Full wwPDB EM Validation Report ⓘ

Jul 6, 2024 – 02:25 PM EDT

PDB ID	:	8UGE
EMDB ID	:	EMD-42222
Title	:	In-situ complex III, state II
Authors	:	Zheng, W.; Zhang, K.; Zhu, J.
Deposited on	:	2023-10-05
Resolution	:	3.50 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:

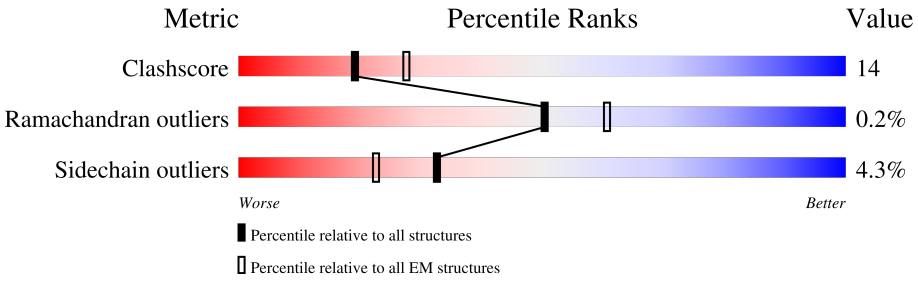
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.50 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.



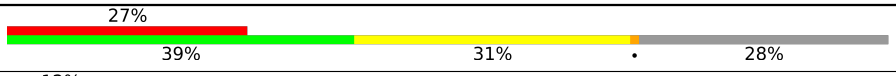
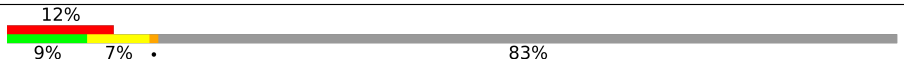
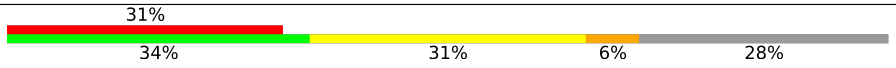
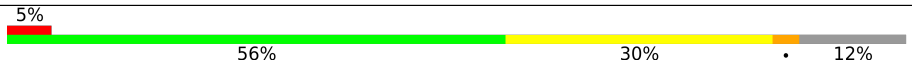
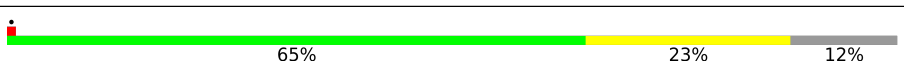
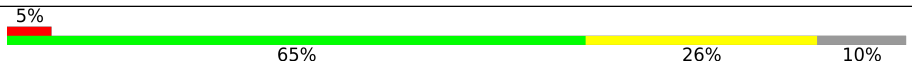
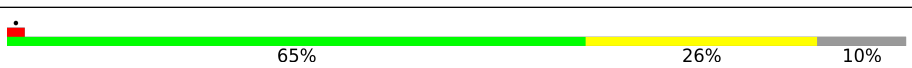
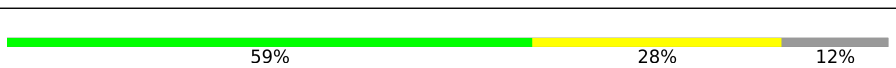
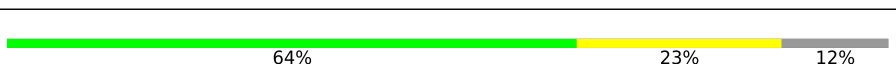
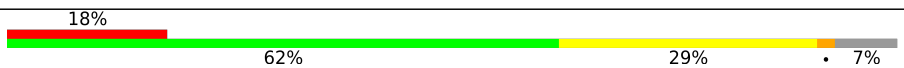
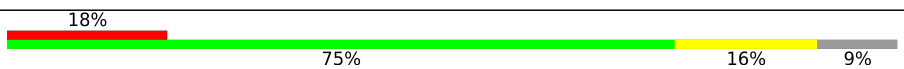
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	3A	480	69% 22% • 8%
1	3N	480	65% 26% • 7%
2	3B	453	67% 24% • 8%
2	3O	453	67% 25% • 8%
3	3C	379	69% 30% •
3	3P	379	75% 23% •
4	3D	325	48% 24% • 27%
4	3Q	325	54% 18% • 26%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	3E	274	
5	3I	274	
5	3R	274	
5	3V	274	
6	3F	111	
6	3S	111	
7	3G	82	
7	3T	82	
8	3H	91	
8	3U	91	
9	3J	64	
9	3W	64	
10	3X	56	
10	3Y	56	

2 Entry composition (i)

There are 17 unique types of molecules in this entry. The entry contains 33534 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	3A	440	Total	C	N	O	S	0	0
			3411	2131	599	662	19		
1	3N	445	Total	C	N	O	S	1	0
			3424	2162	606	637	19		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3B	418	Total	C	N	O	S	0	0
			3138	1965	555	610	8		
2	3O	417	Total	C	N	O	S	0	0
			3124	1960	554	602	8		

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3C	379	Total	C	N	O	S	0	0
			3025	2031	471	502	21		
3	3P	379	Total	C	N	O	S	0	0
			3024	2031	471	501	21		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3D	237	Total	C	N	O	S	0	0
			1888	1205	325	342	16		
4	3Q	239	Total	C	N	O	S	0	0
			1904	1215	327	346	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	3E	196	Total	C	N	O	S	0	0
			1518	955	265	291	7		
5	3I	47	Total	C	N	O	S	0	0
			337	210	62	64	1		
5	3R	196	Total	C	N	O	S	0	0
			1518	955	265	291	7		
5	3V	31	Total	C	N	O	S	0	0
			223	137	45	40	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	3F	98	Total	C	N	O	S	0	0
			868	557	152	157	2		
6	3S	98	Total	C	N	O	S	0	0
			868	557	152	157	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	3G	74	Total	C	N	O	S	0	0
			628	411	116	99	2		
7	3T	74	Total	C	N	O	S	0	0
			628	411	116	99	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	3H	65	Total	C	N	O	S	0	0
			533	325	97	106	5		
8	3U	65	Total	C	N	O	S	0	0
			533	325	97	106	5		

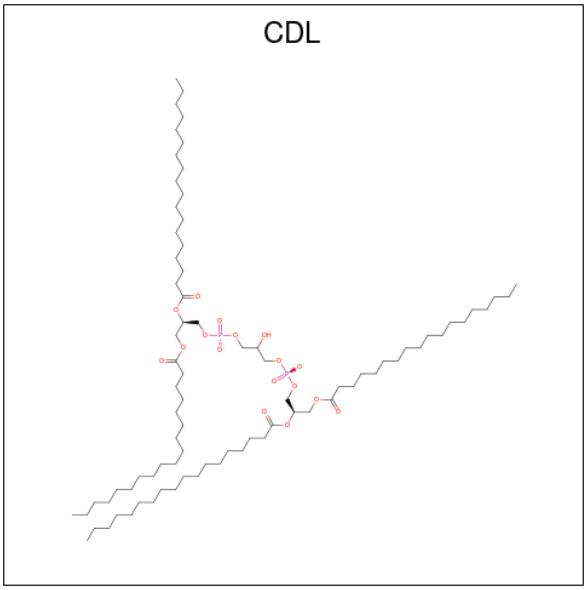
- Molecule 9 is a protein called Ubiquinol-cytochrome c reductase complex 7.2 kDa protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	3J	56	Total	C	N	O	0	0
			464	305	82	77		
9	3W	56	Total	C	N	O	0	0
			464	305	82	77		

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

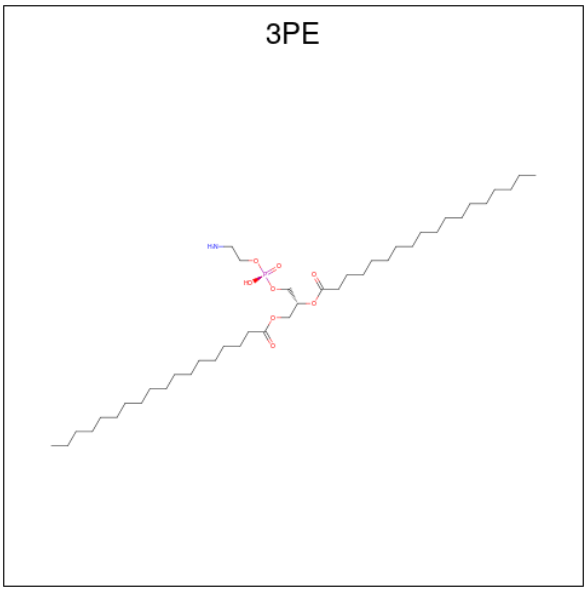
Mol	Chain	Residues	Atoms					AltConf	Trace
10	3X	52	Total	C	N	O	S	0	0
			429	286	75	66	2		
10	3Y	51	Total	C	N	O	S	0	0
			421	281	74	65	1		

- Molecule 11 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



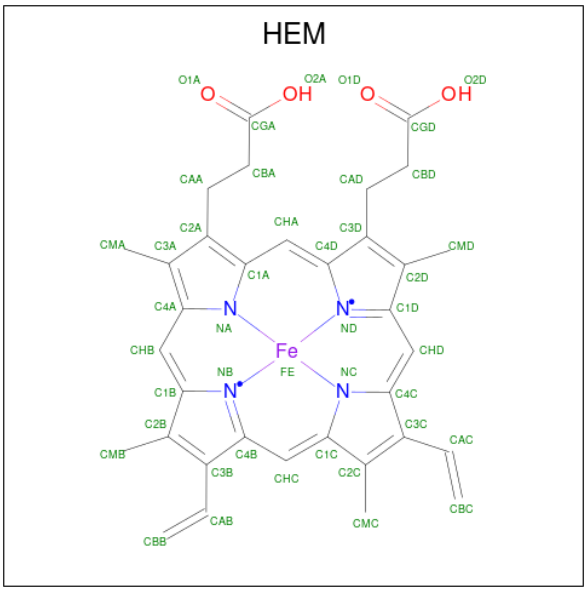
Mol	Chain	Residues	Atoms				AltConf
11	3A	1	Total	C	O	P	0
			58	39	17	2	
11	3C	1	Total	C	O	P	0
			52	33	17	2	
11	3G	1	Total	C	O	P	0
			56	37	17	2	
11	3P	1	Total	C	O	P	0
			56	37	17	2	
11	3P	1	Total	C	O	P	0
			43	24	17	2	
11	3Q	1	Total	C	O	P	0
			57	38	17	2	

- Molecule 12 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



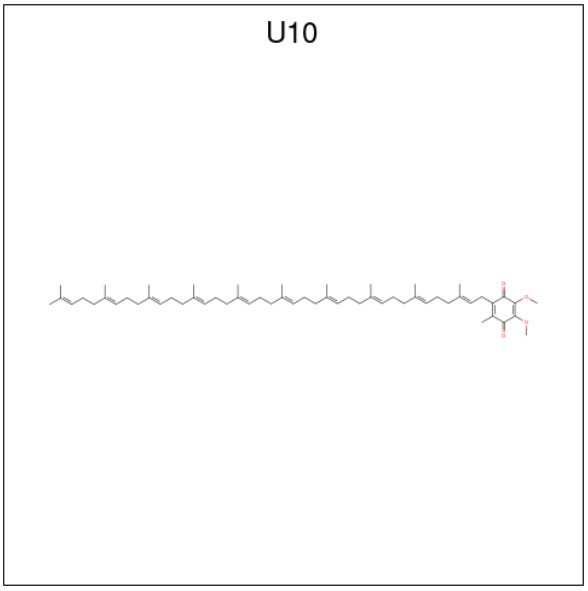
Mol	Chain	Residues	Atoms					AltConf
12	3A	1	Total	C	N	O	P	0
			27	17	1	8	1	
12	3A	1	Total	C	N	O	P	0
			32	22	1	8	1	
12	3C	1	Total	C	N	O	P	0
			35	25	1	8	1	
12	3C	1	Total	C	N	O	P	0
			34	24	1	8	1	
12	3D	1	Total	C	N	O	P	0
			33	23	1	8	1	
12	3G	1	Total	C	N	O	P	0
			29	19	1	8	1	
12	3N	1	Total	C	N	O	P	0
			33	23	1	8	1	
12	3N	1	Total	C	N	O	P	0
			25	15	1	8	1	
12	3P	1	Total	C	N	O	P	0
			33	23	1	8	1	
12	3Q	1	Total	C	N	O	P	0
			47	37	1	8	1	
12	3Y	1	Total	C	N	O	P	0
			30	20	1	8	1	

- Molecule 13 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



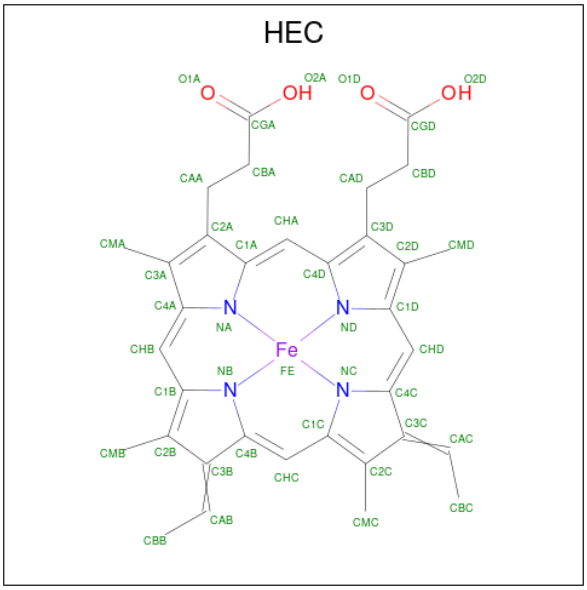
Mol	Chain	Residues	Atoms					AltConf
13	3C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
13	3C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
13	3P	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
13	3P	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 14 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$) (labeled as "Ligand of Interest" by depositor).



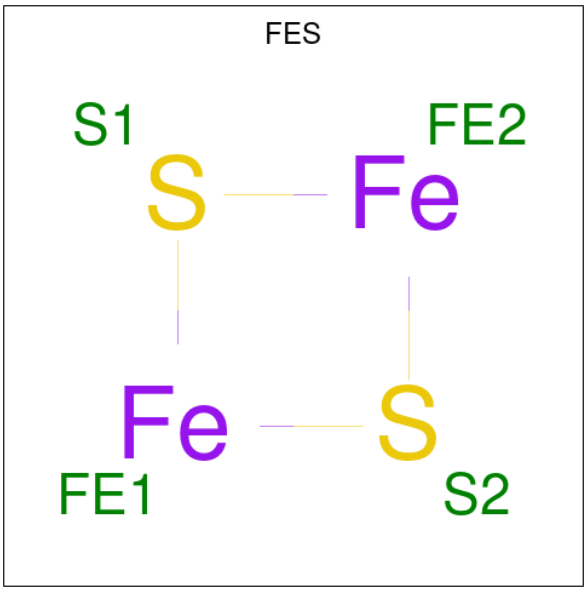
Mol	Chain	Residues	Atoms			AltConf
14	3C	1	Total	C	O	0
			24	20	4	
14	3C	1	Total	C	O	0
			23	19	4	
14	3P	1	Total	C	O	0
			23	19	4	
14	3P	1	Total	C	O	0
			28	24	4	

- Molecule 15 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



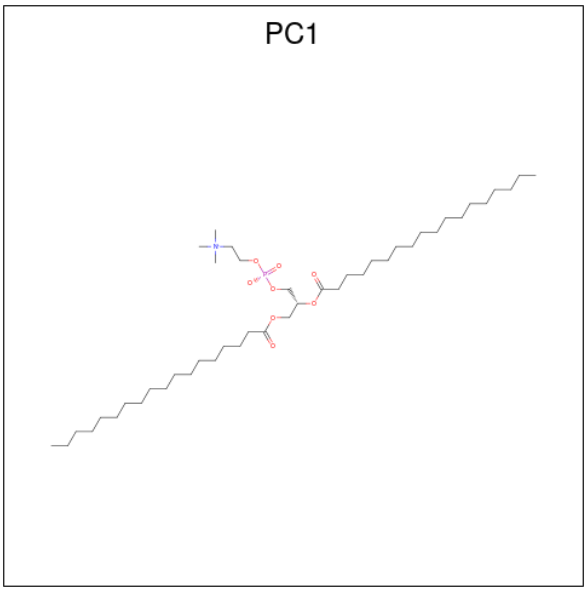
Mol	Chain	Residues	Atoms					AltConf
15	3D	1	Total	C	Fe	N	O	0
			42	34	1	4	3	
15	3Q	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 16 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			AltConf
16	3E	1	Total	Fe	S	0
			4	2	2	
16	3R	1	Total	Fe	S	0
			4	2	2	

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



Mol	Chain	Residues	Atoms					AltConf
17	3E	1	Total	C	N	O	P	0
			47	37	1	8	1	

Continued on next page...

Continued from previous page...

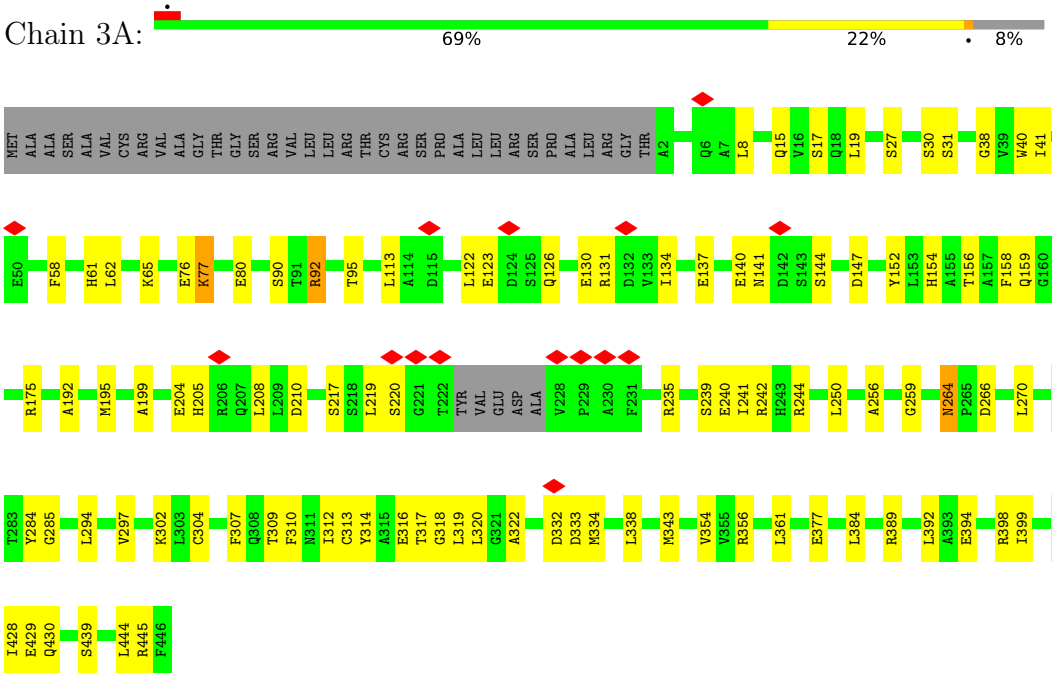
Mol	Chain	Residues	Atoms					AltConf
17	3R	1	Total	C	N	O	P	0
			45	35	1	8	1	
17	3X	1	Total	C	N	O	P	0
			29	19	1	8	1	

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.

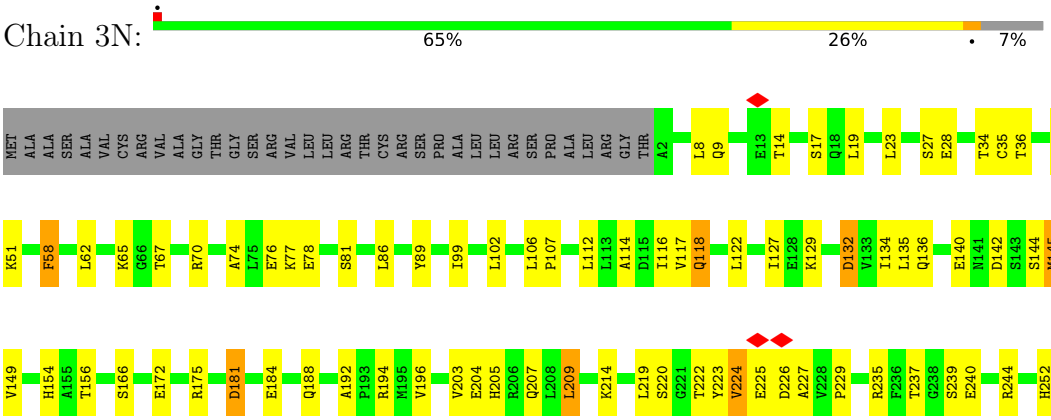
• Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial

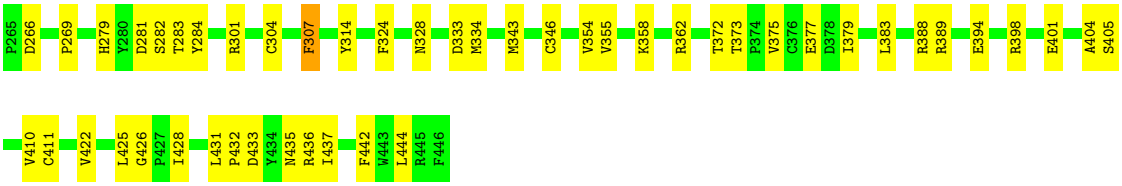
Chain 3A:



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

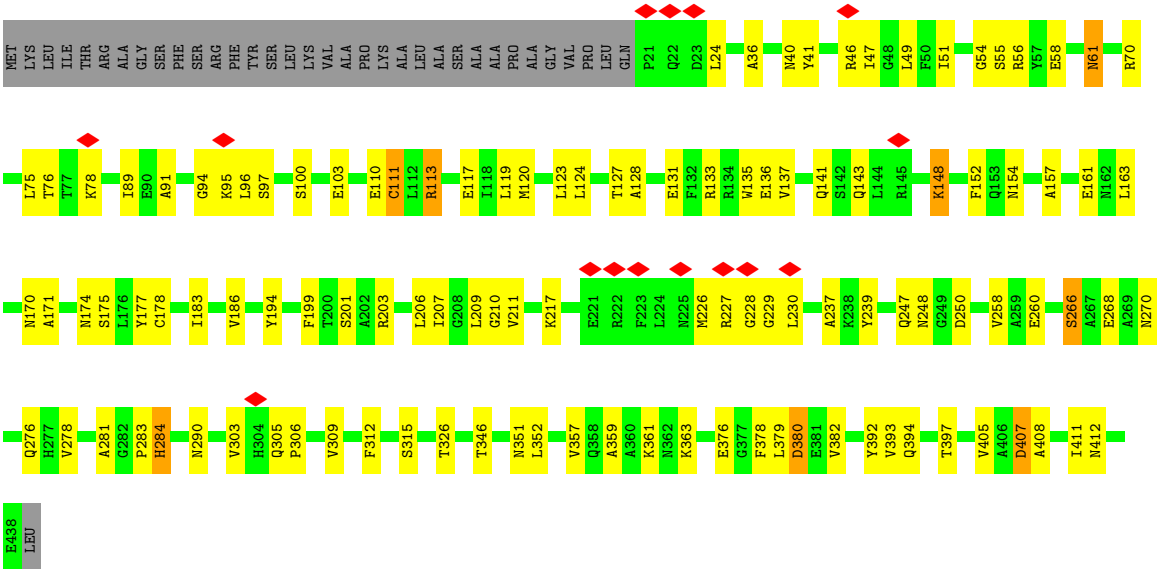
Chain 3N:





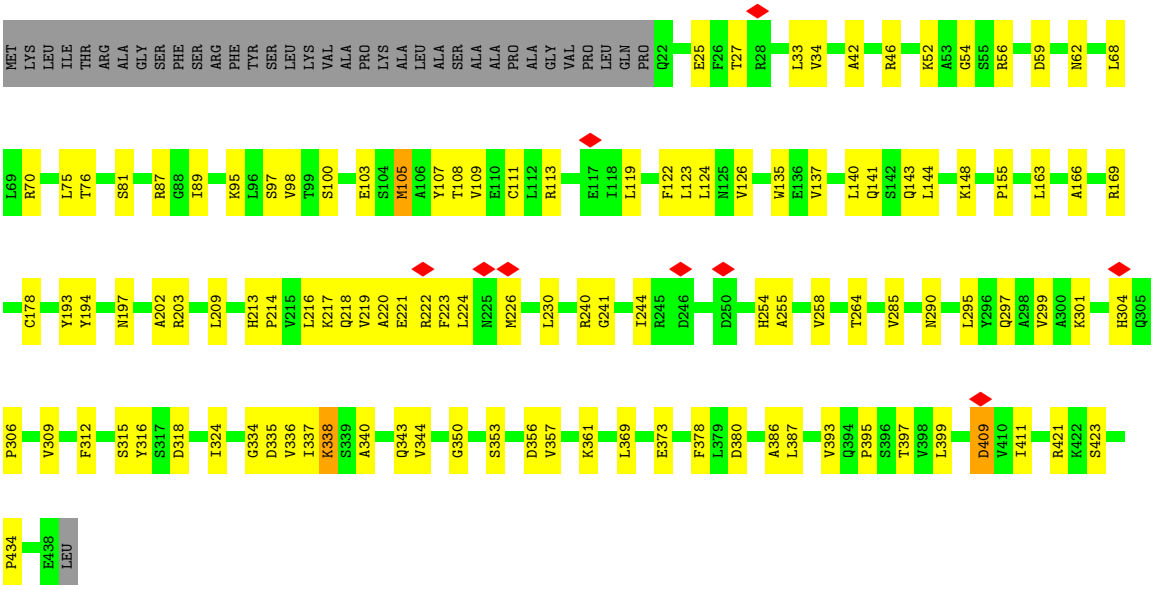
• Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain 3B:



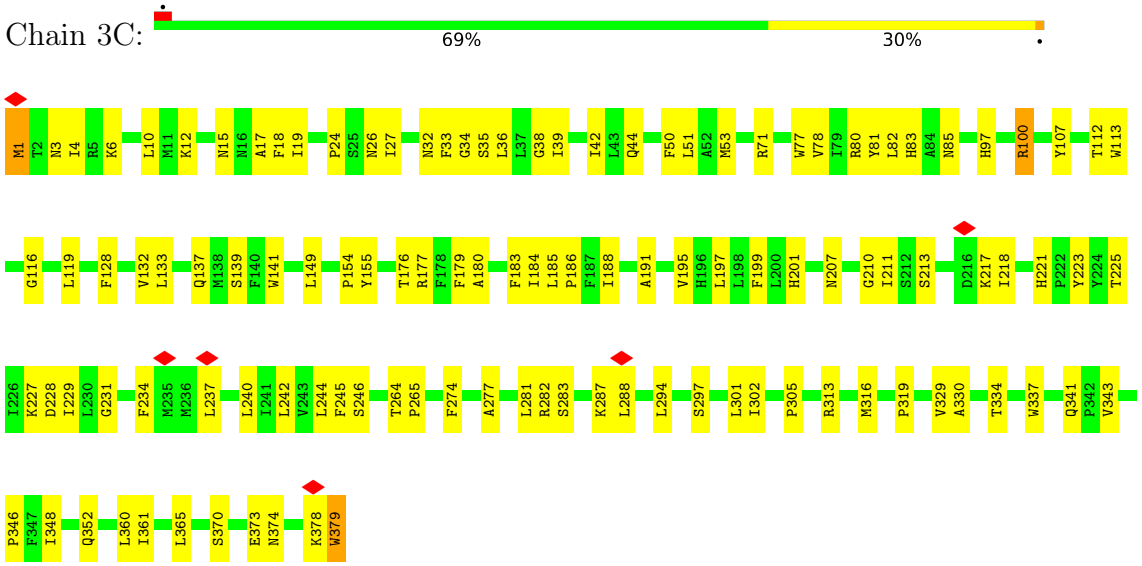
• Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain 3O:



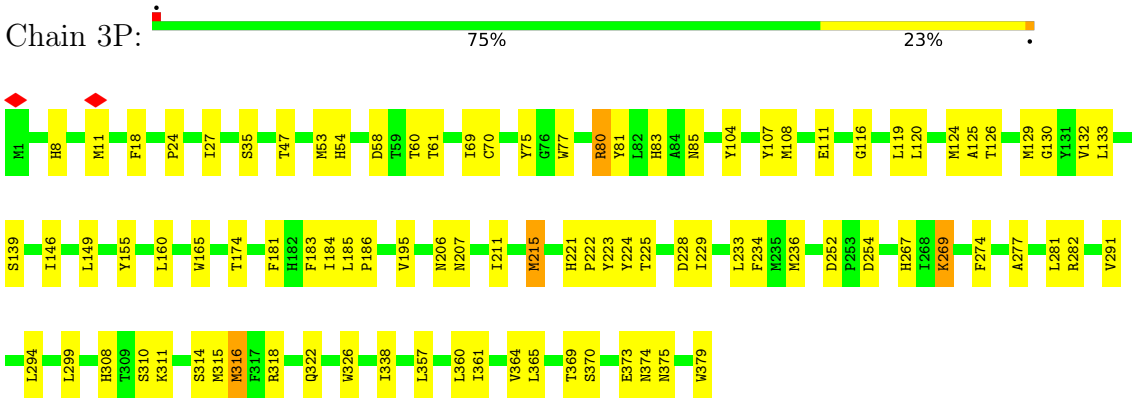
• Molecule 3: Cytochrome b

Chain 3C:



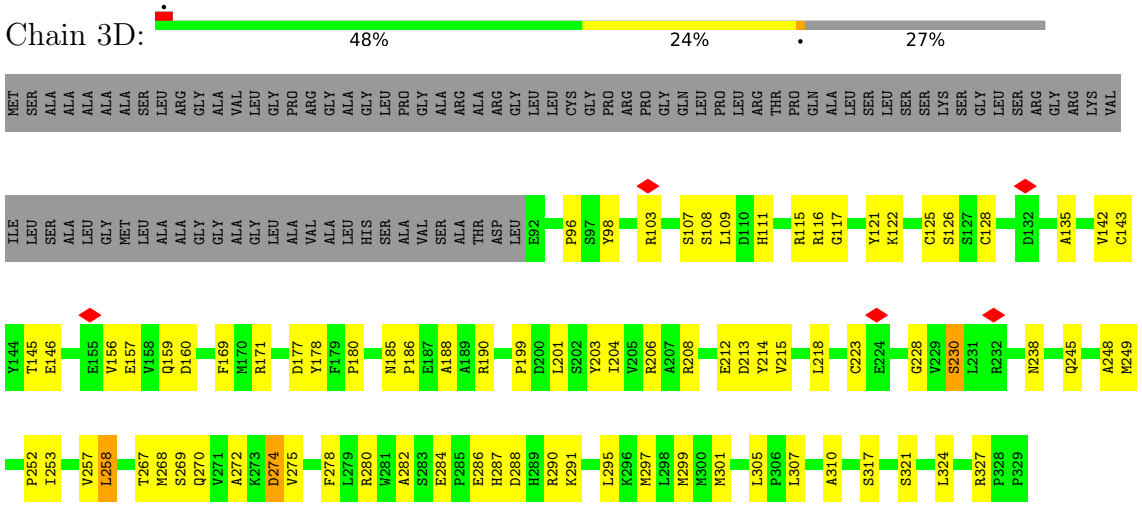
• Molecule 3: Cytochrome b

Chain 3P:



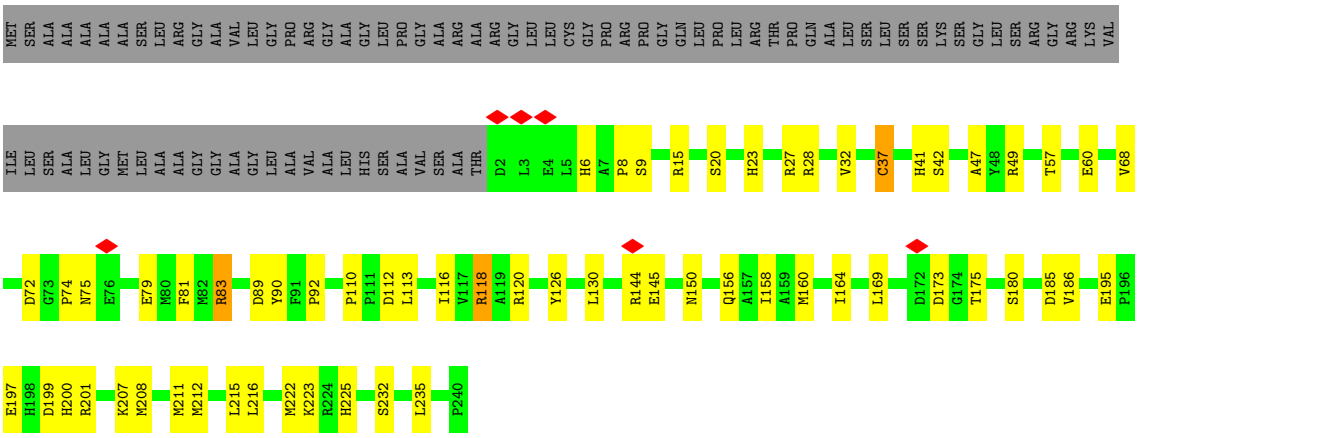
• Molecule 4: Cytochrome c1, heme protein, mitochondrial

Chain 3D:



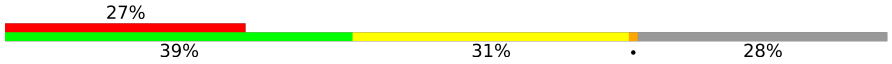
• Molecule 4: Cytochrome c1, heme protein, mitochondrial

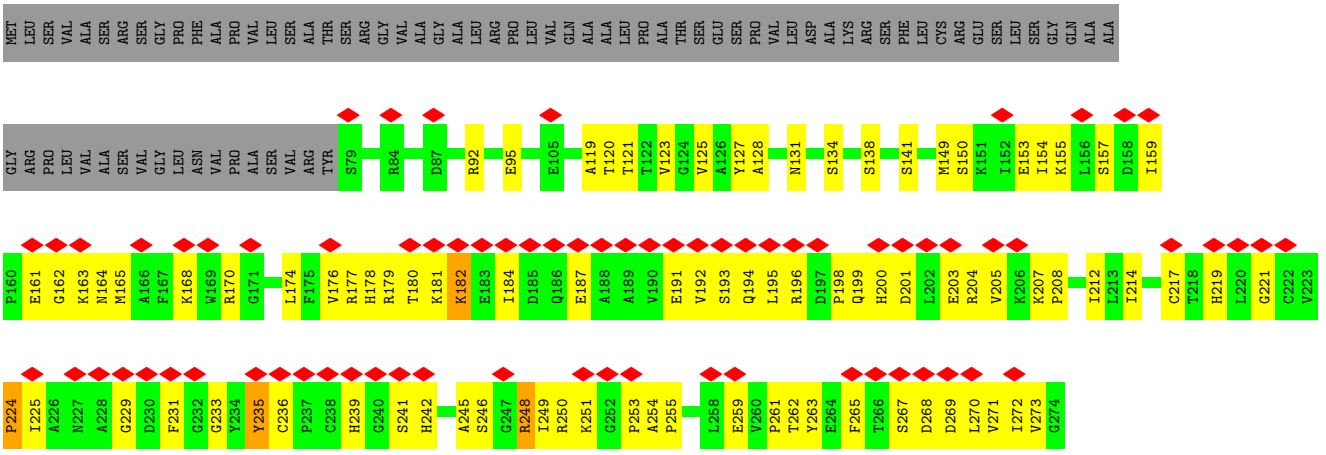
Chain 3Q:



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

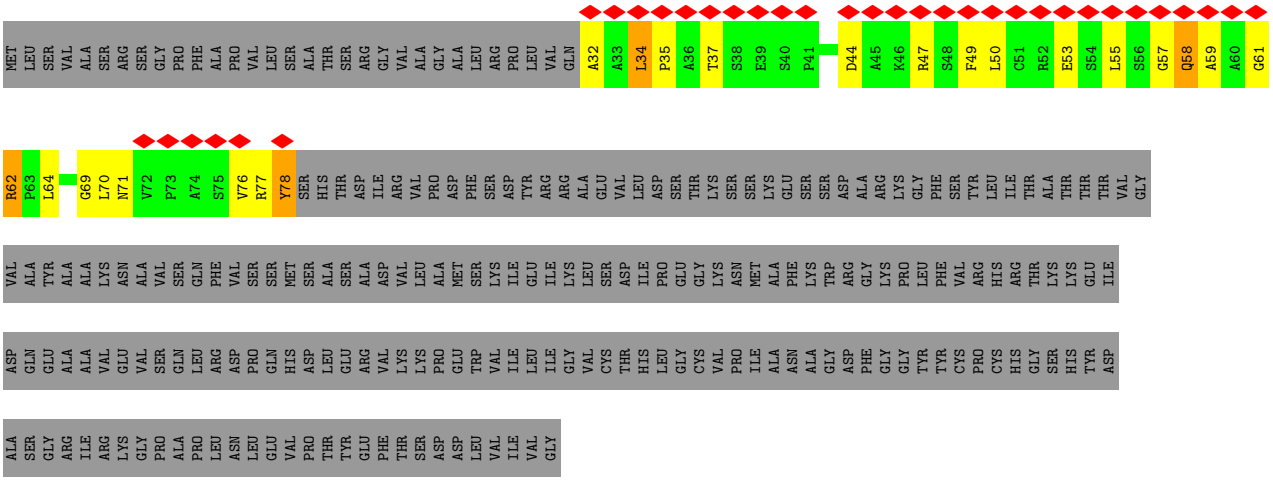
Chain 3E:





