



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2021 – 07:36 PM EDT

PDB ID : 2FYN
Title : Crystal Structure Analysis of the double mutant Rhodobacter Sphaeroides bc1 complex
Authors : Esser, L.; Xia, D.
Deposited on : 2006-02-08
Resolution : 3.20 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : NOT EXECUTED
EDS : NOT EXECUTED
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

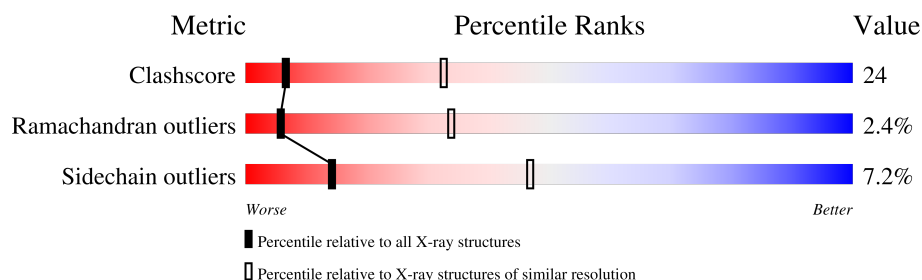
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)










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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	445	
1	D	445	
1	G	445	
1	J	445	
1	M	445	
1	P	445	
2	B	269	
2	E	269	

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Mol	Chain	Length	Quality of chain
2	H	269	
2	K	269	
2	N	269	
2	Q	269	
3	C	187	
3	F	187	
3	I	187	
3	L	187	
3	O	187	
3	R	187	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	FES	C	200	-	-	X	-
7	FES	F	200	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 41688 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 Cytochrome b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	428	Total	C	N	O	S	0	0	0
			3440	2322	548	555	15			
1	D	428	Total	C	N	O	S	0	0	0
			3440	2322	548	555	15			
1	G	428	Total	C	N	O	S	0	0	0
			3440	2322	548	555	15			
1	J	428	Total	C	N	O	S	0	0	0
			3440	2322	548	555	15			
1	M	428	Total	C	N	O	S	0	0	0
			3440	2322	548	555	15			
1	P	428	Total	C	N	O	S	0	0	0
			3440	2322	548	555	15			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q02761
A	287	ARG	SER	engineered mutation	UNP Q02761
D	1	MET	-	initiating methionine	UNP Q02761
D	287	ARG	SER	engineered mutation	UNP Q02761
G	1	MET	-	initiating methionine	UNP Q02761
G	287	ARG	SER	engineered mutation	UNP Q02761
J	1	MET	-	initiating methionine	UNP Q02761
J	287	ARG	SER	engineered mutation	UNP Q02761
M	1	MET	-	initiating methionine	UNP Q02761
M	287	ARG	SER	engineered mutation	UNP Q02761
P	1	MET	-	initiating methionine	UNP Q02761
P	287	ARG	SER	engineered mutation	UNP Q02761

- Molecule 2 is a protein called Cytochrome c1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	256	Total 1953	C 1240	N 326	O 374	S 13	0	0	0
2	E	256	Total 1953	C 1240	N 326	O 374	S 13	0	0	0
2	H	256	Total 1953	C 1240	N 326	O 374	S 13	0	0	0
2	K	256	Total 1953	C 1240	N 326	O 374	S 13	0	0	0
2	N	256	Total 1953	C 1240	N 326	O 374	S 13	0	0	0
2	Q	256	Total 1953	C 1240	N 326	O 374	S 13	0	0	0

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	98	PRO	ALA	conflict	UNP Q02760
E	98	PRO	ALA	conflict	UNP Q02760
H	98	PRO	ALA	conflict	UNP Q02760
K	98	PRO	ALA	conflict	UNP Q02760
N	98	PRO	ALA	conflict	UNP Q02760
Q	98	PRO	ALA	conflict	UNP Q02760
B	264	HIS	-	expression tag	UNP Q02760
B	265	HIS	-	expression tag	UNP Q02760
B	266	HIS	-	expression tag	UNP Q02760
B	267	HIS	-	expression tag	UNP Q02760
B	268	HIS	-	insertion	UNP Q02760
B	269	HIS	-	insertion	UNP Q02760
E	264	HIS	-	insertion	UNP Q02760
E	265	HIS	-	insertion	UNP Q02760
E	266	HIS	-	insertion	UNP Q02760
E	267	HIS	-	insertion	UNP Q02760
E	268	HIS	-	insertion	UNP Q02760
E	269	HIS	-	insertion	UNP Q02760
H	264	HIS	-	insertion	UNP Q02760
H	265	HIS	-	insertion	UNP Q02760
H	266	HIS	-	insertion	UNP Q02760
H	267	HIS	-	insertion	UNP Q02760
H	268	HIS	-	insertion	UNP Q02760
H	269	HIS	-	insertion	UNP Q02760
K	264	HIS	-	insertion	UNP Q02760
K	265	HIS	-	insertion	UNP Q02760
K	266	HIS	-	insertion	UNP Q02760
K	267	HIS	-	insertion	UNP Q02760

