Full wwPDB EM Validation Report ⓘ

Jul 6, 2024 – 04:47 PM EDT

PDB ID	:	8UGG
EMDB ID	:	EMD-42224
Title	:	In-situ complex III, state IV
Authors	:	Zheng, W.; Zhang, K.; Zhu, J.
Deposited on	:	2023-10-05
Resolution	:	3.60 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:

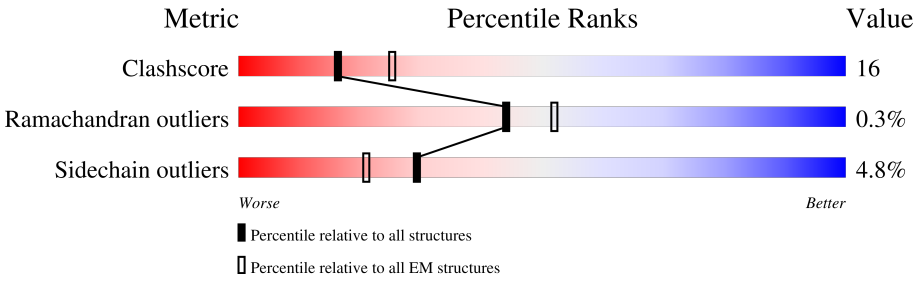
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 3.60 Å.

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



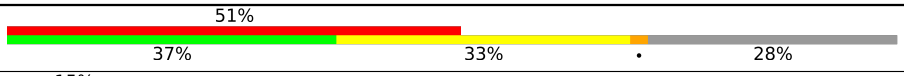
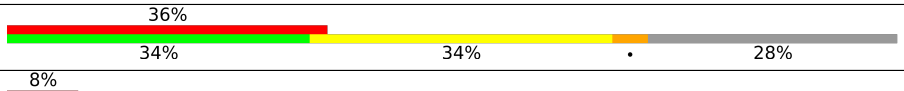
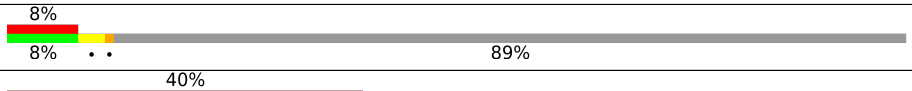
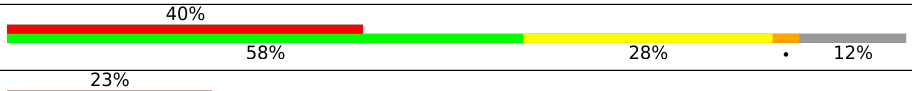
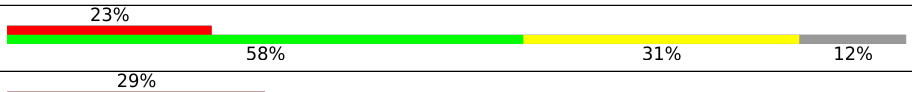
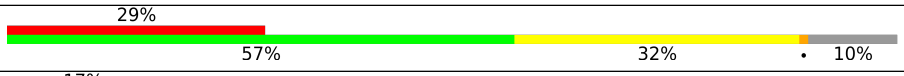
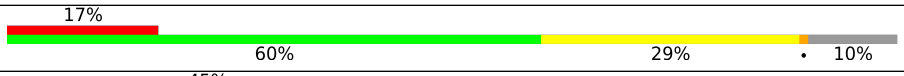
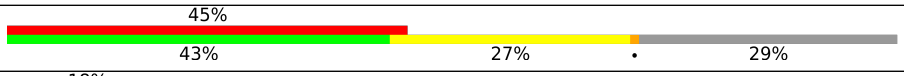
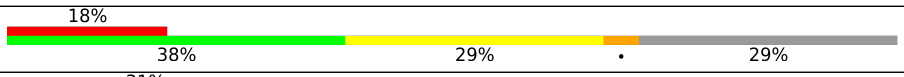
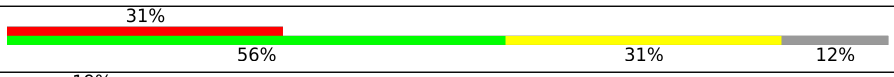
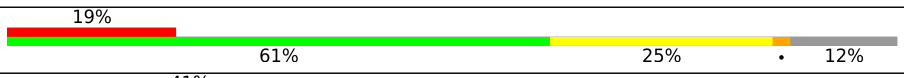
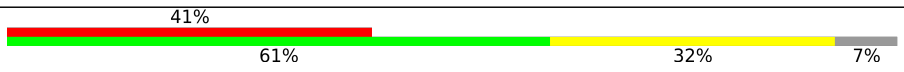
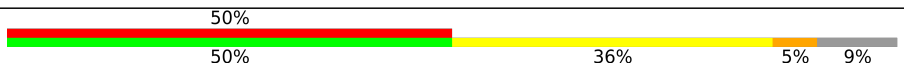
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	28% 64% 27% • 8%
1	3N	480	12% 59% 30% • 7%
2	3B	453	27% 63% 28% • 8%
2	3O	453	19% 68% 23% • 8%
3	3C	379	17% 65% 34% •
3	3P	379	13% 67% 31% •
4	3D	325	18% 51% 20% • 27%
4	3Q	325	11% 51% 22% • 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	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	FES	3E	301	-	-	X	-

2 Entry composition (i)

There are 17 unique types of molecules in this entry. The entry contains 33551 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		

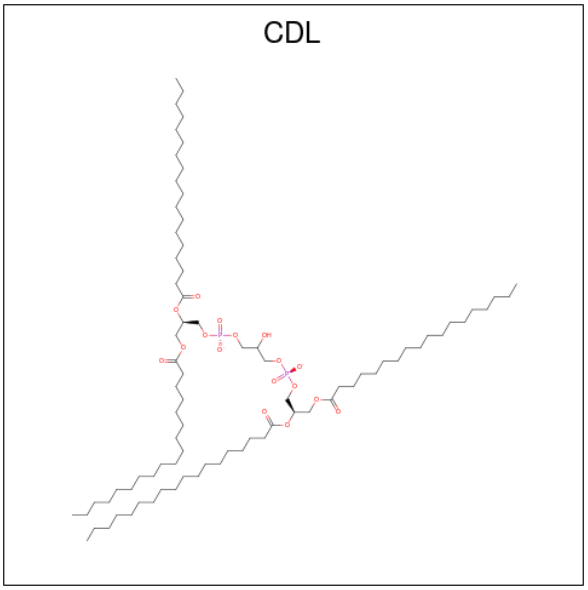
- Molecule 9 is a protein called Ubiquinol-cytochrome c reductase complex 7.2 kDa protein.

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.

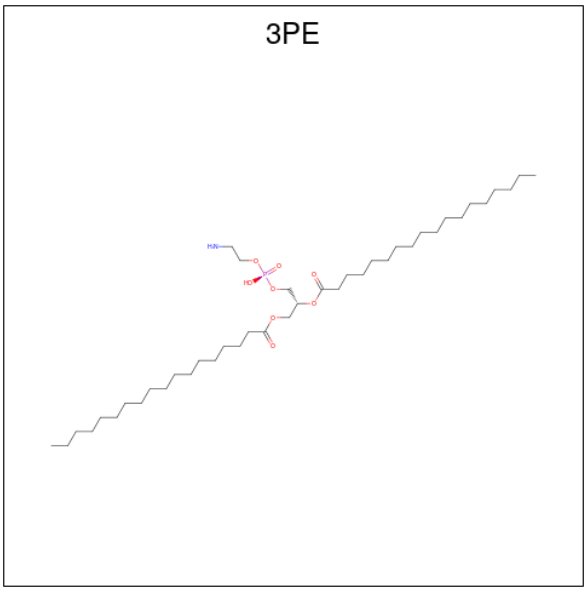
Mol	Chain	Residues	Atoms					AltConf	Trace
10	3X	52	Total	C	N	O	S	0	0
			429	286	75	66	2		
10	3Y	51	Total	C	N	O	S	0	0
			421	281	74	65	1		

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



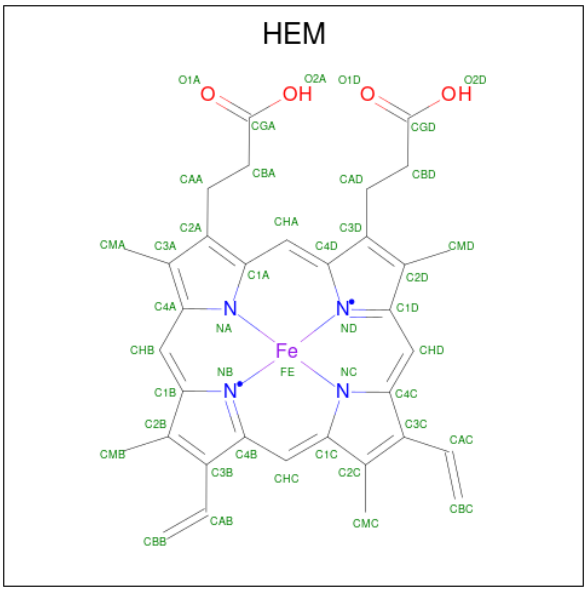
Mol	Chain	Residues	Atoms				AltConf
11	3A	1	Total	C	O	P	0
			58	39	17	2	
11	3D	1	Total	C	O	P	0
			56	37	17	2	
11	3G	1	Total	C	O	P	0
			52	33	17	2	
11	3N	1	Total	C	O	P	0
			43	24	17	2	
11	3P	1	Total	C	O	P	0
			56	37	17	2	
11	3Q	1	Total	C	O	P	0
			57	38	17	2	

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



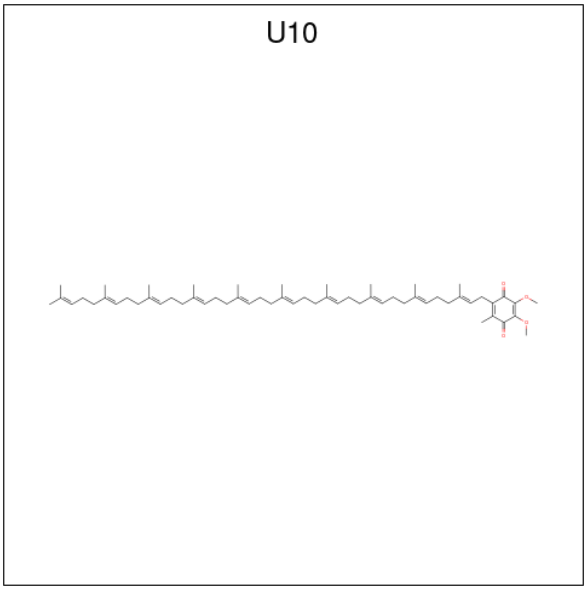
Mol	Chain	Residues	Atoms					AltConf
12	3A	1	Total	C	N	O	P	0
			27	17	1	8	1	
12	3A	1	Total	C	N	O	P	0
			32	22	1	8	1	
12	3C	1	Total	C	N	O	P	0
			35	25	1	8	1	
12	3C	1	Total	C	N	O	P	0
			34	24	1	8	1	
12	3D	1	Total	C	N	O	P	0
			33	23	1	8	1	
12	3G	1	Total	C	N	O	P	0
			29	19	1	8	1	
12	3N	1	Total	C	N	O	P	0
			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	3R	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: $C_{34}H_{32}FeN_4O_4$).



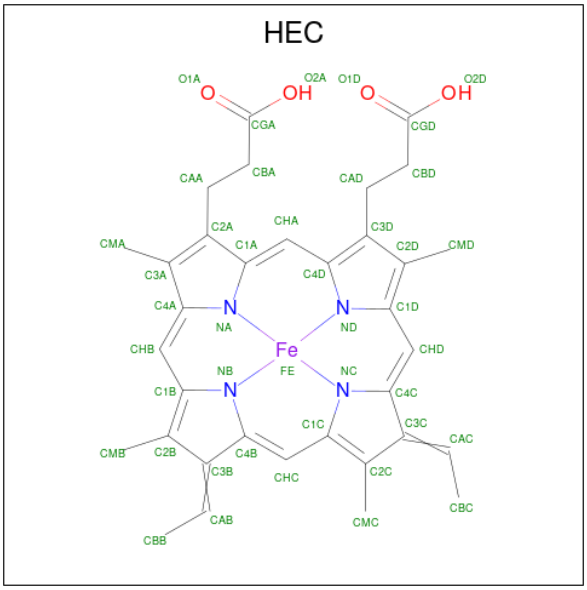
Mol	Chain	Residues	Atoms					AltConf
13	3C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
13	3C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
13	3P	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
13	3P	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

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



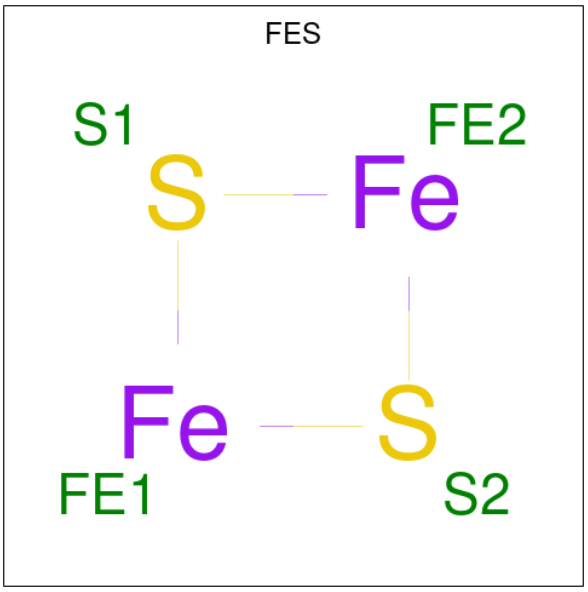
Mol	Chain	Residues	Atoms			AltConf
14	3C	1	Total	C	O	0
			28	24	4	
14	3C	1	Total	C	O	0
			23	19	4	
14	3P	1	Total	C	O	0
			32	28	4	
14	3P	1	Total	C	O	0
			32	28	4	

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



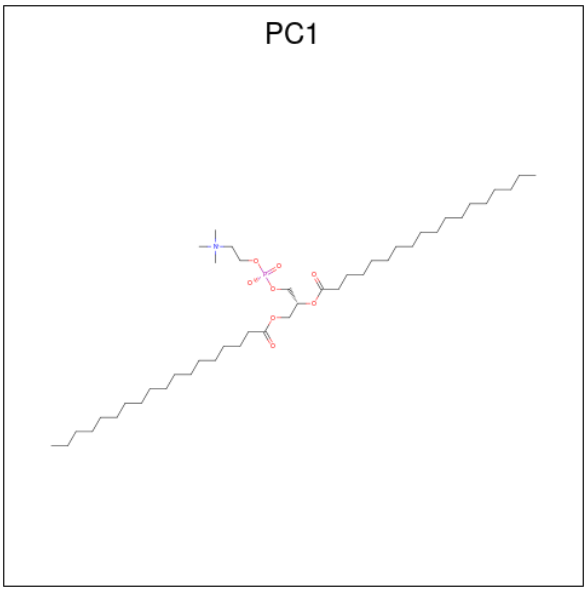
Mol	Chain	Residues	Atoms					AltConf
15	3D	1	Total	C	Fe	N	O	0
			42	34	1	4	3	
15	3Q	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- 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...

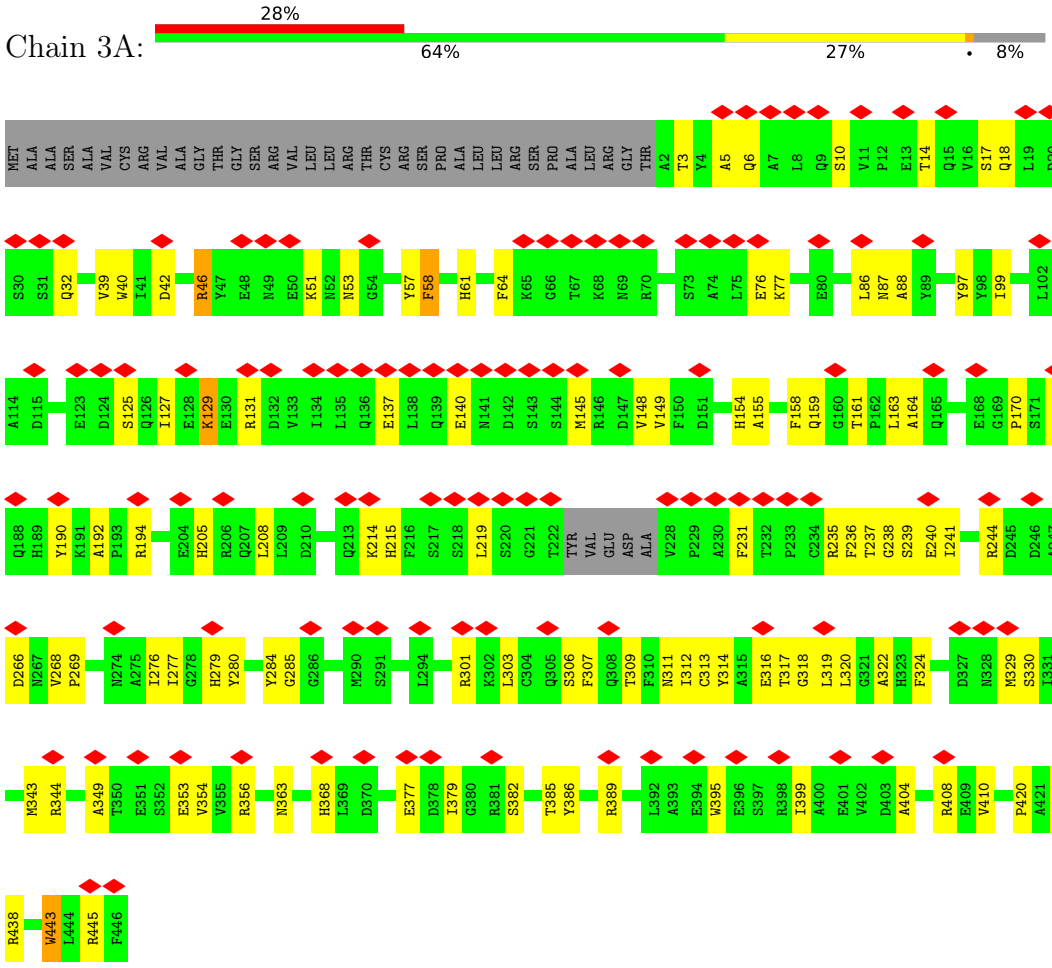
Mol	Chain	Residues	Atoms					AltConf
17	3R	1	Total	C	N	O	P	0
			45	35	1	8	1	
17	3X	1	Total	C	N	O	P	0
			29	19	1	8	1	

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.

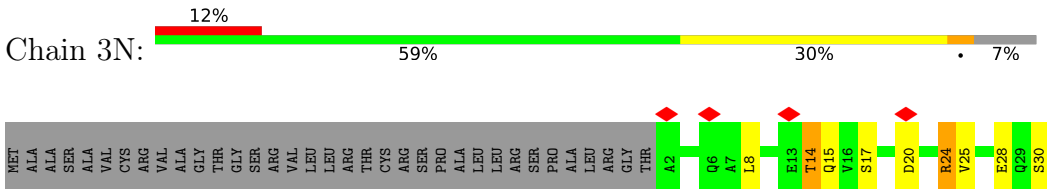
• Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial

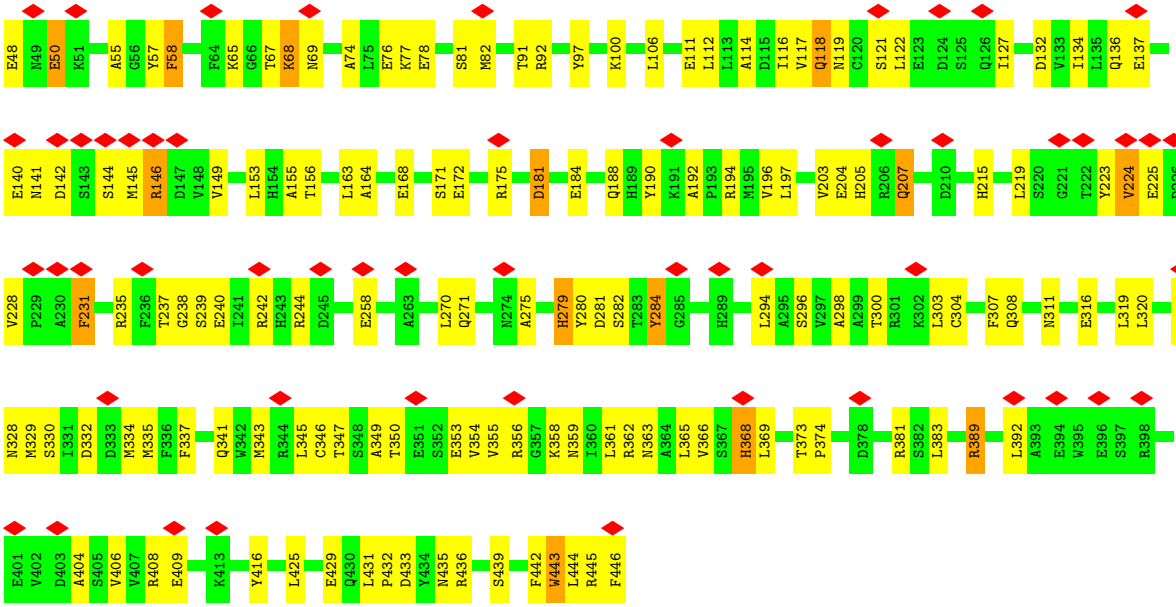
Chain 3A:



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

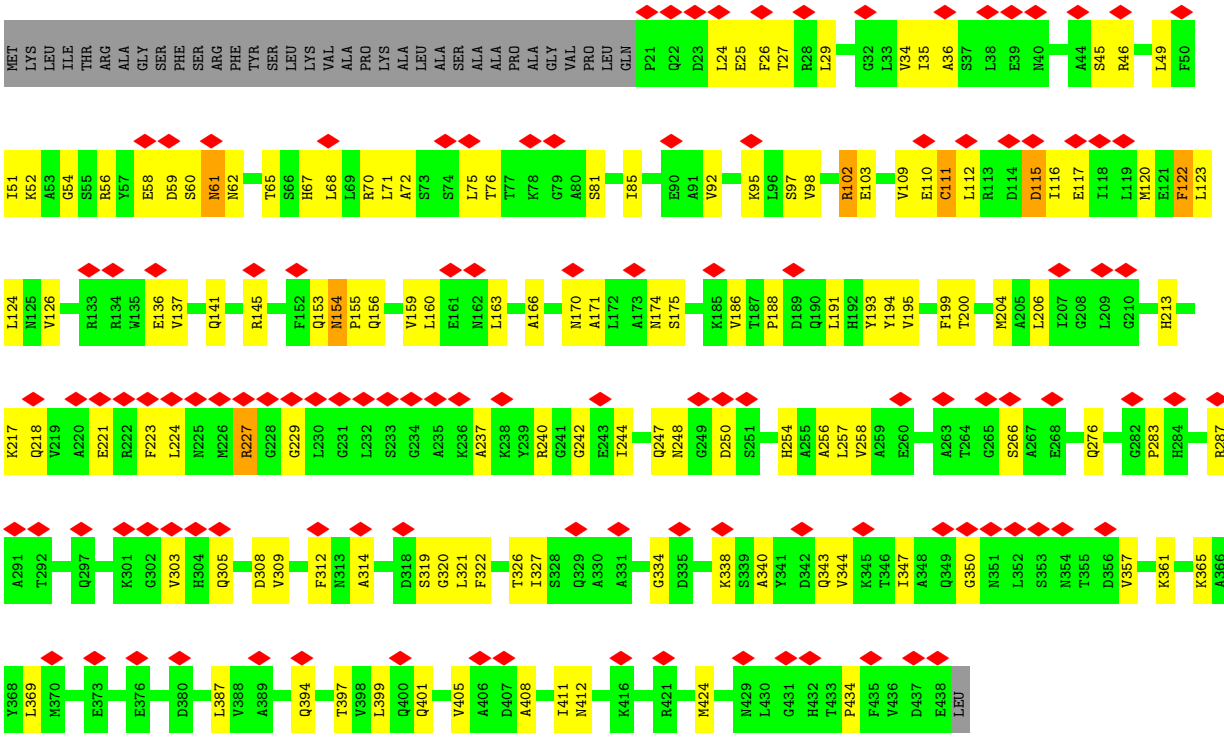
Chain 3N:





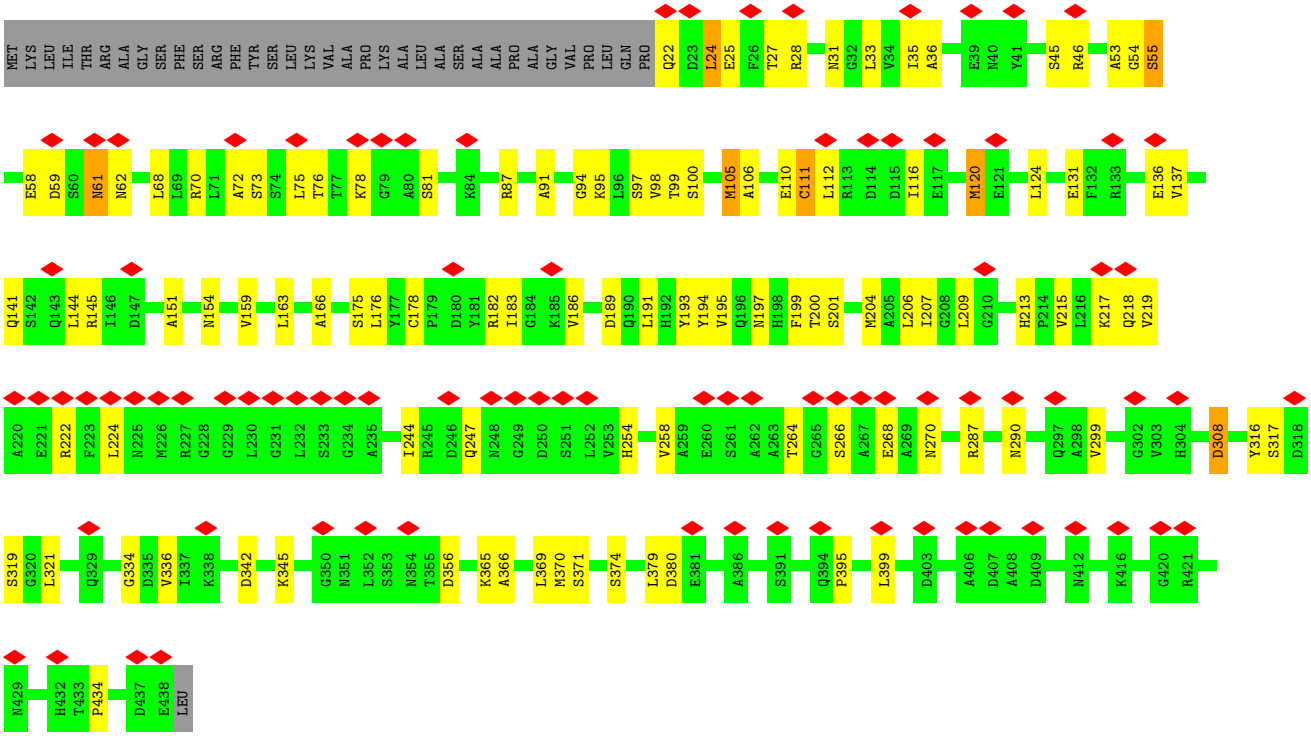
• Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain 3B:



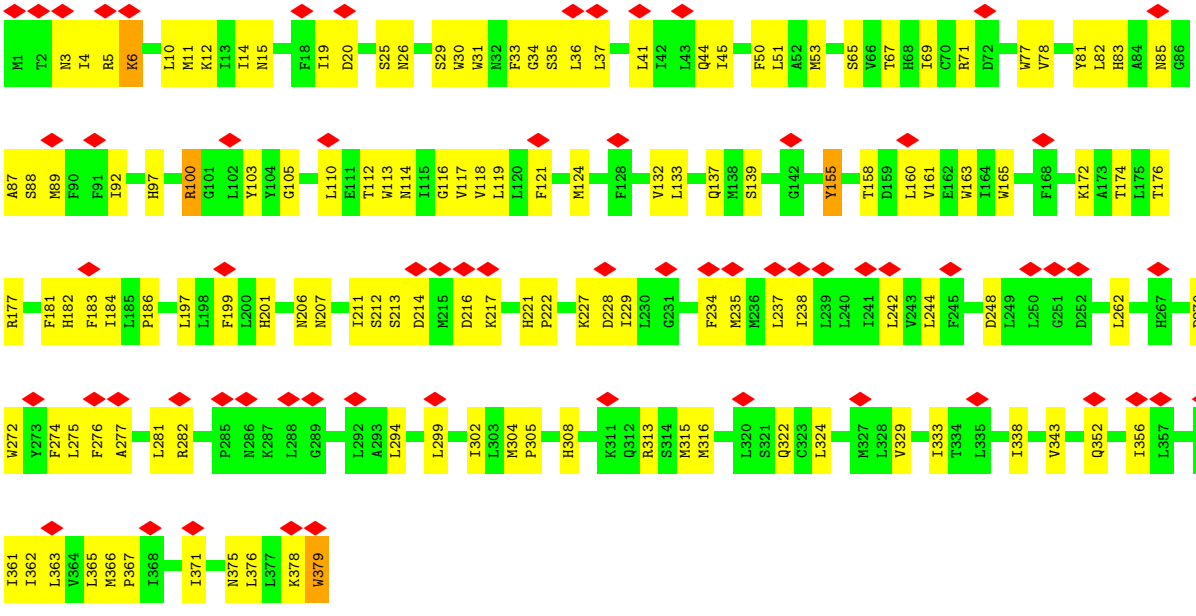
• Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain 3O:



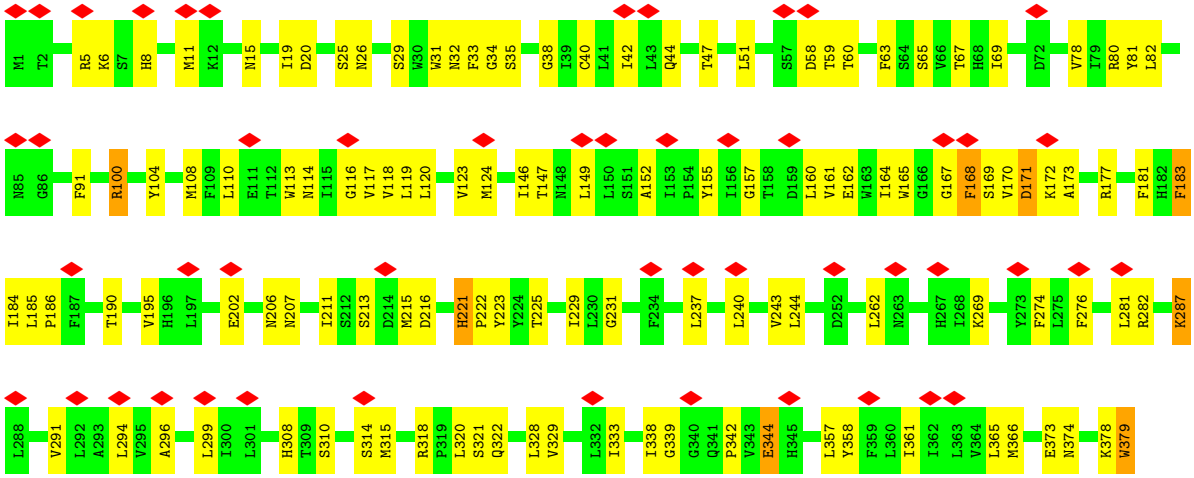
• Molecule 3: Cytochrome b

Chain 3C:



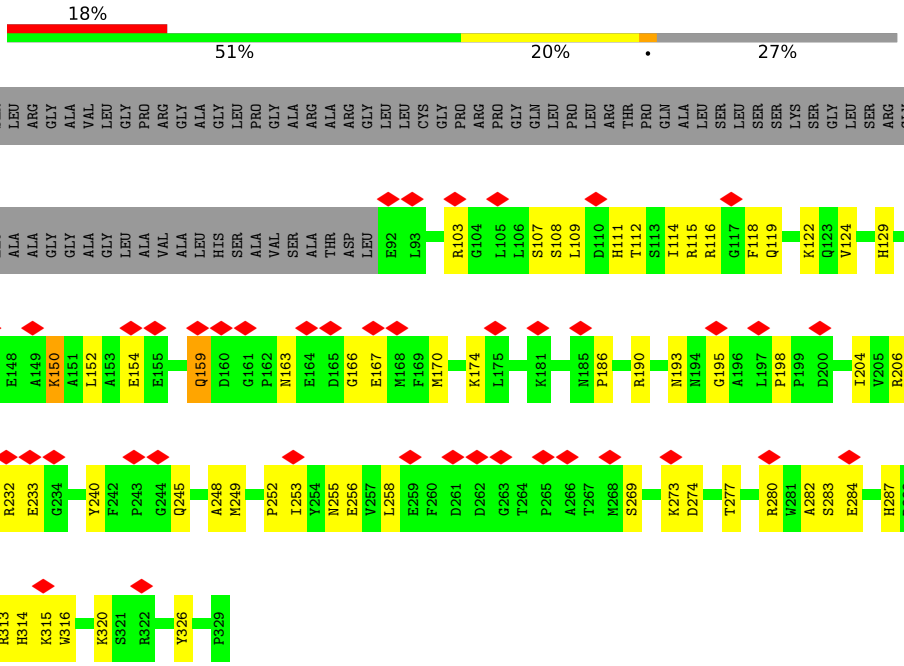
• Molecule 3: Cytochrome b

Chain 3P:



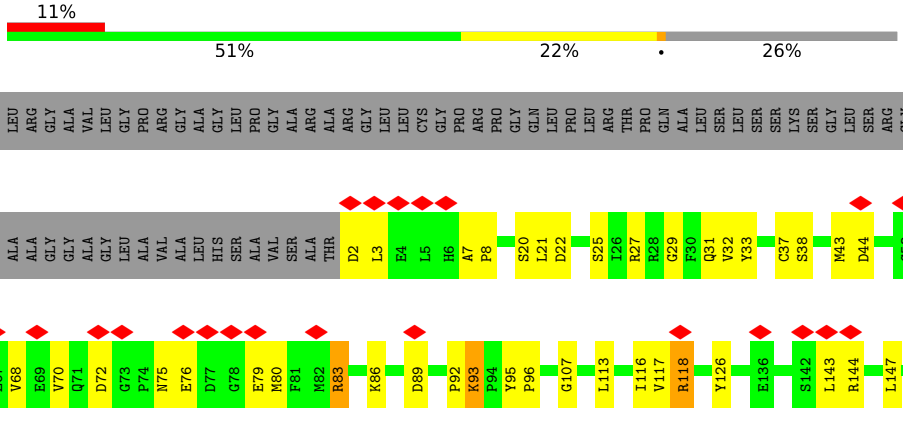
• Molecule 4: Cytochrome c1, heme protein, mitochondrial

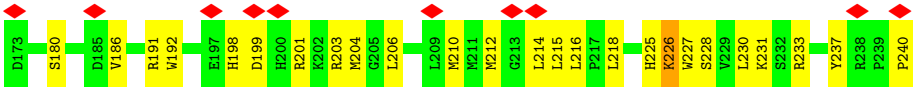
Chain 3D:



• Molecule 4: Cytochrome c1, heme protein, mitochondrial

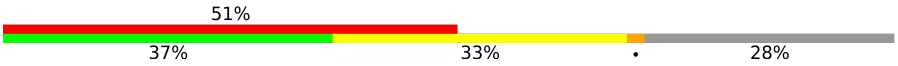
Chain 3Q:

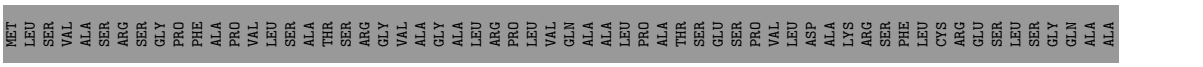


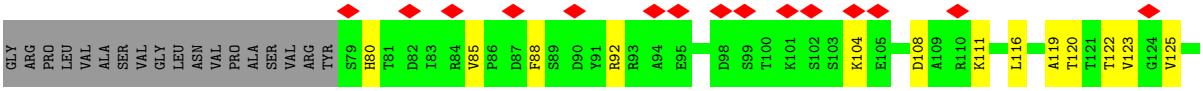


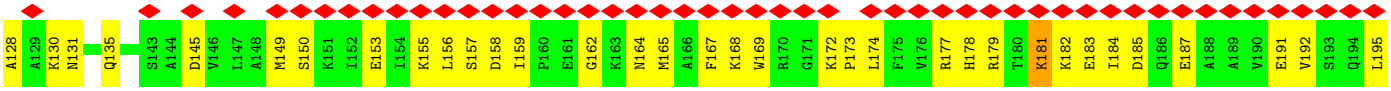
• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

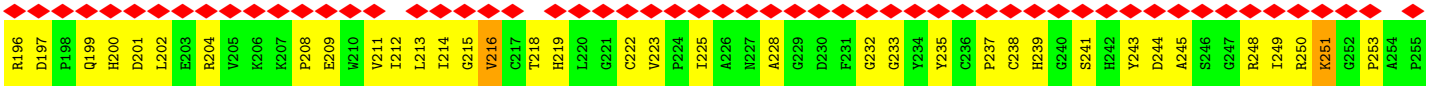
Chain 3E:





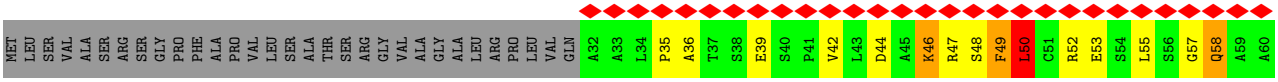


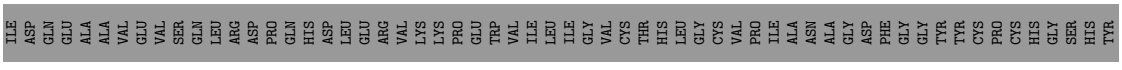


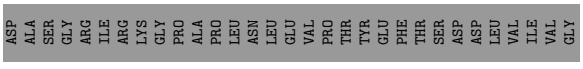


• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain 3I:

