



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 01:31 PM UTC

PDB ID : 2GTL / pdb_00002gtl
Title : Lumbricus Erythrocrutorin at 3.5Å 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

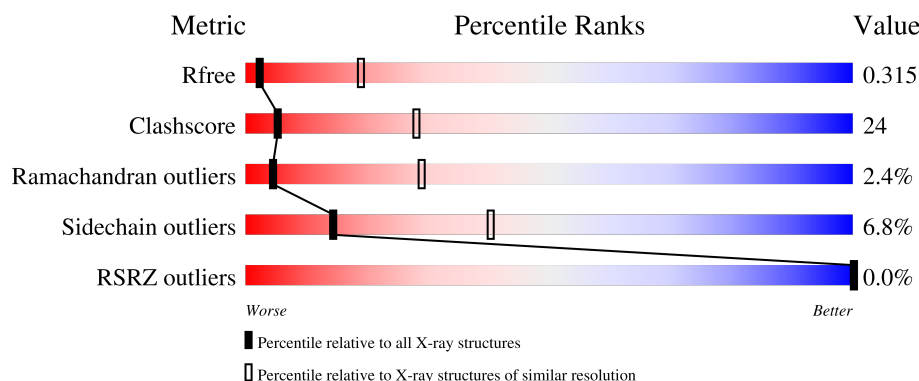
1 Overall quality at a glance

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}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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 $\leq 5\%$. 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	% 47% 44% 5% ...
1	E	151	49% 43% ...
1	I	151	48% 43% 5% ...
2	B	145	65% 33% .
2	F	145	62% 37% .

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Mol	Chain	Length	Quality of chain
2	J	145	 63% 35% .
3	C	153	 57% 35% 6% .
3	G	153	 58% 35% 5% .
3	K	153	 55% 37% 5% .
4	D	140	 56% 39% . .
4	H	140	 57% 38% . .
4	L	140	 59% 36% . .
5	M	217	 45% 43% 10% .
6	N	220	 51% 38% 10% .
7	O	215	 60% 37% . .

2 Entry composition

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			

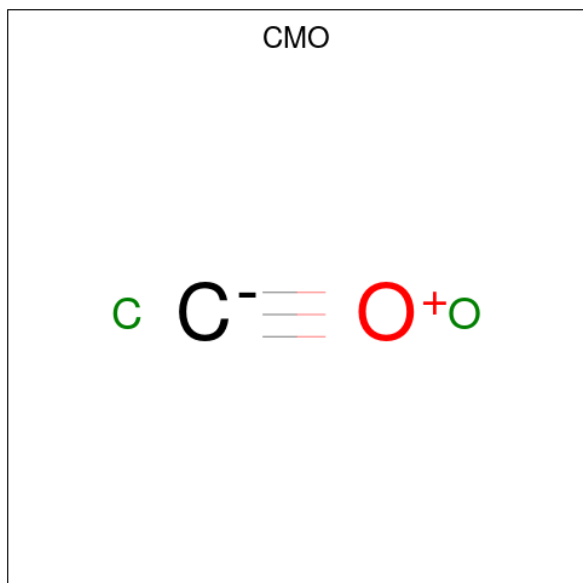
- Molecule 7 is a protein called Extracellular hemoglobin linker L3 subunit.

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 (CCD ID: CMO) (formula: CO).



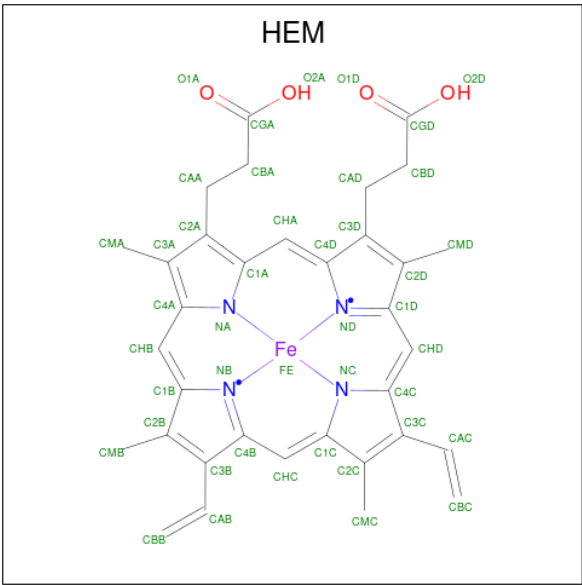
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			2	1	1		
8	B	1	Total	C	O	0	0
			2	1	1		
8	C	1	Total	C	O	0	0
			2	1	1		
8	D	1	Total	C	O	0	0
			2	1	1		
8	E	1	Total	C	O	0	0
			2	1	1		
8	F	1	Total	C	O	0	0
			2	1	1		
8	G	1	Total	C	O	0	0
			2	1	1		
8	H	1	Total	C	O	0	0
			2	1	1		
8	I	1	Total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

- Molecule 9 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄).



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

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

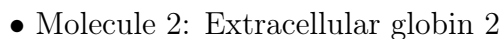
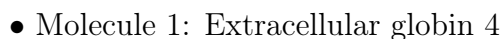
- Molecule 10 is CALCIUM ION (CCD ID: CA) (formula: Ca).

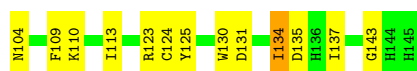
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	M	2	Total 2	Ca 2	0	0
10	N	1	Total 1	Ca 1	0	0
10	O	1	Total 1	Ca 1	0	0

- Molecule 11 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 1: Extracellular globin 4





• Molecule 2: Extracellular globin 2

Chain F: 62% 37% .



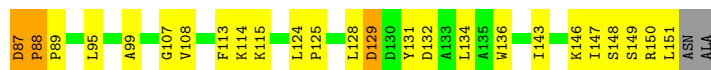
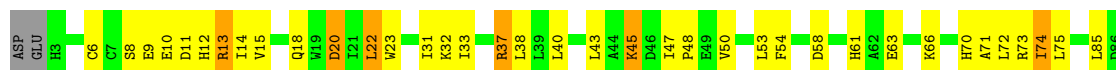
• Molecule 2: Extracellular globin 2

Chain J: 63% 35% .



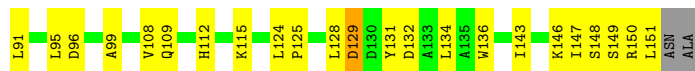
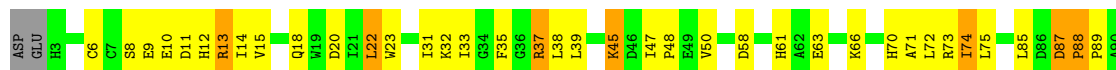
• Molecule 3: Extracellular globin-3

Chain C: 57% 35% 6% .



• Molecule 3: Extracellular globin-3

Chain G: 58% 35% 5% .



• Molecule 3: Extracellular globin-3

Chain K: 55% 37% 5% .





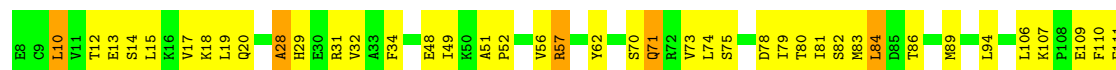
• Molecule 4: Hemoglobin chain d1



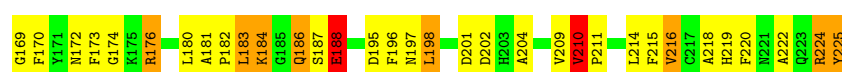
• Molecule 4: Hemoglobin chain d1



• Molecule 4: Hemoglobin chain d1

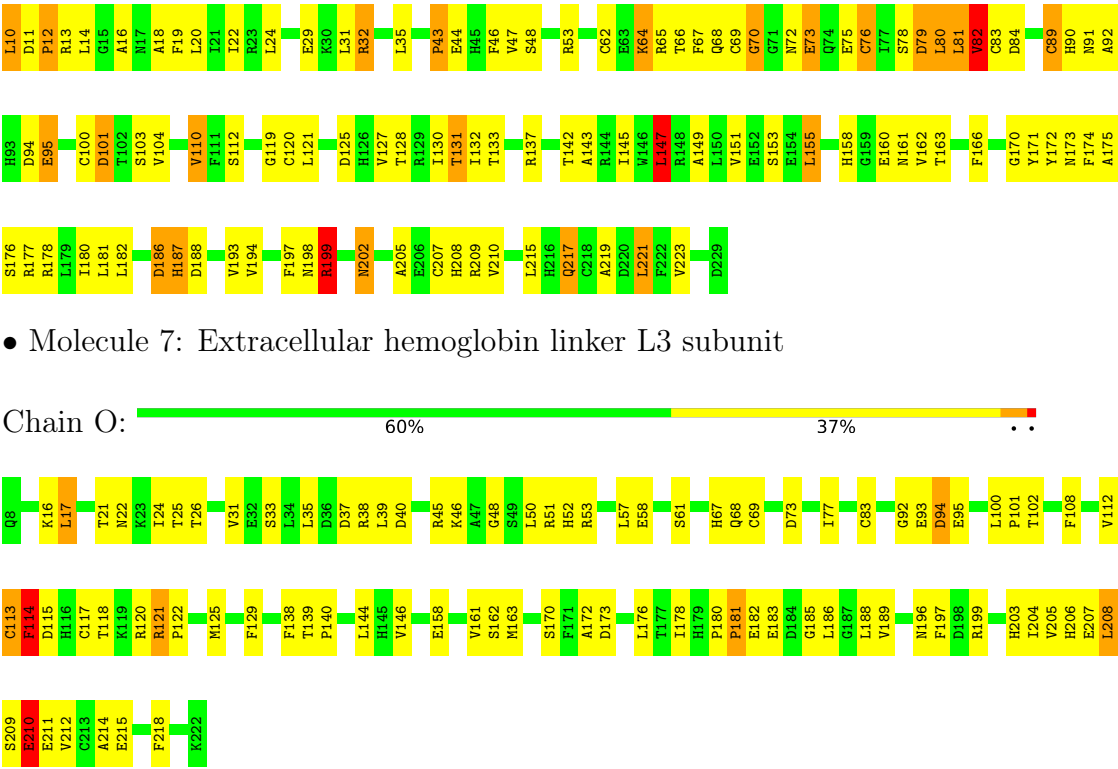


• Molecule 5: Hemoglobin linker chain L1



• Molecule 6: Extracellular hemoglobin linker L2 subunit





• Molecule 7: Extracellular hemoglobin linker L3 subunit

Chain O: 60% 37%

4 Data and refinement statistics

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 – 3.50 100.00 – 3.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (100.00-3.50) 63.7 (100.00-3.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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)	0.28 , 0.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.015 for -h,k,-l	Xtriage
F_o, F_c correlation	0.52	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.61	1/1237 (0.1%)	0.97	3/1670 (0.2%)
1	E	0.58	0/1237	0.95	3/1670 (0.2%)
1	I	0.58	0/1237	0.95	3/1670 (0.2%)
2	B	0.60	0/1176	0.90	2/1587 (0.1%)
2	F	0.60	0/1176	0.90	1/1587 (0.1%)
2	J	0.57	0/1176	0.89	0/1587
3	C	0.58	0/1209	0.93	5/1633 (0.3%)
3	G	0.54	0/1209	0.91	5/1633 (0.3%)
3	K	0.57	0/1209	0.92	5/1633 (0.3%)
4	D	0.58	0/1159	0.90	4/1568 (0.3%)
4	H	0.56	0/1159	0.88	4/1568 (0.3%)
4	L	0.53	0/1159	0.87	4/1568 (0.3%)
5	M	0.63	0/1745	1.03	10/2371 (0.4%)
6	N	0.58	0/1752	0.98	6/2369 (0.3%)
7	O	0.55	0/1699	0.98	6/2298 (0.3%)
All	All	0.58	1/19539 (0.0%)	0.94	61/26412 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	48	THR	N-CA	-5.58	1.39	1.46

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	65	GLU	N-CA-C	-7.94	102.61	111.82
1	A	65	GLU	N-CA-C	-7.89	102.67	111.82
7	O	73	ASP	CA-C-N	7.75	127.68	119.85
7	O	73	ASP	C-N-CA	7.75	127.68	119.85
1	E	65	GLU	N-CA-C	-7.68	102.91	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	138	CYS	N-CA-C	7.44	120.48	111.40
5	M	61	HIS	N-CA-C	7.18	120.15	111.82
5	M	141	PHE	CA-C-N	7.03	126.65	119.19
5	M	141	PHE	C-N-CA	7.03	126.65	119.19
7	O	121	ARG	CA-C-N	6.91	126.87	120.03
7	O	121	ARG	C-N-CA	6.91	126.87	120.03
4	H	138	CYS	N-CA-C	6.84	119.75	111.40
6	N	80	LEU	N-CA-C	-6.49	105.12	113.16
3	K	13	ARG	N-CA-C	-6.26	103.75	111.33
4	D	28	ALA	CB-CA-C	-6.19	109.43	116.54
1	A	109	LYS	N-CA-C	-6.15	104.69	111.82
1	E	109	LYS	N-CA-C	-6.14	104.69	111.82
5	M	222	ALA	N-CA-C	6.14	119.66	110.14
3	C	13	ARG	N-CA-C	-6.00	104.07	111.33
4	L	28	ALA	CB-CA-C	-5.97	109.67	116.54
1	I	109	LYS	N-CA-C	-5.97	104.90	111.82
4	H	28	ALA	CB-CA-C	-5.94	109.71	116.54
3	G	47	ILE	CA-C-N	5.91	125.78	119.28
3	G	47	ILE	C-N-CA	5.91	125.78	119.28
3	G	13	ARG	N-CA-C	-5.89	104.20	111.33
3	K	47	ILE	CA-C-N	5.85	125.72	119.28
3	K	47	ILE	C-N-CA	5.85	125.72	119.28
7	O	17	LEU	N-CA-C	-5.85	106.05	112.72
4	H	86	THR	CA-C-N	5.80	125.00	118.97
4	H	86	THR	C-N-CA	5.80	125.00	118.97
3	K	88	PRO	N-CA-C	5.78	117.75	110.70
1	I	150	LEU	N-CA-C	5.74	122.50	109.81
1	E	150	LEU	N-CA-C	5.71	122.44	109.81
3	C	88	PRO	N-CA-C	5.68	117.63	110.70
7	O	16	LYS	N-CA-C	-5.68	106.89	113.88
6	N	101	ASP	N-CA-C	-5.62	100.66	109.25
1	A	150	LEU	N-CA-C	5.60	122.18	109.81
3	C	47	ILE	CA-C-N	5.59	125.43	119.28
3	C	47	ILE	C-N-CA	5.59	125.43	119.28
5	M	160	HIS	N-CA-C	5.57	119.37	112.24
3	G	22	LEU	N-CA-C	5.56	117.15	111.14
3	C	22	LEU	N-CA-C	5.55	117.14	111.14
5	M	119	SER	N-CA-C	5.54	122.60	110.80
4	L	138	CYS	N-CA-C	5.44	119.88	112.04
6	N	81	LEU	N-CA-C	-5.40	106.56	114.39
4	L	86	THR	CA-C-N	5.36	124.55	118.97
4	L	86	THR	C-N-CA	5.36	124.55	118.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	86	THR	CA-C-N	5.31	124.49	118.97
4	D	86	THR	C-N-CA	5.31	124.49	118.97
3	G	88	PRO	N-CA-C	5.26	117.12	110.70
6	N	147	LEU	N-CA-C	5.25	117.06	109.07
2	B	134	ILE	N-CA-C	-5.22	105.30	110.62
5	M	210	VAL	N-CA-C	-5.18	102.42	107.55
5	M	102	LEU	N-CA-C	-5.17	106.97	113.28
3	K	22	LEU	N-CA-C	5.16	116.71	111.14
5	M	22	ASP	N-CA-C	-5.14	105.65	112.34
6	N	76	CYS	N-CA-C	5.14	118.60	109.96
2	F	53	GLY	N-CA-C	-5.11	108.32	114.66
6	N	217	GLN	N-CA-C	5.05	116.50	108.67
2	B	143	GLY	N-CA-C	-5.05	108.01	114.37
5	M	104	ILE	CB-CA-C	-5.03	105.43	112.02

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	79	0
1	E	1209	0	1194	84	0
1	I	1209	0	1194	85	0
2	B	1148	0	1103	34	0
2	F	1148	0	1103	40	0
2	J	1148	0	1103	36	0
3	C	1185	0	1191	57	0
3	G	1185	0	1191	56	0
3	K	1185	0	1191	55	0
4	D	1129	0	1102	67	0
4	H	1129	0	1102	72	0
4	L	1129	0	1102	64	0
5	M	1705	0	1547	94	0
6	N	1722	0	1632	107	0
7	O	1663	0	1479	87	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
All	All	19648	0	18788	933	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 24.

