



Full wwPDB EM Validation Report ⓘ

Aug 5, 2026 – 12:10 AM EDT

PDB ID : 8EUM / pdb_00008eum
EMDB ID : EMD-28615
Title : MicroED structure of an Aeropyrum pernix protoglobin mutant
Authors : Danelius, E.; Gonen, T.; Unge, J.T.
Deposited on : 2022-10-18
Resolution : 2.10 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : **NOT EXECUTED**
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **NOT EXECUTED**
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

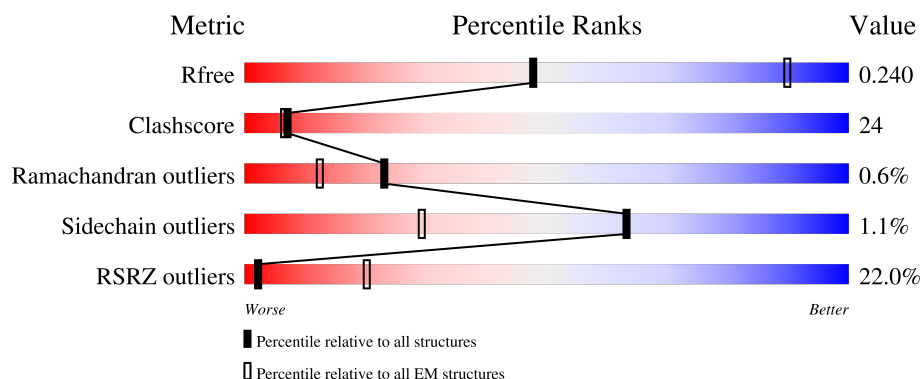
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON CRYSTALLOGRAPHY

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
R_{free}	180332	208
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102
RSRZ outliers	180361	209

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	190	23% 62% 34% ...
1	B	190	24% 64% 32% ...
1	C	190	23% 63% 33% ...
1	D	190	16% 66% 27% .. 5%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6745 atoms, of which 55 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Protogloblin ApPgb.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	187	Total	C	N	O	S	0	0
			1552	1008	260	281	3		
1	B	187	Total	C	N	O	S	0	0
			1551	1008	260	280	3		
1	C	187	Total	C	N	O	S	0	0
			1552	1008	260	281	3		
1	D	180	Total	C	N	O	S	0	0
			1476	961	242	270	3		

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	45	GLY	CYS	engineered mutation	UNP Q9YFF4
A	59	LEU	TRP	engineered mutation	UNP Q9YFF4
A	60	VAL	TYR	engineered mutation	UNP Q9YFF4
A	63	ARG	VAL	engineered mutation	UNP Q9YFF4
A	102	SER	CYS	engineered mutation	UNP Q9YFF4
A	145	GLN	PHE	engineered mutation	UNP Q9YFF4
A	149	LEU	ILE	engineered mutation	UNP Q9YFF4
B	45	GLY	CYS	engineered mutation	UNP Q9YFF4
B	59	LEU	TRP	engineered mutation	UNP Q9YFF4
B	60	VAL	TYR	engineered mutation	UNP Q9YFF4
B	63	ARG	VAL	engineered mutation	UNP Q9YFF4
B	102	SER	CYS	engineered mutation	UNP Q9YFF4
B	145	GLN	PHE	engineered mutation	UNP Q9YFF4
B	149	LEU	ILE	engineered mutation	UNP Q9YFF4
C	45	GLY	CYS	engineered mutation	UNP Q9YFF4
C	59	LEU	TRP	engineered mutation	UNP Q9YFF4
C	60	VAL	TYR	engineered mutation	UNP Q9YFF4
C	63	ARG	VAL	engineered mutation	UNP Q9YFF4
C	102	SER	CYS	engineered mutation	UNP Q9YFF4
C	145	GLN	PHE	engineered mutation	UNP Q9YFF4
C	149	LEU	ILE	engineered mutation	UNP Q9YFF4
D	45	GLY	CYS	engineered mutation	UNP Q9YFF4

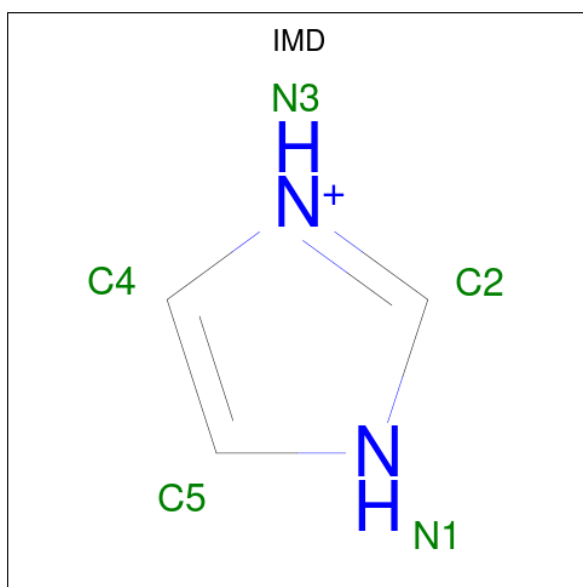
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Chain	Residue	Modelled	Actual	Comment	Reference
D	59	LEU	TRP	engineered mutation	UNP Q9YFF4
D	60	VAL	TYR	engineered mutation	UNP Q9YFF4
D	63	ARG	VAL	engineered mutation	UNP Q9YFF4
D	102	SER	CYS	engineered mutation	UNP Q9YFF4
D	145	GLN	PHE	engineered mutation	UNP Q9YFF4
D	149	LEU	ILE	engineered mutation	UNP Q9YFF4

- # HEM

Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0

- WORLDWIDE
PDB
PROTEIN DATA BANK



Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total 5	C 3	N 2	0	
3	A	1	Total 10	C 3	H 5 N 2	0	
3	A	1	Total 10	C 3	H 5 N 2	0	
3	A	1	Total 10	C 3	H 5 N 2	0	
3	A	1	Total 10	C 3	H 5 N 2	0	
3	B	1	Total 5	C 3	N 2	0	
3	B	1	Total 10	C 3	H 5 N 2	0	
3	C	1	Total 10	C 3	H 5 N 2	0	
3	C	1	Total 10	C 3	H 5 N 2	0	
3	C	1	Total 5	C 3	N 2	0	
3	C	1	Total 10	C 3	H 5 N 2	0	
3	C	1	Total 10	C 3	H 5 N 2	0	
3	C	1	Total 10	C 3	H 5 N 2	0	
3	D	1	Total 5	C 3	N 2	0	

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Mol	Chain	Residues	Atoms				AltConf
3	D	1	Total	C	H	N	0
			10	3	5	2	

- Molecule 4 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Fe	0
			1	1	
4	B	1	Total	Fe	0
			1	1	
4	C	1	Total	Fe	0
			1	1	
4	D	1	Total	Fe	0
			1	1	

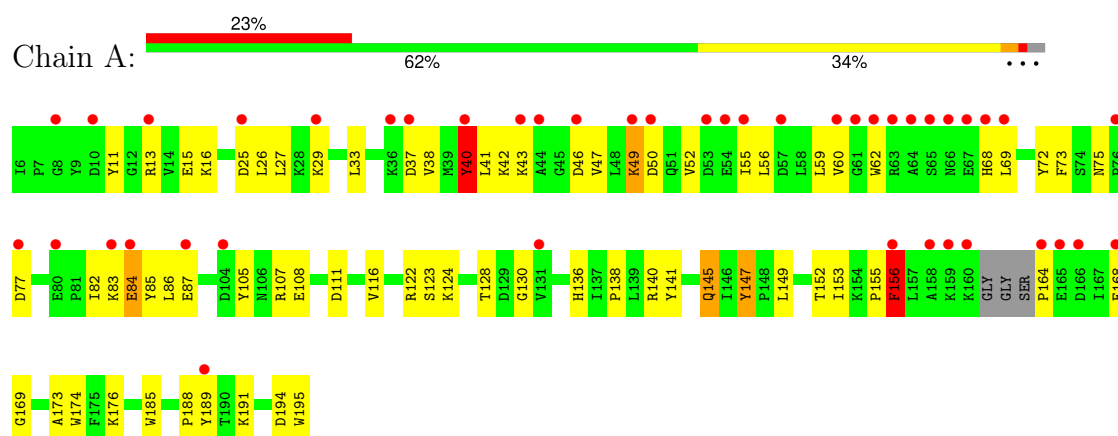
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		AltConf
5	A	68	Total	O	0
			68	68	
5	B	69	Total	O	0
			69	69	
5	C	81	Total	O	0
			81	81	
5	D	90	Total	O	0
			90	90	