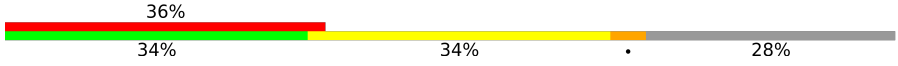


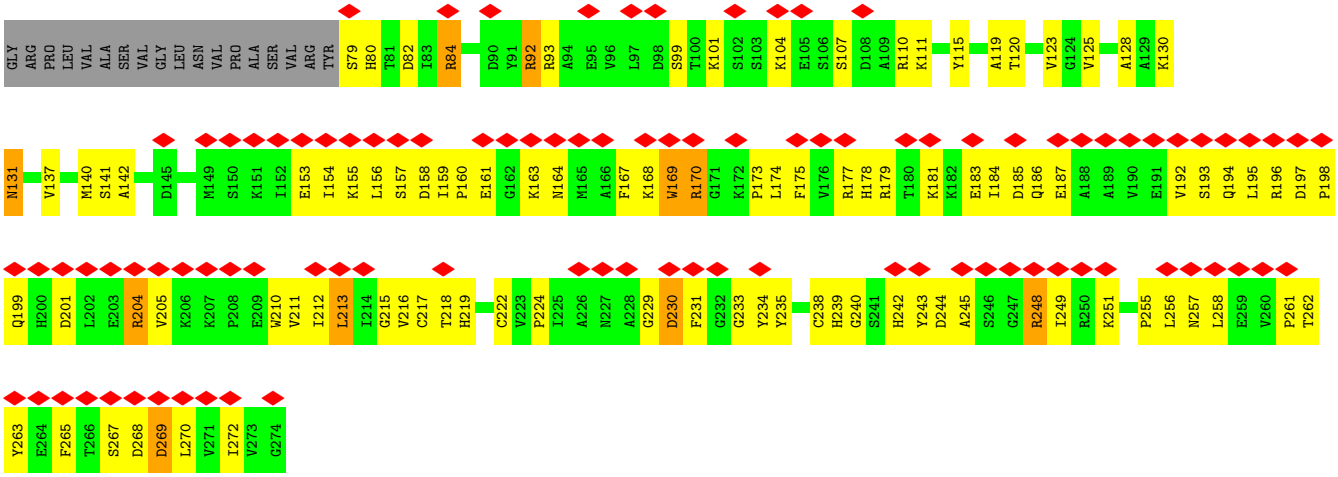




• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

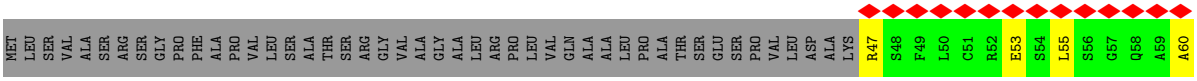
Chain 3R:

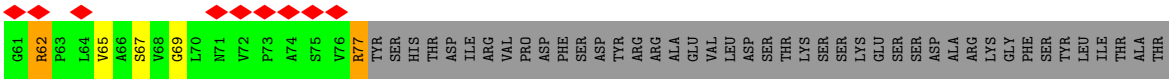




• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

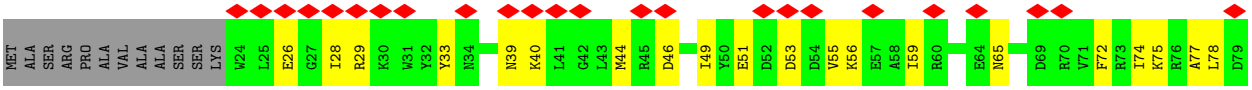
Chain 3V:

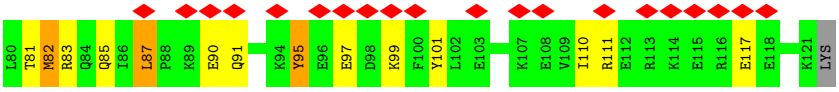




• Molecule 6: Cytochrome b-c1 complex subunit 7

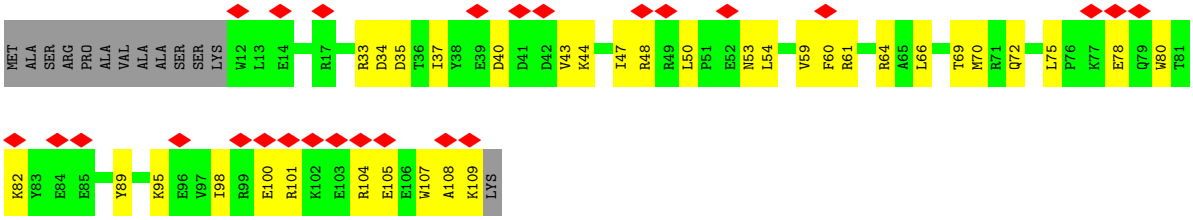
Chain 3F:





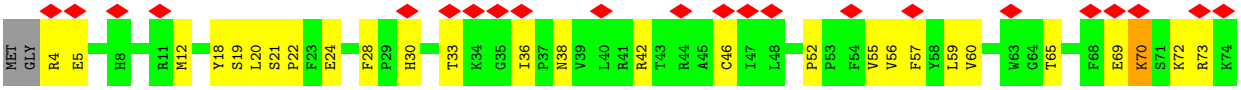
• Molecule 6: Cytochrome b-c1 complex subunit 7

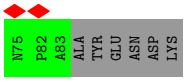
Chain 3S:



• Molecule 7: Cytochrome b-c1 complex subunit 8

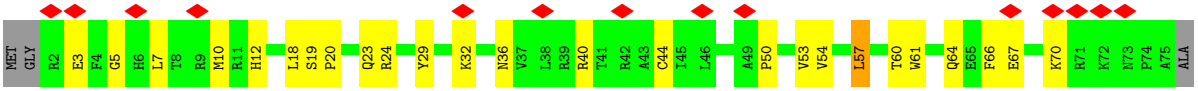
Chain 3G:





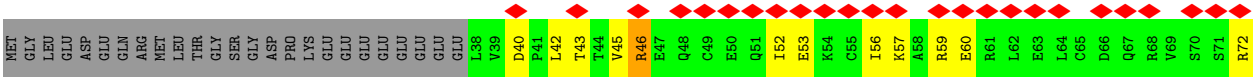
• Molecule 7: Cytochrome b-c1 complex subunit 8

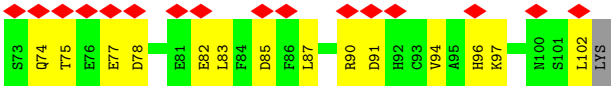
Chain 3T:



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

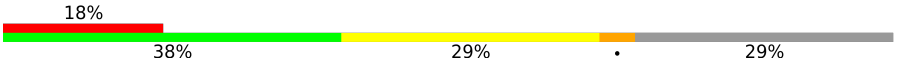
Chain 3H:

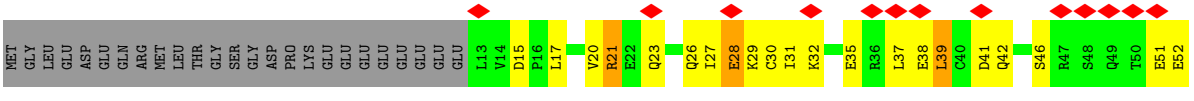


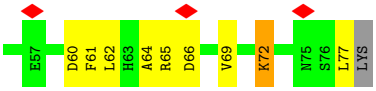


• Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain 3U:

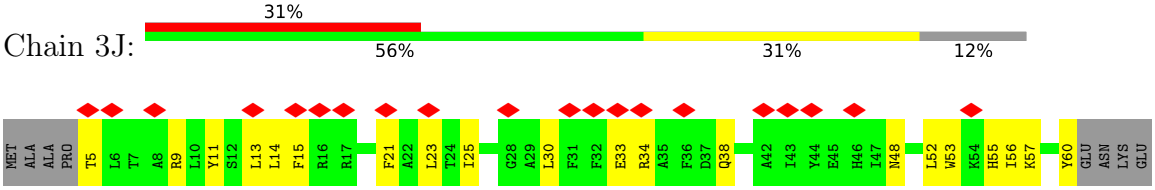






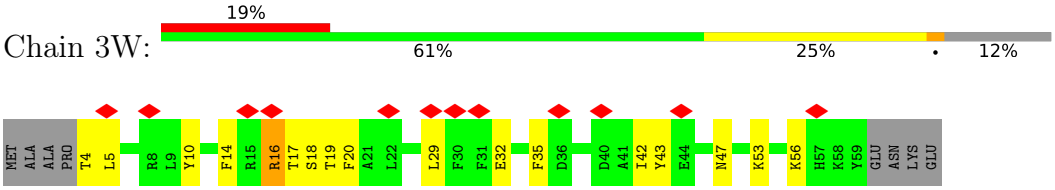
• Molecule 9: Ubiquinol-cytochrome c reductase complex 7.2 kDa protein

Chain 3J:



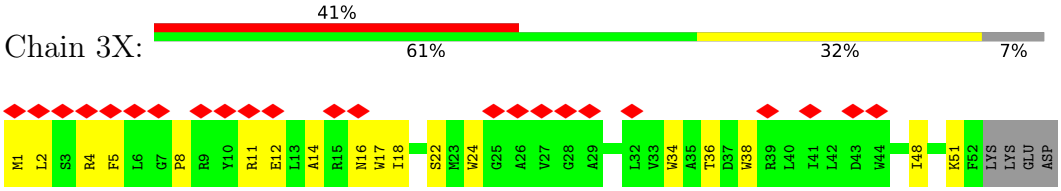
• Molecule 9: Ubiquinol-cytochrome c reductase complex 7.2 kDa protein

Chain 3W:



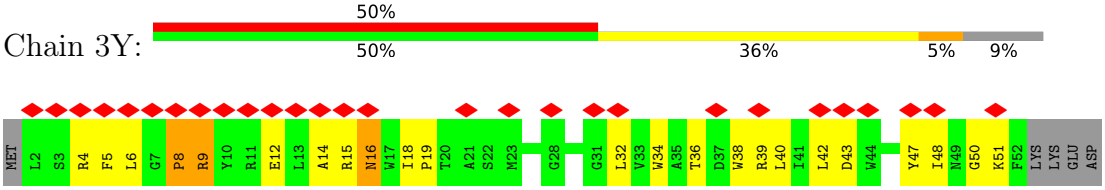
• Molecule 10: Cytochrome b-c1 complex subunit 10

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	45000	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	0.485	Depositor
Minimum map value	-0.190	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.15	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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PC1, U10, FES, HEC, HEM, 3PE, 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	0.25	0/3481	0.49	0/4722
1	3N	0.26	0/3496	0.50	1/4723 (0.0%)
2	3B	0.26	0/3190	0.50	0/4317
2	3O	0.26	0/3175	0.47	0/4292
3	3C	0.26	0/3123	0.48	0/4269
3	3P	0.27	0/3122	0.48	0/4269
4	3D	0.27	0/1946	0.49	0/2641
4	3Q	0.27	0/1962	0.52	0/2663
5	3E	0.26	0/1551	0.55	0/2098
5	3I	1.55	2/342 (0.6%)	1.41	6/465 (1.3%)
5	3R	0.27	0/1551	0.54	0/2098
5	3V	0.27	0/225	0.62	0/303
6	3F	0.27	0/888	0.59	1/1193 (0.1%)
6	3S	0.27	0/888	0.54	0/1193
7	3G	0.27	0/648	0.56	0/874
7	3T	0.27	0/649	0.60	1/878 (0.1%)
8	3H	0.30	0/538	0.66	0/721
8	3U	0.28	0/539	0.66	1/724 (0.1%)
9	3J	0.26	0/476	0.61	0/641
9	3W	0.27	0/476	0.50	0/641
10	3X	0.24	0/445	0.55	0/608
10	3Y	0.28	0/437	0.64	1/598 (0.2%)
All	All	0.31	2/33148 (0.0%)	0.53	11/44931 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	3I	49	PHE	C-N	27.36	1.97	1.34
5	3I	48	SER	C-N	5.86	1.47	1.34

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	3I	48	SER	O-C-N	15.75	147.90	122.70
5	3I	49	PHE	CA-C-N	-15.03	84.13	117.20
5	3I	48	SER	CA-C-N	-12.18	90.41	117.20
5	3I	48	SER	C-N-CA	-7.64	102.61	121.70
8	3U	39	LEU	CA-CB-CG	6.86	131.08	115.30
5	3I	49	PHE	O-C-N	6.24	132.68	122.70
7	3T	57	LEU	CA-CB-CG	6.18	129.52	115.30
6	3F	87	LEU	CA-CB-CG	6.15	129.44	115.30
5	3I	49	PHE	C-N-CA	-6.13	106.38	121.70
1	3N	332	ASP	CB-CG-OD1	5.70	123.43	118.30
10	3Y	8	PRO	CA-N-CD	-5.12	104.33	111.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	3A	3411	0	3309	98	0
1	3N	3424	0	3350	105	0
2	3B	3138	0	3116	87	0
2	3O	3124	0	3108	65	0
3	3C	3025	0	3090	108	0
3	3P	3024	0	3090	106	0
4	3D	1888	0	1834	66	0
4	3Q	1904	0	1849	63	0
5	3E	1518	0	1498	95	0
5	3I	337	0	346	25	0
5	3R	1518	0	1499	83	0
5	3V	223	0	233	12	0
6	3F	868	0	857	34	0
6	3S	868	0	857	29	0
7	3G	628	0	634	23	0
7	3T	628	0	634	29	0
8	3H	533	0	512	19	0
8	3U	533	0	513	24	0
9	3J	464	0	467	39	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	3W	464	0	467	17	0
10	3X	429	0	430	17	0
10	3Y	421	0	418	20	0
11	3A	58	0	60	6	0
11	3D	56	0	56	3	0
11	3G	52	0	48	5	0
11	3N	43	0	30	3	0
11	3P	56	0	56	9	0
11	3Q	57	0	58	11	0
12	3A	59	0	66	10	0
12	3C	69	0	86	6	0
12	3D	33	0	40	4	0
12	3G	29	0	32	1	0
12	3N	58	0	62	7	0
12	3P	33	0	40	0	0
12	3R	47	0	71	5	0
12	3Y	30	0	34	1	0
13	3C	86	0	60	12	0
13	3P	86	0	60	5	0
14	3C	51	0	54	6	0
14	3P	64	0	78	15	0
15	3D	42	0	32	7	0
15	3Q	43	0	32	4	0
16	3E	4	0	0	3	0
16	3R	4	0	0	0	0
17	3E	47	0	68	5	0
17	3R	45	0	64	6	0
17	3X	29	0	32	5	0
All	All	33551	0	33330	1053	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 16.

All (1053) 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:CD1	9:3J:57:LYS:CE	1.75	1.58
9:3J:53:TRP:CD1	9:3J:57:LYS:HE2	0.95	1.47
9:3J:53:TRP:O	9:3J:57:LYS:HE3	1.22	1.33
9:3J:53:TRP:NE1	9:3J:57:LYS:HE2	1.53	1.23
5:3I:49:PHE:C	5:3I:50:LEU:N	1.97	1.18