All (933) 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
4:L:83:MET:HE2	4:L:89:MET:HB3	1.33	1.10
4:H:83:MET:HE2	4:H:89:MET:HB3	1.34	1.07
4:D:83:MET:HE2	4:D:89:MET:HB3	1.35	1.07
7:O:208:LEU:HD23	7:O:208:LEU:H	1.19	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:I:14:GLU:CD	7:O:208:LEU:HD11	1.99	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: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
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
1:E:78:LYS:HZ1	4:H:31:ARG:HH22	1.26	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
1:E:67:LYS:HB3	4:H:89:MET:HE3	1.66	0.77
7:O:138:PHE:C	7:O:140:PRO:HD2	2.10	0.77
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
3:C:10:GLU:HB2	1:I:10:GLU:CD	2.17	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
1:E:126:VAL:CG1	2:F:7:LEU:HD22	2.23	0.69
6:N:162:VAL:HG12	6:N:163:THR:N	2.07	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
1:E:107:VAL:O	1:E:150:LEU:HD22	1.95	0.67
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:10:LEU:HD11	4:L:13:GLU:HG3	1.78	0.66
1:A:13:ARG:HH22	3:G:10:GLU:CD	2.03	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
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
1:E:10:GLU:CD	3:K:10:GLU:HB2	2.21	0.65
4:H:10:LEU:HD11	4:H:13:GLU:HG3	1.77	0.65
6:N:10:LEU:HD22	6:N:13:ARG:HB3	1.77	0.65
5:M:28:LEU:HD23	5:M:28:LEU:C	2.22	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
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
3:C:48:PRO:C	3:C:50:VAL:H	2.05	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
5:M:124:ASN:O	5:M:125:PRO:C	2.41	0.63
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
3:K:48:PRO:C	3:K:50:VAL:H	2.06	0.63
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:ARG:O	1:A:117:GLU:HG3	2.00	0.62
1:I:67:LYS:HB3	4:L:89:MET:HE3	1.82	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
3:K:38:LEU:HD23	3:K:38:LEU:C	2.25	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
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
4:H:20:GLN:NE2	4:H:135:TRP:HE1	1.98	0.61
3:C:38:LEU:C	3:C:38:LEU:HD23	2.26	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
3:G:48:PRO:C	3:G:50:VAL:H	2.08	0.60
6:N:181:LEU:HB2	6:N:193:VAL:CG1	2.31	0.60
3:G:38:LEU:C	3:G:38:LEU:HD23	2.26	0.60
7:O:77:ILE:C	7:O:77:ILE:HD12	2.25	0.60
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:HD12	7:O:77:ILE:O	2.01	0.60
3:C:48:PRO:C	3:C:50:VAL:N	2.58	0.60
3:C:74:ILE:HG23	3:C:75:LEU:N	2.15	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
3:K:48:PRO:C	3:K:50:VAL:N	2.60	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
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
4:H:109:GLU:O	4:H:113:ILE:HG13	2.04	0.58
5:M:172:ASN:HD22	5:M:172:ASN:C	2.10	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
4:D:49:ILE:O	4:D:52:PRO:HD2	2.04	0.57
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
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
3:G:48:PRO:C	3:G:50:VAL:N	2.61	0.57
1:A:28:THR:O	1:A:31:ARG:HG2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
6:N:10:LEU:C	6:N:12:PRO:HD2	2.30	0.57
4:D:125:ARG:HG2	4:D:125:ARG:HH11	1.69	0.57
1:E:78:LYS:HZ3	4:H:31:ARG:HH22	1.48	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
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
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
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
2:B:8:GLU:CD	2:B:8:GLU:H	2.14	0.55
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
4:H:125:ARG:HH11	4:H:125:ARG:HG2	1.71	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
7:O:50:LEU:C	7:O:50:LEU:HD23	2.32	0.55
6:N:16:ALA:C	6:N:18:ALA:H	2.14	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
7:O:93:GLU:C	7:O:95:GLU:H	2.15	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
6:N:198:ASN:O	6:N:198:ASN:CG	2.50	0.54
1:A:67:LYS:HB3	4:D:89:MET:HE3	1.90	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
1:I:78:LYS:HZ1	4:L:31:ARG:HH22	1.54	0.54
6:N:81:LEU:O	6:N:82:VAL:C	2.50	0.54
2:B:89:LEU:HD21	2:B:137:ILE:HG23	1.90	0.54
2:F:8:GLU:CD	2:F:8:GLU:H	2.15	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
3:C:148:SER:C	3:C:150:ARG:H	2.16	0.54
2:B:123:ARG:HD3	2:B:123:ARG:H	1.73	0.53
1:I:23:TRP:CD1	1:I:78:LYS:HZ2	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
7:O:125:MET:HE1	7:O:204:ILE:HD11	1.90	0.53
4:H:51:ALA:HB3	4:H:52:PRO:CD	2.39	0.53
5:M:21:ILE:C	5:M:23:TYR:N	2.66	0.53
7:O:100:LEU:C	7:O:100:LEU:HD23	2.34	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
1:E:23:TRP:CD1	1:E:78:LYS:HZ2	2.27	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
2:J:8:GLU:CD	2:J:8:GLU:H	2.16	0.52
5:M:104:ILE:HG23	5:M:111:TYR:OH	2.09	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
3:G:148:SER:C	3:G:150:ARG:H	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:114:PHE:HD1	7:O:215:GLU:N	2.06	0.52
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
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
1:A:75:ASN:CG	4:D:79:ILE:HG12	2.35	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
3:K:148:SER:C	3:K:150:ARG:H	2.17	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
4:L:56:VAL:O	4:L:57:ARG:C	2.53	0.51
2:J:123:ARG:H	2:J:123:ARG:HD3	1.74	0.51
1:E:15:ILE:C	1:E:17:HIS:N	2.67	0.51
4:H:83:MET:CE	4:H:89:MET:HE2	2.41	0.51
6:N:80:LEU:C	6:N:81:LEU:HD23	2.35	0.51
1:I:53:PHE:HB2	1:I:58:ILE:HG21	1.92	0.51
6:N:16:ALA:C	6:N:18:ALA:N	2.68	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
4:L:83:MET:CE	4:L:89:MET:HE2	2.41	0.51
3:C:87:ASP:C	3:C:89:PRO:HD2	2.36	0.51
1:E:67:LYS:CB	4:H:89:MET:HE3	2.39	0.51
1:I:123:LEU:N	1:I:124:PRO:HD2	2.25	0.51
3:K:87:ASP:C	3:K:89:PRO:HD2	2.36	0.51
6:N:18:ALA:C	6:N:20:LEU:N	2.67	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
5:M:170:PHE:CD1	5:M:170:PHE:C	2.89	0.51
3:C:48:PRO:O	3:C:50:VAL:N	2.45	0.50
4:D:56:VAL:O	4:D:57:ARG:C	2.53	0.50
2:F:110:LYS:HG3	2:F:134:ILE:CG2	2.37	0.50
6:N:46:PHE:CD1	6:N:46:PHE:C	2.88	0.50
1:A:109:LYS:HD2	1:A:151:PRO:HD3	1.93	0.50
2:F:41:VAL:HG23	2:F:41:VAL:O	2.10	0.50
4:H:56:VAL:O	4:H:57:ARG:C	2.54	0.50
1:I:109:LYS:HD2	1:I:151:PRO:HD3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:94:LEU:HD21	4:L:142:ILE:HG23	1.93	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
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:15:ILE:C	1:E:17:HIS:H	2.20	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
1:I:14:GLU:OE2	7:O:208:LEU:HD21	2.12	0.50
1:I:15:ILE:C	1:I:17:HIS:N	2.67	0.50
5:M:115:ALA:O	5:M:125:PRO:HA	2.12	0.50
5:M:172:ASN:C	5:M:172:ASN:ND2	2.67	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
5:M:63:ASP:O	5:M:64:GLU:C	2.53	0.50
2:F:102:PRO:C	2:F:104:ASN:N	2.70	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
2:B:51:VAL:O	2:B:51:VAL:HG22	2.11	0.49
1:E:78:LYS:HZ1	4:H:31:ARG:NH2	2.01	0.49
3:K:72:LEU:O	3:K:73:ARG:C	2.56	0.49
4:D:130:PHE:HD2	4:L:62:TYR:CE2	2.31	0.49
1:I:23:TRP:NE1	1:I:78:LYS:HZ2	2.10	0.49
3:K:108:VAL:HG22	9:K:160:HEM:HBC2	1.93	0.49
5:M:36:ASN:C	5:M:38:LEU:H	2.20	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:120:ARG:O	7:O:121:ARG:C	2.55	0.49
7:O:121:ARG:N	7:O:122:PRO:CD	2.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:G:87:ASP:C	3:G:89:PRO:HD2	2.38	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
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
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
3:C:70:HIS:O	3:C:74:ILE:HG22	2.12	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
1:I:15:ILE:C	1:I:17:HIS:H	2.21	0.48
1:I:28:THR:O	1:I:29:ASP:C	2.56	0.48
7:O:114:PHE:O	7:O:214:ALA:HA	2.12	0.48
1:A:23:TRP:CD1	1:A:78:LYS:HZ2	2.32	0.48
4:D:83:MET:CE	4:D:89:MET:HE2	2.44	0.48
1:E:147:ALA:CB	1:E:150:LEU:HD12	2.43	0.48
5:M:181:ALA:HB1	5:M:182:PRO:HD2	1.95	0.48
6:N:18:ALA:C	6:N:20:LEU:H	2.22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:M:85:GLY:N	5:M:95:GLU:OE2	2.47	0.48
6:N:75:GLU:OE1	6:N:90:HIS:HD2	1.96	0.48
2:B:85:LEU:O	2:B:86:LYS:C	2.56	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: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
1:A:15:ILE:C	1:A:17:HIS:N	2.68	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
5:M:102:LEU:O	5:M:103:ASN:C	2.57	0.47
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
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
2:B:102:PRO:C	2:B:104:ASN:N	2.71	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
7:O:117:CYS:O	7:O:118:THR:C	2.57	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
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: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:31:ILE:O	3:G:32:LYS:C	2.58	0.47
3:G:88:PRO:HG2	3:G:89:PRO:CD	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C	1:A:21:ASP:H	2.23	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
1:I:79:LEU:HD13	1:I:79:LEU:C	2.39	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
6:N:155:LEU:HD23	6:N:155:LEU:H	1.79	0.47
1:A:15:ILE:C	1:A:17:HIS:H	2.23	0.47
1:E:23:TRP:CH2	1:E:74:ALA:HB1	2.50	0.47
2:F:28:ALA:O	2:F:29:PHE:C	2.58	0.47
4:H:110:PHE:O	4:H:113:ILE:HB	2.15	0.47
3:K:31:ILE:O	3:K:32:LYS:C	2.58	0.47
6:N:10:LEU:CD2	6:N:12:PRO:HG2	2.43	0.47
2:F:102:PRO:C	2:F:104:ASN:H	2.22	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
2:B:28:ALA:O	2:B:29:PHE:C	2.56	0.46
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
1:I:19:TRP:HE1	1:I:78:LYS:HD3	1.79	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
5:M:121:GLU:O	5:M:122:ASP:C	2.58	0.46
1:A:79:LEU:HD13	1:A:79:LEU:C	2.40	0.46
4:D:73:VAL:O	4:D:74:LEU:C	2.59	0.46
1:E:22:VAL:CG2	1:E:23:TRP:N	2.78	0.46
1:E:23:TRP:NE1	1:E:78:LYS:HZ2	2.13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:D:110:PHE:O	4:D:113:ILE:HB	2.15	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
1:E:19:TRP:C	1:E:21:ASP:H	2.23	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
1:E:28:THR:O	1:E:29:ASP:C	2.58	0.46
1:E:69:HIS:O	1:E:70:LEU:C	2.59	0.46
1:E:81:ILE:C	1:E:83:LEU:H	2.24	0.46
2:F:85:LEU:O	2:F:86:LYS:C	2.58	0.46
3:K:35:PHE:CE2	3:K:39:LEU:HD11	2.51	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
7:O:100:LEU:C	7:O:100:LEU:CD2	2.89	0.46
3:C:72:LEU:O	3:C:73:ARG:C	2.59	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: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
1:A:23:TRP:NE1	1:A:78:LYS:HZ2	2.14	0.46
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
2:J:24:HIS:O	2:J:25:ASP:C	2.59	0.46
2:J:28:ALA:O	2:J:29:PHE:C	2.58	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:49:ILE:C	4:H:51:ALA:N	2.73	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:LEU:O	1:A:127:LEU:HD23	2.16	0.45
4:D:49:ILE:C	4:D:51:ALA:N	2.73	0.45
1:E:96:HIS:O	1:E:100:GLN:HG3	2.16	0.45
3:G:12:HIS:O	3:G:13:ARG:C	2.59	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
1:I:81:ILE:C	1:I:83:LEU:H	2.24	0.45
2:J:85:LEU:O	2:J:86:LYS:C	2.59	0.45
6:N:10:LEU:HD23	6:N:12:PRO:CG	2.46	0.45
6:N:101:ASP:CG	6:N:103:SER:HG	2.24	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
3:G:72:LEU:O	3:G:73:ARG:C	2.58	0.45
1:I:19:TRP:C	1:I:21:ASP:H	2.24	0.45
1:I:23:TRP:CH2	1:I:74:ALA:HB1	2.51	0.45
7:O:93:GLU:C	7:O:95:GLU:N	2.73	0.45
1:E:128:SER:O	1:E:129:CYS:HB2	2.16	0.45
1:I:69:HIS:O	1:I:70:LEU:C	2.60	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
5:M:187:SER:O	5:M:188:GLU:C	2.60	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
3:K:129:ASP:OD2	3:K:129:ASP:N	2.37	0.45
5:M:12:TYR:CD2	5:M:12:TYR:N	2.85	0.45
5:M:219:HIS:ND1	5:M:219:HIS:C	2.75	0.45
3:C:10:GLU:CD	1:I:13:ARG:HH22	2.25	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
5:M:196:PHE:C	5:M:198:LEU:H	2.25	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
1:A:131:ASN:C	1:A:131:ASN:HD22	2.25	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
4:H:111:PHE:CD1	4:H:111:PHE:N	2.85	0.44
2:J:102:PRO:C	2:J:104:ASN:H	2.26	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
2:B:92:LEU:O	2:B:93:GLN:C	2.58	0.44
2:F:130:TRP:O	2:F:131:ASP:C	2.59	0.44
1:I:14:GLU:CD	7:O:208:LEU:CD1	2.83	0.44
2:J:84:THR:O	2:J:85:LEU:C	2.61	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
1:A:81:ILE:C	1:A:83:LEU:H	2.24	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
4:D:10:LEU:HD11	4:D:13:GLU:H	1.83	0.44
1:E:86:ASP:O	1:E:87:THR:C	2.61	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
5:M:224:ARG:C	5:M:225:TYR:CD2	2.96	0.44
6:N:29:GLU:O	6:N:32:ARG:HB2	2.18	0.44
1:A:86:ASP:O	1:A:87:THR:C	2.61	0.44
1:E:19:TRP:C	1:E:21:ASP:N	2.76	0.44
1:E:131:ASN:C	1:E:131:ASN:HD22	2.25	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
1:A:19:TRP:C	1:A:21:ASP:N	2.75	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:24:ILE:C	7:O:26:THR:N	2.75	0.44
1:A:15:ILE:O	1:A:17:HIS:N	2.51	0.44
3:C:31:ILE:O	3:C:32:LYS:C	2.60	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
3:K:113:PHE:O	3:K:114:LYS:C	2.60	0.44
3:C:129:ASP:CA	4:D:16:LYS:HE3	2.48	0.44
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:E:79:LEU:HD13	1:E:79:LEU:C	2.43	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
6:N:186:ASP:C	6:N:188:ASP:H	2.26	0.43
1:A:22:VAL:CG2	1:A:23:TRP:N	2.81	0.43
2:B:130:TRP:O	2:B:131:ASP:C	2.59	0.43
2:F:73:ASP:O	2:F:74:ILE:C	2.59	0.43
4:H:18:LYS:NZ	4:H:82:SER:HA	2.33	0.43
4:H:79:ILE:O	4:H:80:THR:C	2.61	0.43
1:I:15:ILE:O	1:I:17:HIS:N	2.50	0.43
2:J:130:TRP:O	2:J:131:ASP:C	2.61	0.43
3:K:12:HIS:O	3:K:13:ARG:C	2.58	0.43
6:N:104:VAL:HG22	6:N:202:ASN:HD22	1.83	0.43
6:N:173:ASN:C	6:N:173:ASN:HD22	2.27	0.43
2:F:74:ILE:HG23	3:G:72:LEU:CD1	2.45	0.43
2:J:102:PRO:C	2:J:104:ASN:N	2.72	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
2:B:102:PRO:C	2:B:104:ASN:H	2.25	0.43
4:H:75:SER:O	4:H:78:ASP:HB3	2.19	0.43
1:I:19:TRP:C	1:I:21:ASP:N	2.75	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
1:I:131:ASN:C	1:I:131:ASN:HD22	2.25	0.43
3:K:70:HIS:O	3:K:71:ALA:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:66:GLU:HG3	5:M:78:HIS:HA	2.00	0.43
5:M:114:LEU:HD12	5:M:126:ASP:C	2.42	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:73:ASP:O	2:B:74:ILE:C	2.61	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
1:I:143:VAL:O	1:I:144:ALA:C	2.62	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
1:E:15:ILE:CD1	1:E:138:CYS:HB2	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
4:H:49:ILE:C	4:H:51:ALA:H	2.27	0.43
1:I:80:LEU:HD22	1:I:94:LEU:HD13	2.00	0.43
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
7:O:52:HIS:O	7:O:53:ARG:C	2.62	0.43
2:B:24:HIS:O	2:B:25:ASP:C	2.61	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:HD21	4:L:71:GLN:HG3	2.01	0.43
1:I:86:ASP:O	1:I:87:THR:C	2.62	0.43
1:I:108:THR:H	1:I:111:TYR:HD2	1.65	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
4:D:31:ARG:O	4:D:32:VAL:C	2.60	0.43
2:J:73:ASP:O	2:J:74:ILE:C	2.62	0.43
2:J:92:LEU:O	2:J:93:GLN:C	2.61	0.43
5:M:146:TRP:CD1	5:M:146:TRP:H	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:161:VAL:HG12	7:O:162:SER:N	2.34	0.42
1:A:49:SER:O	1:A:50:LYS:C	2.62	0.42
2:B:76:ILE:C	2:B:78:THR:H	2.27	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:31:VAL:C	7:O:33:SER:N	2.76	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
3:C:14:ILE:O	3:C:15:VAL:C	2.60	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
3:C:113:PHE:O	3:C:114:LYS:C	2.62	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
2:F:24:HIS:O	2:F:25:ASP:C	2.61	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:12:HIS:O	3:C:13:ARG:C	2.60	0.42
3:K:14:ILE:O	3:K:15:VAL:C	2.62	0.42
4:L:49:ILE:C	4:L:51:ALA:N	2.76	0.42
4:L:83:MET:CE	4:L:89:MET:HB3	2.25	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
2:F:92:LEU:O	2:F:93:GLN:C	2.60	0.42
3:G:14:ILE:O	3:G:15:VAL:C	2.62	0.42
4:H:31:ARG:O	4:H:32:VAL:C	2.63	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
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
4:D:49:ILE:C	4:D:51:ALA:H	2.27	0.42
4:D:117:HIS:O	4:D:118:LEU:C	2.63	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: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:92:ALA:C	6:N:94:ASP:N	2.78	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
2:F:84:THR:O	2:F:85:LEU:C	2.61	0.42
3:G:70:HIS:O	3:G:71:ALA:C	2.63	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:119:SER:C	5:M:120:CYS:SG	3.03	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
3:C:20:ASP:C	3:C:22:LEU:N	2.78	0.41
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:83:MET:CE	4:H:89:MET:HB3	2.26	0.41
4:H:134:ALA:O	4:H:138:CYS:HB2	2.20	0.41
4:L:73:VAL:O	4:L:74:LEU:C	2.63	0.41
5:M:18:ASN:HD21	7:O:17:LEU:CB	2.33	0.41
1:A:122:VAL:C	1:A:124:PRO:HD2	2.45	0.41
4:D:19:LEU:O	4:D:22:ALA:HB3	2.20	0.41
4:D:134:ALA:O	4:D:138:CYS:HB2	2.20	0.41
3:G:63:GLU:H	3:G:63:GLU:CD	2.28	0.41
3:G:109:GLN:O	3:G:112:HIS:HB2	2.20	0.41
7:O:92:GLY:O	7:O:93:GLU:C	2.62	0.41
2:F:76:ILE:C	2:F:78:THR:H	2.29	0.41
4:L:14:SER:O	4:L:17:VAL:N	2.53	0.41
6:N:19:PHE:C	6:N:22:ILE:HG22	2.45	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
1:A:28:THR:O	1:A:29:ASP:C	2.62	0.41
2:B:7:LEU:C	2:B:9:GLY:N	2.78	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:57:LYS:HD2	1:E:65:GLU:HG3	2.00	0.41
1:E:122:VAL:C	1:E:124:PRO:HD2	2.45	0.41
1:I:131:ASN:O	1:I:132:VAL:C	2.64	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
1:A:13:ARG:NH2	3:G:10:GLU:CD	2.77	0.41
4:H:14:SER:O	4:H:15:LEU:C	2.64	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
3:C:70:HIS:O	3:C:71:ALA:C	2.64	0.41
4:D:17:VAL:HG13	4:D:135:TRP:CZ2	2.55	0.41
4:H:69:HIS:O	4:H:70:SER:C	2.62	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
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:49:SER:O	1:I:50:LYS:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
4:D:69:HIS:O	4:D:70:SER:C	2.63	0.41
1:E:17:HIS:O	1:E:18:ILE:C	2.64	0.41
1:E:50:LYS:HG2	1:E:58:ILE:HD12	2.02	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:76:ILE:C	2:J:78:THR:H	2.28	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:34:PHE:CD1	4:L:34:PHE:C	2.99	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
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:28:LEU:C	5:M:28:LEU:CD2	2.93	0.41
7:O:209:SER:O	7:O:210:GLU:HB3	2.20	0.41
1:A:16:ARG:NH2	1:A:85:ASP:CG	2.79	0.40
1:A:63:SER:OG	1:A:66:PHE:HB3	2.21	0.40
2:F:68:VAL:O	2:F:69:LEU:C	2.63	0.40
2:F:111:THR:O	2:F:112:ALA:C	2.64	0.40
4:H:73:VAL:O	4:H:74:LEU:C	2.64	0.40
4:H:107:LYS:HD2	4:H:107:LYS:N	2.35	0.40
3:K:109:GLN:O	3:K:112:HIS:HB2	2.21	0.40
1:A:112:PHE:C	1:A:114:GLY:N	2.76	0.40
3:C:150:ARG:O	3:C:151:LEU:HG	2.20	0.40
4:D:79:ILE:O	4:D:80:THR:C	2.63	0.40
1:E:64:GLY:HA2	1:E:67:LYS:HB2	2.02	0.40
1:E:112:PHE:C	1:E:114:GLY:N	2.77	0.40
2:F:127:ARG:O	2:F:128:GLU:C	2.64	0.40
4:L:12:THR:C	4:L:14:SER:N	2.78	0.40
4:L:31:ARG:O	4:L:32:VAL:C	2.65	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:49:ILE:C	4:L:51:ALA:H	2.29	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
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
2:J:105:TYR:O	2:J:106:PHE:C	2.64	0.40
5:M:140:PHE:C	5:M:142:PRO:HD3	2.47	0.40
6:N:19:PHE:HA	6:N:22:ILE:HG22	2.03	0.40
6:N:69:CYS:O	6:N:70:GLY:C	2.64	0.40
6:N:72:ASN:C	6:N:72:ASN:ND2	2.78	0.40
7:O:39:LEU:O	7:O:40:ASP:C	2.64	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:50:LYS:HG2	1:I:58:ILE:HD12	2.03	0.40
1:I:123:LEU:C	1:I:125:GLN:H	2.28	0.40
4:L:79:ILE:O	4:L:80:THR:C	2.63	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
4:D:12:THR:C	4:D:14:SER:N	2.79	0.40
2:J:7:LEU:C	2:J:9:GLY:N	2.79	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:66:GLU:HG2	5:M:77:ILE:C	2.46	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%)	4	26
1	E	145/151 (96%)	119 (82%)	22 (15%)	4 (3%)	4	26
1	I	145/151 (96%)	120 (83%)	21 (14%)	4 (3%)	4	26
2	B	143/145 (99%)	118 (82%)	24 (17%)	1 (1%)	18	51
2	F	143/145 (99%)	120 (84%)	22 (15%)	1 (1%)	18	51
2	J	143/145 (99%)	123 (86%)	18 (13%)	2 (1%)	9	38
3	C	147/153 (96%)	122 (83%)	23 (16%)	2 (1%)	9	38
3	G	147/153 (96%)	124 (84%)	21 (14%)	2 (1%)	9	38
3	K	147/153 (96%)	124 (84%)	21 (14%)	2 (1%)	9	38
4	D	138/140 (99%)	114 (83%)	21 (15%)	3 (2%)	5	30
4	H	138/140 (99%)	114 (83%)	21 (15%)	3 (2%)	5	30
4	L	138/140 (99%)	113 (82%)	23 (17%)	2 (1%)	9	38
5	M	215/217 (99%)	178 (83%)	29 (14%)	8 (4%)	2	21
6	N	218/220 (99%)	177 (81%)	28 (13%)	13 (6%)	1	12
7	O	213/215 (99%)	171 (80%)	37 (17%)	5 (2%)	5	30
All	All	2365/2419 (98%)	1956 (83%)	353 (15%)	56 (2%)	4	29