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Chain	Residue	Modelled	Actual	Comment	Reference
K	268	HIS	-	insertion	UNP Q02760
K	269	HIS	-	insertion	UNP Q02760
N	264	HIS	-	insertion	UNP Q02760
N	265	HIS	-	insertion	UNP Q02760
N	266	HIS	-	insertion	UNP Q02760
N	267	HIS	-	insertion	UNP Q02760
N	268	HIS	-	insertion	UNP Q02760
N	269	HIS	-	insertion	UNP Q02760
Q	264	HIS	-	insertion	UNP Q02760
Q	265	HIS	-	insertion	UNP Q02760
Q	266	HIS	-	insertion	UNP Q02760
Q	267	HIS	-	insertion	UNP Q02760
Q	268	HIS	-	insertion	UNP Q02760
Q	269	HIS	-	insertion	UNP Q02760

- Molecule 3 is a protein called Ubiquinol-cytochrome c reductase iron-sulfur subunit.

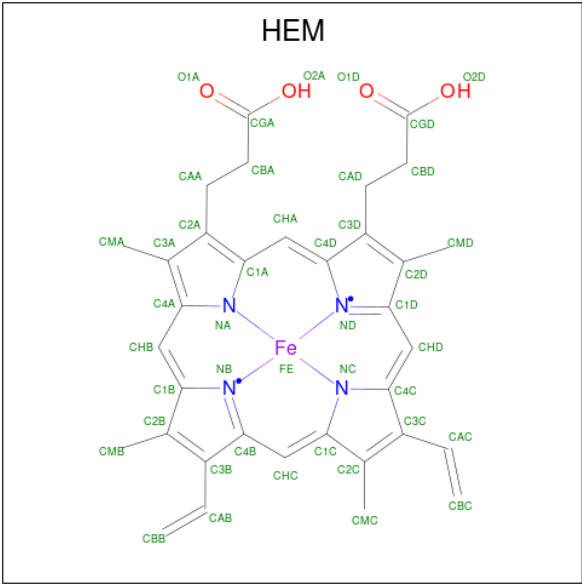
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	179	Total	C	N	O	S	0	0	0
			1340	843	237	254	6			
3	F	179	Total	C	N	O	S	0	0	0
			1340	843	237	254	6			
3	I	179	Total	C	N	O	S	0	0	0
			1340	843	237	254	6			
3	L	179	Total	C	N	O	S	0	0	0
			1340	843	237	254	6			
3	O	179	Total	C	N	O	S	0	0	0
			1340	843	237	254	6			
3	R	179	Total	C	N	O	S	0	0	0
			1340	843	237	254	6			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	135	SER	VAL	engineered mutation	UNP Q02762
F	135	SER	VAL	engineered mutation	UNP Q02762
I	135	SER	VAL	engineered mutation	UNP Q02762
L	135	SER	VAL	engineered mutation	UNP Q02762
O	135	SER	VAL	engineered mutation	UNP Q02762
R	135	SER	VAL	engineered mutation	UNP Q02762

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (for-

mula: C₃₄H₃₂FeN₄O₄).



