Full wwPDB EM Validation Report ⓘ

May 27, 2025 – 12:36 PM JST

PDB ID	:	8ZNO / pdb_00008zno
EMDB ID	:	EMD-60275
Title	:	Cryo-EM structure of Arachis hypogaea bc1 complex
Authors	:	Ye, Y.; Dong, J.Q.; Yang, G.F.
Deposited on	:	2024-05-27
Resolution	:	3.02 Å(reported)

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

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

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

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

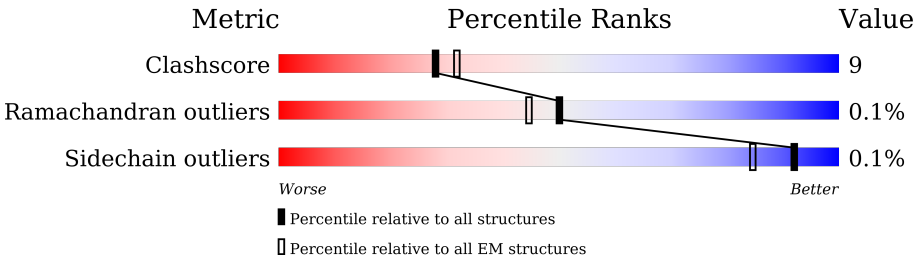
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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 3.02 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	460	49% 86% 14%
1	M	460	47% 77% 23%
2	B	487	23% 78% 22%
2	N	487	21% 82% 18%
3	C	386	5% 84% 15%
3	O	386	6% 79% 20%
4	D	242	7% 80% 19%
4	P	242	7% 81% 19%

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Mol	Chain	Length	Quality of chain
5	E	196	75% 67% 33%
5	Q	196	65% 65% 34%
6	F	117	9% 78% 22%
6	R	117	13% 71% 26%
7	G	70	39% 87% 13%
7	S	70	39% 84% 16%
8	H	64	62% 80% 20%
8	T	64	67% 73% 27%
9	J	60	47% 82% 18%
9	V	60	38% 73% 27%
10	K	29	100% 86% 14%
10	W	29	93% 97%

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
16	FES	E	301	-	-	X	-
16	FES	Q	301	-	-	X	-

2 Entry composition (i)

There are 17 unique types of molecules in this entry. The entry contains 34447 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Mitochondrial-processing peptidase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	460	Total	C	N	O	S	0	0
			3502	2220	591	679	12		
1	M	460	Total	C	N	O	S	0	0
			3502	2220	591	679	12		

- Molecule 2 is a protein called Mitochondrial-processing peptidase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	487	Total	C	N	O	S	0	0
			3855	2426	676	738	15		
2	N	487	Total	C	N	O	S	0	0
			3855	2426	676	738	15		

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	386	Total	C	N	O	S	0	0
			3076	2059	501	502	14		
3	O	385	Total	C	N	O	S	0	0
			3068	2055	500	499	14		

- Molecule 4 is a protein called Cytochrome c domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	242	Total	C	N	O	S	0	0
			1893	1205	323	354	11		
4	P	242	Total	C	N	O	S	0	0
			1893	1205	323	354	11		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	81	GLN	ASN	conflict	UNP A0A445B1W5

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Chain	Residue	Modelled	Actual	Comment	Reference
D	125	GLU	ASP	conflict	UNP A0A445B1W5
D	186	PRO	ARG	conflict	UNP A0A445B1W5
D	246	SER	ALA	conflict	UNP A0A445B1W5
P	81	GLN	ASN	conflict	UNP A0A445B1W5
P	125	GLU	ASP	conflict	UNP A0A445B1W5
P	186	PRO	ARG	conflict	UNP A0A445B1W5
P	246	SER	ALA	conflict	UNP A0A445B1W5

- 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
			1536	986	265	280	5		
5	Q	196	Total	C	N	O	S	0	0
			1536	986	265	280	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	117	Total	C	N	O	S	0	0
			986	628	179	174	5		
6	R	117	Total	C	N	O	S	0	0
			986	628	179	174	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	70	Total	C	N	O	S	0	0
			573	378	95	98	2		
7	S	70	Total	C	N	O	S	0	0
			573	378	95	98	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	64	Total	C	N	O	S	0	0
			519	330	87	96	6		
8	T	64	Total	C	N	O	S	0	0
			519	330	87	96	6		

- Molecule 9 is a protein called Complex III subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	60	Total	C	N	O	S	0	0
			486	312	88	85	1		
9	V	60	Total	C	N	O	S	0	0
			486	312	88	85	1		

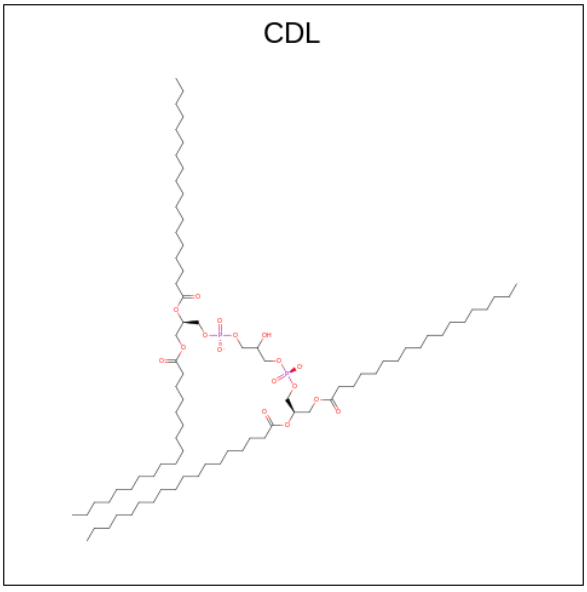
- Molecule 10 is a protein called Ubiquinol-cytochrome c reductase complex 6.7 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	29	Total	C	N	O	S	0	0
			218	145	35	37	1		
10	W	29	Total	C	N	O	S	0	0
			218	145	35	37	1		

- Molecule 11 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
11	B	1	Total	Zn	0
			1	1	
11	N	1	Total	Zn	0
			1	1	

- Molecule 12 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
12	B	1	Total	C	O	P	0
			69	50	17	2	

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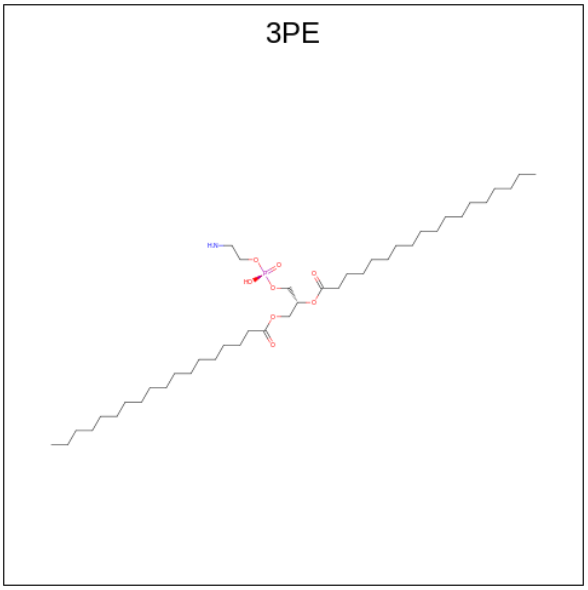
Mol	Chain	Residues	Atoms				AltConf
12	C	1	Total 30	C 21	O 8	P 1	0
12	D	1	Total 64	C 45	O 17	P 2	0
12	N	1	Total 70	C 51	O 17	P 2	0
12	O	1	Total 81	C 62	O 17	P 2	0
12	O	1	Total 58	C 39	O 17	P 2	0
12	P	1	Total 63	C 44	O 17	P 2	0

- Molecule 13 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
13	C	1	Total 28	C 18	N 1	O 8	P 1	0
13	C	1	Total 51	C 41	N 1	O 8	P 1	0
13	C	1	Total 37	C 27	N 1	O 8	P 1	0
13	C	1	Total 33	C 23	N 1	O 8	P 1	0
13	C	1	Total 34	C 24	N 1	O 8	P 1	0

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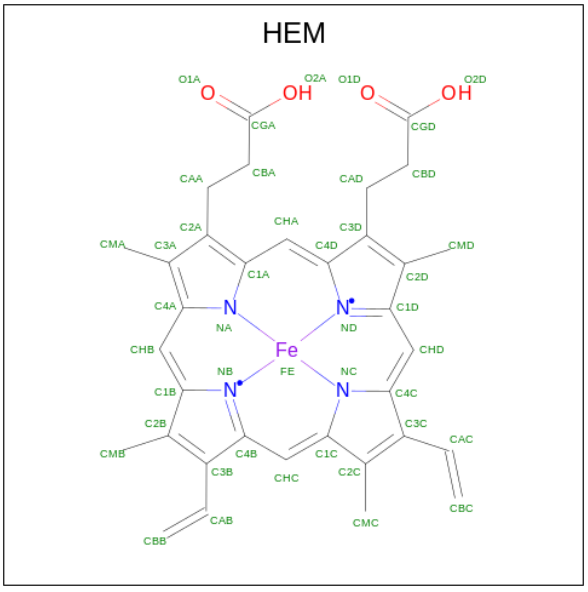
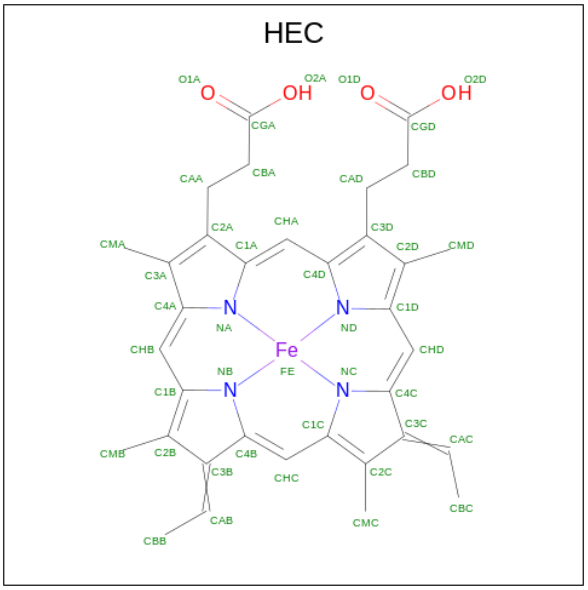
Mol	Chain	Residues	Atoms					AltConf
13	C	1	Total	C	N	O	P	0
			36	26	1	8	1	
13	E	1	Total	C	N	O	P	0
			30	20	1	8	1	
13	G	1	Total	C	N	O	P	0
			32	22	1	8	1	
13	O	1	Total	C	N	O	P	0
			38	28	1	8	1	
13	P	1	Total	C	N	O	P	0
			39	29	1	8	1	
13	R	1	Total	C	N	O	P	0
			48	38	1	8	1	
13	S	1	Total	C	N	O	P	0
			33	23	1	8	1	

- Molecule 14 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



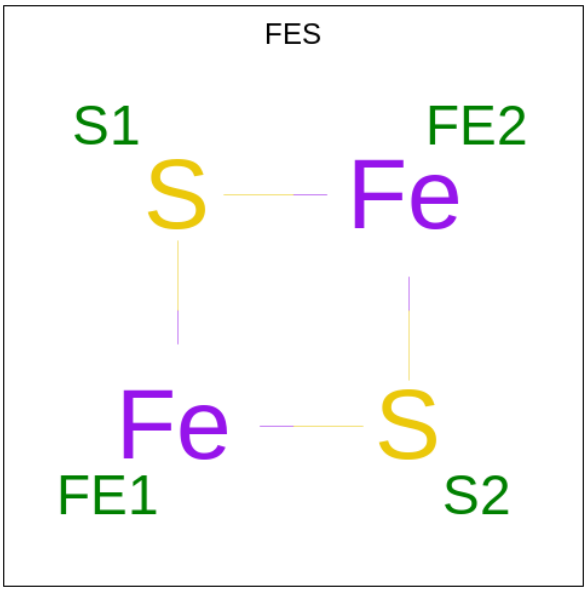
Mol	Chain	Residues	Atoms					AltConf
14	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
14	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
14	O	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
14	O	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 15 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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

- Molecule 16 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



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

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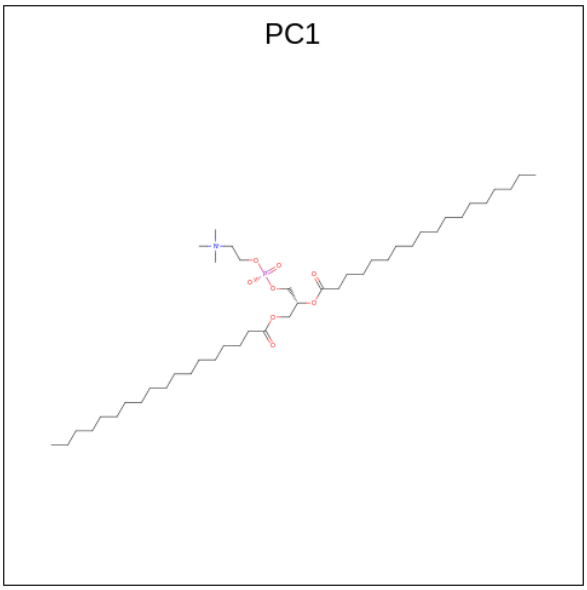
Mol	Chain	Residues	Atoms			AltConf
16	Q	1	Total	Fe	S	0
			4	2	2	

- Molecule 17 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



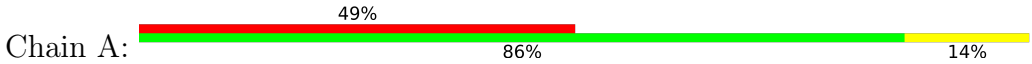
Mol	Chain	Residues	Atoms					AltConf
17	P	1	Total	C	N	O	P	0
			25	17	1	6	1	

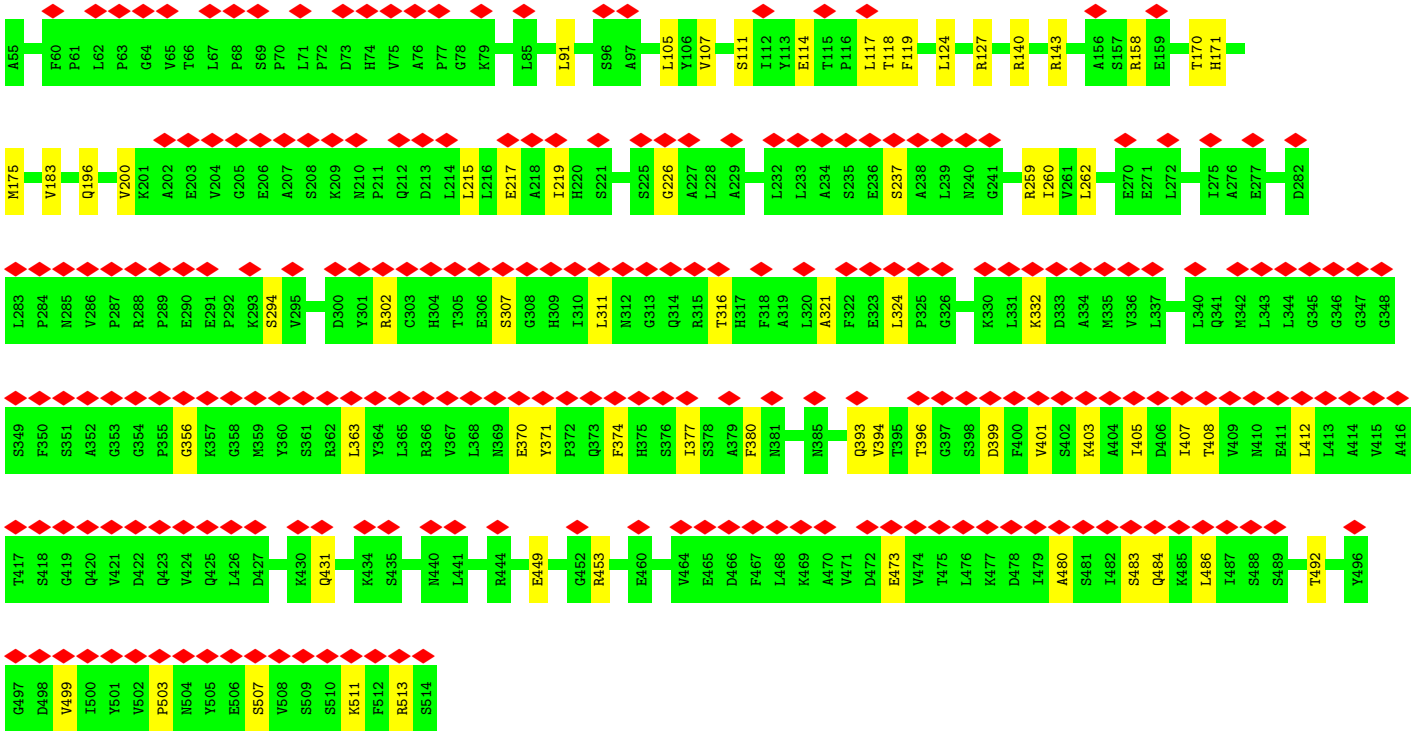
3 Residue-property plots (i)

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: Mitochondrial-processing peptidase subunit alpha

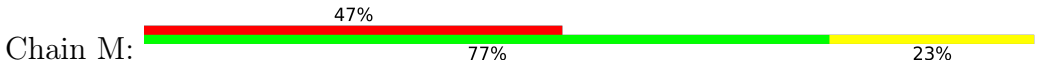
Chain A:

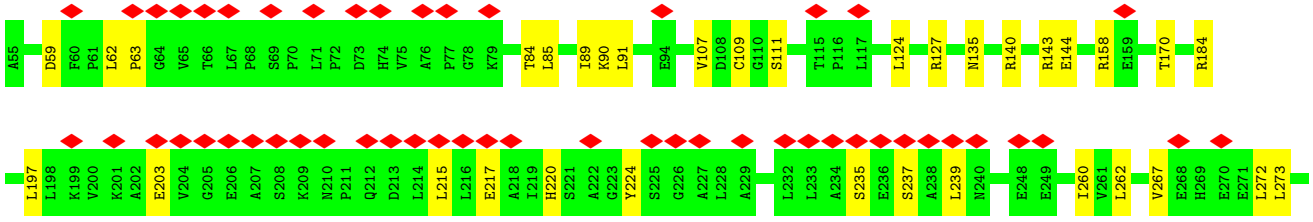


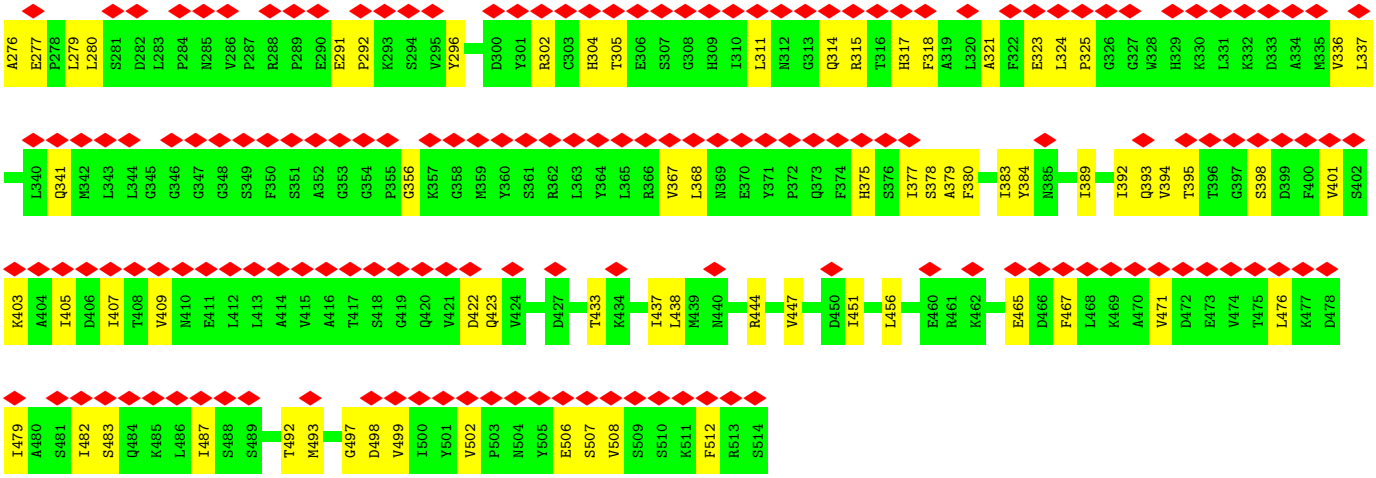


• Molecule 1: Mitochondrial-processing peptidase subunit alpha

Chain M:

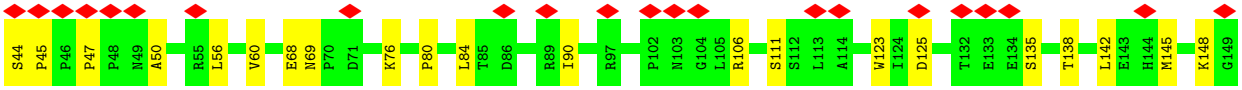


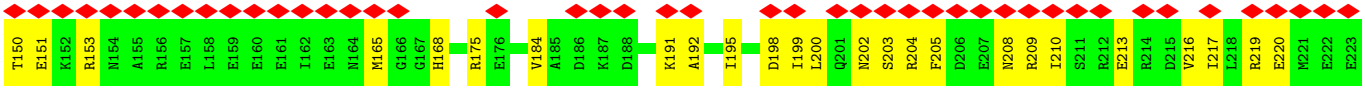




• Molecule 2: Mitochondrial-processing peptidase subunit beta

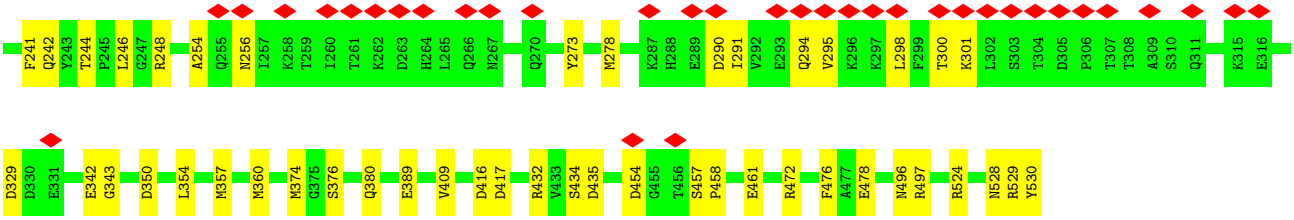
Chain B:



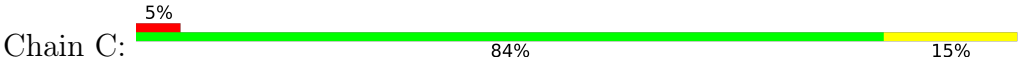


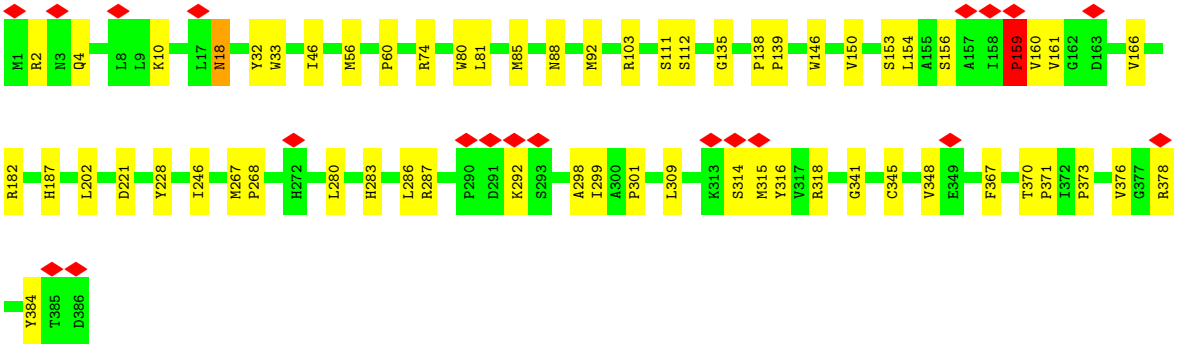
• Molecule 2: Mitochondrial-processing peptidase subunit beta

Chain N:

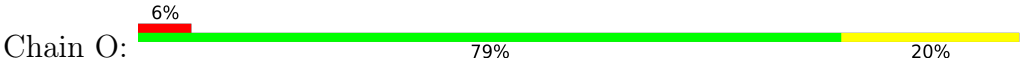


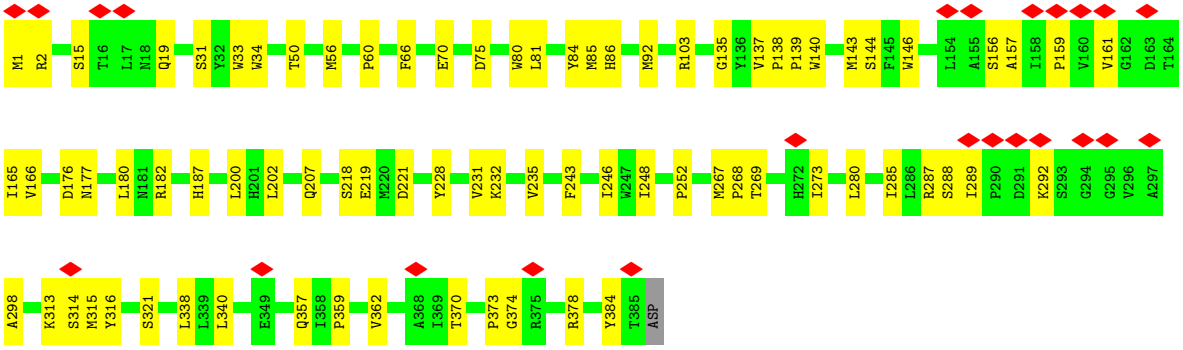
• Molecule 3: Cytochrome b



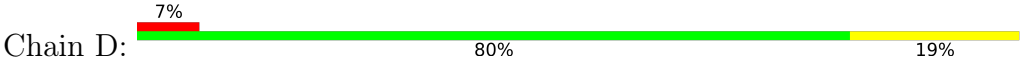


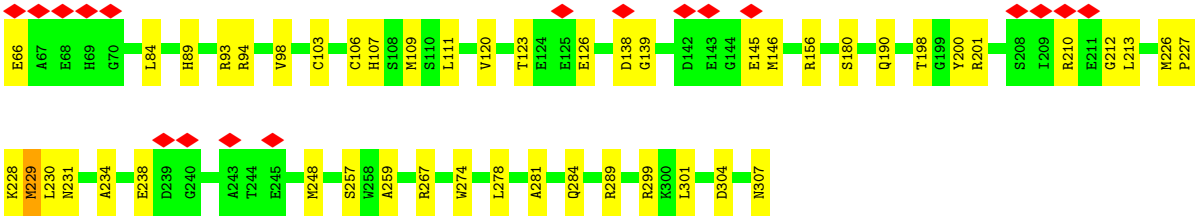
• Molecule 3: Cytochrome b





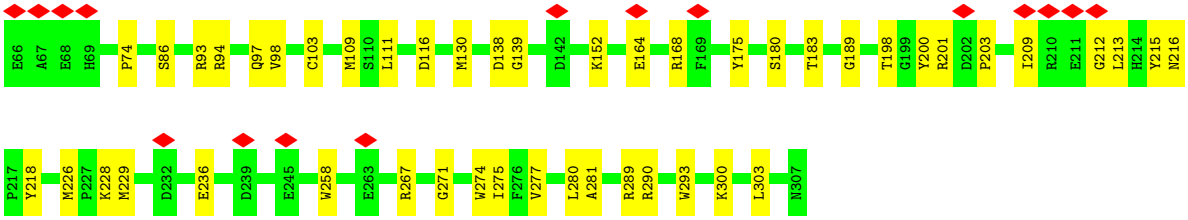
• Molecule 4: Cytochrome c domain-containing protein





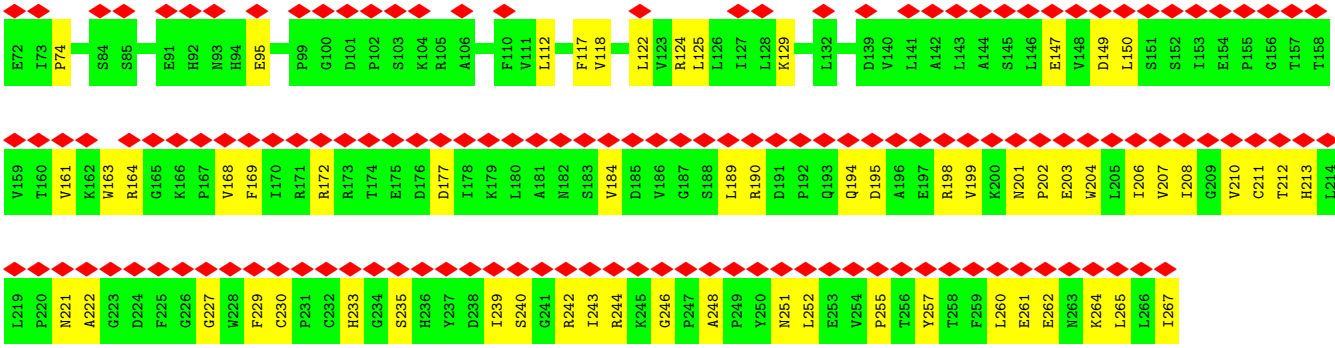
• Molecule 4: Cytochrome c domain-containing protein

Chain P:



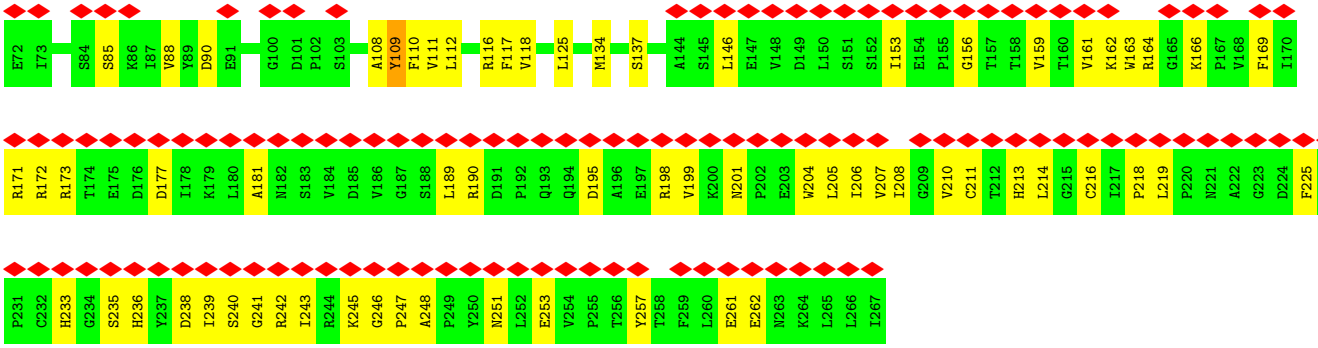
• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain E:



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

Chain Q:



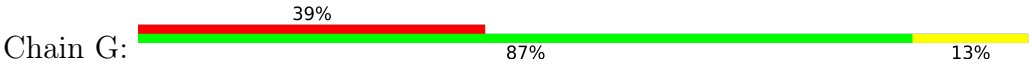
• Molecule 6: Cytochrome b-c1 complex subunit 7

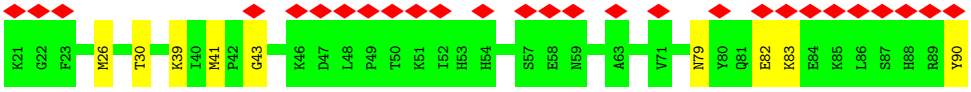
Chain F:

• Molecule 6: Cytochrome b-c1 complex subunit 7

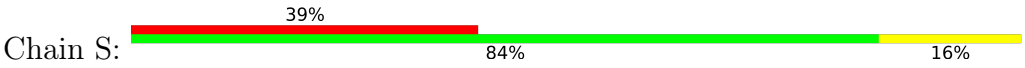
Chain R:

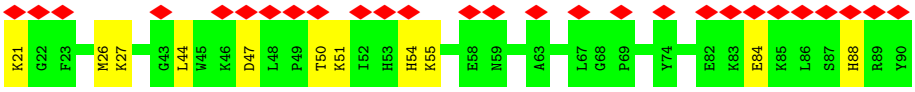
• Molecule 7: Cytochrome b-c1 complex subunit 8