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

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Mol	Chain	Res	Type
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
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 ⓘ

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%)	17	43
1	E	131/134 (98%)	123 (94%)	8 (6%)	17	43
1	I	131/134 (98%)	123 (94%)	8 (6%)	17	43
2	B	117/117 (100%)	111 (95%)	6 (5%)	21	48
2	F	117/117 (100%)	111 (95%)	6 (5%)	21	48
2	J	117/117 (100%)	111 (95%)	6 (5%)	21	48
3	C	127/131 (97%)	119 (94%)	8 (6%)	16	42
3	G	127/131 (97%)	119 (94%)	8 (6%)	16	42
3	K	127/131 (97%)	119 (94%)	8 (6%)	16	42
4	D	121/121 (100%)	115 (95%)	6 (5%)	22	48
4	H	121/121 (100%)	115 (95%)	6 (5%)	22	48
4	L	121/121 (100%)	115 (95%)	6 (5%)	22	48
5	M	182/195 (93%)	153 (84%)	29 (16%)	2	14
6	N	186/193 (96%)	168 (90%)	18 (10%)	8	30
7	O	178/193 (92%)	170 (96%)	8 (4%)	24	50
All	All	2034/2090 (97%)	1895 (93%)	139 (7%)	14	40

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

Mol	Chain	Res	Type
1	A	48	THR
1	A	59	ASP
1	A	65	GLU
1	A	82	ASN
1	A	83	LEU
1	A	121	ARG
1	A	126	VAL
1	A	136	ASN
2	B	8	GLU
2	B	56	THR

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Mol	Chain	Res	Type
2	B	66	ASP
2	B	90	ASP
2	B	125	TYR
2	B	135	ASP
3	C	6	CYS
3	C	20	ASP
3	C	37	ARG
3	C	45	LYS
3	C	74	ILE
3	C	115	LYS
3	C	129	ASP
3	C	146	LYS
4	D	19	LEU
4	D	48	GLU
4	D	71	GLN
4	D	84	LEU
4	D	128	THR
4	D	138	CYS
1	E	48	THR
1	E	59	ASP
1	E	65	GLU
1	E	82	ASN
1	E	83	LEU
1	E	121	ARG
1	E	126	VAL
1	E	136	ASN
2	F	8	GLU
2	F	56	THR
2	F	66	ASP
2	F	90	ASP
2	F	125	TYR
2	F	135	ASP
3	G	6	CYS
3	G	20	ASP
3	G	37	ARG
3	G	45	LYS
3	G	74	ILE
3	G	115	LYS
3	G	129	ASP
3	G	146	LYS
4	H	19	LEU
4	H	48	GLU

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Mol	Chain	Res	Type
4	H	71	GLN
4	H	84	LEU
4	H	128	THR
4	H	138	CYS
1	I	48	THR
1	I	59	ASP
1	I	65	GLU
1	I	82	ASN
1	I	83	LEU
1	I	121	ARG
1	I	126	VAL
1	I	136	ASN
2	J	8	GLU
2	J	56	THR
2	J	66	ASP
2	J	90	ASP
2	J	125	TYR
2	J	135	ASP
3	K	6	CYS
3	K	20	ASP
3	K	37	ARG
3	K	45	LYS
3	K	74	ILE
3	K	115	LYS
3	K	129	ASP
3	K	146	LYS
4	L	19	LEU
4	L	48	GLU
4	L	71	GLN
4	L	84	LEU
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	80	LEU
5	M	95	GLU
5	M	103	ASN
5	M	112	THR
5	M	116	THR

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Mol	Chain	Res	Type
5	M	118	THR
5	M	121	GLU
5	M	124	ASN
5	M	131	THR
5	M	147	LEU
5	M	157	GLU
5	M	159	ASP
5	M	161	THR
5	M	163	SER
5	M	165	THR
5	M	176	ARG
5	M	183	LEU
5	M	188	GLU
5	M	198	LEU
5	M	209	VAL
5	M	210	VAL
5	M	216	VAL
5	M	224	ARG
5	M	225	TYR
6	N	10	LEU
6	N	32	ARG
6	N	64	LYS
6	N	73	GLU
6	N	82	VAL
6	N	89	CYS
6	N	95	GLU
6	N	100	CYS
6	N	110	VAL
6	N	127	VAL
6	N	131	THR
6	N	147	LEU
6	N	155	LEU
6	N	187	HIS
6	N	199	ARG
6	N	202	ASN
6	N	215	LEU
6	N	221	LEU
7	O	37	ASP
7	O	61	SER
7	O	114	PHE
7	O	173	ASP
7	O	176	LEU

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Mol	Chain	Res	Type
7	O	183	GLU
7	O	208	LEU
7	O	210	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (87) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	HIS
1	A	82	ASN
1	A	96	HIS
1	A	125	GLN
1	A	131	ASN
1	A	136	ASN
2	B	52	HIS
2	B	115	HIS
2	B	120	GLN
2	B	145	HIS
3	C	12	HIS
3	C	16	GLN
3	C	18	GLN
3	C	51	ASN
3	C	61	HIS
3	C	70	HIS
3	C	76	ASN
3	C	83	ASN
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	69	HIS
1	E	82	ASN
1	E	131	ASN
1	E	136	ASN
2	F	40	GLN
2	F	52	HIS
2	F	115	HIS
2	F	120	GLN
2	F	145	HIS
3	G	12	HIS
3	G	16	GLN

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Mol	Chain	Res	Type
3	G	18	GLN
3	G	51	ASN
3	G	70	HIS
3	G	76	ASN
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	120	HIS
4	H	141	GLN
1	I	17	HIS
1	I	45	HIS
1	I	69	HIS
1	I	82	ASN
1	I	125	GLN
1	I	131	ASN
1	I	136	ASN
2	J	40	GLN
2	J	52	HIS
2	J	115	HIS
2	J	120	GLN
2	J	145	HIS
3	K	12	HIS
3	K	16	GLN
3	K	18	GLN
3	K	51	ASN
3	K	61	HIS
3	K	70	HIS
3	K	100	HIS
3	K	126	GLN
4	L	20	GLN
4	L	29	HIS
4	L	46	HIS
4	L	117	HIS
4	L	141	GLN
5	M	18	ASN
5	M	36	ASN
5	M	49	GLN
5	M	56	ASN
5	M	103	ASN

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Mol	Chain	Res	Type
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
7	O	174	HIS

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 oligosaccharides 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	$\# Z > 2$
8	CMO	K	161	9	0,1,1	-	-	-		
8	CMO	F	161	9	0,1,1	-	-	-		
9	HEM	C	160	3,8	50,50,50	1.30	5 (10%)	67,82,82	1.12	3 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	HEM	A	160	8,1	50,50,50	1.30	5 (10%)	67,82,82	1.14	4 (5%)
9	HEM	B	160	2,8	50,50,50	1.31	5 (10%)	67,82,82	1.09	3 (4%)
9	HEM	L	160	4,8	50,50,50	1.24	4 (8%)	67,82,82	1.14	4 (5%)
9	HEM	H	160	4,8	50,50,50	1.36	6 (12%)	67,82,82	1.09	3 (4%)
9	HEM	K	160	3,8	50,50,50	1.18	5 (10%)	67,82,82	1.13	3 (4%)
9	HEM	I	160	8,1	50,50,50	1.36	5 (10%)	67,82,82	1.10	4 (5%)
8	CMO	L	161	9	0,1,1	-	-	-		
9	HEM	G	160	3,8	50,50,50	1.22	5 (10%)	67,82,82	1.08	3 (4%)
9	HEM	F	160	2,8	50,50,50	1.29	5 (10%)	67,82,82	1.16	4 (5%)
8	CMO	A	161	9	0,1,1	-	-	-		
8	CMO	C	161	9	0,1,1	-	-	-		
8	CMO	D	161	9	0,1,1	-	-	-		
8	CMO	E	161	9	0,1,1	-	-	-		
8	CMO	I	161	9	0,1,1	-	-	-		
8	CMO	H	161	9	0,1,1	-	-	-		
8	CMO	G	161	9	0,1,1	-	-	-		
9	HEM	J	160	2,8	50,50,50	1.26	6 (12%)	67,82,82	1.08	2 (2%)
8	CMO	J	161	9	0,1,1	-	-	-		
8	CMO	B	161	9	0,1,1	-	-	-		
9	HEM	E	160	8,1	50,50,50	1.37	6 (12%)	67,82,82	1.17	4 (5%)
9	HEM	D	160	4,8	50,50,50	1.26	5 (10%)	67,82,82	1.20	4 (5%)

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	J	160	2,8	-	6/14/54/54	-
9	HEM	A	160	8,1	-	8/14/54/54	-
9	HEM	F	160	2,8	-	6/14/54/54	-
9	HEM	B	160	2,8	-	6/14/54/54	-
9	HEM	L	160	4,8	-	8/14/54/54	-
9	HEM	E	160	8,1	-	8/14/54/54	-
9	HEM	H	160	4,8	-	8/14/54/54	-
9	HEM	K	160	3,8	-	8/14/54/54	-
9	HEM	D	160	4,8	-	8/14/54/54	-
9	HEM	I	160	8,1	-	8/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	HEM	C	160	3,8	-	7/14/54/54	-
9	HEM	G	160	3,8	-	7/14/54/54	-