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:3J:53:TRP:HD1	9:3J:57:LYS:CE	1.33	1.13
9:3J:53:TRP:CD1	9:3J:57:LYS:HE3	1.90	1.03
7:3T:18:LEU:HB3	7:3T:23:GLN:HE21	1.31	0.95
14:3C:504:U10:H4M2	14:3C:504:U10:H3M2	1.48	0.94
9:3J:53:TRP:O	9:3J:57:LYS:CE	2.16	0.92
14:3P:504:U10:H4M3	14:3P:504:U10:H3M3	1.50	0.91
4:3D:115:ARG:CZ	9:3J:60:TYR:CE1	2.55	0.90
14:3C:503:U10:H4M2	14:3C:503:U10:H3M2	1.52	0.90
5:3I:49:PHE:CA	5:3I:50:LEU:N	2.36	0.87
1:3A:86:LEU:HD13	1:3A:99:ILE:HG22	1.58	0.85
5:3E:237:PRO:HG2	4:3Q:144:ARG:HE	1.42	0.84
3:3C:216:ASP:HB2	6:3F:75:LYS:HD2	1.59	0.84
3:3C:316:MET:HG3	12:3C:505:3PE:H111	1.60	0.83
8:3H:72:ARG:HE	8:3H:75:THR:HG21	1.45	0.82
2:3O:111:CYS:SG	2:3O:112:LEU:N	2.54	0.81
1:3N:118:GLN:HE21	1:3N:219:LEU:HG	1.46	0.80
3:3C:71:ARG:NH2	4:3D:282:ALA:O	2.15	0.79
8:3U:21:ARG:HG3	8:3U:65:ARG:HD2	1.67	0.76
9:3J:11:TYR:HA	9:3J:15:PHE:HB2	1.68	0.76
3:3P:310:SER:HA	3:3P:374:ASN:HD21	1.50	0.75
5:3E:181:LYS:HA	5:3E:184:ILE:HD12	1.67	0.74
5:3E:195:LEU:HD12	5:3E:248:ARG:HG2	1.70	0.74
5:3E:219:HIS:HB3	16:3E:301:FES:S1	2.27	0.73
5:3R:181:LYS:HZ1	5:3R:185:ASP:HB3	1.54	0.73
5:3E:225:ILE:HB	5:3E:235:TYR:HB3	1.71	0.72
17:3R:303:PC1:H152	9:3W:17:THR:HG22	1.72	0.72
5:3R:130:LYS:NZ	10:3X:34:TRP:O	2.23	0.72
3:3C:378:LYS:NZ	6:3F:95:TYR:OH	2.23	0.71
9:3J:53:TRP:CE2	9:3J:57:LYS:HG2	2.26	0.71
3:3C:50:PHE:HA	3:3C:53:MET:HE2	1.72	0.71
4:3Q:230:LEU:HD13	4:3Q:233:ARG:HD3	1.70	0.71
4:3D:233:GLU:OE2	4:3D:233:GLU:N	2.23	0.71
3:3P:32:ASN:HD21	3:3P:231:GLY:HA3	1.56	0.71
3:3P:147:THR:HG21	3:3P:165:TRP:HB2	1.71	0.71
5:3E:241:SER:HB2	5:3E:249:ILE:HB	1.74	0.70
3:3C:15:ASN:HA	3:3C:19:ILE:HB	1.73	0.70
2:3O:299:VAL:HG11	2:3O:336:VAL:HG13	1.73	0.70
5:3R:193:SER:OG	5:3R:194:GLN:NE2	2.25	0.70
3:3C:207:ASN:HD22	3:3C:213:SER:HB3	1.56	0.69
2:3O:334:GLY:HA2	2:3O:434:PRO:HD3	1.74	0.69
8:3U:29:LYS:HE2	8:3U:64:ALA:HB2	1.74	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3N:224:VAL:HG12	1:3N:225:GLU:H	1.57	0.69
10:3X:8:PRO:HA	10:3X:11:ARG:HE	1.58	0.69
4:3D:115:ARG:HD3	9:3J:60:TYR:OH	1.93	0.69
5:3R:125:VAL:HG21	17:3R:303:PC1:H372	1.74	0.69
3:3P:221:HIS:O	3:3P:225:THR:OG1	2.12	0.68
1:3A:42:ASP:HB2	1:3A:194:ARG:HB2	1.75	0.68
4:3D:190:ARG:NH2	5:3R:222:CYS:SG	2.65	0.68
14:3P:503:U10:H161	14:3P:503:U10:H112	1.75	0.68
11:3Q:502:CDL:OA4	7:3T:36:ASN:ND2	2.26	0.68
5:3V:60:ALA:HB1	5:3V:77:ARG:HH22	1.56	0.68
6:3F:83:ARG:HG2	6:3F:85:GLN:HB2	1.76	0.68
14:3P:503:U10:H112	14:3P:503:U10:H202	1.76	0.68
9:3J:13:LEU:HD23	9:3J:14:LEU:HB3	1.75	0.68
8:3U:38:GLU:O	8:3U:42:GLN:NE2	2.26	0.68
9:3W:16:ARG:HB2	9:3W:19:THR:HG22	1.75	0.68
2:3B:283:PRO:HD3	5:3I:57:GLY:HA3	1.76	0.68
8:3U:23:GLN:OE1	8:3U:23:GLN:N	2.26	0.68
9:3W:10:TYR:HA	9:3W:14:PHE:HB2	1.75	0.68
2:3B:227:ARG:HD3	2:3B:229:GLY:H	1.59	0.68
6:3F:85:GLN:NE2	7:3G:38:ASN:OD1	2.27	0.67
3:3P:207:ASN:ND2	3:3P:211:ILE:O	2.28	0.67
11:3P:506:CDL:H151	11:3Q:502:CDL:H752	1.76	0.67
1:3A:332:ASP:OD2	3:3C:6:LYS:NZ	2.26	0.67
1:3A:239:SER:HB2	7:3G:20:LEU:HD12	1.77	0.67
3:3C:182:HIS:HE1	13:3C:501:HEM:NB	1.93	0.67
5:3R:183:GLU:HA	5:3R:186:GLN:HG2	1.77	0.66
1:3N:14:THR:HG21	1:3N:389:ARG:HB3	1.76	0.66
12:3A:503:3PE:H122	3:3C:4:ILE:HG12	1.77	0.66
5:3E:244:ASP:OD1	5:3E:245:ALA:N	2.28	0.66
5:3R:128:ALA:HB1	12:3R:302:3PE:H382	1.78	0.66
6:3S:59:VAL:HG11	7:3T:10:MET:HG2	1.76	0.66
4:3D:252:PRO:HB3	15:3D:501:HEC:HHC	1.76	0.66
3:3C:352:GLN:O	3:3C:356:ILE:HG13	1.96	0.66
5:3E:173:PRO:HB2	5:3E:215:GLY:HA3	1.77	0.66
3:3P:379:TRP:HB3	6:3S:33:ARG:HH21	1.61	0.65
2:3B:117:GLU:OE1	2:3B:117:GLU:N	2.28	0.65
3:3C:78:VAL:O	3:3C:82:LEU:HB2	1.95	0.65
4:3Q:117:VAL:HG11	4:3Q:191:ARG:HA	1.76	0.65
1:3A:17:SER:OG	1:3A:205:HIS:NE2	2.27	0.65
2:3O:45:SER:HB2	2:3O:116:ILE:HG21	1.79	0.65
7:3T:3:GLU:N	7:3T:3:GLU:OE2	2.26	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3D:115:ARG:NH1	9:3J:60:TYR:CE1	2.65	0.65
12:3D:502:3PE:H221	12:3D:502:3PE:H331	1.79	0.65
3:3P:42:ILE:HD11	14:3P:503:U10:H201	1.79	0.65
5:3R:229:GLY:O	5:3R:231:PHE:N	2.29	0.65
5:3R:160:PRO:HG2	5:3R:163:LYS:HG3	1.77	0.65
8:3U:35:GLU:O	8:3U:39:LEU:HD22	1.97	0.65
3:3C:51:LEU:HD13	13:3C:501:HEM:HBD1	1.79	0.64
4:3D:107:SER:O	4:3D:291:LYS:NZ	2.30	0.64
8:3U:42:GLN:O	8:3U:46:SER:OG	2.13	0.64
4:3Q:8:PRO:HG3	8:3U:66:ASP:HB3	1.79	0.64
5:3E:172:LYS:HE3	5:3E:214:ILE:HG21	1.80	0.64
8:3H:56:ILE:O	8:3H:60:GLU:HG3	1.97	0.64
1:3N:30:SER:OG	1:3N:32:GLN:OE1	2.16	0.64
1:3N:100:LYS:NZ	2:3O:370:MET:SD	2.69	0.64
3:3C:124:MET:HG2	3:3C:274:PHE:HE1	1.62	0.64
1:3N:153:LEU:HD22	1:3N:319:LEU:HD13	1.80	0.63
7:3G:30:HIS:HB3	7:3G:33:THR:HB	1.80	0.63
1:3A:339:GLN:O	1:3A:343:MET:HG2	1.97	0.63
3:3C:119:LEU:HD22	13:3C:502:HEM:HBB2	1.80	0.63
6:3S:35:ASP:OD1	6:3S:89:TYR:OH	2.14	0.63
8:3H:77:GLU:O	8:3H:78:ASP:N	2.31	0.63
1:3A:354:VAL:HG21	1:3A:404:ALA:HA	1.79	0.63
3:3C:44:GLN:HE22	3:3C:83:HIS:CE1	2.16	0.63
3:3C:237:LEU:HD13	4:3D:301:MET:HG3	1.80	0.63
7:3T:53:VAL:O	7:3T:57:LEU:HD12	1.99	0.63
1:3N:17:SER:HG	1:3N:205:HIS:HE2	1.46	0.62
1:3N:172:GLU:OE1	1:3N:175:ARG:NH2	2.31	0.62
1:3N:242:ARG:HH22	1:3N:433:ASP:HA	1.63	0.62
5:3E:168:LYS:HE2	5:3E:168:LYS:HA	1.80	0.62
2:3B:314:ALA:HB3	2:3B:321:LEU:HB2	1.79	0.62
5:3E:131:ASN:O	5:3E:135:GLN:HG2	1.99	0.62
2:3B:309:VAL:HG12	2:3B:326:THR:HB	1.82	0.62
4:3D:114:ILE:HD13	4:3D:277:THR:HG23	1.79	0.62
9:3J:34:ARG:NH2	10:3Y:50:GLY:HA3	2.15	0.62
1:3N:433:ASP:OD1	3:3P:223:TYR:OH	2.17	0.62
2:3B:254:HIS:HA	2:3B:327:ILE:HG22	1.82	0.62
3:3P:215:MET:SD	3:3P:215:MET:N	2.71	0.62
4:3Q:33:TYR:CZ	4:3Q:43:MET:HG3	2.35	0.62
2:3B:97:SER:HA	5:3I:69:GLY:HA3	1.81	0.62
5:3E:122:THR:HG22	9:3J:25:ILE:HG21	1.81	0.62
1:3A:349:ALA:H	1:3A:408:ARG:HH11	1.47	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:3R:157:SER:OG	5:3R:269:ASP:OD1	2.18	0.61
2:3B:303:VAL:HG22	2:3B:305:GLN:H	1.65	0.61
5:3E:125:VAL:HG21	17:3E:302:PC1:H362	1.81	0.61
1:3N:204:GLU:HG3	1:3N:207[A]:GLN:H	1.65	0.61
1:3A:159:GLN:HE22	5:3E:88:PHE:HD2	1.48	0.61
3:3C:214:ASP:OD1	7:3G:4:ARG:NH1	2.32	0.61
4:3D:245:GLN:N	4:3D:245:GLN:OE1	2.33	0.61
10:3Y:48:ILE:HD12	10:3Y:48:ILE:H	1.64	0.61
4:3D:115:ARG:CZ	9:3J:60:TYR:HE1	2.14	0.61
4:3D:118:PHE:HE2	4:3D:152:LEU:HD21	1.63	0.61
2:3B:327:ILE:HG13	5:3I:55:LEU:HD21	1.83	0.61
3:3P:8:HIS:HB3	3:3P:11:MET:HB2	1.83	0.61
3:3P:29:SER:HB2	11:3Q:502:CDL:H732	1.81	0.61
4:3Q:2:ASP:OD2	7:3T:70:LYS:NZ	2.34	0.61
5:3R:130:LYS:HE3	9:3W:32:GLU:OE1	2.00	0.61
1:3A:158:PHE:O	1:3A:161:THR:OG1	2.17	0.61
5:3E:239:HIS:HD2	5:3E:253:PRO:HD2	1.66	0.61
3:3P:161:VAL:O	3:3P:165:TRP:HB3	2.01	0.61
8:3H:82:GLU:N	8:3H:82:GLU:OE1	2.34	0.60
2:3B:75:LEU:HD22	2:3B:136:GLU:HB3	1.83	0.60
2:3B:350:GLY:HA2	2:3B:411:ILE:HD11	1.82	0.60
3:3C:31:TRP:NE1	13:3C:502:HEM:O2D	2.33	0.60
3:3C:97:HIS:NE2	13:3C:502:HEM:O1A	2.28	0.60
4:3D:115:ARG:NH1	9:3J:60:TYR:CD1	2.70	0.60
12:3N:503:3PE:H32	17:3R:303:PC1:H11	1.83	0.60
4:3Q:72:ASP:OD2	4:3Q:83:ARG:NH1	2.35	0.60
4:3Q:212:MET:HA	4:3Q:215:LEU:HB2	1.83	0.60
5:3E:214:ILE:HB	5:3E:259:GLU:HB3	1.82	0.60
2:3O:100:SER:HB2	2:3O:105:MET:HG3	1.84	0.60
5:3R:242:HIS:HE1	5:3R:251:LYS:HG2	1.67	0.60
2:3O:76:THR:HG23	2:3O:81:SER:HA	1.84	0.60
12:3N:503:3PE:H331	17:3R:303:PC1:H351	1.84	0.60
1:3N:304:CYS:HB3	1:3N:334:MET:SD	2.42	0.60
5:3V:62:ARG:O	5:3V:77:ARG:NH2	2.35	0.60
5:3R:234:TYR:HB2	5:3R:243:TYR:HB2	1.84	0.60
2:3B:95:LYS:NZ	5:3I:71:ASN:O	2.35	0.59
12:3N:501:3PE:H262	11:3N:502:CDL:HB62	1.84	0.59
3:3C:244:LEU:HD23	4:3D:294:GLY:HA2	1.84	0.59
1:3A:303:LEU:HD21	1:3A:333:ASP:HB3	1.85	0.59
3:3P:361:ILE:HA	3:3P:365:LEU:HB2	1.83	0.59
10:3Y:32:LEU:O	10:3Y:36:THR:HG22	2.02	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:3E:150:SER:HB3	3:3P:168:PHE:CE1	2.37	0.59
5:3R:199:GLN:O	5:3R:248:ARG:NH1	2.36	0.59
2:3B:408:ALA:O	2:3B:412:ASN:ND2	2.34	0.59
4:3D:111:HIS:HD2	9:3J:52:LEU:HA	1.68	0.59
5:3E:212:ILE:HD13	5:3E:261:PRO:HD2	1.85	0.59
3:3P:165:TRP:CZ2	3:3P:169:SER:HA	2.37	0.59
3:3P:169:SER:OG	3:3P:171:ASP:OD1	2.20	0.59
1:3A:97:TYR:HH	1:3A:190:TYR:HH	1.48	0.59
5:3E:179:ARG:NH1	5:3E:201:ASP:OD1	2.31	0.59
5:3E:195:LEU:HD13	5:3E:250:ARG:HA	1.84	0.59
3:3P:26:ASN:ND2	6:3S:69:THR:OG1	2.30	0.59
6:3S:53:ASN:OD1	6:3S:54:LEU:N	2.36	0.59
4:3Q:31:GLN:NE2	4:3Q:56:TYR:OH	2.36	0.59
3:3C:262:LEU:HD22	5:3R:216:VAL:HG11	1.84	0.59
3:3C:272:TRP:HA	3:3C:275:LEU:HD12	1.84	0.59
1:3N:30:SER:OG	1:3N:31:SER:N	2.36	0.59
8:3U:27:ILE:HG22	8:3U:30:CYS:HB2	1.84	0.59
5:3E:184:ILE:HG21	5:3E:208:PRO:HB3	1.85	0.58
5:3E:225:ILE:N	5:3E:235:TYR:O	2.35	0.58
2:3B:51:ILE:HG12	2:3B:204:MET:HG2	1.84	0.58
5:3E:162:GLY:H	5:3E:178:HIS:HB3	1.68	0.58
4:3Q:31:GLN:NE2	4:3Q:172:ASP:OD2	2.37	0.58
5:3R:141:SER:OG	5:3R:142:ALA:N	2.36	0.58
12:3R:302:3PE:H232	12:3R:302:3PE:H331	1.84	0.58
6:3S:33:ARG:NH1	6:3S:34:ASP:OD1	2.37	0.58
1:3N:328:ASN:OD1	1:3N:329:MET:N	2.37	0.58
1:3N:329:MET:HE2	7:3T:5:GLY:HA3	1.85	0.58
3:3P:207:ASN:HD22	3:3P:213:SER:HB3	1.68	0.58
1:3A:170:PRO:HG2	1:3A:173:ASN:HB2	1.86	0.58
3:3C:299:LEU:HG	3:3C:302:ILE:HD12	1.85	0.58
2:3O:141:GLN:HE22	2:3O:186:VAL:HG23	1.67	0.58
1:3A:173:ASN:O	1:3A:177:LEU:HD23	2.04	0.57
1:3N:235:ARG:HH21	5:3R:92:ARG:NH1	2.01	0.57
2:3O:166:ALA:HB2	2:3O:244:ILE:HG12	1.85	0.57
4:3Q:144:ARG:HD2	4:3Q:147:LEU:HD22	1.84	0.57
11:3Q:502:CDL:HA21	6:3S:72:GLN:HB2	1.86	0.57
2:3B:95:LYS:HB2	2:3B:110:GLU:H	1.70	0.57
5:3E:116:LEU:O	5:3E:120:THR:HG23	2.02	0.57
11:3Q:502:CDL:OA3	7:3T:40:ARG:NH1	2.37	0.57
3:3P:202:GLU:OE1	3:3P:202:GLU:N	2.27	0.57
10:3Y:8:PRO:HD2	10:3Y:9:ARG:H	1.70	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:3D:502:3PE:H362	5:3E:128:ALA:HB1	1.86	0.57
4:3Q:216:LEU:HB3	11:3Q:502:CDL:H562	1.85	0.57
6:3F:87:LEU:HD21	6:3F:91:GLN:HG2	1.86	0.57
10:3Y:12:GLU:OE1	10:3Y:12:GLU:N	2.25	0.57
6:3S:101:ARG:NH1	6:3S:105:GLU:OE2	2.38	0.57
2:3B:357:VAL:O	2:3B:361:LYS:HG2	2.05	0.56
4:3Q:75:ASN:OD1	4:3Q:76:GLU:N	2.38	0.56
2:3B:319:SER:OG	2:3B:320:GLY:N	2.37	0.56
5:3E:196:ARG:HB2	5:3E:251:LYS:HA	1.87	0.56
1:3A:238:GLY:O	7:3G:21:SER:OG	2.23	0.56
7:3G:38:ASN:O	7:3G:42:ARG:HG3	2.05	0.56
3:3P:164:ILE:HG23	14:3P:504:U10:H152	1.87	0.56
8:3U:31:ILE:O	8:3U:35:GLU:HG2	2.05	0.56
10:3Y:14:ALA:O	10:3Y:18:ILE:HG12	2.04	0.56
6:3F:53:ASP:HA	6:3F:56:LYS:HZ3	1.69	0.56
4:3Q:116:ILE:HG12	15:3Q:501:HEC:HMA3	1.87	0.56
4:3D:115:ARG:NE	9:3J:60:TYR:CE1	2.72	0.56
1:3N:281:ASP:OD1	1:3N:282:SER:N	2.39	0.56
6:3S:100:GLU:HG3	6:3S:104:ARG:HH21	1.70	0.56
1:3A:175:ARG:HB2	1:3A:176:LYS:HZ2	1.70	0.56
1:3A:269:PRO:HB2	1:3A:410:VAL:HG11	1.88	0.56
1:3N:141:ASN:ND2	1:3N:168:GLU:OE2	2.39	0.56
1:3N:142:ASP:OD1	5:3R:80:HIS:ND1	2.38	0.56
2:3B:54:GLY:O	2:3B:194:TYR:OH	2.24	0.56
2:3O:78:LYS:HD2	2:3O:131:GLU:HG2	1.88	0.56
2:3B:312:PHE:HA	5:3I:61:GLY:HA2	1.87	0.56
3:3C:308:HIS:HE1	3:3C:313:ARG:HA	1.71	0.56
4:3D:118:PHE:CE2	4:3D:152:LEU:HD21	2.40	0.56
3:3C:29:SER:HB2	11:3D:503:CDL:H731	1.88	0.56
2:3O:54:GLY:O	2:3O:194:TYR:OH	2.23	0.56
3:3P:124:MET:HG2	3:3P:274:PHE:HE1	1.72	0.55
2:3B:59:ASP:OD1	2:3B:60:SER:N	2.39	0.55
4:3D:240:TYR:OH	8:3H:91:ASP:OD2	2.22	0.55
2:3B:102:ARG:NH1	2:3B:174:ASN:O	2.39	0.55
9:3J:34:ARG:HH22	10:3Y:50:GLY:HA3	1.72	0.55
3:3P:51:LEU:HD21	3:3P:80:ARG:HA	1.89	0.55
9:3J:21:PHE:O	9:3J:25:ILE:HG12	2.05	0.55
3:3P:281:LEU:HB2	3:3P:294:LEU:HD12	1.88	0.55
5:3E:156:LEU:HG	5:3E:158:ASP:H	1.70	0.55
1:3A:244:ARG:HG2	7:3G:12:MET:HG2	1.89	0.55
2:3O:68:LEU:HD23	2:3O:191:LEU:HD21	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:3J:53:TRP:NE1	9:3J:57:LYS:HG2	2.21	0.55
3:3P:119:LEU:HD22	13:3P:502:HEM:HBB2	1.89	0.55
2:3B:25:GLU:O	2:3B:36:ALA:HA	2.06	0.55
3:3C:26:ASN:HD21	3:3C:207:ASN:HB2	1.71	0.55
11:3P:506:CDL:H522	11:3P:506:CDL:HA4	1.89	0.55
1:3A:131:ARG:HD3	1:3A:175:ARG:HA	1.87	0.55
3:3C:282:ARG:HD3	3:3C:343:VAL:HB	1.88	0.55
14:3P:503:U10:H161	14:3P:503:U10:C11	2.37	0.55
1:3A:436:ARG:HH11	3:3C:222:PRO:HD3	1.72	0.55
6:3F:97:GLU:N	6:3F:97:GLU:OE1	2.40	0.55
1:3N:349:ALA:O	1:3N:408:ARG:NH1	2.40	0.55
3:3P:314:SER:O	3:3P:318:ARG:NH1	2.37	0.55
2:3B:24:LEU:HD21	2:3B:36:ALA:HB1	1.89	0.54
3:3C:35:SER:HB3	14:3C:503:U10:H1M1	1.89	0.54
1:3N:77:LYS:O	1:3N:81:SER:OG	2.23	0.54
6:3S:78:GLU:N	6:3S:78:GLU:OE1	2.39	0.54
3:3C:155:TYR:HE1	17:3X:101:PC1:H122	1.72	0.54
4:3D:204:ILE:HG12	15:3D:501:HEC:HMA3	1.89	0.54
1:3N:350:THR:N	1:3N:353:GLU:OE2	2.28	0.54
1:3A:148:VAL:HG22	5:3E:80:HIS:CG	2.41	0.54
1:3N:156:THR:O	1:3N:239:SER:OG	2.24	0.54
3:3P:190:THR:HG23	14:3P:503:U10:H221	1.90	0.54
4:3Q:68:VAL:HG21	4:3Q:92:PRO:HG2	1.89	0.54
2:3O:70:ARG:O	2:3O:98:VAL:HG21	2.07	0.54
4:3D:124:VAL:HG11	4:3D:253:ILE:HG22	1.90	0.54
5:3I:49:PHE:C	5:3I:50:LEU:CA	2.76	0.54
1:3A:154:HIS:NE2	1:3A:314:TYR:OH	2.34	0.54
3:3C:281:LEU:HB2	3:3C:294:LEU:HD12	1.89	0.54
7:3G:28:PHE:HE2	12:3G:101:3PE:H351	1.73	0.54
4:3Q:225:HIS:CE1	7:3T:20:PRO:HB2	2.43	0.54
5:3E:241:SER:N	5:3E:251:LYS:O	2.39	0.54
1:3N:439:SER:HB3	12:3N:503:3PE:H112	1.90	0.54
2:3O:287:ARG:HG2	5:3V:53:GLU:HB3	1.90	0.54
2:3B:365:LYS:HG2	2:3B:399:LEU:HD22	1.88	0.54
3:3C:33:PHE:HA	3:3C:36:LEU:HB2	1.89	0.54
5:3E:222:CYS:HB2	16:3E:301:FES:S2	2.47	0.53
6:3S:98:ILE:HD12	6:3S:101:ARG:HH21	1.73	0.53
1:3A:235:ARG:NH2	5:3E:92:ARG:HH12	2.05	0.53
4:3D:289:HIS:O	4:3D:293:MET:N	2.38	0.53
2:3B:361:LYS:HE2	2:3B:405:VAL:HB	1.90	0.53
8:3H:46:ARG:HD3	8:3H:90:ARG:CZ	2.38	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3O:163:LEU:HD21	2:3O:258:VAL:HG11	1.89	0.53
7:3T:61:TRP:HA	7:3T:64:GLN:HE21	1.73	0.53
2:3B:76:THR:HG23	2:3B:81:SER:HA	1.91	0.53
3:3C:34:GLY:HA2	3:3C:37:LEU:HD12	1.89	0.53
11:3D:503:CDL:H762	11:3G:102:CDL:H312	1.90	0.53
1:3N:279:HIS:HB2	1:3N:308:GLN:HG3	1.90	0.53
3:3P:42:ILE:HG12	14:3P:503:U10:H253	1.90	0.53
5:3E:263:TYR:CE1	5:3E:265:PHE:HB2	2.43	0.53
7:3G:52:PRO:O	7:3G:56:VAL:HG12	2.09	0.53
3:3P:38:GLY:HA3	14:3P:503:U10:H122	1.91	0.53
5:3I:49:PHE:HB3	5:3I:50:LEU:N	2.24	0.53
5:3R:218:THR:HG21	5:3R:256:LEU:HD23	1.90	0.53
6:3S:43:VAL:O	6:3S:47:ILE:HD12	2.09	0.53
8:3H:82:GLU:HA	8:3H:85:ASP:OD2	2.08	0.53
9:3J:5:THR:OG1	9:3J:9:ARG:NH1	2.41	0.53
11:3P:506:CDL:HB31	7:3T:40:ARG:HB3	1.90	0.53
3:3C:97:HIS:CE1	3:3C:100:ARG:HH22	2.26	0.53
6:3F:77:ALA:O	6:3F:81:THR:HG23	2.08	0.53
5:3R:196:ARG:NH1	5:3R:255:PRO:O	2.40	0.53
5:3R:198:PRO:O	5:3R:199:GLN:NE2	2.42	0.53
5:3R:238:CYS:SG	5:3R:239:HIS:N	2.81	0.53
2:3B:166:ALA:HB2	2:3B:244:ILE:HG12	1.91	0.53
5:3R:183:GLU:O	5:3R:187:GLU:HG2	2.08	0.53
10:3Y:38:TRP:HE1	10:3Y:40:LEU:HD23	1.74	0.53
3:3C:177:ARG:NH2	5:3R:140:MET:O	2.36	0.52
1:3N:445:ARG:NH2	12:3N:501:3PE:O12	2.43	0.52
3:3P:181:PHE:HA	3:3P:184:ILE:HG22	1.91	0.52
3:3C:361:ILE:HA	3:3C:365:LEU:HB2	1.92	0.52
9:3J:53:TRP:CD1	9:3J:57:LYS:CD	2.81	0.52
1:3A:131:ARG:NH1	1:3A:175:ARG:O	2.41	0.52
3:3C:158:THR:O	3:3C:161:VAL:HG22	2.09	0.52
1:3N:91:THR:OG1	1:3N:92:ARG:N	2.41	0.52
3:3C:112:THR:HG22	3:3C:199:PHE:HB3	1.92	0.52
5:3E:238:CYS:HB3	16:3E:301:FES:S2	2.49	0.52
5:3R:119:ALA:HB2	9:3W:20:PHE:HE1	1.75	0.52
2:3B:343:GLN:HE21	2:3B:347:ILE:HG13	1.73	0.52
4:3D:273:LYS:HD2	8:3H:102:LEU:HD12	1.90	0.52
4:3D:313:ARG:HG3	7:3G:28:PHE:HE1	1.75	0.52
9:3W:32:GLU:OE2	10:3X:51:LYS:NZ	2.36	0.52
1:3A:61:HIS:CE1	2:3B:287:ARG:HD3	2.45	0.52
2:3B:257:LEU:HD12	2:3B:424:MET:HB2	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3Q:27:ARG:NH2	4:3Q:60:GLU:OE1	2.43	0.52
5:3R:267:SER:O	5:3R:270:LEU:N	2.39	0.52
1:3A:306:SER:OG	5:3I:39:GLU:OE1	2.27	0.52
3:3C:81:TYR:OH	4:3D:206:ARG:NH2	2.42	0.52
5:3E:239:HIS:CD2	5:3E:253:PRO:HD2	2.44	0.52
1:3N:368:HIS:ND1	1:3N:368:HIS:O	2.43	0.52
2:3O:120:MET:SD	2:3O:219:VAL:HG21	2.50	0.52
2:3O:258:VAL:HG21	2:3O:321:LEU:HB3	1.92	0.52
3:3P:357:LEU:HD12	3:3P:361:ILE:HG13	1.91	0.52
5:3R:156:LEU:HG	5:3R:158:ASP:H	1.75	0.52
1:3A:395:TRP:O	1:3A:399:ILE:HG12	2.09	0.52
2:3B:163:LEU:HD21	2:3B:258:VAL:HG21	1.91	0.52
3:3C:163:TRP:HB2	12:3C:506:3PE:H321	1.92	0.52
4:3D:112:THR:HG22	9:3J:56:ILE:HD13	1.92	0.52
1:3N:155:ALA:HA	1:3N:164:ALA:HB1	1.91	0.52
11:3P:506:CDL:H322	11:3P:506:CDL:H152	1.90	0.52
1:3A:324:PHE:CD2	1:3A:334:MET:HG2	2.45	0.51
11:3A:501:CDL:H132	12:3A:503:3PE:H341	1.91	0.51
2:3B:59:ASP:N	2:3B:62:ASN:OD1	2.41	0.51
1:3N:429:GLU:OE2	7:3T:7:LEU:HB2	2.11	0.51
6:3S:105:GLU:O	6:3S:109:LYS:N	2.43	0.51
3:3C:67:THR:O	3:3C:71:ARG:HG3	2.09	0.51
8:3H:96:HIS:C	8:3H:97:LYS:HD2	2.30	0.51
1:3N:359:ASN:O	1:3N:363:ASN:ND2	2.43	0.51
1:3N:444:LEU:HA	9:3W:17:THR:HG21	1.92	0.51
3:3P:33:PHE:HZ	11:3P:506:CDL:H342	1.75	0.51
11:3Q:502:CDL:HA61	7:3T:29:TYR:CE1	2.46	0.51
2:3B:27:THR:OG1	2:3B:213:HIS:NE2	2.31	0.51
5:3I:49:PHE:HA	5:3I:50:LEU:N	2.22	0.51
2:3O:369:LEU:HD11	2:3O:399:LEU:HD11	1.92	0.51
4:3Q:33:TYR:O	4:3Q:38:SER:N	2.42	0.51
1:3N:224:VAL:HG12	1:3N:225:GLU:N	2.24	0.51
2:3O:342:ASP:HA	2:3O:345:LYS:HE2	1.91	0.51
4:3Q:210:MET:O	4:3Q:214:LEU:HD13	2.11	0.51
6:3S:47:ILE:HA	6:3S:50:LEU:HD12	1.92	0.51
1:3A:276:ILE:HD13	1:3A:353:GLU:HB3	1.93	0.51
1:3A:155:ALA:HA	1:3A:164:ALA:HB1	1.93	0.51
2:3B:240:ARG:HG2	2:3B:242:GLY:H	1.75	0.51
3:3C:10:LEU:HD21	3:3P:195:VAL:HG13	1.93	0.51
5:3E:153:GLU:O	5:3E:155:LYS:NZ	2.43	0.51
1:3N:298:ALA:HA	1:3N:303:LEU:HB2	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:3E:241:SER:HA	5:3E:251:LYS:H	1.75	0.51
9:3J:53:TRP:HD1	9:3J:57:LYS:NZ	2.01	0.51
1:3N:15:GLN:OE1	1:3N:15:GLN:N	2.43	0.51
1:3N:67:THR:O	1:3N:69:ASN:N	2.44	0.51
5:3R:164:ASN:OD1	5:3R:177:ARG:HD3	2.11	0.51
1:3N:114:ALA:O	1:3N:118:GLN:HB2	2.11	0.51
11:3P:506:CDL:HA32	11:3Q:502:CDL:HB4	1.92	0.51
2:3B:137:VAL:O	2:3B:141:GLN:HG2	2.11	0.51
1:3N:354:VAL:HG21	1:3N:404:ALA:HA	1.93	0.51
8:3H:53:GLU:O	8:3H:57:LYS:HG2	2.11	0.51
1:3N:362:ARG:O	1:3N:366:VAL:HG22	2.11	0.51
3:3C:367:PRO:O	3:3C:371:ILE:HD13	2.11	0.50
1:3N:373:THR:OG1	1:3N:374:PRO:HD3	2.11	0.50
5:3R:115:TYR:CD1	17:3R:303:PC1:H143	2.44	0.50
8:3U:60:ASP:N	8:3U:60:ASP:OD1	2.44	0.50
2:3B:213:HIS:HD2	2:3B:217:LYS:HD2	1.75	0.50
5:3E:243:TYR:CE1	5:3E:258:LEU:HG	2.47	0.50
1:3N:58:PHE:HE2	1:3N:127:ILE:HG23	1.75	0.50
1:3N:192:ALA:HB2	1:3N:219:LEU:HB3	1.92	0.50
3:3P:342:PRO:HB2	3:3P:344:GLU:OE1	2.10	0.50
1:3N:142:ASP:OD2	5:3R:79:SER:N	2.45	0.50
4:3Q:180:SER:OG	8:3U:17:LEU:HB2	2.11	0.50
1:3A:280:TYR:HB3	1:3A:307:PHE:HE1	1.76	0.50
3:3C:324:LEU:HD12	3:3C:361:ILE:HG23	1.93	0.50
12:3D:502:3PE:H271	12:3D:502:3PE:H232	1.93	0.50
5:3E:150:SER:HB3	3:3P:168:PHE:HE1	1.76	0.50
1:3A:46:ARG:NH1	1:3A:316:GLU:OE2	2.41	0.50
7:3G:69:GLU:O	7:3G:73:ARG:HG2	2.12	0.50
2:3B:276:GLN:HB2	2:3B:322:PHE:HE1	1.77	0.50
3:3P:321:SER:OG	3:3P:373:GLU:OE2	2.28	0.50
3:3P:329:VAL:O	3:3P:333:ILE:HD12	2.12	0.50
5:3R:156:LEU:HD12	5:3R:157:SER:H	1.77	0.50
2:3B:334:GLY:HA2	2:3B:434:PRO:HD3	1.94	0.50
3:3C:211:ILE:HG21	6:3F:74:ILE:HG12	1.94	0.50
3:3C:315:MET:O	3:3C:322:GLN:NE2	2.45	0.50
4:3D:115:ARG:CZ	9:3J:60:TYR:CD1	2.94	0.50
1:3N:258:GLU:HG2	5:3R:104:LYS:HD2	1.94	0.50
1:3N:280:TYR:HB3	1:3N:307:PHE:CE1	2.47	0.50
3:3P:5:ARG:NH1	3:3P:20:ASP:OD2	2.45	0.50
4:3Q:54:VAL:HG21	4:3Q:192:TRP:NE1	2.26	0.50
5:3R:173:PRO:O	5:3R:215:GLY:N	2.45	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:3A:501:CDL:H512	12:3A:503:3PE:H331	1.94	0.49
5:3E:130:LYS:NZ	9:3J:33:GLU:OE2	2.42	0.49
8:3H:42:LEU:HD21	8:3H:46:ARG:NH2	2.27	0.49
5:3I:49:PHE:CB	5:3I:50:LEU:N	2.74	0.49
1:3N:24:ARG:NH2	1:3N:383:LEU:O	2.45	0.49
3:3P:31:TRP:HA	3:3P:100:ARG:HH11	1.77	0.49
3:3P:161:VAL:HG12	3:3P:165:TRP:CE3	2.46	0.49
4:3Q:186:VAL:HG21	15:3Q:501:HEC:HBB3	1.92	0.49
1:3A:137:GLU:HA	1:3A:140:GLU:HG2	1.93	0.49
4:3D:115:ARG:NE	9:3J:60:TYR:HE1	2.10	0.49
3:3P:344:GLU:HG2	7:3T:66:PHE:HE1	1.77	0.49
4:3Q:3:LEU:HD13	7:3T:70:LYS:HE3	1.94	0.49
2:3O:264:THR:HG22	2:3O:317:SER:HA	1.93	0.49
3:3P:244:LEU:HD21	4:3Q:204:MET:HB3	1.93	0.49
5:3R:249:ILE:HG23	5:3R:257:ASN:HA	1.93	0.49
8:3U:28:GLU:O	8:3U:32:LYS:HG2	2.12	0.49
3:3C:14:ILE:HG22	3:3C:19:ILE:HD13	1.94	0.49
3:3C:183:PHE:CE2	3:3P:183:PHE:HB3	2.47	0.49
7:3G:52:PRO:HA	7:3G:55:VAL:HG22	1.92	0.49
3:3P:240:LEU:HA	3:3P:243:VAL:HG12	1.94	0.49
5:3R:181:LYS:NZ	5:3R:185:ASP:HB3	2.24	0.49
1:3A:239:SER:OG	1:3A:240:GLU:N	2.45	0.49
1:3A:240:GLU:OE2	7:3G:19:SER:OG	2.31	0.49
1:3A:285:GLY:HA3	5:3I:70:LEU:HA	1.93	0.49
1:3N:144:SER:HA	5:3V:47:ARG:CZ	2.43	0.49
1:3N:171:SER:N	5:3R:82:ASP:OD1	2.43	0.49
2:3O:195:VAL:O	2:3O:199:PHE:HB2	2.13	0.49
1:3N:381:ARG:HG3	1:3N:381:ARG:HH11	1.78	0.49
3:3P:314:SER:OG	3:3P:315:MET:N	2.46	0.49
9:3J:9:ARG:H	9:3J:9:ARG:HD2	1.77	0.49
2:3O:366:ALA:O	2:3O:370:MET:HB2	2.13	0.49
3:3P:35:SER:HA	14:3P:503:U10:H121	1.93	0.49
4:3Q:228:SER:HB2	7:3T:23:GLN:OE1	2.13	0.49
1:3N:74:ALA:O	1:3N:78:GLU:HG3	2.13	0.49
10:3X:14:ALA:O	10:3X:18:ILE:HG12	2.12	0.49
12:3A:503:3PE:H222	12:3A:503:3PE:H2	1.57	0.49
3:3C:375:ASN:O	6:3F:29:ARG:NH1	2.46	0.49
4:3D:316:TRP:O	4:3D:320:LYS:HG2	2.12	0.49
2:3O:46:ARG:HE	2:3O:110:GLU:HG3	1.76	0.49
3:3P:149:LEU:HD22	3:3P:281:LEU:HD22	1.94	0.49
6:3S:64:ARG:HD2	6:3S:75:LEU:HD21	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3A:445:ARG:HH21	12:3A:503:3PE:H222	1.78	0.49
4:3D:150:LYS:O	4:3D:154:GLU:HG2	2.12	0.49
5:3R:154:ILE:HG23	5:3R:272:ILE:HD12	1.95	0.49
10:3X:48:ILE:HG22	10:3X:51:LYS:HD2	1.95	0.49
5:3E:174:LEU:HD23	5:3E:214:ILE:HA	1.95	0.48
5:3E:204:ARG:HH22	5:3E:248:ARG:HB2	1.77	0.48
4:3Q:230:LEU:HB3	6:3S:70:MET:SD	2.53	0.48
6:3S:40:ASP:O	6:3S:44:LYS:HG2	2.12	0.48
3:3C:163:TRP:CD2	12:3C:506:3PE:H342	2.49	0.48
3:3C:181:PHE:HA	3:3C:184:ILE:HG22	1.94	0.48
5:3E:218:THR:N	5:3E:243:TYR:OH	2.45	0.48
5:3E:250:ARG:HB3	5:3E:251:LYS:HD2	1.95	0.48
4:3Q:20:SER:HB2	4:3Q:199:ASP:OD1	2.13	0.48
1:3A:111:GLU:HB2	1:3A:215:HIS:CE1	2.49	0.48
2:3B:248:ASN:ND2	2:3B:250:ASP:OD2	2.47	0.48
3:3C:165:TRP:O	3:3C:174:THR:OG1	2.29	0.48
1:3N:106:LEU:HD21	1:3N:203:VAL:HG13	1.94	0.48
2:3O:99:THR:HA	5:3V:67:SER:HA	1.94	0.48
6:3S:35:ASP:OD2	6:3S:61:ARG:HD2	2.13	0.48
2:3B:70:ARG:HA	2:3B:98:VAL:HG11	1.95	0.48
2:3B:109:VAL:HG21	2:3B:123:LEU:HB2	1.95	0.48
5:3R:175:PHE:CE2	5:3R:215:GLY:HA2	2.47	0.48
5:3R:217:CYS:HB2	5:3R:224:PRO:HG3	1.96	0.48
8:3U:61:PHE:HD1	8:3U:62:LEU:HD23	1.78	0.48
5:3E:218:THR:HG21	5:3E:249:ILE:HG21	1.95	0.48
11:3G:102:CDL:H712	11:3G:102:CDL:H131	1.94	0.48
3:3P:15:ASN:HA	3:3P:19:ILE:HB	1.95	0.48
3:3P:328:LEU:HD11	3:3P:358:TYR:HD1	1.79	0.48
4:3Q:225:HIS:O	4:3Q:228:SER:OG	2.30	0.48
1:3A:312:ILE:O	1:3A:319:LEU:N	2.47	0.48
4:3D:159:GLN:HA	4:3D:170:MET:HA	1.94	0.48
6:3F:53:ASP:HA	6:3F:56:LYS:NZ	2.29	0.48
11:3G:102:CDL:HB32	11:3G:102:CDL:HB21	1.95	0.48
8:3H:52:ILE:O	8:3H:56:ILE:HG12	2.14	0.48
1:3N:68:LYS:HE2	1:3N:119:ASN:HB3	1.96	0.48
1:3N:181:ASP:OD1	1:3N:181:ASP:N	2.46	0.48
2:3O:365:LYS:HG2	2:3O:399:LEU:HD22	1.96	0.48
2:3B:227:ARG:HD3	2:3B:229:GLY:N	2.28	0.48
7:3G:57:PHE:HA	7:3G:60:VAL:HG12	1.96	0.48
11:3N:502:CDL:H312	11:3N:502:CDL:H121	1.94	0.48
2:3O:97:SER:HA	5:3V:69:GLY:HA2	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:3P:501:HEM:HBC2	13:3P:501:HEM:HMC1	1.96	0.48
7:3T:54:VAL:HA	7:3T:57:LEU:HD13	1.96	0.48
10:3X:4:ARG:HG3	10:3X:5:PHE:HD1	1.78	0.48
5:3E:164:ASN:HB3	5:3E:177:ARG:HG3	1.95	0.48
5:3E:178:HIS:ND1	5:3E:209:GLU:O	2.47	0.48
6:3F:51:GLU:HA	6:3F:55:VAL:HG11	1.96	0.48
2:3O:308:ASP:OD1	5:3V:55:LEU:HB3	2.13	0.48
2:3B:171:ALA:HB3	2:3B:237:ALA:HB2	1.94	0.48
3:3C:88:SER:O	3:3C:92:ILE:HG13	2.14	0.48
3:3C:113:TRP:O	3:3C:117:VAL:HG23	2.14	0.48
3:3C:362:ILE:HG22	3:3C:363:LEU:HD12	1.96	0.48
12:3C:506:3PE:H231	5:3R:137:VAL:HG11	1.95	0.48
4:3D:316:TRP:HD1	4:3D:320:LYS:HD3	1.79	0.48
5:3E:223:VAL:O	4:3Q:144:ARG:NH2	2.47	0.48
1:3N:237:THR:HG22	7:3T:18:LEU:HD11	1.96	0.48
2:3O:124:LEU:HD22	2:3O:224:LEU:CD2	2.44	0.48
5:3R:233:GLY:HA3	5:3R:245:ALA:HA	1.95	0.48
5:3E:120:THR:HA	5:3E:123:VAL:HG12	1.96	0.48
11:3N:502:CDL:H511	11:3N:502:CDL:H122	1.96	0.48
2:3O:99:THR:HG23	2:3O:106:ALA:HB3	1.95	0.48
2:3O:124:LEU:HD22	2:3O:224:LEU:HD23	1.95	0.48
5:3R:204:ARG:HG3	5:3R:248:ARG:HD2	1.95	0.48
1:3A:6:GLN:O	1:3A:10:SER:OG	2.22	0.47
4:3D:314:HIS:CD2	7:3G:22:PRO:HB2	2.49	0.47
5:3E:155:LYS:HD2	5:3E:167:PHE:CE2	2.49	0.47
2:3B:188:PRO:HA	2:3B:191:LEU:HD12	1.96	0.47
3:3C:89:MET:HG2	3:3C:235:MET:SD	2.54	0.47
3:3C:183:PHE:CD1	13:3C:501:HEM:HAC	2.49	0.47
5:3E:130:LYS:HB2	10:3Y:34:TRP:CH2	2.49	0.47
2:3O:218:GLN:O	2:3O:222:ARG:HB2	2.14	0.47
3:3P:59:THR:OG1	3:3P:172:LYS:HA	2.13	0.47
3:3P:119:LEU:O	3:3P:123:VAL:HG12	2.14	0.47