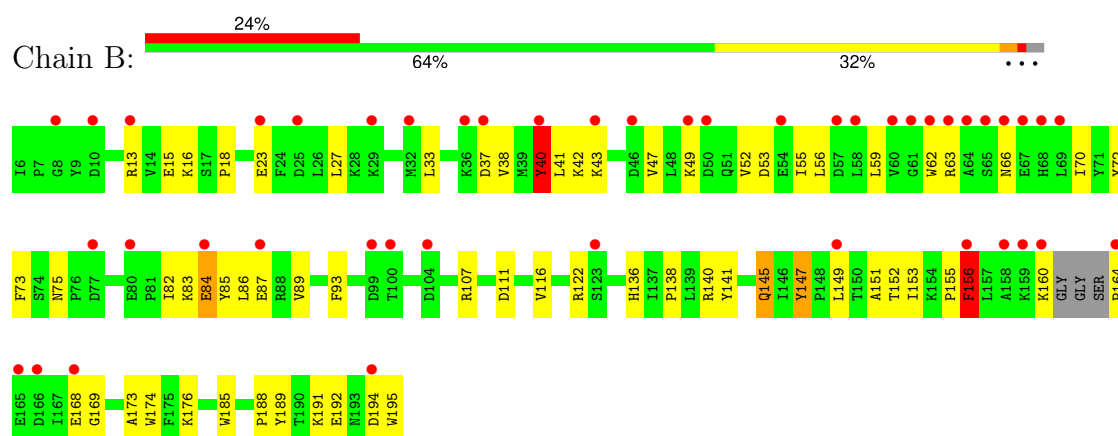
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

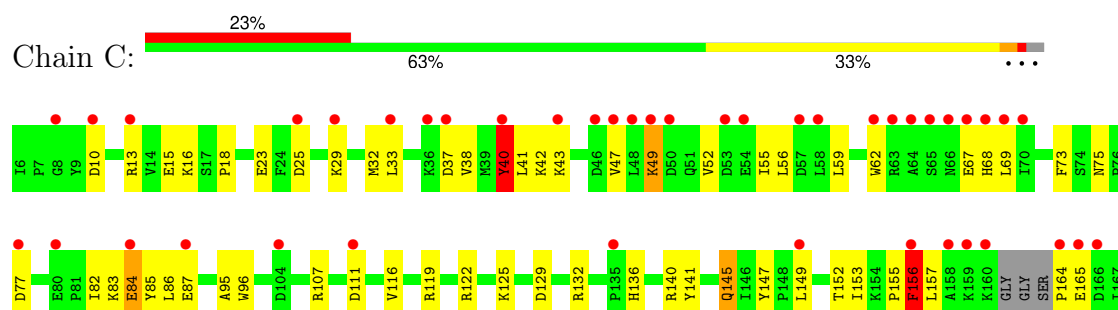
• Molecule 1: Protogloblin ApPgb

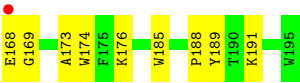


• Molecule 1: Protogloblin ApPgb

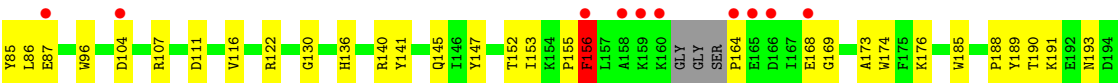
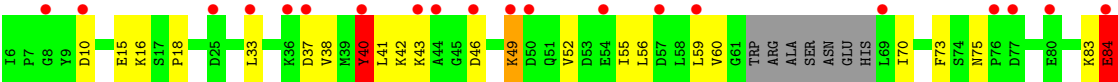


• Molecule 1: Protogloblin ApPgb





● Molecule 1: Protogloblin ApPgb



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	46.23Å 58.27Å 80.73Å 104.09° 98.58° 90.11°	Depositor
Resolution (Å)	24.46 – 2.10 24.46 – 2.10	Depositor EDS
% Data completeness (in resolution range)	71.8 (24.46-2.10) 71.7 (24.46-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.34 (at 2.10Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487)	Depositor
R, R_{free}	0.188 , 0.212 0.223 , 0.240	Depositor DCC
R_{free} test set	1744 reflections (3.70%)	wwPDB-VP
Wilson B-factor (Å ²)	9.1	Xtriage
Anisotropy	1.027	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 41.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	6745	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.87% 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

5.1 Standard geometry

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

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	0.55	0/1595	0.90	7/2163 (0.3%)
1	B	0.55	0/1594	0.89	7/2161 (0.3%)
1	C	0.55	0/1595	0.89	7/2163 (0.3%)
1	D	0.56	0/1515	0.90	7/2055 (0.3%)
All	All	0.55	0/6299	0.90	28/8542 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
1	C	0	2
1	D	0	2
All	All	0	8

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	84	GLU	CA-CB-CG	-5.99	102.12	114.10
1	A	84	GLU	CA-CB-CG	-5.99	102.13	114.10
1	D	84	GLU	CA-CB-CG	-5.99	102.13	114.10
1	C	156	PHE	N-CA-CB	-5.95	100.08	109.78
1	C	84	GLU	CA-CB-CG	-5.95	102.20	114.10
1	A	156	PHE	N-CA-CB	-5.92	100.13	109.78
1	D	156	PHE	N-CA-CB	-5.92	100.13	109.78
1	B	156	PHE	N-CA-CB	-5.91	100.14	109.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	191	LYS	CA-C-O	-5.83	115.36	121.55
1	C	191	LYS	CA-C-O	-5.82	115.38	121.55
1	C	156	PHE	CB-CG-CD1	-5.81	110.83	120.70
1	B	156	PHE	CB-CG-CD1	-5.78	110.88	120.70
1	A	156	PHE	CB-CG-CD1	-5.77	110.89	120.70
1	D	156	PHE	CB-CG-CD1	-5.76	110.90	120.70
1	C	147	TYR	CA-CB-CG	-5.68	103.68	113.90
1	C	40	TYR	N-CA-CB	-5.67	101.49	109.94
1	D	40	TYR	N-CA-CB	-5.67	101.49	109.94
1	B	147	TYR	CA-CB-CG	-5.67	103.70	113.90
1	B	40	TYR	N-CA-CB	-5.65	101.52	109.94
1	A	147	TYR	CA-CB-CG	-5.65	103.73	113.90
1	A	40	TYR	N-CA-CB	-5.65	101.52	109.94
1	D	147	TYR	CA-CB-CG	-5.64	103.75	113.90
1	C	84	GLU	N-CA-CB	-5.58	101.63	110.22
1	A	84	GLU	N-CA-CB	-5.56	101.66	110.22
1	D	84	GLU	N-CA-CB	-5.55	101.67	110.22
1	B	84	GLU	N-CA-CB	-5.55	101.68	110.22
1	B	191	LYS	CA-C-O	-5.46	115.76	121.55
1	D	191	LYS	CA-C-O	-5.40	115.83	121.55

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	156	PHE	Sidechain
1	A	40	TYR	Sidechain
1	B	156	PHE	Sidechain
1	B	40	TYR	Sidechain
1	C	156	PHE	Sidechain
1	C	40	TYR	Sidechain
1	D	156	PHE	Sidechain
1	D	40	TYR	Sidechain

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	1552	0	1537	89	1
1	B	1551	0	1537	80	1
1	C	1552	0	1537	77	1
1	D	1476	0	1453	54	1
2	A	43	0	30	15	0
2	B	43	0	30	8	0
2	C	43	0	30	10	0
2	D	43	0	30	7	0
3	A	25	20	24	2	0
3	B	10	5	9	1	0
3	C	30	25	28	1	0
3	D	10	5	9	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	68	0	0	9	0
5	B	69	0	0	20	0
5	C	81	0	0	18	2
5	D	90	0	0	9	2
All	All	6690	55	6254	301	4

