Full wwPDB EM Validation Report ⓘ

Sep 4, 2023 – 04:23 PM JST

PDB ID	:	8HCR
EMDB ID	:	EMD-34664
Title	:	Cryo-EM structure of the Mycobacterium tuberculosis cytochrome bcc:aa3 supercomplex and a novel inhibitor targeting subunit cytochrome cI
Authors	:	Mathiyazakan, V.; Gruber, G.
Deposited on	:	2022-11-02
Resolution	:	Not provided

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:

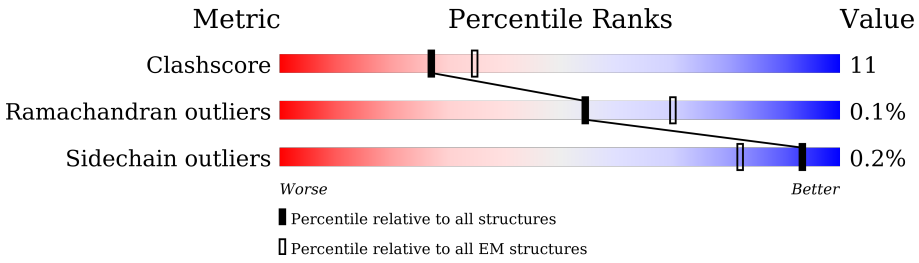
EMDB validation analysis	:	0.0.1.dev50
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance

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

The reported resolution of this entry is unknown.

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%

Mol	Chain	Length	Quality of chain
1	A	429	72% 16% 12%
1	M	429	68% 19% 13%
2	B	573	70% 22% 9%
2	N	573	70% 21% 9%
3	C	280	59% 19% 22%
3	O	280	59% 17% 24%
4	E	363	55% 21% 24%
4	Q	363	55% 23% 22%
5	F	573	66% 30% .

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Mol	Chain	Length	Quality of chain
5	R	573	71% 26%
6	G	203	72% 20% 8%
6	S	203	71% 19% 9%
7	H	139	84% 16%
7	T	139	83% 17%
8	I	79	73% 11% 15%
8	U	79	71% 14% 15%
9	J	155	77% 14% 8%
9	V	155	70% 22% 8%

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
13	HEA	F	601	X	-	-	-
13	HEA	F	602	X	-	-	-
13	HEA	R	601	X	-	-	-
13	HEA	R	602	X	-	-	-

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 38845 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 bc1 complex Rieske iron-sulfur subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	378	Total	C	N	O	S	0	0
			2912	1884	499	518	11		
1	M	372	Total	C	N	O	S	0	0
			2882	1869	494	508	11		

- Molecule 2 is a protein called Cytochrome bc1 complex cytochrome b subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	524	Total	C	N	O	S	0	0
			4130	2729	703	681	17		
2	N	524	Total	C	N	O	S	0	0
			4118	2723	701	677	17		

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	550	GLY	-	expression tag	UNP A0A0K2HYC0
B	551	GLY	-	expression tag	UNP A0A0K2HYC0
B	552	GLY	-	expression tag	UNP A0A0K2HYC0
B	553	GLY	-	expression tag	UNP A0A0K2HYC0
B	554	GLU	-	expression tag	UNP A0A0K2HYC0
B	555	ASN	-	expression tag	UNP A0A0K2HYC0
B	556	LEU	-	expression tag	UNP A0A0K2HYC0
B	557	TYR	-	expression tag	UNP A0A0K2HYC0
B	558	PHE	-	expression tag	UNP A0A0K2HYC0
B	559	GLN	-	expression tag	UNP A0A0K2HYC0
B	560	ASP	-	expression tag	UNP A0A0K2HYC0
B	561	TYR	-	expression tag	UNP A0A0K2HYC0
B	562	LYS	-	expression tag	UNP A0A0K2HYC0
B	563	ASP	-	expression tag	UNP A0A0K2HYC0
B	564	ASP	-	expression tag	UNP A0A0K2HYC0
B	565	ASP	-	expression tag	UNP A0A0K2HYC0
B	566	ASP	-	expression tag	UNP A0A0K2HYC0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	567	LYS	-	expression tag	UNP A0A0K2HYC0
B	568	HIS	-	expression tag	UNP A0A0K2HYC0
B	569	HIS	-	expression tag	UNP A0A0K2HYC0
B	570	HIS	-	expression tag	UNP A0A0K2HYC0
B	571	HIS	-	expression tag	UNP A0A0K2HYC0
B	572	HIS	-	expression tag	UNP A0A0K2HYC0
B	573	HIS	-	expression tag	UNP A0A0K2HYC0
N	550	GLY	-	expression tag	UNP A0A0K2HYC0
N	551	GLY	-	expression tag	UNP A0A0K2HYC0
N	552	GLY	-	expression tag	UNP A0A0K2HYC0
N	553	GLY	-	expression tag	UNP A0A0K2HYC0
N	554	GLU	-	expression tag	UNP A0A0K2HYC0
N	555	ASN	-	expression tag	UNP A0A0K2HYC0
N	556	LEU	-	expression tag	UNP A0A0K2HYC0
N	557	TYR	-	expression tag	UNP A0A0K2HYC0
N	558	PHE	-	expression tag	UNP A0A0K2HYC0
N	559	GLN	-	expression tag	UNP A0A0K2HYC0
N	560	ASP	-	expression tag	UNP A0A0K2HYC0
N	561	TYR	-	expression tag	UNP A0A0K2HYC0
N	562	LYS	-	expression tag	UNP A0A0K2HYC0
N	563	ASP	-	expression tag	UNP A0A0K2HYC0
N	564	ASP	-	expression tag	UNP A0A0K2HYC0
N	565	ASP	-	expression tag	UNP A0A0K2HYC0
N	566	ASP	-	expression tag	UNP A0A0K2HYC0
N	567	LYS	-	expression tag	UNP A0A0K2HYC0
N	568	HIS	-	expression tag	UNP A0A0K2HYC0
N	569	HIS	-	expression tag	UNP A0A0K2HYC0
N	570	HIS	-	expression tag	UNP A0A0K2HYC0
N	571	HIS	-	expression tag	UNP A0A0K2HYC0
N	572	HIS	-	expression tag	UNP A0A0K2HYC0
N	573	HIS	-	expression tag	UNP A0A0K2HYC0

- Molecule 3 is a protein called Cytochrome bc1 complex cytochrome c subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	218	Total	C	N	O	S	0	0
			1487	930	274	274	9		
3	O	213	Total	C	N	O	S	0	0
			1458	921	261	268	8		

- Molecule 4 is a protein called CYTOCHROME AA3 SUBUNIT CtaC.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	276	Total	C	N	O	S	0	0
			2204	1440	365	390	9		
4	Q	283	Total	C	N	O	S	0	0
			2247	1465	375	398	9		

- Molecule 5 is a protein called Probable cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	552	Total	C	N	O	S	0	0
			4358	2926	692	715	25		
5	R	552	Total	C	N	O	S	0	0
			4358	2926	692	715	25		

- Molecule 6 is a protein called Probable cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	186	Total	C	N	O	S	0	0
			1473	987	234	245	7		
6	S	185	Total	C	N	O	S	0	0
			1467	984	233	243	7		

- Molecule 7 is a protein called Cytochrome c oxidase polypeptide 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	139	Total	C	N	O	S	0	0
			1048	699	163	182	4		
7	T	139	Total	C	N	O	S	0	0
			1045	698	163	180	4		

- Molecule 8 is a protein called CYTOCHROME AA3 SUBUNIT CtaJ.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	67	Total	C	N	O	S	0	0
			511	344	82	84	1		
8	U	67	Total	C	N	O	S	0	0
			510	344	82	83	1		

- Molecule 9 is a protein called DUF5130 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	143	Total	C	N	O	S	0	0
			1019	645	177	195	2		

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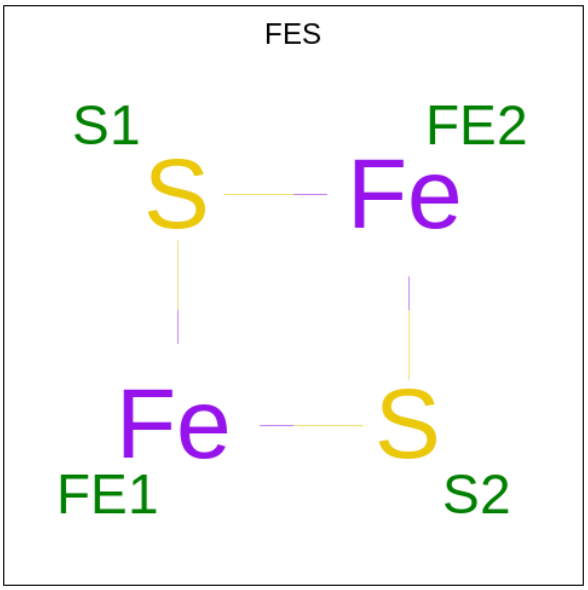
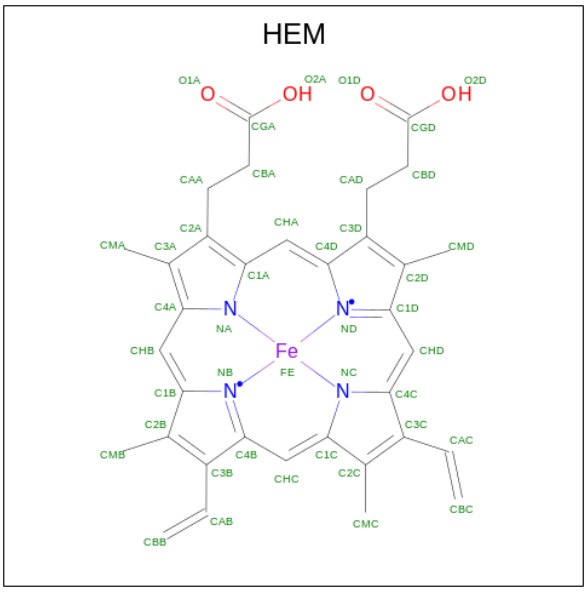
Mol	Chain	Residues	Atoms					AltConf	Trace
9	V	143	Total	C	N	O	S	0	0
			1028	649	180	197	2		

- Molecule 10 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



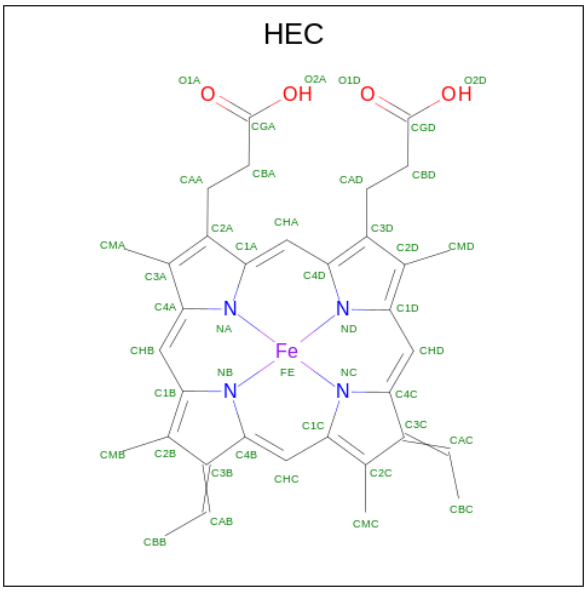
Mol	Chain	Residues	Atoms				AltConf
10	A	1	Total	Fe	S		0
			4	2	2		
10	M	1	Total	Fe	S		0
			4	2	2		

- Molecule 11 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



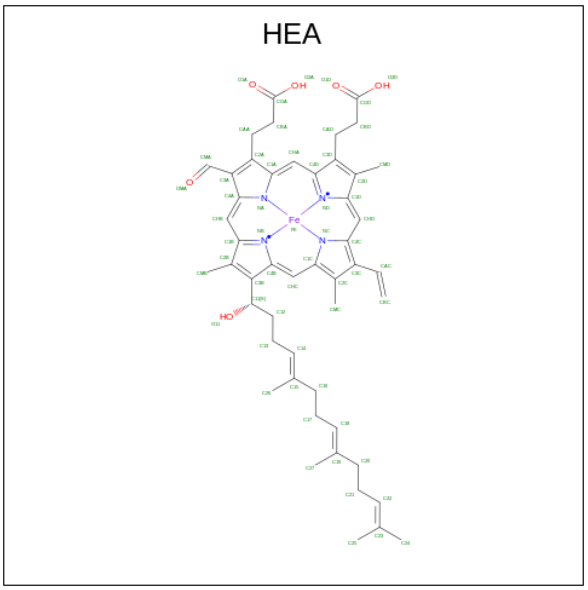
Mol	Chain	Residues	Atoms					AltConf
11	B	1	Total	C	Fe	N	O	0
			42	33	1	4	4	
11	B	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
11	N	1	Total	C	Fe	N	O	0
			42	33	1	4	4	
11	N	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 12 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 13 is HEME-A (three-letter code: HEA) (formula: $C_{49}H_{56}FeN_4O_6$) (labeled as "Ligand of Interest" by depositor).



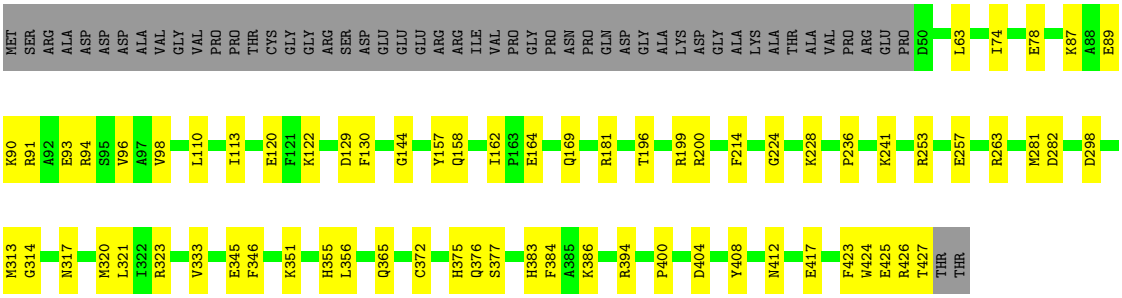
Mol	Chain	Residues	Atoms					AltConf
13	F	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
13	F	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
13	R	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
13	R	1	Total	C	Fe	N	O	0
			60	49	1	4	6	

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

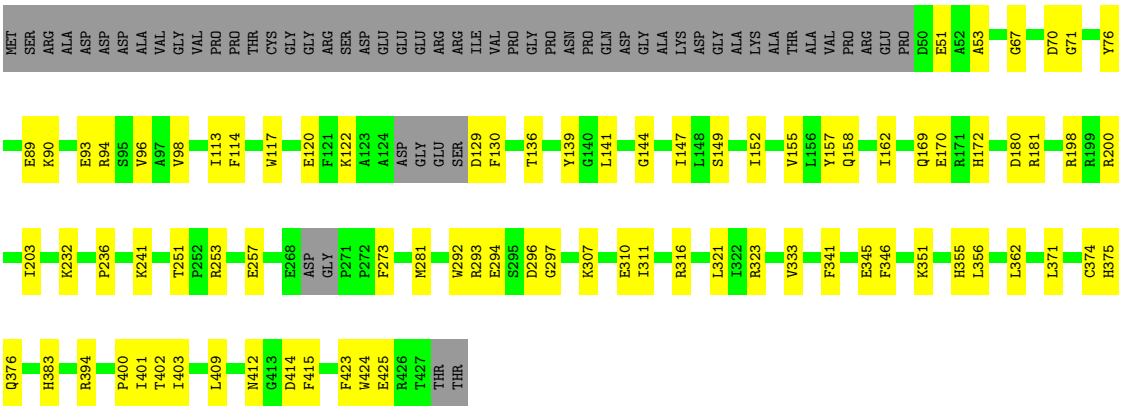
• Molecule 1: Cytochrome bc1 complex Rieske iron-sulfur subunit

Chain A:



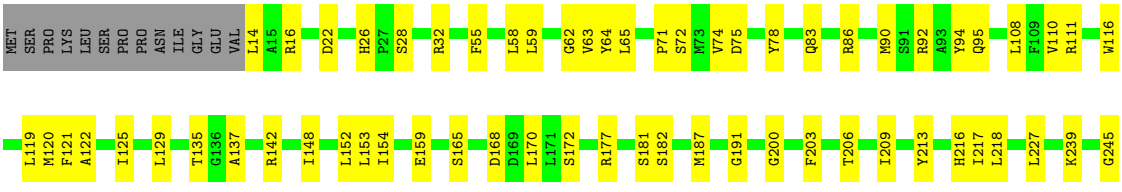
• Molecule 1: Cytochrome bc1 complex Rieske iron-sulfur subunit

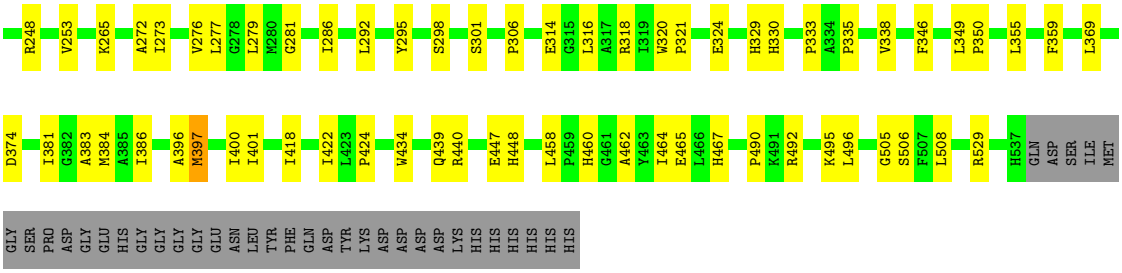
Chain M:



• Molecule 2: Cytochrome bc1 complex cytochrome b subunit

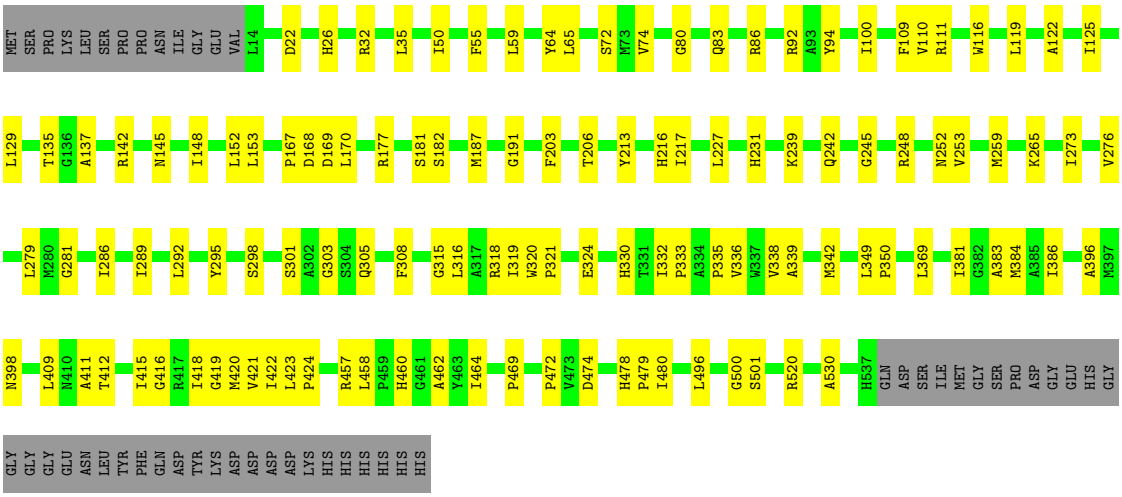
Chain B:





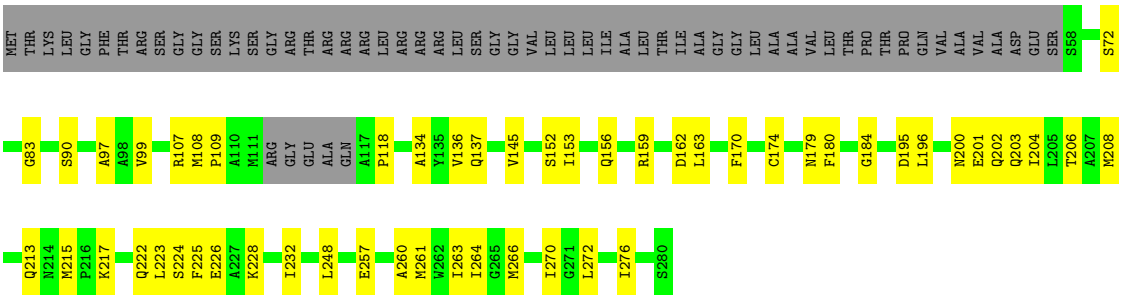
• Molecule 2: Cytochrome bc1 complex cytochrome b subunit

Chain N:



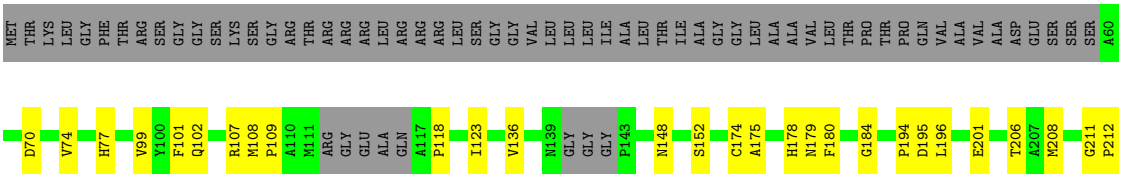
• Molecule 3: Cytochrome bc1 complex cytochrome c subunit

Chain C:



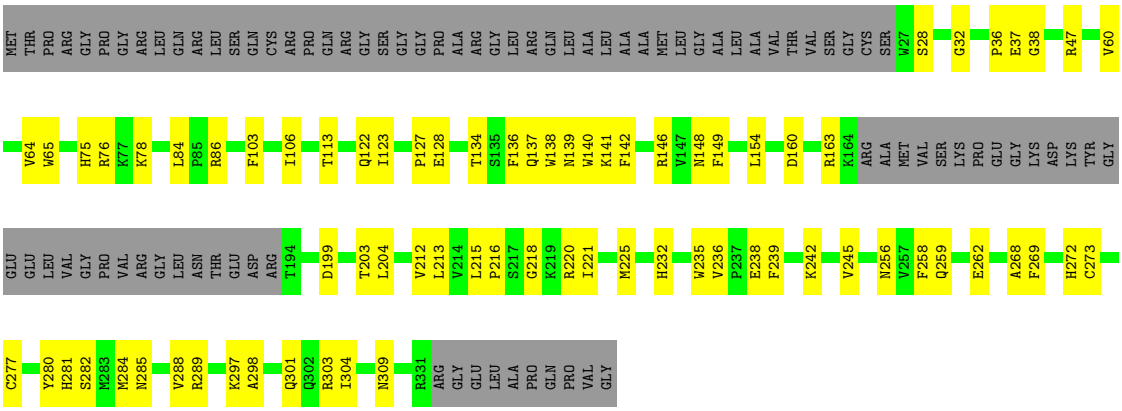
• Molecule 3: Cytochrome bc1 complex cytochrome c subunit

Chain O:



