Full wwPDB X-ray Structure Validation Report ⓘ

Sep 28, 2023 – 11:19 AM EDT

PDB ID	:	2GTL
Title	:	Lumbricus Erythrocruorin at 3.5A resolution
Authors	:	Royer Jr., W.E.; Sharma, H.; Strand, K.; Knapp, J.E.; Bhyravbhatla, B.
Deposited on	:	2006-04-28
Resolution	:	3.50 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:

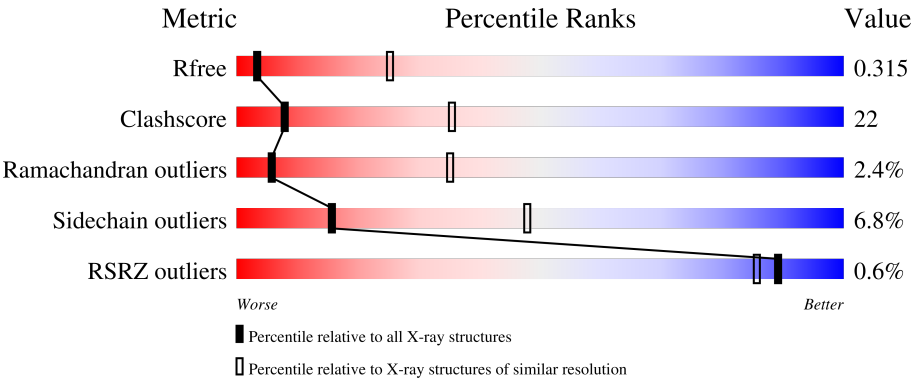
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 3.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	151	50% 44%
1	E	151	52% 42%
1	I	151	52% 43%
2	B	145	70% 28%
2	F	145	71% 28%

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Mol	Chain	Length	Quality of chain
2	J	145	2% 70% 28%
3	C	153	61% 33%
3	G	153	2% 59% 35%
3	K	153	59% 36%
4	D	140	60% 36%
4	H	140	59% 38%
4	L	140	63% 34%
5	M	217	50% 41% 9%
6	N	220	54% 37% 9%
7	O	215	64% 33%

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 19648 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 Extracellular globin 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	147	Total	C	N	O	S	0	0	0
			1209	769	222	214	4			
1	E	147	Total	C	N	O	S	0	0	0
			1209	769	222	214	4			
1	I	147	Total	C	N	O	S	0	0	0
			1209	769	222	214	4			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	78	LYS	ASP	CONFLICT	UNP P13579
E	78	LYS	ASP	CONFLICT	UNP P13579
I	78	LYS	ASP	CONFLICT	UNP P13579

- Molecule 2 is a protein called Extracellular globin 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	145	Total	C	N	O	S	0	0	0
			1148	720	212	213	3			
2	F	145	Total	C	N	O	S	0	0	0
			1148	720	212	213	3			
2	J	145	Total	C	N	O	S	0	0	0
			1148	720	212	213	3			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	66	ASP	GLU	CONFLICT	UNP P02218
F	66	ASP	GLU	CONFLICT	UNP P02218
J	66	ASP	GLU	CONFLICT	UNP P02218

- Molecule 3 is a protein called Extracellular globin-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	149	Total	C	N	O	S	0	0	0
			1185	755	210	217	3			
3	G	149	Total	C	N	O	S	0	0	0
			1185	755	210	217	3			
3	K	149	Total	C	N	O	S	0	0	0
			1185	755	210	217	3			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	49	GLU	ASP	CONFLICT	UNP P11069
G	49	GLU	ASP	CONFLICT	UNP P11069
K	49	GLU	ASP	CONFLICT	UNP P11069

- Molecule 4 is a protein called Hemoglobin chain d1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	140	Total	C	N	O	S	0	0	0
			1129	725	198	202	4			
4	H	140	Total	C	N	O	S	0	0	0
			1129	725	198	202	4			
4	L	140	Total	C	N	O	S	0	0	0
			1129	725	198	202	4			

- Molecule 5 is a protein called Hemoglobin linker chain L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	M	217	Total	C	N	O	S	0	0	0
			1705	1060	302	333	10			

- Molecule 6 is a protein called Extracellular hemoglobin linker L2 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	N	220	Total	C	N	O	S	0	0	0
			1722	1060	316	336	10			

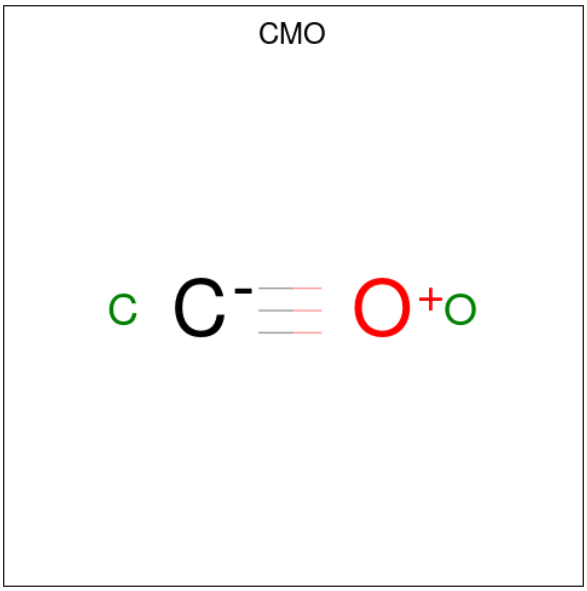
- Molecule 7 is a protein called Extracellular hemoglobin linker L3 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	O	215	Total	C	N	O	S	0	0	0
			1663	1020	292	340	11			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	113	CYS	VAL	CONFLICT	UNP Q2I742

- Molecule 8 is CARBON MONOXIDE (three-letter code: CMO) (formula: CO).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			2	1	1		
8	B	1	Total	C	O	0	0
			2	1	1		
8	C	1	Total	C	O	0	0
			2	1	1		
8	D	1	Total	C	O	0	0
			2	1	1		
8	E	1	Total	C	O	0	0
			2	1	1		
8	F	1	Total	C	O	0	0
			2	1	1		
8	G	1	Total	C	O	0	0
			2	1	1		
8	H	1	Total	C	O	0	0
			2	1	1		
8	I	1	Total	C	O	0	0
			2	1	1		
8	J	1	Total	C	O	0	0
			2	1	1		
8	K	1	Total	C	O	0	0
			2	1	1		

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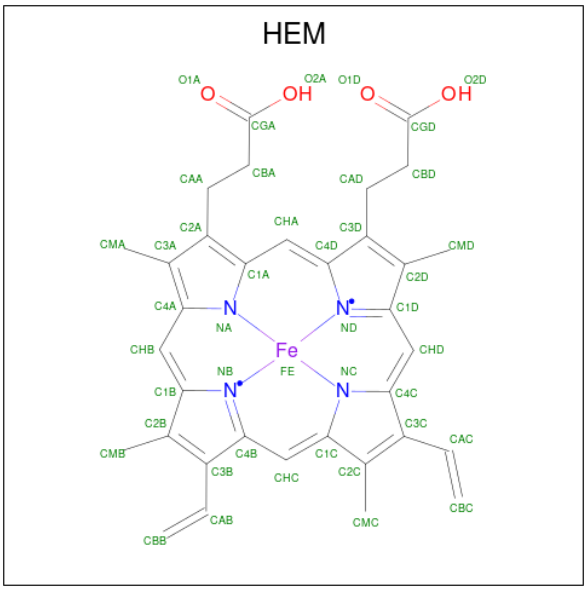
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	L	1	Total C O 2 1 1	0	0

- Molecule 9 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C Fe N O 43 34 1 4 4	0	0
9	B	1	Total C Fe N O 43 34 1 4 4	0	0
9	C	1	Total C Fe N O 43 34 1 4 4	0	0
9	D	1	Total C Fe N O 43 34 1 4 4	0	0
9	E	1	Total C Fe N O 43 34 1 4 4	0	0
9	F	1	Total C Fe N O 43 34 1 4 4	0	0
9	G	1	Total C Fe N O 43 34 1 4 4	0	0
9	H	1	Total C Fe N O 43 34 1 4 4	0	0
9	I	1	Total C Fe N O 43 34 1 4 4	0	0
9	J	1	Total C Fe N O 43 34 1 4 4	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	K	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
9	L	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 10 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	M	2	Total	Ca	0	0
			2	2		
10	N	1	Total	Ca	0	0
			1	1		
10	O	1	Total	Ca	0	0
			1	1		

- Molecule 11 is ZINC ION (three-letter code: ZN) (formula: Zn).

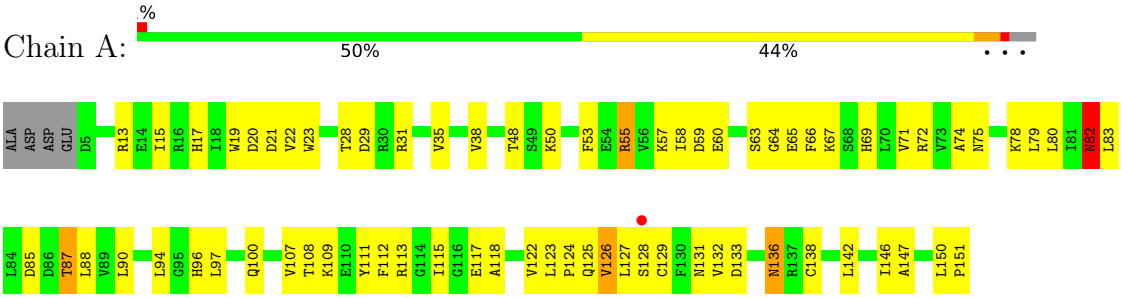
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	M	1	Total	Zn	0	0
			1	1		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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.

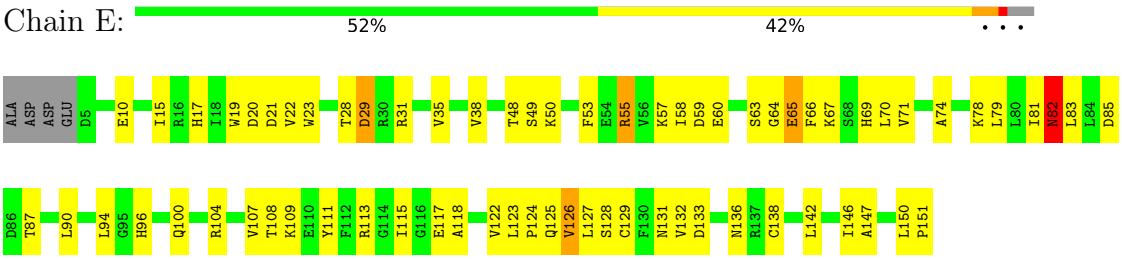
• Molecule 1: Extracellular globin 4

Chain A:



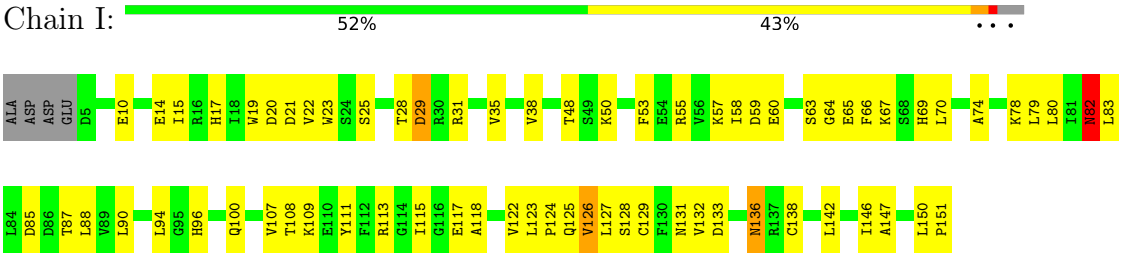
• Molecule 1: Extracellular globin 4

Chain E:



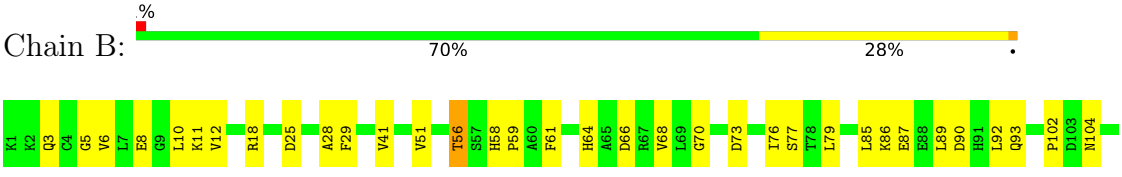
• Molecule 1: Extracellular globin 4

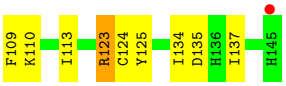
Chain I:



• Molecule 2: Extracellular globin 2

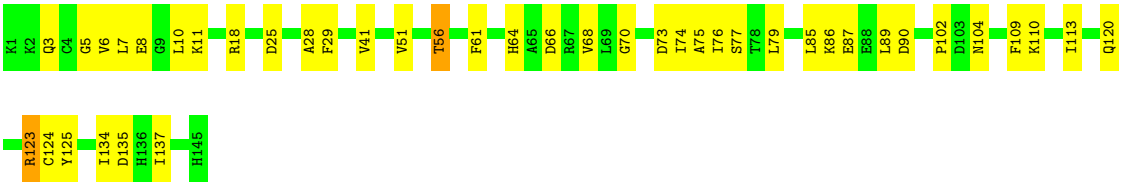
Chain B:





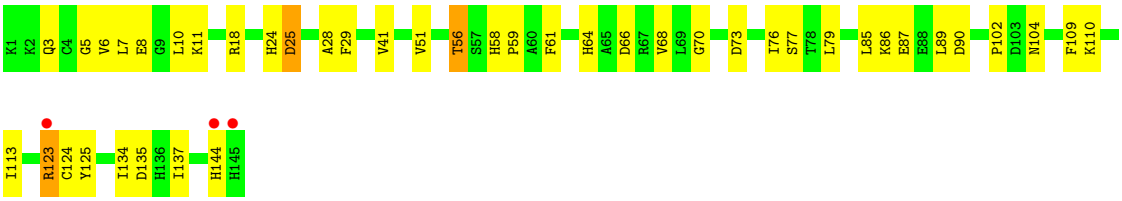
• Molecule 2: Extracellular globin 2

Chain F:



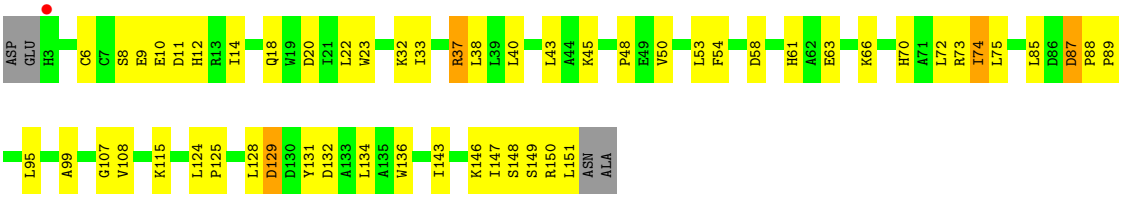
• Molecule 2: Extracellular globin 2

Chain J:



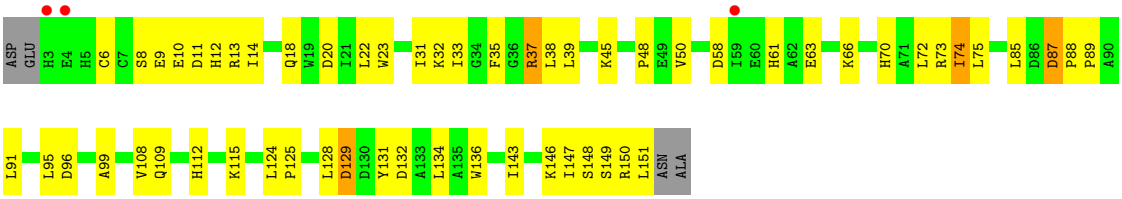
• Molecule 3: Extracellular globin-3

Chain C:



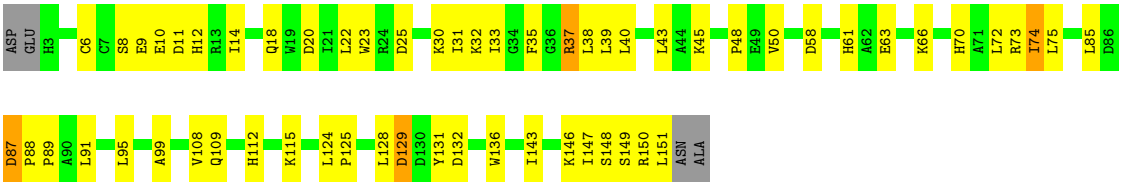
• Molecule 3: Extracellular globin-3

Chain G:



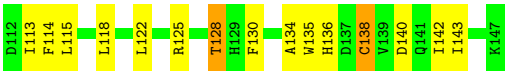
• Molecule 3: Extracellular globin-3

Chain K:



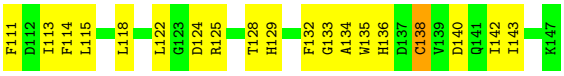
• Molecule 4: Hemoglobin chain d1

Chain D:



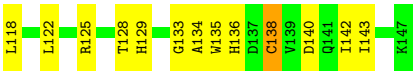
• Molecule 4: Hemoglobin chain d1

Chain H:



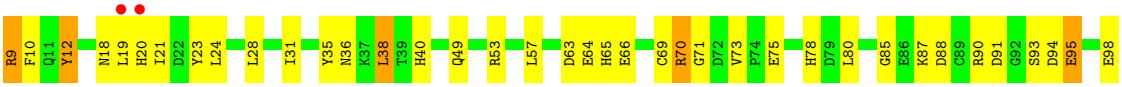
• Molecule 4: Hemoglobin chain d1

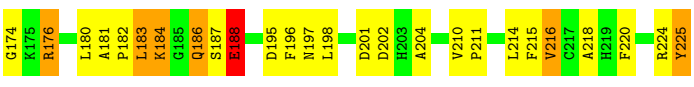
Chain L:



• Molecule 5: Hemoglobin linker chain L1

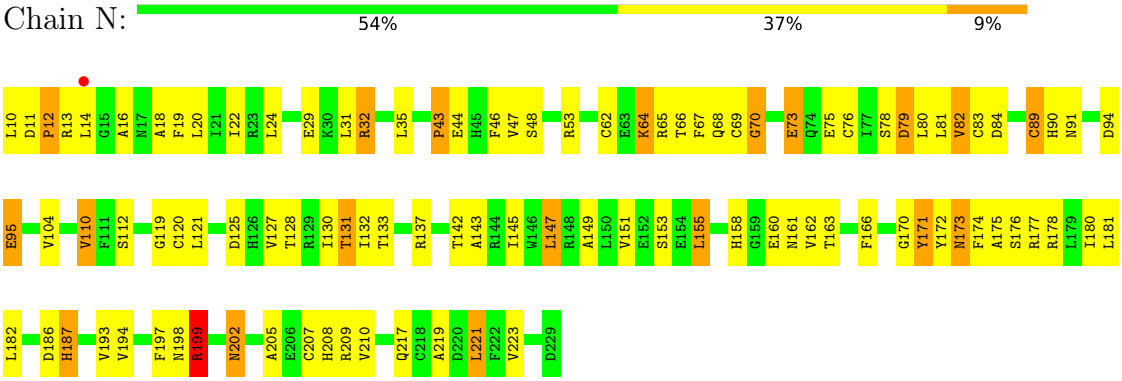
Chain M:





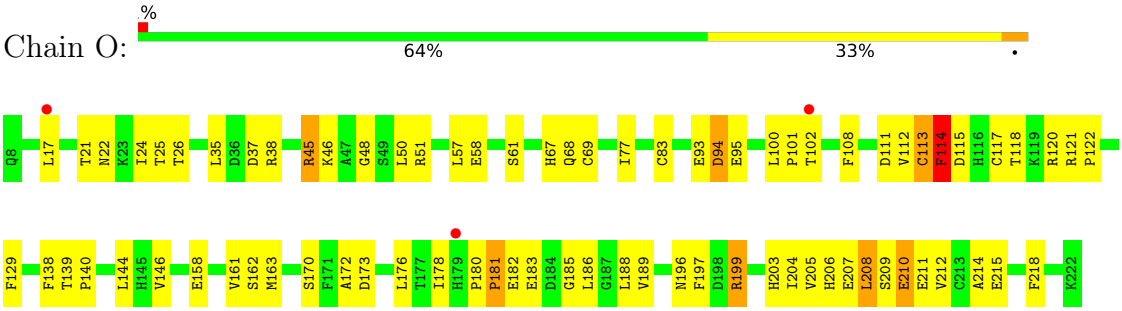
• Molecule 6: Extracellular hemoglobin linker L2 subunit

Chain N:



• Molecule 7: Extracellular hemoglobin linker L3 subunit

Chain O:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	176.08Å 257.96Å 436.53Å 89.69° 97.15° 90.98°	Depositor
Resolution (Å)	100.00 – 3.50 58.80 – 3.34	Depositor EDS
% Data completeness (in resolution range)	(Not available) (100.00-3.50) 76.0 (58.80-3.34)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.87 (at 3.33Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.288 , 0.297 0.310 , 0.315	Depositor DCC
R_{free} test set	45836 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å^2)	79.4	Xtriage
Anisotropy	0.276	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.23 , 37.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.015 for -h,k,-l	Xtriage
F_o,F_c correlation	0.82	EDS
Total number of atoms	19648	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.16% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.44	0/1237	0.60	0/1670
1	E	0.41	0/1237	0.59	0/1670
1	I	0.41	0/1237	0.59	0/1670
2	B	0.43	0/1176	0.54	0/1587
2	F	0.43	0/1176	0.55	0/1587
2	J	0.40	0/1176	0.54	0/1587
3	C	0.41	0/1209	0.56	0/1633
3	G	0.39	0/1209	0.56	0/1633
3	K	0.39	0/1209	0.55	0/1633
4	D	0.41	0/1159	0.53	0/1568
4	H	0.39	0/1159	0.52	0/1568
4	L	0.37	0/1159	0.52	0/1568
5	M	0.48	0/1745	0.70	0/2371
6	N	0.44	0/1752	0.66	0/2369
7	O	0.43	0/1699	0.62	0/2298
All	All	0.42	0/19539	0.59	0/26412

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	1209	0	1194	68	0
1	E	1209	0	1194	75	0
1	I	1209	0	1194	74	0
2	B	1148	0	1103	28	0
2	F	1148	0	1103	31	0
2	J	1148	0	1103	28	0
3	C	1185	0	1191	50	0
3	G	1185	0	1191	52	0
3	K	1185	0	1191	51	0
4	D	1129	0	1102	63	0
4	H	1129	0	1102	66	0
4	L	1129	0	1102	57	0
5	M	1705	0	1547	87	0
6	N	1722	0	1632	100	0
7	O	1663	0	1479	81	0
8	A	2	0	0	0	0
8	B	2	0	0	0	0
8	C	2	0	0	0	0
8	D	2	0	0	0	0
8	E	2	0	0	0	0
8	F	2	0	0	0	0
8	G	2	0	0	0	0
8	H	2	0	0	0	0
8	I	2	0	0	0	0
8	J	2	0	0	0	0
8	K	2	0	0	0	0
8	L	2	0	0	0	0
9	A	43	0	30	0	0
9	B	43	0	30	0	0
9	C	43	0	30	1	0
9	D	43	0	30	3	0
9	E	43	0	30	0	0
9	F	43	0	30	0	0
9	G	43	0	30	1	0
9	H	43	0	30	3	0
9	I	43	0	30	0	0
9	J	43	0	30	0	0
9	K	43	0	30	1	0
9	L	43	0	30	3	0
10	M	2	0	0	0	0
10	N	1	0	0	0	0
10	O	1	0	0	0	0
11	M	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	19648	0	18788	828	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 22.