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 (301) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:145:GLN:HG3	1:C:149:LEU:CD1	1.76	1.15
1:C:145:GLN:HG3	1:C:149:LEU:HD11	1.07	1.07
1:A:145:GLN:HG3	1:A:149:LEU:HD12	1.28	1.06
1:C:13:ARG:NH2	5:C:304:HOH:O	1.96	0.96
1:C:165:GLU:OE2	5:C:301:HOH:O	1.83	0.94
1:A:16:LYS:HA	1:A:111:ASP:OD2	1.68	0.94
1:D:16:LYS:HA	1:D:111:ASP:OD2	1.67	0.94
2:C:203:HEM:O2D	5:C:302:HOH:O	1.85	0.94
1:C:16:LYS:HA	1:C:111:ASP:OD2	1.68	0.94
1:B:16:LYS:HA	1:B:111:ASP:OD2	1.67	0.94
1:C:29:LYS:N	1:C:29:LYS:HE2	1.85	0.91
1:B:84:GLU:HG2	1:B:85:TYR:N	1.86	0.90
1:B:155:PRO:HG2	5:B:317:HOH:O	1.71	0.90
1:C:84:GLU:HG2	1:C:85:TYR:N	1.86	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:GLU:HG2	1:A:85:TYR:N	1.86	0.89
1:A:145:GLN:HG3	1:A:149:LEU:CD1	2.03	0.89
1:A:26:LEU:HA	1:A:29:LYS:HD3	1.55	0.87
1:D:84:GLU:HG2	1:D:85:TYR:N	1.87	0.87
1:C:23:GLU:OE2	5:C:303:HOH:O	1.92	0.87
1:A:185:TRP:O	1:A:188:PRO:HD2	1.76	0.86
1:D:185:TRP:O	1:D:188:PRO:HD2	1.75	0.86
2:C:203:HEM:HMB1	2:C:203:HEM:HBB2	1.55	0.85
1:A:33:LEU:HD12	1:A:37:ASP:CB	2.06	0.85
1:B:185:TRP:O	1:B:188:PRO:HD2	1.75	0.85
1:D:33:LEU:HD12	1:D:37:ASP:CB	2.06	0.85
1:B:63:ARG:NH1	5:B:302:HOH:O	2.09	0.85
1:C:185:TRP:O	1:C:188:PRO:HD2	1.75	0.85
1:B:33:LEU:HD12	1:B:37:ASP:CB	2.06	0.85
1:C:33:LEU:HD12	1:C:37:ASP:CB	2.06	0.84
1:C:141:TYR:HB3	2:C:203:HEM:HBB1	1.57	0.84
1:C:87:GLU:O	5:C:305:HOH:O	1.98	0.81
1:B:15:GLU:HG3	1:C:77:ASP:OD2	1.81	0.81
1:A:26:LEU:HD23	1:A:29:LYS:HD3	1.63	0.81
1:B:72:TYR:OH	5:B:301:HOH:O	1.99	0.80
1:B:145:GLN:HB3	2:B:201:HEM:HMC2	1.63	0.80
1:D:96:TRP:HA	5:D:307:HOH:O	1.82	0.79
1:C:145:GLN:CG	1:C:149:LEU:HD11	2.02	0.79
1:B:66:ASN:HD22	1:B:70:ILE:HD13	1.47	0.79
1:B:53:ASP:CG	5:B:305:HOH:O	2.24	0.79
1:B:66:ASN:HD22	1:B:70:ILE:CD1	1.96	0.78
1:A:75:ASN:ND2	1:D:15:GLU:OE2	2.14	0.78
1:A:77:ASP:OD2	1:D:15:GLU:HG3	1.85	0.77
1:A:33:LEU:HD12	1:A:37:ASP:HB3	1.66	0.77
1:A:72:TYR:HB2	2:A:201:HEM:CBC	2.14	0.77
1:D:33:LEU:HD12	1:D:37:ASP:HB3	1.66	0.77
1:A:72:TYR:HB2	2:A:201:HEM:HBC1	1.67	0.77
1:A:26:LEU:HD23	1:A:29:LYS:CD	2.16	0.76
1:A:26:LEU:HA	1:A:29:LYS:CD	2.16	0.76
1:C:125:LYS:O	5:C:306:HOH:O	2.02	0.76
1:A:87:GLU:O	5:A:301:HOH:O	2.04	0.75
1:D:59:LEU:HD21	1:D:152:THR:HG21	1.68	0.75
1:A:59:LEU:HD21	1:A:152:THR:HG21	1.69	0.75
1:B:59:LEU:HD21	1:B:152:THR:HG21	1.69	0.74
1:C:59:LEU:HD21	1:C:152:THR:HG21	1.69	0.74
1:C:33:LEU:HD12	1:C:37:ASP:HB3	1.67	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:LEU:HD12	1:B:37:ASP:HB3	1.66	0.74
1:C:145:GLN:HB3	2:C:203:HEM:HMC2	1.68	0.74
1:A:25:ASP:OD2	5:A:302:HOH:O	2.06	0.74
1:D:10:ASP:OD2	5:D:302:HOH:O	2.06	0.74
1:B:87:GLU:OE1	5:B:302:HOH:O	2.05	0.73
1:A:108:GLU:OE2	5:A:303:HOH:O	2.07	0.73
1:C:141:TYR:HB3	2:C:203:HEM:CBB	2.17	0.73
1:D:141:TYR:HB3	2:D:201:HEM:HBB1	1.71	0.73
1:B:53:ASP:HB2	5:B:305:HOH:O	1.90	0.71
1:C:10:ASP:HA	1:C:13:ARG:HH11	1.56	0.71
2:B:201:HEM:HMB1	2:B:201:HEM:HBB2	1.73	0.71
2:A:201:HEM:HBC2	2:A:201:HEM:HHB	1.74	0.70
1:B:192:GLU:HB2	5:B:307:HOH:O	1.89	0.70
1:A:26:LEU:HA	1:A:29:LYS:CG	2.21	0.70
1:A:40:TYR:CE2	1:A:169:GLY:HA3	2.27	0.70
1:D:40:TYR:CE2	1:D:169:GLY:HA3	2.27	0.70
1:B:40:TYR:CE2	1:B:169:GLY:HA3	2.27	0.69
1:D:193:ASN:ND2	5:D:301:HOH:O	1.92	0.69
1:C:40:TYR:CE2	1:C:169:GLY:HA3	2.27	0.69
2:D:201:HEM:HBB2	2:D:201:HEM:HMB1	1.74	0.69
1:B:107:ARG:HD3	1:B:111:ASP:OD1	1.93	0.69
1:B:53:ASP:CB	5:B:305:HOH:O	2.41	0.68
1:C:107:ARG:HD3	1:C:111:ASP:OD1	1.93	0.68
1:C:18:PRO:HB2	5:C:339:HOH:O	1.93	0.68
1:A:72:TYR:CD2	2:A:201:HEM:HBC1	2.28	0.68
1:C:157:LEU:O	5:C:307:HOH:O	2.11	0.68
1:A:164:PRO:O	1:A:168:GLU:N	2.23	0.68
1:D:164:PRO:O	1:D:168:GLU:N	2.23	0.68
1:A:107:ARG:HD3	1:A:111:ASP:OD1	1.93	0.68
1:D:107:ARG:HD3	1:D:111:ASP:OD1	1.93	0.68
1:D:84:GLU:HG2	1:D:85:TYR:H	1.59	0.68
1:B:151:ALA:O	5:B:303:HOH:O	2.11	0.67
1:B:13:ARG:O	5:B:304:HOH:O	2.12	0.67
1:C:67:GLU:CD	1:C:68:HIS:H	2.01	0.67
1:A:84:GLU:OE2	5:A:304:HOH:O	2.12	0.67
1:A:62:TRP:CE3	1:A:83:LYS:HA	2.30	0.67
1:A:138:PRO:HB3	5:B:321:HOH:O	1.93	0.67
1:C:49:LYS:HB3	5:C:311:HOH:O	1.93	0.67
1:C:129:ASP:O	5:C:308:HOH:O	2.12	0.67
1:A:11:TYR:O	1:A:13:ARG:HD2	1.94	0.67
1:D:193:ASN:O	5:D:303:HOH:O	2.13	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:ILE:O	1:B:156:PHE:HB2	1.95	0.66
1:B:164:PRO:O	1:B:168:GLU:N	2.23	0.66
1:C:153:ILE:O	1:C:156:PHE:HB2	1.96	0.66
1:C:164:PRO:O	1:C:168:GLU:N	2.23	0.66