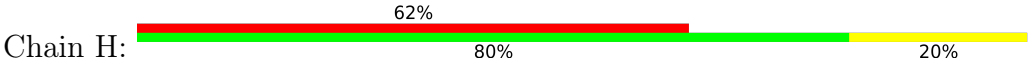


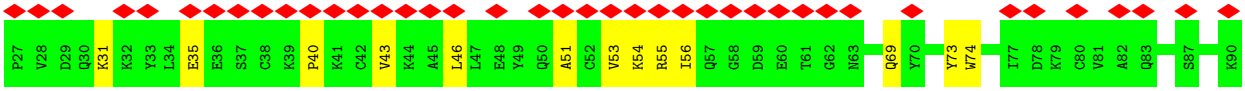
• Molecule 7: Cytochrome b-c1 complex subunit 8



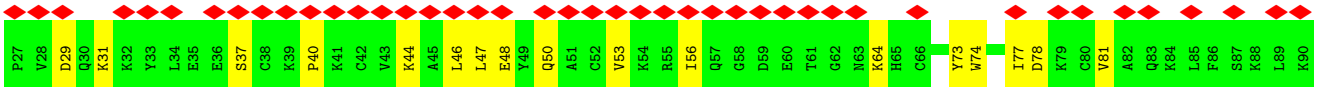


• Molecule 8: Cytochrome b-c1 complex subunit 6

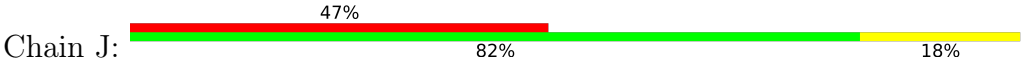


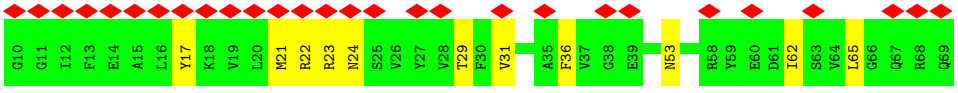


• Molecule 8: Cytochrome b-c1 complex subunit 6

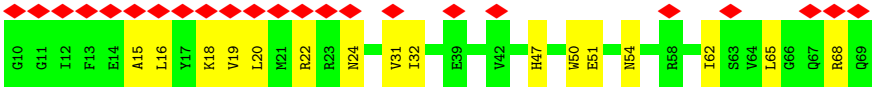


• Molecule 9: Complex III subunit 9



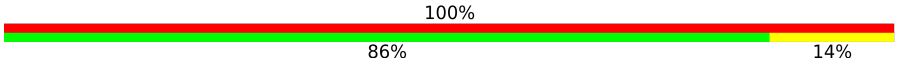


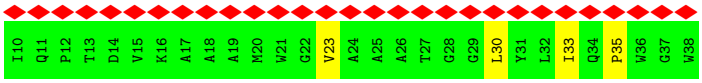
• Molecule 9: Complex III subunit 9



• Molecule 10: Ubiquinol-cytochrome c reductase complex 6.7 kDa protein

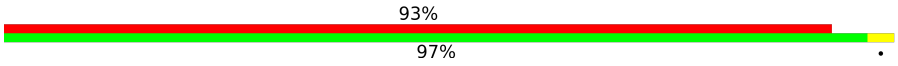
Chain K:

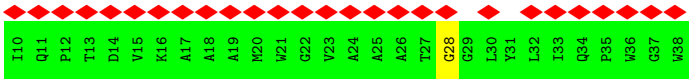




• Molecule 10: Ubiquinol-cytochrome c reductase complex 6.7 kDa protein

Chain W:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	53892	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 ($e^-/Å^2$)	48.42	Depositor
Minimum defocus (nm)	1600	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	130000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	3.544	Depositor
Minimum map value	-2.126	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.117	Depositor
Recommended contour level	0.584	Depositor
Map size (Å)	268.8, 268.8, 268.8	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.96, 0.96, 0.96	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.16	0/3574	0.37	0/4860
1	M	0.17	0/3574	0.41	0/4860
2	B	0.20	0/3933	0.45	0/5332
2	N	0.21	0/3933	0.46	0/5332
3	C	0.26	0/3194	0.47	0/4379
3	O	0.26	0/3186	0.49	0/4368
4	D	0.22	0/1946	0.41	0/2644
4	P	0.22	0/1946	0.44	0/2644
5	E	0.17	0/1576	0.47	0/2144
5	Q	0.49	3/1576 (0.2%)	0.53	0/2144
6	F	0.23	0/1008	0.42	0/1352
6	R	0.66	2/1008 (0.2%)	0.58	1/1352 (0.1%)
7	G	0.19	0/591	0.44	0/799
7	S	0.21	0/591	0.57	0/799
8	H	0.17	0/529	0.40	0/705
8	T	0.27	0/529	0.65	0/705
9	J	0.18	0/496	0.46	0/666
9	V	0.19	0/496	0.47	0/666
10	K	0.13	0/226	0.28	0/310
10	W	0.13	0/226	0.28	0/310
All	All	0.25	5/34138 (0.0%)	0.46	1/46371 (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
3	C	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	Q	108	ALA	C-O	-7.64	1.14	1.24
5	Q	108	ALA	CA-C	-5.90	1.44	1.52
6	R	17	PHE	N-CA	-5.18	1.41	1.46
6	R	120	ARG	C-O	-5.17	1.17	1.23
5	Q	111	VAL	C-O	-5.04	1.16	1.23

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	R	17	PHE	N-CA-C	-9.23	96.73	111.04

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	159	PRO	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	3502	0	3495	48	0
1	M	3502	0	3495	64	0
2	B	3855	0	3817	77	0
2	N	3855	0	3817	64	0
3	C	3076	0	3058	53	0
3	O	3068	0	3054	59	0
4	D	1893	0	1827	43	0
4	P	1893	0	1827	44	0
5	E	1536	0	1539	50	0
5	Q	1536	0	1539	72	0
6	F	986	0	997	18	0
6	R	986	0	997	43	0
7	G	573	0	585	8	0
7	S	573	0	585	14	0
8	H	519	0	517	9	0
8	T	519	0	517	13	0
9	J	486	0	481	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	V	486	0	481	14	0
10	K	218	0	212	3	0
10	W	218	0	212	1	0
11	B	1	0	0	0	0
11	N	1	0	0	0	0
12	B	69	0	85	1	0
12	C	30	0	33	14	0
12	D	64	0	72	2	0
12	N	70	0	87	10	0
12	O	139	0	172	7	0
12	P	63	0	70	2	0
13	C	219	0	288	7	0
13	E	30	0	34	1	0
13	G	32	0	38	0	0
13	O	38	0	50	2	0
13	P	39	0	52	1	0
13	R	48	0	73	3	0
13	S	33	0	40	0	0
14	C	86	0	60	5	0
14	O	86	0	60	5	0
15	D	43	0	32	5	0
15	P	43	0	32	4	0
16	E	4	0	0	3	0
16	Q	4	0	0	2	0
17	P	25	0	31	3	0
All	All	34447	0	34361	647	0