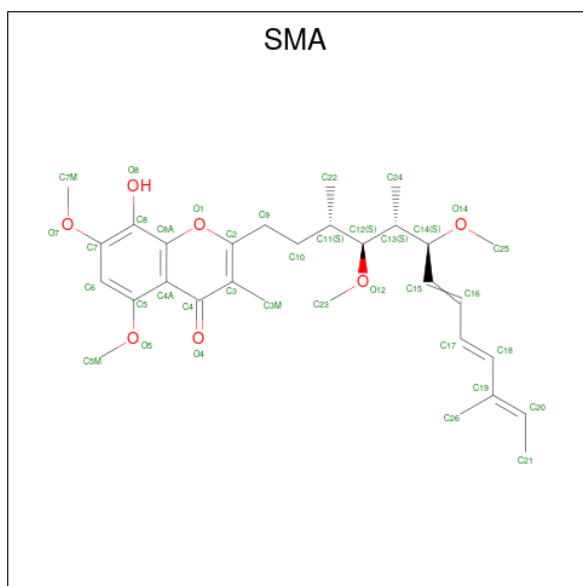
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	G	1	Total 43	C 34	Fe 1	N 4	O 4	0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

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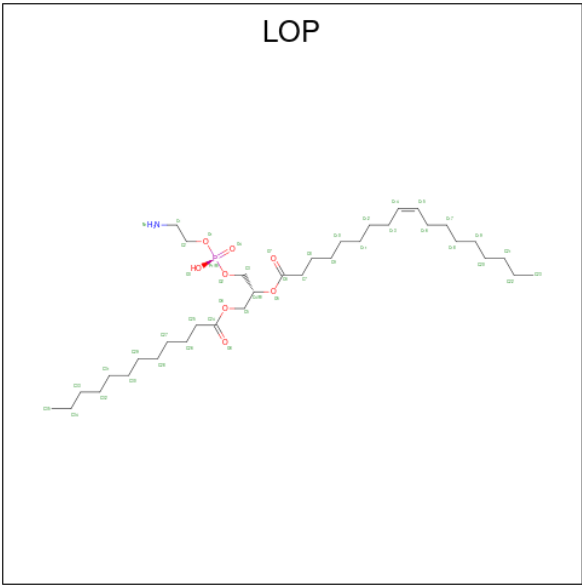
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	M	1	Total	C	Fe	N	O	
			43	34	1	4	4	
4	N	1	Total	C	Fe	N	O	
			43	34	1	4	4	
4	P	1	Total	C	Fe	N	O	
			43	34	1	4	4	
4	P	1	Total	C	Fe	N	O	
			43	34	1	4	4	
4	Q	1	Total	C	Fe	N	O	
			43	34	1	4	4	

- Molecule 5 is STIGMATELLIN A (three-letter code: SMA) (formula: $C_{30}H_{42}O_7$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	C O	0	0
			37	30 7		
5	D	1	Total	C O	0	0
			37	30 7		
5	G	1	Total	C O	0	0
			37	30 7		
5	J	1	Total	C O	0	0
			37	30 7		
5	M	1	Total	C O	0	0
			37	30 7		
5	P	1	Total	C O	0	0
			37	30 7		

- Molecule 6 is (1R)-2-{[(R)-(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(DODECANOYLOXY)METHYL]ETHYL (9Z)-OCTADEC-9-ENOATE (three-letter code: LOP) (formula: C₃₅H₆₈NO₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			45	35	1	8	1		
6	D	1	Total	C	N	O	P	0	0
			45	35	1	8	1		
6	G	1	Total	C	N	O	P	0	0
			45	35	1	8	1		
6	J	1	Total	C	N	O	P	0	0
			45	35	1	8	1		
6	M	1	Total	C	N	O	P	0	0
			45	35	1	8	1		
6	P	1	Total	C	N	O	P	0	0
			45	35	1	8	1		