1:A:84:GLU:HG2	1:A:85:TYR:H	1.61	0.65
5:B:304:HOH:O	1:C:77:ASP:OD2	2.14	0.65
1:C:96:TRP:HA	5:C:332:HOH:O	1.95	0.65
1:A:26:LEU:O	1:A:29:LYS:HG2	1.97	0.65
1:A:128:THR:HA	3:A:206:IMD:H5	1.79	0.65
1:C:132:ARG:O	5:C:309:HOH:O	2.15	0.65
1:C:149:LEU:HD13	2:C:203:HEM:HMC1	1.79	0.65
1:A:140:ARG:HG3	1:B:27:LEU:HD21	1.78	0.64
1:A:153:ILE:O	1:A:156:PHE:HB2	1.95	0.64
2:B:201:HEM:HAA2	5:B:316:HOH:O	1.97	0.64
1:B:53:ASP:OD2	5:B:305:HOH:O	2.14	0.64
1:D:153:ILE:O	1:D:156:PHE:HB2	1.96	0.64
1:A:69:LEU:HB2	2:A:201:HEM:CBC	2.29	0.63
1:B:33:LEU:CD1	1:B:37:ASP:HB3	2.28	0.63
1:C:33:LEU:CD1	1:C:37:ASP:HB3	2.28	0.63
1:A:145:GLN:HB3	2:A:201:HEM:HAB	1.79	0.63
1:B:84:GLU:HG2	1:B:85:TYR:H	1.61	0.63
1:C:145:GLN:O	1:C:149:LEU:HD12	1.99	0.63
1:A:33:LEU:CD1	1:A:37:ASP:HB3	2.28	0.62
1:D:33:LEU:CD1	1:D:37:ASP:HB3	2.28	0.62
1:C:84:GLU:HG2	1:C:85:TYR:H	1.62	0.62
1:B:63:ARG:H	1:B:63:ARG:HD3	1.65	0.62
3:C:207:IMD:H5	5:C:303:HOH:O	1.99	0.61
1:A:124:LYS:O	5:A:306:HOH:O	2.16	0.61
1:D:43:LYS:HD2	1:D:43:LYS:O	2.00	0.61
1:A:26:LEU:HA	1:A:29:LYS:HG2	1.83	0.61
1:B:63:ARG:H	1:B:63:ARG:CD	2.13	0.60
2:D:201:HEM:HHA	5:D:323:HOH:O	2.00	0.60
1:A:149:LEU:HD13	2:A:201:HEM:C3B	2.36	0.60
1:B:141:TYR:HB3	2:B:201:HEM:HBB1	1.83	0.60
1:C:29:LYS:HA	5:C:322:HOH:O	2.01	0.59
1:D:141:TYR:HB3	2:D:201:HEM:CBB	2.33	0.59
1:C:25:ASP:O	1:C:29:LYS:HG2	2.03	0.59
1:C:37:ASP:OD2	1:C:176:LYS:CD	2.51	0.59
1:B:37:ASP:OD2	1:B:176:LYS:CD	2.51	0.59
1:D:37:ASP:OD2	1:D:176:LYS:CD	2.51	0.58
1:A:37:ASP:OD2	1:A:176:LYS:CD	2.51	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:LEU:HD21	1:B:140:ARG:HG3	1.85	0.58
1:C:10:ASP:HA	1:C:13:ARG:NH1	2.19	0.57
1:A:33:LEU:HA	1:A:37:ASP:OD2	2.05	0.57
1:D:33:LEU:HA	1:D:37:ASP:OD2	2.05	0.57
1:C:149:LEU:HD13	2:C:203:HEM:CMC	2.33	0.57
2:A:201:HEM:HMB1	2:A:201:HEM:HBB2	1.87	0.56
1:B:55:ILE:HG12	1:B:156:PHE:CD2	2.41	0.56
1:C:55:ILE:HG12	1:C:156:PHE:CD2	2.41	0.56
1:B:89:VAL:HG21	2:B:201:HEM:HAA1	1.88	0.56
1:C:33:LEU:HA	1:C:37:ASP:OD2	2.05	0.56
1:A:33:LEU:HD12	1:A:37:ASP:HB2	1.87	0.56
1:B:33:LEU:HA	1:B:37:ASP:OD2	2.05	0.55
1:D:33:LEU:HD12	1:D:37:ASP:HB2	1.87	0.55
5:B:304:HOH:O	1:C:77:ASP:CG	2.49	0.55
1:A:55:ILE:HG12	1:A:156:PHE:CD2	2.41	0.55
1:D:55:ILE:HG12	1:D:156:PHE:CD2	2.41	0.55
2:D:201:HEM:HMC2	2:D:201:HEM:HBC2	1.88	0.55
1:C:43:LYS:O	1:C:47:VAL:HG23	2.07	0.55
1:A:26:LEU:HD23	1:A:29:LYS:CE	2.38	0.54
1:A:26:LEU:C	1:A:29:LYS:HG2	2.32	0.54
1:B:93:PHE:HZ	1:B:149:LEU:HD21	1.72	0.54
1:B:18:PRO:HB2	5:B:323:HOH:O	2.06	0.54
1:B:192:GLU:OE1	5:B:307:HOH:O	2.19	0.54
1:B:160:LYS:CD	1:B:160:LYS:C	2.81	0.54
1:C:95:ALA:HB2	5:C:366:HOH:O	2.08	0.54
1:A:195:TRP:OXT	1:B:138:PRO:HB3	2.08	0.53
1:C:145:GLN:HG3	1:C:149:LEU:HD12	1.83	0.53
1:B:192:GLU:CB	5:B:307:HOH:O	2.53	0.53
1:C:25:ASP:O	1:C:29:LYS:CE	2.57	0.53
1:C:33:LEU:HD12	1:C:37:ASP:HB2	1.87	0.52
1:B:33:LEU:HD12	1:B:37:ASP:HB2	1.87	0.52
1:B:40:TYR:CD2	1:B:169:GLY:HA3	2.45	0.52
1:A:138:PRO:HB3	1:B:195:TRP:OXT	2.09	0.52
1:C:40:TYR:CD2	1:C:169:GLY:HA3	2.45	0.52
1:A:152:THR:O	1:A:155:PRO:HD2	2.10	0.52
1:D:37:ASP:OD2	1:D:176:LYS:NZ	2.41	0.52
1:D:152:THR:O	1:D:155:PRO:HD2	2.10	0.52
1:C:37:ASP:OD2	1:C:176:LYS:NZ	2.41	0.51
1:A:40:TYR:CD2	1:A:169:GLY:HA3	2.45	0.51
1:D:40:TYR:CD2	1:D:169:GLY:HA3	2.45	0.51
1:B:37:ASP:OD2	1:B:176:LYS:NZ	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:TYR:HD2	2:A:201:HEM:HBC1	1.75	0.51
1:B:141:TYR:HB3	2:B:201:HEM:CBB	2.40	0.51
1:A:37:ASP:OD1	1:A:37:ASP:N	2.42	0.51
1:B:152:THR:O	1:B:155:PRO:HD2	2.10	0.51
1:C:29:LYS:HE2	1:C:29:LYS:H	1.71	0.51
1:D:70:ILE:HG22	5:D:340:HOH:O	2.11	0.51
1:C:152:THR:O	1:C:155:PRO:HD2	2.10	0.50
1:D:37:ASP:N	1:D:37:ASP:OD1	2.42	0.50
1:A:68:HIS:N	5:A:314:HOH:O	2.44	0.50
1:C:155:PRO:HG2	5:C:335:HOH:O	2.11	0.50
1:A:72:TYR:CB	2:A:201:HEM:HBC1	2.40	0.50
1:D:122:ARG:HB3	1:D:136:HIS:HB2	1.94	0.50
1:A:122:ARG:HB3	1:A:136:HIS:HB2	1.94	0.50
1:B:15:GLU:OE2	1:C:75:ASN:ND2	2.22	0.50
1:D:83:LYS:O	1:D:87:GLU:HG2	2.12	0.49
1:A:83:LYS:O	1:A:87:GLU:HG2	2.12	0.49
1:B:62:TRP:CD1	1:B:83:LYS:HA	2.47	0.49
1:A:26:LEU:CA	1:A:29:LYS:HG2	2.42	0.49
1:A:138:PRO:CB	5:B:321:HOH:O	2.56	0.49
1:B:83:LYS:O	1:B:87:GLU:HG2	2.12	0.49
1:A:145:GLN:HB3	2:A:201:HEM:CAB	2.43	0.49
1:C:37:ASP:OD1	1:C:37:ASP:N	2.42	0.49
1:C:83:LYS:O	1:C:87:GLU:HG2	2.12	0.49
1:C:87:GLU:HA	1:C:87:GLU:OE1	2.13	0.49
1:B:87:GLU:OE1	1:B:87:GLU:HA	2.13	0.49
1:B:37:ASP:N	1:B:37:ASP:OD1	2.42	0.49