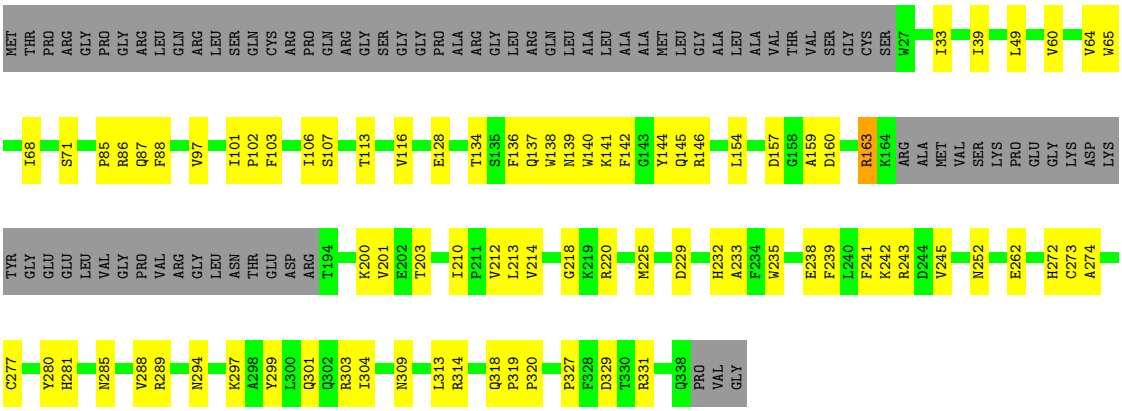
• Molecule 4: CYTOCHROME AA3 SUBUNIT CtaC

Chain E:



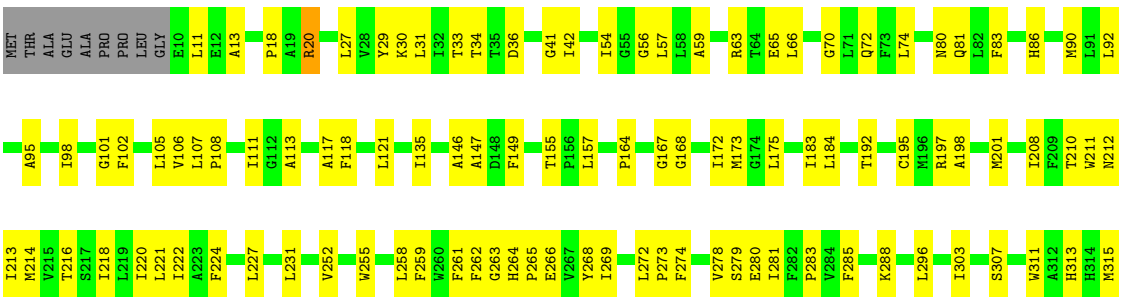
• Molecule 4: CYTOCHROME AA3 SUBUNIT CtaC

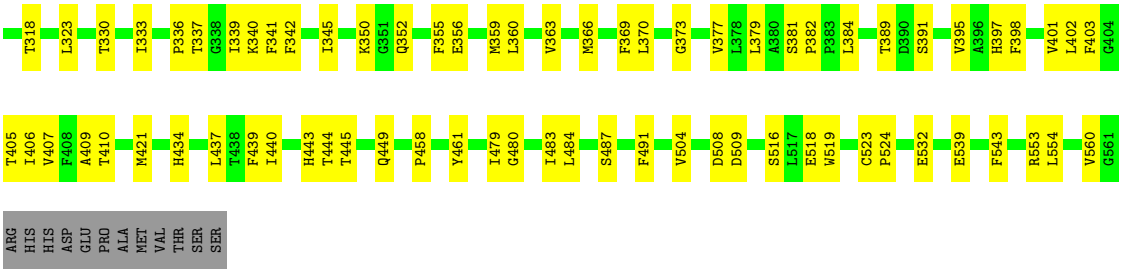
Chain Q:



• Molecule 5: Probable cytochrome c oxidase subunit 1

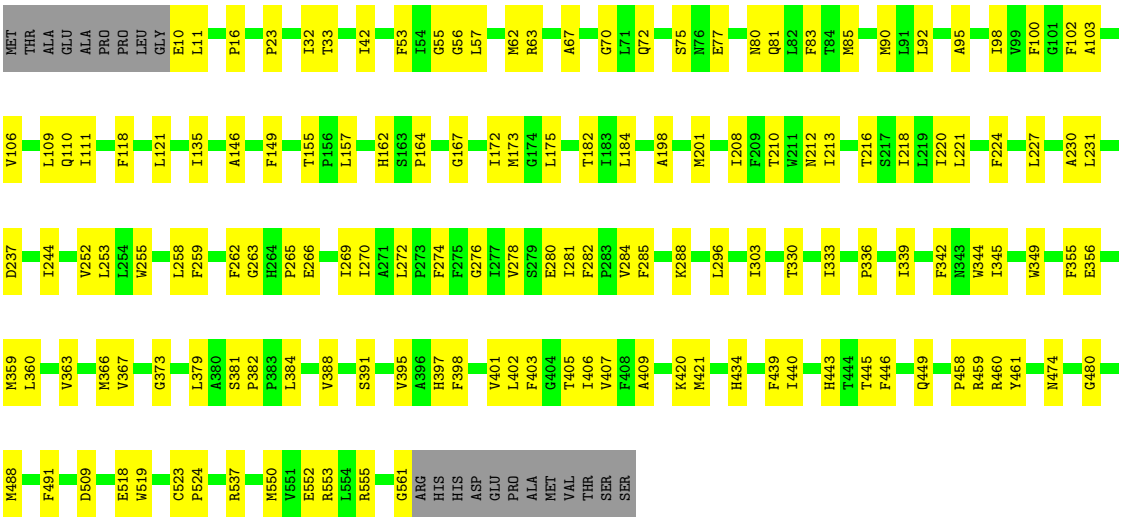
Chain F:





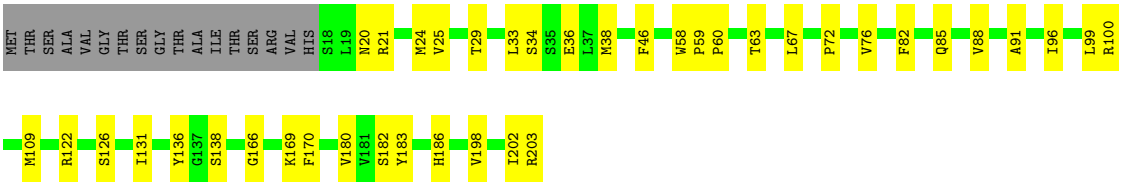
• Molecule 5: Probable cytochrome c oxidase subunit 1

Chain R:



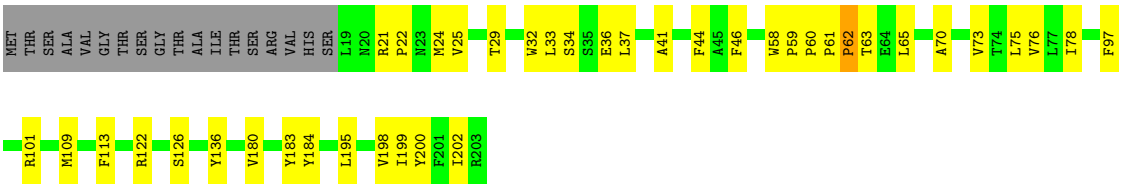
• Molecule 6: Probable cytochrome c oxidase subunit 3

Chain G:



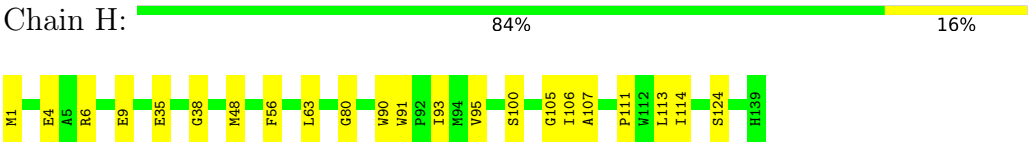
• Molecule 6: Probable cytochrome c oxidase subunit 3

Chain S:



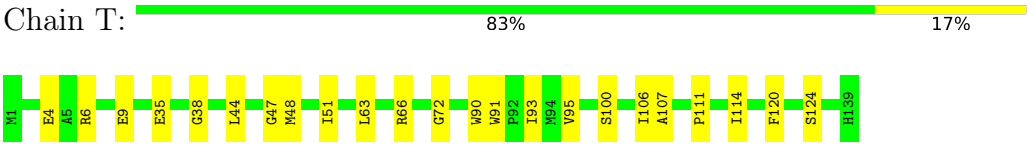
• Molecule 7: Cytochrome c oxidase polypeptide 4

Chain H:



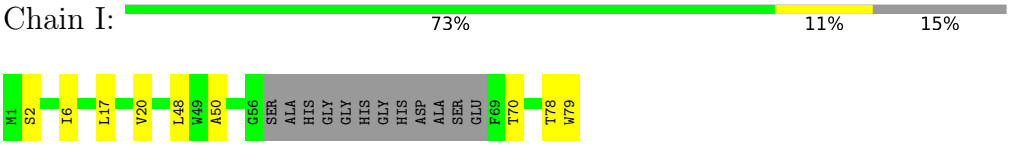
• Molecule 7: Cytochrome c oxidase polypeptide 4

Chain T:



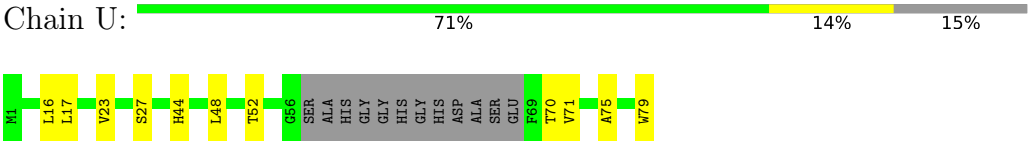
• Molecule 8: CYTOCHROME AA3 SUBUNIT CtaJ

Chain I:



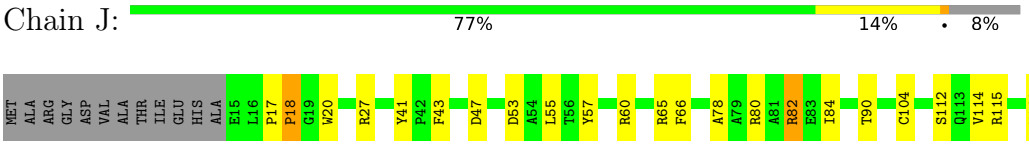
• Molecule 8: CYTOCHROME AA3 SUBUNIT CtaJ

Chain U:



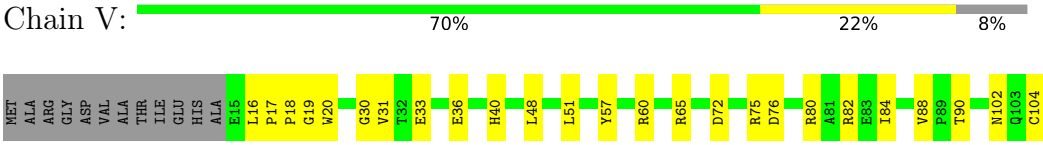
• Molecule 9: DUF5130 domain-containing protein

Chain J:



• Molecule 9: DUF5130 domain-containing protein

Chain V:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	TOMOGRAPHY	Depositor
Imposed symmetry	POINT, Not provided	
Number of tilted images used	100	Depositor
Resolution determination method	Not provided	
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEC, HEM, FES, HEA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.25	0/2989	0.51	0/4056
1	M	0.25	0/2957	0.50	0/4008
2	B	0.25	0/4266	0.49	1/5821 (0.0%)
2	N	0.25	0/4253	0.49	0/5804
3	C	0.25	0/1516	0.51	0/2061
3	O	0.26	0/1487	0.51	0/2022
4	E	0.24	0/2266	0.47	0/3090
4	Q	0.25	0/2310	0.47	0/3151
5	F	0.27	0/4517	0.49	0/6171
5	R	0.27	0/4517	0.49	0/6171
6	G	0.27	0/1523	0.47	0/2078
6	S	0.28	0/1517	0.50	0/2070
7	H	0.25	0/1081	0.45	0/1477
7	T	0.25	0/1078	0.44	0/1473
8	I	0.24	0/530	0.50	0/729
8	U	0.23	0/529	0.49	0/728
9	J	0.25	0/1038	0.51	0/1421
9	V	0.26	0/1047	0.54	0/1432
All	All	0.26	0/39421	0.49	1/53763 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	397	MET	CA-CB-CG	5.04	121.86	113.30

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	A	2912	0	2891	54	0
1	M	2882	0	2877	67	0
2	B	4130	0	4148	94	0
2	N	4118	0	4137	97	0
3	C	1487	0	1398	46	0
3	O	1458	0	1367	51	0
4	E	2204	0	2173	55	0
4	Q	2247	0	2204	56	0
5	F	4358	0	4320	133	0
5	R	4358	0	4321	113	0
6	G	1473	0	1458	29	0
6	S	1467	0	1453	35	0
7	H	1048	0	1027	16	0
7	T	1045	0	1025	22	0
8	I	511	0	516	10	0
8	U	510	0	513	10	0
9	J	1019	0	1019	19	0
9	V	1028	0	1032	26	0
10	A	4	0	0	0	0
10	M	4	0	0	0	0
11	B	85	0	57	8	0
11	N	85	0	57	7	0
12	C	86	0	63	7	0
12	O	86	0	64	20	0
13	F	120	0	107	26	0
13	R	120	0	108	18	0
All	All	38845	0	38335	843	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 11.