- Molecule 7 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



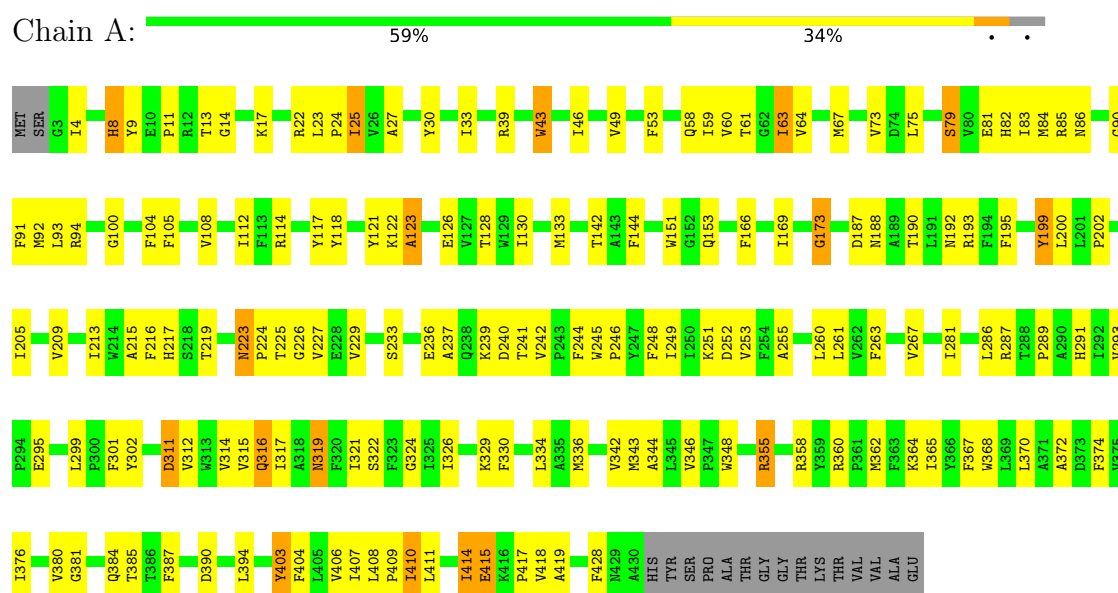
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	Fe	S	0	0
			4	2	2		
7	F	1	Total	Fe	S	0	0
			4	2	2		
7	I	1	Total	Fe	S	0	0
			4	2	2		
7	L	1	Total	Fe	S	0	0
			4	2	2		
7	O	1	Total	Fe	S	0	0
			4	2	2		
7	R	1	Total	Fe	S	0	0
			4	2	2		

3 Residue-property plots [i](#)

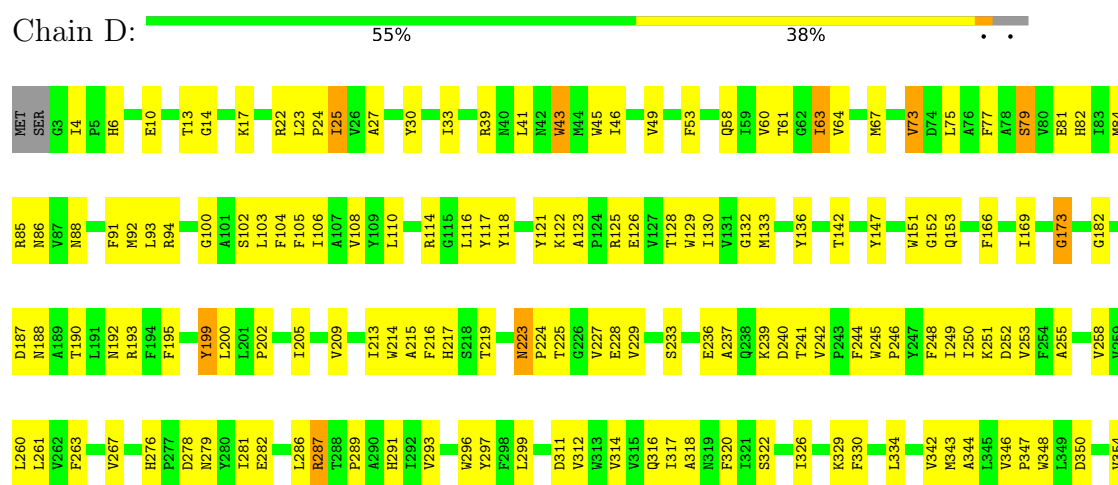
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