All (828) 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:G:129:ASP:HB2	4:H:129:HIS:HB3	1.30	1.12
7:O:208:LEU:HD23	7:O:208:LEU:H	1.19	1.03
1:E:78:LYS:NZ	4:H:31:ARG:HH22	1.60	0.98
4:D:128:THR:HG21	4:L:29:HIS:CE1	2.00	0.96
6:N:66:THR:HG21	6:N:76:CYS:HB3	1.49	0.94
1:A:35:VAL:HG21	1:A:74:ALA:HB2	1.50	0.93
6:N:89:CYS:HB2	6:N:94:ASP:OD2	1.68	0.92
1:I:35:VAL:HG21	1:I:74:ALA:HB2	1.52	0.91
6:N:110:VAL:HG13	6:N:131:THR:HB	1.50	0.91
1:E:35:VAL:HG21	1:E:74:ALA:HB2	1.54	0.89
5:M:69:CYS:HB3	5:M:93:SER:OG	1.73	0.89
4:D:128:THR:HG21	4:L:29:HIS:HE1	1.35	0.88
7:O:209:SER:HB3	7:O:211:GLU:HG2	1.55	0.87
7:O:204:ILE:HB	7:O:214:ALA:HB3	1.54	0.87
1:E:78:LYS:HZ1	4:H:31:ARG:HH22	1.17	0.87
1:I:14:GLU:OE2	7:O:208:LEU:HD11	1.76	0.84
6:N:82:VAL:HG21	6:N:175:ALA:H	1.43	0.83
3:K:74:ILE:HG23	3:K:75:LEU:H	1.44	0.83
1:I:14:GLU:CD	7:O:208:LEU:HD11	1.99	0.83
6:N:82:VAL:HG13	6:N:83:CYS:H	1.43	0.83
2:B:110:LYS:HG3	2:B:134:ILE:HG21	1.62	0.81
1:E:126:VAL:HG13	2:F:7:LEU:HD22	1.61	0.81
3:G:74:ILE:HG23	3:G:75:LEU:H	1.46	0.80
7:O:208:LEU:H	7:O:208:LEU:CD2	1.93	0.80
3:C:74:ILE:HG23	3:C:75:LEU:H	1.46	0.80
2:J:110:LYS:HG3	2:J:134:ILE:HG21	1.64	0.79
2:F:51:VAL:HG21	2:F:64:HIS:HB2	1.65	0.79
5:M:70:ARG:N	5:M:70:ARG:HD2	1.97	0.79
2:F:110:LYS:HG3	2:F:134:ILE:HG21	1.64	0.78
2:B:51:VAL:HG21	2:B:64:HIS:HB2	1.65	0.77
2:J:51:VAL:HG21	2:J:64:HIS:HB2	1.67	0.77
7:O:208:LEU:HD23	7:O:208:LEU:N	1.98	0.77
4:L:83:MET:HE2	4:L:89:MET:HB3	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:38:LEU:HD22	7:O:38:ARG:HH12	1.50	0.76
5:M:115:ALA:HA	5:M:220:PHE:HB3	1.68	0.76
4:D:128:THR:CG2	4:L:29:HIS:HE1	1.98	0.76
4:H:84:LEU:HD11	4:H:142:ILE:HD11	1.67	0.75
1:E:83:LEU:HD23	1:E:90:LEU:HA	1.69	0.75
5:M:88:ASP:HB2	5:M:94:ASP:OD1	1.86	0.75
4:L:84:LEU:HD11	4:L:142:ILE:HD11	1.69	0.74
7:O:180:PRO:HD3	7:O:207:GLU:HG3	1.70	0.73
1:A:83:LEU:HD23	1:A:90:LEU:HA	1.69	0.73
1:I:83:LEU:HD23	1:I:90:LEU:HA	1.69	0.73
4:D:84:LEU:HD11	4:D:142:ILE:HD11	1.69	0.72
7:O:188:LEU:HD12	7:O:189:VAL:H	1.54	0.72
7:O:138:PHE:C	7:O:140:PRO:HD2	2.10	0.72
6:N:82:VAL:HG21	6:N:175:ALA:N	2.05	0.72
5:M:148:ARG:HG3	5:M:148:ARG:HH11	1.55	0.71
4:D:136:HIS:O	4:D:140:ASP:HB2	1.91	0.71
1:A:126:VAL:HG23	1:A:127:LEU:HD23	1.73	0.71
1:A:107:VAL:O	1:A:150:LEU:HD22	1.91	0.71
1:E:126:VAL:HG23	1:E:127:LEU:HD23	1.73	0.71
7:O:139:THR:N	7:O:140:PRO:HD2	2.06	0.70
5:M:135:ALA:HB2	5:M:147:LEU:HB3	1.72	0.70
5:M:20:HIS:O	5:M:24:LEU:HD13	1.91	0.70
1:I:126:VAL:HG13	2:J:7:LEU:HD22	1.74	0.69
3:K:129:ASP:HB2	4:L:129:HIS:HB3	1.74	0.69
4:H:136:HIS:O	4:H:140:ASP:HB2	1.93	0.69
1:I:126:VAL:HG23	1:I:127:LEU:HD23	1.74	0.69
1:A:125:GLN:O	2:B:11:LYS:HE3	1.92	0.69
1:I:78:LYS:NZ	4:L:31:ARG:HH22	1.91	0.69
5:M:135:ALA:CB	5:M:147:LEU:HB3	2.23	0.69
6:N:162:VAL:HG12	6:N:163:THR:N	2.07	0.69
1:E:126:VAL:CG1	2:F:7:LEU:HD22	2.23	0.69
1:I:107:VAL:O	1:I:150:LEU:HD22	1.93	0.69
7:O:45:ARG:NH1	7:O:45:ARG:HB3	2.08	0.68
6:N:10:LEU:HD23	6:N:12:PRO:HG2	1.76	0.68
1:A:58:ILE:HG22	1:A:66:PHE:CE1	2.29	0.68
2:F:18:ARG:HH22	2:F:124:CYS:HB2	1.57	0.68
7:O:209:SER:CB	7:O:211:GLU:HG2	2.22	0.68
1:I:58:ILE:HG22	1:I:66:PHE:CE1	2.29	0.68
4:L:83:MET:CE	4:L:89:MET:HB3	2.25	0.67
4:H:83:MET:HE2	4:H:89:MET:HB3	1.77	0.67
1:E:107:VAL:O	1:E:150:LEU:HD22	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:20:GLN:HE21	4:H:135:TRP:HE1	1.41	0.67
2:F:120:GLN:NE2	6:N:80:LEU:HD21	2.09	0.67
4:L:136:HIS:O	4:L:140:ASP:HB2	1.93	0.67
4:D:115:LEU:HB2	4:D:143:ILE:CD1	2.25	0.67
6:N:162:VAL:HG12	6:N:163:THR:H	1.59	0.67
2:B:87:GLU:HG2	3:C:66:LYS:HA	1.77	0.66
2:B:18:ARG:HH22	2:B:124:CYS:HB2	1.60	0.66
3:G:58:ASP:OD2	3:G:61:HIS:HB2	1.96	0.66
2:J:18:ARG:HH22	2:J:124:CYS:HB2	1.59	0.66
4:L:70:SER:O	4:L:74:LEU:HD23	1.95	0.66
2:F:120:GLN:HE21	6:N:80:LEU:HD21	1.60	0.66
4:L:10:LEU:HD11	4:L:13:GLU:HG3	1.78	0.66
3:C:22:LEU:HG	3:C:128:LEU:HD21	1.78	0.66
4:D:20:GLN:HE21	4:D:135:TRP:HE1	1.43	0.66
4:L:20:GLN:HE21	4:L:135:TRP:HE1	1.44	0.66
4:H:83:MET:CE	4:H:89:MET:HB3	2.26	0.65
6:N:132:ILE:HD12	6:N:147:LEU:HD12	1.78	0.65
7:O:102:THR:HB	7:O:129:PHE:CE2	2.31	0.65
1:E:58:ILE:HG22	1:E:66:PHE:CE1	2.31	0.65
2:F:87:GLU:HG2	3:G:66:LYS:HA	1.77	0.65
3:K:58:ASP:OD2	3:K:61:HIS:HB2	1.96	0.65
4:D:70:SER:O	4:D:74:LEU:HD23	1.96	0.65
4:H:10:LEU:HD11	4:H:13:GLU:HG3	1.77	0.65
3:C:10:GLU:HB2	1:I:10:GLU:CD	2.17	0.65
6:N:10:LEU:HD22	6:N:13:ARG:HB3	1.77	0.65
7:O:22:ASN:O	7:O:26:THR:HG23	1.96	0.64
3:G:22:LEU:HG	3:G:128:LEU:HD21	1.80	0.64
4:L:115:LEU:HB2	4:L:143:ILE:CD1	2.27	0.64
6:N:198:ASN:O	6:N:199:ARG:HD2	1.98	0.64
5:M:155:LEU:HD23	5:M:162:VAL:HA	1.78	0.64
4:D:83:MET:CE	4:D:89:MET:HB3	2.26	0.64
5:M:9:ARG:HH11	5:M:9:ARG:HB3	1.62	0.64
4:D:10:LEU:HD11	4:D:13:GLU:HG3	1.78	0.64
3:C:18:GLN:NE2	3:C:136:TRP:HE1	1.96	0.64
3:C:58:ASP:OD2	3:C:61:HIS:HB2	1.96	0.64
3:K:74:ILE:HG23	3:K:75:LEU:N	2.13	0.64
1:A:126:VAL:HG23	1:A:127:LEU:CD2	2.28	0.64
6:N:10:LEU:HD13	6:N:13:ARG:HH21	1.62	0.64
1:E:126:VAL:HG23	1:E:127:LEU:CD2	2.29	0.63
3:G:22:LEU:HB3	3:G:23:TRP:CE3	2.33	0.63
4:H:115:LEU:HB2	4:H:143:ILE:CD1	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:82:VAL:HB	6:N:175:ALA:HB2	1.79	0.63
2:F:74:ILE:HG23	3:G:72:LEU:HD13	1.80	0.63
3:K:22:LEU:HG	3:K:128:LEU:HD21	1.80	0.63
2:B:6:VAL:O	2:B:10:LEU:HD13	1.99	0.63
1:I:126:VAL:HG23	1:I:127:LEU:CD2	2.29	0.63
3:K:18:GLN:NE2	3:K:136:TRP:HE1	1.97	0.62
5:M:20:HIS:O	5:M:23:TYR:HB3	1.99	0.62
1:A:78:LYS:NZ	4:D:31:ARG:HH22	1.97	0.62
1:A:113:ARG:O	1:A:117:GLU:HG3	2.00	0.62
1:I:150:LEU:N	1:I:151:PRO:HD2	2.14	0.62
3:K:22:LEU:HB3	3:K:23:TRP:CE3	2.34	0.62
4:D:110:PHE:HA	4:D:113:ILE:HD12	1.81	0.62
1:E:150:LEU:N	1:E:151:PRO:HD2	2.14	0.62
3:G:22:LEU:HB3	3:G:23:TRP:CZ3	2.34	0.62
4:H:70:SER:O	4:H:74:LEU:HD23	1.99	0.62
3:K:22:LEU:HB3	3:K:23:TRP:CZ3	2.35	0.62
6:N:82:VAL:HG13	6:N:83:CYS:N	2.12	0.62
1:E:10:GLU:HG3	3:K:10:GLU:HG3	1.80	0.62
1:E:82:ASN:ND2	4:H:28:ALA:H	1.97	0.62
3:G:74:ILE:HG23	3:G:75:LEU:N	2.14	0.62
6:N:24:LEU:HD21	7:O:25:THR:OG1	2.00	0.62
1:A:90:LEU:O	1:A:94:LEU:HB2	2.00	0.62
3:C:22:LEU:HB3	3:C:23:TRP:CZ3	2.35	0.62
6:N:66:THR:CG2	6:N:76:CYS:HB3	2.27	0.62
7:O:196:ASN:O	7:O:197:PHE:HB2	2.00	0.62
4:D:83:MET:HE2	4:D:89:MET:HB3	1.81	0.61
3:C:10:GLU:HG3	1:I:10:GLU:HG3	1.82	0.61
3:C:22:LEU:HB3	3:C:23:TRP:CE3	2.35	0.61
3:G:18:GLN:NE2	3:G:136:TRP:HE1	1.98	0.61
1:A:13:ARG:HH22	3:G:10:GLU:CD	2.03	0.61
4:H:20:GLN:NE2	4:H:135:TRP:HE1	1.98	0.61
1:I:113:ARG:O	1:I:117:GLU:HG3	2.01	0.61
1:A:150:LEU:N	1:A:151:PRO:HD2	2.15	0.61
1:E:90:LEU:O	1:E:94:LEU:HB2	2.01	0.61
1:I:90:LEU:O	1:I:94:LEU:HB2	2.00	0.61
5:M:78:HIS:ND1	5:M:80:LEU:HB2	2.15	0.61
1:E:113:ARG:O	1:E:117:GLU:HG3	2.01	0.61
4:L:110:PHE:HA	4:L:113:ILE:HD12	1.83	0.61
5:M:64:GLU:O	5:M:65:HIS:HB2	2.01	0.61
1:E:10:GLU:CD	3:K:10:GLU:HB2	2.21	0.60
6:N:181:LEU:HB2	6:N:193:VAL:CG1	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:18:GLN:HE21	3:C:136:TRP:HE1	1.50	0.60
2:J:6:VAL:O	2:J:10:LEU:HD13	2.02	0.60
7:O:77:ILE:O	7:O:77:ILE:HD12	2.01	0.60
5:M:28:LEU:HD23	5:M:28:LEU:C	2.22	0.60
3:C:74:ILE:HG23	3:C:75:LEU:N	2.15	0.60
5:M:106:HIS:HD2	5:M:107:VAL:N	1.99	0.60
3:C:10:GLU:HB2	1:I:10:GLU:OE1	2.02	0.59
4:D:20:GLN:NE2	4:D:135:TRP:HE1	2.00	0.59
3:K:18:GLN:HE21	3:K:136:TRP:HE1	1.50	0.59
3:K:108:VAL:O	3:K:151:LEU:HD22	2.02	0.59
3:C:48:PRO:C	3:C:50:VAL:H	2.05	0.59
1:E:66:PHE:O	1:E:69:HIS:HB3	2.02	0.59
7:O:199:ARG:HA	7:O:218:PHE:O	2.03	0.59
4:D:109:GLU:O	4:D:113:ILE:HG13	2.03	0.59
5:M:73:VAL:HG23	5:M:73:VAL:O	2.03	0.59
5:M:78:HIS:CE1	5:M:80:LEU:HB2	2.37	0.59
1:I:66:PHE:O	1:I:69:HIS:HB3	2.03	0.59
7:O:188:LEU:HD12	7:O:189:VAL:N	2.16	0.59
4:H:49:ILE:O	4:H:52:PRO:HD2	2.01	0.59
5:M:124:ASN:O	5:M:125:PRO:C	2.41	0.59
6:N:78:SER:OG	6:N:80:LEU:HD23	2.03	0.59
3:G:18:GLN:HE21	3:G:136:TRP:HE1	1.51	0.58
3:G:129:ASP:OD2	3:G:129:ASP:N	2.36	0.58
6:N:80:LEU:O	6:N:81:LEU:HD23	2.03	0.58
2:B:5:GLY:H	2:B:8:GLU:CG	2.16	0.58
1:E:28:THR:O	1:E:31:ARG:HG2	2.04	0.58
4:L:10:LEU:CD1	4:L:13:GLU:H	2.16	0.58
6:N:210:VAL:HG12	6:N:217:GLN:HA	1.85	0.58
3:C:33:ILE:HG13	3:C:72:LEU:HD21	1.86	0.58
1:E:78:LYS:HZ1	4:H:31:ARG:NH2	1.93	0.58
4:H:109:GLU:O	4:H:113:ILE:HG13	2.04	0.58
6:N:43:PRO:HG2	6:N:44:GLU:H	1.68	0.58
6:N:10:LEU:O	6:N:14:LEU:HD23	2.04	0.58
4:H:110:PHE:HA	4:H:113:ILE:HD12	1.86	0.58
3:C:108:VAL:O	3:C:151:LEU:HD22	2.04	0.57
2:F:3:GLN:O	2:F:8:GLU:HG3	2.03	0.57
2:J:3:GLN:O	2:J:8:GLU:HG3	2.04	0.57
1:A:23:TRP:CZ3	1:A:74:ALA:HB1	2.39	0.57
3:G:108:VAL:O	3:G:151:LEU:HD22	2.03	0.57
3:K:48:PRO:C	3:K:50:VAL:H	2.06	0.57
4:D:49:ILE:O	4:D:52:PRO:HD2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:41:VAL:O	2:J:41:VAL:HG23	2.05	0.57
5:M:202:ASP:OD1	5:M:224:ARG:HD2	2.04	0.57
7:O:205:VAL:HG12	7:O:212:VAL:HA	1.86	0.57
3:K:38:LEU:HD23	3:K:38:LEU:C	2.25	0.57
4:L:20:GLN:NE2	4:L:135:TRP:HE1	2.01	0.57
4:L:109:GLU:O	4:L:113:ILE:HG13	2.04	0.57
1:A:28:THR:O	1:A:31:ARG:HG2	2.04	0.57
4:D:128:THR:CG2	4:L:29:HIS:CE1	2.76	0.57
4:H:10:LEU:CD1	4:H:13:GLU:H	2.17	0.57
2:J:5:GLY:H	2:J:8:GLU:CG	2.17	0.57
5:M:31:ILE:HG23	6:N:35:LEU:HD22	1.86	0.57
2:B:110:LYS:HG3	2:B:134:ILE:CG2	2.34	0.57
2:F:5:GLY:H	2:F:8:GLU:CG	2.17	0.57
2:F:89:LEU:HD21	2:F:137:ILE:HG23	1.86	0.57
4:D:125:ARG:HG2	4:D:125:ARG:HH11	1.69	0.57
5:M:172:ASN:HD22	5:M:173:PHE:N	2.03	0.57
6:N:82:VAL:CG2	6:N:174:PHE:HB2	2.35	0.57
6:N:181:LEU:HB2	6:N:193:VAL:HG13	1.87	0.57
7:O:67:HIS:HB3	7:O:77:ILE:CD1	2.34	0.57
2:B:3:GLN:O	2:B:8:GLU:HG3	2.04	0.57
3:C:48:PRO:C	3:C:50:VAL:N	2.58	0.57
4:D:40:ARG:NH2	4:H:124:ASP:OD2	2.37	0.56
6:N:10:LEU:HD13	6:N:13:ARG:NH2	2.20	0.56
7:O:181:PRO:HG2	7:O:182:GLU:H	1.70	0.56
3:C:38:LEU:C	3:C:38:LEU:HD23	2.26	0.56
1:I:125:GLN:O	2:J:11:LYS:HE3	2.04	0.56
6:N:47:VAL:HG13	6:N:48:SER:N	2.20	0.56
1:A:87:THR:HG21	3:G:134:LEU:H	1.71	0.56
5:M:130:VAL:HG13	5:M:130:VAL:O	2.04	0.56
6:N:147:LEU:N	6:N:147:LEU:HD23	2.20	0.56
2:F:6:VAL:O	2:F:10:LEU:HD13	2.04	0.56
4:D:10:LEU:CD1	4:D:13:GLU:H	2.17	0.56
1:A:66:PHE:O	1:A:69:HIS:HB3	2.05	0.56
1:E:147:ALA:HB2	1:E:150:LEU:HD12	1.88	0.56
1:I:82:ASN:ND2	4:L:28:ALA:H	2.04	0.56
3:C:129:ASP:OD2	3:C:129:ASP:N	2.39	0.56
1:E:67:LYS:HB3	4:H:89:MET:HE3	1.88	0.56
2:J:87:GLU:HG2	3:K:66:LYS:HA	1.88	0.56
7:O:114:PHE:O	7:O:114:PHE:CD1	2.58	0.56
2:B:41:VAL:HG23	2:B:41:VAL:O	2.06	0.56
2:F:123:ARG:H	2:F:123:ARG:HD3	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:48:PRO:C	3:G:50:VAL:H	2.08	0.56
4:D:115:LEU:HB2	4:D:143:ILE:HD11	1.87	0.55
6:N:31:LEU:HD23	6:N:31:LEU:O	2.05	0.55
3:G:38:LEU:C	3:G:38:LEU:HD23	2.26	0.55
4:H:125:ARG:HH11	4:H:125:ARG:HG2	1.71	0.55
7:O:77:ILE:HD12	7:O:77:ILE:C	2.25	0.55
4:L:49:ILE:O	4:L:52:PRO:HD2	2.06	0.55
5:M:57:LEU:HB2	7:O:57:LEU:HD13	1.87	0.55
5:M:131:THR:O	5:M:149:ALA:HB1	2.07	0.55
5:M:168:ARG:HG2	5:M:169:GLY:N	2.20	0.55
4:L:125:ARG:HG2	4:L:125:ARG:HH11	1.71	0.55
6:N:130:ILE:HD11	6:N:193:VAL:HG21	1.88	0.55
3:G:18:GLN:HE22	3:G:132:ASP:H	1.53	0.55
3:K:33:ILE:HG13	3:K:72:LEU:HD21	1.89	0.55
5:M:9:ARG:HB3	5:M:9:ARG:NH1	2.22	0.55
7:O:139:THR:N	7:O:140:PRO:CD	2.69	0.55
1:I:23:TRP:CZ3	1:I:74:ALA:HB1	2.42	0.55
2:J:89:LEU:HD21	2:J:137:ILE:HG23	1.88	0.55
7:O:112:VAL:HG22	7:O:113:CYS:N	2.22	0.55
2:J:64:HIS:O	2:J:68:VAL:HG23	2.07	0.55
1:A:38:VAL:HA	1:A:122:VAL:HG21	1.89	0.54
6:N:35:LEU:HA	7:O:35:LEU:HD11	1.89	0.54
6:N:79:ASP:O	6:N:82:VAL:HG12	2.08	0.54
1:I:28:THR:O	1:I:31:ARG:HG2	2.07	0.54
7:O:21:THR:O	7:O:24:ILE:HG22	2.07	0.54
1:E:38:VAL:HA	1:E:122:VAL:HG21	1.88	0.54
1:E:78:LYS:HE2	4:H:31:ARG:NH1	2.23	0.54
3:G:48:PRO:C	3:G:50:VAL:N	2.61	0.54
1:I:78:LYS:HZ1	4:L:31:ARG:HH22	1.54	0.54
2:B:89:LEU:HD21	2:B:137:ILE:HG23	1.90	0.54
5:M:172:ASN:HD22	5:M:172:ASN:C	2.10	0.54
7:O:67:HIS:HB3	7:O:77:ILE:HD11	1.90	0.54
1:A:83:LEU:HD11	4:D:71:GLN:HG2	1.90	0.54
4:L:115:LEU:HB2	4:L:143:ILE:HD11	1.89	0.54
1:E:23:TRP:CZ3	1:E:74:ALA:HB1	2.43	0.54
2:F:64:HIS:O	2:F:68:VAL:HG23	2.07	0.54
3:G:108:VAL:HG22	9:G:160:HEM:HBC2	1.90	0.54
4:H:115:LEU:HB2	4:H:143:ILE:HD11	1.90	0.54
1:I:38:VAL:HA	1:I:122:VAL:HG21	1.89	0.54
2:J:56:THR:HA	2:J:61:PHE:CD2	2.43	0.54
5:M:224:ARG:HG2	5:M:225:TYR:N	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:123:ARG:HD3	2:B:123:ARG:H	1.73	0.53
1:I:150:LEU:O	1:I:151:PRO:O	2.26	0.53
5:M:143:ASN:O	5:M:144:ARG:HD3	2.07	0.53
6:N:178:ARG:NH2	6:N:180:ILE:HD11	2.23	0.53
7:O:45:ARG:HB3	7:O:45:ARG:HH11	1.71	0.53
1:E:78:LYS:HE2	4:H:31:ARG:HH12	1.73	0.53
3:G:88:PRO:HG2	3:G:89:PRO:HD3	1.90	0.53
2:B:56:THR:HA	2:B:61:PHE:CD2	2.44	0.53
3:K:48:PRO:C	3:K:50:VAL:N	2.60	0.53
6:N:11:ASP:N	6:N:12:PRO:HD2	2.24	0.53
7:O:45:ARG:HH11	7:O:45:ARG:CB	2.22	0.53
7:O:146:VAL:HG21	7:O:178:ILE:HD13	1.89	0.53
3:C:18:GLN:HE22	3:C:132:ASP:H	1.56	0.53
1:E:53:PHE:HB2	1:E:58:ILE:HG21	1.91	0.53
4:L:51:ALA:HB3	4:L:52:PRO:CD	2.39	0.53
4:L:57:ARG:HG2	4:L:57:ARG:HH11	1.73	0.53
5:M:110:SER:OG	5:M:131:THR:HB	2.08	0.53
5:M:143:ASN:ND2	5:M:144:ARG:HE	2.06	0.53
6:N:89:CYS:N	6:N:94:ASP:OD2	2.40	0.53
7:O:158:GLU:O	7:O:158:GLU:HG3	2.09	0.53
3:G:33:ILE:HG13	3:G:72:LEU:HD21	1.91	0.53
3:K:18:GLN:HE22	3:K:132:ASP:H	1.57	0.53
4:H:51:ALA:HB3	4:H:52:PRO:CD	2.39	0.53
3:C:18:GLN:NE2	3:C:131:TYR:HA	2.24	0.53
7:O:114:PHE:HD1	7:O:215:GLU:H	1.56	0.53
6:N:82:VAL:HG21	6:N:174:PHE:HB2	1.90	0.53
2:J:109:PHE:CE1	2:J:113:ILE:HD11	2.44	0.52
1:A:150:LEU:O	1:A:151:PRO:O	2.27	0.52
3:C:22:LEU:HD13	3:C:23:TRP:CH2	2.44	0.52
4:D:51:ALA:HB3	4:D:52:PRO:CD	2.39	0.52
3:G:18:GLN:NE2	3:G:131:TYR:HA	2.24	0.52
5:M:195:ASP:HB3	5:M:197:ASN:ND2	2.25	0.52
3:C:108:VAL:HG22	9:C:160:HEM:HBC2	1.91	0.52
5:M:104:ILE:HG23	5:M:111:TYR:OH	2.09	0.52
6:N:10:LEU:C	6:N:12:PRO:HD2	2.30	0.52
3:C:8:SER:N	3:C:11:ASP:HB2	2.25	0.52
3:G:22:LEU:HD13	3:G:23:TRP:CH2	2.44	0.52
7:O:185:GLY:O	7:O:206:HIS:HA	2.09	0.52
1:E:71:VAL:HG11	4:H:79:ILE:HG23	1.90	0.52
2:J:110:LYS:HG3	2:J:134:ILE:CG2	2.36	0.52
7:O:114:PHE:HD1	7:O:215:GLU:N	2.06	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:161:VAL:HG12	7:O:163:MET:HG3	1.90	0.52
1:A:147:ALA:HB2	1:A:150:LEU:HD12	1.92	0.52
2:F:41:VAL:HG23	2:F:41:VAL:O	2.10	0.52
1:I:25:SER:HA	3:K:25:ASP:HB2	1.90	0.52
1:I:126:VAL:CG1	2:J:7:LEU:HD22	2.39	0.52
3:G:124:LEU:N	3:G:125:PRO:HD2	2.24	0.52
5:M:148:ARG:HG3	5:M:148:ARG:NH1	2.23	0.51
7:O:209:SER:O	7:O:210:GLU:CB	2.58	0.51
1:E:123:LEU:N	1:E:124:PRO:HD2	2.25	0.51
4:D:57:ARG:HH11	4:D:57:ARG:HG2	1.75	0.51
2:F:56:THR:HA	2:F:61:PHE:CD2	2.45	0.51
3:K:124:LEU:N	3:K:125:PRO:HD2	2.25	0.51
2:J:123:ARG:H	2:J:123:ARG:HD3	1.74	0.51
1:A:71:VAL:HG21	4:D:89:MET:HE1	1.93	0.51
2:B:8:GLU:CD	2:B:8:GLU:H	2.14	0.51
1:I:53:PHE:HB2	1:I:58:ILE:HG21	1.92	0.51
6:N:82:VAL:CG2	6:N:175:ALA:N	2.73	0.51
1:I:79:LEU:HD13	1:I:79:LEU:O	2.10	0.51
1:I:123:LEU:N	1:I:124:PRO:HD2	2.25	0.51
1:E:79:LEU:HD21	4:H:71:GLN:HG3	1.92	0.51
3:K:18:GLN:NE2	3:K:131:TYR:HA	2.26	0.51
7:O:180:PRO:HD3	7:O:207:GLU:CG	2.39	0.51
3:C:48:PRO:O	3:C:50:VAL:N	2.45	0.50
2:F:110:LYS:HG3	2:F:134:ILE:CG2	2.37	0.50
1:A:109:LYS:HD2	1:A:151:PRO:HD3	1.93	0.50
1:I:109:LYS:HD2	1:I:151:PRO:HD3	1.94	0.50
4:L:94:LEU:HD21	4:L:142:ILE:HG23	1.93	0.50
7:O:50:LEU:C	7:O:50:LEU:HD23	2.32	0.50
3:C:124:LEU:N	3:C:125:PRO:HD2	2.26	0.50
2:F:76:ILE:O	2:F:79:LEU:HG	2.11	0.50
3:K:8:SER:N	3:K:11:ASP:HB2	2.25	0.50
5:M:106:HIS:CD2	5:M:107:VAL:N	2.79	0.50
6:N:16:ALA:C	6:N:18:ALA:H	2.14	0.50
1:A:123:LEU:N	1:A:124:PRO:HD2	2.26	0.50
3:K:88:PRO:HG2	3:K:89:PRO:HD3	1.94	0.50
2:B:76:ILE:O	2:B:79:LEU:HG	2.10	0.50
3:C:99:ALA:HA	3:C:147:ILE:O	2.12	0.50
1:E:60:GLU:O	1:E:63:SER:HB3	2.12	0.50
3:K:11:ASP:O	3:K:14:ILE:HB	2.12	0.50
5:M:115:ALA:HB2	5:M:128:ALA:HB2	1.94	0.50
1:E:115:ILE:O	1:E:118:ALA:HB3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:93:GLU:C	7:O:95:GLU:H	2.15	0.50
1:I:14:GLU:OE2	7:O:208:LEU:HD21	2.12	0.50
5:M:115:ALA:O	5:M:125:PRO:HA	2.12	0.50
2:B:109:PHE:CE1	2:B:113:ILE:HD11	2.46	0.50
4:H:57:ARG:HG2	4:H:57:ARG:HH11	1.76	0.50
6:N:198:ASN:O	6:N:198:ASN:CG	2.50	0.50
1:I:67:LYS:HB3	4:L:89:MET:HE3	1.94	0.49
3:G:8:SER:N	3:G:11:ASP:HB2	2.27	0.49
4:L:17:VAL:HG13	4:L:135:TRP:CE2	2.47	0.49
7:O:100:LEU:HD23	7:O:101:PRO:N	2.27	0.49
7:O:101:PRO:HG2	7:O:102:THR:H	1.77	0.49
2:B:5:GLY:H	2:B:8:GLU:HG3	1.76	0.49
4:H:94:LEU:HD21	4:H:142:ILE:HG23	1.93	0.49
3:K:22:LEU:HD13	3:K:23:TRP:CH2	2.47	0.49
5:M:114:LEU:HD12	5:M:126:ASP:O	2.11	0.49
6:N:81:LEU:O	6:N:82:VAL:C	2.50	0.49
2:B:51:VAL:O	2:B:51:VAL:HG22	2.11	0.49
4:D:130:PHE:HD2	4:L:62:TYR:CE2	2.31	0.49
3:K:108:VAL:HG22	9:K:160:HEM:HBC2	1.93	0.49
1:E:150:LEU:O	1:E:151:PRO:O	2.30	0.49
2:F:109:PHE:CE1	2:F:113:ILE:HD11	2.48	0.49
7:O:121:ARG:N	7:O:122:PRO:CD	2.75	0.49
1:A:53:PHE:HB2	1:A:58:ILE:HG21	1.93	0.49
3:C:9:GLU:HA	3:C:12:HIS:CE1	2.48	0.49
2:F:51:VAL:HG22	2:F:51:VAL:O	2.13	0.49
5:M:210:VAL:HG12	5:M:215:PHE:O	2.12	0.49
7:O:115:ASP:OD1	7:O:121:ARG:HA	2.12	0.49
3:C:148:SER:C	3:C:150:ARG:H	2.16	0.49
4:L:14:SER:OG	4:L:15:LEU:N	2.45	0.49
4:D:94:LEU:HD21	4:D:142:ILE:HG23	1.94	0.49
1:E:10:GLU:OE1	3:K:10:GLU:HB2	2.12	0.49
1:E:109:LYS:HD2	1:E:151:PRO:HD3	1.95	0.49
3:G:11:ASP:O	3:G:14:ILE:HB	2.13	0.49
1:I:132:VAL:HG13	1:I:133:ASP:N	2.28	0.49
6:N:53:ARG:HD2	7:O:58:GLU:OE1	2.13	0.49
1:E:127:LEU:HD23	1:E:127:LEU:N	2.28	0.49
1:I:147:ALA:HB2	1:I:150:LEU:HD12	1.94	0.49
7:O:24:ILE:HG23	7:O:25:THR:N	2.28	0.49
4:D:60:ASN:HD21	4:H:133:GLY:H	1.61	0.48
7:O:93:GLU:O	7:O:95:GLU:N	2.46	0.48
1:I:127:LEU:HD23	1:I:127:LEU:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:THR:HG22	3:G:134:LEU:HG	1.96	0.48
1:A:115:ILE:O	1:A:118:ALA:HB3	2.13	0.48
2:F:8:GLU:CD	2:F:8:GLU:H	2.15	0.48
3:C:70:HIS:O	3:C:74:ILE:HG22	2.12	0.48
2:J:8:GLU:CD	2:J:8:GLU:H	2.16	0.48
3:K:37:ARG:HH22	3:K:63:GLU:HB3	1.78	0.48
3:K:48:PRO:O	3:K:50:VAL:N	2.46	0.48
4:L:111:PHE:HB3	4:L:143:ILE:HG23	1.95	0.48
3:C:37:ARG:HH22	3:C:63:GLU:HB3	1.79	0.48
1:E:82:ASN:HD22	4:H:31:ARG:HD2	1.79	0.48
3:G:32:LYS:HG2	3:G:75:LEU:HD12	1.95	0.48
4:H:14:SER:O	4:H:17:VAL:N	2.46	0.48
7:O:114:PHE:O	7:O:214:ALA:HA	2.12	0.48
1:E:147:ALA:CB	1:E:150:LEU:HD12	2.43	0.48
5:M:21:ILE:C	5:M:23:TYR:N	2.66	0.48
5:M:181:ALA:HB1	5:M:182:PRO:HD2	1.95	0.48
6:N:137:ARG:NH2	6:N:142:THR:HB	2.28	0.48
1:A:60:GLU:HB2	1:A:63:SER:HB3	1.96	0.48
3:C:11:ASP:O	3:C:14:ILE:HB	2.13	0.48