All (843) 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)
3:O:194:PRO:HD3	12:O:302:HEC:HAD2	1.35	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:36:PRO:O	4:E:47:ARG:NH2	2.09	0.86
3:O:194:PRO:HG2	12:O:302:HEC:HBA1	1.57	0.85
3:O:174:CYS:SG	12:O:302:HEC:HBB3	2.17	0.84
3:O:194:PRO:CD	12:O:302:HEC:HAD2	2.06	0.84
13:F:602:HEA:HBC1	13:F:602:HEA:HMC1	1.67	0.76
13:F:601:HEA:HBC1	13:F:601:HEA:HMC1	1.67	0.76
1:M:356:LEU:HD12	1:M:375:HIS:CE1	2.20	0.76
4:E:154:LEU:HD21	4:E:297:LYS:HG3	1.67	0.76
13:R:602:HEA:HMC1	13:R:602:HEA:HBC1	1.68	0.76
11:N:602:HEM:HHC	11:N:602:HEM:HBB2	1.68	0.75
3:O:263:ILE:HG23	3:O:264:ILE:HG12	1.67	0.75
5:F:216:THR:HG21	5:F:273:PRO:HD3	1.69	0.74
3:C:208:MET:HE2	3:C:228:LYS:HD2	1.69	0.74
4:Q:160:ASP:O	4:Q:163:ARG:NH1	2.20	0.74
1:M:144:GLY:HA3	2:N:279:LEU:HG	1.70	0.73
13:R:601:HEA:HMC1	13:R:601:HEA:HBC1	1.70	0.73
4:Q:101:ILE:HG13	4:Q:102:PRO:HD3	1.70	0.72
5:R:363:VAL:HA	5:R:366:MET:HE3	1.70	0.72
2:N:301:SER:HB3	3:O:180:PHE:HE1	1.54	0.72
3:C:179:ASN:ND2	3:C:184:GLY:O	2.22	0.72
3:O:179:ASN:ND2	3:O:184:GLY:O	2.22	0.72
3:O:225:PHE:HA	3:O:228:LYS:HE2	1.72	0.72
3:O:223:LEU:O	3:O:228:LYS:NZ	2.23	0.71
5:F:149:PHE:HB3	5:F:157:LEU:HD22	1.73	0.71
3:C:223:LEU:O	3:C:228:LYS:NZ	2.24	0.71
5:F:80:ASN:HA	5:F:83:PHE:CE1	2.25	0.71
5:R:80:ASN:HA	5:R:83:PHE:CE1	2.26	0.71
5:F:363:VAL:HA	5:F:366:MET:HE3	1.71	0.71
5:F:377:VAL:HG21	13:F:601:HEA:H251	1.72	0.71
1:A:89:GLU:OE2	1:M:200:ARG:NH2	2.24	0.70
4:Q:159:ALA:HB2	4:Q:200:LYS:HG3	1.73	0.70
3:C:213:GLN:NE2	12:C:301:HEC:O2D	2.24	0.70
9:J:47:ASP:HB3	9:J:140:VAL:HG11	1.73	0.70
6:S:198:VAL:HA	6:S:202:ILE:HD12	1.73	0.70
5:R:149:PHE:HB3	5:R:157:LEU:HD22	1.73	0.70
6:S:41:ALA:HB2	7:T:44:LEU:HD13	1.74	0.69
2:B:152:LEU:HD21	2:B:227:LEU:HB3	1.73	0.69
5:F:198:ALA:HB3	5:F:201:MET:HB2	1.73	0.69
5:F:65:GLU:HG2	5:F:74:LEU:HD23	1.73	0.69
4:E:218:GLY:HA2	4:E:262:GLU:HB2	1.74	0.69
5:R:33:THR:HG22	7:T:90:TRP:HB3	1.72	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:395:VAL:HA	5:R:398:PHE:CE1	2.28	0.68
5:R:198:ALA:HB3	5:R:201:MET:HB2	1.74	0.68
4:Q:145:GLN:HG2	4:Q:146:ARG:HG3	1.74	0.68
4:E:142:PHE:HB2	4:E:203:THR:HB	1.75	0.68
4:E:225:MET:HB3	4:E:245:VAL:HG13	1.75	0.68
4:Q:229:ASP:OD2	5:R:162:HIS:NE2	2.27	0.67
1:A:321:LEU:HD11	1:A:346:PHE:HD2	1.58	0.67
7:H:95:VAL:HG22	7:H:124:SER:HB2	1.74	0.67
3:C:225:PHE:HA	3:C:228:LYS:HE2	1.77	0.66
4:Q:86:ARG:HB3	4:Q:88:PHE:HD1	1.60	0.66
4:Q:65:TRP:HH2	5:R:367:VAL:HG13	1.61	0.66
5:F:146:ALA:HA	5:F:167:GLY:HA3	1.78	0.66
5:F:33:THR:HG22	7:H:90:TRP:HB3	1.78	0.65
5:R:111:ILE:HD11	5:R:210:THR:HG21	1.78	0.65
5:F:440:ILE:HA	5:F:443:HIS:CE1	2.32	0.65
3:C:263:ILE:HG23	3:C:264:ILE:HG12	1.79	0.65
6:S:180:VAL:HA	6:S:183:TYR:CE1	2.32	0.65
4:E:242:LYS:NZ	5:F:389:THR:O	2.30	0.65
3:C:83:GLY:HA3	3:C:90:SER:HA	1.77	0.65
5:F:212:ASN:ND2	5:F:272:LEU:O	2.30	0.65
3:O:101:PHE:HB2	3:O:206:THR:HG23	1.79	0.64
5:F:11:LEU:HD12	8:I:48:LEU:HD22	1.78	0.64
5:F:211:TRP:HA	5:F:214:MET:SD	2.38	0.64
2:N:152:LEU:HD21	2:N:227:LEU:HB3	1.79	0.64
3:O:243:GLN:HG3	3:O:248:LEU:HD13	1.79	0.64
2:B:272:ALA:HB1	3:C:272:LEU:HD13	1.80	0.64
5:R:373:GLY:HA3	13:R:601:HEA:H262	1.79	0.64
6:S:37:LEU:HG	7:T:44:LEU:HD21	1.78	0.64
4:Q:134:THR:HB	4:Q:141:LYS:HB3	1.80	0.64
4:Q:142:PHE:HB2	4:Q:203:THR:HB	1.79	0.64
3:C:97:ALA:HB1	3:C:206:THR:HG23	1.79	0.64
5:R:81:GLN:NE2	5:R:146:ALA:O	2.31	0.63
9:V:75:ARG:HG3	9:V:76:ASP:H	1.64	0.63
1:M:400:PRO:HB2	1:M:412:ASN:HB3	1.81	0.63
4:E:212:VAL:HB	4:E:309:ASN:HD21	1.63	0.63
3:O:108:MET:SD	3:O:109:PRO:HD2	2.39	0.63
5:F:117:ALA:H	5:F:192:THR:HG22	1.64	0.63
5:R:106:VAL:O	5:R:110:GLN:N	2.29	0.62
1:A:376:GLN:OE1	2:B:318:ARG:NH1	2.32	0.62
8:I:2:SER:HA	8:I:6:ILE:HB	1.80	0.62
6:S:76:VAL:HG13	6:S:109:MET:HG3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:405:THR:HG23	5:R:406:ILE:HG12	1.81	0.62
5:F:81:GLN:NE2	5:F:146:ALA:O	2.25	0.62
4:Q:232:HIS:O	4:Q:245:VAL:N	2.32	0.62
6:G:180:VAL:HA	6:G:183:TYR:CE1	2.35	0.62
2:N:242:GLN:NE2	2:N:252:ASN:O	2.33	0.62
1:A:417:GLU:OE2	1:A:417:GLU:N	2.33	0.62
2:N:472:PRO:HB2	2:N:480:ILE:HD12	1.81	0.62
5:F:208:ILE:HG13	5:F:296:LEU:HD23	1.82	0.61
5:F:323:LEU:HD11	5:F:382:PRO:HB3	1.83	0.61
3:O:109:PRO:HG3	12:O:301:HEC:CHC	2.30	0.61
8:U:71:VAL:HG21	9:V:82:ARG:HB2	1.81	0.61
5:F:183:ILE:HG13	5:F:224:PHE:HD2	1.65	0.61
5:R:288:LYS:NZ	5:R:349:TRP:O	2.32	0.61
1:A:424:TRP:O	2:B:330:HIS:ND1	2.30	0.61
1:A:355:HIS:CE1	1:A:356:LEU:HG	2.35	0.61
4:Q:137:GLN:HG3	4:Q:138:TRP:CE3	2.36	0.60
5:R:285:PHE:HE2	5:R:356:GLU:HB2	1.66	0.60
1:M:129:ASP:OD1	1:M:130:PHE:N	2.34	0.60
2:N:83:GLN:HA	2:N:86:ARG:HG3	1.83	0.60
4:Q:218:GLY:HA2	4:Q:262:GLU:HB2	1.83	0.60
4:E:215:LEU:HD12	4:E:216:PRO:HD2	1.82	0.60
5:R:230:ALA:HA	6:S:46:PHE:HZ	1.66	0.60
3:O:212:PRO:HD2	3:O:215:MET:HG2	1.84	0.60
5:F:285:PHE:HE2	5:F:356:GLU:HB2	1.67	0.60
5:R:216:THR:O	5:R:220:ILE:HG12	2.02	0.59
9:V:147:ILE:HD12	9:V:150:LEU:HD21	1.84	0.59
6:G:76:VAL:HG13	6:G:109:MET:HG3	1.83	0.59
6:S:122:ARG:HH21	6:S:126:SER:HB3	1.66	0.59
1:A:158:GLN:HG2	1:A:162:ILE:HD12	1.83	0.59
5:R:173:MET:HG3	7:T:107:ALA:HB2	1.83	0.59
11:N:601:HEM:HMB1	11:N:601:HEM:HBB2	1.85	0.59
2:B:292:LEU:HG	3:C:180:PHE:HD2	1.68	0.59
4:E:86:ARG:HH22	5:F:560:VAL:HG11	1.68	0.59
5:F:509:ASP:HB2	5:F:519:TRP:HB3	1.84	0.59
5:R:95:ALA:HB1	5:R:270:ILE:HG21	1.83	0.59
7:T:95:VAL:HG22	7:T:124:SER:HB2	1.85	0.59
6:G:198:VAL:HA	6:G:202:ILE:HD12	1.85	0.59
4:Q:289:ARG:NH2	4:Q:318:GLN:OE1	2.34	0.59
1:A:400:PRO:HB2	1:A:412:ASN:HB3	1.85	0.58
9:J:65:ARG:HH22	9:J:90:THR:H	1.49	0.58
5:R:100:PHE:HE2	5:R:182:THR:HA	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:35:GLU:OE1	7:T:38:GLY:N	2.31	0.58
2:B:213:TYR:O	2:B:217:ILE:HG12	2.02	0.58
5:R:402:LEU:HD13	13:R:601:HEA:HBC2	1.85	0.58
5:R:445:THR:HB	5:R:480:GLY:HA3	1.85	0.58
1:A:120:GLU:N	1:A:120:GLU:OE1	2.36	0.58
2:B:440:ARG:HH12	5:R:23:PRO:HG2	1.68	0.58
5:F:516:SER:OG	5:F:518:GLU:OE1	2.19	0.58
5:R:42:ILE:HD11	5:R:421:MET:HG2	1.85	0.58
4:E:232:HIS:O	4:E:245:VAL:N	2.32	0.58
5:F:278:VAL:HA	5:F:281:ILE:HG22	1.84	0.58
1:M:158:GLN:HG2	1:M:162:ILE:HD12	1.85	0.58
3:O:214:ASN:O	12:O:302:HEC:HBC3	2.02	0.58
2:B:90:MET:HE3	2:B:94:TYR:HD2	1.69	0.58
3:C:72:SER:HB3	12:C:301:HEC:HBB1	1.85	0.58
2:N:318:ARG:NH1	2:N:396:ALA:O	2.37	0.58
11:B:601:HEM:HMB1	11:B:601:HEM:HBB2	1.84	0.58
2:N:135:THR:HB	2:N:369:LEU:HD13	1.86	0.58
2:B:32:ARG:NH2	1:M:180:ASP:OD1	2.35	0.58
5:R:70:GLY:O	5:R:72:GLN:NE2	2.37	0.57
13:R:601:HEA:HMD1	13:R:601:HEA:HBD2	1.86	0.57
4:Q:329:ASP:OD2	4:Q:331:ARG:HG2	2.04	0.57
7:H:35:GLU:OE1	7:H:38:GLY:N	2.29	0.57
6:S:44:PHE:HE2	6:S:198:VAL:HG21	1.69	0.57
5:F:70:GLY:O	5:F:72:GLN:NE2	2.37	0.57
8:U:75:ALA:HB3	9:V:108:VAL:H	1.69	0.57
5:F:164:PRO:HG2	3:O:118:PRO:HD2	1.87	0.57
8:U:52:THR:HA	9:V:65:ARG:HH21	1.69	0.57
4:E:78:LYS:HD2	5:F:352:GLN:HB3	1.87	0.57
5:F:227:LEU:HD22	5:F:262:PHE:CZ	2.39	0.57
4:Q:113:THR:HG21	5:R:382:PRO:HD2	1.86	0.57
5:R:278:VAL:HA	5:R:281:ILE:HG22	1.87	0.57
5:R:355:PHE:HA	5:R:359:MET:SD	2.45	0.57
2:B:116:TRP:CD1	2:B:281:GLY:HA2	2.40	0.57
4:E:113:THR:HG21	5:F:382:PRO:HD2	1.86	0.57
3:O:211:GLY:HA3	3:O:217:LYS:HB3	1.86	0.57
11:N:602:HEM:HBC2	11:N:602:HEM:HMC2	1.87	0.56
4:Q:225:MET:HB3	4:Q:245:VAL:HG13	1.87	0.56
5:R:62:MET:HE3	5:R:83:PHE:HB3	1.86	0.56
5:R:270:ILE:HG22	5:R:406:ILE:HD11	1.87	0.56
3:C:224:SER:C	3:C:228:LYS:HZ3	2.08	0.56
5:F:341:PHE:HD2	13:F:601:HEA:H273	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:ARG:NH2	2:B:324:GLU:OE1	2.38	0.56
4:E:220:ARG:NH2	4:E:259:GLN:OE1	2.38	0.56
4:E:225:MET:HB2	4:E:256:ASN:HB2	1.88	0.56
8:U:79:TRP:HE1	9:V:106:ILE:HD11	1.69	0.56
2:N:469:PRO:HB3	2:N:479:PRO:HB3	1.88	0.56
5:R:276:GLY:O	5:R:280:GLU:HG2	2.06	0.56
6:S:61:PRO:C	6:S:63:THR:H	2.08	0.56
9:V:72:ASP:OD2	9:V:102:ASN:ND2	2.37	0.56
4:E:128:GLU:O	4:E:146:ARG:NH1	2.39	0.56
1:A:320:MET:HE1	1:A:351:LYS:HE3	1.87	0.56
1:A:426:ARG:HG3	1:A:427:THR:H	1.71	0.56
5:R:379:LEU:HD21	13:R:601:HEA:HBA2	1.88	0.55
1:M:94:ARG:O	1:M:98:VAL:HG23	2.06	0.55
5:R:63:ARG:HH21	5:R:446:PHE:HE1	1.55	0.55
5:F:274:PHE:CD1	5:F:409:ALA:HB3	2.41	0.55
2:B:265:LYS:HE3	3:C:276:ILE:HG23	1.89	0.55
5:F:532:GLU:OE2	9:J:27:ARG:NH1	2.40	0.55
3:C:200:ASN:HB3	3:C:203:GLN:OE1	2.06	0.55
5:F:90:MET:HB3	13:F:602:HEA:CAC	2.37	0.55
5:F:445:THR:O	5:F:449:GLN:NE2	2.39	0.55
6:G:91:ALA:HB2	6:G:99:LEU:HD12	1.87	0.55
4:Q:272:HIS:ND1	4:Q:285:ASN:OD1	2.34	0.55
6:S:58:TRP:CG	6:S:59:PRO:HD3	2.42	0.55
5:F:379:LEU:HD21	13:F:601:HEA:HBA2	1.87	0.55
6:G:58:TRP:CG	6:G:59:PRO:HD3	2.41	0.55
3:O:260:ALA:HA	3:O:263:ILE:HG22	1.89	0.55
2:N:419:GLY:HA2	2:N:423:LEU:HD23	1.88	0.55
4:Q:154:LEU:HD21	4:Q:297:LYS:HB2	1.89	0.55
6:G:63:THR:HG21	6:G:136:TYR:HE2	1.72	0.55
1:M:70:ASP:OD1	2:N:32:ARG:NH1	2.40	0.55
2:B:65:LEU:HB3	11:B:602:HEM:HMD1	1.89	0.55
2:B:170:LEU:HD23	2:B:295:TYR:HA	1.89	0.55
1:A:144:GLY:HA3	2:B:279:LEU:HG	1.89	0.54
1:A:356:LEU:HD22	2:B:182:SER:HB2	1.89	0.54
5:F:173:MET:HG3	7:H:107:ALA:HB2	1.89	0.54
5:F:337:THR:HG21	13:F:601:HEA:H263	1.90	0.54
5:F:90:MET:HB3	13:F:602:HEA:CBC	2.37	0.54
4:Q:103:PHE:HA	4:Q:106:ILE:HG12	1.90	0.54
2:N:72:SER:HB3	2:N:92:ARG:HB3	1.89	0.54
2:N:142:ARG:NH2	2:N:239:LYS:O	2.39	0.54
3:O:99:VAL:HG21	3:O:136:VAL:HG21	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:330:THR:O	5:R:333:ILE:HG22	2.08	0.54
6:S:199:ILE:HG23	6:S:200:TYR:CD2	2.43	0.54
1:M:351:LYS:NZ	2:N:298:SER:O	2.41	0.54
12:O:302:HEC:CBC	12:O:302:HEC:HHD	2.38	0.54
9:J:17:PRO:HD2	9:J:20:TRP:HB2	1.88	0.54
6:S:61:PRO:N	6:S:62:PRO:HD2	2.23	0.54
3:O:215:MET:HE1	12:O:302:HEC:CHB	2.38	0.54
5:F:155:THR:HG22	5:F:255:TRP:HB3	1.89	0.54
1:M:170:GLU:HG3	1:M:172:HIS:CE1	2.43	0.53
2:N:213:TYR:O	2:N:217:ILE:HG12	2.09	0.53
5:F:155:THR:HG21	5:F:252:VAL:HA	1.91	0.53
2:N:501:SER:O	2:N:520:ARG:NH2	2.31	0.53
3:O:148:ASN:N	3:O:152:SER:O	2.35	0.53
1:M:51:GLU:HG2	1:M:53:ALA:H	1.72	0.53
1:M:424:TRP:O	2:N:330:HIS:ND1	2.31	0.53
2:B:187:MET:HB3	2:B:191:GLY:HA2	1.89	0.53
2:N:94:TYR:OH	2:N:289:ILE:O	2.24	0.53
5:R:109:LEU:HB3	5:R:518:GLU:OE1	2.08	0.53
5:F:42:ILE:HD11	5:F:421:MET:HG2	1.89	0.53
3:O:208:MET:HB3	12:O:302:HEC:HMB2	1.91	0.53
5:R:155:THR:HG21	5:R:252:VAL:HA	1.89	0.53
6:S:41:ALA:HB2	7:T:44:LEU:HD22	1.91	0.53
5:F:373:GLY:HA2	13:F:601:HEA:H132	1.91	0.53
3:O:226:GLU:HA	3:O:229:LYS:HG2	1.90	0.53
9:V:19:GLY:O	9:V:30:GLY:HA2	2.08	0.53
8:I:2:SER:H	8:I:6:ILE:HD13	1.73	0.53
2:B:165:SER:HA	2:B:172:SER:HB2	1.91	0.52
5:F:29:TYR:O	5:F:33:THR:OG1	2.16	0.52
6:S:22:PRO:HD3	7:T:66:ARG:HD3	1.90	0.52
1:M:423:PHE:HE2	1:M:425:GLU:HB2	1.73	0.52
2:N:50:ILE:HD11	2:N:273:ILE:HD13	1.91	0.52
5:R:135:ILE:HD11	7:T:100:SER:HB2	1.91	0.52
3:C:99:VAL:HG21	3:C:136:VAL:HG11	1.91	0.52
1:M:376:GLN:HG2	2:N:409:LEU:HD21	1.92	0.52
13:R:602:HEA:HBA1	13:R:602:HEA:HHA	1.91	0.52
5:F:379:LEU:HG	13:F:601:HEA:HMA	1.92	0.52
9:J:65:ARG:NH2	9:J:90:THR:OG1	2.43	0.52
1:A:200:ARG:NH2	1:M:89:GLU:OE2	2.43	0.52
5:F:27:LEU:O	5:F:31:LEU:N	2.40	0.52
5:F:336:PRO:O	5:F:340:LYS:HG2	2.10	0.52
6:G:58:TRP:CD1	6:G:59:PRO:HD3	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:401:VAL:O	5:F:405:THR:HG22	2.09	0.52
6:G:85:GLN:HA	6:G:88:VAL:HG12	1.92	0.52
1:M:423:PHE:CE2	1:M:425:GLU:HB2	2.45	0.52
2:N:458:LEU:HD22	2:N:462:ALA:HB3	1.92	0.52
5:R:401:VAL:O	5:R:405:THR:HG22	2.09	0.52
2:B:301:SER:HB3	3:C:180:PHE:HE1	1.73	0.52
4:Q:136:PHE:CE1	4:Q:139:ASN:HB3	2.44	0.52
4:Q:213:LEU:HB3	4:Q:288:VAL:HG12	1.91	0.52
5:R:16:PRO:HB3	9:V:48:LEU:HD11	1.90	0.52
2:N:316:LEU:HD23	2:N:338:VAL:HG13	1.92	0.52
3:O:215:MET:HE1	12:O:302:HEC:C1B	2.40	0.52
4:Q:65:TRP:CH2	5:R:367:VAL:HG13	2.44	0.52
5:R:155:THR:HG22	5:R:255:TRP:HB3	1.91	0.52
4:E:303:ARG:NH2	4:E:309:ASN:OD1	2.43	0.52
2:N:305:GLN:HE21	2:N:318:ARG:HH22	1.58	0.52
3:O:215:MET:HE1	12:O:302:HEC:NB	2.24	0.52
3:C:72:SER:O	12:C:301:HEC:HHC	2.09	0.51
2:N:129:LEU:HD13	2:N:153:LEU:HD22	1.92	0.51
4:Q:301:GLN:HA	4:Q:304:ILE:HD12	1.92	0.51
5:R:57:LEU:HB3	13:R:602:HEA:H201	1.92	0.51
5:R:272:LEU:HD21	5:R:303:ILE:HG21	1.91	0.51
5:R:388:VAL:O	5:R:391:SER:OG	2.26	0.51
1:A:90:LYS:O	1:A:93:GLU:HG3	2.09	0.51
2:B:490:PRO:HG3	2:B:496:LEU:HD21	1.92	0.51
5:R:90:MET:HB3	13:R:602:HEA:CAC	2.40	0.51
5:R:420:LYS:HE3	5:R:518:GLU:HG3	1.91	0.51
4:E:134:THR:HB	4:E:141:LYS:HB3	1.92	0.51
7:T:111:PRO:HA	7:T:114:ILE:HG12	1.92	0.51
13:F:602:HEA:HBA1	13:F:602:HEA:HHA	1.92	0.51
1:M:362:LEU:HB2	1:M:371:LEU:HB2	1.93	0.51
2:N:305:GLN:NE2	2:N:318:ARG:HH22	2.09	0.51
5:R:336:PRO:HA	5:R:339:ILE:HD12	1.92	0.51
4:E:137:GLN:HG3	4:E:138:TRP:CE3	2.46	0.51
2:N:116:TRP:CD1	2:N:281:GLY:HA2	2.45	0.51
2:N:187:MET:HB3	2:N:191:GLY:H	1.76	0.51
5:R:434:HIS:CD2	5:R:491:PHE:HB2	2.46	0.51
6:S:29:THR:HG21	6:S:180:VAL:HB	1.91	0.51
5:F:107:LEU:HB3	5:F:108:PRO:HD3	1.93	0.51
5:F:484:LEU:HD23	13:F:602:HEA:H11	1.92	0.51
7:T:47:GLY:O	7:T:51:ILE:HG23	2.11	0.51
2:B:318:ARG:HD2	2:B:396:ALA:HA	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:273:PHE:HB2	1:M:292:TRP:HZ3	1.76	0.51
5:R:459:ARG:NH2	13:R:602:HEA:HAD2	2.25	0.51
6:S:21:ARG:HB3	7:T:63:LEU:HD11	1.93	0.51
5:F:523:CYS:HB3	5:F:524:PRO:HD3	1.93	0.51
1:M:120:GLU:N	1:M:120:GLU:OE1	2.44	0.51
13:F:602:HEA:CBD	13:F:602:HEA:HMD1	2.41	0.50
2:N:315:GLY:HA2	2:N:396:ALA:HB2	1.93	0.50
1:A:129:ASP:OD1	1:A:130:PHE:N	2.39	0.50
2:B:135:THR:HB	2:B:369:LEU:HD13	1.92	0.50
9:J:41:TYR:HB3	9:J:43:PHE:HD1	1.77	0.50
1:M:90:LYS:O	1:M:93:GLU:HG3	2.11	0.50
1:M:292:TRP:HE1	1:M:294:GLU:HG3	1.76	0.50
5:R:458:PRO:HG2	5:R:461:TYR:CZ	2.47	0.50
9:V:80:ARG:O	9:V:84:ILE:HG12	2.10	0.50
1:A:63:LEU:HD21	1:A:74:ILE:HD12	1.93	0.50
2:B:62:GLY:C	11:B:602:HEM:HAC	2.32	0.50
4:E:213:LEU:HB3	4:E:288:VAL:HG12	1.93	0.50
1:M:152:ILE:HA	1:M:155:VAL:HG12	1.92	0.50
4:Q:68:ILE:O	4:Q:71:SER:OG	2.25	0.50
5:R:208:ILE:HG13	5:R:296:LEU:HD23	1.92	0.50
5:R:379:LEU:HG	13:R:601:HEA:HMA	1.93	0.50
5:F:264:HIS:CE1	5:F:313:HIS:HE2	2.29	0.50
5:F:355:PHE:HA	5:F:359:MET:SD	2.51	0.50
4:Q:313:LEU:HD22	4:Q:320:PRO:HA	1.94	0.50
4:E:235:TRP:HZ3	5:F:458:PRO:HD3	1.75	0.50
5:F:63:ARG:NH2	5:F:66:LEU:HD23	2.26	0.50
1:M:356:LEU:HD22	2:N:182:SER:HB2	1.93	0.50
3:O:108:MET:HG2	3:O:123:ILE:HD12	1.94	0.50
5:R:81:GLN:O	5:R:85:MET:HG2	2.11	0.50
1:A:94:ARG:O	1:A:98:VAL:HG23	2.11	0.50
1:A:281:MET:HB2	1:A:323:ARG:HH11	1.77	0.50
1:A:351:LYS:NZ	2:B:298:SER:O	2.44	0.50
5:R:172:ILE:HG23	5:R:231:LEU:HG	1.94	0.50
1:M:307:LYS:O	1:M:311:ILE:HG12	2.12	0.49
5:F:395:VAL:HA	5:F:398:PHE:CE1	2.47	0.49
5:F:402:LEU:O	5:F:406:ILE:HG22	2.12	0.49
1:M:323:ARG:HE	1:M:345:GLU:HG3	1.76	0.49
4:Q:138:TRP:CD1	4:Q:280:TYR:HB2	2.47	0.49
5:R:67:ALA:HA	5:R:474:ASN:HD22	1.77	0.49
4:E:268:ALA:HB2	4:E:289:ARG:HE	1.77	0.49
5:F:34:THR:OG1	5:F:36:ASP:OD1	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:129:LEU:HD13	2:B:153:LEU:HD22	1.92	0.49
2:B:316:LEU:HG	2:B:338:VAL:HG22	1.92	0.49
6:S:76:VAL:HA	6:S:109:MET:HE2	1.95	0.49
3:C:108:MET:SD	3:C:109:PRO:HD2	2.52	0.49
4:E:65:TRP:HE1	5:F:370:LEU:HD22	1.76	0.49
1:M:96:VAL:HG21	1:M:157:TYR:HB2	1.93	0.49
4:Q:157:ASP:OD1	4:Q:157:ASP:N	2.45	0.49
5:F:147:ALA:HB2	5:F:168:GLY:HA2	1.94	0.49
1:M:394:ARG:NH2	2:N:324:GLU:OE1	2.45	0.49
2:N:80:GLY:O	2:N:86:ARG:NH1	2.43	0.49
2:N:411:ALA:O	2:N:415:ILE:HG13	2.13	0.49
6:S:73:VAL:HB	6:S:113:PHE:HD1	1.78	0.49
2:B:383:ALA:HA	2:B:386:ILE:HG22	1.95	0.49
2:N:303:GLY:HA3	3:O:180:PHE:CZ	2.48	0.49
5:R:459:ARG:HH21	13:R:602:HEA:HAD2	1.78	0.49
4:E:128:GLU:H	4:E:220:ARG:HB2	1.78	0.48
4:E:277:CYS:SG	4:E:281:HIS:ND1	2.86	0.48
6:G:122:ARG:HH21	6:G:126:SER:HA	1.78	0.48
1:M:355:HIS:ND1	1:M:356:LEU:HG	2.28	0.48
5:R:121:LEU:HD12	5:R:184:LEU:HD12	1.94	0.48
1:A:96:VAL:HG21	1:A:157:TYR:HB2	1.95	0.48
2:B:458:LEU:HD22	2:B:462:ALA:HB3	1.95	0.48
5:R:381:SER:HB3	5:R:384:LEU:HB2	1.95	0.48
7:T:6:ARG:O	7:T:9:GLU:HG3	2.13	0.48
4:E:84:LEU:O	5:F:553:ARG:NH2	2.44	0.48
4:E:236:VAL:HG12	4:E:239:PHE:H	1.78	0.48
2:N:35:LEU:HB3	2:N:259:MET:HE2	1.96	0.48
2:N:474:ASP:OD1	2:N:478:HIS:N	2.46	0.48
5:R:460:ARG:HH21	13:R:602:HEA:CGD	2.25	0.48
7:H:91:TRP:O	7:H:95:VAL:HG23	2.13	0.48
4:Q:299:TYR:OH	4:Q:309:ASN:OD1	2.31	0.48
8:I:70:THR:OG1	9:J:112:SER:HB3	2.13	0.48
2:N:383:ALA:HA	2:N:386:ILE:HG22	1.94	0.48
5:R:284:VAL:HG13	5:R:285:PHE:HD1	1.77	0.48
13:R:601:HEA:HMD1	13:R:601:HEA:CBD	2.43	0.48
1:A:164:GLU:N	1:A:164:GLU:OE1	2.46	0.48
2:B:286:ILE:HG13	3:C:257:GLU:CD	2.34	0.48
5:F:56:GLY:HA3	13:F:602:HEA:H161	1.95	0.48
7:H:1:MET:HE2	7:H:56:PHE:HB3	1.94	0.48
5:R:265:PRO:O	5:R:269:ILE:HG12	2.14	0.48
9:J:57:TYR:HD1	9:J:60:ARG:HH21	1.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:LYS:HE3	2:B:200:GLY:HA2	1.96	0.48
2:B:218:LEU:HD21	11:N:602:HEM:HBC1	1.95	0.48
4:E:225:MET:HE1	4:E:258:PHE:HE1	1.78	0.48
3:O:108:MET:CG	3:O:109:PRO:HD2	2.44	0.48
5:R:537:ARG:HH22	7:T:72:GLY:HA2	1.79	0.48
3:C:170:PHE:HA	3:C:174:CYS:SG	2.54	0.48
4:E:38:GLY:N	4:E:47:ARG:HH22	2.10	0.48
5:F:285:PHE:CE2	5:F:356:GLU:HB2	2.49	0.48
5:F:445:THR:HB	5:F:480:GLY:HA3	1.96	0.48
6:G:29:THR:OG1	6:G:183:TYR:OH	2.31	0.48
1:A:224:GLY:HA3	1:M:114:PHE:HZ	1.79	0.48
1:A:236:PRO:HA	1:A:241:LYS:HG2	1.94	0.48
13:F:601:HEA:CBD	13:F:601:HEA:HMD1	2.43	0.48
2:N:119:LEU:HD22	2:N:308:PHE:HE1	1.79	0.48
2:N:170:LEU:HA	2:N:295:TYR:HD1	1.78	0.48
12:O:301:HEC:HHC	12:O:301:HEC:HBB3	1.96	0.48
5:F:135:ILE:HD11	7:H:100:SER:HB2	1.95	0.47
2:N:137:ALA:HB2	2:N:369:LEU:HD21	1.95	0.47
2:N:216:HIS:HE1	11:N:602:HEM:NB	2.12	0.47
2:B:384:MET:SD	2:B:424:PRO:HB3	2.54	0.47
3:C:152:SER:OG	3:C:153:ILE:N	2.46	0.47
5:F:111:ILE:HG13	5:F:197:ARG:HG3	1.96	0.47
5:F:439:PHE:O	5:F:443:HIS:ND1	2.47	0.47
5:F:458:PRO:HG2	5:F:461:TYR:CZ	2.48	0.47
2:N:458:LEU:O	2:N:460:HIS:N	2.47	0.47
9:V:112:SER:HA	9:V:115:ARG:CZ	2.44	0.47
1:A:282:ASP:HB3	3:C:217:LYS:HD2	1.96	0.47
6:G:169:LYS:N	2:N:500:GLY:O	2.47	0.47
9:J:80:ARG:HH22	9:J:84:ILE:HD11	1.79	0.47
2:N:384:MET:SD	2:N:424:PRO:HB3	2.54	0.47
2:B:206:THR:HB	2:N:92:ARG:HH21	1.78	0.47
2:B:349:LEU:HB3	2:B:350:PRO:HD3	1.96	0.47
4:E:60:VAL:O	4:E:64:VAL:HG23	2.15	0.47
5:R:95:ALA:O	5:R:98:ILE:HG22	2.15	0.47
7:T:91:TRP:O	7:T:95:VAL:HG23	2.14	0.47
2:B:159:GLU:HG3	11:B:602:HEM:HMB3	1.96	0.47
2:B:245:GLY:HA3	2:B:248:ARG:HD3	1.96	0.47
7:H:6:ARG:NE	7:H:9:GLU:OE2	2.47	0.47
4:E:301:GLN:HA	4:E:304:ILE:HD12	1.97	0.47
3:O:215:MET:CE	12:O:302:HEC:NA	2.77	0.47
7:T:4:GLU:OE1	7:T:4:GLU:N	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:THR:HB	1:A:199:ARG:HE	1.78	0.47
2:B:83:GLN:HA	2:B:86:ARG:HG3	1.97	0.47
2:B:397:MET:SD	2:B:401:ILE:HG13	2.54	0.47
2:B:447:GLU:OE1	2:B:448:HIS:NE2	2.47	0.47
3:C:109:PRO:HG3	12:C:301:HEC:C1C	2.44	0.47
5:F:13:ALA:HB1	8:I:50:ALA:HB2	1.96	0.47
5:F:258:LEU:HD22	6:G:46:PHE:HE1	1.79	0.47
7:H:90:TRP:O	7:H:93:ILE:HG22	2.14	0.47
3:O:226:GLU:OE2	3:O:226:GLU:N	2.37	0.47
4:E:272:HIS:ND1	4:E:285:ASN:OD1	2.42	0.47
8:I:17:LEU:HA	8:I:20:VAL:HG22	1.96	0.47
5:R:263:GLY:O	5:R:266:GLU:HB2	2.15	0.47
3:C:226:GLU:OE1	3:C:226:GLU:N	2.36	0.47
5:F:172:ILE:HG23	5:F:231:LEU:HG	1.97	0.47
6:G:131:ILE:O	6:G:138:SER:OG	2.30	0.47
1:M:296:ASP:OD1	1:M:297:GLY:N	2.47	0.47
2:N:245:GLY:HA3	2:N:248:ARG:HD3	1.97	0.47
3:O:219:SER:O	3:O:222:GLN:NE2	2.48	0.47
5:R:440:ILE:HA	5:R:443:HIS:NE2	2.30	0.47
5:R:523:CYS:HB2	5:R:524:PRO:HD3	1.97	0.47
5:F:397:HIS:O	5:F:401:VAL:HG22	2.14	0.46
2:N:418:ILE:O	2:N:422:ILE:HG12	2.14	0.46
1:A:169:GLN:HB3	2:B:253:VAL:HB	1.96	0.46
4:E:138:TRP:CD1	4:E:280:TYR:HB2	2.50	0.46
1:M:333:VAL:HG21	1:M:383:HIS:ND1	2.29	0.46
5:R:220:ILE:HG23	5:R:224:PHE:CD2	2.51	0.46
5:R:269:ILE:HG13	5:R:270:ILE:HG12	1.96	0.46
8:I:79:TRP:CG	9:J:104:CYS:HB3	2.50	0.46
1:M:355:HIS:CE1	1:M:356:LEU:HG	2.50	0.46
2:N:35:LEU:HB3	2:N:259:MET:CE	2.45	0.46
4:Q:97:VAL:O	4:Q:101:ILE:HG12	2.15	0.46
5:R:403:PHE:CE2	5:R:407:VAL:HG21	2.50	0.46
9:V:144:ILE:HG22	9:V:148:ARG:HE	1.80	0.46
2:B:316:LEU:HD23	2:B:338:VAL:HG13	1.97	0.46
2:B:465:GLU:HB3	2:B:467:HIS:CD2	2.50	0.46
3:C:156:GLN:HE22	3:C:159:ARG:HH21	1.64	0.46
2:N:421:VAL:HG13	2:N:422:ILE:HG23	1.98	0.46
2:N:177:ARG:O	2:N:181:SER:HB3	2.16	0.46
3:O:226:GLU:HA	3:O:229:LYS:HZ2	1.80	0.46
1:A:355:HIS:CE1	1:A:375:HIS:ND1	2.84	0.46
9:J:112:SER:HA	9:J:115:ARG:CZ	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:141:LEU:HA	2:N:279:LEU:HD23	1.98	0.46
5:R:237:ASP:OD2	5:R:244:ILE:HB	2.16	0.46
1:A:323:ARG:NE	1:A:345:GLU:HG3	2.31	0.46
5:F:111:ILE:HG23	5:F:113:ALA:H	1.80	0.46
5:F:121:LEU:HD12	5:F:184:LEU:HD12	1.96	0.46
5:F:258:LEU:HD12	5:F:259:PHE:N	2.30	0.46
1:M:198:ARG:HA	1:M:198:ARG:HD2	1.83	0.46
1:M:253:ARG:HB2	1:M:257:GLU:OE2	2.16	0.46
1:M:307:LYS:O	1:M:310:GLU:HG3	2.16	0.46
3:O:196:LEU:HA	12:O:302:HEC:O2A	2.16	0.46
5:R:258:LEU:HD12	5:R:259:PHE:N	2.30	0.46
5:F:212:ASN:O	5:F:216:THR:HG23	2.16	0.46
2:B:92:ARG:NH2	2:N:206:THR:HB	2.31	0.45
2:B:120:MET:HG2	2:B:277:LEU:HD21	1.98	0.45
5:F:449:GLN:OE1	5:F:449:GLN:N	2.49	0.45
2:N:177:ARG:HB2	2:N:203:PHE:CZ	2.50	0.45
6:S:58:TRP:CD1	6:S:59:PRO:HD3	2.51	0.45
1:A:93:GLU:HA	1:A:96:VAL:HG12	1.99	0.45
4:E:146:ARG:NH1	4:E:148:ASN:HB2	2.31	0.45
4:E:215:LEU:HD11	4:E:221:ILE:HD12	1.97	0.45
5:R:173:MET:SD	7:T:106:ILE:HG23	2.56	0.45
5:F:268:TYR:HD2	5:F:307:SER:HB2	1.82	0.45
5:F:373:GLY:HA3	13:F:601:HEA:H262	1.98	0.45
5:R:274:PHE:HD2	5:R:409:ALA:HB3	1.80	0.45
5:R:445:THR:HG23	5:R:446:PHE:CD1	2.51	0.45
6:S:70:ALA:O	6:S:73:VAL:HG22	2.17	0.45
7:T:90:TRP:O	7:T:93:ILE:HG22	2.16	0.45
1:A:78:GLU:HG3	2:B:529:ARG:HH12	1.81	0.45
4:E:122:GLN:HG2	4:E:123:ILE:N	2.32	0.45
7:H:105:GLY:HA2	7:H:113:LEU:HD23	1.98	0.45
2:N:458:LEU:HD11	2:N:464:ILE:HG12	1.97	0.45
2:B:55:PHE:O	2:B:59:LEU:HD23	2.17	0.45
2:B:508:LEU:HD22	6:S:101:ARG:HG2	1.98	0.45
5:F:265:PRO:O	5:F:269:ILE:HG12	2.16	0.45
1:M:321:LEU:HD11	1:M:346:PHE:CD2	2.52	0.45
2:N:398:ASN:OD1	2:N:412:THR:OG1	2.23	0.45
5:R:53:PHE:CE1	5:R:488:MET:HG2	2.52	0.45
5:R:218:ILE:O	5:R:221:LEU:HG	2.17	0.45
1:A:333:VAL:HG21	1:A:383:HIS:ND1	2.31	0.45
2:B:301:SER:HB3	3:C:180:PHE:CE1	2.50	0.45
1:M:130:PHE:H	3:O:242:ARG:HH21	1.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:321:LEU:HD11	1:M:346:PHE:HD2	1.81	0.45
3:O:174:CYS:SG	12:O:302:HEC:CBB	2.98	0.45
1:A:355:HIS:O	1:A:356:LEU:HD23	2.17	0.45
1:A:423:PHE:HD1	1:A:425:GLU:H	1.65	0.45
5:F:195:CYS:SG	6:G:20:ASN:ND2	2.90	0.45
5:F:288:LYS:HB3	5:F:288:LYS:HE2	1.72	0.45
5:F:434:HIS:CD2	5:F:491:PHE:HB2	2.52	0.45
2:N:416:GLY:O	2:N:420:MET:HE3	2.16	0.45
5:R:359:MET:SD	5:R:360:LEU:N	2.90	0.45
1:A:181:ARG:NH1	2:N:22:ASP:OD2	2.39	0.45
2:B:121:PHE:CZ	11:B:601:HEM:HBB1	2.52	0.45
3:C:228:LYS:O	3:C:232:ILE:HG23	2.17	0.45
4:E:139:ASN:OD1	4:E:140:TRP:N	2.46	0.45
2:N:64:TYR:HD2	2:N:65:LEU:HD22	1.80	0.45
5:R:552:GLU:CD	5:R:552:GLU:H	2.19	0.45
6:S:75:LEU:HA	6:S:78:ILE:HG12	1.99	0.45
2:B:116:TRP:CZ2	2:B:286:ILE:HB	2.51	0.45
2:B:119:LEU:HB2	3:C:261:MET:HE3	1.99	0.45
4:E:76:ARG:O	4:E:78:LYS:N	2.49	0.45
5:F:59:ALA:HB2	5:F:86:HIS:CE1	2.52	0.45
2:N:419:GLY:O	2:N:423:LEU:HB2	2.17	0.45
5:R:303:ILE:HG13	5:R:336:PRO:HB2	1.99	0.45
13:R:602:HEA:H271	13:R:602:HEA:H211	1.40	0.45
1:A:426:ARG:HG3	1:A:427:THR:N	2.32	0.45
2:B:75:ASP:OD1	2:B:75:ASP:N	2.50	0.45
3:C:248:LEU:HD23	3:C:248:LEU:H	1.82	0.45
4:E:127:PRO:O	4:E:146:ARG:NH2	2.40	0.45
5:F:381:SER:HB3	5:F:384:LEU:HB2	1.98	0.45
1:M:251:THR:O	1:M:293:ARG:NH2	2.50	0.45
3:O:70:ASP:HA	3:O:74:VAL:HG23	1.99	0.45
3:O:77:HIS:CD2	12:O:301:HEC:NB	2.85	0.45
4:Q:210:ILE:HG13	4:Q:327:PRO:HB3	1.98	0.45
5:R:398:PHE:HA	5:R:401:VAL:HG22	1.99	0.45
2:B:137:ALA:HB2	2:B:369:LEU:HD21	1.99	0.44
4:E:75:HIS:CD2	5:F:350:LYS:H	2.36	0.44
4:E:136:PHE:CZ	4:E:139:ASN:HB3	2.53	0.44
5:F:398:PHE:CE2	13:F:602:HEA:HMD2	2.52	0.44
6:G:82:PHE:HD1	6:G:85:GLN:HE22	1.63	0.44
1:M:155:VAL:HG23	2:N:265:LYS:NZ	2.32	0.44
4:Q:142:PHE:CE2	4:Q:213:LEU:HB2	2.52	0.44
5:R:92:LEU:HD13	5:R:175:LEU:HD22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:CYS:HB3	1:A:377:SER:HB3	1.99	0.44
6:G:21:ARG:HB2	7:H:63:LEU:HD11	1.99	0.44
9:J:55:LEU:HD11	9:J:66:PHE:HB2	1.99	0.44
4:Q:49:LEU:HD22	4:Q:116:VAL:HG21	1.98	0.44
4:Q:128:GLU:H	4:Q:220:ARG:HB3	1.81	0.44
3:C:145:VAL:HG13	3:C:202:GLN:HE21	1.82	0.44
5:F:218:ILE:O	5:F:221:LEU:HG	2.17	0.44
5:F:479:ILE:O	5:F:483:ILE:HG12	2.18	0.44
13:F:602:HEA:HHA	13:F:602:HEA:CBA	2.47	0.44
4:Q:235:TRP:HZ3	5:R:458:PRO:HD3	1.83	0.44
5:R:10:GLU:HB3	5:R:11:LEU:H	1.53	0.44
5:F:336:PRO:HA	5:F:339:ILE:HD12	2.00	0.44
1:M:273:PHE:HB2	1:M:292:TRP:CZ3	2.52	0.44
4:Q:294:ASN:HA	4:Q:297:LYS:HG2	1.99	0.44
5:R:118:PHE:HB3	5:R:121:LEU:HD23	1.98	0.44
3:C:215:MET:CE	12:C:302:HEC:C4B	2.95	0.44
1:M:93:GLU:HA	1:M:96:VAL:HG12	2.00	0.44
2:B:58:LEU:HD23	11:B:602:HEM:C3B	2.53	0.44
6:G:60:PRO:HG2	6:G:63:THR:OG1	2.17	0.44
3:O:178:HIS:ND1	3:O:196:LEU:HD21	2.32	0.44
4:E:37:GLU:HA	4:E:47:ARG:HH12	1.83	0.44
5:F:222:ILE:HA	6:G:38:MET:SD	2.58	0.44
5:F:373:GLY:C	13:F:601:HEA:H162	2.38	0.44
5:F:543:PHE:CE2	5:F:554:LEU:HD11	2.53	0.44
4:E:273:CYS:HB3	4:E:281:HIS:HE1	1.82	0.44
5:F:315:MET:O	5:F:318:THR:OG1	2.34	0.44
6:S:60:PRO:HG2	6:S:63:THR:OG1	2.18	0.44
1:A:93:GLU:HB2	1:M:203:ILE:HD11	1.99	0.43
2:B:492:ARG:HB2	2:B:495:LYS:HG2	2.00	0.43
5:F:41:GLY:HA3	5:F:105:LEU:HD22	2.00	0.43
6:G:96:ILE:HD11	6:G:170:PHE:HB2	1.99	0.43
3:O:178:HIS:HD1	3:O:196:LEU:HD21	1.83	0.43
5:R:212:ASN:ND2	5:R:272:LEU:O	2.47	0.43
2:B:458:LEU:HD11	2:B:464:ILE:HG12	2.00	0.43
2:N:286:ILE:HG13	3:O:257:GLU:CD	2.38	0.43
2:N:316:LEU:HD12	2:N:319:ILE:HD11	2.00	0.43
4:Q:201:VAL:HG11	4:Q:303:ARG:HB3	1.99	0.43
5:R:446:PHE:HA	5:R:449:GLN:OE1	2.17	0.43
5:R:459:ARG:NH2	13:R:602:HEA:O1D	2.50	0.43
3:C:118:PRO:HG2	5:R:164:PRO:HB2	2.01	0.43
5:F:543:PHE:HE2	5:F:554:LEU:HD11	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:232:LYS:HB2	1:M:232:LYS:HE3	1.74	0.43
12:O:302:HEC:HBC3	12:O:302:HEC:HHD	1.98	0.43
4:Q:136:PHE:HE2	4:Q:141:LYS:HB2	1.83	0.43
2:B:92:ARG:HH21	2:N:206:THR:HB	1.82	0.43
5:F:95:ALA:O	5:F:98:ILE:HG22	2.19	0.43
5:F:262:PHE:O	5:F:266:GLU:HG2	2.19	0.43
13:F:602:HEA:H212	13:F:602:HEA:H271	1.69	0.43
9:J:80:ARG:O	9:J:84:ILE:HG12	2.18	0.43
1:M:401:ILE:HD12	1:M:409:LEU:HD12	2.00	0.43
1:A:214:PHE:CZ	1:M:147:ILE:HD12	2.53	0.43
1:A:263:ARG:NH2	3:C:222:GLN:O	2.51	0.43
2:B:59:LEU:O	2:B:63:VAL:HG23	2.17	0.43
2:B:374:ASP:O	2:B:439:GLN:NE2	2.52	0.43
2:B:397:MET:SD	2:B:400:ILE:HB	2.58	0.43
3:C:201:GLU:HA	3:C:204:ILE:HD12	1.99	0.43
4:E:146:ARG:HH11	4:E:148:ASN:HB2	1.83	0.43
13:F:601:HEA:H261	13:F:601:HEA:H172	1.65	0.43
6:G:67:LEU:HD11	6:G:203:ARG:HH22	1.83	0.43
1:M:341:PHE:CG	1:M:400:PRO:HG3	2.54	0.43
2:N:339:ALA:HA	2:N:342:MET:HG2	2.01	0.43
8:U:23:VAL:O	8:U:27:SER:OG	2.32	0.43
2:B:216:HIS:HE1	11:B:602:HEM:C1B	2.37	0.43
2:B:320:TRP:CD2	2:B:321:PRO:HD2	2.54	0.43
2:B:355:LEU:O	2:B:359:PHE:HB2	2.17	0.43
2:B:458:LEU:O	2:B:460:HIS:N	2.52	0.43
7:H:1:MET:SD	7:H:4:GLU:HB2	2.59	0.43
1:M:113:ILE:O	1:M:117:TRP:HB2	2.17	0.43
2:N:64:TYR:CD2	2:N:110:VAL:HG11	2.54	0.43
4:Q:277:CYS:SG	4:Q:281:HIS:ND1	2.85	0.43
5:R:75:SER:OG	5:R:77:GLU:OE1	2.26	0.43
9:V:114:VAL:HG13	9:V:114:VAL:O	2.19	0.43
7:H:80:GLY:H	2:N:457:ARG:HB3	1.83	0.43
9:V:36:GLU:OE1	9:V:36:GLU:N	2.52	0.43
2:B:381:ILE:O	2:B:384:MET:HB3	2.19	0.43
5:F:220:ILE:HG23	5:F:224:PHE:CE2	2.54	0.43
5:F:437:LEU:HD23	5:F:487:SER:HA	2.01	0.43
9:J:114:VAL:O	9:J:114:VAL:HG13	2.19	0.43
1:M:67:GLY:O	1:M:71:GLY:N	2.51	0.43
5:R:439:PHE:O	5:R:443:HIS:CD2	2.72	0.43
5:R:459:ARG:HG3	5:R:460:ARG:HG3	2.00	0.43
5:R:550:MET:SD	5:R:553:ARG:HD3	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:33:LEU:HD11	6:S:184:TYR:HD1	1.84	0.43
6:S:63:THR:HG21	6:S:136:TYR:HE2	1.83	0.43
1:A:122:LYS:HD3	1:A:122:LYS:HA	1.80	0.43
3:C:215:MET:CE	12:C:302:HEC:C1B	2.96	0.43
6:G:182:SER:O	6:G:186:HIS:ND1	2.46	0.43
2:N:320:TRP:CD2	2:N:321:PRO:HD2	2.54	0.43
2:N:333:PRO:HB2	2:N:335:PRO:HD2	2.01	0.43
3:O:195:ASP:OD1	3:O:196:LEU:N	2.52	0.43
9:V:48:LEU:O	9:V:51:LEU:HG	2.19	0.43
9:J:17:PRO:HG2	9:J:20:TRP:CD1	2.54	0.43
1:M:169:GLN:HB3	2:N:253:VAL:HB	2.01	0.43
2:N:332:ILE:HG23	2:N:336:VAL:HG21	2.01	0.43
5:R:227:LEU:HD13	5:R:262:PHE:CE2	2.54	0.43
5:R:342:PHE:HA	5:R:345:ILE:HG22	2.00	0.43
9:V:57:TYR:HA	9:V:60:ARG:HG2	2.01	0.43
1:A:87:LYS:O	1:A:91:ARG:HG3	2.19	0.42
2:B:72:SER:OG	2:B:74:VAL:HG12	2.19	0.42
2:B:177:ARG:O	2:B:181:SER:HB3	2.18	0.42
4:E:103:PHE:HA	4:E:106:ILE:HG12	2.01	0.42
5:F:263:GLY:O	5:F:266:GLU:HB2	2.19	0.42
1:M:136:THR:HG23	2:N:109:PHE:HB2	2.00	0.42
2:N:119:LEU:HD23	2:N:119:LEU:HA	1.90	0.42
2:N:148:ILE:O	2:N:152:LEU:HD23	2.19	0.42
4:Q:101:ILE:HG13	4:Q:102:PRO:CD	2.44	0.42
4:Q:252:ASN:HB3	5:R:253:LEU:HD23	2.00	0.42
5:R:11:LEU:HD12	8:U:48:LEU:HD22	2.01	0.42
2:B:148:ILE:O	2:B:152:LEU:HD23	2.19	0.42
3:C:107:ARG:HB2	3:C:107:ARG:NH1	2.34	0.42
5:F:92:LEU:HD13	5:F:175:LEU:HD22	2.00	0.42
6:G:33:LEU:HA	6:G:36:GLU:OE2	2.19	0.42
6:G:63:THR:HG21	6:G:136:TYR:CE2	2.52	0.42
6:G:100:ARG:NH2	6:G:166:GLY:HA2	2.34	0.42
1:M:281:MET:HB2	1:M:323:ARG:HH11	1.83	0.42
2:N:265:LYS:HE3	3:O:276:ILE:HG23	2.01	0.42
5:R:67:ALA:HA	5:R:474:ASN:ND2	2.33	0.42
3:C:195:ASP:OD1	3:C:196:LEU:N	2.52	0.42
13:F:601:HEA:HMD1	13:F:601:HEA:HBD2	2.00	0.42
1:M:374:CYS:HB3	1:M:375:HIS:CE1	2.54	0.42
3:O:108:MET:HG3	3:O:109:PRO:HD2	2.01	0.42
4:Q:233:ALA:HB3	4:Q:274:ALA:HB3	2.01	0.42
5:R:56:GLY:HA3	13:R:602:HEA:H161	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:103:ALA:HB2	5:R:213:ILE:HD11	2.01	0.42
1:A:298:ASP:N	1:A:298:ASP:OD1	2.49	0.42
4:E:141:LYS:HD2	4:E:204:LEU:HD12	2.01	0.42
5:F:483:ILE:HD12	8:I:17:LEU:HD21	2.02	0.42
1:M:122:LYS:HA	1:M:122:LYS:HD3	1.79	0.42
2:N:111:ARG:NH2	11:N:602:HEM:O2A	2.48	0.42
2:N:273:ILE:HA	2:N:276:VAL:HG12	1.99	0.42
4:Q:319:PRO:HA	4:Q:320:PRO:HD3	1.96	0.42
9:V:75:ARG:HG3	9:V:76:ASP:N	2.32	0.42
2:B:64:TYR:CD2	2:B:110:VAL:HG11	2.55	0.42
5:F:539:GLU:N	5:F:539:GLU:OE1	2.53	0.42
13:F:602:HEA:C18	13:F:602:HEA:H261	2.50	0.42
1:M:76:TYR:CZ	2:N:530:ALA:HB2	2.54	0.42
1:M:323:ARG:NE	1:M:345:GLU:HG3	2.35	0.42
2:N:496:LEU:HD23	2:N:496:LEU:H	1.83	0.42
4:Q:154:LEU:HD11	4:Q:297:LYS:HB3	2.01	0.42
1:A:404:ASP:OD1	1:A:408:TYR:N	2.33	0.42
2:N:458:LEU:HB2	2:N:462:ALA:O	2.19	0.42
8:U:16:LEU:HD12	8:U:17:LEU:N	2.35	0.42
2:B:28:SER:OG	1:M:180:ASP:HB3	2.19	0.42
2:B:434:TRP:HZ3	5:R:32:ILE:HG13	1.85	0.42
3:C:134:ALA:O	3:C:137:GLN:HG3	2.19	0.42
3:C:263:ILE:HD11	7:T:120:PHE:HZ	1.84	0.42
5:F:102:PHE:HZ	5:F:410:THR:HG23	1.85	0.42
2:N:26:HIS:O	2:N:26:HIS:ND1	2.50	0.42
9:V:17:PRO:HG2	9:V:20:TRP:CG	2.54	0.42
2:B:122:ALA:O	2:B:125:ILE:HG22	2.19	0.42
5:F:268:TYR:CD2	5:F:307:SER:HB2	2.55	0.42
5:F:359:MET:SD	5:F:360:LEU:HD22	2.60	0.42
6:G:20:ASN:N	6:G:20:ASN:OD1	2.53	0.42
1:M:114:PHE:HD1	1:M:139:TYR:HH	1.68	0.42
5:R:509:ASP:HB2	5:R:519:TRP:HB3	2.01	0.42
13:R:601:HEA:HHA	13:R:601:HEA:HBA1	2.01	0.42
8:U:70:THR:OG1	9:V:112:SER:HB3	2.20	0.42
1:A:314:GLY:HA3	1:A:317:ASN:OD1	2.19	0.42
2:B:168:ASP:OD1	2:B:168:ASP:N	2.50	0.42
2:B:209:ILE:HD13	2:B:209:ILE:HA	1.91	0.42
5:F:155:THR:HG22	5:F:255:TRP:CD1	2.55	0.42
1:M:236:PRO:HA	1:M:241:LYS:HG2	2.02	0.42
4:Q:85:PRO:O	4:Q:87:GLN:HG2	2.20	0.42
6:S:195:LEU:O	6:S:199:ILE:HG22	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:14:LEU:HD11	2:B:16:ARG:NH2	2.35	0.42
2:B:22:ASP:OD2	1:M:181:ARG:NH1	2.40	0.42
2:B:159:GLU:OE2	2:B:216:HIS:ND1	2.52	0.42
2:B:418:ILE:O	2:B:422:ILE:HG12	2.20	0.42
5:F:18:PRO:HG2	5:F:504:VAL:HG11	2.01	0.42
5:F:210:THR:HG22	5:F:214:MET:HE1	2.02	0.42
5:F:330:THR:O	5:F:333:ILE:HG22	2.20	0.42
4:Q:136:PHE:CZ	4:Q:139:ASN:HB3	2.55	0.42
5:R:55:GLY:HA3	5:R:90:MET:CE	2.50	0.42
5:R:281:ILE:HD12	5:R:281:ILE:HA	1.92	0.42
6:S:61:PRO:O	6:S:63:THR:N	2.52	0.42
2:B:273:ILE:HA	2:B:276:VAL:HG12	2.02	0.41
2:B:306:PRO:HD2	2:B:314:GLU:HG3	2.02	0.41
2:B:333:PRO:HB2	2:B:335:PRO:HD2	2.01	0.41
5:F:118:PHE:HB3	5:F:121:LEU:HD23	2.02	0.41
3:O:102:GLN:OE1	3:O:107:ARG:HG3	2.20	0.41
3:O:228:LYS:O	3:O:232:ILE:HG12	2.20	0.41
4:Q:106:ILE:HG13	4:Q:107:SER:N	2.35	0.41
6:S:24:MET:SD	6:S:25:VAL:HG23	2.60	0.41
8:U:44:HIS:NE2	9:V:40:HIS:O	2.49	0.41
9:V:33:GLU:HB3	9:V:36:GLU:OE1	2.19	0.41
2:B:74:VAL:HG11	2:N:74:VAL:HB	2.01	0.41
5:F:54:ILE:O	5:F:57:LEU:HG	2.20	0.41
8:I:78:THR:HG22	8:I:78:THR:O	2.20	0.41
2:N:381:ILE:O	2:N:384:MET:HB3	2.19	0.41
4:Q:88:PHE:HB2	5:R:561:GLY:H	1.84	0.41
6:S:25:VAL:HG12	6:S:180:VAL:HG11	2.02	0.41
6:S:65:LEU:HB3	6:S:200:TYR:CE1	2.55	0.41
3:C:215:MET:HE3	12:C:302:HEC:C1B	2.35	0.41
5:F:30:LYS:O	5:F:34:THR:HB	2.20	0.41
5:F:107:LEU:HD12	5:F:213:ILE:HG21	2.01	0.41
5:F:261:PHE:HD1	5:F:311:TRP:CD2	2.38	0.41
5:F:337:THR:CG2	13:F:601:HEA:H263	2.49	0.41
5:F:389:THR:C	5:F:391:SER:H	2.24	0.41
6:G:72:PRO:O	6:G:76:VAL:HG23	2.20	0.41
1:M:129:ASP:OD1	3:O:242:ARG:NH2	2.36	0.41
2:N:55:PHE:O	2:N:59:LEU:HD23	2.20	0.41
5:R:98:ILE:HD12	5:R:98:ILE:HA	1.98	0.41
6:S:32:TRP:O	6:S:36:GLU:HG2	2.21	0.41
1:A:253:ARG:HB2	1:A:257:GLU:OE2	2.20	0.41
3:C:266:MET:O	3:C:270:ILE:HG12	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:149:PHE:CE2	4:E:154:LEU:HD12	2.56	0.41
5:F:101:GLY:O	5:F:105:LEU:HD23	2.19	0.41
5:F:342:PHE:HA	5:F:345:ILE:HG22	2.01	0.41
7:H:111:PRO:O	7:H:114:ILE:HG12	2.20	0.41
4:Q:144:TYR:OH	4:Q:214:VAL:O	2.30	0.41
5:R:155:THR:HG22	5:R:255:TRP:CD1	2.56	0.41
5:R:210:THR:O	5:R:213:ILE:HG22	2.21	0.41
1:A:91:ARG:NE	2:B:506:SER:HB3	2.34	0.41
2:B:329:HIS:O	2:B:329:HIS:ND1	2.54	0.41
3:C:201:GLU:HG2	3:C:202:GLN:N	2.35	0.41
3:C:260:ALA:HA	3:C:263:ILE:HG22	2.02	0.41
4:E:28:SER:O	4:E:32:GLY:N	2.53	0.41
2:N:349:LEU:HB3	2:N:350:PRO:HD3	2.01	0.41
4:Q:235:TRP:CD1	4:Q:242:LYS:HE2	2.56	0.41
6:S:34:SER:HB3	7:T:48:MET:CG	2.51	0.41
9:V:17:PRO:O	9:V:18:PRO:C	2.58	0.41
2:B:78:TYR:HB2	2:B:90:MET:SD	2.61	0.41
3:C:162:ASP:OD1	3:C:163:LEU:N	2.54	0.41
5:F:303:ILE:HD12	5:F:340:LYS:HZ3	1.86	0.41
6:G:24:MET:SD	6:G:25:VAL:HG23	2.60	0.41
9:J:17:PRO:HA	9:J:18:PRO:HD2	1.87	0.41
1:M:356:LEU:HD22	2:N:182:SER:CB	2.51	0.41
1:M:402:THR:OG1	1:M:403:ILE:N	2.54	0.41
4:Q:39:ILE:HD13	4:Q:238:GLU:HB3	2.02	0.41
8:U:79:TRP:CG	9:V:104:CYS:HB3	2.56	0.41
4:E:273:CYS:HB3	4:E:281:HIS:CE1	2.55	0.41
4:E:282:SER:HB2	5:F:461:TYR:CD1	2.56	0.41
5:F:341:PHE:HZ	5:F:369:PHE:HD2	1.68	0.41
2:N:35:LEU:HD23	2:N:35:LEU:HA	1.93	0.41
4:Q:212:VAL:HB	4:Q:309:ASN:ND2	2.35	0.41
5:R:270:ILE:O	5:R:406:ILE:HD11	2.20	0.41
1:A:365:GLN:HE22	3:C:215:MET:N	2.19	0.41
2:B:108:LEU:HA	2:B:111:ARG:HG2	2.01	0.41
2:B:177:ARG:HB2	2:B:203:PHE:CZ	2.55	0.41
2:N:145:ASN:OD1	2:N:231:HIS:ND1	2.50	0.41
4:Q:241:PHE:HZ	4:Q:243:ARG:HH21	1.68	0.41
5:R:282:PHE:HE2	5:R:344:TRP:HB3	1.85	0.41
1:A:313:MET:SD	1:A:313:MET:N	2.94	0.41
1:A:356:LEU:HD12	1:A:375:HIS:CE1	2.56	0.41
2:B:26:HIS:O	2:B:26:HIS:ND1	2.51	0.41
2:B:71:PRO:HG3	2:B:213:TYR:CD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:505:GLY:HA3	6:S:97:PHE:HE2	1.86	0.41
5:F:224:PHE:HE1	5:F:266:GLU:OE2	2.04	0.41
5:F:274:PHE:CD1	5:F:406:ILE:HA	2.56	0.41
9:J:78:ALA:HB1	9:J:82:ARG:NH1	2.36	0.41
1:M:414:ASP:OD1	1:M:415:PHE:N	2.50	0.41
2:N:167:PRO:O	2:N:169:ASP:N	2.52	0.41
2:N:168:ASP:N	2:N:168:ASP:OD1	2.53	0.41
2:N:213:TYR:CZ	2:N:217:ILE:HD13	2.56	0.41
3:O:109:PRO:HG3	12:O:301:HEC:HHC	2.02	0.41
3:O:215:MET:HE1	12:O:302:HEC:C4A	2.51	0.41
5:R:102:PHE:O	5:R:106:VAL:HG22	2.21	0.41
5:R:397:HIS:O	5:R:401:VAL:HG22	2.21	0.41
5:R:550:MET:O	5:R:550:MET:HG3	2.21	0.41
9:V:19:GLY:CA	9:V:31:VAL:HG22	2.51	0.41
9:V:144:ILE:O	9:V:147:ILE:HG22	2.21	0.41
2:B:458:LEU:HB2	2:B:462:ALA:O	2.21	0.41
4:E:142:PHE:CE2	4:E:213:LEU:HB2	2.56	0.41
4:E:235:TRP:CE2	4:E:242:LYS:HE2	2.55	0.41
5:F:173:MET:SD	7:H:106:ILE:HG23	2.61	0.41
8:I:6:ILE:HD12	8:I:6:ILE:H	1.85	0.41
2:N:100:ILE:HD12	2:N:100:ILE:HA	1.93	0.41
4:E:277:CYS:SG	4:E:284:MET:HE1	2.62	0.40
5:F:208:ILE:N	5:F:280:GLU:OE2	2.54	0.40
6:G:82:PHE:HA	6:G:85:GLN:CD	2.41	0.40
2:N:129:LEU:HD12	11:N:601:HEM:HMC2	2.03	0.40
2:N:301:SER:OG	3:O:175:ALA:O	2.23	0.40
2:N:316:LEU:HG	2:N:338:VAL:HG22	2.03	0.40
1:A:110:LEU:HA	1:A:113:ILE:HG22	2.02	0.40
2:B:92:ARG:NH1	2:B:95:GLN:OE1	2.53	0.40
11:B:602:HEM:O1D	11:B:602:HEM:HHA	2.22	0.40
5:F:403:PHE:CE2	5:F:407:VAL:HG21	2.57	0.40
5:F:405:THR:HG23	5:F:406:ILE:N	2.36	0.40
5:F:440:ILE:O	5:F:444:THR:OG1	2.32	0.40
5:F:508:ASP:OD2	9:J:27:ARG:NH2	2.55	0.40
13:F:602:HEA:HBA1	13:F:602:HEA:CHA	2.51	0.40
13:F:602:HEA:HMD1	13:F:602:HEA:HBD2	2.02	0.40
2:N:119:LEU:HD22	2:N:308:PHE:CE1	2.56	0.40
2:N:316:LEU:HA	2:N:319:ILE:HG12	2.03	0.40
4:Q:60:VAL:O	4:Q:64:VAL:HG23	2.21	0.40
4:Q:139:ASN:OD1	4:Q:140:TRP:N	2.51	0.40
7:T:111:PRO:O	7:T:114:ILE:HG12	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:PHE:CE1	1:A:386:LYS:HB2	2.57	0.40
5:F:20:ARG:NH2	9:J:53:ASP:OD1	2.54	0.40
5:F:102:PHE:O	5:F:106:VAL:HG22	2.21	0.40
1:M:149:SER:HA	1:M:152:ILE:HG12	2.03	0.40
2:N:169:ASP:OD2	2:N:292:LEU:HD22	2.22	0.40
4:Q:39:ILE:HD11	4:Q:239:PHE:HD1	1.86	0.40
6:S:61:PRO:C	6:S:63:THR:N	2.73	0.40
2:B:142:ARG:NH2	2:B:239:LYS:O	2.51	0.40
4:E:160:ASP:HB2	4:E:199:ASP:HA	2.04	0.40
5:F:279:SER:O	5:F:283:PRO:HD3	2.20	0.40
6:G:34:SER:HB3	7:H:48:MET:CG	2.51	0.40
3:O:201:GLU:OE1	3:O:201:GLU:N	2.38	0.40
6:S:21:ARG:HB2	7:T:66:ARG:HD3	2.03	0.40
9:V:88:VAL:HG12	9:V:90:THR:H	1.87	0.40
2:B:154:ILE:HG13	2:B:346:PHE:CD2	2.57	0.40
3:C:208:MET:HE1	3:C:223:LEU:HD23	2.03	0.40
4:E:238:GLU:HG3	4:E:269:PHE:CD1	2.57	0.40
4:E:298:ALA:HA	4:E:301:GLN:NE2	2.36	0.40
2:N:122:ALA:O	2:N:125:ILE:HG22	2.22	0.40
3:O:215:MET:HE2	12:O:302:HEC:NA	2.36	0.40
4:Q:273:CYS:HB3	4:Q:281:HIS:CE1	2.57	0.40
5:R:146:ALA:HA	5:R:167:GLY:HA3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	376/429 (88%)	345 (92%)	31 (8%)	0	100	100
1	M	366/429 (85%)	338 (92%)	28 (8%)	0	100	100
2	B	522/573 (91%)	477 (91%)	45 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	N	522/573 (91%)	482 (92%)	40 (8%)	0	100	100
3	C	214/280 (76%)	198 (92%)	16 (8%)	0	100	100
3	O	207/280 (74%)	192 (93%)	15 (7%)	0	100	100
4	E	272/363 (75%)	256 (94%)	16 (6%)	0	100	100
4	Q	279/363 (77%)	260 (93%)	18 (6%)	1 (0%)	34	34
5	F	550/573 (96%)	528 (96%)	22 (4%)	0	100	100
5	R	550/573 (96%)	528 (96%)	22 (4%)	0	100	100
6	G	184/203 (91%)	179 (97%)	5 (3%)	0	100	100
6	S	183/203 (90%)	177 (97%)	5 (3%)	1 (0%)	29	29
7	H	137/139 (99%)	132 (96%)	5 (4%)	0	100	100
7	T	137/139 (99%)	133 (97%)	4 (3%)	0	100	100
8	I	63/79 (80%)	58 (92%)	5 (8%)	0	100	100
8	U	63/79 (80%)	62 (98%)	1 (2%)	0	100	100
9	J	141/155 (91%)	135 (96%)	5 (4%)	1 (1%)	22	22
9	V	141/155 (91%)	137 (97%)	4 (3%)	0	100	100
All	All	4907/5588 (88%)	4617 (94%)	287 (6%)	3 (0%)	54	51