• Molecule 1: Cytochrome b

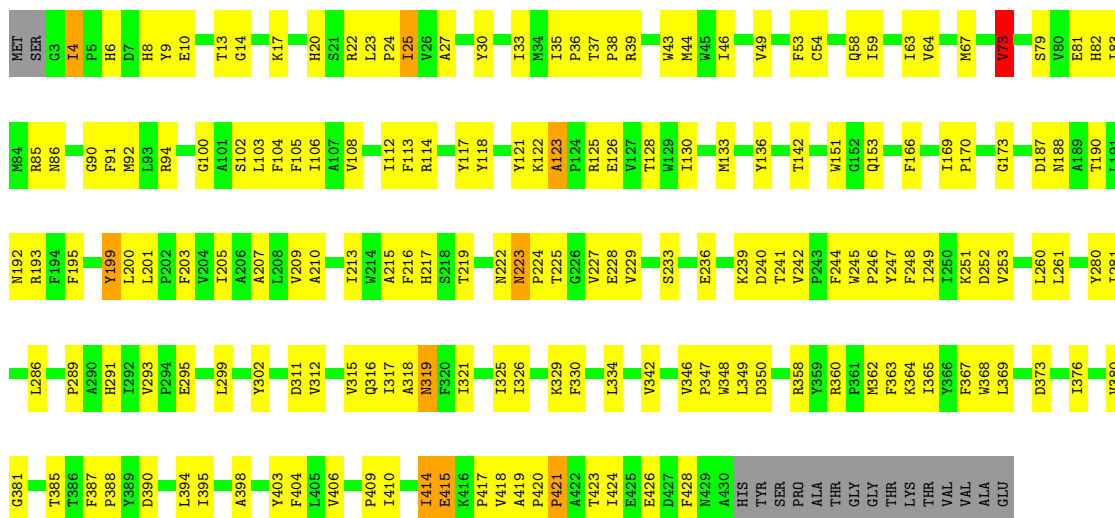


• Molecule 1: Cytochrome b

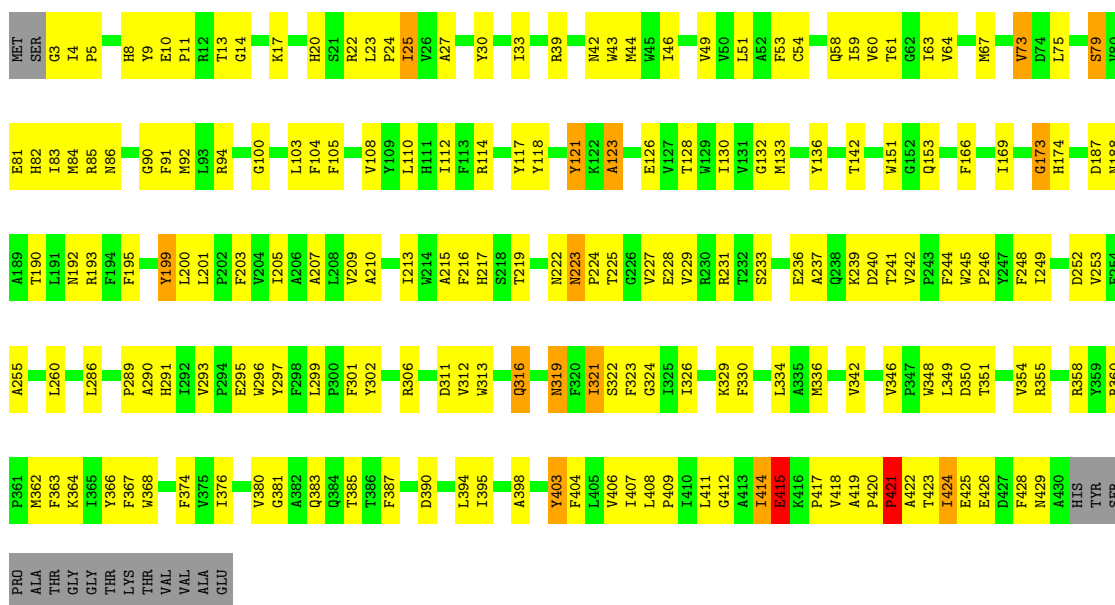




- Molecule 1: Cytochrome b

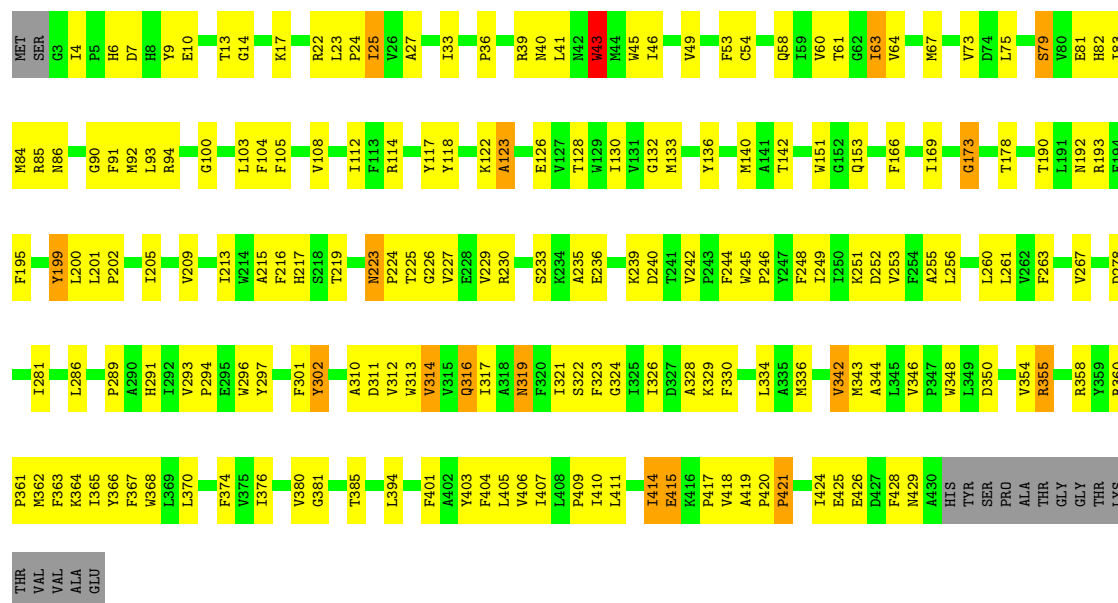


- Molecule 1: Cytochrome b