3:C:129:ASP:HA	4:D:16:LYS:HE3	1.95	0.48
1:I:142:LEU:O	1:I:146:ILE:HG13	2.14	0.48
3:K:9:GLU:HA	3:K:12:HIS:CE1	2.49	0.48
7:O:100:LEU:HD23	7:O:100:LEU:C	2.34	0.48
5:M:85:GLY:N	5:M:95:GLU:OE2	2.47	0.48
6:N:18:ALA:C	6:N:20:LEU:N	2.67	0.48
6:N:75:GLU:OE1	6:N:90:HIS:HD2	1.96	0.48
4:H:111:PHE:HB3	4:H:143:ILE:HG23	1.96	0.48
1:E:53:PHE:HB2	1:E:58:ILE:CG2	2.44	0.48
1:E:108:THR:HG23	1:E:111:TYR:CE2	2.49	0.48
1:I:15:ILE:C	1:I:17:HIS:N	2.67	0.48
1:I:115:ILE:O	1:I:118:ALA:HB3	2.13	0.48
1:E:19:TRP:HE1	1:E:78:LYS:HD3	1.79	0.47
3:G:70:HIS:O	3:G:74:ILE:HG22	2.14	0.47
5:M:28:LEU:O	5:M:31:ILE:HB	2.15	0.47
5:M:172:ASN:C	5:M:172:ASN:ND2	2.67	0.47
2:B:64:HIS:O	2:B:68:VAL:HG23	2.15	0.47
1:E:15:ILE:O	1:E:17:HIS:N	2.47	0.47
3:G:37:ARG:HH22	3:G:63:GLU:HB3	1.79	0.47
1:I:53:PHE:HB2	1:I:58:ILE:CG2	2.44	0.47
1:I:60:GLU:HB2	1:I:63:SER:HB3	1.96	0.47
2:J:51:VAL:HG22	2:J:51:VAL:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:117:TRP:HA	5:M:218:ALA:CB	2.44	0.47
6:N:120:CYS:O	6:N:121:LEU:HG	2.13	0.47
1:A:60:GLU:O	1:A:63:SER:HB3	2.14	0.47
1:E:118:ALA:O	1:E:122:VAL:HG23	2.14	0.47
3:G:148:SER:C	3:G:150:ARG:H	2.18	0.47
1:I:29:ASP:OD2	3:K:30:LYS:HE3	2.14	0.47
2:J:5:GLY:H	2:J:8:GLU:HG3	1.79	0.47
1:E:60:GLU:HB2	1:E:63:SER:HB3	1.95	0.47
5:M:183:LEU:O	5:M:184:LYS:HB3	2.13	0.47
5:M:196:PHE:CE2	5:M:204:ALA:HB2	2.49	0.47
1:A:127:LEU:HD23	1:A:127:LEU:N	2.29	0.47
3:K:12:HIS:HB2	3:K:85:LEU:HD13	1.97	0.47
1:A:96:HIS:O	1:A:100:GLN:HG3	2.14	0.47
1:E:15:ILE:C	1:E:17:HIS:N	2.67	0.47
7:O:120:ARG:N	7:O:120:ARG:HD2	2.29	0.47
7:O:181:PRO:HD2	7:O:186:LEU:O	2.14	0.47
1:A:23:TRP:CH2	1:A:74:ALA:HB1	2.50	0.47
1:A:75:ASN:CG	4:D:79:ILE:HG12	2.35	0.47
1:A:79:LEU:HD13	1:A:79:LEU:O	2.14	0.47
4:D:51:ALA:HB3	4:D:52:PRO:HD3	1.97	0.47
3:G:88:PRO:HG2	3:G:89:PRO:CD	2.43	0.47
1:I:108:THR:HG23	1:I:111:TYR:CE2	2.50	0.47
5:M:176:ARG:NH2	5:M:201:ASP:OD2	2.48	0.47
5:M:210:VAL:HG13	5:M:210:VAL:O	2.15	0.47
1:A:19:TRP:HE1	1:A:78:LYS:HD3	1.79	0.47
3:C:87:ASP:OD1	3:C:89:PRO:HG2	2.15	0.47
3:G:48:PRO:O	3:G:50:VAL:N	2.48	0.47
2:J:76:ILE:O	2:J:79:LEU:HG	2.15	0.47
3:K:88:PRO:N	3:K:89:PRO:HD2	2.30	0.47
5:M:69:CYS:HB3	5:M:93:SER:HG	1.74	0.47
6:N:155:LEU:HD23	6:N:155:LEU:H	1.79	0.47
1:E:23:TRP:CH2	1:E:74:ALA:HB1	2.50	0.47
4:H:110:PHE:O	4:H:113:ILE:HB	2.15	0.47
3:K:148:SER:C	3:K:150:ARG:H	2.17	0.47
6:N:10:LEU:CD2	6:N:12:PRO:HG2	2.43	0.47
6:N:80:LEU:C	6:N:81:LEU:HD23	2.35	0.47
4:D:56:VAL:O	4:D:57:ARG:C	2.53	0.47
1:I:118:ALA:O	1:I:122:VAL:HG23	2.15	0.47
6:N:80:LEU:N	6:N:80:LEU:HD22	2.30	0.47
1:E:132:VAL:HG13	1:E:133:ASP:N	2.29	0.46
3:G:88:PRO:N	3:G:89:PRO:HD2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:19:TRP:HE1	1:I:78:LYS:HD3	1.79	0.46
4:L:56:VAL:O	4:L:57:ARG:C	2.53	0.46
5:M:152:SER:HA	5:M:163:SER:O	2.15	0.46
1:A:53:PHE:HB2	1:A:58:ILE:CG2	2.45	0.46
1:A:142:LEU:O	1:A:146:ILE:HG13	2.14	0.46
3:C:88:PRO:HG2	3:C:89:PRO:HD3	1.96	0.46
4:H:31:ARG:HB3	4:H:71:GLN:HE22	1.80	0.46
6:N:208:HIS:HA	6:N:219:ALA:O	2.15	0.46
7:O:203:HIS:CD2	7:O:215:GLU:HG3	2.49	0.46
4:D:14:SER:OG	4:D:15:LEU:N	2.47	0.46
4:D:118:LEU:O	4:D:122:LEU:HG	2.16	0.46
4:H:118:LEU:O	4:H:122:LEU:HG	2.15	0.46
6:N:16:ALA:C	6:N:18:ALA:N	2.68	0.46
1:A:15:ILE:C	1:A:17:HIS:N	2.68	0.46
1:E:22:VAL:CG2	1:E:23:TRP:N	2.78	0.46
5:M:71:GLY:HA3	5:M:91:ASP:OD1	2.15	0.46
5:M:152:SER:OG	5:M:164:THR:HG23	2.16	0.46
7:O:68:GLN:OE1	7:O:69:CYS:N	2.48	0.46
1:A:108:THR:HG23	1:A:111:TYR:CE2	2.50	0.46
3:C:87:ASP:C	3:C:89:PRO:HD2	2.36	0.46
4:D:110:PHE:O	4:D:113:ILE:HB	2.15	0.46
3:K:87:ASP:C	3:K:89:PRO:HD2	2.36	0.46
3:K:99:ALA:HA	3:K:147:ILE:O	2.16	0.46
6:N:10:LEU:HD22	6:N:13:ARG:CB	2.42	0.46
4:L:51:ALA:HB3	4:L:52:PRO:HD3	1.97	0.46
6:N:197:PHE:CD2	6:N:205:ALA:HB2	2.51	0.46
4:D:83:MET:HE1	4:D:89:MET:HB3	1.96	0.46
3:K:35:PHE:CE2	3:K:39:LEU:HD11	2.51	0.46
3:K:129:ASP:N	3:K:129:ASP:OD2	2.37	0.46
5:M:170:PHE:CD1	5:M:170:PHE:C	2.89	0.46
5:M:183:LEU:O	5:M:184:LYS:CB	2.64	0.46
6:N:64:LYS:O	6:N:65:ARG:HB2	2.15	0.46
4:D:107:LYS:HB3	4:D:109:GLU:HG2	1.98	0.46
4:H:14:SER:OG	4:H:15:LEU:N	2.49	0.46
6:N:46:PHE:CD1	6:N:46:PHE:C	2.88	0.46
1:E:78:LYS:NZ	4:H:31:ARG:NH2	2.45	0.46
3:G:45:LYS:HA	3:G:45:LYS:HE3	1.98	0.46
3:G:99:ALA:HA	3:G:147:ILE:O	2.16	0.46
4:H:56:VAL:O	4:H:57:ARG:C	2.54	0.46
4:L:110:PHE:O	4:L:113:ILE:HB	2.16	0.46
6:N:162:VAL:CG1	6:N:163:THR:N	2.76	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:LYS:HD2	1:A:65:GLU:HG3	1.98	0.46
3:C:12:HIS:HB2	3:C:85:LEU:HD13	1.98	0.46
4:D:18:LYS:NZ	4:D:82:SER:HA	2.31	0.46
4:L:107:LYS:HB3	4:L:109:GLU:HG2	1.98	0.46
5:M:114:LEU:HB2	6:N:73:GLU:HA	1.97	0.46
5:M:149:ALA:HB3	5:M:180:LEU:HD13	1.98	0.46
6:N:180:ILE:HG22	6:N:182:LEU:CD1	2.46	0.46
2:F:5:GLY:H	2:F:8:GLU:HG3	1.80	0.45
3:G:35:PHE:CE2	3:G:39:LEU:HD11	2.51	0.45
4:H:51:ALA:HB3	4:H:52:PRO:HD3	1.98	0.45
4:H:107:LYS:HB3	4:H:109:GLU:HG2	1.98	0.45
6:N:14:LEU:N	6:N:14:LEU:HD22	2.31	0.45
6:N:147:LEU:CD2	6:N:171:TYR:HA	2.47	0.45
1:A:123:LEU:O	1:A:127:LEU:HD23	2.16	0.45
1:E:96:HIS:O	1:E:100:GLN:HG3	2.16	0.45
1:I:64:GLY:HA2	1:I:67:LYS:HB2	1.98	0.45
1:I:94:LEU:HD12	1:I:94:LEU:HA	1.84	0.45
6:N:133:THR:H	6:N:149:ALA:HA	1.80	0.45
1:A:132:VAL:HG13	1:A:133:ASP:N	2.32	0.45
3:G:9:GLU:HA	3:G:12:HIS:CE1	2.52	0.45
6:N:10:LEU:HD23	6:N:12:PRO:CG	2.46	0.45
3:C:88:PRO:N	3:C:89:PRO:HD2	2.31	0.45
3:K:87:ASP:OD1	3:K:89:PRO:HG2	2.16	0.45
6:N:62:CYS:HB3	6:N:66:THR:HB	1.99	0.45
1:I:23:TRP:CH2	1:I:74:ALA:HB1	2.51	0.45
5:M:63:ASP:O	5:M:64:GLU:C	2.53	0.45
1:E:15:ILE:C	1:E:17:HIS:H	2.20	0.45
1:E:128:SER:O	1:E:129:CYS:HB2	2.16	0.45
4:L:75:SER:O	4:L:78:ASP:HB3	2.17	0.45
4:H:17:VAL:HG13	4:H:135:TRP:CE2	2.52	0.45
4:L:111:PHE:N	4:L:111:PHE:CD1	2.85	0.45
5:M:176:ARG:HG2	5:M:176:ARG:HH11	1.82	0.45
1:E:108:THR:H	1:E:111:TYR:HD2	1.63	0.45
3:G:96:ASP:O	3:G:99:ALA:HB3	2.17	0.45
5:M:12:TYR:CD2	5:M:12:TYR:N	2.85	0.45
3:C:32:LYS:HG2	3:C:75:LEU:HD12	1.99	0.45
4:D:10:LEU:HG	4:D:13:GLU:OE1	2.16	0.45
1:E:123:LEU:HA	1:E:126:VAL:CG2	2.47	0.45
6:N:82:VAL:CG1	6:N:83:CYS:H	2.22	0.45
6:N:84:ASP:HA	6:N:142:THR:OG1	2.16	0.45
1:A:15:ILE:CD1	1:A:138:CYS:HB2	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:111:PHE:HB3	4:D:143:ILE:HG23	1.98	0.44
1:E:79:LEU:HD13	1:E:79:LEU:O	2.15	0.44
3:G:87:ASP:C	3:G:89:PRO:HD2	2.38	0.44
4:H:111:PHE:CD1	4:H:111:PHE:N	2.85	0.44
3:K:72:LEU:O	3:K:73:ARG:C	2.56	0.44
5:M:36:ASN:C	5:M:38:LEU:H	2.20	0.44
7:O:161:VAL:CG1	7:O:163:MET:HG3	2.46	0.44
1:A:108:THR:H	1:A:111:TYR:HD2	1.65	0.44
3:K:148:SER:O	3:K:150:ARG:N	2.50	0.44
6:N:70:GLY:N	6:N:91:ASN:HD21	2.15	0.44
7:O:120:ARG:O	7:O:121:ARG:C	2.55	0.44
1:A:123:LEU:HA	1:A:126:VAL:CG2	2.47	0.44
3:C:148:SER:O	3:C:150:ARG:N	2.50	0.44
1:I:60:GLU:O	1:I:63:SER:HB3	2.17	0.44
3:K:70:HIS:O	3:K:74:ILE:HG22	2.16	0.44
4:H:17:VAL:HG13	4:H:135:TRP:CZ2	2.53	0.44
4:L:10:LEU:HD13	4:L:12:THR:H	1.82	0.44
5:M:210:VAL:CG1	5:M:215:PHE:HB3	2.48	0.44
6:N:147:LEU:HD23	6:N:171:TYR:HA	1.99	0.44
1:A:78:LYS:HZ1	4:D:31:ARG:HH22	1.63	0.44
4:D:10:LEU:HD11	4:D:13:GLU:H	1.83	0.44
2:F:102:PRO:C	2:F:104:ASN:N	2.70	0.44
1:I:22:VAL:CG2	1:I:23:TRP:N	2.80	0.44
4:L:17:VAL:HG13	4:L:135:TRP:CZ2	2.52	0.44
4:L:134:ALA:O	4:L:138:CYS:HB2	2.18	0.44
5:M:114:LEU:CB	6:N:73:GLU:HA	2.48	0.44
5:M:132:ILE:HD13	5:M:149:ALA:HB2	1.99	0.44
6:N:29:GLU:O	6:N:32:ARG:HB2	2.18	0.44
3:G:87:ASP:OD1	3:G:89:PRO:HG2	2.17	0.44
4:H:60:ASN:HD21	4:L:133:GLY:H	1.63	0.44
3:K:32:LYS:HG2	3:K:75:LEU:HD12	2.00	0.44
3:K:150:ARG:O	3:K:151:LEU:HG	2.18	0.44
4:D:17:VAL:HG13	4:D:135:TRP:CE2	2.53	0.44
1:E:123:LEU:O	1:E:127:LEU:HD23	2.18	0.44
6:N:153:SER:O	6:N:155:LEU:HD22	2.18	0.44
1:A:15:ILE:O	1:A:17:HIS:N	2.51	0.44
4:D:31:ARG:HB3	4:D:71:GLN:HE22	1.83	0.44
4:D:114:PHE:CZ	9:D:160:HEM:HAB	2.53	0.44
4:H:10:LEU:HG	4:H:13:GLU:OE1	2.18	0.44
4:H:83:MET:HE1	4:H:89:MET:HB3	1.99	0.44
3:C:129:ASP:CA	4:D:16:LYS:HE3	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:75:SER:O	4:D:78:ASP:HB3	2.18	0.44
4:D:111:PHE:CD1	4:D:111:PHE:N	2.86	0.44
1:A:80:LEU:HD22	1:A:94:LEU:HD13	2.00	0.43
1:A:147:ALA:CB	1:A:150:LEU:HD12	2.48	0.43
3:K:95:LEU:HD21	3:K:143:ILE:HG23	2.00	0.43
4:L:10:LEU:HG	4:L:13:GLU:OE1	2.18	0.43
1:A:22:VAL:CG2	1:A:23:TRP:N	2.81	0.43
4:H:18:LYS:NZ	4:H:82:SER:HA	2.33	0.43
1:I:15:ILE:O	1:I:17:HIS:N	2.50	0.43
1:I:28:THR:O	1:I:29:ASP:C	2.56	0.43
6:N:104:VAL:HG22	6:N:202:ASN:HD22	1.83	0.43
2:F:74:ILE:HG23	3:G:72:LEU:CD1	2.45	0.43
5:M:147:LEU:HD12	5:M:169:GLY:O	2.18	0.43
6:N:162:VAL:CG1	6:N:163:THR:H	2.28	0.43
4:H:75:SER:O	4:H:78:ASP:HB3	2.19	0.43
1:I:57:LYS:HD2	1:I:65:GLU:HG3	1.99	0.43
3:K:45:LYS:HE3	3:K:45:LYS:HA	1.99	0.43
3:K:88:PRO:HG2	3:K:89:PRO:CD	2.48	0.43
1:A:64:GLY:HA2	1:A:67:LYS:HB2	2.00	0.43
4:D:114:PHE:CE2	9:D:160:HEM:HAB	2.53	0.43
1:E:60:GLU:CB	1:E:63:SER:HB3	2.49	0.43
5:M:66:GLU:HG3	5:M:78:HIS:HA	2.00	0.43
6:N:18:ALA:C	6:N:20:LEU:H	2.22	0.43
7:O:45:ARG:HG3	7:O:46:LYS:N	2.34	0.43
1:A:55:ARG:HD2	1:A:55:ARG:O	2.19	0.43
2:B:85:LEU:O	2:B:86:LYS:C	2.56	0.43
4:D:106:LEU:HD22	9:D:160:HEM:HBC2	2.00	0.43
4:H:114:PHE:CE2	9:H:160:HEM:HAB	2.54	0.43
6:N:20:LEU:HD23	6:N:20:LEU:O	2.19	0.43
6:N:207:CYS:HB2	6:N:221:LEU:HB3	2.00	0.43
7:O:102:THR:HG22	7:O:108:PHE:CE2	2.53	0.43
2:B:102:PRO:C	2:B:104:ASN:N	2.71	0.43
1:E:15:ILE:CD1	1:E:138:CYS:HB2	2.48	0.43
1:E:67:LYS:HB3	4:H:89:MET:CE	2.48	0.43
1:I:96:HIS:O	1:I:100:GLN:HG3	2.18	0.43
6:N:47:VAL:CG1	6:N:48:SER:N	2.81	0.43
6:N:176:SER:HB2	6:N:178:ARG:HG3	2.01	0.43
1:A:23:TRP:HZ3	1:A:74:ALA:HB1	1.81	0.43
1:A:72:ARG:HD2	4:D:93:GLN:OE1	2.18	0.43
1:A:128:SER:O	1:A:129:CYS:HB2	2.19	0.43
1:I:80:LEU:HD22	1:I:94:LEU:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:136:ASN:HD22	1:I:136:ASN:HA	1.56	0.43
5:M:182:PRO:HD2	5:M:211:PRO:HB3	2.01	0.43
3:G:148:SER:O	3:G:150:ARG:N	2.51	0.43
3:G:150:ARG:O	3:G:151:LEU:HG	2.19	0.43
1:I:79:LEU:HD13	1:I:79:LEU:C	2.39	0.43
1:I:79:LEU:HD21	4:L:71:GLN:HG3	2.01	0.43
1:I:108:THR:H	1:I:111:TYR:HD2	1.65	0.43
5:M:102:LEU:O	5:M:103:ASN:C	2.57	0.43
6:N:53:ARG:NH1	7:O:58:GLU:OE2	2.52	0.43
6:N:82:VAL:CB	6:N:175:ALA:HB2	2.49	0.43
1:A:136:ASN:HD22	1:A:136:ASN:HA	1.56	0.43
5:M:196:PHE:CD2	5:M:204:ALA:HB2	2.54	0.43
6:N:128:THR:HB	6:N:221:LEU:HD11	2.01	0.43
6:N:160:GLU:HB3	6:N:161:ASN:H	1.73	0.43
1:E:142:LEU:O	1:E:146:ILE:HG13	2.18	0.42
4:H:10:LEU:HD13	4:H:12:THR:H	1.84	0.42
4:H:80:THR:O	4:H:84:LEU:HD13	2.19	0.42
1:I:128:SER:O	1:I:129:CYS:HB2	2.19	0.42
2:J:102:PRO:C	2:J:104:ASN:N	2.72	0.42
4:L:57:ARG:HG2	4:L:57:ARG:NH1	2.32	0.42
4:L:114:PHE:CZ	9:L:160:HEM:HAB	2.54	0.42
6:N:194:VAL:O	6:N:207:CYS:HA	2.19	0.42
7:O:117:CYS:O	7:O:118:THR:C	2.57	0.42
7:O:161:VAL:HG12	7:O:162:SER:N	2.34	0.42
1:A:15:ILE:C	1:A:17:HIS:H	2.23	0.42
4:H:106:LEU:HD22	9:H:160:HEM:HBC2	2.01	0.42
4:L:118:LEU:O	4:L:122:LEU:HG	2.18	0.42
7:O:129:PHE:HE2	7:O:144:LEU:HD13	1.84	0.42
7:O:209:SER:HB3	7:O:211:GLU:CG	2.39	0.42
2:F:75:ALA:HB1	2:F:137:ILE:HD13	2.02	0.42
3:G:12:HIS:HB2	3:G:85:LEU:HD13	1.99	0.42
5:M:38:LEU:HD22	7:O:38:ARG:NH1	2.26	0.42
5:M:80:LEU:HA	5:M:143:ASN:ND2	2.35	0.42
7:O:67:HIS:HB3	7:O:77:ILE:HD12	2.01	0.42
2:B:123:ARG:HH21	5:M:214:LEU:HG	1.84	0.42
1:E:22:VAL:HG23	1:E:23:TRP:N	2.34	0.42
1:E:55:ARG:HD2	1:E:55:ARG:O	2.19	0.42
3:G:95:LEU:HD21	3:G:143:ILE:HG23	2.01	0.42
5:M:90:ARG:NH1	7:O:113:CYS:HA	2.35	0.42
5:M:172:ASN:ND2	5:M:174:GLY:H	2.17	0.42
1:E:19:TRP:O	1:E:21:ASP:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:78:LYS:HZ3	4:H:31:ARG:HH22	1.56	0.42
3:G:31:ILE:O	3:G:32:LYS:C	2.58	0.42
4:L:18:LYS:NZ	4:L:82:SER:HA	2.34	0.42
5:M:131:THR:HG23	5:M:150:THR:OG1	2.20	0.42
6:N:155:LEU:HD23	6:N:155:LEU:O	2.19	0.42
1:A:19:TRP:O	1:A:21:ASP:N	2.53	0.42
1:A:19:TRP:C	1:A:21:ASP:H	2.23	0.42
1:A:118:ALA:O	1:A:122:VAL:HG23	2.20	0.42
2:B:8:GLU:O	2:B:12:VAL:HG23	2.20	0.42
3:C:45:LYS:HE3	3:C:45:LYS:HA	2.00	0.42
1:I:123:LEU:HA	1:I:126:VAL:CG2	2.48	0.42
4:L:81:ILE:HA	4:L:84:LEU:HD13	2.01	0.42
4:L:114:PHE:CE2	9:L:160:HEM:HAB	2.54	0.42
6:N:151:VAL:HB	6:N:166:PHE:CE2	2.55	0.42
1:A:60:GLU:CB	1:A:63:SER:HB3	2.49	0.42
2:B:58:HIS:CE1	2:B:59:PRO:HG2	2.54	0.42
2:F:28:ALA:O	2:F:29:PHE:C	2.58	0.42
3:K:31:ILE:O	3:K:32:LYS:C	2.58	0.42
5:M:49:GLN:HE21	5:M:49:GLN:HB2	1.65	0.42
5:M:75:GLU:OE1	5:M:90:ARG:HB2	2.20	0.42
1:A:109:LYS:HB2	1:A:151:PRO:HD3	2.01	0.42
4:D:107:LYS:HD2	4:D:107:LYS:N	2.34	0.42
4:L:10:LEU:HD12	4:L:13:GLU:H	1.85	0.42
7:O:101:PRO:HB3	7:O:197:PHE:CD2	2.55	0.42
1:A:82:ASN:ND2	4:D:31:ARG:CZ	2.82	0.42
1:A:112:PHE:O	1:A:115:ILE:HG22	2.20	0.42
2:B:28:ALA:O	2:B:29:PHE:C	2.56	0.42
3:C:88:PRO:HG2	3:C:89:PRO:CD	2.49	0.42
4:D:10:LEU:HD13	4:D:12:THR:H	1.84	0.42
2:F:70:GLY:O	2:F:73:ASP:HB3	2.20	0.42
4:H:10:LEU:HD11	4:H:13:GLU:H	1.84	0.42
1:I:15:ILE:C	1:I:17:HIS:H	2.21	0.42
1:I:60:GLU:CB	1:I:63:SER:HB3	2.50	0.42
3:K:85:LEU:HA	3:K:91:LEU:HD22	2.02	0.42
6:N:112:SER:O	6:N:223:VAL:HA	2.20	0.42
1:E:63:SER:OG	1:E:66:PHE:HB3	2.20	0.42
3:G:72:LEU:O	3:G:73:ARG:C	2.58	0.42
1:I:19:TRP:O	1:I:21:ASP:N	2.53	0.42
1:I:147:ALA:CB	1:I:150:LEU:HD12	2.49	0.42
5:M:155:LEU:HD13	5:M:155:LEU:HA	1.91	0.42
6:N:170:GLY:HA3	6:N:180:ILE:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:85:LEU:HA	3:G:91:LEU:HD22	2.02	0.41
2:J:70:GLY:O	2:J:73:ASP:HB3	2.20	0.41
5:M:121:GLU:O	5:M:122:ASP:C	2.58	0.41
5:M:183:LEU:HB2	5:M:186:GLN:NE2	2.35	0.41
6:N:173:ASN:HD22	6:N:174:PHE:N	2.18	0.41
7:O:48:GLY:O	7:O:51:ARG:HB3	2.20	0.41
1:A:79:LEU:HD13	1:A:79:LEU:C	2.40	0.41
3:C:134:LEU:HD23	3:C:134:LEU:HA	1.92	0.41
4:D:60:ASN:ND2	4:H:132:PHE:HB3	2.35	0.41
4:D:73:VAL:O	4:D:74:LEU:C	2.59	0.41
2:F:102:PRO:C	2:F:104:ASN:H	2.22	0.41
4:H:134:ALA:O	4:H:138:CYS:HB2	2.20	0.41
5:M:18:ASN:HD21	7:O:17:LEU:CB	2.33	0.41
4:D:19:LEU:O	4:D:22:ALA:HB3	2.20	0.41
4:D:49:ILE:C	4:D:51:ALA:N	2.73	0.41
4:D:134:ALA:O	4:D:138:CYS:HB2	2.20	0.41
1:E:81:ILE:C	1:E:83:LEU:H	2.24	0.41
3:G:109:GLN:O	3:G:112:HIS:HB2	2.20	0.41
4:L:14:SER:O	4:L:17:VAL:N	2.53	0.41
6:N:177:ARG:NH1	6:N:177:ARG:HG2	2.35	0.41
7:O:83:CYS:O	7:O:139:THR:HB	2.20	0.41
7:O:102:THR:HB	7:O:129:PHE:CD2	2.55	0.41
2:B:87:GLU:OE2	3:C:66:LYS:HE3	2.20	0.41
3:C:95:LEU:HD21	3:C:143:ILE:HG23	2.02	0.41
4:D:125:ARG:HG2	4:D:125:ARG:NH1	2.34	0.41
1:E:19:TRP:C	1:E:21:ASP:H	2.23	0.41
1:E:28:THR:O	1:E:29:ASP:C	2.58	0.41
1:E:57:LYS:HD2	1:E:65:GLU:HG3	2.00	0.41
1:E:69:HIS:O	1:E:70:LEU:C	2.59	0.41
2:F:85:LEU:O	2:F:86:LYS:C	2.58	0.41
6:N:155:LEU:H	6:N:155:LEU:CD2	2.33	0.41
7:O:94:ASP:N	7:O:94:ASP:OD2	2.53	0.41
4:H:19:LEU:O	4:H:22:ALA:HB3	2.21	0.41
4:L:10:LEU:HD11	4:L:13:GLU:H	1.83	0.41
6:N:64:LYS:HB3	6:N:64:LYS:NZ	2.35	0.41
7:O:93:GLU:C	7:O:95:GLU:N	2.73	0.41
7:O:100:LEU:C	7:O:100:LEU:CD2	2.89	0.41
3:C:72:LEU:O	3:C:73:ARG:C	2.59	0.41
4:D:17:VAL:HG13	4:D:135:TRP:CZ2	2.55	0.41
4:H:114:PHE:CZ	9:H:160:HEM:HAB	2.55	0.41
6:N:68:GLN:OE1	6:N:69:CYS:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:LYS:HG2	1:A:58:ILE:HD12	2.02	0.41
4:D:57:ARG:HG2	4:D:57:ARG:NH1	2.35	0.41
4:D:81:ILE:HA	4:D:84:LEU:HD13	2.03	0.41
1:E:83:LEU:HD11	4:H:71:GLN:HG2	2.03	0.41
1:I:19:TRP:C	1:I:21:ASP:H	2.24	0.41
1:I:63:SER:OG	1:I:66:PHE:HB3	2.20	0.41
1:I:109:LYS:HB2	1:I:151:PRO:HD3	2.02	0.41
2:J:28:ALA:O	2:J:29:PHE:C	2.58	0.41
2:B:70:GLY:O	2:B:73:ASP:HB3	2.21	0.41
3:C:53:LEU:HD21	3:C:107:GLY:HA3	2.03	0.41
1:E:50:LYS:HG2	1:E:58:ILE:HD12	2.02	0.41
3:G:12:HIS:O	3:G:13:ARG:C	2.59	0.41
4:H:49:ILE:C	4:H:51:ALA:N	2.73	0.41
4:H:57:ARG:HG2	4:H:57:ARG:NH1	2.36	0.41
4:H:111:PHE:HD1	4:H:111:PHE:H	1.69	0.41
1:I:15:ILE:CD1	1:I:138:CYS:HB2	2.51	0.41
1:I:88:LEU:HD23	1:I:88:LEU:HA	1.92	0.41
1:I:123:LEU:O	1:I:127:LEU:HD23	2.20	0.41
2:J:24:HIS:O	2:J:25:ASP:C	2.59	0.41
3:K:40:LEU:O	3:K:43:LEU:HB3	2.21	0.41
4:L:31:ARG:HB3	4:L:71:GLN:HE22	1.85	0.41
4:L:106:LEU:HD22	9:L:160:HEM:HBC2	2.02	0.41
4:L:111:PHE:HD1	4:L:111:PHE:H	1.68	0.41
6:N:66:THR:HG22	6:N:67:PHE:N	2.36	0.41
6:N:209:ARG:HA	6:N:209:ARG:HD2	1.78	0.41
1:A:88:LEU:HD23	1:A:88:LEU:HA	1.93	0.41
1:A:97:LEU:HD23	1:A:146:ILE:CD1	2.50	0.41
2:B:92:LEU:O	2:B:93:GLN:C	2.58	0.41
4:H:25:PHE:CE2	4:H:31:ARG:NE	2.89	0.41
2:J:134:ILE:HD13	2:J:134:ILE:HA	1.97	0.41
5:M:118:THR:O	5:M:118:THR:OG1	2.39	0.41
7:O:209:SER:O	7:O:210:GLU:HB3	2.20	0.41
1:A:63:SER:OG	1:A:66:PHE:HB3	2.21	0.40
4:H:107:LYS:HD2	4:H:107:LYS:N	2.35	0.40
2:J:85:LEU:O	2:J:86:LYS:C	2.59	0.40
3:K:109:GLN:O	3:K:112:HIS:HB2	2.21	0.40
4:L:18:LYS:HZ2	4:L:82:SER:HA	1.86	0.40
3:C:150:ARG:O	3:C:151:LEU:HG	2.20	0.40
1:E:64:GLY:HA2	1:E:67:LYS:HB2	2.02	0.40
5:M:130:VAL:O	5:M:130:VAL:CG1	2.68	0.40
6:N:145:ILE:HB	6:N:172:TYR:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:147:LEU:N	6:N:147:LEU:CD2	2.83	0.40
1:E:125:GLN:O	2:F:11:LYS:HE3	2.21	0.40
1:I:78:LYS:HZ3	4:L:31:ARG:HH22	1.67	0.40
6:N:19:PHE:HA	6:N:22:ILE:HG22	2.03	0.40
7:O:170:SER:OG	7:O:172:ALA:HB3	2.20	0.40
1:E:49:SER:HB3	1:E:111:TYR:CD1	2.56	0.40
1:E:104:ARG:HG2	1:E:104:ARG:HH11	1.86	0.40
1:I:14:GLU:CD	7:O:208:LEU:CD1	2.83	0.40
1:I:50:LYS:HG2	1:I:58:ILE:HD12	2.03	0.40
5:M:35:TYR:O	5:M:38:LEU:HB2	2.21	0.40
3:C:40:LEU:O	3:C:43:LEU:HB3	2.21	0.40
3:C:40:LEU:HD22	3:C:54:PHE:CE1	2.57	0.40
1:I:69:HIS:O	1:I:70:LEU:C	2.60	0.40
2:J:58:HIS:CE1	2:J:59:PRO:HG2	2.57	0.40
5:M:53:ARG:HG3	5:M:53:ARG:HH11	1.87	0.40
5:M:187:SER:O	5:M:188:GLU:C	2.60	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	145/151 (96%)	119 (82%)	22 (15%)	4 (3%)	5 32
1	E	145/151 (96%)	119 (82%)	22 (15%)	4 (3%)	5 32
1	I	145/151 (96%)	120 (83%)	21 (14%)	4 (3%)	5 32
2	B	143/145 (99%)	118 (82%)	24 (17%)	1 (1%)	22 61
2	F	143/145 (99%)	120 (84%)	22 (15%)	1 (1%)	22 61
2	J	143/145 (99%)	123 (86%)	18 (13%)	2 (1%)	11 46
3	C	147/153 (96%)	122 (83%)	23 (16%)	2 (1%)	11 46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	G	147/153 (96%)	124 (84%)	21 (14%)	2 (1%)	11	46
3	K	147/153 (96%)	124 (84%)	21 (14%)	2 (1%)	11	46
4	D	138/140 (99%)	114 (83%)	21 (15%)	3 (2%)	6	37
4	H	138/140 (99%)	114 (83%)	21 (15%)	3 (2%)	6	37
4	L	138/140 (99%)	113 (82%)	23 (17%)	2 (1%)	11	46
5	M	215/217 (99%)	178 (83%)	29 (14%)	8 (4%)	3	26
6	N	218/220 (99%)	177 (81%)	28 (13%)	13 (6%)	1	15
7	O	213/215 (99%)	171 (80%)	37 (17%)	5 (2%)	6	36
All	All	2365/2419 (98%)	1956 (83%)	353 (15%)	56 (2%)	6	35