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	J	18	PRO
4	Q	33	ILE
6	S	62	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	A	296/343 (86%)	296 (100%)	0	100	100
1	M	294/343 (86%)	293 (100%)	1 (0%)	92	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	422/466 (91%)	422 (100%)	0	100 100
2	N	419/466 (90%)	419 (100%)	0	100 100
3	C	131/207 (63%)	131 (100%)	0	100 100
3	O	128/207 (62%)	128 (100%)	0	100 100
4	E	236/306 (77%)	235 (100%)	1 (0%)	91 91
4	Q	238/306 (78%)	236 (99%)	2 (1%)	81 81
5	F	449/466 (96%)	448 (100%)	1 (0%)	93 93
5	R	449/466 (96%)	448 (100%)	1 (0%)	93 93
6	G	153/166 (92%)	153 (100%)	0	100 100
6	S	152/166 (92%)	152 (100%)	0	100 100
7	H	100/101 (99%)	100 (100%)	0	100 100
7	T	99/101 (98%)	99 (100%)	0	100 100
8	I	54/62 (87%)	54 (100%)	0	100 100
8	U	53/62 (86%)	53 (100%)	0	100 100
9	J	103/115 (90%)	102 (99%)	1 (1%)	76 76
9	V	105/115 (91%)	104 (99%)	1 (1%)	76 76
All	All	3881/4464 (87%)	3873 (100%)	8 (0%)	93 93

