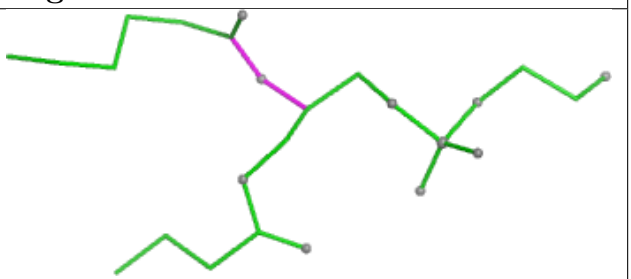


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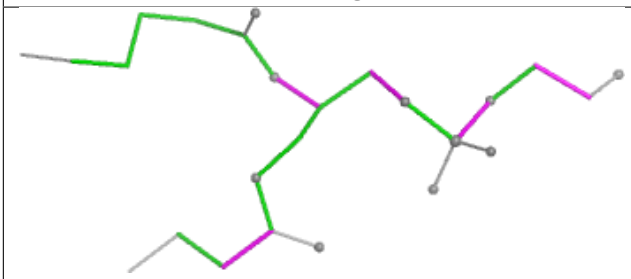
Ligand 3PE g 303



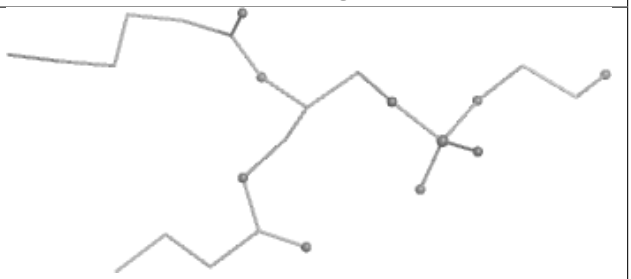
Bond lengths



Bond angles

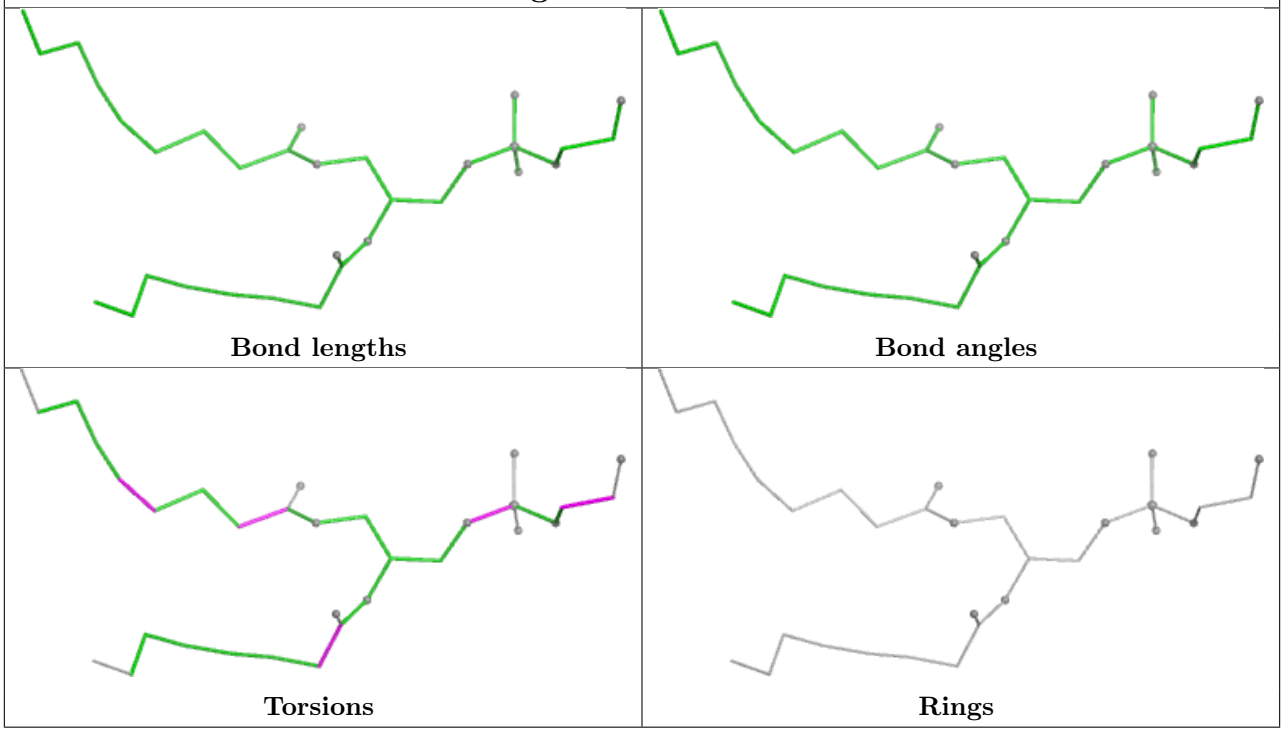


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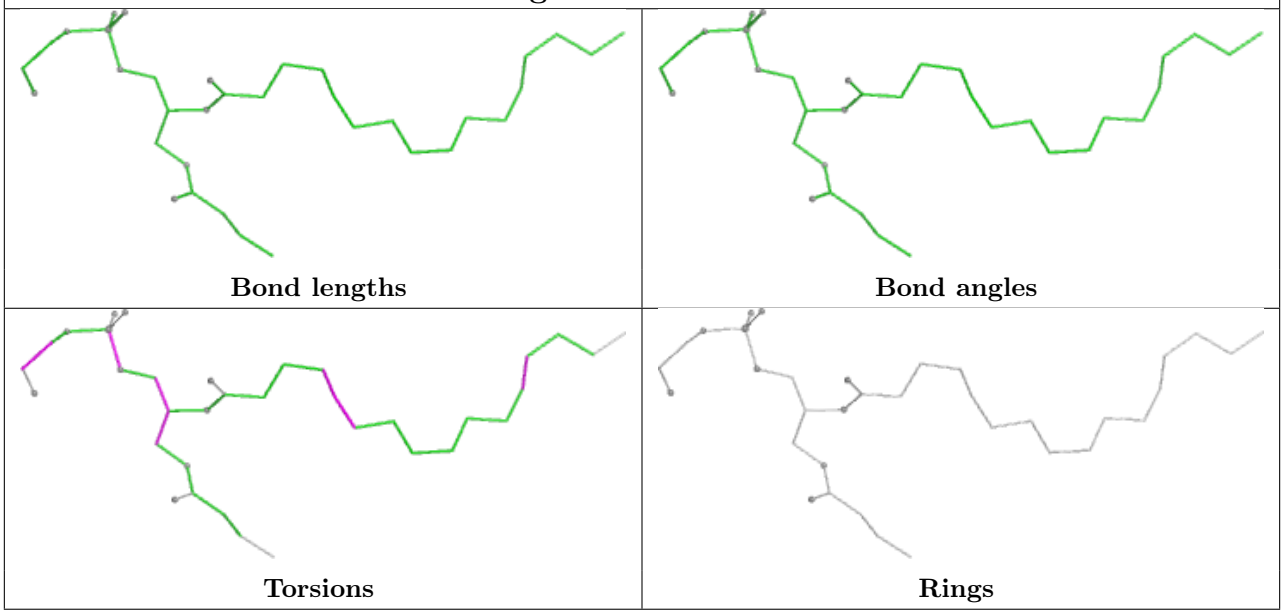


