Full wwPDB X-ray Structure Validation Report ⓘ

Jan 27, 2024 – 08:50 AM EST

PDB ID	:	1BCF
Title	:	THE STRUCTURE OF A UNIQUE, TWO-FOLD SYMMETRIC, HAEM-BINDING SITE
Authors	:	Frolow, F.; Kalb(Gilboa), A.J.; Yariv, J.
Deposited on	:	1993-12-06
Resolution	:	2.90 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp
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:

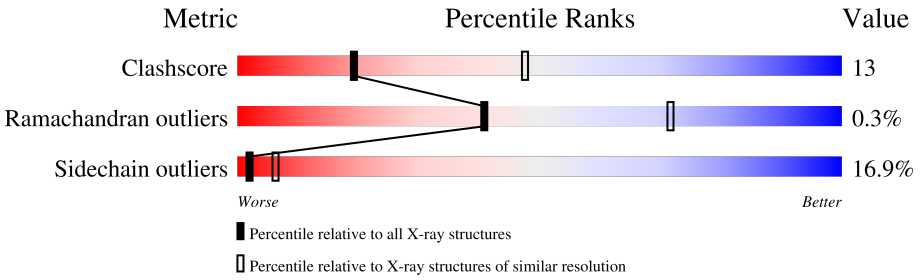
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	158	59% 33% 8%
1	B	158	59% 34% 6%
1	C	158	59% 35% 6%
1	D	158	60% 33% 7%
1	E	158	61% 32% 6%
1	F	158	59% 34% 6%
1	G	158	61% 32% 6%
1	H	158	60% 34% 6%

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Mol	Chain	Length	Quality of chain
1	I	158	61% 33% 6%
1	J	158	59% 35% 6%
1	K	158	61% 33% 6%
1	L	158	58% 36% 6%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 15846 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 BACTERIOFERRITIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	158	Total	C	N	O	S	0	0	0
			1297	818	222	250	7			
1	B	158	Total	C	N	O	S	0	0	0
			1297	818	222	250	7			
1	C	158	Total	C	N	O	S	0	0	0
			1297	818	222	250	7			
1	D	158	Total	C	N	O	S	0	0	0
			1297	818	222	250	7			
1	E	158	Total	C	N	O	S	0	0	0
			1297	818	222	250	7			
1	F	158	Total	C	N	O	S	0	0	0
			1297	818	222	250	7			
1	G	158	Total	C	N	O	S	0	0	0
			1297	818	222	250	7			
1	H	158	Total	C	N	O	S	0	0	0
			1297	818	222	250	7			
1	I	158	Total	C	N	O	S	0	0	0
			1297	818	222	250	7			
1	J	158	Total	C	N	O	S	0	0	0
			1297	818	222	250	7			
1	K	158	Total	C	N	O	S	0	0	0
			1297	818	222	250	7			
1	L	158	Total	C	N	O	S	0	0	0
			1297	818	222	250	7			

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mn	0	0
			2	2		
2	B	2	Total	Mn	0	0
			2	2		

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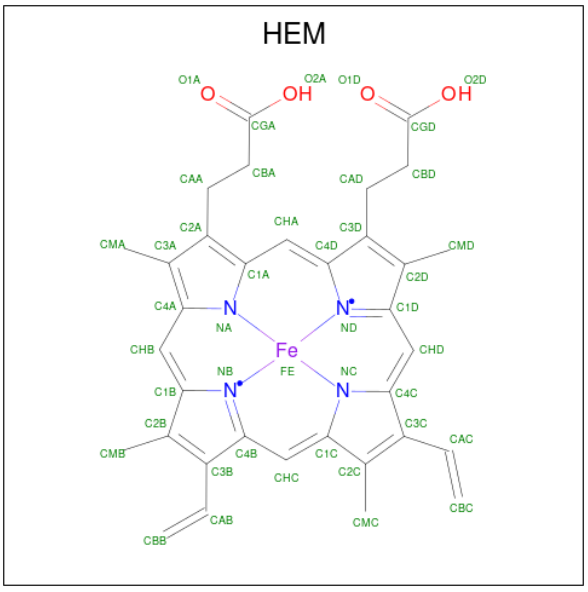
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	2	Total Mn 2 2	0	0
2	D	2	Total Mn 2 2	0	0
2	E	2	Total Mn 2 2	0	0
2	F	2	Total Mn 2 2	0	0
2	G	2	Total Mn 2 2	0	0
2	H	2	Total Mn 2 2	0	0
2	I	2	Total Mn 2 2	0	0
2	J	2	Total Mn 2 2	0	0
2	K	2	Total Mn 2 2	0	0
2	L	2	Total Mn 2 2	0	0

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	E	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	G	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	I	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	K	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

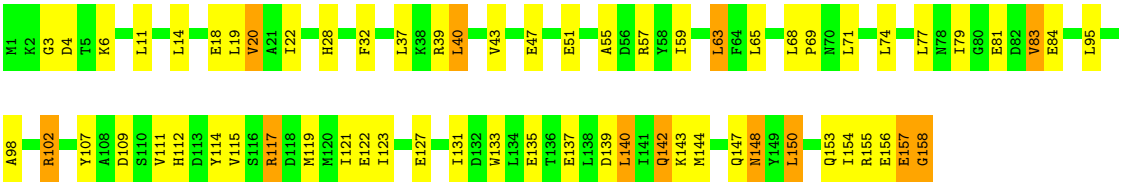
3 Residue-property plots (i)

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.

Note EDS was not executed.

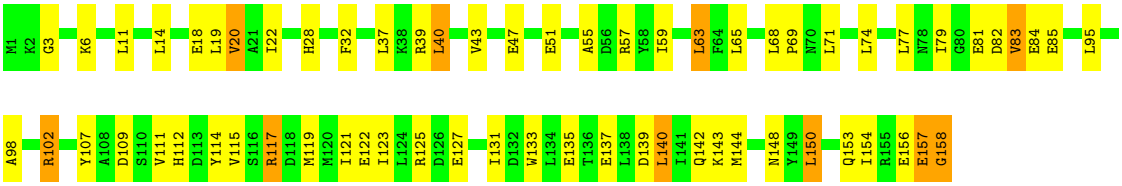
• Molecule 1: BACTERIOFERRITIN

Chain A:



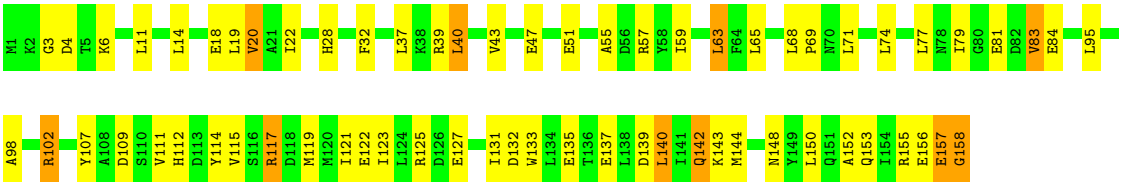
• Molecule 1: BACTERIOFERRITIN

Chain B:



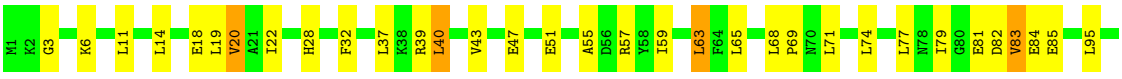
• Molecule 1: BACTERIOFERRITIN

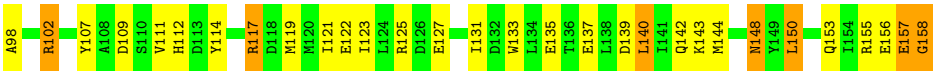
Chain C:



• Molecule 1: BACTERIOFERRITIN

Chain D:



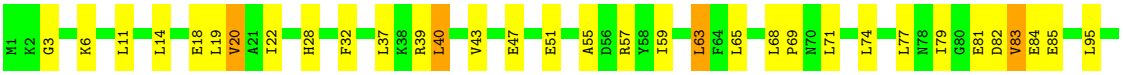


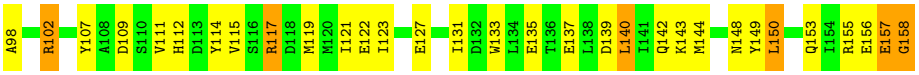
• Molecule 1: BACTERIOFERRITIN

Chain E:

• Molecule 1: BACTERIOFERRITIN

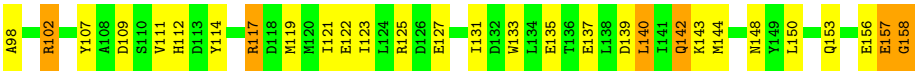
Chain F:





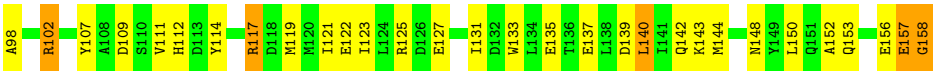
• Molecule 1: BACTERIOFERRITIN

Chain G:



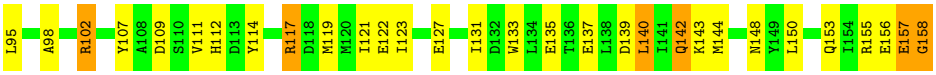
• Molecule 1: BACTERIOFERRITIN

Chain H:



• Molecule 1: BACTERIOFERRITIN

Chain I:

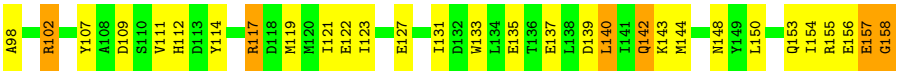


• Molecule 1: BACTERIOFERRITIN

Chain J:

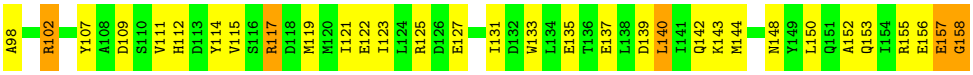
• Molecule 1: BACTERIOFERRITIN

Chain K:



• Molecule 1: BACTERIOFERRITIN

Chain L:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α, β, γ	211.10Å 211.10Å 145.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.208 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	15846	wwPDB-VP
Average B, all atoms (Å^2)	7.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.77	1/1316 (0.1%)	0.83	2/1769 (0.1%)
1	B	0.76	1/1316 (0.1%)	0.83	2/1769 (0.1%)
1	C	0.77	1/1316 (0.1%)	0.83	2/1769 (0.1%)
1	D	0.76	1/1316 (0.1%)	0.83	2/1769 (0.1%)
1	E	0.77	1/1316 (0.1%)	0.83	2/1769 (0.1%)
1	F	0.76	1/1316 (0.1%)	0.83	2/1769 (0.1%)
1	G	0.77	1/1316 (0.1%)	0.83	2/1769 (0.1%)
1	H	0.76	1/1316 (0.1%)	0.83	2/1769 (0.1%)
1	I	0.77	1/1316 (0.1%)	0.83	2/1769 (0.1%)
1	J	0.76	1/1316 (0.1%)	0.83	2/1769 (0.1%)
1	K	0.77	1/1316 (0.1%)	0.83	2/1769 (0.1%)
1	L	0.76	1/1316 (0.1%)	0.83	2/1769 (0.1%)
All	All	0.77	12/15792 (0.1%)	0.83	24/21228 (0.1%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	81	GLU	CG-CD	6.28	1.61	1.51
1	A	81	GLU	CG-CD	6.27	1.61	1.51
1	E	81	GLU	CG-CD	6.26	1.61	1.51
1	I	81	GLU	CG-CD	6.24	1.61	1.51
1	G	81	GLU	CG-CD	6.23	1.61	1.51
1	K	81	GLU	CG-CD	6.22	1.61	1.51
1	F	81	GLU	CG-CD	6.10	1.61	1.51
1	J	81	GLU	CG-CD	6.09	1.61	1.51
1	D	81	GLU	CG-CD	6.07	1.61	1.51
1	B	81	GLU	CG-CD	6.06	1.61	1.51
1	H	81	GLU	CG-CD	6.01	1.60	1.51
1	L	81	GLU	CG-CD	6.01	1.60	1.51