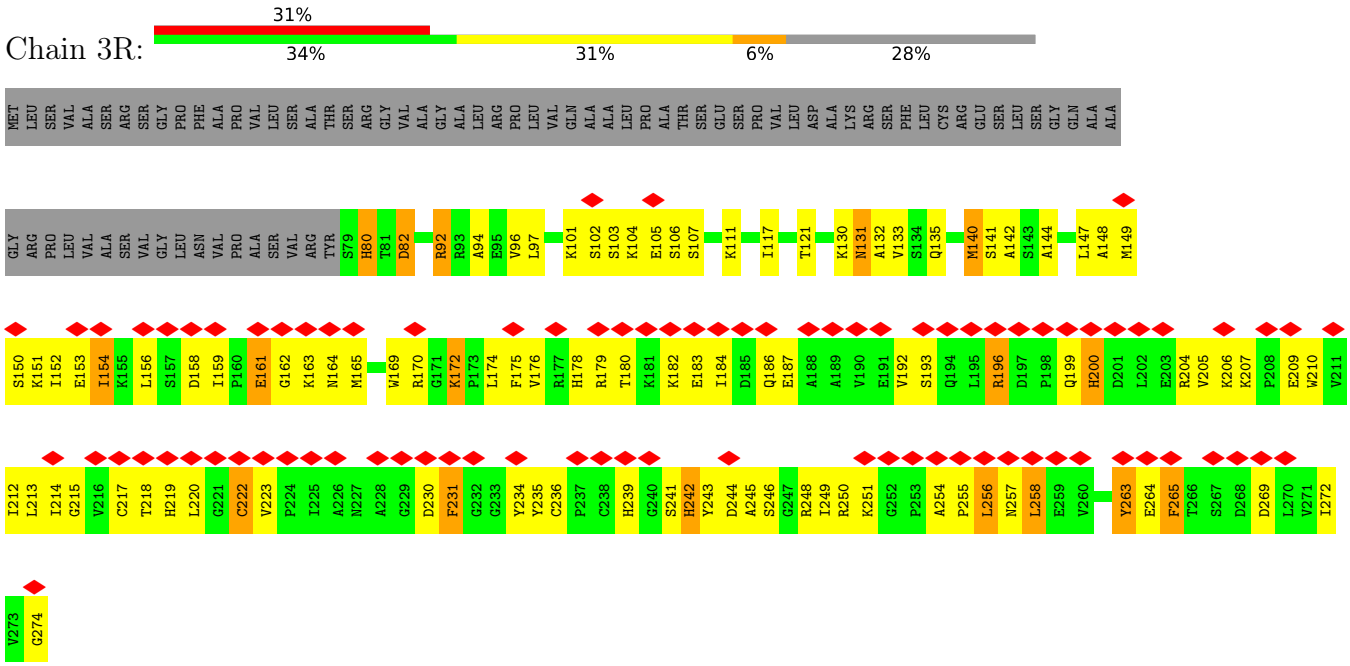
• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain 3I:



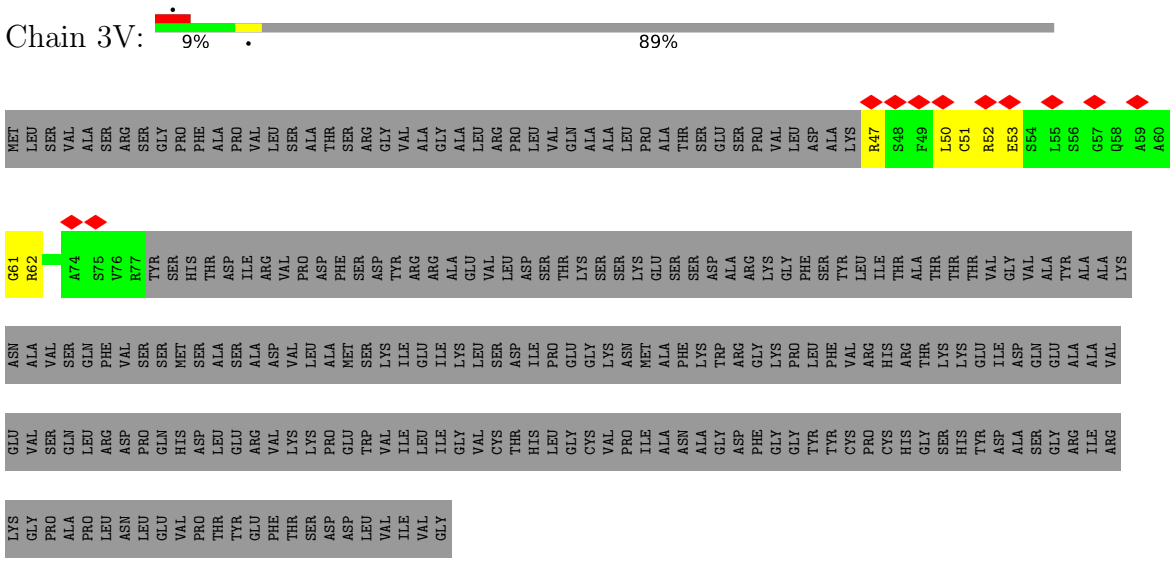
• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain 3R:



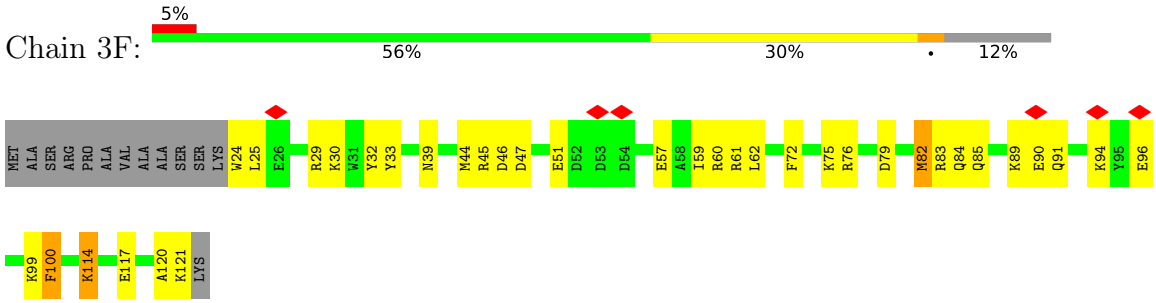
• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain 3V:



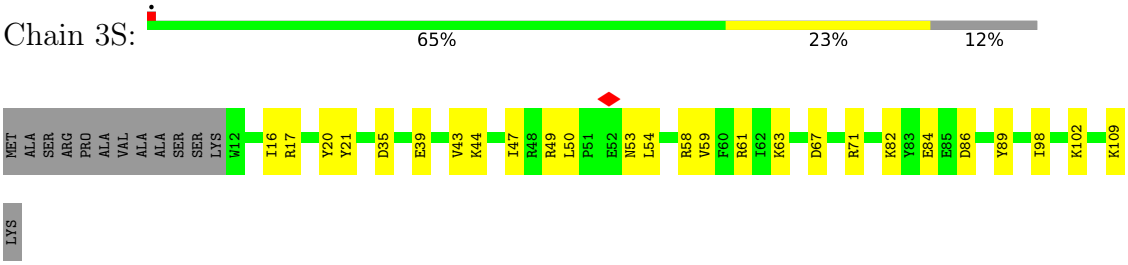
• Molecule 6: Cytochrome b-c1 complex subunit 7

Chain 3F:



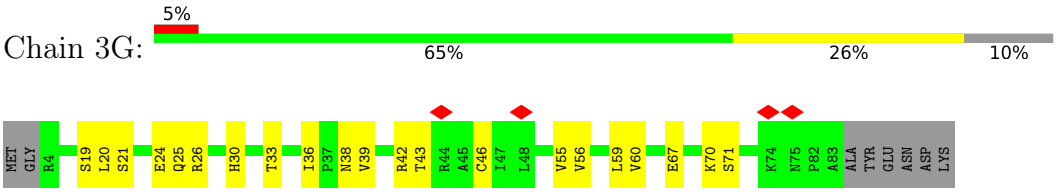
• Molecule 6: Cytochrome b-c1 complex subunit 7

Chain 3S:



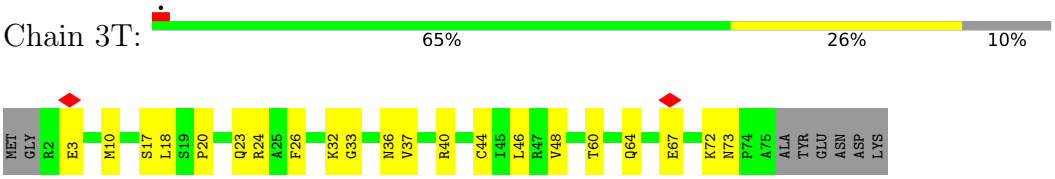
• Molecule 7: Cytochrome b-c1 complex subunit 8

Chain 3G:



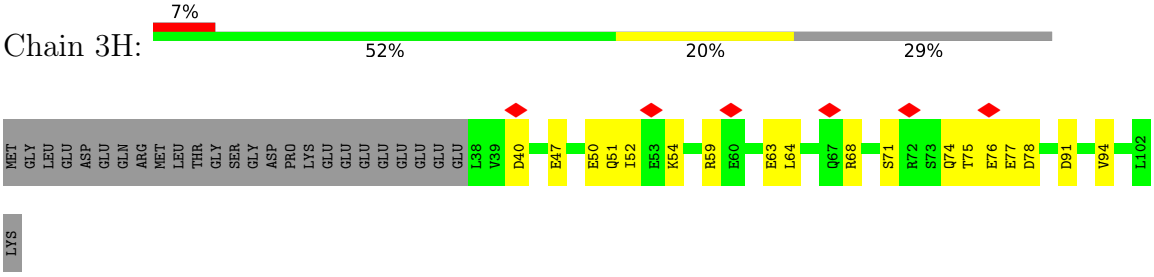
• Molecule 7: Cytochrome b-c1 complex subunit 8

Chain 3T:



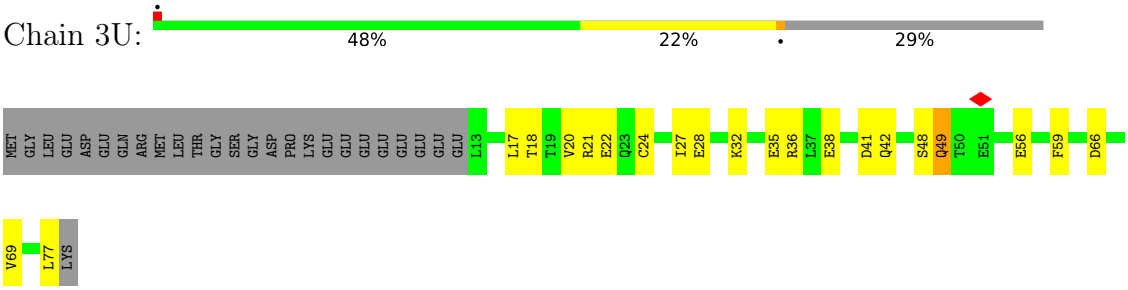
• Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain 3H:



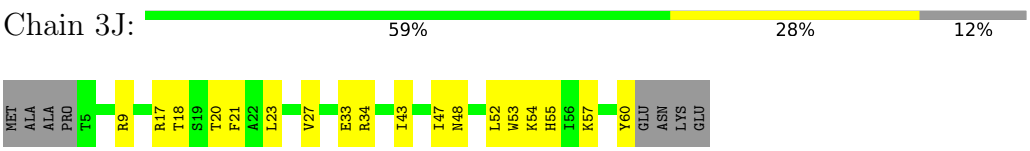
• Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain 3U:



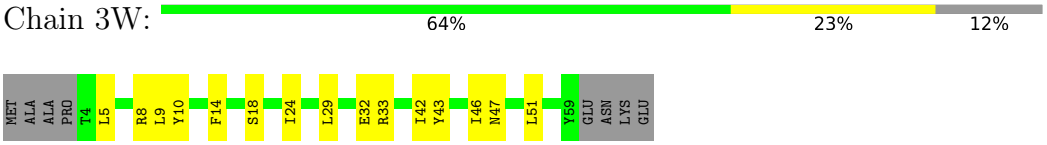
• Molecule 9: Ubiquinol-cytochrome c reductase complex 7.2 kDa protein

Chain 3J:



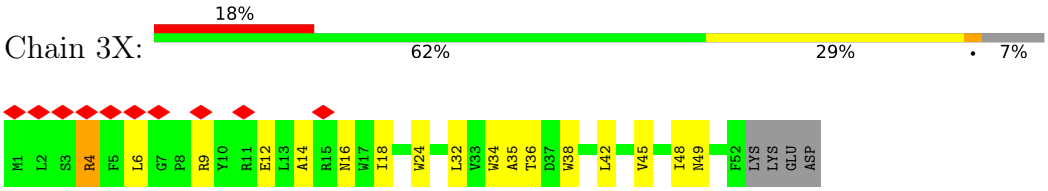
• Molecule 9: Ubiquinol-cytochrome c reductase complex 7.2 kDa protein

Chain 3W:



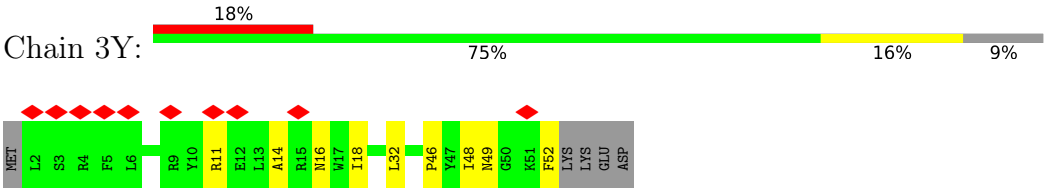
• Molecule 10: Cytochrome b-c1 complex subunit 10

Chain 3X:



• Molecule 10: Cytochrome b-c1 complex subunit 10

Chain 3Y:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	50000	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.599	Depositor
Minimum map value	-0.248	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	425.6, 425.6, 425.6	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.33, 1.33, 1.33	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEC, FES, PC1, U10, 3PE, HEM, CDL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	3A	0.33	0/3481	0.51	0/4722
1	3N	0.34	0/3496	0.51	0/4723
2	3B	0.32	0/3190	0.50	0/4317
2	3O	0.32	0/3175	0.49	0/4292
3	3C	0.37	0/3123	0.47	0/4269
3	3P	0.35	0/3122	0.47	0/4269
4	3D	0.38	0/1946	0.51	0/2641
4	3Q	0.36	0/1962	0.53	0/2663
5	3E	0.31	0/1551	0.57	1/2098 (0.0%)
5	3I	0.33	0/342	0.64	0/465
5	3R	0.32	0/1551	0.61	0/2098
5	3V	0.30	0/225	0.60	0/303
6	3F	0.36	0/888	0.54	0/1193
6	3S	0.35	0/888	0.53	0/1193
7	3G	0.34	0/649	0.56	0/878
7	3T	0.36	0/649	0.57	0/878
8	3H	0.31	0/538	0.62	0/721
8	3U	0.33	0/539	0.57	0/724
9	3J	0.33	0/476	0.52	0/641
9	3W	0.35	0/476	0.53	0/641
10	3X	0.30	0/445	0.58	0/608
10	3Y	0.32	0/437	0.58	0/598
All	All	0.34	0/33149	0.52	1/44935 (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
5	3R	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	3E	224	PRO	CA-N-CD	-5.86	103.30	111.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	3R	148	ALA	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	3A	3411	0	3309	80	0
1	3N	3424	0	3350	85	0
2	3B	3138	0	3116	86	0
2	3O	3124	0	3108	75	0
3	3C	3025	0	3090	94	0
3	3P	3024	0	3090	70	0
4	3D	1888	0	1834	81	0
4	3Q	1904	0	1849	49	0
5	3E	1518	0	1498	79	0
5	3I	337	0	347	25	0
5	3R	1518	0	1498	111	0
5	3V	223	0	233	5	0
6	3F	868	0	857	31	0
6	3S	868	0	857	20	0
7	3G	628	0	634	17	0
7	3T	628	0	634	23	0
8	3H	533	0	512	15	0
8	3U	533	0	513	16	0
9	3J	464	0	467	28	0
9	3W	464	0	467	11	0
10	3X	429	0	430	19	0
10	3Y	421	0	418	6	0
11	3A	58	0	60	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	3C	52	0	48	5	0
11	3G	56	0	56	3	0
11	3P	99	0	86	12	0
11	3Q	57	0	58	13	0
12	3A	59	0	66	12	0
12	3C	69	0	86	5	0
12	3D	33	0	40	4	0
12	3G	29	0	32	1	0
12	3N	58	0	62	6	0
12	3P	33	0	40	3	0
12	3Q	47	0	71	8	0
12	3Y	30	0	34	0	0
13	3C	86	0	60	9	0
13	3P	86	0	60	4	0
14	3C	47	0	48	11	0
14	3P	51	0	54	5	0
15	3D	42	0	32	16	0
15	3Q	43	0	32	4	0
16	3E	4	0	0	1	0
16	3R	4	0	0	1	0
17	3E	47	0	68	7	0
17	3R	45	0	64	5	0
17	3X	29	0	32	5	0
All	All	33534	0	33300	948	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 14.