1:D:43:LYS:HD2	1:D:43:LYS:C	2.36	0.49
1:B:160:LYS:C	1:B:160:LYS:HD3	2.38	0.48
1:A:194:ASP:OD1	1:B:136:HIS:CE1	2.66	0.48
1:A:62:TRP:CE3	1:A:83:LYS:CA	2.97	0.48
1:A:87:GLU:OE1	1:A:87:GLU:HA	2.13	0.48
1:C:122:ARG:HB3	1:C:136:HIS:HB2	1.94	0.48
1:C:41:LEU:HG	1:C:173:ALA:HB1	1.95	0.48
1:D:87:GLU:OE1	1:D:87:GLU:HA	2.13	0.48
1:B:41:LEU:HG	1:B:173:ALA:HB1	1.95	0.48
1:B:122:ARG:HB3	1:B:136:HIS:HB2	1.94	0.48
1:C:25:ASP:O	1:C:29:LYS:HE2	2.13	0.48
1:D:130:GLY:HA2	5:D:313:HOH:O	2.14	0.48
1:D:41:LEU:HG	1:D:173:ALA:HB1	1.95	0.47
1:A:41:LEU:HG	1:A:173:ALA:HB1	1.96	0.47
1:A:147:TYR:CE2	1:B:176:LYS:HE2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:ARG:CD	1:B:63:ARG:N	2.77	0.46
1:B:23:GLU:OE1	3:B:203:IMD:N1	2.48	0.46
1:D:185:TRP:HH2	2:D:201:HEM:C4C	2.34	0.46
1:B:145:GLN:HG3	1:B:149:LEU:HD12	1.98	0.45
1:B:93:PHE:HZ	1:B:149:LEU:CD2	2.29	0.45
1:A:37:ASP:OD2	1:A:176:LYS:NZ	2.41	0.45
1:D:73:PHE:CD2	1:D:86:LEU:HD23	2.52	0.45
1:A:73:PHE:CD2	1:A:86:LEU:HD23	2.52	0.45
1:C:32:MET:HA	5:C:322:HOH:O	2.16	0.45
1:A:72:TYR:CB	2:A:201:HEM:CBC	2.92	0.45
1:A:82:ILE:HG22	1:A:84:GLU:CD	2.42	0.45
1:B:40:TYR:CD2	1:B:169:GLY:CA	3.00	0.45
1:B:185:TRP:HH2	2:B:201:HEM:C4C	2.35	0.45
1:C:40:TYR:CD2	1:C:169:GLY:CA	3.00	0.45
1:C:119:ARG:HB3	2:C:203:HEM:O1A	2.16	0.45
1:A:62:TRP:CE2	1:A:83:LYS:HD2	2.52	0.45
1:C:73:PHE:CD2	1:C:86:LEU:HD23	2.52	0.45
1:C:82:ILE:HG22	1:C:84:GLU:CD	2.42	0.45
1:B:82:ILE:HG22	1:B:84:GLU:CD	2.41	0.44
1:B:93:PHE:CZ	1:B:149:LEU:HD21	2.51	0.44
1:B:73:PHE:CD2	1:B:86:LEU:HD23	2.52	0.44
1:D:37:ASP:OD2	1:D:176:LYS:HD2	2.17	0.44
1:A:37:ASP:OD2	1:A:176:LYS:HD2	2.17	0.44
1:A:122:ARG:HB3	1:A:122:ARG:NH1	2.33	0.44
1:D:122:ARG:HB3	1:D:122:ARG:NH1	2.33	0.44
1:D:96:TRP:CZ2	2:D:201:HEM:HAC	2.53	0.44
1:B:149:LEU:HD13	2:B:201:HEM:C3C	2.52	0.44
1:A:105:TYR:HB2	5:A:323:HOH:O	2.17	0.44
1:A:176:LYS:HE2	1:B:147:TYR:CE2	2.52	0.44
1:B:122:ARG:HB3	1:B:122:ARG:NH1	2.33	0.44
1:B:43:LYS:O	1:B:47:VAL:HG23	2.18	0.44
1:D:40:TYR:CD2	1:D:169:GLY:CA	3.00	0.44
1:A:40:TYR:CD2	1:A:169:GLY:CA	3.00	0.43
1:C:37:ASP:OD2	1:C:176:LYS:HD2	2.17	0.43
1:C:122:ARG:HB3	1:C:122:ARG:NH1	2.33	0.43
2:A:201:HEM:HBB2	2:A:201:HEM:CMB	2.48	0.43
1:B:52:VAL:O	1:B:56:LEU:HG	2.18	0.43
1:B:37:ASP:OD2	1:B:176:LYS:HD2	2.17	0.43
1:C:52:VAL:O	1:C:56:LEU:HG	2.18	0.43
1:D:52:VAL:O	1:D:56:LEU:HG	2.18	0.43
1:A:52:VAL:O	1:A:56:LEU:HG	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:HIS:CE1	1:B:194:ASP:OD1	2.72	0.43
1:A:130:GLY:HA2	5:A:326:HOH:O	2.17	0.42
1:A:62:TRP:CZ3	1:A:83:LYS:HB2	2.53	0.42
1:B:62:TRP:HA	1:B:86:LEU:HD13	2.00	0.42
1:A:43:LYS:O	1:A:47:VAL:HG23	2.20	0.42
5:A:326:HOH:O	1:D:18:PRO:HB2	2.18	0.42
1:C:67:GLU:HB3	1:C:69:LEU:HG	2.00	0.42
1:D:38:VAL:O	1:D:42:LYS:HG3	2.20	0.42
1:D:87:GLU:OE1	5:D:304:HOH:O	2.22	0.42
1:A:38:VAL:O	1:A:42:LYS:HG3	2.20	0.42
1:B:153:ILE:HD13	1:B:174:TRP:CZ2	2.55	0.42
2:C:203:HEM:HAA2	5:C:312:HOH:O	2.19	0.42
1:C:153:ILE:HD13	1:C:174:TRP:CZ2	2.55	0.42
1:A:140:ARG:HG2	1:A:141:TYR:N	2.35	0.41
1:D:140:ARG:HG2	1:D:141:TYR:N	2.35	0.41
1:A:138:PRO:HA	5:B:321:HOH:O	2.21	0.41
1:B:38:VAL:O	1:B:42:LYS:HG3	2.20	0.41
1:C:38:VAL:O	1:C:42:LYS:HG3	2.20	0.41
1:D:153:ILE:HD13	1:D:174:TRP:CZ2	2.55	0.41
1:A:136:HIS:CE1	1:A:189:TYR:CE2	3.09	0.41
1:A:153:ILE:HD13	1:A:174:TRP:CZ2	2.55	0.41
1:A:149:LEU:HD13	2:A:201:HEM:C2B	2.56	0.41
1:D:104:ASP:OD2	5:D:305:HOH:O	2.22	0.41
1:D:136:HIS:CE1	1:D:189:TYR:CE2	3.09	0.41
1:C:140:ARG:HG2	1:C:141:TYR:N	2.35	0.41
1:B:140:ARG:HG2	1:B:141:TYR:N	2.35	0.41
1:C:136:HIS:CE1	1:C:189:TYR:CE2	3.09	0.41
1:A:116:VAL:HG12	1:A:185:TRP:CZ2	2.56	0.41
1:B:136:HIS:CE1	1:B:189:TYR:CE2	3.09	0.41
1:C:62:TRP:CE3	1:C:83:LYS:HA	2.56	0.41
1:D:116:VAL:HG12	1:D:185:TRP:CZ2	2.56	0.41
1:A:46:ASP:O	1:A:49:LYS:HB2	2.21	0.41
1:D:46:ASP:O	1:D:49:LYS:HB2	2.21	0.41
1:C:116:VAL:HG12	1:C:185:TRP:CZ2	2.56	0.40
1:B:116:VAL:HG12	1:B:185:TRP:CZ2	2.56	0.40
1:D:190:THR:HG21	1:D:195:TRP:N	2.36	0.40
1:A:72:TYR:CG	2:A:201:HEM:HBC1	2.56	0.40
1:D:60:VAL:HB	3:D:202:IMD:H5	2.02	0.40
1:A:60:VAL:HB	3:A:202:IMD:H5	2.02	0.40
2:C:203:HEM:HMB1	2:C:203:HEM:CBB	2.40	0.40
1:C:165:GLU:H	1:C:165:GLU:HG3	1.39	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:380:HOH:O	5:D:367:HOH:O[1_445]	1.92	0.28
5:C:380:HOH:O	5:D:373:HOH:O[1_445]	2.03	0.17
1:A:15:GLU:OE2	1:D:75:ASN:ND2[1_455]	2.15	0.05
1:B:75:ASN:ND2	1:C:15:GLU:OE2[1_455]	2.15	0.05