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	3	GLY	N-CA-C	6.68	129.80	113.10
1	K	3	GLY	N-CA-C	6.67	129.78	113.10
1	C	3	GLY	N-CA-C	6.67	129.78	113.10
1	A	3	GLY	N-CA-C	6.66	129.76	113.10
1	I	3	GLY	N-CA-C	6.66	129.76	113.10
1	E	3	GLY	N-CA-C	6.66	129.75	113.10
1	J	3	GLY	N-CA-C	6.54	129.44	113.10
1	B	3	GLY	N-CA-C	6.54	129.44	113.10
1	D	3	GLY	N-CA-C	6.53	129.43	113.10
1	L	3	GLY	N-CA-C	6.53	129.43	113.10
1	F	3	GLY	N-CA-C	6.53	129.42	113.10
1	H	3	GLY	N-CA-C	6.52	129.41	113.10
1	E	158	GLY	N-CA-C	-5.34	99.75	113.10
1	C	158	GLY	N-CA-C	-5.33	99.77	113.10
1	A	158	GLY	N-CA-C	-5.33	99.78	113.10
1	K	158	GLY	N-CA-C	-5.33	99.78	113.10
1	G	158	GLY	N-CA-C	-5.33	99.79	113.10
1	I	158	GLY	N-CA-C	-5.33	99.78	113.10
1	F	158	GLY	N-CA-C	-5.06	100.46	113.10
1	D	158	GLY	N-CA-C	-5.04	100.49	113.10
1	J	158	GLY	N-CA-C	-5.04	100.50	113.10
1	B	158	GLY	N-CA-C	-5.04	100.51	113.10
1	L	158	GLY	N-CA-C	-5.04	100.51	113.10
1	H	158	GLY	N-CA-C	-5.03	100.52	113.10

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	1297	0	1280	44	0
1	B	1297	0	1280	43	0
1	C	1297	0	1280	39	0
1	D	1297	0	1280	43	0
1	E	1297	0	1280	28	0
1	F	1297	0	1280	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	1297	0	1280	35	0
1	H	1297	0	1280	31	0
1	I	1297	0	1280	33	0
1	J	1297	0	1280	34	0
1	K	1297	0	1280	30	0
1	L	1297	0	1280	46	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
2	I	2	0	0	0	0
2	J	2	0	0	0	0
2	K	2	0	0	0	0
2	L	2	0	0	0	0
3	A	43	0	30	3	0
3	C	43	0	30	3	0
3	E	43	0	30	3	0
3	G	43	0	30	3	0
3	I	43	0	30	3	0
3	K	43	0	30	3	0
All	All	15846	0	15540	405	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 13.