All (948) 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)
9:3J:53:TRP:CE2	9:3J:57:LYS:HG2	1.79	1.18
5:3R:219:HIS:CE1	5:3R:239:HIS:ND1	2.18	1.11
4:3D:115:ARG:CD	9:3J:60:TYR:OH	2.02	1.07
4:3D:115:ARG:CZ	9:3J:60:TYR:CE1	2.39	1.05
9:3J:53:TRP:O	9:3J:57:LYS:HE3	1.57	1.04
5:3R:219:HIS:HE1	5:3R:239:HIS:ND1	1.57	1.00
14:3C:503:U10:H4M2	14:3C:503:U10:H3M2	1.47	0.92
4:3D:115:ARG:HD2	9:3J:60:TYR:OH	1.69	0.90
4:3D:115:ARG:CZ	9:3J:60:TYR:HE1	1.79	0.88
5:3E:242:HIS:HB2	5:3E:251:LYS:HB3	1.54	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:3R:196:ARG:HD2	5:3R:249:ILE:HD13	1.53	0.88
2:3B:226:MET:HG3	2:3B:227:ARG:H	1.39	0.86
12:3D:502:3PE:H31	5:3E:131:ASN:HD22	1.42	0.85
9:3J:53:TRP:NE1	9:3J:57:LYS:HG2	1.79	0.84
2:3B:95:LYS:HB3	2:3B:110:GLU:H	1.43	0.83
2:3B:95:LYS:NZ	5:3I:71:ASN:O	2.12	0.82
4:3D:249:MET:SD	15:3D:501:HEC:FE	1.72	0.82
5:3R:204:ARG:NH2	5:3R:258:LEU:O	2.12	0.82
4:3D:115:ARG:HD3	9:3J:60:TYR:OH	1.79	0.81
7:3T:18:LEU:HB3	7:3T:23:GLN:HE21	1.46	0.81
5:3R:101:LYS:HD3	5:3R:103:SER:H	1.45	0.80
1:3N:184:GLU:OE2	1:3N:184:GLU:N	2.15	0.79
3:3C:264:THR:HG23	5:3R:223:VAL:HG22	1.65	0.79
3:3C:177:ARG:NH2	5:3R:140:MET:O	2.17	0.77
9:3J:53:TRP:NE1	9:3J:57:LYS:CG	2.37	0.76
12:3A:503:3PE:H32	3:3C:4:ILE:HD11	1.68	0.76
11:3Q:502:CDL:HA62	7:3T:33:GLY:HA3	1.66	0.76
5:3I:32:ALA:C	5:3I:34:LEU:H	1.89	0.75
3:3C:264:THR:OG1	5:3R:222:CYS:SG	2.43	0.74
4:3D:111:HIS:ND1	4:3D:142:VAL:O	2.21	0.74
11:3A:501:CDL:H132	12:3A:503:3PE:H381	1.70	0.73
2:3O:350:GLY:HA2	2:3O:411:ILE:HD13	1.70	0.73
5:3R:156:LEU:HG	5:3R:176:VAL:HG22	1.70	0.72
6:3S:59:VAL:HG11	7:3T:10:MET:HG2	1.72	0.72
8:3H:50:GLU:OE1	8:3H:51:GLN:NE2	2.23	0.71
4:3D:249:MET:SD	15:3D:501:HEC:NB	2.63	0.71
3:3P:149:LEU:HD11	3:3P:281:LEU:HD22	1.71	0.71
1:3A:285:GLY:HA3	5:3I:70:LEU:HA	1.72	0.71
3:3P:314:SER:O	3:3P:318:ARG:NH1	2.22	0.71
1:3A:126:GLN:NE2	1:3A:130:GLU:OE1	2.23	0.71
3:3P:316:MET:HB2	12:3P:505:3PE:H112	1.73	0.71
2:3B:111:CYS:HB3	2:3B:119:LEU:HD22	1.73	0.70
1:3N:422:VAL:HG21	1:3N:437:ILE:HD13	1.74	0.70
3:3C:229:ILE:HD12	17:3E:302:PC1:H3A1	1.73	0.70
3:3C:316:MET:HG3	12:3C:506:3PE:H112	1.73	0.70
4:3D:267:THR:OG1	8:3H:40:ASP:OD1	2.10	0.70
4:3D:115:ARG:NH1	9:3J:60:TYR:CE1	2.60	0.70
4:3D:249:MET:SD	15:3D:501:HEC:NC	2.65	0.70
5:3R:264:GLU:HB2	5:3R:272:ILE:HG23	1.73	0.70
4:3Q:232:SER:OG	7:3T:23:GLN:NE2	2.25	0.69
2:3O:306:PRO:HA	5:3V:52:ARG:HG3	1.74	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:3X:36:THR:HG21	17:3X:101:PC1:H332	1.75	0.69
11:3Q:502:CDL:OA4	7:3T:36:ASN:ND2	2.26	0.68
11:3G:102:CDL:H532	11:3G:102:CDL:H722	1.74	0.68
5:3R:207:LYS:HD2	5:3R:210:TRP:HB3	1.75	0.68
1:3N:14:THR:HG21	1:3N:389:ARG:HB3	1.75	0.68
1:3A:17:SER:OG	1:3A:205:HIS:NE2	2.26	0.68
9:3J:53:TRP:O	9:3J:57:LYS:CE	2.39	0.68
1:3N:204:GLU:HG3	1:3N:207[A]:GLN:H	1.57	0.68
1:3N:145:MET:HG3	1:3N:425:LEU:HD23	1.75	0.68
10:3X:32:LEU:HD11	17:3X:101:PC1:H341	1.76	0.67
2:3B:141:GLN:HE22	2:3B:186:VAL:HB	1.59	0.67
4:3D:111:HIS:NE2	4:3D:288:ASP:OD2	2.28	0.67
5:3R:204:ARG:HH12	5:3R:257:ASN:HB3	1.58	0.67
5:3E:181:LYS:HA	5:3E:184:ILE:HD12	1.75	0.67
6:3F:121:LYS:NZ	10:3X:4:ARG:O	2.28	0.67
2:3B:227:ARG:HE	2:3B:229:GLY:HA3	1.58	0.66
5:3R:209:GLU:HB2	5:3R:210:TRP:HE3	1.61	0.66
2:3B:408:ALA:O	2:3B:412:ASN:ND2	2.29	0.66
5:3E:154:ILE:HB	5:3E:272:ILE:HG22	1.77	0.66
5:3E:229:GLY:HA2	5:3E:235:TYR:HD2	1.58	0.66
10:3Y:48:ILE:HD12	10:3Y:48:ILE:H	1.60	0.66
11:3Q:502:CDL:H311	7:3T:37:VAL:HG21	1.77	0.66
3:3C:33:PHE:HA	3:3C:36:LEU:HB2	1.77	0.66
3:3P:229:ILE:HG23	17:3R:302:PC1:H3C1	1.78	0.66
6:3F:84:GLN:OE1	7:3G:42:ARG:NH1	2.29	0.65
5:3R:107:SER:HB2	5:3R:111:LYS:HZ1	1.60	0.65
5:3R:214:ILE:HD12	5:3R:214:ILE:H	1.61	0.65
11:3P:506:CDL:H541	11:3P:506:CDL:HA61	1.78	0.65
10:3X:12:GLU:O	10:3X:16:ASN:ND2	2.28	0.65
2:3B:89:ILE:HD13	2:3B:119:LEU:HG	1.76	0.65
1:3A:304:CYS:HB3	1:3A:334:MET:HE3	1.78	0.65
4:3D:204:ILE:HG12	15:3D:501:HEC:HMA3	1.79	0.65
5:3I:64:LEU:HD11	5:3I:76:VAL:HG12	1.79	0.65
5:3V:53:GLU:N	5:3V:53:GLU:OE1	2.29	0.65
2:3B:346:THR:O	2:3B:351:ASN:ND2	2.29	0.65
3:3P:126:THR:HG21	13:3P:501:HEM:HBB2	1.78	0.65
12:3A:502:3PE:H32	17:3E:302:PC1:H31	1.79	0.65
6:3F:72:PHE:HE2	6:3F:76:ARG:HH21	1.45	0.65
3:3C:282:ARG:HD3	3:3C:343:VAL:HG22	1.77	0.64
5:3R:169:TRP:CD1	5:3R:174:LEU:HB2	2.32	0.64
8:3U:56:GLU:OE1	8:3U:56:GLU:N	2.20	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3C:149:LEU:HD21	3:3C:281:LEU:HD11	1.80	0.64
5:3E:155:LYS:HZ1	5:3E:273:VAL:HG22	1.62	0.64
12:3A:503:3PE:O11	12:3A:503:3PE:N	2.31	0.63
8:3U:56:GLU:HA	8:3U:59:PHE:HB2	1.80	0.63
2:3B:201:SER:HB2	2:3B:228:GLY:HA2	1.81	0.63
2:3O:76:THR:HG23	2:3O:81:SER:HA	1.80	0.63
2:3O:240:ARG:O	2:3O:421:ARG:NH2	2.31	0.63
3:3C:38:GLY:HA3	14:3C:503:U10:H13	1.81	0.63
3:3C:379:TRP:HB3	6:3F:45:ARG:HH21	1.61	0.63
5:3E:153:GLU:O	5:3E:155:LYS:NZ	2.22	0.63
2:3O:226:MET:SD	2:3O:226:MET:N	2.71	0.63
5:3R:144:ALA:HA	5:3R:147:LEU:HB2	1.80	0.63
9:3W:10:TYR:HA	9:3W:14:PHE:HB2	1.81	0.63
5:3R:152:ILE:HD12	5:3R:169:TRP:HA	1.79	0.63
5:3E:157:SER:HB2	5:3E:269:ASP:HB3	1.80	0.63
8:3U:32:LYS:HB2	8:3U:36:ARG:HH12	1.62	0.63
4:3D:109:LEU:HD11	4:3D:287:HIS:HB3	1.79	0.63
8:3H:76:GLU:OE2	8:3H:76:GLU:N	2.32	0.63
5:3I:32:ALA:C	5:3I:34:LEU:N	2.51	0.62
2:3O:56:ARG:HD2	2:3O:103:GLU:HG2	1.82	0.62
3:3P:125:ALA:O	3:3P:129:MET:HG3	1.98	0.62
3:3P:35:SER:OG	14:3P:503:U10:O5	2.15	0.62
5:3R:210:TRP:NE1	5:3R:269:ASP:OD1	2.27	0.62
5:3R:175:PHE:CE2	5:3R:215:GLY:HA2	2.34	0.62
11:3C:505:CDL:H122	11:3C:505:CDL:H321	1.82	0.62
6:3F:117:GLU:HG2	10:3X:4:ARG:HD3	1.81	0.62
9:3J:53:TRP:CE2	9:3J:57:LYS:CG	2.68	0.62
5:3E:267:SER:HB3	5:3E:270:LEU:HD12	1.81	0.62
4:3D:257:VAL:HG13	4:3D:258:LEU:HG	1.81	0.62
8:3H:75:THR:HG22	8:3H:77:GLU:H	1.64	0.62
4:3Q:28:ARG:NE	4:3Q:185:ASP:OD2	2.27	0.62
2:3O:100:SER:HB2	2:3O:105:MET:HG3	1.81	0.61
5:3E:125:VAL:HG21	17:3E:302:PC1:H362	1.81	0.61
2:3O:219:VAL:HG12	2:3O:222:ARG:HH22	1.65	0.61
5:3R:105:GLU:OE1	5:3R:105:GLU:N	2.25	0.61
1:3N:258:GLU:OE1	5:3R:101:LYS:NZ	2.34	0.61
3:3P:361:ILE:HA	3:3P:365:LEU:HB2	1.81	0.61
11:3Q:502:CDL:OA3	7:3T:40:ARG:NH1	2.33	0.61
1:3A:131:ARG:HD3	1:3A:175:ARG:HA	1.82	0.61
3:3C:207:ASN:ND2	3:3C:211:ILE:O	2.34	0.61
2:3B:157:ALA:O	2:3B:161:GLU:HG2	2.00	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3Q:120:ARG:NE	15:3Q:501:HEC:O1A	2.32	0.61
4:3D:295:LEU:O	4:3D:299:MET:HG2	2.01	0.60
1:3A:158:PHE:O	1:3A:161:THR:OG1	2.19	0.60
5:3R:182:LYS:HE2	5:3R:186:GLN:OE1	2.01	0.60
7:3T:60:THR:O	7:3T:64:GLN:HG2	2.02	0.60
1:3A:61:HIS:CG	1:3A:134:ILE:HD11	2.37	0.60
4:3D:284:GLU:HG3	4:3D:286:GLU:HG2	1.83	0.60
3:3C:15:ASN:HA	3:3C:19:ILE:HB	1.82	0.60
3:3C:1:MET:SD	3:3C:1:MET:N	2.73	0.60
2:3B:58:GLU:O	2:3B:174:ASN:ND2	2.35	0.60
2:3B:207:ILE:HD13	2:3B:382:VAL:HG12	1.83	0.60
2:3O:141:GLN:HA	2:3O:144:LEU:HD12	1.84	0.60
3:3P:360:LEU:HG	3:3P:365:LEU:HD23	1.83	0.60
3:3P:373:GLU:OE1	6:3S:20:TYR:OH	2.17	0.60
2:3B:47:ILE:HD11	2:3B:211:VAL:HG21	1.83	0.60
2:3B:248:ASN:ND2	2:3B:250:ASP:OD2	2.35	0.60
10:3X:45:VAL:O	10:3X:49:ASN:ND2	2.34	0.60
4:3Q:23:HIS:NE2	4:3Q:199:ASP:OD2	2.35	0.59
1:3A:30:SER:OG	1:3A:31:SER:N	2.35	0.59
3:3C:51:LEU:HD13	13:3C:501:HEM:HBD1	1.84	0.59
1:3N:281:ASP:OD1	1:3N:282:SER:N	2.35	0.59
3:3C:32:ASN:ND2	11:3G:102:CDL:OB9	2.35	0.59
3:3C:244:LEU:O	4:3D:290:ARG:NE	2.32	0.59
5:3E:225:ILE:HD11	4:3Q:144:ARG:HH12	1.67	0.59
5:3R:162:GLY:HA3	5:3R:180:THR:HG23	1.84	0.59
1:3A:147:ASP:OD2	5:3I:47:ARG:NH2	2.35	0.59
3:3P:149:LEU:HD22	3:3P:291:VAL:HG22	1.84	0.59
10:3X:38:TRP:HA	17:3X:101:PC1:H32	1.85	0.59
6:3F:45:ARG:NH1	6:3F:46:ASP:OD1	2.34	0.59
6:3S:16:ILE:HD12	6:3S:16:ILE:H	1.68	0.59
1:3A:76:GLU:OE2	2:3B:290:ASN:N	2.36	0.59
3:3P:314:SER:OG	3:3P:315:MET:N	2.34	0.59
5:3R:149:MET:SD	5:3R:150:SER:N	2.75	0.59
2:3O:89:ILE:HD13	2:3O:119:LEU:HD22	1.85	0.59
1:3A:195:MET:HE2	1:3A:219:LEU:HD21	1.83	0.59
1:3A:354:VAL:HG21	1:3A:404:ALA:HA	1.85	0.59
3:3C:246:SER:O	3:3C:246:SER:OG	2.21	0.59
1:3N:192:ALA:HB2	1:3N:219:LEU:HB3	1.83	0.58
5:3R:184:ILE:HG12	5:3R:209:GLU:HG3	1.85	0.58
3:3C:50:PHE:HA	3:3C:53:MET:HE2	1.83	0.58
3:3C:34:GLY:HA3	13:3C:502:HEM:HBA2	1.86	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3O:290:ASN:O	2:3O:297:GLN:NE2	2.36	0.58
2:3O:334:GLY:HA2	2:3O:434:PRO:HD3	1.84	0.58
3:3C:119:LEU:HD22	13:3C:502:HEM:HBB2	1.84	0.58
4:3D:230:SER:O	4:3D:230:SER:OG	2.22	0.58
1:3A:279:HIS:CG	5:3I:35:PRO:HB3	2.38	0.58
11:3A:501:CDL:H321	11:3A:501:CDL:H131	1.86	0.58
2:3B:56:ARG:HD2	2:3B:103:GLU:HG2	1.85	0.58
5:3E:241:SER:HA	5:3E:249:ILE:HD11	1.85	0.58
5:3E:242:HIS:HD2	5:3E:251:LYS:HD2	1.69	0.58
3:3C:373:GLU:CD	6:3F:32:TYR:HH	2.07	0.58
4:3D:249:MET:SD	15:3D:501:HEC:NA	2.76	0.58
5:3E:161:GLU:HG3	5:3E:180:THR:HG22	1.85	0.58
1:3N:237:THR:HG22	7:3T:18:LEU:HD11	1.84	0.58
1:3N:304:CYS:HB3	1:3N:334:MET:SD	2.43	0.58
8:3U:32:LYS:HA	8:3U:35:GLU:HG2	1.85	0.58
5:3R:153:GLU:N	5:3R:153:GLU:OE2	2.37	0.58
3:3C:81:TYR:OH	4:3D:206:ARG:NH1	2.36	0.57
1:3A:144:SER:HB3	5:3I:47:ARG:CZ	2.34	0.57
3:3C:107:TYR:HB2	3:3C:305:PRO:HG3	1.86	0.57
5:3E:195:LEU:HD21	5:3E:248:ARG:HB3	1.87	0.57
1:3N:172:GLU:OE1	1:3N:175:ARG:NH2	2.36	0.57
2:3B:96:LEU:HB3	5:3I:70:LEU:HB3	1.86	0.57
2:3B:239:TYR:CD2	2:3B:260:GLU:HB2	2.39	0.57
5:3R:179:ARG:NH1	5:3R:183:GLU:OE1	2.37	0.57
6:3S:35:ASP:OD1	6:3S:89:TYR:OH	2.19	0.57
3:3C:360:LEU:HG	3:3C:365:LEU:HD23	1.86	0.57
11:3P:506:CDL:HB31	7:3T:40:ARG:HB3	1.87	0.57
1:3N:74:ALA:O	1:3N:78:GLU:HG2	2.04	0.57
5:3R:199:GLN:O	5:3R:248:ARG:NE	2.36	0.57
2:3B:394:GLN:O	2:3B:397:THR:OG1	2.22	0.57
4:3D:245:GLN:N	4:3D:245:GLN:OE1	2.38	0.57
1:3N:34:THR:OG1	2:3O:373:GLU:OE2	2.19	0.57
2:3B:133:ARG:HD2	2:3B:135:TRP:CZ2	2.38	0.57
4:3Q:37:CYS:HB2	15:3Q:501:HEC:CAB	2.35	0.57
2:3O:357:VAL:HG12	2:3O:361:LYS:HD2	1.87	0.57
2:3B:97:SER:HA	5:3I:69:GLY:HA3	1.85	0.57
8:3U:18:THR:O	8:3U:22:GLU:HG2	2.05	0.57
3:3P:81:TYR:OH	4:3Q:118:ARG:NH2	2.34	0.56
1:3A:297:VAL:HG22	3:3C:1:MET:HG3	1.87	0.56
2:3B:361:LYS:NZ	2:3B:405:VAL:O	2.33	0.56
4:3D:249:MET:SD	15:3D:501:HEC:ND	2.79	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3P:119:LEU:HD22	13:3P:502:HEM:HBB2	1.87	0.56
4:3Q:144:ARG:HD2	4:3Q:145:GLU:N	2.21	0.56
5:3R:231:PHE:H	5:3R:242:HIS:CE1	2.23	0.56
3:3C:237:LEU:HD13	4:3D:301:MET:HG2	1.86	0.56
4:3D:324:LEU:HD21	6:3F:75:LYS:HE3	1.86	0.56
2:3O:124:LEU:HD13	2:3O:223:PHE:HB2	1.87	0.56
1:3N:354:VAL:HG21	1:3N:404:ALA:HA	1.88	0.56
4:3Q:110:PRO:HG3	15:3Q:501:HEC:HMD3	1.88	0.56
7:3T:18:LEU:HB3	7:3T:23:GLN:NE2	2.18	0.56
4:3D:252:PRO:HB3	15:3D:501:HEC:HHC	1.88	0.56
5:3E:235:TYR:HB2	5:3E:242:HIS:ND1	2.21	0.56
2:3B:226:MET:HG3	2:3B:227:ARG:N	2.17	0.56
4:3D:214:TYR:OH	15:3D:501:HEC:O2A	2.15	0.56
5:3E:191:GLU:OE2	5:3E:194:GLN:N	2.38	0.56
6:3F:79:ASP:OD2	6:3F:83:ARG:NH2	2.38	0.56
6:3F:85:GLN:HG2	7:3G:38:ASN:HD21	1.70	0.56
3:3P:322:GLN:HE22	12:3P:505:3PE:H111	1.69	0.56
4:3Q:225:HIS:CE1	7:3T:20:PRO:HB2	2.41	0.56
2:3B:54:GLY:O	2:3B:194:TYR:OH	2.24	0.56
5:3R:101:LYS:HD3	5:3R:101:LYS:C	2.26	0.56
7:3T:24:ARG:HH12	7:3T:26:PHE:HD2	1.54	0.56
1:3A:144:SER:H	5:3I:47:ARG:NH1	2.04	0.56
4:3D:201:LEU:HA	4:3D:204:ILE:HB	1.87	0.56
7:3G:67:GLU:O	7:3G:71:SER:OG	2.19	0.56
1:3A:235:ARG:CZ	5:3E:92:ARG:HH22	2.19	0.55
5:3E:229:GLY:HA2	5:3E:235:TYR:CD2	2.40	0.55
1:3N:106:LEU:HD21	1:3N:203:VAL:HG23	1.88	0.55
3:3C:361:ILE:HA	3:3C:365:LEU:HB2	1.88	0.55
1:3N:19:LEU:HD13	1:3N:23:LEU:HB3	1.87	0.55
3:3P:252:ASP:OD2	3:3P:269:LYS:NZ	2.39	0.55
4:3Q:158:ILE:HG23	4:3Q:160:MET:H	1.70	0.55
5:3E:239:HIS:HB3	16:3E:301:FES:S2	2.45	0.55
5:3R:153:GLU:C	5:3R:154:ILE:HG13	2.26	0.55
8:3U:48:SER:OG	8:3U:49:GLN:OE1	2.24	0.55
3:3P:360:LEU:HD12	3:3P:364:VAL:HB	1.89	0.55
4:3D:108:SER:HB2	4:3D:288:ASP:OD1	2.07	0.55
7:3G:30:HIS:HB3	7:3G:33:THR:HB	1.89	0.55
3:3P:181:PHE:HA	3:3P:184:ILE:HG22	1.89	0.55
3:3C:319:PRO:HD2	6:3F:32:TYR:OH	2.07	0.55
5:3R:156:LEU:HD13	5:3R:210:TRP:CD1	2.41	0.55
7:3T:3:GLU:N	7:3T:3:GLU:OE2	2.40	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:3E:246:SER:O	5:3E:246:SER:OG	2.25	0.55
1:3A:38:GLY:HA2	1:3A:113:LEU:HD21	1.89	0.54
4:3D:107:SER:O	4:3D:291:LYS:NZ	2.40	0.54
12:3D:502:3PE:H372	5:3E:128:ALA:HB1	1.89	0.54
5:3E:242:HIS:CD2	5:3E:251:LYS:HD2	2.42	0.54
1:3N:156:THR:OG1	1:3N:239:SER:OG	2.23	0.54
2:3O:68:LEU:HD21	2:3O:137:VAL:HG13	1.89	0.54
8:3U:28:GLU:O	8:3U:32:LYS:NZ	2.40	0.54
1:3A:444:LEU:HD11	12:3A:502:3PE:H12	1.88	0.54
2:3B:148:LYS:HG3	2:3B:177:TYR:HB3	1.88	0.54
5:3E:239:HIS:O	5:3E:241:SER:OG	2.24	0.54
5:3R:102:SER:O	5:3R:106:SER:OG	2.13	0.54
10:3X:14:ALA:O	10:3X:18:ILE:HG12	2.08	0.54
9:3J:23:LEU:O	9:3J:27:VAL:HG23	2.08	0.54
9:3J:52:LEU:HD13	9:3J:55:HIS:HE1	1.73	0.54
3:3P:215:MET:HB2	7:3T:10:MET:SD	2.48	0.54
4:3Q:83:ARG:NH1	4:3Q:89:ASP:OD2	2.41	0.54
3:3C:378:LYS:HZ1	6:3F:29:ARG:HD3	1.73	0.54
12:3Q:503:3PE:H2H1	5:3R:133:VAL:HG13	1.88	0.54
5:3R:117:ILE:O	5:3R:121:THR:HG22	2.08	0.54
8:3U:28:GLU:OE1	8:3U:28:GLU:N	2.41	0.54
9:3W:33:ARG:HD3	10:3X:48:ILE:HA	1.90	0.54
2:3B:46:ARG:HG2	2:3B:379:LEU:HD22	1.88	0.54
3:3C:97:HIS:NE2	13:3C:502:HEM:O1A	2.36	0.54
7:3G:39:VAL:O	7:3G:43:THR:HG22	2.07	0.54
3:3P:207:ASN:ND2	3:3P:211:ILE:O	2.39	0.54
3:3P:369:THR:O	3:3P:373:GLU:HG2	2.07	0.54
5:3R:156:LEU:HB3	5:3R:210:TRP:NE1	2.22	0.54
5:3E:225:ILE:HG13	5:3E:235:TYR:CZ	2.43	0.54
4:3Q:156:GLN:HG2	8:3U:59:PHE:HZ	1.73	0.54
4:3Q:222:MET:SD	5:3R:121:THR:HG21	2.47	0.54
1:3A:219:LEU:HG	1:3A:220:SER:H	1.72	0.54
3:3P:229:ILE:HG21	17:3R:302:PC1:H362	1.90	0.54
4:3Q:74:PRO:HA	4:3Q:79:GLU:O	2.08	0.54
2:3B:305:GLN:HG3	2:3B:306:PRO:HD2	1.88	0.54
1:3N:269:PRO:HB2	1:3N:410:VAL:HG11	1.90	0.54
4:3D:249:MET:HG3	15:3D:501:HEC:C4C	2.38	0.53
6:3F:120:ALA:O	10:3X:9:ARG:NH1	2.41	0.53
2:3B:133:ARG:HB2	2:3B:136:GLU:HG3	1.91	0.53
1:3N:301:ARG:NH2	1:3N:333:ASP:OD2	2.40	0.53
1:3N:394:GLU:O	1:3N:398:ARG:HG3	2.07	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3P:221:HIS:O	3:3P:225:THR:OG1	2.16	0.53
10:3Y:14:ALA:O	10:3Y:18:ILE:HG12	2.07	0.53
3:3C:128:PHE:CD1	14:3C:504:U10:H4M1	2.43	0.53
4:3D:122:LYS:O	4:3D:126:SER:OG	2.19	0.53
4:3D:128:CYS:SG	15:3D:501:HEC:HBC3	2.49	0.53
11:3P:506:CDL:OB4	7:3T:40:ARG:NE	2.36	0.53
3:3C:116:GLY:C	13:3C:502:HEM:HBC2	2.28	0.53
1:3N:36:THR:HG21	1:3N:373:THR:HA	1.91	0.53
2:3B:283:PRO:HD3	5:3I:57:GLY:HA2	1.90	0.53
2:3O:209:LEU:HD11	2:3O:378:PHE:HD2	1.73	0.53
5:3R:179:ARG:HH22	5:3R:246:SER:HA	1.74	0.53
5:3R:217:CYS:SG	5:3R:218:THR:N	2.82	0.53
4:3D:96:PRO:HG3	8:3H:91:ASP:HB3	1.91	0.53
2:3O:166:ALA:HB2	2:3O:244:ILE:HG12	1.91	0.53
3:3P:375:ASN:O	6:3S:17:ARG:NH1	2.38	0.53
4:3Q:113:LEU:HA	4:3Q:116:ILE:HB	1.91	0.53
4:3D:115:ARG:NE	9:3J:60:TYR:CE1	2.76	0.53
4:3D:157:GLU:N	4:3D:157:GLU:OE1	2.42	0.53
1:3N:132:ASP:HA	1:3N:135:LEU:HD12	1.91	0.53
4:3D:307:LEU:HB3	5:3E:121:THR:OG1	2.09	0.53
4:3Q:116:ILE:HG12	15:3Q:501:HEC:HMA3	1.91	0.53
1:3N:279:HIS:ND1	1:3N:284:TYR:OH	2.41	0.53
3:3P:75:TYR:HE1	4:3Q:200:HIS:HE1	1.56	0.53
3:3C:185:LEU:HD23	3:3C:188:ILE:HD12	1.91	0.52
1:3N:76:GLU:OE2	2:3O:290:ASN:N	2.42	0.52
2:3O:42:ALA:O	2:3O:113:ARG:NH1	2.38	0.52
3:3P:277:ALA:HB1	3:3P:294:LEU:HD11	1.91	0.52
5:3E:200:HIS:HB3	5:3E:203:GLU:HG2	1.90	0.52
5:3E:212:ILE:HG22	5:3E:261:PRO:HD2	1.91	0.52
2:3O:34:VAL:HG21	2:3O:386:ALA:HB1	1.91	0.52
5:3R:176:VAL:HG23	5:3R:212:ILE:CG2	2.40	0.52
2:3B:163:LEU:HD21	2:3B:258:VAL:HG21	1.90	0.52
2:3B:266:SER:O	2:3B:270:ASN:ND2	2.42	0.52
7:3G:21:SER:HB2	7:3G:24:GLU:HG3	1.91	0.52
1:3N:436:ARG:HD3	3:3P:222:PRO:HD3	1.90	0.52
3:3P:35:SER:OG	3:3P:228:ASP:OD2	2.28	0.52
6:3S:53:ASN:OD1	6:3S:54:LEU:N	2.43	0.52
3:3P:111:GLU:HA	3:3P:111:GLU:OE1	2.09	0.52
6:3S:67:ASP:OD2	6:3S:71:ARG:NH1	2.42	0.52
1:3N:19:LEU:H	1:3N:19:LEU:HD12	1.74	0.52
3:3C:207:ASN:HD22	3:3C:213:SER:HB3	1.74	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3P:8:HIS:HB3	3:3P:11:MET:HB2	1.92	0.52
5:3R:151:LYS:NZ	5:3R:274:GLY:OXT	2.42	0.52
4:3D:171:ARG:NH2	4:3D:177:ASP:OD2	2.30	0.52
5:3E:199:GLN:HG2	5:3E:204:ARG:HE	1.75	0.52
2:3O:304:HIS:HA	5:3V:52:ARG:HH22	1.75	0.52
4:3Q:173:ASP:HB3	4:3Q:175:THR:HG23	1.92	0.52
1:3A:80:GLU:HG2	2:3B:284:HIS:HB2	1.91	0.52
1:3A:280:TYR:HB3	1:3A:307:PHE:CE1	2.45	0.52
1:3A:282:SER:O	2:3B:143:GLN:NE2	2.43	0.52
2:3O:369:LEU:HD11	2:3O:399:LEU:HD11	1.92	0.52
4:3Q:47:ALA:HA	4:3Q:90:TYR:HA	1.91	0.52
4:3D:253:ILE:HG22	4:3D:268:MET:HG3	1.92	0.51
5:3E:212:ILE:HG21	5:3E:263:TYR:HB3	1.92	0.51
9:3W:18:SER:HB3	10:3X:24:TRP:CE2	2.45	0.51
8:3H:77:GLU:O	8:3H:78:ASP:N	2.43	0.51
2:3B:357:VAL:HG12	2:3B:361:LYS:HD2	1.91	0.51
6:3F:90:GLU:H	6:3F:90:GLU:CD	2.12	0.51
1:3N:181:ASP:OD1	1:3N:181:ASP:N	2.42	0.51
4:3Q:72:ASP:HB3	4:3Q:81:PHE:CE1	2.45	0.51
2:3B:24:LEU:HD11	2:3B:36:ALA:HB1	1.93	0.51
1:3N:343:MET:HE1	1:3N:442:PHE:HA	1.92	0.51
5:3R:176:VAL:HG23	5:3R:212:ILE:HG22	1.93	0.51
1:3A:46:ARG:HH22	1:3A:316:GLU:CD	2.13	0.51
5:3E:219:HIS:O	5:3E:219:HIS:ND1	2.43	0.51
4:3Q:208:MET:HA	12:3Q:503:3PE:H341	1.92	0.51
5:3R:222:CYS:HB3	5:3R:236:CYS:SG	2.51	0.51
1:3A:204:GLU:OE1	1:3A:204:GLU:N	2.42	0.51
4:3D:186:PRO:O	4:3D:190:ARG:HG3	2.11	0.51
5:3E:214:ILE:HG22	5:3E:259:GLU:HB3	1.93	0.51
6:3F:51:GLU:N	6:3F:51:GLU:OE1	2.44	0.51
8:3H:59:ARG:NE	8:3H:59:ARG:HA	2.26	0.51
2:3O:107:TYR:HB3	2:3O:123:LEU:HD11	1.91	0.51
10:3X:12:GLU:CD	10:3X:16:ASN:HD21	2.13	0.51
2:3O:353:SER:OG	2:3O:356:ASP:OD1	2.21	0.51
12:3C:507:3PE:H2B2	5:3R:130:LYS:HA	1.92	0.51
5:3E:134:SER:O	5:3E:138:SER:OG	2.21	0.51
2:3O:70:ARG:O	2:3O:98:VAL:HG21	2.11	0.51
1:3A:62:LEU:HD23	1:3A:122:LEU:HA	1.92	0.51
4:3D:125:CYS:HB3	15:3D:501:HEC:C3B	2.41	0.51
9:3J:34:ARG:HG2	10:3Y:48:ILE:HG23	1.92	0.51
4:3Q:9:SER:HB2	4:3Q:15:ARG:HH12	1.75	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:3R:255:PRO:HB2	5:3R:256:LEU:HD23	1.93	0.51
1:3N:235:ARG:CZ	5:3R:92:ARG:HH22	2.24	0.50
3:3C:346:PRO:HG3	7:3G:67:GLU:HB3	1.93	0.50
4:3D:156:VAL:HG21	4:3D:180:PRO:HG2	1.92	0.50
3:3P:234:PHE:HB3	11:3Q:502:CDL:H762	1.93	0.50
3:3P:326:TRP:HZ2	12:3P:505:3PE:H31	1.76	0.50
12:3Q:503:3PE:H3A1	12:3Q:503:3PE:H362	1.94	0.50
5:3R:101:LYS:HD2	5:3R:104:LYS:H	1.75	0.50
8:3H:91:ASP:HA	8:3H:94:VAL:HG12	1.94	0.50
1:3A:280:TYR:HB3	1:3A:307:PHE:HE1	1.77	0.50
3:3C:373:GLU:OE2	6:3F:32:TYR:CZ	2.65	0.50
12:3C:507:3PE:H291	5:3R:133:VAL:HB	1.93	0.50
5:3E:119:ALA:HB2	9:3J:21:PHE:CE1	2.47	0.50
5:3E:217:CYS:SG	5:3E:221:GLY:HA2	2.51	0.50
4:3Q:164:ILE:HG13	4:3Q:164:ILE:O	2.12	0.50
4:3D:145:THR:OG1	4:3D:146:GLU:OE1	2.30	0.50
7:3G:20:LEU:HB3	7:3G:25:GLN:NE2	2.26	0.50
2:3B:36:ALA:O	2:3B:207:ILE:HA	2.12	0.50
2:3B:41:TYR:HA	2:3B:113:ARG:HH12	1.76	0.50
4:3D:117:GLY:HA3	4:3D:278:PHE:HB2	1.94	0.50
2:3O:155:PRO:HB2	2:3O:254:HIS:CE1	2.46	0.50
3:3P:165:TRP:O	3:3P:174:THR:OG1	2.29	0.50
11:3C:505:CDL:OB3	7:3G:42:ARG:NH1	2.44	0.50
5:3E:196:ARG:NH1	5:3E:255:PRO:O	2.45	0.50
4:3D:109:LEU:HD12	4:3D:109:LEU:H	1.75	0.50
5:3E:125:VAL:HG11	17:3E:302:PC1:H381	1.93	0.50
1:3N:375:VAL:O	1:3N:379:ILE:HG13	2.12	0.50
4:3Q:207:LYS:NZ	12:3Q:503:3PE:O12	2.35	0.50
1:3A:140:GLU:HG2	5:3I:50:LEU:HD23	1.93	0.49
5:3E:164:ASN:HB3	5:3E:177:ARG:HB2	1.93	0.49
1:3N:196:VAL:HG21	1:3N:383:LEU:HB3	1.94	0.49
5:3R:217:CYS:SG	5:3R:243:TYR:OH	2.69	0.49
11:3A:501:CDL:H151	12:3A:502:3PE:H242	1.93	0.49
3:3C:221:HIS:O	3:3C:225:THR:OG1	2.18	0.49
1:3N:240:GLU:HG2	7:3T:17:SER:HB2	1.92	0.49
4:3Q:32:VAL:HG11	4:3Q:186:VAL:HB	1.94	0.49
1:3A:322:ALA:HB3	1:3A:338:LEU:HD21	1.94	0.49
5:3E:236:CYS:O	5:3E:241:SER:OG	2.30	0.49
4:3Q:42:SER:OG	4:3Q:112:ASP:OD2	2.30	0.49
5:3R:219:HIS:CE1	5:3R:220:LEU:HD12	2.47	0.49
2:3B:123:LEU:O	2:3B:127:THR:HG23	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3B:312:PHE:HA	5:3I:61:GLY:HA2	1.95	0.49
4:3D:310:ALA:HB2	12:3G:101:3PE:H342	1.94	0.49
2:3O:312:PHE:HA	5:3V:61:GLY:HA2	1.94	0.49
5:3R:92:ARG:HB3	5:3R:97:LEU:HD13	1.94	0.49
2:3B:276:GLN:HG2	2:3B:281:ALA:HB2	1.93	0.49
3:3C:154:PRO:HG3	3:3C:288:LEU:HD11	1.94	0.49
2:3O:52:LYS:HB3	2:3O:203:ARG:HB2	1.94	0.49
2:3O:214:PRO:O	2:3O:218:GLN:HG2	2.12	0.49
3:3P:124:MET:HB3	3:3P:274:PHE:HE1	1.77	0.49
4:3Q:223:LYS:NZ	11:3Q:502:CDL:OB4	2.26	0.49
12:3Q:503:3PE:H232	12:3Q:503:3PE:H332	1.95	0.49
1:3N:244:ARG:HB2	1:3N:428:ILE:HD11	1.95	0.49
2:3O:148:LYS:HE3	2:3O:178:CYS:O	2.13	0.49
2:3O:264:THR:HB	2:3O:315:SER:HB2	1.95	0.49
1:3N:372:THR:OG1	2:3O:373:GLU:OE2	2.20	0.49
2:3B:36:ALA:HB3	2:3B:207:ILE:HG23	1.94	0.49
5:3R:159:ILE:HD13	5:3R:163:LYS:H	1.77	0.49
3:3C:245:PHE:O	4:3D:290:ARG:NH2	2.46	0.49
5:3R:187:GLU:HG3	5:3R:248:ARG:HH22	1.78	0.49
1:3A:156:THR:OG1	1:3A:239:SER:HB2	2.13	0.49
3:3C:35:SER:HB3	14:3C:503:U10:H1M1	1.95	0.49
4:3D:199:PRO:HG2	15:3D:501:HEC:HAA1	1.95	0.49
9:3J:43:ILE:O	9:3J:47:ILE:HG13	2.13	0.49
11:3P:507:CDL:H312	11:3P:507:CDL:H121	1.94	0.49
1:3A:141:ASN:ND2	1:3A:168:GLU:OE2	2.45	0.48
1:3A:154:HIS:NE2	1:3A:314:TYR:OH	2.35	0.48
2:3B:393:VAL:HG22	2:3B:397:THR:OG1	2.12	0.48
5:3R:183:GLU:HB3	5:3R:187:GLU:HB2	1.95	0.48
1:3A:356:ARG:HG3	2:3B:91:ALA:HA	1.94	0.48
12:3N:501:3PE:O12	12:3N:501:3PE:N	2.34	0.48
5:3R:179:ARG:HD2	5:3R:184:ILE:HG13	1.95	0.48
7:3T:67:GLU:N	7:3T:67:GLU:OE1	2.44	0.48
9:3W:46:ILE:HG22	9:3W:47:ASN:ND2	2.28	0.48
3:3C:10:LEU:HD21	3:3P:195:VAL:HG13	1.95	0.48
3:3C:44:GLN:O	3:3C:83:HIS:HE1	1.96	0.48
1:3N:145:MET:HA	1:3N:148:VAL:HG22	1.95	0.48
3:3P:186:PRO:HG2	13:3P:501:HEM:HMC3	1.95	0.48
2:3B:113:ARG:NH2	2:3B:210:GLY:O	2.46	0.48
3:3C:78:VAL:O	3:3C:82:LEU:HB2	2.13	0.48
8:3U:24:CYS:O	8:3U:27:ILE:HG22	2.13	0.48
13:3C:501:HEM:O1D	13:3C:501:HEM:HHA	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:3E:174:LEU:HD22	5:3E:214:ILE:HG13	1.95	0.48
2:3O:220:ALA:HA	2:3O:224:LEU:HD23	1.96	0.48
4:3Q:27:ARG:NH2	4:3Q:60:GLU:OE1	2.47	0.48
5:3R:210:TRP:HE1	5:3R:269:ASP:CG	2.14	0.48
12:3A:503:3PE:H2	12:3A:503:3PE:H221	1.50	0.48
3:3C:370:SER:HA	3:3C:373:GLU:HB2	1.96	0.48
5:3E:204:ARG:HG3	5:3E:205:VAL:HG23	1.95	0.48
6:3F:57:GLU:OE1	6:3F:60:ARG:NH1	2.46	0.48
1:3A:384:LEU:HD23	1:3A:384:LEU:HA	1.70	0.48
2:3B:227:ARG:HD2	2:3B:229:GLY:H	1.79	0.48
1:3A:192:ALA:H	1:3A:220:SER:HB3	1.79	0.48
4:3D:116:ARG:NE	4:3D:274:ASP:OD2	2.41	0.48
4:3D:284:GLU:HG2	4:3D:287:HIS:HB2	1.95	0.48
5:3R:209:GLU:HB2	5:3R:210:TRP:CE3	2.46	0.48
5:3R:213:LEU:HD13	5:3R:258:LEU:HB3	1.94	0.48
8:3U:20:VAL:HG12	8:3U:69:VAL:HG22	1.95	0.48
1:3A:27:SER:HB3	1:3A:208:LEU:HD22	1.96	0.48
2:3B:137:VAL:O	2:3B:141:GLN:HG2	2.14	0.48
3:3C:197:LEU:HD11	14:3C:503:U10:H111	1.95	0.48
4:3D:115:ARG:HD2	9:3J:60:TYR:CZ	2.49	0.48
5:3E:191:GLU:OE1	5:3E:193:SER:N	2.45	0.48
6:3F:44:MET:HB2	6:3F:47:ASP:OD1	2.14	0.48
8:3U:38:GLU:HA	8:3U:41:ASP:OD1	2.13	0.48