All (56) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	87	THR
1	E	29	ASP
1	E	87	THR
1	I	87	THR
5	M	123	LEU
6	N	82	VAL
1	A	29	ASP
3	C	149	SER
3	G	149	SER
1	I	29	ASP
3	K	149	SER
6	N	70	GLY
6	N	187	HIS
7	O	94	ASP
3	C	87	ASP
4	D	10	LEU
4	H	10	LEU
4	L	10	LEU
5	M	87	LYS
5	M	125	PRO
6	N	143	ALA
6	N	158	HIS
7	O	114	PHE
7	O	210	GLU
2	B	77	SER
4	D	103	GLU

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Mol	Chain	Res	Type
1	E	20	ASP
2	F	77	SER
3	G	87	ASP
4	H	57	ARG
1	I	20	ASP
2	J	77	SER
3	K	87	ASP
5	M	186	GLN
6	N	79	ASP
6	N	186	ASP
6	N	199	ARG
7	O	113	CYS
1	A	20	ASP
1	A	82	ASN
4	D	57	ARG
4	H	103	GLU
4	L	57	ARG
5	M	119	SER
5	M	184	LYS
5	M	188	GLU
6	N	43	PRO
6	N	95	GLU
6	N	125	ASP
1	E	82	ASN
1	I	82	ASN
2	J	144	HIS
6	N	12	PRO
6	N	119	GLY
5	M	216	VAL
7	O	181	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 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	131/134 (98%)	123 (94%)	8 (6%)	18 51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	E	131/134 (98%)	122 (93%)	9 (7%)	15 47
1	I	131/134 (98%)	123 (94%)	8 (6%)	18 51
2	B	117/117 (100%)	110 (94%)	7 (6%)	19 52
2	F	117/117 (100%)	110 (94%)	7 (6%)	19 52
2	J	117/117 (100%)	110 (94%)	7 (6%)	19 52
3	C	127/131 (97%)	120 (94%)	7 (6%)	21 54
3	G	127/131 (97%)	120 (94%)	7 (6%)	21 54
3	K	127/131 (97%)	120 (94%)	7 (6%)	21 54
4	D	121/121 (100%)	115 (95%)	6 (5%)	24 58
4	H	121/121 (100%)	115 (95%)	6 (5%)	24 58
4	L	121/121 (100%)	114 (94%)	7 (6%)	20 53
5	M	182/195 (93%)	155 (85%)	27 (15%)	3 17
6	N	186/193 (96%)	170 (91%)	16 (9%)	10 38
7	O	178/193 (92%)	168 (94%)	10 (6%)	21 54
All	All	2034/2090 (97%)	1895 (93%)	139 (7%)	16 48

All (139) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	THR
1	A	55	ARG
1	A	59	ASP
1	A	82	ASN
1	A	85	ASP
1	A	126	VAL
1	A	131	ASN
1	A	136	ASN
2	B	25	ASP
2	B	56	THR
2	B	66	ASP
2	B	90	ASP
2	B	123	ARG
2	B	125	TYR
2	B	135	ASP
3	C	6	CYS
3	C	20	ASP
3	C	37	ARG

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Mol	Chain	Res	Type
3	C	74	ILE
3	C	115	LYS
3	C	129	ASP
3	C	146	LYS
4	D	19	LEU
4	D	41	ASP
4	D	48	GLU
4	D	71	GLN
4	D	128	THR
4	D	138	CYS
1	E	48	THR
1	E	55	ARG
1	E	59	ASP
1	E	65	GLU
1	E	82	ASN
1	E	85	ASP
1	E	126	VAL
1	E	131	ASN
1	E	136	ASN
2	F	25	ASP
2	F	56	THR
2	F	66	ASP
2	F	90	ASP
2	F	123	ARG
2	F	125	TYR
2	F	135	ASP
3	G	6	CYS
3	G	20	ASP
3	G	37	ARG
3	G	74	ILE
3	G	115	LYS
3	G	129	ASP
3	G	146	LYS
4	H	10	LEU
4	H	19	LEU
4	H	41	ASP
4	H	48	GLU
4	H	128	THR
4	H	138	CYS
1	I	48	THR
1	I	55	ARG
1	I	59	ASP