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	183/190 (96%)	175 (96%)	7 (4%)	1 (0%)	24	22
1	B	183/190 (96%)	175 (96%)	7 (4%)	1 (0%)	24	22
1	C	183/190 (96%)	174 (95%)	8 (4%)	1 (0%)	24	22
1	D	174/190 (92%)	168 (97%)	5 (3%)	1 (1%)	21	18
All	All	723/760 (95%)	692 (96%)	27 (4%)	4 (1%)	23	18

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	49	LYS
1	B	49	LYS
1	C	49	LYS
1	D	49	LYS

5.3.2 Protein sidechains [i](#)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	166/168 (99%)	163 (98%)	3 (2%)	51	60
1	B	166/168 (99%)	165 (99%)	1 (1%)	78	86
1	C	166/168 (99%)	165 (99%)	1 (1%)	78	86
1	D	157/168 (94%)	155 (99%)	2 (1%)	61	69
All	All	655/672 (98%)	648 (99%)	7 (1%)	63	74

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	ASP
1	A	123	SER
1	A	145	GLN
1	B	145	GLN
1	C	145	GLN
1	D	84	GLU
1	D	145	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	GLN
1	A	172	ASN
1	B	51	GLN
1	B	66	ASN
1	C	51	GLN
1	C	172	ASN
1	D	51	GLN
1	D	172	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 23 ligands modelled in this entry, 4 are monoatomic - leaving 19 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	IMD	A	206	-	5,5,5	0.56	0	5,5,5	0.42	0
3	IMD	C	201	-	5,5,5	0.67	0	5,5,5	0.33	0
3	IMD	A	202	2	5,5,5	0.65	0	5,5,5	0.65	0
3	IMD	C	205	4	5,5,5	0.53	0	5,5,5	0.43	0
3	IMD	C	206	4	5,5,5	0.67	0	5,5,5	0.45	0
2	HEM	D	201	3,1	50,50,50	1.48	7 (14%)	67,82,82	1.70	11 (16%)
2	HEM	C	203	3,1	50,50,50	1.59	10 (20%)	67,82,82	1.87	17 (25%)
3	IMD	D	202	2	5,5,5	0.66	0	5,5,5	0.64	0
2	HEM	B	201	3,1	50,50,50	1.61	10 (20%)	67,82,82	1.49	13 (19%)
3	IMD	C	204	2	5,5,5	0.65	0	5,5,5	0.63	0
3	IMD	B	202	2	5,5,5	0.65	0	5,5,5	0.63	0
3	IMD	B	203	4	5,5,5	0.77	0	5,5,5	0.38	0
3	IMD	A	203	4	5,5,5	0.60	0	5,5,5	0.50	0
3	IMD	C	207	4	5,5,5	0.49	0	5,5,5	0.64	0
3	IMD	C	202	-	5,5,5	0.59	0	5,5,5	0.47	0
2	HEM	A	201	3,1	50,50,50	1.40	7 (14%)	67,82,82	1.53	11 (16%)
3	IMD	A	204	4	5,5,5	0.65	0	5,5,5	0.42	0
3	IMD	A	205	-	5,5,5	0.48	0	5,5,5	0.14	0
3	IMD	D	203	4	5,5,5	0.47	0	5,5,5	0.49	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	IMD	A	206	-	-	-	0/1/1/1
3	IMD	C	201	-	-	-	0/1/1/1
3	IMD	A	202	2	-	-	0/1/1/1
3	IMD	C	205	4	-	-	0/1/1/1
3	IMD	C	206	4	-	-	0/1/1/1
2	HEM	D	201	3,1	-	4/14/54/54	-
2	HEM	C	203	3,1	-	6/14/54/54	-
3	IMD	D	202	2	-	-	0/1/1/1
2	HEM	B	201	3,1	-	4/14/54/54	-
3	IMD	C	204	2	-	-	0/1/1/1
3	IMD	B	202	2	-	-	0/1/1/1
3	IMD	B	203	4	-	-	0/1/1/1
3	IMD	A	203	4	-	-	0/1/1/1
3	IMD	C	207	4	-	-	0/1/1/1
3	IMD	C	202	-	-	-	0/1/1/1
2	HEM	A	201	3,1	-	4/14/54/54	-
3	IMD	A	204	4	-	-	0/1/1/1
3	IMD	A	205	-	-	-	0/1/1/1
3	IMD	D	203	4	-	-	0/1/1/1

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	201	HEM	FE-ND	5.16	2.10	1.94
2	C	203	HEM	FE-NB	4.58	2.09	1.94
2	A	201	HEM	FE-NB	3.95	2.07	1.94
2	C	203	HEM	CMC-C2C	3.85	1.58	1.50
2	B	201	HEM	FE-NA	-3.81	1.82	1.95
2	B	201	HEM	FE-NC	3.62	2.07	1.95
2	B	201	HEM	CMC-C2C	3.59	1.58	1.50
2	C	203	HEM	CMA-C3A	3.47	1.57	1.50
2	A	201	HEM	CAB-C3B	3.26	1.56	1.47
2	A	201	HEM	CMD-C2D	2.94	1.56	1.50
2	D	201	HEM	CMA-C3A	2.83	1.56	1.50
2	D	201	HEM	FE-NC	2.75	2.04	1.95
2	D	201	HEM	CAC-C3C	2.75	1.54	1.47
2	C	203	HEM	FE-ND	2.74	2.03	1.94
2	A	201	HEM	FE-NA	2.70	2.04	1.95
2	C	203	HEM	CAC-C3C	2.62	1.54	1.47
2	B	201	HEM	C4A-NA	-2.60	1.34	1.39
2	C	203	HEM	CAB-C3B	2.58	1.54	1.47
2	B	201	HEM	CAC-C3C	2.54	1.54	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	201	HEM	C4C-NC	-2.54	1.34	1.39
2	C	203	HEM	CMD-C2D	2.46	1.55	1.50
2	C	203	HEM	FE-NC	2.43	2.03	1.95
2	A	201	HEM	CAC-C3C	2.37	1.53	1.47
2	B	201	HEM	CAB-C3B	2.24	1.53	1.47
2	A	201	HEM	C2A-C3A	-2.24	1.33	1.38
2	D	201	HEM	CMB-C2B	2.22	1.55	1.50
2	B	201	HEM	CMA-C3A	2.21	1.55	1.50
2	D	201	HEM	C4C-NC	-2.18	1.35	1.39
2	C	203	HEM	FE-NA	2.14	2.02	1.95
2	A	201	HEM	CMC-C2C	2.13	1.55	1.50
2	B	201	HEM	CMB-C2B	2.10	1.55	1.50
2	C	203	HEM	C4D-ND	-2.02	1.36	1.40
2	B	201	HEM	C1B-NB	-2.01	1.36	1.40
2	D	201	HEM	CAB-C3B	2.00	1.52	1.47

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	203	HEM	C3B-C4B-NB	-5.68	105.39	109.47
2	D	201	HEM	CBA-CAA-C2A	-5.50	97.32	112.53
2	C	203	HEM	C1B-NB-C4B	4.83	110.92	105.21
2	C	203	HEM	C4C-C3C-C2C	4.51	110.72	106.81
2	B	201	HEM	CBD-CAD-C3D	-4.35	100.52	112.53
2	D	201	HEM	C3B-C4B-NB	-4.20	106.45	109.47
2	D	201	HEM	CBD-CAD-C3D	-4.06	101.30	112.53
2	C	203	HEM	C4D-ND-C1D	3.59	109.45	105.21
2	B	201	HEM	CBA-CAA-C2A	-3.55	102.71	112.53
2	A	201	HEM	CBD-CAD-C3D	-3.41	103.09	112.53
2	A	201	HEM	C1B-NB-C4B	3.29	109.10	105.21
2	B	201	HEM	C4C-C3C-C2C	3.22	109.61	106.81
2	D	201	HEM	C1B-NB-C4B	3.11	108.89	105.21
2	A	201	HEM	C3B-C2B-C1B	3.05	108.70	106.41
2	C	203	HEM	C3D-C4D-ND	-3.05	106.83	110.17
2	D	201	HEM	CHD-C4C-NC	2.99	127.71	124.45
2	D	201	HEM	CHC-C4B-NB	2.97	127.62	124.42
2	C	203	HEM	CBA-CAA-C2A	-2.96	104.35	112.53
2	C	203	HEM	CMC-C2C-C1C	2.89	129.83	124.73
2	B	201	HEM	CHC-C4B-NB	2.75	127.38	124.42
2	D	201	HEM	C2A-C1A-NA	-2.74	107.12	110.15
2	A	201	HEM	C2B-C1B-NB	-2.73	106.70	109.84
2	C	203	HEM	C2A-C1A-NA	-2.72	107.13	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	201	HEM	C3C-C2C-C1C	-2.72	104.47	107.05
2	C	203	HEM	C2B-C1B-NB	-2.72	106.72	109.84
2	B	201	HEM	CAA-C2A-C3A	2.69	133.11	127.07
2	C	203	HEM	CAD-CBD-CGD	-2.63	106.69	113.67
2	B	201	HEM	CAA-C2A-C1A	-2.60	119.87	124.94
2	D	201	HEM	C1A-CHA-C4D	-2.55	120.25	126.25
2	A	201	HEM	C3D-C4D-ND	-2.47	107.46	110.17
2	A	201	HEM	C4C-NC-C1C	2.45	109.81	105.82
2	D	201	HEM	C4B-C3B-C2B	2.43	109.52	107.28
2	C	203	HEM	C3B-C2B-C1B	2.43	108.23	106.41
2	C	203	HEM	CHD-C4C-NC	2.42	127.09	124.45
2	A	201	HEM	CHB-C4A-NA	2.41	128.22	123.86
2	D	201	HEM	C1A-C2A-C3A	2.39	110.56	106.87
2	A	201	HEM	CAD-CBD-CGD	-2.35	107.44	113.67
2	C	203	HEM	CHA-C1A-NA	2.35	128.12	123.86
2	B	201	HEM	C1B-NB-C4B	2.21	107.82	105.21
2	A	201	HEM	O2A-CGA-CBA	2.17	120.85	114.00
2	B	201	HEM	CAD-CBD-CGD	-2.17	107.92	113.67
2	D	201	HEM	CHA-C1A-NA	2.16	127.78	123.86
2	B	201	HEM	C3B-C4B-NB	-2.14	107.93	109.47
2	B	201	HEM	CMA-C3A-C2A	2.14	130.16	125.62
2	A	201	HEM	C4D-ND-C1D	2.13	107.73	105.21
2	C	203	HEM	CHC-C4B-C3B	2.13	129.32	125.07
2	B	201	HEM	CHB-C1B-NB	-2.13	121.74	124.37
2	B	201	HEM	C1A-CHA-C4D	-2.12	121.27	126.25
2	A	201	HEM	C1A-CHA-C4D	-2.09	121.33	126.25
2	C	203	HEM	C3C-C2C-C1C	-2.08	105.07	107.05
2	C	203	HEM	CHD-C1D-ND	2.04	126.61	124.42
2	C	203	HEM	C1A-CHA-C4D	-2.01	121.52	126.25