5:3R:219:HIS:CE1	5:3R:239:HIS:ND1	2.82	0.47
4:3D:159:GLN:HB2	4:3D:170:MET:HG3	1.96	0.47
3:3P:108:MET:SD	3:3P:308:HIS:ND1	2.87	0.47
10:3Y:9:ARG:HA	10:3Y:12:GLU:OE1	2.14	0.47
2:3B:223:PHE:HB2	2:3B:224:LEU:HD12	1.96	0.47
3:3C:105:GLY:HA3	3:3C:313:ARG:HG2	1.95	0.47
4:3D:109:LEU:HD21	4:3D:280:ARG:HG3	1.96	0.47
5:3E:199:GLN:HB2	5:3E:204:ARG:HH11	1.79	0.47
7:3G:65:THR:O	7:3G:69:GLU:HG2	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3P:146:ILE:O	3:3P:149:LEU:HB3	2.13	0.47
5:3R:179:ARG:NH1	5:3R:184:ILE:HG12	2.29	0.47
5:3R:235:TYR:HE1	5:3R:240:GLY:HA2	1.79	0.47
5:3V:53:GLU:N	5:3V:53:GLU:OE1	2.46	0.47
3:3C:26:ASN:ND2	3:3C:207:ASN:HB2	2.30	0.47
5:3E:119:ALA:HB2	9:3J:21:PHE:HE1	1.80	0.47
5:3I:63:PRO:O	5:3I:77:ARG:NH2	2.47	0.47
9:3J:52:LEU:HD22	9:3J:55:HIS:HE1	1.80	0.47
3:3P:120:LEU:O	3:3P:124:MET:HB2	2.14	0.47
3:3P:231:GLY:HA2	11:3Q:502:CDL:H751	1.96	0.47
5:3R:93:ARG:HD2	5:3R:110:ARG:HD2	1.94	0.47
8:3U:35:GLU:O	8:3U:38:GLU:HG2	2.14	0.47
10:3X:1:MET:HB3	10:3X:2:LEU:H	1.58	0.47
3:3C:30:TRP:HB3	3:3C:100:ARG:HG3	1.96	0.47
5:3E:235:TYR:HA	5:3E:243:TYR:HB2	1.97	0.47
5:3I:36:ALA:HB3	5:3I:73:PRO:HG2	1.96	0.47
3:3P:186:PRO:HG2	13:3P:501:HEM:HHC	1.96	0.47
5:3R:192:VAL:HG12	5:3R:198:PRO:HB3	1.96	0.47
8:3U:38:GLU:HA	8:3U:41:ASP:OD2	2.14	0.47
1:3A:192:ALA:HB2	1:3A:219:LEU:HG	1.97	0.47
2:3B:56:ARG:HD2	2:3B:103:GLU:HG2	1.97	0.47
3:3C:19:ILE:HA	3:3C:221:HIS:HB2	1.96	0.47
3:3C:212:SER:OG	6:3F:51:GLU:OE1	2.27	0.47
5:3E:153:GLU:HG2	5:3E:169:TRP:CD2	2.49	0.47
5:3E:243:TYR:CZ	5:3E:258:LEU:HG	2.49	0.47
9:3J:23:LEU:HD12	9:3J:23:LEU:HA	1.77	0.47
1:3N:343:MET:O	1:3N:347:THR:N	2.46	0.47
5:3R:235:TYR:CE1	5:3R:240:GLY:HA2	2.50	0.47
6:3S:80:TRP:O	6:3S:82:LYS:HD3	2.13	0.47
1:3A:311:ASN:OD1	1:3A:320:LEU:HD12	2.15	0.47
4:3D:248:ALA:HB3	15:3D:501:HEC:HBD2	1.97	0.47
8:3H:87:LEU:O	8:3H:90:ARG:N	2.48	0.47
1:3N:431:LEU:HD12	1:3N:432:PRO:HD2	1.97	0.47
3:3P:81:TYR:OH	4:3Q:118:ARG:NH1	2.34	0.47
4:3Q:7:ALA:HA	4:3Q:152:TYR:HE2	1.79	0.47
4:3Q:203:ARG:HB2	9:3W:43:TYR:CE2	2.50	0.47
5:3R:154:ILE:O	5:3R:155:LYS:HD3	2.14	0.47
2:3B:49:LEU:HD13	2:3B:206:LEU:HD13	1.95	0.47
1:3A:175:ARG:HB2	1:3A:176:LYS:NZ	2.30	0.47
1:3A:313:CYS:HA	1:3A:318:GLY:HA3	1.97	0.47
3:3C:227:LYS:HB2	4:3D:316:TRP:CH2	2.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3C:379:TRP:CH2	6:3F:49:ILE:HB	2.49	0.47
5:3E:159:ILE:HG22	5:3E:159:ILE:O	2.15	0.47
1:3N:25:VAL:HG22	1:3N:197:LEU:HB3	1.97	0.47
1:3N:244:ARG:HD3	7:3T:10:MET:HB2	1.97	0.47
1:3A:241:ILE:HD11	5:3E:85:VAL:HG22	1.97	0.46
2:3B:195:VAL:O	2:3B:199:PHE:HB2	2.15	0.46
5:3E:183:GLU:O	5:3E:187:GLU:HG2	2.15	0.46
1:3N:196:VAL:HG21	1:3N:383:LEU:HB3	1.98	0.46
3:3P:168:PHE:HB3	3:3P:169:SER:H	1.50	0.46
7:3G:5:GLU:OE2	7:3G:5:GLU:N	2.48	0.46
1:3N:356:ARG:HG3	2:3O:91:ALA:HA	1.97	0.46
2:3O:70:ARG:HD3	2:3O:100:SER:HB3	1.97	0.46
3:3P:32:ASN:ND2	11:3Q:502:CDL:H721	2.30	0.46
8:3U:20:VAL:HA	8:3U:23:GLN:HE22	1.79	0.46
17:3X:101:PC1:H32	17:3X:101:PC1:H321	1.42	0.46
4:3D:108:SER:N	9:3J:48:ASN:OD1	2.48	0.46
4:3D:252:PRO:HB3	15:3D:501:HEC:CHC	2.44	0.46
5:3E:174:LEU:HD11	5:3E:273:VAL:HG21	1.96	0.46
6:3F:33:TYR:HE2	6:3F:95:TYR:HA	1.80	0.46
4:3Q:206:LEU:O	4:3Q:210:MET:HG3	2.16	0.46
1:3A:76:GLU:OE1	2:3B:289:SER:N	2.45	0.46
1:3A:420:PRO:O	1:3A:434:TYR:OH	2.18	0.46
5:3E:212:ILE:HD12	5:3E:212:ILE:O	2.15	0.46
4:3Q:93:LYS:NZ	4:3Q:96:PRO:O	2.47	0.46
10:3Y:4:ARG:HH21	10:3Y:5:PHE:HE1	1.63	0.46
3:3C:186:PRO:HG2	13:3C:501:HEM:HMC1	1.97	0.46
5:3I:42:VAL:C	5:3I:44:ASP:H	2.18	0.46
2:3O:94:GLY:CA	2:3O:111:CYS:HB2	2.46	0.46
3:3P:173:ALA:O	3:3P:177:ARG:HG2	2.16	0.46
2:3B:52:LYS:HB2	2:3B:387:LEU:HD22	1.98	0.46
2:3B:111:CYS:SG	2:3B:112:LEU:N	2.89	0.46
2:3B:218:GLN:O	2:3B:221:GLU:HG3	2.15	0.46
3:3P:379:TRP:CZ3	6:3S:37:ILE:HD13	2.50	0.46
4:3D:186:PRO:O	4:3D:190:ARG:HG3	2.15	0.46
2:3O:62:ASN:HA	2:3O:182:ARG:HH21	1.81	0.46
3:3P:152:ALA:HB2	3:3P:287:LYS:HB3	1.97	0.46
6:3S:109:LYS:N	10:3Y:9:ARG:HH12	2.13	0.46
1:3N:97:TYR:HH	1:3N:190:TYR:HH	1.51	0.46
1:3A:40:TRP:CZ2	1:3A:377:GLU:HA	2.51	0.46
1:3A:268:VAL:HG13	1:3A:399:ILE:HD13	1.98	0.46
3:3C:172:LYS:O	3:3C:176:THR:HG22	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3D:255:ASN:O	4:3D:256:GLU:HG3	2.16	0.46
9:3J:53:TRP:CG	9:3J:57:LYS:HE3	2.46	0.46
2:3O:31:ASN:HD22	2:3O:201:SER:HB3	1.80	0.46
3:3P:244:LEU:HD12	4:3Q:201:ARG:HG3	1.96	0.46
4:3Q:86:LYS:HB3	4:3Q:86:LYS:HE3	1.75	0.46
2:3B:123:LEU:HG	2:3B:124:LEU:HD22	1.98	0.46
4:3D:258:LEU:HD12	4:3D:258:LEU:HA	1.78	0.46
4:3D:290:ARG:O	4:3D:293:MET:HB2	2.15	0.46
1:3N:436:ARG:HD3	3:3P:222:PRO:HD3	1.97	0.46
3:3P:315:MET:O	3:3P:322:GLN:NE2	2.43	0.46
5:3R:167:PHE:O	5:3R:173:PRO:HA	2.16	0.46
5:3R:178:HIS:CD2	5:3R:210:TRP:HE1	2.33	0.46
1:3A:445:ARG:NH2	12:3A:503:3PE:H2	2.31	0.45
4:3D:218:LEU:HD23	4:3D:219:LEU:HD23	1.98	0.45
5:3E:216:VAL:HG21	3:3P:262:LEU:HD22	1.98	0.45
5:3I:64:LEU:HA	5:3I:77:ARG:O	2.16	0.45
9:3J:30:LEU:HD21	10:3Y:34:TRP:HB2	1.97	0.45
1:3N:76:GLU:OE1	2:3O:290:ASN:N	2.48	0.45
2:3O:266:SER:OG	2:3O:268:GLU:OE1	2.22	0.45
5:3V:77:ARG:HE	5:3V:77:ARG:C	2.19	0.45
2:3B:153:GLN:HB3	5:3I:46:LYS:HE3	1.97	0.45
5:3E:179:ARG:HB2	5:3E:211:VAL:HG12	1.99	0.45
8:3H:91:ASP:N	8:3H:91:ASP:OD1	2.49	0.45
5:3R:197:ASP:OD1	5:3R:197:ASP:N	2.49	0.45
5:3R:213:LEU:HD11	5:3R:234:TYR:HE2	1.81	0.45
1:3N:231:PHE:HZ	1:3N:316:GLU:HB3	1.81	0.45
4:3Q:75:ASN:HB3	4:3Q:79:GLU:H	1.79	0.45
4:3D:163:ASN:OD1	4:3D:167:GLU:HG3	2.16	0.45
5:3E:125:VAL:HG11	17:3E:302:PC1:H381	1.99	0.45
6:3F:53:ASP:OD1	6:3F:56:LYS:NZ	2.48	0.45
6:3F:65:ASN:OD1	6:3F:65:ASN:N	2.42	0.45
8:3H:45:VAL:HG12	8:3H:94:VAL:HG22	1.98	0.45
1:3N:358:LYS:O	1:3N:362:ARG:HG3	2.16	0.45
2:3O:24:LEU:HD11	2:3O:36:ALA:HB1	1.97	0.45
4:3Q:218:LEU:HD13	5:3R:120:THR:HG22	1.99	0.45
1:3A:58:PHE:CE2	1:3A:127:ILE:HG23	2.51	0.45
12:3C:505:3PE:H12	11:3G:102:CDL:OB4	2.15	0.45
5:3E:196:ARG:N	5:3E:250:ARG:O	2.48	0.45
5:3E:223:VAL:HB	4:3Q:107:GLY:HA3	1.99	0.45
6:3F:33:TYR:CE2	6:3F:95:TYR:HA	2.52	0.45
1:3N:184:GLU:OE1	1:3N:184:GLU:N	2.50	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3P:31:TRP:HA	3:3P:100:ARG:NH1	2.31	0.45
3:3P:328:LEU:HD11	3:3P:358:TYR:CD1	2.52	0.45
5:3R:119:ALA:HB2	9:3W:20:PHE:CE1	2.51	0.45
5:3R:177:ARG:O	5:3R:210:TRP:HA	2.16	0.45
9:3W:18:SER:HB3	10:3X:24:TRP:CE2	2.52	0.45
1:3A:240:GLU:HB2	1:3A:422:VAL:HB	1.99	0.45
1:3A:279:HIS:ND1	5:3I:35:PRO:HB3	2.31	0.45
11:3A:501:CDL:H331	11:3A:501:CDL:H372	1.98	0.45
2:3B:115:ASP:OD1	2:3B:115:ASP:N	2.49	0.45
2:3B:160:LEU:HD13	5:3I:64:LEU:HB3	1.97	0.45
3:3C:116:GLY:C	13:3C:502:HEM:HBC2	2.36	0.45
11:3P:506:CDL:HB32	7:3T:44:CYS:SG	2.56	0.45
4:3Q:113:LEU:HA	4:3Q:116:ILE:HB	1.98	0.45
1:3A:39:VAL:HG23	1:3A:113:LEU:HD13	1.98	0.45
1:3A:149:VAL:HG21	1:3A:252:HIS:HB3	1.98	0.45
1:3A:353:GLU:HG2	1:3A:356:ARG:NH2	2.32	0.45
3:3C:110:LEU:HD12	3:3C:110:LEU:H	1.82	0.45
4:3D:290:ARG:HA	4:3D:293:MET:HB2	1.99	0.45
1:3N:46:ARG:HH21	1:3N:163:LEU:HD11	1.81	0.45
2:3O:200:THR:O	2:3O:204:MET:HG2	2.17	0.45
3:3P:113:TRP:O	3:3P:117:VAL:HG23	2.17	0.45
3:3P:223:TYR:HB3	4:3Q:227:TRP:NE1	2.32	0.45
6:3S:107:TRP:O	10:3Y:9:ARG:NH1	2.50	0.45
8:3U:37:LEU:HD23	8:3U:37:LEU:HA	1.83	0.45
10:3X:38:TRP:CD2	17:3X:101:PC1:H331	2.52	0.45
2:3B:154:ASN:HD22	2:3B:156:GLN:H	1.64	0.45
4:3D:190:ARG:O	4:3D:195:GLY:N	2.42	0.45
1:3N:355:VAL:HA	1:3N:358:LYS:HD3	1.99	0.45
1:3N:146:ARG:O	1:3N:149:VAL:HG12	2.16	0.45
3:3P:58:ASP:OD1	3:3P:60:THR:N	2.46	0.45
3:3P:78:VAL:O	3:3P:82:LEU:HB2	2.17	0.45
5:3R:107:SER:HB2	5:3R:111:LYS:HZ1	1.81	0.45
5:3R:258:LEU:HD12	5:3R:258:LEU:HA	1.82	0.45
2:3B:120:MET:O	2:3B:124:LEU:N	2.43	0.45
3:3C:229:ILE:HD12	17:3E:302:PC1:H372	1.99	0.45
17:3E:302:PC1:H111	17:3E:302:PC1:H11	2.00	0.45
1:3N:294:LEU:HB2	1:3N:341:GLN:HG3	1.98	0.45
3:3P:25:SER:HB3	3:3P:216:ASP:O	2.17	0.45
7:3G:36:ILE:HD13	7:3G:36:ILE:HA	1.88	0.44
8:3H:59:ARG:HE	8:3H:59:ARG:HB3	1.56	0.44
1:3N:435:ASN:ND2	3:3P:223:TYR:OH	2.37	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:3P:504:U10:H3M3	14:3P:504:U10:C4M	2.33	0.44
5:3R:159:ILE:HD12	5:3R:160:PRO:HD2	1.98	0.44
5:3R:230:ASP:OD1	5:3R:231:PHE:N	2.46	0.44
1:3A:363:ASN:ND2	2:3B:92:VAL:O	2.49	0.44
2:3B:61:ASN:OD1	2:3B:61:ASN:N	2.50	0.44
2:3B:68:LEU:O	2:3B:72:ALA:N	2.50	0.44
2:3O:75:LEU:HD23	2:3O:136:GLU:HB2	1.99	0.44
3:3P:124:MET:HE2	3:3P:124:MET:HB3	1.91	0.44
3:3P:344:GLU:HG2	7:3T:66:PHE:CE1	2.52	0.44
1:3A:322:ALA:HB3	1:3A:338:LEU:HD21	1.99	0.44
2:3B:394:GLN:O	2:3B:397:THR:OG1	2.34	0.44
5:3E:263:TYR:HE1	5:3E:265:PHE:HB2	1.82	0.44
6:3F:51:GLU:HA	6:3F:55:VAL:CG1	2.48	0.44
2:3O:36:ALA:HB3	2:3O:207:ILE:HG13	2.00	0.44
14:3P:503:U10:H1M1	14:3P:503:U10:H72	1.67	0.44
5:3V:55:LEU:HD23	5:3V:55:LEU:HA	1.81	0.44
1:3A:316:GLU:HG2	1:3A:317:THR:HG22	1.99	0.44
1:3A:329:MET:HA	1:3A:430:GLN:HE22	1.82	0.44
1:3A:445:ARG:HH22	12:3A:503:3PE:P	2.40	0.44
3:3C:114:ASN:O	3:3C:118:VAL:HG23	2.17	0.44
3:3C:376:LEU:HD21	6:3F:28:ILE:HG22	2.00	0.44
5:3E:197:ASP:OD1	5:3E:248:ARG:HG3	2.17	0.44
9:3J:30:LEU:CD2	10:3Y:34:TRP:HB2	2.47	0.44
3:3P:162:GLU:OE2	3:3P:167:GLY:HA2	2.17	0.44
4:3Q:70:VAL:HG11	4:3Q:89:ASP:OD2	2.17	0.44
5:3R:168:LYS:H	5:3R:168:LYS:HG2	1.69	0.44
6:3S:47:ILE:HD12	6:3S:47:ILE:H	1.81	0.44
4:3D:326:TYR:HB2	6:3F:72:PHE:CZ	2.51	0.44
5:3E:111:LYS:NZ	9:3J:11:TYR:OH	2.51	0.44
5:3E:182:LYS:HA	5:3E:185:ASP:OD2	2.17	0.44
7:3G:55:VAL:O	7:3G:59:LEU:HG	2.18	0.44
1:3N:194:ARG:H	1:3N:194:ARG:HG2	1.58	0.44
5:3R:201:ASP:HA	5:3R:204:ARG:HB2	1.99	0.44
1:3A:240:GLU:HA	1:3A:422:VAL:O	2.17	0.44
2:3B:123:LEU:O	2:3B:126:VAL:HG12	2.17	0.44
1:3N:303:LEU:HD23	1:3N:303:LEU:HA	1.83	0.44
1:3A:125:SER:O	1:3A:129:LYS:NZ	2.42	0.44
2:3B:58:GLU:OE2	2:3B:65:THR:N	2.50	0.44
2:3B:141:GLN:HE22	2:3B:186:VAL:HB	1.82	0.44
3:3C:308:HIS:CE1	3:3C:313:ARG:HA	2.53	0.44
5:3E:269:ASP:O	5:3E:270:LEU:HD23	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3N:296:SER:O	1:3N:300:THR:OG1	2.33	0.44
4:3Q:231:LYS:NZ	11:3Q:502:CDL:O1	2.45	0.44
5:3R:153:GLU:O	5:3R:155:LYS:HE2	2.17	0.44
5:3V:62:ARG:HG2	5:3V:77:ARG:CZ	2.48	0.44
1:3A:14:THR:HG22	1:3A:28:GLU:HG3	2.00	0.44
1:3A:27:SER:HB2	1:3A:208:LEU:HD22	1.99	0.44
1:3A:264:ASN:O	1:3A:266:ASP:N	2.51	0.44
3:3C:65:SER:O	3:3C:69:ILE:HG13	2.18	0.44
4:3D:174:LYS:HD3	4:3D:174:LYS:HA	1.76	0.44
5:3E:196:ARG:HA	5:3E:196:ARG:HD2	1.77	0.44
5:3R:195:LEU:HD23	5:3R:196:ARG:N	2.33	0.44
5:3R:213:LEU:HA	5:3R:261:PRO:HD3	1.99	0.44
10:3X:18:ILE:O	10:3X:22:SER:HB3	2.18	0.44
1:3A:237:THR:HG22	7:3G:20:LEU:HD11	1.98	0.44
5:3E:145:ASP:O	5:3E:149:MET:HB2	2.18	0.44
2:3B:338:LYS:HE2	2:3B:338:LYS:HB2	1.84	0.43
3:3C:229:ILE:HG23	17:3E:302:PC1:H3A1	2.00	0.43
6:3F:91:GLN:OE1	6:3F:91:GLN:N	2.36	0.43
8:3H:40:ASP:HB3	8:3H:43:THR:HG22	2.00	0.43
1:3N:439:SER:HA	1:3N:442:PHE:CE2	2.53	0.43
3:3P:146:ILE:HD12	14:3P:504:U10:H4M2	1.99	0.43
3:3P:185:LEU:HD23	3:3P:185:LEU:HA	1.88	0.43
7:3T:64:GLN:HA	7:3T:67:GLU:HG3	1.99	0.43
3:3C:5:ARG:HD2	3:3C:19:ILE:HG21	2.01	0.43
4:3D:193:ASN:HD22	15:3D:501:HEC:HMD3	1.84	0.43
5:3E:249:ILE:HG23	5:3E:257:ASN:HA	2.00	0.43
6:3F:55:VAL:O	6:3F:59:ILE:HG13	2.18	0.43
3:3P:104:TYR:O	3:3P:206:ASN:ND2	2.52	0.43
1:3A:214:LYS:HG2	1:3A:215:HIS:CD2	2.53	0.43
1:3A:303:LEU:HG	1:3A:330:SER:HB2	2.00	0.43
3:3C:44:GLN:OE1	3:3C:87:ALA:N	2.51	0.43
5:3I:42:VAL:C	5:3I:44:ASP:N	2.72	0.43
1:3N:145:MET:HG3	1:3N:425:LEU:HD23	1.99	0.43
2:3O:68:LEU:O	2:3O:72:ALA:N	2.51	0.43
3:3P:26:ASN:HD21	6:3S:66:LEU:HD22	1.84	0.43
5:3R:156:LEU:HD12	5:3R:157:SER:N	2.34	0.43
1:3A:163:LEU:HD23	1:3A:163:LEU:HA	1.76	0.43
4:3D:212:GLU:CD	4:3D:280:ARG:HE	2.21	0.43
5:3E:192:VAL:HG11	5:3E:200:HIS:HA	2.01	0.43
1:3N:223:TYR:CD2	1:3N:228:VAL:HG12	2.53	0.43
4:3Q:20:SER:HB3	9:3W:47:ASN:ND2	2.34	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:3R:161:GLU:HA	5:3R:178:HIS:CG	2.53	0.43
5:3R:212:ILE:HG21	5:3R:263:TYR:HB3	2.00	0.43
9:3W:53:LYS:HA	9:3W:56:LYS:NZ	2.33	0.43
3:3C:302:ILE:O	3:3C:305:PRO:HD2	2.19	0.43
4:3D:212:GLU:HG2	4:3D:280:ARG:HB2	2.00	0.43
5:3E:241:SER:HA	5:3E:251:LYS:N	2.33	0.43
6:3F:117:GLU:OE1	10:3X:4:ARG:HB2	2.19	0.43
1:3N:77:LYS:HE3	1:3N:77:LYS:HB2	1.58	0.43
4:3Q:204:MET:HG2	12:3R:302:3PE:H2	2.01	0.43
5:3R:131:ASN:OD1	12:3R:302:3PE:H12	2.18	0.43
3:3C:85:ASN:HD22	3:3C:242:LEU:HB3	1.83	0.43
1:3N:50:GLU:OE2	5:3R:84:ARG:NH2	2.51	0.43
1:3N:238:GLY:O	7:3T:19:SER:HB2	2.18	0.43
1:3N:240:GLU:CD	1:3N:242:ARG:HE	2.21	0.43
1:3N:327:ASP:OD1	1:3N:330:SER:OG	2.20	0.43
12:3R:302:3PE:H231	12:3R:302:3PE:H272	2.01	0.43
1:3A:236:PHE:HB2	1:3A:258:GLU:OE1	2.19	0.43
1:3A:382:SER:HA	1:3A:386:TYR:HD2	1.83	0.43
3:3C:37:LEU:O	3:3C:41:LEU:N	2.52	0.43
4:3D:116:ARG:NE	4:3D:274:ASP:OD2	2.48	0.43
4:3D:118:PHE:CZ	4:3D:139:LEU:HD11	2.54	0.43
5:3E:196:ARG:O	5:3E:196:ARG:NH1	2.47	0.43
1:3N:280:TYR:HA	1:3N:284:TYR:CE2	2.53	0.43
1:3N:369:LEU:HD23	1:3N:369:LEU:HA	1.79	0.43
2:3O:68:LEU:HD13	2:3O:144:LEU:HD11	2.00	0.43
2:3O:151:ALA:O	2:3O:154:ASN:ND2	2.50	0.43
3:3P:287:LYS:O	3:3P:291:VAL:HG23	2.18	0.43
8:3U:52:GLU:H	8:3U:52:GLU:HG2	1.65	0.43
1:3A:258:GLU:HG2	5:3E:104:LYS:HD2	2.00	0.43
1:3A:277:ILE:HB	1:3A:309:THR:HG21	2.01	0.43
3:3C:45:ILE:HA	13:3C:501:HEM:HMC3	2.00	0.43
3:3C:201:HIS:CD2	14:3C:503:U10:H4M1	2.54	0.43
4:3D:252:PRO:HB2	4:3D:253:ILE:HG23	2.01	0.43
1:3N:242:ARG:NH2	1:3N:433:ASP:HA	2.33	0.43
11:3P:506:CDL:H1	11:3P:506:CDL:H521	1.99	0.43
11:3P:506:CDL:HB62	11:3P:506:CDL:H712	1.33	0.43
5:3R:181:LYS:NZ	5:3R:181:LYS:O	2.50	0.43
8:3U:72:LYS:HB2	8:3U:72:LYS:HE2	1.80	0.43
2:3B:155:PRO:O	2:3B:159:VAL:HG23	2.19	0.43
3:3C:67:THR:HG23	3:3C:71:ARG:HH11	1.84	0.43
3:3C:304:MET:HE1	3:3C:362:ILE:HG23	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3D:115:ARG:CD	9:3J:60:TYR:OH	2.66	0.43
5:3E:264:GLU:O	5:3E:271:VAL:HA	2.19	0.43
1:3N:188:GLN:HE22	1:3N:227:ALA:HB3	1.84	0.43
1:3N:270:LEU:HD13	1:3N:320:LEU:HD22	2.00	0.43
3:3P:47:THR:O	3:3P:51:LEU:HD12	2.19	0.43
4:3Q:33:TYR:CE1	4:3Q:43:MET:HG3	2.54	0.43
4:3Q:206:LEU:HD11	9:3W:42:ILE:HG22	2.01	0.43
6:3F:26:GLU:OE1	6:3F:26:GLU:N	2.50	0.43
6:3F:40:LYS:O	6:3F:87:LEU:HB3	2.19	0.43
7:3G:70:LYS:HB3	7:3G:70:LYS:HE3	1.85	0.43
2:3O:53:ALA:HB1	2:3O:194:TYR:HE1	1.84	0.43
3:3P:32:ASN:ND2	3:3P:231:GLY:HA3	2.29	0.43
10:3X:38:TRP:HA	17:3X:101:PC1:H11	2.01	0.43
1:3A:344:ARG:NH2	1:3A:353:GLU:OE2	2.52	0.42
3:3C:103:TYR:CE2	12:3C:505:3PE:H222	2.55	0.42
13:3C:501:HEM:O1D	13:3C:501:HEM:HHA	2.19	0.42
4:3D:284:GLU:OE2	4:3D:287:HIS:ND1	2.51	0.42
1:3N:136:GLN:O	1:3N:140:GLU:HG3	2.19	0.42
1:3N:240:GLU:OE2	1:3N:242:ARG:NE	2.50	0.42
2:3O:87:ARG:HA	2:3O:87:ARG:HD3	1.58	0.42
4:3Q:126:TYR:OH	15:3Q:501:HEC:O2A	2.31	0.42
6:3S:108:ALA:C	10:3Y:9:ARG:HH12	2.23	0.42
10:3Y:39:ARG:O	10:3Y:43:ASP:HB2	2.18	0.42
1:3A:172:GLU:O	1:3A:176:LYS:NZ	2.49	0.42
1:3A:238:GLY:N	7:3G:24:GLU:OE1	2.51	0.42
2:3B:102:ARG:HH12	2:3B:175:SER:HA	1.84	0.42
3:3C:77:TRP:CZ3	4:3D:290:ARG:HG3	2.53	0.42
3:3C:270:PRO:HD2	3:3C:275:LEU:HD23	2.02	0.42
3:3P:229:ILE:HG23	17:3R:303:PC1:H381	2.00	0.42
4:3Q:22:ASP:HB3	4:3Q:25:SER:HB3	2.02	0.42
5:3R:244:ASP:H	5:3R:249:ILE:HA	1.83	0.42
7:3T:32:LYS:HE3	7:3T:32:LYS:HB2	1.79	0.42
10:3X:12:GLU:O	10:3X:16:ASN:ND2	2.47	0.42
2:3B:369:LEU:HD21	2:3B:399:LEU:HD11	2.01	0.42
1:3N:392:LEU:HD12	1:3N:392:LEU:H	1.84	0.42
2:3O:35:ILE:HD12	2:3O:206:LEU:HB3	2.00	0.42
3:3P:124:MET:HE1	14:3P:504:U10:C2	2.49	0.42
4:3Q:33:TYR:CD1	4:3Q:37:CYS:HB3	2.54	0.42
10:3Y:38:TRP:O	10:3Y:42:LEU:HB2	2.20	0.42
1:3A:3:THR:O	1:3A:5:ALA:N	2.50	0.42
1:3A:301:ARG:NH2	1:3A:333:ASP:OD2	2.52	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3C:5:ARG:NH1	3:3C:20:ASP:OD2	2.52	0.42
3:3C:197:LEU:HD22	14:3C:503:U10:H161	2.01	0.42
1:3N:343:MET:HG3	1:3N:443:TRP:CD1	2.54	0.42
3:3P:215:MET:HB2	7:3T:10:MET:SD	2.58	0.42
3:3P:237:LEU:HB2	4:3Q:212:MET:HE1	2.01	0.42
3:3P:357:LEU:O	3:3P:361:ILE:HG13	2.19	0.42
4:3Q:29:GLY:HA2	4:3Q:32:VAL:HG12	2.01	0.42
5:3R:179:ARG:NH2	5:3R:205:VAL:HG11	2.34	0.42
6:3S:61:ARG:HG3	6:3S:64:ARG:HH21	1.84	0.42
9:3W:18:SER:HB3	10:3X:24:TRP:NE1	2.35	0.42
2:3B:327:ILE:HD11	5:3I:58:GLN:HB2	2.01	0.42
2:3B:340:ALA:O	2:3B:344:VAL:HG23	2.19	0.42
3:3C:234:PHE:O	3:3C:238:ILE:HG12	2.20	0.42
1:3N:361:LEU:O	1:3N:365:LEU:HG	2.19	0.42
3:3P:91:PHE:HZ	3:3P:124:MET:HA	1.84	0.42
4:3Q:166:ASN:ND2	8:3U:15:ASP:HB2	2.35	0.42
5:3R:101:LYS:HE3	5:3R:101:LYS:HB3	1.84	0.42
8:3U:21:ARG:HE	8:3U:69:VAL:HG21	1.84	0.42
1:3A:280:TYR:HB3	1:3A:307:PHE:CE1	2.54	0.42
1:3A:329:MET:HA	1:3A:430:GLN:NE2	2.34	0.42
4:3D:129:HIS:NE2	4:3D:198:PRO:HB3	2.34	0.42
5:3E:167:PHE:HB2	5:3E:174:LEU:HB2	2.02	0.42
6:3F:44:MET:HE1	6:3F:99:LYS:HG2	2.02	0.42
1:3N:436:ARG:HA	1:3N:436:ARG:HD2	1.84	0.42
2:3O:25:GLU:HB2	2:3O:213:HIS:ND1	2.34	0.42
4:3Q:226:LYS:HD3	4:3Q:226:LYS:HA	1.86	0.42
1:3A:58:PHE:HE2	1:3A:127:ILE:HG23	1.85	0.42
5:3E:173:PRO:O	5:3E:215:GLY:N	2.36	0.42
6:3F:110:ILE:HD13	6:3F:110:ILE:HA	1.89	0.42
3:3P:282:ARG:NH2	3:3P:339:GLY:O	2.47	0.42
4:3Q:21:LEU:HD21	4:3Q:198:HIS:CG	2.54	0.42
4:3D:137:ARG:O	4:3D:140:VAL:HG12	2.20	0.42
1:3A:99:ILE:HD11	1:3A:109:ALA:HB1	2.01	0.42
11:3A:501:CDL:H712	11:3A:501:CDL:HB62	1.58	0.42
3:3C:12:LYS:HB2	3:3C:12:LYS:HE3	1.84	0.42
2:3O:95:LYS:HG3	2:3O:110:GLU:OE2	2.20	0.42
2:3O:215:VAL:O	2:3O:219:VAL:HG13	2.20	0.42
3:3P:296:ALA:HA	3:3P:299:LEU:HB2	2.01	0.42
5:3R:179:ARG:HG2	5:3R:183:GLU:HG3	2.02	0.42
1:3A:53:ASN:HD22	1:3A:170:PRO:HD3	1.85	0.42
12:3A:503:3PE:N	3:3C:3:ASN:HA	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3B:45:SER:HB2	2:3B:116:ILE:HG21	2.01	0.42
4:3D:163:ASN:OD1	4:3D:166:GLY:N	2.52	0.42
3:3P:338:ILE:HD13	3:3P:338:ILE:HA	1.84	0.42
12:3A:502:3PE:H222	12:3A:502:3PE:H2	1.39	0.41
3:3C:25:SER:OG	3:3C:216:ASP:OD1	2.24	0.41
5:3E:88:PHE:O	5:3E:92:ARG:HG2	2.20	0.41
1:3N:111:GLU:HB2	1:3N:215:HIS:NE2	2.35	0.41
1:3N:235:ARG:NH1	5:3R:99:SER:HA	2.34	0.41
5:3R:179:ARG:HE	5:3R:211:VAL:CG2	2.33	0.41
7:3T:24:ARG:HA	7:3T:24:ARG:HD2	1.85	0.41
1:3A:86:LEU:HD12	1:3A:87:ASN:N	2.35	0.41
2:3B:334:GLY:O	2:3B:338:LYS:HD3	2.20	0.41
8:3H:87:LEU:HD13	8:3H:87:LEU:HA	1.86	0.41
1:3N:48:GLU:OE2	1:3N:55:ALA:N	2.53	0.41
3:3P:165:TRP:HE1	3:3P:170:VAL:N	2.19	0.41
6:3S:98:ILE:HD13	6:3S:98:ILE:HA	1.84	0.41
2:3B:46:ARG:NH2	2:3B:110:GLU:HG3	2.35	0.41
2:3B:124:LEU:HD11	2:3B:224:LEU:HD11	2.02	0.41
5:3E:157:SER:N	5:3E:269:ASP:HB3	2.35	0.41
5:3E:232:GLY:HA3	5:3E:245:ALA:HB2	2.02	0.41
8:3H:83:LEU:HD13	8:3H:87:LEU:HD23	2.01	0.41
1:3N:294:LEU:HD23	1:3N:337:PHE:HB3	2.02	0.41
4:3Q:237:TYR:HB2	6:3S:60:PHE:CE1	2.55	0.41
5:3R:262:THR:O	5:3R:262:THR:OG1	2.36	0.41
1:3N:57:TYR:OH	1:3N:137:GLU:OE1	2.39	0.41
1:3N:346:CYS:SG	1:3N:416:TYR:HB2	2.60	0.41
2:3O:46:ARG:HB2	2:3O:379:LEU:HD22	2.03	0.41
2:3O:395:PRO:O	2:3O:399:LEU:HG	2.20	0.41
3:3P:34:GLY:HA3	13:3P:502:HEM:HBA2	2.02	0.41
9:3W:29:LEU:CD2	10:3X:34:TRP:HB2	2.50	0.41
12:3A:503:3PE:H351	3:3C:11:MET:SD	2.60	0.41
2:3B:141:GLN:NE2	2:3B:186:VAL:O	2.53	0.41
3:3C:160:LEU:HD23	3:3C:160:LEU:HA	1.88	0.41
3:3C:376:LEU:HA	3:3C:376:LEU:HD23	1.83	0.41
4:3D:122:LYS:HE3	4:3D:122:LYS:HB3	1.77	0.41
12:3D:502:3PE:O32	5:3E:131:ASN:ND2	2.46	0.41
2:3O:193:TYR:O	2:3O:197:ASN:HB2	2.19	0.41
4:3Q:160:MET:HE2	15:3Q:501:HEC:ND	2.35	0.41
5:3R:92:ARG:HE	5:3R:92:ARG:HB2	1.73	0.41
11:3A:501:CDL:HB31	11:3A:501:CDL:H122	2.03	0.41
4:3D:115:ARG:HG2	4:3D:119:GLN:NE2	2.36	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:3E:191:GLU:OE1	5:3E:192:VAL:N	2.54	0.41
4:3Q:215:LEU:HD23	4:3Q:215:LEU:HA	1.87	0.41
5:3R:119:ALA:O	5:3R:123:VAL:HG12	2.20	0.41
5:3R:155:LYS:NZ	5:3R:169:TRP:HE1	2.19	0.41
8:3U:23:GLN:HA	8:3U:26:GLN:HG2	2.03	0.41
1:3A:46:ARG:HH12	1:3A:316:GLU:CD	2.24	0.41
1:3A:64:PHE:CZ	1:3A:88:ALA:HB2	2.56	0.41
1:3A:317:THR:OG1	1:3A:318:GLY:N	2.52	0.41
3:3C:276:PHE:CG	3:3C:277:ALA:N	2.88	0.41
5:3E:222:CYS:HB3	5:3E:238:CYS:HB2	1.84	0.41
2:3O:209:LEU:HD23	2:3O:209:LEU:HA	1.83	0.41
3:3P:116:GLY:C	13:3P:502:HEM:HBC2	2.40	0.41
3:3P:320:LEU:HD12	3:3P:373:GLU:HG2	2.03	0.41
5:3R:161:GLU:HA	5:3R:178:HIS:HB3	2.03	0.41
7:3T:50:PRO:O	7:3T:54:VAL:HG13	2.20	0.41
9:3W:4:THR:HG22	9:3W:5:LEU:HD23	2.03	0.41
1:3A:86:LEU:HD12	1:3A:87:ASN:H	1.86	0.41
2:3B:305:GLN:O	5:3I:52:ARG:NH1	2.52	0.41
5:3E:202:LEU:HD23	5:3E:202:LEU:HA	1.94	0.41
5:3E:235:TYR:CZ	5:3E:237:PRO:HB3	2.56	0.41
7:3G:69:GLU:HA	7:3G:72:LYS:HZ2	1.86	0.41
2:3O:27:THR:HG21	2:3O:217:LYS:HZ2	1.86	0.41
2:3O:75:LEU:H	2:3O:75:LEU:HD12	1.86	0.41
10:3Y:38:TRP:HA	12:3Y:101:3PE:H11	2.02	0.41
1:3A:51:LYS:HD2	1:3A:51:LYS:HA	1.83	0.41
1:3A:438:ARG:NH2	5:3E:111:LYS:HE2	2.36	0.41
2:3B:26:PHE:CZ	2:3B:34:VAL:HG21	2.56	0.41
2:3B:256:ALA:O	2:3B:424:MET:HA	2.20	0.41
3:3C:121:PHE:HD1	3:3C:121:PHE:HA	1.77	0.41
3:3C:132:VAL:HA	3:3C:139:SER:HB3	2.03	0.41
3:3C:329:VAL:O	3:3C:333:ILE:HG13	2.21	0.41
3:3C:366:MET:HB2	3:3C:367:PRO:HD3	2.03	0.41
4:3D:249:MET:HB2	15:3D:501:HEC:C1D	2.51	0.41
5:3E:92:ARG:HG2	5:3E:92:ARG:H	1.67	0.41
5:3E:213:LEU:HD22	5:3E:258:LEU:HB2	2.03	0.41
1:3N:271:GLN:O	1:3N:275:ALA:N	2.52	0.41
1:3N:439:SER:HB3	12:3N:503:3PE:C11	2.51	0.41
2:3O:55:SER:HA	2:3O:58:GLU:HG3	2.02	0.41
2:3O:61:ASN:N	2:3O:61:ASN:OD1	2.54	0.41
3:3P:160:LEU:HD12	3:3P:160:LEU:HA	1.90	0.41
3:3P:162:GLU:OE2	3:3P:162:GLU:HA	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:3P:504:U10:H4M3	14:3P:504:U10:C3M	2.37	0.41
4:3Q:144:ARG:CD	4:3Q:147:LEU:HD22	2.50	0.41
5:3V:65:VAL:N	5:3V:77:ARG:O	2.54	0.41
1:3A:145:MET:H	5:3I:47:ARG:NH1	2.18	0.41
1:3A:438:ARG:HH21	5:3E:111:LYS:HE2	1.86	0.41
11:3A:501:CDL:H131	11:3A:501:CDL:OA9	2.21	0.41
2:3B:170:ASN:OD1	2:3B:170:ASN:N	2.53	0.41
3:3C:26:ASN:HA	6:3F:82:MET:HB2	2.03	0.41
6:3F:90:GLU:OE1	6:3F:91:GLN:N	2.54	0.41
1:3N:122:LEU:HD23	1:3N:122:LEU:HA	1.85	0.41
1:3N:235:ARG:HH11	5:3R:99:SER:HA	1.86	0.41
1:3N:345:LEU:HA	1:3N:345:LEU:HD23	1.87	0.41
12:3N:501:3PE:H361	3:3P:5:ARG:HD3	2.02	0.41
3:3P:65:SER:O	3:3P:69:ILE:HG13	2.21	0.41
3:3P:157:GLY:O	3:3P:161:VAL:HG23	2.20	0.41
4:3Q:240:PRO:HD3	7:3T:12:HIS:CD2	2.56	0.41
6:3S:44:LYS:HG2	6:3S:44:LYS:H	1.72	0.41
1:3A:379:ILE:HG12	1:3A:389:ARG:HE	1.86	0.40
2:3B:67:HIS:O	2:3B:71:LEU:HD12	2.21	0.40
3:3C:133:LEU:HD12	13:3C:501:HEM:C3D	2.56	0.40
5:3E:200:HIS:NE2	5:3E:202:LEU:HB2	2.35	0.40
3:3P:63:PHE:O	3:3P:67:THR:HG23	2.21	0.40
7:3T:60:THR:O	7:3T:64:GLN:HG3	2.21	0.40
1:3A:262:TRP:CG	1:3A:385:THR:HB	2.56	0.40
3:3C:182:HIS:HE1	13:3C:501:HEM:C4B	2.39	0.40
3:3C:197:LEU:HD12	3:3C:197:LEU:HA	1.84	0.40
4:3D:139:LEU:HD22	4:3D:143:CYS:SG	2.62	0.40
6:3F:39:ASN:OD1	6:3F:40:LYS:N	2.54	0.40
11:3G:102:CDL:H522	11:3G:102:CDL:HA31	2.03	0.40
1:3N:406:VAL:O	1:3N:409:GLU:HG3	2.22	0.40
2:3O:68:LEU:HD21	2:3O:137:VAL:HG13	2.03	0.40
2:3O:70:ARG:NH2	2:3O:176:LEU:O	2.40	0.40
2:3O:159:VAL:HG21	2:3O:254:HIS:HB2	2.02	0.40
2:3O:316:TYR:HB2	2:3O:319:SER:O	2.22	0.40
10:3Y:16:ASN:O	10:3Y:19:PRO:HD2	2.22	0.40
1:3A:436:ARG:HA	1:3A:436:ARG:HD2	1.86	0.40
2:3B:200:THR:HG22	2:3B:227:ARG:HB3	2.02	0.40
3:3C:338:ILE:HD13	3:3C:338:ILE:HA	1.86	0.40
6:3F:74:ILE:O	6:3F:78:LEU:HG	2.21	0.40
4:3Q:172:ASP:OD1	4:3Q:172:ASP:N	2.53	0.40
8:3U:42:GLN:CD	8:3U:42:GLN:H	2.25	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:3W:29:LEU:HD21	10:3X:34:TRP:HB2	2.02	0.40
1:3A:145:MET:SD	1:3A:248:LEU:HD13	2.61	0.40
1:3A:443:TRP:CE3	1:3A:445:ARG:HD2	2.57	0.40
2:3B:29:LEU:HD11	2:3B:35:ILE:HD11	2.04	0.40
2:3B:124:LEU:HA	2:3B:124:LEU:HD13	1.76	0.40
3:3C:227:LYS:HE2	11:3D:503:CDL:CB7	2.51	0.40
3:3C:379:TRP:CZ3	6:3F:49:ILE:HB	2.56	0.40
5:3E:150:SER:HB3	3:3P:168:PHE:CZ	2.56	0.40
5:3E:228:ALA:N	5:3E:233:GLY:O	2.54	0.40
2:3O:73:SER:HB3	2:3O:98:VAL:HG11	2.04	0.40
3:3P:40:CYS:O	3:3P:44:GLN:HB3	2.22	0.40
4:3Q:180:SER:HB3	8:3U:77:LEU:HD11	2.04	0.40
10:3X:36:THR:O	17:3X:101:PC1:H2	2.22	0.40
2:3B:85:ILE:HA	2:3B:122:PHE:CE1	2.57	0.40
2:3B:116:ILE:HD12	2:3B:117:GLU:N	2.37	0.40
2:3B:308:ASP:OD1	2:3B:327:ILE:HG12	2.22	0.40
14:3C:504:U10:H72	14:3C:504:U10:H1M1	1.94	0.40
4:3D:208:ARG:HH21	15:3D:501:HEC:CGA	2.35	0.40
6:3F:46:ASP:HB2	6:3F:101:TYR:CZ	2.56	0.40
5:3I:55:LEU:HA	5:3I:58:GLN:OE1	2.22	0.40
2:3O:33:LEU:HG	2:3O:35:ILE:HD11	2.04	0.40
3:3P:114:ASN:O	3:3P:118:VAL:HG23	2.21	0.40
3:3P:237:LEU:HD13	4:3Q:212:MET:HE2	2.02	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%)	409 (94%)	26 (6%)	1 (0%)	47 79
1	3N	444/480 (92%)	412 (93%)	29 (6%)	3 (1%)	22 61