All (62) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	160	HEM	CAC-C3C	-4.11	1.36	1.47
9	D	160	HEM	CAC-C3C	-4.06	1.36	1.47
9	H	160	HEM	CAC-C3C	-3.84	1.37	1.47
9	E	160	HEM	CAC-C3C	-3.80	1.37	1.47
9	F	160	HEM	CAB-C3B	-3.70	1.37	1.47
9	G	160	HEM	CAB-C3B	-3.66	1.37	1.47
9	C	160	HEM	CAC-C3C	-3.59	1.37	1.47
9	J	160	HEM	CAB-C3B	-3.51	1.38	1.47
9	F	160	HEM	CAC-C3C	-3.45	1.38	1.47
9	I	160	HEM	CAB-C3B	-3.41	1.38	1.47
9	H	160	HEM	CAB-C3B	-3.41	1.38	1.47
9	C	160	HEM	CAB-C3B	-3.40	1.38	1.47
9	A	160	HEM	CAC-C3C	-3.40	1.38	1.47
9	L	160	HEM	CAC-C3C	-3.35	1.38	1.47
9	J	160	HEM	CAC-C3C	-3.33	1.38	1.47
9	K	160	HEM	CAB-C3B	-3.32	1.38	1.47
9	A	160	HEM	CAB-C3B	-3.25	1.38	1.47
9	L	160	HEM	CAB-C3B	-3.25	1.38	1.47
9	K	160	HEM	CAC-C3C	-3.17	1.38	1.47
9	E	160	HEM	CAB-C3B	-3.09	1.39	1.47
9	A	160	HEM	CBB-CAB	3.06	1.45	1.30
9	I	160	HEM	CBB-CAB	3.02	1.44	1.30
9	G	160	HEM	CAC-C3C	-2.96	1.39	1.47
9	I	160	HEM	CAC-C3C	-2.96	1.39	1.47
9	D	160	HEM	CBB-CAB	2.96	1.44	1.30
9	B	160	HEM	CAB-C3B	-2.96	1.39	1.47
9	C	160	HEM	CBC-CAC	2.95	1.44	1.30
9	G	160	HEM	CBC-CAC	2.95	1.44	1.30
9	J	160	HEM	CBB-CAB	2.94	1.44	1.30
9	D	160	HEM	CAB-C3B	-2.91	1.39	1.47
9	I	160	HEM	CBC-CAC	2.90	1.44	1.30
9	L	160	HEM	CBB-CAB	2.87	1.44	1.30
9	H	160	HEM	CBB-CAB	2.81	1.43	1.30
9	K	160	HEM	CBC-CAC	2.80	1.43	1.30
9	A	160	HEM	CBC-CAC	2.78	1.43	1.30
9	E	160	HEM	CBB-CAB	2.77	1.43	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	L	160	HEM	CBC-CAC	2.74	1.43	1.30
9	F	160	HEM	C4D-ND	-2.74	1.35	1.40
9	G	160	HEM	CBB-CAB	2.74	1.43	1.30
9	B	160	HEM	CBB-CAB	2.69	1.43	1.30
9	F	160	HEM	CBC-CAC	2.69	1.43	1.30
9	H	160	HEM	CBC-CAC	2.68	1.43	1.30
9	B	160	HEM	CBC-CAC	2.61	1.42	1.30
9	F	160	HEM	CBB-CAB	2.61	1.42	1.30
9	D	160	HEM	CBC-CAC	2.55	1.42	1.30
9	K	160	HEM	CBB-CAB	2.53	1.42	1.30
9	C	160	HEM	C2A-C3A	-2.53	1.32	1.38
9	J	160	HEM	CBC-CAC	2.52	1.42	1.30
9	E	160	HEM	CBC-CAC	2.50	1.42	1.30
9	K	160	HEM	C2A-C3A	-2.46	1.32	1.38
9	G	160	HEM	C2A-C3A	-2.45	1.32	1.38
9	J	160	HEM	C2A-C3A	-2.35	1.32	1.38
9	E	160	HEM	FE-NB	2.32	2.02	1.94
9	B	160	HEM	C4D-ND	-2.31	1.36	1.40
9	A	160	HEM	C2A-C3A	-2.30	1.32	1.38
9	D	160	HEM	C2A-C3A	-2.29	1.32	1.38
9	H	160	HEM	C4D-ND	-2.23	1.36	1.40
9	C	160	HEM	CBB-CAB	2.21	1.41	1.30
9	E	160	HEM	C2A-C3A	-2.19	1.33	1.38
9	H	160	HEM	C3B-C2B	-2.09	1.32	1.37
9	J	160	HEM	C4D-ND	-2.05	1.36	1.40
9	I	160	HEM	C2A-C3A	-2.00	1.33	1.38

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	160	HEM	CMB-C2B-C1B	3.17	129.98	125.03
9	K	160	HEM	CMA-C3A-C4A	2.97	129.95	125.42
9	C	160	HEM	CMA-C3A-C4A	2.87	129.79	125.42
9	H	160	HEM	CMB-C2B-C1B	2.85	129.49	125.03
9	G	160	HEM	CMA-C3A-C4A	2.74	129.59	125.42
9	E	160	HEM	CMB-C2B-C1B	2.71	129.27	125.03
9	A	160	HEM	CMB-C2B-C1B	2.70	129.26	125.03
9	E	160	HEM	C3B-C4B-NB	2.62	111.35	109.47
9	L	160	HEM	CMC-C2C-C1C	2.60	129.31	124.73
9	I	160	HEM	CMB-C2B-C1B	2.57	129.04	125.03
9	I	160	HEM	CAD-C3D-C4D	2.53	129.11	124.70
9	K	160	HEM	CAA-C2A-C1A	2.51	129.84	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	L	160	HEM	CMB-C2B-C1B	2.48	128.91	125.03
9	D	160	HEM	CMC-C2C-C1C	2.47	129.09	124.73
9	E	160	HEM	CAD-C3D-C4D	2.46	128.98	124.70
9	B	160	HEM	CMD-C2D-C1D	2.44	128.85	125.03
9	C	160	HEM	C3B-C4B-NB	2.44	111.22	109.47
9	C	160	HEM	CAA-C2A-C1A	2.43	129.69	124.94
9	G	160	HEM	CAA-C2A-C1A	2.41	129.65	124.94
9	A	160	HEM	CAD-C3D-C4D	2.38	128.84	124.70
9	F	160	HEM	CMA-C3A-C4A	2.35	129.00	125.42
9	F	160	HEM	C2B-C1B-NB	2.34	112.53	109.84
9	E	160	HEM	CMB-C2B-C3B	-2.25	122.97	128.43
9	B	160	HEM	C2B-C1B-NB	2.22	112.40	109.84
9	G	160	HEM	C2A-C1A-NA	2.18	112.57	110.15
9	J	160	HEM	CMA-C3A-C4A	2.18	128.74	125.42
9	B	160	HEM	CHA-C4D-C3D	-2.17	121.23	125.23
9	J	160	HEM	CMD-C2D-C1D	2.15	128.40	125.03
9	L	160	HEM	CHA-C4D-C3D	-2.14	121.28	125.23
9	F	160	HEM	CMD-C2D-C1D	2.12	128.35	125.03
9	I	160	HEM	C3B-C4B-NB	2.12	110.99	109.47
9	L	160	HEM	CMA-C3A-C4A	2.11	128.63	125.42
9	H	160	HEM	CMA-C3A-C4A	2.10	128.62	125.42
9	D	160	HEM	CMA-C3A-C4A	2.09	128.59	125.42
9	A	160	HEM	C2A-C1A-NA	2.07	112.45	110.15
9	D	160	HEM	CAC-C3C-C2C	-2.06	121.75	128.43
9	I	160	HEM	CMB-C2B-C3B	-2.05	123.48	128.43
9	A	160	HEM	C3B-C4B-NB	2.04	110.93	109.47
9	F	160	HEM	CHA-C4D-C3D	-2.03	121.48	125.23
9	K	160	HEM	CAD-C3D-C4D	2.02	128.21	124.70
9	H	160	HEM	C2B-C1B-NB	2.01	112.14	109.84

There are no chirality outliers.

All (88) 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	A	160	HEM	C2C-C3C-CAC-CBC
9	A	160	HEM	C4C-C3C-CAC-CBC
9	B	160	HEM	C2C-C3C-CAC-CBC
9	D	160	HEM	C2B-C3B-CAB-CBB
9	E	160	HEM	C2B-C3B-CAB-CBB
9	E	160	HEM	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
9	E	160	HEM	C2C-C3C-CAC-CBC
9	E	160	HEM	C4C-C3C-CAC-CBC
9	F	160	HEM	C2C-C3C-CAC-CBC
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	I	160	HEM	C2C-C3C-CAC-CBC
9	I	160	HEM	C4C-C3C-CAC-CBC
9	J	160	HEM	C2C-C3C-CAC-CBC
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	H	160	HEM	C2C-C3C-CAC-CBC
9	K	160	HEM	C2B-C3B-CAB-CBB
9	L	160	HEM	C2C-C3C-CAC-CBC
9	B	160	HEM	C4C-C3C-CAC-CBC
9	D	160	HEM	C4B-C3B-CAB-CBB
9	D	160	HEM	C4C-C3C-CAC-CBC
9	F	160	HEM	C4C-C3C-CAC-CBC
9	H	160	HEM	C4B-C3B-CAB-CBB
9	H	160	HEM	C4C-C3C-CAC-CBC
9	J	160	HEM	C4C-C3C-CAC-CBC
9	L	160	HEM	C4B-C3B-CAB-CBB
9	L	160	HEM	C4C-C3C-CAC-CBC
9	D	160	HEM	C2C-C3C-CAC-CBC
9	G	160	HEM	C4C-C3C-CAC-CBC
9	K	160	HEM	C4C-C3C-CAC-CBC
9	K	160	HEM	CAD-CBD-CGD-O2D
9	G	160	HEM	CAD-CBD-CGD-O2D
9	C	160	HEM	C4C-C3C-CAC-CBC
9	C	160	HEM	CAD-CBD-CGD-O2D
9	G	160	HEM	CAD-CBD-CGD-O1D
9	K	160	HEM	CAD-CBD-CGD-O1D
9	L	160	HEM	CAD-CBD-CGD-O2D
9	C	160	HEM	CAD-CBD-CGD-O1D
9	D	160	HEM	CAD-CBD-CGD-O2D
9	I	160	HEM	CAD-CBD-CGD-O2D
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	F	160	HEM	CAD-CBD-CGD-O2D

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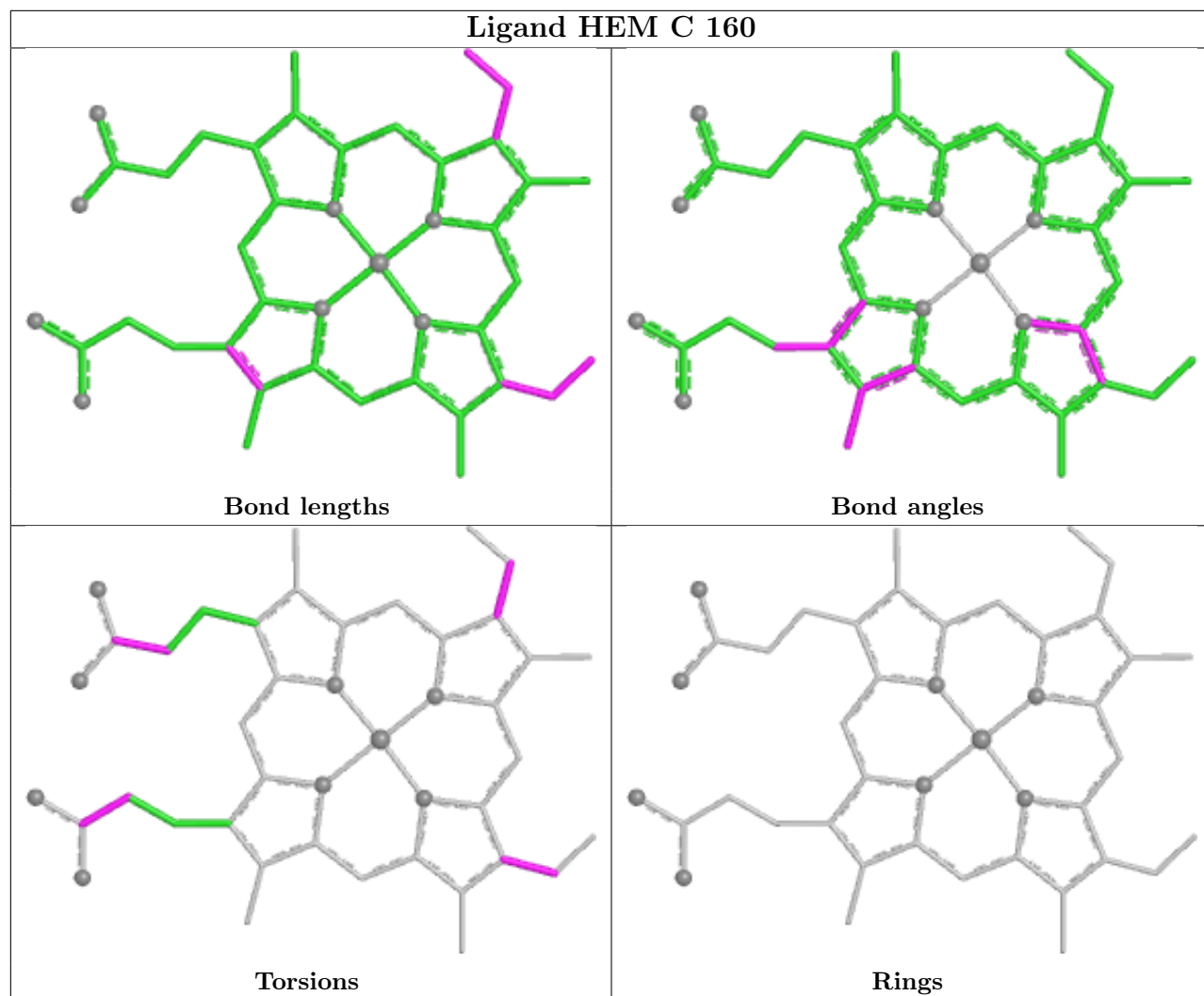
Mol	Chain	Res	Type	Atoms
9	J	160	HEM	CAD-CBD-CGD-O2D
9	L	160	HEM	CAD-CBD-CGD-O1D
9	D	160	HEM	CAD-CBD-CGD-O1D
9	A	160	HEM	CAA-CBA-CGA-O2A
9	H	160	HEM	CAD-CBD-CGD-O1D
9	I	160	HEM	CAD-CBD-CGD-O1D
9	A	160	HEM	CAD-CBD-CGD-O1D
9	F	160	HEM	CAD-CBD-CGD-O1D
9	E	160	HEM	CAD-CBD-CGD-O1D
9	F	160	HEM	CAA-CBA-CGA-O2A
9	J	160	HEM	CAD-CBD-CGD-O1D
9	B	160	HEM	CAD-CBD-CGD-O1D
9	E	160	HEM	CAA-CBA-CGA-O2A
9	I	160	HEM	CAA-CBA-CGA-O2A
9	J	160	HEM	CAA-CBA-CGA-O2A
9	L	160	HEM	CAA-CBA-CGA-O2A
9	D	160	HEM	CAA-CBA-CGA-O2A
9	C	160	HEM	CAA-CBA-CGA-O2A
9	G	160	HEM	CAA-CBA-CGA-O2A
9	K	160	HEM	CAA-CBA-CGA-O2A
9	B	160	HEM	CAA-CBA-CGA-O2A
9	H	160	HEM	CAA-CBA-CGA-O2A
9	A	160	HEM	CAA-CBA-CGA-O1A
9	F	160	HEM	CAA-CBA-CGA-O1A
9	K	160	HEM	CAA-CBA-CGA-O1A
9	C	160	HEM	CAA-CBA-CGA-O1A
9	D	160	HEM	CAA-CBA-CGA-O1A
9	G	160	HEM	CAA-CBA-CGA-O1A
9	J	160	HEM	CAA-CBA-CGA-O1A
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	L	160	HEM	CAA-CBA-CGA-O1A
9	H	160	HEM	CAA-CBA-CGA-O1A
9	E	160	HEM	CAA-CBA-CGA-O1A
9	I	160	HEM	CAA-CBA-CGA-O1A
9	K	160	HEM	C2C-C3C-CAC-CBC