1:3A:445:ARG:NH1	11:3A:501:CDL:OB3	2.46	0.48
2:3B:135:TRP:CG	6:3S:49:ARG:HD3	2.49	0.48
8:3H:47:GLU:CD	8:3H:47:GLU:H	2.17	0.48
5:3R:131:ASN:O	5:3R:131:ASN:ND2	2.39	0.48
8:3U:17:LEU:HD11	8:3U:21:ARG:CZ	2.44	0.48
17:3X:101:PC1:H31	17:3X:101:PC1:H112	1.95	0.48
2:3B:135:TRP:CD2	6:3S:49:ARG:HD3	2.49	0.47
4:3D:125:CYS:HB3	15:3D:501:HEC:CAB	2.43	0.47
5:3E:196:ARG:HB2	5:3E:253:PRO:HA	1.96	0.47
1:3N:156:THR:HG1	1:3N:239:SER:HG	1.60	0.47
5:3R:161:GLU:HG2	5:3R:180:THR:HA	1.94	0.47
2:3B:96:LEU:O	5:3I:70:LEU:N	2.47	0.47
3:3C:24:PRO:HB2	3:3C:27:ILE:HG12	1.96	0.47
3:3P:357:LEU:O	3:3P:361:ILE:HG13	2.14	0.47
1:3A:15:GLN:HB2	1:3A:205:HIS:ND1	2.30	0.47
8:3H:54:LYS:HE2	8:3H:54:LYS:HA	1.96	0.47
12:3N:502:3PE:H242	17:3R:302:PC1:H241	1.97	0.47
2:3O:255:ALA:HB3	2:3O:337:ILE:HD11	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3P:277:ALA:HB1	3:3P:294:LEU:CD1	2.44	0.47
5:3R:162:GLY:N	5:3R:178:HIS:O	2.41	0.47
1:3A:279:HIS:ND1	1:3A:284:TYR:OH	2.38	0.47
11:3C:505:CDL:H112	11:3C:505:CDL:HA4	1.47	0.47
1:3N:224:VAL:HG13	1:3N:225:GLU:N	2.28	0.47
5:3R:176:VAL:HA	5:3R:212:ILE:HG22	1.95	0.47
1:3A:163:LEU:HD23	1:3A:163:LEU:HA	1.73	0.47
3:3C:71:ARG:NH2	4:3D:282:ALA:O	2.46	0.47
4:3D:98:TYR:O	4:3D:103:ARG:NH1	2.47	0.47
1:3N:433:ASP:CG	3:3P:223:TYR:HH	2.13	0.47
4:3Q:235:LEU:HD21	6:3S:63:LYS:HE3	1.95	0.47
12:3Q:503:3PE:H231	12:3Q:503:3PE:H272	1.97	0.47
5:3R:159:ILE:HD12	5:3R:161:GLU:N	2.29	0.47
3:3C:185:LEU:HD23	3:3C:185:LEU:HA	1.74	0.47
1:3N:58:PHE:HE2	1:3N:127:ILE:HG23	1.79	0.47
2:3O:122:PHE:O	2:3O:126:VAL:HG23	2.14	0.47
2:3O:395:PRO:O	2:3O:399:LEU:HG	2.15	0.47
3:3P:47:THR:HG1	3:3P:83:HIS:HD1	1.62	0.47
4:3Q:20:SER:HB2	4:3Q:199:ASP:OD1	2.14	0.47
5:3R:249:ILE:HG22	5:3R:254:ALA:HB1	1.95	0.47
1:3A:312:ILE:O	1:3A:319:LEU:N	2.46	0.47
4:3D:287:HIS:O	4:3D:291:LYS:HG2	2.14	0.47
12:3N:501:3PE:O21	11:3P:507:CDL:H512	2.15	0.47
5:3R:214:ILE:HG22	5:3R:215:GLY:H	1.79	0.47
10:3Y:46:PRO:O	10:3Y:49:ASN:ND2	2.48	0.47
3:3C:240:LEU:HD21	12:3D:502:3PE:H251	1.97	0.47
5:3E:163:LYS:HD3	5:3E:164:ASN:H	1.80	0.47
9:3J:34:ARG:HG3	10:3Y:48:ILE:HA	1.95	0.47
1:3N:144:SER:HA	5:3V:47:ARG:NH1	2.30	0.47
2:3O:393:VAL:HG13	2:3O:397:THR:HB	1.95	0.47
5:3R:103:SER:O	5:3R:107:SER:HB3	2.15	0.47
3:3C:85:ASN:HB3	3:3C:242:LEU:HD23	1.97	0.47
1:3N:224:VAL:HG13	1:3N:225:GLU:H	1.80	0.47
1:3A:250:LEU:HD12	5:3I:44:ASP:HB2	1.98	0.46
1:3N:435:ASN:ND2	3:3P:223:TYR:OH	2.48	0.46
11:3Q:502:CDL:HA62	7:3T:33:GLY:CA	2.42	0.46
5:3R:249:ILE:O	5:3R:249:ILE:HD12	2.15	0.46
3:3C:337:TRP:HE1	3:3C:341:GLN:HE21	1.62	0.46
5:3E:162:GLY:H	5:3E:178:HIS:HB3	1.80	0.46
6:3F:24:TRP:CG	6:3F:25:LEU:N	2.83	0.46
6:3S:44:LYS:HA	6:3S:47:ILE:HD12	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3A:294:LEU:HD12	1:3A:307:PHE:CE2	2.49	0.46
3:3C:3:ASN:HB2	3:3C:6:LYS:HG2	1.97	0.46
3:3C:113:TRP:NE1	3:3C:301:LEU:O	2.28	0.46
3:3C:128:PHE:O	3:3C:132:VAL:HG23	2.15	0.46
1:3N:184:GLU:O	1:3N:188:GLN:HB2	2.14	0.46
2:3O:25:GLU:HB2	2:3O:213:HIS:ND1	2.30	0.46
2:3B:239:TYR:CE2	2:3B:260:GLU:HB2	2.50	0.46
5:3E:164:ASN:OD1	5:3E:164:ASN:N	2.47	0.46
5:3E:165:MET:HA	5:3E:165:MET:HE2	1.97	0.46
5:3E:182:LYS:HE2	5:3E:182:LYS:HB2	1.56	0.46
1:3A:242:ARG:HB3	1:3A:428:ILE:HD11	1.98	0.46
1:3A:444:LEU:HA	9:3J:18:THR:HG21	1.98	0.46
2:3B:178:CYS:SG	2:3B:183:ILE:HG12	2.56	0.46
17:3E:302:PC1:H111	17:3E:302:PC1:H11	1.98	0.46
5:3R:205:VAL:HG22	5:3R:207:LYS:H	1.80	0.46
11:3A:501:CDL:H351	3:3C:225:THR:HG21	1.96	0.46
4:3D:228:GLY:HA3	8:3H:78:ASP:N	2.30	0.46
5:3E:199:GLN:O	5:3E:248:ARG:NH1	2.49	0.46
7:3G:67:GLU:OE1	7:3G:67:GLU:HA	2.15	0.46
2:3O:409:ASP:N	2:3O:409:ASP:OD1	2.48	0.46
7:3T:72:LYS:HE2	8:3U:56:GLU:OE2	2.16	0.46
1:3A:279:HIS:ND1	5:3I:35:PRO:HB3	2.29	0.46
3:3C:231:GLY:HA2	11:3G:102:CDL:H711	1.97	0.46
5:3E:120:THR:HA	5:3E:123:VAL:HG12	1.97	0.46
4:3Q:32:VAL:HG22	4:3Q:169:LEU:HD21	1.97	0.46
5:3R:206:LYS:HE3	5:3R:263:TYR:HE1	1.80	0.46
1:3A:259:GLY:N	1:3A:318:GLY:O	2.37	0.46
1:3A:439:SER:O	12:3A:502:3PE:N	2.48	0.46
5:3R:159:ILE:HD13	5:3R:163:LYS:N	2.31	0.46
1:3A:40:TRP:CZ2	1:3A:377:GLU:HA	2.50	0.46
2:3B:124:LEU:O	2:3B:128:ALA:HB3	2.16	0.46
4:3D:212:GLU:HA	4:3D:215:VAL:HG12	1.98	0.46
5:3E:249:ILE:HD12	5:3E:249:ILE:HA	1.79	0.46
7:3G:56:VAL:O	7:3G:60:VAL:HG23	2.16	0.46
2:3O:202:ALA:HB3	2:3O:230:LEU:HA	1.97	0.46
5:3R:184:ILE:HD12	5:3R:184:ILE:H	1.80	0.46
1:3A:264:ASN:O	1:3A:266:ASP:N	2.49	0.45
4:3D:108:SER:N	9:3J:48:ASN:OD1	2.48	0.45
2:3O:169:ARG:HG3	2:3O:240:ARG:HB3	1.98	0.45
5:3R:241:SER:HB3	5:3R:254:ALA:HB2	1.99	0.45
4:3D:115:ARG:NH2	9:3J:60:TYR:HE1	2.10	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3D:280:ARG:O	4:3D:280:ARG:HD3	2.16	0.45
1:3N:431:LEU:HD12	1:3N:432:PRO:HD2	1.98	0.45
12:3A:502:3PE:C3	17:3E:302:PC1:H31	2.45	0.45
4:3D:160:ASP:HB2	4:3D:171:ARG:HE	1.82	0.45
6:3F:59:ILE:HA	6:3F:62:LEU:HD12	1.99	0.45
3:3P:58:ASP:HB3	3:3P:61:THR:HG22	1.97	0.45
3:3P:254:ASP:OD2	3:3P:267:HIS:NE2	2.50	0.45
1:3A:61:HIS:CD2	1:3A:134:ILE:HD11	2.51	0.45
2:3B:76:THR:HG21	2:3B:133:ARG:NH2	2.31	0.45
2:3B:309:VAL:HG23	2:3B:326:THR:HG22	1.97	0.45
2:3O:137:VAL:O	2:3O:141:GLN:HG2	2.16	0.45
2:3B:94:GLY:HA3	2:3B:119:LEU:HD21	1.99	0.45
3:3C:186:PRO:HG2	13:3C:501:HEM:HMC3	1.98	0.45
3:3C:277:ALA:HB1	3:3C:294:LEU:CD1	2.46	0.45
5:3E:154:ILE:HA	5:3E:271:VAL:O	2.17	0.45
1:3N:77:LYS:HE3	1:3N:77:LYS:HB2	1.63	0.45
1:3N:114:ALA:O	1:3N:118:GLN:HB2	2.15	0.45
2:3O:193:TYR:O	2:3O:197:ASN:HB2	2.16	0.45
2:3O:299:VAL:HG11	2:3O:336:VAL:HG13	1.98	0.45
3:3P:18:PHE:CE1	14:3P:503:U10:H72	2.51	0.45
6:3S:35:ASP:OD2	6:3S:61:ARG:NH1	2.49	0.45
6:3S:43:VAL:O	6:3S:47:ILE:HD12	2.16	0.45
6:3S:84:GLU:OE1	6:3S:84:GLU:N	2.40	0.45
2:3B:131:GLU:OE1	2:3B:133:ARG:NH1	2.49	0.45
2:3B:278:VAL:HG11	2:3B:352:LEU:HD11	1.98	0.45
5:3E:268:ASP:O	5:3E:270:LEU:HG	2.16	0.45
1:3N:283:THR:HA	2:3O:143:GLN:NE2	2.32	0.45
11:3P:506:CDL:H312	11:3Q:502:CDL:H731	1.99	0.45
4:3Q:130:LEU:HA	4:3Q:150:ASN:HD21	1.80	0.45
5:3R:132:ALA:O	5:3R:135:GLN:HB2	2.17	0.45
5:3R:164:ASN:HD22	5:3R:175:PHE:HB3	1.82	0.45
3:3C:277:ALA:HB1	3:3C:294:LEU:HD11	1.99	0.45
4:3D:208:ARG:HA	4:3D:208:ARG:HD3	1.65	0.45
8:3H:63:GLU:OE2	8:3H:63:GLU:HA	2.16	0.45
1:3N:209:LEU:HD23	1:3N:209:LEU:HA	1.70	0.45
1:3N:220:SER:OG	1:3N:222:THR:HG22	2.17	0.45
5:3R:219:HIS:ND1	5:3R:239:HIS:ND1	2.59	0.45
2:3B:303:VAL:HG22	2:3B:305:GLN:H	1.82	0.45
2:3B:359:ALA:O	2:3B:363:LYS:HG3	2.16	0.45
3:3C:302:ILE:O	3:3C:305:PRO:HD2	2.17	0.45
3:3C:329:VAL:HG22	12:3C:506:3PE:H2E1	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:3C:507:3PE:H281	10:3X:35:ALA:HB1	1.97	0.45
5:3E:179:ARG:NH1	5:3E:208:PRO:O	2.50	0.45
5:3E:233:GLY:H	5:3E:245:ALA:HA	1.82	0.45
2:3O:124:LEU:HB3	2:3O:223:PHE:HD2	1.81	0.45
5:3R:92:ARG:HG2	5:3R:96:VAL:O	2.17	0.45
10:3X:18:ILE:HD13	10:3X:18:ILE:HA	1.83	0.45
1:3A:394:GLU:OE2	1:3A:398:ARG:NH1	2.44	0.45
2:3B:40:ASN:HD21	2:3B:209:LEU:HD21	1.81	0.45
3:3C:378:LYS:NZ	6:3F:29:ARG:HD3	2.32	0.45
2:3O:241:GLY:HA2	2:3O:423:SER:OG	2.17	0.45
1:3N:40:TRP:CZ2	1:3N:377:GLU:HA	2.52	0.45
3:3P:54:HIS:HB2	3:3P:69:ILE:HG12	1.98	0.45
5:3R:249:ILE:H	5:3R:249:ILE:HG13	1.54	0.45
5:3E:176:VAL:HG12	5:3E:212:ILE:CD1	2.47	0.44
1:3N:77:LYS:O	1:3N:81:SER:OG	2.24	0.44
1:3N:149:VAL:HG21	1:3N:252:HIS:CB	2.47	0.44
5:3R:141:SER:OG	5:3R:142:ALA:N	2.49	0.44
5:3R:242:HIS:CB	5:3R:251:LYS:HB3	2.48	0.44
1:3A:361:LEU:HD23	1:3A:399:ILE:HG12	1.99	0.44
3:3C:132:VAL:O	3:3C:139:SER:OG	2.32	0.44
3:3C:374:ASN:HB3	3:3C:379:TRP:O	2.17	0.44
5:3I:70:LEU:HD23	5:3I:71:ASN:HB3	1.98	0.44
4:3Q:37:CYS:SG	4:3Q:41:HIS:HB2	2.57	0.44
10:3X:6:LEU:HD12	10:3X:6:LEU:HA	1.79	0.44
1:3A:156:THR:HB	1:3A:241:ILE:HG13	1.99	0.44
6:3F:114:LYS:HE3	6:3F:114:LYS:HB2	1.77	0.44
5:3I:62:ARG:HB2	5:3I:77:ARG:HH12	1.82	0.44
1:3N:34:THR:HA	1:3N:102:LEU:HA	1.99	0.44
12:3N:502:3PE:H322	17:3R:302:PC1:H351	1.98	0.44
5:3R:207:LYS:HD3	5:3R:265:PHE:CE2	2.52	0.44
1:3A:159:GLN:O	1:3A:235:ARG:NH2	2.47	0.44
11:3A:501:CDL:HB61	12:3A:503:3PE:H242	2.00	0.44
9:3J:53:TRP:CD2	9:3J:57:LYS:HG2	2.44	0.44
1:3N:17:SER:OG	1:3N:205:HIS:NE2	2.46	0.44
1:3N:148:VAL:HG12	5:3R:80:HIS:ND1	2.32	0.44
3:3P:108:MET:HE1	3:3P:308:HIS:HB3	2.00	0.44
14:3P:504:U10:O5	14:3P:504:U10:H4M2	2.17	0.44
11:3Q:502:CDL:HB61	11:3Q:502:CDL:H711	1.81	0.44
2:3B:203:ARG:HD2	2:3B:230:LEU:O	2.17	0.44
3:3C:35:SER:HB3	14:3C:503:U10:H71	1.98	0.44
3:3P:24:PRO:O	3:3P:224:TYR:OH	2.23	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3P:70:CYS:SG	3:3P:80:ARG:NH1	2.90	0.44
11:3P:506:CDL:HA32	11:3Q:502:CDL:HB4	2.00	0.44
2:3B:70:ARG:HD3	2:3B:100:SER:OG	2.18	0.44
3:3C:176:THR:OG1	3:3P:53:MET:O	2.36	0.44
5:3E:192:VAL:HB	5:3E:198:PRO:HB3	2.00	0.44
1:3N:346:CYS:SG	1:3N:411:CYS:HB3	2.57	0.44
2:3O:95:LYS:O	2:3O:109:VAL:HA	2.18	0.44
3:3P:160:LEU:HD23	3:3P:160:LEU:HA	1.83	0.44
3:3P:185:LEU:HD23	3:3P:185:LEU:HA	1.74	0.44
1:3A:62:LEU:HD12	1:3A:130:GLU:HG2	2.00	0.44
5:3E:262:THR:O	5:3E:262:THR:OG1	2.30	0.44
1:3N:148:VAL:HG12	5:3R:80:HIS:CG	2.53	0.44
1:3N:264:ASN:O	1:3N:266:ASP:N	2.51	0.44
2:3O:338:LYS:HB2	2:3O:338:LYS:HE3	1.76	0.44
3:3P:120:LEU:O	3:3P:124:MET:HG3	2.18	0.44
4:3Q:208:MET:O	4:3Q:212:MET:HG2	2.17	0.44
3:3C:141:TRP:CD1	3:3C:265:PRO:HD3	2.53	0.44
6:3F:33:TYR:HE1	6:3F:39:ASN:HB3	1.83	0.44
2:3O:27:THR:HG21	2:3O:217:LYS:HZ2	1.82	0.44
4:3Q:126:TYR:CZ	4:3Q:130:LEU:HD12	2.52	0.44
3:3P:75:TYR:CG	5:3R:135:GLN:OE1	2.71	0.44
1:3A:277:ILE:HB	1:3A:309:THR:HG21	1.99	0.43
2:3B:49:LEU:HD13	2:3B:206:LEU:HD13	2.00	0.43
3:3C:39:ILE:HG23	17:3E:302:PC1:H3F1	2.00	0.43
4:3D:272:ALA:O	4:3D:275:VAL:HG12	2.18	0.43
6:3F:30:LYS:NZ	6:3F:96:GLU:OE1	2.43	0.43
14:3P:504:U10:C13	14:3P:504:U10:H101	2.48	0.43
1:3A:317:THR:OG1	1:3A:318:GLY:N	2.50	0.43
3:3C:201:HIS:CD2	14:3C:503:U10:H4M1	2.53	0.43
14:3C:504:U10:H121	14:3C:504:U10:H101	1.81	0.43
5:3E:187:GLU:HG2	5:3E:246:SER:HB3	1.99	0.43
1:3N:188:GLN:HE22	1:3N:227:ALA:HB3	1.83	0.43
5:3R:222:CYS:HB2	16:3R:301:FES:S2	2.59	0.43
9:3W:8:ARG:HD2	9:3W:8:ARG:N	2.33	0.43
2:3B:407:ASP:N	2:3B:407:ASP:OD1	2.49	0.43
7:3T:32:LYS:HE3	7:3T:32:LYS:HB2	1.85	0.43
7:3T:44:CYS:O	7:3T:48:VAL:HG12	2.18	0.43
1:3A:141:ASN:HA	5:3I:47:ARG:NH1	2.33	0.43
3:3C:97:HIS:CE1	3:3C:100:ARG:HH22	2.37	0.43
6:3F:94:LYS:H	6:3F:94:LYS:HG2	1.57	0.43
1:3N:343:MET:HE3	1:3N:343:MET:HB3	1.93	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3N:398:ARG:O	1:3N:401:GLU:HG2	2.18	0.43
2:3O:301:LYS:HB2	2:3O:301:LYS:HE2	1.83	0.43
11:3P:506:CDL:H121	11:3Q:502:CDL:H521	1.99	0.43
5:3R:169:TRP:HD1	5:3R:174:LEU:HB2	1.82	0.43
5:3R:192:VAL:HG13	5:3R:193:SER:H	1.83	0.43
1:3A:41:ILE:HB	1:3A:95:THR:HB	2.00	0.43
1:3A:240:GLU:HA	1:3A:422:VAL:O	2.18	0.43
1:3A:244:ARG:CZ	1:3A:429:GLU:HB2	2.49	0.43
4:3D:115:ARG:NH2	9:3J:60:TYR:CE1	2.84	0.43
3:3P:107:TYR:HE2	3:3P:308:HIS:HB2	1.82	0.43
3:3P:130:GLY:HA2	3:3P:133:LEU:HD23	2.00	0.43
1:3A:19:LEU:HD23	1:3A:19:LEU:HA	1.82	0.43
1:3A:27:SER:HA	1:3A:199:ALA:O	2.18	0.43
2:3B:380:ASP:OD1	2:3B:380:ASP:N	2.51	0.43
2:3B:408:ALA:O	2:3B:411:ILE:HG22	2.18	0.43
5:3E:242:HIS:O	5:3E:250:ARG:N	2.41	0.43
8:3H:52:ILE:HD13	8:3H:52:ILE:HA	1.85	0.43
5:3R:196:ARG:HH11	5:3R:249:ILE:HD13	1.82	0.43
6:3S:21:TYR:OH	6:3S:86:ASP:OD2	2.20	0.43
9:3W:42:ILE:O	9:3W:46:ILE:HG13	2.18	0.43
1:3A:137:GLU:HA	1:3A:140:GLU:HG3	2.01	0.43
1:3A:239:SER:HB3	7:3G:19:SER:O	2.19	0.43
1:3A:430:GLN:O	1:3A:430:GLN:HG3	2.18	0.43
12:3A:502:3PE:H32	12:3A:502:3PE:H322	1.43	0.43
3:3C:133:LEU:HD21	3:3C:179:PHE:HA	2.01	0.43
4:3D:317:SER:O	4:3D:321:SER:OG	2.36	0.43
1:3N:426:GLY:O	1:3N:428:ILE:HG13	2.18	0.43
2:3B:148:LYS:HE3	2:3B:152:PHE:HE2	1.83	0.43
8:3H:47:GLU:OE2	8:3H:47:GLU:N	2.47	0.43
2:3O:54:GLY:O	2:3O:194:TYR:OH	2.36	0.43
3:3P:104:TYR:O	3:3P:206:ASN:ND2	2.52	0.43
5:3R:235:TYR:CD1	5:3R:242:HIS:HD2	2.37	0.43
1:3A:240:GLU:HG2	7:3G:19:SER:HB3	1.99	0.43
2:3B:171:ALA:HB3	2:3B:237:ALA:HB2	2.00	0.43
4:3D:121:TYR:HA	4:3D:125:CYS:SG	2.59	0.43
4:3D:249:MET:HG3	15:3D:501:HEC:NC	2.33	0.43
1:3N:106:LEU:CD2	1:3N:203:VAL:HG23	2.48	0.43
1:3N:328:ASN:OD1	1:3N:328:ASN:N	2.50	0.43
3:3P:116:GLY:C	13:3P:502:HEM:HBC2	2.38	0.43
2:3B:217:LYS:HE3	2:3B:217:LYS:HB3	1.79	0.43
2:3B:315:SER:O	2:3B:315:SER:OG	2.31	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3C:51:LEU:HD23	3:3C:51:LEU:HA	1.78	0.43
3:3C:71:ARG:HE	4:3D:203:TYR:HE1	1.67	0.43
5:3E:150:SER:O	5:3E:170:ARG:NH2	2.52	0.43
7:3G:55:VAL:O	7:3G:59:LEU:HG	2.19	0.43
12:3N:502:3PE:H2	12:3N:502:3PE:H221	1.52	0.43
1:3A:256:ALA:HB2	1:3A:310:PHE:CZ	2.53	0.42
11:3C:505:CDL:OB3	7:3G:42:ARG:HD2	2.19	0.42
4:3D:115:ARG:CD	9:3J:60:TYR:CZ	2.99	0.42
4:3D:135:ALA:HB2	4:3D:178:TYR:CD2	2.53	0.42
7:3G:67:GLU:HA	7:3G:70:LYS:NZ	2.34	0.42
2:3O:87:ARG:HD3	2:3O:87:ARG:HA	1.78	0.42
3:3P:24:PRO:HB2	3:3P:27:ILE:HG23	2.00	0.42
3:3P:338:ILE:HD13	3:3P:338:ILE:HA	1.83	0.42
4:3Q:120:ARG:HD3	4:3Q:120:ARG:HA	1.67	0.42
6:3S:39:GLU:OE1	6:3S:39:GLU:N	2.48	0.42
2:3B:51:ILE:HG21	2:3B:199:PHE:CD1	2.54	0.42
8:3H:64:LEU:O	8:3H:68:ARG:HG3	2.18	0.42
1:3A:313:CYS:HA	1:3A:318:GLY:HA3	2.00	0.42
2:3B:124:LEU:HD13	2:3B:124:LEU:HA	1.84	0.42
2:3B:227:ARG:CD	2:3B:229:GLY:H	2.32	0.42
3:3C:112:THR:HG22	3:3C:199:PHE:HB3	2.01	0.42
6:3F:83:ARG:HG3	6:3F:85:GLN:HB2	2.01	0.42
1:3N:136:GLN:O	1:3N:140:GLU:HG3	2.19	0.42
1:3N:258:GLU:CD	5:3R:101:LYS:HZ1	2.20	0.42
4:3Q:180:SER:OG	8:3U:77:LEU:HD11	2.19	0.42
1:3A:294:LEU:HD12	1:3A:307:PHE:CZ	2.54	0.42
3:3C:180:ALA:O	3:3C:184:ILE:HG22	2.20	0.42
1:3N:86:LEU:HD13	1:3N:99:ILE:HG13	2.02	0.42
1:3N:154:HIS:NE2	1:3N:314:TYR:OH	2.52	0.42
3:3P:373:GLU:OE1	6:3S:20:TYR:CZ	2.72	0.42
10:3X:38:TRP:CD1	17:3X:101:PC1:H32	2.54	0.42
5:3I:32:ALA:O	5:3I:34:LEU:N	2.52	0.42
1:3N:149:VAL:HG21	1:3N:252:HIS:HB2	2.00	0.42
4:3Q:200:HIS:NE2	12:3Q:503:3PE:O14	2.44	0.42
3:3C:26:ASN:HA	6:3F:82:MET:HB2	2.00	0.42
3:3C:348:ILE:HG22	3:3C:352:GLN:OE1	2.18	0.42
2:3O:216:LEU:HD12	2:3O:216:LEU:HA	1.89	0.42
3:3P:146:ILE:O	3:3P:149:LEU:HB2	2.19	0.42
4:3Q:216:LEU:HD23	4:3Q:216:LEU:HA	1.87	0.42
1:3A:65:LYS:HA	1:3A:65:LYS:HD3	1.73	0.42
1:3A:130:GLU:O	1:3A:134:ILE:HD13	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3C:77:TRP:CZ3	4:3D:290:ARG:HG3	2.55	0.42
3:3C:177:ARG:HH21	5:3R:140:MET:HG3	1.85	0.42
13:3C:502:HEM:HBA1	14:3C:503:U10:C2	2.49	0.42
5:3E:95:GLU:OE1	5:3E:95:GLU:N	2.42	0.42
5:3E:194:GLN:HE22	5:3E:250:ARG:HA	1.83	0.42
3:3P:132:VAL:HA	3:3P:139:SER:OG	2.20	0.42
9:3W:32:GLU:OE2	10:3X:34:TRP:NE1	2.45	0.42
5:3E:231:PHE:CD1	5:3E:231:PHE:N	2.87	0.42
5:3E:231:PHE:N	5:3E:231:PHE:HD1	2.18	0.42
5:3E:239:HIS:O	5:3E:241:SER:N	2.53	0.42
5:3R:131:ASN:O	5:3R:135:GLN:HG2	2.20	0.42
2:3B:378:PHE:O	2:3B:382:VAL:HG23	2.20	0.42
6:3F:45:ARG:CZ	6:3F:100:PHE:HE1	2.32	0.42
2:3O:217:LYS:O	2:3O:221:GLU:HG3	2.19	0.42
3:3P:18:PHE:HE1	14:3P:503:U10:H72	1.85	0.42
5:3R:150:SER:HB2	5:3R:169:TRP:CE3	2.54	0.42
1:3A:161:THR:HG21	1:3A:235:ARG:H	1.85	0.42
2:3B:227:ARG:HD2	2:3B:227:ARG:C	2.41	0.42
3:3C:218:ILE:HD12	3:3C:223:TYR:CD2	2.55	0.42
3:3C:274:PHE:HB3	14:3C:504:U10:H3M3	2.02	0.42
1:3N:67:THR:OG1	1:3N:70:ARG:N	2.51	0.42
1:3N:129:LYS:NZ	1:3N:129:LYS:HB3	2.34	0.42
1:3N:223:TYR:CD2	1:3N:229:PRO:HD2	2.55	0.42
3:3C:330:ALA:O	3:3C:334:THR:OG1	2.34	0.41
4:3D:218:LEU:HD21	15:3D:501:HEC:HBA1	2.02	0.41
5:3E:187:GLU:HB3	5:3E:201:ASP:HB2	2.02	0.41
5:3E:224:PRO:HA	5:3E:236:CYS:HA	2.02	0.41
1:3N:40:TRP:NE1	1:3N:89:TYR:OH	2.45	0.41
2:3O:340:ALA:O	2:3O:343:GLN:HB3	2.20	0.41
3:3P:370:SER:O	3:3P:373:GLU:HB2	2.19	0.41
11:3P:506:CDL:H111	11:3Q:502:CDL:H132	2.02	0.41
4:3Q:211:MET:HG3	4:3Q:215:LEU:HD12	2.02	0.41
5:3R:170:ARG:HD2	5:3R:172:LYS:NZ	2.35	0.41
5:3R:250:ARG:O	5:3R:250:ARG:HG2	2.19	0.41
2:3B:61:ASN:OD1	2:3B:61:ASN:N	2.53	0.41
5:3E:159:ILE:HD11	5:3E:163:LYS:C	2.40	0.41
5:3E:176:VAL:HG12	5:3E:212:ILE:HD13	2.02	0.41
1:3N:76:GLU:HG3	2:3O:285:VAL:HG21	2.01	0.41
1:3N:307:PHE:HB2	1:3N:324:PHE:HB3	2.02	0.41
2:3O:46:ARG:HH21	2:3O:108:THR:HG21	1.84	0.41
2:3O:209:LEU:HD23	2:3O:209:LEU:HA	1.88	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:3R:183:GLU:OE2	5:3R:245:ALA:HB3	2.20	0.41
11:3A:501:CDL:H511	11:3A:501:CDL:H141	2.02	0.41
12:3A:502:3PE:H2	12:3A:502:3PE:H222	1.47	0.41
11:3C:505:CDL:OB5	11:3C:505:CDL:O1	2.35	0.41
1:3N:145:MET:SD	1:3N:252:HIS:CD2	3.14	0.41
11:3P:506:CDL:CA6	11:3P:506:CDL:H522	2.50	0.41
5:3R:150:SER:HB3	5:3R:170:ARG:HG3	2.02	0.41
5:3R:156:LEU:HD22	5:3R:210:TRP:CG	2.55	0.41
5:3R:230:ASP:N	5:3R:242:HIS:NE2	2.62	0.41
1:3A:45:SER:OG	1:3A:92:ARG:HG2	2.20	0.41
1:3N:122:LEU:HD23	1:3N:122:LEU:HA	1.89	0.41
2:3O:318:ASP:OD1	2:3O:318:ASP:N	2.43	0.41
3:3P:77:TRP:CD2	4:3Q:197:GLU:HG3	2.56	0.41
5:3R:101:LYS:HD2	5:3R:104:LYS:N	2.34	0.41
5:3R:234:TYR:N	5:3R:243:TYR:O	2.53	0.41
5:3R:251:LYS:HZ2	5:3R:251:LYS:HG3	1.76	0.41
1:3A:332:ASP:H	1:3A:430:GLN:HG2	1.85	0.41
3:3C:213:SER:O	3:3C:217:LYS:HG2	2.21	0.41
4:3D:185:ASN:OD1	4:3D:188:ALA:N	2.39	0.41
1:3N:62:LEU:HA	1:3N:65:LYS:HG2	2.03	0.41
2:3O:25:GLU:OE1	2:3O:25:GLU:N	2.48	0.41
2:3O:137:VAL:HG12	2:3O:141:GLN:HE21	1.85	0.41
4:3Q:195:GLU:OE2	4:3Q:201:ARG:NE	2.53	0.41
5:3R:104:LYS:HD2	5:3R:104:LYS:HA	1.71	0.41
14:3C:504:U10:O2	14:3C:504:U10:C3M	2.68	0.41
4:3D:297:MET:HA	12:3D:502:3PE:H321	2.03	0.41
5:3E:225:ILE:HD11	4:3Q:144:ARG:NH1	2.36	0.41
5:3I:47:ARG:O	5:3I:49:PHE:CE2	2.74	0.41
3:3P:58:ASP:OD1	3:3P:60:THR:HG22	2.21	0.41
5:3R:218:THR:HG23	5:3R:258:LEU:HD22	2.02	0.41
2:3B:170:ASN:OD1	2:3B:170:ASN:N	2.54	0.41
3:3C:137:GLN:HB3	3:3C:265:PRO:HG3	2.02	0.41
4:3D:305:LEU:HD23	4:3D:305:LEU:HA	1.83	0.41
5:3E:249:ILE:HG12	5:3E:254:ALA:HB3	2.02	0.41
2:3O:33:LEU:HD23	2:3O:33:LEU:HA	1.82	0.41
2:3O:59:ASP:N	2:3O:62:ASN:OD1	2.54	0.41
3:3P:299:LEU:HD12	3:3P:299:LEU:HA	1.89	0.41
4:3Q:212:MET:HE2	4:3Q:212:MET:HB3	1.96	0.41
6:3S:109:LYS:H	6:3S:109:LYS:HG3	1.75	0.41
3:3C:282:ARG:HD3	3:3C:343:VAL:CG2	2.46	0.41
5:3E:207:LYS:HA	5:3E:207:LYS:HD2	1.82	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:3I:55:LEU:HA	5:3I:58:GLN:OE1	2.20	0.41
9:3J:17:ARG:HB2	9:3J:20:THR:OG1	2.20	0.41
1:3N:358:LYS:O	1:3N:362:ARG:HG3	2.21	0.41
12:3Q:503:3PE:H12	5:3R:131:ASN:ND2	2.36	0.41
6:3S:98:ILE:O	6:3S:102:LYS:HG2	2.21	0.41
9:3W:5:LEU:HD23	9:3W:5:LEU:HA	1.88	0.41
1:3A:77:LYS:HB2	1:3A:77:LYS:HE3	1.67	0.41
2:3B:24:LEU:HD23	2:3B:392:TYR:CD2	2.56	0.41
3:3C:42:ILE:HD13	3:3C:42:ILE:HA	1.91	0.41
3:3C:81:TYR:O	3:3C:85:ASN:ND2	2.37	0.41
3:3C:197:LEU:HD21	13:3C:502:HEM:HMA3	2.03	0.41
4:3D:218:LEU:HD12	4:3D:238:ASN:OD1	2.21	0.41
5:3E:231:PHE:HB3	5:3E:250:ARG:NH1	2.36	0.41
6:3F:61:ARG:HD3	2:3O:135:TRP:CE2	2.56	0.41
7:3G:36:ILE:HA	7:3G:36:ILE:HD13	1.80	0.41
1:3N:106:LEU:HB3	1:3N:107:PRO:HD3	2.03	0.41
3:3P:311:LYS:H	3:3P:374:ASN:HD21	1.69	0.41
11:3P:506:CDL:HA32	11:3Q:502:CDL:OB7	2.20	0.41
4:3Q:68:VAL:HG21	4:3Q:92:PRO:HG2	2.03	0.41
5:3R:97:LEU:HD12	5:3R:97:LEU:HA	1.91	0.41
7:3T:46:LEU:HD23	7:3T:46:LEU:HA	1.76	0.41
10:3X:42:LEU:HD23	10:3X:42:LEU:HA	1.88	0.41
2:3B:78:LYS:HE2	2:3B:78:LYS:HB2	1.59	0.41
3:3C:378:LYS:HZ3	6:3F:29:ARG:CZ	2.33	0.41
4:3D:96:PRO:O	4:3D:213:ASP:HB3	2.20	0.41
4:3D:111:HIS:CE1	4:3D:142:VAL:HG23	2.57	0.41
1:3N:444:LEU:HD13	12:3N:502:3PE:H122	2.03	0.41
2:3O:163:LEU:HD11	2:3O:258:VAL:HG22	2.02	0.41
5:3R:82:ASP:OD1	5:3R:82:ASP:N	2.54	0.41
9:3W:29:LEU:CD1	10:3X:34:TRP:HB2	2.51	0.41
1:3A:270:LEU:HD22	1:3A:320:LEU:HD21	2.03	0.40
2:3B:154:ASN:ND2	5:3I:78:TYR:OH	2.36	0.40
3:3C:191:ALA:O	3:3C:195:VAL:HG23	2.21	0.40
6:3F:99:LYS:HD3	6:3F:99:LYS:HA	1.75	0.40
1:3N:225:GLU:HG2	1:3N:226:ASP:N	2.35	0.40
1:3N:240:GLU:HA	1:3N:422:VAL:O	2.21	0.40
2:3O:219:VAL:HA	2:3O:222:ARG:NH1	2.37	0.40
2:3O:324:ILE:HD11	2:3O:344:VAL:HG21	2.03	0.40
5:3R:200:HIS:O	5:3R:204:ARG:HG3	2.21	0.40
1:3A:8:LEU:HD22	1:3A:392:LEU:HB3	2.03	0.40
2:3B:199:PHE:O	2:3B:226:MET:HG2	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3D:270:GLN:O	4:3D:274:ASP:OD1	2.39	0.40
5:3E:127:TYR:CE1	9:3J:33:GLU:HG3	2.56	0.40
2:3O:295:LEU:HD13	2:3O:309:VAL:HG22	2.03	0.40
3:3P:81:TYR:O	3:3P:85:ASN:ND2	2.48	0.40
3:3P:233:LEU:HD12	3:3P:233:LEU:HA	1.80	0.40
6:3S:50:LEU:HD23	6:3S:50:LEU:HA	1.91	0.40
10:3Y:32:LEU:HA	10:3Y:32:LEU:HD12	1.80	0.40
2:3B:75:LEU:HD23	2:3B:75:LEU:HA	1.89	0.40
2:3B:95:LYS:HZ3	5:3I:32:ALA:N	2.20	0.40
2:3B:96:LEU:HD12	2:3B:96:LEU:HA	1.83	0.40
2:3B:227:ARG:HD2	2:3B:227:ARG:O	2.21	0.40
5:3E:194:GLN:HE22	5:3E:250:ARG:HE	1.68	0.40
1:3N:355:VAL:HA	1:3N:358:LYS:HD3	2.03	0.40
2:3O:75:LEU:HD11	2:3O:140:LEU:HD12	2.04	0.40
2:3O:217:LYS:HE2	2:3O:217:LYS:HB2	1.60	0.40
11:3P:506:CDL:H522	11:3P:506:CDL:HA4	2.04	0.40
4:3Q:8:PRO:HG3	8:3U:66:ASP:HB3	2.04	0.40
4:3Q:130:LEU:O	4:3Q:150:ASN:ND2	2.54	0.40
5:3R:158:ASP:OD1	5:3R:159:ILE:HG23	2.21	0.40
3:3C:207:ASN:ND2	3:3C:213:SER:HB3	2.34	0.40
4:3D:248:ALA:HB3	15:3D:501:HEC:HBD2	2.04	0.40
4:3D:307:LEU:HD21	5:3E:120:THR:HG22	2.02	0.40
1:3N:223:TYR:CE2	1:3N:229:PRO:HD2	2.56	0.40
2:3O:98:VAL:HG12	2:3O:107:TYR:CD2	2.57	0.40
4:3Q:57:THR:HG22	4:3Q:60:GLU:HB2	2.04	0.40
5:3R:151:LYS:HE3	5:3R:272:ILE:HD11	2.02	0.40
5:3R:244:ASP:OD2	5:3R:250:ARG:HB2	2.22	0.40
1:3A:152:TYR:O	1:3A:156:THR:HG22	2.21	0.40
3:3C:17:ALA:HA	3:3C:201:HIS:CE1	2.57	0.40
3:3C:210:GLY:O	3:3C:313:ARG:HD2	2.22	0.40
5:3E:159:ILE:HD11	5:3E:163:LYS:O	2.21	0.40
5:3E:225:ILE:N	5:3E:235:TYR:O	2.52	0.40
2:3O:264:THR:HG22	2:3O:316:TYR:O	2.20	0.40
2:3O:387:LEU:HD23	2:3O:387:LEU:HA	1.75	0.40
17:3R:302:PC1:H281	9:3W:24:ILE:HG21	2.04	0.40
9:3W:5:LEU:O	9:3W:9:LEU:HD12	2.21	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	3A	436/480 (91%)	410 (94%)	26 (6%)	0	100	100
1	3N	444/480 (92%)	412 (93%)	30 (7%)	2 (0%)	29	68
2	3B	414/453 (91%)	398 (96%)	16 (4%)	0	100	100
2	3O	413/453 (91%)	394 (95%)	19 (5%)	0	100	100
3	3C	377/379 (100%)	366 (97%)	10 (3%)	1 (0%)	41	75
3	3P	377/379 (100%)	359 (95%)	17 (4%)	1 (0%)	41	75
4	3D	235/325 (72%)	217 (92%)	18 (8%)	0	100	100
4	3Q	237/325 (73%)	219 (92%)	18 (8%)	0	100	100
5	3E	194/274 (71%)	172 (89%)	22 (11%)	0	100	100
5	3I	45/274 (16%)	37 (82%)	7 (16%)	1 (2%)	6	37
5	3R	194/274 (71%)	158 (81%)	32 (16%)	4 (2%)	7	38
5	3V	29/274 (11%)	28 (97%)	1 (3%)	0	100	100
6	3F	96/111 (86%)	95 (99%)	1 (1%)	0	100	100
6	3S	96/111 (86%)	96 (100%)	0	0	100	100
7	3G	72/82 (88%)	71 (99%)	1 (1%)	0	100	100
7	3T	72/82 (88%)	72 (100%)	0	0	100	100
8	3H	61/91 (67%)	55 (90%)	6 (10%)	0	100	100
8	3U	63/91 (69%)	58 (92%)	5 (8%)	0	100	100
9	3J	54/64 (84%)	51 (94%)	3 (6%)	0	100	100
9	3W	54/64 (84%)	52 (96%)	2 (4%)	0	100	100
10	3X	50/56 (89%)	47 (94%)	3 (6%)	0	100	100
10	3Y	49/56 (88%)	44 (90%)	5 (10%)	0	100	100
All	All	4062/5178 (78%)	3811 (94%)	242 (6%)	9 (0%)	50	81