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

All (647) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:R:13:LYS:O	6:R:14:LYS:HE2	1.37	1.21
4:D:229:MET:SD	15:D:402:HEC:HMC2	1.93	1.09
6:R:17:PHE:O	6:R:19:ALA:N	1.94	1.00
12:C:408:CDL:H112	4:D:289:ARG:NH1	1.81	0.96
4:D:229:MET:SD	15:D:402:HEC:CMC	2.54	0.93
2:N:151:GLU:HB3	2:N:204:ARG:HE	1.34	0.92
6:R:43:TYR:HH	7:S:21:LYS:N	1.67	0.91
6:R:13:LYS:O	6:R:14:LYS:CE	2.19	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:R:13:LYS:C	6:R:14:LYS:CE	2.45	0.90
6:R:13:LYS:C	6:R:14:LYS:HE2	1.96	0.89
4:D:103:CYS:HB2	15:D:402:HEC:HAB	1.54	0.88
1:M:401:VAL:HG11	1:M:502:VAL:HG22	1.57	0.87
6:R:15:ASN:OD1	6:R:16:TRP:N	2.11	0.84
1:M:215:LEU:HD11	1:M:317:HIS:HB3	1.62	0.81
4:P:116:ASP:OD2	4:P:258:TRP:CH2	2.33	0.81
6:R:15:ASN:OD1	6:R:17:PHE:N	2.14	0.81
3:O:176:ASP:OD1	3:O:177:ASN:N	2.15	0.80
6:R:17:PHE:O	6:R:20:GLN:N	2.15	0.79
5:E:213:HIS:ND1	16:E:301:FES:S2	2.57	0.77
2:B:217:ILE:HA	2:B:220:GLU:HG2	1.67	0.77
6:R:13:LYS:C	6:R:14:LYS:HE3	2.09	0.77
6:R:17:PHE:O	6:R:18:ALA:C	2.26	0.77
5:Q:117:PHE:HE1	9:V:31:VAL:HA	1.50	0.76
2:N:152:LYS:HD3	2:N:153:ARG:HH21	1.50	0.76
2:N:175:ARG:NH1	2:N:248:ARG:O	2.19	0.76
5:Q:163:TRP:CD1	5:Q:164:ARG:H	2.04	0.76
4:D:278:LEU:HD21	5:E:122:LEU:HD11	1.69	0.75
4:P:281:ALA:HB2	5:Q:118:VAL:HG11	1.68	0.74
4:P:280:LEU:HD13	17:P:401:PC1:H262	1.68	0.73
4:D:229:MET:SD	15:D:402:HEC:C2C	2.77	0.72
5:Q:213:HIS:ND1	16:Q:301:FES:S2	2.62	0.72
12:C:408:CDL:C11	4:D:289:ARG:NH1	2.52	0.72
7:G:82:GLU:OE2	7:G:83:LYS:HE2	1.89	0.72
4:D:93:ARG:NH2	4:D:238:GLU:OE2	2.23	0.72
3:C:32:TYR:HB2	12:C:408:CDL:H312	1.72	0.71
5:E:230:CYS:HB3	5:E:235:SER:HB2	1.72	0.71
5:E:95:GLU:OE1	7:G:39:LYS:NZ	2.22	0.70
3:O:267:MET:HB3	3:O:268:PRO:HD3	1.73	0.70
12:N:602:CDL:HA62	12:N:602:CDL:OA7	1.91	0.70
3:C:32:TYR:HB2	12:C:408:CDL:H331	1.74	0.70
9:J:22:ARG:HG2	9:J:23:ARG:HH21	1.56	0.70
5:Q:161:VAL:HG12	5:Q:162:LYS:H	1.57	0.70
5:E:117:PHE:HE1	9:J:31:VAL:HA	1.55	0.70
4:P:103:CYS:HB2	15:P:403:HEC:HAB	1.73	0.70
1:A:449:GLU:OE2	1:A:453:ARG:NH1	2.26	0.69
1:A:321:ALA:HB3	1:A:492:THR:HB	1.75	0.69
12:C:408:CDL:H112	4:D:289:ARG:HH12	1.56	0.69
3:O:33:TRP:HB3	3:O:103:ARG:HG3	1.73	0.69
4:D:299:ARG:NH1	6:F:72:ASP:OD1	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:210:VAL:HG13	5:E:215:GLY:HA2	1.75	0.68
13:E:302:3PE:H232	3:O:165:ILE:HG12	1.75	0.67
12:C:408:CDL:H132	12:C:408:CDL:OA7	1.95	0.67
3:O:232:LYS:HE3	4:P:289:ARG:HH21	1.60	0.67
1:A:311:LEU:HG	1:M:237:SER:HB3	1.77	0.67
1:M:321:ALA:HB3	1:M:492:THR:HB	1.75	0.67
14:O:403:HEM:HBC2	14:O:403:HEM:HHD	1.77	0.67
3:O:316:TYR:OH	6:R:45:ASP:OD2	2.11	0.66
1:M:184:ARG:NH1	1:M:279:LEU:O	2.28	0.66
1:M:324:LEU:HD12	1:M:325:PRO:HD2	1.78	0.66
5:Q:181:ALA:HB1	5:Q:240:SER:HB2	1.76	0.66
5:Q:236:HIS:HB2	5:Q:245:LYS:HB3	1.77	0.66
3:C:32:TYR:HB2	12:C:408:CDL:C31	2.26	0.66
2:B:175:ARG:NH1	2:B:248:ARG:O	2.29	0.66
3:C:32:TYR:HD2	12:C:408:CDL:H312	1.59	0.66
6:R:43:TYR:OH	7:S:21:LYS:N	2.27	0.66
4:D:281:ALA:HB2	5:E:118:VAL:HG11	1.79	0.65
5:E:163:TRP:CG	5:E:164:ARG:H	2.13	0.65
8:H:31:LYS:O	8:H:35:GLU:HG3	1.96	0.65
6:F:120:ARG:NH1	6:F:121:THR:O	2.29	0.65
5:Q:206:ILE:HB	5:Q:257:TYR:CZ	2.31	0.65
2:B:350:ASP:OD2	2:B:497:ARG:NH1	2.29	0.65
3:C:292:LYS:HD3	5:Q:213:HIS:CD2	2.32	0.65
6:R:14:LYS:HE2	6:R:14:LYS:HA	1.79	0.64
5:E:150:LEU:HG	5:E:161:VAL:HG11	1.78	0.64
1:A:324:LEU:HD21	1:A:486:LEU:HG	1.79	0.64
1:M:140:ARG:O	1:M:144:GLU:HG3	1.98	0.64
2:B:529:ARG:NH2	12:B:602:CDL:OB3	2.30	0.64
2:N:528:ASN:O	9:V:24:ASN:ND2	2.27	0.64
5:Q:163:TRP:CG	5:Q:164:ARG:H	2.16	0.63
5:E:217:ILE:HB	3:O:269:THR:HG21	1.79	0.63
5:E:198:ARG:NH1	5:E:240:SER:O	2.31	0.63
2:B:153:ARG:NH2	2:B:198:ASP:OD2	2.30	0.63
12:N:602:CDL:HA21	12:N:602:CDL:CA3	2.28	0.63
5:E:184:VAL:HG21	5:E:244:ARG:HH22	1.62	0.63
1:A:302:ARG:NH2	1:A:503:PRO:O	2.31	0.63
12:P:404:CDL:HB32	7:S:51:LYS:HD3	1.80	0.63
1:A:237:SER:HB2	1:M:311:LEU:HG	1.81	0.62
2:B:433:VAL:HG12	2:B:492:LYS:HE3	1.79	0.62
3:O:315:MET:HB2	3:O:374:GLY:HA2	1.81	0.62
4:D:111:LEU:HA	4:D:156:ARG:HH21	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Q:173:ARG:HB3	5:Q:177:ASP:HB3	1.80	0.62
1:M:158:ARG:NH2	1:M:217:GLU:OE1	2.32	0.62
2:B:151:GLU:HB3	2:B:204:ARG:HD3	1.81	0.62
2:N:191:LYS:O	2:N:195:ILE:HG12	2.00	0.62
5:Q:181:ALA:O	5:Q:242:ARG:NH2	2.33	0.62
4:D:200:TYR:HD2	4:D:228:LYS:HB2	1.65	0.61
1:M:403:LYS:O	1:M:407:ILE:HG13	2.00	0.61
2:N:221:MET:HE1	2:N:254:ALA:HB2	1.82	0.61
2:B:416:ASP:OD2	3:C:10:LYS:NZ	2.32	0.61
3:C:314:SER:HA	3:C:378:ARG:HH21	1.65	0.61
1:M:220:HIS:NE2	1:M:384:TYR:OH	2.27	0.61
5:Q:117:PHE:CE1	9:V:31:VAL:HA	2.35	0.61
1:A:484:GLN:HE22	1:A:513:ARG:HH12	1.49	0.61
2:B:286:VAL:HB	2:B:291:ILE:HD11	1.83	0.61
2:B:106:ARG:NH2	2:B:276:PRO:O	2.34	0.61
4:P:201:ARG:HD3	8:T:74:TRP:CE2	2.36	0.61
5:Q:190:ARG:NH2	5:Q:246:GLY:O	2.34	0.61
8:H:40:PRO:HA	8:H:43:VAL:HG23	1.83	0.60
5:Q:198:ARG:NH1	5:Q:240:SER:O	2.29	0.60
4:P:116:ASP:OD2	4:P:258:TRP:HH2	1.82	0.60
14:O:403:HEM:HBB2	14:O:403:HEM:HMB1	1.83	0.60
4:P:97:GLN:NE2	4:P:236:GLU:O	2.34	0.60
1:A:91:LEU:HD22	1:A:262:LEU:HD12	1.84	0.60
12:N:602:CDL:H752	12:N:602:CDL:H712	1.82	0.60
14:C:404:HEM:HBC2	14:C:404:HEM:HMC2	1.84	0.60
2:N:350:ASP:OD2	2:N:497:ARG:NH1	2.34	0.60
7:S:84:GLU:HG2	7:S:88:HIS:CE1	2.37	0.60
5:Q:169:PHE:HZ	5:Q:218:PRO:HD2	1.65	0.60
3:O:157:ALA:HB2	3:O:292:LYS:HE2	1.84	0.59
3:O:314:SER:C	3:O:378:ARG:HH12	2.09	0.59
4:D:284:GLN:HE21	5:E:112:LEU:HA	1.68	0.59
4:P:164:GLU:OE2	4:P:168:ARG:NE	2.35	0.59
3:O:143:MET:HA	3:O:143:MET:HE2	1.85	0.59
14:C:403:HEM:HMC1	14:C:403:HEM:HBC2	1.84	0.59
5:E:235:SER:OG	16:E:301:FES:S2	2.52	0.59
12:N:602:CDL:H151	12:O:402:CDL:OA7	2.03	0.59
4:P:86:SER:OG	9:V:54:ASN:ND2	2.36	0.59
3:C:32:TYR:CD2	12:C:408:CDL:H312	2.37	0.59
4:D:228:LYS:NZ	4:D:230:LEU:O	2.33	0.59
3:C:112:SER:O	3:C:318:ARG:NH2	2.33	0.58
4:D:190:GLN:OE1	4:D:257:SER:OG	2.20	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:229:MET:HE1	15:P:403:HEC:C2C	2.34	0.58
1:M:476:LEU:HD23	1:M:479:ILE:HD11	1.85	0.58
14:O:404:HEM:HMC2	14:O:404:HEM:HBC2	1.84	0.58
3:C:32:TYR:CB	12:C:408:CDL:H331	2.32	0.58
3:C:154:LEU:HD21	3:C:286:LEU:HD11	1.85	0.58
5:Q:172:ARG:HA	5:Q:204:TRP:HA	1.86	0.58
2:N:209:ARG:HH12	2:N:212:ARG:HH21	1.49	0.58
8:T:56:ILE:HD11	8:T:64:LYS:HB3	1.86	0.58
5:E:117:PHE:CE1	9:J:31:VAL:HA	2.38	0.58
2:B:308:THR:HG23	2:B:310:SER:H	1.69	0.58
14:C:403:HEM:HBB2	14:C:403:HEM:HMB1	1.85	0.57
2:N:528:ASN:N	12:N:602:CDL:OB3	2.36	0.57
8:T:44:LYS:O	8:T:47:LEU:HG	2.04	0.57
4:D:227:PRO:O	4:D:229:MET:HE3	2.03	0.57
3:C:46:ILE:HD11	12:D:401:CDL:H201	1.84	0.57
2:N:221:MET:O	2:N:224:VAL:HG12	2.04	0.57
9:J:62:ILE:HG13	9:J:65:LEU:HB2	1.86	0.57
1:M:304:HIS:CE1	1:M:498:ASP:HA	2.40	0.57
5:Q:236:HIS:N	5:Q:245:LYS:O	2.38	0.57
2:B:148:LYS:HZ1	2:B:205:PHE:HA	1.69	0.57
2:B:274:THR:HG22	2:B:276:PRO:HD2	1.85	0.57
2:B:202:ASN:OD1	2:B:301:LYS:NZ	2.33	0.57
4:D:228:LYS:NZ	4:D:231:ASN:OD1	2.37	0.57
1:M:170:THR:HG23	2:N:90:ILE:HD13	1.86	0.57
5:E:190:ARG:NH1	5:E:246:GLY:O	2.37	0.57
5:Q:90:ASP:OD2	6:R:76:LYS:NZ	2.28	0.57
3:C:373:PRO:HA	3:C:376:VAL:HG12	1.87	0.56
7:G:79:ASN:O	7:G:83:LYS:HG2	2.05	0.56
4:P:138:ASP:OD1	4:P:139:GLY:N	2.38	0.56
1:M:107:VAL:HG12	1:M:109:CYS:H	1.71	0.56
4:D:84:LEU:O	9:J:53:ASN:ND2	2.38	0.56
4:D:138:ASP:OD1	4:D:139:GLY:N	2.39	0.56
2:N:209:ARG:NH1	2:N:212:ARG:HH21	2.04	0.56
1:A:143:ARG:NH1	2:B:375:GLY:HA2	2.20	0.56
2:N:128:SER:HB3	2:N:175:ARG:HA	1.87	0.56
5:Q:213:HIS:NE2	5:Q:247:PRO:HG2	2.21	0.56
8:T:46:LEU:O	8:T:50:GLN:HG3	2.04	0.56
2:B:199:ILE:HG13	2:B:200:LEU:HD12	1.88	0.55
6:R:120:ARG:HG2	6:R:121:THR:N	2.21	0.55
1:A:401:VAL:O	1:A:405:ILE:HD12	2.06	0.55
3:C:292:LYS:HD3	5:Q:213:HIS:NE2	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:198:THR:OG1	8:H:31:LYS:NZ	2.36	0.55
1:M:467:PHE:O	1:M:471:VAL:HG23	2.07	0.55
1:M:341:GLN:NE2	1:M:379:ALA:O	2.39	0.55
5:E:217:ILE:HB	3:O:269:THR:CG2	2.36	0.55
4:P:200:TYR:HE1	4:P:216:ASN:HD22	1.53	0.55
8:T:77:ILE:O	8:T:81:VAL:HG23	2.07	0.55
1:M:91:LEU:HD22	1:M:262:LEU:HD12	1.89	0.55
5:E:206:ILE:HD11	5:E:265:LEU:HD23	1.87	0.55
1:M:302:ARG:HG3	1:M:499:VAL:HG11	1.88	0.55
12:N:602:CDL:CA3	12:N:602:CDL:CA2	2.85	0.55
6:R:14:LYS:CE	6:R:14:LYS:CA	2.85	0.55
6:R:47:ASP:OD2	6:R:103:LYS:NZ	2.40	0.54
2:B:148:LYS:NZ	2:B:205:PHE:HA	2.22	0.54
2:B:151:GLU:HB3	2:B:204:ARG:HH11	1.73	0.54
4:D:210:ARG:HG3	4:D:213:LEU:HD13	1.89	0.54
5:E:203:GLU:HG3	5:E:204:TRP:CD1	2.43	0.54
4:P:274:TRP:CE2	5:Q:125:LEU:HD22	2.42	0.54
3:C:60:PRO:HD2	3:O:60:PRO:HD2	1.90	0.54
3:O:218:SER:HA	6:R:71:MET:HE1	1.90	0.54
3:C:56:MET:HG2	3:O:182:ARG:HA	1.90	0.54
1:M:273:LEU:O	1:M:277:GLU:HG2	2.08	0.54
6:F:101:LEU:O	6:F:105:GLU:HG3	2.08	0.54
6:R:17:PHE:C	6:R:19:ALA:N	2.65	0.54
1:M:493:MET:HE1	1:M:508:VAL:HG21	1.90	0.54
3:O:81:LEU:HG	3:O:85:MET:HE2	1.91	0.53
5:E:147:GLU:HB2	5:E:267:ILE:HB	1.89	0.53
2:B:501:ASP:OD2	9:J:17:TYR:OH	2.22	0.53
5:E:149:ASP:HB2	5:E:264:LYS:HE3	1.91	0.53
5:E:163:TRP:CD1	5:E:164:ARG:H	2.26	0.53
2:N:155:ALA:HA	2:N:158:LEU:HD12	1.89	0.53
2:B:199:ILE:O	2:B:203:SER:OG	2.27	0.53
1:M:375:HIS:HB2	1:M:395:THR:HG23	1.91	0.53
2:N:432:ARG:NH2	2:N:530:TYR:OH	2.29	0.53
2:N:496:ASN:OD1	9:V:22:ARG:NH2	2.41	0.53
3:O:246:ILE:HG21	13:P:402:3PE:H372	1.91	0.53
5:Q:153:ILE:HG23	5:Q:172:ARG:HD3	1.91	0.53
1:M:356:GLY:HA3	2:N:168:HIS:HB3	1.90	0.52
2:B:213:GLU:HA	2:B:216:VAL:HG12	1.90	0.52
2:B:289:GLU:CD	2:B:289:GLU:H	2.18	0.52
5:E:260:LEU:HB2	5:E:264:LYS:HB2	1.91	0.52
4:P:86:SER:HB3	9:V:50:TRP:CZ2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Q:169:PHE:CZ	5:Q:218:PRO:HD2	2.44	0.52
3:C:182:ARG:HA	3:O:56:MET:HG3	1.90	0.52
4:D:123:THR:HG22	4:D:126:GLU:HG3	1.91	0.52
3:O:289:ILE:HD12	3:O:298:ALA:HB2	1.90	0.52
3:C:135:GLY:HA3	3:C:187:HIS:CE1	2.44	0.52
3:O:285:ILE:HG13	3:O:340:LEU:HD21	1.91	0.52
3:O:370:THR:O	3:O:373:PRO:HD2	2.10	0.52
4:P:218:TYR:OH	8:T:78:ASP:OD2	2.28	0.52
6:R:98:MET:O	6:R:102:VAL:HG23	2.10	0.52
3:C:146:TRP:O	3:C:150:VAL:HG23	2.10	0.52
1:M:291:GLU:HG2	1:M:292:PRO:HD2	1.91	0.52
2:N:227:GLN:OE1	2:N:227:GLN:N	2.43	0.52
2:N:228:THR:HA	2:N:231:VAL:HB	1.92	0.52
2:B:111:SER:OG	2:B:286:VAL:O	2.23	0.52
2:B:148:LYS:HE2	2:B:209:ARG:HG2	1.91	0.52
12:N:602:CDL:HA21	12:N:602:CDL:HA32	1.91	0.52
4:P:109:MET:O	4:P:180:SER:OG	2.27	0.52
2:N:416:ASP:OD1	2:N:417:ASP:N	2.43	0.51
4:P:200:TYR:CD2	4:P:228:LYS:HB2	2.45	0.51
4:D:201:ARG:HD3	8:H:74:TRP:CZ2	2.45	0.51
5:Q:156:GLY:N	5:Q:172:ARG:O	2.44	0.51
8:T:50:GLN:HA	8:T:53:VAL:HG12	1.91	0.51
5:E:161:VAL:HG22	5:E:168:VAL:HB	1.91	0.51
2:N:201:GLN:HE22	2:N:300:THR:H	1.59	0.51
2:N:224:VAL:HA	2:N:227:GLN:HE22	1.76	0.51
5:Q:161:VAL:HG12	5:Q:162:LYS:N	2.24	0.51
1:A:158:ARG:NH2	1:A:217:GLU:OE1	2.44	0.51
1:M:422:ASP:OD1	1:M:423:GLN:N	2.43	0.51
3:O:75:ASP:O	5:Q:137:SER:OG	2.29	0.51
4:P:209:ILE:HD11	4:P:215:TYR:HD1	1.74	0.51
6:R:14:LYS:CE	6:R:14:LYS:N	2.73	0.51
1:A:307:SER:O	1:M:237:SER:N	2.44	0.51
3:C:280:LEU:HD13	3:C:345:CYS:HB2	1.93	0.51
1:M:377:ILE:HD12	1:M:394:VAL:HB	1.92	0.51
2:N:89:ARG:H	2:N:89:ARG:HD3	1.76	0.51
3:O:156:SER:HB3	3:O:166:VAL:HG21	1.93	0.51
2:B:191:LYS:O	2:B:195:ILE:HG12	2.11	0.51
1:A:316:THR:OG1	1:A:396:THR:O	2.27	0.51
3:C:81:LEU:HG	3:C:85:MET:HE3	1.92	0.51
1:A:332:LYS:NZ	1:A:473:GLU:OE1	2.44	0.50
4:D:304:ASP:OD2	5:E:74:PRO:HB3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:283:HIS:CD2	3:C:287:ARG:HE	2.28	0.50
2:B:125:ASP:O	2:B:277:ARG:NH2	2.43	0.50
1:M:314:GLN:O	1:M:398:SER:OG	2.29	0.50
4:P:93:ARG:HH22	9:V:65:LEU:HA	1.74	0.50
3:C:159:PRO:O	3:C:161:VAL:N	2.45	0.50
3:O:92:MET:HE1	3:O:243:PHE:HD2	1.76	0.50
4:D:307:ASN:O	6:F:66:ARG:NH1	2.42	0.50
6:F:68:LYS:HD3	7:G:26:MET:HE2	1.93	0.50
2:N:342:GLU:HG2	2:N:343:GLY:H	1.76	0.50
6:R:27:LYS:HE3	6:R:31:ARG:HH22	1.77	0.50
1:A:117:LEU:HG	1:A:118:THR:HG23	1.94	0.50
2:B:84:LEU:HD21	2:B:484:ASP:HB2	1.94	0.50
4:P:226:MET:HB3	15:P:403:HEC:C1D	2.42	0.50
3:C:88:ASN:O	3:C:92:MET:HG2	2.12	0.50
6:F:83:ASP:OD1	6:F:83:ASP:N	2.44	0.50
2:N:209:ARG:NH2	2:N:213:GLU:OE2	2.45	0.50
6:R:14:LYS:HE2	6:R:14:LYS:CA	2.41	0.50
1:M:401:VAL:O	1:M:405:ILE:HG12	2.12	0.49
2:N:124:ILE:HG12	2:N:278:MET:HG2	1.93	0.49
6:R:68:LYS:HD3	7:S:26:MET:HE2	1.94	0.49
2:N:434:SER:OG	2:N:435:ASP:N	2.41	0.49
3:O:228:TYR:O	4:P:293:TRP:NE1	2.39	0.49
1:A:363:LEU:HD12	1:A:377:ILE:HD12	1.94	0.49
4:D:145:GLU:C	4:D:146:MET:HE2	2.36	0.49
10:K:33:ILE:HG22	10:K:35:PRO:HD3	1.94	0.49
3:C:150:VAL:HG22	5:Q:216:CYS:SG	2.52	0.49
5:E:243:ILE:HD13	5:E:248:ALA:HB3	1.93	0.49
1:M:433:THR:O	1:M:437:ILE:HG12	2.12	0.49
4:P:200:TYR:HD2	4:P:228:LYS:HB2	1.77	0.49
3:C:309:LEU:HD21	3:C:367:PHE:HD1	1.77	0.49
5:Q:199:VAL:HG12	5:Q:205:LEU:HD12	1.94	0.49
1:A:431:GLN:NE2	2:B:165:MET:O	2.46	0.49
3:O:321:SER:O	6:R:28:ARG:NH1	2.45	0.49
5:Q:171:ARG:O	5:Q:205:LEU:N	2.44	0.49
2:N:241:PHE:O	2:N:244:THR:HG22	2.13	0.49
2:N:376:SER:O	2:N:380:GLN:HG3	2.12	0.49
1:A:324:LEU:HD11	1:A:486:LEU:HD12	1.94	0.49
3:C:221:ASP:HB3	6:F:71:MET:SD	2.53	0.49
1:A:215:LEU:O	1:A:219:ILE:HG12	2.13	0.49
1:A:403:LYS:O	1:A:407:ILE:HG12	2.13	0.49
3:C:267:MET:HB2	3:C:268:PRO:HD3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:62:LEU:HG	1:M:63:PRO:HD2	1.95	0.49
3:O:200:LEU:HG	13:O:401:3PE:H3A1	1.93	0.49
4:P:183:THR:O	4:P:189:GLY:HA3	2.13	0.49
2:N:186:ASP:OD1	2:N:186:ASP:N	2.45	0.48
6:R:14:LYS:CE	6:R:14:LYS:HA	2.40	0.48
4:D:226:MET:HB3	15:D:402:HEC:C1D	2.43	0.48
1:M:318:PHE:CE2	1:M:401:VAL:HG13	2.48	0.48
1:M:465:GLU:OE1	1:M:465:GLU:N	2.42	0.48
5:Q:213:HIS:HB2	5:Q:248:ALA:HB2	1.94	0.48
2:B:263:ASP:OD1	2:B:264:HIS:ND1	2.41	0.48
3:O:84:TYR:CE1	3:O:252:PRO:HB2	2.48	0.48
3:O:103:ARG:HH12	14:O:404:HEM:HBD2	1.78	0.48
3:O:135:GLY:O	3:O:138:PRO:HD2	2.14	0.48
3:O:137:VAL:HA	3:O:144:SER:HB3	1.96	0.48
3:O:221:ASP:HB3	6:R:71:MET:SD	2.53	0.48
14:O:404:HEM:HMB1	14:O:404:HEM:HBB2	1.95	0.48
5:Q:201:ASN:HD22	5:Q:204:TRP:HB2	1.77	0.48
1:A:170:THR:HG23	2:B:90:ILE:HD13	1.95	0.48
1:M:378:SER:O	1:M:392:ILE:HG13	2.14	0.48
5:Q:261:GLU:HG2	5:Q:262:GLU:H	1.78	0.48
1:M:85:LEU:HD13	1:M:89:ILE:HG23	1.95	0.48
3:O:135:GLY:HA3	3:O:187:HIS:CE1	2.48	0.48
1:A:114:GLU:HG2	1:A:119:PHE:HD1	1.78	0.48
5:Q:110:PHE:CZ	9:V:16:LEU:HD23	2.49	0.48
3:O:80:TRP:CZ3	4:P:267:ARG:HG3	2.49	0.48
3:O:384:TYR:CD1	6:R:12:PRO:HG3	2.48	0.48
6:F:73:LEU:HD11	6:F:80:LEU:HG	1.96	0.48
6:R:65:GLN:HA	7:S:26:MET:HE1	1.95	0.48
2:B:376:SER:O	2:B:380:GLN:HG3	2.13	0.48
5:E:211:CYS:HB3	16:E:301:FES:S1	2.54	0.48
2:N:63:LYS:O	2:N:66:GLN:HG3	2.14	0.48
2:N:201:GLN:NE2	2:N:300:THR:O	2.47	0.48
4:P:94:ARG:O	4:P:98:VAL:HG23	2.14	0.47
6:R:84:LEU:O	6:R:88:GLN:HG2	2.14	0.47
6:F:37:ASP:OD2	6:F:93:GLY:HA2	2.14	0.47
3:O:362:VAL:HG13	13:R:201:3PE:H2E2	1.97	0.47
5:Q:163:TRP:CG	5:Q:164:ARG:N	2.78	0.47
1:A:377:ILE:HG22	1:A:394:VAL:HG23	1.96	0.47
2:B:254:ALA:HA	2:B:257:ILE:HG22	1.96	0.47
2:N:357:MET:HA	2:N:360:MET:HG2	1.95	0.47
5:Q:211:CYS:HB2	5:Q:218:PRO:HD3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:256:ASN:O	2:B:256:ASN:ND2	2.47	0.47
3:C:246:ILE:HG21	13:C:406:3PE:H241	1.96	0.47
14:C:404:HEM:HMB1	14:C:404:HEM:HBB2	1.96	0.47
4:P:103:CYS:CB	15:P:403:HEC:HAB	2.44	0.47
1:A:483:SER:HA	1:A:486:LEU:HD13	1.97	0.47
3:C:315:MET:O	6:F:44:TYR:OH	2.29	0.47
4:D:94:ARG:O	4:D:98:VAL:HG23	2.15	0.47
2:N:209:ARG:NH2	2:N:212:ARG:HE	2.12	0.47
2:N:389:GLU:HB2	2:N:409:VAL:HG13	1.95	0.47
3:O:31:SER:HG	3:O:34:TRP:HZ3	1.62	0.47
6:R:15:ASN:CG	6:R:16:TRP:N	2.73	0.47
1:A:105:LEU:HD23	1:A:183:VAL:HG21	1.97	0.47
3:C:74:ARG:NH2	4:D:259:ALA:O	2.47	0.47
2:N:159:GLU:HA	2:N:162:ILE:HG12	1.95	0.47
1:A:105:LEU:HD11	1:A:260:ILE:HG23	1.97	0.47
2:B:290:ASP:O	2:B:293:GLU:HG3	2.14	0.47
2:N:294:GLN:HB2	2:N:298:LEU:HD13	1.96	0.47
4:P:200:TYR:OH	4:P:226:MET:HG3	2.15	0.47
5:Q:238:ASP:OD1	5:Q:242:ARG:N	2.48	0.47
2:B:237:HIS:NE2	2:B:398:TYR:OH	2.44	0.47
3:C:156:SER:HB3	3:C:166:VAL:HG21	1.96	0.47
12:C:408:CDL:H132	12:C:408:CDL:H162	1.62	0.47
4:D:109:MET:O	4:D:180:SER:OG	2.33	0.47
5:E:198:ARG:HH12	5:E:240:SER:C	2.23	0.47
2:B:262:LYS:HA	2:B:265:LEU:HD13	1.96	0.46
5:Q:213:HIS:ND1	5:Q:235:SER:OG	2.49	0.46
7:G:82:GLU:OE2	7:G:83:LYS:CE	2.61	0.46
3:C:286:LEU:HD13	3:C:299:ILE:HD11	1.98	0.46
3:O:340:LEU:HD13	3:O:359:PRO:HB2	1.98	0.46
12:O:402:CDL:H532	12:O:402:CDL:H561	1.65	0.46
5:Q:169:PHE:HB2	5:Q:207:VAL:HG23	1.96	0.46
12:N:602:CDL:H582	12:O:402:CDL:H722	1.97	0.46
3:O:66:PHE:O	3:O:70:GLU:HG2	2.15	0.46
3:O:85:MET:HG2	3:O:248:ILE:HD13	1.98	0.46
2:B:68:GLU:HG3	2:B:69:ASN:N	2.30	0.46
2:B:205:PHE:HB2	2:B:262:LYS:HG3	1.97	0.46
4:P:152:LYS:HE3	5:Q:146:LEU:HD21	1.97	0.46
4:P:277:VAL:HG12	5:Q:118:VAL:HG13	1.98	0.46
5:Q:153:ILE:HD13	5:Q:159:VAL:HG23	1.98	0.46
5:Q:229:PHE:HD1	5:Q:236:HIS:HA	1.80	0.46
5:Q:243:ILE:HG12	5:Q:248:ALA:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:374:MET:O	2:B:374:MET:HG2	2.16	0.46
1:A:302:ARG:HB3	1:A:499:VAL:HG11	1.97	0.46
2:B:208:ASN:OD1	2:B:209:ARG:N	2.48	0.46
5:E:261:GLU:HG2	5:E:262:GLU:N	2.31	0.46
6:R:118:TYR:O	6:R:118:TYR:CD2	2.69	0.46
1:M:305:THR:HG23	1:M:497:GLY:HA2	1.97	0.46
5:Q:235:SER:OG	16:Q:301:FES:S2	2.70	0.46
2:N:329:ASP:HA	7:S:27:LYS:HD2	1.98	0.45
3:C:370:THR:OG1	3:C:371:PRO:HD3	2.16	0.45
1:M:506:GLU:HG3	1:M:507:SER:N	2.30	0.45
3:C:341:GLY:HA3	13:C:405:3PE:H342	1.98	0.45
13:C:405:3PE:H232	13:C:405:3PE:H262	1.79	0.45
13:R:201:3PE:H392	13:R:201:3PE:H362	1.64	0.45
8:T:44:LYS:O	8:T:48:GLU:OE1	2.34	0.45
2:B:508:ALA:HB1	2:B:512:ILE:HG21	1.99	0.45
1:A:356:GLY:HA3	2:B:168:HIS:HB3	1.99	0.45
2:N:123:TRP:CZ2	2:N:461:GLU:HA	2.51	0.45
2:N:291:ILE:O	2:N:295:VAL:HG23	2.16	0.45
8:T:29:ASP:OD2	8:T:31:LYS:HB3	2.17	0.45
13:C:405:3PE:H2	13:C:405:3PE:H221	1.72	0.45
5:E:207:VAL:HG21	5:E:252:LEU:HB3	1.99	0.45
1:M:84:THR:HG22	1:M:90:LYS:HG2	1.97	0.45
1:M:315:ARG:HB2	1:M:317:HIS:CE1	2.51	0.45
3:O:146:TRP:CH2	3:O:269:THR:HG22	2.51	0.45
6:R:89:THR:O	6:R:89:THR:HG23	2.17	0.45
6:F:98:MET:O	6:F:102:VAL:HG23	2.16	0.45
9:V:15:ALA:O	9:V:18:LYS:HG2	2.17	0.45
5:Q:166:LYS:NZ	5:Q:210:VAL:HG21	2.32	0.45
7:S:50:THR:O	7:S:54:HIS:ND1	2.48	0.45
12:C:408:CDL:C11	4:D:289:ARG:HH11	2.28	0.45
8:H:69:GLN:OE1	8:H:69:GLN:N	2.47	0.45
1:M:304:HIS:HE1	1:M:498:ASP:HA	1.81	0.45
1:A:140:ARG:HG3	2:B:80:PRO:HG3	1.98	0.44
2:B:357:MET:HA	2:B:360:MET:HG2	1.99	0.44
3:C:348:VAL:O	3:C:348:VAL:HG13	2.17	0.44
5:E:206:ILE:HB	5:E:257:TYR:CZ	2.51	0.44
12:N:602:CDL:H712	12:N:602:CDL:C75	2.43	0.44
1:A:484:GLN:OE1	1:A:513:ARG:NH2	2.26	0.44
2:B:380:GLN:HE22	6:R:114:GLY:HA2	1.82	0.44
2:B:474:ILE:HG23	2:B:478:GLU:OE1	2.17	0.44
5:E:195:ASP:O	5:E:199:VAL:HG22	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:242:GLN:HA	5:Q:85:SER:HB2	1.98	0.44
1:A:111:SER:HB3	1:A:158:ARG:HA	1.99	0.44
4:D:111:LEU:HA	4:D:156:ARG:NH2	2.31	0.44
10:K:30:LEU:HD23	10:K:30:LEU:HA	1.86	0.44
4:P:271:GLY:O	4:P:275:ILE:HG12	2.17	0.44
2:B:388:ALA:HB2	2:B:418:LEU:HD13	1.98	0.44
3:O:288:SER:OG	3:O:357:GLN:HA	2.18	0.44
4:P:290:ARG:HH12	7:S:44:LEU:HD21	1.82	0.44
5:Q:134:MET:HE2	5:Q:134:MET:HB3	1.85	0.44
6:R:16:TRP:O	6:R:16:TRP:CD2	2.70	0.44
3:C:138:PRO:N	3:C:139:PRO:HD2	2.33	0.44
1:M:409:VAL:HG13	1:M:512:PHE:HE1	1.82	0.44
2:N:374:MET:O	2:N:374:MET:HG2	2.18	0.44
2:N:529:ARG:NH2	12:N:602:CDL:OB4	2.51	0.44
4:P:116:ASP:OD2	4:P:258:TRP:CZ2	2.71	0.44
5:Q:177:ASP:OD2	5:Q:239:ILE:HG21	2.17	0.44
2:B:517:ASP:OD2	3:C:228:TYR:OH	2.28	0.44
1:M:127:ARG:NH2	1:M:203:GLU:OE1	2.51	0.44
12:P:404:CDL:H552	7:S:44:LEU:HD13	1.98	0.44
2:B:384:ILE:CD1	6:R:117:LEU:HD23	2.47	0.44
5:E:163:TRP:CG	5:E:164:ARG:N	2.82	0.44
1:A:380:PHE:HE2	1:A:393:GLN:HB2	1.82	0.44
1:A:507:SER:O	1:A:511:LYS:NZ	2.37	0.44
1:M:267:VAL:HG11	1:M:272:LEU:HB2	2.00	0.44
1:M:483:SER:O	1:M:487:ILE:HG12	2.18	0.44
3:C:135:GLY:O	3:C:138:PRO:HD2	2.18	0.43
3:C:154:LEU:CD2	3:C:286:LEU:HD21	2.48	0.43
2:N:300:THR:HG23	2:N:301:LYS:HG3	1.99	0.43
5:E:184:VAL:HG21	5:E:244:ARG:NH2	2.30	0.43
6:F:21:HIS:O	6:F:25:ILE:HG12	2.18	0.43
1:M:124:LEU:HD11	1:M:197:LEU:HD21	1.99	0.43
4:P:130:MET:HG3	9:V:68:ARG:NH2	2.32	0.43
5:Q:238:ASP:OD1	5:Q:241:GLY:N	2.51	0.43
2:N:91:LEU:HD22	2:N:476:PHE:HB3	2.00	0.43
3:O:140:TRP:CE3	3:O:180:LEU:HD13	2.53	0.43
4:P:203:PRO:HB3	4:P:209:ILE:HD11	1.99	0.43
6:R:101:LEU:HD12	6:R:104:ARG:HH21	1.82	0.43
2:B:44:SER:N	2:B:45:PRO:HD2	2.33	0.43
2:B:76:LYS:HE3	2:B:76:LYS:HB2	1.85	0.43
2:B:305:ASP:OD1	2:B:307:THR:OG1	2.26	0.43
5:E:124:ARG:HD3	9:J:36:PHE:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:194:GLN:HA	5:E:242:ARG:NH1	2.34	0.43
1:M:59:ASP:OD1	1:M:59:ASP:N	2.45	0.43
3:O:50:THR:OG1	3:O:86:HIS:ND1	2.37	0.43
6:R:45:ASP:O	6:R:46:LEU:HB2	2.17	0.43
7:S:84:GLU:HG2	7:S:88:HIS:HE1	1.82	0.43
3:C:32:TYR:HB2	12:C:408:CDL:C33	2.47	0.43
3:C:316:TYR:OH	6:F:45:ASP:OD2	2.29	0.43
8:H:53:VAL:HA	8:H:56:ILE:HG22	2.00	0.43
2:N:145:MET:SD	2:N:213:GLU:HG3	2.59	0.43
4:P:198:THR:HG21	8:T:31:LYS:HD3	2.00	0.43
5:Q:198:ARG:HH21	5:Q:251:ASN:HB3	1.83	0.43
9:V:19:VAL:HG12	9:V:20:LEU:HD12	1.99	0.43
1:A:408:THR:O	1:A:412:LEU:HD23	2.19	0.43
4:D:66:GLU:OE1	4:D:66:GLU:N	2.51	0.43
2:N:120:VAL:HG11	2:N:193:LEU:HD13	2.00	0.43
3:O:146:TRP:HB3	3:O:273:ILE:HD12	2.01	0.43
5:Q:214:LEU:HD23	5:Q:214:LEU:HA	1.72	0.43
1:A:370:GLU:HG2	1:A:371:TYR:CE2	2.53	0.43
2:B:123:TRP:CZ2	2:B:461:GLU:HA	2.54	0.43
2:B:165:MET:HE2	2:B:191:LYS:HE2	1.99	0.43
3:C:80:TRP:CZ3	4:D:267:ARG:HG3	2.54	0.43
2:N:56:LEU:O	2:N:60:VAL:HG23	2.18	0.43
3:O:1:MET:HG2	3:O:2:ARG:H	1.83	0.43
4:P:209:ILE:HD11	4:P:215:TYR:CD1	2.53	0.43
2:B:142:LEU:HD22	2:B:268:TYR:HD2	1.84	0.43
5:E:150:LEU:HB2	5:E:265:LEU:O	2.19	0.43
5:E:222:ALA:HB3	5:E:229:PHE:HB3	2.00	0.43
3:O:202:LEU:HD12	3:O:202:LEU:HA	1.82	0.43
4:P:303:LEU:HD23	4:P:303:LEU:HA	1.86	0.43
5:Q:218:PRO:HB3	5:Q:230:CYS:HB2	2.01	0.43
1:A:480:ALA:O	1:A:484:GLN:HG2	2.18	0.43
2:B:148:LYS:CD	2:B:209:ARG:HG2	2.49	0.43
2:B:254:ALA:O	2:B:257:ILE:HG22	2.18	0.43
2:B:266:GLN:O	2:B:270:GLN:HG2	2.19	0.43
2:N:86:ASP:O	2:N:89:ARG:NH2	2.52	0.43
2:N:131:GLU:N	2:N:131:GLU:OE1	2.52	0.43
4:P:164:GLU:HG2	4:P:175:TYR:CE1	2.53	0.43
1:A:399:ASP:OD1	1:A:399:ASP:N	2.50	0.43
3:C:18:ASN:ND2	3:C:18:ASN:C	2.77	0.43
3:C:292:LYS:NZ	5:Q:213:HIS:O	2.51	0.43
3:O:159:PRO:O	3:O:161:VAL:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:177:ASP:OD1	5:E:239:ILE:HG21	2.19	0.42
5:E:210:VAL:CG1	5:E:215:GLY:HA2	2.47	0.42
1:M:337:LEU:HD22	1:M:383:ILE:HD11	2.00	0.42
3:O:314:SER:HB3	3:O:315:MET:H	1.70	0.42
4:P:212:GLY:O	4:P:213:LEU:HD23	2.19	0.42
17:P:401:PC1:H152	17:P:401:PC1:H112	1.77	0.42
5:Q:161:VAL:CG1	5:Q:162:LYS:H	2.30	0.42
5:Q:206:ILE:HB	5:Q:257:TYR:CE2	2.54	0.42
13:R:201:3PE:H232	13:R:201:3PE:H261	1.81	0.42
2:N:472:ARG:HH22	2:N:478:GLU:CD	2.26	0.42
13:C:402:3PE:H2E1	13:C:402:3PE:H2H2	1.69	0.42
5:E:129:LYS:HA	5:E:129:LYS:HD3	1.75	0.42
2:N:290:ASP:O	2:N:294:GLN:OE1	2.38	0.42
3:O:138:PRO:N	3:O:139:PRO:HD2	2.35	0.42
5:Q:153:ILE:O	5:Q:172:ARG:NH1	2.53	0.42
1:A:114:GLU:HG2	1:A:119:PHE:CD1	2.54	0.42
2:B:135:SER:HB2	2:B:138:THR:OG1	2.19	0.42
2:B:219:ARG:HE	2:B:219:ARG:HB3	1.76	0.42
3:C:287:ARG:HG2	5:Q:233:HIS:CD2	2.54	0.42
4:D:301:LEU:HB3	7:G:30:THR:HG22	2.01	0.42
7:G:90:TYR:OXT	8:H:55:ARG:NE	2.52	0.42
1:M:224:TYR:HE2	1:M:389:ILE:HD11	1.83	0.42
1:M:438:LEU:HD23	1:M:438:LEU:HA	1.81	0.42
2:N:184:VAL:HG22	2:N:185:ALA:H	1.83	0.42
2:B:184:VAL:HG11	2:B:192:ALA:HB2	2.02	0.42
2:B:354:LEU:HD23	2:B:354:LEU:HA	1.82	0.42
2:B:385:ASN:HB2	2:B:387:VAL:HG23	2.01	0.42
3:C:33:TRP:HB3	3:C:103:ARG:HG3	2.02	0.42
1:M:111:SER:HB3	1:M:158:ARG:HA	2.01	0.42
2:N:524:ARG:HD3	2:N:524:ARG:HA	1.84	0.42
12:O:405:CDL:H162	12:O:405:CDL:H131	1.89	0.42
1:A:117:LEU:H	1:A:117:LEU:HD23	1.84	0.42
2:B:490:THR:O	2:B:494:VAL:HG23	2.19	0.42
5:E:208:ILE:H	5:E:255:PRO:HD3	1.84	0.42
8:H:51:ALA:O	8:H:54:LYS:HG2	2.20	0.42
1:M:444:ARG:HH12	2:N:454:ASP:HB2	1.85	0.42
1:M:456:LEU:HD23	1:M:456:LEU:HA	1.91	0.42
4:P:229:MET:HE2	4:P:229:MET:HB3	1.86	0.42
1:A:171:HIS:O	1:A:175:MET:HG3	2.20	0.42
4:D:212:GLY:C	4:D:213:LEU:HD12	2.45	0.42
5:E:189:LEU:HD13	5:E:242:ARG:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:212:THR:HG21	5:E:251:ASN:O	2.20	0.42
1:M:235:SER:O	1:M:239:LEU:HG	2.19	0.42
1:M:447:VAL:O	1:M:451:ILE:HG13	2.20	0.42
12:O:402:CDL:H152	12:O:402:CDL:H122	1.74	0.42
6:R:16:TRP:O	6:R:16:TRP:CG	2.72	0.42
3:C:384:TYR:CE1	6:F:12:PRO:HG3	2.55	0.42
4:D:200:TYR:OH	4:D:226:MET:HG3	2.19	0.42
4:D:200:TYR:CD2	4:D:228:LYS:HB2	2.49	0.42
1:A:307:SER:CB	1:M:235:SER:HB2	2.50	0.42
1:A:371:TYR:HB2	1:A:374:PHE:CE2	2.54	0.42
2:B:387:VAL:HG13	2:B:414:CYS:HB3	2.01	0.42
4:D:89:HIS:ND1	4:D:120:VAL:O	2.52	0.42
2:N:209:ARG:HE	2:N:213:GLU:HG2	1.85	0.42
3:O:231:VAL:O	3:O:235:VAL:HG23	2.20	0.42
5:Q:208:ILE:HD12	5:Q:253:GLU:HG2	2.01	0.42
9:V:32:ILE:HD13	10:W:28:GLY:HA2	2.02	0.42
4:D:106:CYS:SG	4:D:107:HIS:N	2.92	0.42
2:N:354:LEU:HD23	2:N:354:LEU:HA	1.85	0.42
2:B:449:LEU:HD23	2:B:449:LEU:HA	1.87	0.41
7:G:41:MET:O	7:G:43:GLY:N	2.53	0.41
8:H:46:LEU:HD13	8:H:73:TYR:CZ	2.55	0.41
1:M:296:TYR:CD2	1:M:323:GLU:HG2	2.55	0.41
2:N:256:ASN:O	2:N:256:ASN:ND2	2.52	0.41
3:O:219:GLU:HG3	7:S:21:LYS:HA	2.01	0.41
3:O:313:LYS:HD2	3:O:313:LYS:HA	1.85	0.41
3:O:338:LEU:HD23	12:O:405:CDL:H181	2.02	0.41
4:P:109:MET:C	4:P:111:LEU:H	2.28	0.41
1:A:196:GLN:O	1:A:200:VAL:HG13	2.20	0.41
3:C:111:SER:HB3	3:C:315:MET:HE3	2.03	0.41
13:C:402:3PE:H241	6:F:123:PRO:HD2	2.01	0.41
1:M:107:VAL:HG22	1:M:260:ILE:HG12	2.02	0.41
2:N:124:ILE:HG21	2:N:273:TYR:CE1	2.55	0.41
5:Q:162:LYS:HD3	5:Q:163:TRP:O	2.20	0.41
5:Q:195:ASP:O	5:Q:199:VAL:N	2.28	0.41
5:Q:195:ASP:HA	5:Q:198:ARG:HD3	2.02	0.41
9:V:47:HIS:O	9:V:51:GLU:OE1	2.38	0.41
2:B:47:PRO:HG2	2:B:50:ALA:HB2	2.02	0.41
6:F:50:GLU:HG3	6:F:118:TYR:CE2	2.56	0.41
2:B:145:MET:HE1	2:B:210:ILE:HA	2.03	0.41
3:C:153:SER:OG	5:Q:214:LEU:O	2.25	0.41
5:E:201:ASN:OD1	5:E:202:PRO:HD2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:45:ASP:HB3	6:F:48:VAL:HG23	2.01	0.41
3:O:15:SER:O	3:O:19:GLN:HG2	2.20	0.41
4:P:74:PRO:HG3	8:T:78:ASP:HB3	2.03	0.41
8:T:37:SER:O	8:T:40:PRO:HD2	2.19	0.41
2:B:263:ASP:OD1	2:B:264:HIS:N	2.53	0.41
3:C:2:ARG:O	3:C:4:GLN:N	2.53	0.41
13:C:402:3PE:H292	13:C:402:3PE:H262	1.90	0.41
5:Q:219:LEU:N	5:Q:229:PHE:O	2.54	0.41
8:T:46:LEU:HB2	8:T:73:TYR:CE1	2.55	0.41
4:D:234:ALA:HB3	4:D:248:MET:HE1	2.03	0.41
5:E:172:ARG:HA	5:E:203:GLU:O	2.21	0.41
5:E:233:HIS:CD2	3:O:287:ARG:HG2	2.56	0.41
3:O:280:LEU:HD12	12:O:405:CDL:H112	2.03	0.41
1:A:124:LEU:HD23	1:A:124:LEU:HA	1.90	0.41
1:A:226:GLY:HA3	1:A:294:SER:HA	2.03	0.41
12:C:408:CDL:H151	12:C:408:CDL:H181	1.90	0.41
9:J:21:MET:O	9:J:21:MET:HG2	2.21	0.41
3:O:370:THR:C	3:O:373:PRO:HD2	2.46	0.41
4:P:300:LYS:HD3	5:Q:88:VAL:O	2.20	0.41
5:Q:201:ASN:HB3	5:Q:204:TRP:H	1.86	0.41
2:B:148:LYS:CE	2:B:209:ARG:HG2	2.50	0.41
4:D:274:TRP:CE2	5:E:125:LEU:HD22	2.56	0.41
1:M:336:VAL:HG11	1:M:482:ILE:HG13	2.02	0.41
1:M:367:VAL:HG12	1:M:368:LEU:HD22	2.03	0.41
2:N:129:ARG:NH1	2:N:246:LEU:HD11	2.35	0.41
2:N:256:ASN:C	2:N:256:ASN:HD22	2.28	0.41
9:V:62:ILE:HG13	9:V:65:LEU:HB3	2.03	0.41
1:A:107:VAL:HA	1:A:259:ARG:O	2.21	0.41
2:B:150:THR:O	2:B:153:ARG:N	2.36	0.41
2:B:528:ASN:O	9:J:24:ASN:ND2	2.54	0.41
12:D:401:CDL:HA21	12:D:401:CDL:HB32	2.03	0.41
6:F:27:LYS:O	6:F:31:ARG:HG3	2.20	0.41
1:M:276:ALA:HB1	1:M:280:LEU:HD12	2.02	0.41
5:Q:213:HIS:HE1	5:Q:233:HIS:HB2	1.85	0.41
6:R:14:LYS:HE3	6:R:14:LYS:N	2.32	0.41
6:R:118:TYR:O	6:R:118:TYR:HD2	2.04	0.41
5:E:221:ASN:N	5:E:227:GLY:O	2.53	0.41
9:J:22:ARG:CG	9:J:23:ARG:HH21	2.30	0.41
1:M:135:ASN:OD1	2:N:71:ASP:N	2.46	0.41
7:S:47:ASP:O	7:S:50:THR:HG22	2.20	0.41
2:B:429:LEU:HD23	2:B:429:LEU:HA	1.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:380:PHE:HE2	1:M:393:GLN:HB2	1.86	0.40
2:N:184:VAL:HG22	2:N:185:ALA:N	2.36	0.40
2:N:457:SER:HB2	2:N:458:PRO:HD3	2.03	0.40
7:S:55:LYS:HA	7:S:55:LYS:HD2	1.69	0.40
2:B:256:ASN:C	2:B:256:ASN:HD22	2.24	0.40
2:B:392:MET:O	2:B:392:MET:HG3	2.21	0.40
3:C:202:LEU:HD11	14:C:404:HEM:HMA1	2.03	0.40
9:J:29:THR:OG1	10:K:23:VAL:HG22	2.21	0.40
5:Q:189:LEU:HD13	5:Q:242:ARG:HD2	2.03	0.40
2:B:261:THR:HG23	2:B:263:ASP:OD1	2.21	0.40
5:E:169:PHE:CZ	5:E:218:PRO:HD2	2.56	0.40
3:O:207:GLN:HG3	13:O:401:3PE:O11	2.21	0.40
5:Q:112:LEU:HB3	5:Q:116:ARG:NH2	2.36	0.40
2:B:56:LEU:O	2:B:60:VAL:HG23	2.22	0.40
1:M:143:ARG:HA	1:M:143:ARG:HD3	1.95	0.40
1:A:107:VAL:HG22	1:A:260:ILE:HG12	2.03	0.40
1:A:127:ARG:HD3	1:A:127:ARG:HA	1.87	0.40
3:C:298:ALA:C	3:C:301:PRO:HD2	2.46	0.40
1:M:476:LEU:HA	1:M:479:ILE:HG12	2.04	0.40
17:P:401:PC1:O14	17:P:401:PC1:C2	2.70	0.40
5:Q:172:ARG:HB3	5:Q:204:TRP:CD1	2.56	0.40
5:Q:211:CYS:SG	5:Q:213:HIS:HB3	2.61	0.40
5:Q:225:PHE:HB3	5:Q:238:ASP:HA	2.03	0.40
6:R:120:ARG:NH2	6:R:123:PRO:HG3	2.36	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	458/460 (100%)	429 (94%)	29 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	M	458/460 (100%)	442 (96%)	16 (4%)	0	100 100
2	B	485/487 (100%)	448 (92%)	37 (8%)	0	100 100
2	N	485/487 (100%)	453 (93%)	32 (7%)	0	100 100
3	C	384/386 (100%)	360 (94%)	22 (6%)	2 (0%)	25 59
3	O	383/386 (99%)	357 (93%)	26 (7%)	0	100 100
4	D	240/242 (99%)	222 (92%)	18 (8%)	0	100 100
4	P	240/242 (99%)	224 (93%)	16 (7%)	0	100 100
5	E	194/196 (99%)	171 (88%)	23 (12%)	0	100 100
5	Q	194/196 (99%)	174 (90%)	19 (10%)	1 (0%)	25 59
6	F	115/117 (98%)	110 (96%)	5 (4%)	0	100 100
6	R	115/117 (98%)	109 (95%)	5 (4%)	1 (1%)	14 47
7	G	68/70 (97%)	64 (94%)	4 (6%)	0	100 100
7	S	68/70 (97%)	61 (90%)	7 (10%)	0	100 100
8	H	62/64 (97%)	58 (94%)	4 (6%)	0	100 100
8	T	62/64 (97%)	56 (90%)	6 (10%)	0	100 100
9	J	58/60 (97%)	55 (95%)	3 (5%)	0	100 100
9	V	58/60 (97%)	57 (98%)	1 (2%)	0	100 100
10	K	27/29 (93%)	27 (100%)	0	0	100 100
10	W	27/29 (93%)	26 (96%)	1 (4%)	0	100 100
All	All	4181/4222 (99%)	3903 (93%)	274 (7%)	4 (0%)	50 80

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	R	18	ALA
5	Q	109	TYR
3	C	159	PRO
3	C	160	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	384/384 (100%)	384 (100%)	0	100 100
1	M	384/384 (100%)	384 (100%)	0	100 100
2	B	409/409 (100%)	409 (100%)	0	100 100
2	N	409/409 (100%)	409 (100%)	0	100 100
3	C	331/331 (100%)	330 (100%)	1 (0%)	91 96
3	O	330/331 (100%)	330 (100%)	0	100 100
4	D	197/197 (100%)	196 (100%)	1 (0%)	86 94
4	P	197/197 (100%)	197 (100%)	0	100 100
5	E	169/169 (100%)	169 (100%)	0	100 100
5	Q	169/169 (100%)	168 (99%)	1 (1%)	84 92
6	F	104/104 (100%)	104 (100%)	0	100 100
6	R	104/104 (100%)	103 (99%)	1 (1%)	73 88
7	G	63/63 (100%)	63 (100%)	0	100 100
7	S	63/63 (100%)	63 (100%)	0	100 100
8	H	58/58 (100%)	58 (100%)	0	100 100
8	T	58/58 (100%)	58 (100%)	0	100 100
9	J	49/49 (100%)	49 (100%)	0	100 100
9	V	49/49 (100%)	49 (100%)	0	100 100
10	K	19/19 (100%)	19 (100%)	0	100 100
10	W	19/19 (100%)	19 (100%)	0	100 100
All	All	3565/3566 (100%)	3561 (100%)	4 (0%)	92 97

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	18	ASN
4	D	229	MET
5	Q	109	TYR
6	R	14	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	160	GLN
1	A	309	HIS
2	B	395	ASN
3	C	4	GLN
3	C	19	GLN
3	C	142	GLN
3	C	177	ASN
4	D	80	HIS
5	E	251	ASN
6	F	20	GLN
6	F	21	HIS
6	F	88	GLN
1	M	160	GLN
1	M	369	ASN
2	N	201	GLN
2	N	395	ASN
2	N	397	ASN
3	O	4	GLN
3	O	177	ASN
3	O	181	ASN
3	O	188	HIS
3	O	326	HIS
4	P	171	ASN
5	Q	93	ASN
5	Q	182	ASN
7	S	37	GLN
7	S	79	ASN
9	V	54	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 (i)