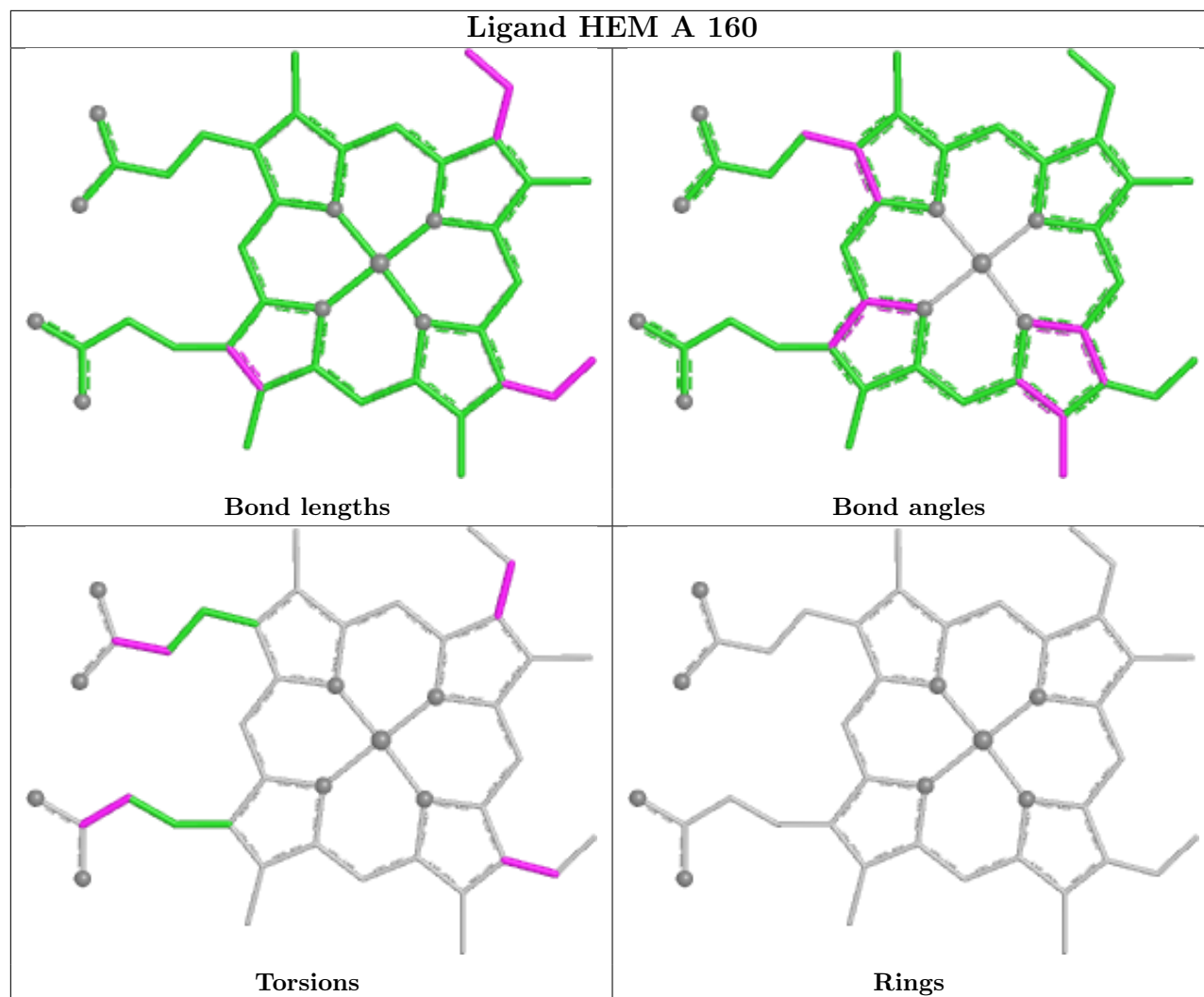
There are no ring outliers.

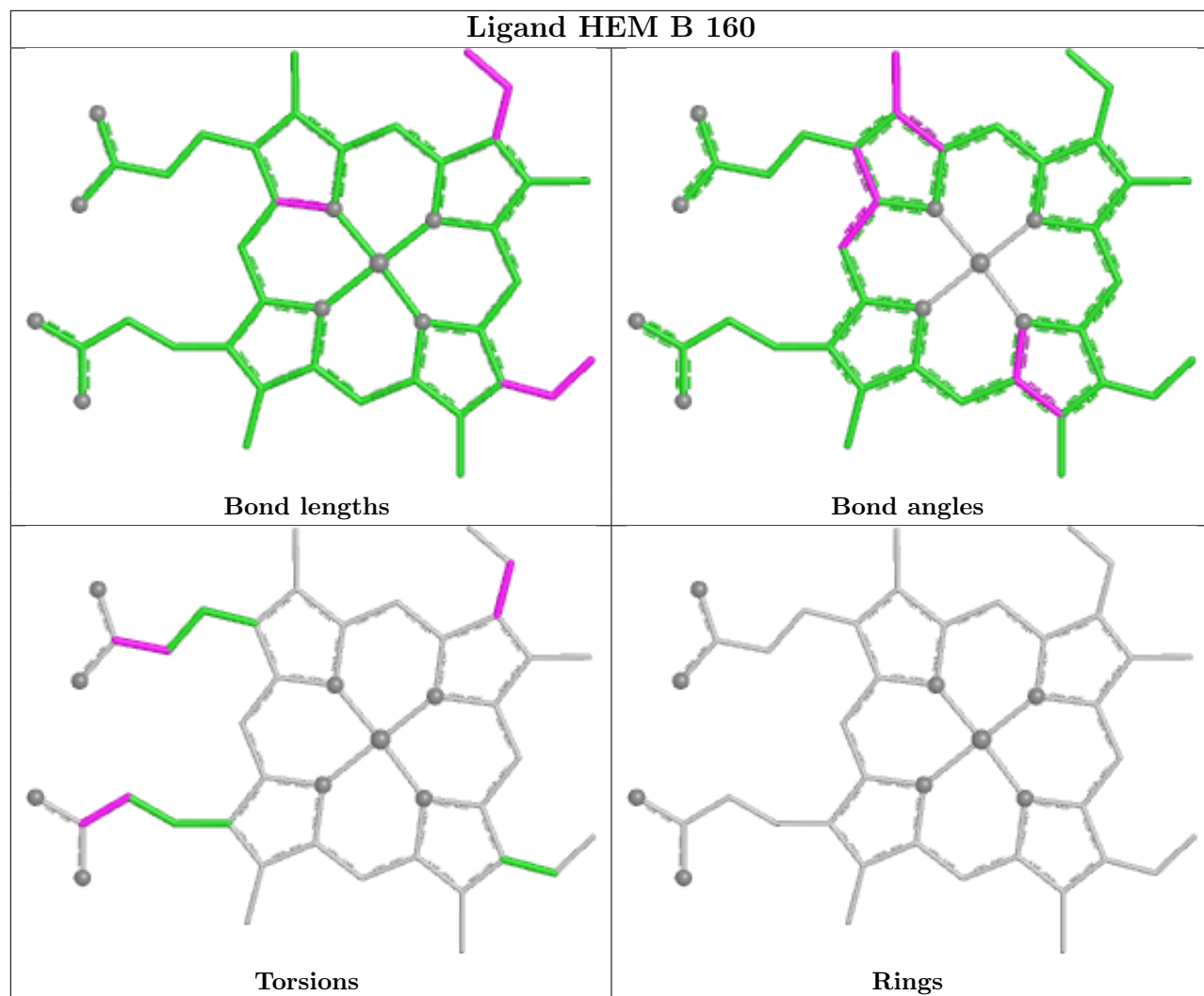
6 monomers are involved in 12 short contacts:

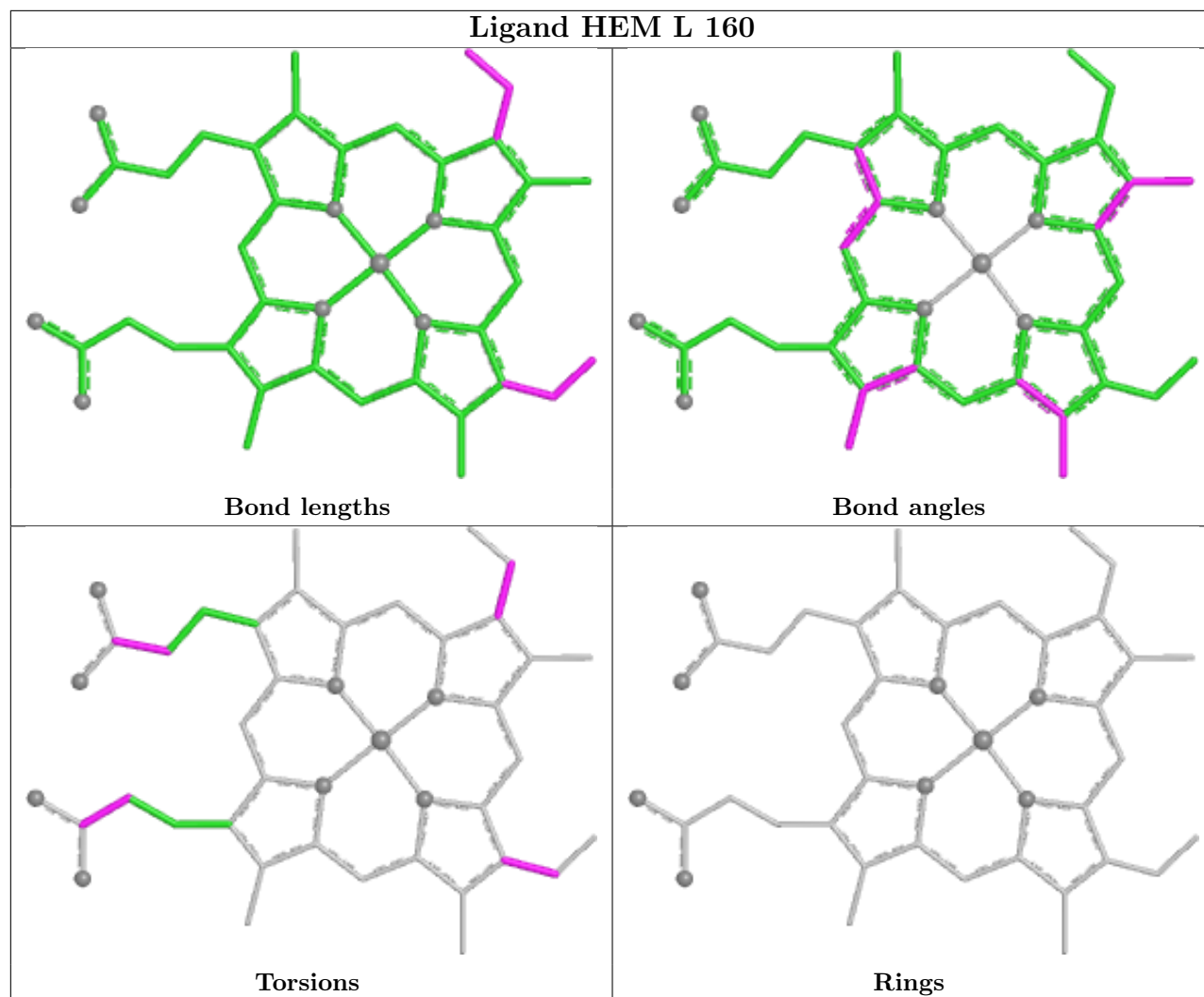
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	C	160	HEM	1	0
9	L	160	HEM	3	0
9	H	160	HEM	3	0
9	K	160	HEM	1	0
9	G	160	HEM	1	0
9	D	160	HEM	3	0

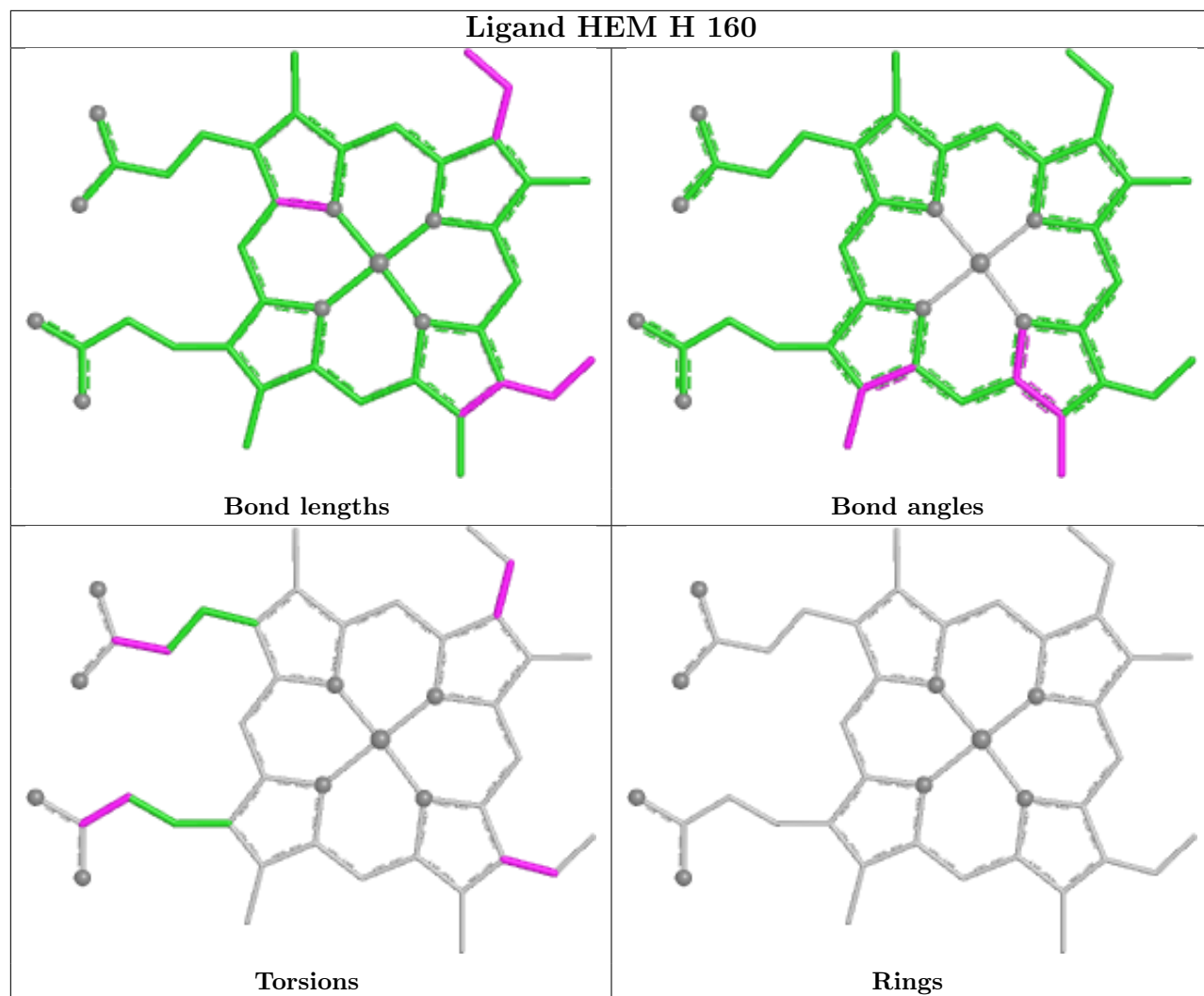
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