Rings

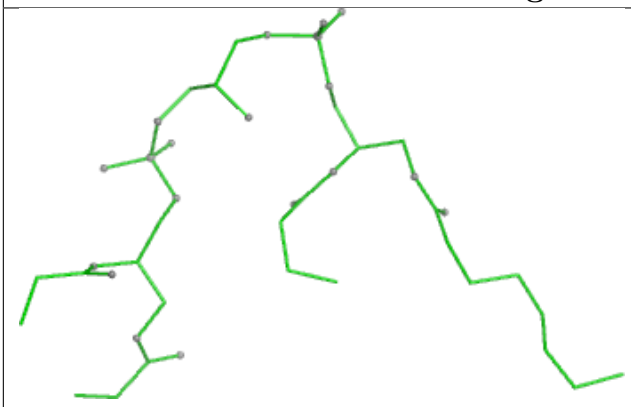
Ligand 3PE E 201



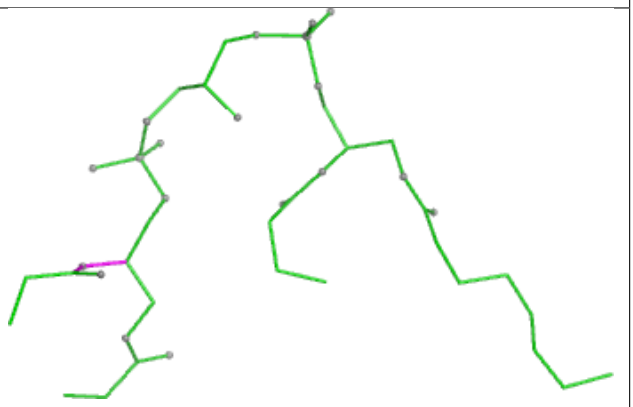
Ligand 3PE C 403



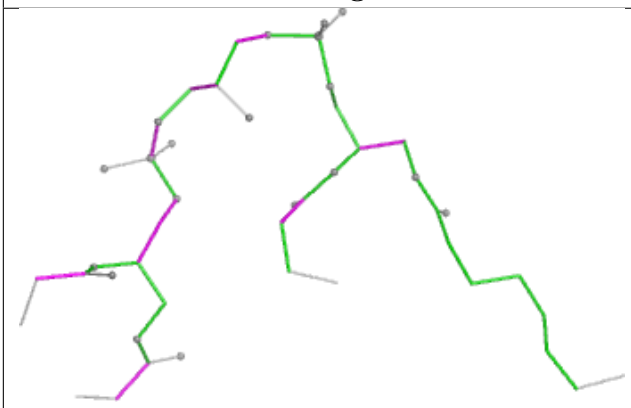
Ligand CDL L 502



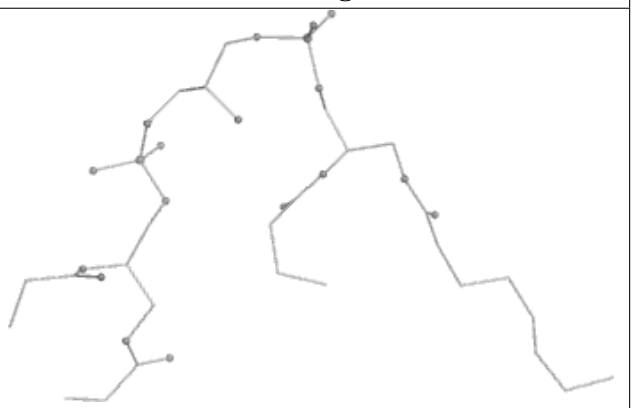
Bond lengths



Bond angles

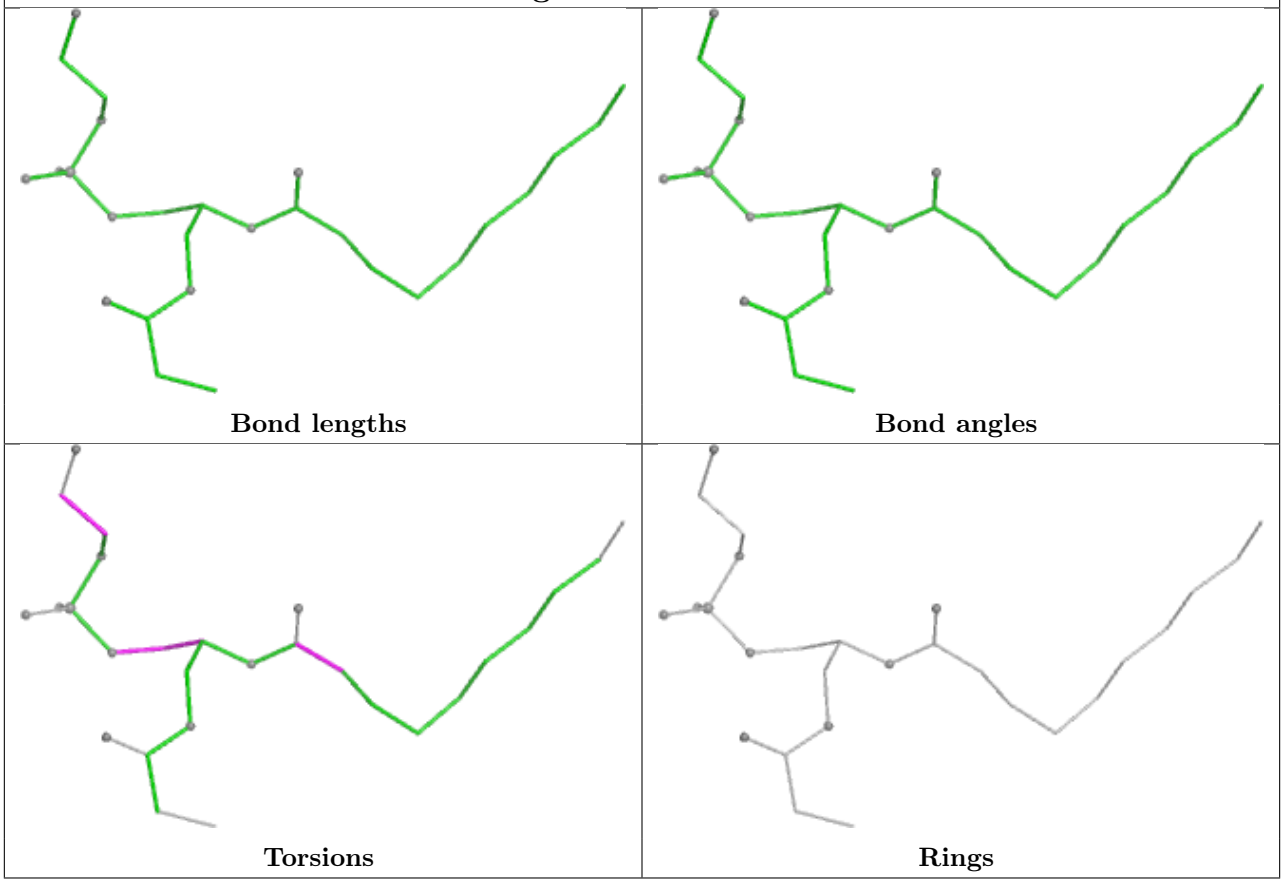


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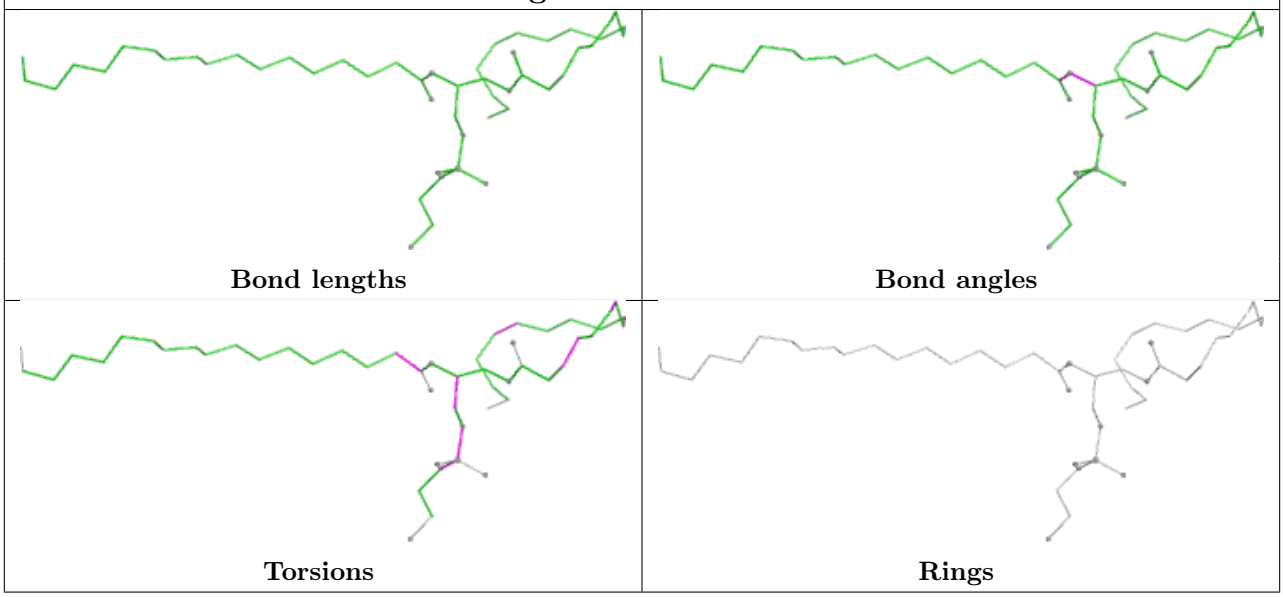


Rings

Ligand 3PE b 304



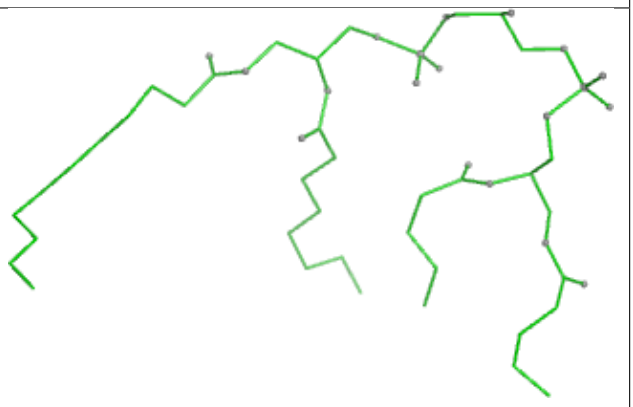
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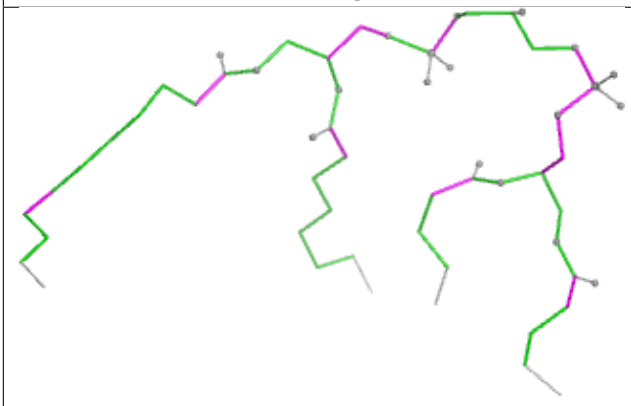
Ligand CDL O 301



Bond lengths



Bond angles

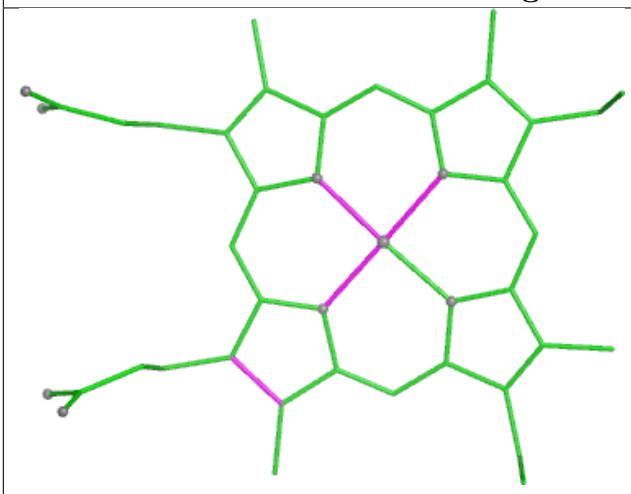


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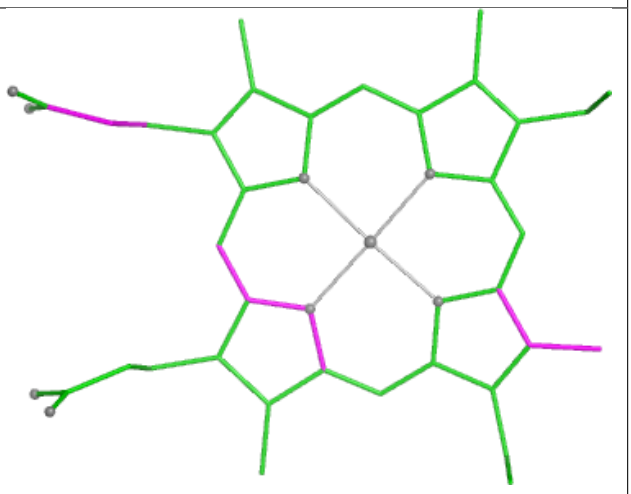


Rings

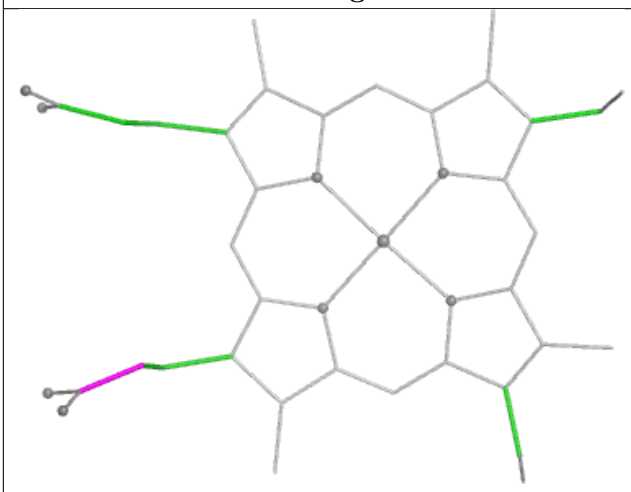
Ligand HEC D 302



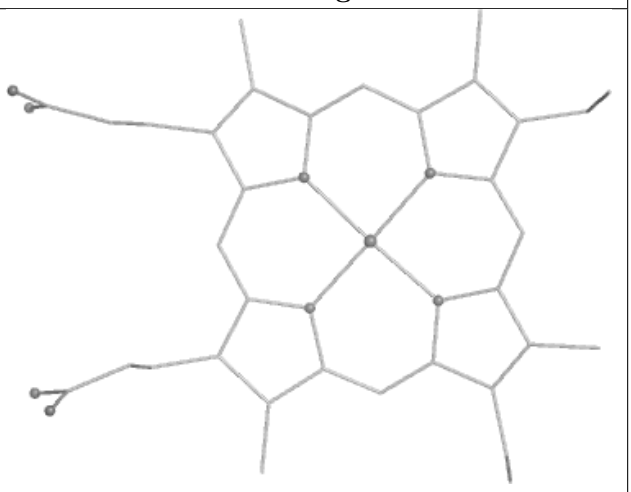
Bond lengths



Bond angles

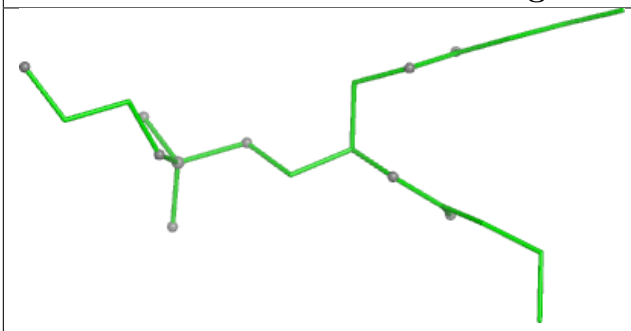


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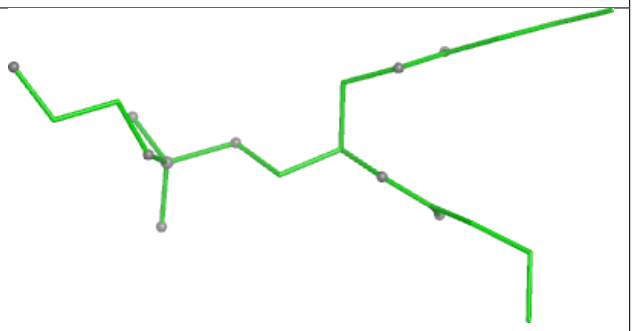


Rings

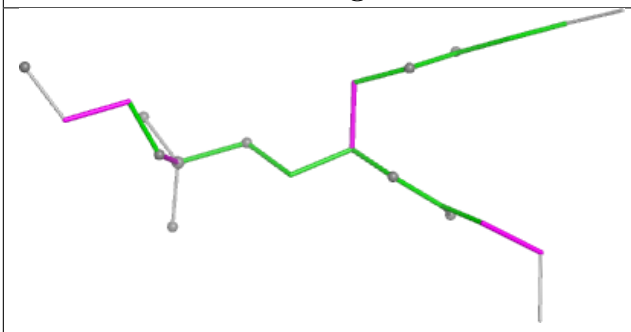
Ligand 3PE O 302



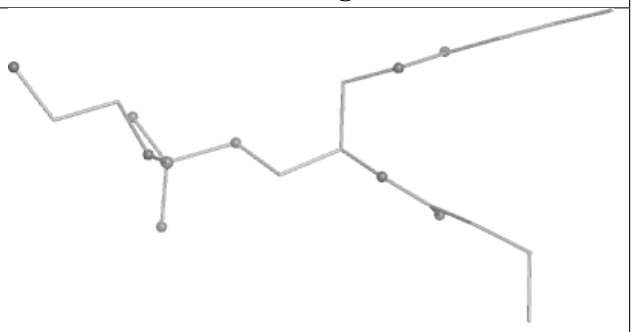
Bond lengths



Bond angles

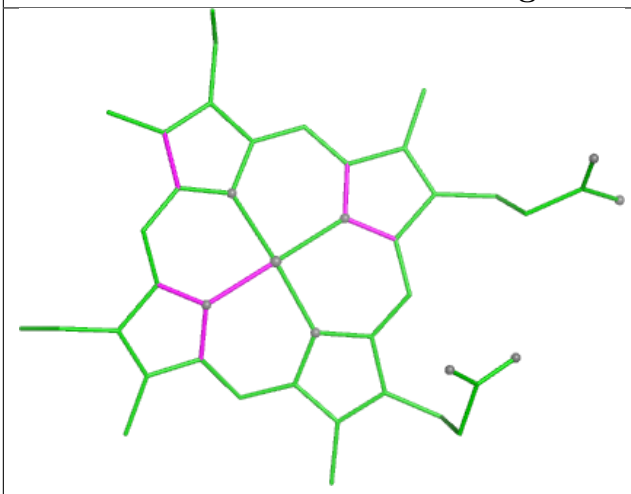


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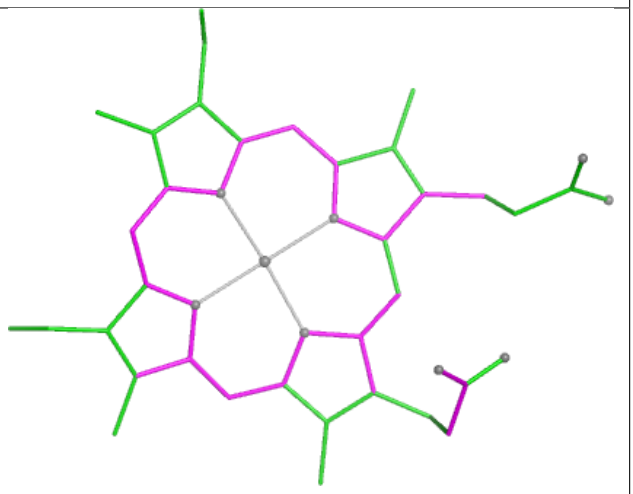


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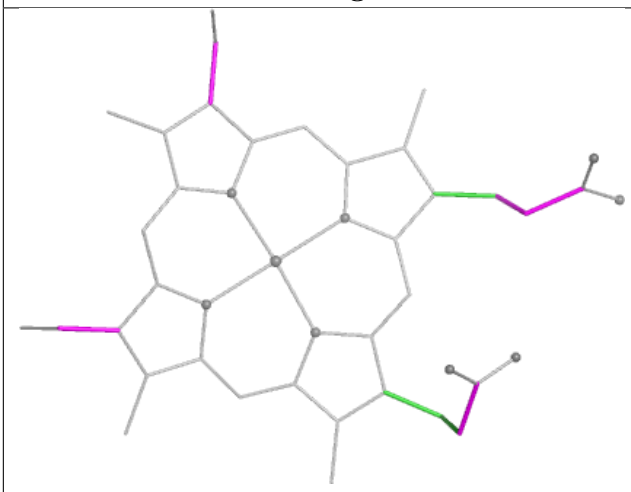
Ligand HEM C 402