Of 30 ligands modelled in this entry, 2 are monoatomic - leaving 28 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	$\#\|Z\| > 2$
13	3PE	P	402	-	38,38,50	0.97	3 (7%)	41,43,55	1.11	2 (4%)
15	HEC	D	402	4	32,50,50	2.19	3 (9%)	24,82,82	1.78	5 (20%)
13	3PE	C	407	-	33,33,50	1.06	4 (12%)	36,38,55	1.14	2 (5%)
13	3PE	C	406	-	32,32,50	1.05	4 (12%)	35,37,55	1.16	2 (5%)
14	HEM	O	404	3	41,50,50	1.44	4 (9%)	45,82,82	1.58	10 (22%)
12	CDL	D	401	-	63,63,99	1.07	8 (12%)	69,75,111	1.22	4 (5%)
13	3PE	C	402	-	50,50,50	0.86	4 (8%)	53,55,55	1.06	2 (3%)
13	3PE	S	101	-	32,32,50	1.08	4 (12%)	35,37,55	1.10	2 (5%)
12	CDL	N	602	-	69,69,99	0.42	0	75,81,111	0.74	3 (4%)
13	3PE	C	405	-	36,36,50	1.00	4 (11%)	39,41,55	1.17	2 (5%)
13	3PE	R	201	-	47,47,50	0.89	4 (8%)	50,52,55	1.05	2 (4%)
14	HEM	C	404	3	41,50,50	1.44	3 (7%)	45,82,82	1.57	10 (22%)
16	FES	E	301	5	0,4,4	-	-	-		
12	CDL	O	402	-	80,80,99	0.96	7 (8%)	86,92,111	1.13	4 (4%)
12	CDL	O	405	-	57,57,99	1.13	8 (14%)	63,69,111	1.20	4 (6%)
12	CDL	P	404	-	62,62,99	1.09	8 (12%)	68,74,111	1.15	4 (5%)
14	HEM	C	403	3	41,50,50	1.43	3 (7%)	45,82,82	1.52	12 (26%)
17	PC1	P	401	-	24,24,53	0.53	0	29,30,61	0.65	1 (3%)
12	CDL	C	408	-	29,29,99	0.55	0	33,34,111	0.97	3 (9%)
13	3PE	G	201	-	31,31,50	1.06	4 (12%)	34,36,55	1.14	2 (5%)
13	3PE	C	409	-	35,35,50	1.02	4 (11%)	38,40,55	1.09	2 (5%)
13	3PE	O	401	-	37,37,50	1.00	4 (10%)	40,42,55	1.11	2 (5%)
16	FES	Q	301	5	0,4,4	-	-	-		
12	CDL	B	602	-	68,68,99	1.05	8 (11%)	74,80,111	1.16	4 (5%)
15	HEC	P	403	4	32,50,50	2.24	3 (9%)	24,82,82	1.46	4 (16%)
14	HEM	O	403	3	41,50,50	1.48	3 (7%)	45,82,82	1.42	7 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	3PE	E	302	-	29,29,50	1.10	4 (13%)	32,34,55	1.19	2 (6%)
13	3PE	C	401	-	27,27,50	1.13	4 (14%)	30,32,55	1.14	2 (6%)

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
13	3PE	P	402	-	-	16/42/42/54	-
15	HEC	D	402	4	-	2/10/54/54	-
13	3PE	C	407	-	-	14/37/37/54	-
13	3PE	C	406	-	-	10/36/36/54	-
14	HEM	O	404	3	-	4/12/54/54	-
12	CDL	D	401	-	-	33/74/74/110	-
13	3PE	C	402	-	-	20/54/54/54	-
13	3PE	S	101	-	-	15/36/36/54	-
12	CDL	N	602	-	-	46/80/80/110	-
13	3PE	C	405	-	-	22/40/40/54	-
13	3PE	R	201	-	-	23/51/51/54	-
14	HEM	C	404	3	-	4/12/54/54	-
16	FES	E	301	5	-	-	0/1/1/1
12	CDL	O	402	-	-	43/91/91/110	-
12	CDL	O	405	-	-	40/68/68/110	-
12	CDL	P	404	-	-	42/73/73/110	-
14	HEM	C	403	3	-	3/12/54/54	-
17	PC1	P	401	-	-	12/25/25/57	-
12	CDL	C	408	-	-	14/31/31/110	-
13	3PE	G	201	-	-	20/35/35/54	-
13	3PE	C	409	-	-	22/39/39/54	-
13	3PE	O	401	-	-	18/41/41/54	-
16	FES	Q	301	5	-	-	0/1/1/1
12	CDL	B	602	-	-	45/79/79/110	-
15	HEC	P	403	4	-	0/10/54/54	-
14	HEM	O	403	3	-	5/12/54/54	-
13	3PE	E	302	-	-	11/33/33/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	3PE	C	401	-	-	13/31/31/54	-

All (105) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	P	403	HEC	C2B-C3B	-6.93	1.33	1.40
15	P	403	HEC	C3C-C2C	-6.67	1.33	1.40
15	D	402	HEC	C2B-C3B	-6.60	1.33	1.40
15	D	402	HEC	C3C-C2C	-6.41	1.34	1.40
15	D	402	HEC	C3D-C2D	5.28	1.53	1.37
14	O	403	HEM	C3C-C2C	-5.24	1.33	1.40
15	P	403	HEC	C3D-C2D	5.22	1.53	1.37
14	C	403	HEM	C3C-C2C	-4.16	1.34	1.40
14	O	404	HEM	C3C-C2C	-4.11	1.34	1.40
14	C	404	HEM	C3C-C2C	-4.08	1.34	1.40
14	C	404	HEM	C3C-CAC	3.67	1.55	1.47
14	C	403	HEM	C3C-CAC	3.66	1.55	1.47
14	O	404	HEM	C3C-CAC	3.55	1.55	1.47
14	O	403	HEM	C3C-CAC	3.40	1.54	1.47
14	C	404	HEM	CAB-C3B	2.90	1.55	1.47
14	O	404	HEM	CAB-C3B	2.88	1.55	1.47
14	O	403	HEM	CAB-C3B	2.84	1.55	1.47
14	C	403	HEM	CAB-C3B	2.83	1.55	1.47
13	C	409	3PE	O21-C2	-2.63	1.40	1.46
13	C	407	3PE	O21-C2	-2.62	1.40	1.46
13	P	402	3PE	O21-C2	-2.61	1.40	1.46
13	S	101	3PE	O21-C2	-2.59	1.40	1.46
13	R	201	3PE	O21-C2	-2.57	1.40	1.46
12	O	402	CDL	OB6-CB4	-2.57	1.40	1.46
13	C	405	3PE	O21-C2	-2.56	1.40	1.46
13	C	402	3PE	O21-C2	-2.56	1.40	1.46
12	O	402	CDL	OA6-CA4	-2.52	1.40	1.46
12	O	405	CDL	OA6-CA4	-2.52	1.40	1.46
12	P	404	CDL	OA6-CA4	-2.52	1.40	1.46
13	O	401	3PE	O31-C31	2.52	1.40	1.33
12	O	402	CDL	OB8-CB7	2.52	1.40	1.33
12	P	404	CDL	OB8-CB7	2.51	1.40	1.33
12	B	602	CDL	OB6-CB4	-2.50	1.40	1.46
12	B	602	CDL	OB8-CB7	2.49	1.40	1.33
13	E	302	3PE	O31-C31	2.48	1.40	1.33
13	C	406	3PE	O21-C2	-2.48	1.40	1.46
12	P	404	CDL	OB6-CB4	-2.48	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	P	402	3PE	O31-C31	2.47	1.40	1.33
12	B	602	CDL	OA6-CA4	-2.47	1.40	1.46
13	O	401	3PE	O21-C2	-2.47	1.40	1.46
12	O	405	CDL	OB6-CB5	2.46	1.41	1.34
13	E	302	3PE	O21-C2	-2.46	1.40	1.46
13	R	201	3PE	O31-C31	2.46	1.40	1.33
12	D	401	CDL	OB6-CB4	-2.45	1.40	1.46
12	O	402	CDL	OA8-CA7	2.44	1.40	1.33
12	O	405	CDL	OA8-CA7	2.43	1.40	1.33
12	D	401	CDL	OA6-CA4	-2.42	1.40	1.46
12	B	602	CDL	OA8-CA7	2.42	1.40	1.33
12	O	405	CDL	OB8-CB7	2.42	1.40	1.33
13	C	409	3PE	O31-C31	2.40	1.40	1.33
12	D	401	CDL	OA8-CA7	2.40	1.40	1.33
13	S	101	3PE	O31-C3	-2.39	1.39	1.45
12	D	401	CDL	OB8-CB7	2.39	1.40	1.33
13	C	402	3PE	O31-C31	2.38	1.40	1.33
12	P	404	CDL	OA8-CA7	2.37	1.40	1.33
13	C	407	3PE	O31-C31	2.36	1.40	1.33
13	C	406	3PE	O31-C31	2.36	1.40	1.33
13	G	201	3PE	O31-C31	2.35	1.40	1.33
13	G	201	3PE	O21-C21	2.33	1.40	1.34
13	S	101	3PE	O31-C31	2.32	1.40	1.33
13	C	405	3PE	O31-C31	2.32	1.40	1.33
13	C	401	3PE	O21-C2	-2.31	1.40	1.46
13	C	401	3PE	O21-C21	2.30	1.40	1.34
13	G	201	3PE	O31-C3	-2.28	1.40	1.45
13	C	401	3PE	O31-C31	2.25	1.39	1.33
12	B	602	CDL	OA6-CA5	2.24	1.40	1.34
12	D	401	CDL	OA6-CA5	2.23	1.40	1.34
13	C	401	3PE	O31-C3	-2.23	1.40	1.45
13	C	406	3PE	O31-C3	-2.20	1.40	1.45
13	C	405	3PE	O31-C3	-2.19	1.40	1.45
13	C	402	3PE	O31-C3	-2.19	1.40	1.45
13	S	101	3PE	O21-C21	2.18	1.40	1.34
12	P	404	CDL	OB6-CB5	2.17	1.40	1.34
13	C	409	3PE	O31-C3	-2.17	1.40	1.45
12	O	405	CDL	OB8-CB6	-2.17	1.40	1.45
12	P	404	CDL	OA6-CA5	2.15	1.40	1.34
12	D	401	CDL	OB8-CB6	-2.14	1.40	1.45
12	D	401	CDL	OB6-CB5	2.14	1.40	1.34
13	C	405	3PE	O21-C21	2.14	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	602	CDL	OB6-CB5	2.14	1.40	1.34
12	D	401	CDL	OA8-CA6	-2.14	1.40	1.45
12	B	602	CDL	OA8-CA6	-2.13	1.40	1.45
13	O	401	3PE	O21-C21	2.13	1.40	1.34
13	C	407	3PE	O21-C21	2.13	1.40	1.34
13	C	407	3PE	O31-C3	-2.12	1.40	1.45
13	R	201	3PE	O21-C21	2.11	1.40	1.34
12	O	405	CDL	OA6-CA5	2.11	1.40	1.34
12	B	602	CDL	OB8-CB6	-2.10	1.40	1.45
12	P	404	CDL	OB8-CB6	-2.10	1.40	1.45
13	R	201	3PE	O31-C3	-2.09	1.40	1.45
13	E	302	3PE	O21-C21	2.09	1.40	1.34
12	O	402	CDL	OA6-CA5	2.08	1.40	1.34
12	O	405	CDL	OA8-CA6	-2.07	1.40	1.45
13	P	402	3PE	O31-C3	-2.07	1.40	1.45
12	P	404	CDL	OA8-CA6	-2.07	1.40	1.45
13	G	201	3PE	O21-C2	-2.06	1.41	1.46
13	C	402	3PE	O21-C21	2.05	1.40	1.34
13	C	406	3PE	O21-C21	2.04	1.40	1.34
13	E	302	3PE	O31-C3	-2.04	1.40	1.45
12	O	402	CDL	OA8-CA6	-2.04	1.40	1.45
14	O	404	HEM	FE-ND	2.02	2.06	1.96
12	O	402	CDL	OB6-CB5	2.02	1.40	1.34
13	C	409	3PE	O21-C21	2.02	1.40	1.34
12	O	405	CDL	OB6-CB4	-2.01	1.41	1.46
13	O	401	3PE	O31-C3	-2.00	1.40	1.45

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	O	405	CDL	OA6-CA5-C11	4.38	120.94	111.50
12	D	401	CDL	OA6-CA5-C11	4.36	120.89	111.50
13	C	405	3PE	O21-C21-C22	4.33	120.83	111.50
12	B	602	CDL	OA6-CA5-C11	4.23	120.63	111.50
13	E	302	3PE	O21-C21-C22	4.23	120.61	111.50
12	B	602	CDL	OB6-CB5-C51	4.09	120.33	111.50
12	P	404	CDL	OA6-CA5-C11	4.07	120.26	111.50
12	D	401	CDL	OB6-CB5-C51	4.02	120.16	111.50
13	C	409	3PE	O21-C21-C22	4.01	120.14	111.50
12	O	402	CDL	OB6-CB5-C51	4.00	120.12	111.50
12	O	405	CDL	OB6-CB5-C51	3.97	120.05	111.50
13	C	406	3PE	O21-C21-C22	3.96	120.03	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	P	404	CDL	OB6-CB5-C51	3.96	120.03	111.50
12	O	402	CDL	OA6-CA5-C11	3.91	119.92	111.50
13	O	401	3PE	O21-C21-C22	3.90	119.91	111.50
13	P	402	3PE	O21-C21-C22	3.88	119.85	111.50
13	S	101	3PE	O21-C21-C22	3.80	119.69	111.50
13	C	402	3PE	O21-C21-C22	3.78	119.65	111.50
13	R	201	3PE	O21-C21-C22	3.75	119.59	111.50
15	D	402	HEC	CMC-C2C-C3C	-3.68	121.49	125.82
13	C	407	3PE	O21-C21-C22	3.64	119.34	111.50
13	C	401	3PE	O21-C21-C22	3.48	118.99	111.50
15	D	402	HEC	CBD-CAD-C3D	-3.39	106.83	112.62
12	D	401	CDL	OA8-CA7-C31	3.20	119.77	111.38
13	C	407	3PE	O31-C31-C32	3.11	121.66	111.91
14	O	404	HEM	C4D-ND-C1D	3.10	108.27	105.07
13	G	201	3PE	O21-C21-C22	3.05	118.07	111.50
14	C	404	HEM	CMA-C3A-C4A	-3.02	123.82	128.46
14	O	404	HEM	C4C-CHD-C1D	3.01	126.54	122.56
14	C	404	HEM	C4D-ND-C1D	3.00	108.18	105.07
12	N	602	CDL	OB6-CB5-C51	2.96	117.88	111.50
14	O	404	HEM	CAD-C3D-C4D	2.93	129.78	124.66
12	C	408	CDL	OA4-PA1-OA5	2.90	114.46	106.73
14	O	403	HEM	C3B-C2B-C1B	2.88	108.62	106.49
13	C	401	3PE	O31-C31-C32	2.83	120.78	111.91
15	D	402	HEC	CMC-C2C-C1C	-2.81	124.15	128.46
14	O	404	HEM	CAD-C3D-C2D	-2.80	122.66	127.88
15	D	402	HEC	CMB-C2B-C1B	-2.79	124.17	128.46
13	G	201	3PE	O31-C31-C32	2.78	120.63	111.91
14	C	403	HEM	C4D-ND-C1D	2.77	107.94	105.07
13	O	401	3PE	O31-C31-C32	2.77	120.60	111.91
15	P	403	HEC	CBD-CAD-C3D	-2.75	107.93	112.62
15	P	403	HEC	C1D-C2D-C3D	-2.73	105.10	107.00
13	E	302	3PE	O31-C31-C32	2.71	120.41	111.91
14	C	403	HEM	CAD-CBD-CGD	-2.70	107.80	113.60
14	O	403	HEM	C4D-ND-C1D	2.70	107.86	105.07
14	O	403	HEM	C4C-CHD-C1D	2.69	126.11	122.56
12	B	602	CDL	OA8-CA7-C31	2.69	120.34	111.91
13	C	405	3PE	O31-C31-C32	2.68	120.32	111.91
12	O	405	CDL	OA8-CA7-C31	2.67	120.29	111.91
14	C	404	HEM	C4B-CHC-C1C	2.67	126.08	122.56
14	C	404	HEM	C4C-CHD-C1D	2.67	126.08	122.56
12	O	402	CDL	OA8-CA7-C31	2.67	120.27	111.91
13	R	201	3PE	O31-C31-C32	2.63	120.17	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	B	602	CDL	OB8-CB7-C71	2.62	120.12	111.91
12	O	405	CDL	OB8-CB7-C71	2.61	120.09	111.91
15	D	402	HEC	C1D-C2D-C3D	-2.60	105.19	107.00
13	C	402	3PE	O31-C31-C32	2.58	120.01	111.91
14	C	403	HEM	C4C-CHD-C1D	2.57	125.96	122.56
12	P	404	CDL	OB8-CB7-C71	2.57	119.98	111.91
12	D	401	CDL	OB8-CB7-C71	2.55	119.92	111.91
12	C	408	CDL	OA4-PA1-OA3	2.52	120.55	110.68
12	P	404	CDL	OA8-CA7-C31	2.52	119.81	111.91
12	O	402	CDL	OB8-CB7-C71	2.50	119.74	111.91
14	O	404	HEM	CMA-C3A-C4A	-2.49	124.63	128.46
13	C	406	3PE	O31-C31-C32	2.47	119.65	111.91
14	C	404	HEM	CAD-C3D-C4D	2.46	128.96	124.66
14	O	403	HEM	C4B-CHC-C1C	2.45	125.79	122.56
14	C	403	HEM	CAD-C3D-C2D	-2.44	123.33	127.88
15	P	403	HEC	CMB-C2B-C1B	-2.44	124.71	128.46
13	S	101	3PE	O31-C31-C32	2.43	119.53	111.91
14	C	404	HEM	CAD-C3D-C2D	-2.42	123.37	127.88
12	C	408	CDL	OA2-PA1-OA3	-2.39	101.31	110.68
14	O	404	HEM	C4B-CHC-C1C	2.39	125.71	122.56
14	C	403	HEM	C4B-CHC-C1C	2.36	125.67	122.56
12	N	602	CDL	OA6-CA4-CA6	2.35	116.91	108.40
14	O	404	HEM	C3D-C4D-ND	-2.33	107.57	110.17
14	C	403	HEM	CMC-C2C-C3C	2.33	129.04	124.68
14	C	403	HEM	C3D-C4D-ND	-2.33	107.58	110.17
14	O	404	HEM	CMC-C2C-C3C	2.32	129.02	124.68
13	C	409	3PE	O31-C31-C32	2.32	119.18	111.91
13	P	402	3PE	O31-C31-C32	2.31	119.17	111.91
14	C	404	HEM	C3D-C4D-ND	-2.31	107.60	110.17
14	C	404	HEM	C1B-NB-C4B	2.29	107.44	105.07
14	O	403	HEM	C1B-NB-C4B	2.28	107.43	105.07
14	O	403	HEM	CAD-CBD-CGD	-2.26	108.73	113.60
14	O	404	HEM	C1B-NB-C4B	2.22	107.36	105.07
14	C	403	HEM	CAD-C3D-C4D	2.21	128.53	124.66
14	C	403	HEM	C1B-NB-C4B	2.20	107.34	105.07
14	O	404	HEM	CHD-C1D-ND	2.18	126.80	124.43
15	P	403	HEC	CAA-CBA-CGA	-2.18	107.64	113.76
14	O	403	HEM	CAA-CBA-CGA	-2.18	107.64	113.76
14	C	404	HEM	CHD-C1D-ND	2.16	126.77	124.43
14	C	403	HEM	C3B-C2B-C1B	2.14	108.07	106.49
14	C	404	HEM	CMB-C2B-C1B	-2.09	121.85	125.04
14	C	403	HEM	CAA-CBA-CGA	-2.08	107.93	113.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	P	401	PC1	O12-P-O14	2.07	122.46	112.24
14	C	403	HEM	CBA-CAA-C2A	-2.03	109.15	112.62
12	N	602	CDL	OA4-PA1-OA3	2.03	122.27	112.24

There are no chirality outliers.

All (497) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	B	602	CDL	O1-C1-CA2-OA2
12	B	602	CDL	CB2-C1-CA2-OA2
12	B	602	CDL	CA2-C1-CB2-OB2
12	B	602	CDL	CA2-OA2-PA1-OA3
12	B	602	CDL	CA2-OA2-PA1-OA4
12	B	602	CDL	CA2-OA2-PA1-OA5
12	B	602	CDL	CB2-OB2-PB2-OB3
12	B	602	CDL	CB3-OB5-PB2-OB3
12	B	602	CDL	CB3-OB5-PB2-OB4
12	D	401	CDL	CA2-OA2-PA1-OA3
12	D	401	CDL	CA2-OA2-PA1-OA4
12	D	401	CDL	CA3-OA5-PA1-OA4
12	D	401	CDL	CB2-OB2-PB2-OB3
12	D	401	CDL	CB2-OB2-PB2-OB4
12	D	401	CDL	CB3-OB5-PB2-OB3
12	D	401	CDL	CB3-OB5-PB2-OB4
12	N	602	CDL	CA3-OA5-PA1-OA3
12	N	602	CDL	CB2-OB2-PB2-OB4
12	N	602	CDL	CB3-OB5-PB2-OB3
12	N	602	CDL	CB3-CB4-OB6-CB5
12	N	602	CDL	C51-CB5-OB6-CB4
12	O	402	CDL	CA2-C1-CB2-OB2
12	O	402	CDL	CA2-OA2-PA1-OA3
12	O	402	CDL	CB2-OB2-PB2-OB3
12	O	402	CDL	CB2-OB2-PB2-OB4
12	O	402	CDL	CB2-OB2-PB2-OB5
12	O	402	CDL	CB3-OB5-PB2-OB2
12	O	402	CDL	CB3-OB5-PB2-OB3
12	O	402	CDL	CB3-OB5-PB2-OB4
12	O	405	CDL	CA2-C1-CB2-OB2
12	O	405	CDL	CA2-OA2-PA1-OA3
12	O	405	CDL	CB3-OB5-PB2-OB3
12	P	404	CDL	CB2-C1-CA2-OA2
12	P	404	CDL	CA2-C1-CB2-OB2

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Mol	Chain	Res	Type	Atoms
12	P	404	CDL	CA3-OA5-PA1-OA2
12	P	404	CDL	CA3-OA5-PA1-OA3
12	P	404	CDL	CA3-OA5-PA1-OA4
12	P	404	CDL	OA7-CA5-OA6-CA4
12	P	404	CDL	CB3-OB5-PB2-OB2
12	P	404	CDL	CB3-OB5-PB2-OB3
12	P	404	CDL	CB3-OB5-PB2-OB4
13	C	401	3PE	C11-O13-P-O11
13	C	401	3PE	C11-O13-P-O14
13	C	401	3PE	C2-C1-O11-P
13	C	402	3PE	C11-O13-P-O12
13	C	402	3PE	C11-O13-P-O14
13	C	405	3PE	C11-O13-P-O11
13	C	405	3PE	C11-O13-P-O12
13	C	405	3PE	C11-O13-P-O14
13	C	405	3PE	O13-C11-C12-N
13	C	405	3PE	O11-C1-C2-O21
13	C	405	3PE	O22-C21-O21-C2
13	C	405	3PE	C22-C21-O21-C2
13	C	406	3PE	C11-O13-P-O12
13	C	406	3PE	C11-O13-P-O14
13	C	407	3PE	C1-O11-P-O12
13	C	407	3PE	C1-O11-P-O14
13	C	407	3PE	O13-C11-C12-N
13	C	409	3PE	C11-O13-P-O12
13	C	409	3PE	O22-C21-O21-C2
13	E	302	3PE	C11-O13-P-O12
13	G	201	3PE	C1-O11-P-O14
13	G	201	3PE	C11-O13-P-O12
13	G	201	3PE	C11-O13-P-O14
13	O	401	3PE	C11-O13-P-O14
13	O	401	3PE	O22-C21-O21-C2
13	P	402	3PE	C1-O11-P-O12
13	P	402	3PE	C1-O11-P-O13
13	P	402	3PE	C1-O11-P-O14
13	P	402	3PE	C11-O13-P-O11
13	P	402	3PE	C11-O13-P-O12
13	P	402	3PE	C11-O13-P-O14
13	P	402	3PE	O13-C11-C12-N
13	R	201	3PE	C1-O11-P-O14
13	R	201	3PE	C11-O13-P-O11
13	R	201	3PE	C11-O13-P-O14

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Mol	Chain	Res	Type	Atoms
13	R	201	3PE	O13-C11-C12-N
17	P	401	PC1	O13-C11-C12-N
17	P	401	PC1	C2-C1-O11-P
12	O	402	CDL	OA9-CA7-OA8-CA6
13	E	302	3PE	C32-C31-O31-C3
12	B	602	CDL	OB9-CB7-OB8-CB6
12	O	402	CDL	OB9-CB7-OB8-CB6
13	E	302	3PE	O32-C31-O31-C3
12	O	402	CDL	C31-CA7-OA8-CA6
12	O	402	CDL	C71-CB7-OB8-CB6
12	P	404	CDL	C71-CB7-OB8-CB6
12	P	404	CDL	C11-CA5-OA6-CA4
13	C	409	3PE	C22-C21-O21-C2
13	O	401	3PE	C22-C21-O21-C2
14	O	404	HEM	C2D-C3D-CAD-CBD
12	B	602	CDL	C71-CB7-OB8-CB6
13	R	201	3PE	C32-C31-O31-C3
14	O	404	HEM	C4D-C3D-CAD-CBD
12	N	602	CDL	OB7-CB5-OB6-CB4
12	O	405	CDL	OA9-CA7-OA8-CA6
12	B	602	CDL	O1-C1-CB2-OB2
12	D	401	CDL	O1-C1-CB2-OB2
12	O	402	CDL	O1-C1-CB2-OB2
12	O	405	CDL	O1-C1-CB2-OB2
12	P	404	CDL	O1-C1-CA2-OA2
12	P	404	CDL	O1-C1-CB2-OB2
12	O	405	CDL	C71-CB7-OB8-CB6
12	P	404	CDL	OB9-CB7-OB8-CB6
13	R	201	3PE	O32-C31-O31-C3
12	D	401	CDL	C16-C17-C18-C19
12	O	405	CDL	C31-CA7-OA8-CA6
12	O	405	CDL	OB9-CB7-OB8-CB6
12	D	401	CDL	CA2-C1-CB2-OB2
12	N	602	CDL	CA2-C1-CB2-OB2
12	O	405	CDL	CB2-C1-CA2-OA2
12	O	405	CDL	O1-C1-CA2-OA2
12	C	408	CDL	C13-C14-C15-C16
12	D	401	CDL	CA5-C11-C12-C13
14	C	403	HEM	C2A-CAA-CBA-CGA
14	O	403	HEM	C2A-CAA-CBA-CGA
12	C	408	CDL	CA7-C31-C32-C33
17	P	401	PC1	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
14	C	404	HEM	C4D-C3D-CAD-CBD
12	N	602	CDL	CB7-C71-C72-C73
12	O	402	CDL	CB7-C71-C72-C73
12	O	405	CDL	CA5-C11-C12-C13
12	O	405	CDL	CB7-C71-C72-C73
12	P	404	CDL	CA5-C11-C12-C13
13	C	407	3PE	C31-C32-C33-C34
12	N	602	CDL	C1-CB2-OB2-PB2
13	E	302	3PE	C21-C22-C23-C24
12	O	402	CDL	C60-C61-C62-C63
12	P	404	CDL	CA7-C31-C32-C33
12	N	602	CDL	O1-C1-CB2-OB2
12	P	404	CDL	CB7-C71-C72-C73
12	O	405	CDL	C13-C14-C15-C16
12	B	602	CDL	CB3-OB5-PB2-OB2
12	D	401	CDL	CA2-OA2-PA1-OA5
12	D	401	CDL	CA3-OA5-PA1-OA2
12	D	401	CDL	CB2-OB2-PB2-OB5
12	D	401	CDL	CB3-OB5-PB2-OB2
12	N	602	CDL	CB2-OB2-PB2-OB5
12	N	602	CDL	CB3-OB5-PB2-OB2
12	O	402	CDL	CA2-OA2-PA1-OA5
12	O	405	CDL	CA3-OA5-PA1-OA2
12	O	405	CDL	CB2-OB2-PB2-OB5
12	O	405	CDL	CB3-OB5-PB2-OB2
13	C	401	3PE	C1-O11-P-O13
13	C	402	3PE	C11-O13-P-O11
13	C	406	3PE	C11-O13-P-O11
13	C	407	3PE	C1-O11-P-O13
13	C	409	3PE	C11-O13-P-O11
13	G	201	3PE	C1-O11-P-O13
13	G	201	3PE	C11-O13-P-O11
12	P	404	CDL	CB5-C51-C52-C53
13	C	402	3PE	C31-C32-C33-C34
13	O	401	3PE	C31-C32-C33-C34
13	R	201	3PE	C33-C34-C35-C36
12	N	602	CDL	C13-C14-C15-C16
12	P	404	CDL	C52-C53-C54-C55
12	N	602	CDL	C12-C13-C14-C15
12	N	602	CDL	C16-C17-C18-C19
12	O	402	CDL	C11-C12-C13-C14
12	O	402	CDL	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
12	P	404	CDL	C15-C16-C17-C18
13	C	402	3PE	C29-C2A-C2B-C2C
14	C	404	HEM	C2D-C3D-CAD-CBD
12	N	602	CDL	C14-C15-C16-C17
13	O	401	3PE	C34-C35-C36-C37
17	P	401	PC1	C23-C24-C25-C26
17	P	401	PC1	C24-C25-C26-C27
12	N	602	CDL	CA6-CA4-OA6-CA5
12	N	602	CDL	CB5-C51-C52-C53
12	N	602	CDL	C21-C22-C23-C24
12	O	405	CDL	C1-CB2-OB2-PB2
12	N	602	CDL	C31-C32-C33-C34
17	P	401	PC1	C22-C23-C24-C25
12	B	602	CDL	C51-C52-C53-C54
12	O	402	CDL	C57-C58-C59-C60
12	P	404	CDL	C31-C32-C33-C34
13	C	409	3PE	C22-C23-C24-C25
13	G	201	3PE	C22-C23-C24-C25
12	N	602	CDL	CA7-C31-C32-C33
12	O	402	CDL	C19-C20-C21-C22
12	B	602	CDL	C20-C21-C22-C23
12	P	404	CDL	C71-C72-C73-C74
12	B	602	CDL	C15-C16-C17-C18
12	B	602	CDL	C22-C23-C24-C25
13	C	409	3PE	C32-C33-C34-C35
12	N	602	CDL	OA7-CA5-OA6-CA4
12	N	602	CDL	C11-CA5-OA6-CA4
12	N	602	CDL	C17-C18-C19-C20
13	E	302	3PE	C25-C26-C27-C28
13	C	405	3PE	C21-C22-C23-C24
12	B	602	CDL	C16-C17-C18-C19
13	E	302	3PE	C23-C24-C25-C26
12	N	602	CDL	C20-C21-C22-C23
13	C	402	3PE	C37-C38-C39-C3A
13	C	402	3PE	C23-C24-C25-C26
13	C	409	3PE	C33-C34-C35-C36
13	P	402	3PE	C25-C26-C27-C28
13	R	201	3PE	C35-C36-C37-C38
13	C	409	3PE	O13-C11-C12-N
13	S	101	3PE	O13-C11-C12-N
12	B	602	CDL	C23-C24-C25-C26
12	D	401	CDL	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
12	D	401	CDL	C57-C58-C59-C60
13	C	406	3PE	C21-C22-C23-C24
13	C	402	3PE	C32-C33-C34-C35
12	O	405	CDL	C15-C16-C17-C18
12	C	408	CDL	C14-C15-C16-C17
12	D	401	CDL	C52-C53-C54-C55
13	O	401	3PE	C3A-C3B-C3C-C3D
12	D	401	CDL	C54-C55-C56-C57
13	C	405	3PE	C26-C27-C28-C29
12	B	602	CDL	CB5-C51-C52-C53
13	R	201	3PE	C31-C32-C33-C34
12	D	401	CDL	C31-CA7-OA8-CA6
12	C	408	CDL	C18-C19-C20-C21
12	D	401	CDL	C58-C59-C60-C61
12	O	402	CDL	C73-C74-C75-C76
13	C	402	3PE	C2A-C2B-C2C-C2D
13	C	409	3PE	C23-C24-C25-C26
13	C	402	3PE	C28-C29-C2A-C2B
12	P	404	CDL	C12-C13-C14-C15
13	C	401	3PE	C22-C21-O21-C2
13	C	406	3PE	C22-C21-O21-C2
12	O	402	CDL	C74-C75-C76-C77
13	C	402	3PE	C36-C37-C38-C39
13	C	407	3PE	C36-C37-C38-C39
12	O	402	CDL	CB5-C51-C52-C53
13	S	101	3PE	C24-C25-C26-C27
12	D	401	CDL	OA9-CA7-OA8-CA6
12	B	602	CDL	C13-C14-C15-C16
13	G	201	3PE	C33-C34-C35-C36
13	P	402	3PE	C26-C27-C28-C29
12	D	401	CDL	C12-C13-C14-C15
12	P	404	CDL	C17-C18-C19-C20
12	O	402	CDL	CA5-C11-C12-C13
12	O	405	CDL	C51-CB5-OB6-CB4
12	B	602	CDL	OB5-CB3-CB4-OB6
12	C	408	CDL	OA5-CA3-CA4-OA6
12	O	405	CDL	OB7-CB5-OB6-CB4
12	B	602	CDL	CB7-C71-C72-C73
12	B	602	CDL	C72-C73-C74-C75
12	O	405	CDL	C54-C55-C56-C57
13	P	402	3PE	C35-C36-C37-C38
13	G	201	3PE	O21-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
12	O	405	CDL	C72-C73-C74-C75
12	N	602	CDL	CA4-CA6-OA8-CA7
12	N	602	CDL	C72-C73-C74-C75
13	O	401	3PE	C33-C34-C35-C36
12	N	602	CDL	C54-C55-C56-C57
14	C	403	HEM	C4D-C3D-CAD-CBD
13	C	409	3PE	C36-C37-C38-C39
13	C	401	3PE	O22-C21-O21-C2
13	C	406	3PE	O22-C21-O21-C2
13	E	302	3PE	C11-O13-P-O11
13	C	402	3PE	C2B-C2C-C2D-C2E
13	C	405	3PE	O11-C1-C2-C3
13	C	405	3PE	C28-C29-C2A-C2B
13	R	201	3PE	C28-C29-C2A-C2B
13	C	405	3PE	C32-C31-O31-C3
12	N	602	CDL	C22-C23-C24-C25
12	O	402	CDL	C14-C15-C16-C17
12	P	404	CDL	C72-C73-C74-C75
12	N	602	CDL	C71-C72-C73-C74
12	O	405	CDL	CB3-CB4-CB6-OB8
13	C	407	3PE	C1-C2-C3-O31
13	G	201	3PE	C1-C2-C3-O31
12	D	401	CDL	C20-C21-C22-C23
17	P	401	PC1	C27-C28-C29-C2A
13	O	401	3PE	C36-C37-C38-C39
13	C	407	3PE	C21-C22-C23-C24
13	C	409	3PE	C27-C28-C29-C2A
12	O	402	CDL	C24-C25-C26-C27
12	N	602	CDL	C32-C33-C34-C35
12	O	402	CDL	C62-C63-C64-C65
13	O	401	3PE	C37-C38-C39-C3A
12	O	402	CDL	C15-C16-C17-C18
13	G	201	3PE	C31-C32-C33-C34
12	O	402	CDL	C58-C59-C60-C61
13	O	401	3PE	C23-C24-C25-C26
12	C	408	CDL	C31-C32-C33-C34
12	N	602	CDL	C56-C57-C58-C59
12	O	405	CDL	OB5-CB3-CB4-OB6
12	P	404	CDL	OA5-CA3-CA4-OA6
13	G	201	3PE	O11-C1-C2-O21
12	P	404	CDL	C19-C20-C21-C22
13	C	409	3PE	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
13	C	405	3PE	C34-C35-C36-C37
12	B	602	CDL	OB6-CB4-CB6-OB8
12	O	405	CDL	C73-C74-C75-C76
12	O	402	CDL	C76-C77-C78-C79
13	C	401	3PE	O21-C21-C22-C23
13	C	409	3PE	C31-C32-C33-C34
12	D	401	CDL	C15-C16-C17-C18
13	C	405	3PE	C32-C33-C34-C35
12	O	402	CDL	C63-C64-C65-C66
12	B	602	CDL	OB5-CB3-CB4-CB6
12	C	408	CDL	OA5-CA3-CA4-CA6
12	O	402	CDL	OB5-CB3-CB4-CB6
13	O	401	3PE	O11-C1-C2-C3
13	S	101	3PE	O11-C1-C2-C3
14	C	403	HEM	C2D-C3D-CAD-CBD
13	C	401	3PE	C32-C33-C34-C35
13	C	405	3PE	O32-C31-O31-C3
12	B	602	CDL	C11-CA5-OA6-CA4
13	C	406	3PE	C33-C34-C35-C36
12	D	401	CDL	C60-C61-C62-C63
12	D	401	CDL	C13-C14-C15-C16
13	S	101	3PE	C26-C27-C28-C29
12	O	402	CDL	C13-C14-C15-C16
13	S	101	3PE	C33-C34-C35-C36
13	C	405	3PE	C1-C2-C3-O31
13	C	409	3PE	C1-C2-C3-O31
13	E	302	3PE	C1-C2-C3-O31
13	R	201	3PE	C1-C2-C3-O31
13	C	409	3PE	C37-C38-C39-C3A
12	O	402	CDL	C55-C56-C57-C58
12	D	401	CDL	C56-C57-C58-C59
12	D	401	CDL	C19-C20-C21-C22
12	N	602	CDL	C19-C20-C21-C22
13	R	201	3PE	C1-O11-P-O13
12	N	602	CDL	OB5-CB3-CB4-OB6
12	O	402	CDL	OB5-CB3-CB4-OB6
12	O	402	CDL	C23-C24-C25-C26
13	C	407	3PE	C24-C25-C26-C27
12	D	401	CDL	C53-C54-C55-C56
12	B	602	CDL	C21-C22-C23-C24
12	O	402	CDL	C33-C34-C35-C36
12	N	602	CDL	C55-C56-C57-C58