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	203	HEM	C2C-C3C-CAC-CBC
2	C	203	HEM	C4C-C3C-CAC-CBC
2	B	201	HEM	CAD-CBD-CGD-O2D
2	D	201	HEM	CAA-CBA-CGA-O1A
2	D	201	HEM	CAD-CBD-CGD-O1D
2	B	201	HEM	CAD-CBD-CGD-O1D
2	D	201	HEM	CAD-CBD-CGD-O2D
2	C	203	HEM	CAD-CBD-CGD-O2D

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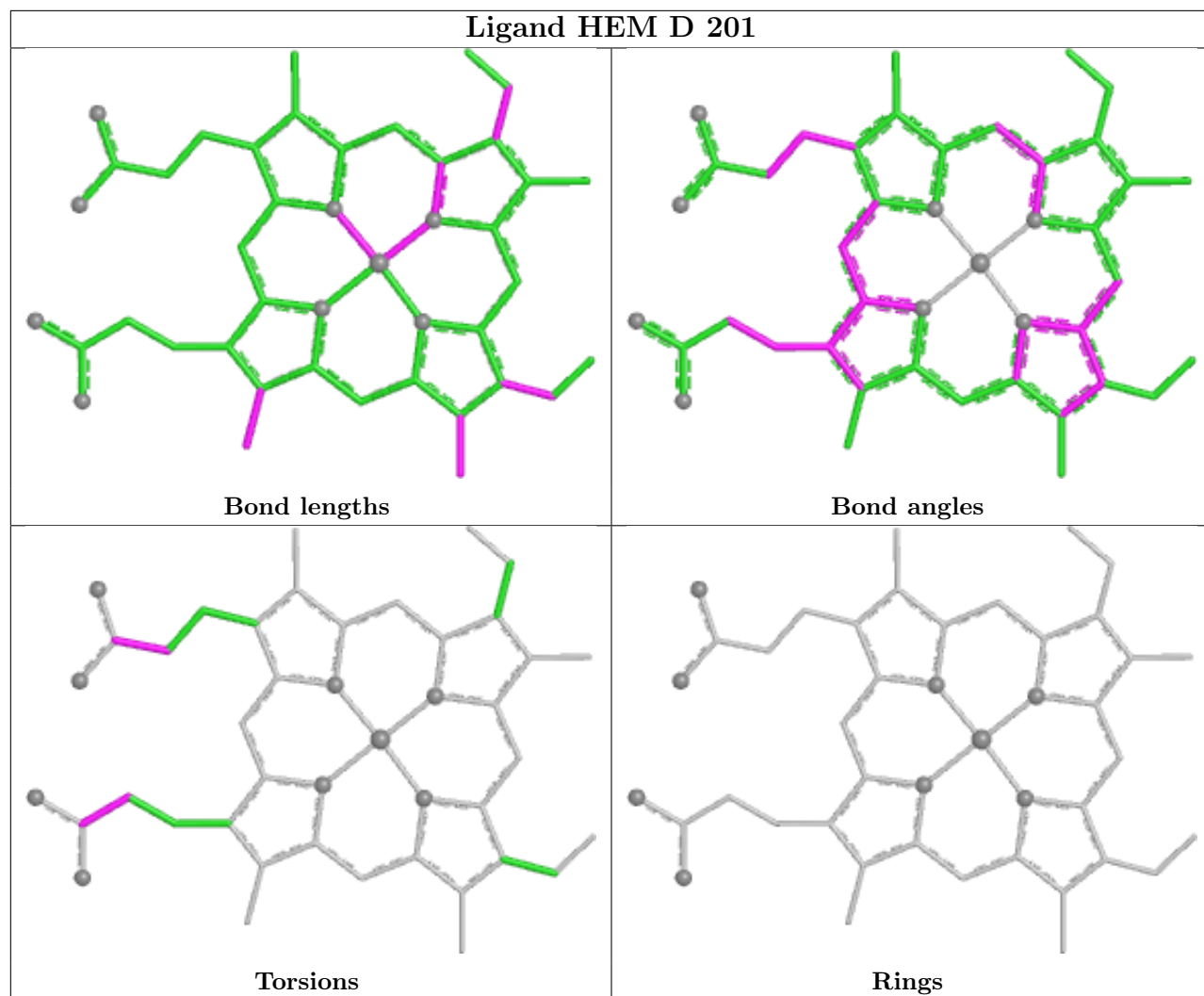
Mol	Chain	Res	Type	Atoms
2	D	201	HEM	CAA-CBA-CGA-O2A
2	B	201	HEM	CAA-CBA-CGA-O2A
2	A	201	HEM	CAD-CBD-CGD-O2D
2	A	201	HEM	CAD-CBD-CGD-O1D
2	C	203	HEM	CAD-CBD-CGD-O1D
2	C	203	HEM	CAA-CBA-CGA-O1A
2	B	201	HEM	CAA-CBA-CGA-O1A
2	C	203	HEM	CAA-CBA-CGA-O2A
2	A	201	HEM	CAA-CBA-CGA-O2A
2	A	201	HEM	CAA-CBA-CGA-O1A

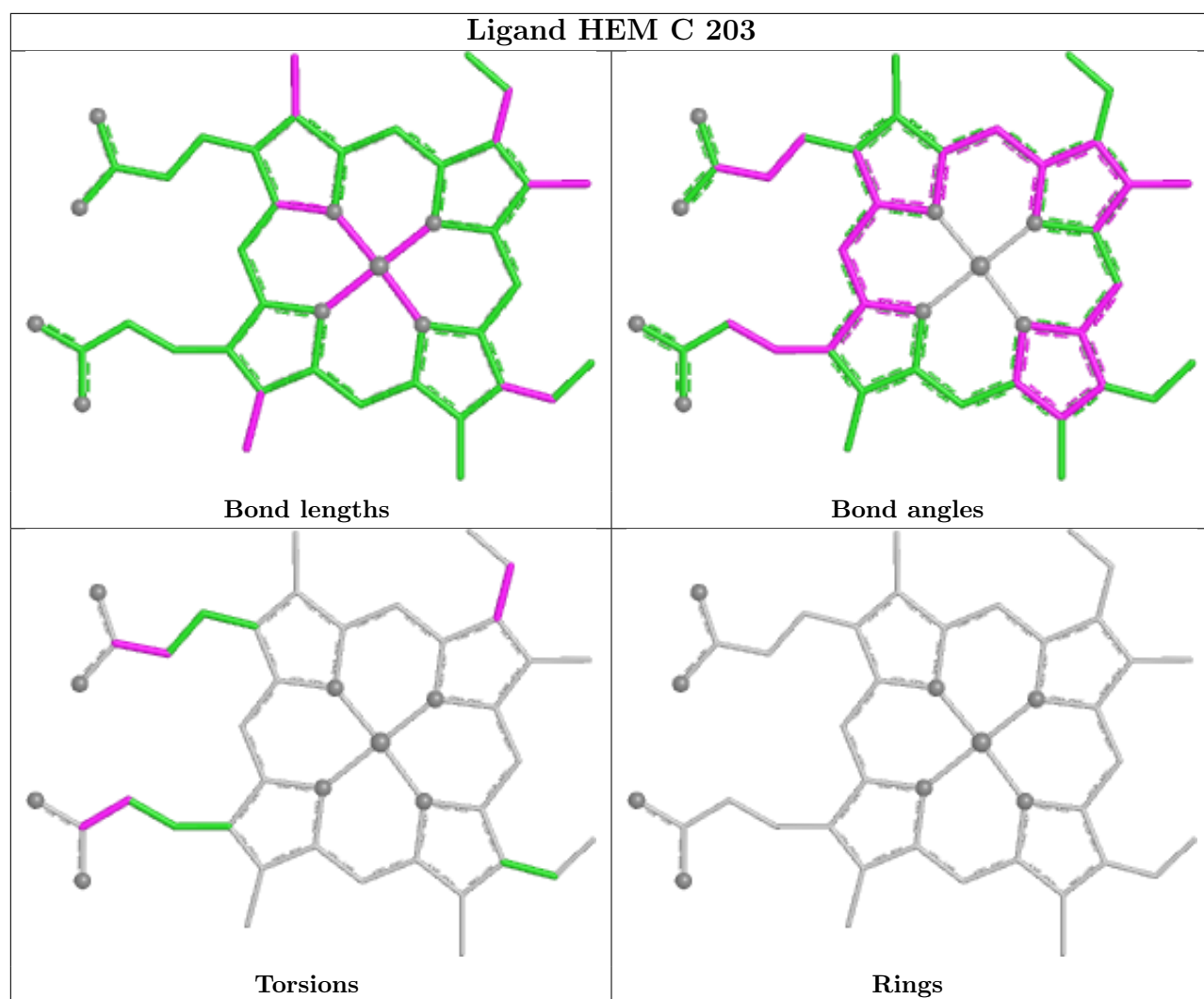
There are no ring outliers.