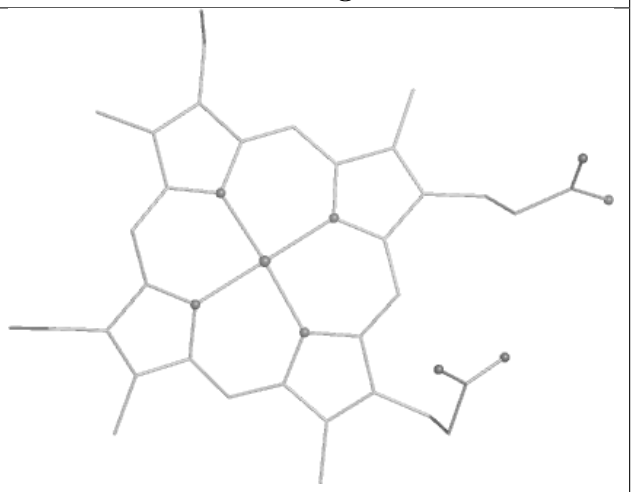
Bond lengths



Bond angles

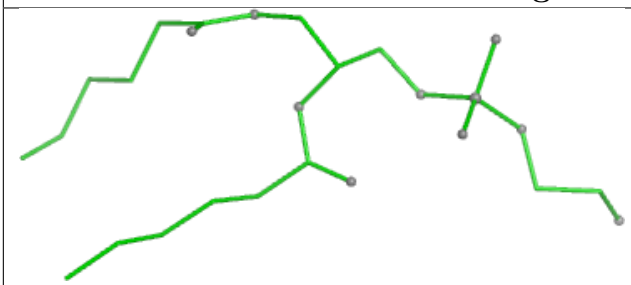


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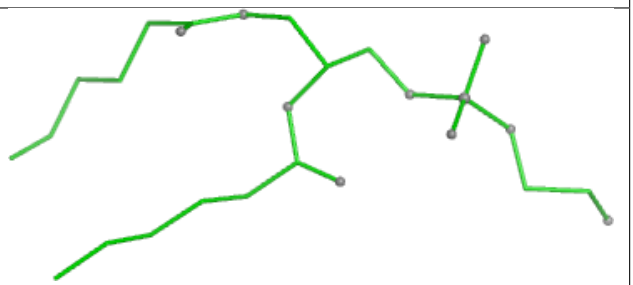


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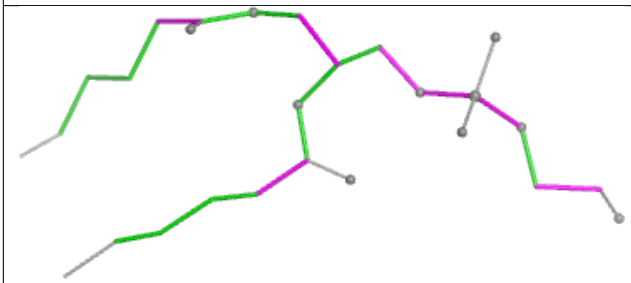
Ligand 3PE a 607



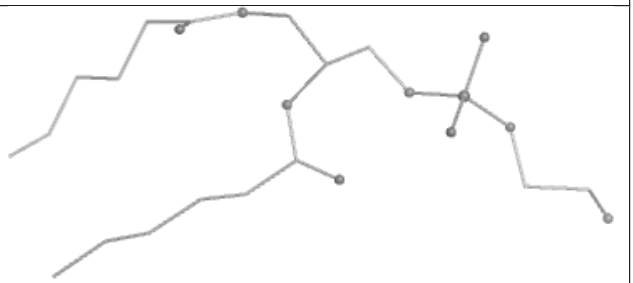
Bond lengths



Bond angles

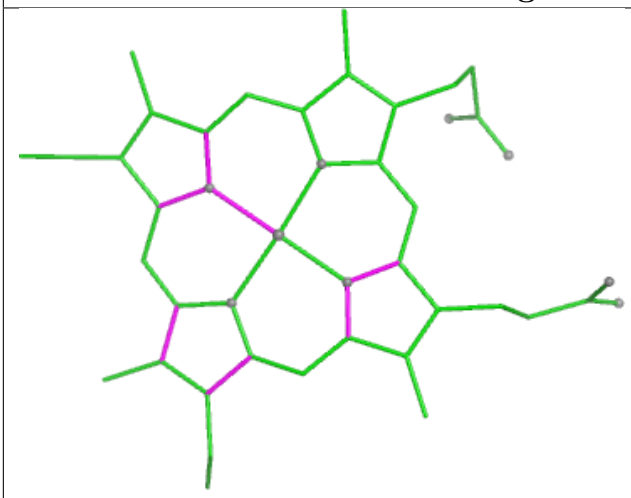


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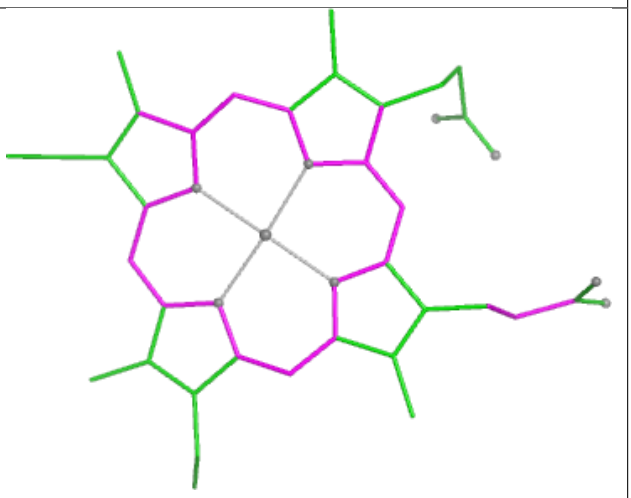


Rings

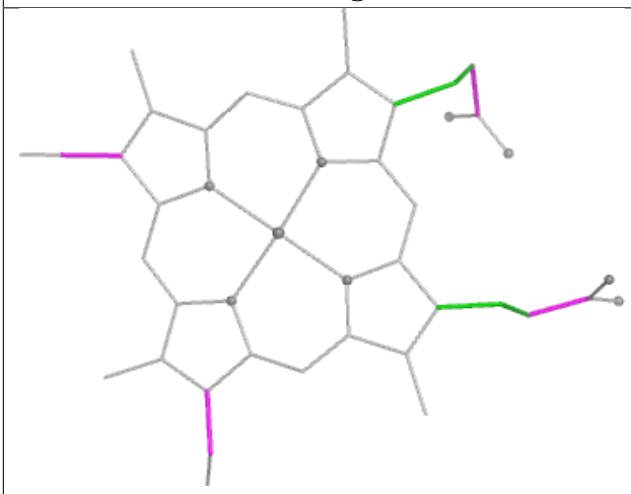
Ligand HEM N 402



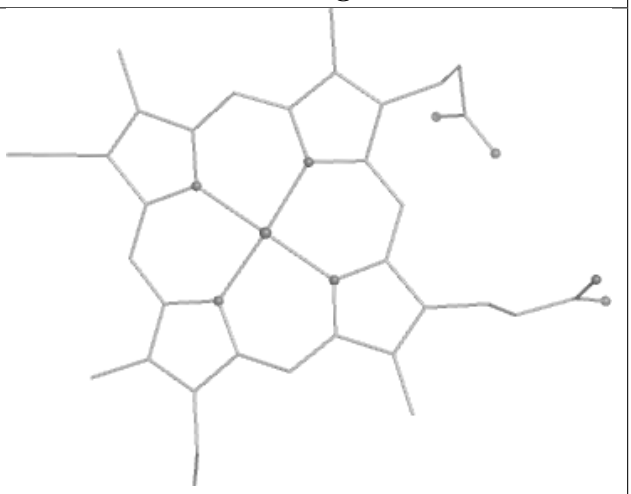
Bond lengths



Bond angles

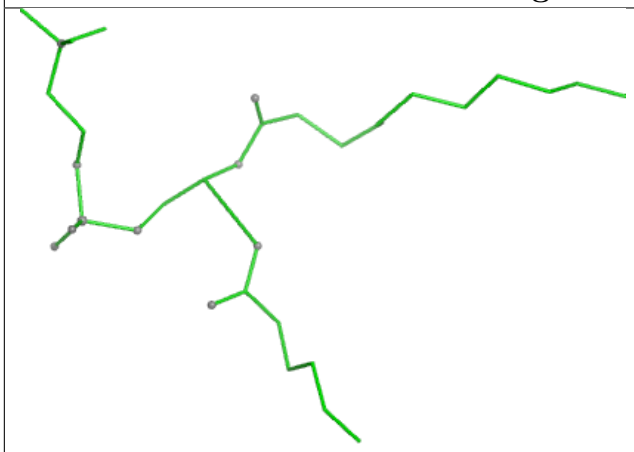


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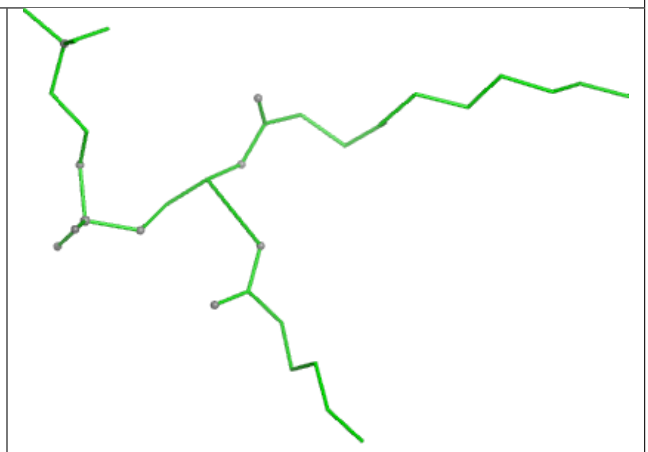


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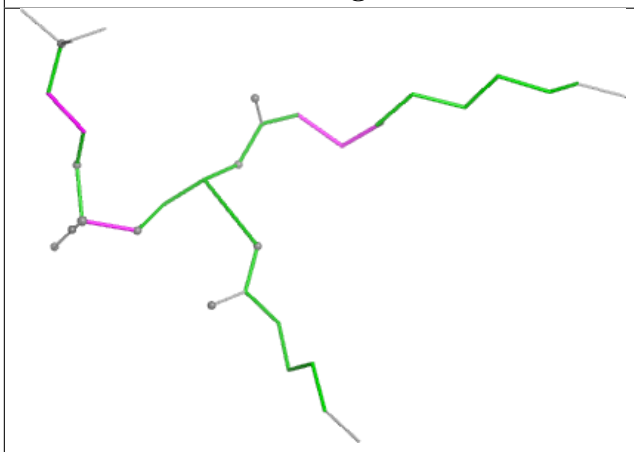
Ligand PC1 J 101



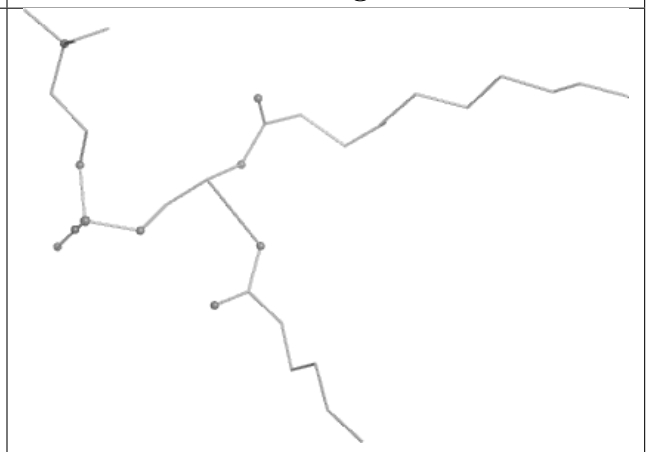
Bond lengths



Bond angles

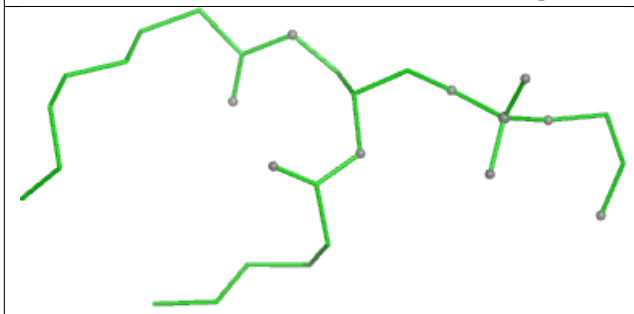


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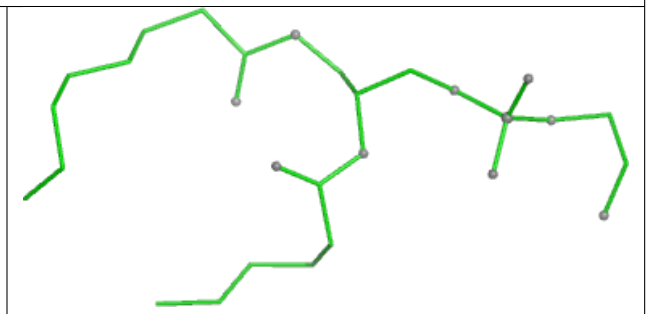


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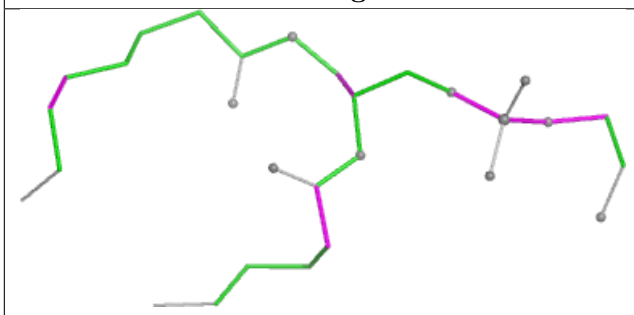
Ligand 3PE b 302