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	3N	118	GLN
5	3R	94	ALA
5	3R	154	ILE
1	3N	224	VAL
3	3P	155	TYR
5	3R	161	GLU
5	3I	59	ALA
5	3R	196	ARG
3	3C	155	TYR

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	3A	367/397 (92%)	355 (97%)	12 (3%)	38 68
1	3N	372/397 (94%)	348 (94%)	24 (6%)	17 50
2	3B	328/355 (92%)	313 (95%)	15 (5%)	27 61
2	3O	327/355 (92%)	320 (98%)	7 (2%)	53 79
3	3C	332/332 (100%)	319 (96%)	13 (4%)	32 64
3	3P	332/332 (100%)	323 (97%)	9 (3%)	44 73
4	3D	202/258 (78%)	193 (96%)	9 (4%)	27 61
4	3Q	204/258 (79%)	198 (97%)	6 (3%)	42 71
5	3E	166/225 (74%)	159 (96%)	7 (4%)	30 63
5	3I	36/225 (16%)	30 (83%)	6 (17%)	2 12
5	3R	166/225 (74%)	151 (91%)	15 (9%)	9 37
5	3V	24/225 (11%)	21 (88%)	3 (12%)	4 23
6	3F	90/99 (91%)	85 (94%)	5 (6%)	21 54
6	3S	90/99 (91%)	88 (98%)	2 (2%)	52 78
7	3G	67/73 (92%)	65 (97%)	2 (3%)	41 71
7	3T	67/73 (92%)	66 (98%)	1 (2%)	65 84
8	3H	62/85 (73%)	60 (97%)	2 (3%)	39 69

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
8	3U	62/85 (73%)	60 (97%)	2 (3%)	39 69
9	3J	46/52 (88%)	44 (96%)	2 (4%)	29 62
9	3W	46/52 (88%)	44 (96%)	2 (4%)	29 62
10	3X	42/46 (91%)	41 (98%)	1 (2%)	49 76
10	3Y	41/46 (89%)	38 (93%)	3 (7%)	14 45
All	All	3469/4294 (81%)	3321 (96%)	148 (4%)	33 62

All (148) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	3A	58	PHE
1	3A	77	LYS
1	3A	90	SER
1	3A	92	ARG
1	3A	123	GLU
1	3A	210	ASP
1	3A	217	SER
1	3A	264	ASN
1	3A	302	LYS
1	3A	333	ASP
1	3A	343	MET
1	3A	389	ARG
2	3B	55	SER
2	3B	61	ASN
2	3B	111	CYS
2	3B	113	ARG
2	3B	117	GLU
2	3B	120	MET
2	3B	148	LYS
2	3B	175	SER
2	3B	247	GLN
2	3B	266	SER
2	3B	268	GLU
2	3B	284	HIS
2	3B	376	GLU
2	3B	380	ASP
2	3B	407	ASP
3	3C	1	MET
3	3C	12	LYS
3	3C	18	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	3C	80	ARG
3	3C	100	ARG
3	3C	183	PHE
3	3C	227	LYS
3	3C	228	ASP
3	3C	234	PHE
3	3C	283	SER
3	3C	287	LYS
3	3C	297	SER
3	3C	379	TRP
4	3D	143	CYS
4	3D	159	GLN
4	3D	169	PHE
4	3D	223	CYS
4	3D	230	SER
4	3D	258	LEU
4	3D	269	SER
4	3D	274	ASP
4	3D	327	ARG
5	3E	141	SER
5	3E	149	MET
5	3E	168	LYS
5	3E	182	LYS
5	3E	235	TYR
5	3E	248	ARG
5	3E	265	PHE
6	3F	82	MET
6	3F	89	LYS
6	3F	91	GLN
6	3F	100	PHE
6	3F	114	LYS
7	3G	26	ARG
7	3G	46	CYS
8	3H	71	SER
8	3H	74	GLN
5	3I	34	LEU
5	3I	37	THR
5	3I	53	GLU
5	3I	58	GLN
5	3I	62	ARG
5	3I	78	TYR
9	3J	9	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	3J	54	LYS
1	3N	8	LEU
1	3N	9	GLN
1	3N	27	SER
1	3N	28	GLU
1	3N	35	CYS
1	3N	42	ASP
1	3N	51	LYS
1	3N	58	PHE
1	3N	112	LEU
1	3N	116	ILE
1	3N	117	VAL
1	3N	132	ASP
1	3N	134	ILE
1	3N	142	ASP
1	3N	145	MET
1	3N	146	ARG
1	3N	166	SER
1	3N	181	ASP
1	3N	194	ARG
1	3N	209	LEU
1	3N	214	LYS
1	3N	307	PHE
1	3N	388	ARG
1	3N	405	SER
2	3O	97	SER
2	3O	105	MET
2	3O	111	CYS
2	3O	335	ASP
2	3O	338	LYS
2	3O	380	ASP
2	3O	409	ASP
3	3P	80	ARG
3	3P	183	PHE
3	3P	215	MET
3	3P	236	MET
3	3P	269	LYS
3	3P	282	ARG
3	3P	310	SER
3	3P	316	MET
3	3P	379	TRP
4	3Q	6	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	3Q	37	CYS
4	3Q	49	ARG
4	3Q	75	ASN
4	3Q	83	ARG
4	3Q	118	ARG
5	3R	80	HIS
5	3R	82	ASP
5	3R	92	ARG
5	3R	131	ASN
5	3R	140	MET
5	3R	165	MET
5	3R	172	LYS
5	3R	200	HIS
5	3R	222	CYS
5	3R	231	PHE
5	3R	242	HIS
5	3R	256	LEU
5	3R	258	LEU
5	3R	263	TYR
5	3R	265	PHE
6	3S	58	ARG
6	3S	82	LYS
7	3T	73	ASN
8	3U	42	GLN
8	3U	49	GLN
5	3V	50	LEU
5	3V	51	CYS
5	3V	62	ARG
9	3W	43	TYR
9	3W	51	LEU
10	3X	4	ARG
10	3Y	11	ARG
10	3Y	16	ASN
10	3Y	52	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	3A	126	GLN
3	3C	44	GLN
3	3C	201	HIS
5	3E	242	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	3H	51	GLN
1	3N	9	GLN
1	3N	435	ASN
4	3Q	121	HIS
5	3R	219	HIS
8	3U	67	HIS
8	3U	71	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

32 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
17	PC1	3R	302	-	44,44,53	0.29	0	50,52,61	0.35	0
11	CDL	3C	505	-	51,51,99	0.36	0	57,63,111	0.55	1 (1%)
13	HEM	3P	502	3	41,50,50	1.39	6 (14%)	45,82,82	1.79	9 (20%)
14	U10	3P	504	-	28,28,63	0.82	1 (3%)	34,37,79	1.06	4 (11%)
12	3PE	3A	502	-	26,26,50	0.36	0	29,31,55	0.55	0
11	CDL	3G	102	-	55,55,99	0.35	0	61,67,111	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	3PE	3N	501	-	31,31,50	0.34	0	34,36,55	0.37	0
12	3PE	3C	507	-	33,33,50	0.33	0	36,38,55	0.40	0
17	PC1	3X	101	-	28,28,53	0.37	0	34,36,61	0.41	0
13	HEM	3C	501	3	41,50,50	1.39	6 (14%)	45,82,82	1.91	11 (24%)
16	FES	3E	301	5	0,4,4	-	-	-		
12	3PE	3C	506	-	34,34,50	0.33	0	37,39,55	0.48	0
12	3PE	3N	502	-	24,24,50	0.37	0	27,29,55	0.70	1 (3%)
12	3PE	3Q	503	-	46,46,50	0.28	0	49,51,55	0.37	0
13	HEM	3P	501	3	41,50,50	1.39	6 (14%)	45,82,82	1.91	9 (20%)
12	3PE	3D	502	-	32,32,50	0.35	0	35,37,55	0.40	0
14	U10	3C	504	-	23,23,63	0.91	2 (8%)	28,31,79	1.19	4 (14%)
12	3PE	3Y	101	-	29,29,50	0.36	0	32,34,55	0.42	0
14	U10	3C	503	-	24,24,63	1.00	2 (8%)	29,32,79	1.22	5 (17%)
11	CDL	3A	501	-	57,57,99	0.34	0	63,69,111	0.43	0
11	CDL	3P	507	-	42,42,99	0.39	0	48,54,111	0.66	1 (2%)
11	CDL	3P	506	-	55,55,99	0.35	0	61,67,111	0.48	1 (1%)
11	CDL	3Q	502	-	56,56,99	0.35	0	62,68,111	0.46	0
13	HEM	3C	502	-	41,50,50	1.40	6 (14%)	45,82,82	1.81	9 (20%)
12	3PE	3A	503	-	31,31,50	0.34	0	34,36,55	0.58	1 (2%)
15	HEC	3D	501	4	31,49,50	2.33	12 (38%)	22,80,82	2.33	5 (22%)
12	3PE	3P	505	-	32,32,50	0.34	0	35,37,55	0.40	0
16	FES	3R	301	5	0,4,4	-	-	-		
15	HEC	3Q	501	4	32,50,50	2.30	12 (37%)	24,82,82	2.32	5 (20%)
12	3PE	3G	101	-	28,28,50	0.33	0	31,33,55	0.45	0
17	PC1	3E	302	-	46,46,53	0.29	0	52,54,61	0.30	0
14	U10	3P	503	-	23,23,63	0.90	2 (8%)	28,31,79	1.24	4 (14%)

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
17	PC1	3R	302	-	-	7/48/48/57	-
11	CDL	3C	505	-	-	15/62/62/110	-
13	HEM	3P	502	3	-	6/12/54/54	-
14	U10	3P	504	-	-	5/21/45/87	0/1/1/1
12	3PE	3A	502	-	-	5/30/30/54	-
11	CDL	3G	102	-	-	12/66/66/110	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	3PE	3N	501	-	-	12/35/35/54	-
12	3PE	3C	507	-	-	12/37/37/54	-
17	PC1	3X	101	-	-	6/32/32/57	-
13	HEM	3C	501	3	-	5/12/54/54	-
16	FES	3E	301	5	-	-	0/1/1/1
12	3PE	3C	506	-	-	9/38/38/54	-
12	3PE	3N	502	-	-	6/28/28/54	-
12	3PE	3Q	503	-	-	5/50/50/54	-
13	HEM	3P	501	3	-	4/12/54/54	-
12	3PE	3D	502	-	-	2/36/36/54	-
14	U10	3C	504	-	-	5/15/39/87	0/1/1/1
12	3PE	3Y	101	-	-	9/33/33/54	-
14	U10	3C	503	-	-	1/17/41/87	0/1/1/1
11	CDL	3A	501	-	-	2/68/68/110	-
11	CDL	3P	507	-	-	11/53/53/110	-
11	CDL	3P	506	-	-	15/66/66/110	-
11	CDL	3Q	502	-	-	19/67/67/110	-
13	HEM	3C	502	-	-	4/12/54/54	-
12	3PE	3A	503	-	-	9/35/35/54	-
15	HEC	3D	501	4	-	2/8/53/54	-
12	3PE	3P	505	-	-	11/36/36/54	-
16	FES	3R	301	5	-	-	0/1/1/1
15	HEC	3Q	501	4	-	5/10/54/54	-
12	3PE	3G	101	-	-	1/32/32/54	-
17	PC1	3E	302	-	-	2/50/50/57	-
14	U10	3P	503	-	-	6/15/39/87	0/1/1/1