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Mol	Chain	Res	Type
1	I	82	ASN
1	I	85	ASP
1	I	126	VAL
1	I	131	ASN
1	I	136	ASN
2	J	25	ASP
2	J	56	THR
2	J	66	ASP
2	J	90	ASP
2	J	123	ARG
2	J	125	TYR
2	J	135	ASP
3	K	6	CYS
3	K	20	ASP
3	K	37	ARG
3	K	74	ILE
3	K	115	LYS
3	K	129	ASP
3	K	146	LYS
4	L	10	LEU
4	L	19	LEU
4	L	41	ASP
4	L	48	GLU
4	L	71	GLN
4	L	128	THR
4	L	138	CYS
5	M	9	ARG
5	M	10	PHE
5	M	12	TYR
5	M	19	LEU
5	M	38	LEU
5	M	40	HIS
5	M	70	ARG
5	M	95	GLU
5	M	98	GLU
5	M	112	THR
5	M	116	THR
5	M	118	THR
5	M	121	GLU
5	M	124	ASN
5	M	131	THR
5	M	147	LEU

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Mol	Chain	Res	Type
5	M	159	ASP
5	M	161	THR
5	M	163	SER
5	M	165	THR
5	M	172	ASN
5	M	176	ARG
5	M	183	LEU
5	M	188	GLU
5	M	198	LEU
5	M	216	VAL
5	M	225	TYR
6	N	32	ARG
6	N	64	LYS
6	N	73	GLU
6	N	89	CYS
6	N	95	GLU
6	N	110	VAL
6	N	127	VAL
6	N	131	THR
6	N	147	LEU
6	N	155	LEU
6	N	171	TYR
6	N	173	ASN
6	N	187	HIS
6	N	199	ARG
6	N	202	ASN
6	N	221	LEU
7	O	37	ASP
7	O	45	ARG
7	O	61	SER
7	O	111	ASP
7	O	114	PHE
7	O	173	ASP
7	O	176	LEU
7	O	183	GLU
7	O	199	ARG
7	O	208	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	ASN

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Mol	Chain	Res	Type
1	A	131	ASN
1	A	136	ASN
2	B	31	GLN
2	B	52	HIS
2	B	120	GLN
3	C	12	HIS
3	C	16	GLN
3	C	18	GLN
3	C	100	HIS
3	C	126	GLN
4	D	20	GLN
4	D	46	HIS
4	D	117	HIS
4	D	141	GLN
1	E	82	ASN
1	E	131	ASN
1	E	136	ASN
2	F	52	HIS
2	F	81	GLN
2	F	120	GLN
3	G	12	HIS
3	G	16	GLN
3	G	18	GLN
3	G	97	HIS
3	G	100	HIS
3	G	126	GLN
4	H	20	GLN
4	H	46	HIS
4	H	117	HIS
4	H	141	GLN
1	I	17	HIS
1	I	82	ASN
1	I	131	ASN
1	I	136	ASN
3	K	12	HIS
3	K	16	GLN
3	K	18	GLN
3	K	100	HIS
3	K	126	GLN
4	L	20	GLN
4	L	29	HIS
4	L	46	HIS

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Mol	Chain	Res	Type
4	L	117	HIS
4	L	141	GLN
5	M	18	ASN
5	M	20	HIS
5	M	49	GLN
5	M	56	ASN
5	M	103	ASN
5	M	106	HIS
5	M	143	ASN
5	M	172	ASN
6	N	72	ASN
6	N	74	GLN
6	N	86	HIS
6	N	90	HIS
6	N	173	ASN
6	N	217	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 29 ligands modelled in this entry, 5 are monoatomic - leaving 24 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	$\#\|Z\|>2$
9	HEM	K	160	3,8	41,50,50	1.45	5 (12%)	45,82,82	1.07	2 (4%)
8	CMO	I	161	9	0,1,1	-	-	-		
9	HEM	D	160	4,8	41,50,50	1.63	5 (12%)	45,82,82	1.12	1 (2%)
9	HEM	G	160	3,8	41,50,50	1.46	6 (14%)	45,82,82	0.97	0
9	HEM	J	160	2,8	41,50,50	1.54	5 (12%)	45,82,82	1.03	1 (2%)
9	HEM	L	160	4,8	41,50,50	1.54	5 (12%)	45,82,82	1.09	2 (4%)
8	CMO	B	161	9	0,1,1	-	-	-		
8	CMO	F	161	9	0,1,1	-	-	-		
8	CMO	H	161	9	0,1,1	-	-	-		
9	HEM	C	160	3,8	41,50,50	1.58	5 (12%)	45,82,82	1.05	2 (4%)
8	CMO	C	161	9	0,1,1	-	-	-		
8	CMO	G	161	9	0,1,1	-	-	-		
9	HEM	H	160	4,8	41,50,50	1.62	7 (17%)	45,82,82	1.05	1 (2%)
9	HEM	I	160	8,1	41,50,50	1.55	6 (14%)	45,82,82	1.14	3 (6%)
9	HEM	B	160	2,8	41,50,50	1.58	7 (17%)	45,82,82	1.08	3 (6%)
9	HEM	F	160	2,8	41,50,50	1.58	6 (14%)	45,82,82	1.11	3 (6%)
8	CMO	K	161	9	0,1,1	-	-	-		
9	HEM	A	160	8,1	41,50,50	1.52	5 (12%)	45,82,82	1.13	2 (4%)
8	CMO	A	161	9	0,1,1	-	-	-		
8	CMO	D	161	9	0,1,1	-	-	-		
9	HEM	E	160	8,1	41,50,50	1.62	5 (12%)	45,82,82	1.21	4 (8%)
8	CMO	J	161	9	0,1,1	-	-	-		
8	CMO	L	161	9	0,1,1	-	-	-		
8	CMO	E	161	9	0,1,1	-	-	-		

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
9	HEM	B	160	2,8	-	4/12/54/54	-
9	HEM	A	160	8,1	-	6/12/54/54	-
9	HEM	K	160	3,8	-	6/12/54/54	-
9	HEM	C	160	3,8	-	6/12/54/54	-
9	HEM	L	160	4,8	-	6/12/54/54	-
9	HEM	D	160	4,8	-	6/12/54/54	-
9	HEM	E	160	8,1	-	6/12/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	HEM	F	160	2,8	-	4/12/54/54	-
9	HEM	G	160	3,8	-	6/12/54/54	-
9	HEM	J	160	2,8	-	4/12/54/54	-
9	HEM	I	160	8,1	-	6/12/54/54	-
9	HEM	H	160	4,8	-	6/12/54/54	-

All (67) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	160	HEM	C3C-CAC	-5.55	1.36	1.47
9	D	160	HEM	C3C-CAC	-5.48	1.36	1.47
9	H	160	HEM	C3C-CAC	-5.20	1.37	1.47
9	E	160	HEM	C3C-CAC	-5.15	1.37	1.47
9	C	160	HEM	C3C-CAC	-4.87	1.37	1.47
9	C	160	HEM	C3C-C2C	-4.81	1.33	1.40
9	D	160	HEM	C3C-C2C	-4.80	1.33	1.40
9	F	160	HEM	C3C-CAC	-4.70	1.38	1.47
9	E	160	HEM	C3C-C2C	-4.70	1.33	1.40
9	A	160	HEM	C3C-CAC	-4.63	1.38	1.47
9	L	160	HEM	C3C-CAC	-4.56	1.38	1.47
9	J	160	HEM	C3C-CAC	-4.54	1.38	1.47
9	K	160	HEM	C3C-CAC	-4.33	1.38	1.47
9	I	160	HEM	C3C-C2C	-4.26	1.34	1.40
9	H	160	HEM	C3C-C2C	-4.19	1.34	1.40
9	L	160	HEM	C3C-C2C	-4.18	1.34	1.40
9	J	160	HEM	C3C-C2C	-4.07	1.34	1.40
9	G	160	HEM	C3C-CAC	-4.06	1.39	1.47
9	I	160	HEM	C3C-CAC	-4.06	1.39	1.47
9	A	160	HEM	C3C-C2C	-3.98	1.34	1.40
9	F	160	HEM	C3C-C2C	-3.96	1.34	1.40
9	K	160	HEM	C3C-C2C	-3.81	1.35	1.40
9	B	160	HEM	C3C-C2C	-3.71	1.35	1.40
9	F	160	HEM	CAB-C3B	-3.64	1.37	1.47
9	G	160	HEM	CAB-C3B	-3.60	1.37	1.47
9	G	160	HEM	C3C-C2C	-3.51	1.35	1.40
9	J	160	HEM	CAB-C3B	-3.46	1.38	1.47
9	I	160	HEM	CAB-C3B	-3.36	1.38	1.47
9	H	160	HEM	CAB-C3B	-3.36	1.38	1.47
9	C	160	HEM	CAB-C3B	-3.35	1.38	1.47
9	K	160	HEM	CAB-C3B	-3.27	1.38	1.47
9	A	160	HEM	CAB-C3B	-3.20	1.38	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	L	160	HEM	CAB-C3B	-3.20	1.38	1.47
9	E	160	HEM	CAB-C3B	-3.04	1.39	1.47
9	A	160	HEM	CBB-CAB	2.99	1.45	1.30
9	I	160	HEM	CBB-CAB	2.95	1.44	1.30
9	B	160	HEM	CAB-C3B	-2.91	1.39	1.47
9	D	160	HEM	CBB-CAB	2.89	1.44	1.30
9	J	160	HEM	CBB-CAB	2.87	1.44	1.30
9	D	160	HEM	CAB-C3B	-2.86	1.39	1.47
9	L	160	HEM	CBB-CAB	2.81	1.44	1.30
9	F	160	HEM	C4D-ND	-2.79	1.35	1.40
9	H	160	HEM	CBB-CAB	2.75	1.43	1.30
9	E	160	HEM	CBB-CAB	2.71	1.43	1.30
9	G	160	HEM	CBB-CAB	2.68	1.43	1.30
9	B	160	HEM	CBB-CAB	2.63	1.43	1.30
9	F	160	HEM	CBB-CAB	2.55	1.42	1.30
9	K	160	HEM	CBB-CAB	2.48	1.42	1.30
9	B	160	HEM	C4D-ND	-2.36	1.36	1.40
9	G	160	HEM	CHA-C4D	2.35	1.41	1.35
9	C	160	HEM	CBC-CAC	2.31	1.44	1.29
9	G	160	HEM	CBC-CAC	2.31	1.44	1.29
9	H	160	HEM	C4D-ND	-2.28	1.36	1.40
9	I	160	HEM	CBC-CAC	2.28	1.44	1.29
9	K	160	HEM	CBC-CAC	2.20	1.43	1.29
9	A	160	HEM	CBC-CAC	2.18	1.43	1.29
9	C	160	HEM	CBB-CAB	2.16	1.41	1.30
9	H	160	HEM	C3B-C2B	-2.16	1.32	1.37
9	L	160	HEM	CBC-CAC	2.16	1.43	1.29
9	B	160	HEM	C1A-CHA	-2.13	1.35	1.41
9	F	160	HEM	CBC-CAC	2.12	1.43	1.29
9	H	160	HEM	CBC-CAC	2.12	1.43	1.29
9	J	160	HEM	C4D-ND	-2.10	1.36	1.40
9	B	160	HEM	CBC-CAC	2.07	1.42	1.29
9	E	160	HEM	C3B-C2B	-2.05	1.33	1.37
9	I	160	HEM	C3B-C2B	-2.03	1.33	1.37
9	D	160	HEM	CBC-CAC	2.02	1.42	1.29

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	D	160	HEM	CMB-C2B-C1B	3.25	129.98	125.04
9	H	160	HEM	CMB-C2B-C1B	2.92	129.49	125.04
9	E	160	HEM	CMB-C2B-C1B	2.78	129.27	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	160	HEM	CMB-C2B-C1B	2.77	129.26	125.04
9	I	160	HEM	CMB-C2B-C1B	2.63	129.04	125.04
9	I	160	HEM	CAD-C3D-C4D	2.55	129.11	124.66
9	L	160	HEM	CMB-C2B-C1B	2.54	128.91	125.04
9	B	160	HEM	CMD-C2D-C1D	2.50	128.85	125.04
9	E	160	HEM	CAD-C3D-C4D	2.47	128.98	124.66
9	A	160	HEM	CAD-C3D-C4D	2.40	128.84	124.66
9	I	160	HEM	CBA-CAA-C2A	2.37	116.67	112.62
9	E	160	HEM	CBA-CAA-C2A	2.34	116.61	112.62
9	C	160	HEM	C4B-CHC-C1C	2.30	125.60	122.56
9	F	160	HEM	C2B-C1B-NB	2.27	112.53	109.84
9	J	160	HEM	CMD-C2D-C1D	2.20	128.40	125.04
9	B	160	HEM	CHA-C4D-C3D	-2.19	121.23	125.33
9	E	160	HEM	CMB-C2B-C3B	-2.18	122.97	128.30
9	F	160	HEM	CMD-C2D-C1D	2.18	128.35	125.04
9	B	160	HEM	C2B-C1B-NB	2.16	112.40	109.84
9	L	160	HEM	CHA-C4D-C3D	-2.16	121.28	125.33
9	C	160	HEM	CBA-CAA-C2A	2.08	116.18	112.62
9	K	160	HEM	CBA-CAA-C2A	2.06	116.14	112.62
9	F	160	HEM	CHA-C4D-C3D	-2.05	121.48	125.33
9	K	160	HEM	CAD-C3D-C4D	2.03	128.21	124.66

There are no chirality outliers.

All (66) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	160	HEM	C2B-C3B-CAB-CBB
9	A	160	HEM	C4B-C3B-CAB-CBB
9	D	160	HEM	C2B-C3B-CAB-CBB
9	E	160	HEM	C2B-C3B-CAB-CBB
9	E	160	HEM	C4B-C3B-CAB-CBB
9	H	160	HEM	C2B-C3B-CAB-CBB
9	I	160	HEM	C2B-C3B-CAB-CBB
9	I	160	HEM	C4B-C3B-CAB-CBB
9	L	160	HEM	C2B-C3B-CAB-CBB
9	C	160	HEM	C2B-C3B-CAB-CBB
9	G	160	HEM	C2B-C3B-CAB-CBB
9	K	160	HEM	C2B-C3B-CAB-CBB
9	D	160	HEM	C4B-C3B-CAB-CBB
9	H	160	HEM	C4B-C3B-CAB-CBB
9	L	160	HEM	C4B-C3B-CAB-CBB
9	K	160	HEM	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
9	G	160	HEM	CAD-CBD-CGD-O2D
9	G	160	HEM	CAD-CBD-CGD-O1D
9	K	160	HEM	CAD-CBD-CGD-O1D
9	C	160	HEM	CAD-CBD-CGD-O2D
9	C	160	HEM	CAD-CBD-CGD-O1D
9	L	160	HEM	CAD-CBD-CGD-O2D
9	D	160	HEM	CAD-CBD-CGD-O2D
9	I	160	HEM	CAD-CBD-CGD-O2D
9	A	160	HEM	CAA-CBA-CGA-O2A
9	A	160	HEM	CAD-CBD-CGD-O2D
9	B	160	HEM	CAD-CBD-CGD-O2D
9	E	160	HEM	CAD-CBD-CGD-O2D
9	H	160	HEM	CAD-CBD-CGD-O2D
9	L	160	HEM	CAD-CBD-CGD-O1D
9	F	160	HEM	CAD-CBD-CGD-O2D
9	D	160	HEM	CAD-CBD-CGD-O1D
9	J	160	HEM	CAD-CBD-CGD-O2D
9	H	160	HEM	CAD-CBD-CGD-O1D
9	I	160	HEM	CAD-CBD-CGD-O1D
9	E	160	HEM	CAA-CBA-CGA-O2A
9	I	160	HEM	CAA-CBA-CGA-O2A
9	A	160	HEM	CAD-CBD-CGD-O1D
9	F	160	HEM	CAA-CBA-CGA-O2A
9	F	160	HEM	CAD-CBD-CGD-O1D
9	E	160	HEM	CAD-CBD-CGD-O1D
9	J	160	HEM	CAD-CBD-CGD-O1D
9	B	160	HEM	CAD-CBD-CGD-O1D
9	D	160	HEM	CAA-CBA-CGA-O2A
9	J	160	HEM	CAA-CBA-CGA-O2A
9	L	160	HEM	CAA-CBA-CGA-O2A
9	A	160	HEM	CAA-CBA-CGA-O1A
9	C	160	HEM	CAA-CBA-CGA-O2A
9	K	160	HEM	CAA-CBA-CGA-O2A
9	B	160	HEM	CAA-CBA-CGA-O2A
9	G	160	HEM	CAA-CBA-CGA-O1A
9	G	160	HEM	CAA-CBA-CGA-O2A
9	H	160	HEM	CAA-CBA-CGA-O2A
9	C	160	HEM	C4B-C3B-CAB-CBB
9	G	160	HEM	C4B-C3B-CAB-CBB
9	K	160	HEM	C4B-C3B-CAB-CBB
9	B	160	HEM	CAA-CBA-CGA-O1A
9	F	160	HEM	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
9	D	160	HEM	CAA-CBA-CGA-O1A
9	H	160	HEM	CAA-CBA-CGA-O1A
9	J	160	HEM	CAA-CBA-CGA-O1A
9	K	160	HEM	CAA-CBA-CGA-O1A
9	C	160	HEM	CAA-CBA-CGA-O1A
9	L	160	HEM	CAA-CBA-CGA-O1A
9	E	160	HEM	CAA-CBA-CGA-O1A
9	I	160	HEM	CAA-CBA-CGA-O1A

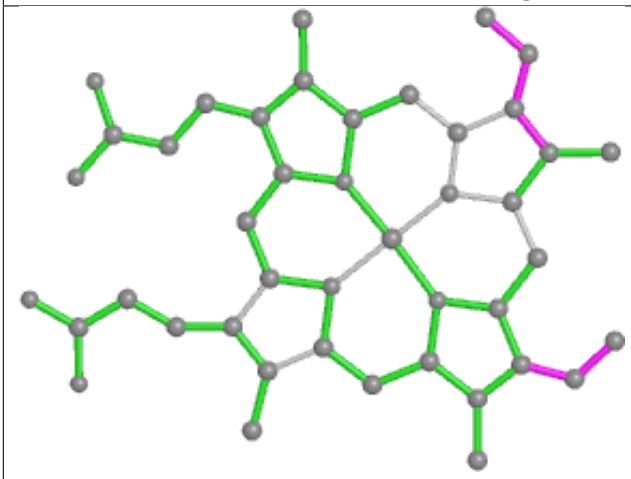
There are no ring outliers.

6 monomers are involved in 12 short contacts:

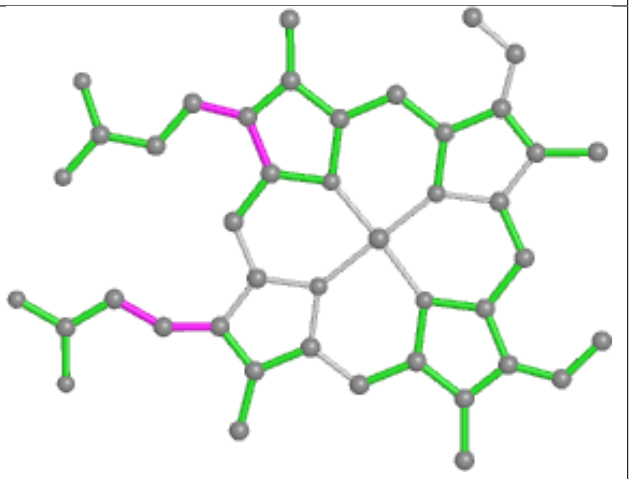
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	K	160	HEM	1	0
9	D	160	HEM	3	0
9	G	160	HEM	1	0
9	L	160	HEM	3	0
9	C	160	HEM	1	0
9	H	160	HEM	3	0

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.

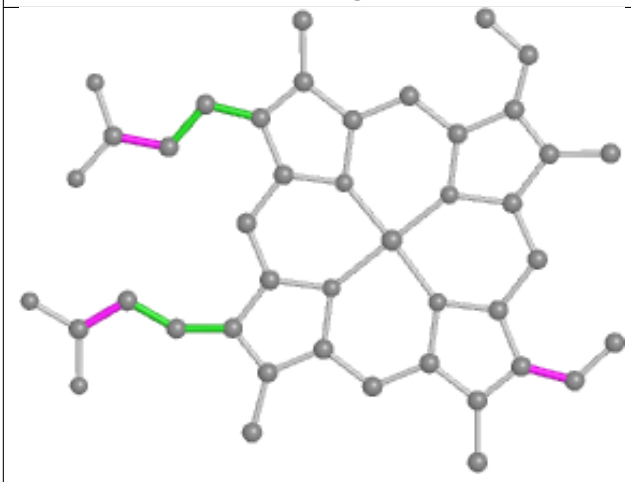
Ligand HEM K 160



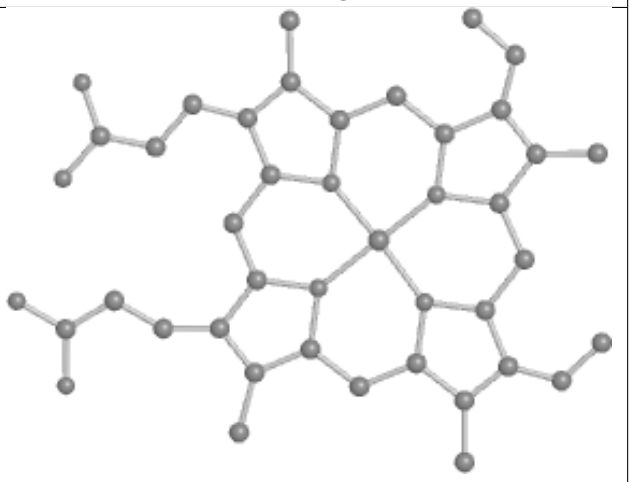
Bond lengths



Bond angles

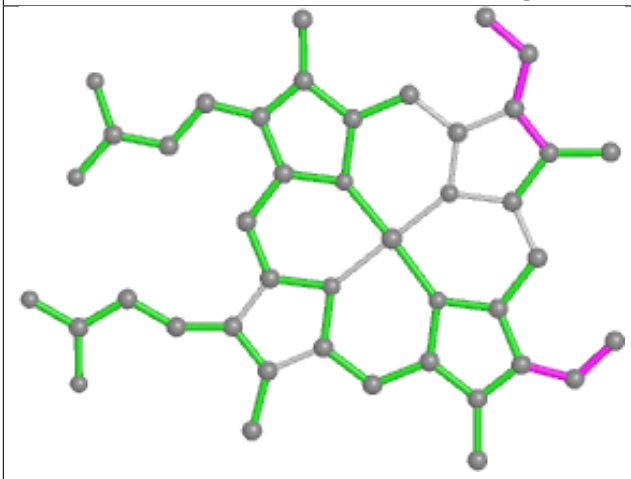


Torsions

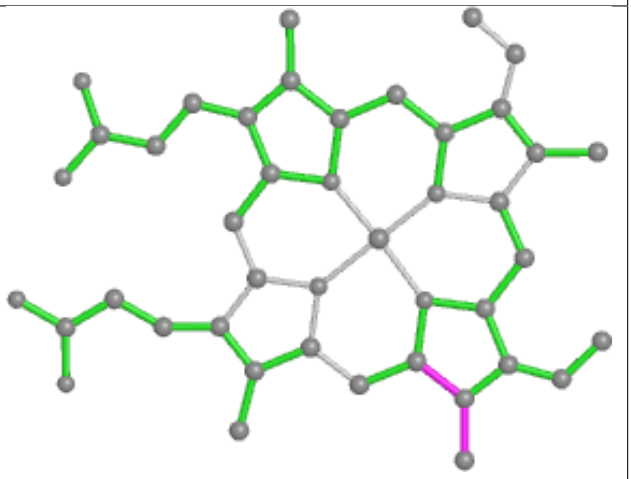


Rings

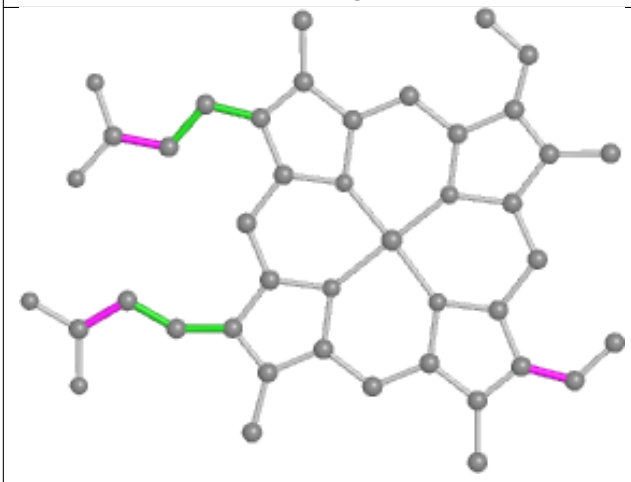
Ligand HEM D 160



Bond lengths



Bond angles



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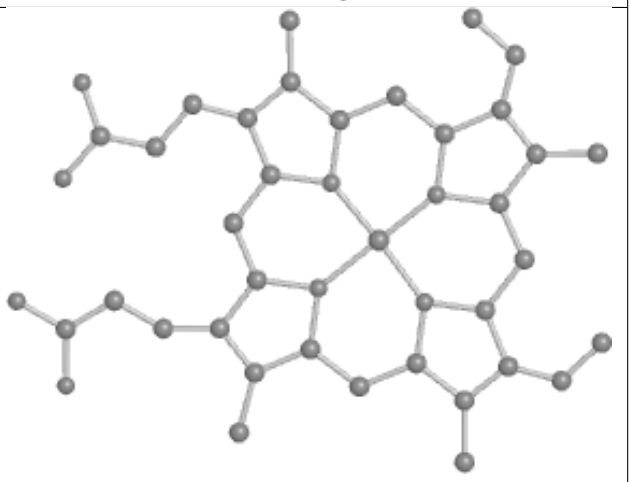
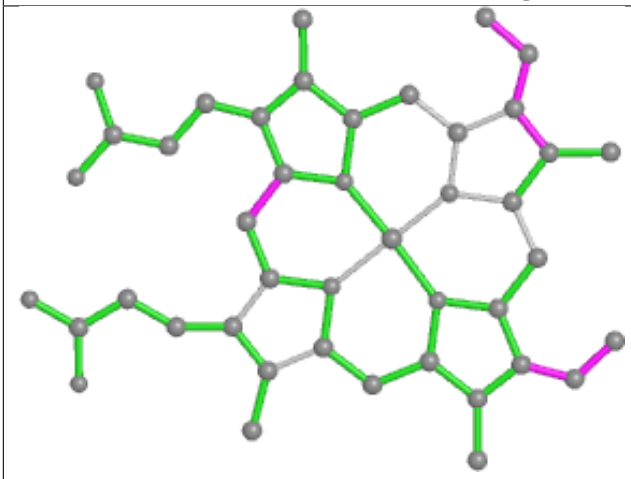
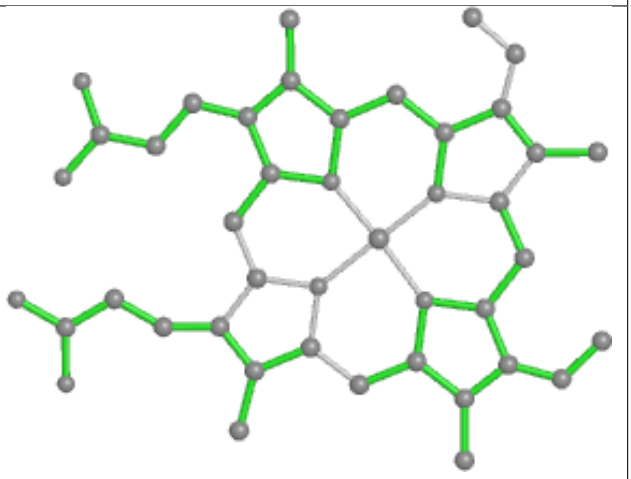