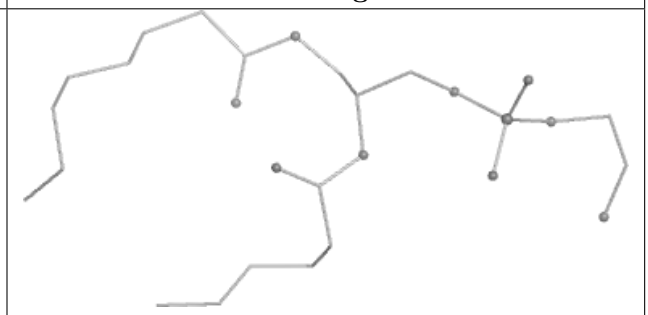
Bond lengths



Bond angles

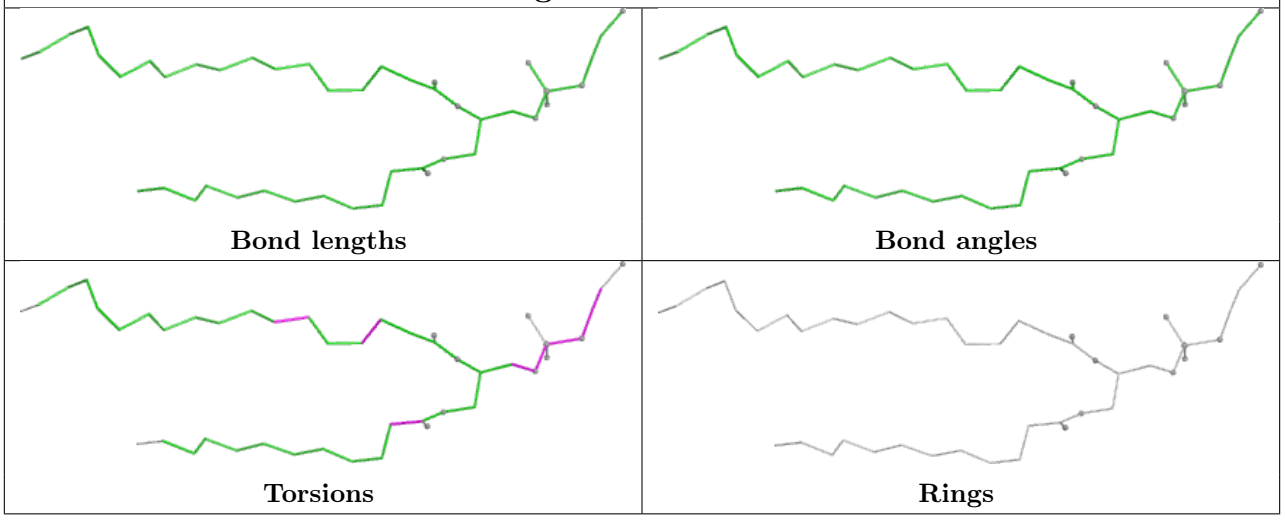


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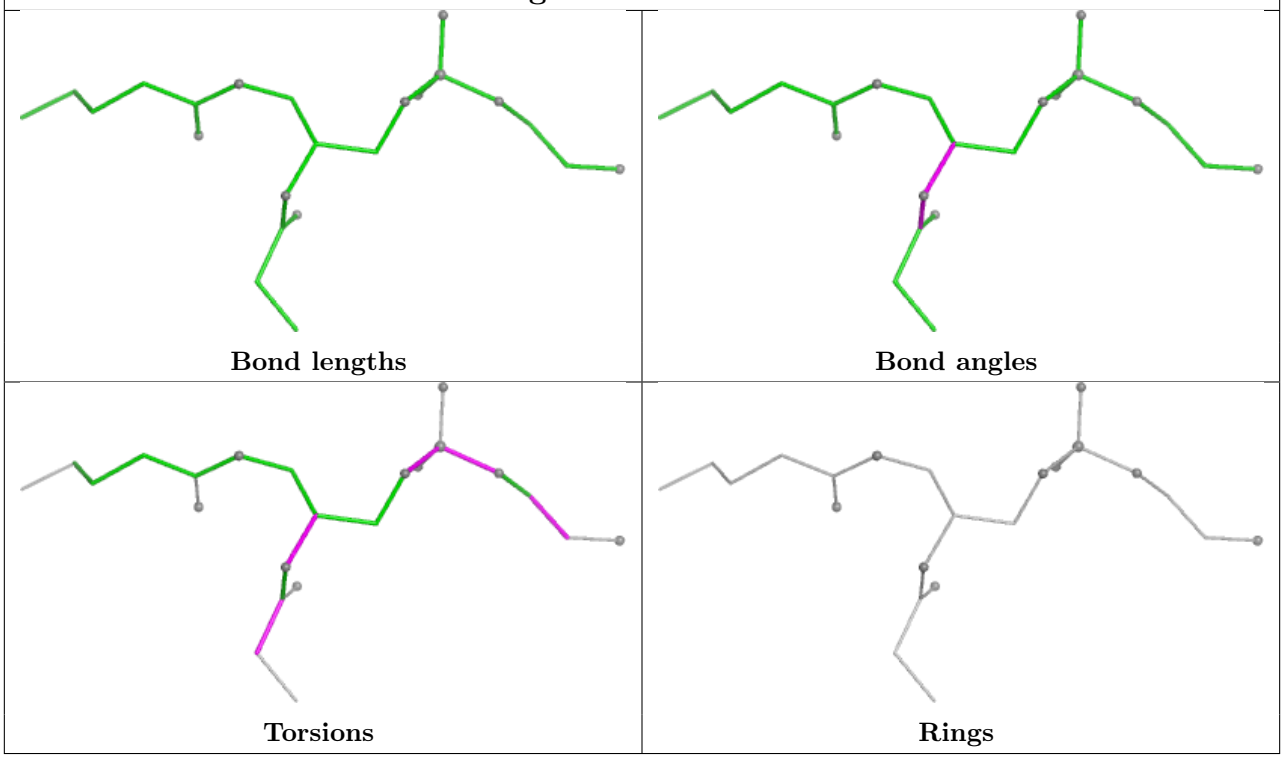


Rings

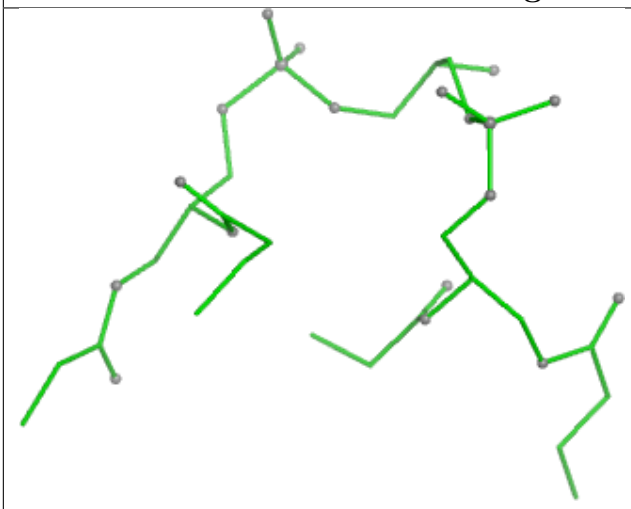
Ligand 3PE c 301



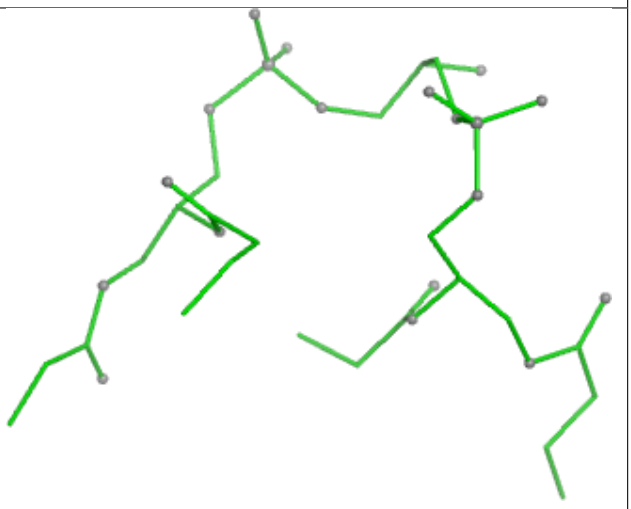
Ligand 3PE A 501



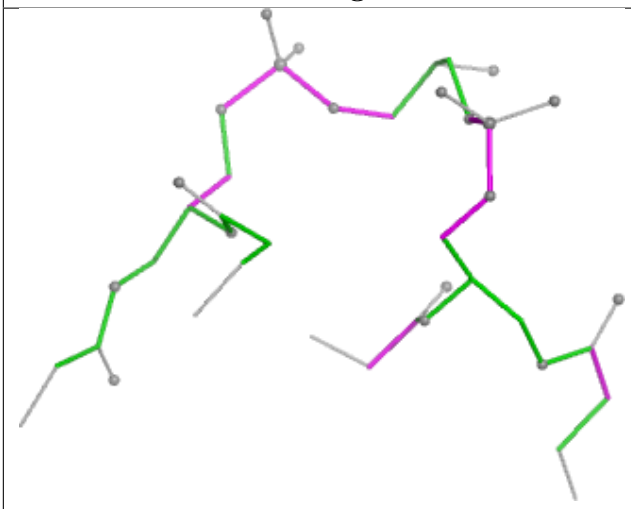
Ligand CDL C 404



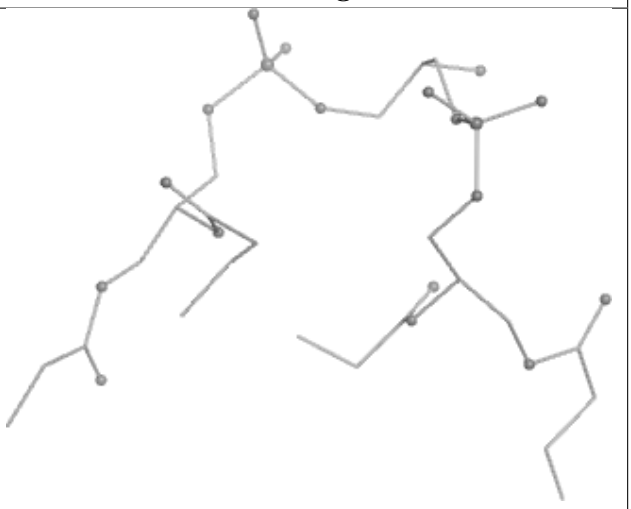
Bond lengths



Bond angles

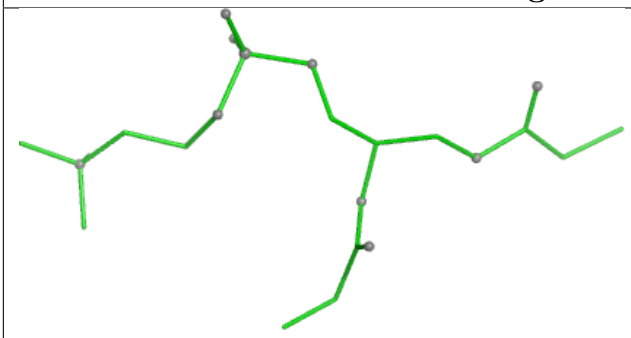


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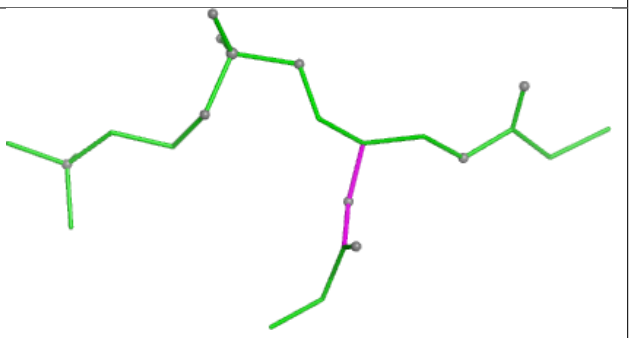


Rings

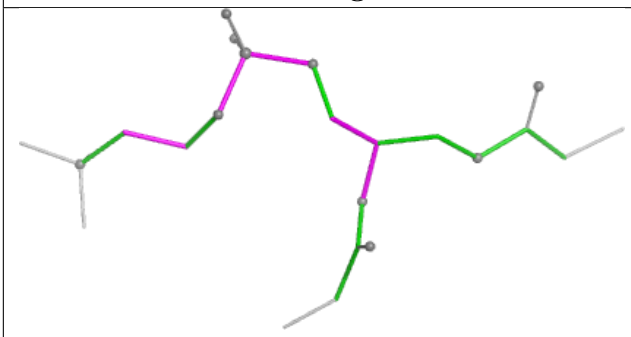
Ligand PC1 P 202



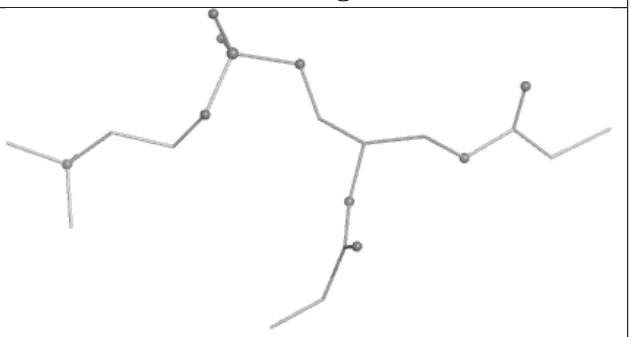
Bond lengths



Bond angles

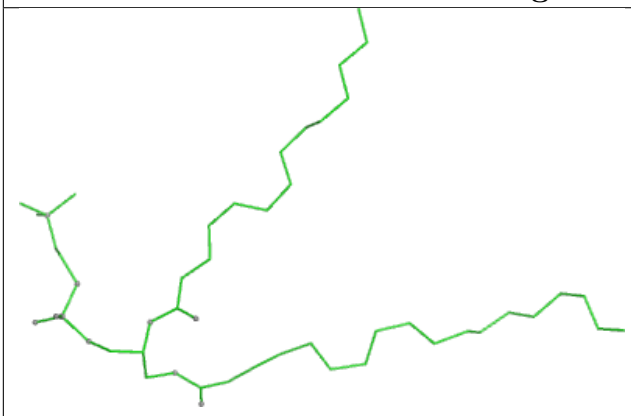


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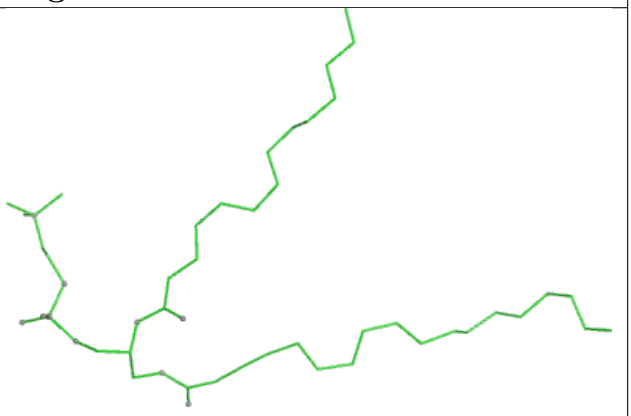