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Mol	Chain	Res	Type	Atoms
13	C	405	3PE	C25-C26-C27-C28
12	B	602	CDL	OA7-CA5-OA6-CA4
13	O	401	3PE	C24-C25-C26-C27
13	R	201	3PE	C34-C35-C36-C37
12	N	602	CDL	OB5-CB3-CB4-CB6
13	G	201	3PE	O22-C21-O21-C2
12	P	404	CDL	C31-CA7-OA8-CA6
12	B	602	CDL	CA3-CA4-CA6-OA8
12	C	408	CDL	CA3-CA4-CA6-OA8
12	N	602	CDL	CA3-CA4-CA6-OA8
12	O	405	CDL	CA3-CA4-CA6-OA8
12	P	404	CDL	CA3-CA4-CA6-OA8
13	C	402	3PE	O11-C1-C2-O21
13	S	101	3PE	O21-C21-C22-C23
13	C	405	3PE	O21-C2-C3-O31
13	E	302	3PE	O21-C2-C3-O31
13	R	201	3PE	O21-C2-C3-O31
12	N	602	CDL	C23-C24-C25-C26
13	R	201	3PE	C24-C25-C26-C27
13	G	201	3PE	C22-C21-O21-C2
13	C	405	3PE	C29-C2A-C2B-C2C
13	G	201	3PE	C23-C24-C25-C26
12	B	602	CDL	CB2-OB2-PB2-OB5
12	O	405	CDL	CA2-OA2-PA1-OA5
13	O	401	3PE	C11-O13-P-O11
12	O	405	CDL	C51-C52-C53-C54
12	B	602	CDL	C1-CB2-OB2-PB2
12	B	602	CDL	CB4-CB3-OB5-PB2
12	N	602	CDL	CA3-OA5-PA1-OA4
12	N	602	CDL	CB2-OB2-PB2-OB3
12	N	602	CDL	CB3-OB5-PB2-OB4
12	O	402	CDL	CA2-OA2-PA1-OA4
12	O	405	CDL	CA3-OA5-PA1-OA4
12	O	405	CDL	CB2-OB2-PB2-OB4
12	O	405	CDL	CB3-OB5-PB2-OB4
13	C	401	3PE	C1-O11-P-O12
13	C	405	3PE	C1-O11-P-O12
13	C	407	3PE	C11-O13-P-O12
13	C	409	3PE	C11-O13-P-O14
13	E	302	3PE	C11-O13-P-O14
13	S	101	3PE	C1-O11-P-O14
12	B	602	CDL	OA5-CA3-CA4-CA6

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Mol	Chain	Res	Type	Atoms
12	O	405	CDL	OB5-CB3-CB4-CB6
12	P	404	CDL	OA5-CA3-CA4-CA6
13	C	407	3PE	O11-C1-C2-C3
13	G	201	3PE	O11-C1-C2-C3
13	O	401	3PE	C35-C36-C37-C38
13	R	201	3PE	C3A-C3B-C3C-C3D
12	P	404	CDL	OA9-CA7-OA8-CA6
13	P	402	3PE	C33-C34-C35-C36
13	C	405	3PE	C12-C11-O13-P
13	O	401	3PE	C12-C11-O13-P
13	P	402	3PE	C12-C11-O13-P
13	R	201	3PE	C12-C11-O13-P
17	P	401	PC1	C12-C11-O13-P
13	R	201	3PE	C37-C38-C39-C3A
12	O	405	CDL	C52-C51-CB5-OB6
13	G	201	3PE	C32-C33-C34-C35
13	C	406	3PE	C31-C32-C33-C34
13	C	407	3PE	O11-C1-C2-O21
13	O	401	3PE	O11-C1-C2-O21
13	S	101	3PE	O11-C1-C2-O21
12	B	602	CDL	C52-C53-C54-C55
13	C	405	3PE	O31-C31-C32-C33
12	B	602	CDL	CB3-CB4-CB6-OB8
12	N	602	CDL	OA6-CA4-CA6-OA8
12	O	405	CDL	OA6-CA4-CA6-OA8
12	P	404	CDL	OA6-CA4-CA6-OA8
13	C	407	3PE	O21-C2-C3-O31
13	C	409	3PE	O21-C2-C3-O31
12	D	401	CDL	C71-CB7-OB8-CB6
13	C	402	3PE	O31-C31-C32-C33
12	D	401	CDL	OB9-CB7-OB8-CB6
13	C	402	3PE	C39-C3A-C3B-C3C
13	R	201	3PE	C3C-C3D-C3E-C3F
12	O	405	CDL	CA7-C31-C32-C33
12	P	404	CDL	C32-C31-CA7-OA8
13	P	402	3PE	C2B-C2C-C2D-C2E
13	S	101	3PE	C32-C33-C34-C35
12	C	408	CDL	CA3-CA4-OA6-CA5
12	O	405	CDL	CB6-CB4-OB6-CB5
13	C	401	3PE	C3-C2-O21-C21
13	G	201	3PE	C1-C2-O21-C21
13	C	402	3PE	O11-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
13	C	402	3PE	C2-C1-O11-P
12	P	404	CDL	OB5-CB3-CB4-OB6
12	C	408	CDL	C12-C13-C14-C15
12	N	602	CDL	CA3-OA5-PA1-OA2
13	C	402	3PE	C1-O11-P-O13
13	S	101	3PE	C1-O11-P-O13
17	P	401	PC1	C11-O13-P-O11
17	P	401	PC1	C1-O11-P-O13
13	C	409	3PE	C35-C36-C37-C38
12	P	404	CDL	C16-C17-C18-C19
13	C	406	3PE	C2-C1-O11-P
12	O	402	CDL	C12-C13-C14-C15
13	C	409	3PE	O31-C31-C32-C33
13	G	201	3PE	O13-C11-C12-N
13	R	201	3PE	C36-C37-C38-C39
13	C	401	3PE	C22-C23-C24-C25
13	S	101	3PE	C2-C1-O11-P
12	B	602	CDL	C35-C36-C37-C38
12	P	404	CDL	C72-C71-CB7-OB8
12	C	408	CDL	CA5-C11-C12-C13
13	R	201	3PE	C3D-C3E-C3F-C3G
13	P	402	3PE	C31-C32-C33-C34
12	O	402	CDL	C22-C23-C24-C25
12	O	405	CDL	C11-C12-C13-C14
13	C	407	3PE	C11-O13-P-O11
13	C	401	3PE	O22-C21-C22-C23
12	B	602	CDL	OA5-CA3-CA4-OA6
14	O	403	HEM	C2D-C3D-CAD-CBD
14	O	403	HEM	C4D-C3D-CAD-CBD
12	P	404	CDL	C13-C14-C15-C16
13	C	402	3PE	C21-C22-C23-C24
12	O	402	CDL	CA7-C31-C32-C33
13	C	402	3PE	O21-C2-C3-O31
12	B	602	CDL	C31-CA7-OA8-CA6
13	C	406	3PE	C38-C39-C3A-C3B
12	B	602	CDL	OA9-CA7-OA8-CA6
13	E	302	3PE	C22-C23-C24-C25
13	C	409	3PE	C24-C25-C26-C27
12	C	408	CDL	C15-C16-C17-C18
13	R	201	3PE	C2C-C2D-C2E-C2F
12	N	602	CDL	C52-C53-C54-C55
12	O	405	CDL	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
13	P	402	3PE	O31-C31-C32-C33
14	O	404	HEM	C3D-CAD-CBD-CGD
14	O	403	HEM	CAD-CBD-CGD-O1D
13	G	201	3PE	C2-C1-O11-P
12	B	602	CDL	C73-C74-C75-C76
12	N	602	CDL	CA2-OA2-PA1-OA5
12	B	602	CDL	C19-C20-C21-C22
12	B	602	CDL	CA7-C31-C32-C33
14	O	404	HEM	C2A-CAA-CBA-CGA
13	G	201	3PE	O31-C31-C32-C33
13	C	401	3PE	C1-C2-O21-C21
12	D	401	CDL	C17-C18-C19-C20
12	P	404	CDL	C54-C55-C56-C57
12	O	402	CDL	C20-C21-C22-C23
12	O	402	CDL	C31-C32-C33-C34
13	C	409	3PE	C32-C31-O31-C3
13	C	409	3PE	O32-C31-O31-C3
14	C	404	HEM	CAA-CBA-CGA-O2A
12	P	404	CDL	OB5-CB3-CB4-CB6
13	S	101	3PE	O21-C2-C3-O31
13	O	401	3PE	C21-C22-C23-C24
13	P	402	3PE	C36-C37-C38-C39
12	B	602	CDL	C24-C25-C26-C27
12	C	408	CDL	C19-C20-C21-C22
12	O	405	CDL	C12-C13-C14-C15
13	O	401	3PE	C32-C33-C34-C35
14	C	404	HEM	CAA-CBA-CGA-O1A
14	O	403	HEM	CAD-CBD-CGD-O2D
12	B	602	CDL	CA3-OA5-PA1-OA4
12	O	405	CDL	CA3-OA5-PA1-OA3
13	S	101	3PE	C11-O13-P-O14
12	N	602	CDL	OA5-CA3-CA4-CA6
15	D	402	HEC	CAD-CBD-CGD-O2D
15	D	402	HEC	CAD-CBD-CGD-O1D
12	C	408	CDL	CA6-CA4-OA6-CA5
12	P	404	CDL	C52-C51-CB5-OB6
13	S	101	3PE	O31-C31-C32-C33
17	P	401	PC1	O21-C21-C22-C23
13	R	201	3PE	C32-C33-C34-C35
12	P	404	CDL	C73-C74-C75-C76
17	P	401	PC1	O22-C21-C22-C23
12	P	404	CDL	C52-C51-CB5-OB7

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Mol	Chain	Res	Type	Atoms
13	S	101	3PE	O32-C31-C32-C33

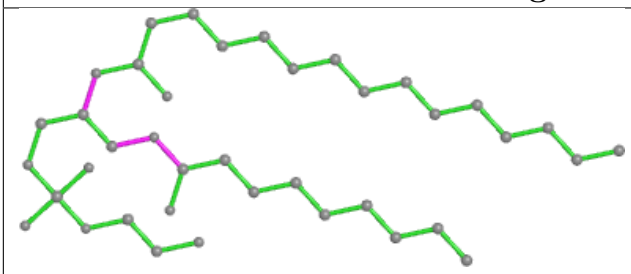
There are no ring outliers.

23 monomers are involved in 75 short contacts:

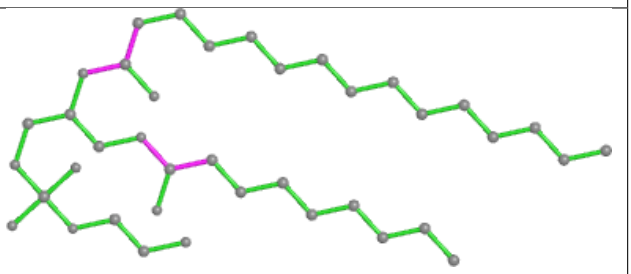
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	P	402	3PE	1	0
15	D	402	HEC	5	0
13	C	406	3PE	1	0
14	O	404	HEM	3	0
12	D	401	CDL	2	0
13	C	402	3PE	3	0
12	N	602	CDL	10	0
13	C	405	3PE	3	0
13	R	201	3PE	3	0
14	C	404	HEM	3	0
16	E	301	FES	3	0
12	O	402	CDL	4	0
12	O	405	CDL	3	0
12	P	404	CDL	2	0
14	C	403	HEM	2	0
17	P	401	PC1	3	0
12	C	408	CDL	14	0
13	O	401	3PE	2	0
16	Q	301	FES	2	0
12	B	602	CDL	1	0
15	P	403	HEC	4	0
14	O	403	HEM	2	0
13	E	302	3PE	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

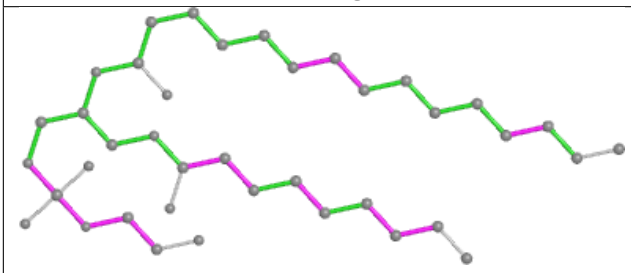
Ligand 3PE P 402



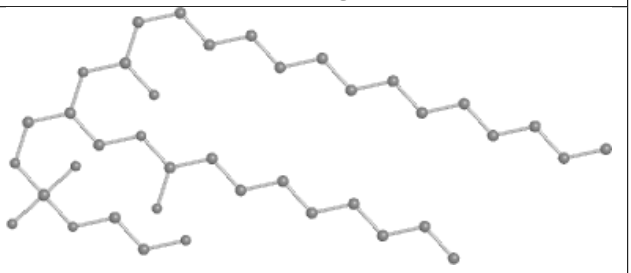
Bond lengths



Bond angles

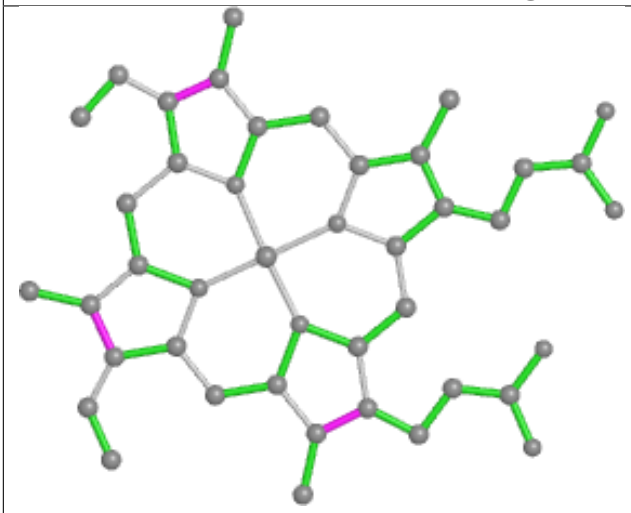


Torsions

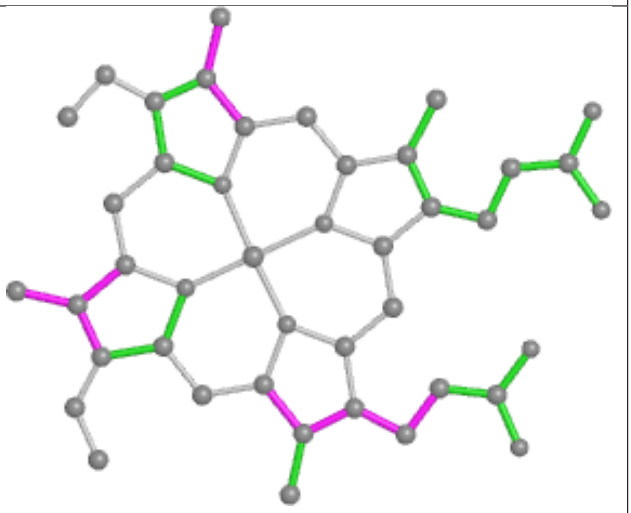


Rings

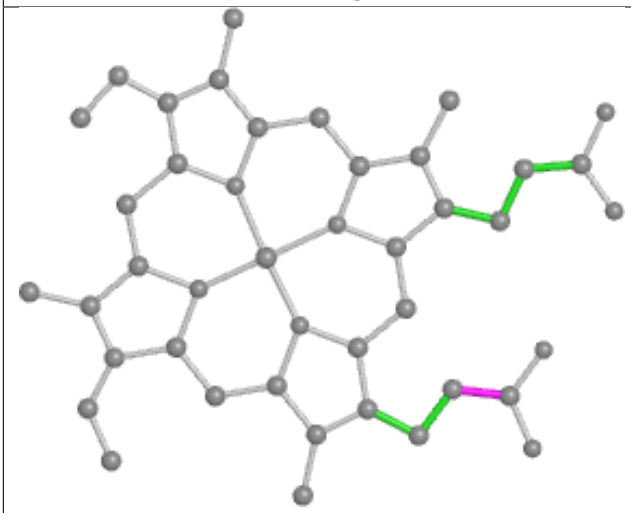
Ligand HEC D 402



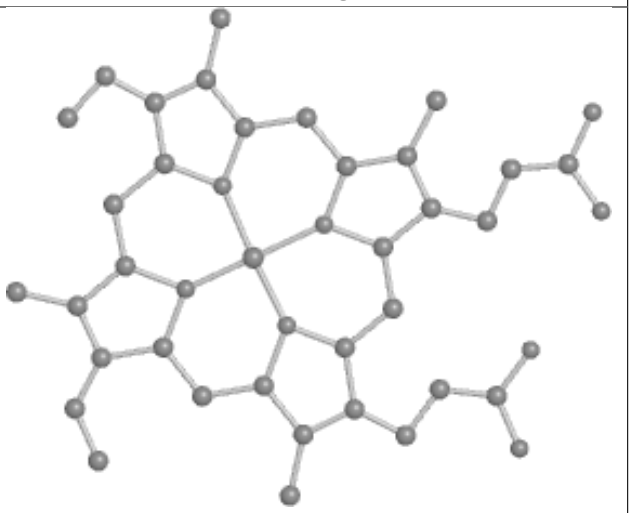
Bond lengths



Bond angles

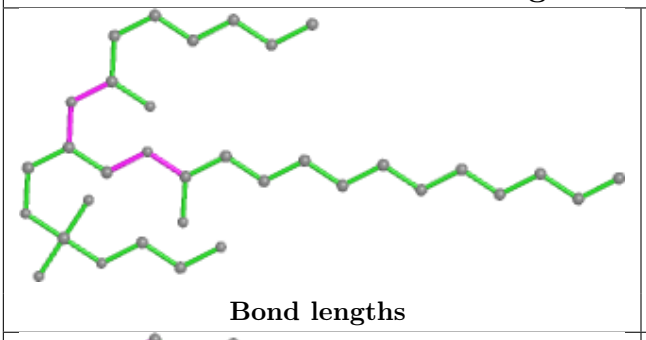


Torsions

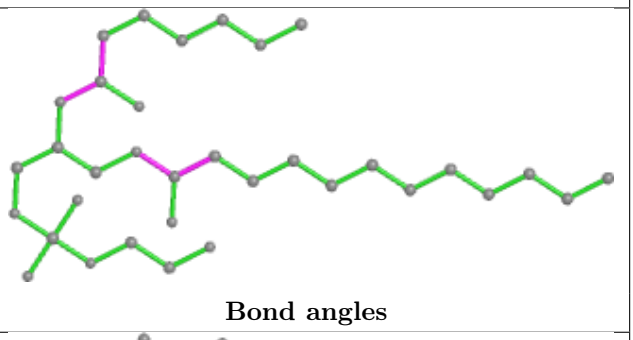


Rings

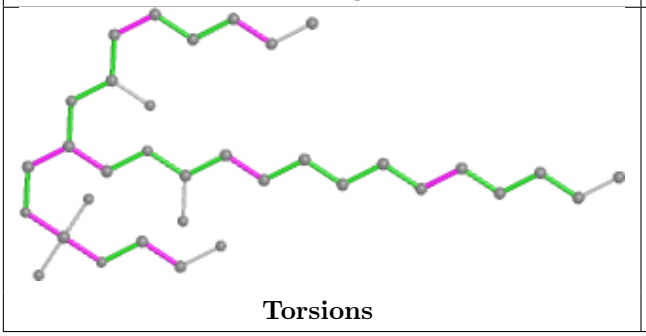
Ligand 3PE C 407



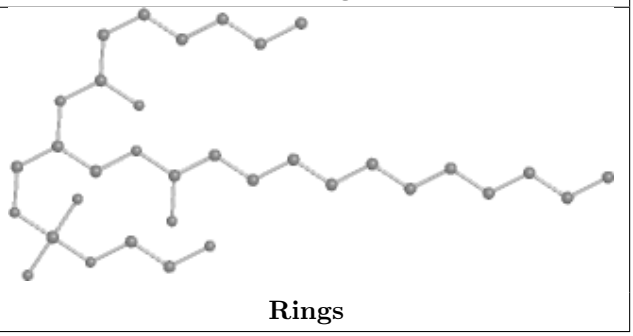
Bond lengths



Bond angles

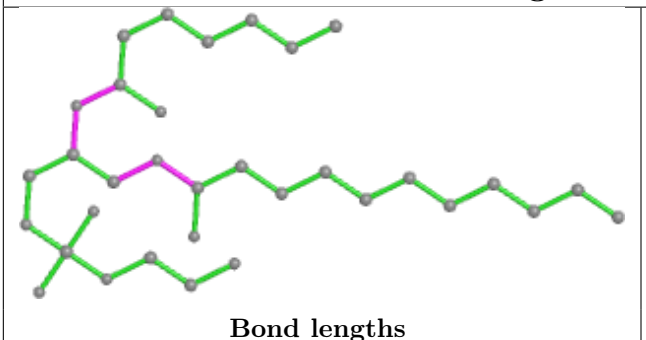


Torsions



Rings

Ligand 3PE C 406



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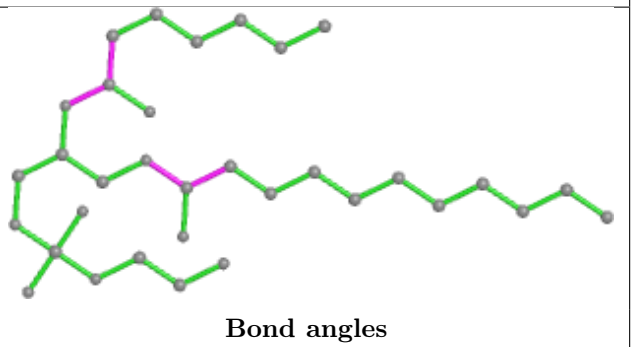
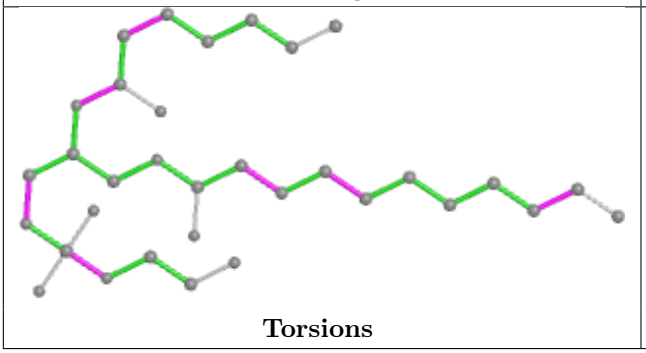
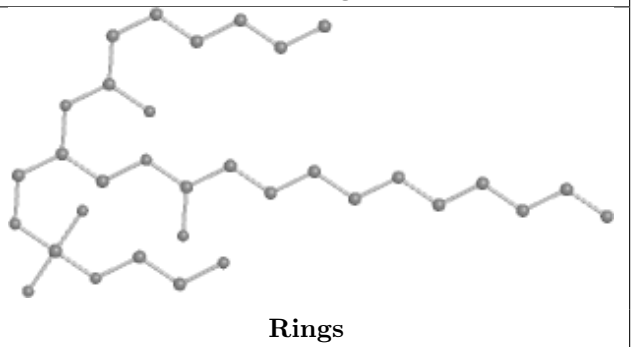