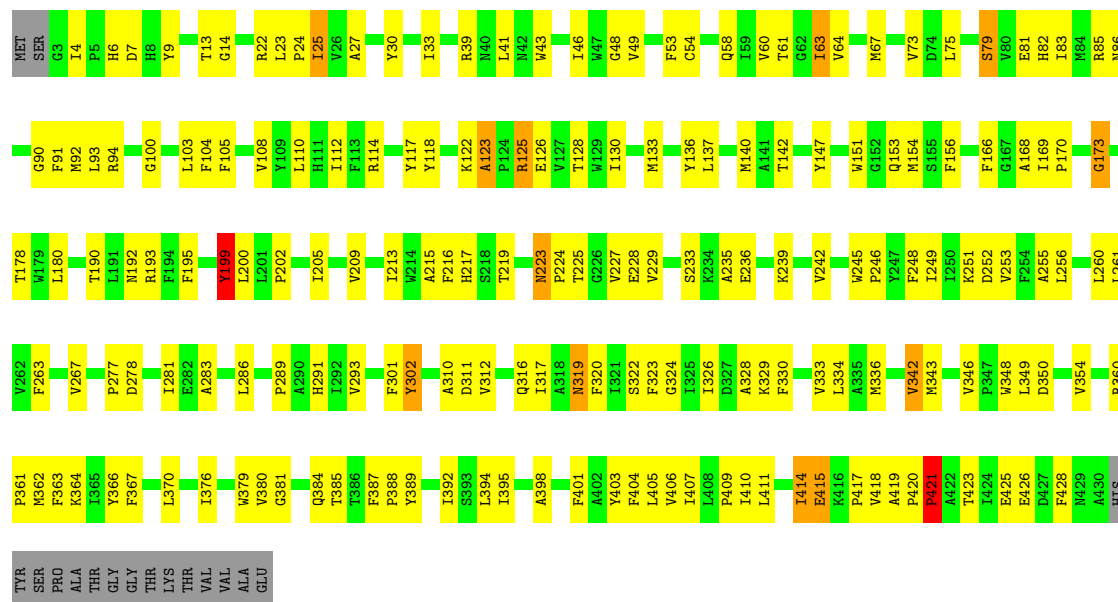
- Molecule 1: Cytochrome b





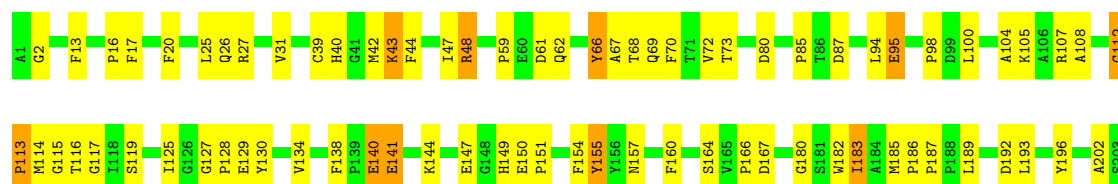
• Molecule 1: Cytochrome b

Chain P: 54% 39%



• Molecule 2: Cytochrome c1

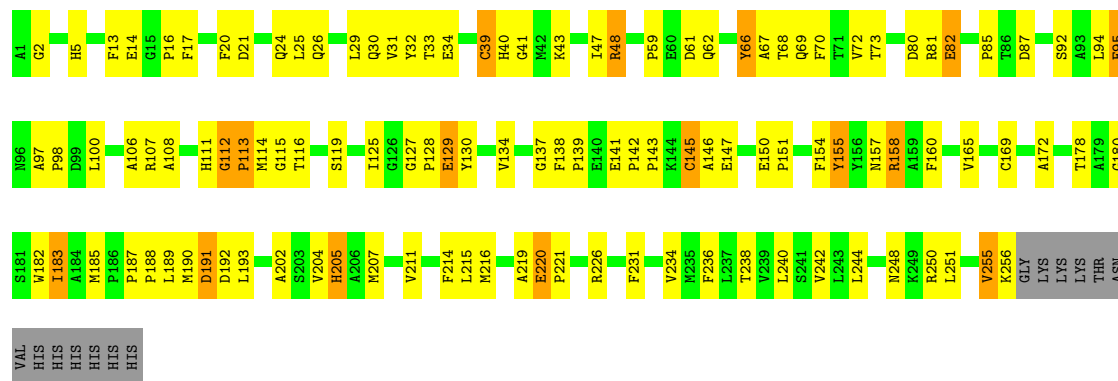