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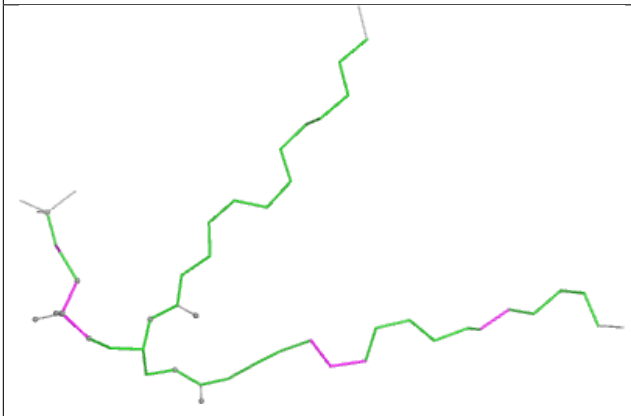
Ligand PC1 g 302



Bond lengths



Bond angles

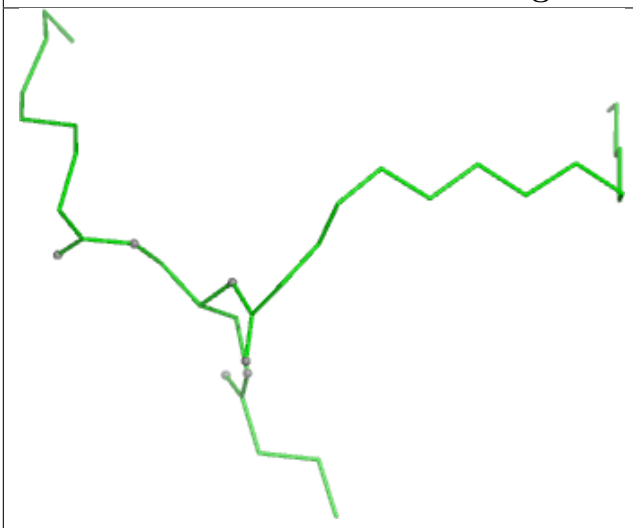


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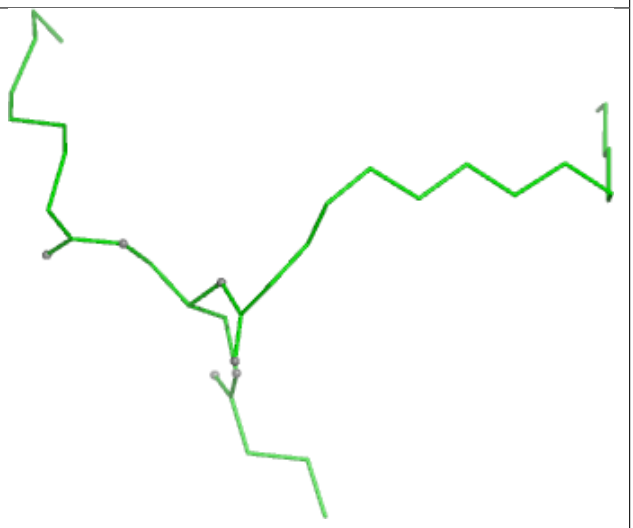


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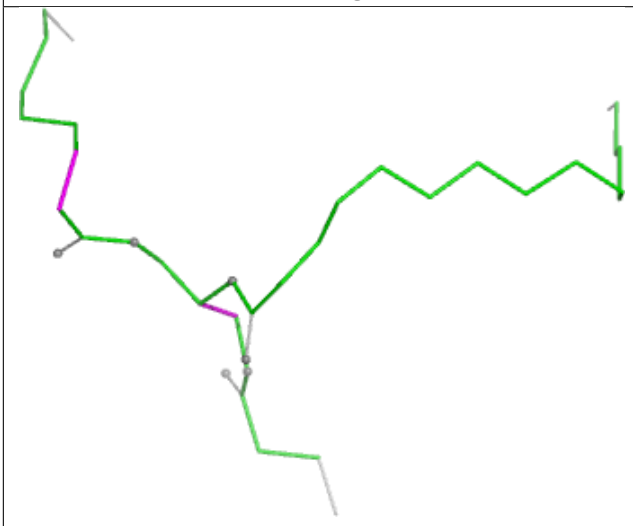
Ligand TGL l 601



Bond lengths



Bond angles

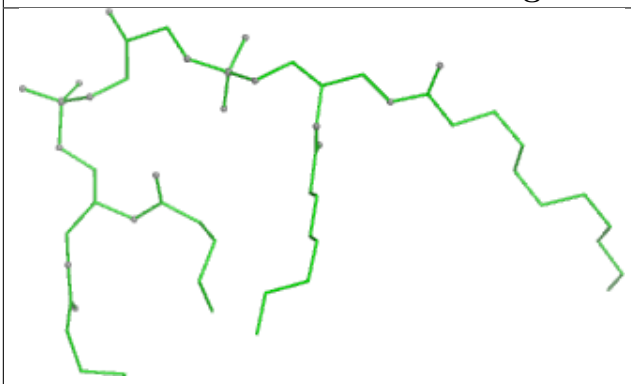


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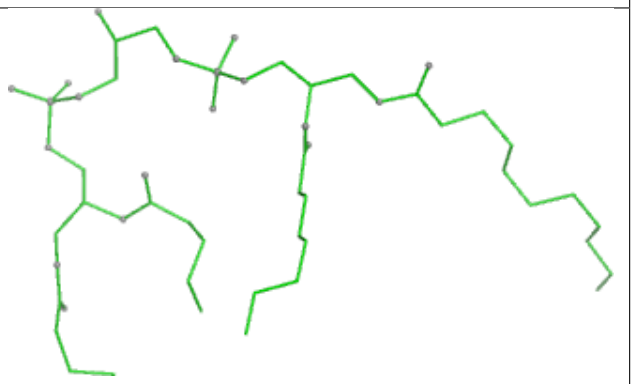


Rings

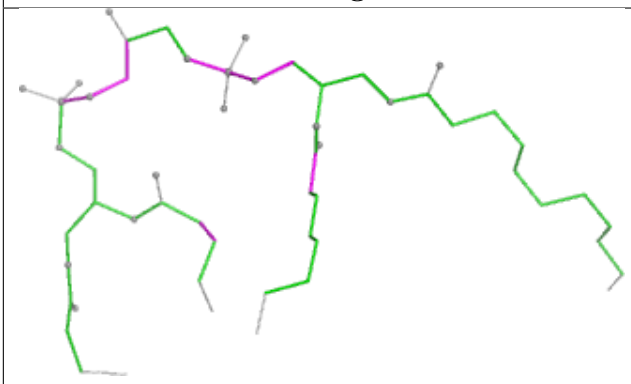
Ligand CDL D 301



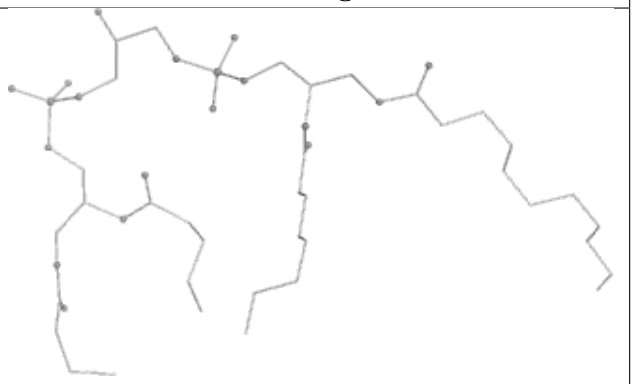
Bond lengths



Bond angles

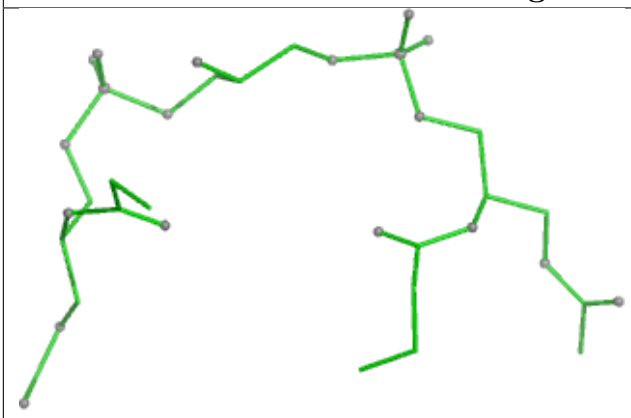


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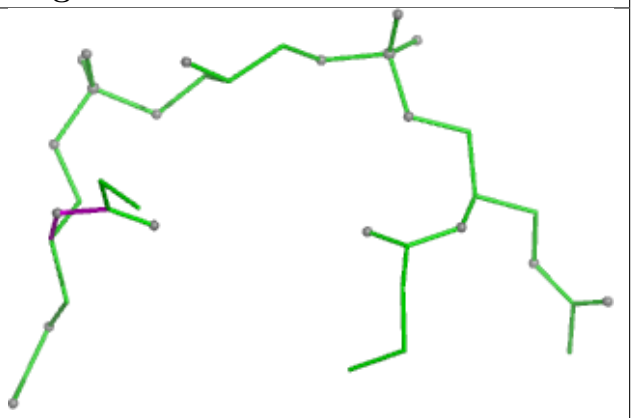


Rings

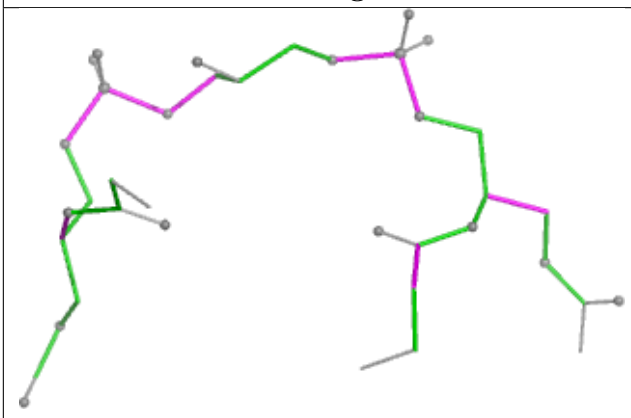
Ligand CDL g 301



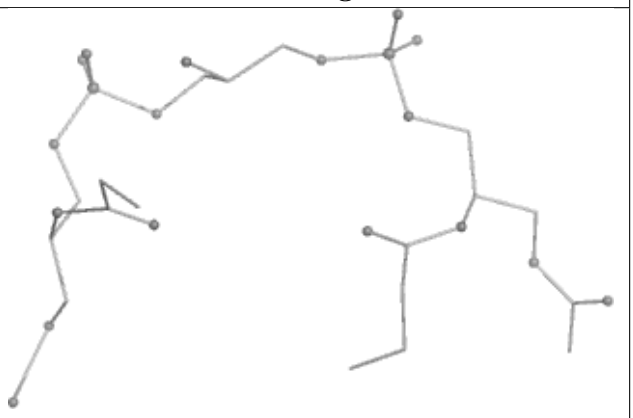
Bond lengths



Bond angles

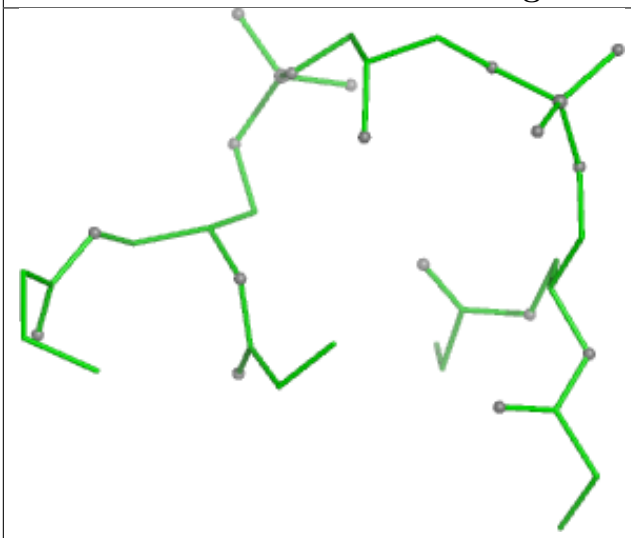


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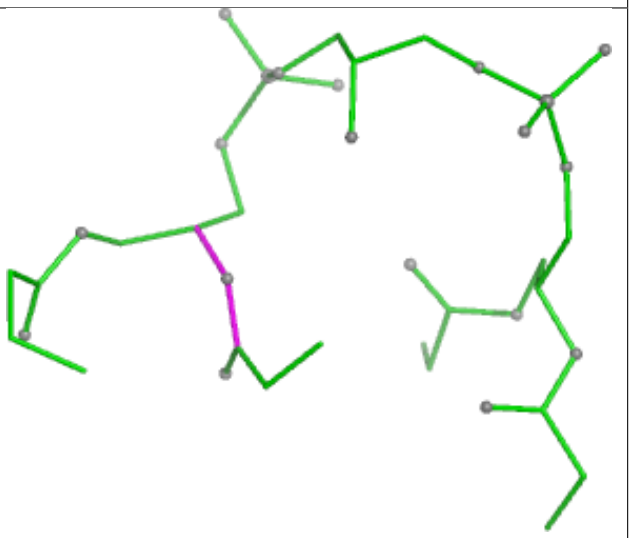