Bond angles

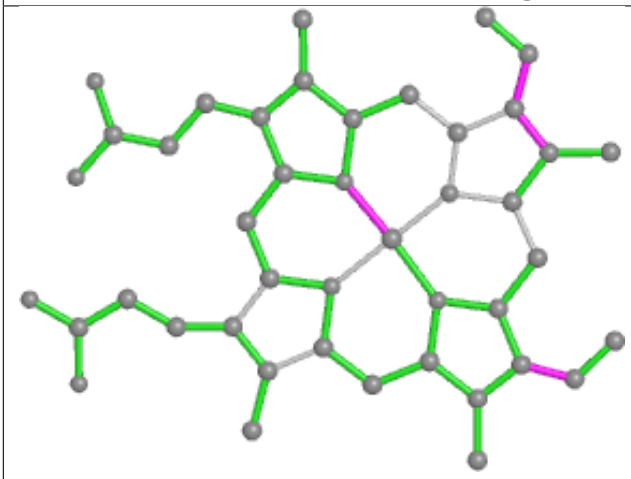


Torsions

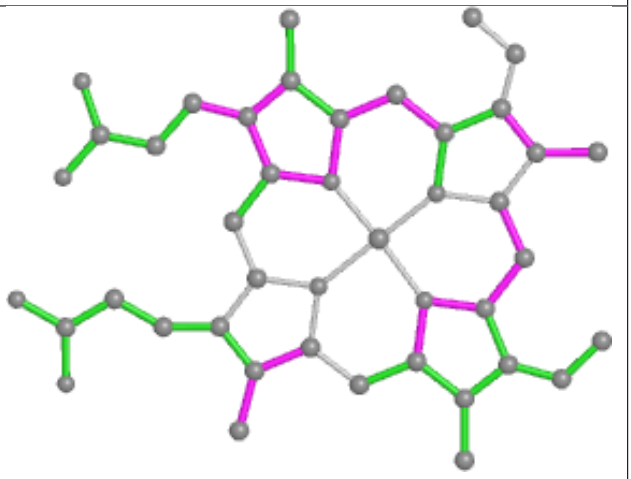


Rings

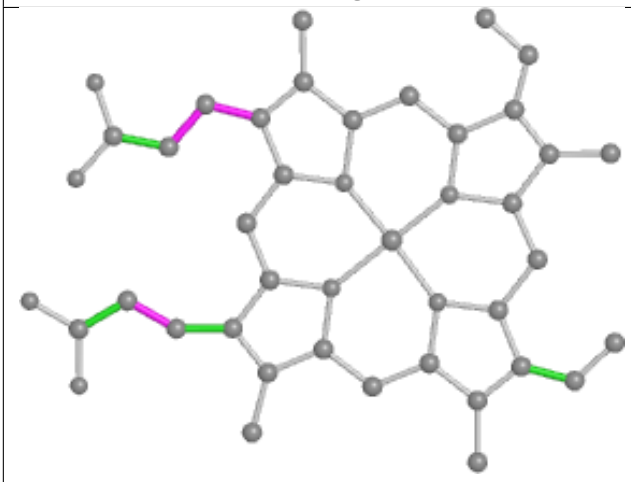
Ligand HEM O 404



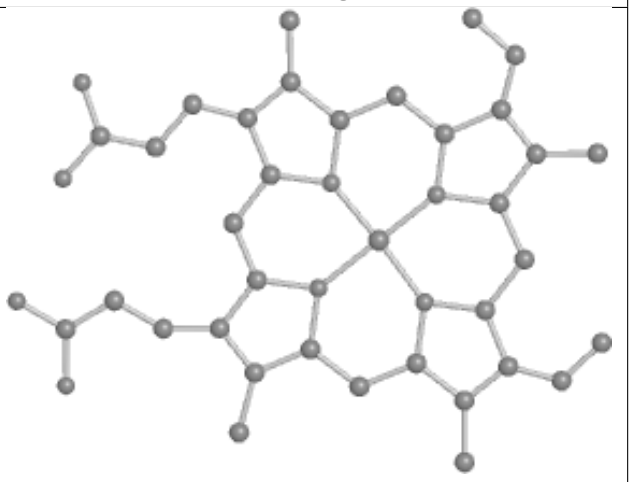
Bond lengths



Bond angles

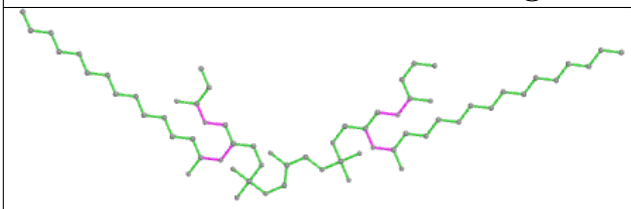


Torsions

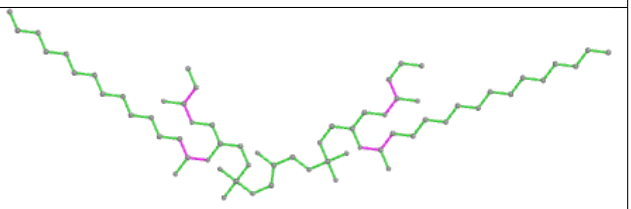


Rings

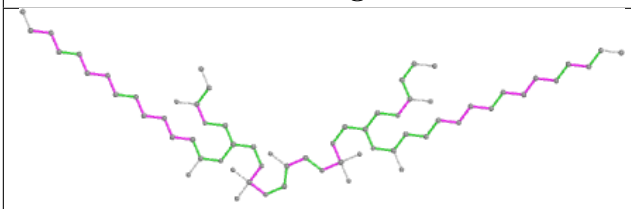
Ligand CDL D 401



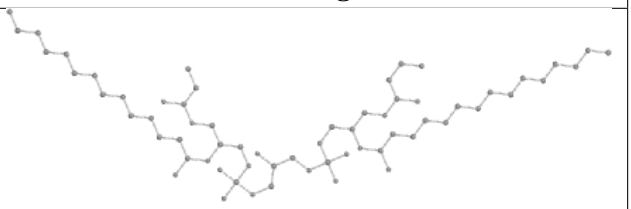
Bond lengths



Bond angles

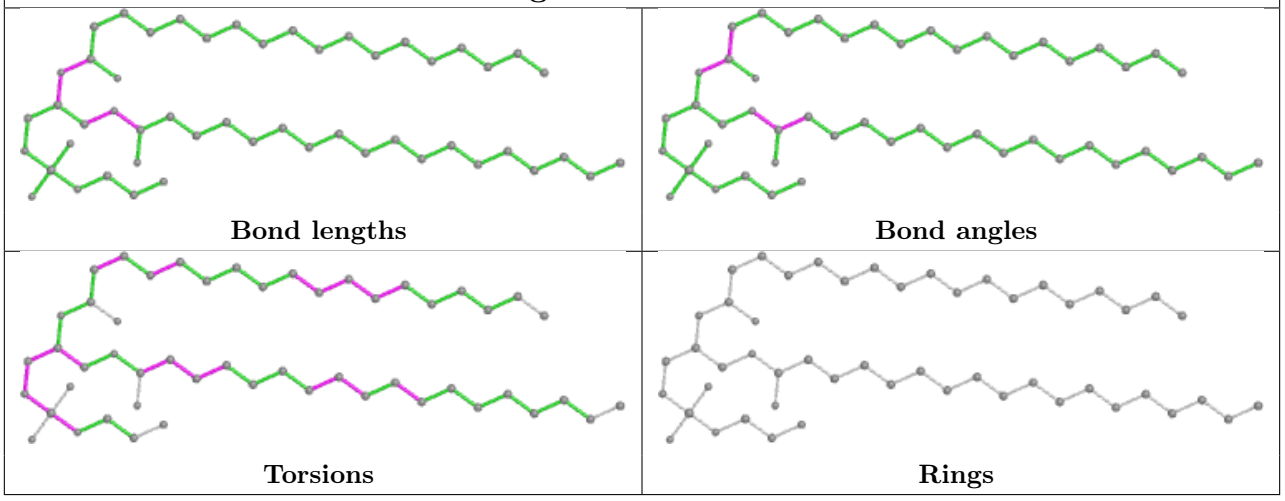


Torsions

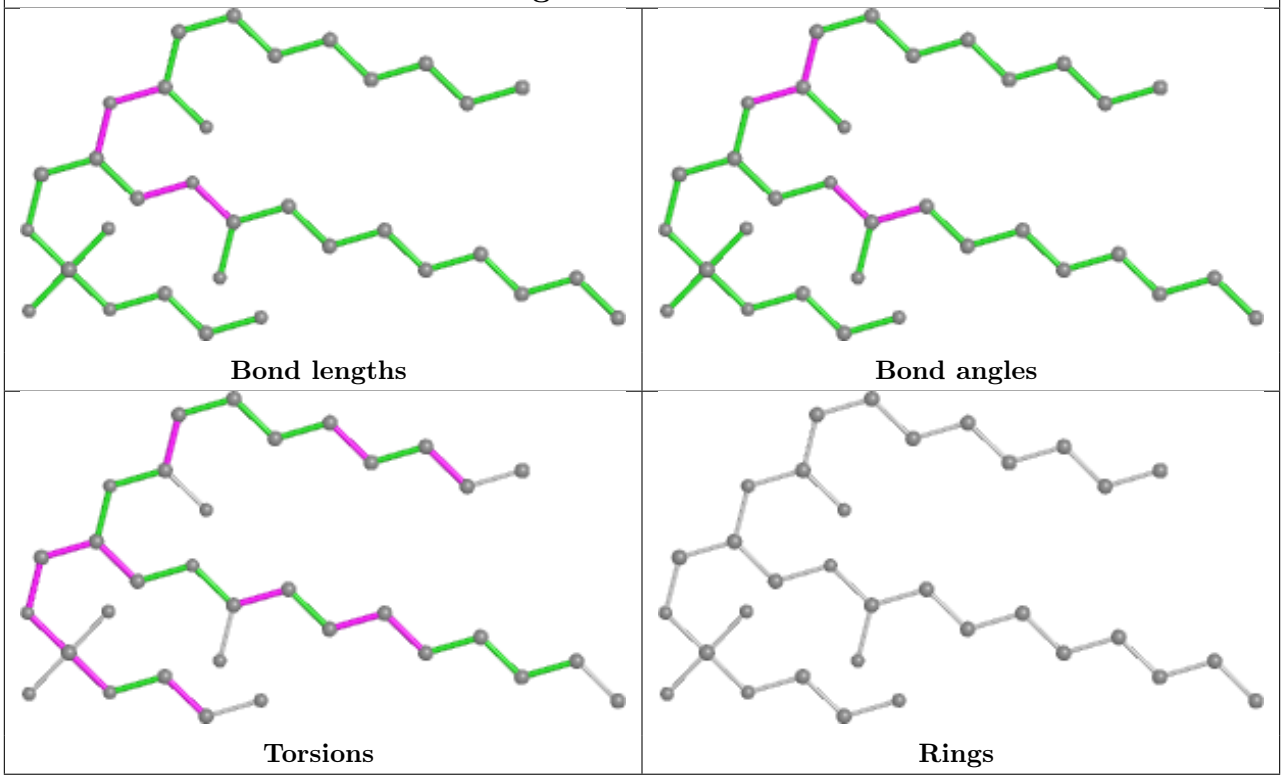


Rings

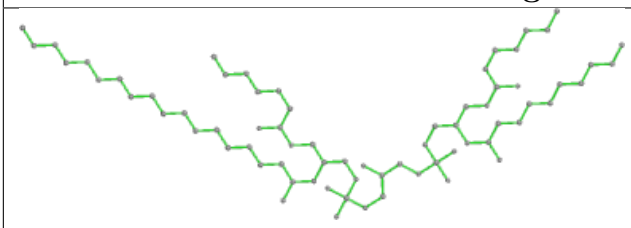
Ligand 3PE C 402



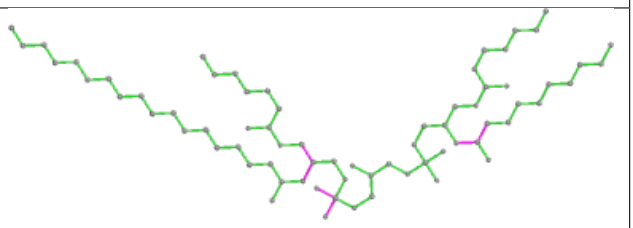
Ligand 3PE S 101



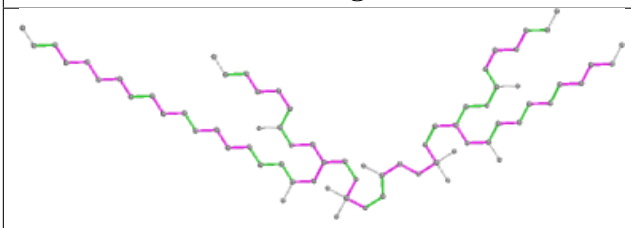
Ligand CDL N 602



Bond lengths



Bond angles



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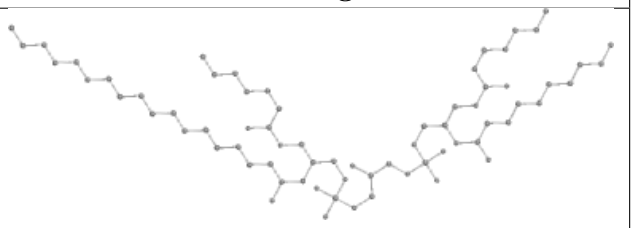
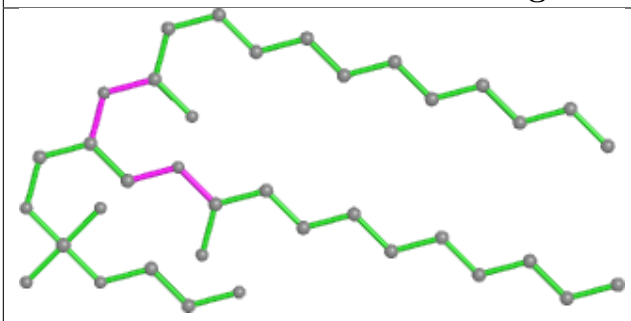
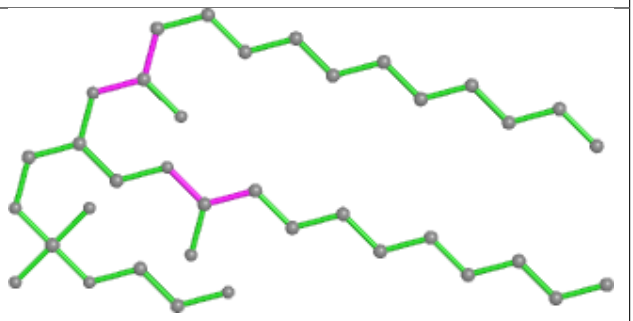


Rings

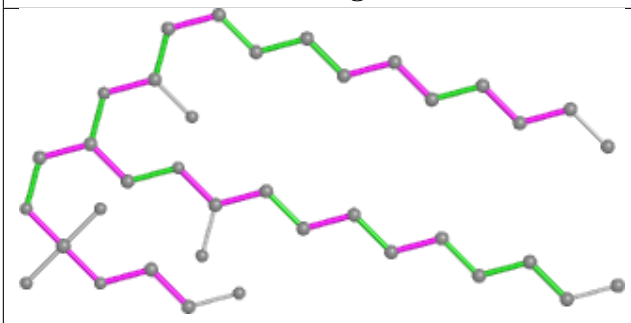
Ligand 3PE C 405



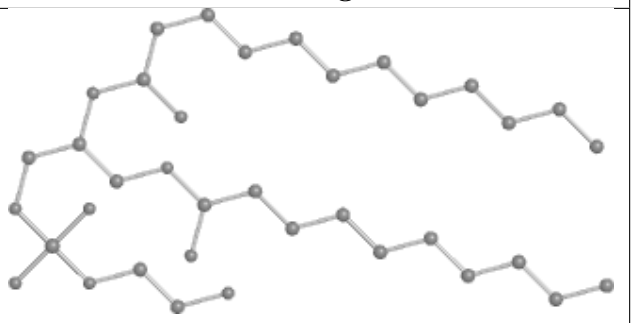
Bond lengths



Bond angles

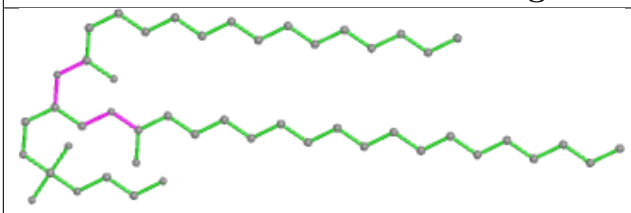


Torsions

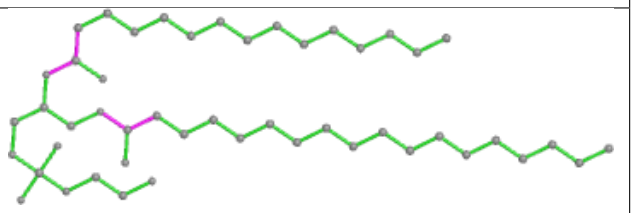


Rings

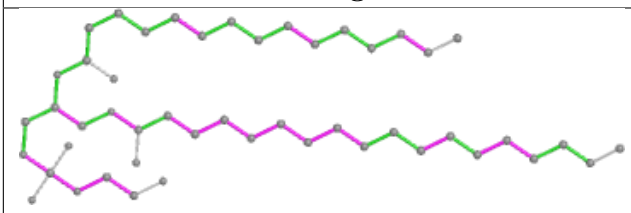
Ligand 3PE R 201



Bond lengths



Bond angles



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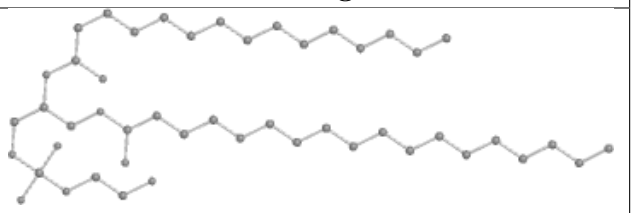
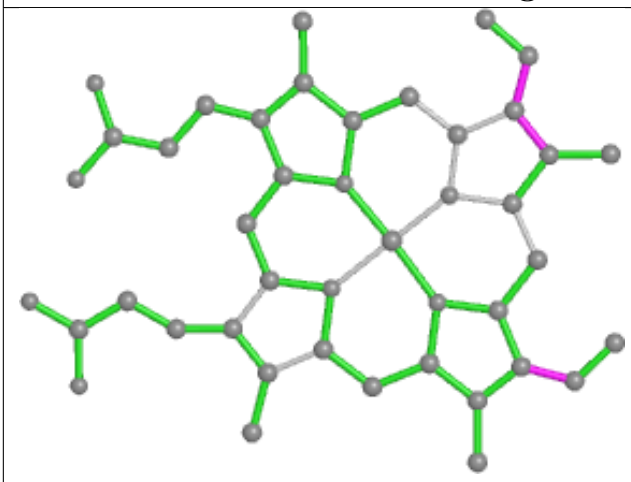
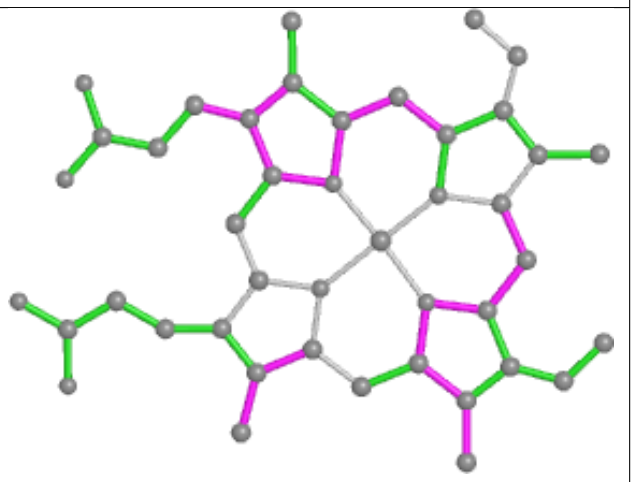


Rings

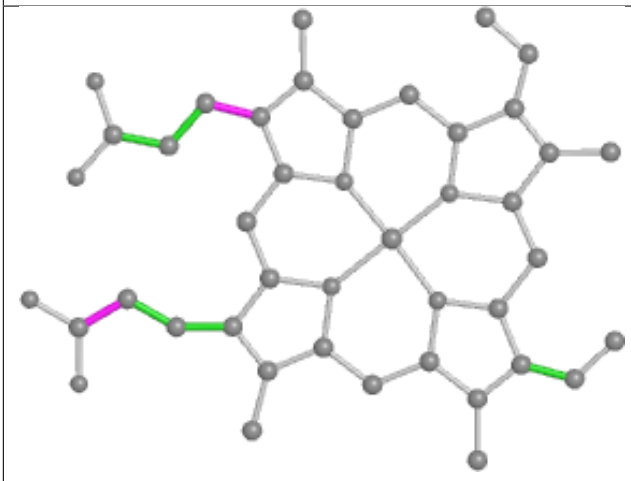
Ligand HEM C 404



Bond lengths



Bond angles



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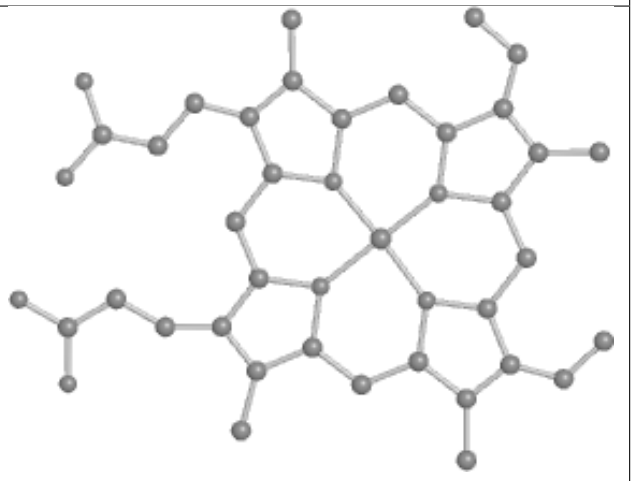
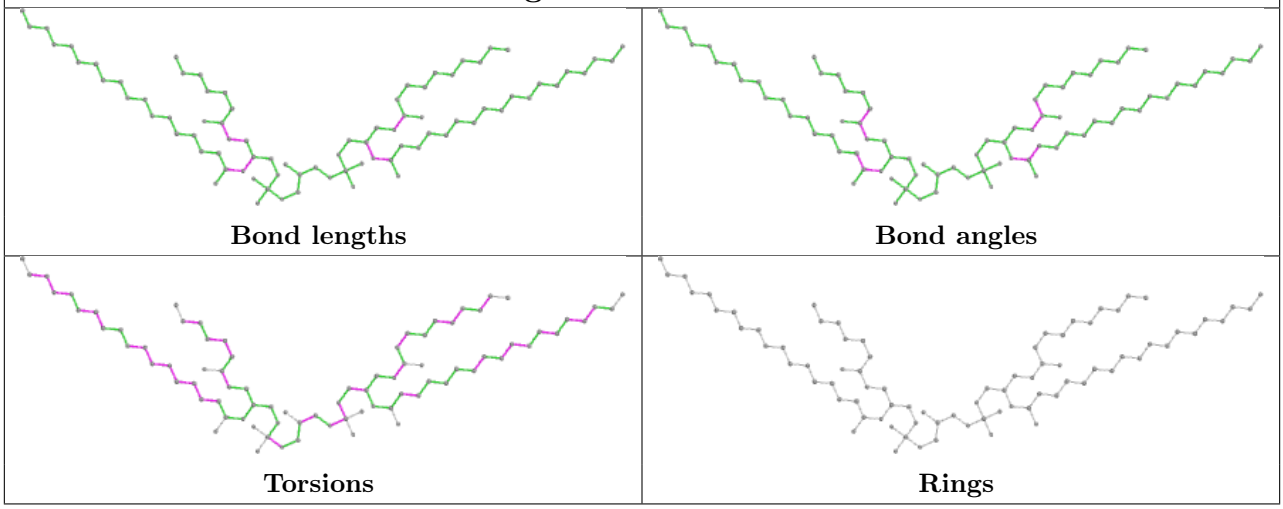
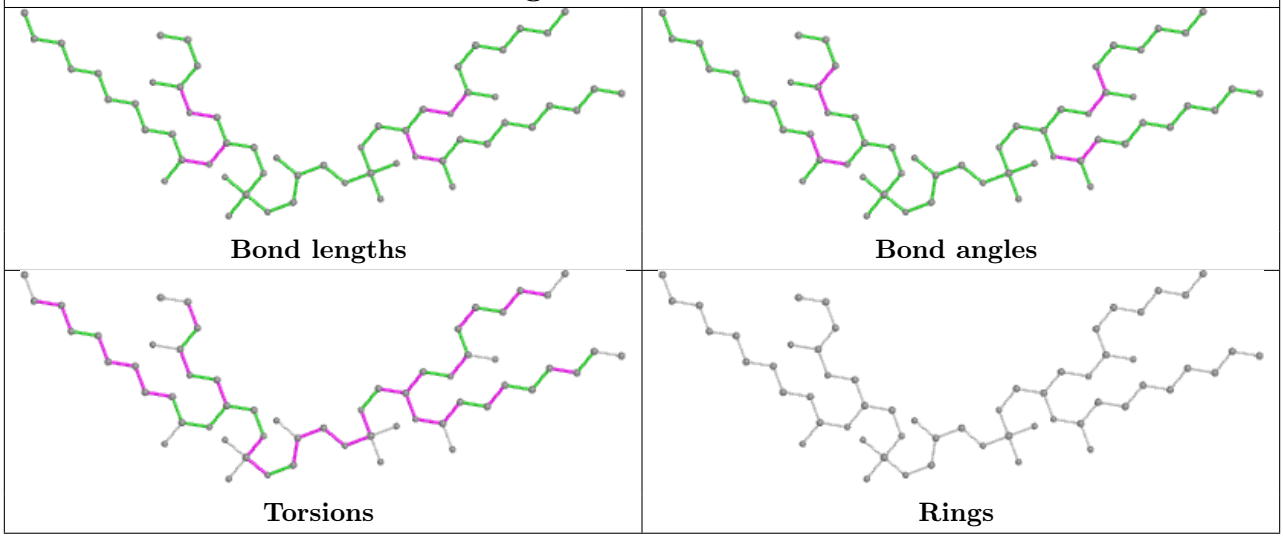


Rings

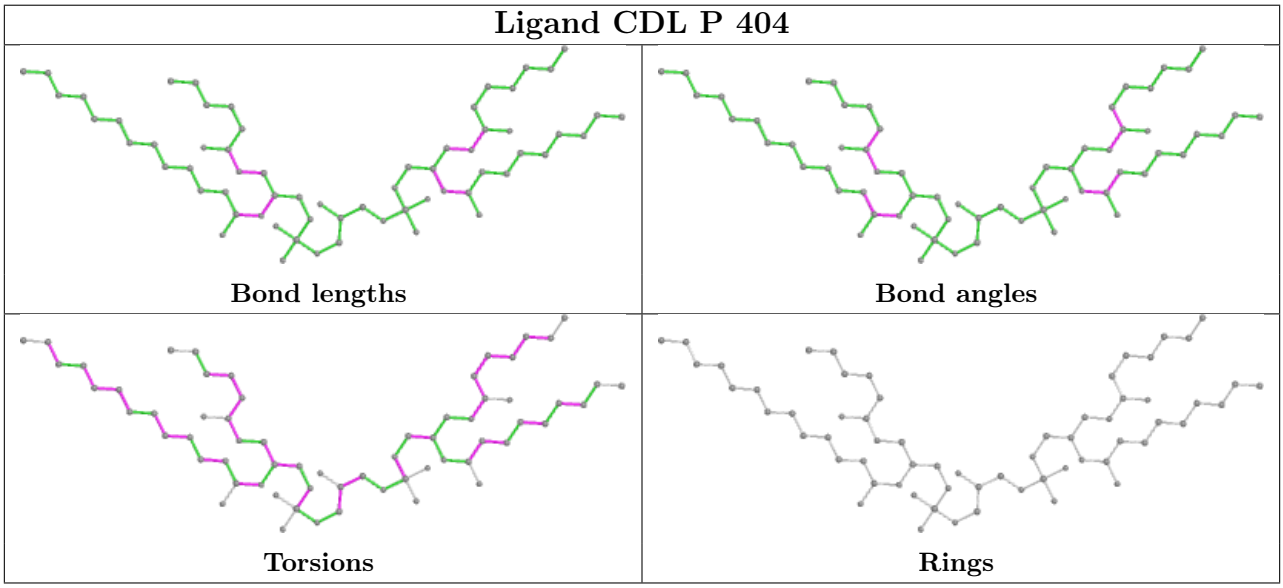
Ligand CDL O 402



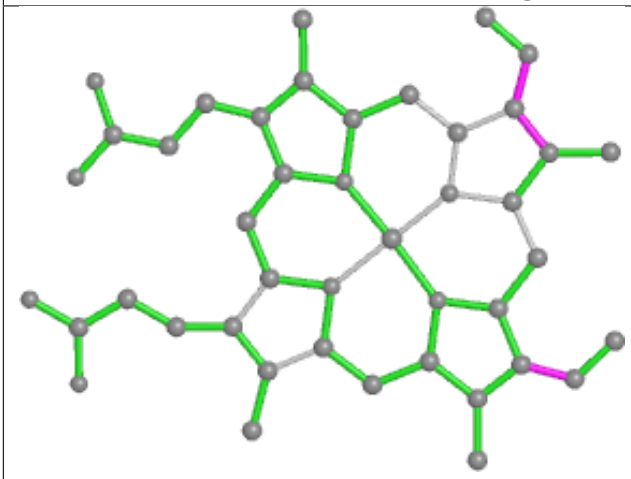
Ligand CDL O 405



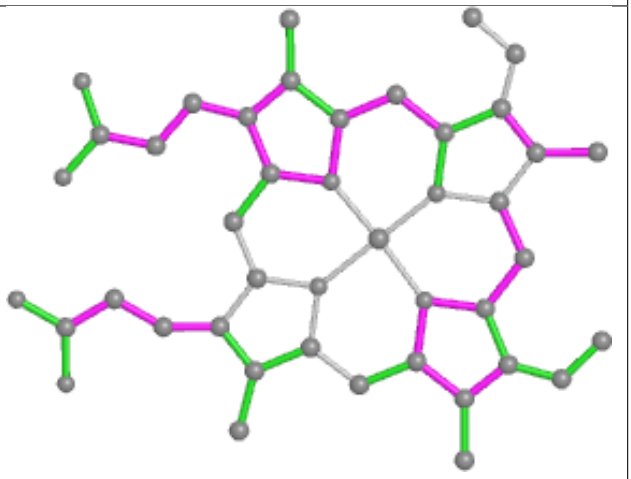
Ligand CDL P 404



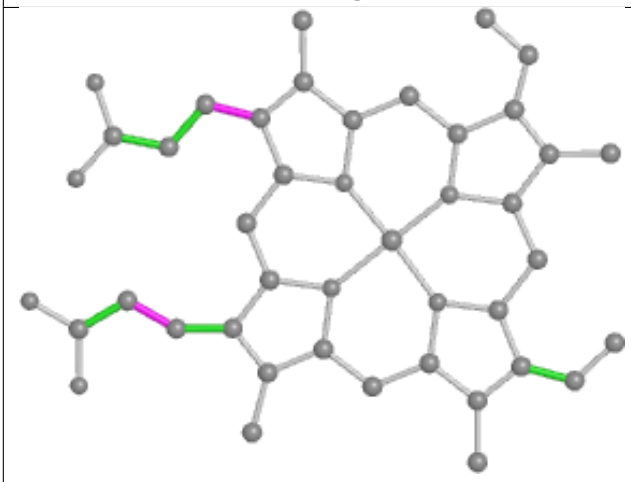
Ligand HEM C 403



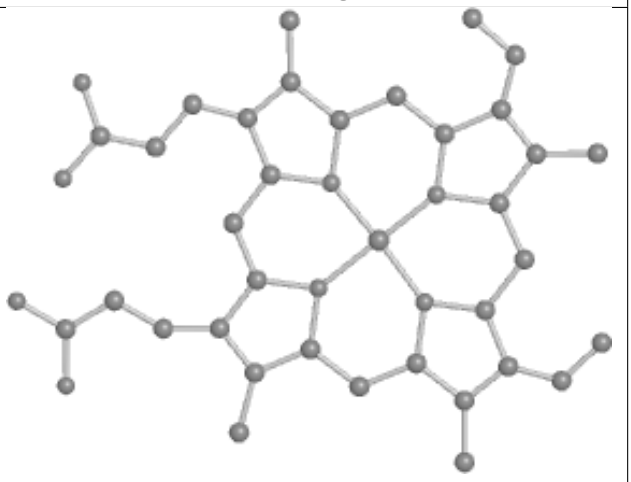
Bond lengths



Bond angles

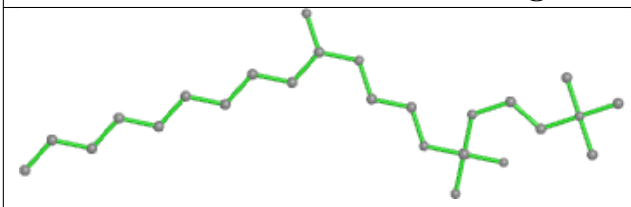


Torsions

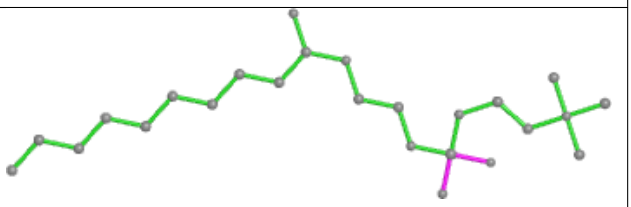


Rings

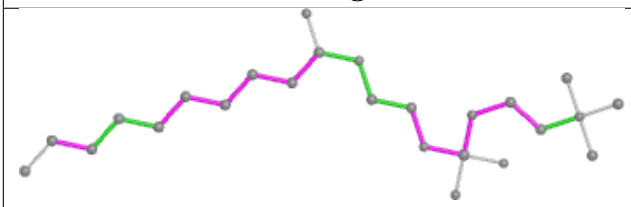
Ligand PC1 P 401



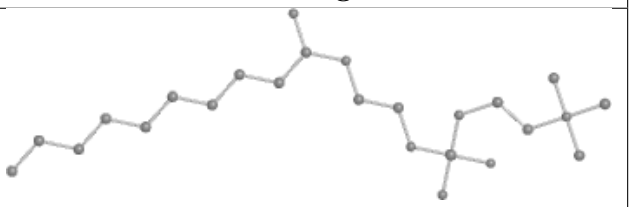
Bond lengths



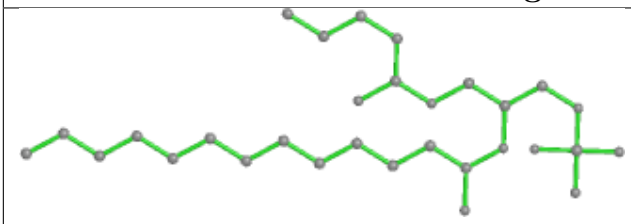
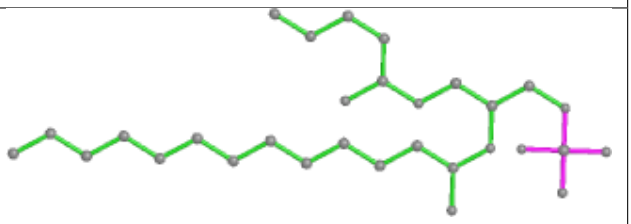
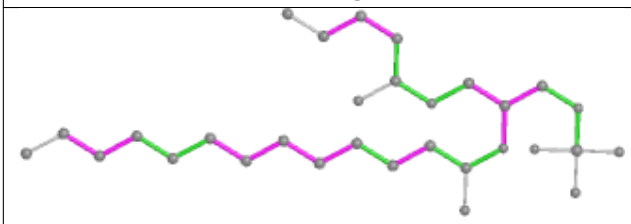
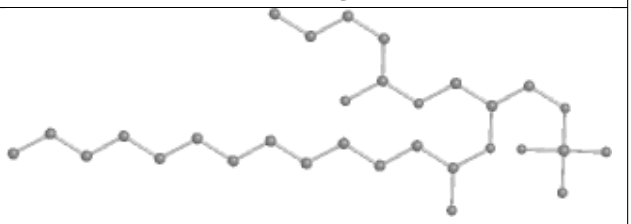
Bond angles