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	3B	414/453 (91%)	395 (95%)	19 (5%)	0	100	100
2	3O	413/453 (91%)	397 (96%)	16 (4%)	0	100	100
3	3C	377/379 (100%)	361 (96%)	16 (4%)	0	100	100
3	3P	377/379 (100%)	363 (96%)	12 (3%)	2 (0%)	29	68
4	3D	235/325 (72%)	216 (92%)	19 (8%)	0	100	100
4	3Q	237/325 (73%)	218 (92%)	18 (8%)	1 (0%)	34	71
5	3E	194/274 (71%)	169 (87%)	24 (12%)	1 (0%)	29	68
5	3I	45/274 (16%)	36 (80%)	8 (18%)	1 (2%)	6	39
5	3R	194/274 (71%)	175 (90%)	17 (9%)	2 (1%)	15	55
5	3V	29/274 (11%)	29 (100%)	0	0	100	100
6	3F	96/111 (86%)	95 (99%)	1 (1%)	0	100	100
6	3S	96/111 (86%)	94 (98%)	2 (2%)	0	100	100
7	3G	70/82 (85%)	67 (96%)	3 (4%)	0	100	100
7	3T	72/82 (88%)	69 (96%)	3 (4%)	0	100	100
8	3H	61/91 (67%)	59 (97%)	2 (3%)	0	100	100
8	3U	63/91 (69%)	58 (92%)	5 (8%)	0	100	100
9	3J	54/64 (84%)	50 (93%)	4 (7%)	0	100	100
9	3W	54/64 (84%)	53 (98%)	1 (2%)	0	100	100
10	3X	50/56 (89%)	47 (94%)	3 (6%)	0	100	100
10	3Y	49/56 (88%)	44 (90%)	4 (8%)	1 (2%)	7	41
All	All	4060/5178 (78%)	3816 (94%)	232 (6%)	12 (0%)	44	75

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	3N	118	GLN
5	3R	230	ASP
10	3Y	6	LEU
5	3I	50	LEU
1	3N	68	LYS
4	3Q	44	ASP
1	3N	224	VAL
5	3E	216	VAL
3	3P	155	TYR
3	3P	110	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	3R	170	ARG
1	3A	265	PRO

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%)	352 (96%)	15 (4%)	30 64
1	3N	372/397 (94%)	344 (92%)	28 (8%)	13 45
2	3B	328/355 (92%)	316 (96%)	12 (4%)	34 66
2	3O	327/355 (92%)	306 (94%)	21 (6%)	17 52
3	3C	332/332 (100%)	323 (97%)	9 (3%)	44 73
3	3P	332/332 (100%)	319 (96%)	13 (4%)	32 65
4	3D	202/258 (78%)	192 (95%)	10 (5%)	24 59
4	3Q	204/258 (79%)	195 (96%)	9 (4%)	28 63
5	3E	166/225 (74%)	159 (96%)	7 (4%)	30 63
5	3I	36/225 (16%)	29 (81%)	7 (19%)	1 9
5	3R	166/225 (74%)	154 (93%)	12 (7%)	14 47
5	3V	24/225 (11%)	22 (92%)	2 (8%)	11 42
6	3F	90/99 (91%)	87 (97%)	3 (3%)	38 69
6	3S	90/99 (91%)	88 (98%)	2 (2%)	52 77
7	3G	67/73 (92%)	64 (96%)	3 (4%)	27 62
7	3T	67/73 (92%)	67 (100%)	0	100 100
8	3H	62/85 (73%)	60 (97%)	2 (3%)	39 70
8	3U	62/85 (73%)	58 (94%)	4 (6%)	17 51
9	3J	46/52 (88%)	45 (98%)	1 (2%)	52 77
9	3W	46/52 (88%)	44 (96%)	2 (4%)	29 63
10	3X	42/46 (91%)	41 (98%)	1 (2%)	49 75
10	3Y	41/46 (89%)	36 (88%)	5 (12%)	5 26

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3469/4294 (81%)	3301 (95%)	168 (5%)	29 60

All (168) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	3A	18	GLN
1	3A	32	GLN
1	3A	46	ARG
1	3A	57	TYR
1	3A	58	PHE
1	3A	77	LYS
1	3A	129	LYS
1	3A	177	LEU
1	3A	231	PHE
1	3A	258	GLU
1	3A	284	TYR
1	3A	333	ASP
1	3A	368	HIS
1	3A	429	GLU
1	3A	443	TRP
2	3B	61	ASN
2	3B	102	ARG
2	3B	111	CYS
2	3B	115	ASP
2	3B	122	PHE
2	3B	145	ARG
2	3B	154	ASN
2	3B	193	TYR
2	3B	227	ARG
2	3B	247	GLN
2	3B	266	SER
2	3B	401	GLN
3	3C	6	LYS
3	3C	100	ARG
3	3C	137	GLN
3	3C	155	TYR
3	3C	206	ASN
3	3C	217	LYS
3	3C	228	ASP
3	3C	248	ASP
3	3C	379	TRP
4	3D	103	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	3D	143	CYS
4	3D	150	LYS
4	3D	159	GLN
4	3D	208	ARG
4	3D	218	LEU
4	3D	232	ARG
4	3D	269	SER
4	3D	283	SER
4	3D	315	LYS
5	3E	108	ASP
5	3E	165	MET
5	3E	181	LYS
5	3E	251	LYS
5	3E	263	TYR
5	3E	265	PHE
5	3E	267	SER
6	3F	82	MET
6	3F	95	TYR
6	3F	111	ARG
7	3G	18	TYR
7	3G	46	CYS
7	3G	70	LYS
8	3H	46	ARG
8	3H	74	GLN
5	3I	46	LYS
5	3I	50	LEU
5	3I	53	GLU
5	3I	58	GLN
5	3I	62	ARG
5	3I	77	ARG
5	3I	78	TYR
9	3J	38	GLN
1	3N	8	LEU
1	3N	14	THR
1	3N	20	ASP
1	3N	24	ARG
1	3N	28	GLU
1	3N	50	GLU
1	3N	58	PHE
1	3N	65	LYS
1	3N	82	MET
1	3N	112	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	3N	116	ILE
1	3N	117	VAL
1	3N	121	SER
1	3N	132	ASP
1	3N	134	ILE
1	3N	146	ARG
1	3N	181	ASP
1	3N	207[A]	GLN
1	3N	207[B]	GLN
1	3N	231	PHE
1	3N	279	HIS
1	3N	284	TYR
1	3N	311	ASN
1	3N	335	MET
1	3N	368	HIS
1	3N	389	ARG
1	3N	443	TRP
1	3N	446	PHE
2	3O	22	GLN
2	3O	24	LEU
2	3O	28	ARG
2	3O	55	SER
2	3O	59	ASP
2	3O	61	ASN
2	3O	105	MET
2	3O	111	CYS
2	3O	120	MET
2	3O	145	ARG
2	3O	175	SER
2	3O	178	CYS
2	3O	183	ILE
2	3O	189	ASP
2	3O	247	GLN
2	3O	270	ASN
2	3O	308	ASP
2	3O	356	ASP
2	3O	371	SER
2	3O	374	SER
2	3O	380	ASP
3	3P	6	LYS
3	3P	100	ARG
3	3P	168	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	3P	171	ASP
3	3P	183	PHE
3	3P	221	HIS
3	3P	269	LYS
3	3P	276	PHE
3	3P	287	LYS
3	3P	344	GLU
3	3P	366	MET
3	3P	378	LYS
3	3P	379	TRP
4	3Q	55	CYS
4	3Q	80	MET
4	3Q	83	ARG
4	3Q	93	LYS
4	3Q	95	TYR
4	3Q	118	ARG
4	3Q	143	LEU
4	3Q	167	GLU
4	3Q	226	LYS
5	3R	84	ARG
5	3R	92	ARG
5	3R	131	ASN
5	3R	169	TRP
5	3R	170	ARG
5	3R	174	LEU
5	3R	204	ARG
5	3R	213	LEU
5	3R	248	ARG
5	3R	265	PHE
5	3R	268	ASP
5	3R	269	ASP
6	3S	48	ARG
6	3S	95	LYS
8	3U	21	ARG
8	3U	28	GLU
8	3U	51	GLU
8	3U	72	LYS
5	3V	62	ARG
5	3V	77	ARG
9	3W	16	ARG
9	3W	35	PHE
10	3X	17	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	3Y	9	ARG
10	3Y	15	ARG
10	3Y	16	ASN
10	3Y	47	TYR
10	3Y	51	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
2	3B	154	ASN
2	3B	254	HIS
3	3C	83	HIS
5	3E	239	HIS
6	3F	85	GLN
8	3H	88	HIS
1	3N	9	GLN
1	3N	69	ASN
1	3N	118	GLN
2	3O	141	GLN
3	3P	32	ASN
3	3P	374	ASN
4	3Q	31	GLN
5	3R	194	GLN
7	3T	23	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
11	CDL	3D	503	-	55,55,99	0.34	0	61,67,111	0.49	1 (1%)
12	3PE	3G	101	-	28,28,50	0.33	0	31,33,55	0.37	0
12	3PE	3A	502	-	26,26,50	0.36	0	29,31,55	0.55	0
13	HEM	3C	501	3	41,50,50	1.33	5 (12%)	45,82,82	1.78	8 (17%)
14	U10	3P	503	-	32,32,63	0.77	1 (3%)	38,41,79	1.32	6 (15%)
12	3PE	3N	503	-	24,24,50	0.37	0	27,29,55	0.66	1 (3%)
12	3PE	3N	501	-	31,31,50	0.33	0	34,36,55	0.45	0
17	PC1	3E	302	-	46,46,53	0.28	0	52,54,61	0.36	0
13	HEM	3P	501	3	41,50,50	1.31	5 (12%)	45,82,82	1.80	9 (20%)
17	PC1	3R	303	-	44,44,53	0.29	0	50,52,61	0.35	0
12	3PE	3C	506	-	33,33,50	0.33	0	36,38,55	0.47	0
12	3PE	3P	505	-	32,32,50	0.32	0	35,37,55	0.36	0
17	PC1	3X	101	-	28,28,53	0.35	0	34,36,61	0.36	0
12	3PE	3D	502	-	32,32,50	0.33	0	35,37,55	0.46	0
14	U10	3P	504	-	32,32,63	0.83	2 (6%)	38,41,79	1.35	4 (10%)
11	CDL	3N	502	-	42,42,99	0.38	0	48,54,111	0.54	0
12	3PE	3C	505	-	34,34,50	0.31	0	37,39,55	0.46	0
11	CDL	3A	501	-	57,57,99	0.34	0	63,69,111	0.47	0
11	CDL	3Q	502	-	56,56,99	0.34	0	62,68,111	0.49	0
12	3PE	3A	503	-	31,31,50	0.33	0	34,36,55	0.55	1 (2%)
14	U10	3C	504	-	23,23,63	0.99	2 (8%)	28,31,79	1.25	5 (17%)
11	CDL	3G	102	-	51,51,99	0.36	0	57,63,111	0.46	0
16	FES	3E	301	5	0,4,4	-	-	-		
14	U10	3C	503	-	28,28,63	0.90	2 (7%)	34,37,79	1.05	4 (11%)
15	HEC	3Q	501	4	32,50,50	2.37	12 (37%)	24,82,82	2.39	6 (25%)
15	HEC	3D	501	4	31,49,50	2.46	12 (38%)	22,80,82	2.34	4 (18%)
12	3PE	3Y	101	-	29,29,50	0.34	0	32,34,55	0.39	0
11	CDL	3P	506	-	55,55,99	0.36	0	61,67,111	0.47	0
13	HEM	3P	502	3	41,50,50	1.33	5 (12%)	45,82,82	1.75	7 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	3PE	3R	302	-	46,46,50	0.28	0	49,51,55	0.33	0
16	FES	3R	301	5	0,4,4	-	-	-		
13	HEM	3C	502	3	41,50,50	1.33	5 (12%)	45,82,82	1.74	8 (17%)