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	3Q	501	HEC	C2B-C3B	6.78	1.47	1.40
15	3D	501	HEC	C3C-C2C	6.64	1.47	1.40
15	3D	501	HEC	C2B-C3B	6.58	1.47	1.40
15	3Q	501	HEC	C3C-C2C	6.34	1.47	1.40
13	3C	502	HEM	C1B-NB	-3.75	1.33	1.40
13	3C	502	HEM	C4D-ND	-3.72	1.33	1.40
13	3P	501	HEM	C1B-NB	-3.68	1.34	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	3P	502	HEM	C1B-NB	-3.66	1.34	1.40
13	3P	501	HEM	C4D-ND	-3.66	1.34	1.40
13	3C	501	HEM	C1B-NB	-3.64	1.34	1.40
13	3P	502	HEM	C4D-ND	-3.61	1.34	1.40
13	3C	501	HEM	C4D-ND	-3.56	1.34	1.40
15	3Q	501	HEC	C2A-C3A	3.48	1.48	1.37
15	3D	501	HEC	C3D-C2D	3.20	1.47	1.37
15	3D	501	HEC	C2A-C3A	3.19	1.47	1.37
15	3Q	501	HEC	C3D-C2D	3.09	1.46	1.37
15	3D	501	HEC	C4B-C3B	3.00	1.48	1.43
14	3P	504	U10	C3-C2	-2.95	1.40	1.48
14	3C	503	U10	C3-C2	-2.84	1.40	1.48
13	3C	501	HEM	FE-NB	2.74	2.10	1.96
15	3Q	501	HEC	C3A-C4A	2.74	1.48	1.42
13	3P	501	HEM	FE-NB	2.70	2.10	1.96
13	3P	502	HEM	FE-NB	2.69	2.10	1.96
13	3C	502	HEM	FE-NB	2.68	2.10	1.96
14	3C	504	U10	C4-C5	-2.63	1.41	1.48
15	3D	501	HEC	C2A-C1A	2.62	1.48	1.42
15	3Q	501	HEC	C4B-C3B	2.61	1.47	1.43
15	3D	501	HEC	C3C-C4C	2.60	1.47	1.43
15	3D	501	HEC	C3A-C4A	2.60	1.48	1.42
14	3P	503	U10	C4-C5	-2.58	1.41	1.48
15	3Q	501	HEC	C3C-C4C	2.58	1.47	1.43
15	3Q	501	HEC	C2A-C1A	2.56	1.48	1.42
14	3C	503	U10	C4-C5	-2.48	1.41	1.48
15	3D	501	HEC	C1C-CHC	2.48	1.47	1.41
15	3Q	501	HEC	C1B-CHB	2.46	1.47	1.41
15	3D	501	HEC	C1D-CHD	2.42	1.47	1.41
15	3Q	501	HEC	C1D-CHD	2.37	1.47	1.41
15	3D	501	HEC	C1B-CHB	2.35	1.47	1.41
15	3Q	501	HEC	C1C-CHC	2.35	1.47	1.41
15	3Q	501	HEC	C4D-CHA	2.34	1.47	1.41
15	3D	501	HEC	C4D-CHA	2.29	1.47	1.41
13	3C	501	HEM	C1D-ND	-2.27	1.34	1.38
13	3C	502	HEM	C1D-ND	-2.27	1.34	1.38
13	3P	502	HEM	C1D-ND	-2.26	1.34	1.38
13	3P	501	HEM	C1D-ND	-2.22	1.34	1.38
13	3P	502	HEM	C4B-NB	-2.19	1.34	1.38
13	3C	502	HEM	C4B-NB	-2.14	1.34	1.38
13	3P	501	HEM	FE-ND	-2.12	1.86	1.96
13	3C	501	HEM	FE-ND	-2.10	1.86	1.96

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	3P	502	HEM	FE-ND	-2.09	1.86	1.96
13	3C	502	HEM	FE-ND	-2.07	1.86	1.96
13	3C	501	HEM	C4B-NB	-2.07	1.34	1.38
14	3C	504	U10	C6-C5	-2.06	1.40	1.46
13	3P	501	HEM	C4B-NB	-2.05	1.34	1.38
14	3P	503	U10	C6-C5	-2.02	1.41	1.46

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	3D	501	HEC	C1D-C2D-C3D	-6.08	102.77	107.00
15	3Q	501	HEC	C1D-C2D-C3D	-5.79	102.97	107.00
15	3D	501	HEC	CMB-C2B-C3B	5.47	132.25	125.82
13	3P	501	HEM	CHC-C4B-NB	5.33	130.22	124.43
15	3Q	501	HEC	CMB-C2B-C3B	5.32	132.08	125.82
13	3C	501	HEM	CHC-C4B-NB	5.26	130.14	124.43
15	3Q	501	HEC	CMC-C2C-C3C	5.08	131.80	125.82
13	3C	502	HEM	CHC-C4B-NB	5.05	129.92	124.43
13	3P	502	HEM	CHC-C4B-NB	5.01	129.87	124.43
13	3P	501	HEM	CHD-C1D-ND	4.92	129.78	124.43
13	3C	501	HEM	CHD-C1D-ND	4.61	129.44	124.43
15	3D	501	HEC	CMC-C2C-C3C	4.51	131.12	125.82
13	3C	502	HEM	CHD-C1D-ND	4.11	128.89	124.43
13	3P	502	HEM	CHD-C1D-ND	4.10	128.88	124.43
13	3C	502	HEM	C1B-NB-C4B	4.04	109.24	105.07
13	3P	502	HEM	C1B-NB-C4B	3.94	109.14	105.07
13	3P	501	HEM	C1B-NB-C4B	3.81	109.01	105.07
13	3C	501	HEM	C1B-NB-C4B	3.66	108.85	105.07
13	3C	501	HEM	CHB-C1B-NB	3.64	128.88	124.38
13	3P	502	HEM	CHA-C4D-ND	3.60	128.82	124.38
13	3C	502	HEM	CHA-C4D-ND	3.47	128.67	124.38
13	3C	501	HEM	CHA-C4D-ND	3.44	128.63	124.38
13	3P	501	HEM	CHA-C4D-ND	3.40	128.58	124.38
13	3P	501	HEM	CHB-C1B-NB	3.28	128.43	124.38
13	3P	502	HEM	CHB-C1B-NB	3.25	128.39	124.38
13	3C	502	HEM	CHB-C1B-NB	3.12	128.23	124.38
13	3P	501	HEM	CHD-C1D-C2D	-3.05	120.21	124.98
13	3C	501	HEM	CBA-CAA-C2A	-3.03	107.45	112.62
14	3C	503	U10	O3-C3-C4	2.96	134.79	123.64
14	3P	503	U10	O4-C4-C5	-2.89	106.78	116.56
13	3P	501	HEM	CAD-CBD-CGD	-2.84	107.50	113.60
14	3C	504	U10	O4-C4-C5	-2.80	107.10	116.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	3C	501	HEM	CHD-C1D-C2D	-2.77	120.65	124.98
14	3P	503	U10	O3-C3-C2	2.76	125.90	116.56
14	3C	504	U10	O3-C3-C2	2.67	125.60	116.56
11	3P	507	CDL	OA6-CA5-C11	2.67	117.26	111.50
14	3C	503	U10	O4-C4-C3	2.60	133.44	123.64
12	3N	502	3PE	O21-C21-C22	2.55	117.00	111.50
13	3C	502	HEM	C4D-ND-C1D	2.55	107.70	105.07
14	3C	503	U10	O3-C3-C2	-2.54	107.97	116.56
15	3Q	501	HEC	CMA-C3A-C2A	2.50	129.65	124.94
13	3C	501	HEM	CAD-CBD-CGD	-2.45	108.33	113.60
13	3P	502	HEM	CHD-C1D-C2D	-2.44	121.17	124.98
13	3P	502	HEM	C4D-ND-C1D	2.43	107.59	105.07
14	3P	503	U10	O4-C4-C3	2.43	132.80	123.64
14	3P	504	U10	O3-C3-C2	-2.39	108.49	116.56
15	3D	501	HEC	CAA-CBA-CGA	-2.36	107.15	113.76
14	3C	503	U10	O4-C4-C5	-2.36	108.59	116.56
15	3Q	501	HEC	CAD-CBD-CGD	-2.35	107.18	113.76
13	3C	502	HEM	CHD-C1D-C2D	-2.34	121.33	124.98
13	3C	502	HEM	CBA-CAA-C2A	-2.33	108.65	112.62
13	3C	501	HEM	C4D-ND-C1D	2.30	107.44	105.07
14	3P	504	U10	O4-C4-C5	2.29	124.30	116.56
13	3P	501	HEM	C4D-ND-C1D	2.26	107.41	105.07
14	3P	504	U10	O3-C3-C4	2.25	132.13	123.64
14	3P	504	U10	C3-C4-C5	-2.23	116.30	120.68
14	3C	504	U10	O4-C4-C3	2.22	132.01	123.64
14	3C	504	U10	C4-C3-C2	-2.21	116.34	120.68
14	3C	503	U10	C4-C3-C2	-2.14	116.47	120.68
13	3P	502	HEM	CHA-C4D-C3D	-2.13	121.32	125.33
13	3C	501	HEM	CHB-C1B-C2B	-2.12	120.85	126.72
14	3P	503	U10	C4-C3-C2	-2.12	116.52	120.68
11	3C	505	CDL	OA6-CA5-C11	2.10	116.02	111.50
13	3C	501	HEM	CHA-C4D-C3D	-2.10	121.39	125.33
13	3C	502	HEM	CHA-C4D-C3D	-2.09	121.40	125.33
15	3D	501	HEC	CMD-C2D-C3D	2.08	128.86	124.94
13	3P	501	HEM	CBA-CAA-C2A	-2.04	109.13	112.62
13	3P	502	HEM	CAD-CBD-CGD	-2.04	109.21	113.60
11	3P	506	CDL	OA6-CA5-C11	2.04	115.90	111.50
12	3A	503	3PE	O21-C21-C22	2.03	115.87	111.50

There are no chirality outliers.

All (213) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	3C	505	CDL	OA7-CA5-OA6-CA4
11	3C	505	CDL	C11-CA5-OA6-CA4
11	3C	505	CDL	CB3-OB5-PB2-OB4
11	3C	505	CDL	CB4-CB3-OB5-PB2
11	3G	102	CDL	CA3-OA5-PA1-OA3
11	3G	102	CDL	CA4-CA3-OA5-PA1
11	3G	102	CDL	OA7-CA5-OA6-CA4
11	3G	102	CDL	C11-CA5-OA6-CA4
11	3G	102	CDL	OA9-CA7-OA8-CA6
11	3G	102	CDL	C31-CA7-OA8-CA6
11	3P	506	CDL	C1-CA2-OA2-PA1
11	3P	506	CDL	CA2-OA2-PA1-OA3
11	3P	507	CDL	OA7-CA5-OA6-CA4
11	3P	507	CDL	C11-CA5-OA6-CA4
11	3Q	502	CDL	CA2-OA2-PA1-OA5
11	3Q	502	CDL	CA3-OA5-PA1-OA3
11	3Q	502	CDL	OA6-CA4-CA6-OA8
11	3Q	502	CDL	CB3-OB5-PB2-OB3
11	3Q	502	CDL	OB9-CB7-OB8-CB6
11	3Q	502	CDL	C71-CB7-OB8-CB6
12	3A	502	3PE	O32-C31-O31-C3
12	3A	502	3PE	C32-C31-O31-C3
12	3A	502	3PE	O22-C21-O21-C2
12	3A	502	3PE	C22-C21-O21-C2
12	3A	503	3PE	C1-O11-P-O14
12	3A	503	3PE	O32-C31-O31-C3
12	3A	503	3PE	C32-C31-O31-C3
12	3A	503	3PE	O22-C21-O21-C2
12	3A	503	3PE	C22-C21-O21-C2
12	3C	506	3PE	C11-O13-P-O11
12	3C	507	3PE	C11-O13-P-O11
12	3C	507	3PE	C2-C1-O11-P
12	3C	507	3PE	C12-C11-O13-P
12	3N	502	3PE	C11-O13-P-O14
12	3N	502	3PE	O22-C21-O21-C2
12	3N	502	3PE	C22-C21-O21-C2
12	3P	505	3PE	C11-O13-P-O14
13	3C	501	HEM	C2B-C3B-CAB-CBB
13	3C	501	HEM	C4B-C3B-CAB-CBB
13	3C	502	HEM	C2B-C3B-CAB-CBB
13	3P	501	HEM	C2B-C3B-CAB-CBB
13	3P	501	HEM	C4B-C3B-CAB-CBB
13	3P	502	HEM	C2B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	3Q	501	HEC	C1A-C2A-CAA-CBA
15	3Q	501	HEC	C3A-C2A-CAA-CBA
17	3X	101	PC1	C1-O11-P-O14
17	3X	101	PC1	C1-O11-P-O13
14	3C	504	U10	C12-C11-C9-C10
14	3C	504	U10	C12-C11-C9-C8
14	3C	504	U10	C4-C3-O3-C3M
14	3P	503	U10	C4-C3-O3-C3M
14	3P	504	U10	C3-C4-O4-C4M
11	3C	505	CDL	CB3-OB5-PB2-OB2
11	3P	507	CDL	CB3-OB5-PB2-OB2
11	3Q	502	CDL	CA3-OA5-PA1-OA2
17	3R	302	PC1	C1-O11-P-O13
12	3N	501	3PE	C2-C1-O11-P
11	3C	505	CDL	O1-C1-CB2-OB2
11	3G	102	CDL	C51-C52-C53-C54
12	3P	505	3PE	C33-C34-C35-C36
12	3N	501	3PE	C32-C33-C34-C35
14	3P	503	U10	C2-C3-O3-C3M
11	3Q	502	CDL	CA7-C31-C32-C33
12	3P	505	3PE	C31-C32-C33-C34
12	3Q	503	3PE	C38-C39-C3A-C3B
11	3P	506	CDL	OB5-CB3-CB4-OB6
13	3C	502	HEM	C4B-C3B-CAB-CBB
13	3P	502	HEM	C4B-C3B-CAB-CBB
12	3C	507	3PE	O21-C2-C3-O31
12	3Y	101	3PE	C34-C35-C36-C37
12	3A	503	3PE	C1-O11-P-O13
11	3Q	502	CDL	CA4-CA3-OA5-PA1
11	3Q	502	CDL	CB4-CB3-OB5-PB2
13	3C	501	HEM	C3D-CAD-CBD-CGD
14	3C	504	U10	C2-C3-O3-C3M
11	3C	505	CDL	CA3-CA4-CA6-OA8
12	3C	507	3PE	C1-C2-C3-O31
12	3Y	101	3PE	C2-C1-O11-P
12	3P	505	3PE	O11-C1-C2-O21
17	3X	101	PC1	O21-C21-C22-C23
12	3C	506	3PE	C25-C26-C27-C28
11	3C	505	CDL	C52-C51-CB5-OB6
12	3C	507	3PE	O21-C21-C22-C23
11	3A	501	CDL	C32-C33-C34-C35
11	3P	506	CDL	OA5-CA3-CA4-CA6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	3P	506	CDL	OB5-CB3-CB4-CB6
12	3P	505	3PE	O11-C1-C2-C3
12	3C	507	3PE	C22-C23-C24-C25
11	3P	507	CDL	C1-CA2-OA2-PA1
11	3Q	502	CDL	C1-CB2-OB2-PB2
17	3R	302	PC1	C2-C1-O11-P
11	3Q	502	CDL	CA3-CA4-CA6-OA8
12	3N	501	3PE	C1-C2-C3-O31
11	3G	102	CDL	CA3-OA5-PA1-OA2
11	3Q	502	CDL	CB3-OB5-PB2-OB2
11	3P	506	CDL	OA5-CA3-CA4-OA6
12	3C	506	3PE	O11-C1-C2-O21
11	3P	506	CDL	C12-C11-CA5-OA6
11	3C	505	CDL	C1-CB2-OB2-PB2
11	3P	507	CDL	CA4-CA3-OA5-PA1
11	3A	501	CDL	C1-CB2-OB2-PB2
12	3C	507	3PE	O11-C1-C2-O21
11	3C	505	CDL	C52-C53-C54-C55
11	3P	506	CDL	CA4-CA3-OA5-PA1
11	3P	507	CDL	CB3-OB5-PB2-OB3
11	3Q	502	CDL	CA2-OA2-PA1-OA4
11	3Q	502	CDL	CA3-OA5-PA1-OA4
12	3C	506	3PE	C11-O13-P-O12
12	3C	507	3PE	C11-O13-P-O12
17	3R	302	PC1	C1-O11-P-O14
17	3R	302	PC1	C38-C39-C3A-C3B
12	3C	506	3PE	C12-C11-O13-P
12	3D	502	3PE	C12-C11-O13-P
12	3N	501	3PE	C12-C11-O13-P
12	3N	502	3PE	C12-C11-O13-P
12	3P	505	3PE	C12-C11-O13-P
12	3Y	101	3PE	C12-C11-O13-P
12	3G	101	3PE	C31-C32-C33-C34
11	3C	505	CDL	OA6-CA4-CA6-OA8
12	3N	501	3PE	O21-C2-C3-O31
12	3Y	101	3PE	O21-C2-C3-O31
14	3P	504	U10	C1-C6-C7-C8
17	3X	101	PC1	O31-C31-C32-C33
17	3R	302	PC1	C32-C33-C34-C35
12	3N	502	3PE	C31-C32-C33-C34
11	3P	506	CDL	C72-C71-CB7-OB8
12	3Q	503	3PE	C23-C24-C25-C26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
12	3C	507	3PE	O11-C1-C2-C3
12	3D	502	3PE	C31-C32-C33-C34
11	3G	102	CDL	CB2-OB2-PB2-OB5
11	3P	506	CDL	CA2-OA2-PA1-OA5
11	3P	506	CDL	CB3-OB5-PB2-OB2
11	3P	507	CDL	CA2-OA2-PA1-OA5
12	3C	507	3PE	C1-O11-P-O13
12	3N	501	3PE	C11-O13-P-O11
12	3N	502	3PE	C11-O13-P-O11
12	3P	505	3PE	C1-O11-P-O13
12	3P	505	3PE	C11-O13-P-O11
12	3Y	101	3PE	C1-O11-P-O13
12	3Y	101	3PE	C11-O13-P-O11
11	3G	102	CDL	CB4-CB3-OB5-PB2
12	3N	501	3PE	O11-C1-C2-C3
13	3P	501	HEM	CAD-CBD-CGD-O1D
12	3P	505	3PE	O21-C2-C3-O31
13	3C	501	HEM	CAA-CBA-CGA-O2A
13	3C	501	HEM	CAA-CBA-CGA-O1A
13	3C	502	HEM	CAA-CBA-CGA-O1A
13	3P	502	HEM	CAD-CBD-CGD-O1D
12	3C	506	3PE	C21-C22-C23-C24
13	3P	502	HEM	CAA-CBA-CGA-O1A
12	3C	506	3PE	C1-C2-O21-C21
13	3P	502	HEM	CAD-CBD-CGD-O2D
14	3P	503	U10	C12-C11-C9-C10
17	3E	302	PC1	C38-C39-C3A-C3B
17	3R	302	PC1	C36-C37-C38-C39
14	3C	504	U10	C5-C4-O4-C4M
14	3P	503	U10	C5-C4-O4-C4M
14	3P	504	U10	C5-C4-O4-C4M
11	3Q	502	CDL	CA5-C11-C12-C13
12	3Q	503	3PE	C21-C22-C23-C24
13	3C	502	HEM	CAA-CBA-CGA-O2A
13	3P	501	HEM	CAD-CBD-CGD-O2D
12	3Q	503	3PE	C37-C38-C39-C3A
12	3C	507	3PE	O22-C21-C22-C23
11	3P	507	CDL	C72-C71-CB7-OB9
13	3P	502	HEM	CAA-CBA-CGA-O2A
12	3N	501	3PE	O11-C1-C2-O21
11	3P	506	CDL	C52-C51-CB5-OB6
14	3P	503	U10	C12-C11-C9-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	3P	507	CDL	C72-C71-CB7-OB8
12	3N	501	3PE	O31-C31-C32-C33
15	3D	501	HEC	CAA-CBA-CGA-O2A
12	3A	503	3PE	C33-C34-C35-C36
14	3P	504	U10	C5-C6-C7-C8
15	3Q	501	HEC	CAA-CBA-CGA-O2A
11	3P	507	CDL	CB6-CB4-OB6-CB5
11	3C	505	CDL	C52-C51-CB5-OB7
12	3P	505	3PE	C1-C2-C3-O31
11	3P	506	CDL	C12-C11-CA5-OA7
15	3D	501	HEC	CAA-CBA-CGA-O1A
11	3G	102	CDL	OB6-CB4-CB6-OB8
14	3P	504	U10	C2-C3-O3-C3M
15	3Q	501	HEC	CAA-CBA-CGA-O1A
17	3X	101	PC1	C2-C1-O11-P
12	3N	501	3PE	O32-C31-C32-C33
11	3P	506	CDL	CB3-OB5-PB2-OB3
12	3C	506	3PE	C1-O11-P-O14
12	3N	501	3PE	C11-O13-P-O14
12	3P	505	3PE	C1-O11-P-O14
12	3C	506	3PE	C29-C2A-C2B-C2C
12	3A	503	3PE	C34-C35-C36-C37
17	3X	101	PC1	O22-C21-C22-C23
14	3C	503	U10	C5-C4-O4-C4M
11	3P	507	CDL	CB3-CB4-OB6-CB5
12	3A	503	3PE	C12-C11-O13-P
17	3E	302	PC1	C12-C11-O13-P
17	3R	302	PC1	C12-C11-O13-P
11	3C	505	CDL	C12-C11-CA5-OA6
11	3P	506	CDL	C32-C31-CA7-OA8
15	3Q	501	HEC	CAD-CBD-CGD-O1D
11	3Q	502	CDL	C32-C31-CA7-OA8
11	3C	505	CDL	CA2-C1-CB2-OB2
11	3C	505	CDL	C12-C11-CA5-OA7
12	3A	502	3PE	O21-C21-C22-C23
11	3Q	502	CDL	C32-C31-CA7-OA9
12	3Y	101	3PE	O31-C31-C32-C33
11	3Q	502	CDL	C11-C12-C13-C14
14	3P	503	U10	C3-C4-O4-C4M
12	3Y	101	3PE	O32-C31-C32-C33
12	3N	501	3PE	C22-C23-C24-C25
11	3G	102	CDL	C32-C31-CA7-OA8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
12	3Q	503	3PE	C36-C37-C38-C39
12	3Y	101	3PE	C32-C33-C34-C35

There are no ring outliers.

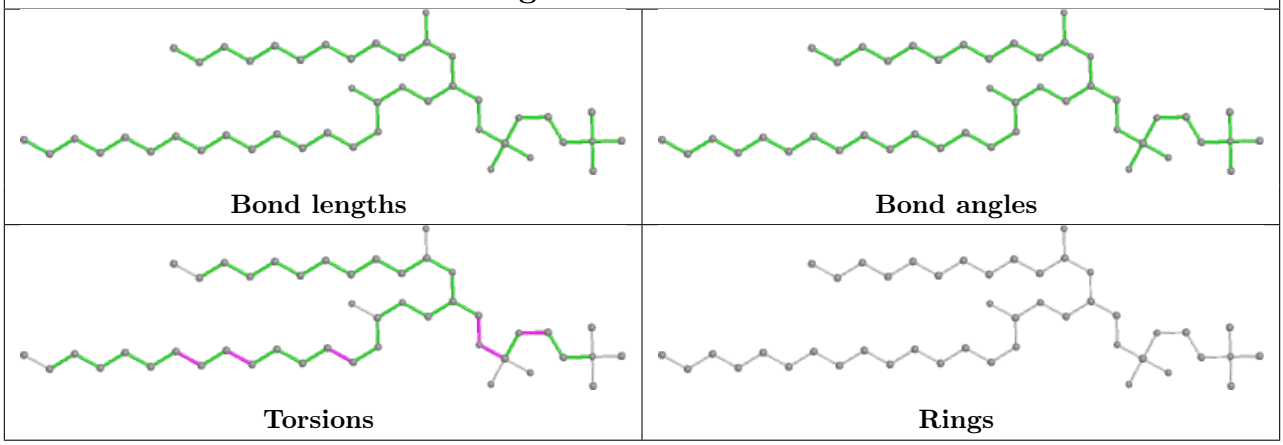
31 monomers are involved in 133 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	3R	302	PC1	5	0
11	3C	505	CDL	5	0
13	3P	502	HEM	2	0
14	3P	504	U10	2	0
12	3A	502	3PE	7	0
11	3G	102	CDL	3	0
12	3N	501	3PE	2	0
12	3C	507	3PE	3	0
17	3X	101	PC1	5	0
13	3C	501	HEM	3	0
16	3E	301	FES	1	0
12	3C	506	3PE	2	0
12	3N	502	3PE	4	0
12	3Q	503	3PE	8	0
13	3P	501	HEM	2	0
12	3D	502	3PE	4	0
14	3C	504	U10	4	0
14	3C	503	U10	7	0
11	3A	501	CDL	7	0
11	3P	507	CDL	2	0
11	3P	506	CDL	10	0
11	3Q	502	CDL	13	0
13	3C	502	HEM	6	0
12	3A	503	3PE	5	0
15	3D	501	HEC	16	0
12	3P	505	3PE	3	0
16	3R	301	FES	1	0
15	3Q	501	HEC	4	0
12	3G	101	3PE	1	0
17	3E	302	PC1	7	0
14	3P	503	U10	3	0

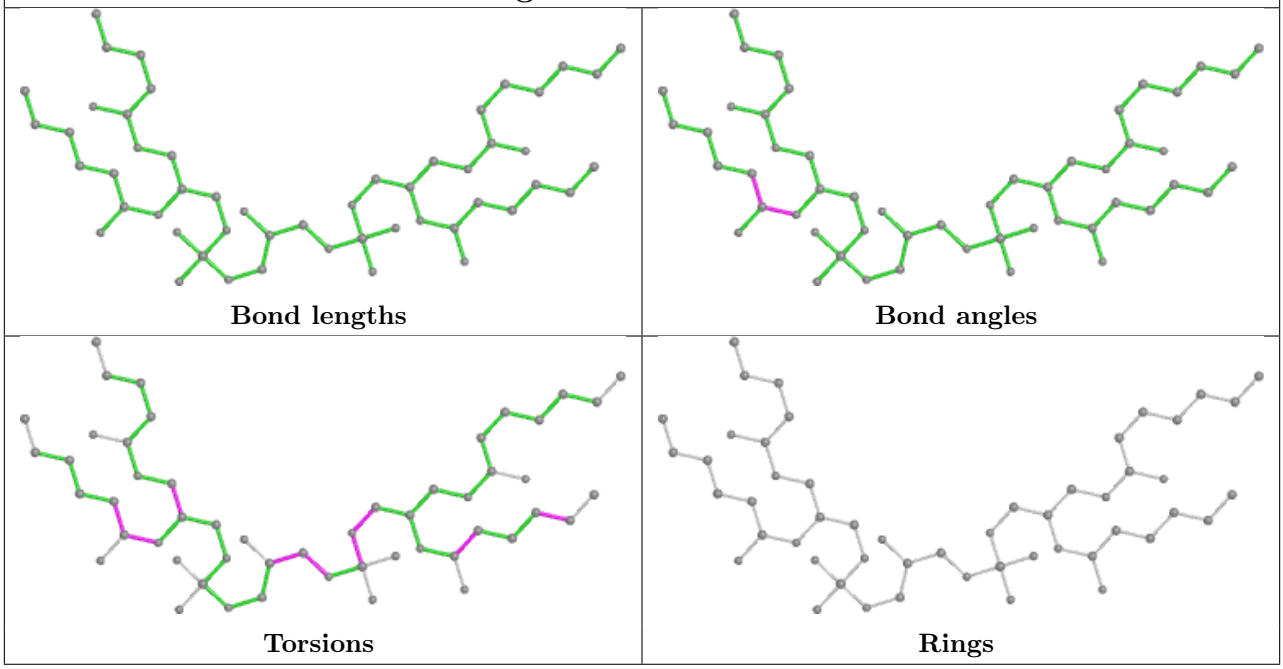
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less 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.