Chain B: 59% 31% 5% 5%





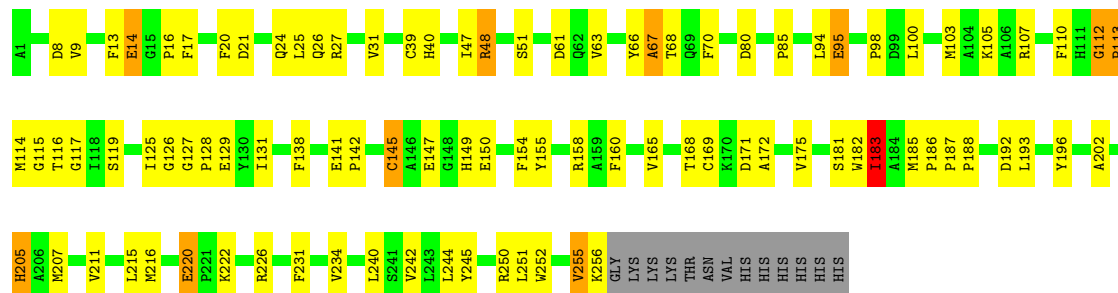
• Molecule 2: Cytochrome c1

Chain E: 52% 37% 6% 5%



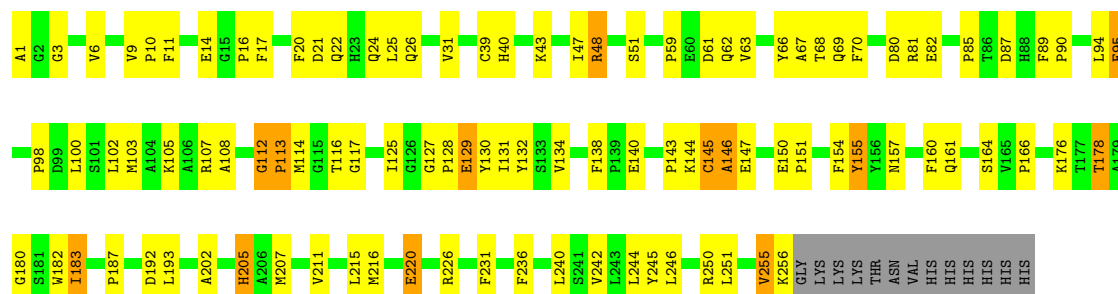
• Molecule 2: Cytochrome c1

Chain H: 60% 31% 5%



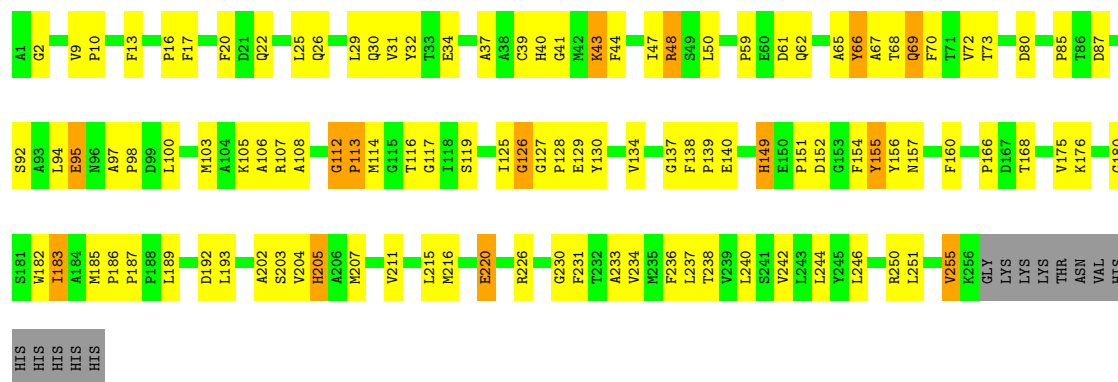