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	E	163	ARG
5	F	20	ARG
9	J	82	ARG
1	M	316	ARG
4	Q	163	ARG
4	Q	314	ARG
5	R	555	ARG
9	V	16	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	179	ASN
3	C	213	GLN

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Mol	Chain	Res	Type
5	F	474	ASN
3	O	179	ASN
5	R	434	HIS
6	S	186	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

14 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	$\#\|Z\| > 2$
10	FES	A	501	1	0,4,4	-	-	-		
11	HEM	N	601	2	41,49,50	1.28	3 (7%)	46,81,82	1.21	3 (6%)
11	HEM	B	601	2	41,49,50	1.27	3 (7%)	46,81,82	1.21	3 (6%)
12	HEC	O	301	3	32,50,50	2.22	3 (9%)	24,82,82	1.33	2 (8%)
13	HEA	F	601	5	57,67,67	1.99	14 (24%)	61,103,103	2.43	26 (42%)
10	FES	M	501	1	0,4,4	-	-	-		
11	HEM	B	602	2	41,50,50	1.33	5 (12%)	45,82,82	1.76	8 (17%)
12	HEC	C	302	3	32,50,50	2.24	3 (9%)	24,82,82	1.37	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	HEM	N	602	2	41,50,50	1.47	3 (7%)	45,82,82	1.43	7 (15%)
13	HEA	R	602	5	57,67,67	1.98	14 (24%)	61,103,103	2.38	23 (37%)
13	HEA	F	602	5	57,67,67	2.03	14 (24%)	61,103,103	2.33	24 (39%)
12	HEC	C	301	-	32,50,50	2.25	4 (12%)	24,82,82	1.27	2 (8%)
12	HEC	O	302	3	32,50,50	2.38	12 (37%)	24,82,82	2.11	6 (25%)
13	HEA	R	601	5	57,67,67	1.99	14 (24%)	61,103,103	2.43	24 (39%)

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
10	FES	A	501	1	-	-	0/1/1/1
11	HEM	B	601	2	-	0/12/52/54	-
11	HEM	N	601	2	-	0/12/52/54	-
12	HEC	O	301	3	-	3/10/54/54	-
13	HEA	F	601	5	3/3/7/16	15/32/76/76	-
10	FES	M	501	1	-	-	0/1/1/1
11	HEM	B	602	2	-	4/12/54/54	-
12	HEC	C	302	3	-	0/10/54/54	-
11	HEM	N	602	2	-	2/12/54/54	-
13	HEA	R	602	5	3/3/7/16	17/32/76/76	-
13	HEA	F	602	5	3/3/7/16	19/32/76/76	-
12	HEC	C	301	-	-	3/10/54/54	-
12	HEC	O	302	3	-	1/10/54/54	-
13	HEA	R	601	5	3/3/7/16	11/32/76/76	-