Rings

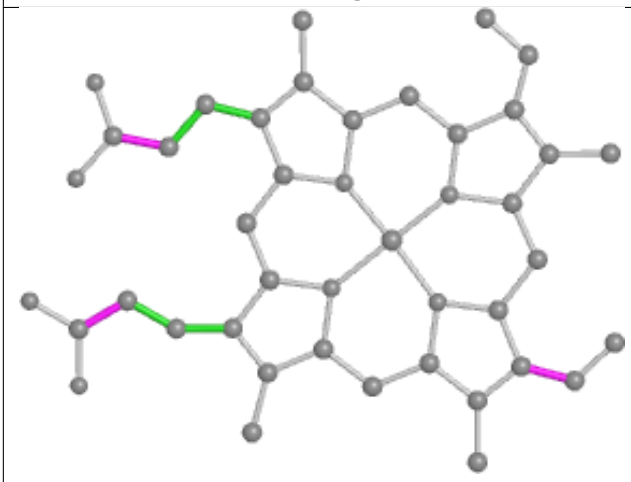
Ligand HEM G 160



Bond lengths



Bond angles



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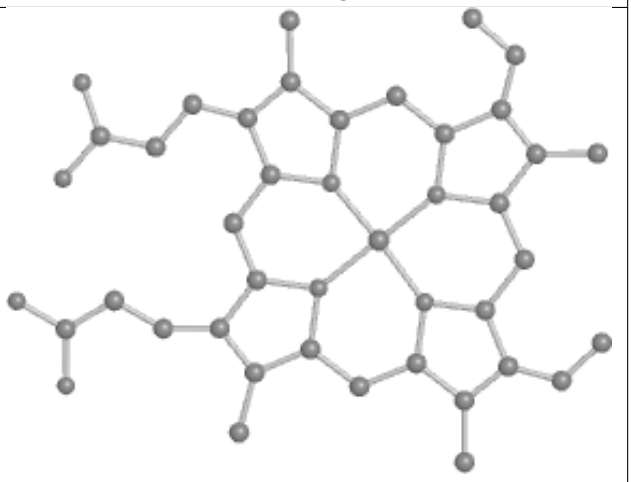
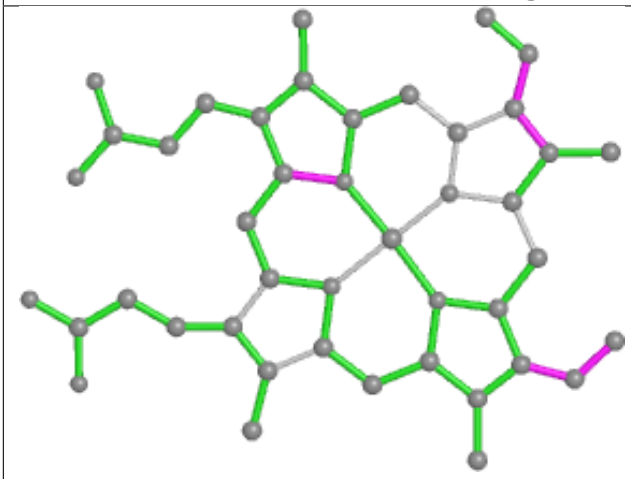
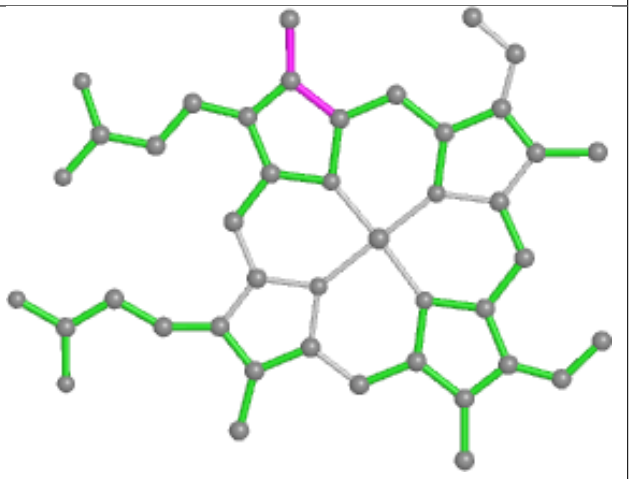


Rings

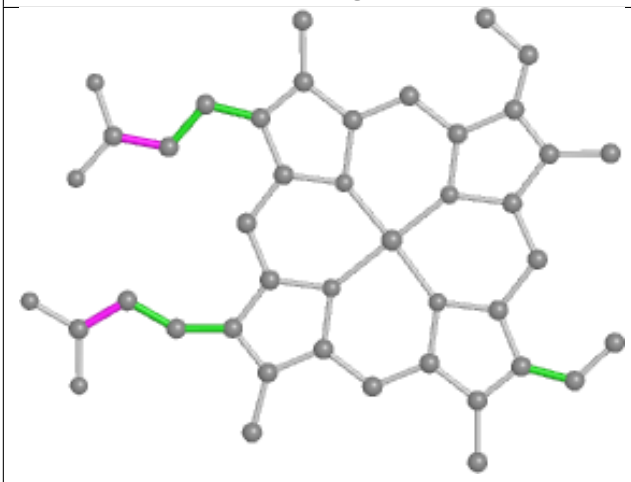
Ligand HEM J 160



Bond lengths



Bond angles



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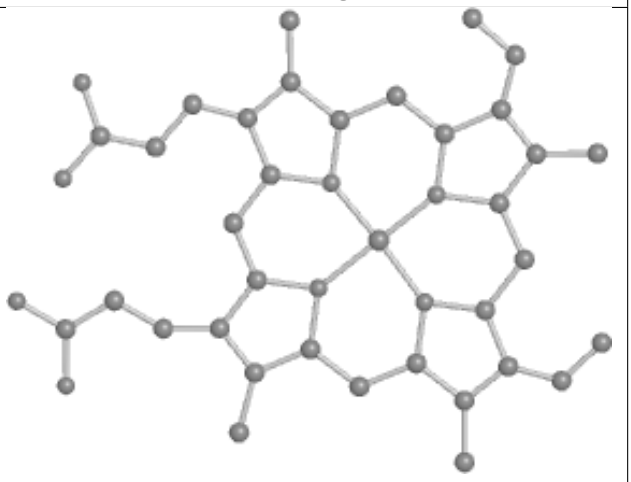
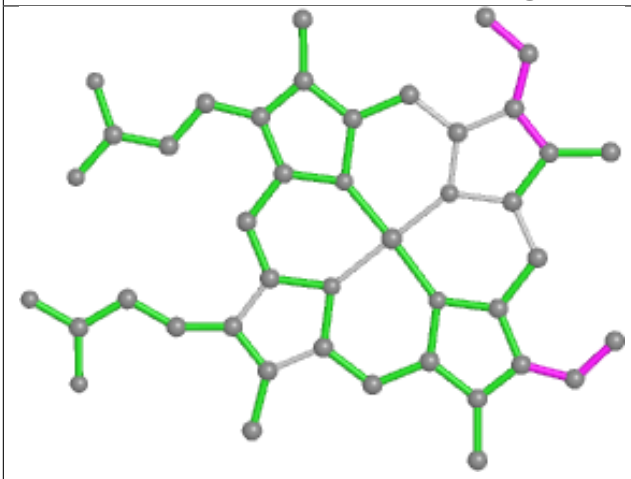
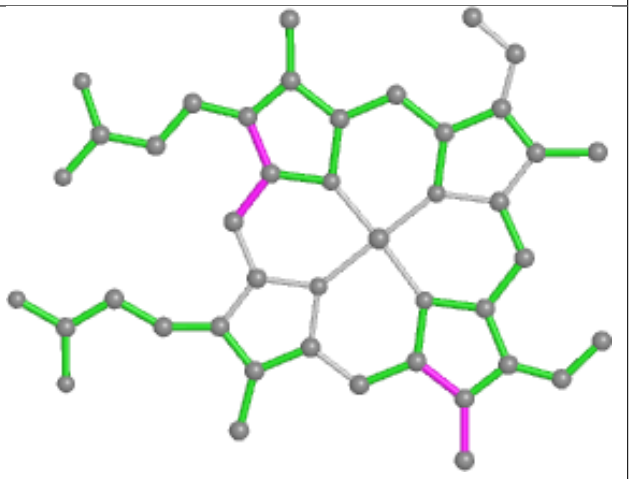