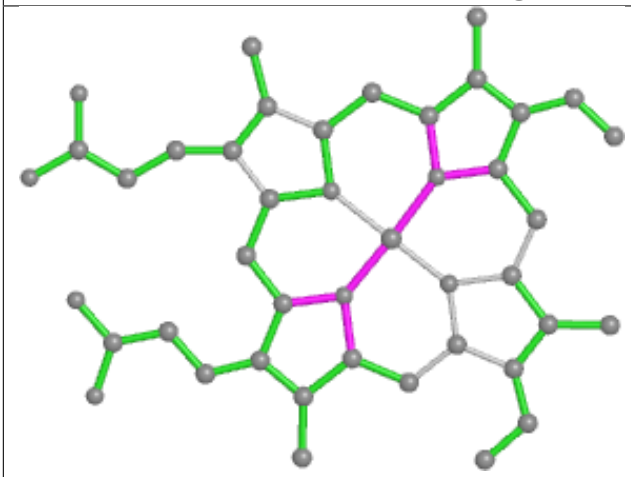
Ligand PC1 3R 302



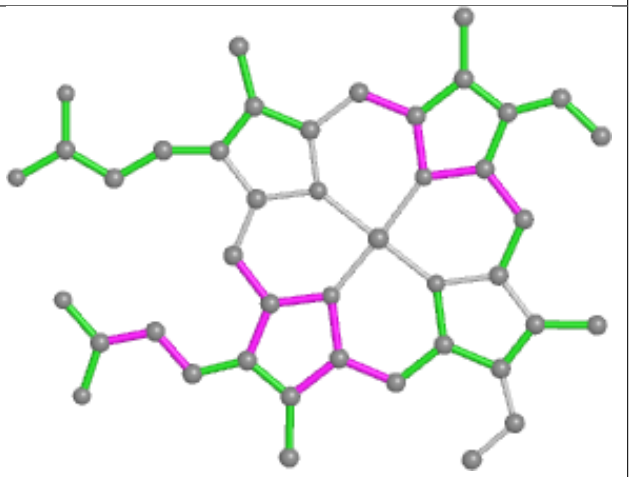
Ligand CDL 3C 505



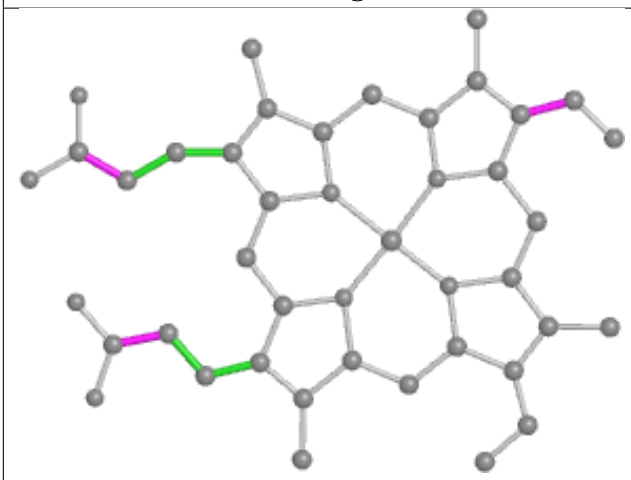
Ligand HEM 3P 502



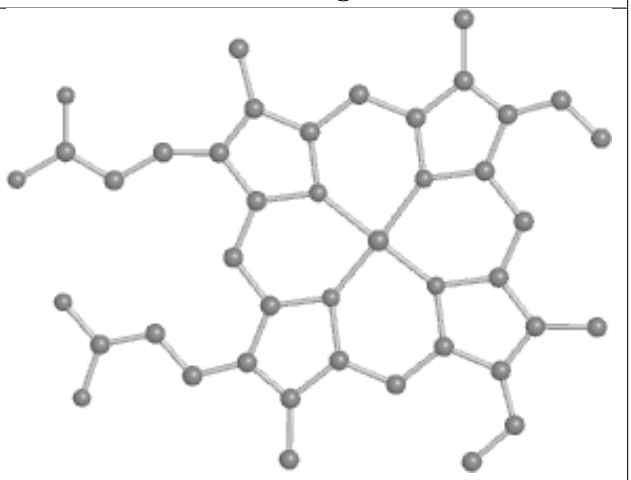
Bond lengths



Bond angles

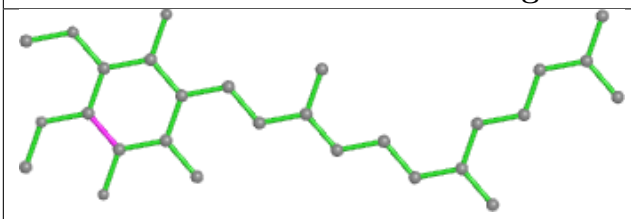


Torsions

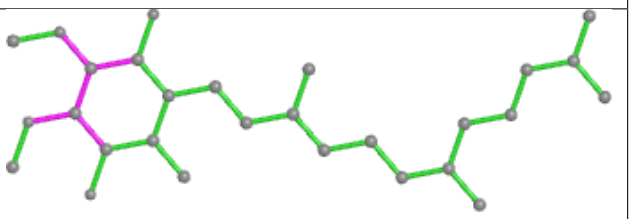


Rings

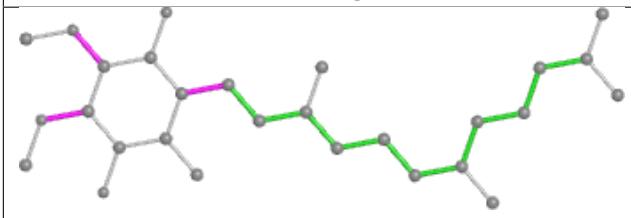
Ligand U10 3P 504



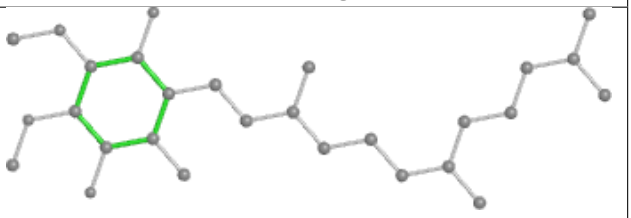
Bond lengths



Bond angles

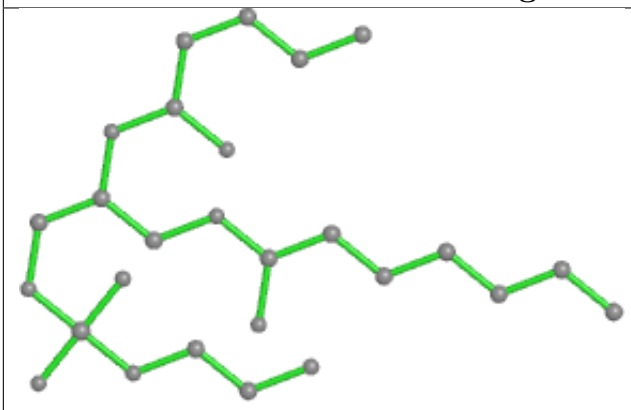


Torsions

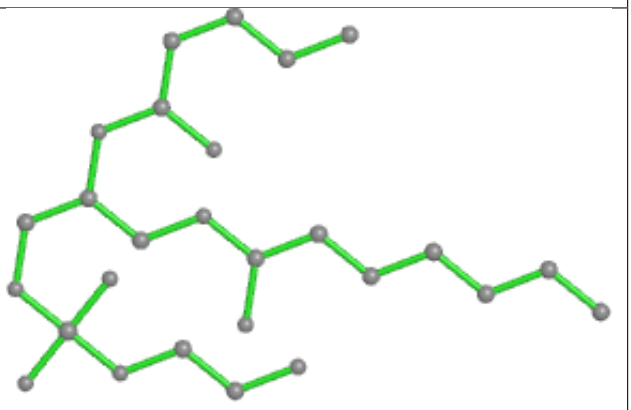


Rings

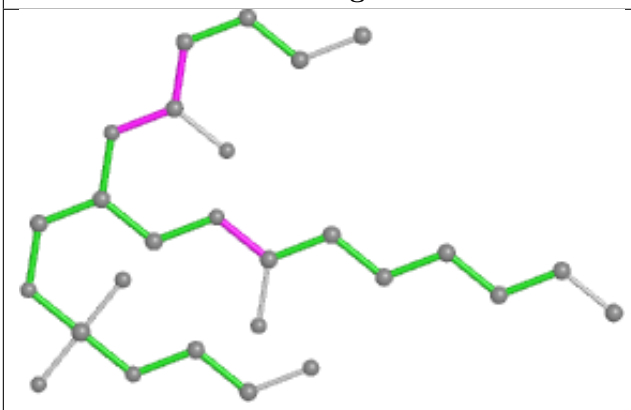
Ligand 3PE 3A 502



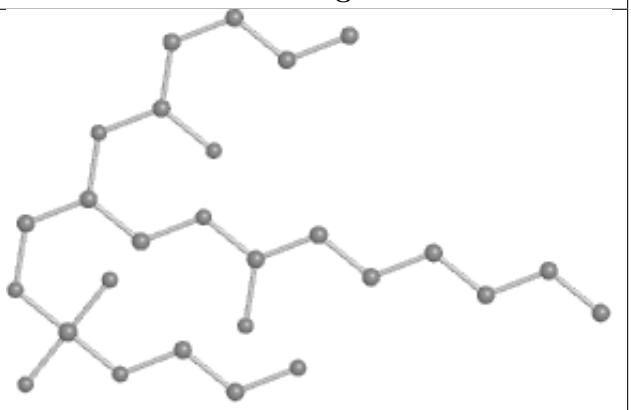
Bond lengths



Bond angles

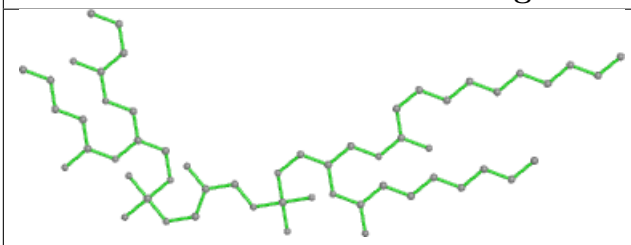


Torsions

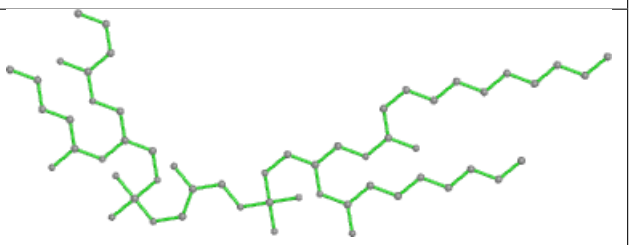


Rings

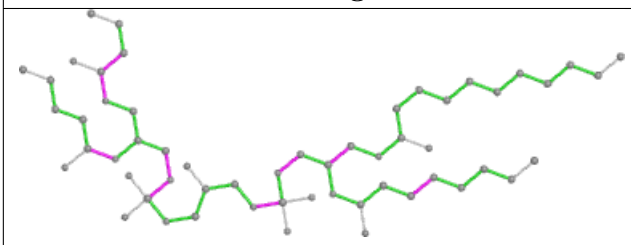
Ligand CDL 3G 102



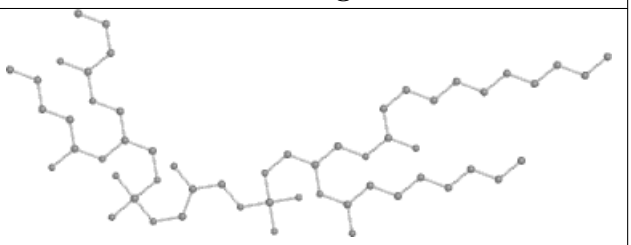
Bond lengths



Bond angles

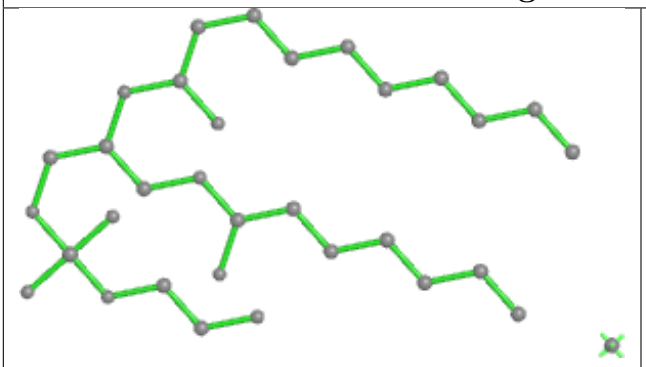


Torsions

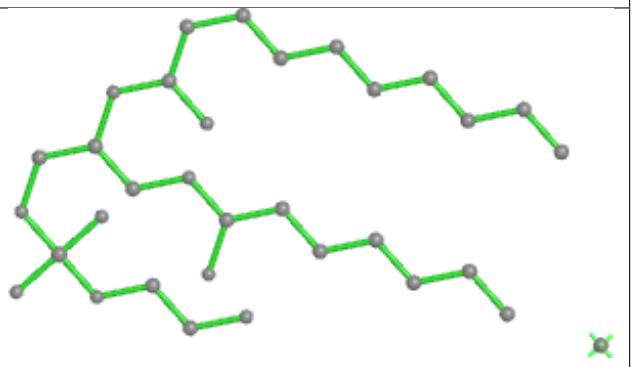


Rings

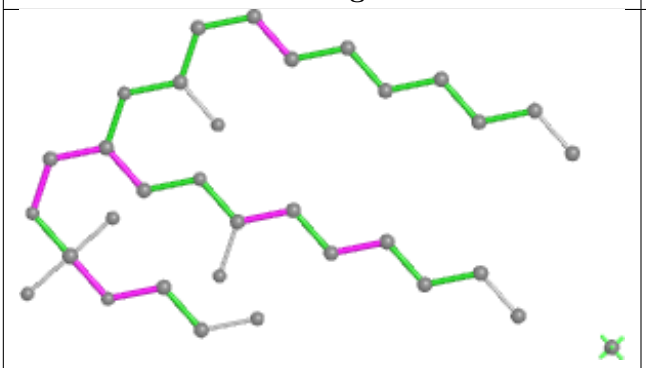
Ligand 3PE 3N 501



Bond lengths



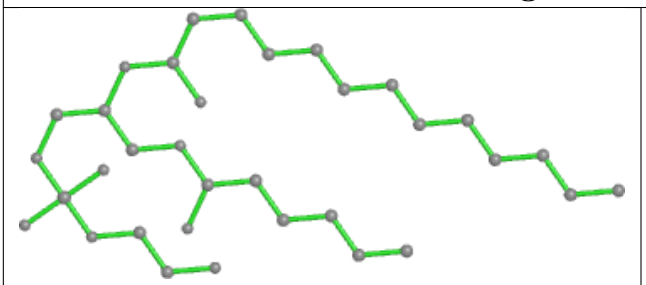
Bond angles



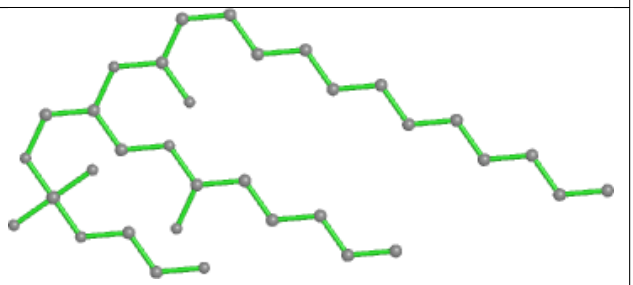
Torsions

Rings

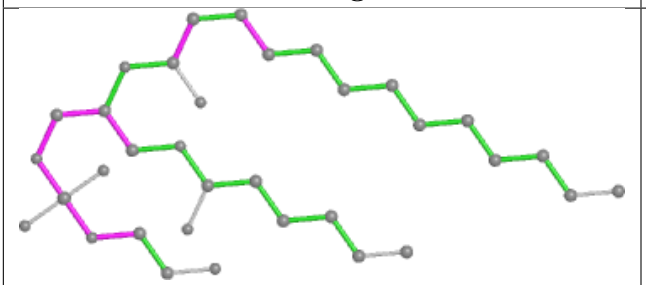
Ligand 3PE 3C 507



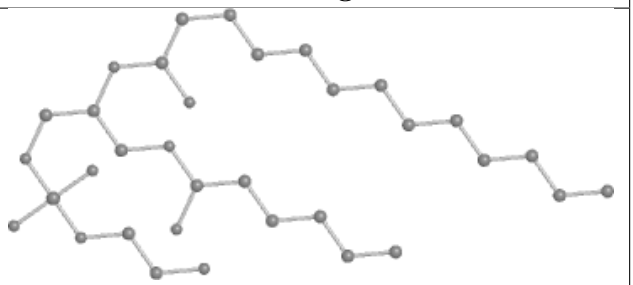
Bond lengths



Bond angles

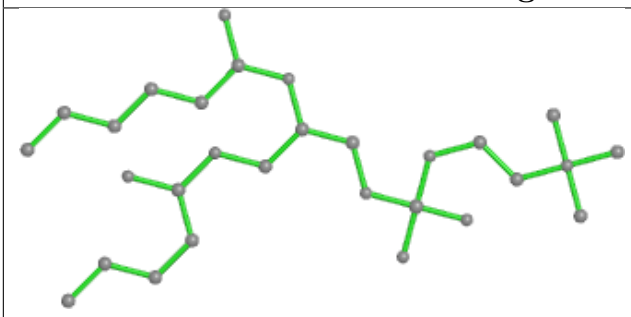


Torsions

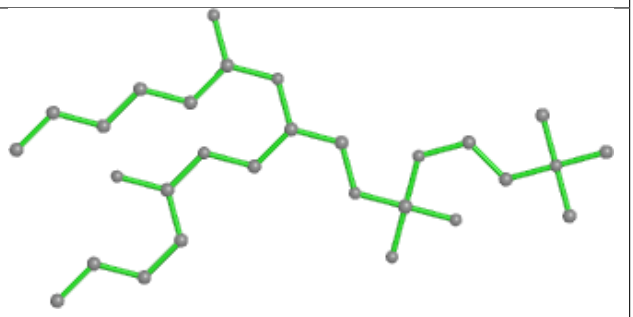


Rings

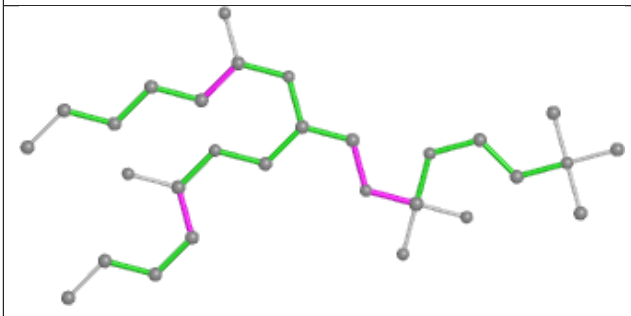
Ligand PC1 3X 101



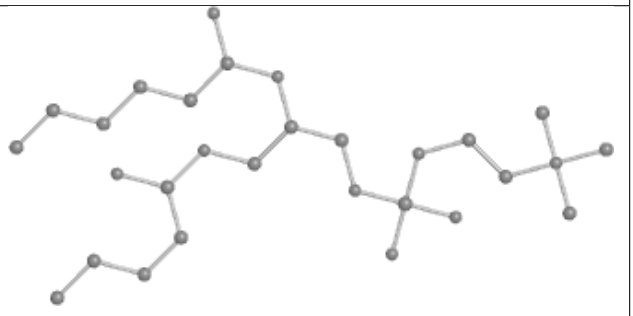
Bond lengths



Bond angles

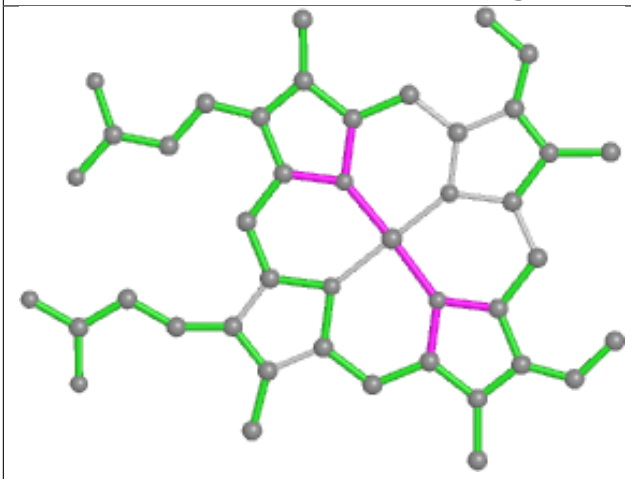


Torsions

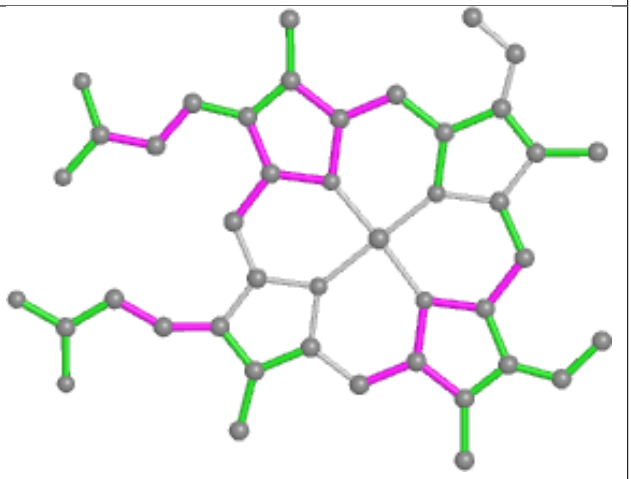


Rings

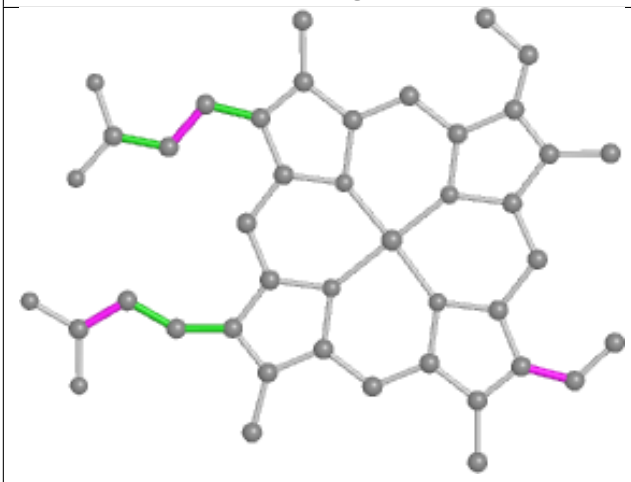
Ligand HEM 3C 501



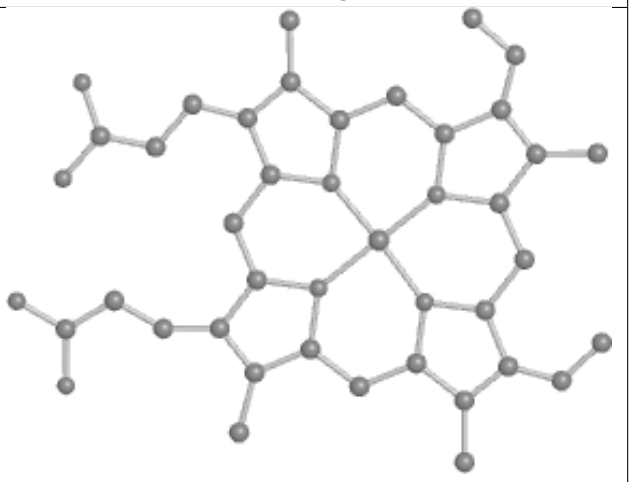
Bond lengths



Bond angles

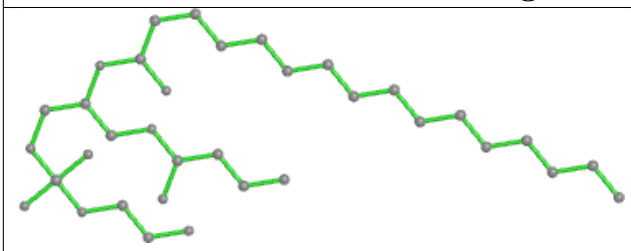


Torsions

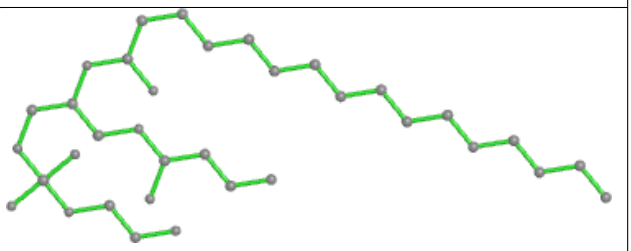


Rings

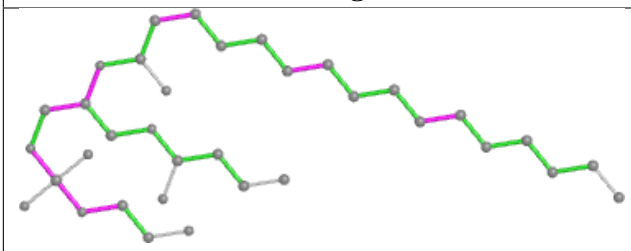
Ligand 3PE 3C 506



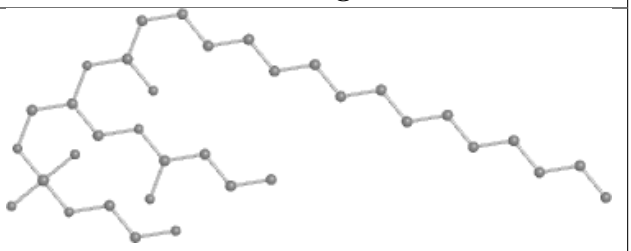
Bond lengths



Bond angles

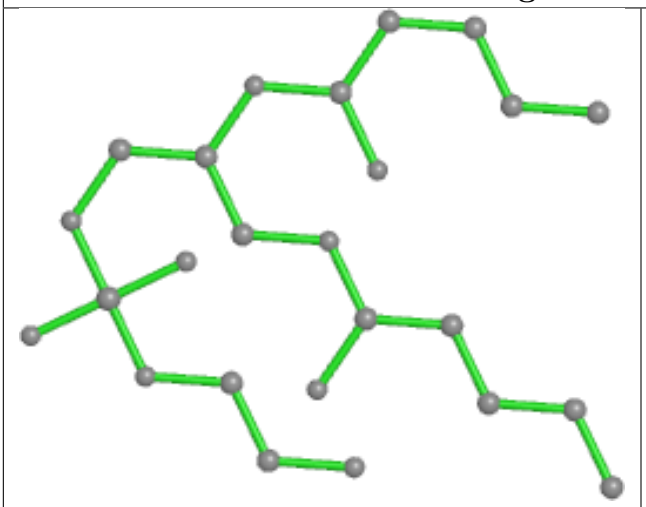


Torsions

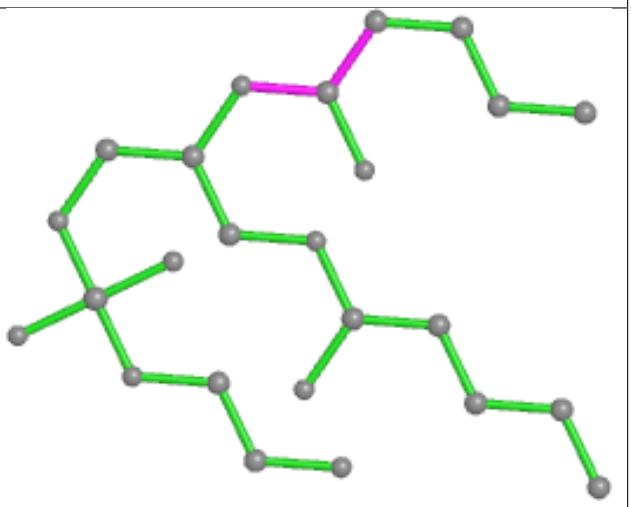


Rings

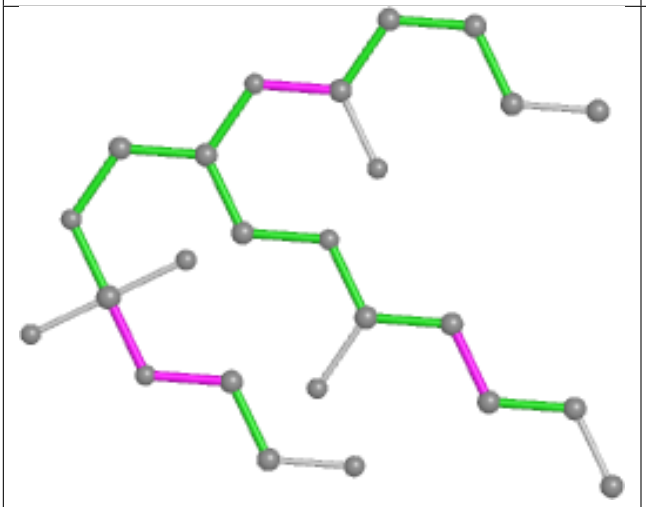
Ligand 3PE 3N 502



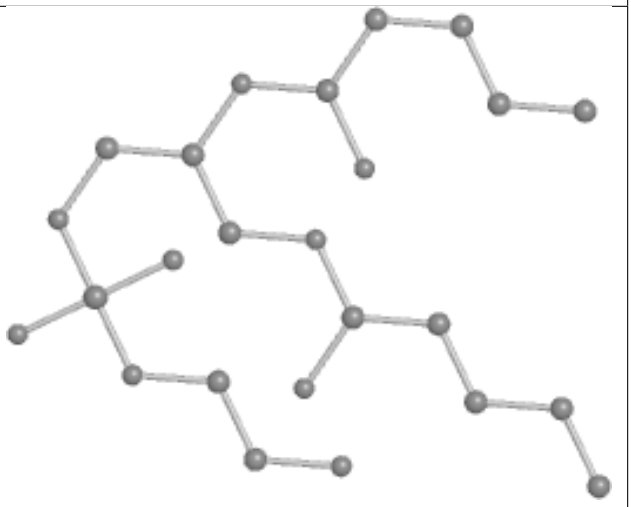
Bond lengths



Bond angles

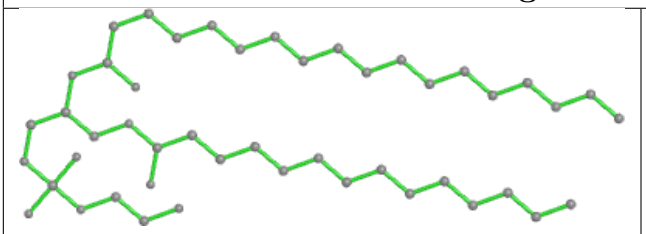


Torsions

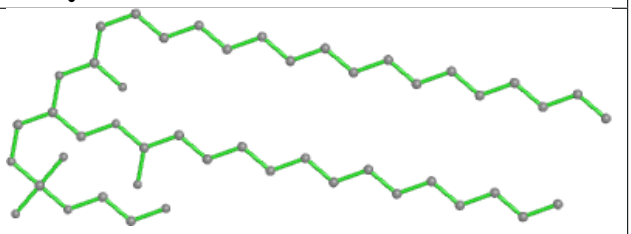


Rings

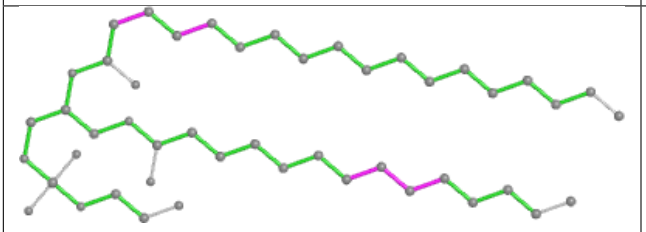
Ligand 3PE 3Q 503



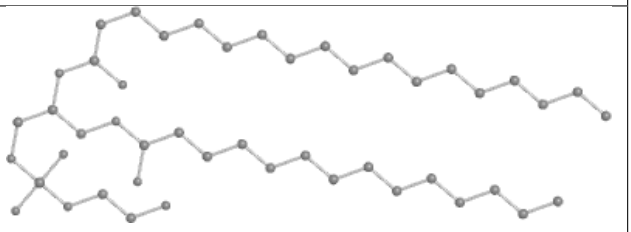
Bond lengths



Bond angles

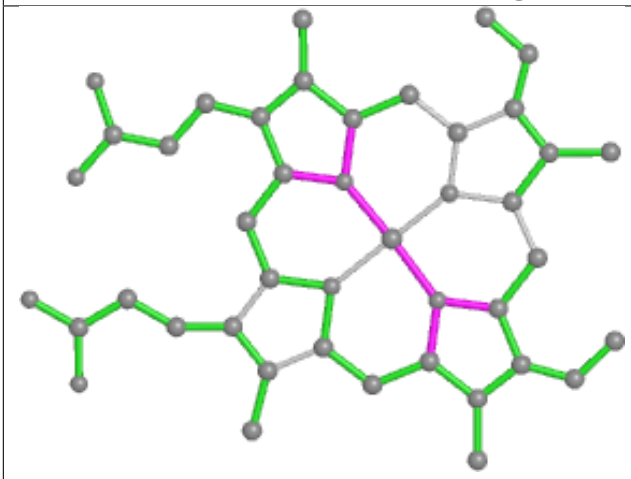


Torsions

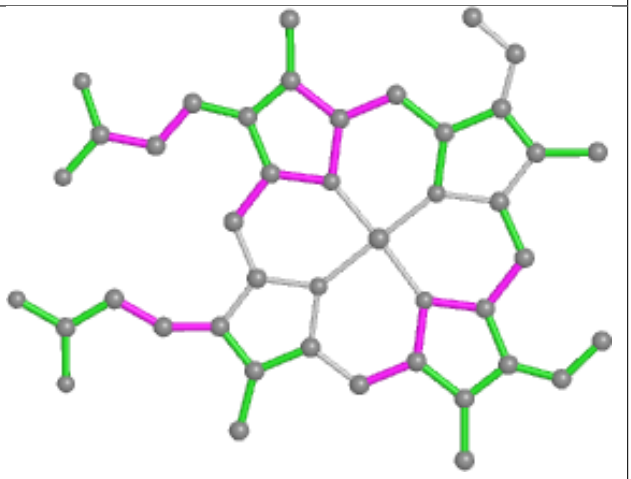


Rings

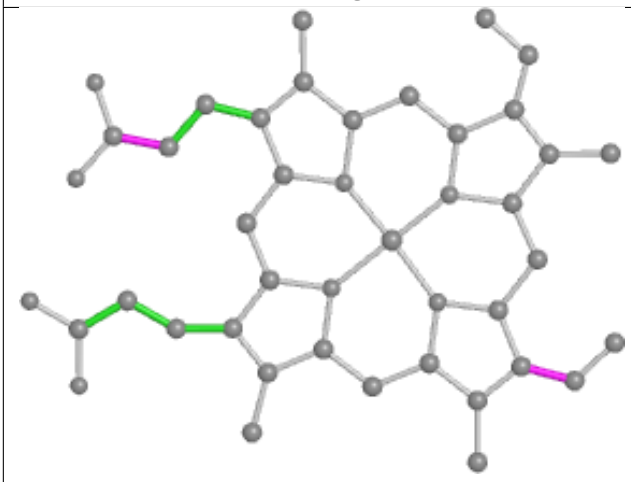
Ligand HEM 3P 501



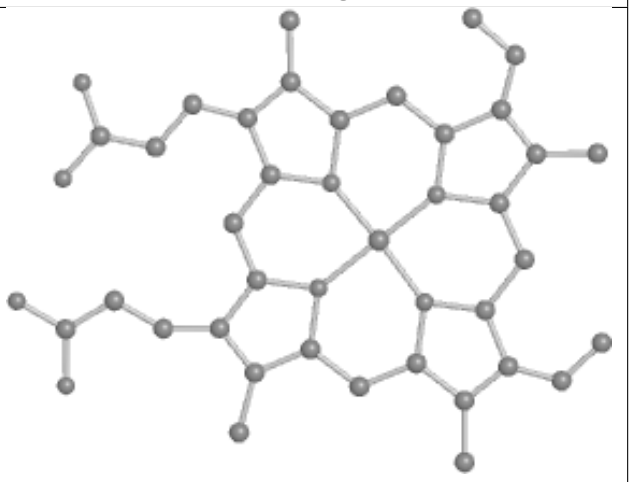
Bond lengths



Bond angles

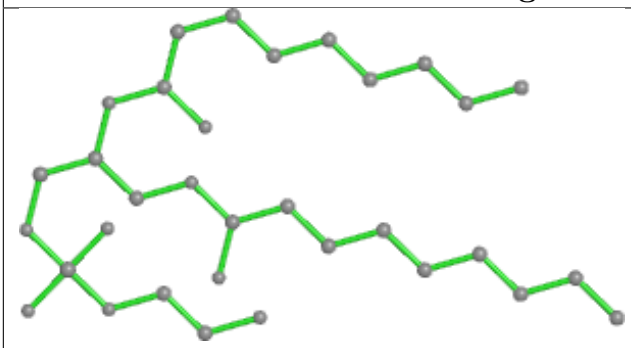


Torsions

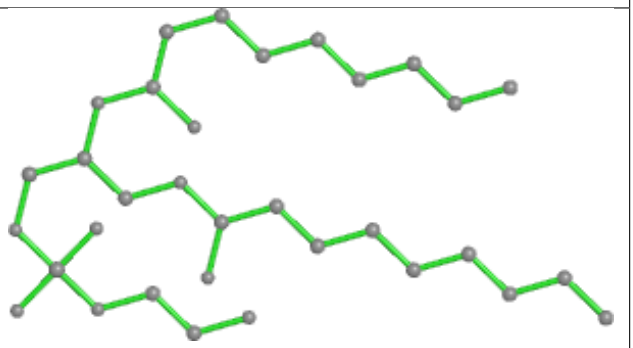


Rings

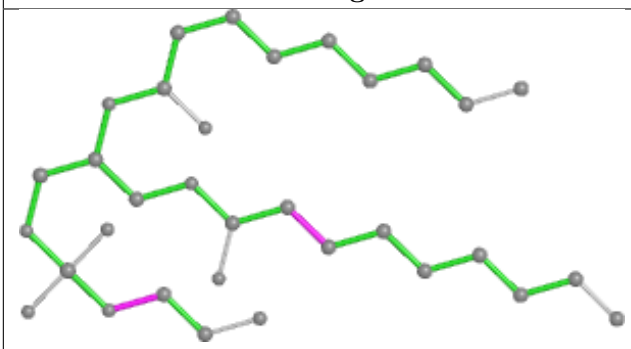
Ligand 3PE 3D 502



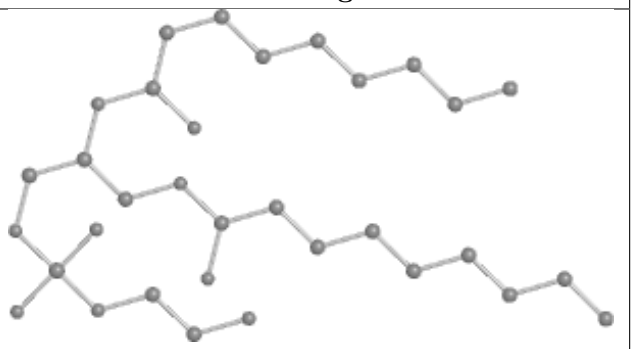
Bond lengths



Bond angles

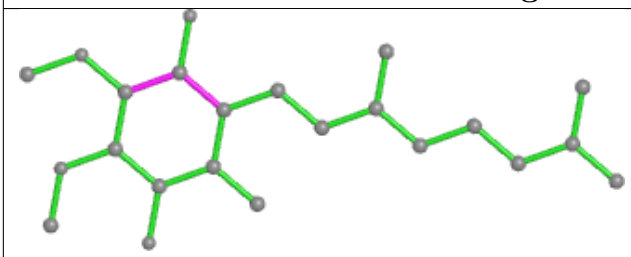


Torsions

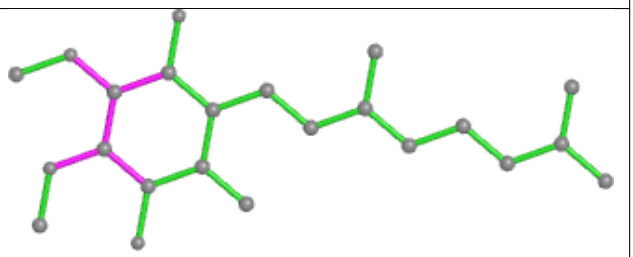


Rings

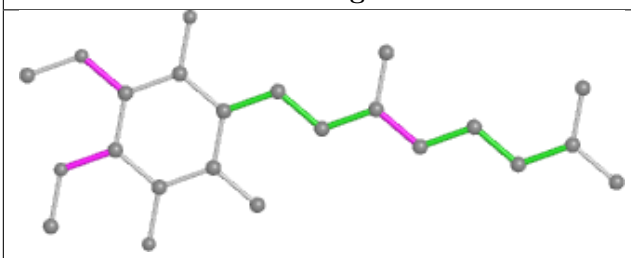
Ligand U10 3C 504



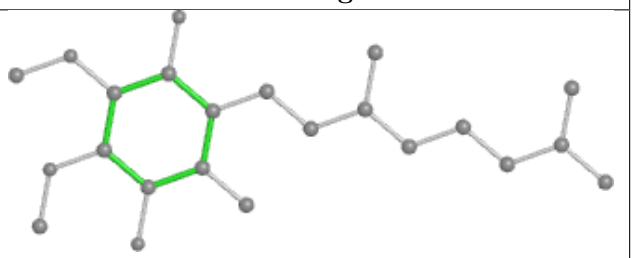
Bond lengths



Bond angles

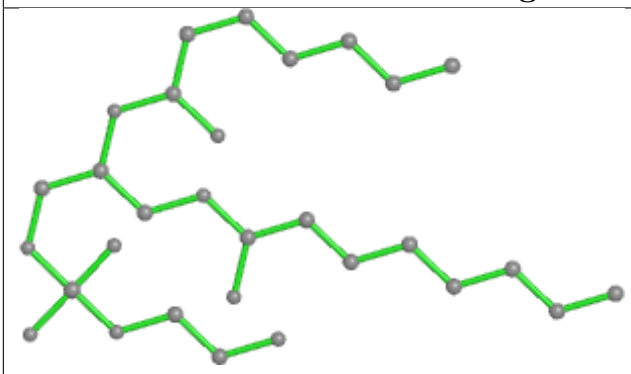


Torsions

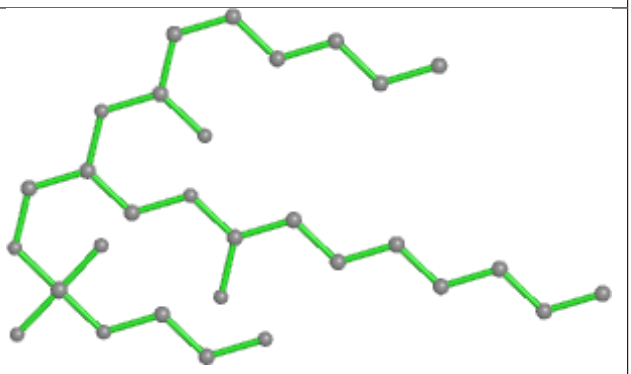


Rings

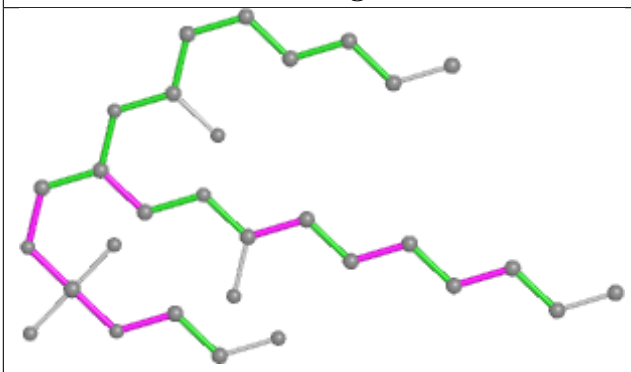
Ligand 3PE 3Y 101



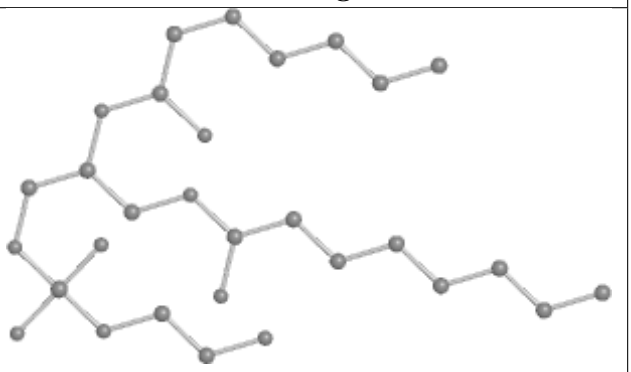
Bond lengths



Bond angles

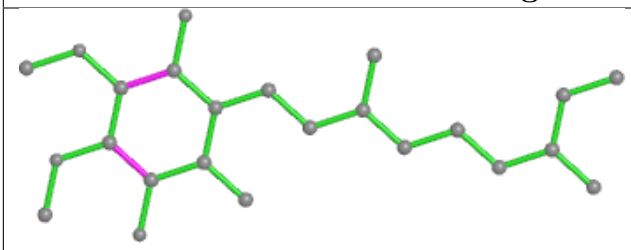


Torsions

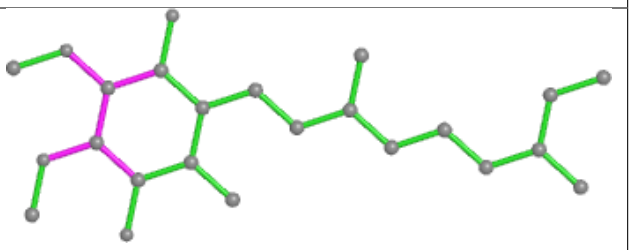


Rings

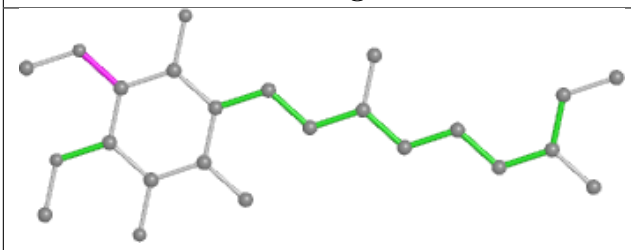
Ligand U10 3C 503



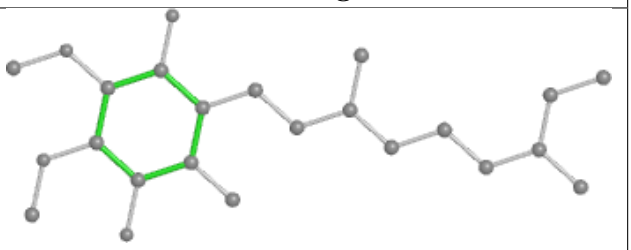
Bond lengths



Bond angles

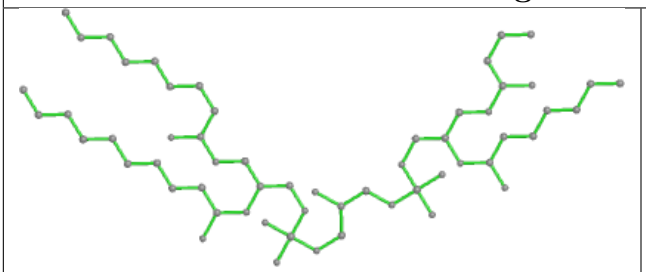


Torsions

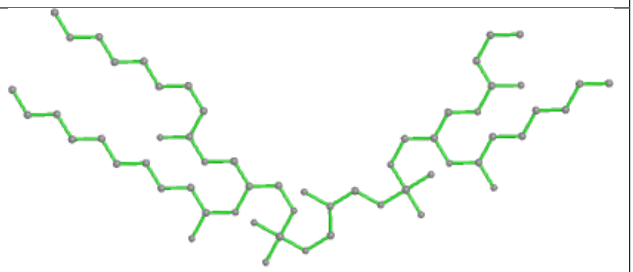


Rings

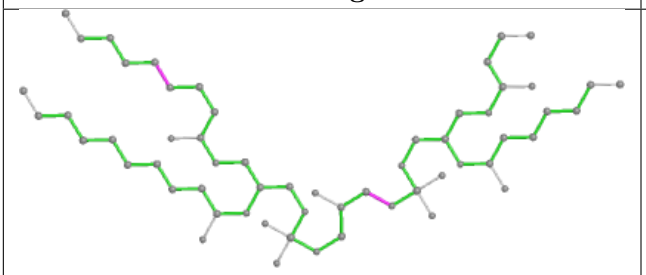
Ligand CDL 3A 501



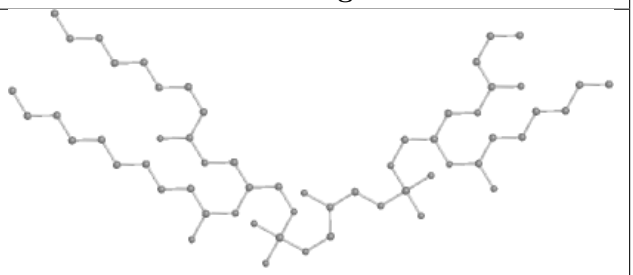
Bond lengths



Bond angles

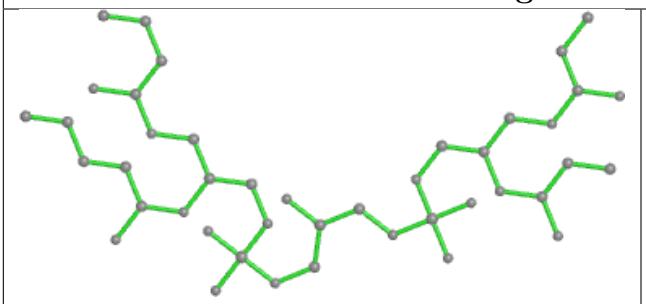


Torsions

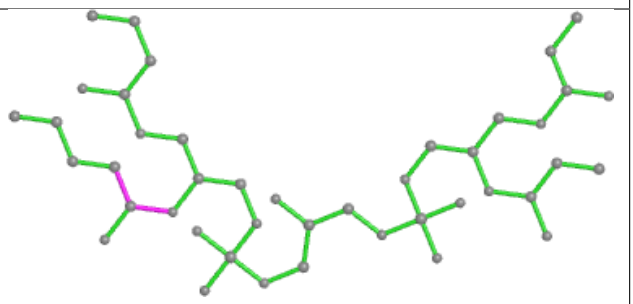


Rings

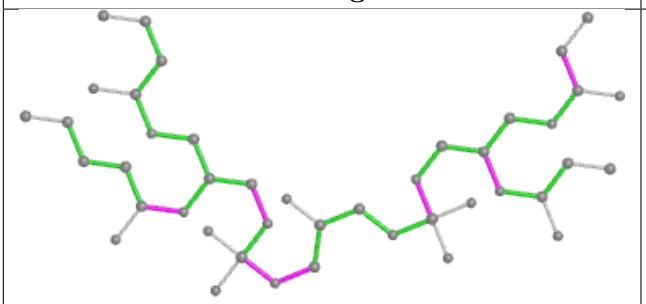
Ligand CDL 3P 507



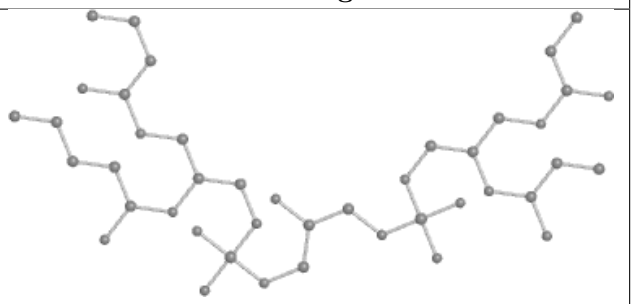
Bond lengths



Bond angles

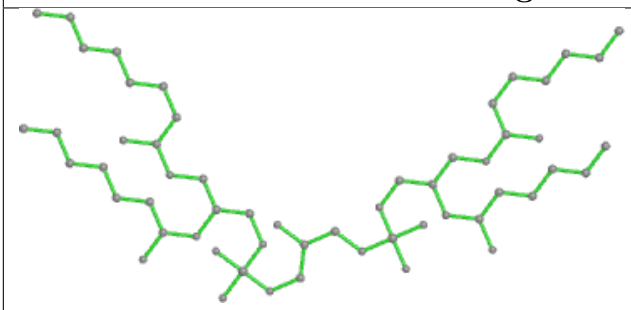


Torsions

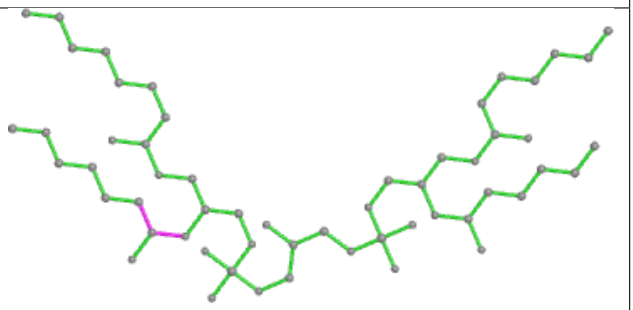


Rings

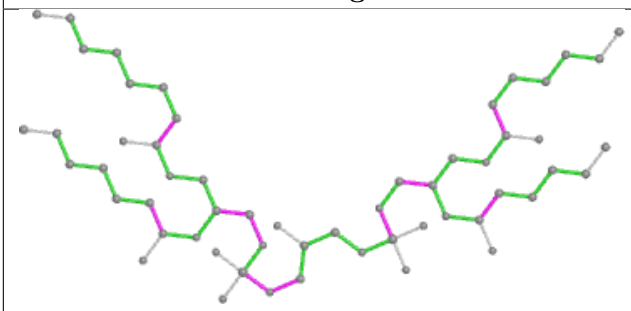
Ligand CDL 3P 506



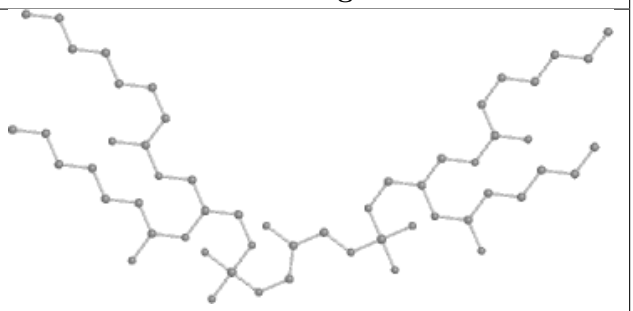
Bond lengths



Bond angles

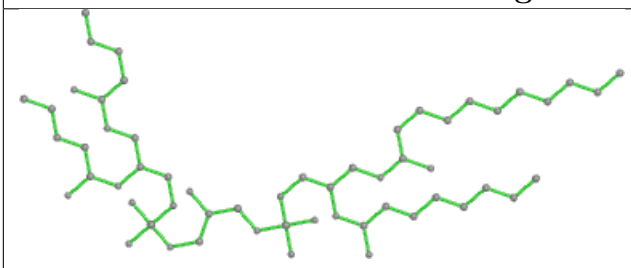


Torsions

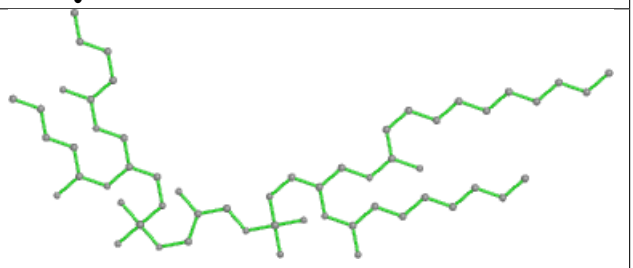


Rings

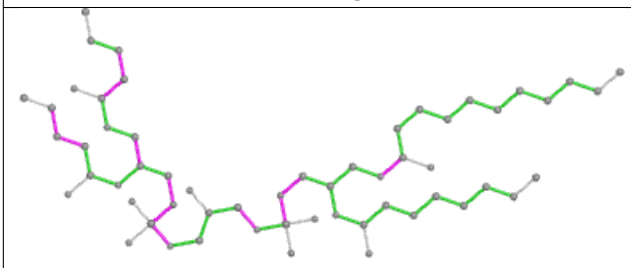
Ligand CDL 3Q 502



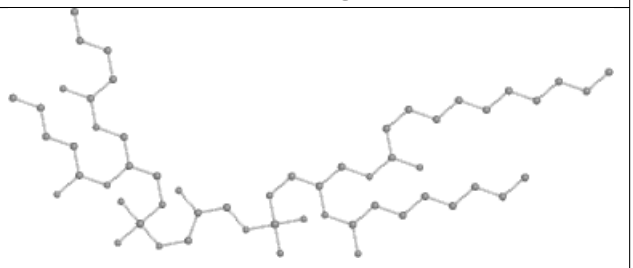
Bond lengths



Bond angles

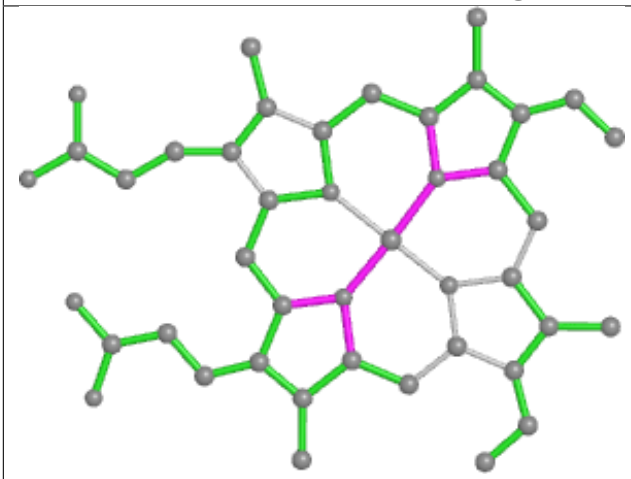


Torsions

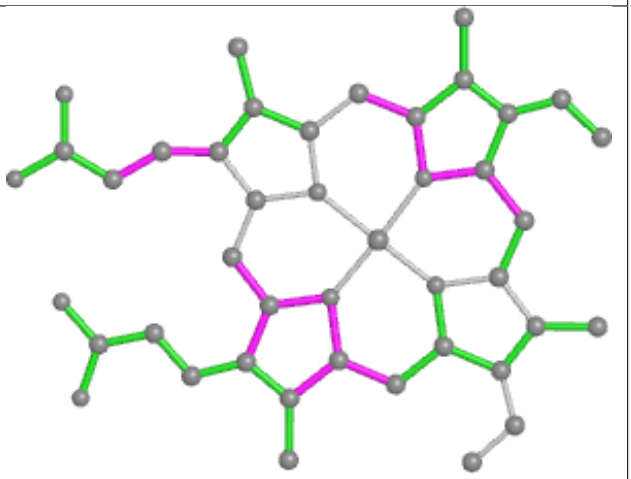


Rings

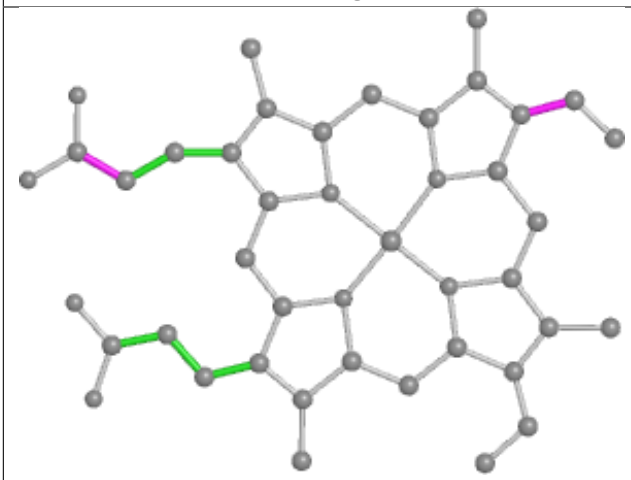
Ligand HEM 3C 502



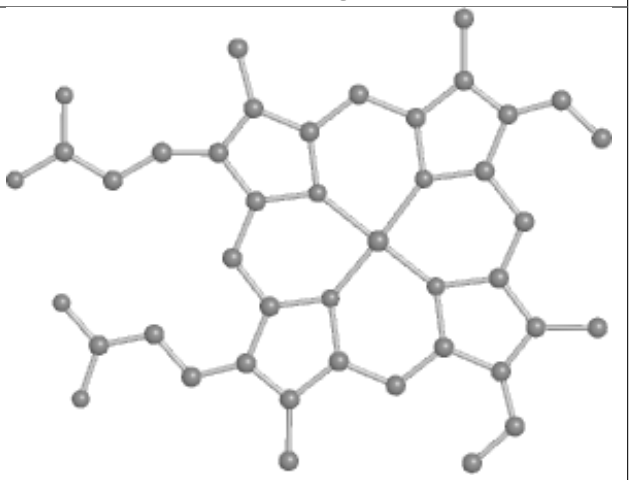
Bond lengths



Bond angles

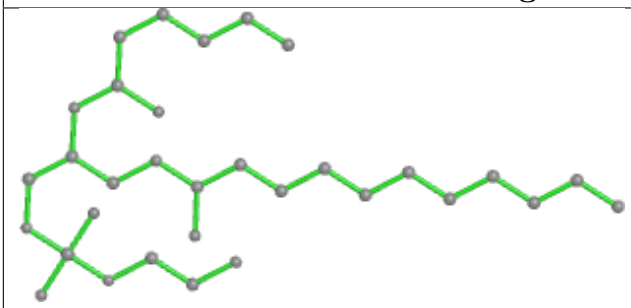


Torsions

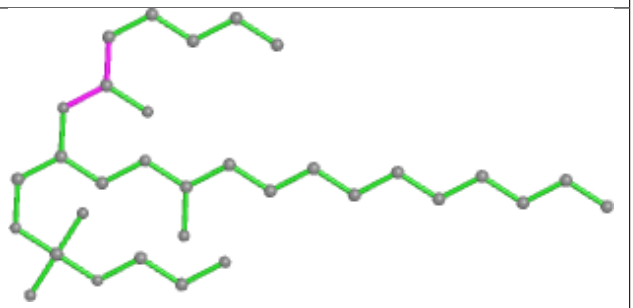


Rings

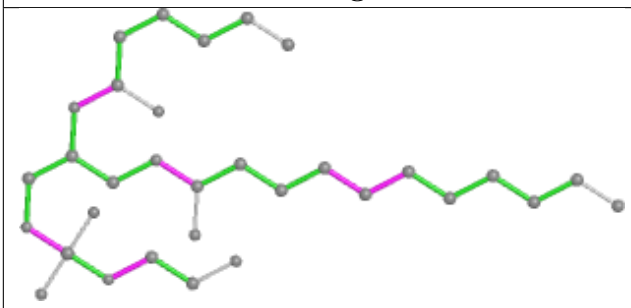
Ligand 3PE 3A 503



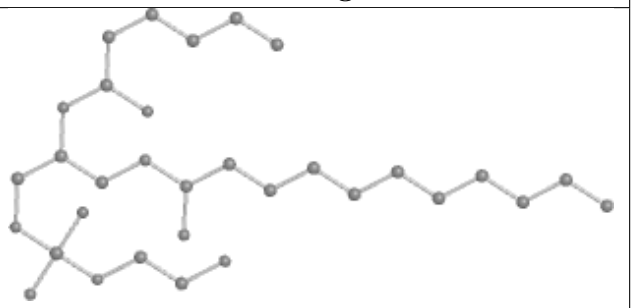
Bond lengths



Bond angles

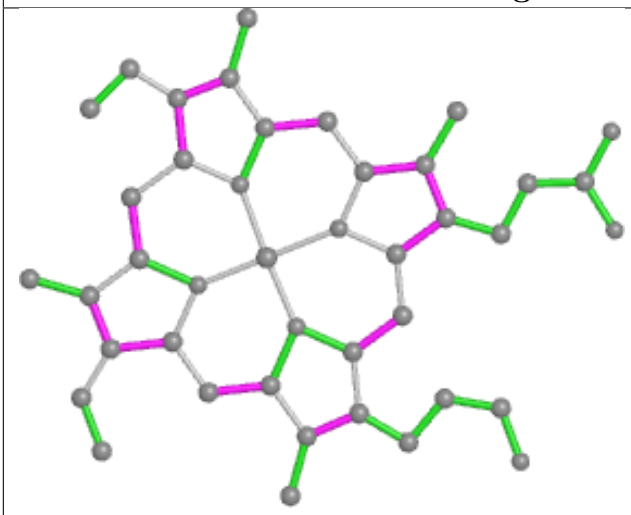


Torsions

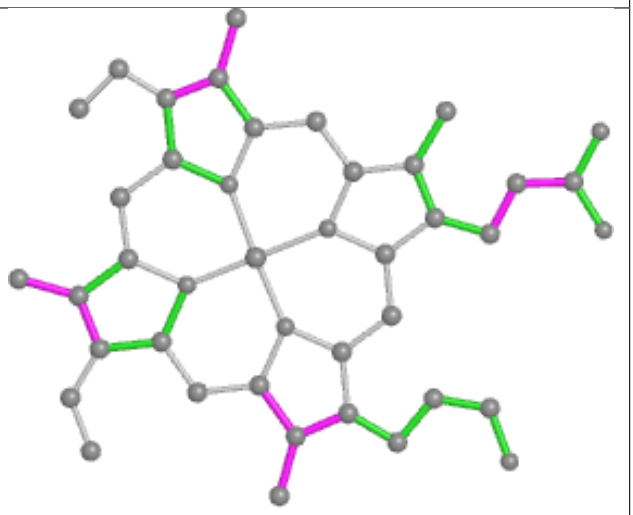


Rings

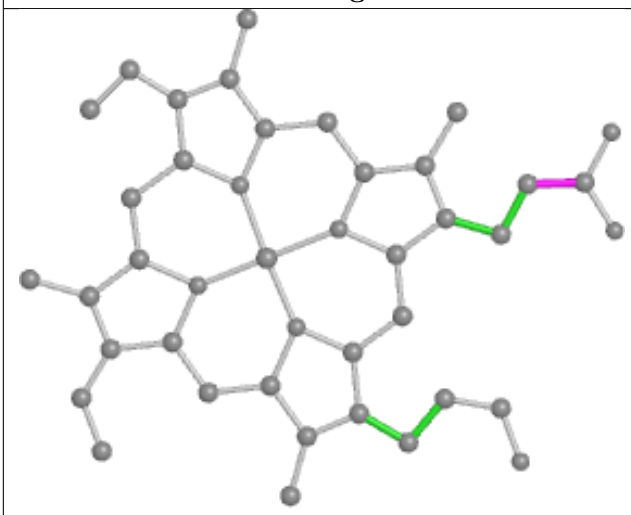
Ligand HEC 3D 501



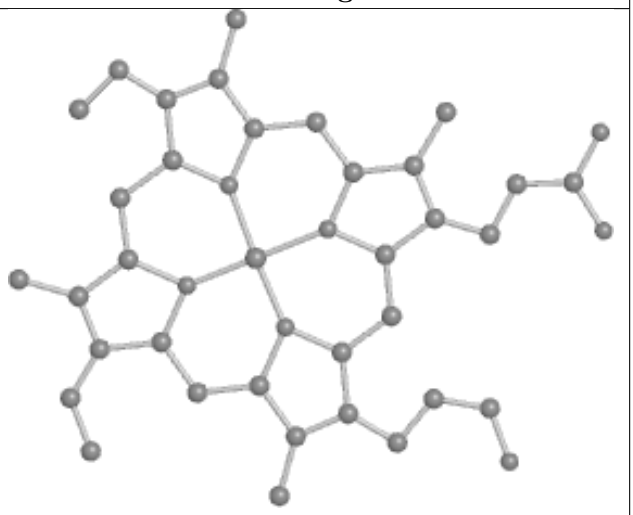
Bond lengths



Bond angles

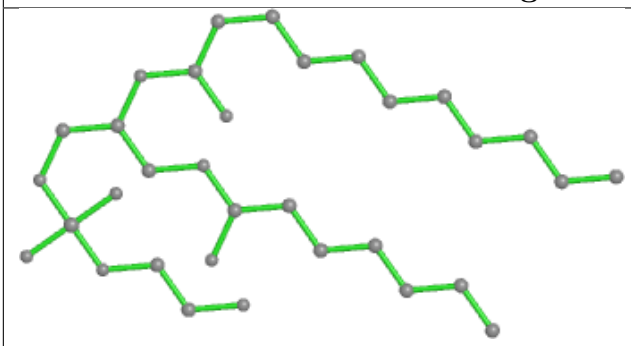


Torsions

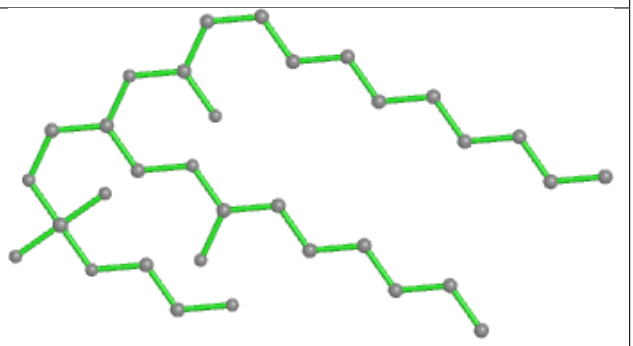


Rings

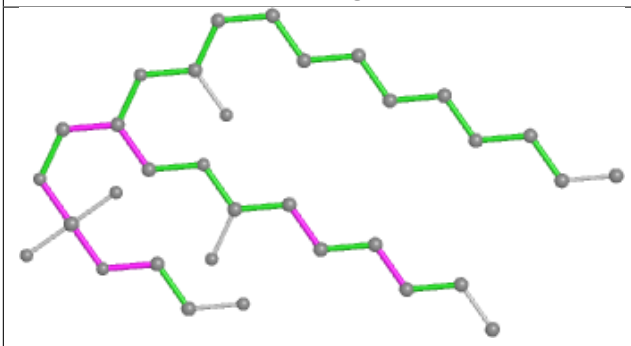
Ligand 3PE 3P 505



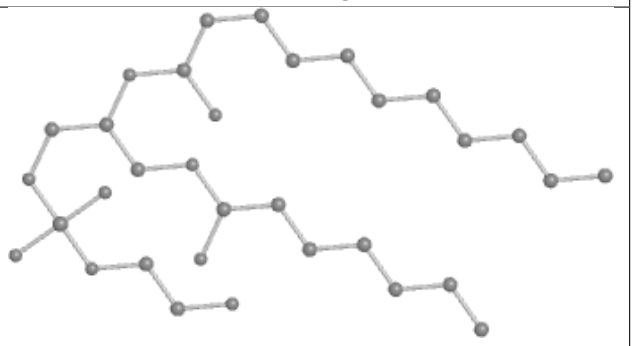
Bond lengths



Bond angles

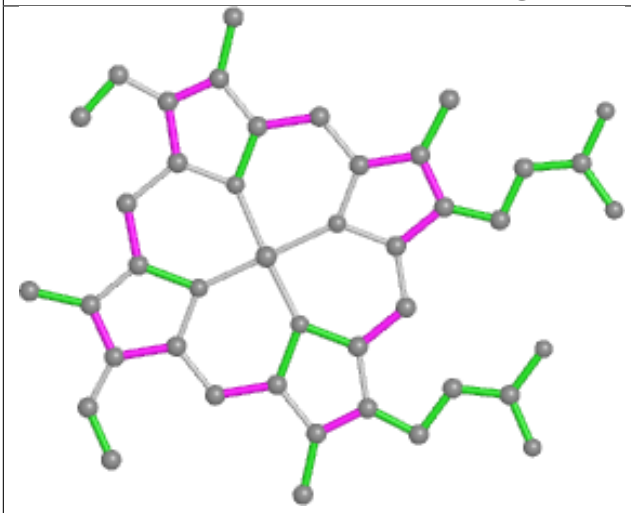


Torsions

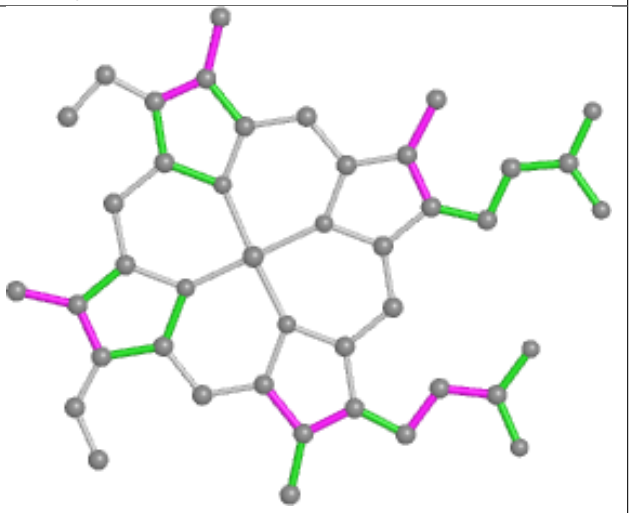


Rings

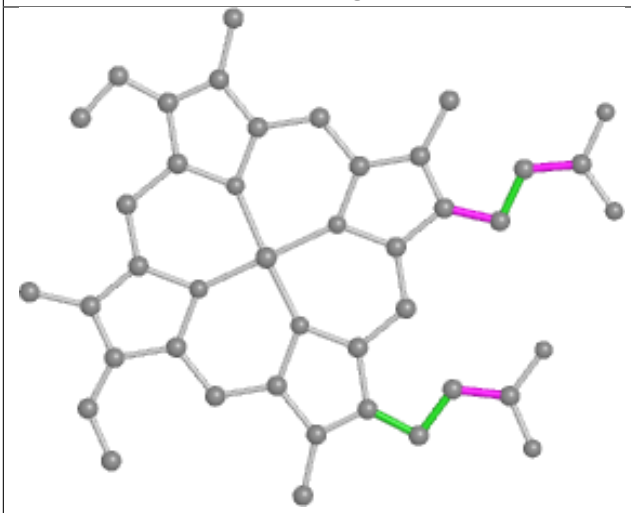
Ligand HEC 3Q 501



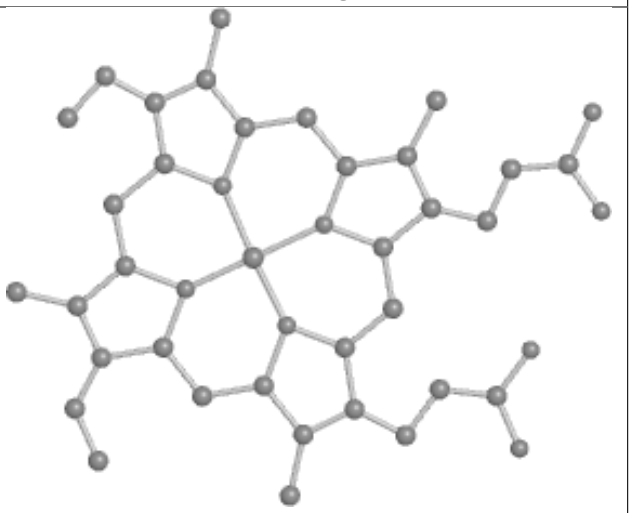
Bond lengths



Bond angles

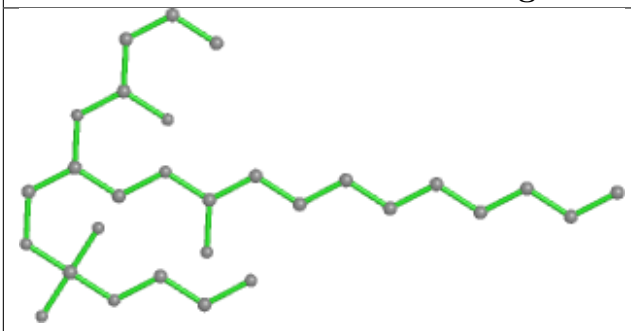


Torsions

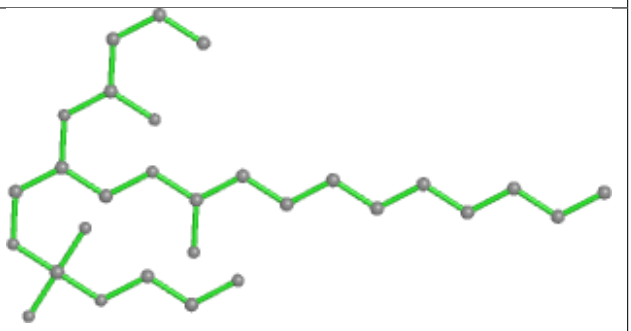


Rings

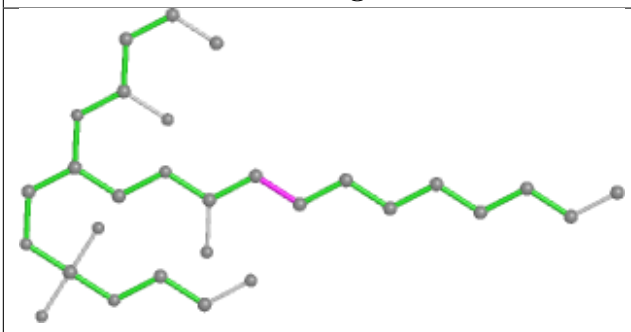
Ligand 3PE 3G 101



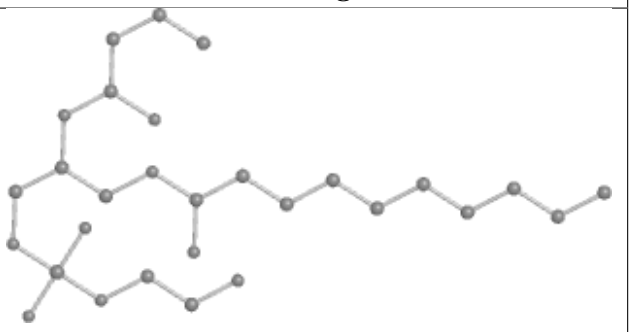
Bond lengths



Bond angles

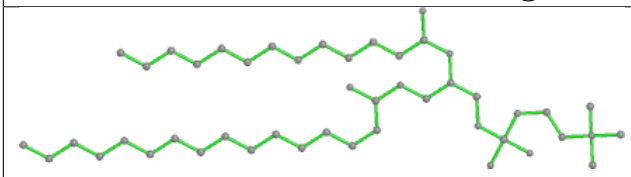


Torsions

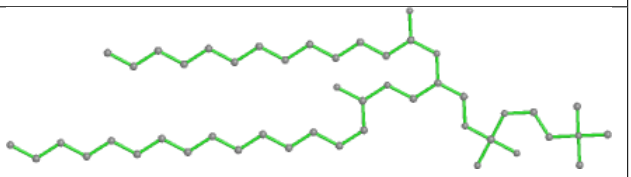


Rings

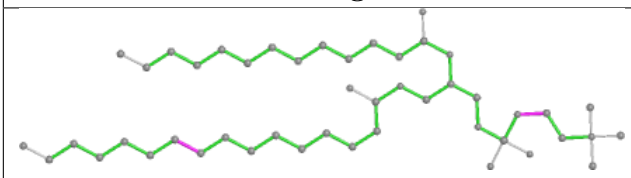
Ligand PC1 3E 302



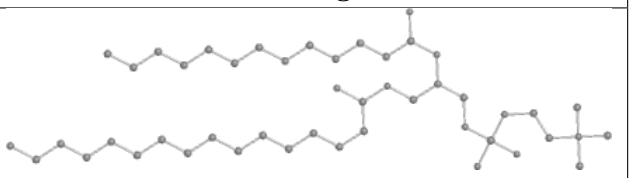
Bond lengths



Bond angles

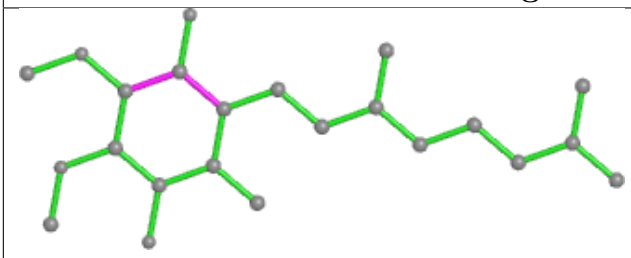


Torsions

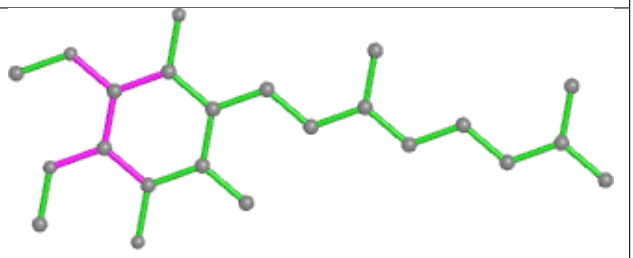


Rings

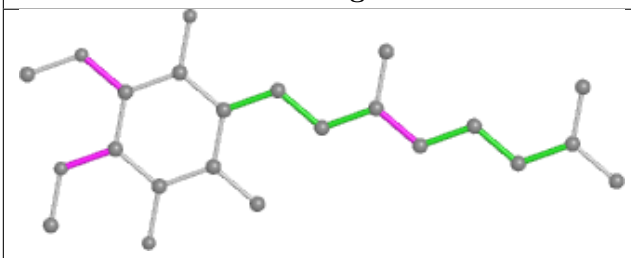
Ligand U10 3P 503



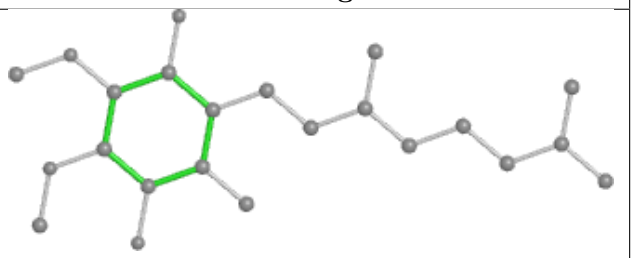
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
8	3H	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	3H	77:GLU	C	78:ASP	N	3.32

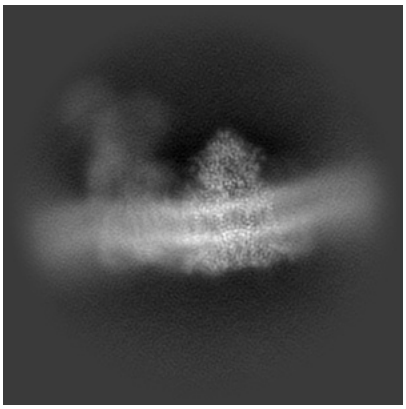
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-42222. These allow visual inspection of the internal detail of the map and identification of artifacts.