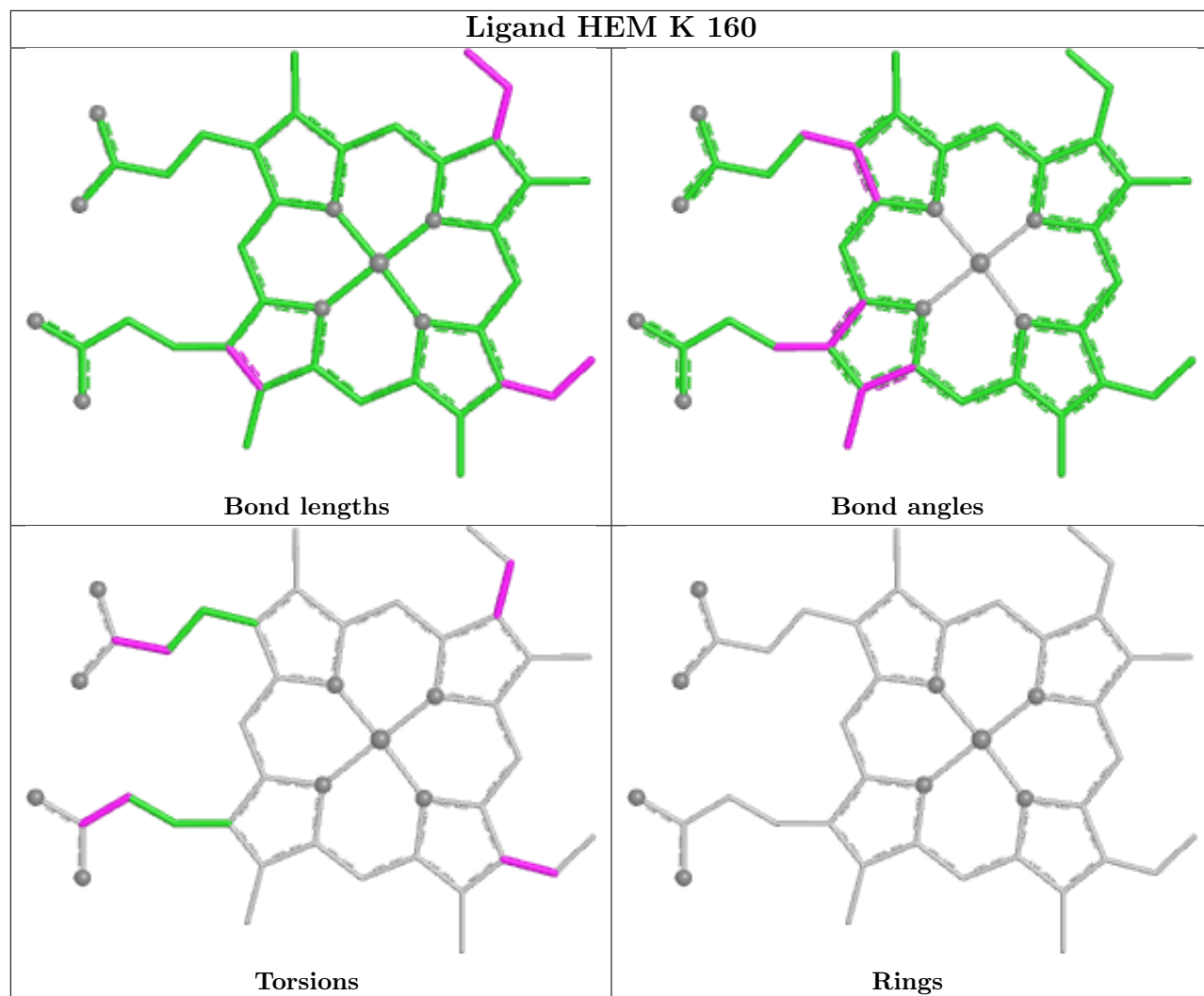




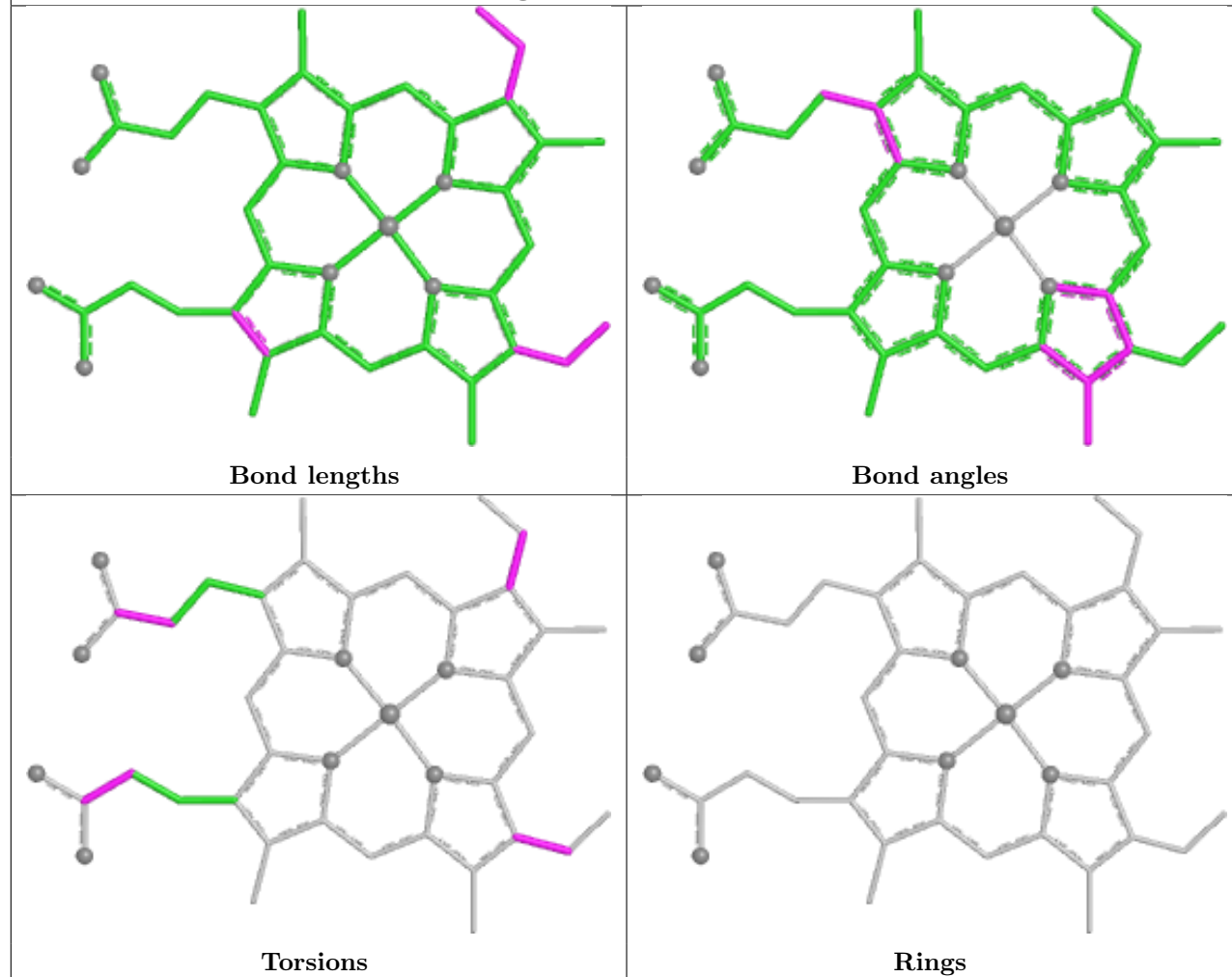


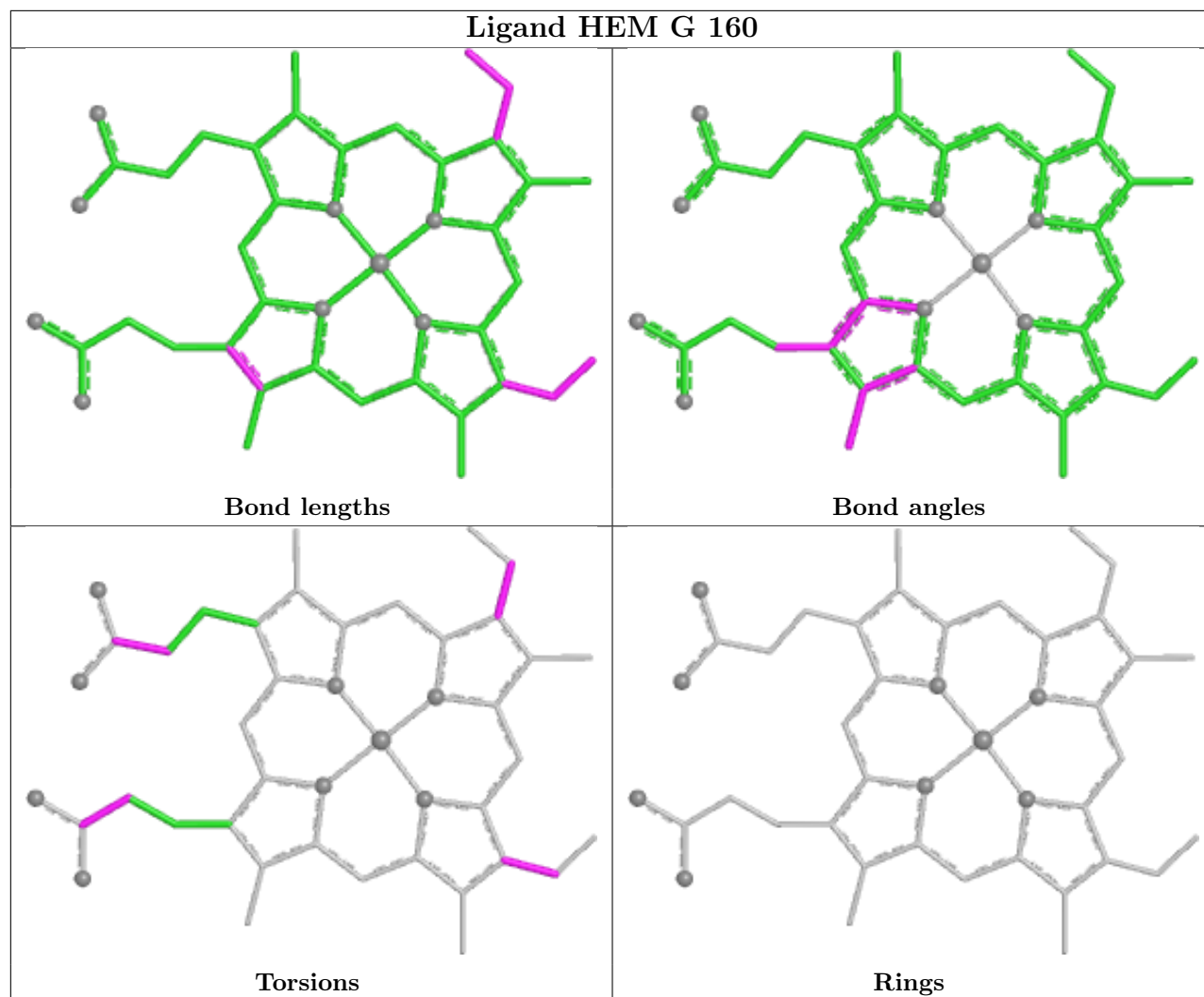


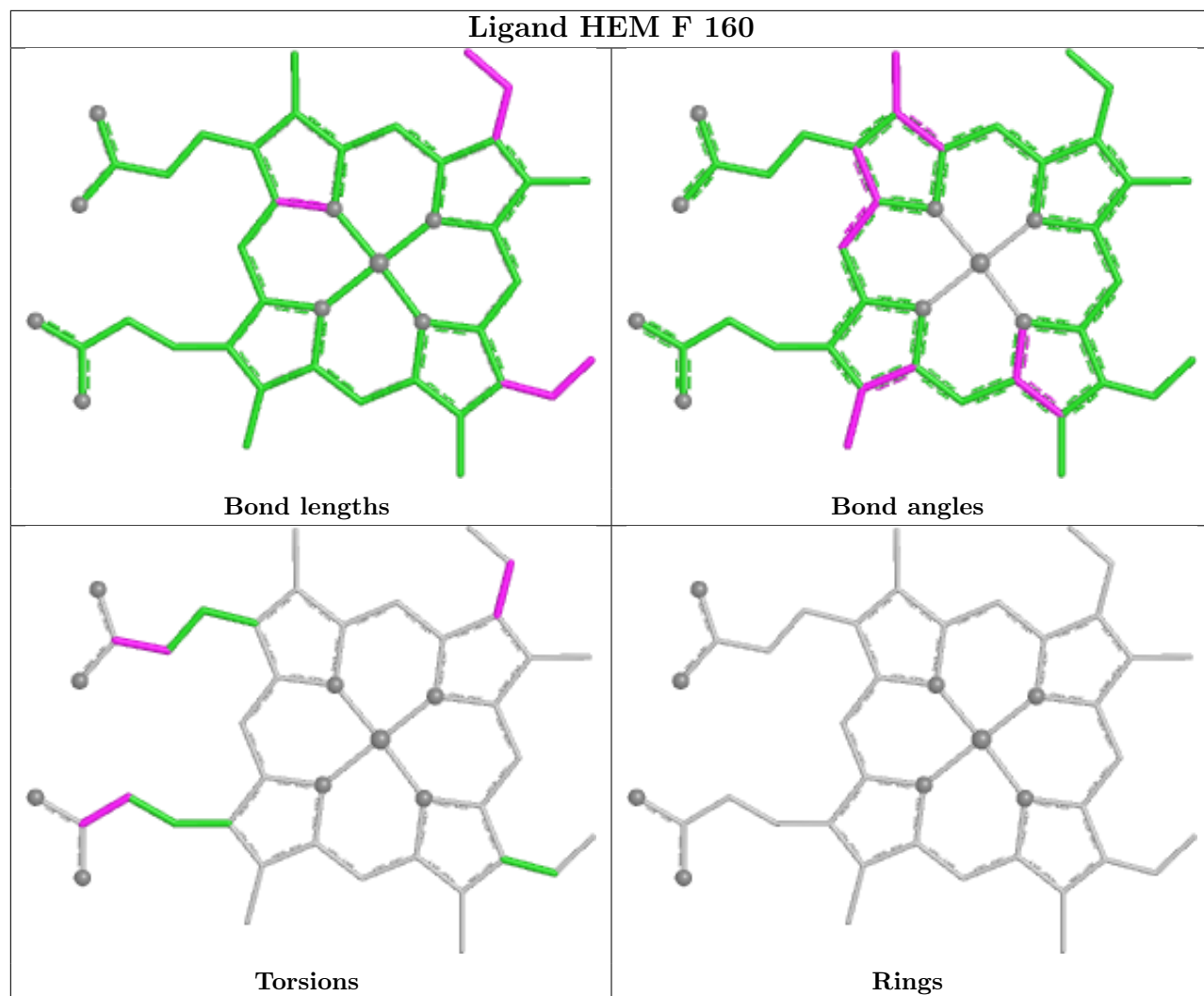




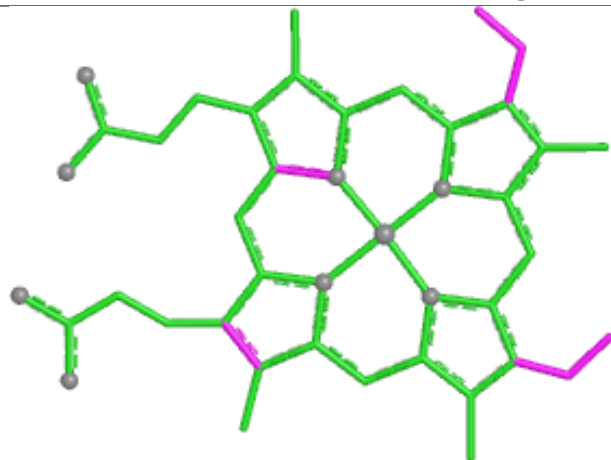
Ligand HEM I 160



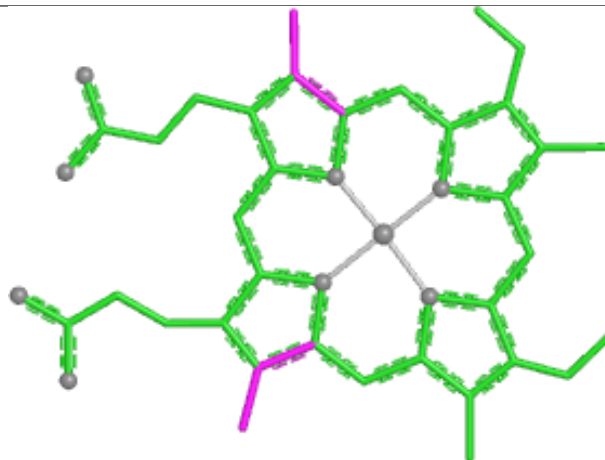




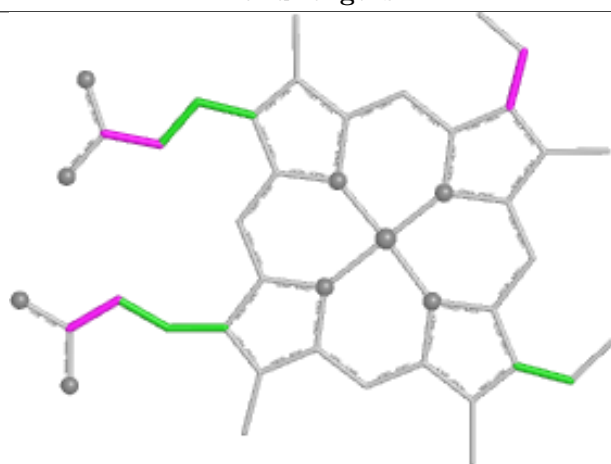
Ligand HEM J 160



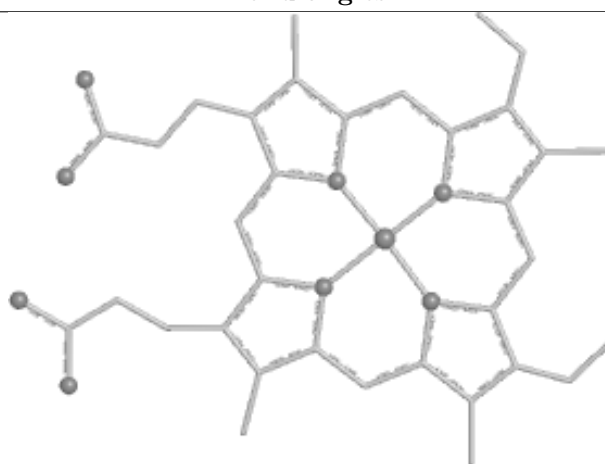
Bond lengths



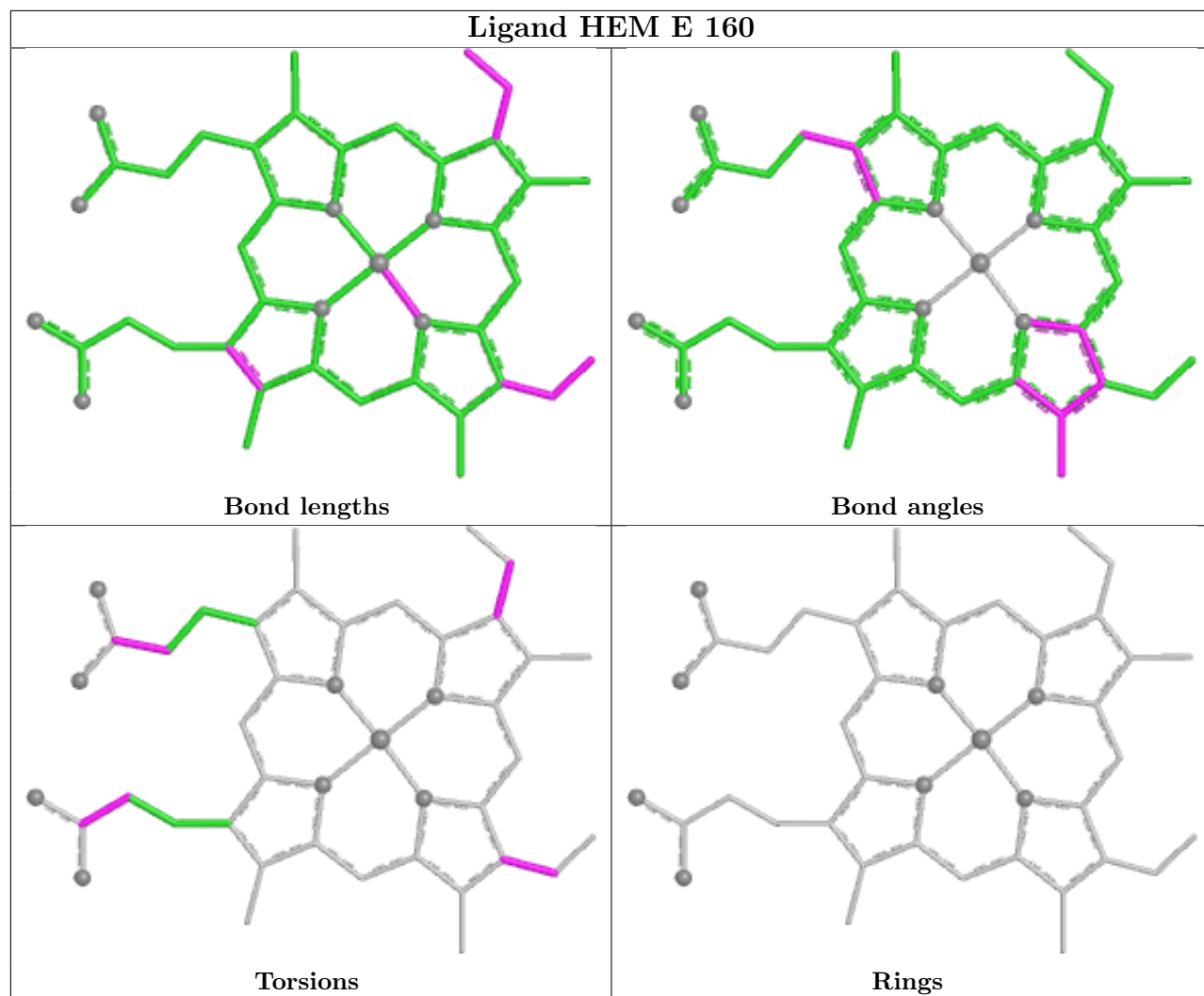
Bond angles

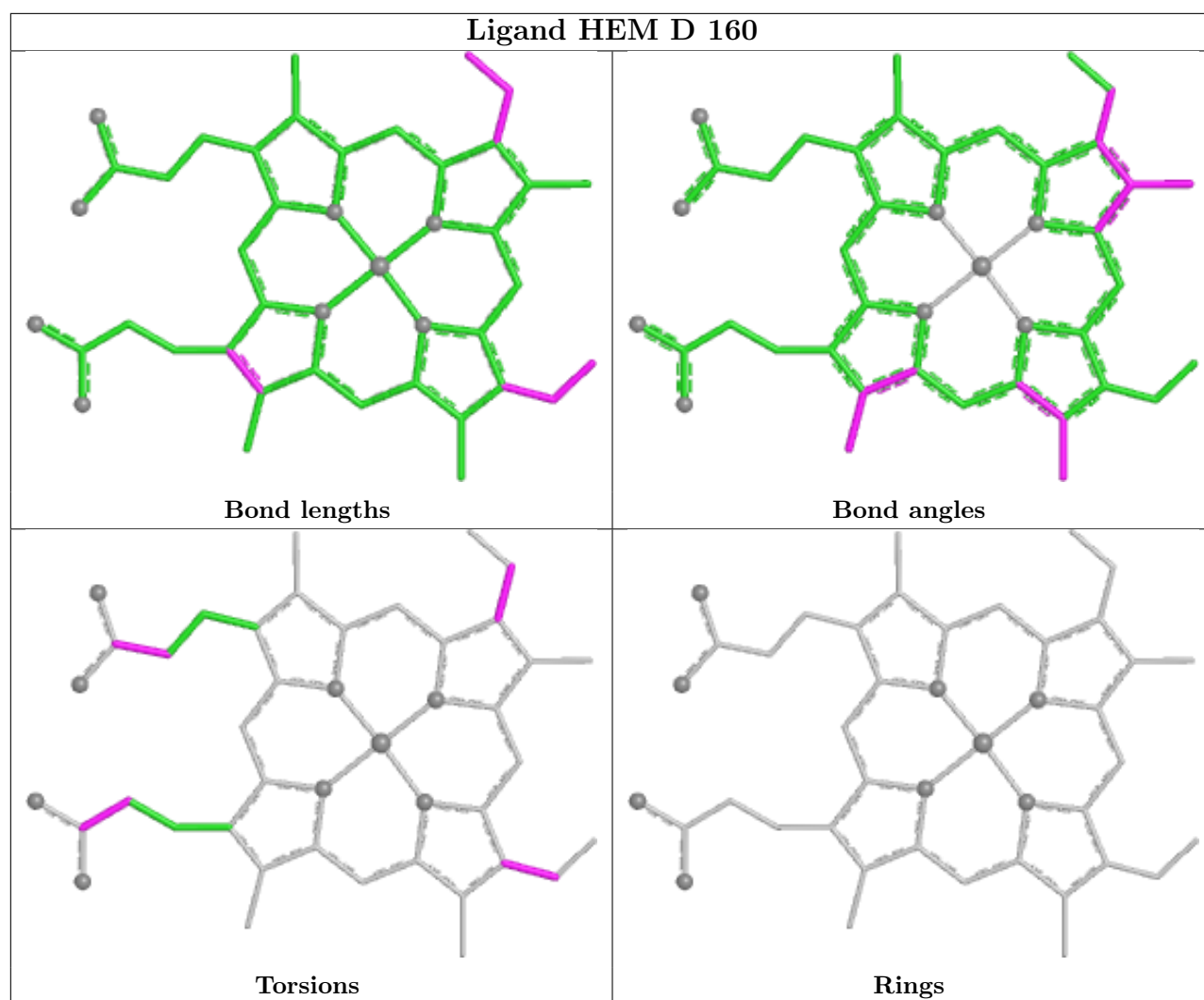


Torsions



Rings





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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th 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%)	-0.31	1 (0%) 84 63	20, 66, 108, 122	0
1	E	147/151 (97%)	-0.40	0 100 100	31, 71, 113, 122	0
1	I	147/151 (97%)	-0.21	0 100 100	22, 69, 109, 122	0
2	B	145/145 (100%)	-0.37	0 100 100	10, 54, 102, 122	0
2	F	145/145 (100%)	-0.29	0 100 100	13, 49, 96, 116	0
2	J	145/145 (100%)	-0.29	0 100 100	25, 69, 114, 122	0
3	C	149/153 (97%)	-0.20	0 100 100	18, 62, 104, 122	0
3	G	149/153 (97%)	-0.32	0 100 100	15, 63, 111, 122	0
3	K	149/153 (97%)	-0.27	0 100 100	33, 85, 122, 122	0
4	D	140/140 (100%)	-0.42	0 100 100	33, 66, 107, 122	0
4	H	140/140 (100%)	-0.39	0 100 100	31, 69, 107, 122	0
4	L	140/140 (100%)	-0.42	0 100 100	31, 72, 108, 122	0
5	M	217/217 (100%)	-0.38	0 100 100	10, 48, 117, 122	0
6	N	220/220 (100%)	-0.39	0 100 100	9, 64, 120, 122	0
7	O	215/215 (100%)	-0.35	0 100 100	16, 69, 114, 122	0
All	All	2395/2419 (99%)	-0.34	1 (0%) 100 100	9, 66, 114, 122	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	5	ASP	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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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, 95th 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.