All (92) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	O	302	HEC	C2B-C3B	7.01	1.48	1.40
12	C	301	HEC	C3C-C2C	-6.61	1.33	1.40
12	C	302	HEC	C3C-C2C	-6.57	1.33	1.40
12	C	301	HEC	C2B-C3B	-6.56	1.33	1.40
12	O	301	HEC	C2B-C3B	-6.56	1.33	1.40
12	C	302	HEC	C2B-C3B	-6.51	1.34	1.40
12	O	301	HEC	C3C-C2C	-6.38	1.34	1.40
12	O	302	HEC	C3C-C2C	6.31	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	302	HEC	C3D-C2D	5.43	1.53	1.37
12	O	301	HEC	C3D-C2D	5.39	1.53	1.37
12	C	301	HEC	C3D-C2D	5.38	1.53	1.37
13	F	602	HEA	C3B-C2B	5.31	1.46	1.34
13	R	602	HEA	C3B-C2B	5.31	1.46	1.34
13	R	601	HEA	C3B-C2B	5.27	1.46	1.34
13	F	601	HEA	C3B-C2B	5.26	1.46	1.34
13	F	601	HEA	CHC-C4B	4.98	1.47	1.35
13	R	601	HEA	CHC-C4B	4.97	1.47	1.35
13	F	602	HEA	C3D-C2D	4.90	1.47	1.36
13	R	602	HEA	CHC-C4B	4.90	1.47	1.35
13	F	602	HEA	CHC-C4B	4.89	1.47	1.35
13	R	601	HEA	C3D-C2D	4.80	1.46	1.36
13	F	601	HEA	C3D-C2D	4.80	1.46	1.36
13	F	602	HEA	C3A-C2A	4.73	1.46	1.40
13	R	602	HEA	C3D-C2D	4.66	1.46	1.36
13	F	602	HEA	CHD-C1D	4.55	1.46	1.35
13	R	601	HEA	C3A-C2A	4.51	1.46	1.40
13	F	601	HEA	C3A-C2A	4.48	1.46	1.40
13	R	602	HEA	C3A-C2A	4.47	1.46	1.40
13	R	601	HEA	CHD-C1D	4.42	1.46	1.35
13	F	601	HEA	CHD-C1D	4.42	1.46	1.35
13	R	602	HEA	CHD-C1D	4.40	1.46	1.35
13	F	601	HEA	C3C-C2C	4.38	1.46	1.40
13	F	602	HEA	C3C-C2C	4.37	1.46	1.40
13	R	601	HEA	C3C-C2C	4.33	1.46	1.40
13	R	602	HEA	C3C-C2C	4.29	1.46	1.40
11	N	602	HEM	C3C-C2C	-4.00	1.34	1.40
11	N	602	HEM	C3C-CAC	3.64	1.55	1.47
12	O	302	HEC	C2A-C3A	3.45	1.47	1.37
11	B	602	HEM	C1B-NB	-3.35	1.34	1.40
11	B	602	HEM	C4D-ND	-3.35	1.34	1.40
13	F	602	HEA	C1D-ND	-3.34	1.34	1.40
13	R	602	HEA	C1D-ND	-3.32	1.34	1.40
12	O	302	HEC	C3D-C2D	3.32	1.47	1.37
13	F	601	HEA	C1D-ND	-3.28	1.34	1.40
13	R	601	HEA	C1D-ND	-3.28	1.34	1.40
12	O	302	HEC	C3C-C4C	3.22	1.48	1.43
11	N	602	HEM	CAB-C3B	2.99	1.55	1.47
13	R	601	HEA	FE-NB	2.99	2.11	1.96
13	F	602	HEA	C4B-NB	-2.99	1.35	1.40
13	R	602	HEA	FE-NB	2.97	2.11	1.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	F	601	HEA	FE-NB	2.97	2.11	1.96
13	F	602	HEA	FE-NB	2.97	2.11	1.96
11	N	601	HEM	CAB-C3B	2.94	1.55	1.47
13	R	602	HEA	C4B-NB	-2.89	1.35	1.40
11	B	601	HEM	CAB-C3B	2.89	1.55	1.47
12	O	302	HEC	C2A-C1A	2.87	1.49	1.42
13	F	601	HEA	C4B-NB	-2.86	1.35	1.40
12	O	302	HEC	C3A-C4A	2.84	1.49	1.42
13	F	601	HEA	FE-ND	2.81	2.10	1.96
12	O	302	HEC	C4D-CHA	2.81	1.48	1.41
11	B	602	HEM	FE-NB	2.81	2.10	1.96
12	O	302	HEC	C1B-CHB	2.80	1.48	1.41
13	R	601	HEA	FE-ND	2.80	2.10	1.96
13	R	601	HEA	C4B-NB	-2.78	1.35	1.40
13	R	602	HEA	FE-ND	2.75	2.10	1.96
13	F	602	HEA	FE-ND	2.74	2.10	1.96
12	O	302	HEC	C4B-C3B	2.71	1.48	1.43
13	F	602	HEA	C2A-C1A	2.71	1.48	1.42
13	F	601	HEA	C4B-C3B	2.70	1.49	1.44
13	R	601	HEA	C4B-C3B	2.66	1.49	1.44
13	R	602	HEA	C4B-C3B	2.51	1.48	1.44
13	R	602	HEA	C2A-C1A	2.51	1.48	1.42
13	F	602	HEA	C4B-C3B	2.50	1.48	1.44
13	F	601	HEA	C2A-C1A	2.47	1.48	1.42
13	R	601	HEA	C2A-C1A	2.46	1.48	1.42
13	F	601	HEA	C1C-CHC	2.42	1.47	1.41
13	R	601	HEA	C1C-CHC	2.42	1.47	1.41
11	N	601	HEM	C2C-C3C	-2.40	1.33	1.41
13	F	602	HEA	C1C-CHC	2.39	1.47	1.41
11	B	601	HEM	C2C-C3C	-2.39	1.33	1.41
13	R	602	HEA	C1C-CHC	2.36	1.47	1.41
12	O	302	HEC	C1D-CHD	2.33	1.47	1.41
12	O	302	HEC	C1C-CHC	2.29	1.47	1.41
11	B	602	HEM	CHB-C1B	2.19	1.40	1.35
13	F	602	HEA	C4C-CHD	2.16	1.47	1.41
11	N	601	HEM	CAA-C2A	2.08	1.55	1.52
12	C	301	HEC	CAD-C3D	2.06	1.55	1.52
13	R	601	HEA	C4C-CHD	2.06	1.46	1.41
13	F	601	HEA	C4C-CHD	2.05	1.46	1.41
11	B	601	HEM	CAA-C2A	2.05	1.55	1.52
11	B	602	HEM	C1D-ND	-2.05	1.34	1.38
13	R	602	HEA	C4C-CHD	2.02	1.46	1.41

All (130) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	R	601	HEA	C3D-C4D-ND	6.46	116.61	110.36
13	F	601	HEA	C3D-C4D-ND	6.46	116.61	110.36
12	O	302	HEC	C1D-C2D-C3D	-6.43	102.52	107.00
13	F	602	HEA	C3D-C4D-ND	6.05	116.22	110.36
13	R	602	HEA	C3D-C4D-ND	6.03	116.20	110.36
13	R	601	HEA	C2D-C1D-ND	5.71	116.60	109.84
13	F	601	HEA	C2D-C1D-ND	5.66	116.55	109.84
13	R	602	HEA	C2D-C1D-ND	5.52	116.38	109.84
13	R	602	HEA	C2B-C1B-NB	5.40	116.34	109.88
13	F	601	HEA	C2B-C1B-NB	5.39	116.34	109.88
13	R	601	HEA	C2B-C1B-NB	5.39	116.33	109.88
13	F	602	HEA	C2B-C1B-NB	5.32	116.26	109.88
13	F	602	HEA	C2D-C1D-ND	5.27	116.08	109.84
13	R	602	HEA	C3B-C4B-NB	5.25	116.06	109.84
13	F	602	HEA	C3B-C4B-NB	5.25	116.06	109.84
13	R	601	HEA	C3B-C4B-NB	5.04	115.82	109.84
13	F	601	HEA	C3B-C4B-NB	5.02	115.78	109.84
11	B	602	HEM	CHC-C4B-NB	4.81	129.66	124.43
13	F	601	HEA	C1D-C2D-C3D	-4.56	102.16	106.96
13	R	602	HEA	C1D-C2D-C3D	-4.56	102.17	106.96
13	R	601	HEA	C1D-C2D-C3D	-4.54	102.18	106.96
11	B	602	HEM	C1B-NB-C4B	4.48	109.70	105.07
13	F	602	HEA	C1D-C2D-C3D	-4.36	102.38	106.96
13	R	602	HEA	C3C-C4C-NC	3.91	114.26	109.21
11	B	602	HEM	CHD-C1D-ND	3.88	128.64	124.43
13	F	601	HEA	C3C-C4C-NC	3.87	114.21	109.21
13	R	601	HEA	C3C-C4C-NC	3.86	114.20	109.21
12	O	302	HEC	CMB-C2B-C3B	3.74	130.21	125.82
13	F	601	HEA	CHA-C4D-C3D	-3.67	119.44	124.84
13	R	601	HEA	CHA-C4D-C3D	-3.65	119.48	124.84
13	F	602	HEA	C3C-C4C-NC	3.60	113.87	109.21
12	O	302	HEC	CMC-C2C-C3C	3.46	129.89	125.82
13	R	602	HEA	CAD-CBD-CGD	-3.46	106.16	113.60
13	R	602	HEA	CHA-C4D-C3D	-3.38	119.87	124.84
13	F	602	HEA	C1B-C2B-C3B	-3.30	102.85	106.80
13	R	602	HEA	C1B-C2B-C3B	-3.30	102.85	106.80
13	F	601	HEA	C1B-C2B-C3B	-3.26	102.90	106.80
13	R	601	HEA	C1B-C2B-C3B	-3.24	102.92	106.80
13	F	602	HEA	CMC-C2C-C3C	3.24	130.74	124.68
13	R	602	HEA	CMC-C2C-C3C	3.18	130.63	124.68
13	F	601	HEA	CMC-C2C-C3C	3.18	130.62	124.68
13	F	601	HEA	CAD-CBD-CGD	-3.17	106.77	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	R	601	HEA	CAD-CBD-CGD	-3.16	106.79	113.60
13	R	601	HEA	CMC-C2C-C3C	3.16	130.59	124.68
13	R	601	HEA	C4D-C3D-C2D	-3.08	102.41	106.90
13	F	602	HEA	C4B-C3B-C2B	-3.08	102.16	107.41
11	B	602	HEM	CHA-C4D-ND	3.07	128.17	124.38
13	F	602	HEA	C4D-C3D-C2D	-3.06	102.43	106.90
13	F	601	HEA	C4D-C3D-C2D	-3.06	102.44	106.90
13	R	602	HEA	C4B-C3B-C2B	-3.06	102.19	107.41
13	R	601	HEA	CHB-C1B-C2B	-3.05	120.21	124.98
13	R	602	HEA	CHB-C1B-C2B	-3.04	120.23	124.98
13	F	601	HEA	CHB-C1B-C2B	-3.04	120.23	124.98
13	R	601	HEA	C4B-C3B-C2B	-3.01	102.27	107.41
13	F	601	HEA	C4B-C3B-C2B	-3.01	102.27	107.41
13	F	602	HEA	CHA-C4D-C3D	-3.00	120.42	124.84
13	F	602	HEA	CAD-CBD-CGD	-2.98	107.18	113.60
13	F	602	HEA	C27-C19-C20	2.95	120.23	115.27
11	B	602	HEM	C4D-ND-C1D	2.93	108.10	105.07
13	R	601	HEA	C27-C19-C20	2.89	120.13	115.27
13	R	602	HEA	C4D-C3D-C2D	-2.88	102.70	106.90
13	F	602	HEA	CHB-C1B-C2B	-2.87	120.50	124.98
11	B	602	HEM	CHB-C1B-NB	2.83	127.88	124.38
13	R	601	HEA	C1D-ND-C4D	-2.78	102.20	105.07
13	R	601	HEA	C17-C18-C19	-2.78	120.98	127.66
11	N	602	HEM	C4B-CHC-C1C	2.74	126.18	122.56
13	F	601	HEA	C17-C18-C19	-2.74	121.06	127.66
13	F	601	HEA	C1D-ND-C4D	-2.74	102.25	105.07
13	R	602	HEA	C27-C19-C20	2.72	119.84	115.27
13	R	602	HEA	C17-C18-C19	-2.69	121.18	127.66
13	F	601	HEA	C27-C19-C20	2.67	119.76	115.27
11	N	602	HEM	C3B-C2B-C1B	2.62	108.43	106.49
13	F	602	HEA	C17-C18-C19	-2.62	121.34	127.66
11	N	602	HEM	C4D-ND-C1D	2.61	107.76	105.07
11	N	601	HEM	C4D-ND-C1D	2.59	107.75	105.07
13	R	601	HEA	CBA-CAA-C2A	-2.58	108.26	112.60
11	N	602	HEM	C1B-NB-C4B	2.57	107.72	105.07
12	O	302	HEC	CBA-CAA-C2A	-2.57	108.28	112.60
13	F	601	HEA	CAD-C3D-C2D	2.56	132.64	127.88
13	R	601	HEA	CAD-C3D-C2D	2.55	132.63	127.88
13	F	601	HEA	CBA-CAA-C2A	-2.51	108.37	112.60
11	B	601	HEM	C4D-ND-C1D	2.51	107.67	105.07
13	R	601	HEA	OMA-CMA-C3A	-2.49	119.48	124.91
11	N	602	HEM	CMC-C2C-C3C	2.49	129.33	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	O	301	HEC	CMC-C2C-C1C	-2.46	124.69	128.46
13	R	602	HEA	C4B-NB-C1B	-2.44	102.55	105.07
13	R	602	HEA	C1D-ND-C4D	-2.44	102.55	105.07
11	B	601	HEM	CMA-C3A-C4A	-2.43	124.72	128.46
13	F	601	HEA	OMA-CMA-C3A	-2.43	119.61	124.91
12	O	301	HEC	C1D-C2D-C3D	-2.42	105.31	107.00
11	N	601	HEM	CMA-C3A-C4A	-2.40	124.78	128.46
11	B	602	HEM	CBA-CAA-C2A	-2.39	108.54	112.62
12	O	302	HEC	CBD-CAD-C3D	-2.39	108.54	112.62
12	C	301	HEC	CMB-C2B-C1B	-2.39	124.80	128.46
13	R	601	HEA	C4B-NB-C1B	-2.34	102.66	105.07
13	F	602	HEA	CAD-C3D-C2D	2.33	132.22	127.88
13	F	602	HEA	C4B-NB-C1B	-2.32	102.67	105.07
12	C	301	HEC	C1D-C2D-C3D	-2.31	105.39	107.00
13	R	602	HEA	CBA-CAA-C2A	-2.30	108.72	112.60
13	F	601	HEA	C4B-NB-C1B	-2.30	102.70	105.07
13	R	601	HEA	C17-C16-C15	-2.30	105.43	112.98
12	C	302	HEC	CMC-C2C-C1C	-2.24	125.02	128.46
13	F	602	HEA	CHC-C4B-NB	-2.24	121.62	124.38
13	R	602	HEA	CHD-C1D-C2D	-2.23	120.56	126.72
11	N	601	HEM	C1B-NB-C4B	2.22	107.36	105.07
12	O	302	HEC	CMD-C2D-C3D	2.22	129.12	124.94
13	F	601	HEA	C17-C16-C15	-2.21	105.69	112.98
13	R	601	HEA	CHD-C1D-C2D	-2.20	120.63	126.72
13	R	602	HEA	C17-C16-C15	-2.19	105.78	112.98
11	N	602	HEM	CBA-CAA-C2A	-2.18	108.90	112.62
13	F	601	HEA	CHD-C1D-C2D	-2.16	120.75	126.72
11	B	601	HEM	C1B-NB-C4B	2.16	107.30	105.07
12	C	302	HEC	C1D-C2D-C3D	-2.16	105.50	107.00
13	F	601	HEA	C26-C15-C14	-2.14	118.19	123.68
13	F	602	HEA	C1D-ND-C4D	-2.11	102.89	105.07
13	F	602	HEA	C17-C16-C15	-2.11	106.03	112.98
11	N	602	HEM	CMA-C3A-C4A	-2.11	125.22	128.46
13	F	601	HEA	C12-C13-C14	-2.10	106.68	112.23
13	R	602	HEA	CMB-C2B-C1B	2.08	128.21	125.04
11	B	602	HEM	CHD-C1D-C2D	-2.08	121.74	124.98
13	F	602	HEA	CMB-C2B-C1B	2.05	128.17	125.04
13	F	601	HEA	CMB-C2B-C1B	2.05	128.16	125.04
13	R	602	HEA	CMD-C2D-C1D	2.05	128.16	125.04
13	F	602	HEA	C26-C15-C14	-2.05	118.43	123.68
13	R	602	HEA	CAD-C3D-C2D	2.04	131.68	127.88
13	F	602	HEA	CHD-C1D-C2D	-2.04	121.09	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	F	601	HEA	C25-C23-C24	2.02	119.07	114.60
13	R	601	HEA	CMB-C2B-C1B	2.02	128.11	125.04
13	F	602	HEA	CBA-CAA-C2A	-2.01	109.22	112.60
13	R	601	HEA	C25-C23-C24	2.01	119.03	114.60

All (12) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	F	601	HEA	ND
13	F	601	HEA	NA
13	F	601	HEA	NB
13	F	602	HEA	ND
13	F	602	HEA	NA
13	F	602	HEA	NB
13	R	601	HEA	ND
13	R	601	HEA	NA
13	R	601	HEA	NB
13	R	602	HEA	ND
13	R	602	HEA	NA
13	R	602	HEA	NB

All (75) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	O	301	HEC	C2A-CAA-CBA-CGA
13	F	601	HEA	C4D-C3D-CAD-CBD
13	F	601	HEA	C13-C14-C15-C16
13	F	601	HEA	C13-C14-C15-C26
13	F	601	HEA	C14-C15-C16-C17
13	F	601	HEA	C17-C18-C19-C27
13	F	601	HEA	C21-C22-C23-C24
13	F	601	HEA	C21-C22-C23-C25
13	F	602	HEA	C1A-C2A-CAA-CBA
13	F	602	HEA	C3A-C2A-CAA-CBA
13	F	602	HEA	C2A-CAA-CBA-CGA
13	F	602	HEA	C4D-C3D-CAD-CBD
13	F	602	HEA	C13-C14-C15-C26
13	F	602	HEA	C14-C15-C16-C17
13	F	602	HEA	C15-C16-C17-C18
13	F	602	HEA	C17-C18-C19-C20
13	F	602	HEA	C17-C18-C19-C27
13	R	601	HEA	C4D-C3D-CAD-CBD

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Mol	Chain	Res	Type	Atoms
13	R	601	HEA	C3B-C11-C12-C13
13	R	601	HEA	O11-C11-C12-C13
13	R	601	HEA	C13-C14-C15-C16
13	R	601	HEA	C13-C14-C15-C26
13	R	601	HEA	C21-C22-C23-C25
13	R	602	HEA	C2D-C3D-CAD-CBD
13	R	602	HEA	C4D-C3D-CAD-CBD
13	R	602	HEA	C13-C14-C15-C26
13	R	602	HEA	C14-C15-C16-C17
13	R	602	HEA	C15-C16-C17-C18
13	R	602	HEA	C17-C18-C19-C27
13	R	602	HEA	C27-C19-C20-C21
13	R	602	HEA	C21-C22-C23-C25
13	R	601	HEA	C21-C22-C23-C24
13	R	602	HEA	C21-C22-C23-C24
13	F	601	HEA	C2D-C3D-CAD-CBD
13	F	602	HEA	C2D-C3D-CAD-CBD
13	R	601	HEA	C2D-C3D-CAD-CBD
13	F	602	HEA	C27-C19-C20-C21
13	F	602	HEA	C21-C22-C23-C24
13	F	602	HEA	C21-C22-C23-C25
13	F	601	HEA	C17-C18-C19-C20
13	R	602	HEA	C17-C18-C19-C20
11	B	602	HEM	C3D-CAD-CBD-CGD
13	R	602	HEA	C18-C19-C20-C21
13	F	602	HEA	C19-C20-C21-C22
13	R	602	HEA	C19-C20-C21-C22
12	C	301	HEC	C3D-CAD-CBD-CGD
12	O	302	HEC	C2A-CAA-CBA-CGA
13	F	601	HEA	C19-C20-C21-C22
11	N	602	HEM	C3D-CAD-CBD-CGD
11	B	602	HEM	C2B-C3B-CAB-CBB
11	B	602	HEM	C4B-C3B-CAB-CBB
13	F	601	HEA	C11-C12-C13-C14
11	N	602	HEM	C4B-C3B-CAB-CBB
12	O	301	HEC	C1A-C2A-CAA-CBA
12	O	301	HEC	C3A-C2A-CAA-CBA
13	R	602	HEA	C1A-C2A-CAA-CBA
13	R	602	HEA	C3A-C2A-CAA-CBA
13	F	601	HEA	CAA-CBA-CGA-O1A
13	R	602	HEA	CAA-CBA-CGA-O1A
13	F	602	HEA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
13	F	601	HEA	CAA-CBA-CGA-O2A
13	R	601	HEA	CAA-CBA-CGA-O1A
12	C	301	HEC	CAA-CBA-CGA-O2A
12	C	301	HEC	CAA-CBA-CGA-O1A
13	R	601	HEA	CAA-CBA-CGA-O2A
13	F	601	HEA	CAD-CBD-CGD-O2D
13	R	601	HEA	CAD-CBD-CGD-O2D
11	B	602	HEM	C4D-C3D-CAD-CBD
13	F	602	HEA	CAA-CBA-CGA-O2A
13	F	602	HEA	CAD-CBD-CGD-O2D
13	R	602	HEA	CAD-CBD-CGD-O2D
13	F	602	HEA	CAD-CBD-CGD-O1D
13	F	601	HEA	C3B-C11-C12-C13
13	F	602	HEA	C3B-C11-C12-C13
13	R	602	HEA	CAA-CBA-CGA-O2A

There are no ring outliers.

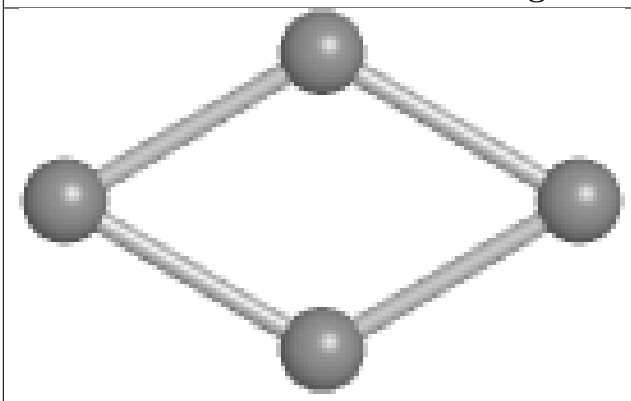
12 monomers are involved in 86 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	N	601	HEM	2	0
11	B	601	HEM	2	0
12	O	301	HEC	4	0
13	F	601	HEA	13	0
11	B	602	HEM	6	0
12	C	302	HEC	3	0
11	N	602	HEM	5	0
13	R	602	HEA	10	0
13	F	602	HEA	13	0
12	C	301	HEC	4	0
12	O	302	HEC	16	0
13	R	601	HEA	8	0

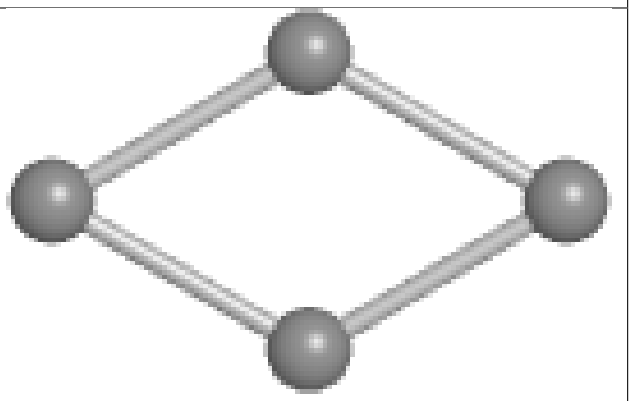
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

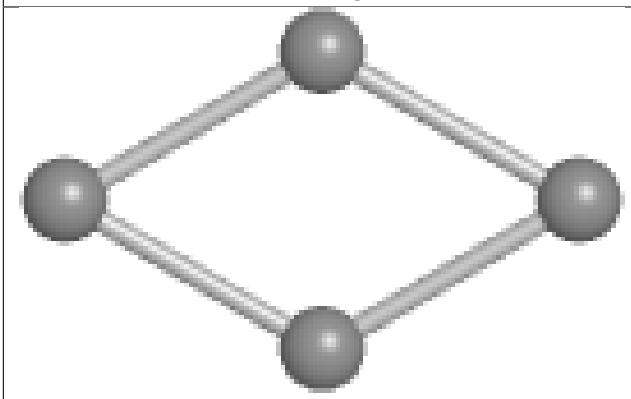
Ligand FES A 501



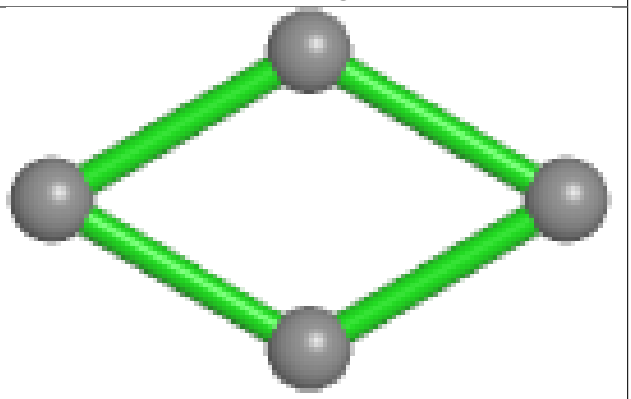
Bond lengths



Bond angles

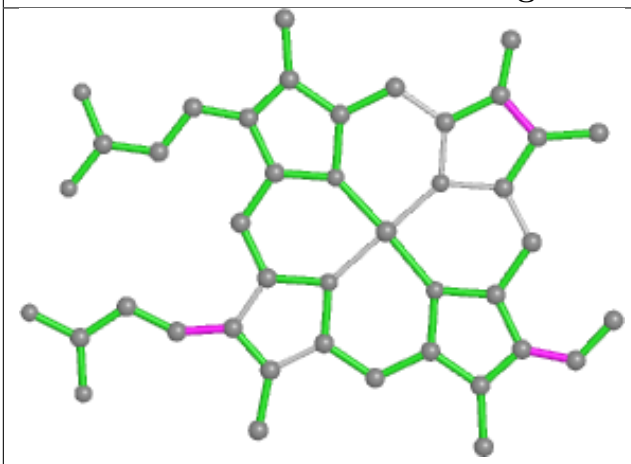


Torsions



Rings

Ligand HEM N 601



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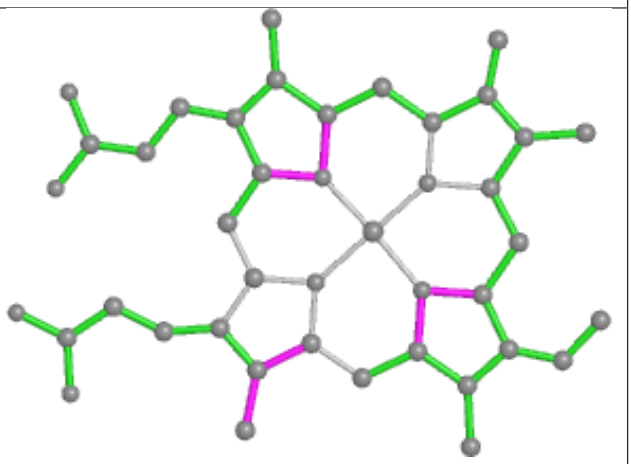