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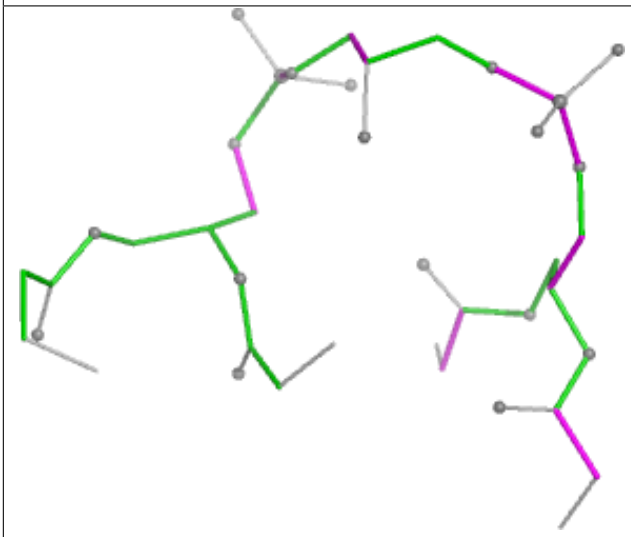
Ligand CDL N 404



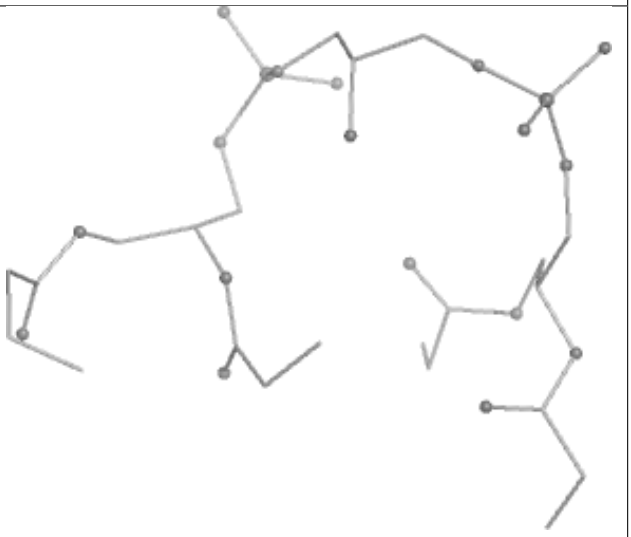
Bond lengths



Bond angles

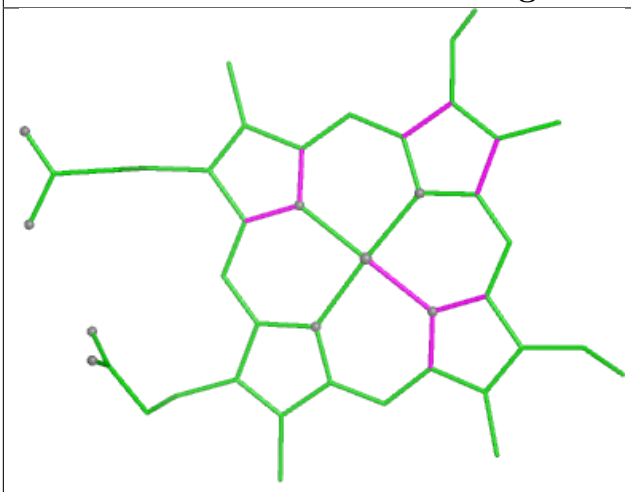


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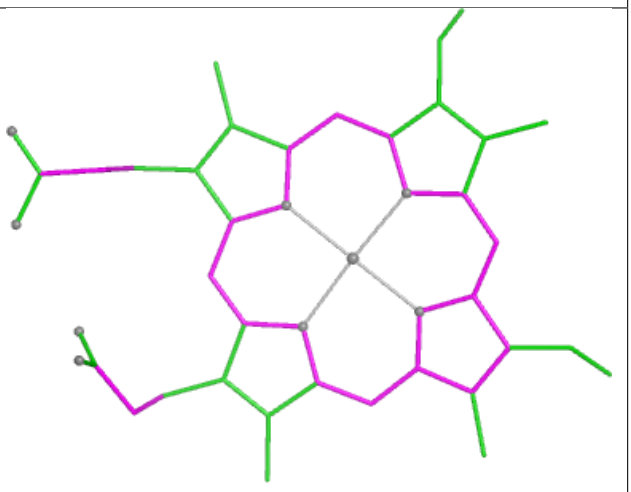


Rings

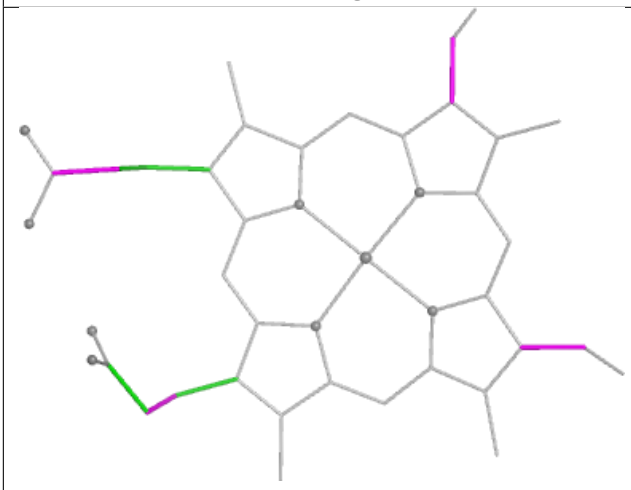
Ligand HEM C 401



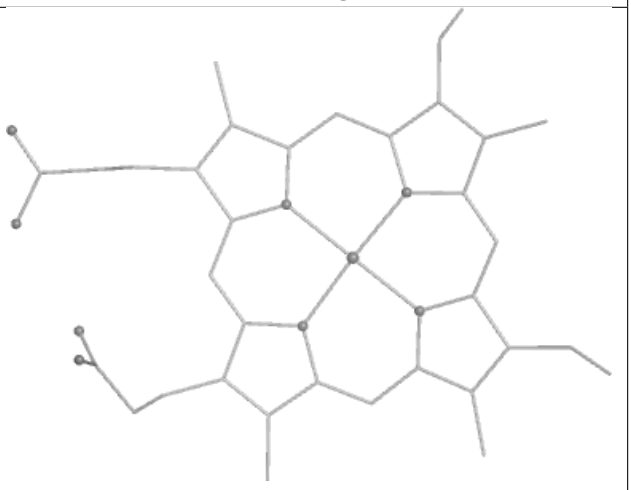
Bond lengths



Bond angles

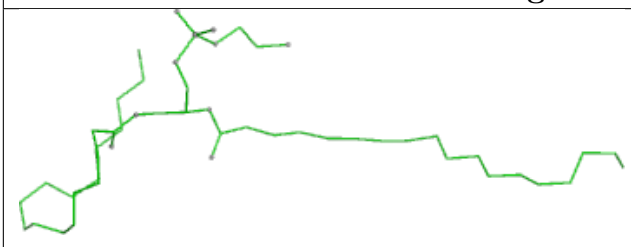


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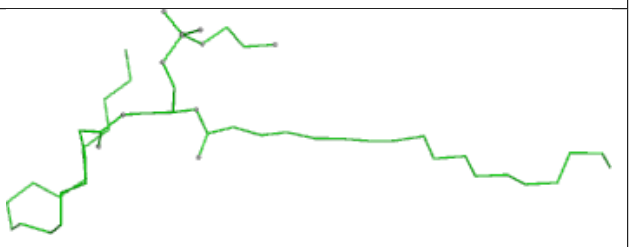


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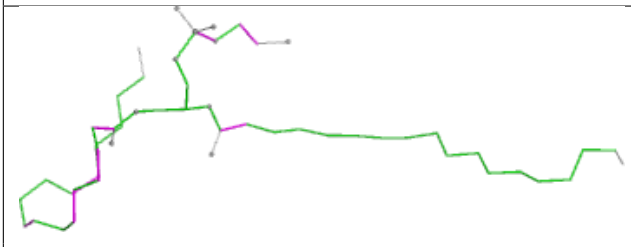
Ligand 3PE G 101



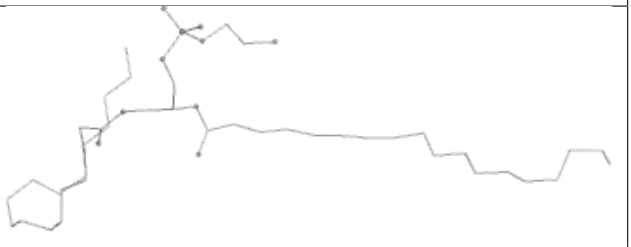
Bond lengths



Bond angles

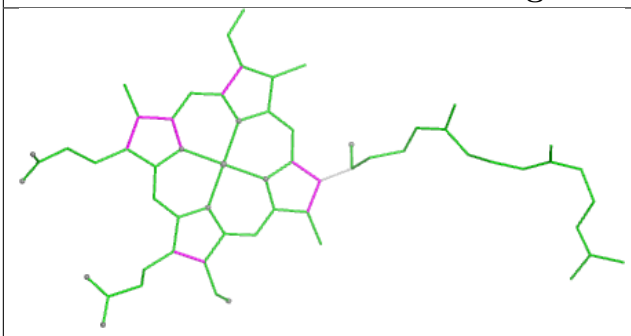


Torsions

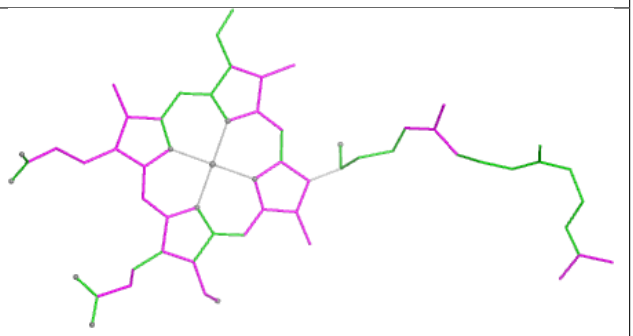


Rings

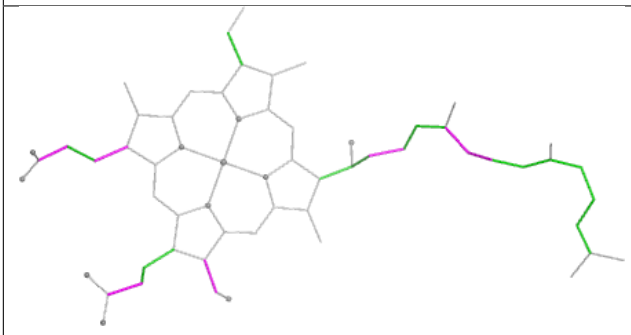
Ligand HEA a 604



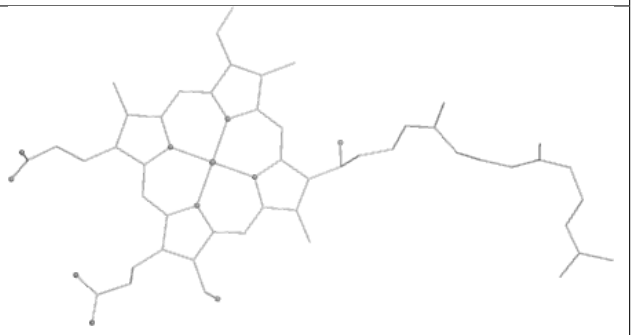
Bond lengths



Bond angles

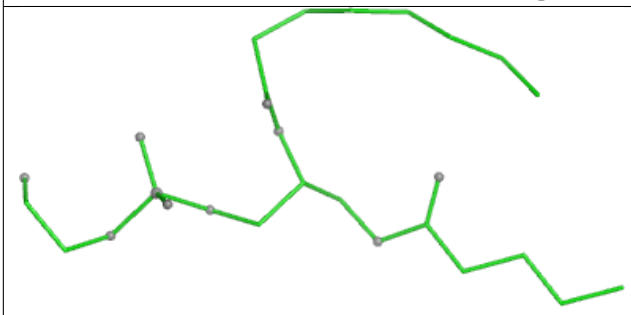


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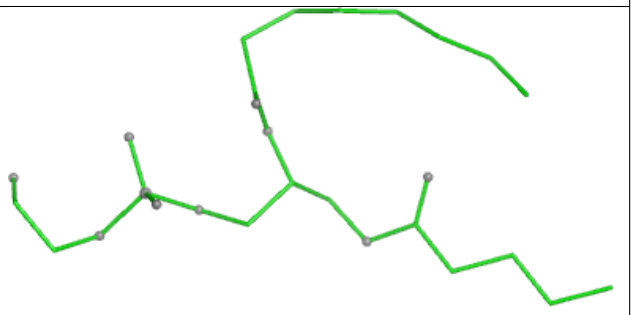