All (405) 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)
1:B:157:GLU:HA	1:D:155:ARG:NH1	1.75	1.02
1:G:157:GLU:HA	1:I:155:ARG:NH1	1.91	0.85
1:J:20:VAL:HG23	1:J:77:LEU:HD23	1.60	0.84
1:K:20:VAL:HG23	1:K:77:LEU:HD23	1.61	0.83
1:F:20:VAL:HG23	1:F:77:LEU:HD23	1.60	0.83
1:D:20:VAL:HG23	1:D:77:LEU:HD23	1.60	0.82
1:L:20:VAL:HG23	1:L:77:LEU:HD23	1.60	0.82
1:E:20:VAL:HG23	1:E:77:LEU:HD23	1.61	0.82
1:I:20:VAL:HG23	1:I:77:LEU:HD23	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:20:VAL:HG23	1:C:77:LEU:HD23	1.61	0.81
1:B:20:VAL:HG23	1:B:77:LEU:HD23	1.60	0.81
1:H:20:VAL:HG23	1:H:77:LEU:HD23	1.60	0.80
1:A:20:VAL:HG23	1:A:77:LEU:HD23	1.61	0.80
1:G:20:VAL:HG23	1:G:77:LEU:HD23	1.61	0.80
1:A:155:ARG:NH1	1:L:157:GLU:HA	1.98	0.79
1:B:157:GLU:CA	1:D:155:ARG:NH1	2.50	0.74
1:D:157:GLU:HA	1:F:155:ARG:NH1	2.02	0.74
1:C:125:ARG:NH1	1:L:115:VAL:HG13	2.06	0.69
1:C:125:ARG:HH11	1:L:115:VAL:HG13	1.57	0.69
1:B:157:GLU:HG2	1:D:155:ARG:CD	2.24	0.67
1:B:125:ARG:NH1	1:C:115:VAL:HG13	2.09	0.67
1:A:115:VAL:HG13	1:H:125:ARG:NH1	2.10	0.67
1:C:125:ARG:HA	1:L:115:VAL:HG21	1.76	0.67
1:B:125:ARG:HH11	1:C:115:VAL:HG13	1.60	0.65
1:F:142:GLN:NE2	1:F:143:LYS:HG3	2.12	0.64
1:B:142:GLN:NE2	1:B:143:LYS:HG3	2.12	0.64
1:H:142:GLN:NE2	1:H:143:LYS:HG3	2.12	0.64
1:G:142:GLN:NE2	1:G:143:LYS:HG3	2.13	0.64
1:A:142:GLN:NE2	1:A:143:LYS:HG3	2.13	0.64
1:J:142:GLN:NE2	1:J:143:LYS:HG3	2.12	0.63
1:L:142:GLN:NE2	1:L:143:LYS:HG3	2.12	0.63
1:C:142:GLN:NE2	1:C:143:LYS:HG3	2.13	0.63
1:I:142:GLN:NE2	1:I:143:LYS:HG3	2.13	0.63
1:E:142:GLN:NE2	1:E:143:LYS:HG3	2.13	0.63
1:D:142:GLN:NE2	1:D:143:LYS:HG3	2.12	0.63
1:K:142:GLN:NE2	1:K:143:LYS:HG3	2.13	0.63
1:A:155:ARG:CD	1:L:157:GLU:HG2	2.30	0.61
1:F:115:VAL:HG13	1:J:125:ARG:NH1	2.15	0.61
1:B:157:GLU:HA	1:D:155:ARG:HH12	1.63	0.60
1:F:19:LEU:HD11	1:F:71:LEU:HD23	1.86	0.58
1:D:19:LEU:HD11	1:D:71:LEU:HD23	1.86	0.57
1:G:125:ARG:NH1	1:J:115:VAL:HG13	2.19	0.57
1:L:19:LEU:HD11	1:L:71:LEU:HD23	1.86	0.57
1:A:155:ARG:NH1	1:L:157:GLU:CA	2.66	0.57
1:B:19:LEU:HD11	1:B:71:LEU:HD23	1.86	0.57
1:G:157:GLU:CA	1:I:155:ARG:NH1	2.67	0.56
1:H:19:LEU:HD11	1:H:71:LEU:HD23	1.86	0.56
1:J:19:LEU:HD11	1:J:71:LEU:HD23	1.86	0.56
1:A:155:ARG:HH21	1:L:39:ARG:HD2	1.70	0.56
1:B:55:ALA:O	1:B:59:ILE:HG13	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:115:VAL:HG13	1:J:125:ARG:HH11	1.69	0.56
1:L:55:ALA:O	1:L:59:ILE:HG13	2.06	0.56
1:D:55:ALA:O	1:D:59:ILE:HG13	2.06	0.55
1:B:157:GLU:HG2	1:D:155:ARG:HG2	1.88	0.55
1:G:19:LEU:HD11	1:G:71:LEU:HD23	1.89	0.55
1:E:19:LEU:HD11	1:E:71:LEU:HD23	1.89	0.55
1:F:55:ALA:O	1:F:59:ILE:HG13	2.06	0.55
1:C:19:LEU:HD11	1:C:71:LEU:HD23	1.89	0.55
1:H:55:ALA:O	1:H:59:ILE:HG13	2.06	0.55
1:A:19:LEU:HD11	1:A:71:LEU:HD23	1.89	0.54
1:I:19:LEU:HD11	1:I:71:LEU:HD23	1.89	0.54
1:L:157:GLU:CD	1:L:158:GLY:H	2.11	0.54
1:G:157:GLU:HG2	1:I:155:ARG:CD	2.37	0.54
1:B:157:GLU:CD	1:B:158:GLY:H	2.11	0.54
1:D:157:GLU:CD	1:D:158:GLY:H	2.11	0.54
1:G:157:GLU:HA	1:I:155:ARG:HH12	1.71	0.54
1:J:55:ALA:O	1:J:59:ILE:HG13	2.06	0.54
1:A:39:ARG:HD3	1:A:153:GLN:OE1	2.08	0.54
1:J:157:GLU:CD	1:J:158:GLY:H	2.11	0.54
1:K:19:LEU:HD11	1:K:71:LEU:HD23	1.89	0.54
1:D:39:ARG:HD3	1:D:153:GLN:OE1	2.08	0.54
1:I:39:ARG:HD3	1:I:153:GLN:OE1	2.08	0.54
1:L:63:LEU:HD13	1:L:69:PRO:HD3	1.90	0.54
1:C:98:ALA:O	1:C:102:ARG:HG3	2.08	0.54
1:H:39:ARG:HD3	1:H:153:GLN:OE1	2.08	0.54
1:H:157:GLU:CD	1:H:158:GLY:H	2.11	0.54
1:A:157:GLU:CD	1:A:158:GLY:H	2.12	0.53
1:B:157:GLU:CG	1:D:155:ARG:HG2	2.37	0.53
1:C:39:ARG:HD3	1:C:153:GLN:OE1	2.08	0.53
1:G:39:ARG:HD3	1:G:153:GLN:OE1	2.08	0.53
1:E:98:ALA:O	1:E:102:ARG:HG3	2.08	0.53
1:I:157:GLU:CD	1:I:158:GLY:H	2.12	0.53
1:L:39:ARG:HD3	1:L:153:GLN:OE1	2.08	0.53
1:I:98:ALA:O	1:I:102:ARG:HG3	2.08	0.53
1:B:39:ARG:HD3	1:B:153:GLN:OE1	2.08	0.53
1:E:39:ARG:HD3	1:E:153:GLN:OE1	2.08	0.53
1:F:157:GLU:CD	1:F:158:GLY:H	2.11	0.53
1:H:63:LEU:HD13	1:H:69:PRO:HD3	1.90	0.53
1:K:157:GLU:CD	1:K:158:GLY:H	2.12	0.53
1:J:63:LEU:HD13	1:J:69:PRO:HD3	1.90	0.53
1:K:98:ALA:O	1:K:102:ARG:HG3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:157:GLU:CD	1:E:158:GLY:H	2.12	0.53
1:K:39:ARG:HD3	1:K:153:GLN:OE1	2.08	0.53
1:C:157:GLU:CD	1:C:158:GLY:H	2.12	0.53
1:G:98:ALA:O	1:G:102:ARG:HG3	2.08	0.53
1:D:63:LEU:HD13	1:D:69:PRO:HD3	1.90	0.53
1:J:39:ARG:HD3	1:J:153:GLN:OE1	2.08	0.53
1:B:63:LEU:HD13	1:B:69:PRO:HD3	1.90	0.52
1:C:132:ASP:HB2	1:L:64:PHE:CE1	2.44	0.52
1:F:39:ARG:HD3	1:F:153:GLN:OE1	2.08	0.52
1:I:63:LEU:HD13	1:I:69:PRO:HD3	1.92	0.52
1:C:140:LEU:O	1:C:144:MET:HG2	2.10	0.52
1:G:157:GLU:CD	1:G:158:GLY:H	2.12	0.52
1:A:98:ALA:O	1:A:102:ARG:HG3	2.08	0.52
1:G:63:LEU:HD13	1:G:69:PRO:HD3	1.92	0.52
1:A:155:ARG:NH2	1:L:39:ARG:HD2	2.25	0.52
1:C:63:LEU:HD13	1:C:69:PRO:HD3	1.92	0.52
1:I:140:LEU:O	1:I:144:MET:HG2	2.10	0.52
1:A:63:LEU:HD13	1:A:69:PRO:HD3	1.92	0.52
1:H:140:LEU:O	1:H:144:MET:HG2	2.10	0.52
1:E:63:LEU:HD13	1:E:69:PRO:HD3	1.92	0.52
1:K:140:LEU:O	1:K:144:MET:HG2	2.10	0.51
1:L:140:LEU:O	1:L:144:MET:HG2	2.10	0.51
1:E:55:ALA:O	1:E:59:ILE:HG13	2.10	0.51
1:G:55:ALA:O	1:G:59:ILE:HG13	2.10	0.51
1:K:63:LEU:HD13	1:K:69:PRO:HD3	1.92	0.51
1:A:55:ALA:O	1:A:59:ILE:HG13	2.10	0.51
1:B:140:LEU:O	1:B:144:MET:HG2	2.10	0.51
1:C:55:ALA:O	1:C:59:ILE:HG13	2.10	0.51
1:E:131:ILE:O	1:E:135:GLU:HG3	2.11	0.51
1:F:63:LEU:HD13	1:F:69:PRO:HD3	1.90	0.51
1:I:55:ALA:O	1:I:59:ILE:HG13	2.10	0.51
1:J:140:LEU:O	1:J:144:MET:HG2	2.10	0.51
1:G:131:ILE:O	1:G:135:GLU:HG3	2.11	0.51
1:G:140:LEU:O	1:G:144:MET:HG2	2.10	0.51
1:A:140:LEU:O	1:A:144:MET:HG2	2.10	0.51
1:D:140:LEU:O	1:D:144:MET:HG2	2.10	0.51
1:K:131:ILE:O	1:K:135:GLU:HG3	2.11	0.51
1:A:131:ILE:O	1:A:135:GLU:HG3	2.11	0.51
1:K:55:ALA:O	1:K:59:ILE:HG13	2.10	0.51
1:F:98:ALA:O	1:F:102:ARG:HG3	2.11	0.51
1:B:98:ALA:O	1:B:102:ARG:HG3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:140:LEU:O	1:F:144:MET:HG2	2.10	0.50
1:E:140:LEU:O	1:E:144:MET:HG2	2.10	0.50
1:C:125:ARG:HG3	1:L:115:VAL:HG13	1.93	0.50
1:D:98:ALA:O	1:D:102:ARG:HG3	2.11	0.50
1:D:125:ARG:NH1	1:E:115:VAL:HG13	2.26	0.50
1:K:6:LYS:HB3	1:K:107:TYR:CE2	2.47	0.50
1:G:6:LYS:HB3	1:G:107:TYR:CE2	2.47	0.50
1:H:98:ALA:O	1:H:102:ARG:HG3	2.11	0.50
1:A:6:LYS:HB3	1:A:107:TYR:CE2	2.47	0.50
1:C:131:ILE:O	1:C:135:GLU:HG3	2.11	0.50
1:E:133:TRP:O	1:E:137:GLU:HG2	2.12	0.50
1:G:133:TRP:O	1:G:137:GLU:HG2	2.12	0.50
1:I:133:TRP:O	1:I:137:GLU:HG2	2.12	0.50
1:C:6:LYS:HB3	1:C:107:TYR:CE2	2.47	0.50
1:C:133:TRP:O	1:C:137:GLU:HG2	2.12	0.49
1:B:18:GLU:OE1	1:B:18:GLU:HA	2.13	0.49
1:J:98:ALA:O	1:J:102:ARG:HG3	2.11	0.49
1:B:123:ILE:O	1:B:127:GLU:HG2	2.12	0.49
1:I:6:LYS:HB3	1:I:107:TYR:CE2	2.47	0.49
1:J:18:GLU:HA	1:J:18:GLU:OE1	2.13	0.49
1:J:123:ILE:O	1:J:127:GLU:HG2	2.12	0.49
1:D:18:GLU:OE1	1:D:18:GLU:HA	2.12	0.49
1:E:6:LYS:HB3	1:E:107:TYR:CE2	2.47	0.49
1:I:131:ILE:O	1:I:135:GLU:HG3	2.11	0.49
1:F:123:ILE:O	1:F:127:GLU:HG2	2.12	0.49
1:A:150:LEU:HD23	1:L:143:LYS:HB3	1.94	0.49
1:A:155:ARG:HD3	1:L:157:GLU:HG2	1.94	0.49
1:B:157:GLU:HG2	1:D:155:ARG:NE	2.27	0.49
1:H:18:GLU:HA	1:H:18:GLU:OE1	2.13	0.49
1:L:98:ALA:O	1:L:102:ARG:HG3	2.11	0.49
1:D:131:ILE:O	1:D:135:GLU:HG3	2.13	0.48
1:J:131:ILE:O	1:J:135:GLU:HG3	2.13	0.48
1:F:18:GLU:OE1	1:F:18:GLU:HA	2.13	0.48
1:J:6:LYS:HB3	1:J:107:TYR:CE2	2.49	0.48
1:K:133:TRP:O	1:K:137:GLU:HG2	2.12	0.48
1:B:43:VAL:HG11	1:B:133:TRP:CE2	2.49	0.48
1:D:123:ILE:O	1:D:127:GLU:HG2	2.12	0.48
1:F:43:VAL:HG11	1:F:133:TRP:CE2	2.49	0.48
1:F:127:GLU:OE1	1:F:127:GLU:HA	2.14	0.48
1:H:6:LYS:HB3	1:H:107:TYR:CE2	2.49	0.48
1:H:123:ILE:O	1:H:127:GLU:HG2	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:TRP:O	1:A:137:GLU:HG2	2.12	0.48
1:C:127:GLU:OE1	1:C:127:GLU:HA	2.14	0.48
1:E:117:ARG:O	1:E:121:ILE:HG13	2.14	0.48
1:F:131:ILE:O	1:F:135:GLU:HG3	2.13	0.48
1:L:123:ILE:O	1:L:127:GLU:HG2	2.12	0.48
1:B:157:GLU:HG2	1:D:155:ARG:CG	2.43	0.48
1:K:127:GLU:OE1	1:K:127:GLU:HA	2.13	0.48
1:A:147:GLN:HB3	1:L:144:MET:O	2.12	0.48
1:G:117:ARG:O	1:G:121:ILE:HG13	2.14	0.48
1:H:43:VAL:HG11	1:H:133:TRP:CE2	2.49	0.48
1:L:18:GLU:HA	1:L:18:GLU:OE1	2.13	0.48
1:D:127:GLU:OE1	1:D:127:GLU:HA	2.14	0.48
1:H:127:GLU:OE1	1:H:127:GLU:HA	2.14	0.48
1:J:43:VAL:HG11	1:J:133:TRP:CE2	2.49	0.48
1:L:6:LYS:HB3	1:L:107:TYR:CE2	2.49	0.48
1:A:115:VAL:HG13	1:H:125:ARG:HH11	1.76	0.48
1:F:6:LYS:HB3	1:F:107:TYR:CE2	2.49	0.48
1:G:127:GLU:HA	1:G:127:GLU:OE1	2.14	0.48
1:I:127:GLU:OE1	1:I:127:GLU:HA	2.14	0.48
1:A:127:GLU:OE1	1:A:127:GLU:HA	2.14	0.48
1:B:6:LYS:HB3	1:B:107:TYR:CE2	2.49	0.48
1:D:43:VAL:HG11	1:D:133:TRP:CE2	2.49	0.48
1:C:117:ARG:O	1:C:121:ILE:HG13	2.14	0.47
1:C:157:GLU:HA	1:K:155:ARG:NH1	2.29	0.47
1:D:6:LYS:HB3	1:D:107:TYR:CE2	2.49	0.47
1:G:125:ARG:HH11	1:J:115:VAL:HG13	1.78	0.47
1:J:127:GLU:OE1	1:J:127:GLU:HA	2.14	0.47
1:L:127:GLU:HA	1:L:127:GLU:OE1	2.14	0.47
1:A:117:ARG:O	1:A:121:ILE:HG13	2.14	0.47
1:B:127:GLU:HA	1:B:127:GLU:OE1	2.14	0.47