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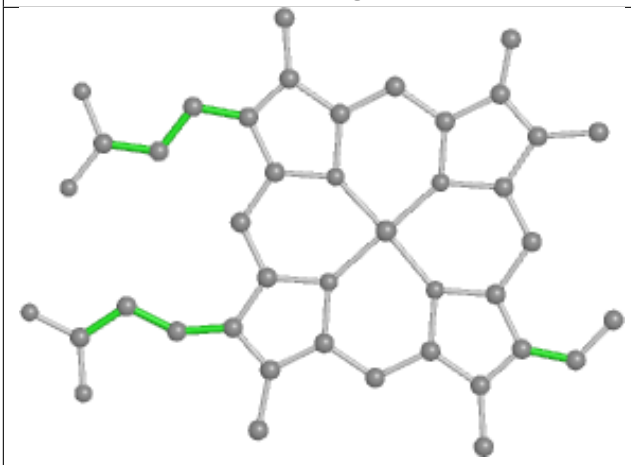

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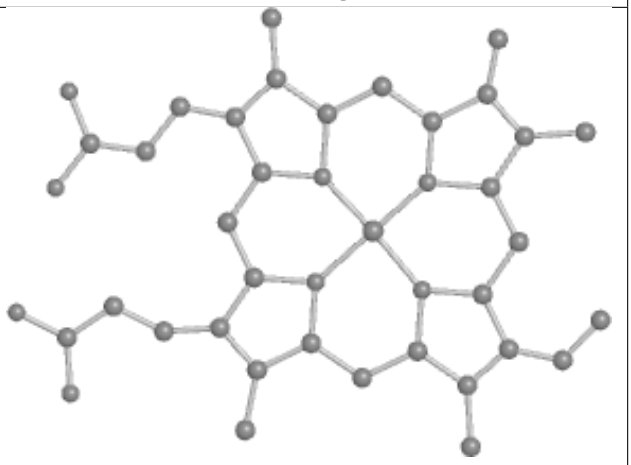
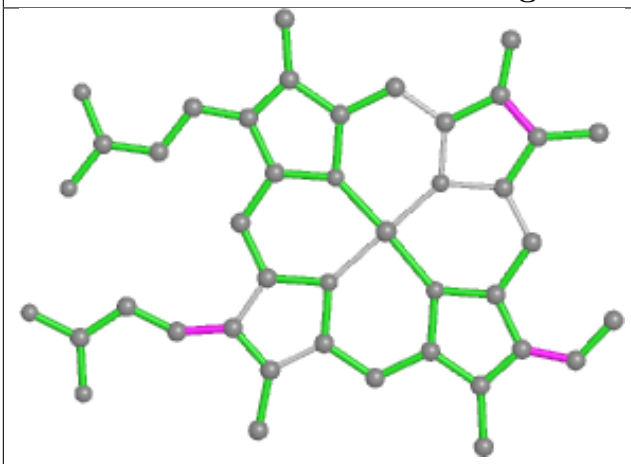


Rings

Ligand HEM B 601



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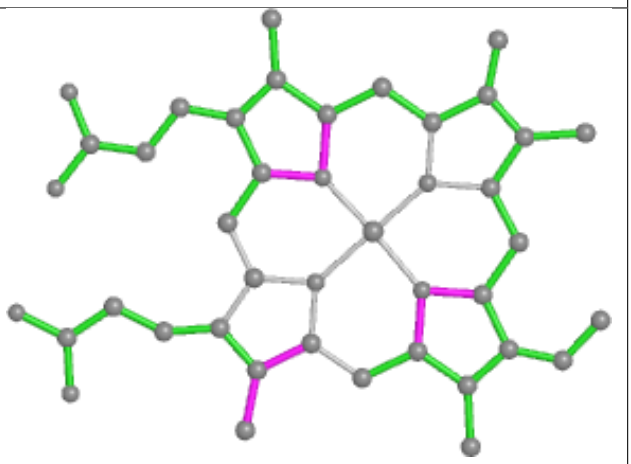
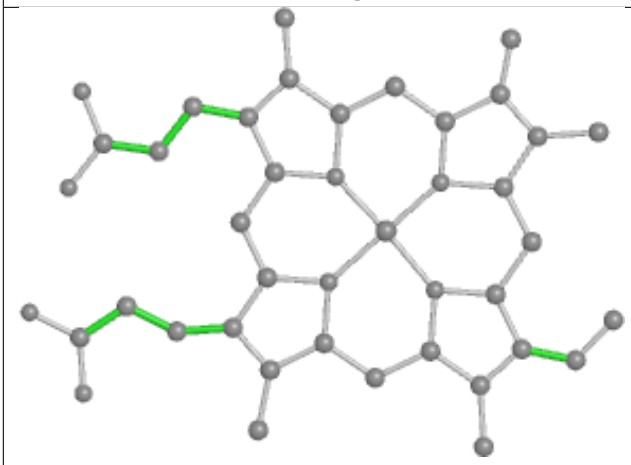


Bond angles



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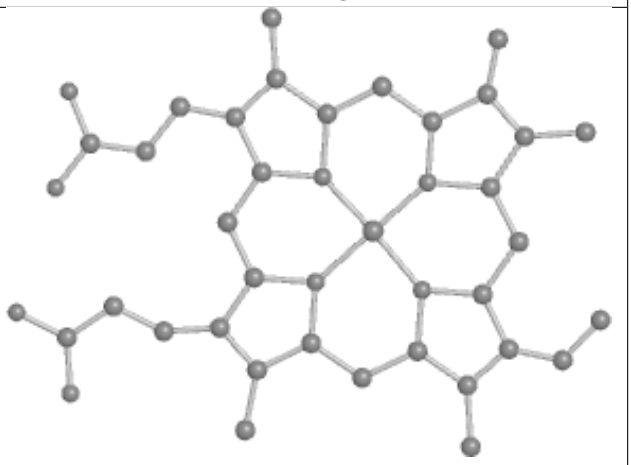
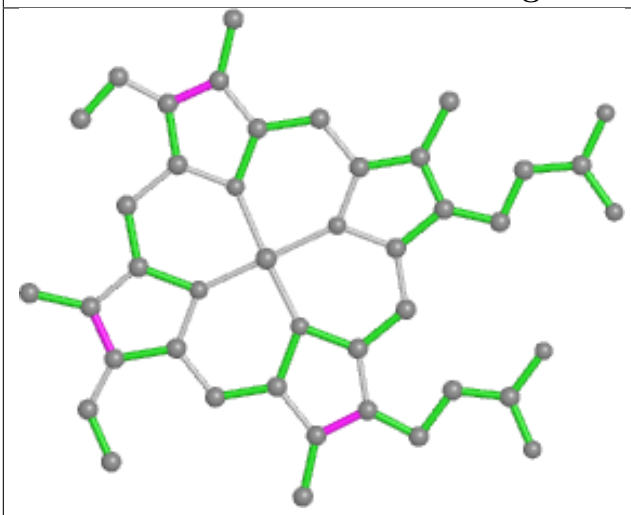


Rings

Ligand HEC O 301



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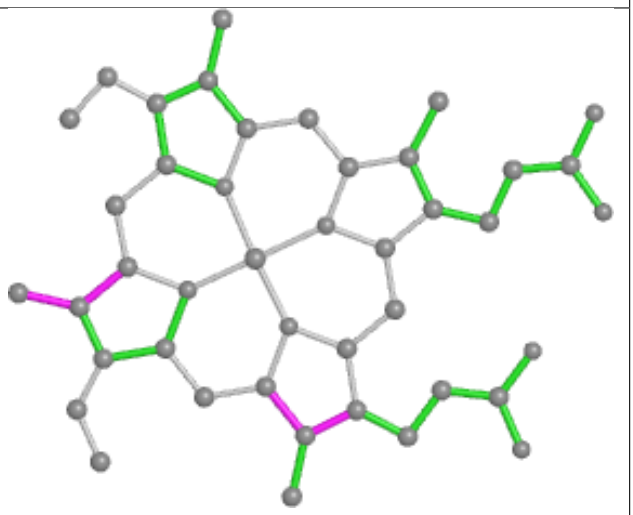

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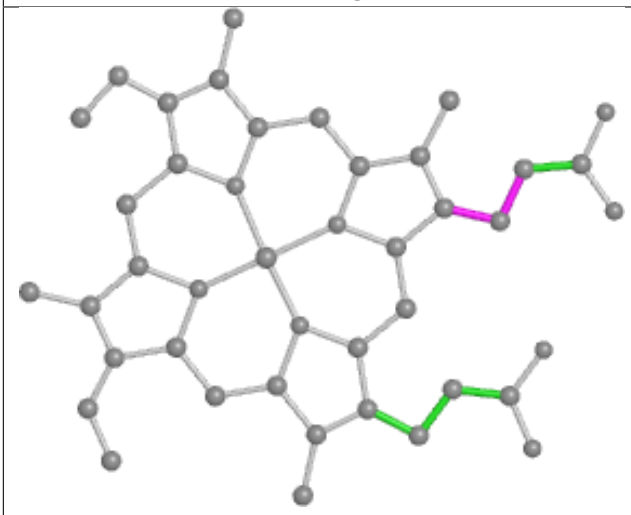

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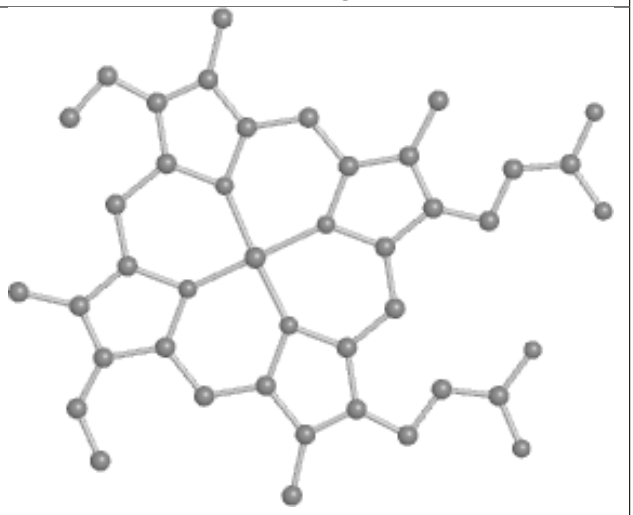
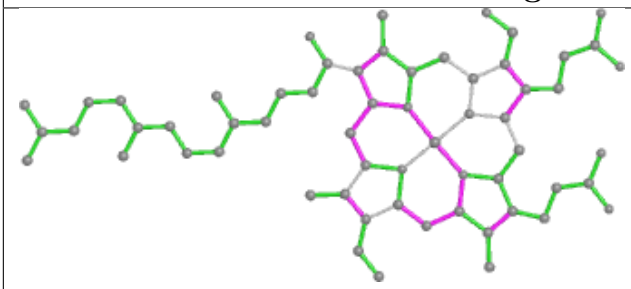


Rings

Ligand HEA F 601



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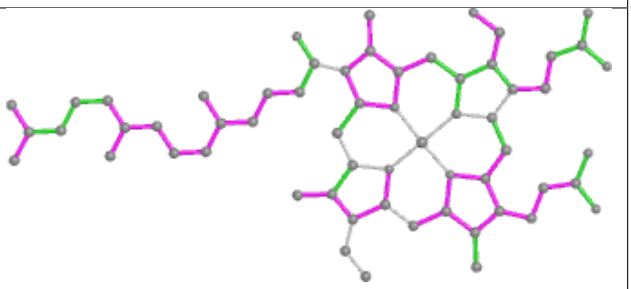

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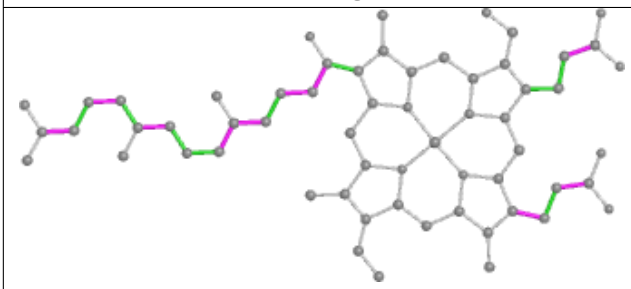

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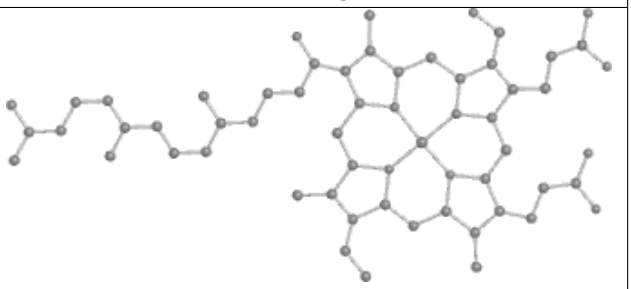
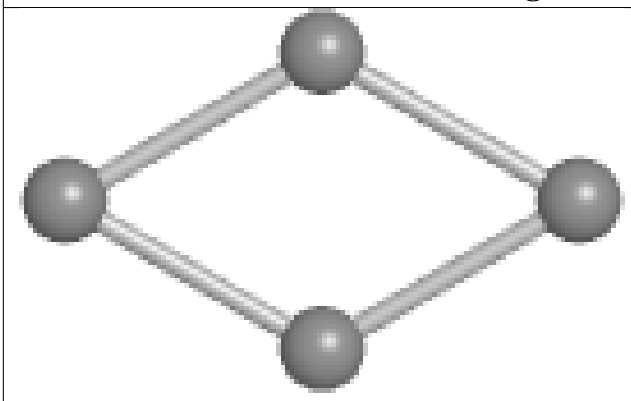


Rings

Ligand FES M 501



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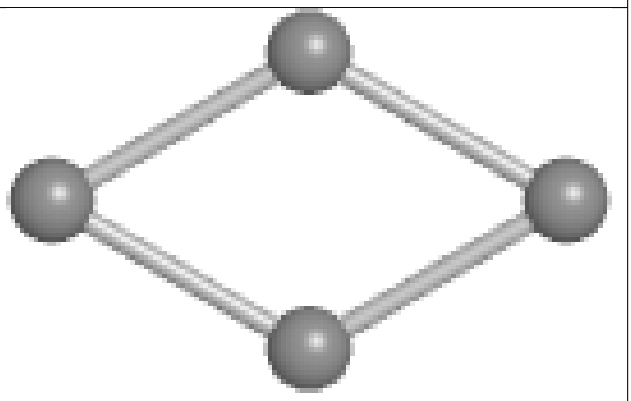

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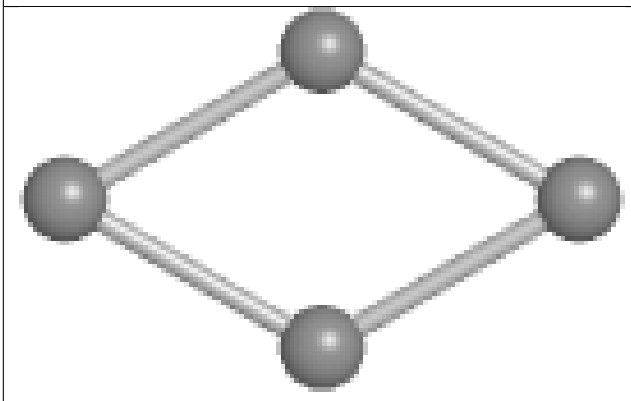

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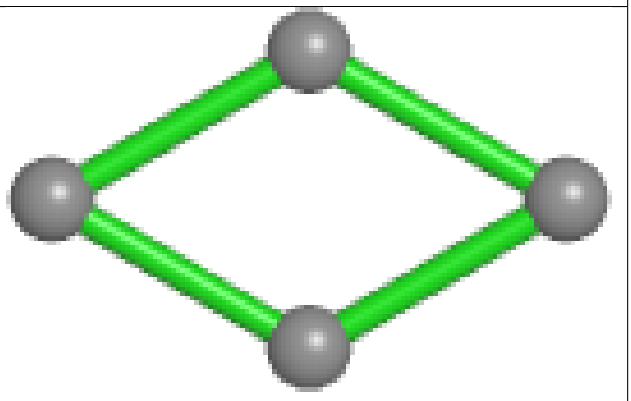
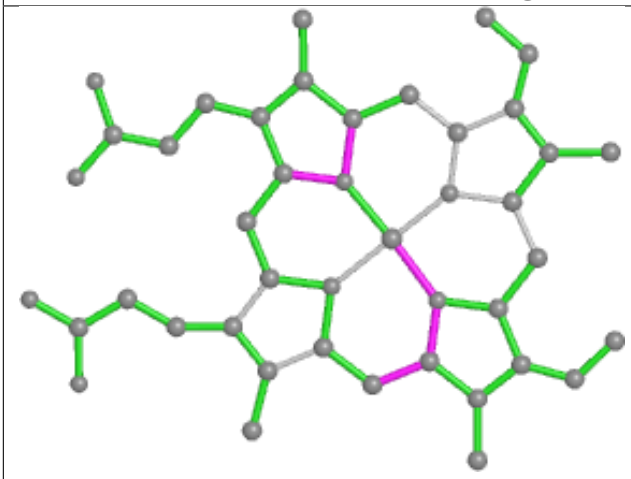


Rings

Ligand HEM B 602



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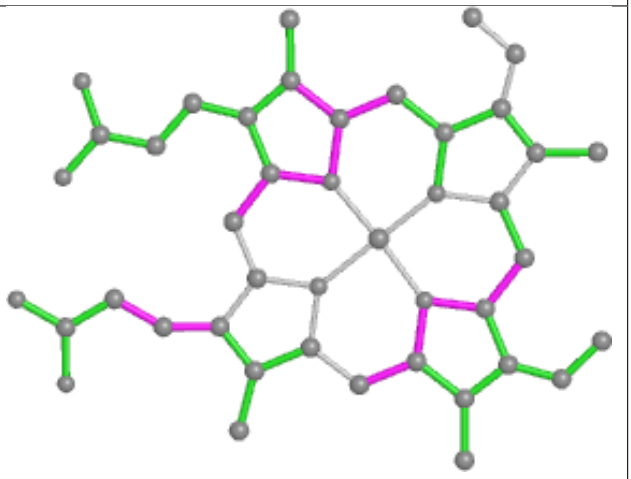

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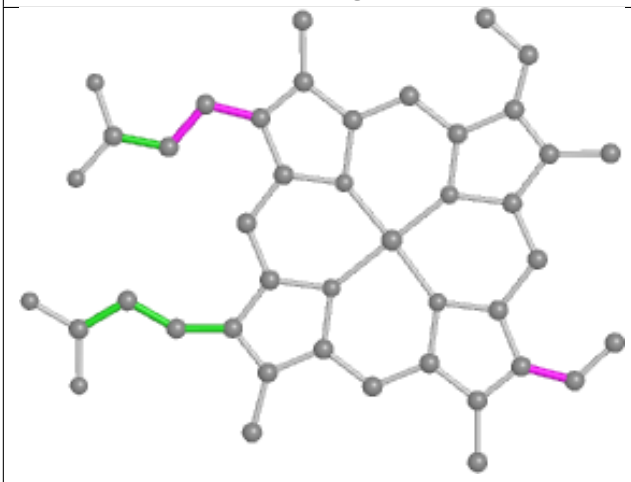

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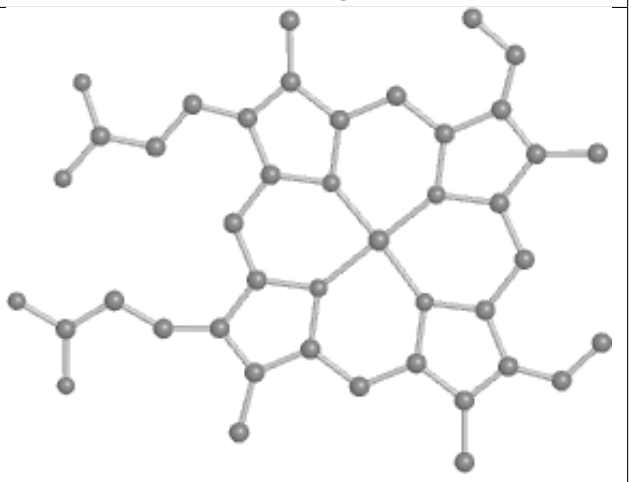
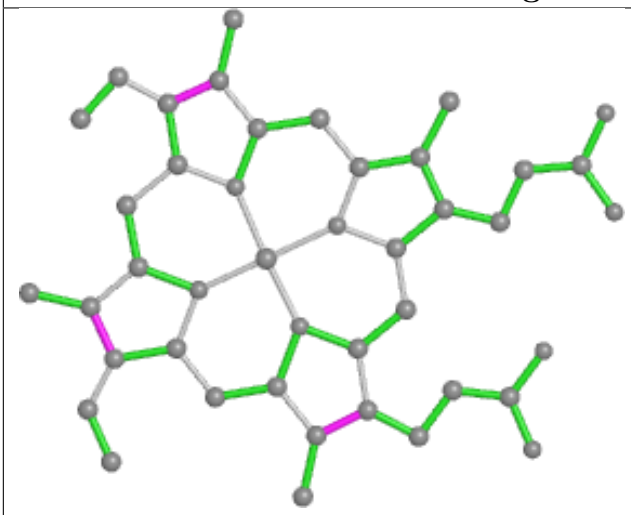


Rings

Ligand HEC C 302



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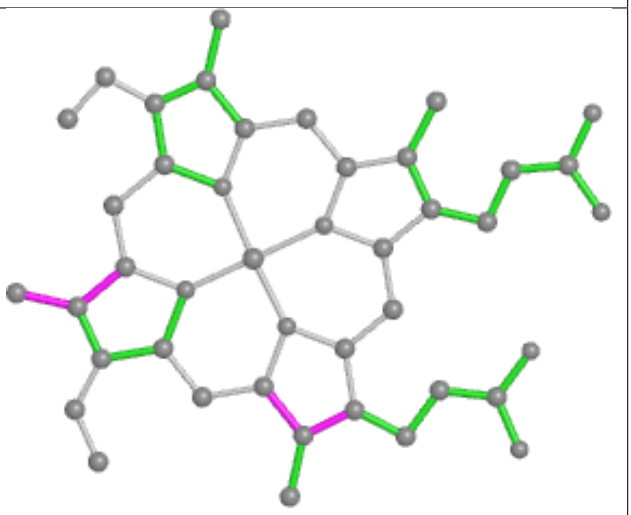