Rings

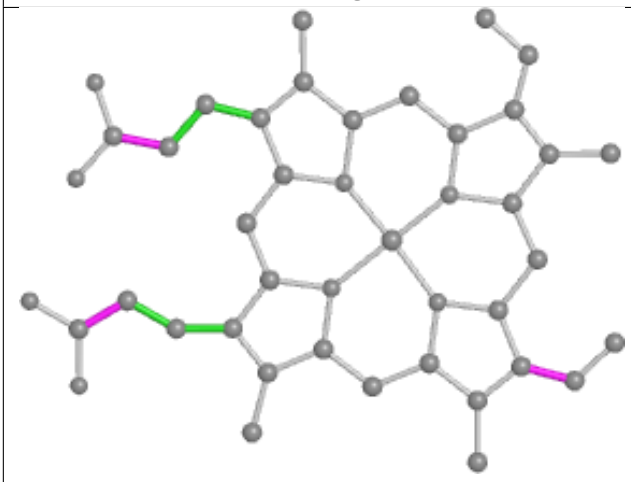
Ligand HEM L 160



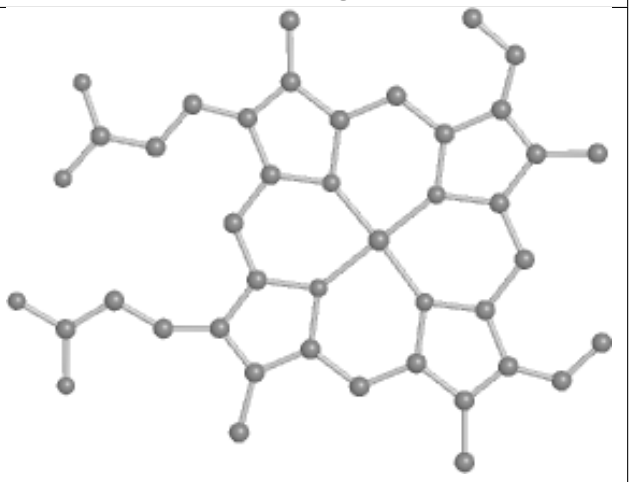
Bond lengths



Bond angles

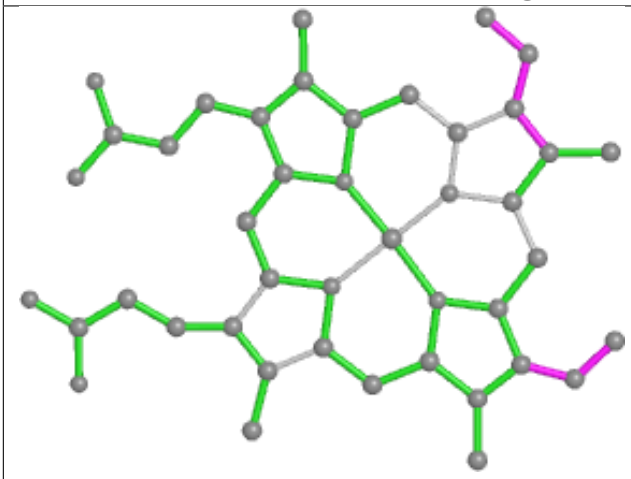


Torsions

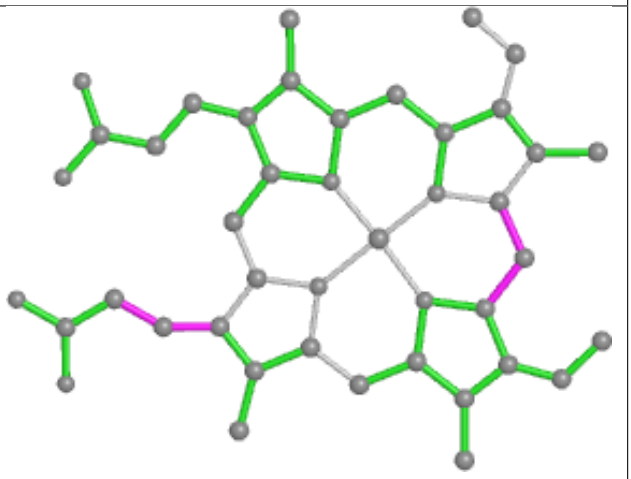


Rings

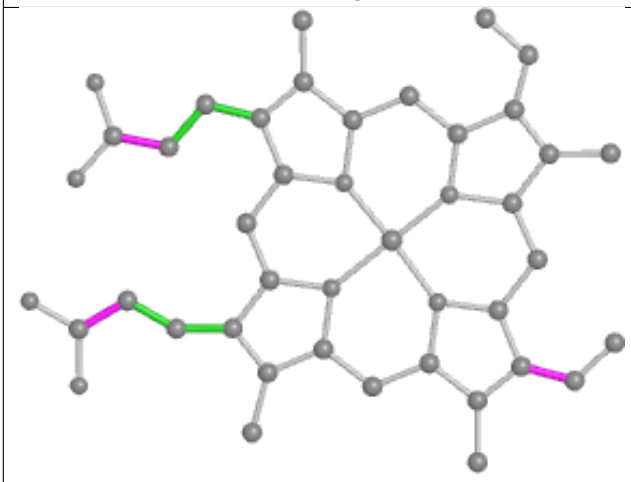
Ligand HEM C 160



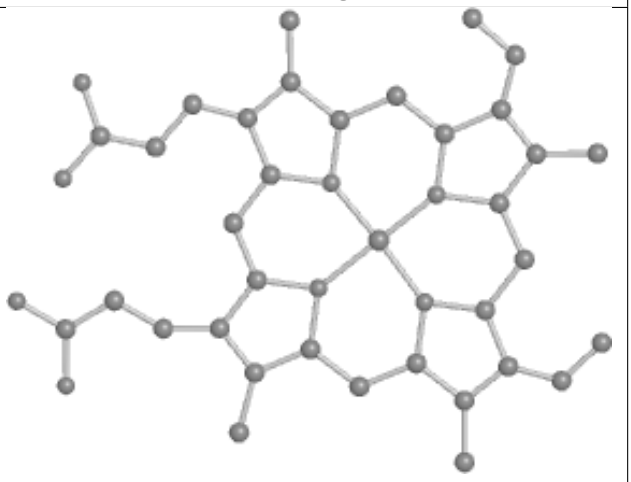
Bond lengths



Bond angles

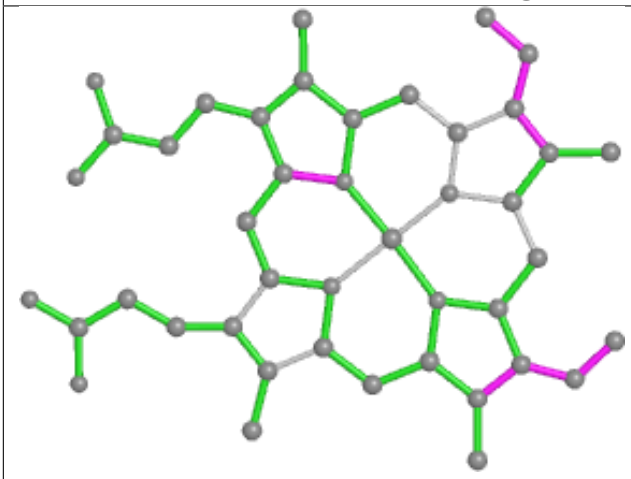


Torsions

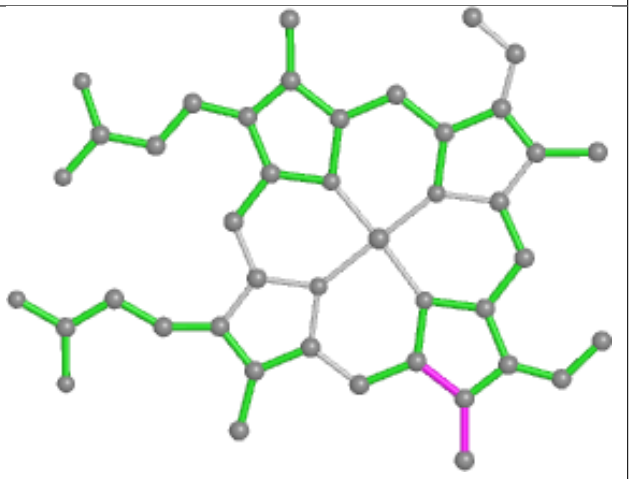


Rings

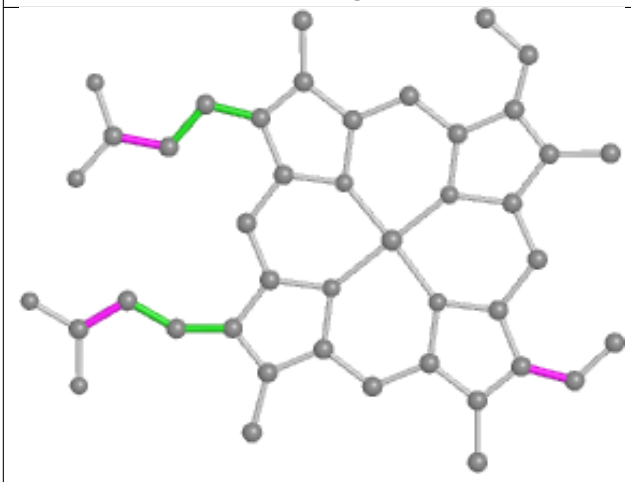
Ligand HEM H 160



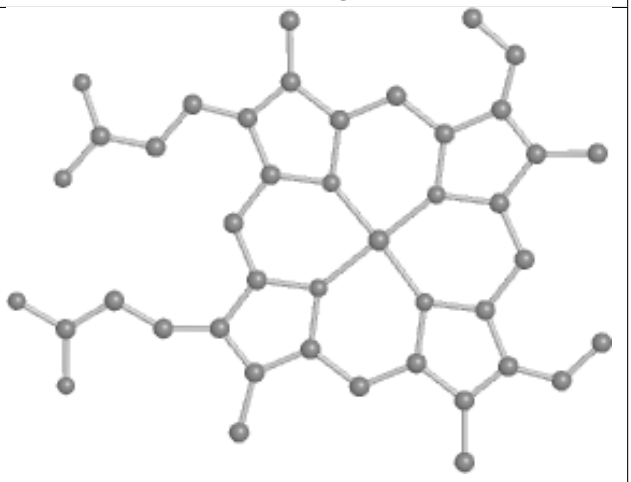
Bond lengths



Bond angles

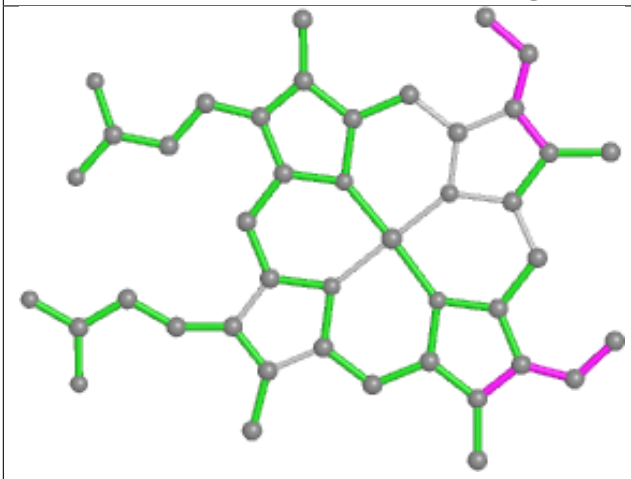


Torsions

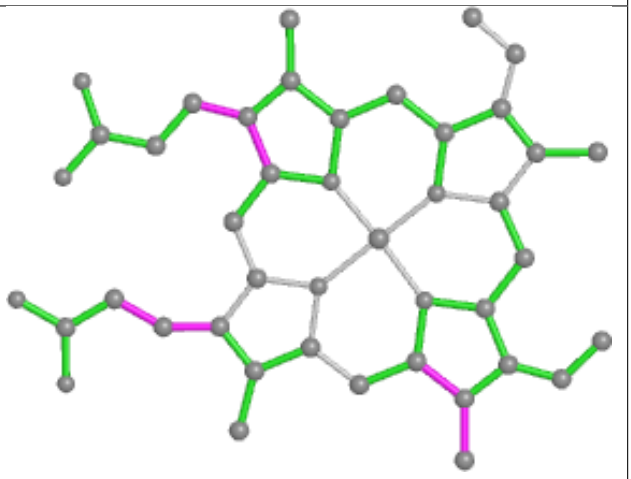


Rings

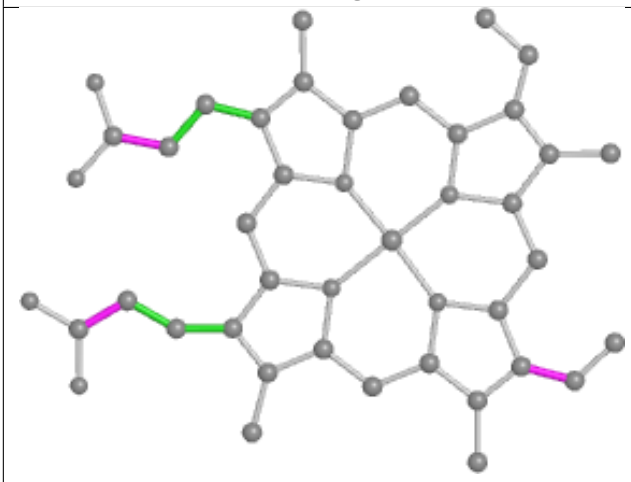
Ligand HEM I 160



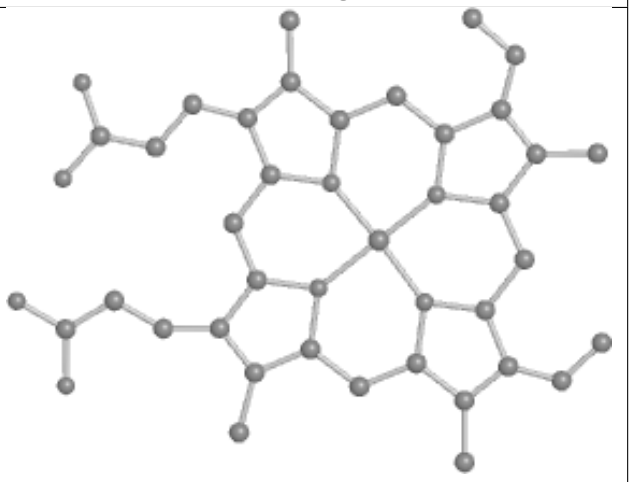
Bond lengths



Bond angles

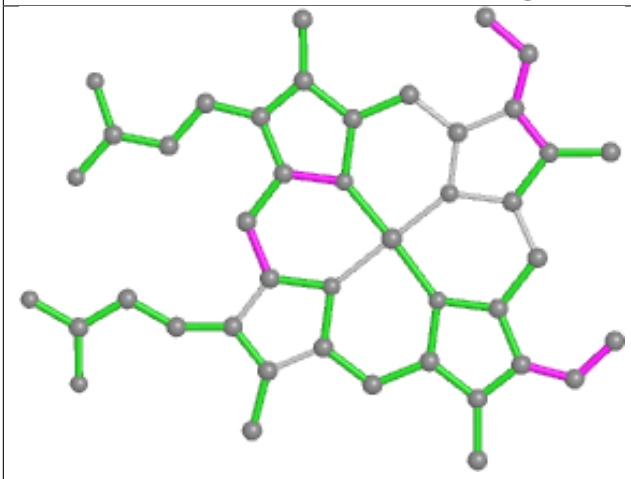


Torsions

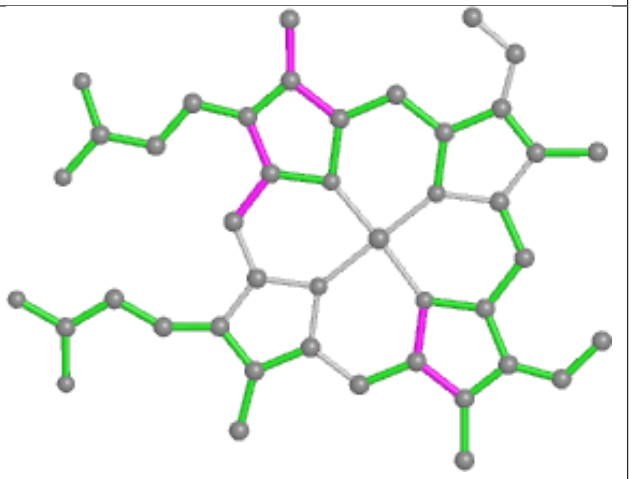


Rings

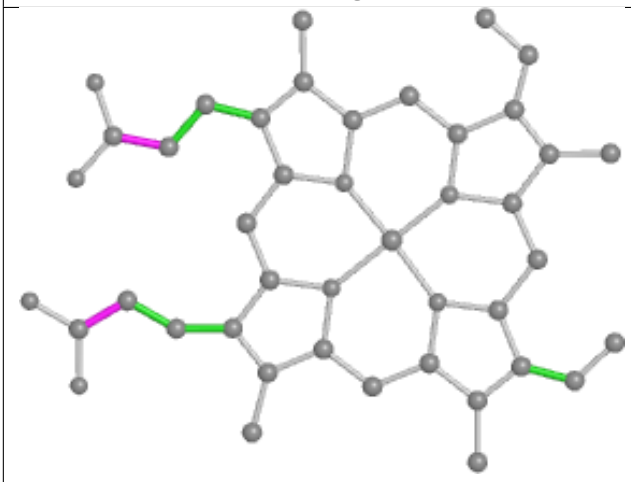
Ligand HEM B 160



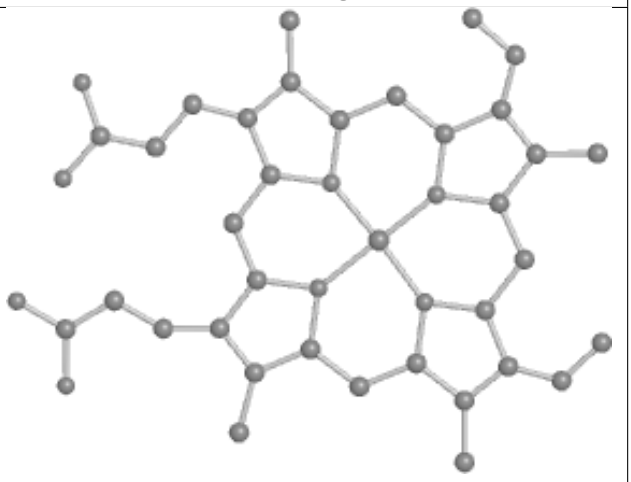
Bond lengths



Bond angles

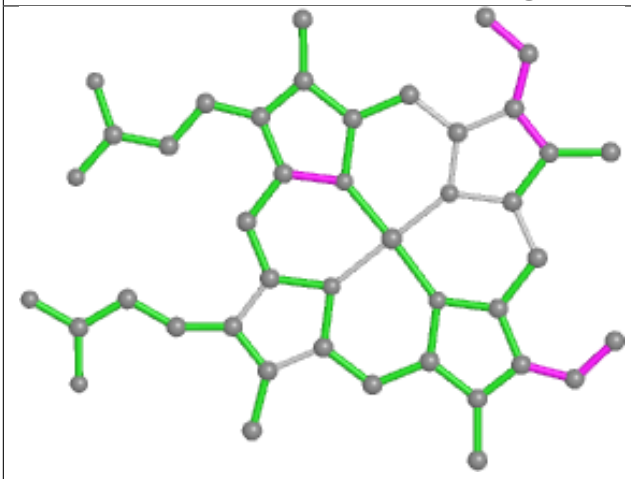


Torsions

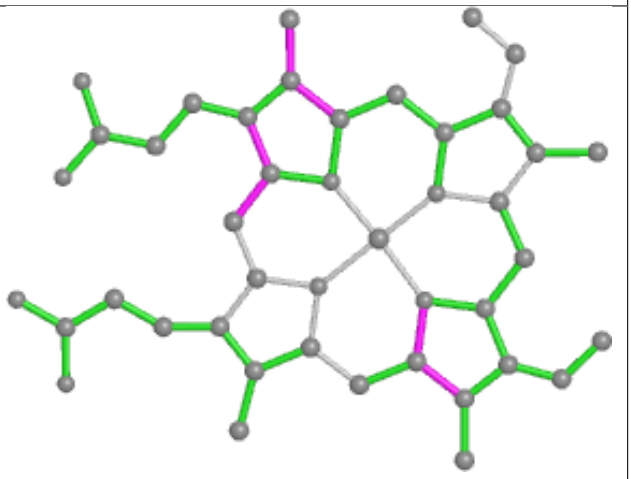


Rings

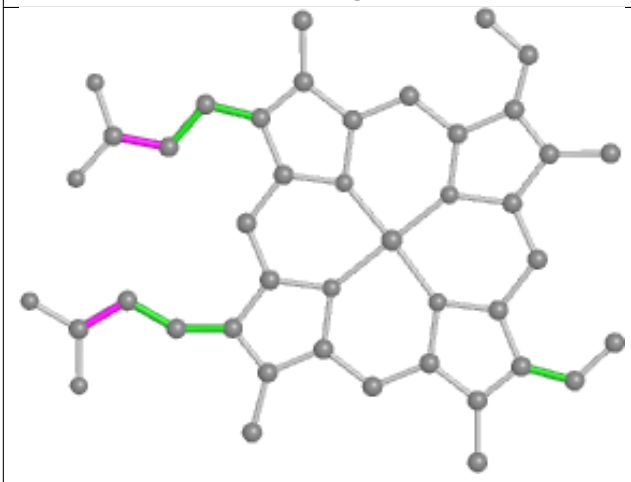
Ligand HEM F 160



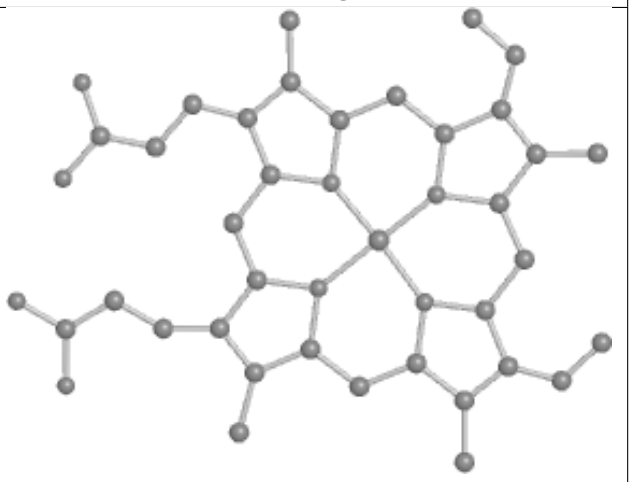
Bond lengths



Bond angles

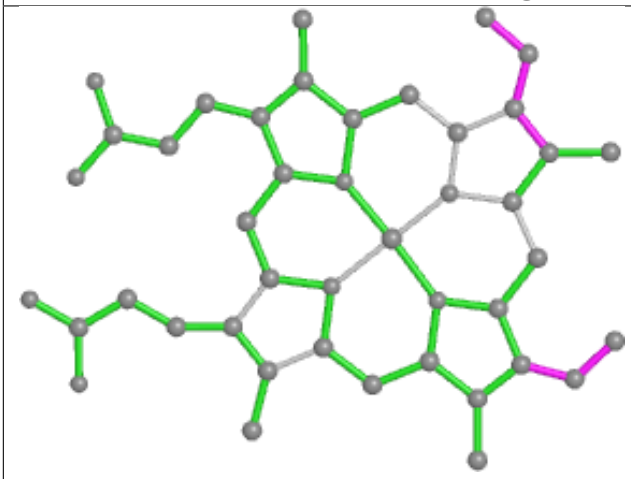


Torsions

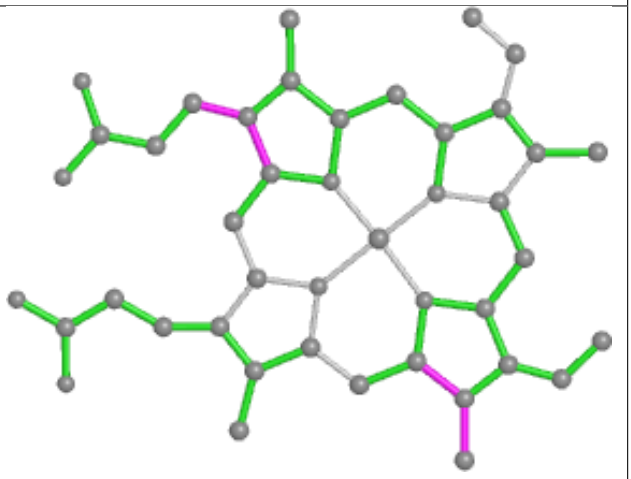


Rings

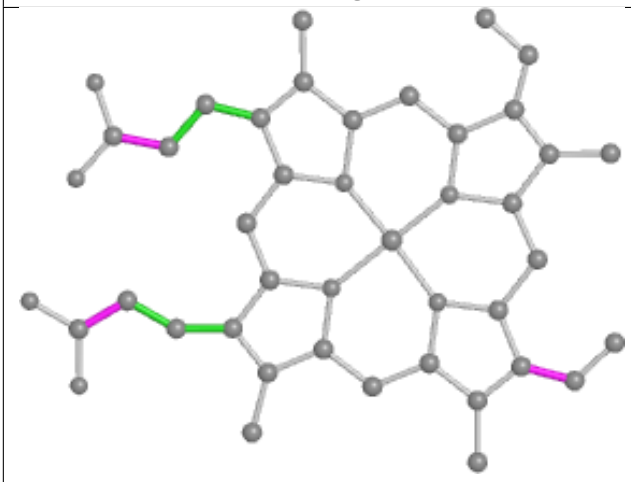
Ligand HEM A 160



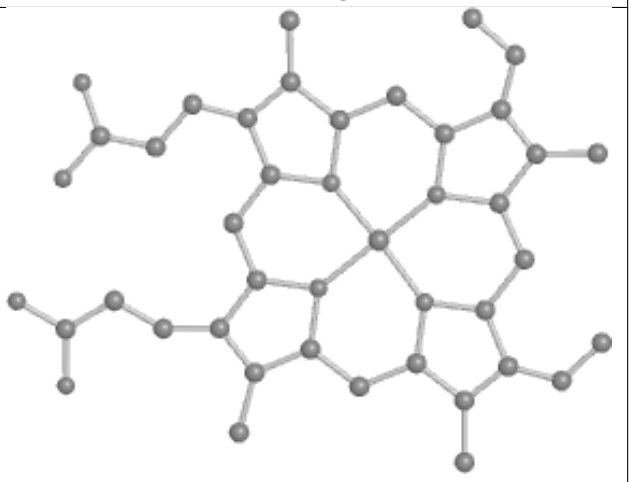
Bond lengths



Bond angles

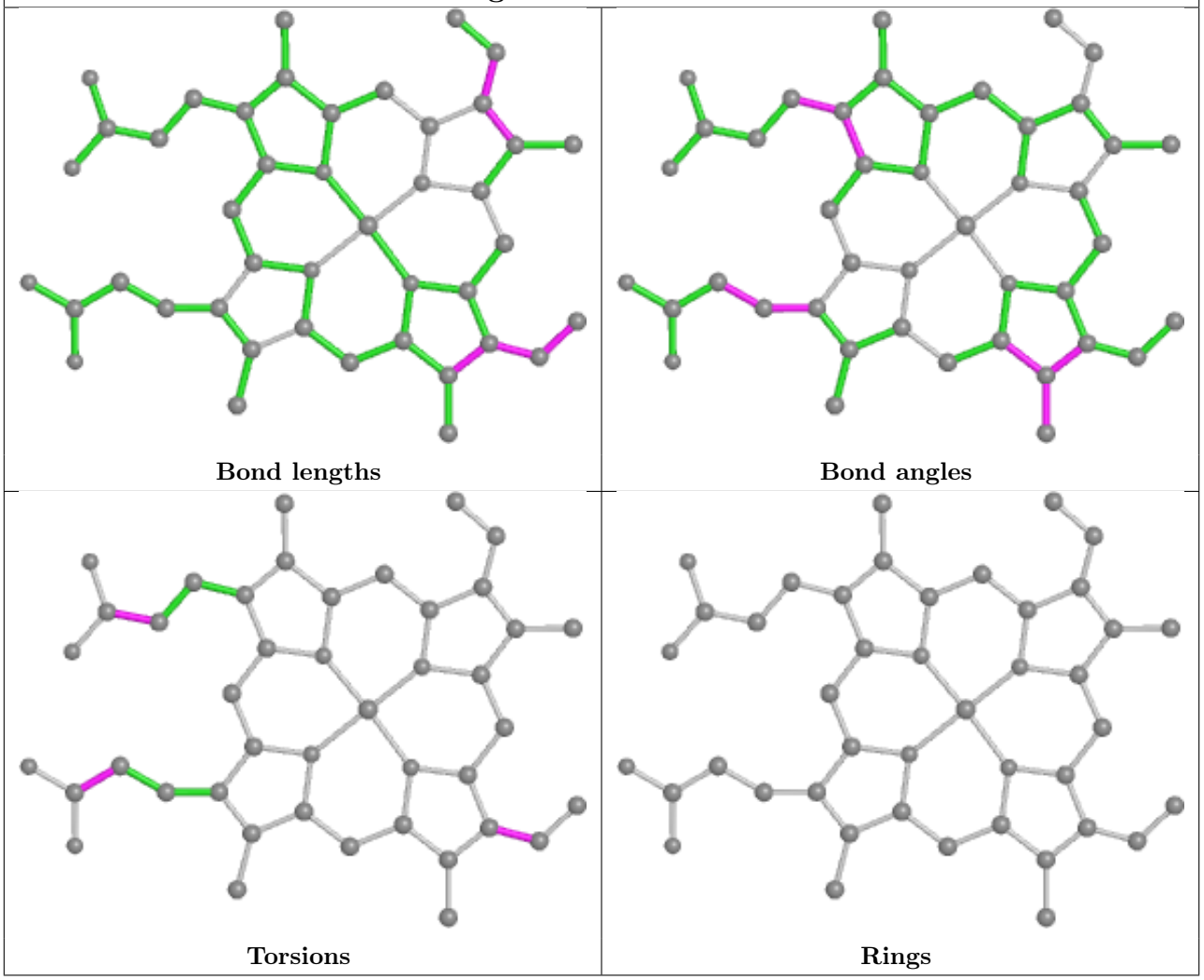


Torsions



Rings

Ligand HEM E 160



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

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	147/151 (97%)	-0.35	1 (0%) 87 83	20, 66, 108, 122	0
1	E	147/151 (97%)	-0.27	0 100 100	31, 71, 113, 122	0
1	I	147/151 (97%)	-0.38	0 100 100	22, 69, 109, 122	0
2	B	145/145 (100%)	-0.26	1 (0%) 87 83	10, 54, 102, 122	0
2	F	145/145 (100%)	-0.41	0 100 100	13, 49, 96, 116	0
2	J	145/145 (100%)	-0.04	3 (2%) 63 58	25, 69, 114, 122	0
3	C	149/153 (97%)	-0.39	1 (0%) 87 83	18, 62, 104, 122	0
3	G	149/153 (97%)	-0.02	3 (2%) 65 60	15, 63, 111, 122	0
3	K	149/153 (97%)	-0.22	0 100 100	33, 85, 122, 122	0
4	D	140/140 (100%)	-0.31	0 100 100	33, 66, 107, 122	0
4	H	140/140 (100%)	-0.29	0 100 100	31, 69, 107, 122	0
4	L	140/140 (100%)	-0.15	0 100 100	31, 72, 108, 122	0
5	M	217/217 (100%)	-0.22	2 (0%) 84 79	10, 48, 117, 122	0
6	N	220/220 (100%)	-0.18	1 (0%) 91 88	9, 64, 120, 122	0
7	O	215/215 (100%)	0.10	3 (1%) 75 69	16, 69, 114, 122	0
All	All	2395/2419 (99%)	-0.21	15 (0%) 89 86	9, 66, 114, 122	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	J	144	HIS	3.5
2	J	145	HIS	3.3
3	G	4	GLU	3.2
3	G	3	HIS	2.9
5	M	20	HIS	2.8
7	O	179	HIS	2.6
2	B	145	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
6	N	14	LEU	2.6
3	C	3	HIS	2.5
7	O	17	LEU	2.4
2	J	123	ARG	2.2
7	O	102	THR	2.2
5	M	19	LEU	2.2
3	G	59	ILE	2.2
1	A	128	SER	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
10	CA	M	250	1/1	0.92	0.06	20,20,20,20	0
9	HEM	K	160	43/43	0.94	0.31	91,91,91,91	0
9	HEM	A	160	43/43	0.94	0.29	60,60,60,60	0
10	CA	N	250	1/1	0.94	0.08	15,15,15,15	0
9	HEM	H	160	43/43	0.95	0.32	52,52,52,52	0
11	ZN	M	252	1/1	0.95	0.07	58,58,58,58	0
9	HEM	J	160	43/43	0.96	0.34	54,54,54,54	0
9	HEM	E	160	43/43	0.96	0.29	71,71,71,71	0
9	HEM	L	160	43/43	0.96	0.34	46,46,46,46	0
9	HEM	G	160	43/43	0.96	0.41	66,66,66,66	0
10	CA	M	251	1/1	0.96	0.15	43,43,43,43	0
9	HEM	C	160	43/43	0.96	0.28	39,39,39,39	0
10	CA	O	250	1/1	0.96	0.06	23,23,23,23	0
9	HEM	I	160	43/43	0.96	0.30	64,64,64,64	0
9	HEM	F	160	43/43	0.97	0.27	37,37,37,37	0

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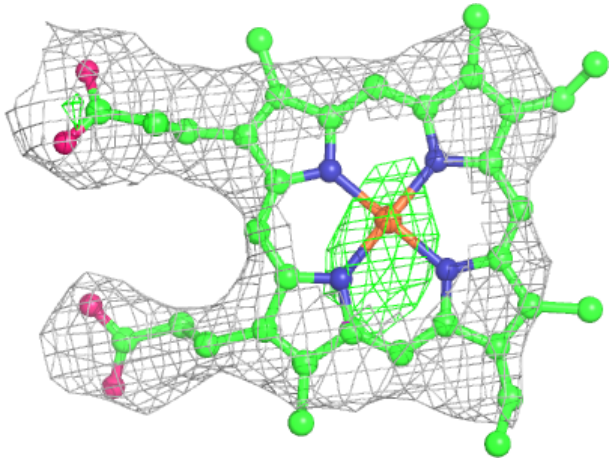
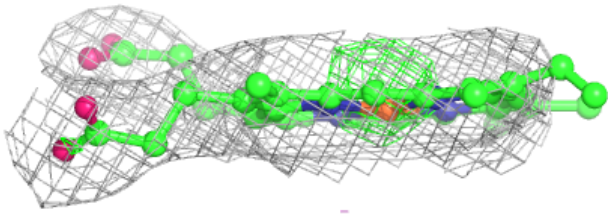
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	HEM	D	160	43/43	0.97	0.25	38,38,38,38	0
9	HEM	B	160	43/43	0.97	0.24	26,26,26,26	0
8	CMO	E	161	2/2	0.98	0.43	54,54,54,54	0
8	CMO	L	161	2/2	0.99	0.18	72,72,72,72	0
8	CMO	B	161	2/2	0.99	0.12	46,46,46,46	0
8	CMO	C	161	2/2	0.99	0.36	46,46,46,46	0
8	CMO	A	161	2/2	0.99	0.25	82,82,82,82	0
8	CMO	F	161	2/2	0.99	0.20	64,64,64,64	0
8	CMO	G	161	2/2	0.99	0.20	38,38,38,38	0
8	CMO	H	161	2/2	0.99	0.29	68,68,68,68	0
8	CMO	J	161	2/2	0.99	0.22	69,69,69,69	0
8	CMO	K	161	2/2	0.99	0.31	69,69,69,69	0
8	CMO	D	161	2/2	1.00	0.19	74,74,74,74	0
8	CMO	I	161	2/2	1.00	0.17	80,80,80,80	0

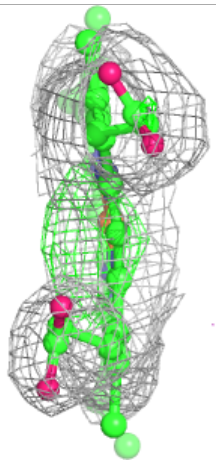
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around HEM K 160:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