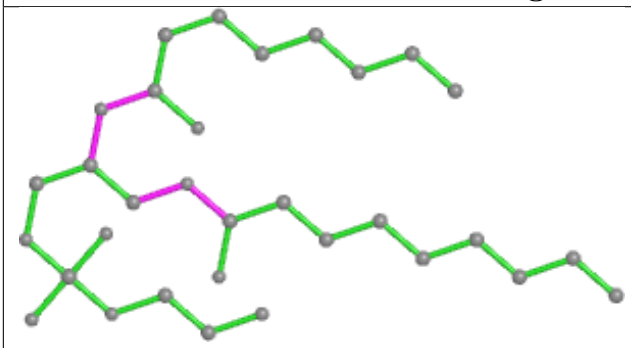
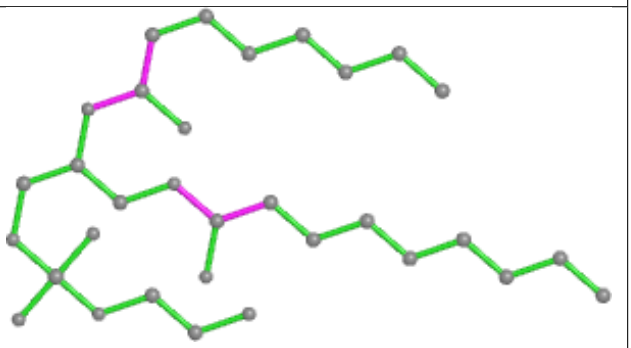
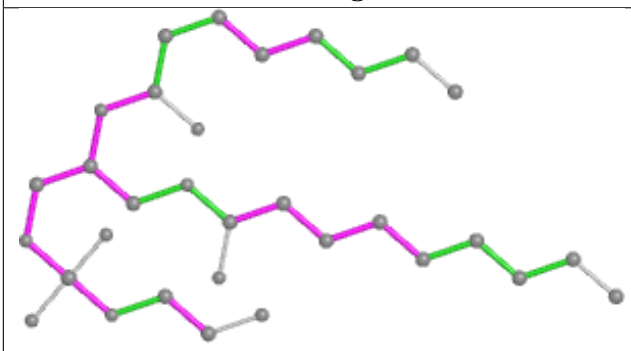
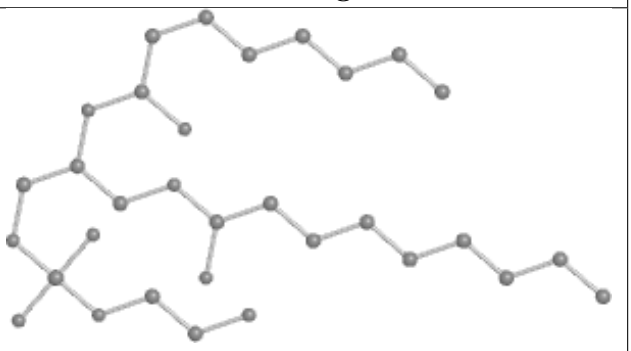


Torsions

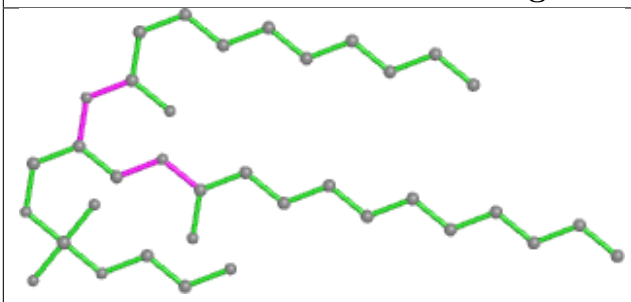


Rings

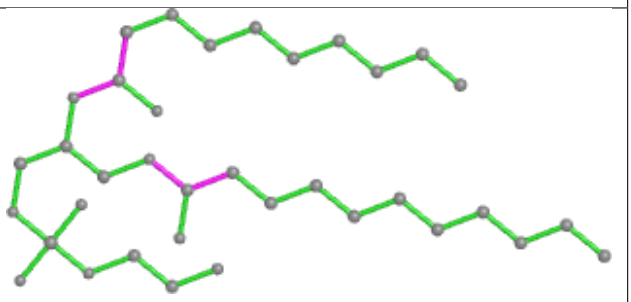
Ligand CDL C 408	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 3PE G 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

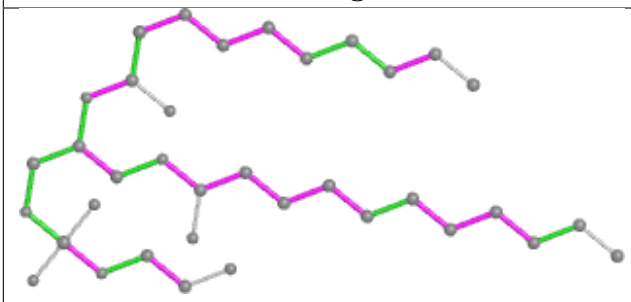
Ligand 3PE C 409



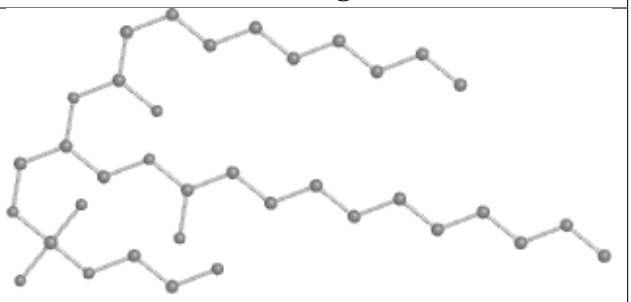
Bond lengths



Bond angles

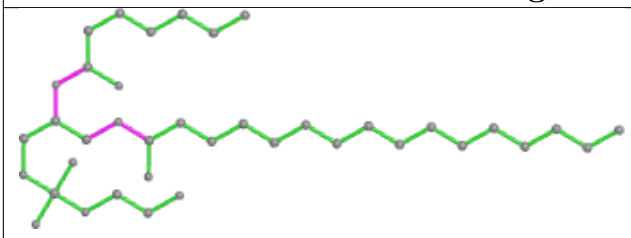


Torsions

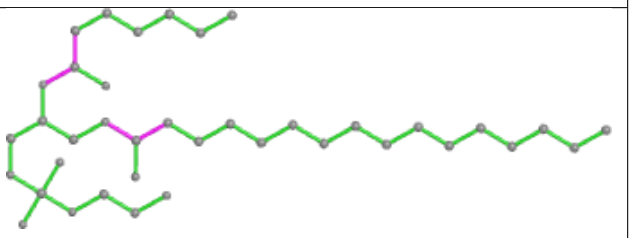


Rings

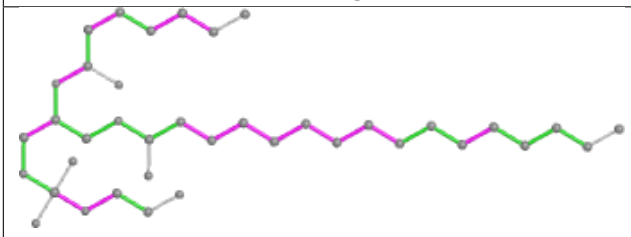
Ligand 3PE O 401



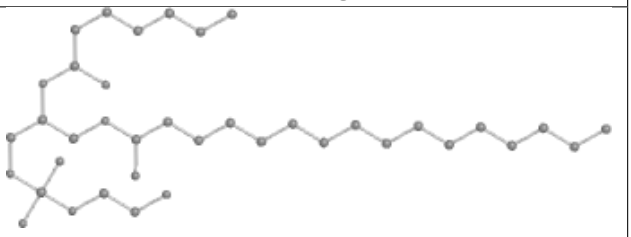
Bond lengths



Bond angles

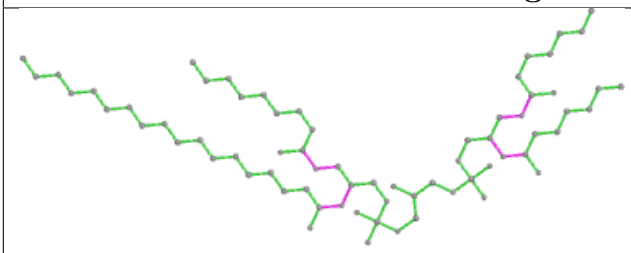


Torsions

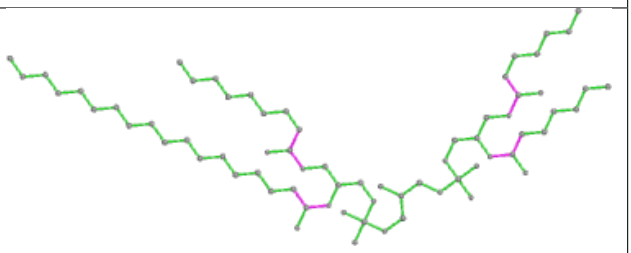


Rings

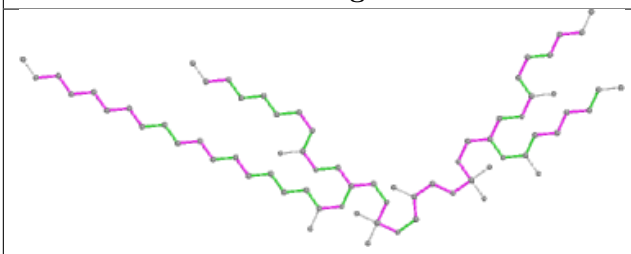
Ligand CDL B 602



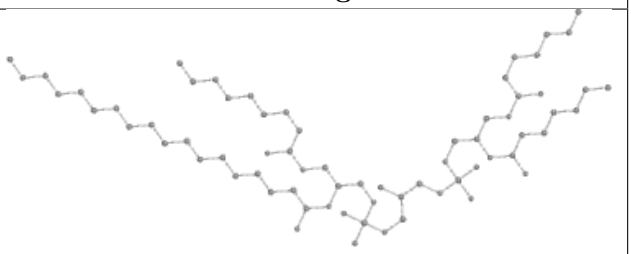
Bond lengths



Bond angles

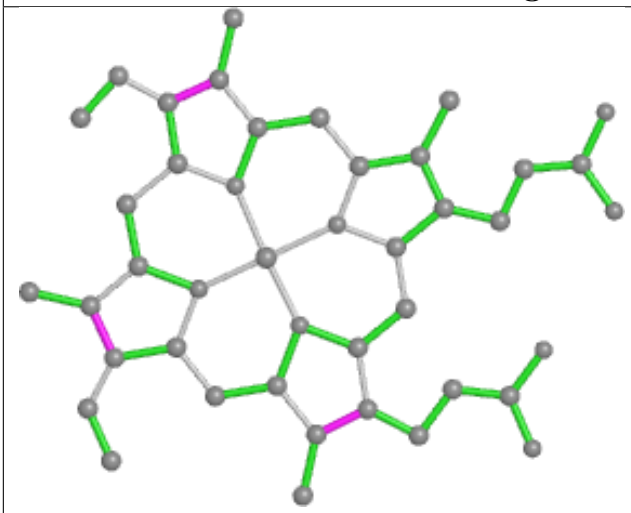


Torsions

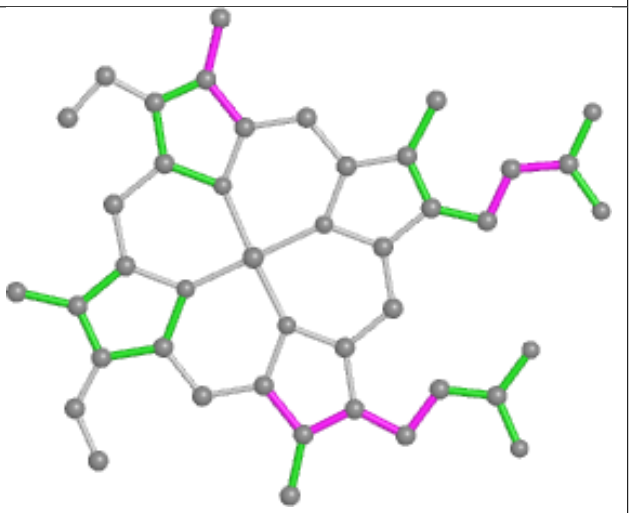


Rings

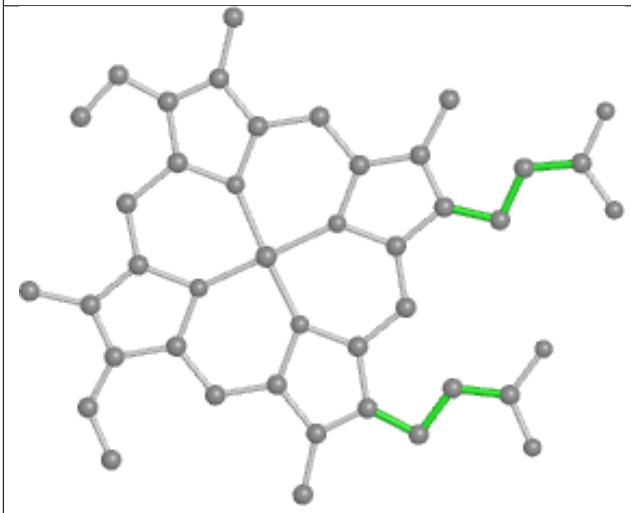
Ligand HEC P 403



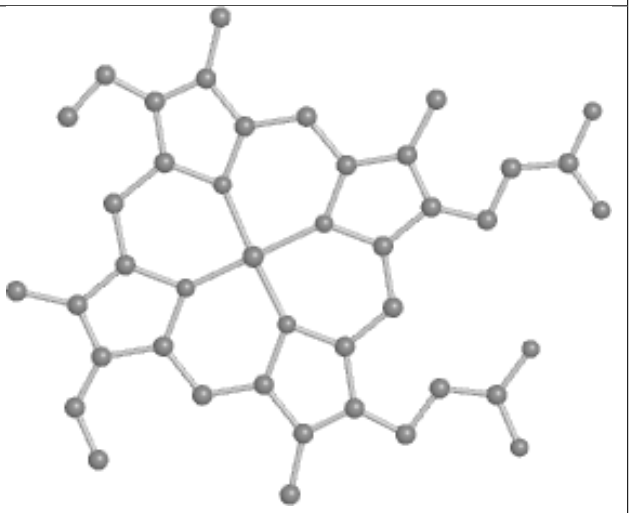
Bond lengths



Bond angles

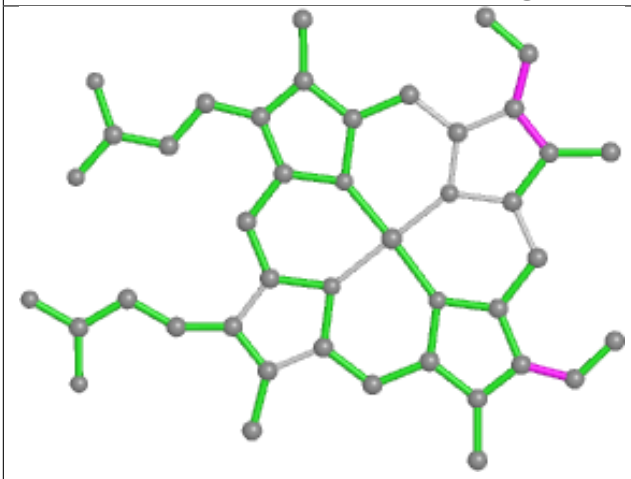


Torsions

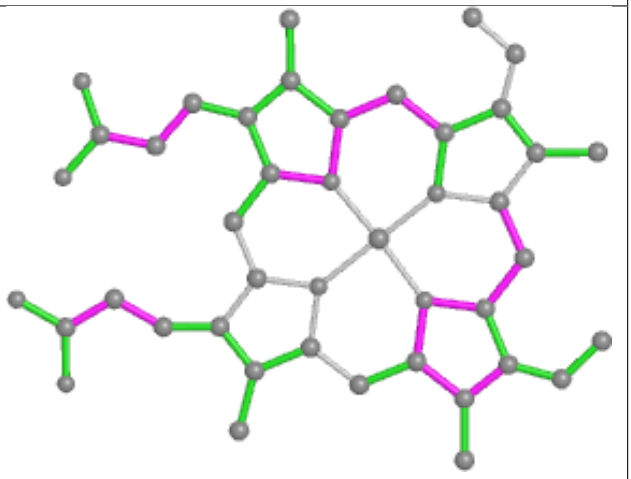


Rings

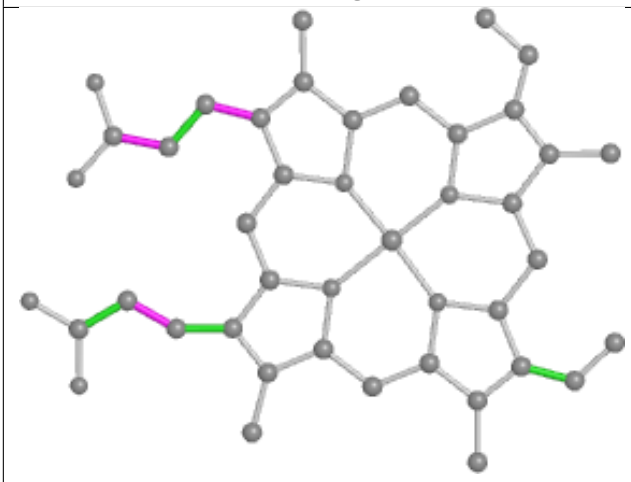
Ligand HEM O 403



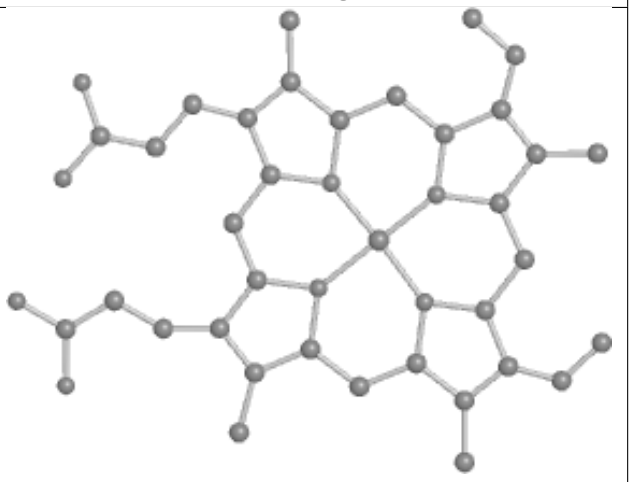
Bond lengths



Bond angles

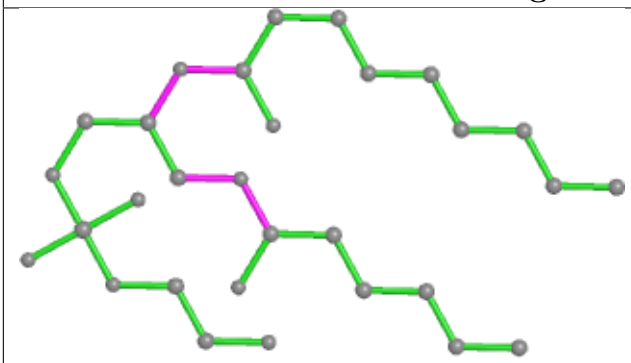


Torsions

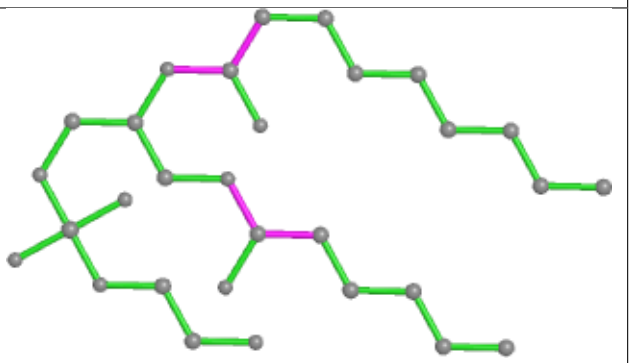


Rings

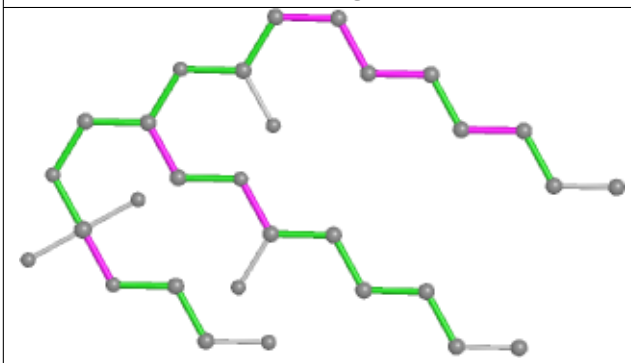
Ligand 3PE E 302



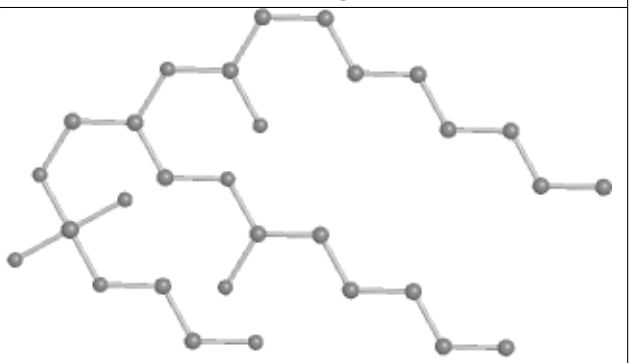
Bond lengths



Bond angles

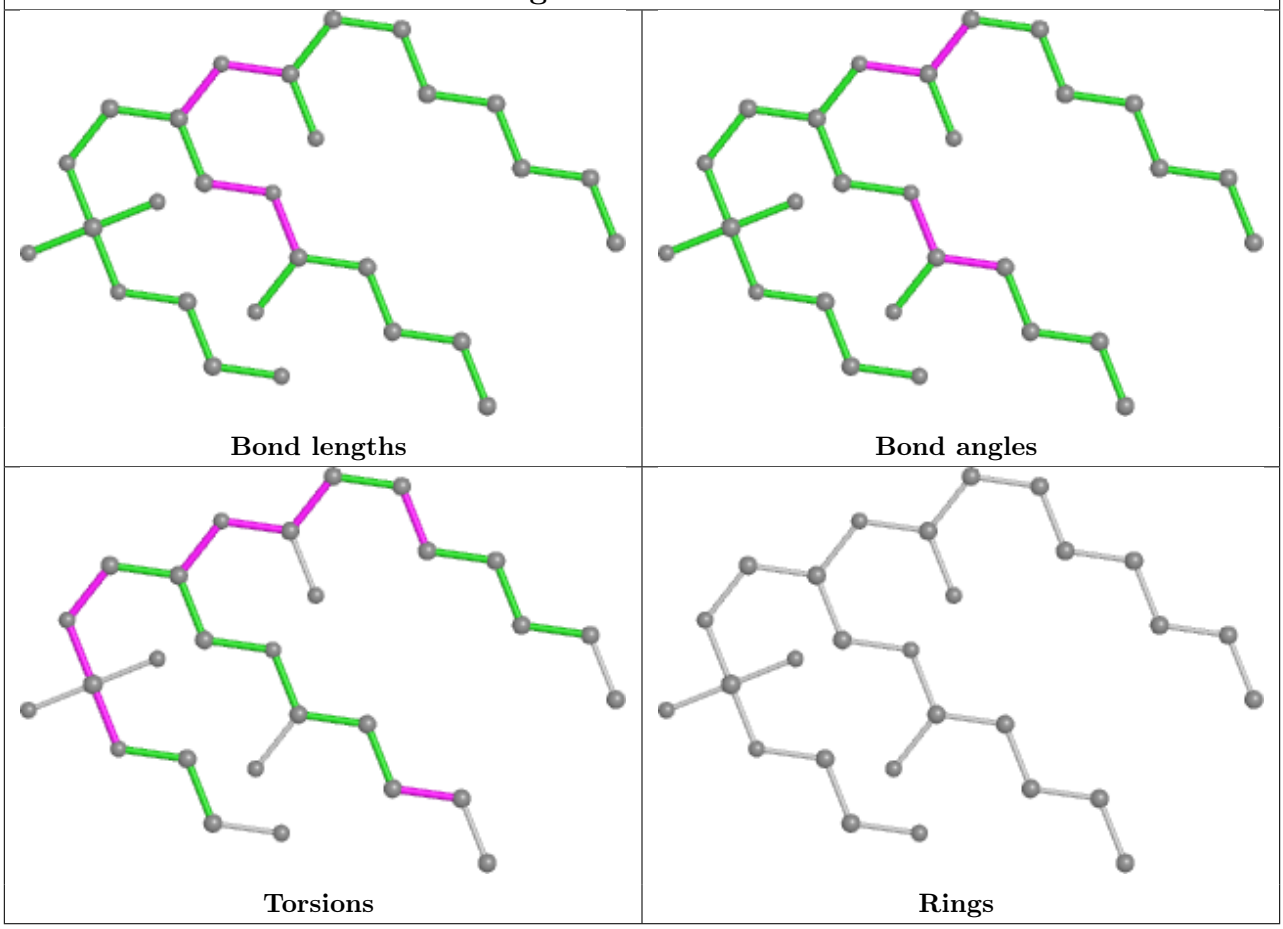


Torsions



Rings

Ligand 3PE C 401



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

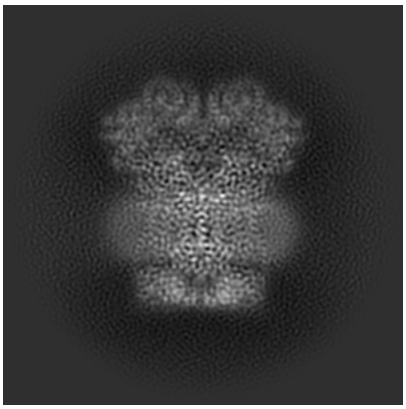
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-60275. These allow visual inspection of the internal detail of the map and identification of artifacts.

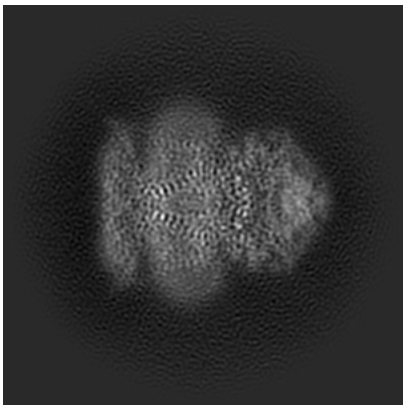
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

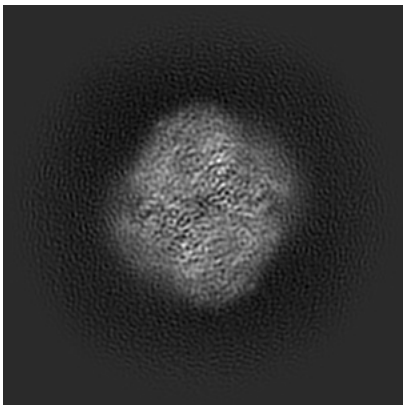
6.1.1 Primary map



X

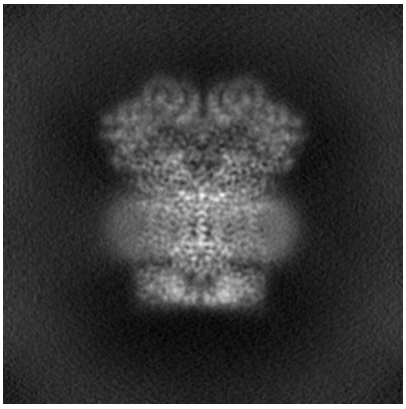


Y

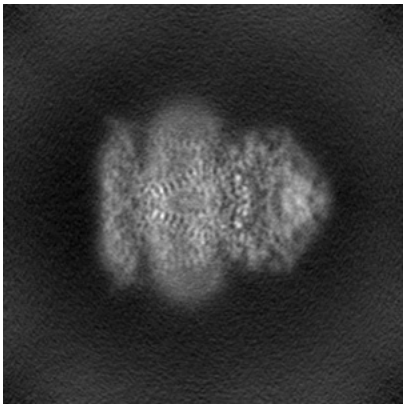


Z

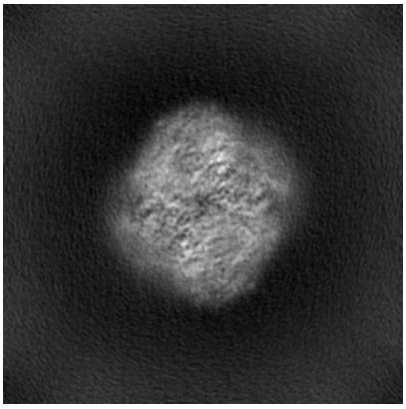
6.1.2 Raw map



X



Y

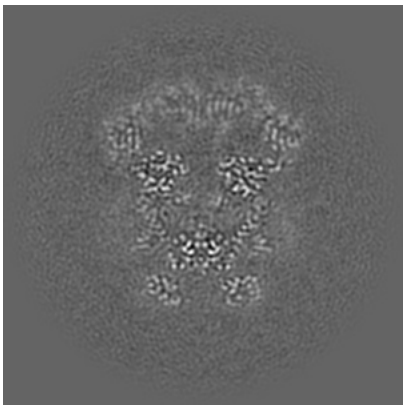


Z

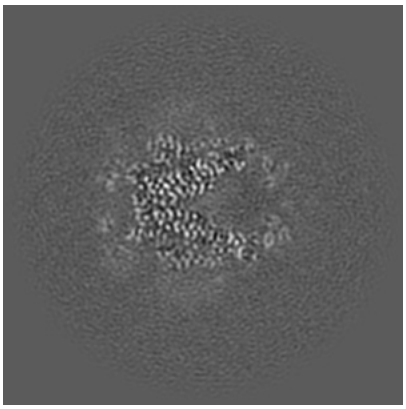
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

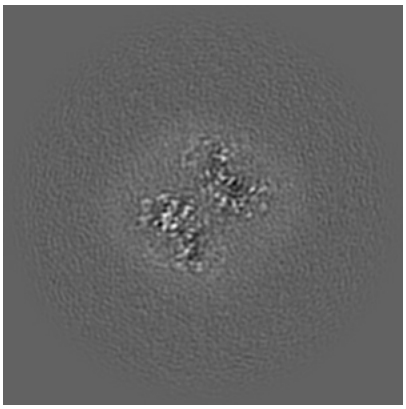
6.2.1 Primary map



X Index: 140

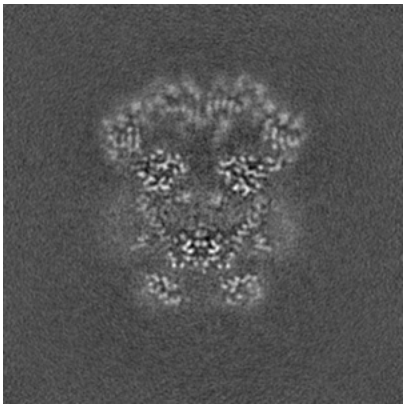


Y Index: 140

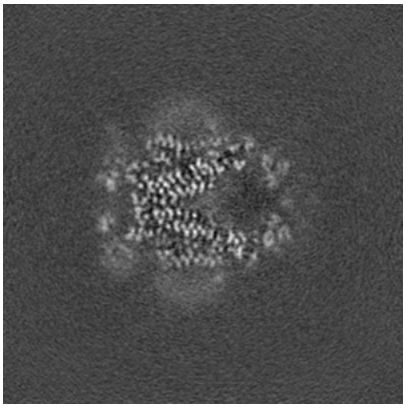


Z Index: 140

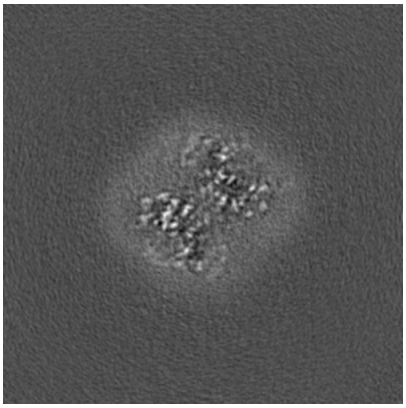
6.2.2 Raw map



X Index: 140



Y Index: 140

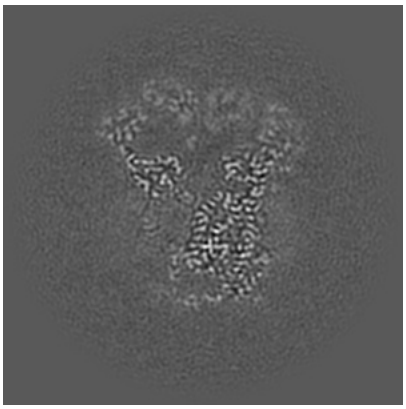


Z Index: 140

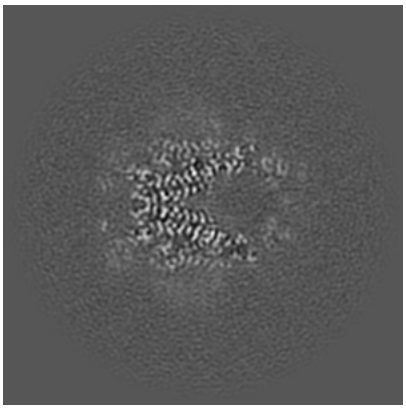
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

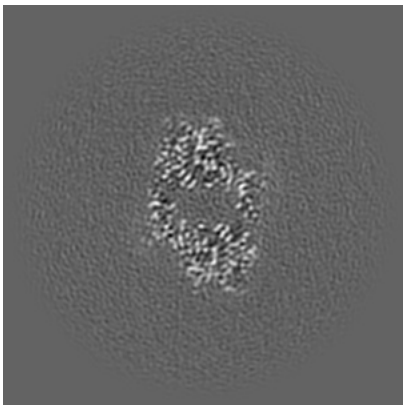
6.3.1 Primary map



X Index: 149

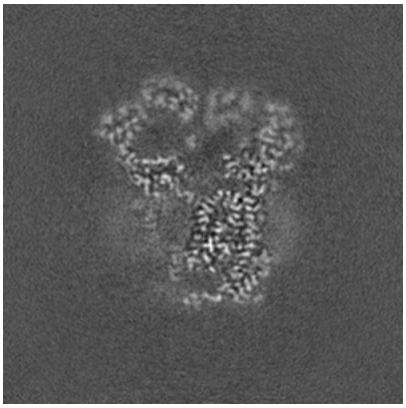


Y Index: 138

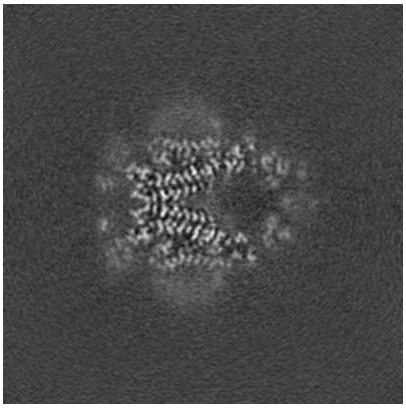


Z Index: 165

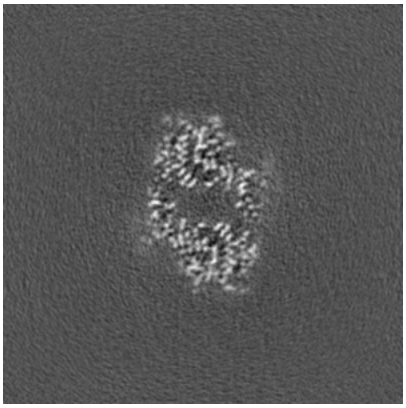
6.3.2 Raw map



X Index: 150



Y Index: 138

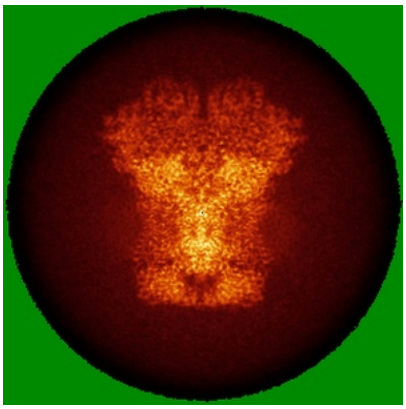


Z Index: 165

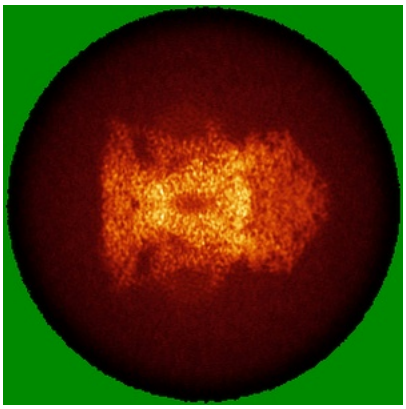
The images above show the largest variance slices of the map in three orthogonal directions.