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
11	CDL	3D	503	-	-	17/66/66/110	-
12	3PE	3G	101	-	-	6/32/32/54	-
12	3PE	3A	502	-	-	11/30/30/54	-
13	HEM	3C	501	3	-	5/12/54/54	-
14	U10	3P	503	-	-	9/26/50/87	0/1/1/1
12	3PE	3N	503	-	-	4/28/28/54	-
12	3PE	3N	501	-	-	5/35/35/54	-
17	PC1	3E	302	-	-	4/50/50/57	-
13	HEM	3P	501	3	-	4/12/54/54	-
17	PC1	3R	303	-	-	8/48/48/57	-
12	3PE	3C	506	-	-	8/37/37/54	-
12	3PE	3P	505	-	-	5/36/36/54	-
17	PC1	3X	101	-	-	4/32/32/57	-
12	3PE	3D	502	-	-	6/36/36/54	-
14	U10	3P	504	-	-	4/26/50/87	0/1/1/1
11	CDL	3N	502	-	-	15/53/53/110	-
12	3PE	3C	505	-	-	9/38/38/54	-
11	CDL	3A	501	-	-	18/68/68/110	-
11	CDL	3Q	502	-	-	20/67/67/110	-
12	3PE	3A	503	-	-	6/35/35/54	-
14	U10	3C	504	-	-	3/15/39/87	0/1/1/1
11	CDL	3G	102	-	-	10/62/62/110	-
16	FES	3E	301	5	-	-	0/1/1/1
14	U10	3C	503	-	-	5/21/45/87	0/1/1/1
15	HEC	3Q	501	4	-	5/10/54/54	-
15	HEC	3D	501	4	-	3/8/53/54	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	3PE	3Y	101	-	-	5/33/33/54	-
11	CDL	3P	506	-	-	22/66/66/110	-
13	HEM	3P	502	3	-	6/12/54/54	-
12	3PE	3R	302	-	-	5/50/50/54	-
16	FES	3R	301	5	-	-	0/1/1/1
13	HEM	3C	502	3	-	4/12/54/54	-

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	3D	501	HEC	C2B-C3B	7.05	1.48	1.40
15	3D	501	HEC	C3C-C2C	6.93	1.48	1.40
15	3Q	501	HEC	C2B-C3B	6.91	1.48	1.40
15	3Q	501	HEC	C3C-C2C	6.71	1.47	1.40
15	3D	501	HEC	C2A-C3A	3.42	1.47	1.37
13	3P	502	HEM	C1B-NB	-3.41	1.34	1.40
13	3C	502	HEM	C1B-NB	-3.40	1.34	1.40
15	3D	501	HEC	C3D-C2D	3.40	1.47	1.37
13	3C	502	HEM	C4D-ND	-3.36	1.34	1.40
13	3P	502	HEM	C4D-ND	-3.35	1.34	1.40
15	3Q	501	HEC	C2A-C3A	3.31	1.47	1.37
13	3C	501	HEM	C1B-NB	-3.30	1.34	1.40
13	3P	501	HEM	C1B-NB	-3.30	1.34	1.40
15	3Q	501	HEC	C3D-C2D	3.27	1.47	1.37
13	3C	501	HEM	C4D-ND	-3.24	1.34	1.40
13	3P	501	HEM	C4D-ND	-3.15	1.34	1.40
15	3D	501	HEC	C3C-C4C	3.11	1.48	1.43
15	3D	501	HEC	C4B-C3B	3.11	1.48	1.43
15	3Q	501	HEC	C3C-C4C	2.98	1.48	1.43
15	3Q	501	HEC	C4B-C3B	2.95	1.48	1.43
13	3C	501	HEM	FE-NB	2.90	2.11	1.96
13	3P	501	HEM	FE-NB	2.88	2.11	1.96
15	3D	501	HEC	C2A-C1A	2.87	1.49	1.42
14	3C	504	U10	C3-C2	-2.82	1.40	1.48
13	3C	502	HEM	FE-NB	2.81	2.10	1.96
13	3P	502	HEM	FE-NB	2.81	2.10	1.96
15	3Q	501	HEC	C2A-C1A	2.80	1.48	1.42
14	3C	503	U10	C3-C2	-2.73	1.41	1.48
15	3Q	501	HEC	C3A-C4A	2.72	1.48	1.42
15	3D	501	HEC	C3A-C4A	2.71	1.48	1.42
14	3P	504	U10	C3-C2	-2.61	1.41	1.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	3D	501	HEC	C4D-CHA	2.59	1.48	1.41
14	3P	503	U10	C4-C5	-2.58	1.41	1.48
15	3D	501	HEC	C1D-CHD	2.57	1.48	1.41
15	3Q	501	HEC	C4D-CHA	2.53	1.48	1.41
15	3D	501	HEC	C1C-CHC	2.47	1.47	1.41
15	3D	501	HEC	C1B-CHB	2.46	1.47	1.41
14	3C	504	U10	C4-C5	-2.44	1.41	1.48
15	3Q	501	HEC	C1B-CHB	2.44	1.47	1.41
14	3C	503	U10	C4-C5	-2.42	1.41	1.48
15	3Q	501	HEC	C1D-CHD	2.42	1.47	1.41
15	3Q	501	HEC	C1C-CHC	2.39	1.47	1.41
14	3P	504	U10	C4-C5	-2.36	1.42	1.48
13	3C	502	HEM	C1D-ND	-2.11	1.34	1.38
13	3P	502	HEM	C1D-ND	-2.09	1.34	1.38
13	3C	501	HEM	CHB-C1B	2.08	1.40	1.35
13	3P	501	HEM	CHB-C1B	2.05	1.40	1.35
13	3C	501	HEM	C1D-ND	-2.05	1.34	1.38
13	3P	501	HEM	C4B-NB	-2.03	1.34	1.38
13	3C	502	HEM	CHB-C1B	2.02	1.40	1.35
13	3P	502	HEM	CHB-C1B	2.01	1.40	1.35

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	3Q	501	HEC	C1D-C2D-C3D	-6.21	102.68	107.00
15	3D	501	HEC	C1D-C2D-C3D	-5.94	102.86	107.00
15	3Q	501	HEC	CMB-C2B-C3B	5.29	132.04	125.82
15	3D	501	HEC	CMB-C2B-C3B	5.26	132.00	125.82
15	3Q	501	HEC	CMC-C2C-C3C	5.19	131.92	125.82
15	3D	501	HEC	CMC-C2C-C3C	5.15	131.87	125.82
13	3P	502	HEM	CHC-C4B-NB	5.02	129.88	124.43
13	3C	501	HEM	CHC-C4B-NB	4.99	129.85	124.43
13	3C	502	HEM	CHC-C4B-NB	4.96	129.82	124.43
13	3P	501	HEM	CHC-C4B-NB	4.60	129.43	124.43
13	3P	501	HEM	CHD-C1D-ND	4.56	129.39	124.43
13	3C	501	HEM	CHD-C1D-ND	4.20	129.00	124.43
13	3P	502	HEM	C1B-NB-C4B	4.09	109.30	105.07
13	3C	502	HEM	C1B-NB-C4B	4.03	109.24	105.07
13	3P	502	HEM	CHD-C1D-ND	3.89	128.66	124.43
13	3C	502	HEM	CHD-C1D-ND	3.82	128.58	124.43
13	3P	501	HEM	C1B-NB-C4B	3.81	109.00	105.07
13	3C	501	HEM	C1B-NB-C4B	3.74	108.93	105.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	3P	504	U10	O3-C3-C4	3.64	137.35	123.64
14	3P	503	U10	C11-C12-C13	3.62	123.77	111.88
14	3P	504	U10	O4-C4-C3	3.49	136.80	123.64
13	3C	501	HEM	CHA-C4D-ND	3.46	128.65	124.38
14	3P	504	U10	O4-C4-C5	-3.44	104.93	116.56
13	3C	502	HEM	CHA-C4D-ND	3.42	128.60	124.38
14	3P	504	U10	O3-C3-C2	-3.41	105.04	116.56
13	3P	502	HEM	CHA-C4D-ND	3.37	128.54	124.38
13	3P	501	HEM	CHA-C4D-ND	3.31	128.47	124.38
13	3P	501	HEM	CHB-C1B-NB	3.24	128.38	124.38
13	3C	501	HEM	CHB-C1B-NB	3.19	128.32	124.38
14	3C	504	U10	O3-C3-C4	3.03	135.06	123.64
14	3P	503	U10	O4-C4-C5	-2.90	106.76	116.56
13	3P	502	HEM	CHB-C1B-NB	2.86	127.92	124.38
13	3C	502	HEM	CHB-C1B-NB	2.85	127.90	124.38
13	3P	501	HEM	CHD-C1D-C2D	-2.76	120.67	124.98
14	3P	503	U10	O3-C3-C2	2.70	125.69	116.56
14	3C	504	U10	O3-C3-C2	-2.65	107.61	116.56
13	3P	501	HEM	CBA-CAA-C2A	-2.64	108.11	112.62
14	3C	503	U10	O3-C3-C4	2.63	133.56	123.64
13	3P	502	HEM	C4D-ND-C1D	2.59	107.75	105.07
14	3C	504	U10	O4-C4-C3	2.51	133.09	123.64
13	3C	501	HEM	CHD-C1D-C2D	-2.48	121.11	124.98
13	3C	502	HEM	C4D-ND-C1D	2.47	107.62	105.07
14	3P	503	U10	C12-C13-C14	2.42	133.49	127.66
15	3Q	501	HEC	CBD-CAD-C3D	-2.40	108.52	112.62
13	3P	501	HEM	C4D-ND-C1D	2.39	107.55	105.07
14	3C	503	U10	O4-C4-C3	2.37	132.57	123.64
13	3C	501	HEM	C4D-ND-C1D	2.37	107.52	105.07
14	3P	503	U10	O4-C4-C3	2.36	132.54	123.64
14	3C	504	U10	O4-C4-C5	-2.35	108.60	116.56
14	3C	503	U10	C4-C3-C2	-2.30	116.16	120.68
15	3D	501	HEC	CMA-C3A-C2A	2.30	129.28	124.94
15	3Q	501	HEC	CBA-CAA-C2A	-2.30	108.73	112.60
13	3P	502	HEM	CHD-C1D-C2D	-2.27	121.43	124.98
12	3N	503	3PE	O21-C21-C22	2.25	116.35	111.50
13	3C	502	HEM	CHD-C1D-C2D	-2.22	121.52	124.98
14	3C	503	U10	O3-C3-C2	-2.11	109.42	116.56
12	3A	503	3PE	O21-C21-C22	2.10	116.02	111.50
13	3C	501	HEM	CHA-C4D-C3D	-2.10	121.39	125.33
14	3P	503	U10	C4-C3-C2	-2.09	116.58	120.68
14	3C	504	U10	C4-C3-C2	-2.08	116.58	120.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	3Q	501	HEC	CMA-C3A-C2A	2.08	128.86	124.94
13	3C	502	HEM	CHA-C4D-C3D	-2.03	121.51	125.33
11	3D	503	CDL	OA6-CA5-C11	2.03	115.88	111.50
13	3P	501	HEM	CAD-CBD-CGD	-2.02	109.26	113.60

There are no chirality outliers.

All (236) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	3A	501	CDL	C1-CA2-OA2-PA1
11	3A	501	CDL	OB9-CB7-OB8-CB6
11	3A	501	CDL	C71-CB7-OB8-CB6
11	3D	503	CDL	CA3-OA5-PA1-OA3
11	3D	503	CDL	CA4-CA3-OA5-PA1
11	3D	503	CDL	OA7-CA5-OA6-CA4
11	3D	503	CDL	C11-CA5-OA6-CA4
11	3D	503	CDL	OA9-CA7-OA8-CA6
11	3D	503	CDL	C31-CA7-OA8-CA6
11	3D	503	CDL	C1-CB2-OB2-PB2
11	3D	503	CDL	CB4-CB3-OB5-PB2
11	3G	102	CDL	CA4-CA3-OA5-PA1
11	3N	502	CDL	C1-CA2-OA2-PA1
11	3N	502	CDL	CA2-OA2-PA1-OA4
11	3P	506	CDL	C1-CA2-OA2-PA1
11	3P	506	CDL	C1-CB2-OB2-PB2
11	3P	506	CDL	OB9-CB7-OB8-CB6
11	3P	506	CDL	C71-CB7-OB8-CB6
11	3Q	502	CDL	CA3-OA5-PA1-OA4
11	3Q	502	CDL	OB9-CB7-OB8-CB6
11	3Q	502	CDL	C71-CB7-OB8-CB6
12	3A	502	3PE	C2-C1-O11-P
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	C2-C1-O11-P
12	3A	503	3PE	O22-C21-O21-C2
12	3A	503	3PE	C22-C21-O21-C2
12	3C	505	3PE	C1-O11-P-O14
12	3C	506	3PE	C1-O11-P-O14
12	3C	506	3PE	C2-C1-O11-P
12	3G	101	3PE	O32-C31-O31-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
12	3G	101	3PE	C32-C31-O31-C3
12	3N	501	3PE	C2-C1-O11-P
12	3N	503	3PE	O22-C21-O21-C2
12	3N	503	3PE	C22-C21-O21-C2
12	3Y	101	3PE	C1-O11-P-O13
12	3Y	101	3PE	C2-C1-O11-P
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	3C	502	HEM	C4B-C3B-CAB-CBB
13	3P	501	HEM	C2B-C3B-CAB-CBB
13	3P	502	HEM	C2B-C3B-CAB-CBB
13	3P	502	HEM	C4B-C3B-CAB-CBB
14	3P	503	U10	C11-C12-C13-C14
17	3R	303	PC1	C2-C1-O11-P
17	3R	303	PC1	O32-C31-O31-C3
17	3R	303	PC1	C32-C31-O31-C3
17	3X	101	PC1	O32-C31-O31-C3
17	3X	101	PC1	C32-C31-O31-C3
14	3C	503	U10	C12-C11-C9-C10
14	3C	503	U10	C12-C11-C9-C8
11	3N	502	CDL	CA2-C1-CB2-OB2
11	3N	502	CDL	O1-C1-CB2-OB2
11	3N	502	CDL	C1-CB2-OB2-PB2
14	3P	503	U10	C4-C3-O3-C3M
14	3P	504	U10	C14-C16-C17-C18
11	3D	503	CDL	CA3-OA5-PA1-OA2
11	3G	102	CDL	CA3-OA5-PA1-OA2
11	3N	502	CDL	CA2-OA2-PA1-OA5
11	3Q	502	CDL	CA3-OA5-PA1-OA2
12	3N	501	3PE	C1-O11-P-O13
12	3C	506	3PE	C22-C23-C24-C25
12	3C	505	3PE	C25-C26-C27-C28
12	3D	502	3PE	C21-C22-C23-C24
17	3R	303	PC1	C31-C32-C33-C34
11	3N	502	CDL	CA3-CA4-CA6-OA8
14	3P	503	U10	C2-C3-O3-C3M
11	3G	102	CDL	CB4-CB3-OB5-PB2
11	3Q	502	CDL	OB5-CB3-CB4-OB6
13	3P	501	HEM	C4B-C3B-CAB-CBB
11	3N	502	CDL	OA6-CA4-CA6-OA8
11	3Q	502	CDL	OA6-CA4-CA6-OA8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	3Q	502	CDL	OB6-CB4-CB6-OB8
11	3A	501	CDL	CA2-OA2-PA1-OA5
12	3A	502	3PE	C1-O11-P-O13
12	3C	505	3PE	C1-O11-P-O13
12	3C	506	3PE	C1-O11-P-O13
11	3G	102	CDL	CB7-C71-C72-C73
11	3Q	502	CDL	CA7-C31-C32-C33
17	3X	101	PC1	C21-C22-C23-C24
14	3P	504	U10	C6-C7-C8-C9
11	3P	506	CDL	OA5-CA3-CA4-CA6
12	3A	503	3PE	O11-C1-C2-C3
12	3C	506	3PE	O11-C1-C2-C3
15	3Q	501	HEC	C3D-CAD-CBD-CGD
12	3P	505	3PE	C1-C2-C3-O31
11	3P	506	CDL	CB7-C71-C72-C73
12	3R	302	3PE	C35-C36-C37-C38
12	3N	503	3PE	C31-C32-C33-C34
11	3D	503	CDL	C72-C73-C74-C75
11	3A	501	CDL	C32-C31-CA7-OA8
11	3N	502	CDL	C12-C11-CA5-OA6
12	3D	502	3PE	O21-C21-C22-C23
12	3N	501	3PE	O21-C21-C22-C23
13	3C	501	HEM	C3D-CAD-CBD-CGD
11	3Q	502	CDL	CB5-C51-C52-C53
11	3Q	502	CDL	OB5-CB3-CB4-CB6
11	3G	102	CDL	C52-C51-CB5-OB6
11	3Q	502	CDL	CA4-CA3-OA5-PA1
11	3Q	502	CDL	CA3-CA4-CA6-OA8
11	3Q	502	CDL	CB3-CB4-CB6-OB8
12	3C	505	3PE	C21-C22-C23-C24
11	3A	501	CDL	OB5-CB3-CB4-OB6
12	3A	503	3PE	O11-C1-C2-O21
11	3P	506	CDL	OB6-CB4-CB6-OB8
11	3P	506	CDL	CB2-C1-CA2-OA2
11	3P	506	CDL	CB4-CB3-OB5-PB2
11	3Q	502	CDL	CB4-CB3-OB5-PB2
12	3P	505	3PE	C2-C1-O11-P
12	3A	502	3PE	O11-C1-C2-O21
12	3C	505	3PE	C23-C24-C25-C26
11	3A	501	CDL	OB6-CB4-CB6-OB8
12	3P	505	3PE	O21-C2-C3-O31
12	3C	505	3PE	C11-O13-P-O11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
12	3C	506	3PE	C11-O13-P-O11
11	3P	506	CDL	CA4-CA3-OA5-PA1
11	3D	503	CDL	CA3-OA5-PA1-OA4
11	3G	102	CDL	CA3-OA5-PA1-OA3
11	3Q	502	CDL	CA3-OA5-PA1-OA3
12	3N	501	3PE	C1-O11-P-O12
12	3Y	101	3PE	C1-O11-P-O12
12	3C	506	3PE	C12-C11-O13-P
12	3D	502	3PE	C12-C11-O13-P
17	3R	303	PC1	C12-C11-O13-P
12	3C	506	3PE	O11-C1-C2-O21
15	3D	501	HEC	C2A-CAA-CBA-CGA
12	3R	302	3PE	C21-C22-C23-C24
11	3N	502	CDL	CA5-C11-C12-C13
11	3P	506	CDL	C12-C11-CA5-OA6
11	3A	501	CDL	OB5-CB3-CB4-CB6
12	3P	505	3PE	C31-C32-C33-C34
11	3A	501	CDL	CA4-CA3-OA5-PA1
11	3P	506	CDL	OA5-CA3-CA4-OA6
11	3A	501	CDL	CB2-OB2-PB2-OB5
11	3D	503	CDL	CA2-OA2-PA1-OA5
11	3D	503	CDL	CB3-OB5-PB2-OB2
11	3G	102	CDL	CA2-OA2-PA1-OA5
11	3N	502	CDL	CB3-OB5-PB2-OB2
11	3P	506	CDL	CA2-OA2-PA1-OA5
11	3P	506	CDL	CB3-OB5-PB2-OB2
11	3Q	502	CDL	CA2-OA2-PA1-OA5
12	3N	503	3PE	C11-O13-P-O11
12	3Y	101	3PE	C11-O13-P-O11
17	3X	101	PC1	C1-O11-P-O13
12	3R	302	3PE	C23-C24-C25-C26
11	3A	501	CDL	CB5-C51-C52-C53
11	3A	501	CDL	C33-C34-C35-C36
11	3A	501	CDL	C32-C31-CA7-OA9
11	3Q	502	CDL	C72-C73-C74-C75
13	3C	502	HEM	CAA-CBA-CGA-O1A
13	3P	502	HEM	CAD-CBD-CGD-O1D
12	3R	302	3PE	C22-C23-C24-C25
12	3Y	101	3PE	O11-C1-C2-C3
11	3P	506	CDL	OB5-CB3-CB4-OB6
12	3C	505	3PE	O11-C1-C2-O21
14	3P	503	U10	C12-C11-C9-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	3P	501	HEM	CAD-CBD-CGD-O1D
13	3C	501	HEM	CAA-CBA-CGA-O2A
13	3P	502	HEM	CAA-CBA-CGA-O1A
13	3C	501	HEM	CAA-CBA-CGA-O1A
13	3P	502	HEM	CAD-CBD-CGD-O2D
12	3C	505	3PE	C1-C2-O21-C21
14	3P	503	U10	C12-C11-C9-C10
12	3D	502	3PE	C24-C25-C26-C27
13	3P	501	HEM	CAD-CBD-CGD-O2D
12	3N	501	3PE	O22-C21-C22-C23
13	3P	502	HEM	CAA-CBA-CGA-O2A
12	3G	101	3PE	C32-C33-C34-C35
14	3P	503	U10	C5-C4-O4-C4M
13	3C	502	HEM	CAA-CBA-CGA-O2A
12	3G	101	3PE	O21-C2-C3-O31
15	3D	501	HEC	CAA-CBA-CGA-O2A
15	3Q	501	HEC	CAD-CBD-CGD-O2D
14	3P	503	U10	C16-C17-C18-C19
12	3P	505	3PE	C23-C24-C25-C26
12	3C	505	3PE	C1-C2-C3-O31
12	3D	502	3PE	O22-C21-C22-C23
14	3P	503	U10	C20-C19-C21-C22
15	3D	501	HEC	CAA-CBA-CGA-O1A
11	3Q	502	CDL	C75-C76-C77-C78
15	3Q	501	HEC	CAD-CBD-CGD-O1D
12	3A	502	3PE	O11-C1-C2-C3
12	3A	502	3PE	C32-C33-C34-C35
11	3D	503	CDL	C74-C75-C76-C77
11	3N	502	CDL	OB6-CB4-CB6-OB8
15	3Q	501	HEC	CAA-CBA-CGA-O2A
12	3D	502	3PE	C33-C34-C35-C36
14	3P	503	U10	C18-C19-C21-C22
11	3N	502	CDL	CB3-CB4-OB6-CB5
11	3D	503	CDL	C52-C51-CB5-OB6
17	3R	303	PC1	C36-C37-C38-C39
11	3P	506	CDL	CB3-CB4-CB6-OB8
11	3P	506	CDL	CB5-C51-C52-C53
11	3P	506	CDL	OB5-CB3-CB4-CB6
12	3A	502	3PE	O21-C2-C3-O31
11	3G	102	CDL	C52-C51-CB5-OB7
14	3C	504	U10	C3-C4-O4-C4M
17	3E	302	PC1	C36-C37-C38-C39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	3Q	501	HEC	CAA-CBA-CGA-O1A
11	3D	503	CDL	C52-C51-CB5-OB7
14	3P	504	U10	C21-C22-C23-C24
11	3A	501	CDL	CB3-CB4-CB6-OB8
11	3N	502	CDL	CA4-CA6-OA8-CA7
17	3E	302	PC1	C29-C2A-C2B-C2C
11	3A	501	CDL	CA2-OA2-PA1-OA4
11	3A	501	CDL	CB2-OB2-PB2-OB3
11	3A	501	CDL	CB3-OB5-PB2-OB3
11	3D	503	CDL	CA2-OA2-PA1-OA3
11	3G	102	CDL	CA3-OA5-PA1-OA4
11	3P	506	CDL	CA2-OA2-PA1-OA3
12	3A	502	3PE	C1-O11-P-O12
17	3R	303	PC1	C1-O11-P-O14
17	3E	302	PC1	C24-C25-C26-C27
11	3P	506	CDL	C72-C71-CB7-OB8
12	3G	101	3PE	O31-C31-C32-C33
17	3R	303	PC1	C38-C39-C3A-C3B
14	3C	503	U10	C2-C3-O3-C3M
14	3C	503	U10	C5-C4-O4-C4M
14	3C	504	U10	C2-C3-O3-C3M
14	3C	504	U10	C5-C4-O4-C4M
14	3P	504	U10	C2-C3-O3-C3M
17	3E	302	PC1	C12-C11-O13-P
11	3N	502	CDL	C12-C11-CA5-OA7
11	3A	501	CDL	C52-C51-CB5-OB6
11	3Q	502	CDL	C32-C31-CA7-OA8
11	3Q	502	CDL	C32-C31-CA7-OA9
14	3C	503	U10	C11-C12-C13-C14
11	3P	506	CDL	O1-C1-CA2-OA2
12	3R	302	3PE	O31-C31-C32-C33
11	3P	506	CDL	C72-C71-CB7-OB9
12	3G	101	3PE	O32-C31-C32-C33
11	3G	102	CDL	C12-C11-CA5-OA6
12	3A	503	3PE	O21-C21-C22-C23

There are no ring outliers.

30 monomers are involved in 130 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	3D	503	CDL	3	0
12	3G	101	3PE	1	0

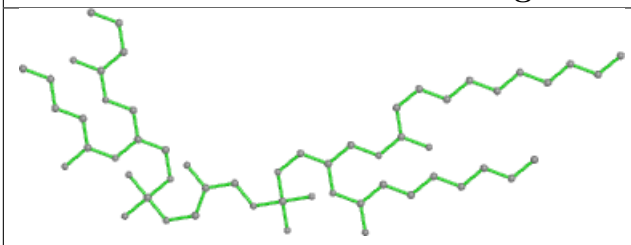
Continued on next page...

Continued from previous page...

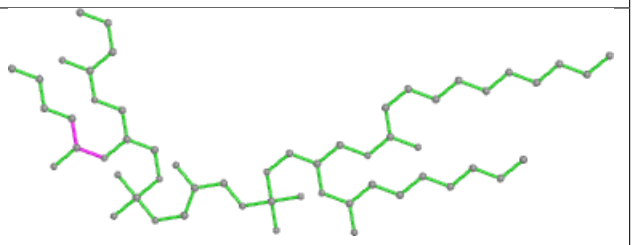
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	3A	502	3PE	1	0
13	3C	501	HEM	8	0
14	3P	503	U10	9	0
12	3N	503	3PE	4	0
12	3N	501	3PE	3	0
17	3E	302	PC1	5	0
13	3P	501	HEM	2	0
17	3R	303	PC1	6	0
12	3C	506	3PE	3	0
17	3X	101	PC1	5	0
12	3D	502	3PE	4	0
14	3P	504	U10	6	0
11	3N	502	CDL	3	0
12	3C	505	3PE	3	0
11	3A	501	CDL	6	0
11	3Q	502	CDL	11	0
12	3A	503	3PE	9	0
14	3C	504	U10	2	0
11	3G	102	CDL	5	0
16	3E	301	FES	3	0
14	3C	503	U10	4	0
15	3Q	501	HEC	4	0
15	3D	501	HEC	7	0
12	3Y	101	3PE	1	0
11	3P	506	CDL	9	0
13	3P	502	HEM	3	0
12	3R	302	3PE	5	0
13	3C	502	HEM	4	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.