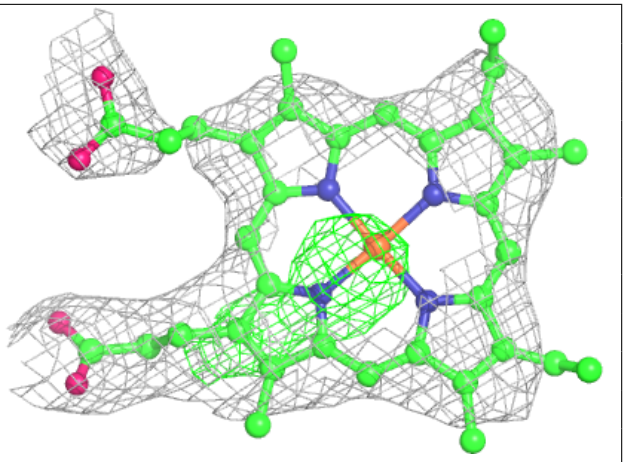


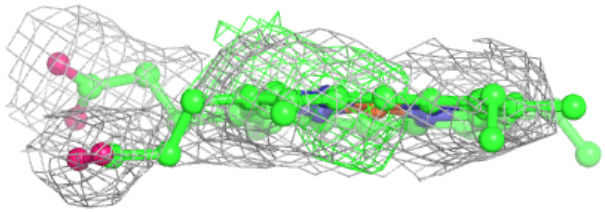


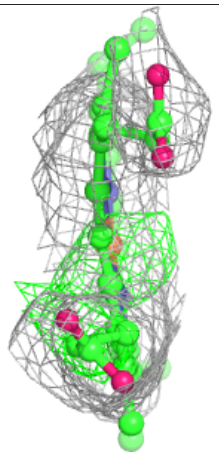


Electron density around HEM A 160:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

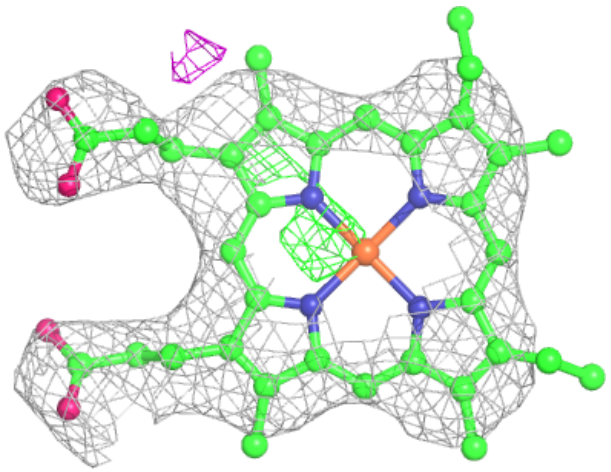


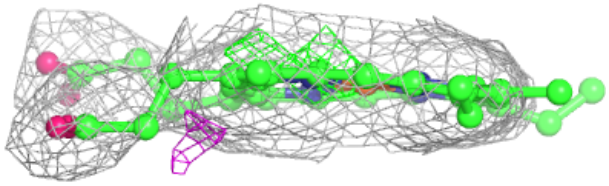


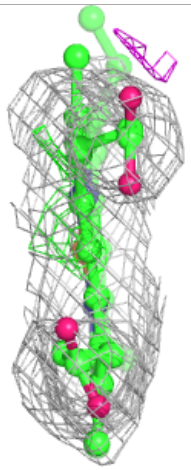


Electron density around HEM H 160:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

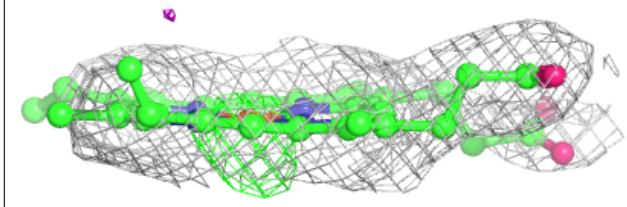


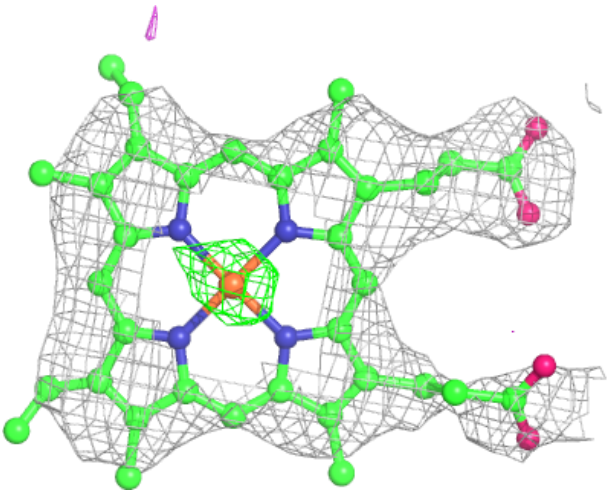


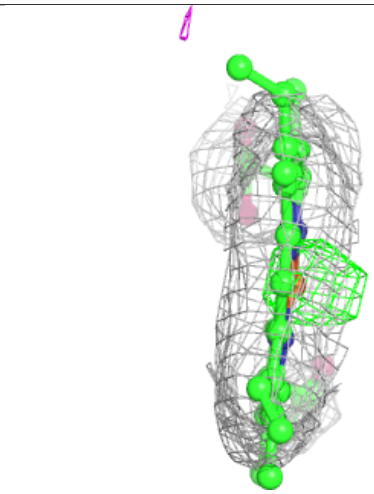


Electron density around HEM J 160:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

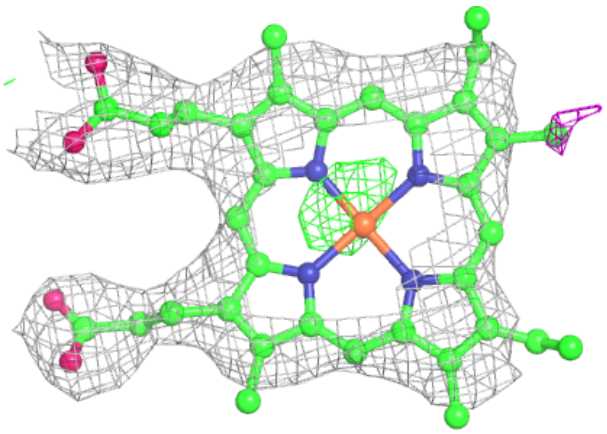


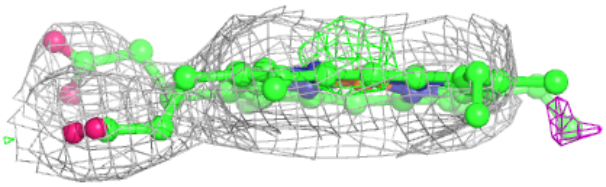


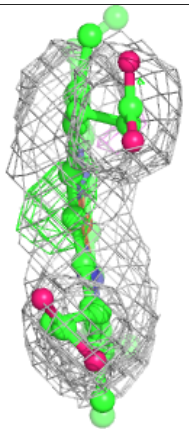


Electron density around HEM E 160:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

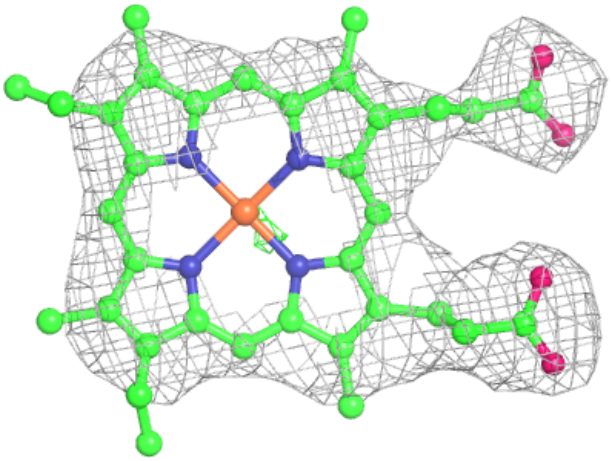


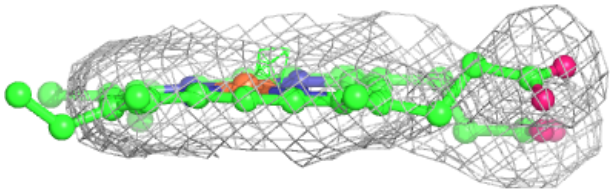


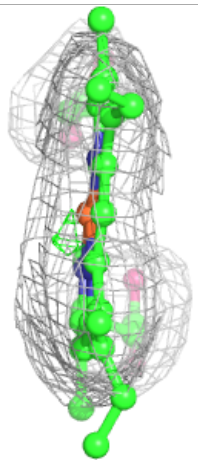


Electron density around HEM L 160:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

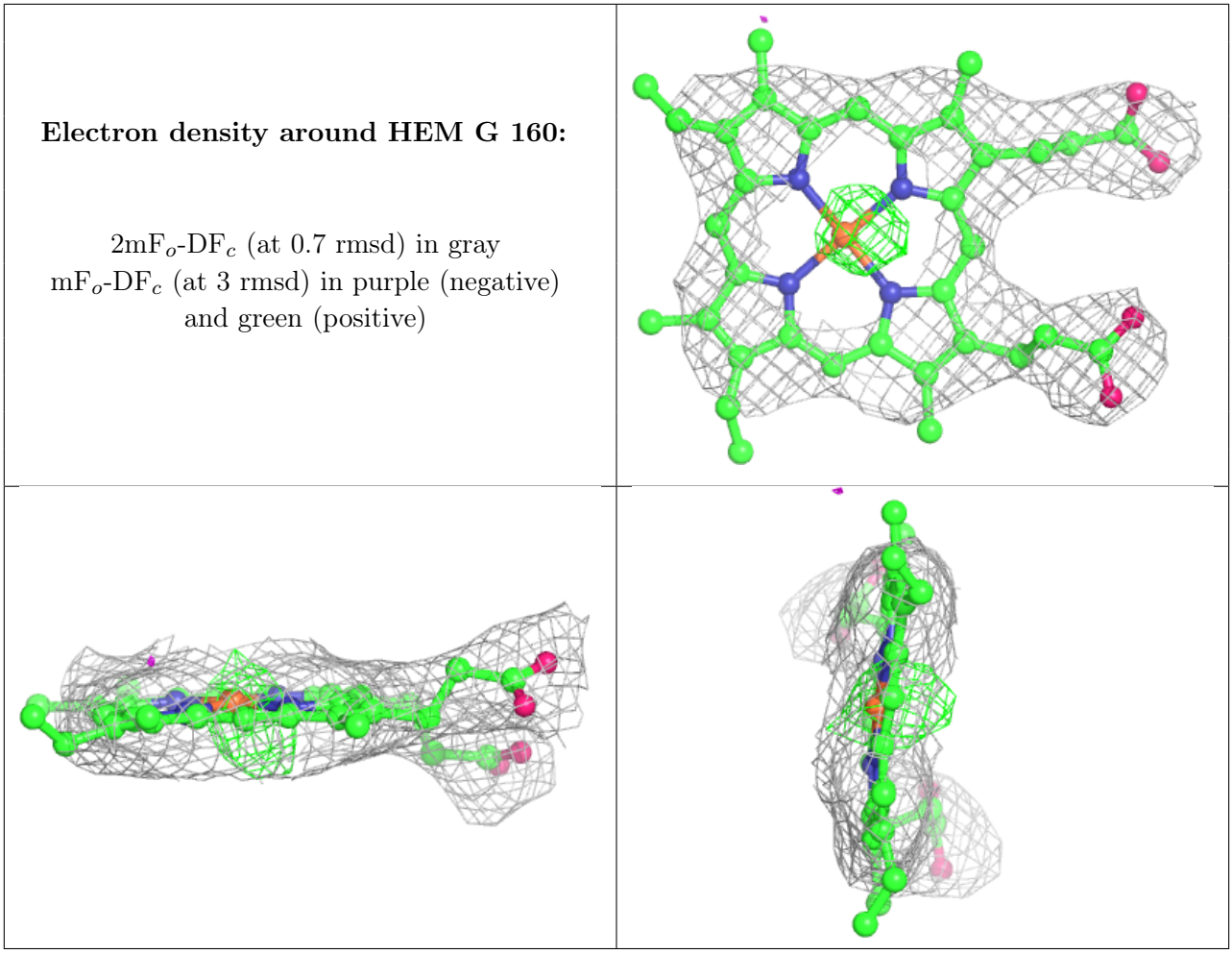






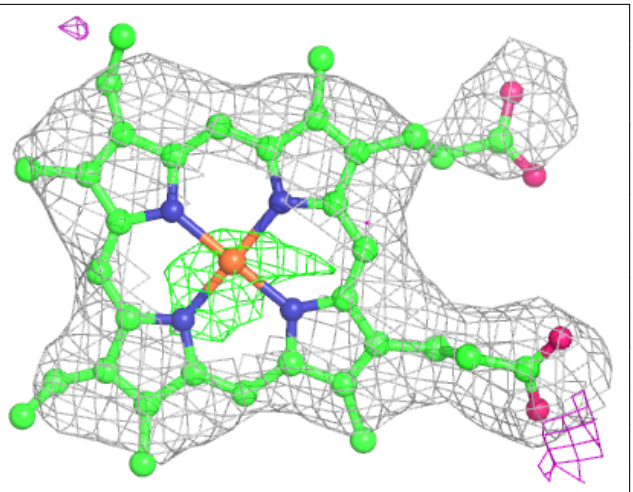
Electron density around HEM G 160:

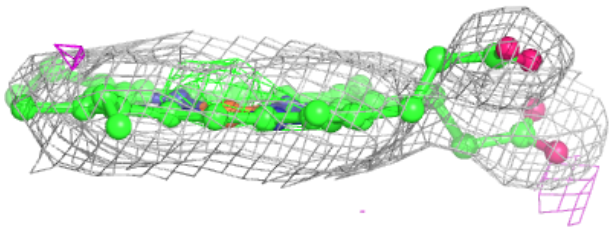
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

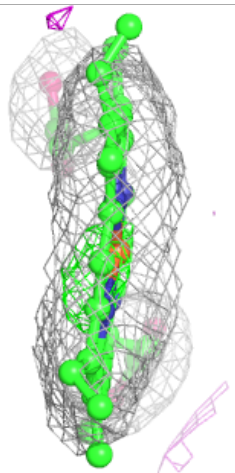


Electron density around HEM C 160:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

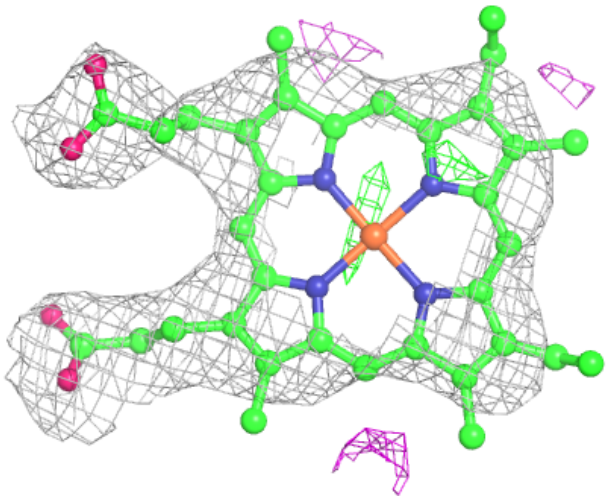


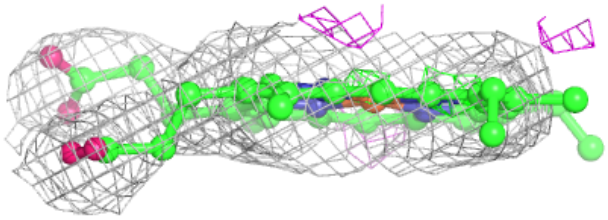


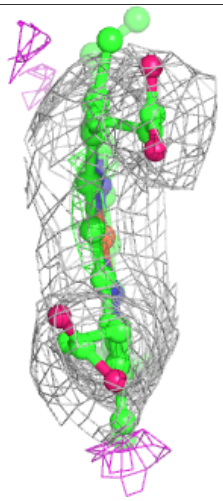


Electron density around HEM I 160:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

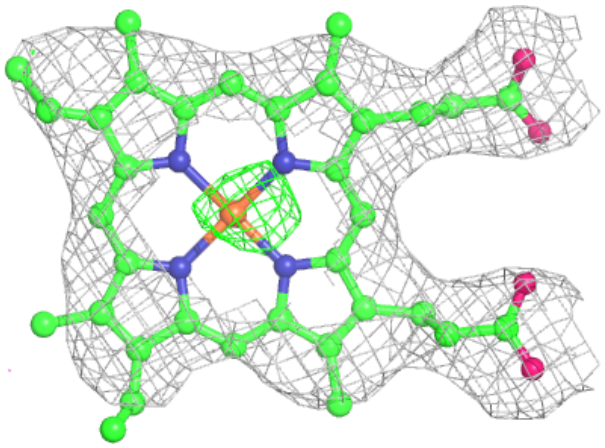


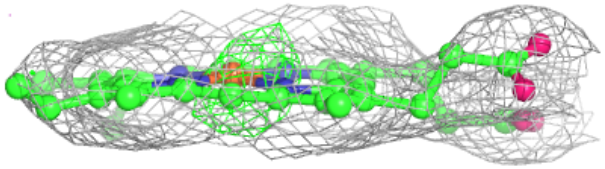


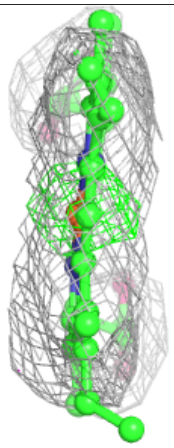


Electron density around HEM F 160:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

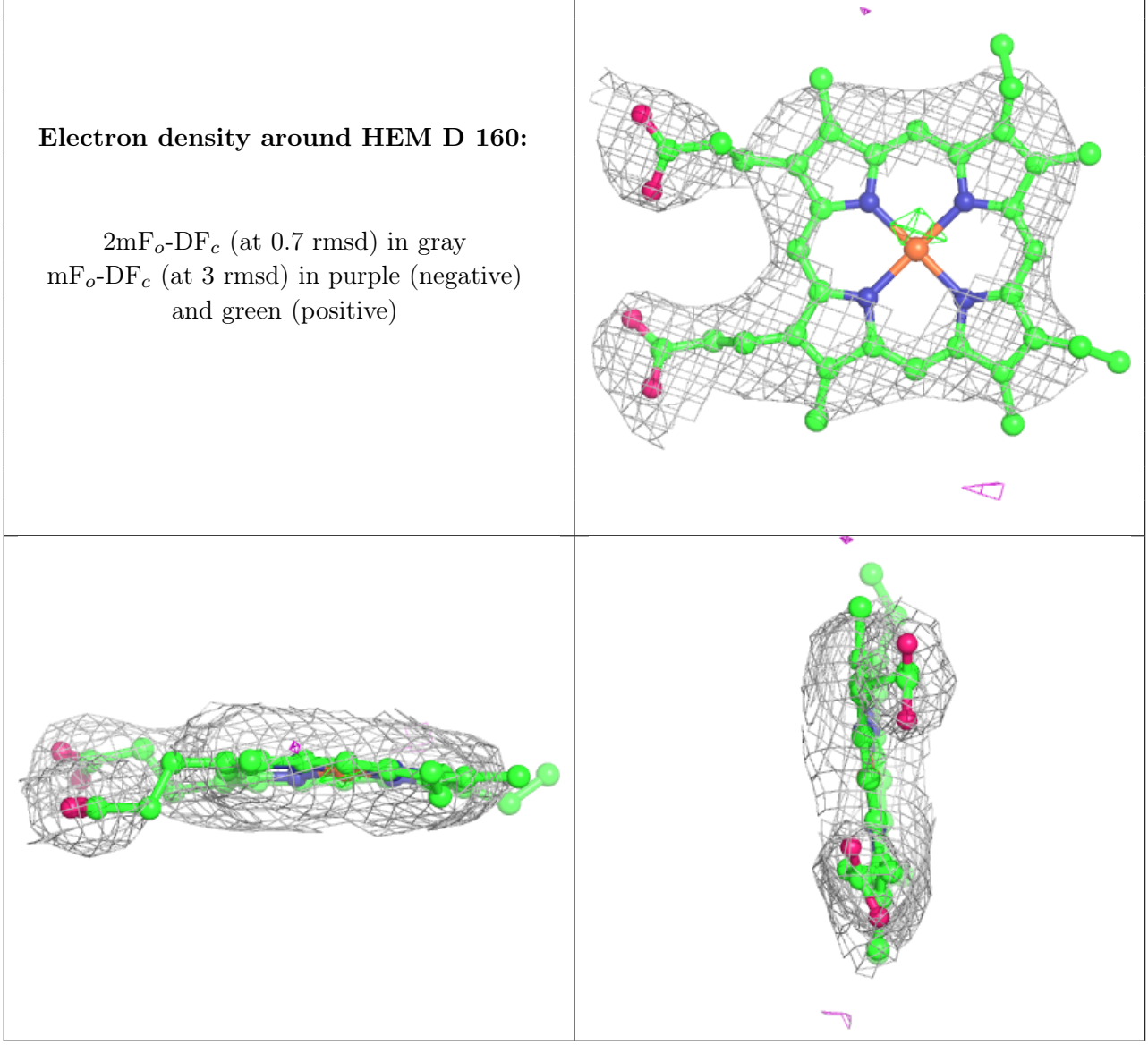






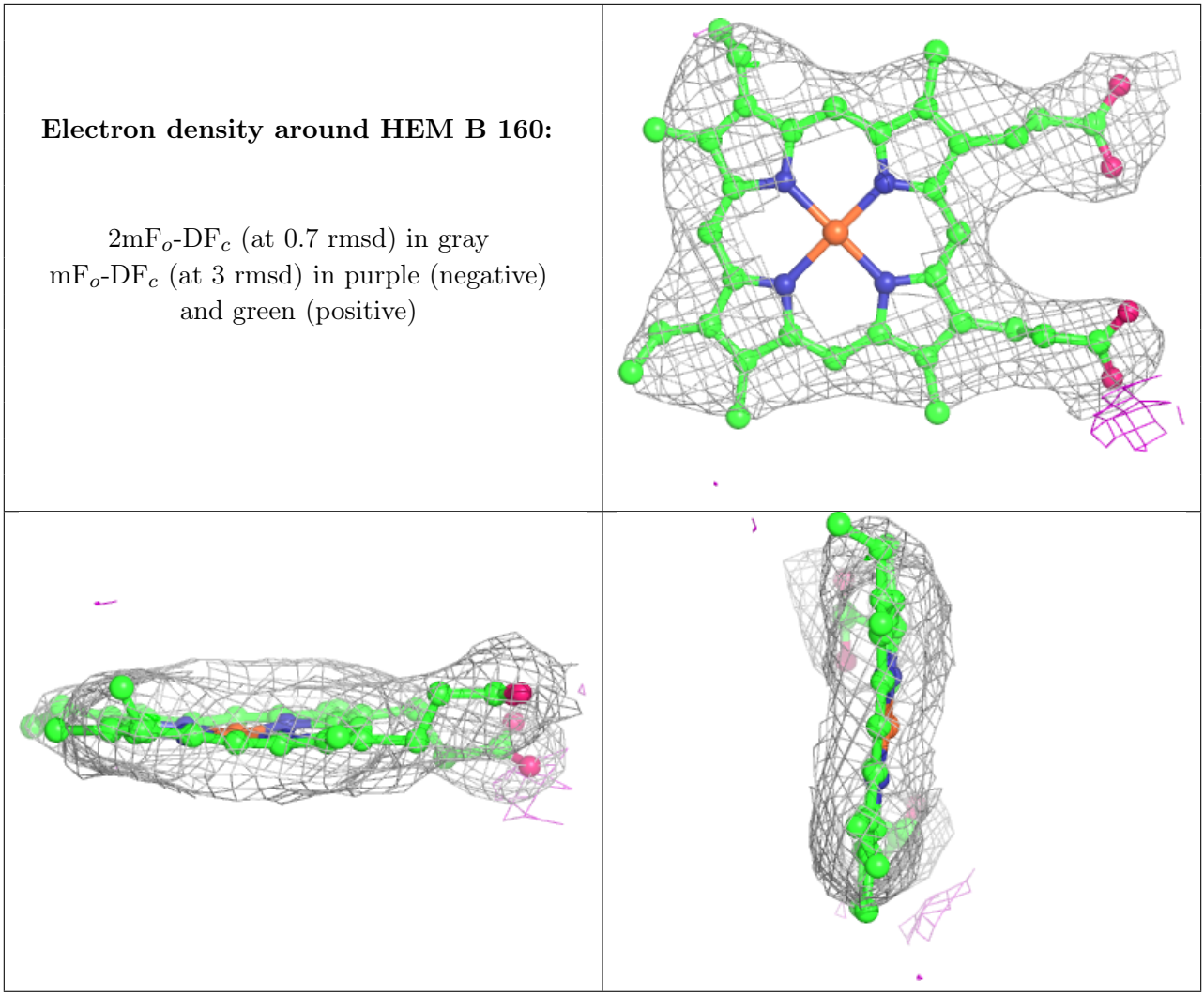
Electron density around HEM D 160:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around HEM B 160:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers

There are no such residues in this entry.