1:H:40:LEU:HD13	1:H:153:GLN:OE1	2.15	0.47
1:H:131:ILE:O	1:H:135:GLU:HG3	2.13	0.47
1:L:43:VAL:HG11	1:L:133:TRP:CE2	2.49	0.47
1:E:127:GLU:HA	1:E:127:GLU:OE1	2.13	0.47
1:L:131:ILE:O	1:L:135:GLU:HG3	2.13	0.47
1:F:40:LEU:HD13	1:F:153:GLN:OE1	2.15	0.47
1:I:117:ARG:O	1:I:121:ILE:HG13	2.14	0.47
1:K:117:ARG:O	1:K:121:ILE:HG13	2.14	0.47
3:K:205:HEM:HMB1	3:K:205:HEM:HBB2	1.97	0.47
1:G:43:VAL:HG11	1:G:133:TRP:CE2	2.50	0.47
1:K:43:VAL:HG11	1:K:133:TRP:CE2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:40:LEU:HD13	1:L:153:GLN:OE1	2.15	0.47
1:D:40:LEU:HD13	1:D:153:GLN:OE1	2.15	0.47
1:B:117:ARG:O	1:B:121:ILE:HG13	2.16	0.46
1:D:117:ARG:O	1:D:121:ILE:HG13	2.16	0.46
3:E:202:HEM:HBB2	3:E:202:HEM:HMB1	1.97	0.46
1:B:131:ILE:O	1:B:135:GLU:HG3	2.13	0.46
1:E:43:VAL:HG11	1:E:133:TRP:CE2	2.50	0.46
3:G:203:HEM:HBB2	3:G:203:HEM:HMB1	1.97	0.46
1:H:117:ARG:O	1:H:121:ILE:HG13	2.16	0.46
1:C:18:GLU:HA	1:C:18:GLU:OE1	2.16	0.46
1:J:40:LEU:HD13	1:J:153:GLN:OE1	2.15	0.46
1:L:133:TRP:O	1:L:137:GLU:HG2	2.16	0.46
1:H:133:TRP:O	1:H:137:GLU:HG2	2.16	0.46
1:K:18:GLU:OE1	1:K:18:GLU:HA	2.16	0.46
1:B:133:TRP:O	1:B:137:GLU:HG2	2.16	0.46
1:F:117:ARG:O	1:F:121:ILE:HG13	2.15	0.46
1:C:157:GLU:HG2	1:K:155:ARG:HG2	1.98	0.46
1:K:123:ILE:O	1:K:127:GLU:HG2	2.16	0.46
1:C:112:HIS:HD2	1:C:114:TYR:OH	1.99	0.46
1:E:112:HIS:HD2	1:E:114:TYR:OH	1.99	0.46
1:E:123:ILE:O	1:E:127:GLU:HG2	2.16	0.46
1:G:18:GLU:OE1	1:G:18:GLU:HA	2.16	0.46
1:A:112:HIS:HD2	1:A:114:TYR:OH	1.99	0.46
1:F:133:TRP:O	1:F:137:GLU:HG2	2.16	0.46
1:G:40:LEU:HD13	1:G:153:GLN:OE1	2.16	0.46
1:A:43:VAL:HG11	1:A:133:TRP:CE2	2.50	0.46
3:A:200:HEM:HMB1	3:A:200:HEM:HBB2	1.97	0.46
1:G:112:HIS:HD2	1:G:114:TYR:OH	1.99	0.46
3:I:204:HEM:HMB1	3:I:204:HEM:HBB2	1.97	0.46
3:C:201:HEM:HMB1	3:C:201:HEM:HBB2	1.97	0.45
1:D:133:TRP:O	1:D:137:GLU:HG2	2.16	0.45
1:I:43:VAL:HG11	1:I:133:TRP:CE2	2.50	0.45
1:L:117:ARG:O	1:L:121:ILE:HG13	2.15	0.45
1:B:40:LEU:HD13	1:B:153:GLN:OE1	2.15	0.45
1:C:43:VAL:HG11	1:C:133:TRP:CE2	2.50	0.45
1:G:123:ILE:O	1:G:127:GLU:HG2	2.16	0.45
1:D:112:HIS:HD2	1:D:114:TYR:OH	1.99	0.45
1:J:117:ARG:O	1:J:121:ILE:HG13	2.15	0.45
1:A:18:GLU:OE1	1:A:18:GLU:HA	2.16	0.45
1:C:123:ILE:O	1:C:127:GLU:HG2	2.16	0.45
1:E:18:GLU:HA	1:E:18:GLU:OE1	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:40:LEU:HD13	1:E:153:GLN:OE1	2.16	0.45
3:G:203:HEM:HBC2	3:G:203:HEM:HMC1	1.99	0.45
1:J:112:HIS:HD2	1:J:114:TYR:OH	1.99	0.45
3:C:201:HEM:HMC1	3:C:201:HEM:HBC2	1.99	0.45
1:I:112:HIS:HD2	1:I:114:TYR:OH	1.99	0.45
1:J:133:TRP:O	1:J:137:GLU:HG2	2.16	0.45
1:I:40:LEU:HD13	1:I:153:GLN:OE1	2.16	0.45
1:K:40:LEU:HD13	1:K:153:GLN:OE1	2.16	0.45
1:A:123:ILE:O	1:A:127:GLU:HG2	2.16	0.45
1:A:154:ILE:HD11	1:L:152:ALA:HB1	1.97	0.45
3:A:200:HEM:HMC1	3:A:200:HEM:HBC2	1.99	0.45
1:B:112:HIS:HD2	1:B:114:TYR:OH	1.99	0.45
1:C:152:ALA:HB1	1:K:154:ILE:HD11	1.99	0.45
1:D:125:ARG:HH11	1:E:115:VAL:HG13	1.81	0.45
1:G:157:GLU:HG2	1:I:155:ARG:CZ	2.47	0.45
3:K:205:HEM:HMC1	3:K:205:HEM:HBC2	1.99	0.45
1:C:125:ARG:HA	1:L:115:VAL:CG2	2.46	0.45
1:K:109:ASP:HB2	1:K:117:ARG:HH21	1.82	0.45
1:L:43:VAL:HG11	1:L:133:TRP:CZ2	2.52	0.45
1:A:40:LEU:HD13	1:A:153:GLN:OE1	2.16	0.44
1:D:43:VAL:HG11	1:D:133:TRP:CZ2	2.52	0.44
1:B:43:VAL:HG11	1:B:133:TRP:CZ2	2.52	0.44
3:E:202:HEM:HMC1	3:E:202:HEM:HBC2	1.99	0.44
1:F:43:VAL:HG11	1:F:133:TRP:CZ2	2.52	0.44
1:J:43:VAL:HG11	1:J:133:TRP:CZ2	2.52	0.44
1:C:40:LEU:HD13	1:C:153:GLN:OE1	2.16	0.44
1:F:115:VAL:HG21	1:J:125:ARG:HA	1.99	0.44
1:I:18:GLU:OE1	1:I:18:GLU:HA	2.16	0.44
1:I:109:ASP:HB2	1:I:117:ARG:HH21	1.82	0.44
1:I:123:ILE:O	1:I:127:GLU:HG2	2.16	0.44
1:A:109:ASP:HB2	1:A:117:ARG:HH21	1.82	0.44
1:C:109:ASP:HB2	1:C:117:ARG:HH21	1.82	0.44
1:K:112:HIS:HD2	1:K:114:TYR:OH	1.99	0.44
1:L:112:HIS:HD2	1:L:114:TYR:OH	1.99	0.44
1:E:28:HIS:CE1	1:E:79:ILE:O	2.71	0.44
3:I:204:HEM:HMC1	3:I:204:HEM:HBC2	1.99	0.44
1:A:28:HIS:CE1	1:A:79:ILE:O	2.71	0.44
1:F:112:HIS:HD2	1:F:114:TYR:OH	1.99	0.44
1:G:28:HIS:CE1	1:G:79:ILE:O	2.71	0.44
1:K:28:HIS:CE1	1:K:79:ILE:O	2.71	0.44
1:A:119:MET:O	1:A:122:GLU:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:119:MET:O	1:E:122:GLU:HB2	2.18	0.44
1:G:119:MET:O	1:G:122:GLU:HB2	2.18	0.44
1:H:43:VAL:HG11	1:H:133:TRP:CZ2	2.52	0.44
1:I:119:MET:O	1:I:122:GLU:HB2	2.18	0.44
1:A:155:ARG:HG2	1:L:157:GLU:HG2	2.00	0.43
1:C:119:MET:O	1:C:122:GLU:HB2	2.18	0.43
1:H:112:HIS:HD2	1:H:114:TYR:OH	1.99	0.43
1:I:43:VAL:HG11	1:I:133:TRP:CZ2	2.54	0.43
1:C:28:HIS:CE1	1:C:79:ILE:O	2.71	0.43
1:G:109:ASP:HB2	1:G:117:ARG:HH21	1.82	0.43
1:E:109:ASP:HB2	1:E:117:ARG:HH21	1.82	0.43
1:K:43:VAL:HG11	1:K:133:TRP:CZ2	2.53	0.43
1:C:43:VAL:HG11	1:C:133:TRP:CZ2	2.54	0.43
3:K:205:HEM:HBB2	3:K:205:HEM:CMB	2.49	0.43
3:A:200:HEM:HBB2	3:A:200:HEM:CMB	2.49	0.43
1:E:43:VAL:HG11	1:E:133:TRP:CZ2	2.54	0.43
1:G:43:VAL:HG11	1:G:133:TRP:CZ2	2.53	0.43
1:I:28:HIS:CE1	1:I:79:ILE:O	2.71	0.43
1:K:47:GLU:O	1:K:51:GLU:HG2	2.19	0.43
1:B:150:LEU:HD12	1:B:150:LEU:HA	1.85	0.43
1:A:43:VAL:HG11	1:A:133:TRP:CZ2	2.54	0.43
1:C:155:ARG:O	1:K:155:ARG:NH2	2.36	0.43
1:G:47:GLU:O	1:G:51:GLU:HG2	2.19	0.43
3:I:204:HEM:HBB2	3:I:204:HEM:CMB	2.49	0.43
1:B:157:GLU:HG2	1:D:155:ARG:CZ	2.49	0.43
1:D:47:GLU:O	1:D:51:GLU:HG2	2.19	0.43
1:F:51:GLU:OE1	1:F:51:GLU:HA	2.19	0.43
1:L:51:GLU:OE1	1:L:51:GLU:HA	2.19	0.43
1:B:47:GLU:O	1:B:51:GLU:HG2	2.19	0.43
3:C:201:HEM:HBB2	3:C:201:HEM:CMB	2.49	0.43
1:D:63:LEU:HD12	1:D:63:LEU:HA	1.88	0.43
1:J:47:GLU:O	1:J:51:GLU:HG2	2.19	0.43
1:B:51:GLU:OE1	1:B:51:GLU:HA	2.19	0.43
1:B:109:ASP:HB2	1:B:117:ARG:HH21	1.84	0.43
1:D:148:ASN:HD22	1:D:148:ASN:HA	1.65	0.43
1:K:119:MET:O	1:K:122:GLU:HB2	2.18	0.43
3:E:202:HEM:HBB2	3:E:202:HEM:CMB	2.49	0.42
3:G:203:HEM:HBB2	3:G:203:HEM:CMB	2.49	0.42
1:I:47:GLU:O	1:I:51:GLU:HG2	2.19	0.42
1:D:150:LEU:HD12	1:D:150:LEU:HA	1.85	0.42
1:J:109:ASP:HB2	1:J:117:ARG:HH21	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:28:HIS:CE1	1:F:79:ILE:O	2.73	0.42
1:E:47:GLU:O	1:E:51:GLU:HG2	2.19	0.42
1:L:109:ASP:HB2	1:L:117:ARG:HH21	1.84	0.42
1:A:155:ARG:NH2	1:L:155:ARG:O	2.47	0.42
1:A:47:GLU:O	1:A:51:GLU:HG2	2.19	0.42
1:L:47:GLU:O	1:L:51:GLU:HG2	2.19	0.42
1:A:28:HIS:HE1	1:A:79:ILE:O	2.03	0.42
1:H:51:GLU:HA	1:H:51:GLU:OE1	2.19	0.42
1:J:28:HIS:CE1	1:J:79:ILE:O	2.73	0.42
1:K:28:HIS:HE1	1:K:79:ILE:O	2.03	0.42
1:B:28:HIS:CE1	1:B:79:ILE:O	2.73	0.42
1:D:82:ASP:OD1	1:D:85:GLU:HB2	2.20	0.42
1:F:47:GLU:O	1:F:51:GLU:HG2	2.19	0.42
1:H:28:HIS:CE1	1:H:79:ILE:O	2.73	0.42
1:H:47:GLU:O	1:H:51:GLU:HG2	2.19	0.42
1:A:63:LEU:HD12	1:A:63:LEU:HA	1.89	0.42
1:D:109:ASP:HB2	1:D:117:ARG:HH21	1.84	0.42
1:H:82:ASP:OD1	1:H:85:GLU:HB2	2.20	0.42
1:I:28:HIS:HE1	1:I:79:ILE:O	2.03	0.42
1:A:32:PHE:HE1	1:A:83:VAL:HB	1.85	0.42
1:B:82:ASP:OD1	1:B:85:GLU:HB2	2.20	0.42
1:B:154:ILE:HD11	1:H:152:ALA:HB1	2.02	0.42
1:C:47:GLU:O	1:C:51:GLU:HG2	2.19	0.42
1:D:51:GLU:OE1	1:D:51:GLU:HA	2.19	0.42
1:I:32:PHE:HE1	1:I:83:VAL:HB	1.85	0.42
1:K:32:PHE:HE1	1:K:83:VAL:HB	1.85	0.42
1:D:32:PHE:HE1	1:D:83:VAL:HB	1.85	0.41
1:J:32:PHE:HE1	1:J:83:VAL:HB	1.85	0.41
1:L:32:PHE:HE1	1:L:83:VAL:HB	1.85	0.41
1:D:28:HIS:CE1	1:D:79:ILE:O	2.73	0.41
1:I:61:ARG:HA	1:I:61:ARG:HD2	1.90	0.41
1:J:51:GLU:HA	1:J:51:GLU:OE1	2.19	0.41
1:L:28:HIS:CE1	1:L:79:ILE:O	2.73	0.41
1:F:109:ASP:HB2	1:F:117:ARG:HH21	1.85	0.41
1:A:150:LEU:HD12	1:A:150:LEU:HA	1.86	0.41
1:A:155:ARG:CG	1:L:157:GLU:HG2	2.50	0.41
1:L:119:MET:O	1:L:122:GLU:HB2	2.21	0.41
1:G:32:PHE:HE1	1:G:83:VAL:HB	1.85	0.41
1:L:82:ASP:OD1	1:L:85:GLU:HB2	2.20	0.41
1:G:63:LEU:HD12	1:G:63:LEU:HA	1.89	0.41
1:H:109:ASP:HB2	1:H:117:ARG:HH21	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:MET:O	1:B:122:GLU:HB2	2.21	0.41
1:G:28:HIS:HE1	1:G:79:ILE:O	2.03	0.41
1:H:32:PHE:HE1	1:H:83:VAL:HB	1.85	0.41
1:J:82:ASP:OD1	1:J:85:GLU:HB2	2.20	0.41
1:D:119:MET:O	1:D:122:GLU:HB2	2.21	0.41
1:F:32:PHE:HE1	1:F:83:VAL:HB	1.85	0.41
1:F:150:LEU:HD12	1:F:150:LEU:HA	1.85	0.41
1:G:157:GLU:HG2	1:I:155:ARG:NE	2.36	0.41
1:B:32:PHE:HE1	1:B:83:VAL:HB	1.85	0.41
1:E:28:HIS:HE1	1:E:79:ILE:O	2.03	0.41
1:H:119:MET:O	1:H:122:GLU:HB2	2.21	0.41
1:J:28:HIS:HE1	1:J:79:ILE:O	2.05	0.41
1:B:28:HIS:HE1	1:B:79:ILE:O	2.04	0.40
1:C:28:HIS:HE1	1:C:79:ILE:O	2.03	0.40
1:C:32:PHE:HE1	1:C:83:VAL:HB	1.85	0.40
1:E:32:PHE:HE1	1:E:83:VAL:HB	1.85	0.40
1:H:28:HIS:HE1	1:H:79:ILE:O	2.04	0.40
1:C:40:LEU:HD12	1:C:40:LEU:HA	1.94	0.40
1:F:82:ASP:OD1	1:F:85:GLU:HB2	2.20	0.40
1:A:148:ASN:HD22	1:A:148:ASN:HA	1.67	0.40
1:B:115:VAL:HG13	1:L:125:ARG:NH1	2.36	0.40
1:F:119:MET:O	1:F:122:GLU:HB2	2.21	0.40
1:B:157:GLU:HA	1:D:155:ARG:HH11	1.76	0.40
1:F:149:TYR:O	1:F:153:GLN:HG2	2.22	0.40
1:A:51:GLU:OE1	1:A:51:GLU:HA	2.22	0.40
1:J:119:MET:O	1:J:122:GLU:HB2	2.21	0.40
1:J:149:TYR:O	1:J:153:GLN:HG2	2.22	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 X-ray entries followed by that with respect to entries of similar resolution.