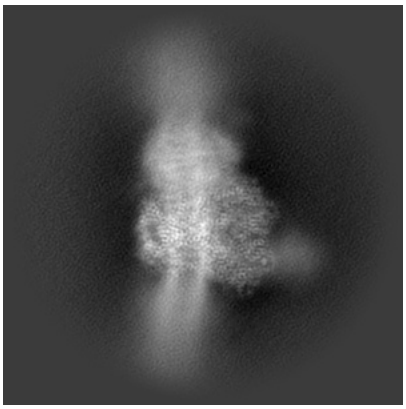
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

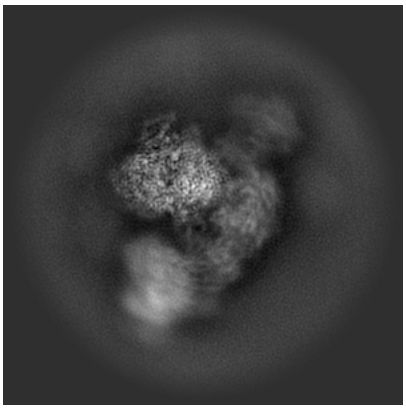
6.1.1 Primary map



X

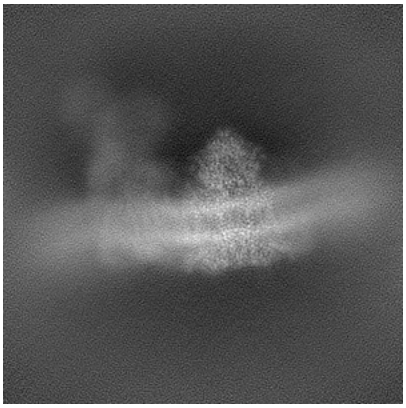


Y

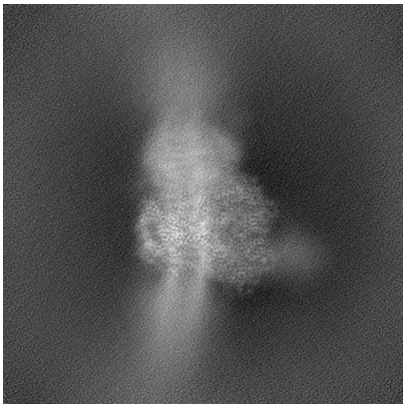


Z

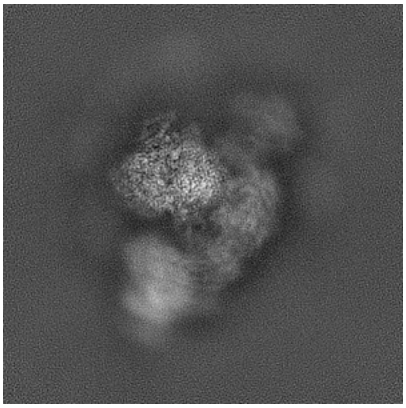
6.1.2 Raw map



X



Y

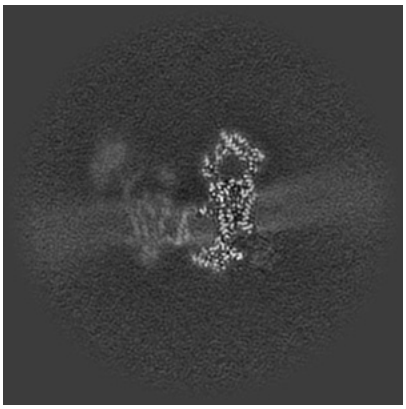


Z

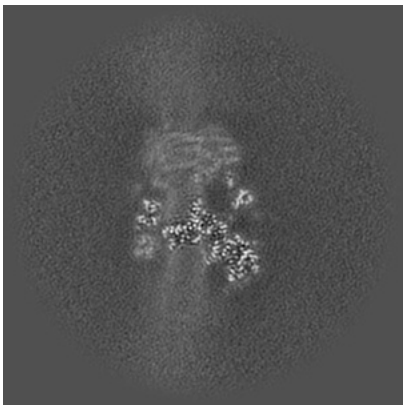
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

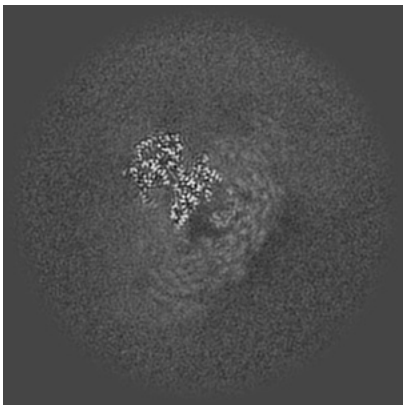
6.2.1 Primary map



X Index: 160

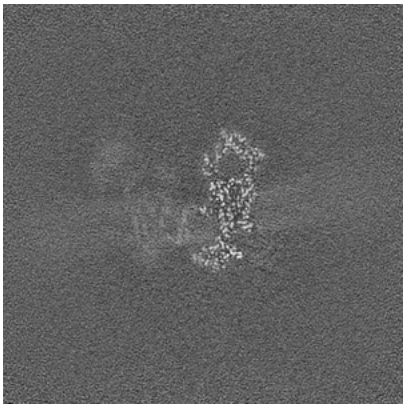


Y Index: 160

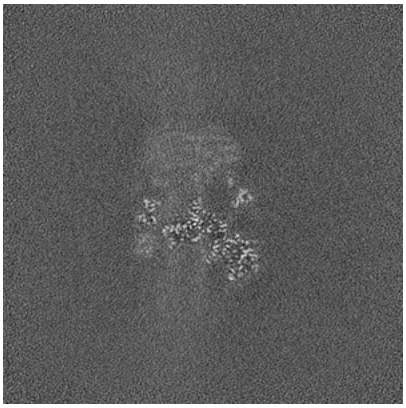


Z Index: 160

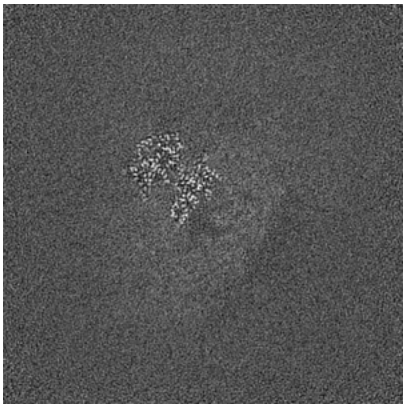
6.2.2 Raw map



X Index: 160



Y Index: 160

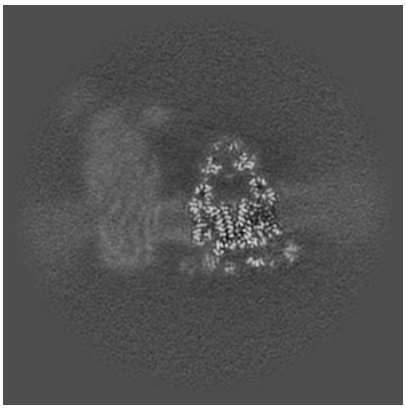


Z Index: 160

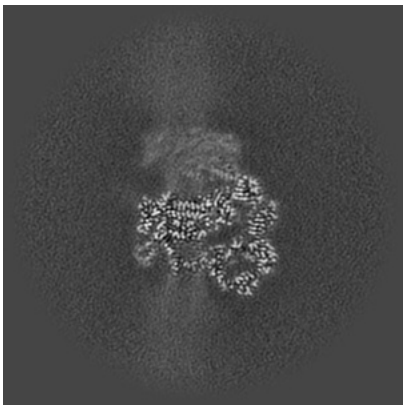
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

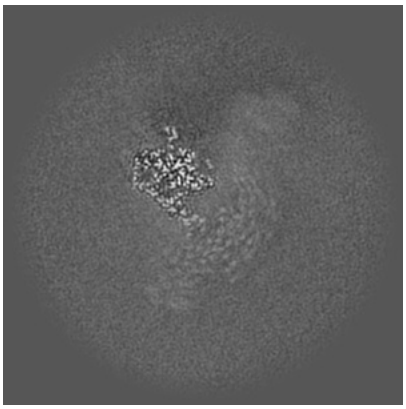
6.3.1 Primary map



X Index: 135

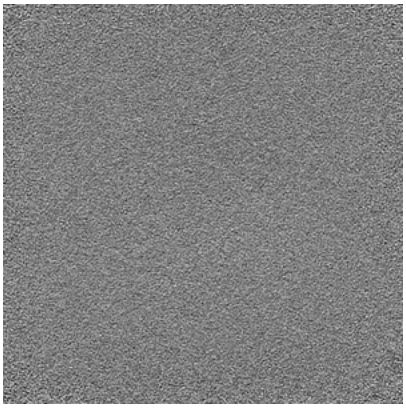


Y Index: 175

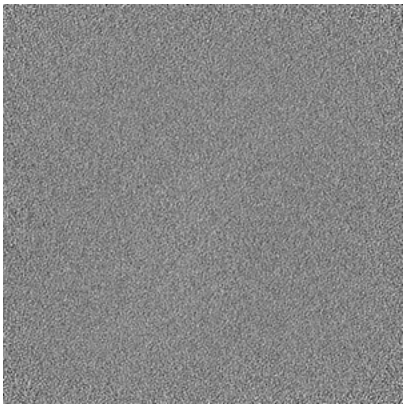


Z Index: 136

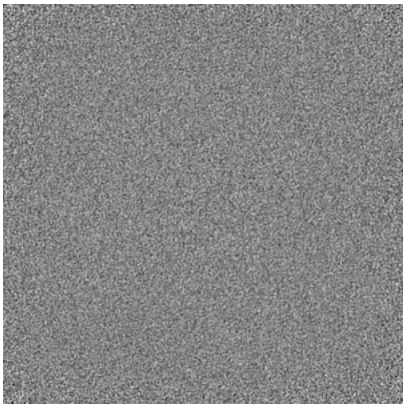
6.3.2 Raw map



X Index: 0



Y Index: 0

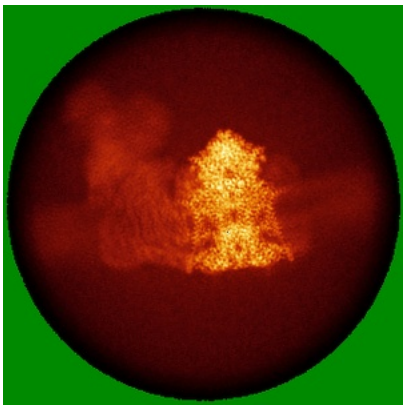


Z Index: 0

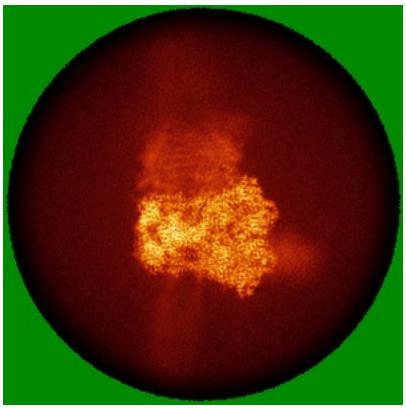
The images above show the largest variance slices of the map in three orthogonal directions.

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

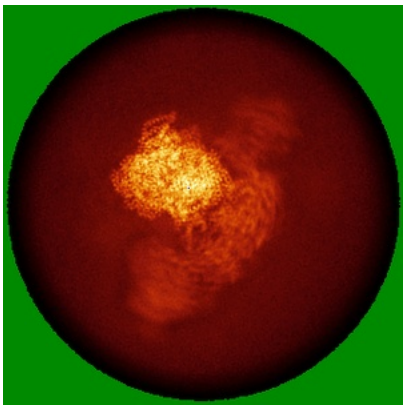
6.4.1 Primary map



X

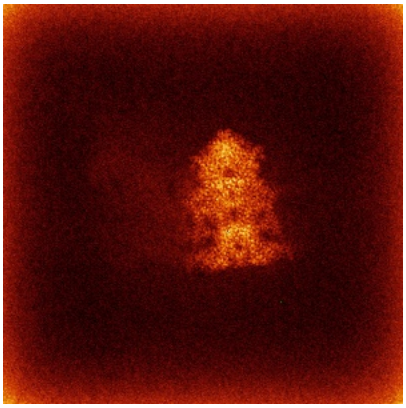


Y

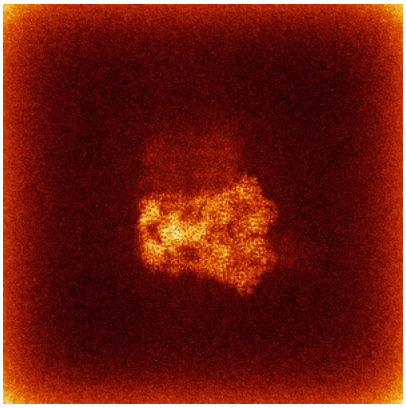


Z

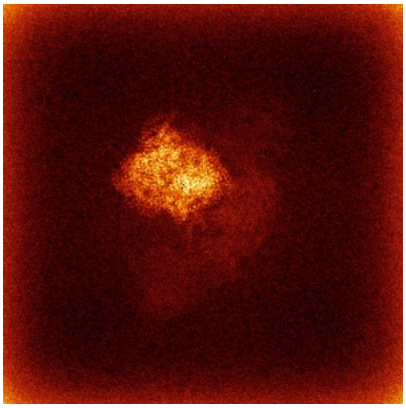
6.4.2 Raw map



X



Y

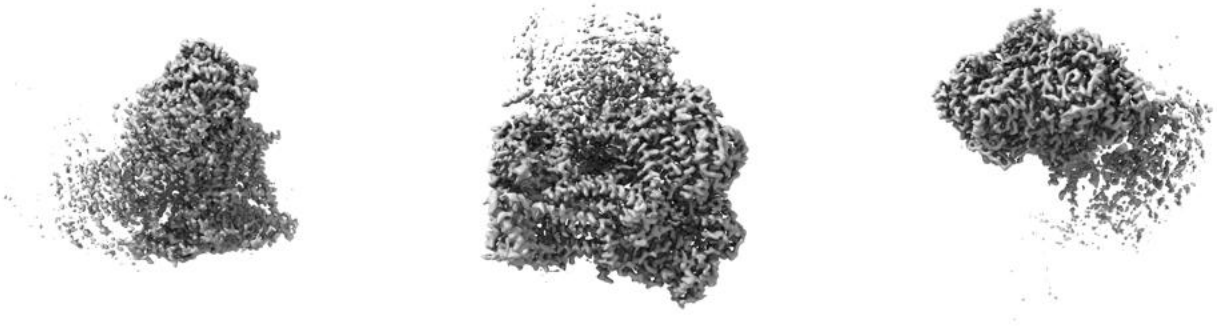


Z

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 0.12. 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.

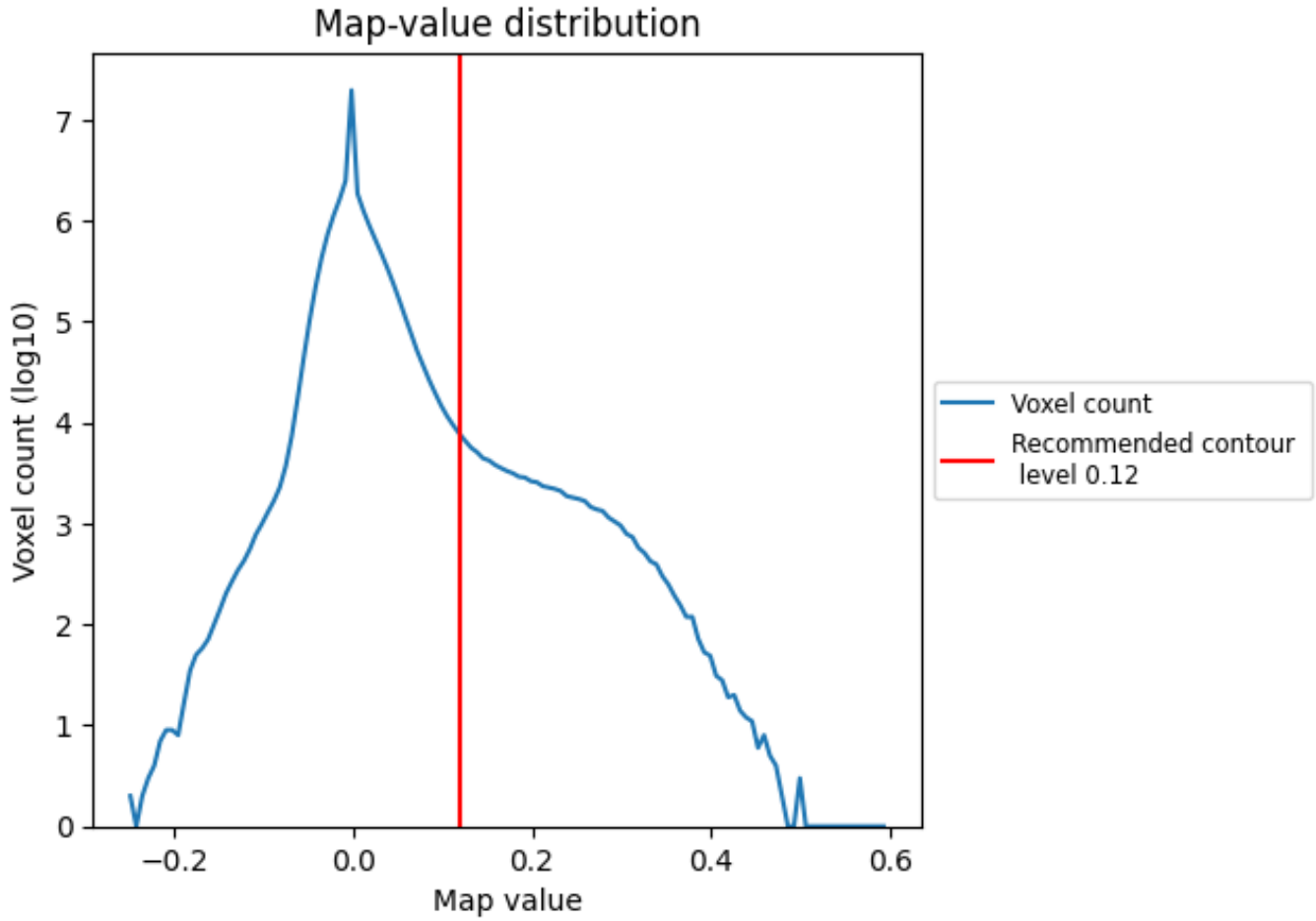
6.6 Mask visualisation (i)

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

7 Map analysis

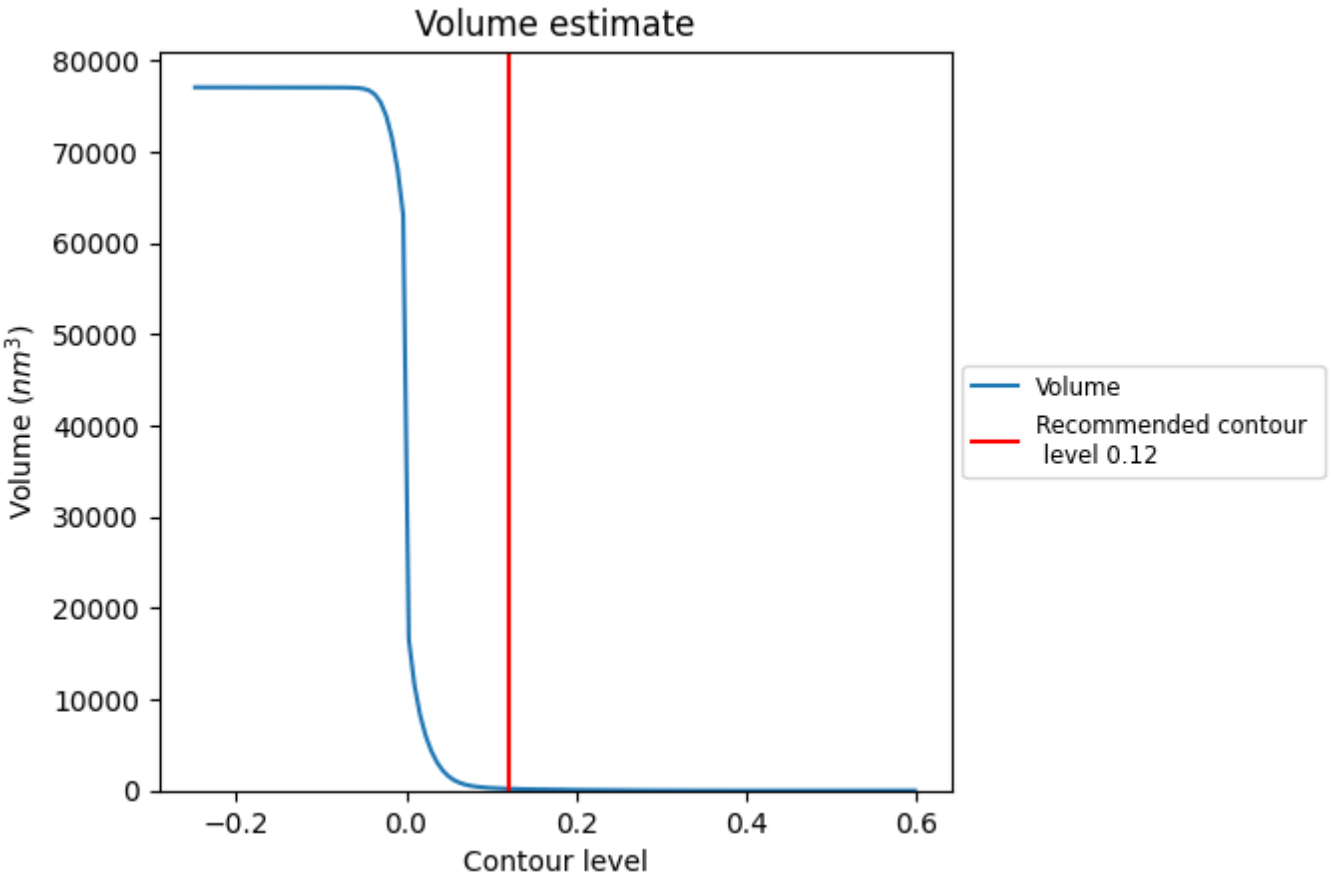
This section contains the results of statistical analysis of the map.

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.

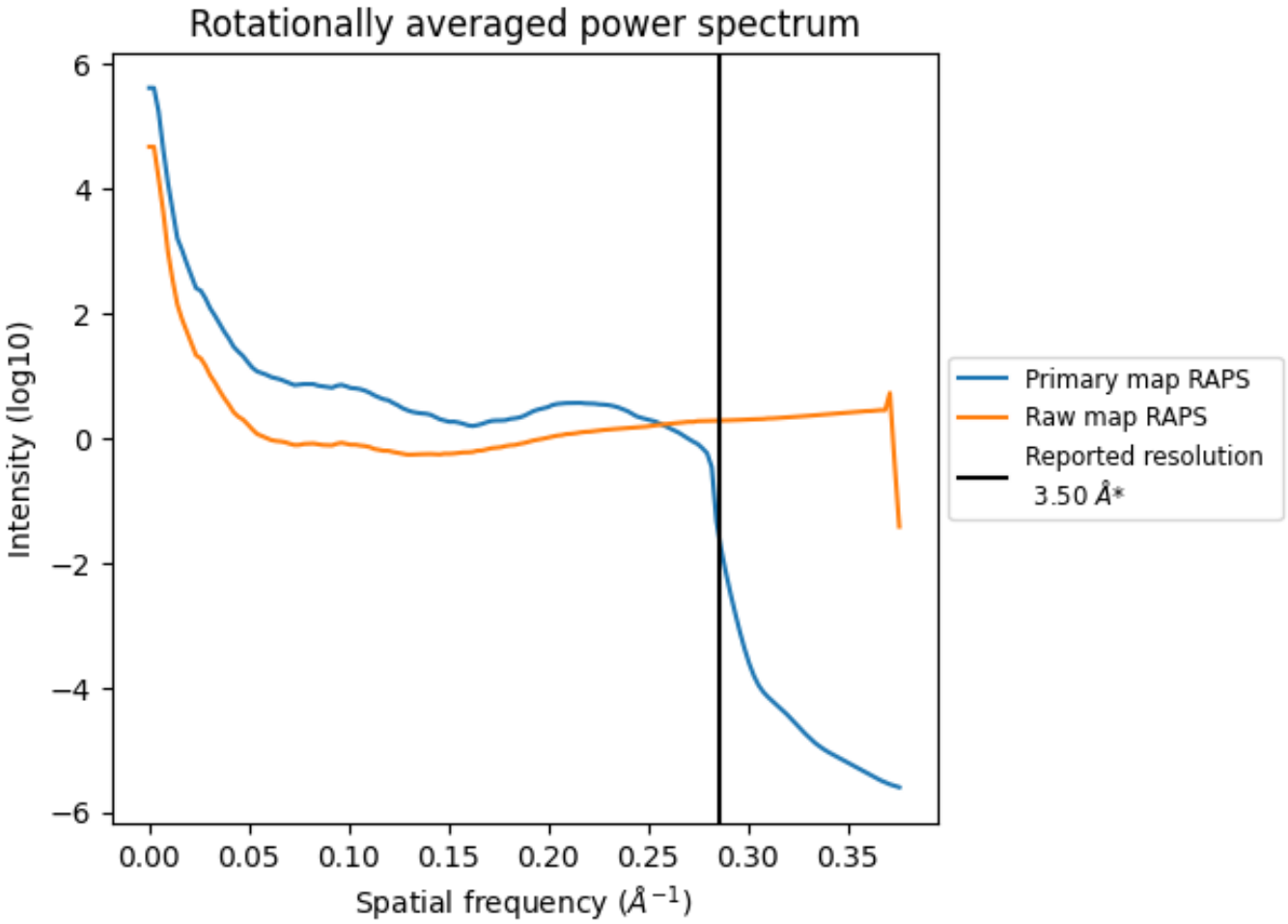
7.2 Volume estimate



The volume at the recommended contour level is 201 nm^3; this corresponds to an approximate mass of 181 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)

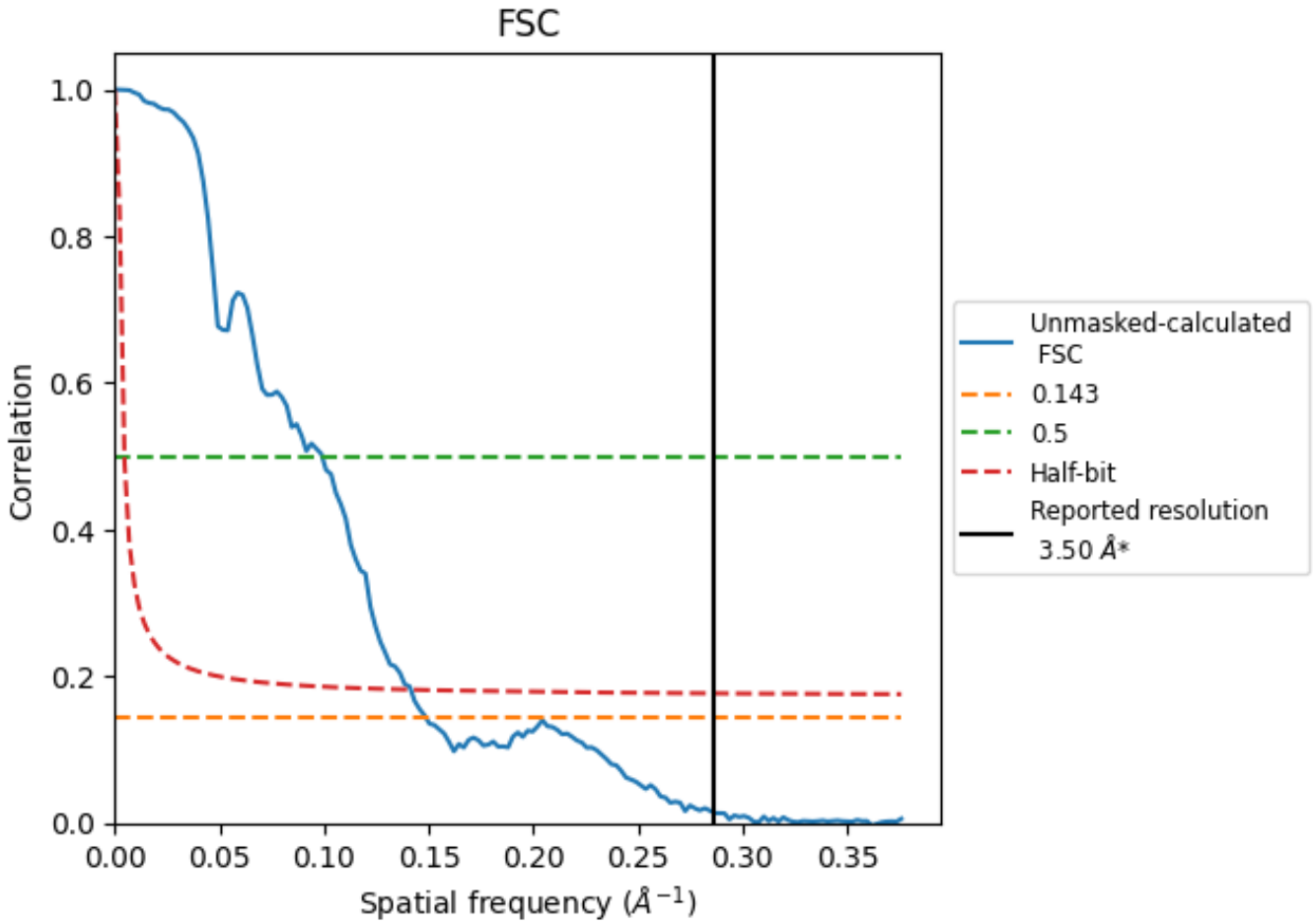


*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

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 0.286 Å^{-1}

8.2 Resolution estimates (i)

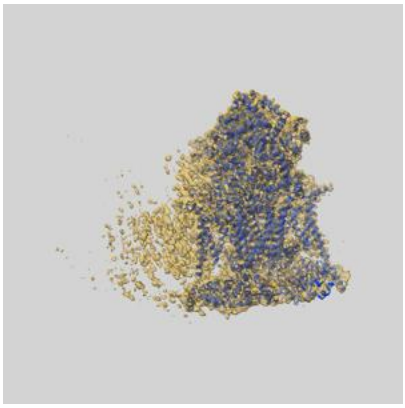
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.72	10.10	7.07

*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 6.72 differs from the reported value 3.5 by more than 10 %

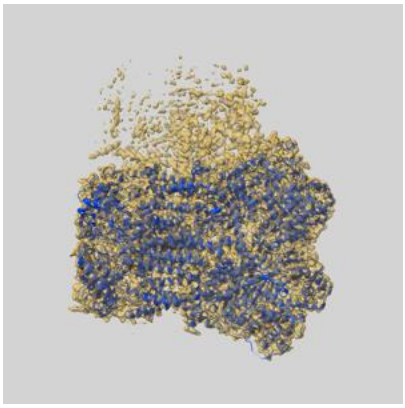
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-42222 and PDB model 8UGE. Per-residue inclusion information can be found in section 3 on page 12.

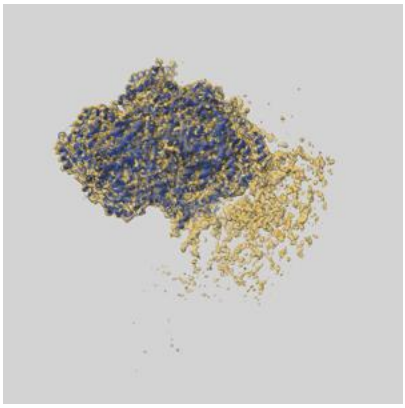
9.1 Map-model overlay



X



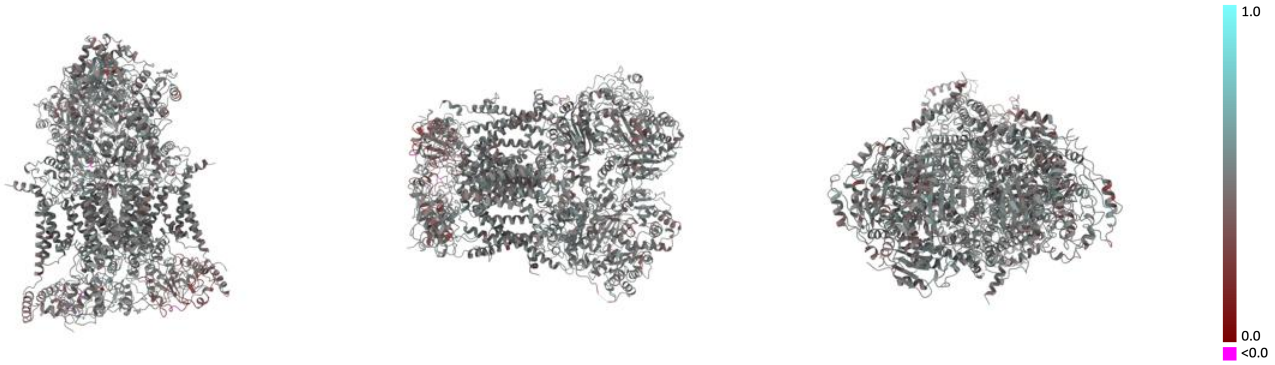
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.12 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.

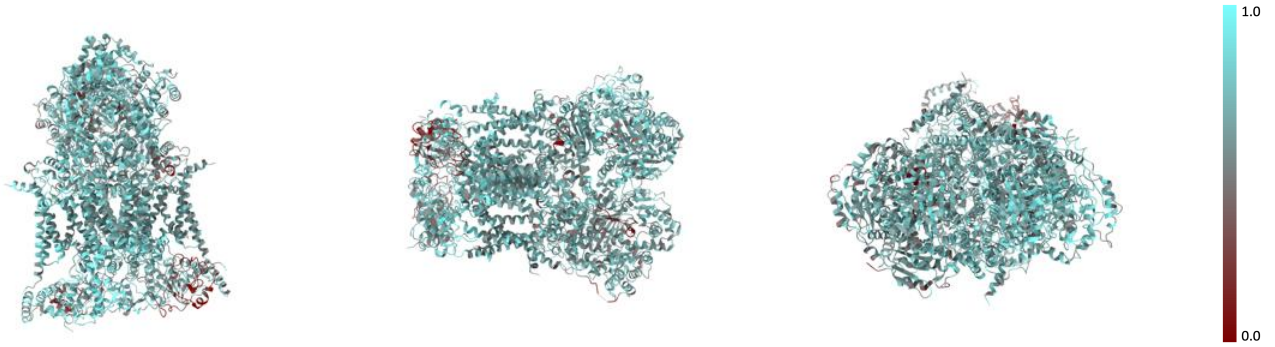
9.2 Q-score mapped to coordinate model (i)



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.

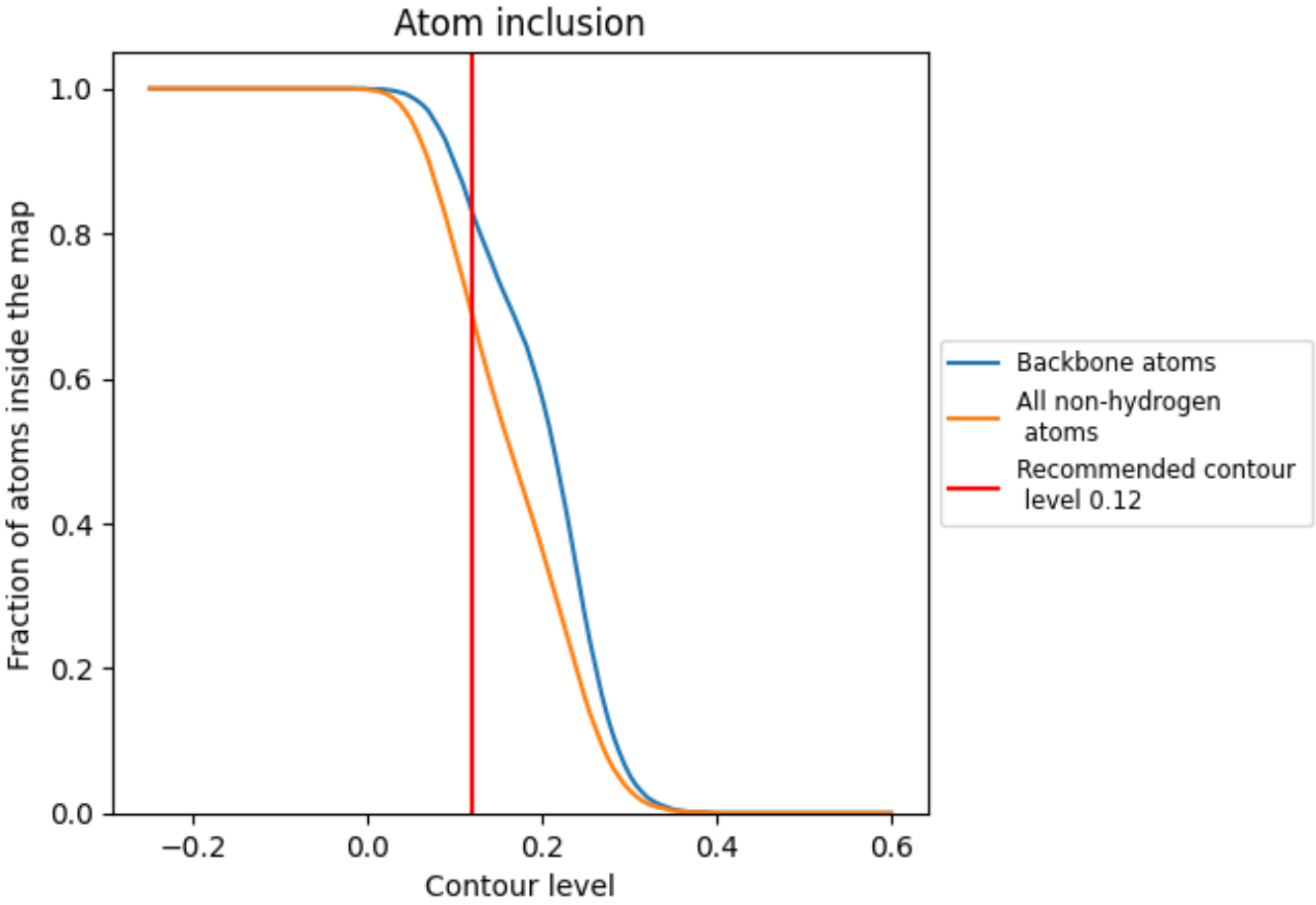
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.12).

9.4 Atom inclusion (i)



At the recommended contour level, 83% of all backbone atoms, 69% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6860	0.4780
3A	0.6670	0.4890
3B	0.6840	0.4880
3C	0.7050	0.4930
3D	0.7530	0.4970
3E	0.4800	0.4050
3F	0.6740	0.4900
3G	0.6330	0.4870
3H	0.6830	0.4360
3I	0.2410	0.3820
3J	0.6990	0.4880
3N	0.7470	0.4860
3O	0.7290	0.4840
3P	0.7440	0.4920
3Q	0.7690	0.4930
3R	0.4620	0.3790
3S	0.7560	0.5010
3T	0.7970	0.4960
3U	0.7060	0.4460
3V	0.4610	0.4500
3W	0.7790	0.4950
3X	0.6240	0.4740
3Y	0.5580	0.4900