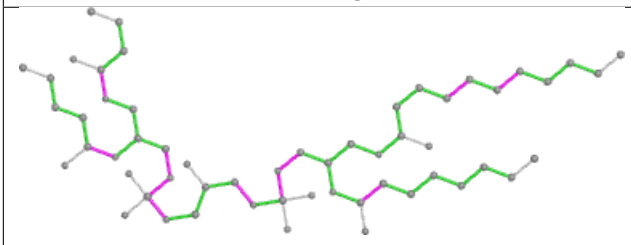
Ligand CDL 3D 503



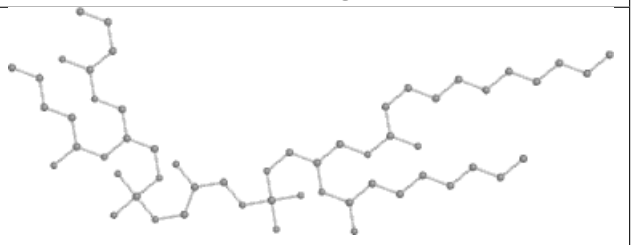
Bond lengths



Bond angles

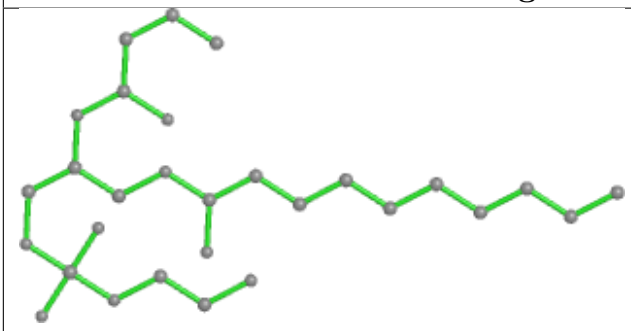


Torsions

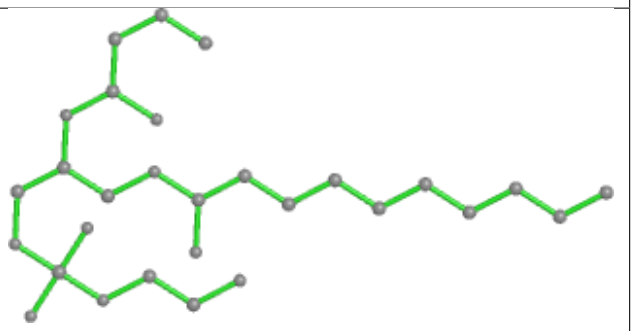


Rings

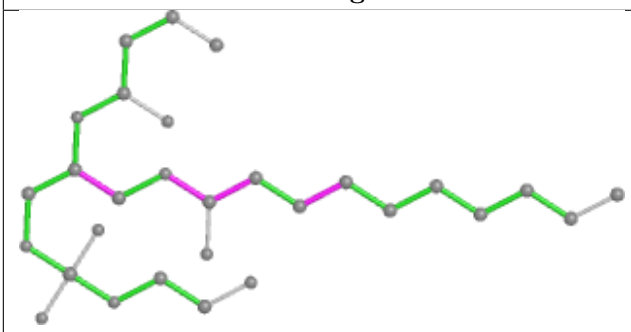
Ligand 3PE 3G 101



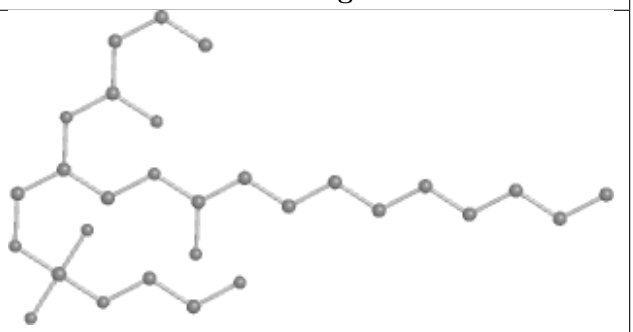
Bond lengths



Bond angles

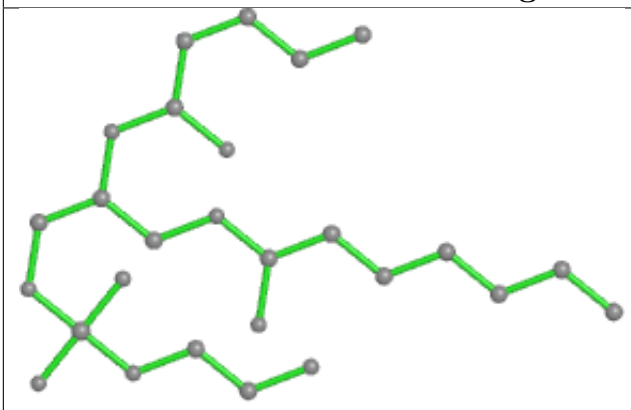


Torsions

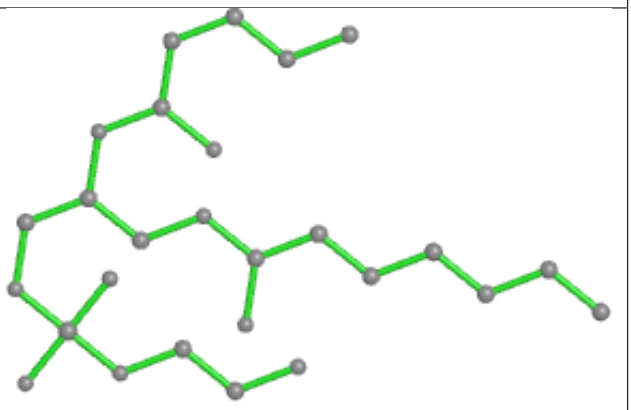


Rings

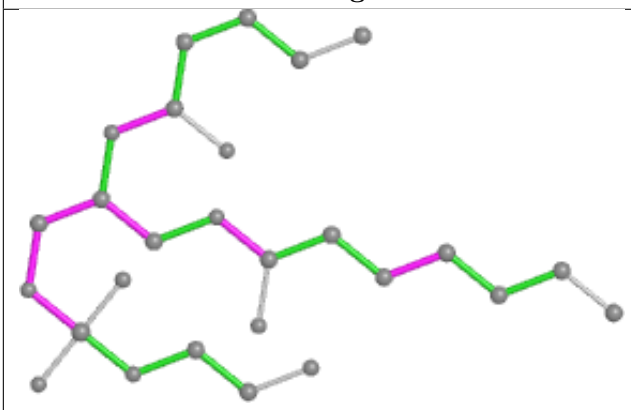
Ligand 3PE 3A 502



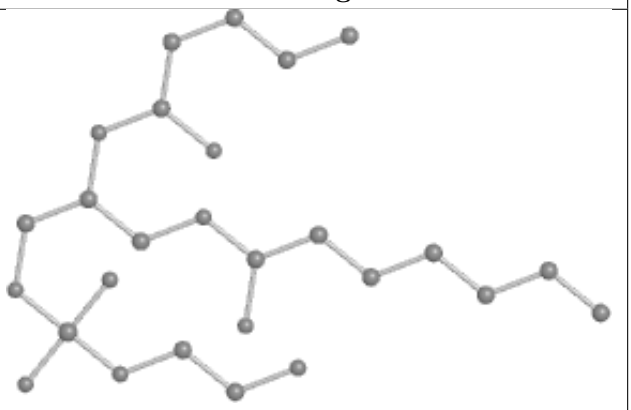
Bond lengths



Bond angles

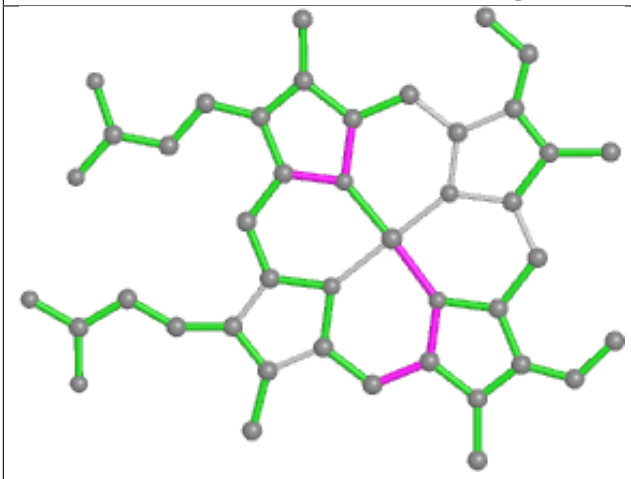


Torsions

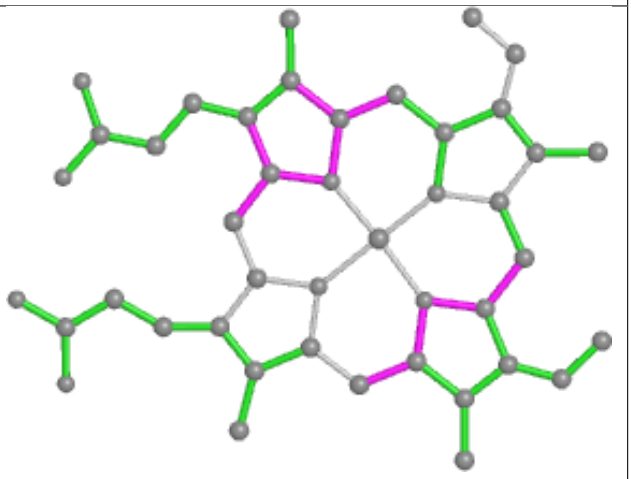


Rings

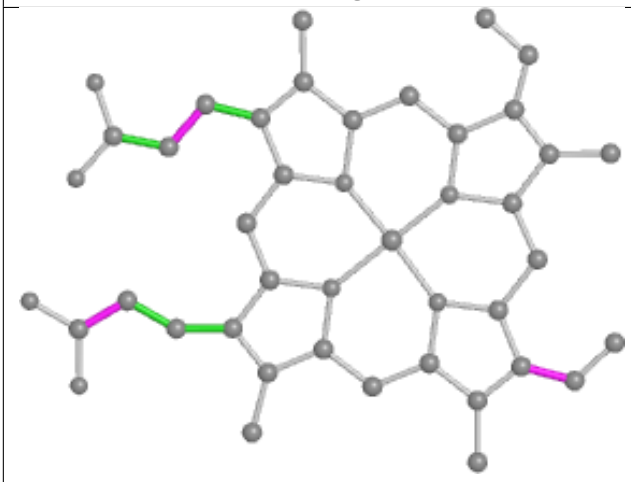
Ligand HEM 3C 501



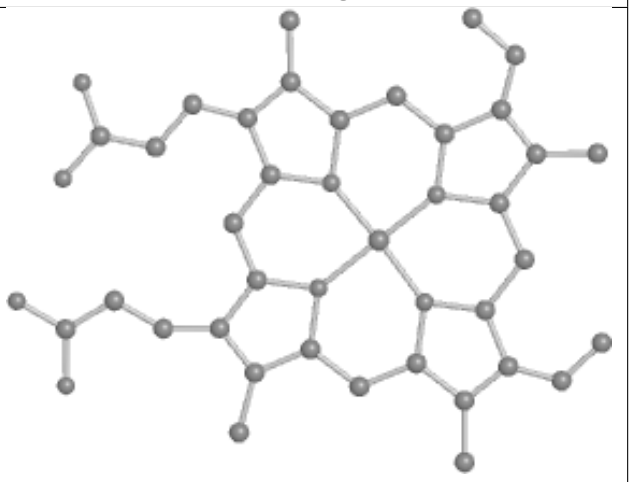
Bond lengths



Bond angles

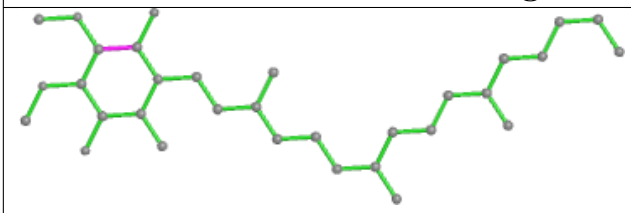


Torsions

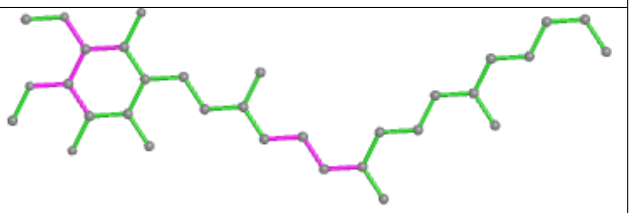


Rings

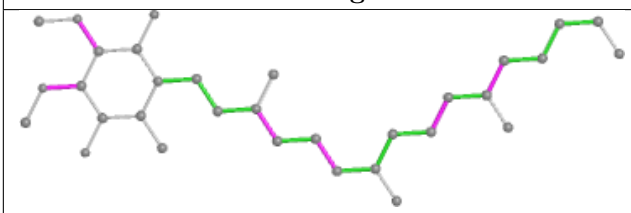
Ligand U10 3P 503



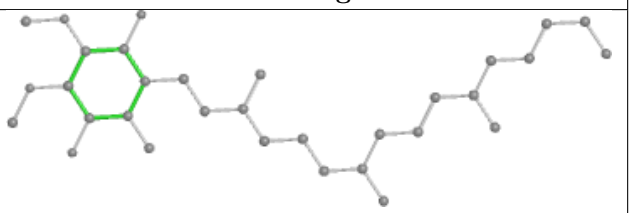
Bond lengths



Bond angles

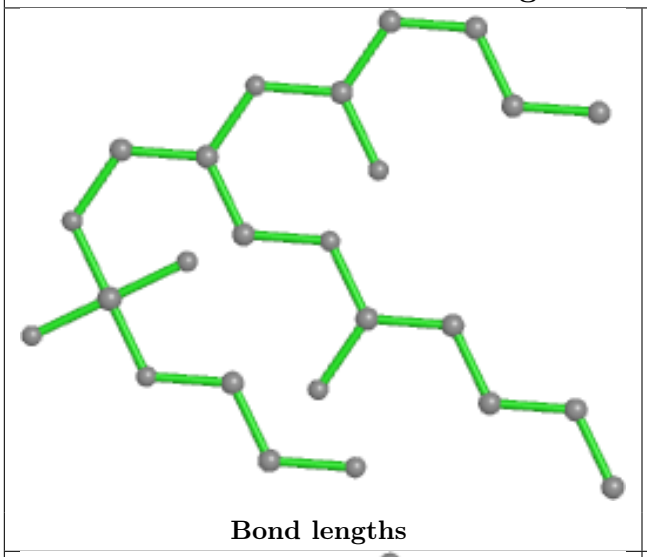


Torsions

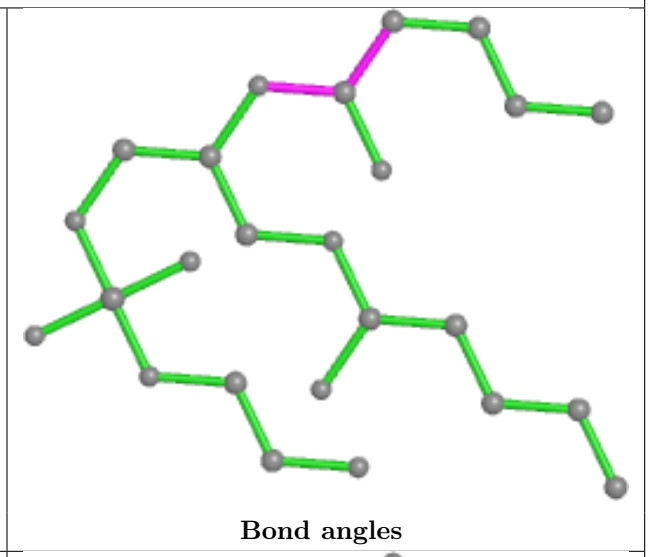


Rings

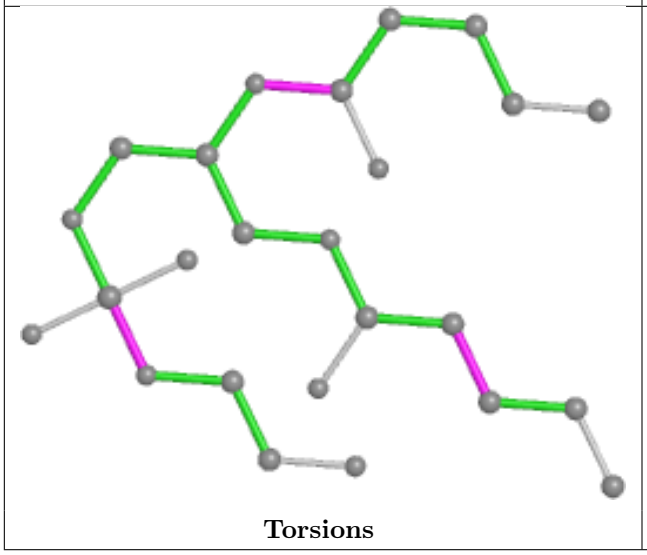
Ligand 3PE 3N 503



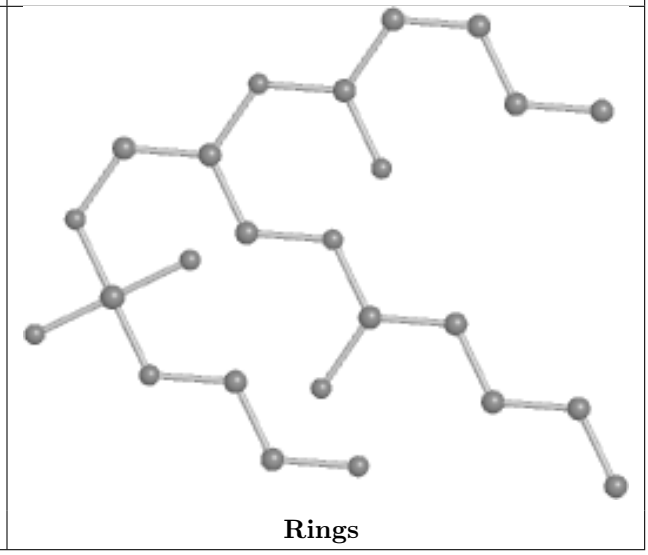
Bond lengths



Bond angles

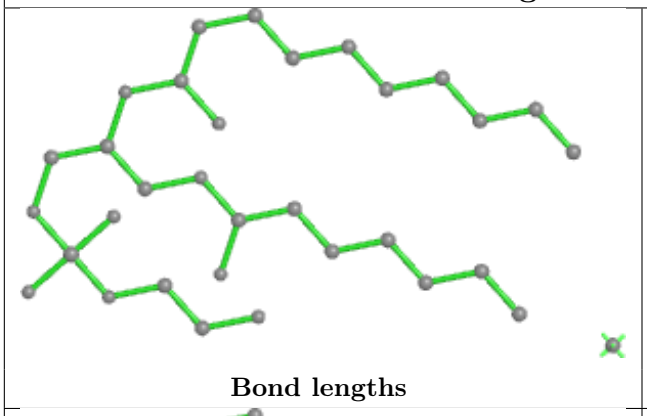


Torsions

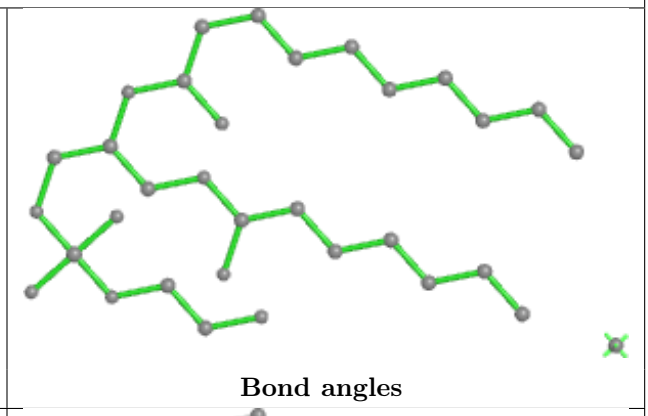


Rings

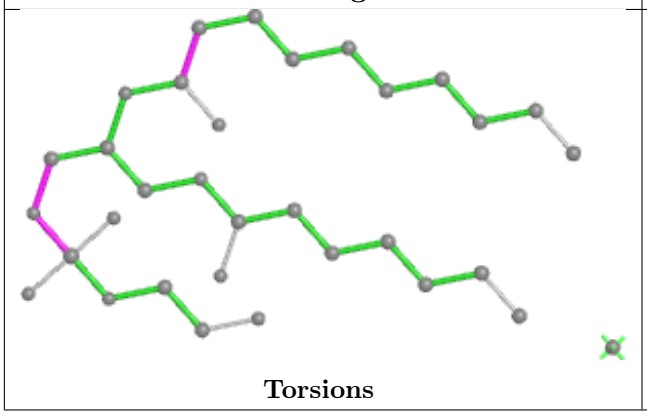
Ligand 3PE 3N 501



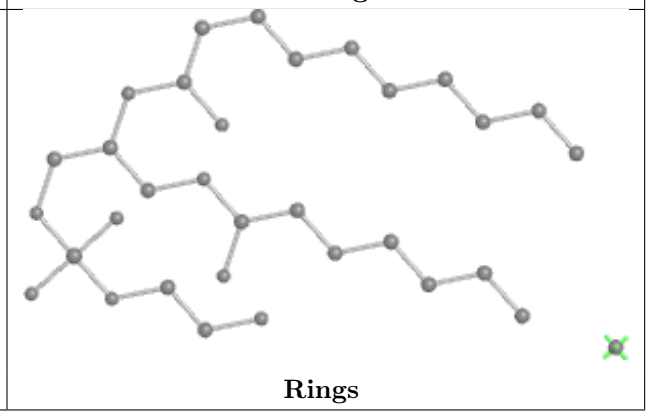
Bond lengths



Bond angles

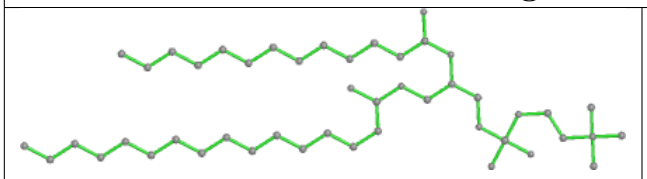


Torsions

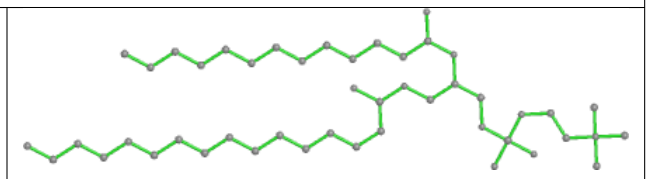


Rings

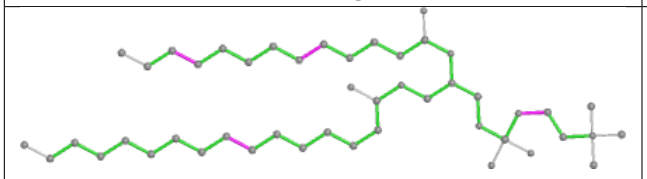
Ligand PC1 3E 302



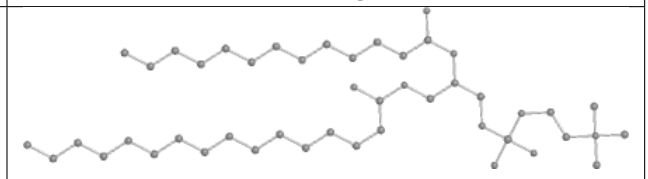
Bond lengths



Bond angles

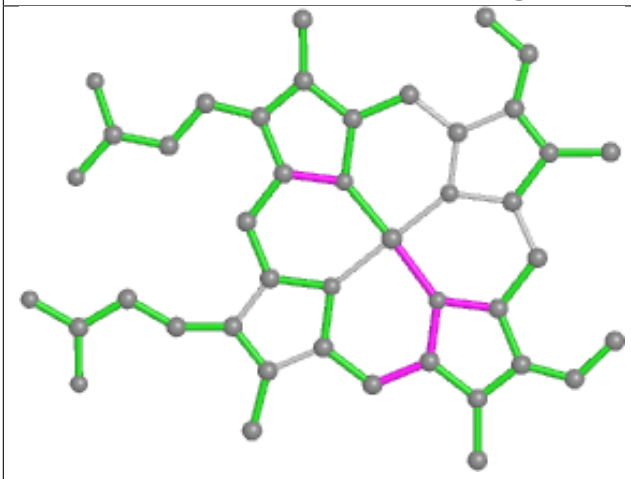


Torsions

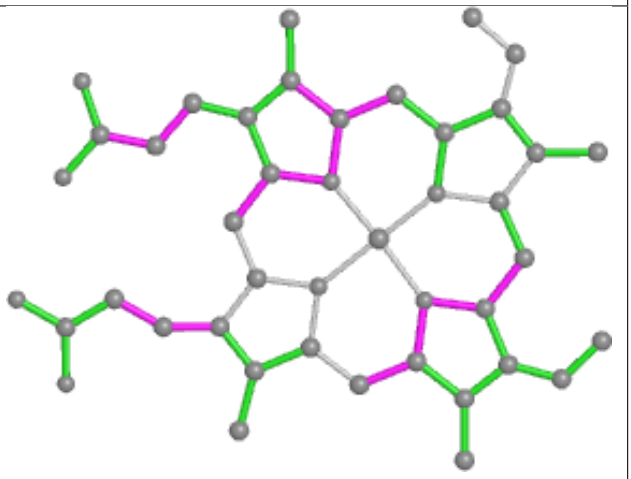


Rings

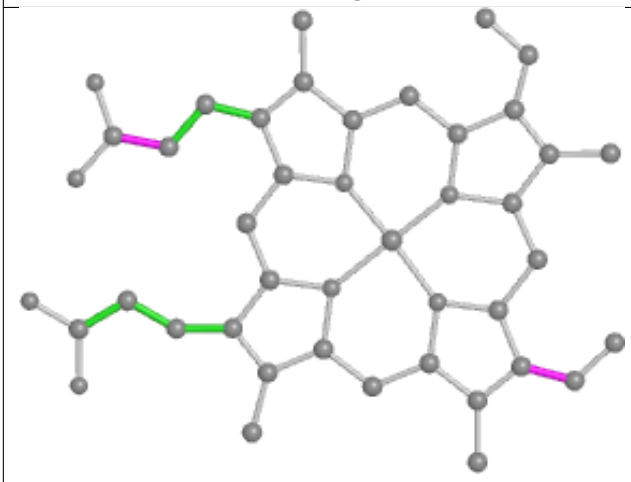
Ligand HEM 3P 501



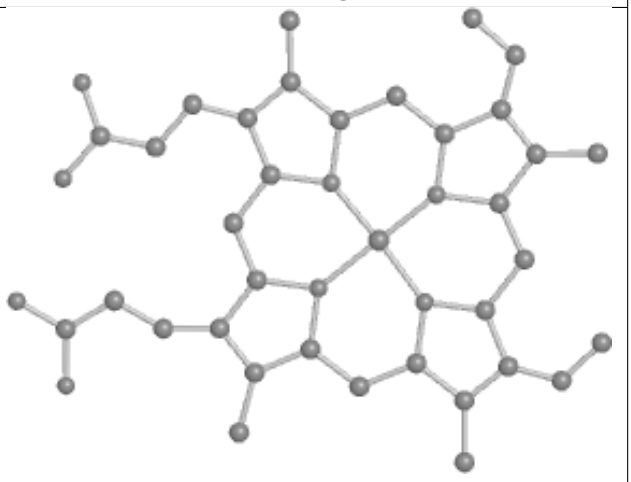
Bond lengths



Bond angles

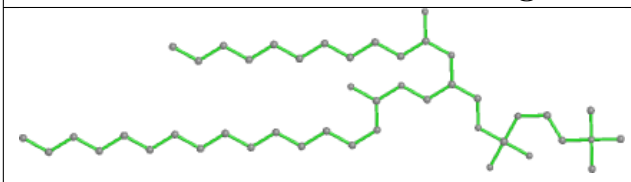


Torsions

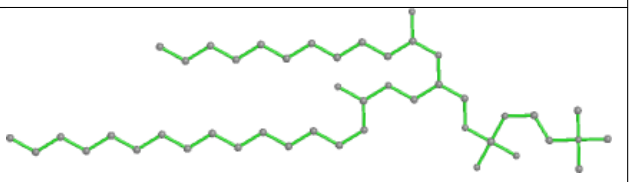


Rings

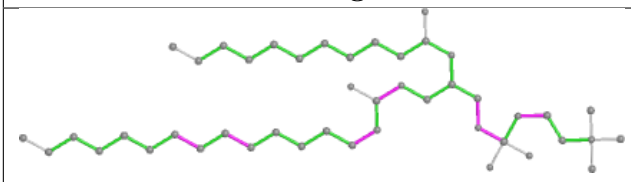
Ligand PC1 3R 303



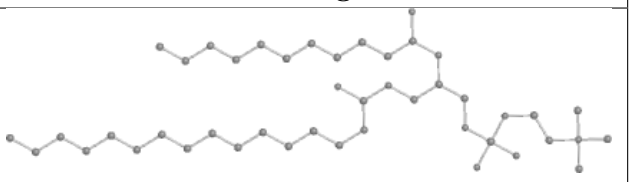
Bond lengths



Bond angles

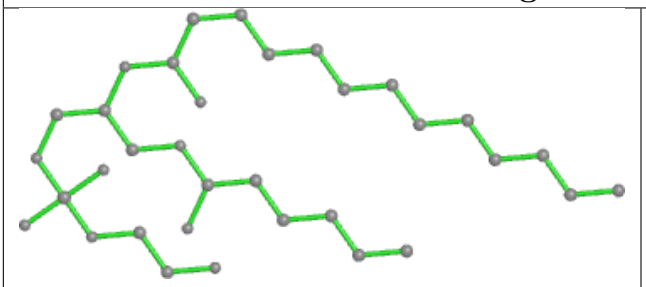


Torsions

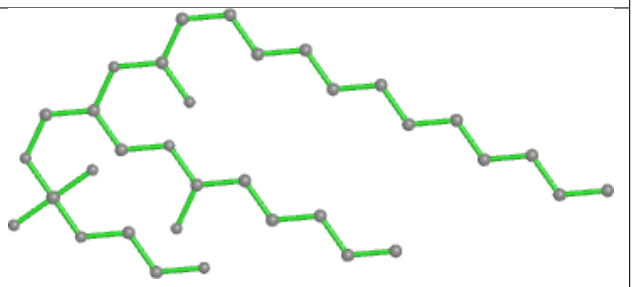


Rings

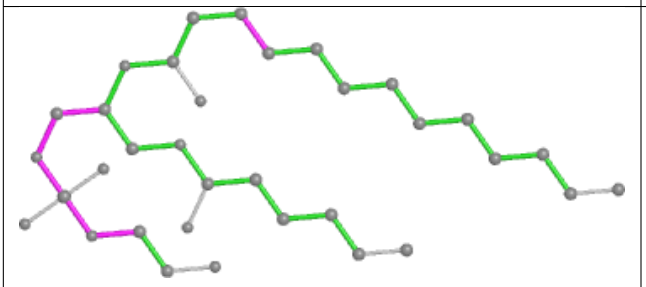
Ligand 3PE 3C 506



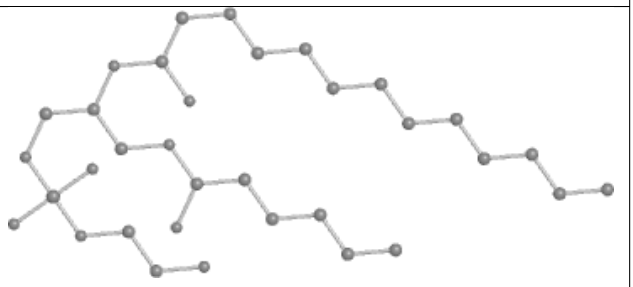
Bond lengths



Bond angles

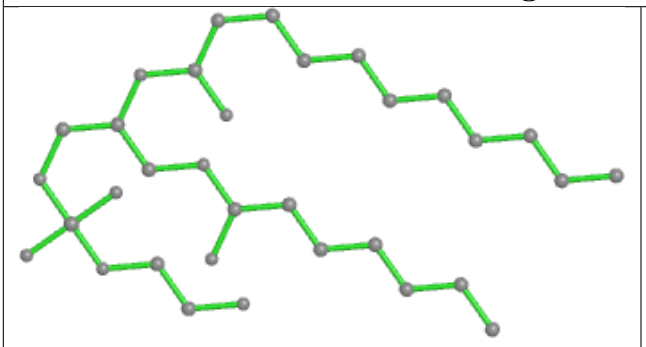


Torsions

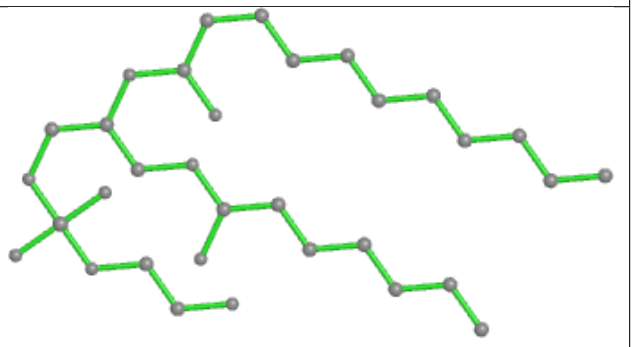


Rings

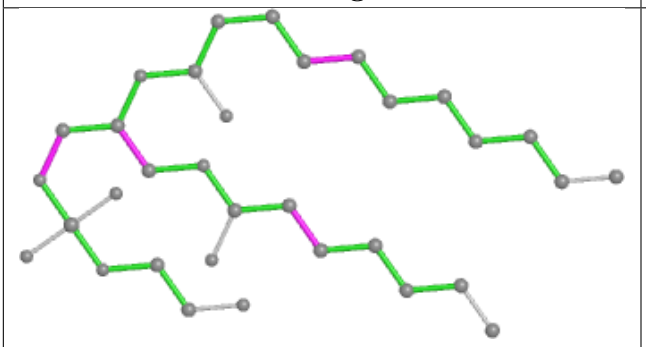
Ligand 3PE 3P 505



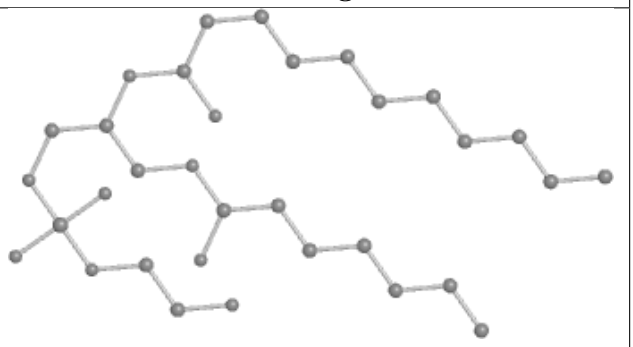
Bond lengths



Bond angles

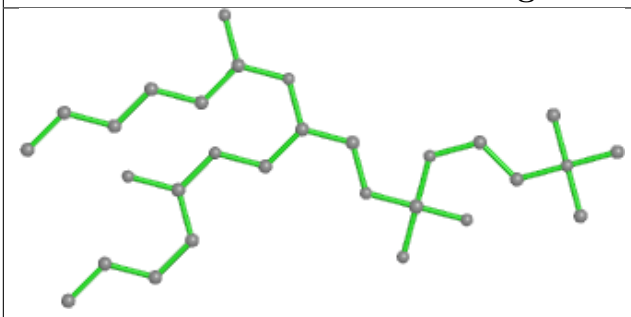


Torsions

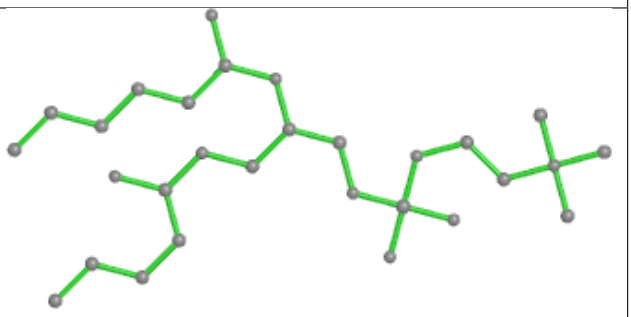


Rings

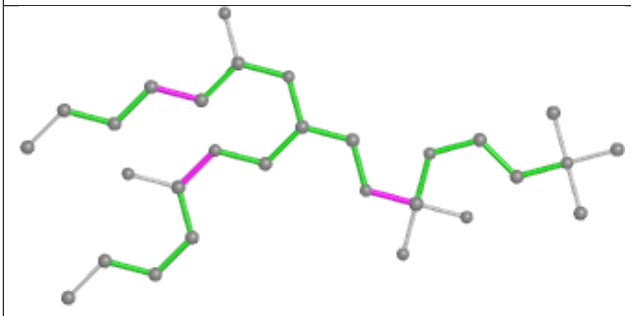
Ligand PC1 3X 101



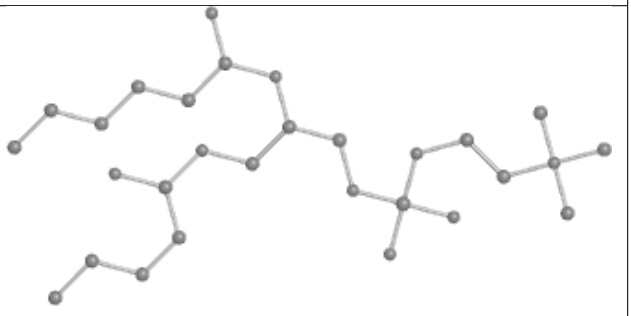
Bond lengths



Bond angles

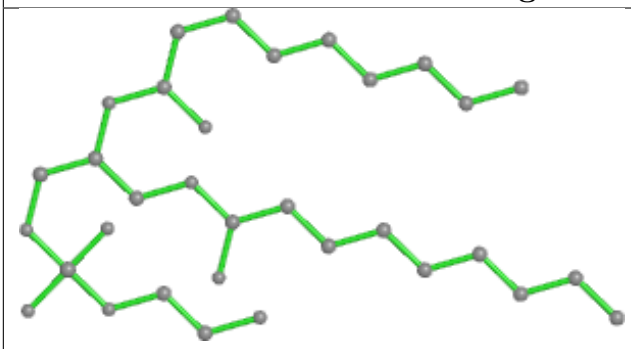


Torsions

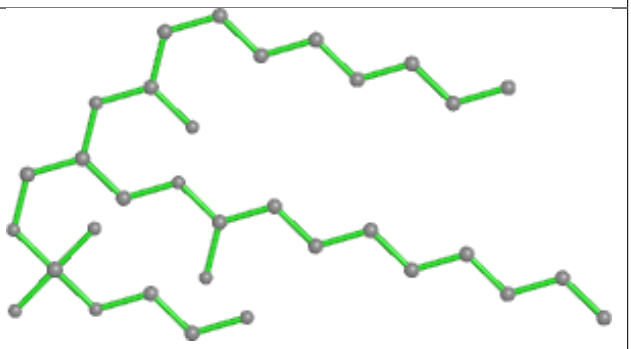


Rings

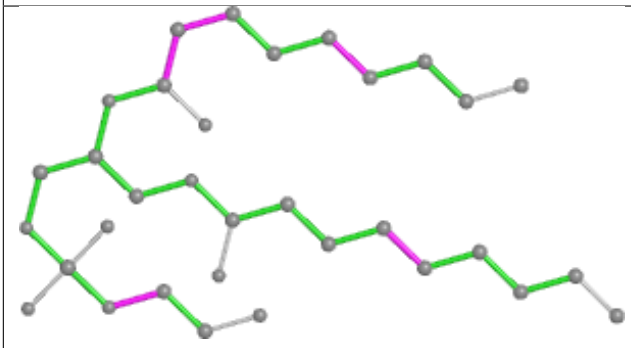
Ligand 3PE 3D 502



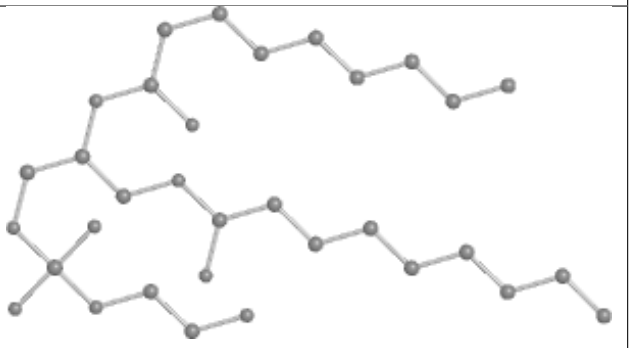
Bond lengths



Bond angles

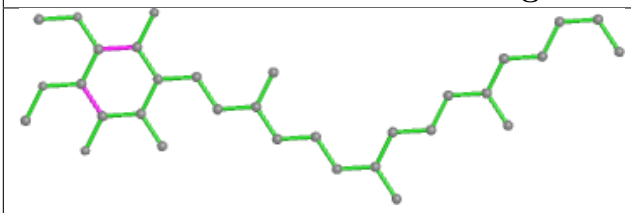


Torsions

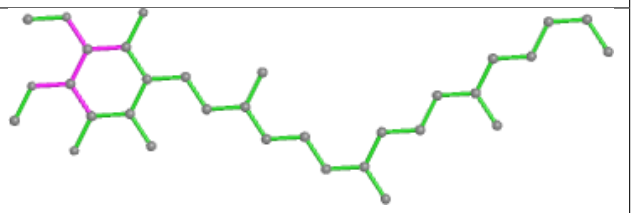


Rings

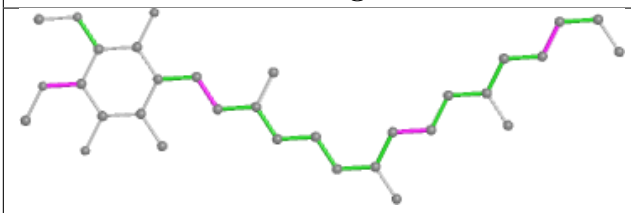
Ligand U10 3P 504



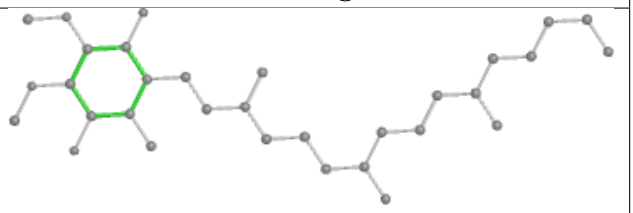
Bond lengths



Bond angles

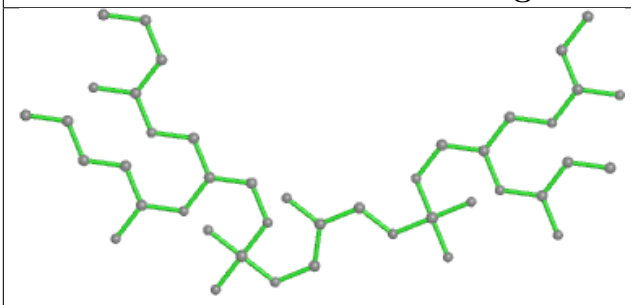


Torsions

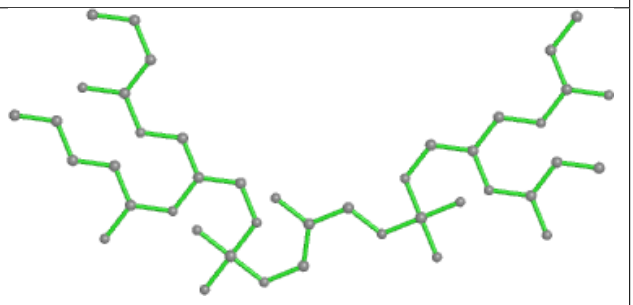


Rings

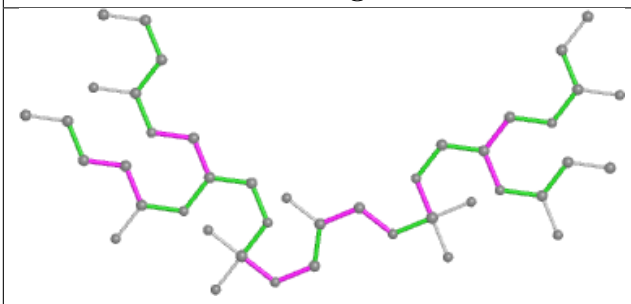
Ligand CDL 3N 502



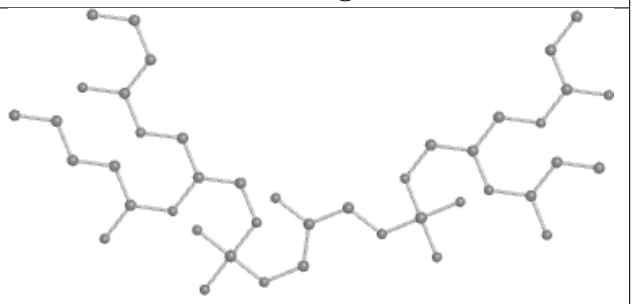
Bond lengths



Bond angles

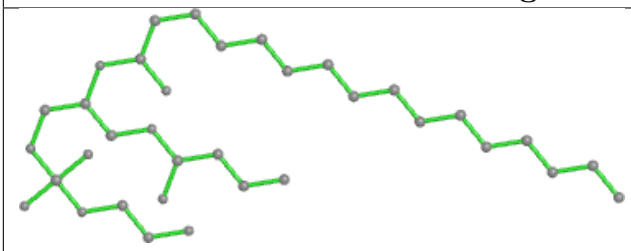


Torsions

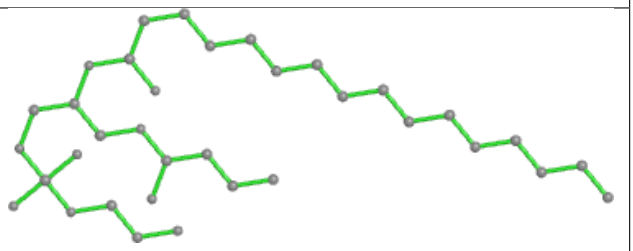


Rings

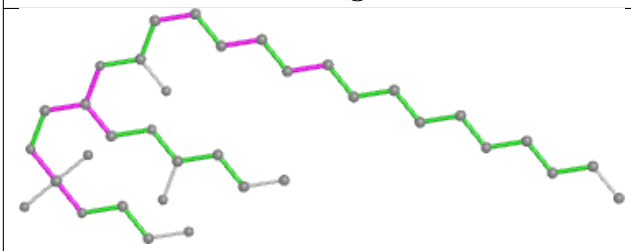
Ligand 3PE 3C 505



Bond lengths



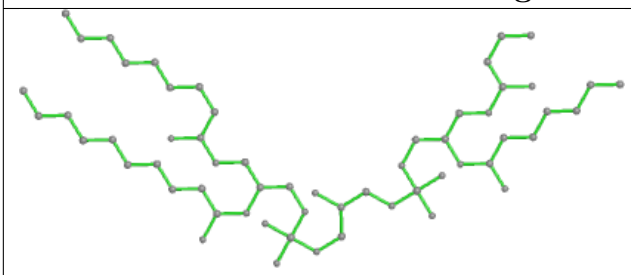
Bond angles



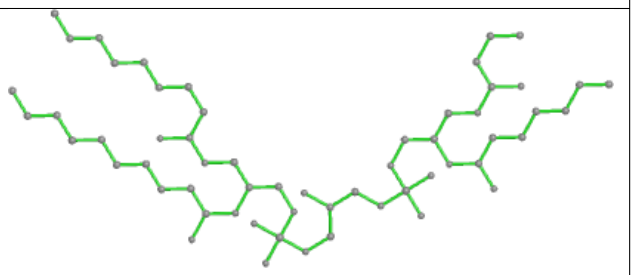
Torsions

Rings

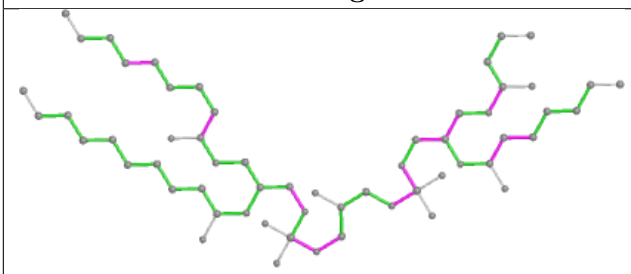
Ligand CDL 3A 501



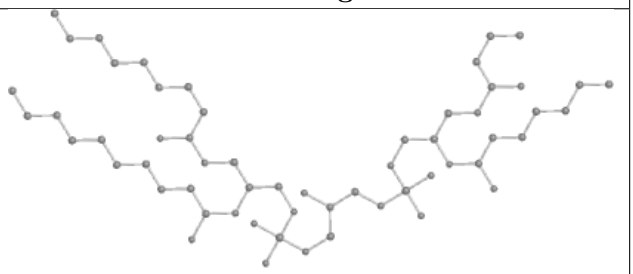
Bond lengths



Bond angles

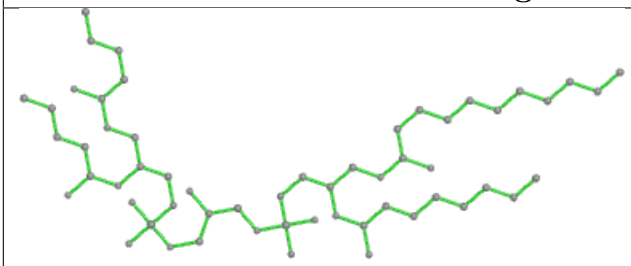


Torsions

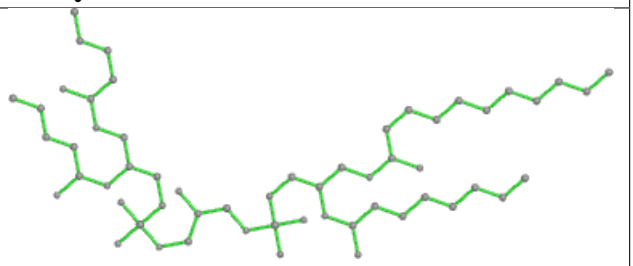


Rings

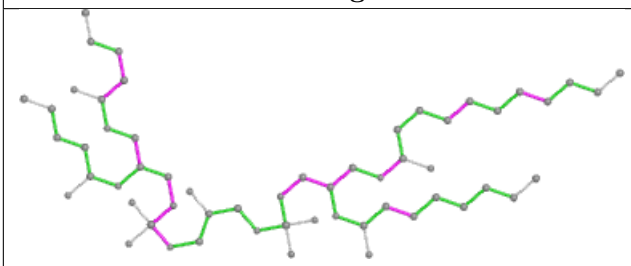
Ligand CDL 3Q 502



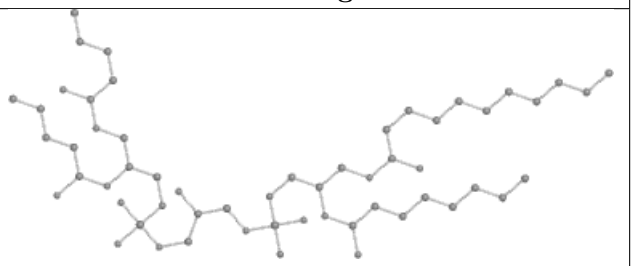
Bond lengths



Bond angles

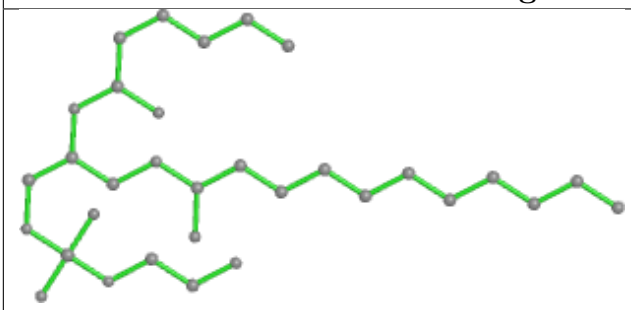


Torsions

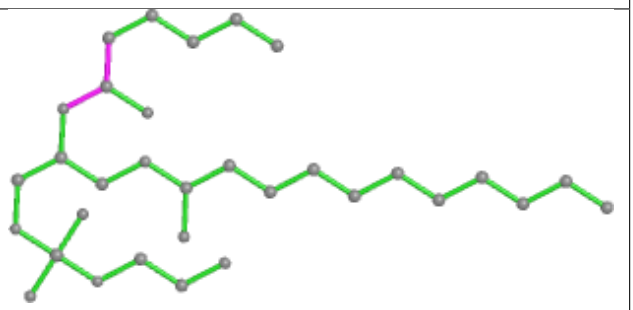


Rings

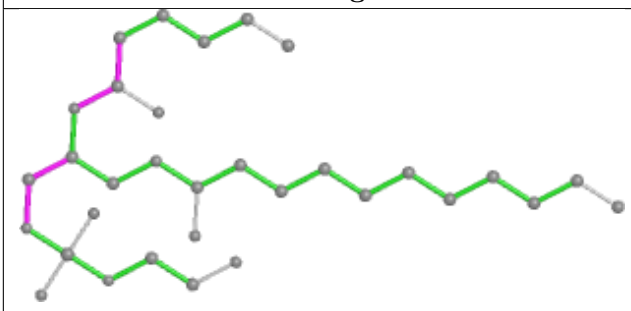
Ligand 3PE 3A 503



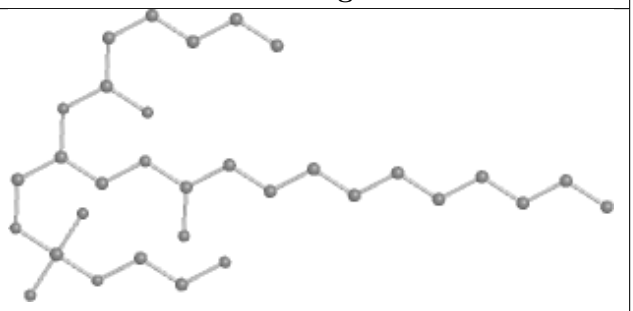
Bond lengths



Bond angles

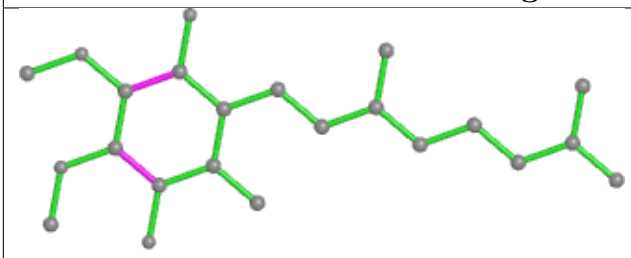


Torsions

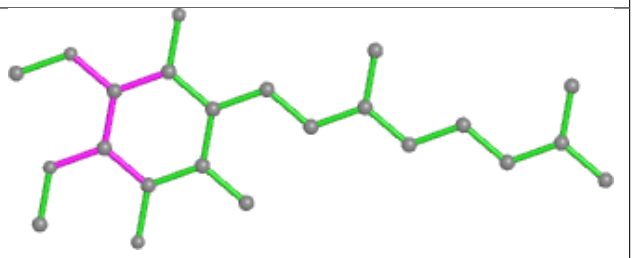


Rings

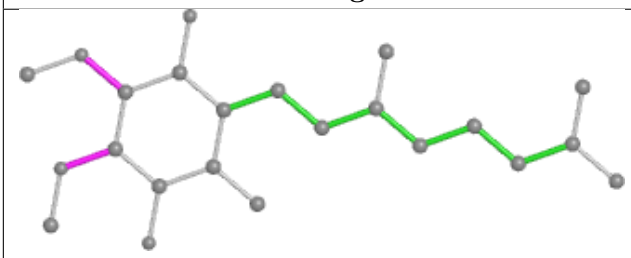
Ligand U10 3C 504



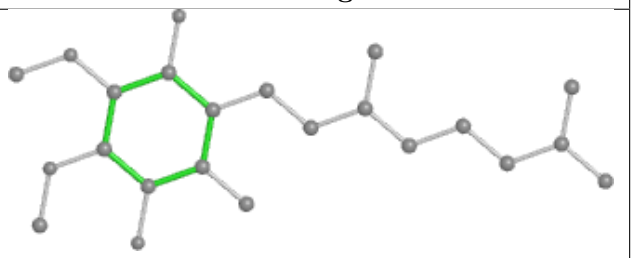
Bond lengths



Bond angles

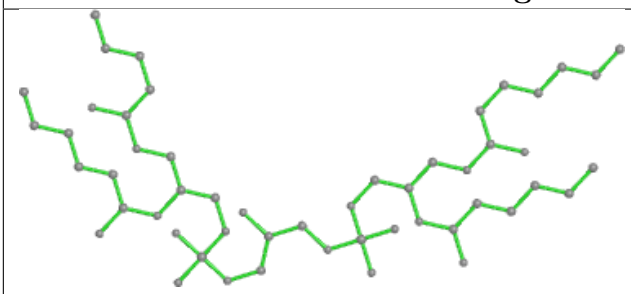


Torsions

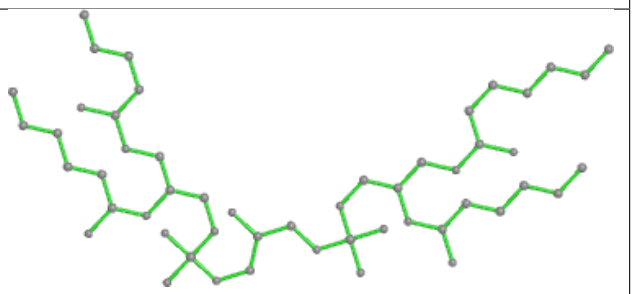


Rings

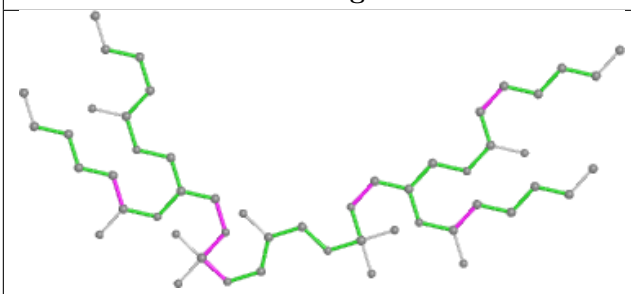
Ligand CDL 3G 102



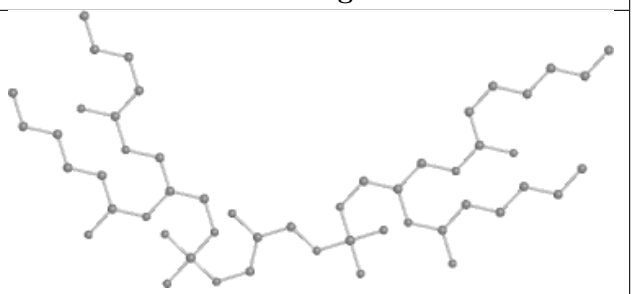
Bond lengths



Bond angles

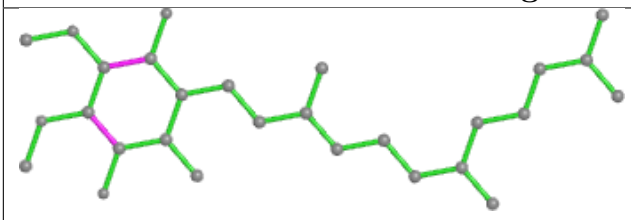


Torsions

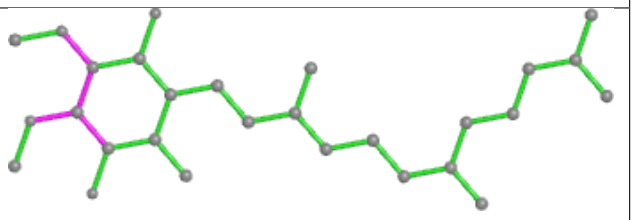


Rings

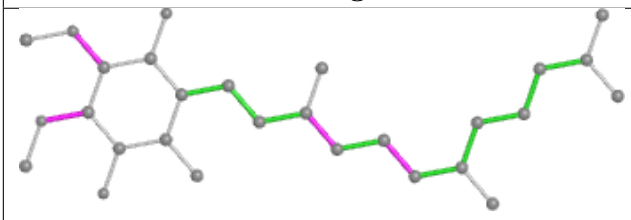
Ligand U10 3C 503



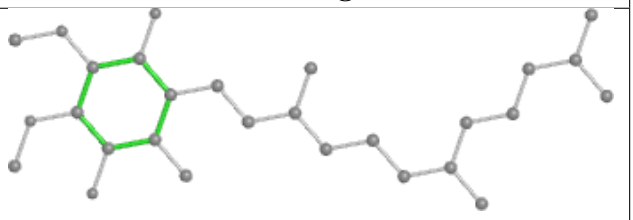
Bond lengths



Bond angles

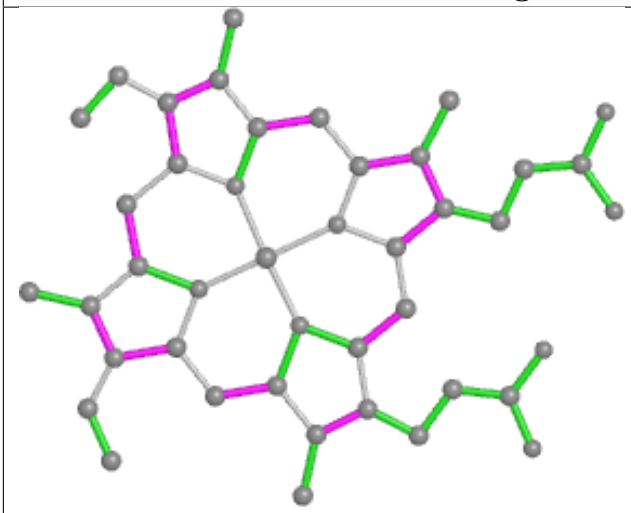


Torsions

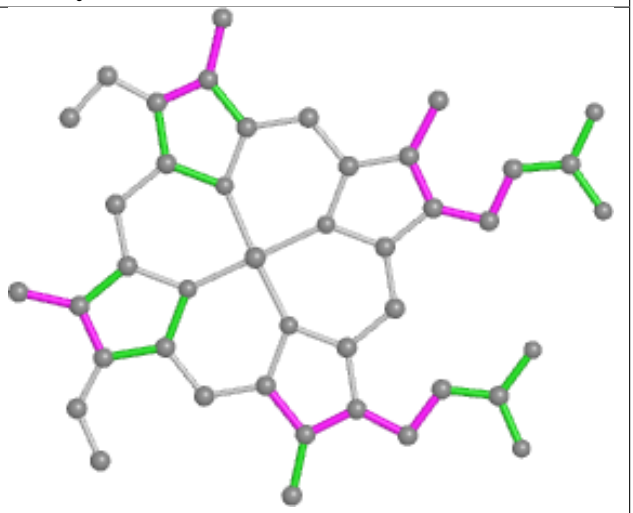


Rings

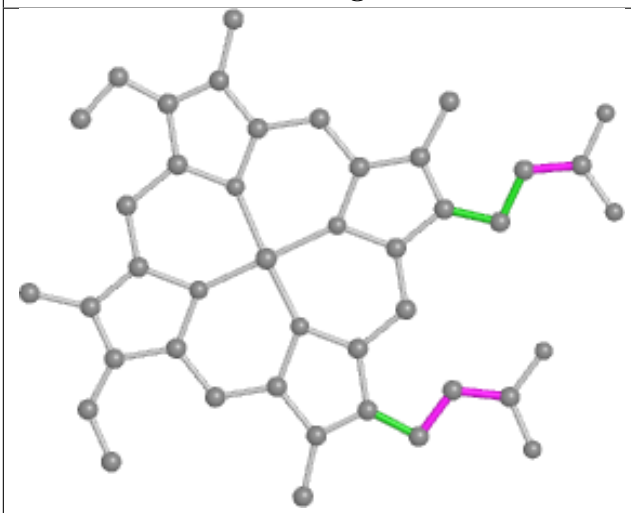
Ligand HEC 3Q 501



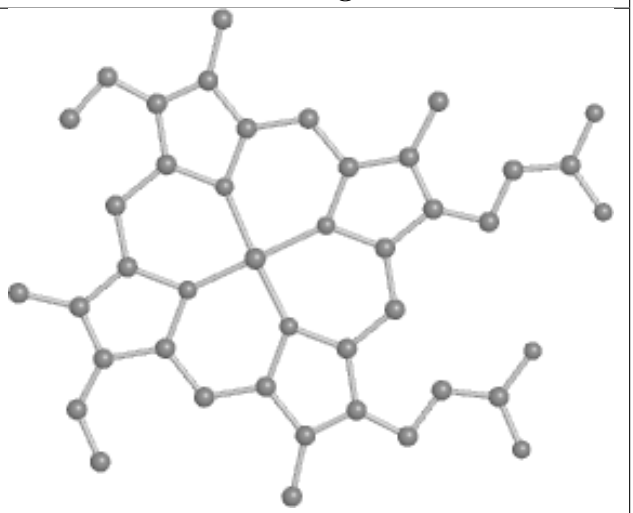
Bond lengths



Bond angles

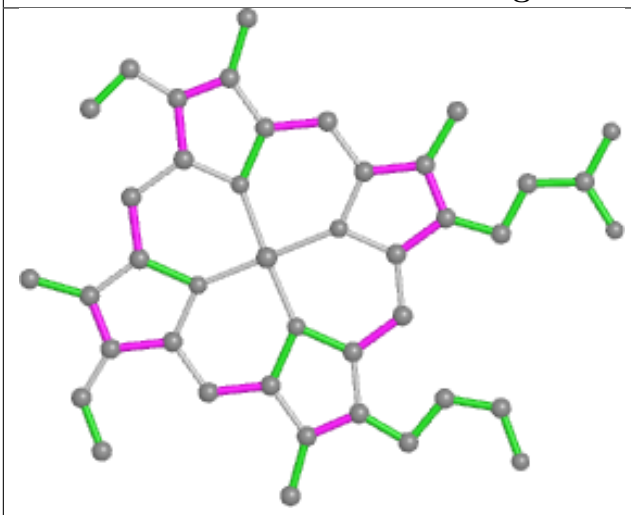


Torsions

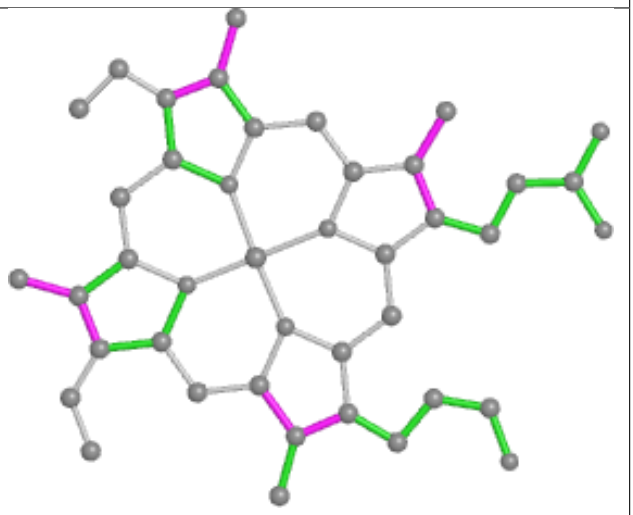


Rings

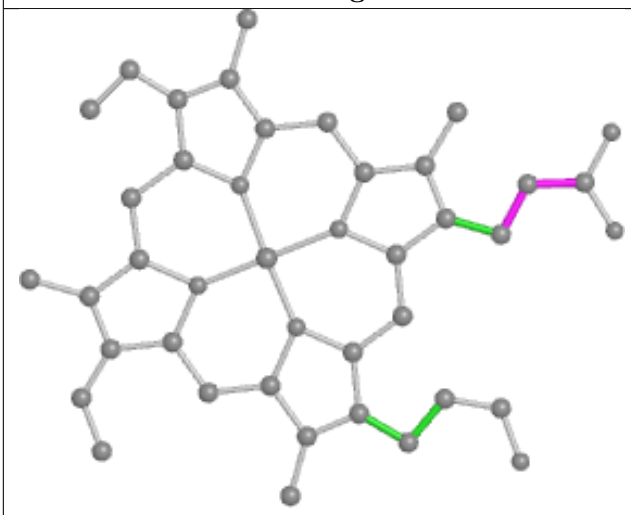
Ligand HEC 3D 501



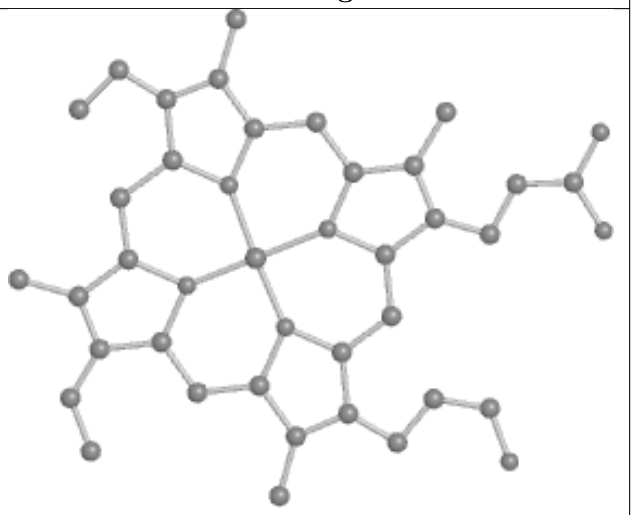
Bond lengths



Bond angles

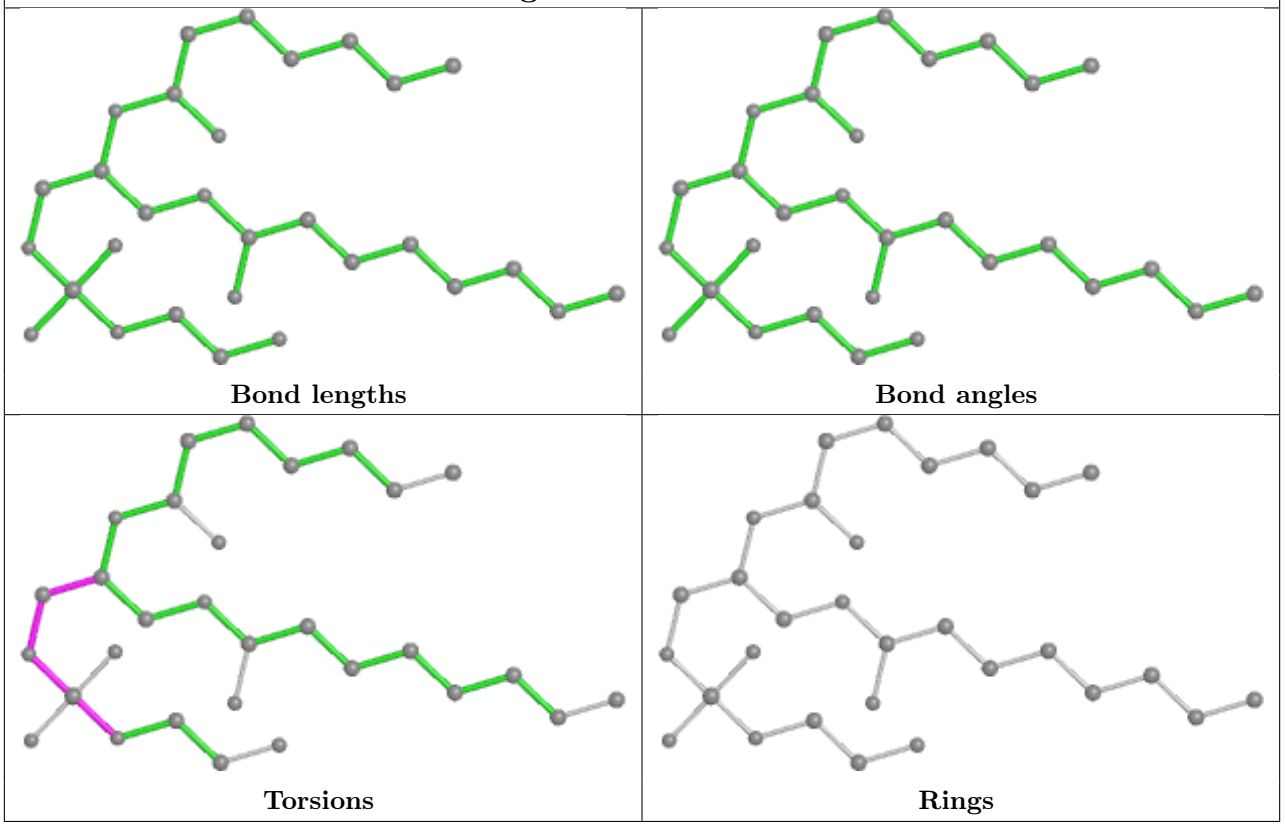


Torsions

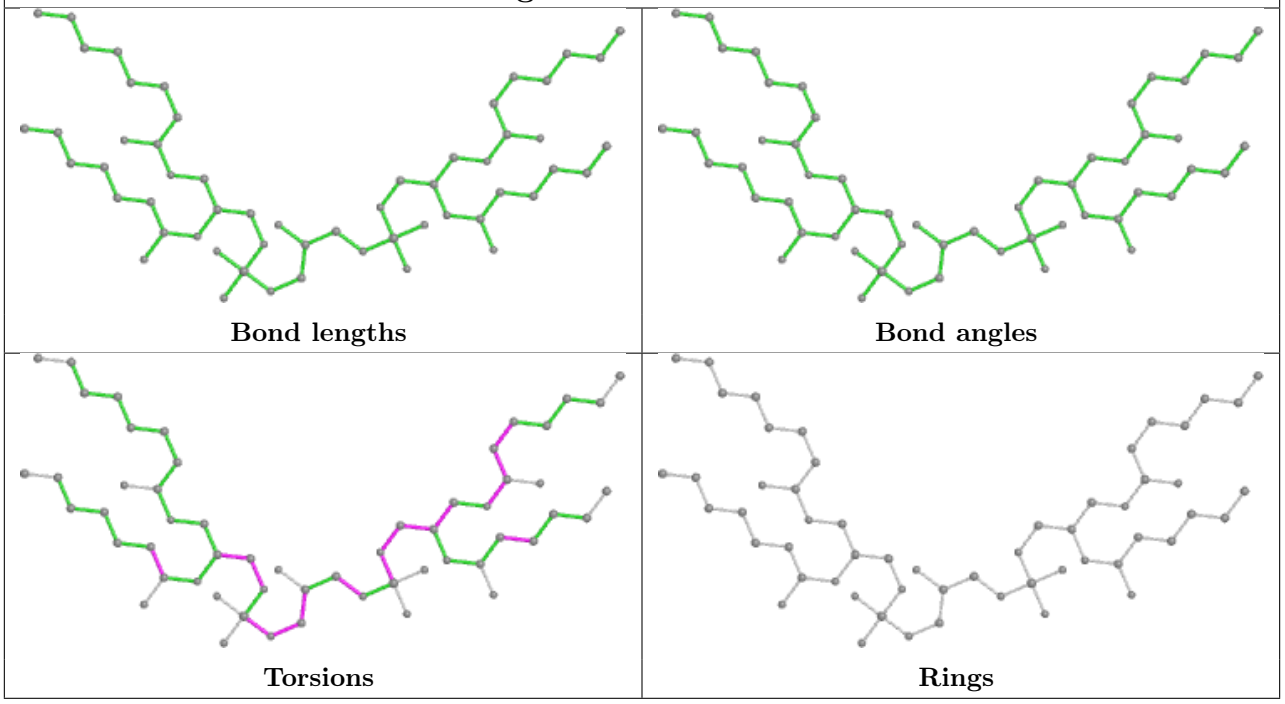


Rings

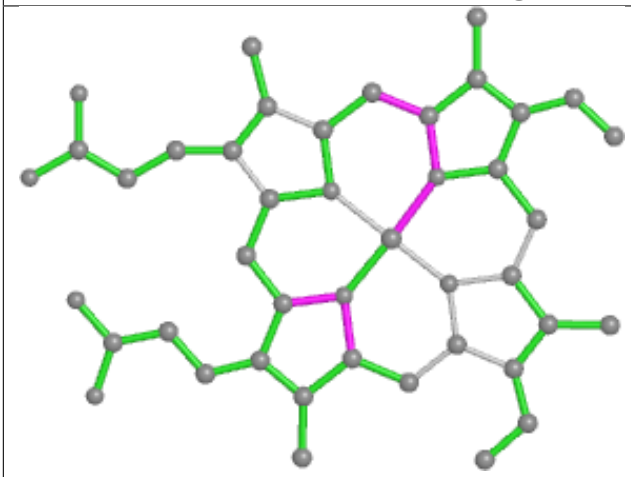
Ligand 3PE 3Y 101



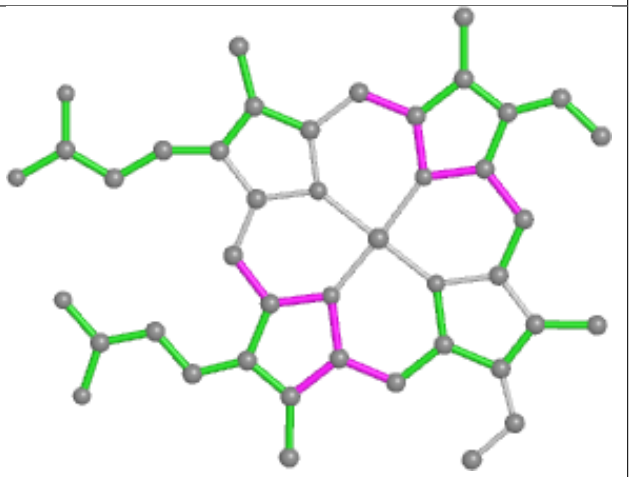
Ligand CDL 3P 506



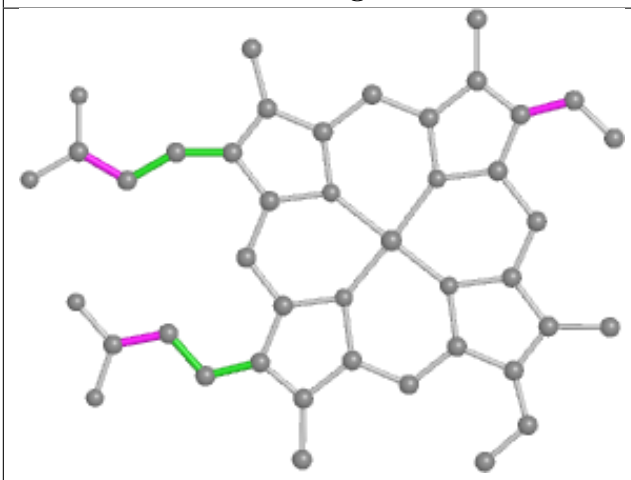
Ligand HEM 3P 502



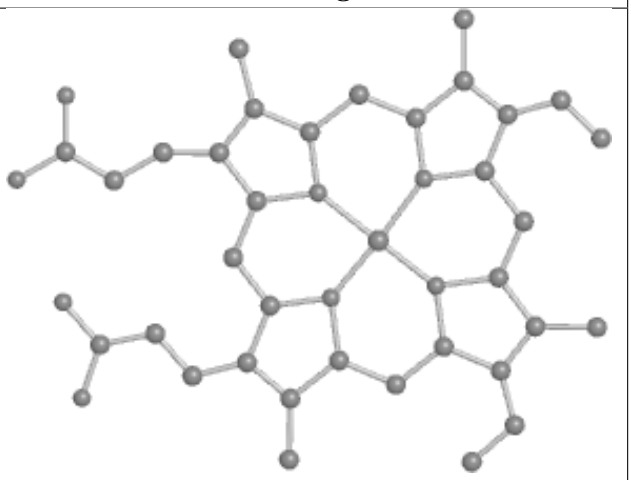
Bond lengths



Bond angles

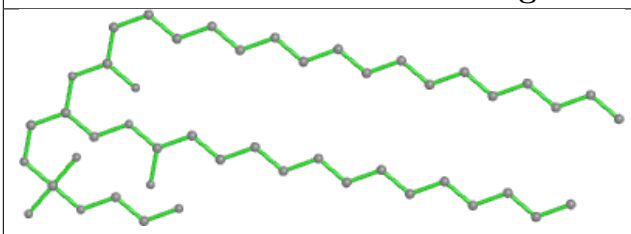


Torsions

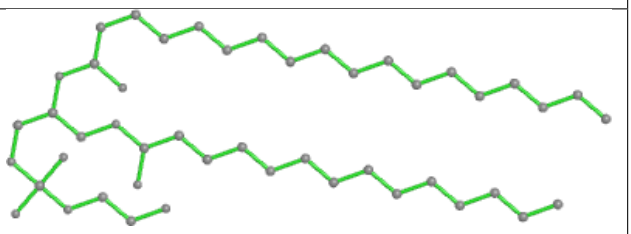


Rings

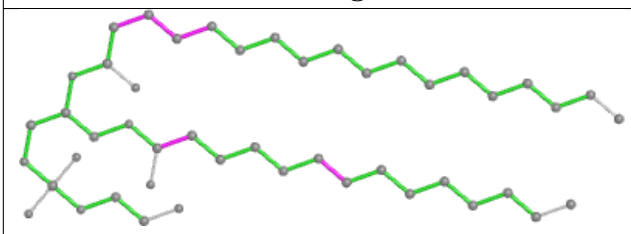
Ligand 3PE 3R 302



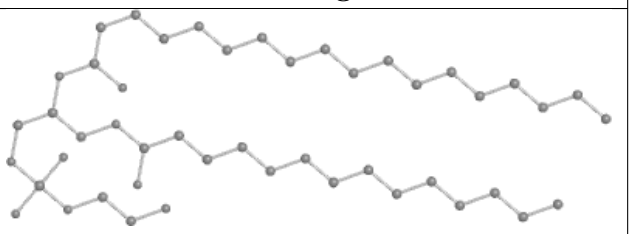
Bond lengths



Bond angles

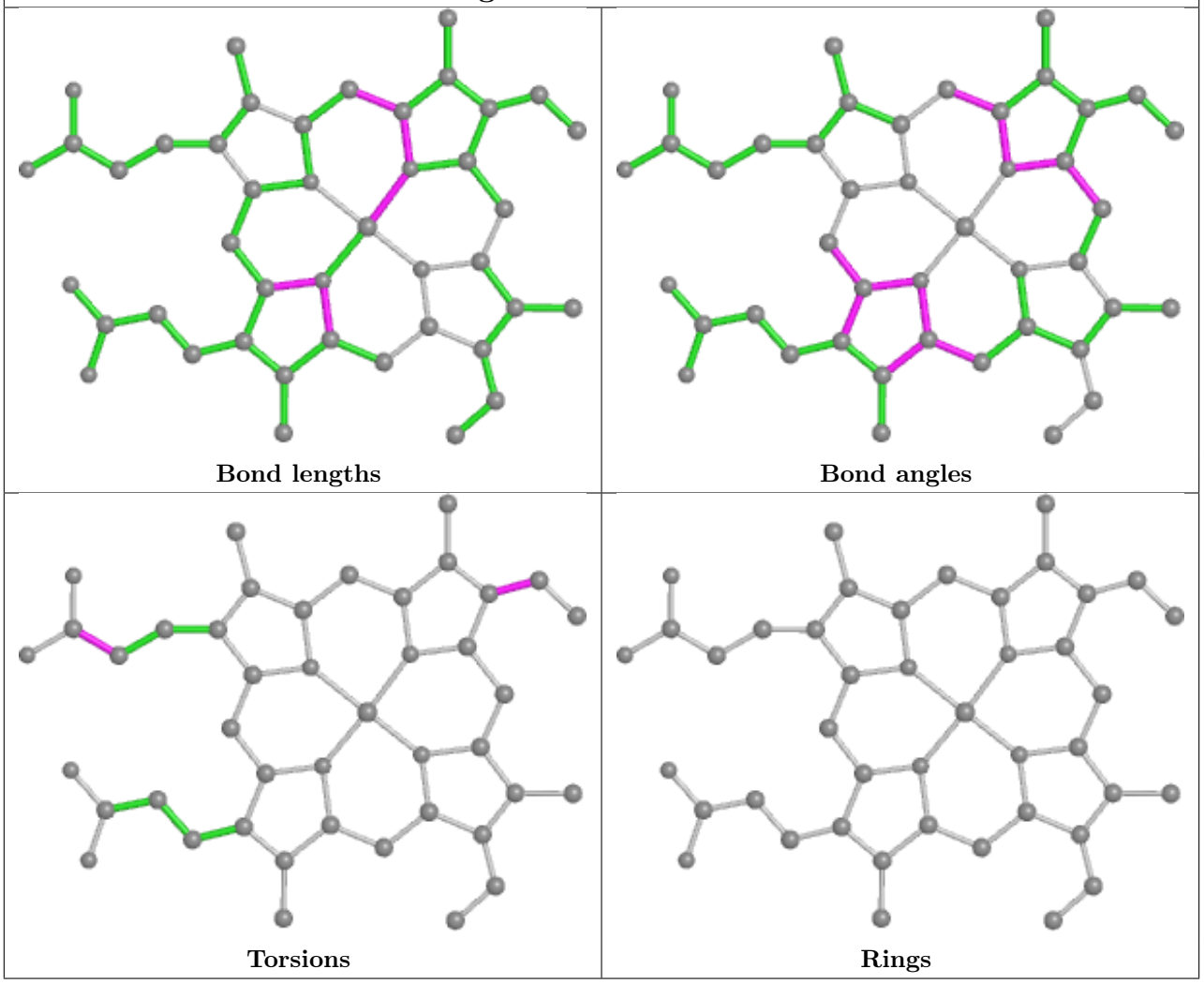


Torsions



Rings

Ligand HEM 3C 502



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
7	3G	1
8	3H	1
5	3I	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	3G	75:ASN	C	82:PRO	N	3.36
1	3H	77:GLU	C	78:ASP	N	3.12
1	3I	49:PHE	C	50:LEU	N	1.97

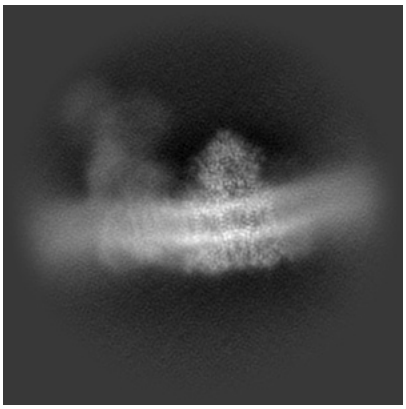
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-42224. These allow visual inspection of the internal detail of the map and identification of artifacts.