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	156/158 (99%)	151 (97%)	4 (3%)	1 (1%)	25 58
1	B	156/158 (99%)	151 (97%)	5 (3%)	0	100 100
1	C	156/158 (99%)	151 (97%)	4 (3%)	1 (1%)	25 58
1	D	156/158 (99%)	151 (97%)	5 (3%)	0	100 100
1	E	156/158 (99%)	151 (97%)	4 (3%)	1 (1%)	25 58
1	F	156/158 (99%)	151 (97%)	5 (3%)	0	100 100
1	G	156/158 (99%)	151 (97%)	4 (3%)	1 (1%)	25 58
1	H	156/158 (99%)	151 (97%)	5 (3%)	0	100 100
1	I	156/158 (99%)	151 (97%)	4 (3%)	1 (1%)	25 58
1	J	156/158 (99%)	151 (97%)	5 (3%)	0	100 100
1	K	156/158 (99%)	151 (97%)	4 (3%)	1 (1%)	25 58
1	L	156/158 (99%)	151 (97%)	5 (3%)	0	100 100
All	All	1872/1896 (99%)	1812 (97%)	54 (3%)	6 (0%)	41 71

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	ASP
1	C	4	ASP
1	E	4	ASP
1	G	4	ASP
1	I	4	ASP
1	K	4	ASP

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 X-ray entries followed by that with respect to entries of similar resolution.

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	139/139 (100%)	115 (83%)	24 (17%)	2 6
1	B	139/139 (100%)	116 (84%)	23 (16%)	2 7
1	C	139/139 (100%)	115 (83%)	24 (17%)	2 6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	139/139 (100%)	116 (84%)	23 (16%)	2 7
1	E	139/139 (100%)	115 (83%)	24 (17%)	2 6
1	F	139/139 (100%)	116 (84%)	23 (16%)	2 7
1	G	139/139 (100%)	115 (83%)	24 (17%)	2 6
1	H	139/139 (100%)	116 (84%)	23 (16%)	2 7
1	I	139/139 (100%)	115 (83%)	24 (17%)	2 6
1	J	139/139 (100%)	116 (84%)	23 (16%)	2 7
1	K	139/139 (100%)	115 (83%)	24 (17%)	2 6
1	L	139/139 (100%)	116 (84%)	23 (16%)	2 7
All	All	1668/1668 (100%)	1386 (83%)	282 (17%)	2 6

All (282) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	14	LEU
1	A	20	VAL
1	A	22	ILE
1	A	37	LEU
1	A	40	LEU
1	A	57	ARG
1	A	63	LEU
1	A	65	LEU
1	A	68	LEU
1	A	74	LEU
1	A	83	VAL
1	A	84	GLU
1	A	95	LEU
1	A	102	ARG
1	A	111	VAL
1	A	117	ARG
1	A	139	ASP
1	A	140	LEU
1	A	142	GLN
1	A	148	ASN
1	A	150	LEU
1	A	156	GLU
1	A	157	GLU
1	B	11	LEU

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Mol	Chain	Res	Type
1	B	14	LEU
1	B	20	VAL
1	B	22	ILE
1	B	37	LEU
1	B	40	LEU
1	B	57	ARG
1	B	63	LEU
1	B	65	LEU
1	B	68	LEU
1	B	74	LEU
1	B	83	VAL
1	B	84	GLU
1	B	95	LEU
1	B	102	ARG
1	B	111	VAL
1	B	117	ARG
1	B	139	ASP
1	B	140	LEU
1	B	148	ASN
1	B	150	LEU
1	B	156	GLU
1	B	157	GLU
1	C	11	LEU
1	C	14	LEU
1	C	20	VAL
1	C	22	ILE
1	C	37	LEU
1	C	40	LEU
1	C	57	ARG
1	C	63	LEU
1	C	65	LEU
1	C	68	LEU
1	C	74	LEU
1	C	83	VAL
1	C	84	GLU
1	C	95	LEU
1	C	102	ARG
1	C	111	VAL
1	C	117	ARG
1	C	139	ASP
1	C	140	LEU
1	C	142	GLN

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Mol	Chain	Res	Type
1	C	148	ASN
1	C	150	LEU
1	C	156	GLU
1	C	157	GLU
1	D	11	LEU
1	D	14	LEU
1	D	20	VAL
1	D	22	ILE
1	D	37	LEU
1	D	40	LEU
1	D	57	ARG
1	D	63	LEU
1	D	65	LEU
1	D	68	LEU
1	D	74	LEU
1	D	83	VAL
1	D	84	GLU
1	D	95	LEU
1	D	102	ARG
1	D	111	VAL
1	D	117	ARG
1	D	139	ASP
1	D	140	LEU
1	D	148	ASN
1	D	150	LEU
1	D	156	GLU
1	D	157	GLU
1	E	11	LEU
1	E	14	LEU
1	E	20	VAL
1	E	22	ILE
1	E	37	LEU
1	E	40	LEU
1	E	57	ARG
1	E	63	LEU
1	E	65	LEU
1	E	68	LEU
1	E	74	LEU
1	E	83	VAL
1	E	84	GLU
1	E	95	LEU
1	E	102	ARG

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Mol	Chain	Res	Type
1	E	111	VAL
1	E	117	ARG
1	E	139	ASP
1	E	140	LEU
1	E	142	GLN
1	E	148	ASN
1	E	150	LEU
1	E	156	GLU
1	E	157	GLU
1	F	11	LEU
1	F	14	LEU
1	F	20	VAL
1	F	22	ILE
1	F	37	LEU
1	F	40	LEU
1	F	57	ARG
1	F	63	LEU
1	F	65	LEU
1	F	68	LEU
1	F	74	LEU
1	F	83	VAL
1	F	84	GLU
1	F	95	LEU
1	F	102	ARG
1	F	111	VAL
1	F	117	ARG
1	F	139	ASP
1	F	140	LEU
1	F	148	ASN
1	F	150	LEU
1	F	156	GLU
1	F	157	GLU
1	G	11	LEU
1	G	14	LEU
1	G	20	VAL
1	G	22	ILE
1	G	37	LEU
1	G	40	LEU
1	G	57	ARG
1	G	63	LEU
1	G	65	LEU
1	G	68	LEU

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Mol	Chain	Res	Type
1	G	74	LEU
1	G	83	VAL
1	G	84	GLU
1	G	95	LEU
1	G	102	ARG
1	G	111	VAL
1	G	117	ARG
1	G	139	ASP
1	G	140	LEU
1	G	142	GLN
1	G	148	ASN
1	G	150	LEU
1	G	156	GLU
1	G	157	GLU
1	H	11	LEU
1	H	14	LEU
1	H	20	VAL
1	H	22	ILE
1	H	37	LEU
1	H	40	LEU
1	H	57	ARG
1	H	63	LEU
1	H	65	LEU
1	H	68	LEU
1	H	74	LEU
1	H	83	VAL
1	H	84	GLU
1	H	95	LEU
1	H	102	ARG
1	H	111	VAL
1	H	117	ARG
1	H	139	ASP
1	H	140	LEU
1	H	148	ASN
1	H	150	LEU
1	H	156	GLU
1	H	157	GLU
1	I	11	LEU
1	I	14	LEU
1	I	20	VAL
1	I	22	ILE
1	I	37	LEU

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Mol	Chain	Res	Type
1	I	40	LEU
1	I	57	ARG
1	I	63	LEU
1	I	65	LEU
1	I	68	LEU
1	I	74	LEU
1	I	83	VAL
1	I	84	GLU
1	I	95	LEU
1	I	102	ARG
1	I	111	VAL
1	I	117	ARG
1	I	139	ASP
1	I	140	LEU
1	I	142	GLN
1	I	148	ASN
1	I	150	LEU
1	I	156	GLU
1	I	157	GLU
1	J	11	LEU
1	J	14	LEU
1	J	20	VAL
1	J	22	ILE
1	J	37	LEU
1	J	40	LEU
1	J	57	ARG
1	J	63	LEU
1	J	65	LEU
1	J	68	LEU
1	J	74	LEU
1	J	83	VAL
1	J	84	GLU
1	J	95	LEU
1	J	102	ARG
1	J	111	VAL
1	J	117	ARG
1	J	139	ASP
1	J	140	LEU
1	J	148	ASN
1	J	150	LEU
1	J	156	GLU
1	J	157	GLU

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Mol	Chain	Res	Type
1	K	11	LEU
1	K	14	LEU
1	K	20	VAL
1	K	22	ILE
1	K	37	LEU
1	K	40	LEU
1	K	57	ARG
1	K	63	LEU
1	K	65	LEU
1	K	68	LEU
1	K	74	LEU
1	K	83	VAL
1	K	84	GLU
1	K	95	LEU
1	K	102	ARG
1	K	111	VAL
1	K	117	ARG
1	K	139	ASP
1	K	140	LEU
1	K	142	GLN
1	K	148	ASN
1	K	150	LEU
1	K	156	GLU
1	K	157	GLU
1	L	11	LEU
1	L	14	LEU
1	L	20	VAL
1	L	22	ILE
1	L	37	LEU
1	L	40	LEU
1	L	57	ARG
1	L	63	LEU
1	L	65	LEU
1	L	68	LEU
1	L	74	LEU
1	L	83	VAL
1	L	84	GLU
1	L	95	LEU
1	L	102	ARG
1	L	111	VAL
1	L	117	ARG
1	L	139	ASP

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Mol	Chain	Res	Type
1	L	140	LEU
1	L	148	ASN
1	L	150	LEU
1	L	156	GLU
1	L	157	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	28	HIS
1	A	78	ASN
1	A	112	HIS
1	A	142	GLN
1	A	148	ASN
1	B	24	GLN
1	B	28	HIS
1	B	78	ASN
1	B	112	HIS
1	B	148	ASN
1	C	24	GLN
1	C	28	HIS
1	C	78	ASN
1	C	112	HIS
1	C	142	GLN
1	C	148	ASN
1	D	24	GLN
1	D	28	HIS
1	D	78	ASN
1	D	112	HIS
1	D	148	ASN
1	E	24	GLN
1	E	28	HIS
1	E	78	ASN
1	E	112	HIS
1	E	142	GLN
1	E	148	ASN
1	F	24	GLN
1	F	28	HIS
1	F	78	ASN
1	F	112	HIS
1	F	148	ASN

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Mol	Chain	Res	Type
1	G	24	GLN
1	G	28	HIS
1	G	78	ASN
1	G	112	HIS
1	G	142	GLN
1	G	148	ASN
1	H	24	GLN
1	H	28	HIS
1	H	78	ASN
1	H	112	HIS
1	H	148	ASN
1	I	24	GLN
1	I	28	HIS
1	I	78	ASN
1	I	112	HIS
1	I	142	GLN
1	I	148	ASN
1	J	24	GLN
1	J	28	HIS
1	J	78	ASN
1	J	112	HIS
1	J	148	ASN
1	K	24	GLN
1	K	28	HIS
1	K	78	ASN
1	K	112	HIS
1	K	142	GLN
1	K	148	ASN
1	L	24	GLN
1	L	28	HIS
1	L	78	ASN
1	L	112	HIS
1	L	148	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 30 ligands modelled in this entry, 24 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	HEM	K	205	1	41,50,50	1.85	12 (29%)	45,82,82	1.59	8 (17%)
3	HEM	A	200	1	41,50,50	1.85	13 (31%)	45,82,82	1.60	8 (17%)
3	HEM	G	203	1	41,50,50	1.85	12 (29%)	45,82,82	1.60	8 (17%)
3	HEM	C	201	1	41,50,50	1.85	14 (34%)	45,82,82	1.60	8 (17%)
3	HEM	I	204	1	41,50,50	1.85	12 (29%)	45,82,82	1.60	8 (17%)
3	HEM	E	202	1	41,50,50	1.85	14 (34%)	45,82,82	1.60	8 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEM	K	205	1	-	4/12/54/54	-
3	HEM	A	200	1	-	4/12/54/54	-
3	HEM	G	203	1	-	4/12/54/54	-
3	HEM	C	201	1	-	4/12/54/54	-
3	HEM	I	204	1	-	4/12/54/54	-
3	HEM	E	202	1	-	4/12/54/54	-