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

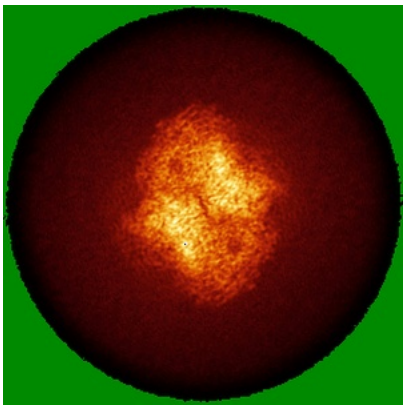
6.4.1 Primary map



X

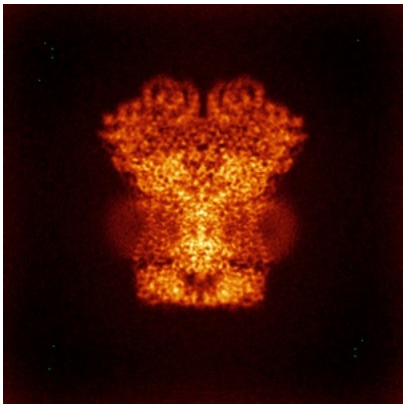


Y

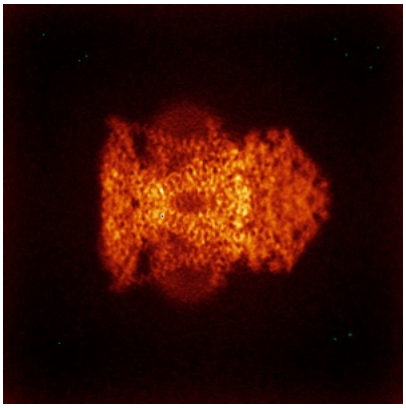


Z

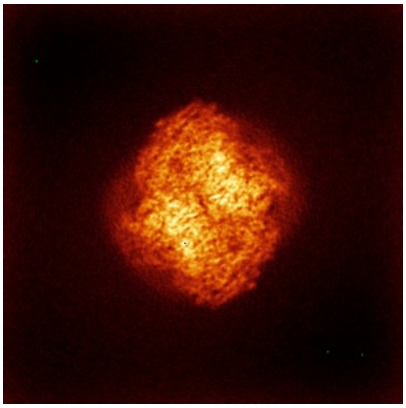
6.4.2 Raw map



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.

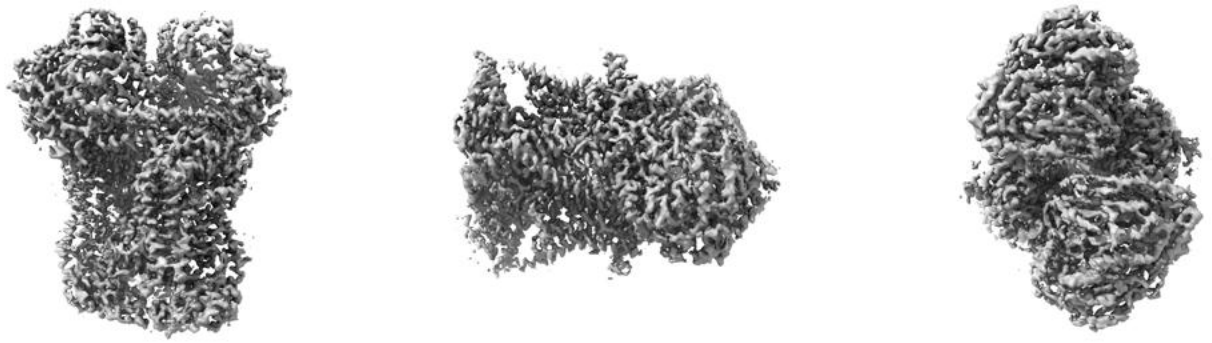
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.584. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

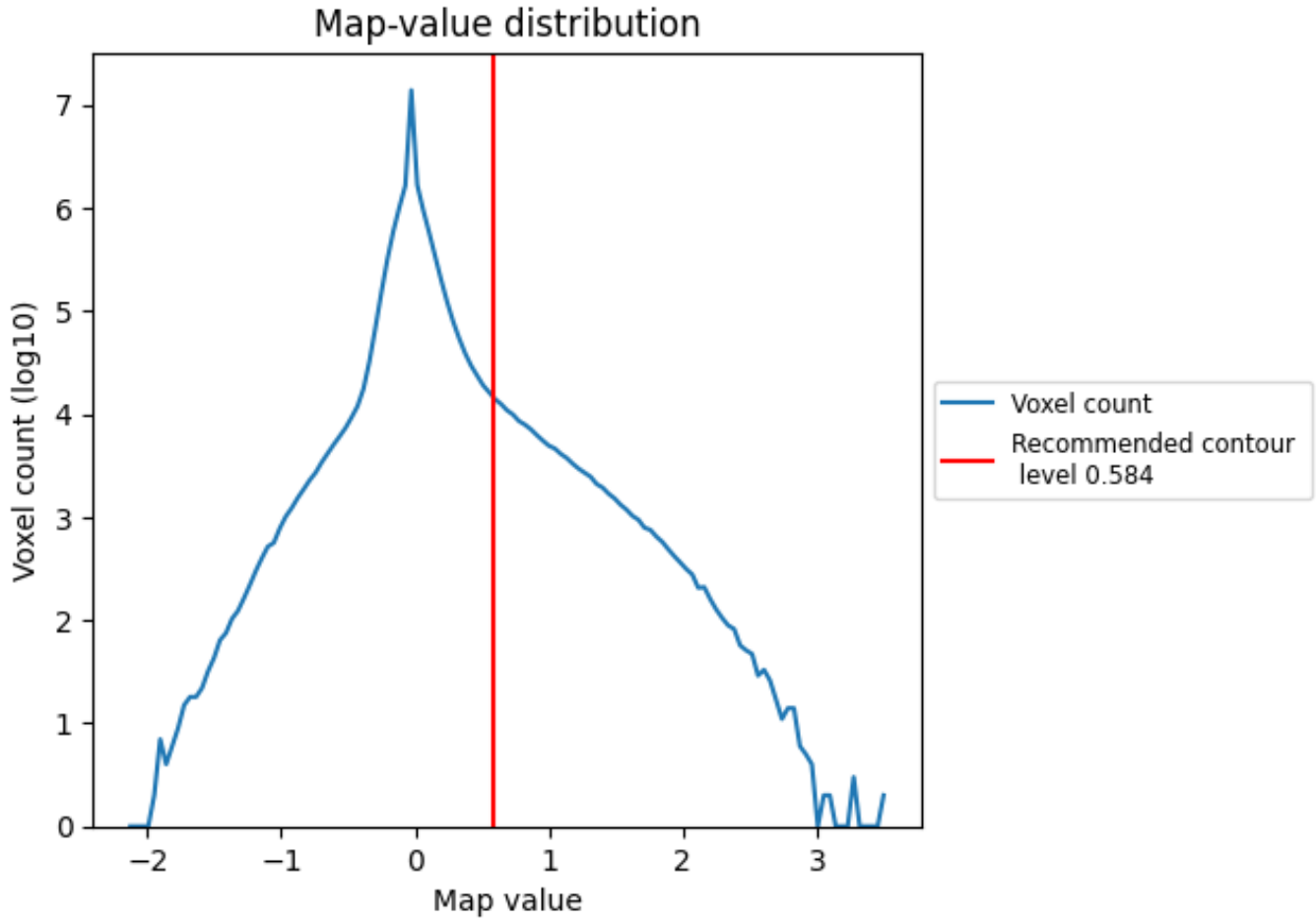
6.6 Mask visualisation (i)

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

7 Map analysis

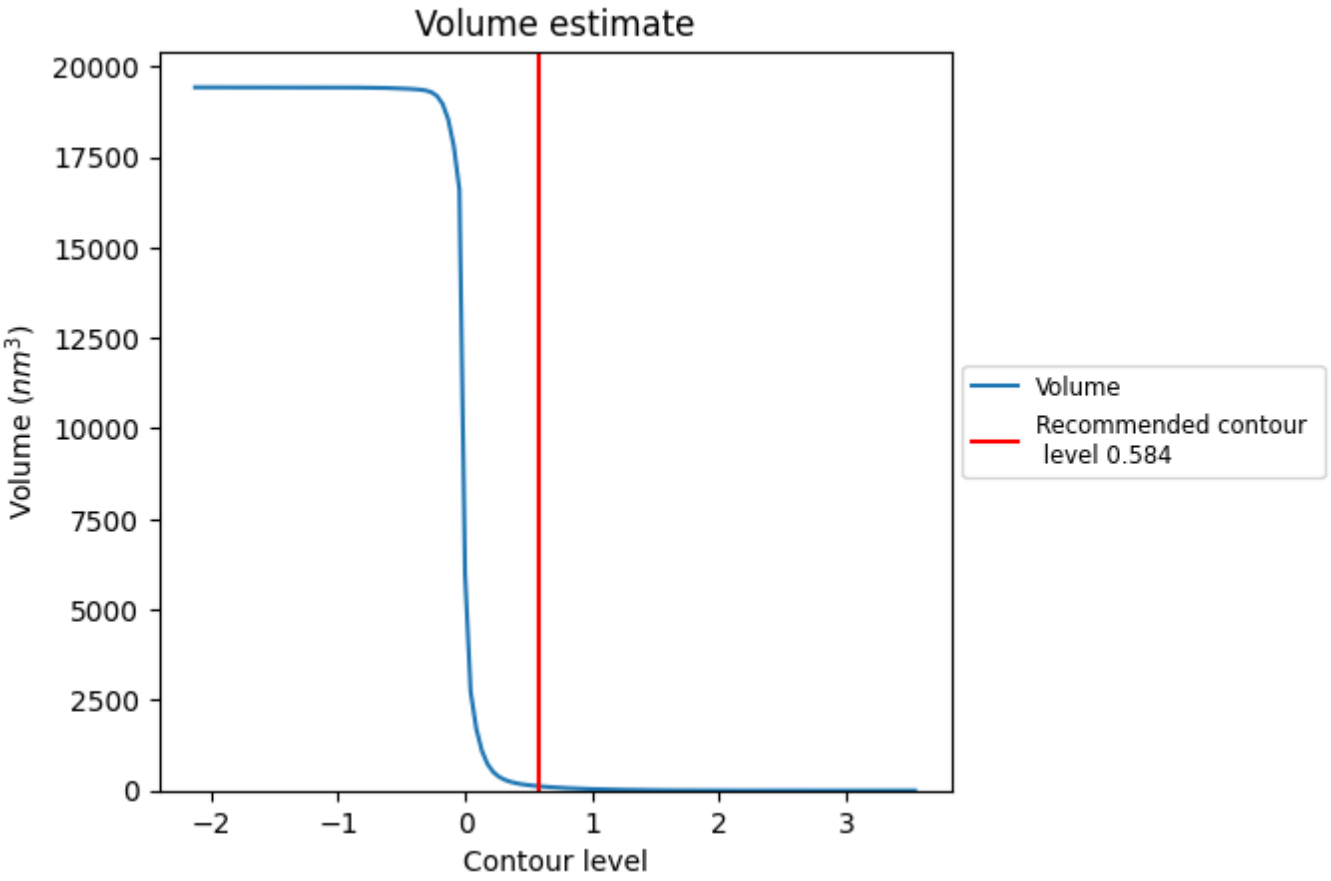
This section contains the results of statistical analysis of the map.

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.

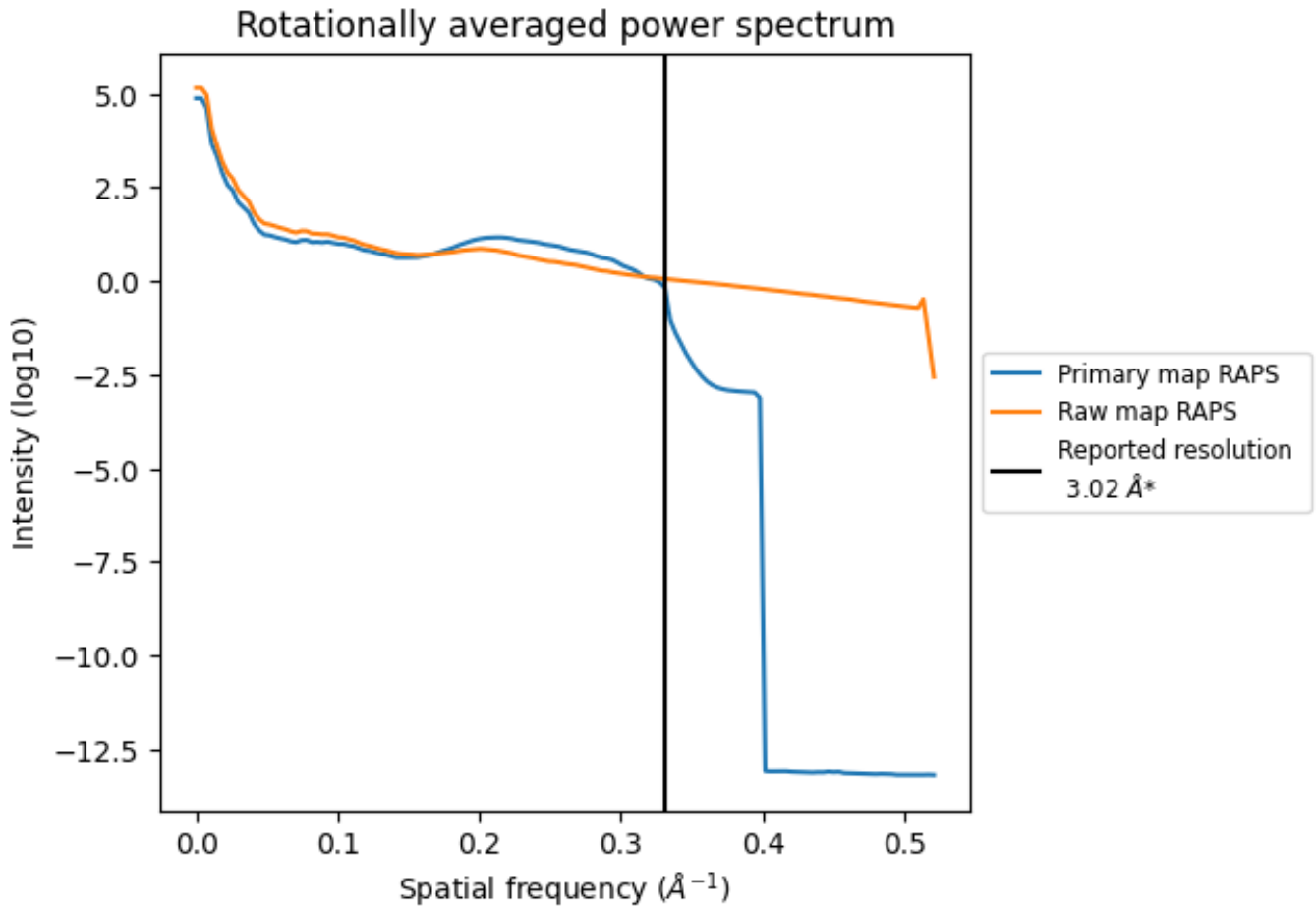
7.2 Volume estimate



The volume at the recommended contour level is 118 nm^3; this corresponds to an approximate mass of 107 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

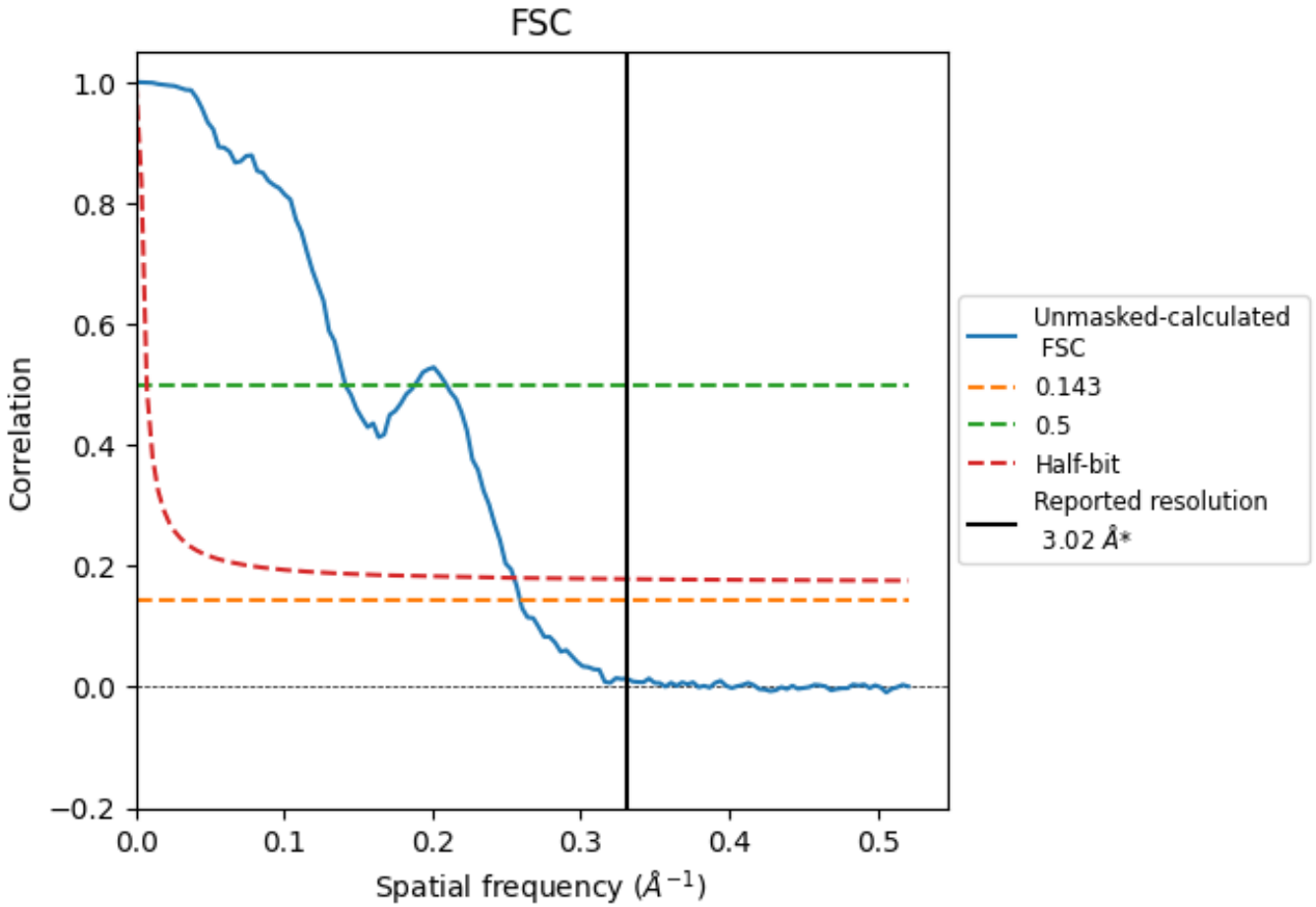


*Reported resolution corresponds to spatial frequency of 0.331 $Å^{-1}$

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 0.331 Å^{-1}

8.2 Resolution estimates (i)

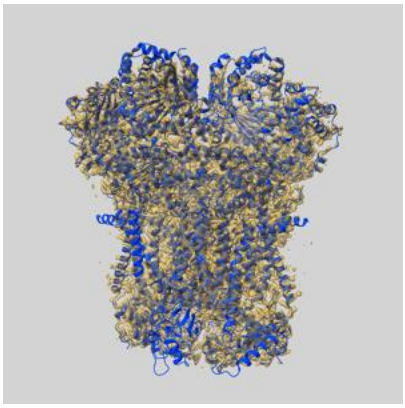
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.02	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.86	7.09	3.92

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.86 differs from the reported value 3.02 by more than 10 %

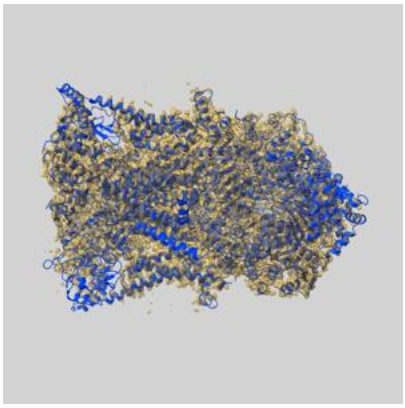
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-60275 and PDB model 8ZNO. Per-residue inclusion information can be found in section 3 on page 11.

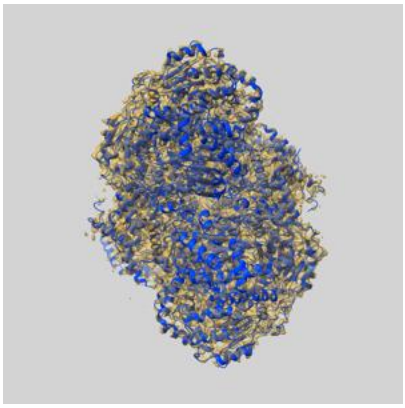
9.1 Map-model overlay



X



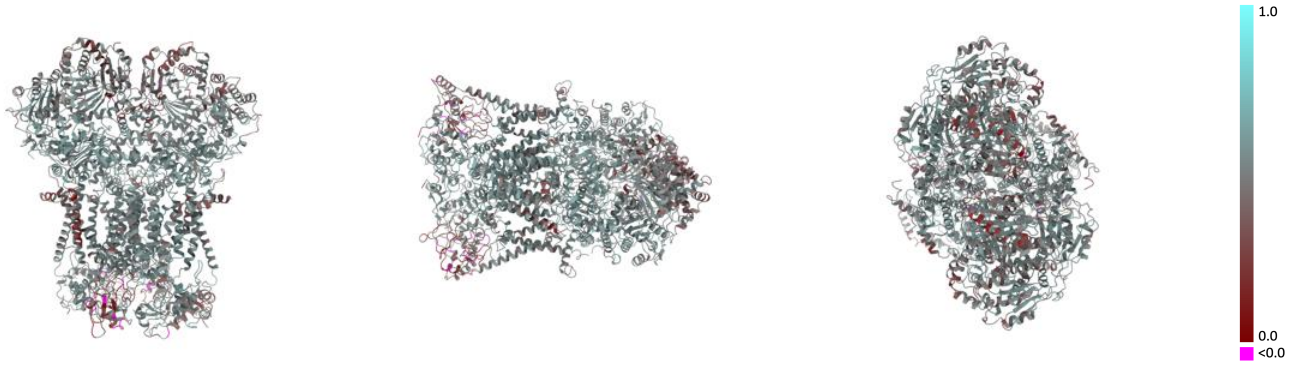
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.584 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

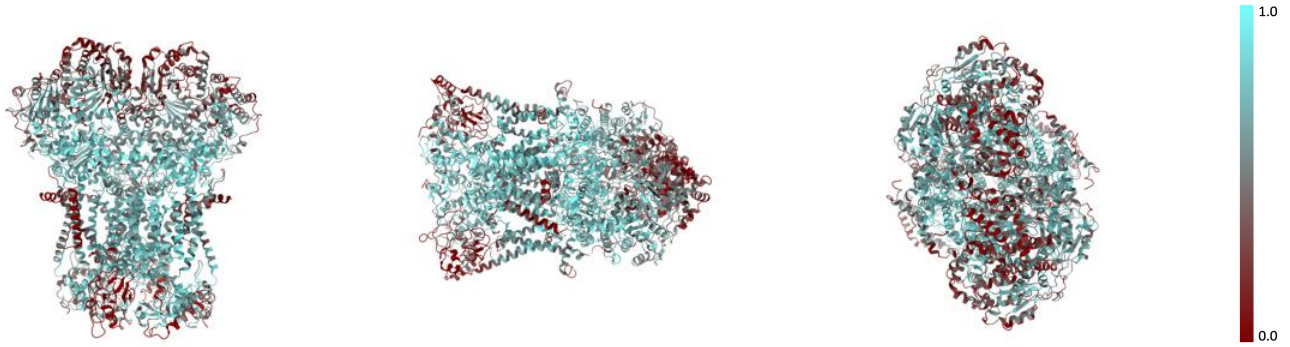
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

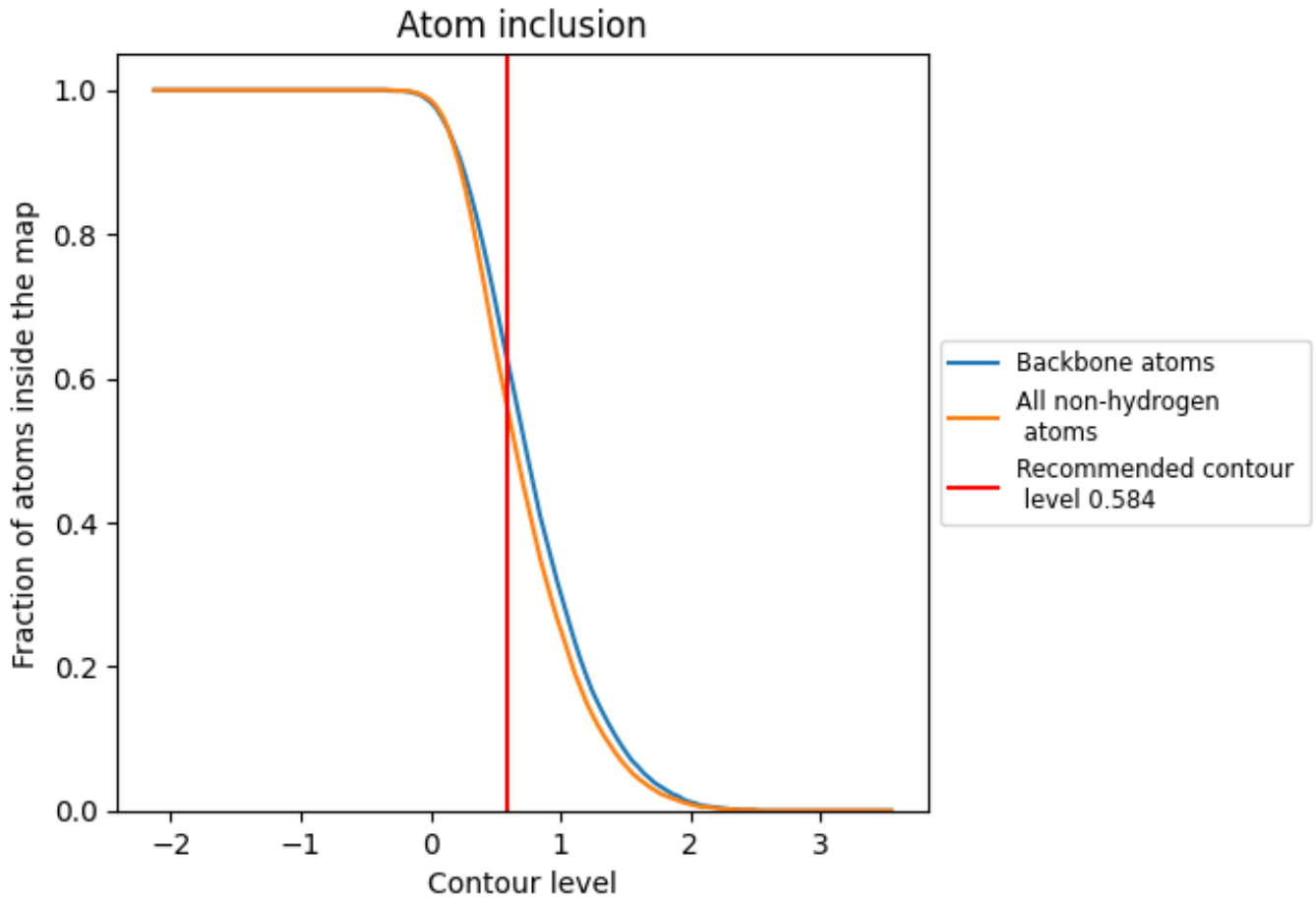
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.584).

9.4 Atom inclusion (i)



At the recommended contour level, 63% of all backbone atoms, 56% 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 (0.584) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5640	0.5020
A	0.4140	0.4740
B	0.6080	0.5290
C	0.7540	0.5590
D	0.7240	0.5430
E	0.1890	0.3410
F	0.7330	0.5510
G	0.4810	0.4850
H	0.3180	0.4580
J	0.3860	0.4670
K	0.0050	0.2690
M	0.4350	0.4770
N	0.6310	0.5310
O	0.7540	0.5560
P	0.7290	0.5470
Q	0.2700	0.3400
R	0.7160	0.5500
S	0.5060	0.4920
T	0.3220	0.4170
V	0.4820	0.4740
W	0.1260	0.3900