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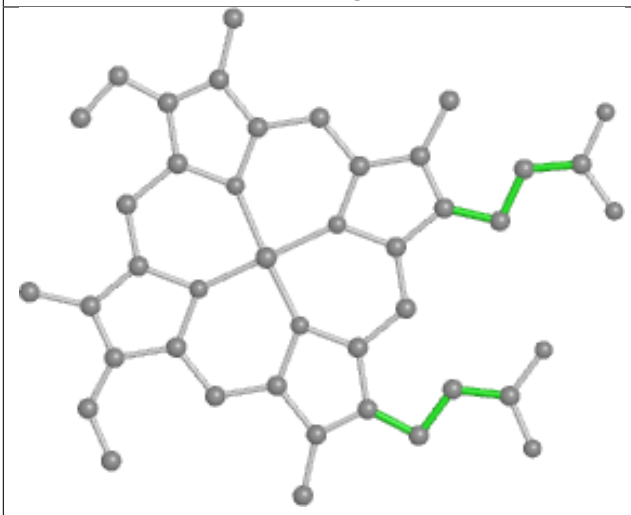

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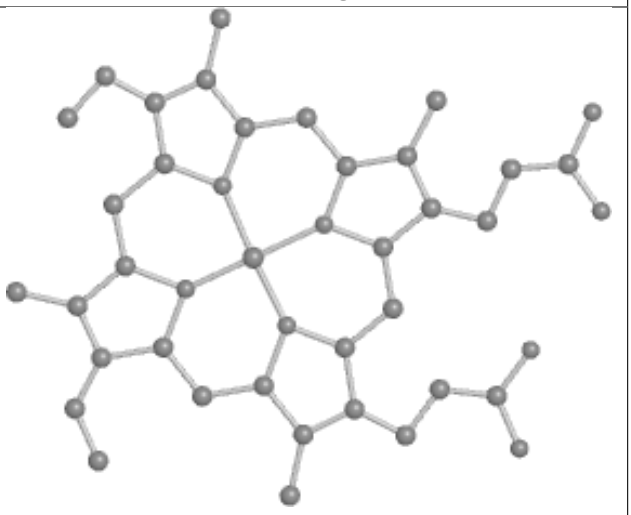
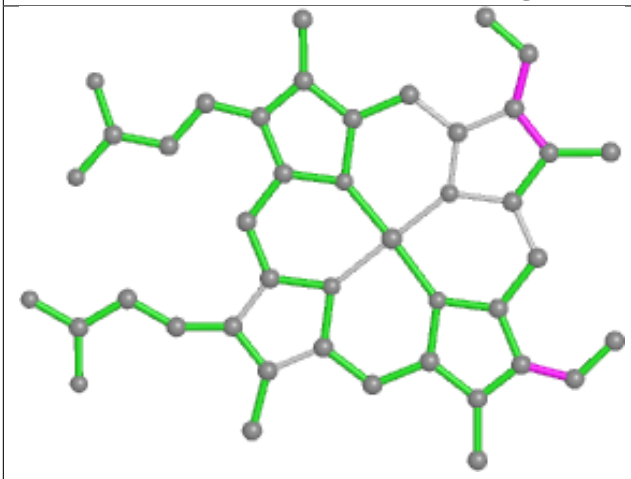


Rings

Ligand HEM N 602



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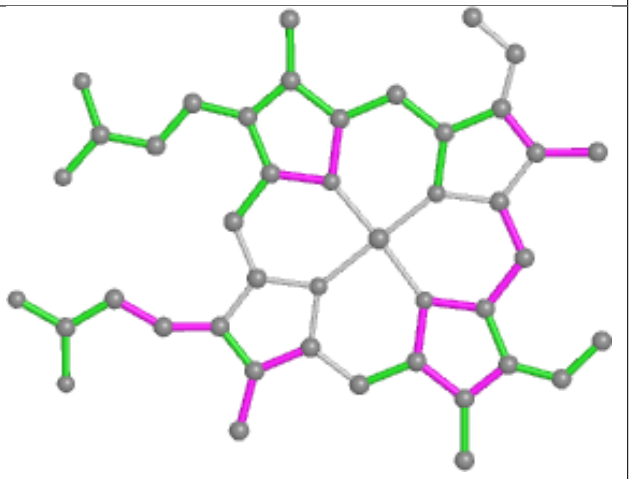

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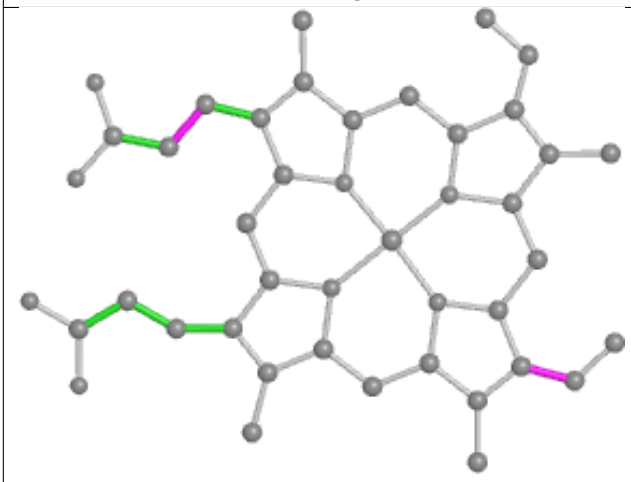

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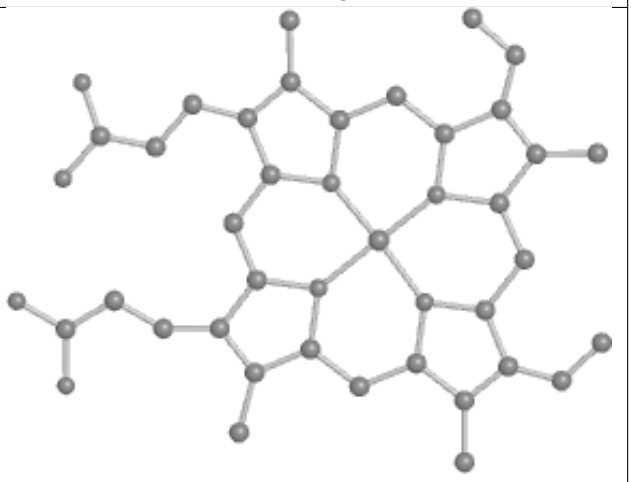
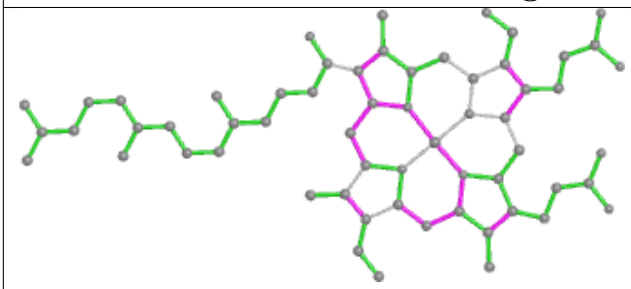


Rings

Ligand HEA R 602



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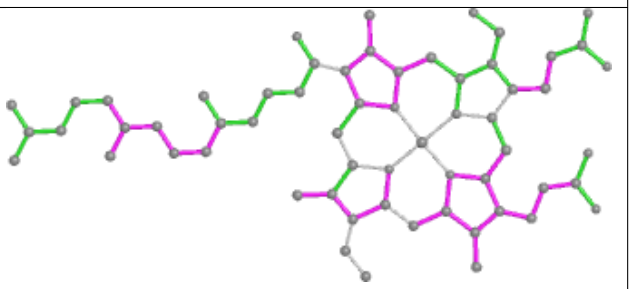

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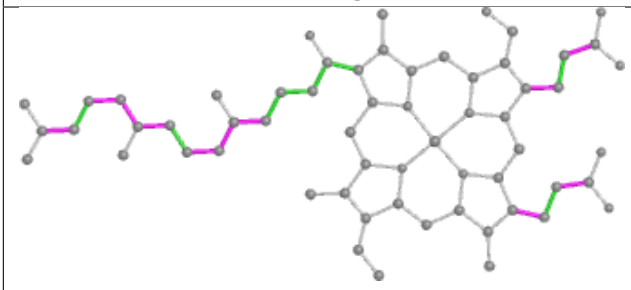

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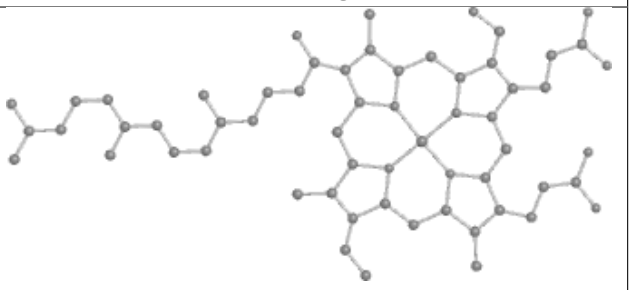
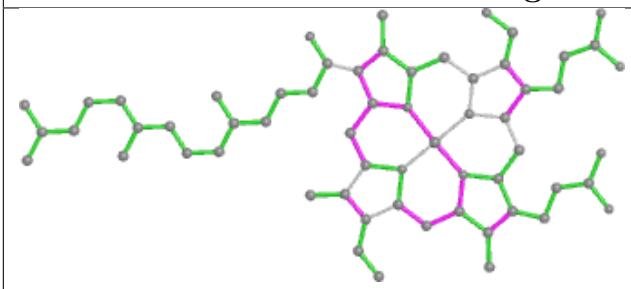


Rings

Ligand HEA F 602



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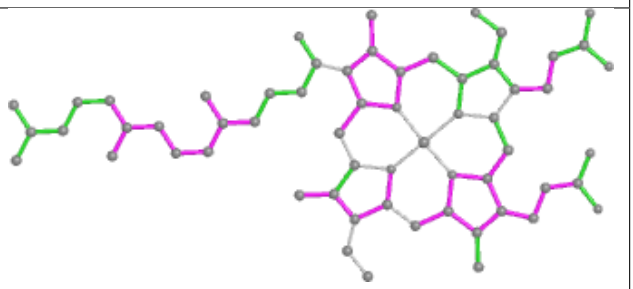

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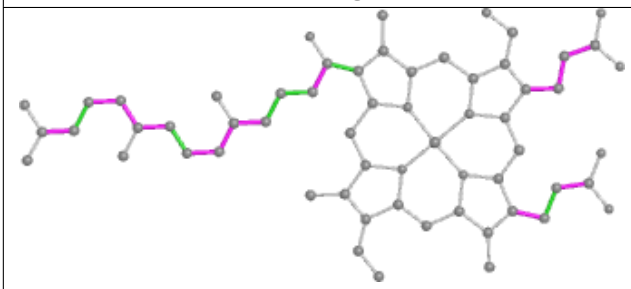

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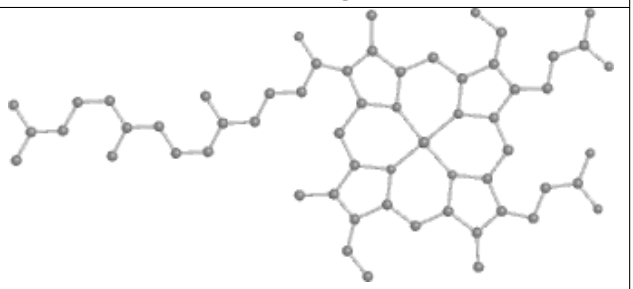
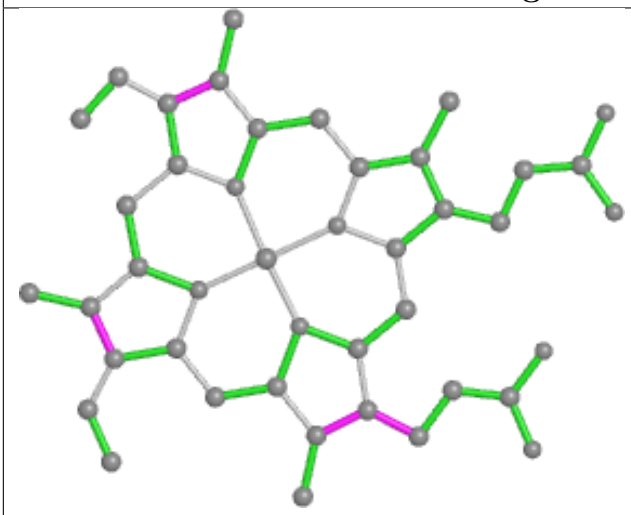


Rings

Ligand HEC C 301



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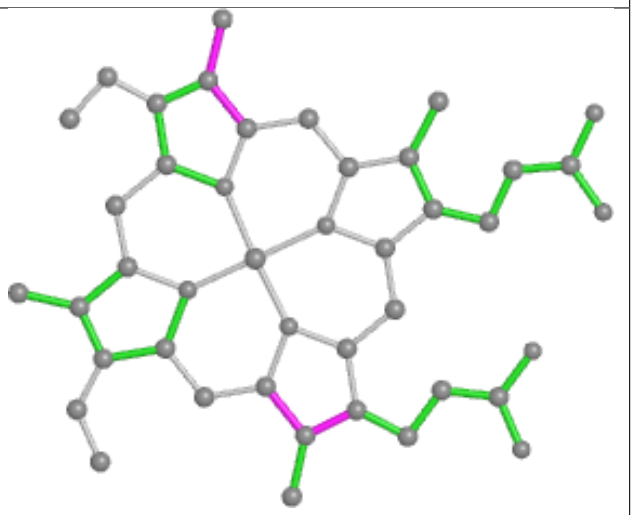
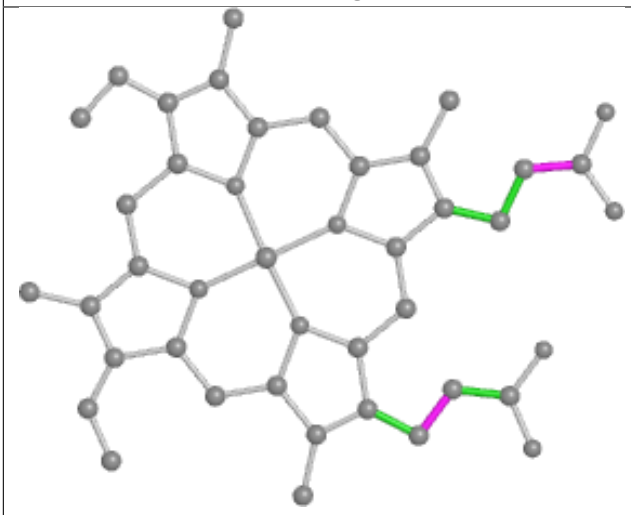
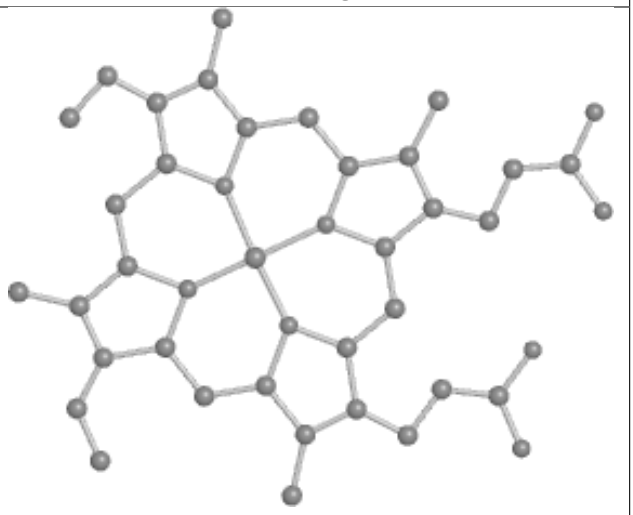


Bond angles

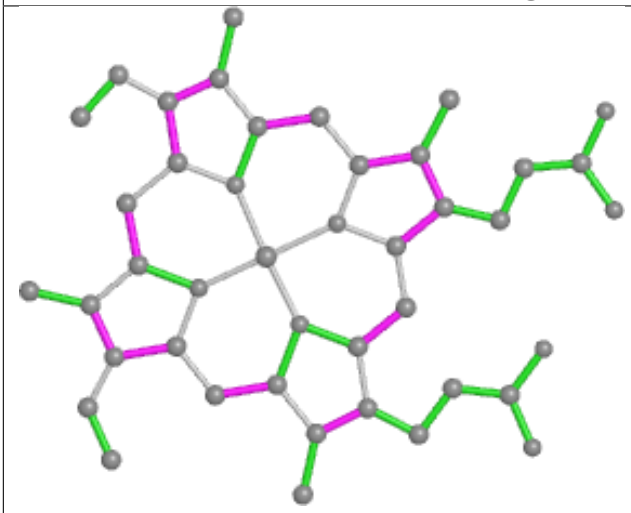


Torsions

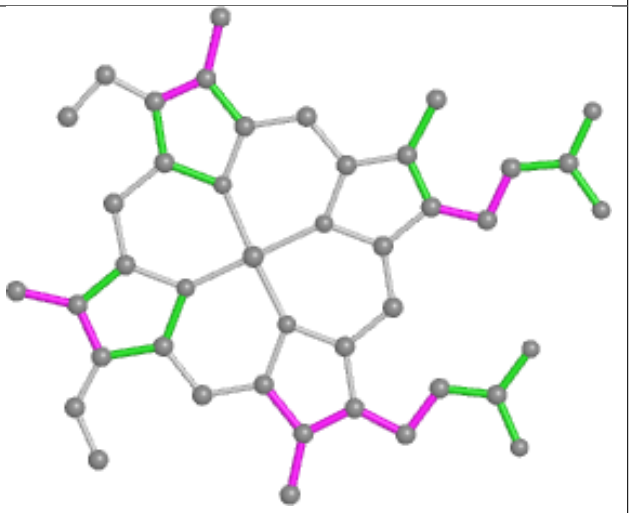


Rings

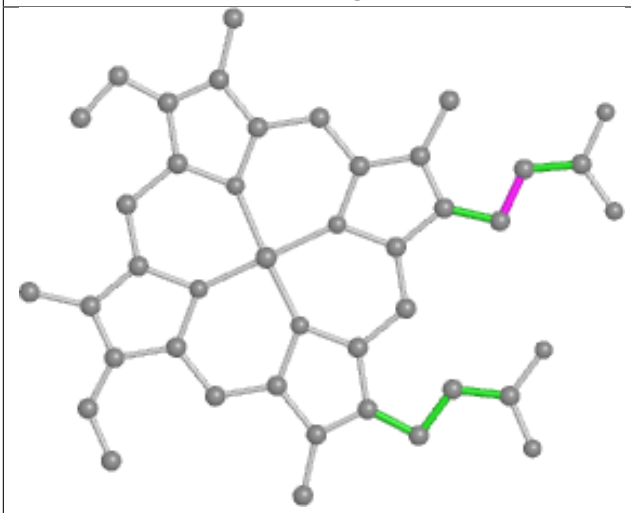
Ligand HEC O 302



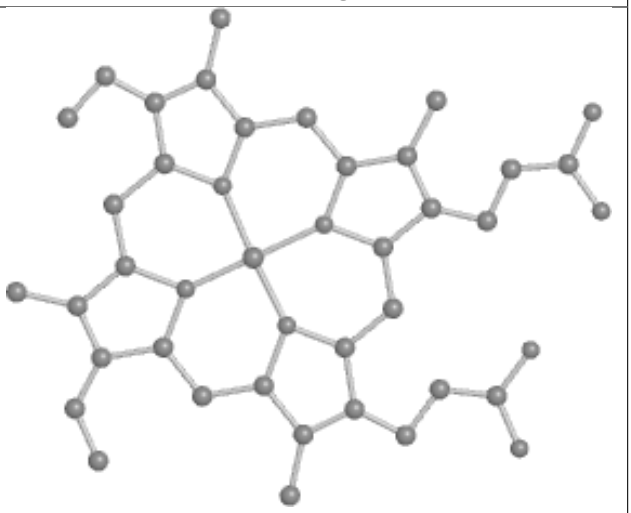
Bond lengths



Bond angles

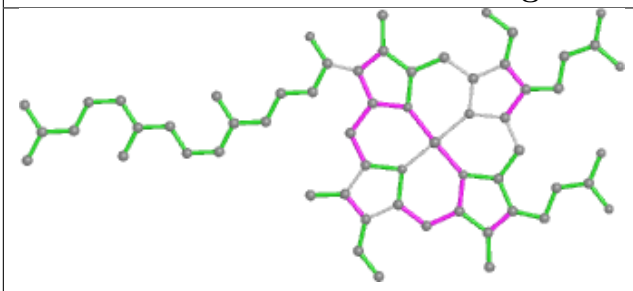


Torsions

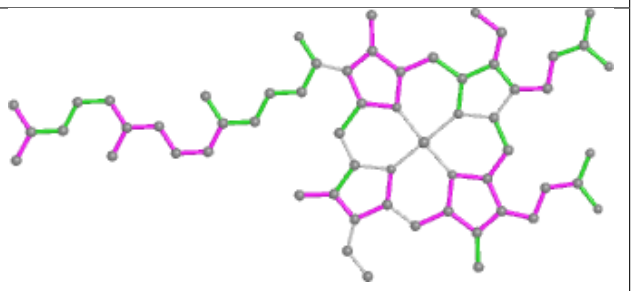


Rings

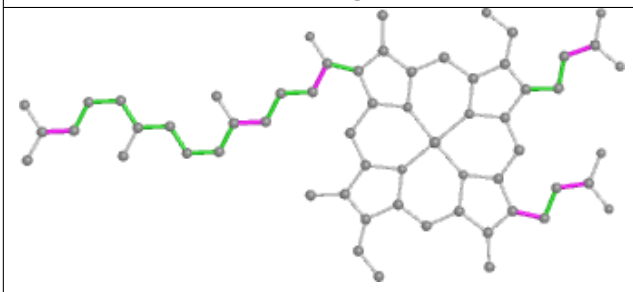
Ligand HEA R 601



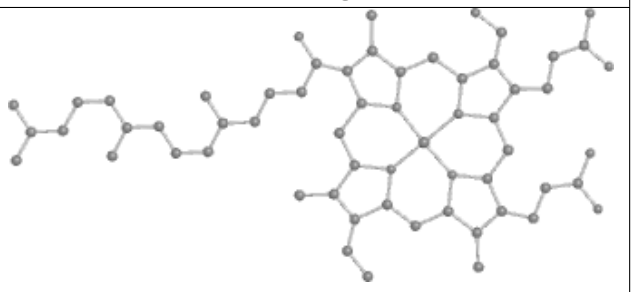
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Tomogram visualisation

This section contains visualisations of the EMDB entry EMD-34664. These allow visual inspection of the internal detail of the tomogram and identification of artifacts.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Mask visualisation

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

7 Tomogram analysis

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

7.1 Map-value distribution

This section was not generated.

8 Map-model fit

This section was not generated.