All (77) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	205	HEM	C3C-CAC	-4.85	1.37	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	203	HEM	C3C-CAC	-4.83	1.37	1.47
3	I	204	HEM	C3C-CAC	-4.82	1.37	1.47
3	A	200	HEM	C3C-CAC	-4.82	1.37	1.47
3	C	201	HEM	C3C-CAC	-4.81	1.37	1.47
3	E	202	HEM	C3C-CAC	-4.80	1.38	1.47
3	G	203	HEM	CAA-C2A	-3.47	1.47	1.52
3	C	201	HEM	CAA-C2A	-3.46	1.47	1.52
3	I	204	HEM	CAA-C2A	-3.44	1.47	1.52
3	E	202	HEM	CAA-C2A	-3.43	1.47	1.52
3	A	200	HEM	CAA-C2A	-3.43	1.47	1.52
3	K	205	HEM	CAA-C2A	-3.42	1.47	1.52
3	C	201	HEM	CBB-CAB	3.31	1.46	1.30
3	K	205	HEM	CBB-CAB	3.31	1.46	1.30
3	A	200	HEM	CBB-CAB	3.30	1.46	1.30
3	I	204	HEM	CBB-CAB	3.30	1.46	1.30
3	G	203	HEM	CBB-CAB	3.30	1.46	1.30
3	E	202	HEM	CBB-CAB	3.29	1.46	1.30
3	C	201	HEM	C2C-C1C	3.10	1.49	1.42
3	A	200	HEM	C2C-C1C	3.07	1.49	1.42
3	E	202	HEM	C2C-C1C	3.06	1.49	1.42
3	G	203	HEM	C2C-C1C	3.05	1.49	1.42
3	K	205	HEM	C2C-C1C	3.05	1.49	1.42
3	I	204	HEM	C2C-C1C	3.05	1.49	1.42
3	C	201	HEM	C3B-C4B	2.97	1.50	1.44
3	I	204	HEM	C3B-C4B	2.94	1.50	1.44
3	E	202	HEM	C3B-C4B	2.94	1.50	1.44
3	K	205	HEM	C3B-C4B	2.93	1.50	1.44
3	A	200	HEM	C3B-C4B	2.93	1.50	1.44
3	G	203	HEM	C3B-C4B	2.93	1.50	1.44
3	G	203	HEM	CHA-C4D	2.83	1.42	1.35
3	I	204	HEM	CHA-C4D	2.82	1.42	1.35
3	K	205	HEM	CHA-C4D	2.82	1.42	1.35
3	C	201	HEM	CHA-C4D	2.81	1.42	1.35
3	A	200	HEM	CHA-C4D	2.81	1.42	1.35
3	E	202	HEM	CHA-C4D	2.81	1.42	1.35
3	G	203	HEM	CAB-C3B	-2.72	1.40	1.47
3	C	201	HEM	CAB-C3B	-2.72	1.40	1.47
3	K	205	HEM	CAB-C3B	-2.72	1.40	1.47
3	A	200	HEM	CAB-C3B	-2.72	1.40	1.47
3	E	202	HEM	CAB-C3B	-2.71	1.40	1.47
3	I	204	HEM	CAB-C3B	-2.70	1.40	1.47
3	G	203	HEM	CHB-C1B	2.63	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	200	HEM	CHB-C1B	2.63	1.41	1.35
3	C	201	HEM	CHB-C1B	2.63	1.41	1.35
3	K	205	HEM	CHB-C1B	2.62	1.41	1.35
3	I	204	HEM	CHB-C1B	2.61	1.41	1.35
3	E	202	HEM	CHB-C1B	2.60	1.41	1.35
3	I	204	HEM	C1B-NB	2.52	1.44	1.40
3	I	204	HEM	C1A-NA	2.51	1.41	1.36
3	E	202	HEM	C1B-NB	2.51	1.44	1.40
3	C	201	HEM	C1A-NA	2.51	1.41	1.36
3	K	205	HEM	C1B-NB	2.50	1.44	1.40
3	A	200	HEM	C1B-NB	2.50	1.44	1.40
3	E	202	HEM	C1A-NA	2.49	1.41	1.36
3	A	200	HEM	C1A-NA	2.49	1.41	1.36
3	G	203	HEM	C1B-NB	2.49	1.44	1.40
3	G	203	HEM	C1A-NA	2.48	1.41	1.36
3	K	205	HEM	C1A-NA	2.48	1.41	1.36
3	C	201	HEM	C1B-NB	2.48	1.44	1.40
3	G	203	HEM	C4B-NB	2.04	1.43	1.38
3	E	202	HEM	C4A-NA	2.03	1.40	1.36
3	C	201	HEM	C2A-C3A	-2.02	1.31	1.37
3	K	205	HEM	C2A-C3A	-2.01	1.31	1.37
3	A	200	HEM	C2A-C3A	-2.01	1.31	1.37
3	E	202	HEM	C2A-C3A	-2.01	1.31	1.37
3	C	201	HEM	C4A-NA	2.01	1.40	1.36
3	A	200	HEM	C3B-C2B	2.01	1.41	1.37
3	C	201	HEM	C4B-NB	2.01	1.42	1.38
3	I	204	HEM	C3B-C2B	2.01	1.41	1.37
3	I	204	HEM	C2A-C3A	-2.01	1.31	1.37
3	C	201	HEM	C3B-C2B	2.01	1.41	1.37
3	E	202	HEM	C3B-C2B	2.01	1.41	1.37
3	K	205	HEM	C3B-C2B	2.01	1.41	1.37
3	A	200	HEM	C4B-NB	2.00	1.42	1.38
3	E	202	HEM	C4B-NB	2.00	1.42	1.38
3	G	203	HEM	C2A-C3A	-2.00	1.31	1.37

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	I	204	HEM	C4B-C3B-C2B	3.93	110.23	107.11
3	K	205	HEM	C4B-C3B-C2B	3.89	110.21	107.11
3	G	203	HEM	C4B-C3B-C2B	3.88	110.20	107.11
3	A	200	HEM	C4B-C3B-C2B	3.88	110.20	107.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	202	HEM	C4B-C3B-C2B	3.88	110.20	107.11
3	C	201	HEM	C4B-C3B-C2B	3.87	110.19	107.11
3	C	201	HEM	C2C-C3C-C4C	3.58	109.40	106.90
3	I	204	HEM	C4A-C3A-C2A	-3.55	104.52	107.00
3	A	200	HEM	C2C-C3C-C4C	3.55	109.38	106.90
3	C	201	HEM	C4A-C3A-C2A	-3.54	104.53	107.00
3	E	202	HEM	C2C-C3C-C4C	3.54	109.37	106.90
3	G	203	HEM	C4A-C3A-C2A	-3.53	104.54	107.00
3	A	200	HEM	C4A-C3A-C2A	-3.53	104.54	107.00
3	G	203	HEM	C2C-C3C-C4C	3.53	109.36	106.90
3	I	204	HEM	C2C-C3C-C4C	3.53	109.36	106.90
3	K	205	HEM	C4A-C3A-C2A	-3.52	104.55	107.00
3	E	202	HEM	C4A-C3A-C2A	-3.51	104.55	107.00
3	K	205	HEM	C2C-C3C-C4C	3.47	109.32	106.90
3	C	201	HEM	CMB-C2B-C1B	-3.45	119.78	125.04
3	A	200	HEM	CMB-C2B-C1B	-3.44	119.80	125.04
3	G	203	HEM	CMB-C2B-C1B	-3.44	119.80	125.04
3	I	204	HEM	CMB-C2B-C1B	-3.44	119.80	125.04
3	K	205	HEM	CMB-C2B-C1B	-3.43	119.81	125.04
3	E	202	HEM	CMB-C2B-C1B	-3.43	119.82	125.04
3	I	204	HEM	C3B-C2B-C1B	-3.11	104.18	106.49
3	E	202	HEM	C3B-C2B-C1B	-3.08	104.20	106.49
3	A	200	HEM	C3B-C2B-C1B	-3.07	104.21	106.49
3	G	203	HEM	C3B-C2B-C1B	-3.06	104.22	106.49
3	K	205	HEM	C3B-C2B-C1B	-3.06	104.22	106.49
3	C	201	HEM	C3B-C2B-C1B	-3.04	104.23	106.49
3	I	204	HEM	CMB-C2B-C3B	2.38	134.13	128.30
3	C	201	HEM	CMB-C2B-C3B	2.37	134.11	128.30
3	G	203	HEM	C2B-C1B-NB	2.37	112.64	109.84
3	A	200	HEM	CMB-C2B-C3B	2.37	134.09	128.30
3	G	203	HEM	CMB-C2B-C3B	2.37	134.09	128.30
3	E	202	HEM	C2B-C1B-NB	2.36	112.64	109.84
3	E	202	HEM	CMB-C2B-C3B	2.36	134.08	128.30
3	K	205	HEM	CMB-C2B-C3B	2.36	134.08	128.30
3	C	201	HEM	CMC-C2C-C3C	2.35	129.08	124.68
3	A	200	HEM	C2B-C1B-NB	2.35	112.63	109.84
3	A	200	HEM	CMC-C2C-C3C	2.34	129.05	124.68
3	I	204	HEM	C2B-C1B-NB	2.34	112.61	109.84
3	K	205	HEM	C2B-C1B-NB	2.33	112.60	109.84
3	I	204	HEM	CMC-C2C-C3C	2.33	129.04	124.68
3	E	202	HEM	CMC-C2C-C3C	2.33	129.04	124.68
3	C	201	HEM	C2B-C1B-NB	2.32	112.59	109.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	K	205	HEM	CMC-C2C-C3C	2.32	129.02	124.68
3	G	203	HEM	CMC-C2C-C3C	2.32	129.01	124.68

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	200	HEM	CAA-CBA-CGA-O1A
3	C	201	HEM	CAA-CBA-CGA-O1A
3	E	202	HEM	CAA-CBA-CGA-O1A
3	G	203	HEM	CAA-CBA-CGA-O1A
3	I	204	HEM	CAA-CBA-CGA-O1A
3	K	205	HEM	CAA-CBA-CGA-O1A
3	A	200	HEM	CAA-CBA-CGA-O2A
3	C	201	HEM	CAA-CBA-CGA-O2A
3	E	202	HEM	CAA-CBA-CGA-O2A
3	G	203	HEM	CAA-CBA-CGA-O2A
3	I	204	HEM	CAA-CBA-CGA-O2A
3	K	205	HEM	CAA-CBA-CGA-O2A
3	A	200	HEM	CAD-CBD-CGD-O1D
3	C	201	HEM	CAD-CBD-CGD-O1D
3	E	202	HEM	CAD-CBD-CGD-O1D
3	G	203	HEM	CAD-CBD-CGD-O1D
3	I	204	HEM	CAD-CBD-CGD-O1D
3	K	205	HEM	CAD-CBD-CGD-O1D
3	A	200	HEM	CAD-CBD-CGD-O2D
3	C	201	HEM	CAD-CBD-CGD-O2D
3	E	202	HEM	CAD-CBD-CGD-O2D
3	G	203	HEM	CAD-CBD-CGD-O2D
3	I	204	HEM	CAD-CBD-CGD-O2D
3	K	205	HEM	CAD-CBD-CGD-O2D

There are no ring outliers.