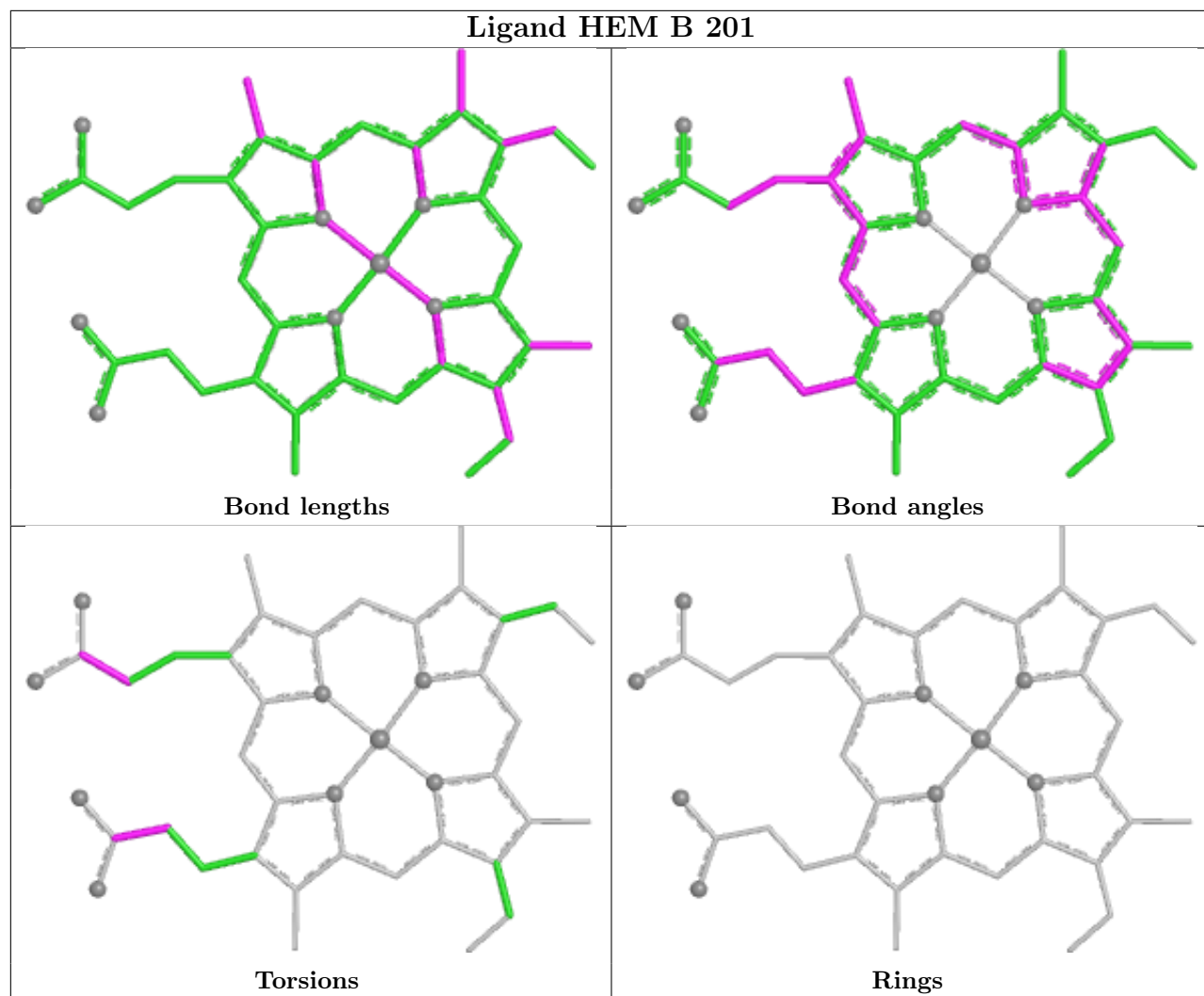
9 monomers are involved in 45 short contacts:

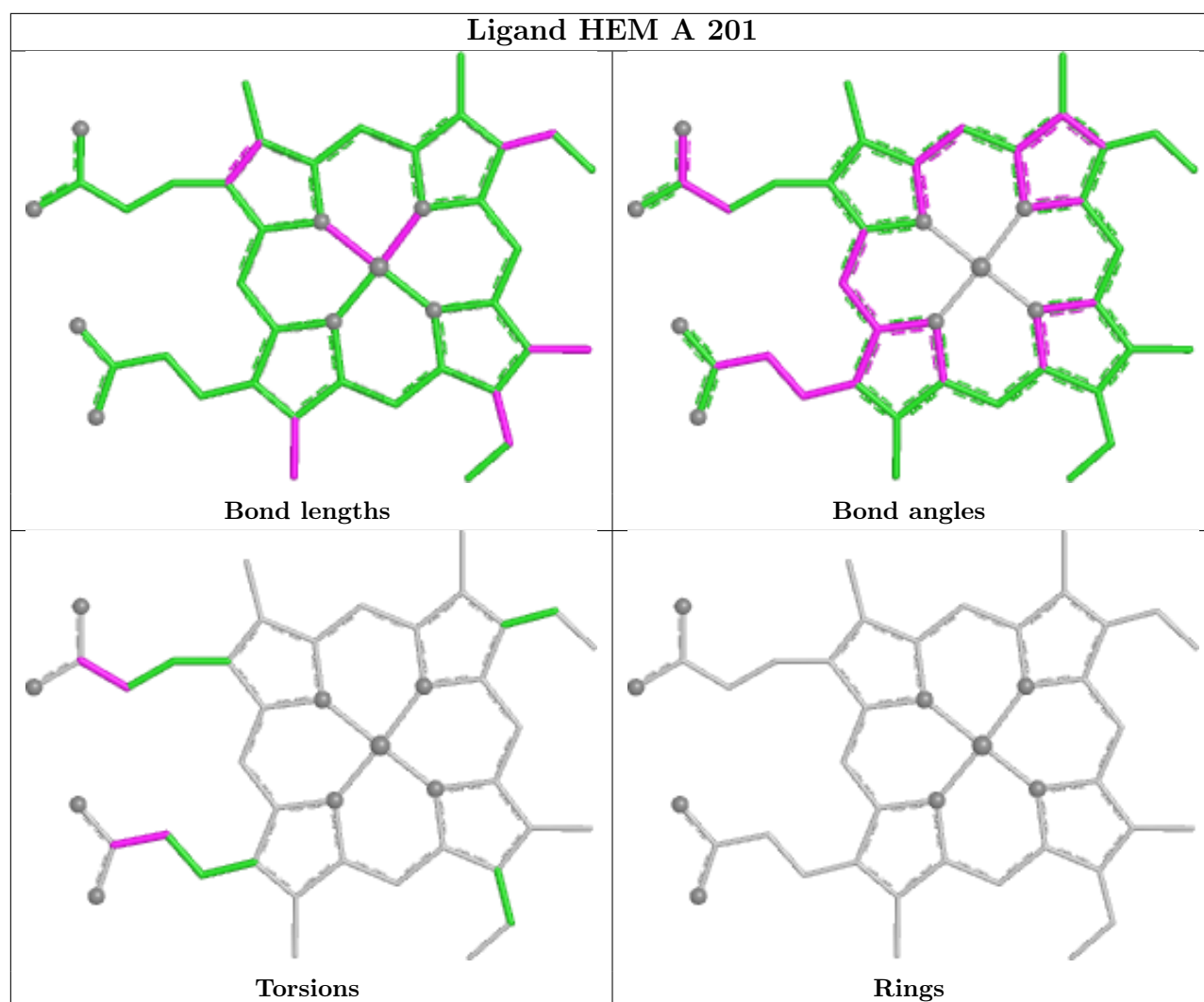
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	206	IMD	1	0
3	A	202	IMD	1	0
2	D	201	HEM	7	0
2	C	203	HEM	10	0
3	D	202	IMD	1	0
2	B	201	HEM	8	0
3	B	203	IMD	1	0
3	C	207	IMD	1	0
2	A	201	HEM	15	0

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.









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.