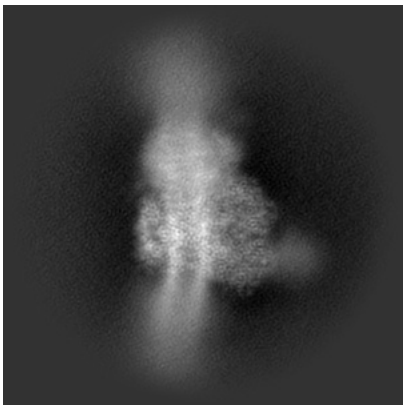
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

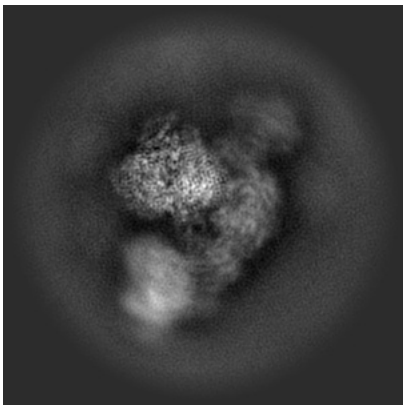
6.1.1 Primary map



X

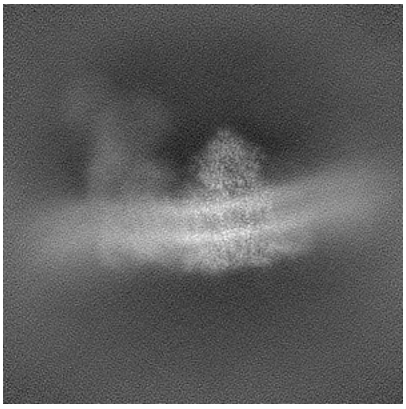


Y

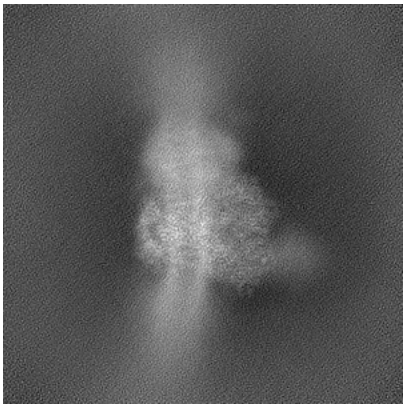


Z

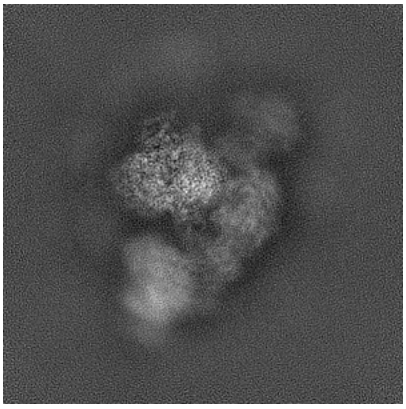
6.1.2 Raw map



X



Y

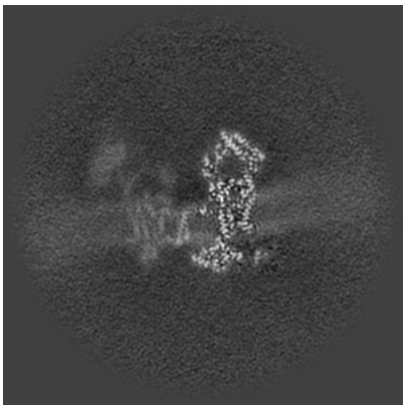


Z

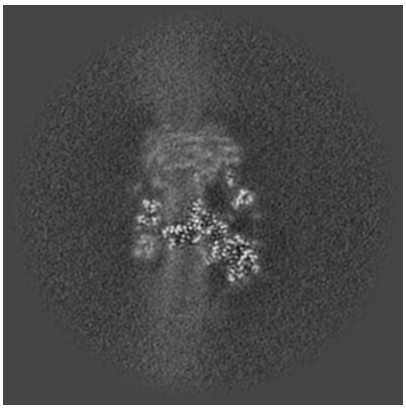
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

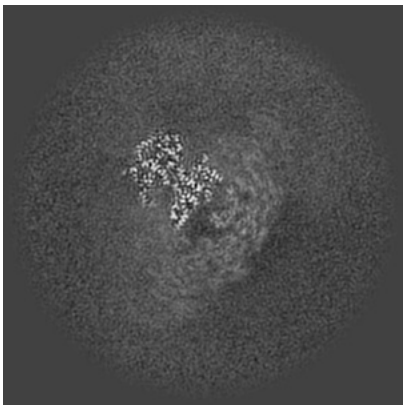
6.2.1 Primary map



X Index: 160

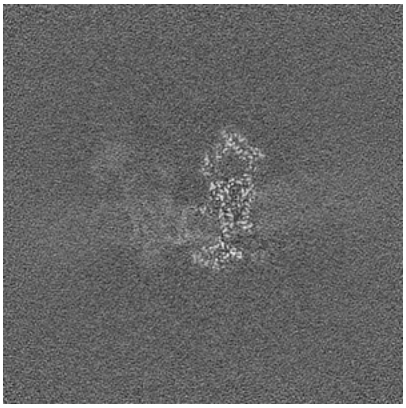


Y Index: 160

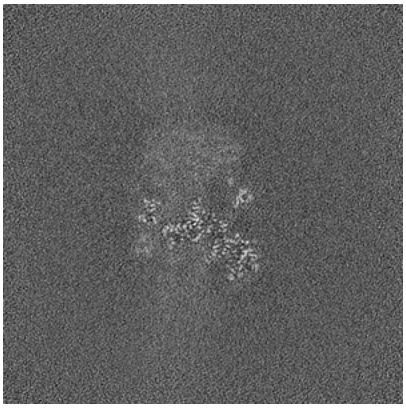


Z Index: 160

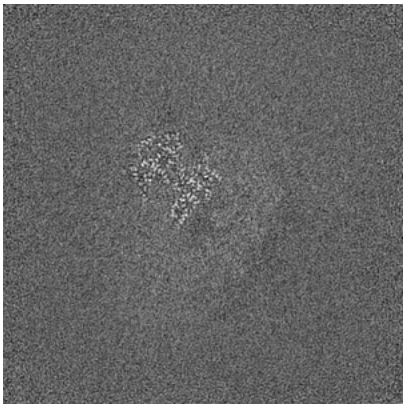
6.2.2 Raw map



X Index: 160



Y Index: 160

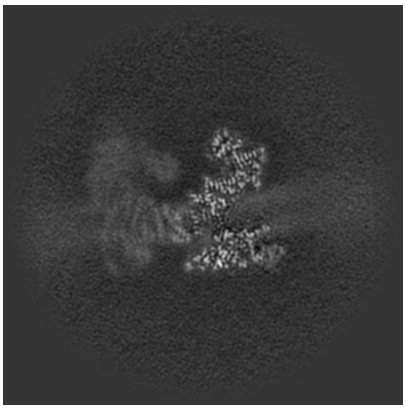


Z Index: 160

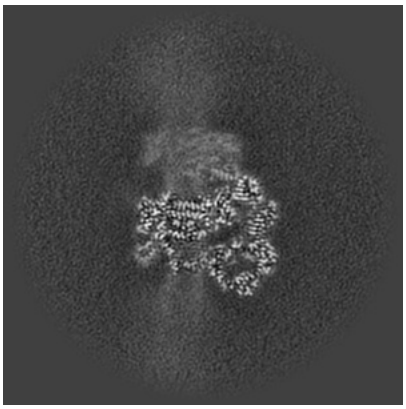
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

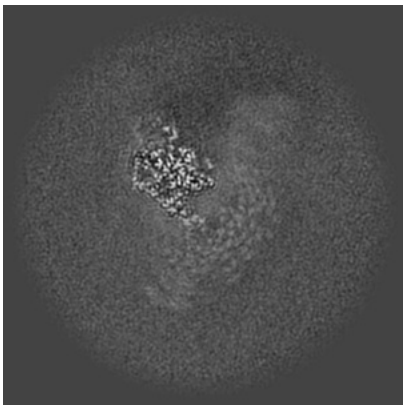
6.3.1 Primary map



X Index: 148

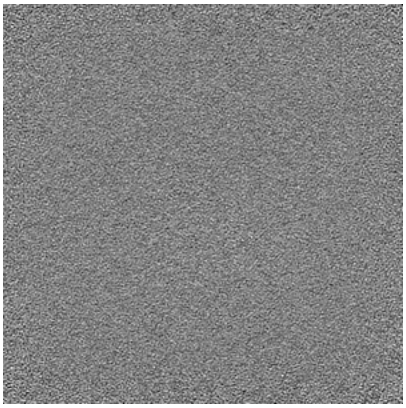


Y Index: 175

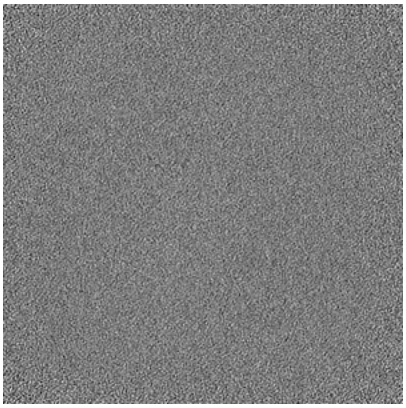


Z Index: 136

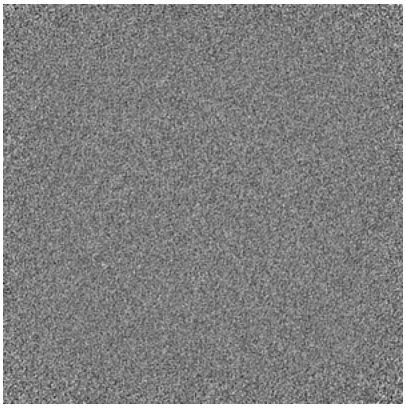
6.3.2 Raw map



X Index: 0



Y Index: 0

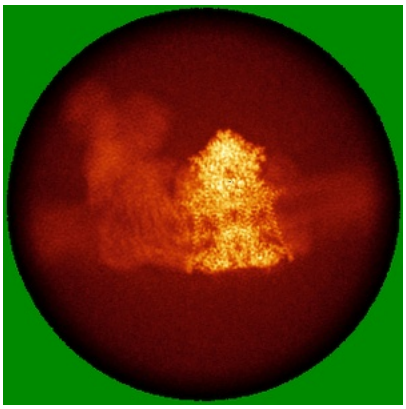


Z Index: 0

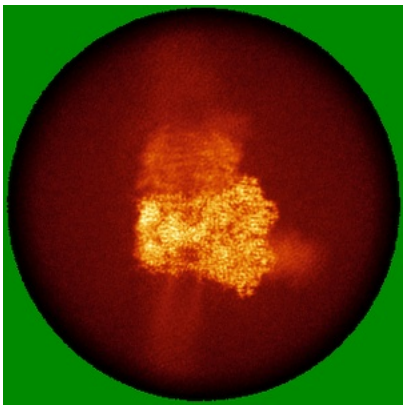
The images above show the largest variance slices of the map in three orthogonal directions.

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

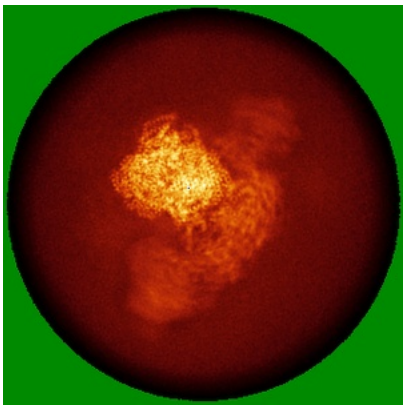
6.4.1 Primary map



X

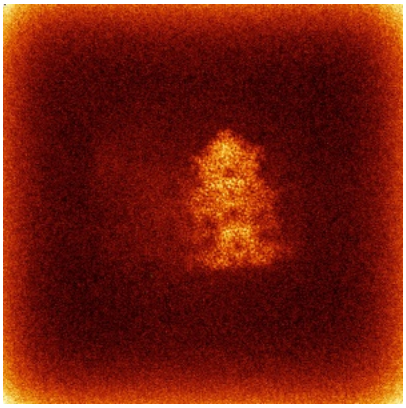


Y

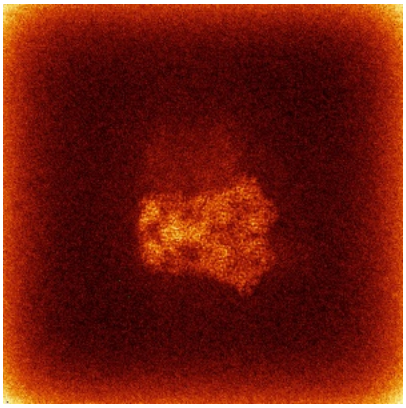


Z

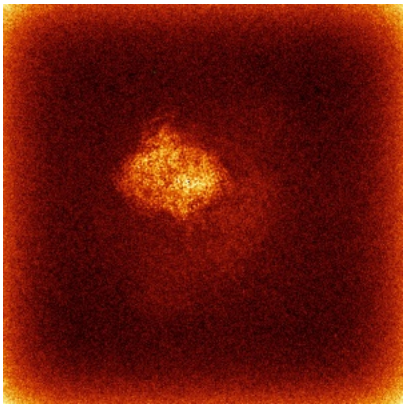
6.4.2 Raw map



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.

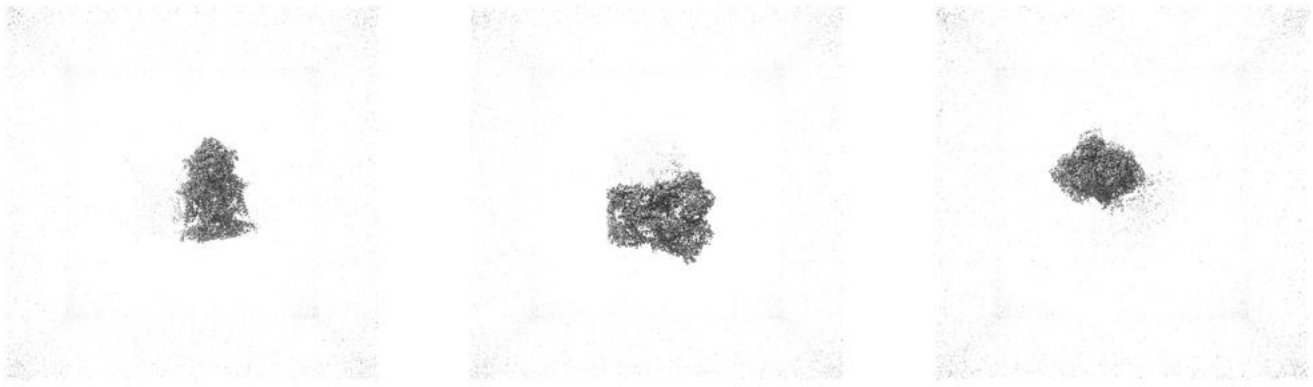
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.15. 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.

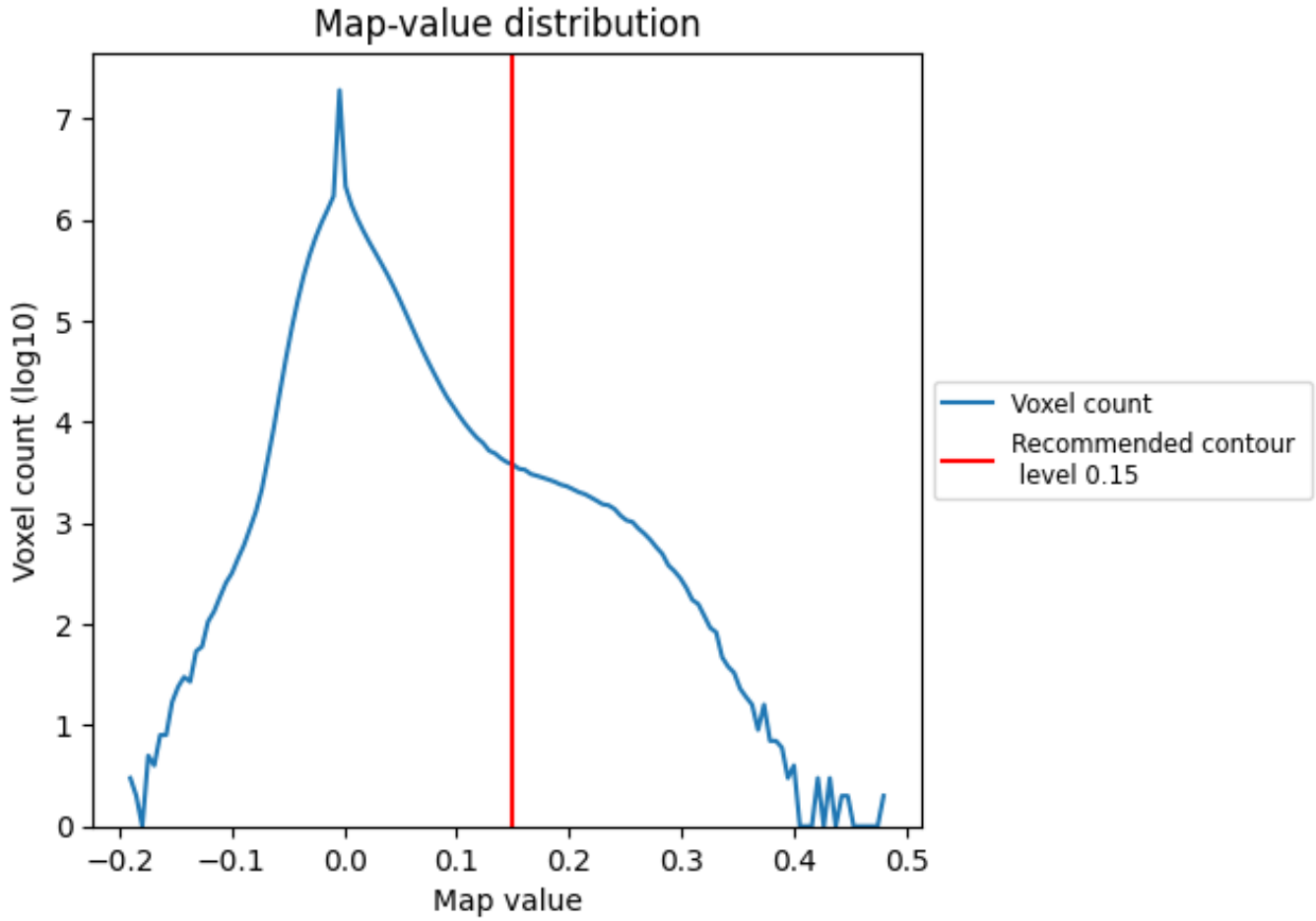
6.6 Mask visualisation (i)

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

7 Map analysis

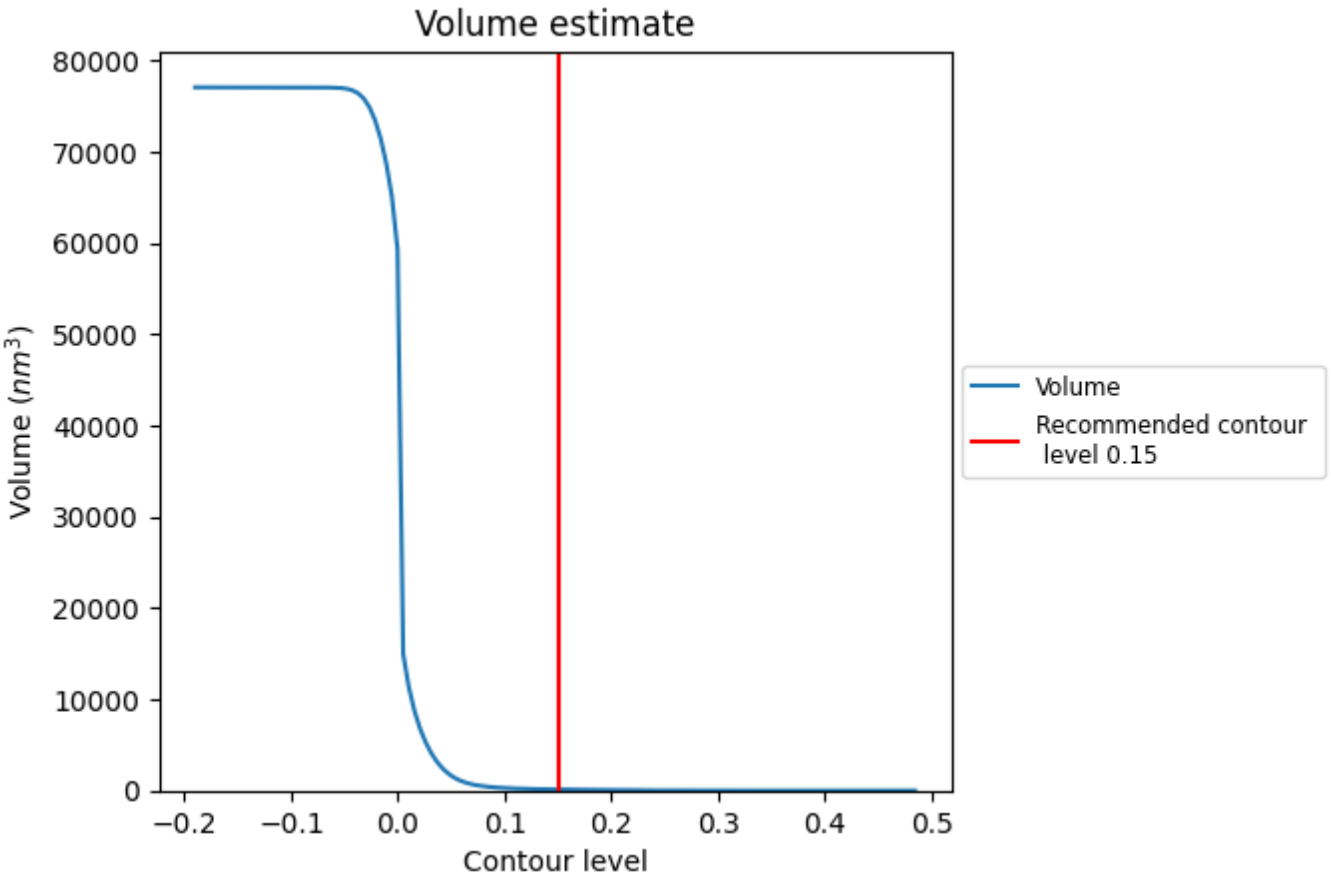
This section contains the results of statistical analysis of the map.

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.

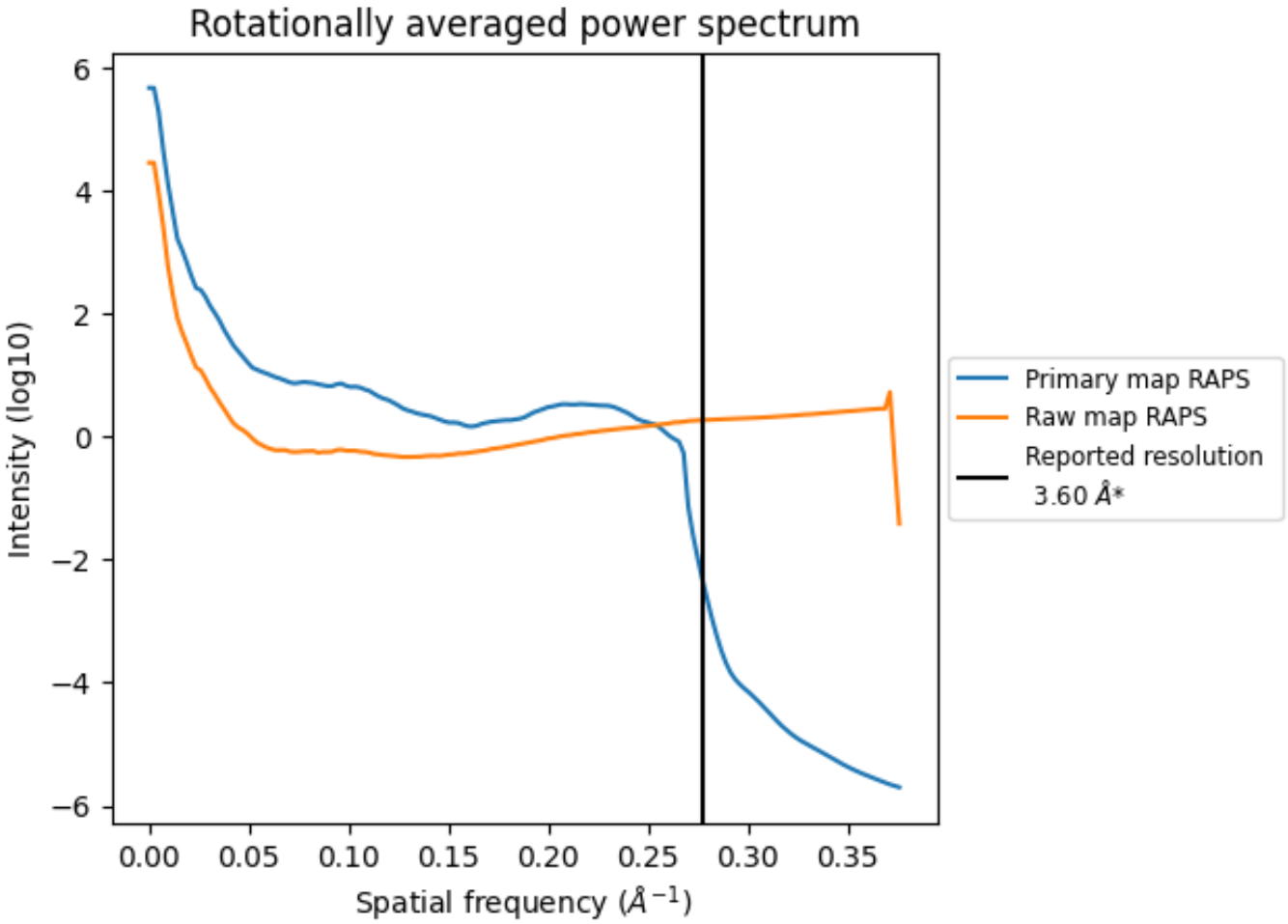
7.2 Volume estimate



The volume at the recommended contour level is 123 nm^3; this corresponds to an approximate mass of 111 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)

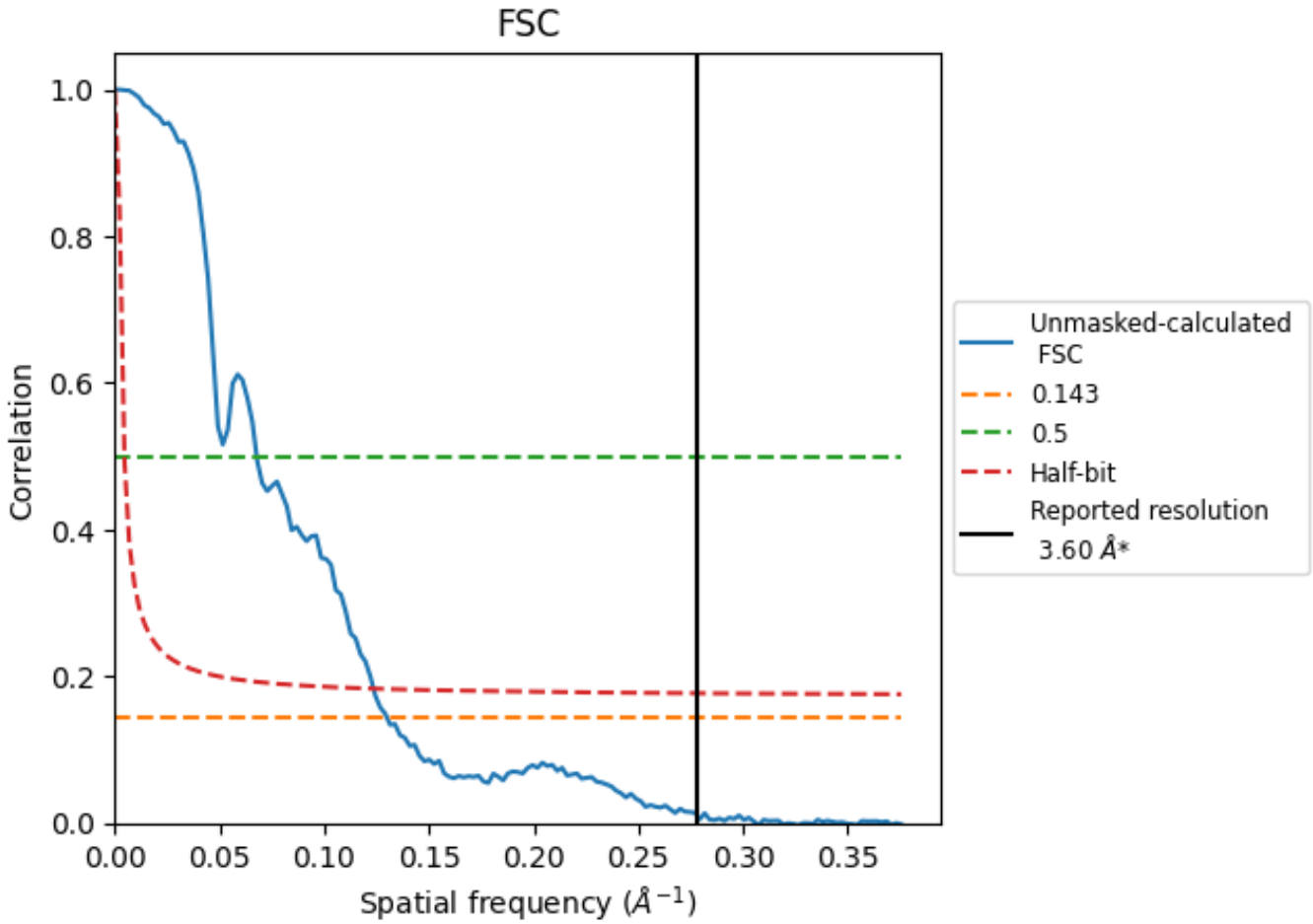


*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

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 0.278 Å^{-1}

8.2 Resolution estimates (i)

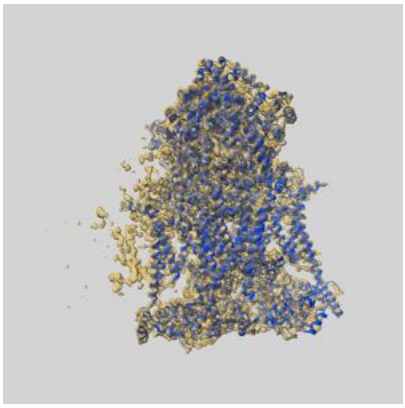
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.69	14.75	8.09

*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 7.69 differs from the reported value 3.6 by more than 10 %

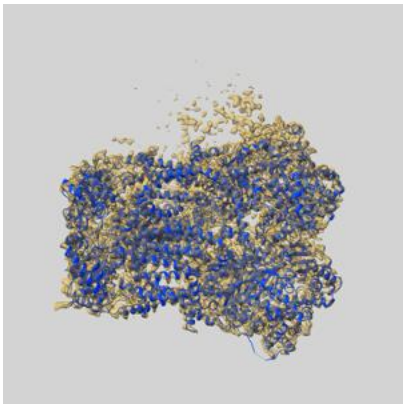
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-42224 and PDB model 8UGG. Per-residue inclusion information can be found in section 3 on page 12.

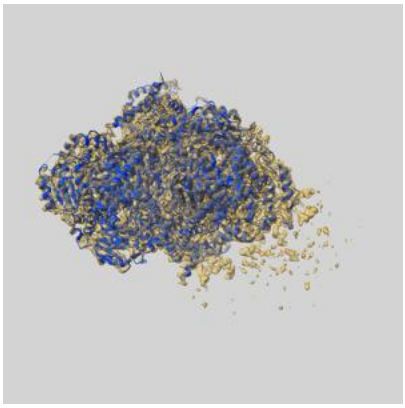
9.1 Map-model overlay



X



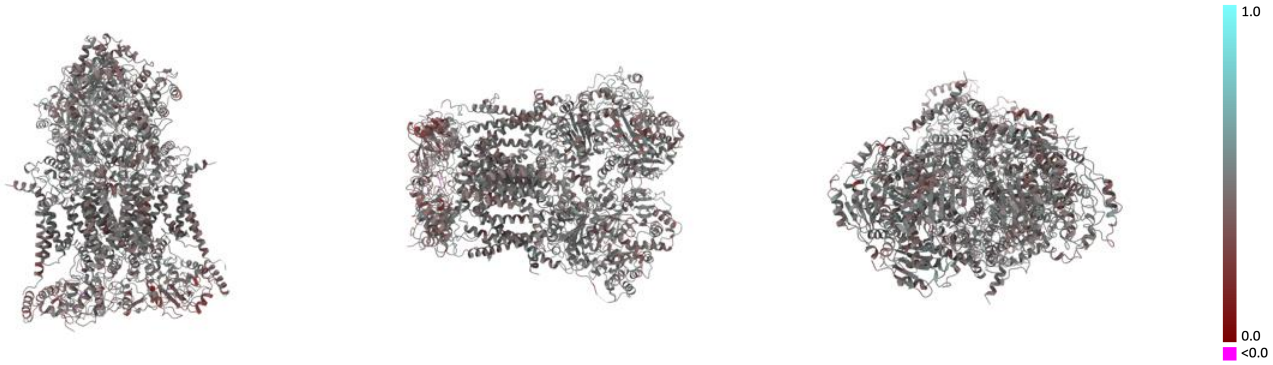
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.15 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.

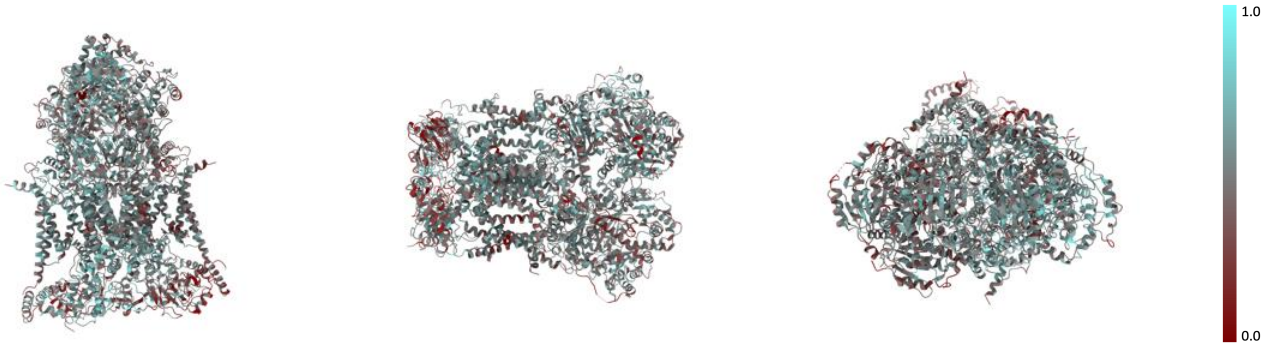
9.2 Q-score mapped to coordinate model (i)



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.

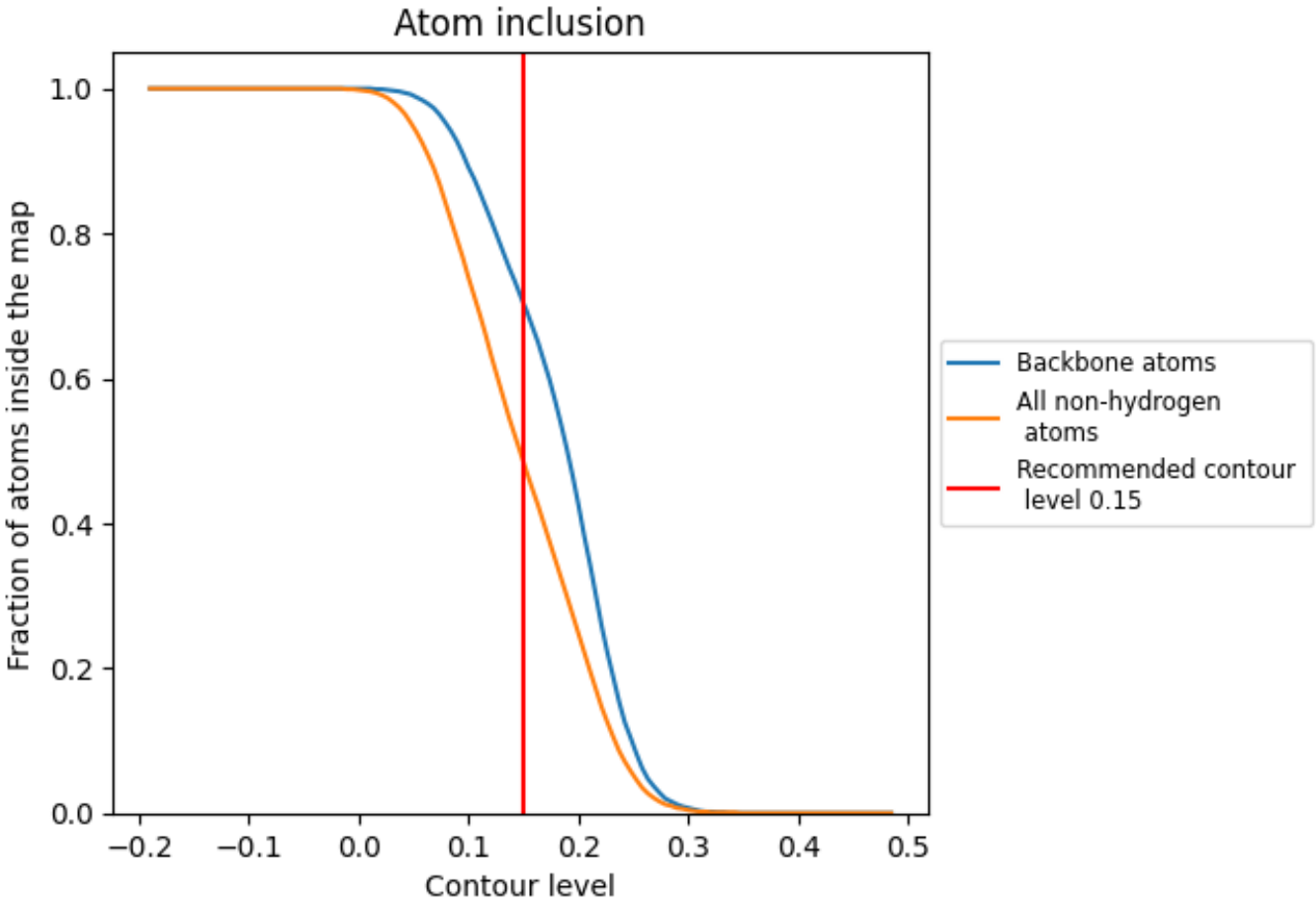
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.15).

9.4 Atom inclusion (i)



At the recommended contour level, 70% of all backbone atoms, 48% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4840	0.4470
3A	0.4700	0.4580
3B	0.4810	0.4600
3C	0.5220	0.4560
3D	0.5070	0.4580
3E	0.2290	0.3590
3F	0.4590	0.4580
3G	0.4150	0.4460
3H	0.3450	0.4190
3I	0.1070	0.3810
3J	0.4650	0.4420
3N	0.5570	0.4580
3O	0.5240	0.4550
3P	0.5510	0.4580
3Q	0.5730	0.4500
3R	0.3770	0.3970
3S	0.5420	0.4670
3T	0.5540	0.4650
3U	0.5010	0.4210
3V	0.2090	0.4240
3W	0.5510	0.4610
3X	0.3830	0.4470
3Y	0.3500	0.4520