6 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	K	205	HEM	3	0
3	A	200	HEM	3	0
3	G	203	HEM	3	0
3	C	201	HEM	3	0
3	I	204	HEM	3	0

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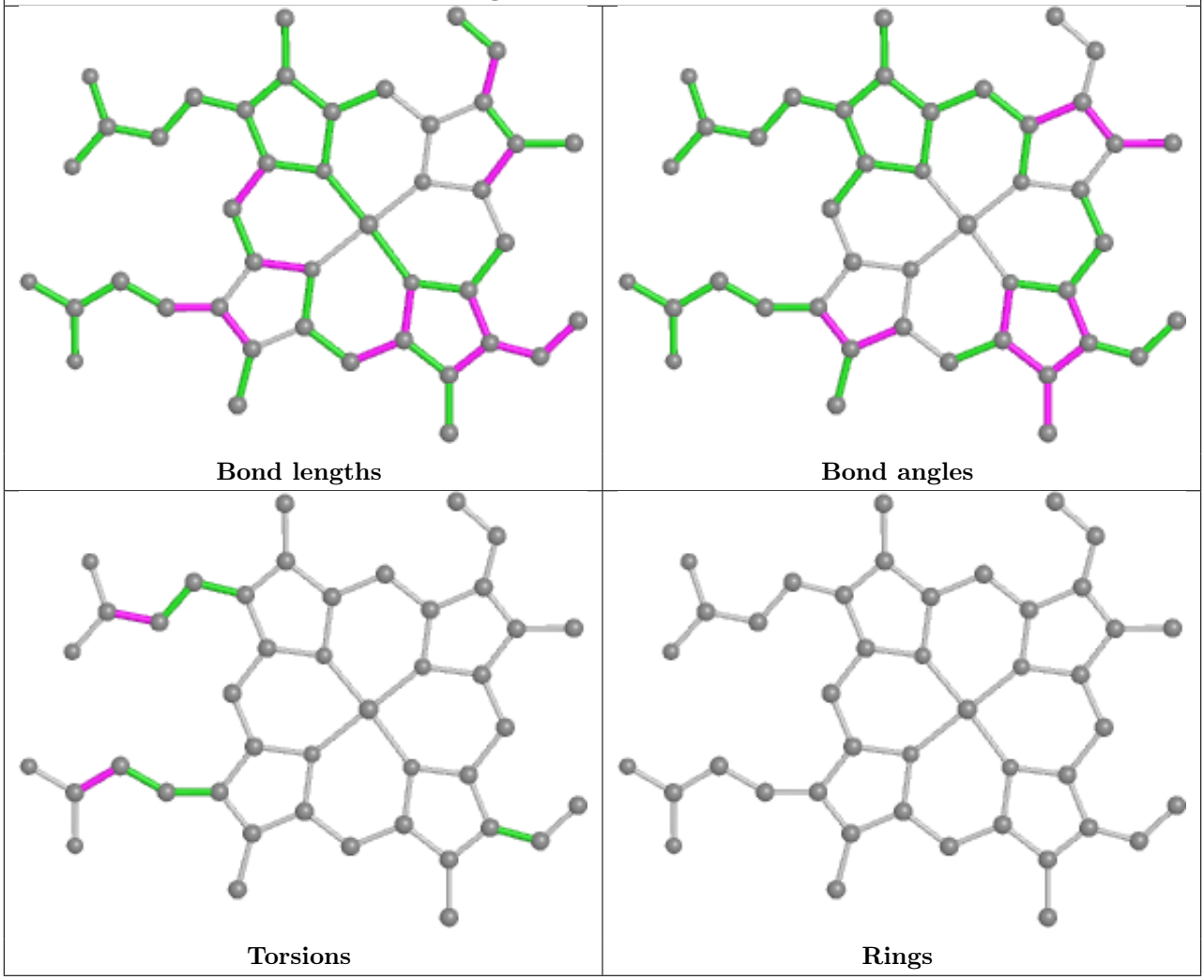
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	202	HEM	3	0