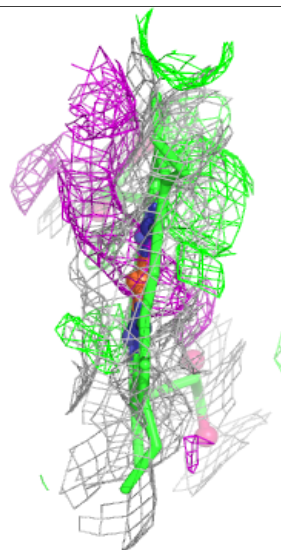
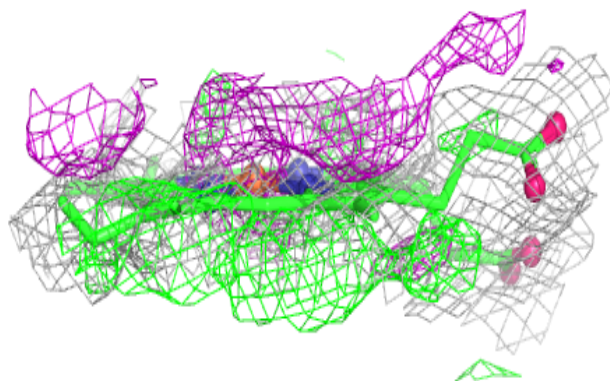
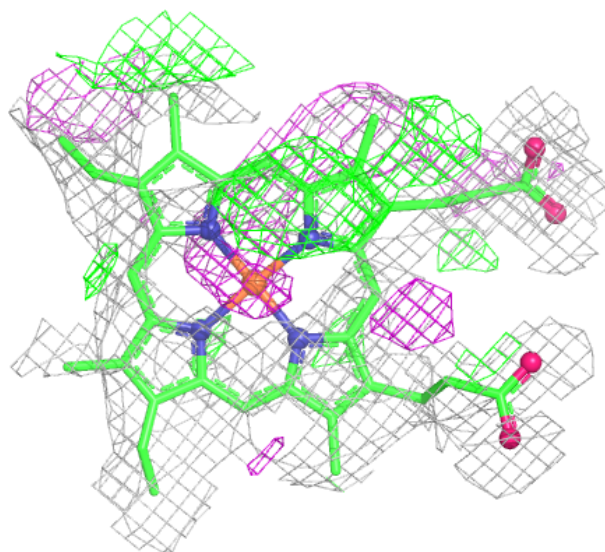
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	CMO	C	161	2/2	0.96	0.16	46,46,46,46	0
8	CMO	B	161	2/2	0.97	0.14	46,46,46,46	0
9	HEM	G	160	43/43	0.97	0.12	66,66,66,66	0
8	CMO	E	161	2/2	0.98	0.07	54,54,54,54	0
8	CMO	L	161	2/2	0.98	0.10	72,72,72,72	0
9	HEM	A	160	43/43	0.98	0.09	60,60,60,60	0
9	HEM	B	160	43/43	0.98	0.10	26,26,26,26	0
9	HEM	C	160	43/43	0.98	0.07	39,39,39,39	0
9	HEM	D	160	43/43	0.98	0.09	38,38,38,38	0
9	HEM	F	160	43/43	0.98	0.08	37,37,37,37	0
8	CMO	A	161	2/2	0.98	0.10	82,82,82,82	0
9	HEM	I	160	43/43	0.98	0.09	64,64,64,64	0
9	HEM	J	160	43/43	0.98	0.09	54,54,54,54	0
9	HEM	K	160	43/43	0.98	0.09	91,91,91,91	0
8	CMO	H	161	2/2	0.99	0.09	68,68,68,68	0
8	CMO	I	161	2/2	0.99	0.08	80,80,80,80	0
9	HEM	E	160	43/43	0.99	0.08	71,71,71,71	0
8	CMO	J	161	2/2	0.99	0.09	69,69,69,69	0
8	CMO	K	161	2/2	0.99	0.08	69,69,69,69	0
9	HEM	H	160	43/43	0.99	0.07	52,52,52,52	0
8	CMO	D	161	2/2	0.99	0.09	74,74,74,74	0
8	CMO	F	161	2/2	0.99	0.08	64,64,64,64	0
8	CMO	G	161	2/2	0.99	0.10	38,38,38,38	0
9	HEM	L	160	43/43	0.99	0.08	46,46,46,46	0
10	CA	M	250	1/1	0.99	0.04	20,20,20,20	0
10	CA	M	251	1/1	0.99	0.14	43,43,43,43	0
10	CA	O	250	1/1	0.99	0.12	23,23,23,23	0
11	ZN	M	252	1/1	0.99	0.05	58,58,58,58	0
10	CA	N	250	1/1	1.00	0.09	15,15,15,15	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.

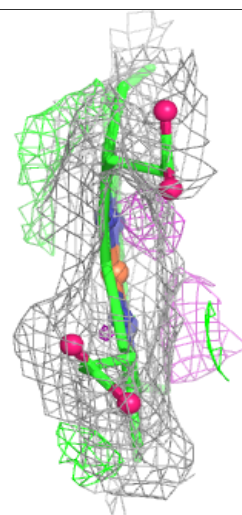
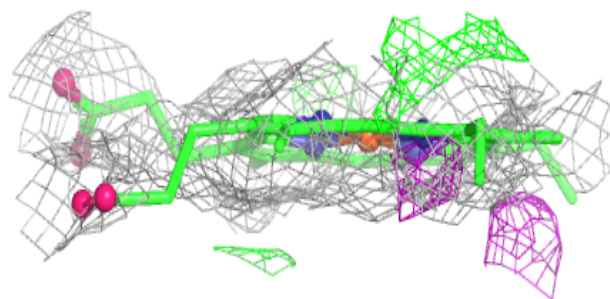
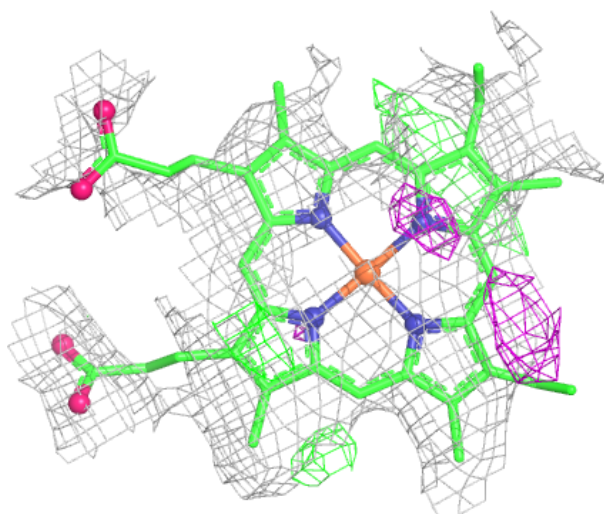
Electron density around HEM G 160:

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



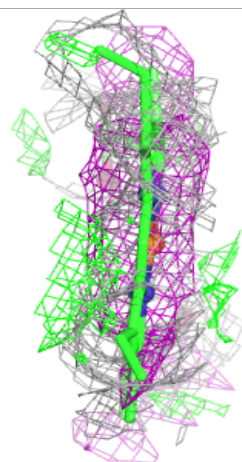
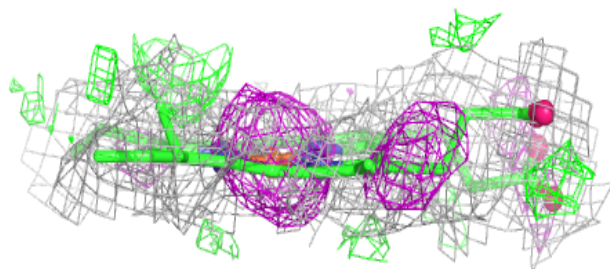
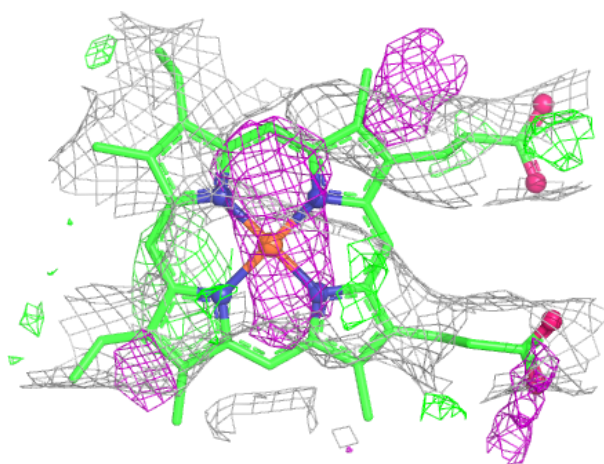
Electron density around HEM A 160:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