Rings

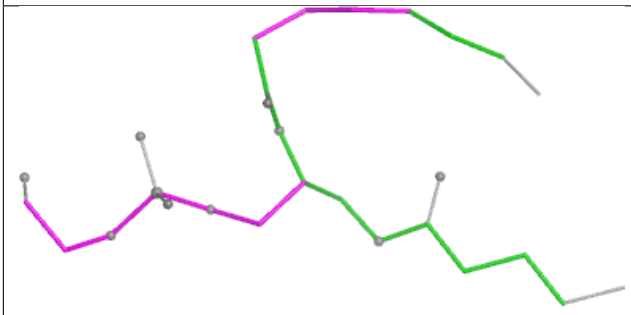
Ligand 3PE a 606



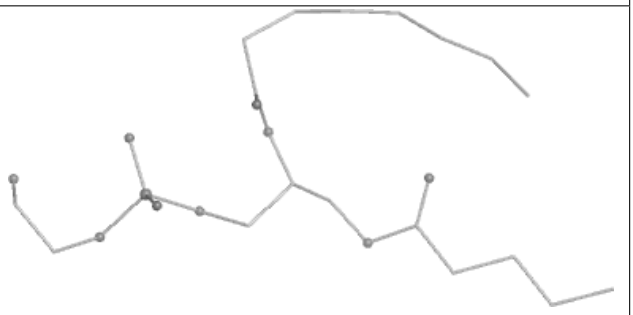
Bond lengths



Bond angles

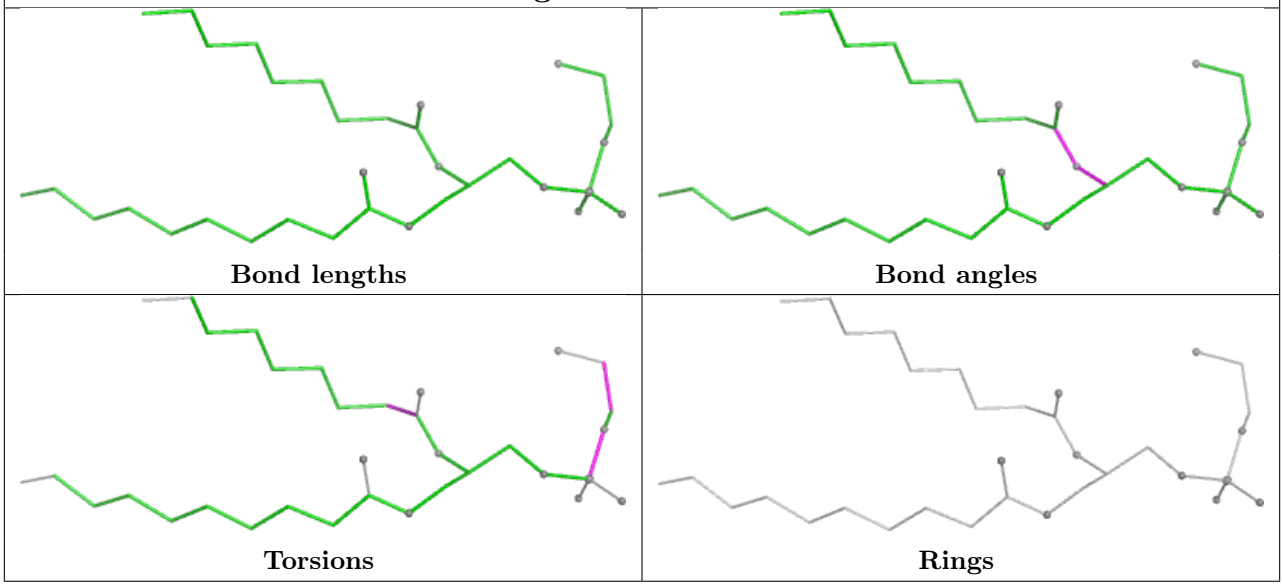


Torsions



Rings

Ligand 3PE a 605



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

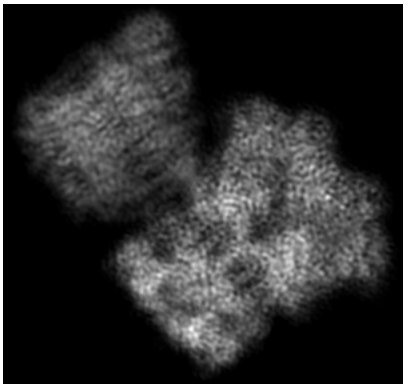
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-12703. These allow visual inspection of the internal detail of the map and identification of artifacts.

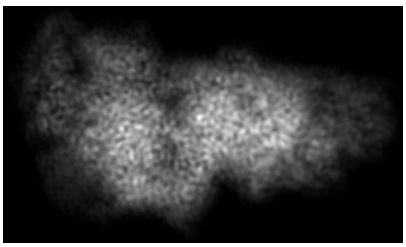
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

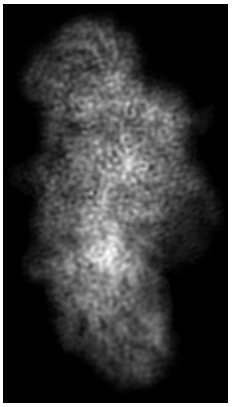
6.1.1 Primary map



X



Y

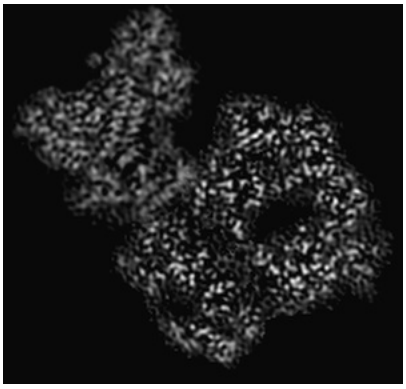


Z

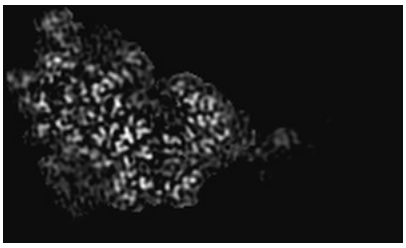
The images above show the map projected in three orthogonal directions.

6.2 Central slices

6.2.1 Primary map



X Index: 61



Y Index: 108

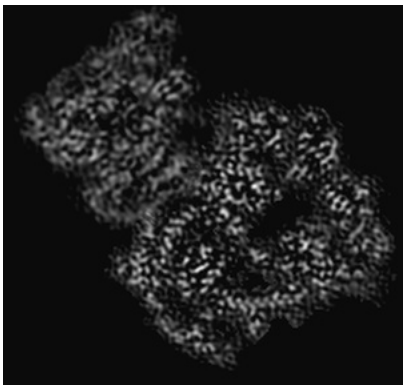


Z Index: 103

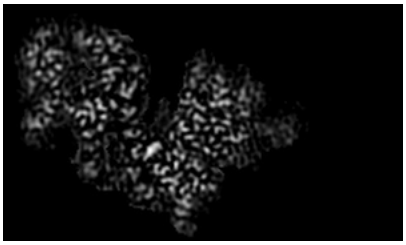
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

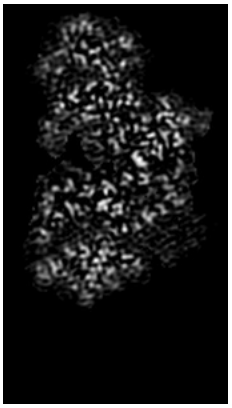
6.3.1 Primary map



X Index: 57



Y Index: 120

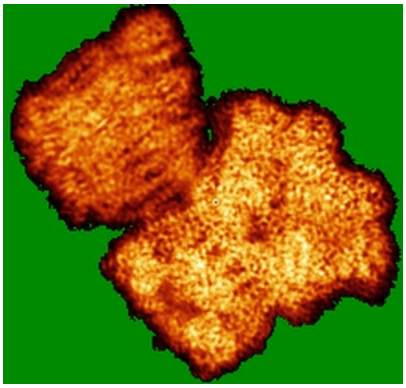


Z Index: 65

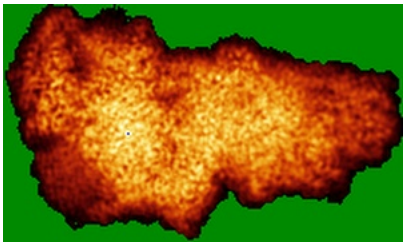
The images above show the largest variance slices of the map in three orthogonal directions.

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

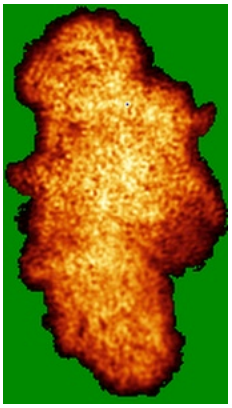
6.4.1 Primary map



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.

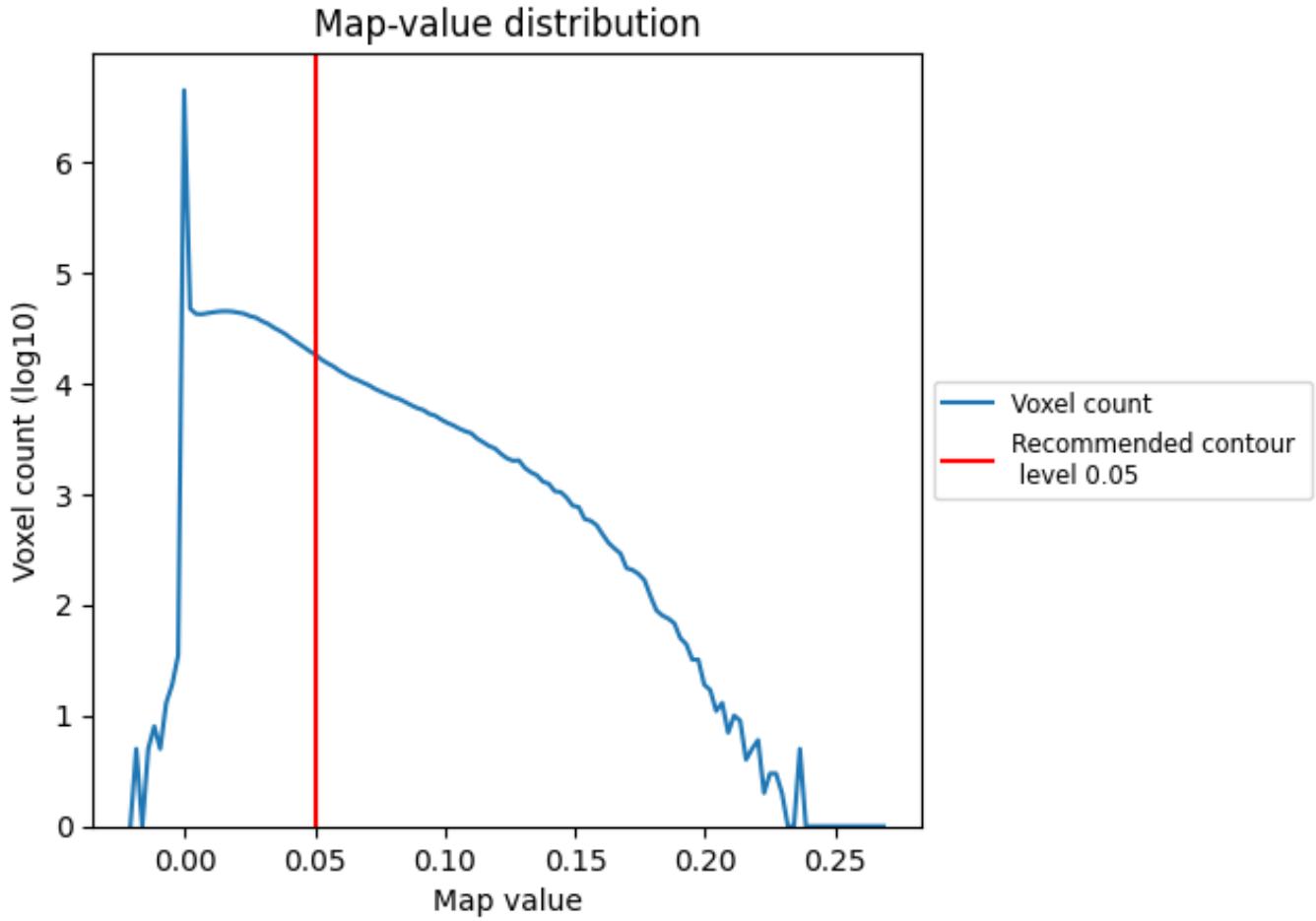
6.6 Mask visualisation (i)

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

7 Map analysis

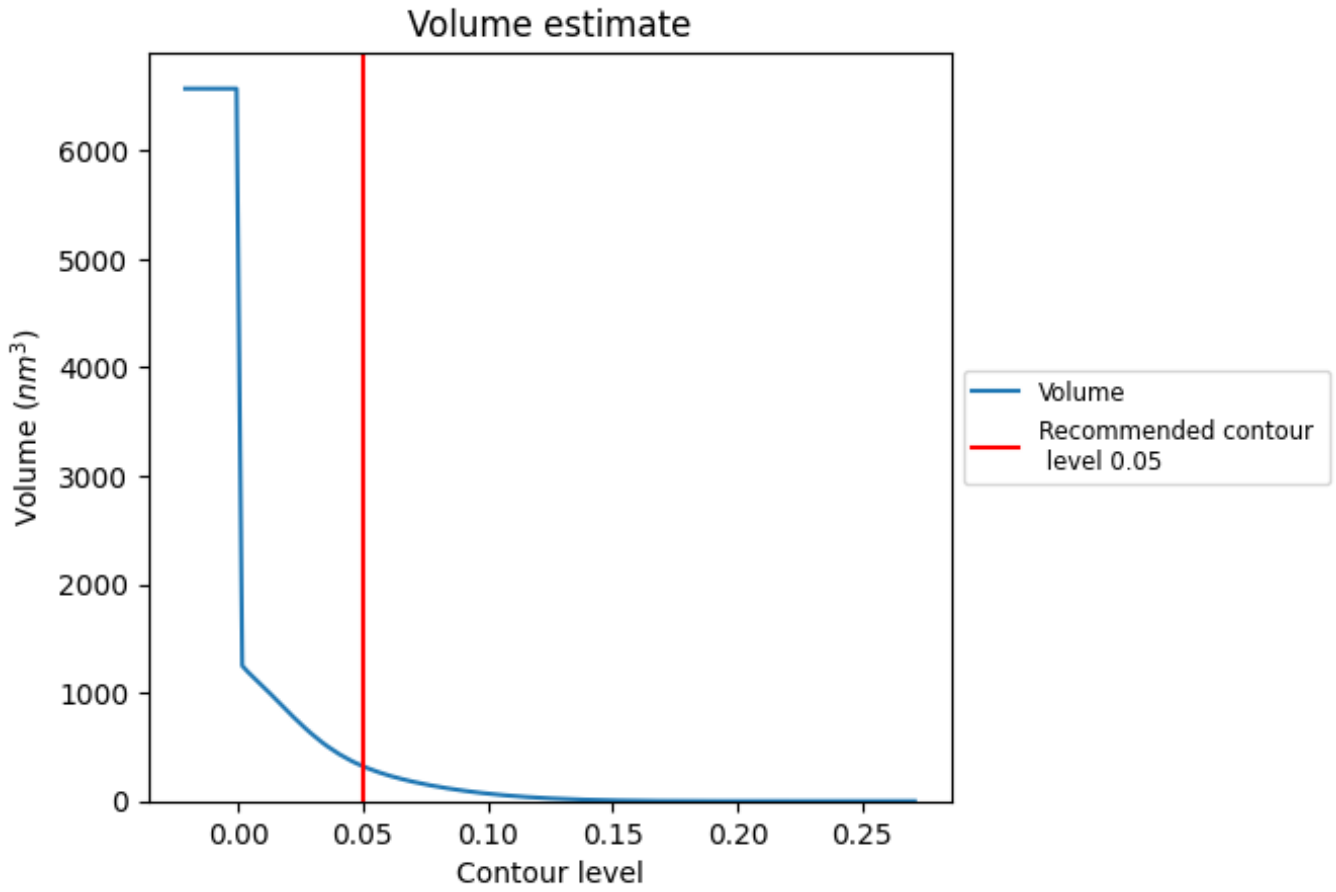
This section contains the results of statistical analysis of the map.