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

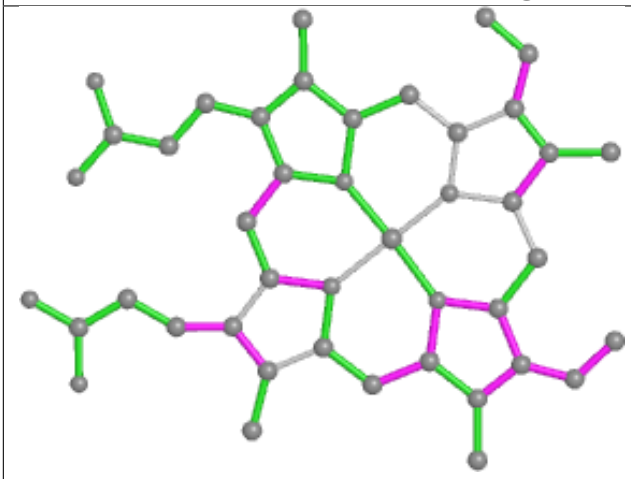
Ligand HEM K 205



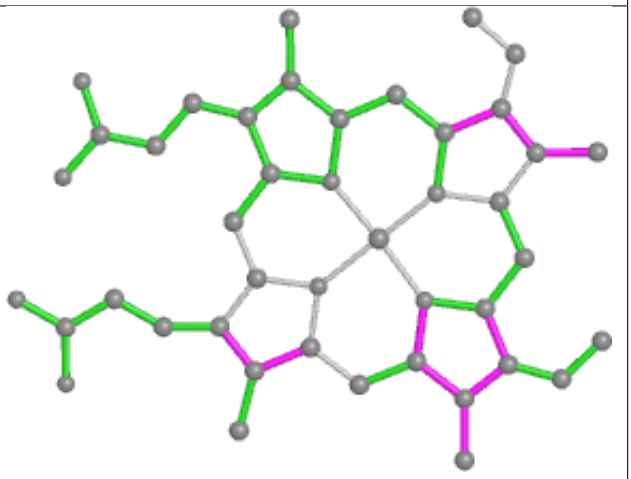
Bond lengths **Bond angles**

Torsions **Rings**

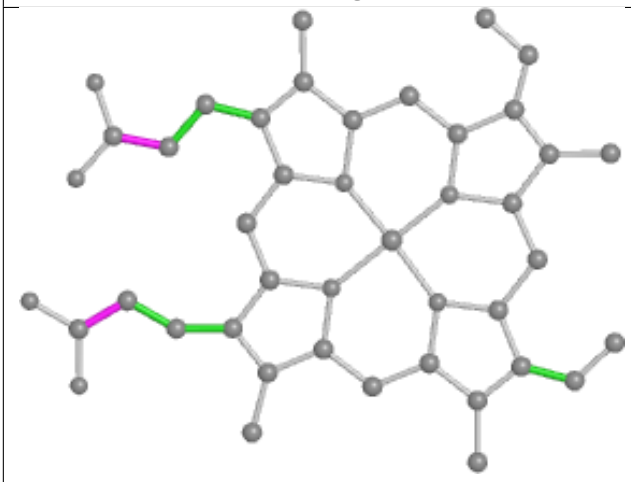
Ligand HEM A 200



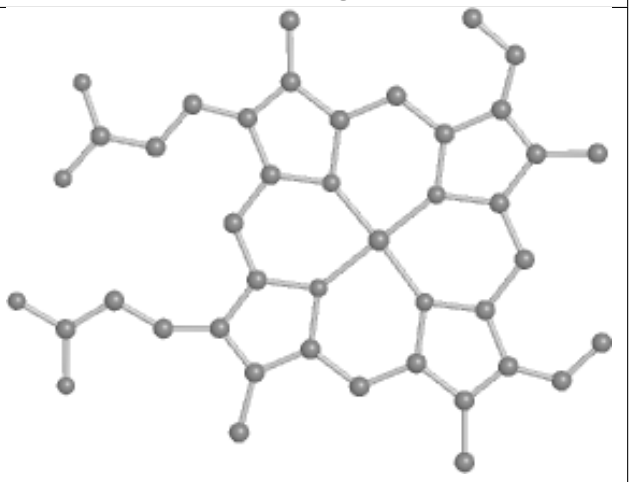
Bond lengths



Bond angles

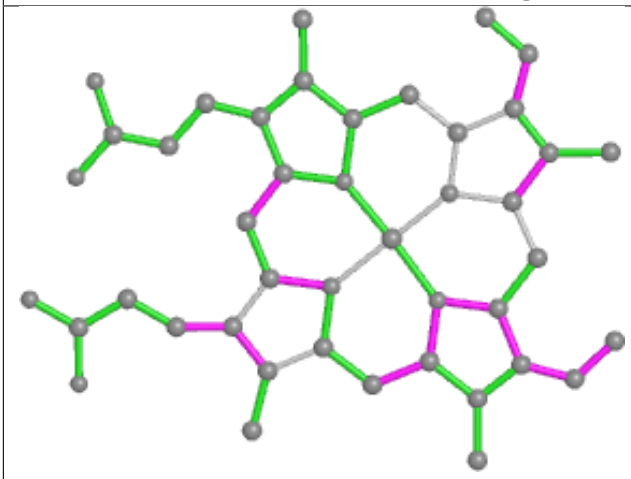


Torsions

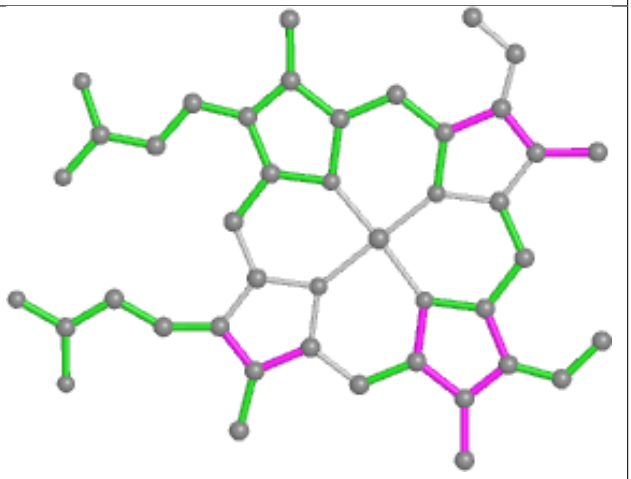


Rings

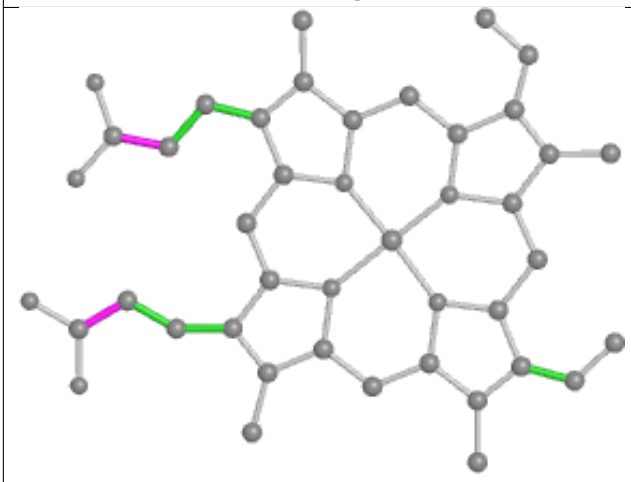
Ligand HEM G 203



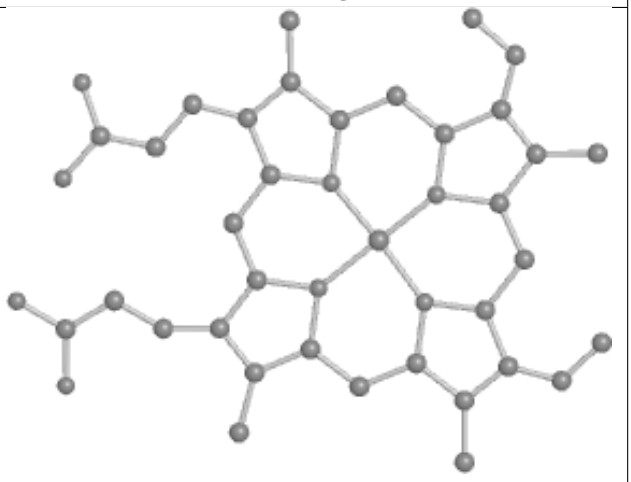
Bond lengths



Bond angles

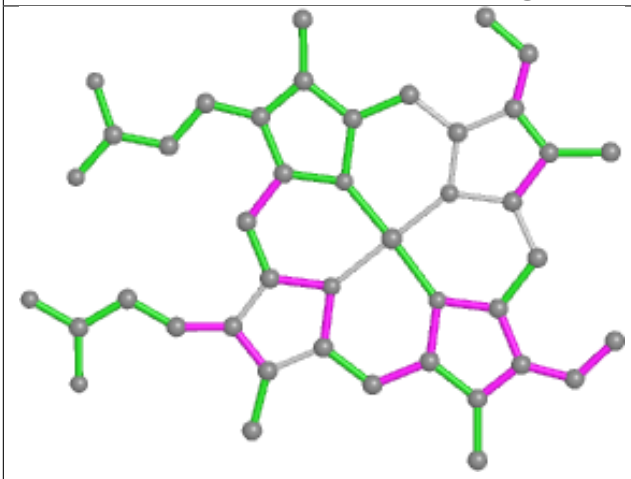


Torsions

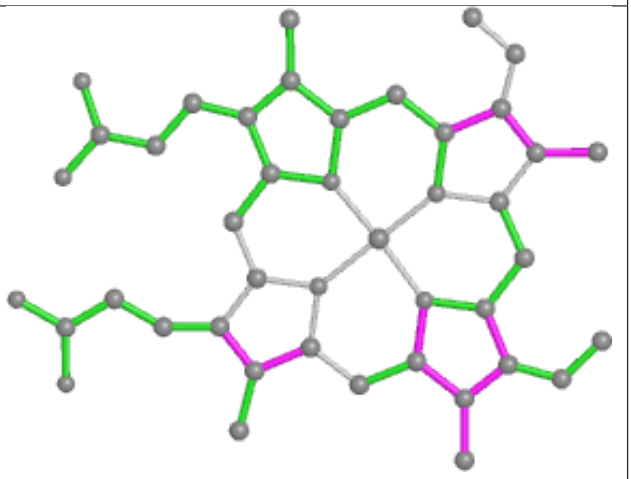


Rings

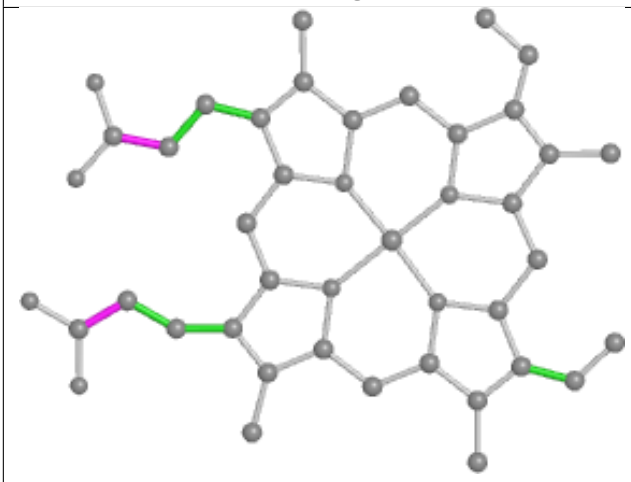
Ligand HEM C 201



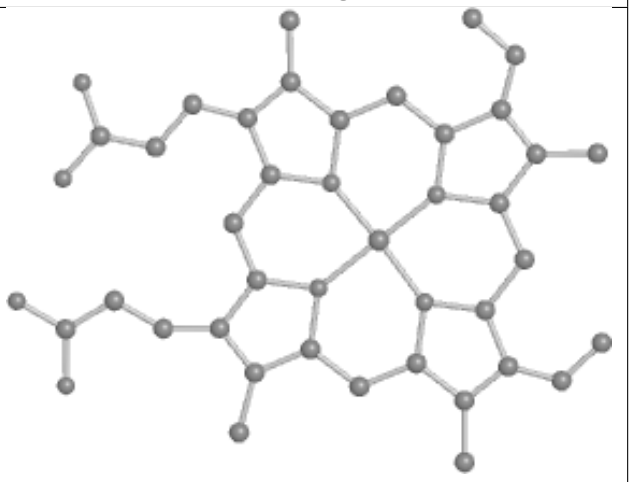
Bond lengths



Bond angles

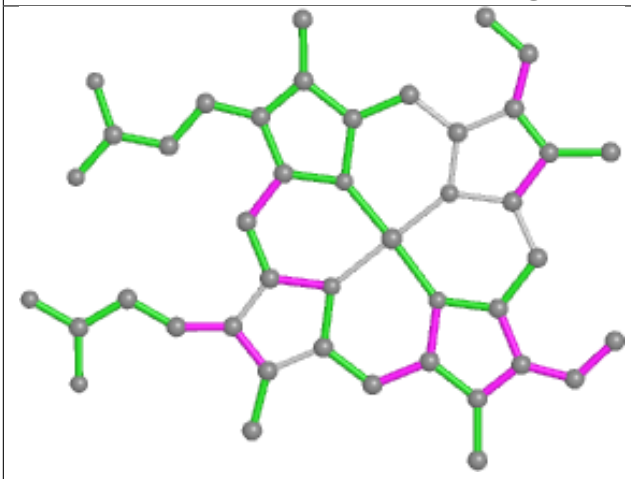


Torsions

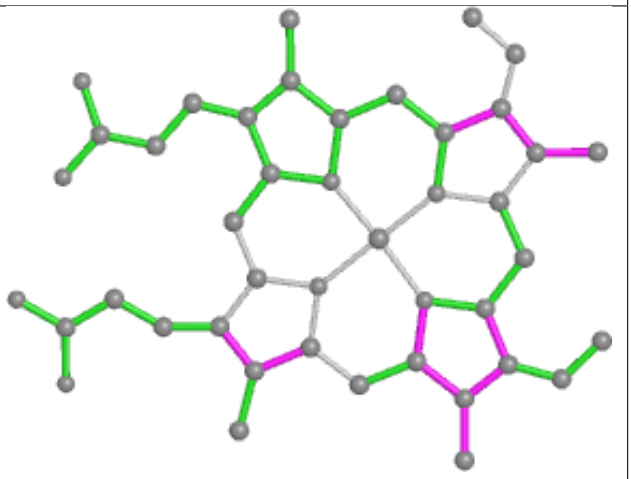


Rings

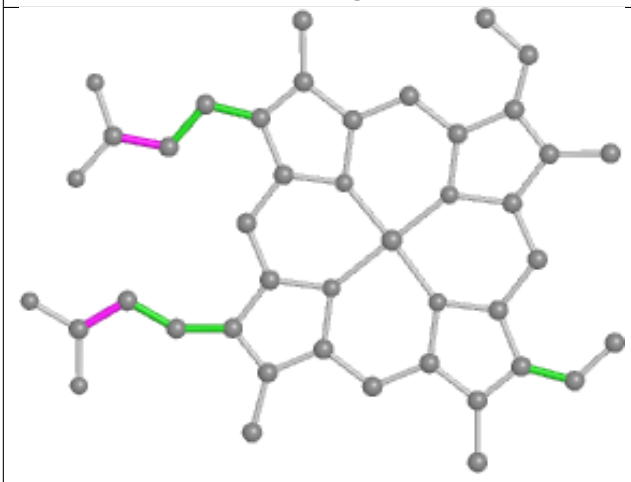
Ligand HEM I 204



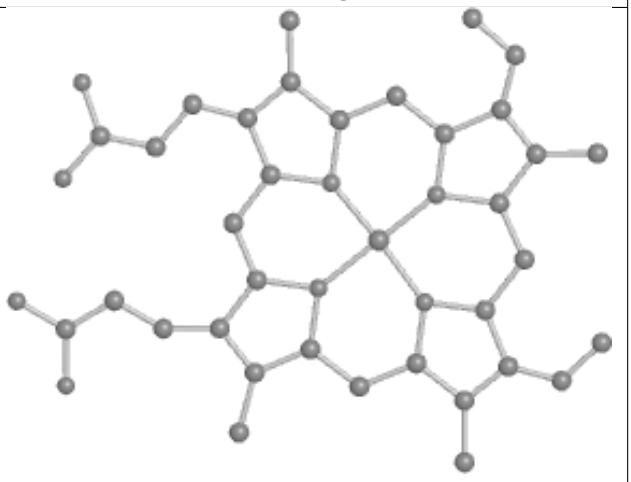
Bond lengths



Bond angles

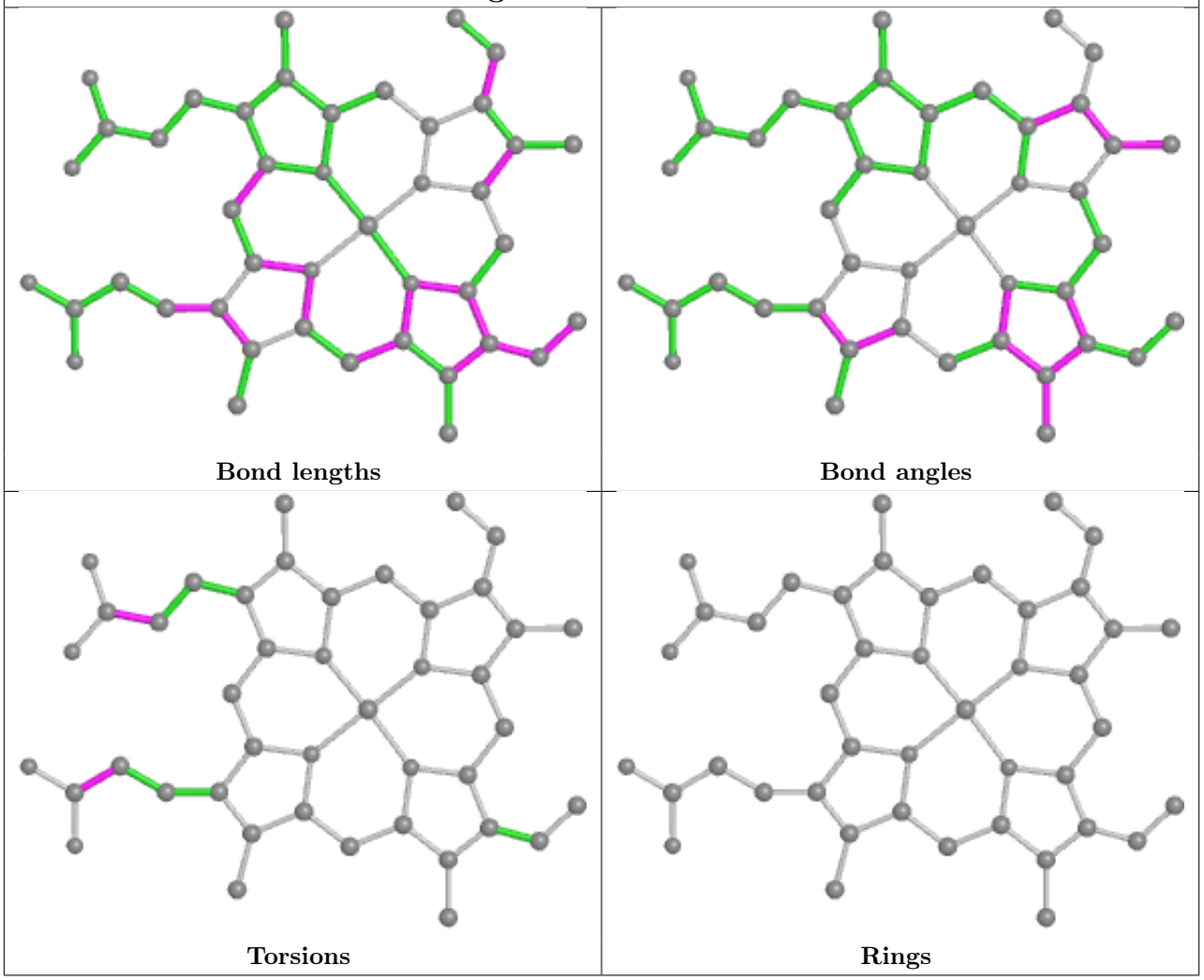


Torsions



Rings

Ligand HEM E 202



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.