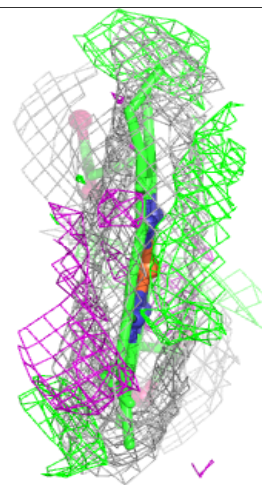
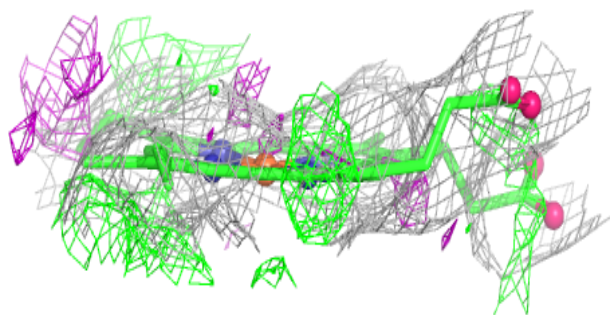
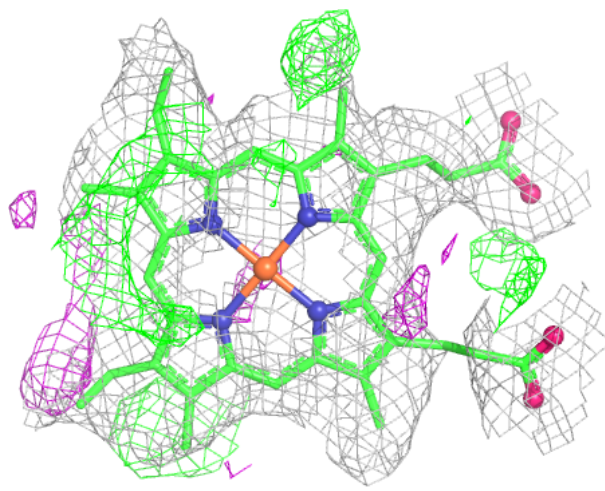
Electron density around HEM B 160:

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



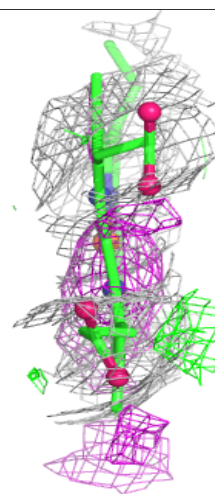
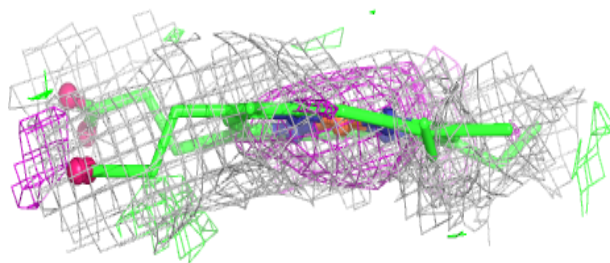
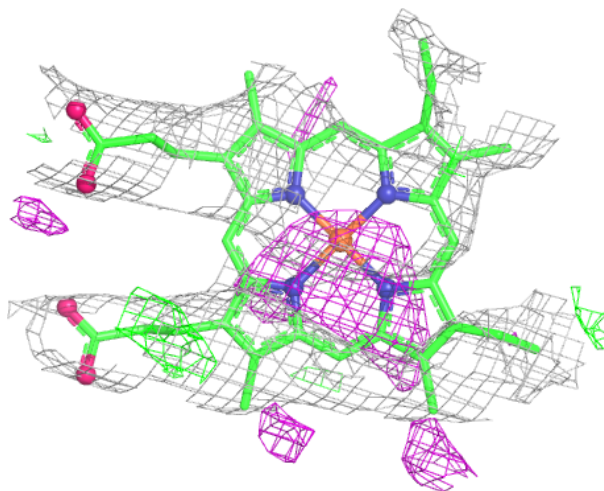
Electron density around HEM C 160:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



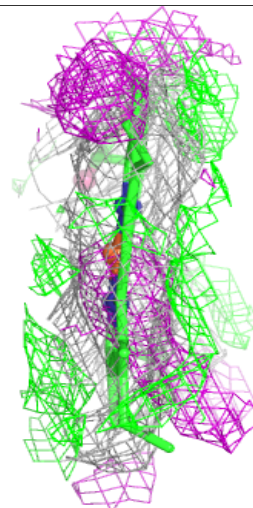
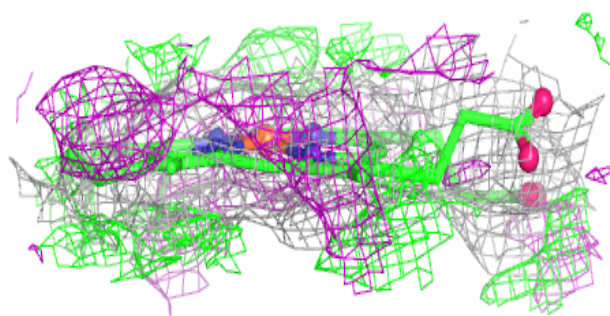
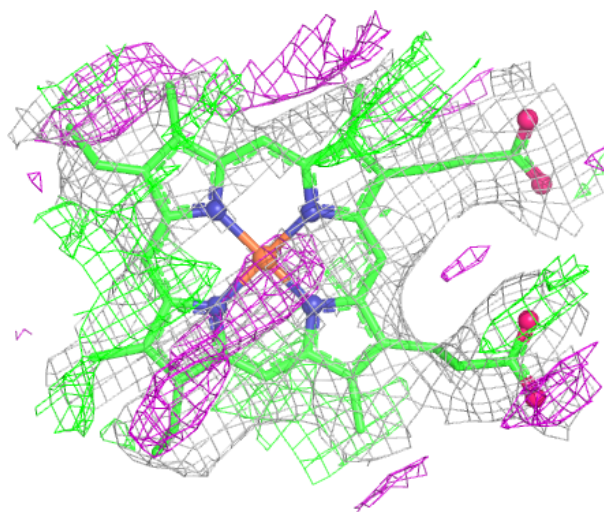
Electron density around HEM D 160:

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and green (positive)



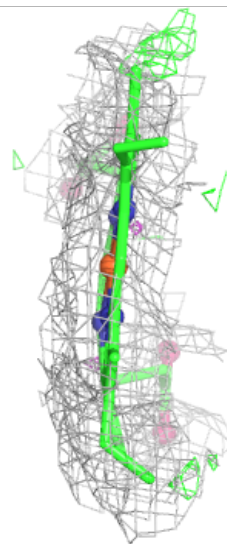
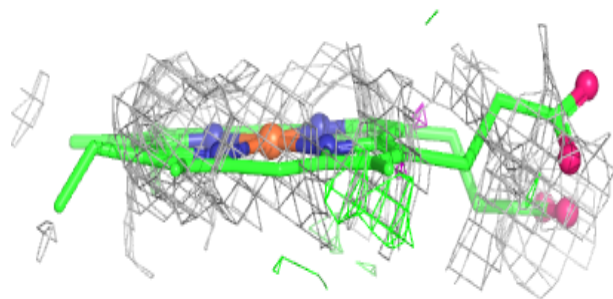
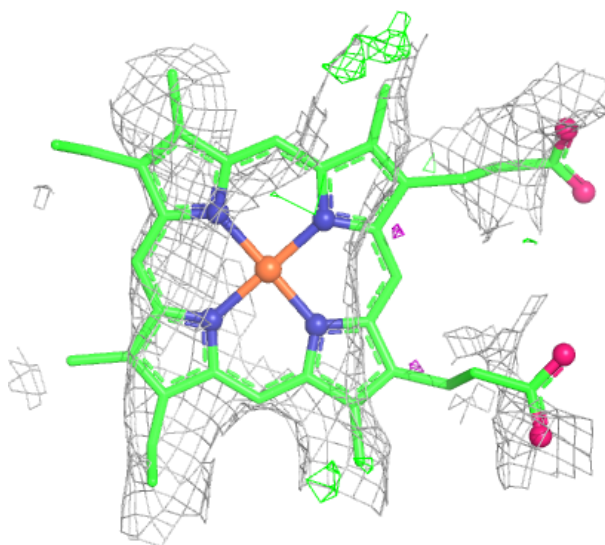
Electron density around HEM F 160:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



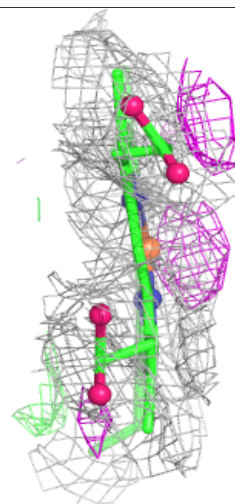
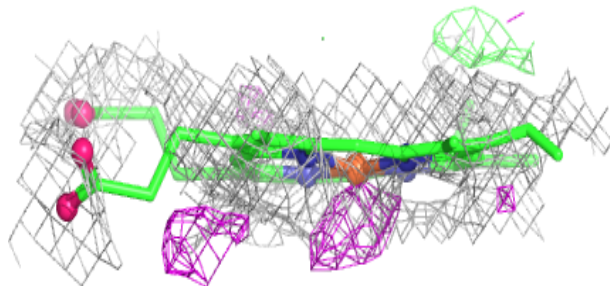
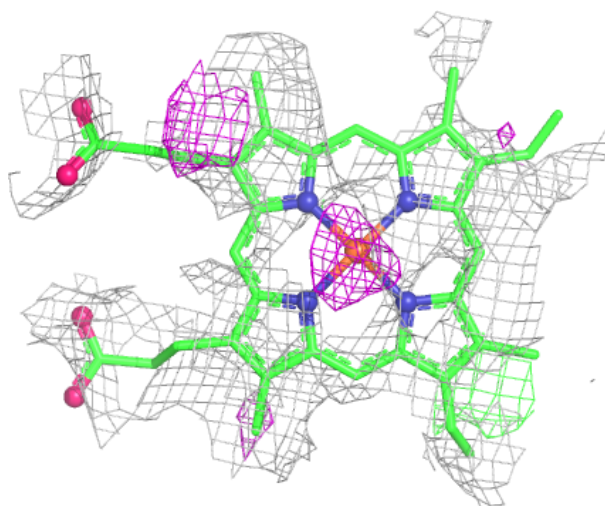
Electron density around HEM I 160:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



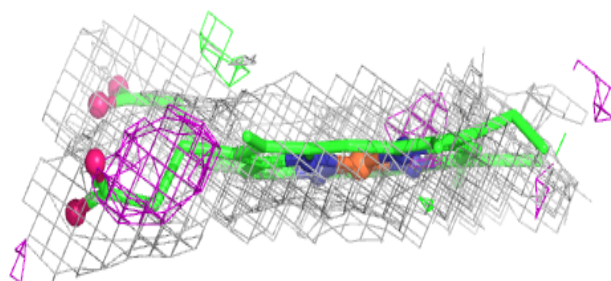
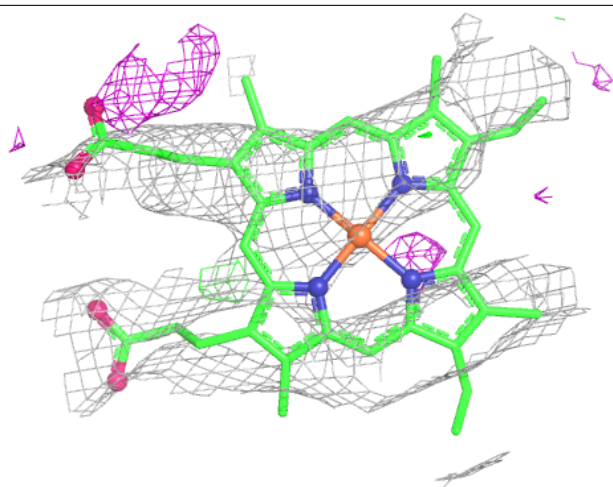
Electron density around HEM J 160:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



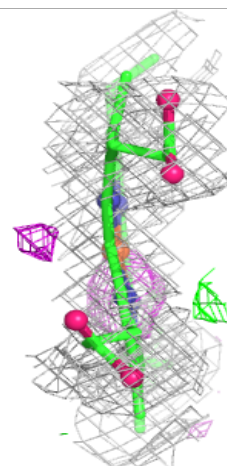
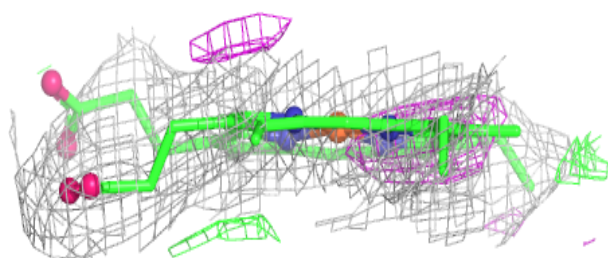
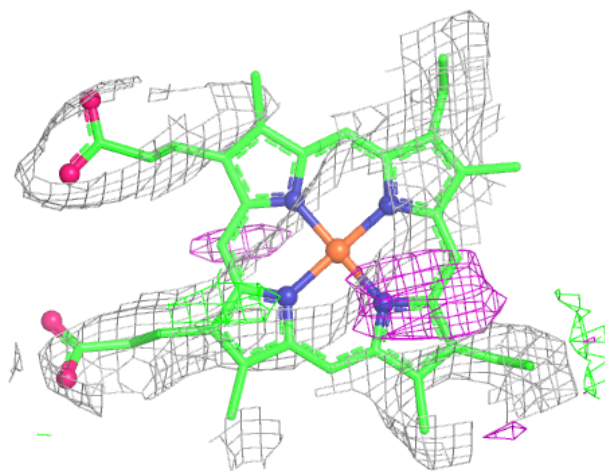
Electron density around HEM K 160:

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



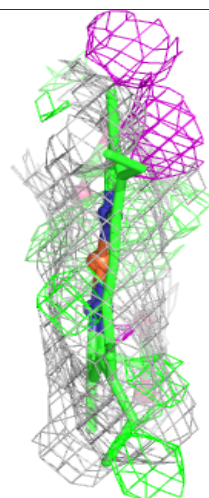
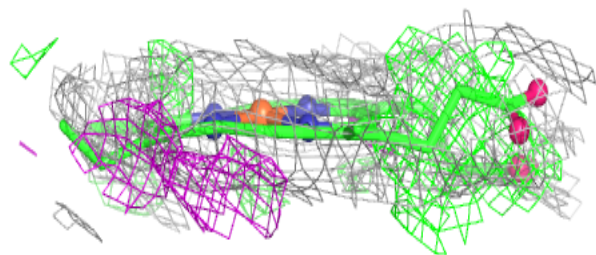
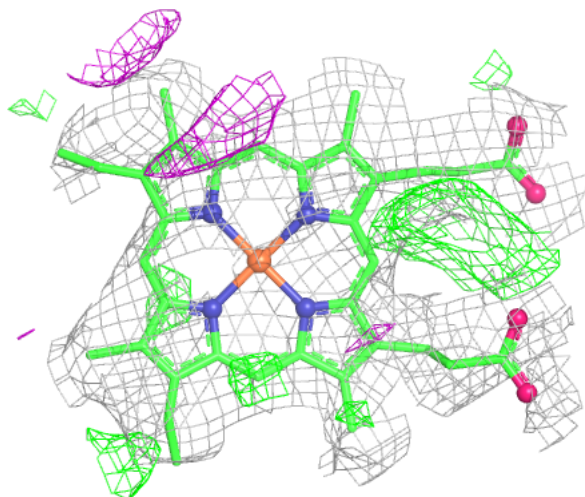
Electron density around HEM E 160:

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



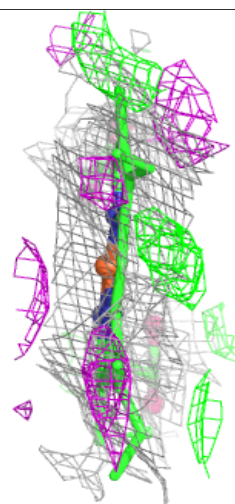
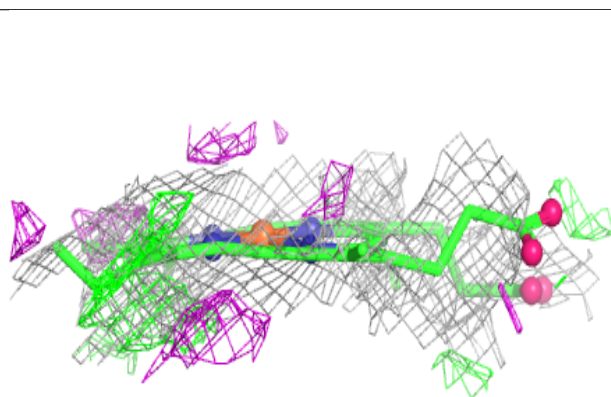
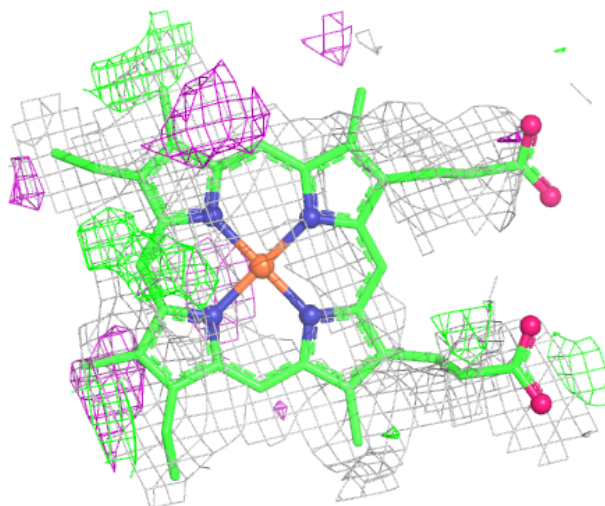
Electron density around HEM H 160:

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



Electron density around HEM 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)



6.5 Other polymers ⓘ

There are no such residues in this entry.