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



The volume at the recommended contour level is 322 nm^3; this corresponds to an approximate mass of 291 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.

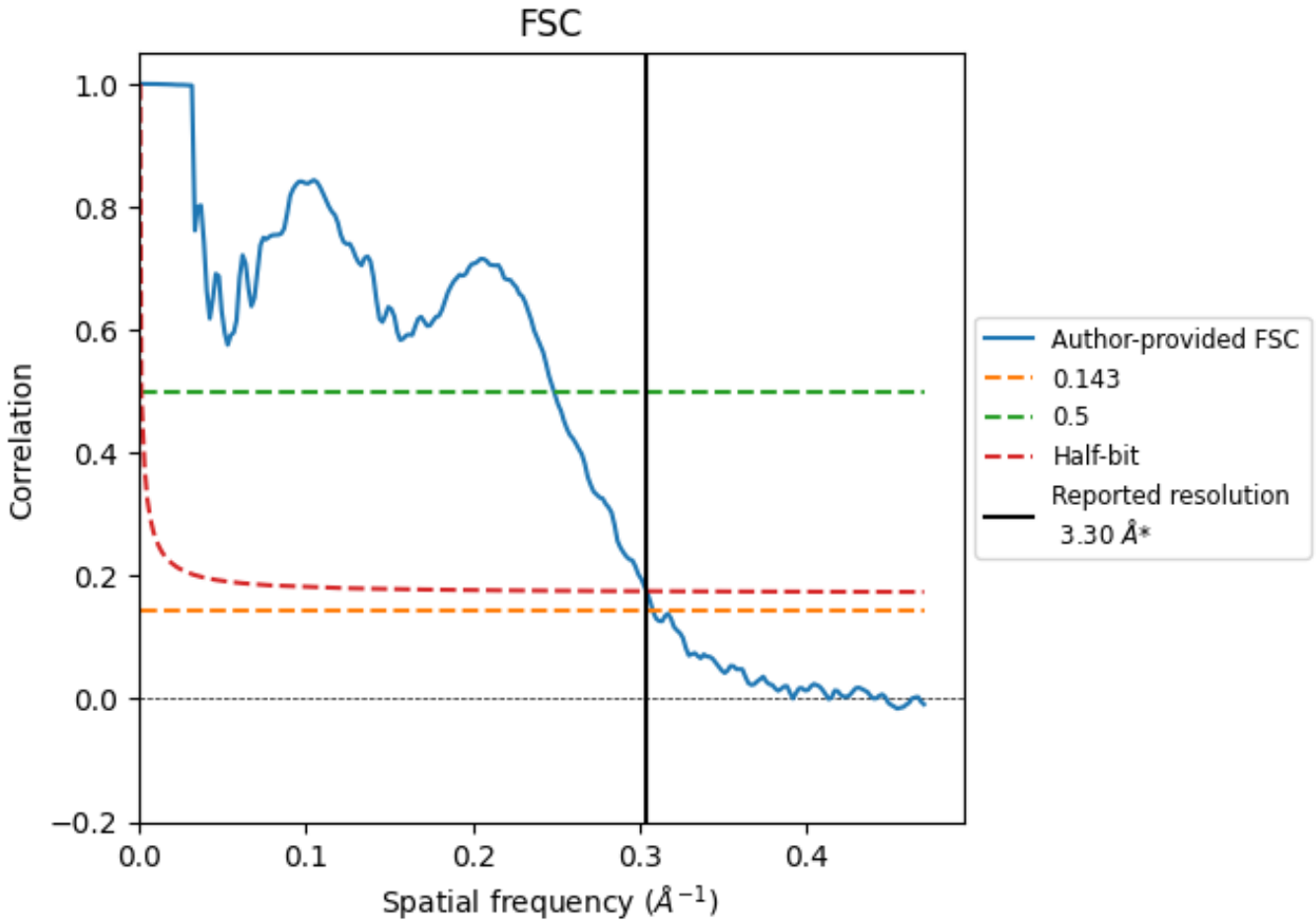
7.3 Rotationally averaged power spectrum

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

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.303 $Å^{-1}$

8.2 Resolution estimates (i)

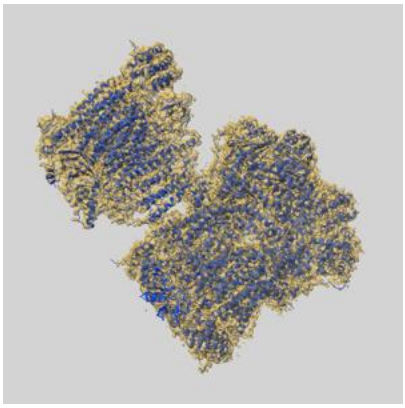
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.25	4.02	3.29
Unmasked-calculated*	-	-	-

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

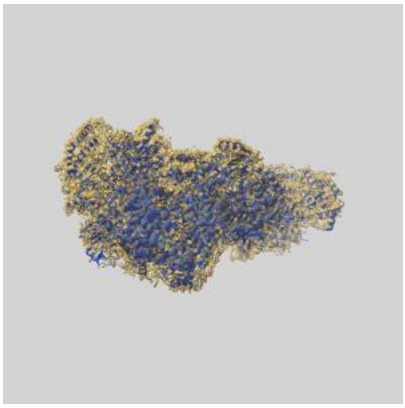
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-12703 and PDB model 7O3C. Per-residue inclusion information can be found in section 3 on page 16.

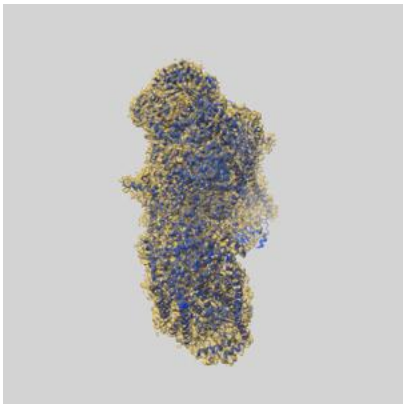
9.1 Map-model overlay



X



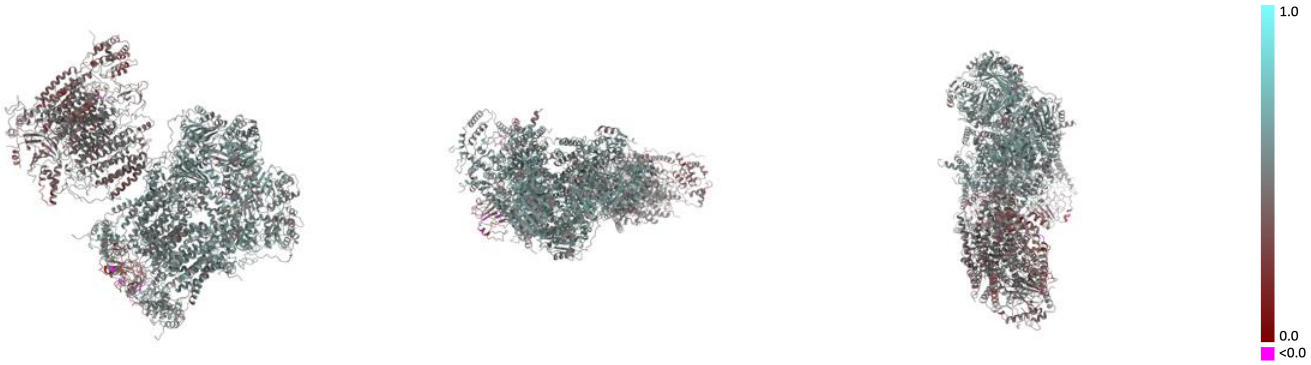
Y



Z

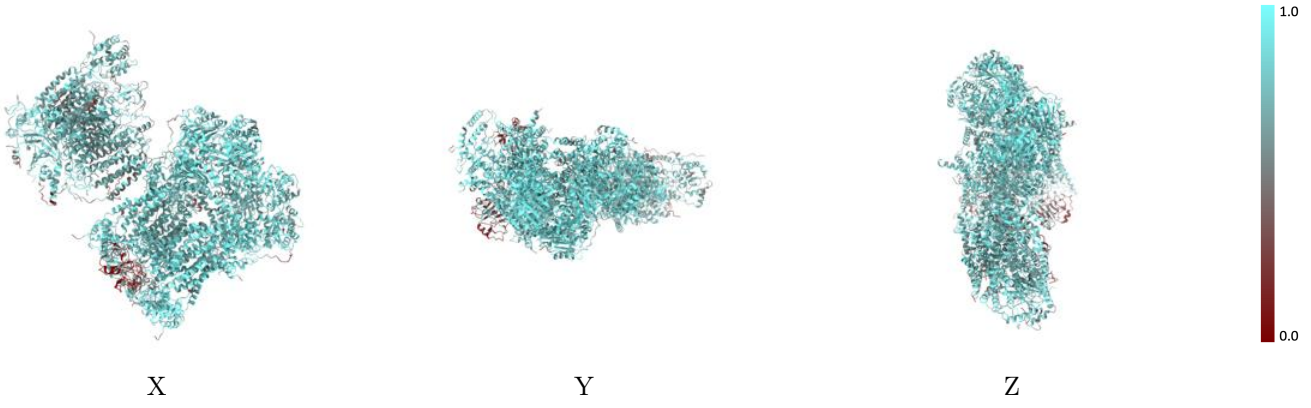
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



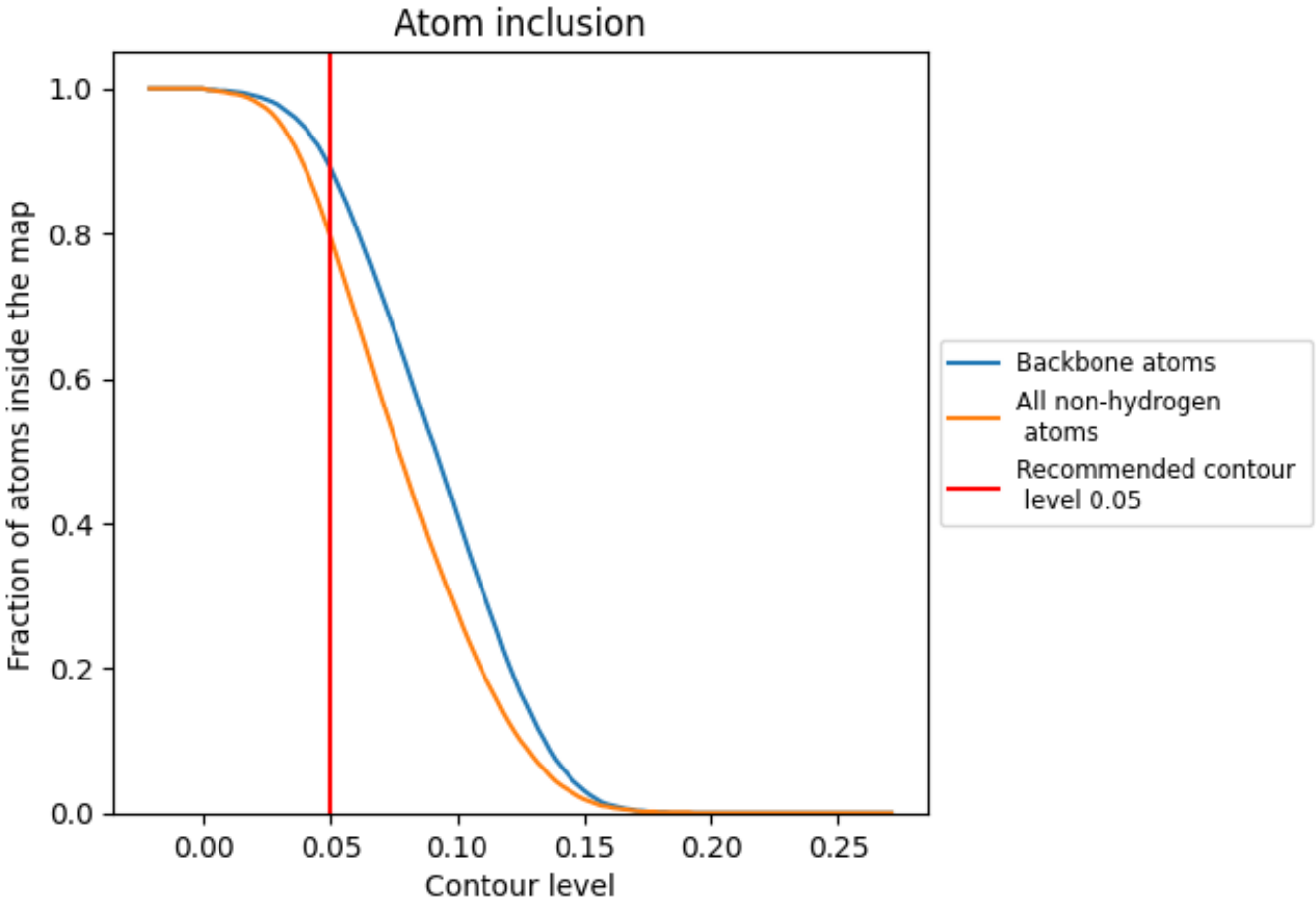
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model (i)



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

9.4 Atom inclusion (i)



At the recommended contour level, 89% of all backbone atoms, 80% 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	0.7960	0.4930
A	0.8580	0.5430
B	0.8630	0.5420
C	0.8670	0.5500
D	0.8800	0.5500
E	0.4730	0.3860
F	0.8550	0.5480
G	0.8550	0.5490
H	0.7370	0.4580
I	0.7190	0.4430
J	0.8710	0.5460
K	0.7600	0.4900
L	0.8490	0.5360
M	0.8520	0.5360
N	0.8690	0.5490
O	0.8790	0.5380
P	0.4980	0.3800
Q	0.8600	0.5380
R	0.8580	0.5410
S	0.7640	0.4630
T	0.8070	0.5140
U	0.8530	0.5310
V	0.6700	0.4620
a	0.7850	0.4580
b	0.7250	0.4050
c	0.7770	0.4390
d	0.6980	0.4040
e	0.7200	0.3620
f	0.6980	0.4120
g	0.7080	0.4360
h	0.7090	0.3820
i	0.7070	0.4020
k	0.7510	0.4030
l	0.7560	0.4390
m	0.6600	0.3980