• Molecule 2: Cytochrome c1

Chain K: 57% 33% 5% 5%



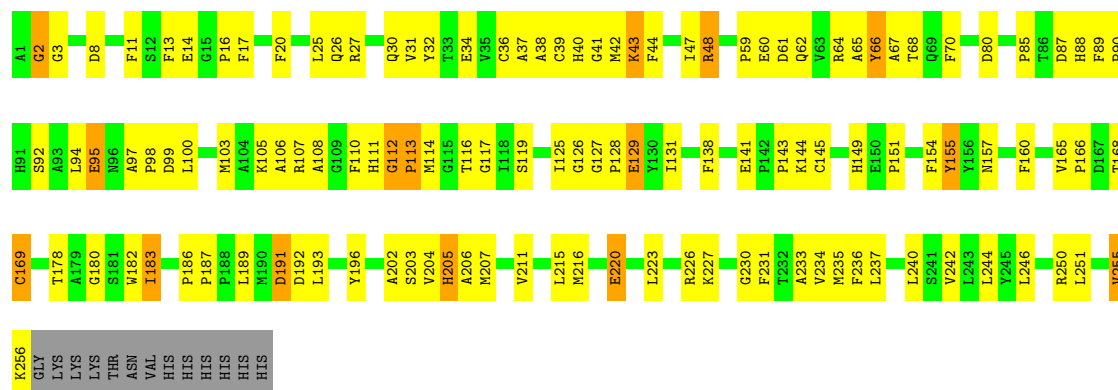
• Molecule 2: Cytochrome c1

Chain N: 54% 36% 5% 5%



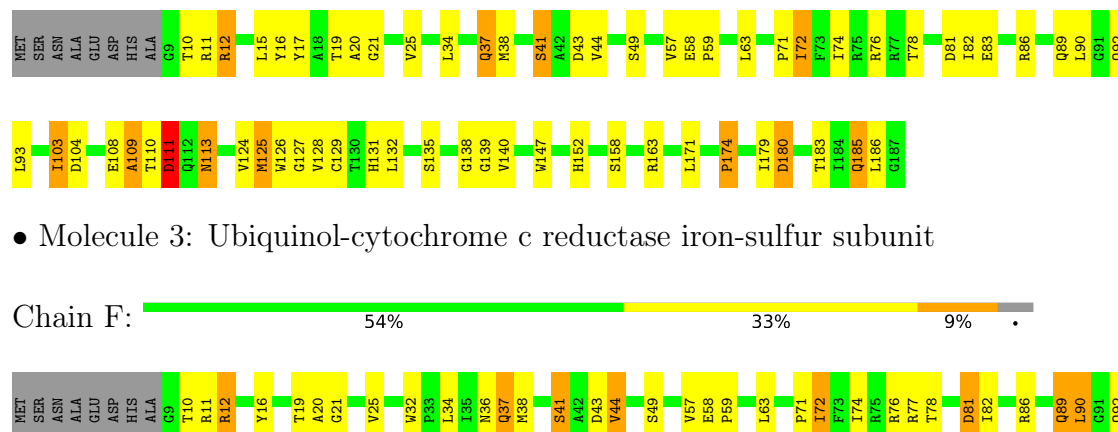
• Molecule 2: Cytochrome c1

Chain Q: 49% 40% 6% 5%



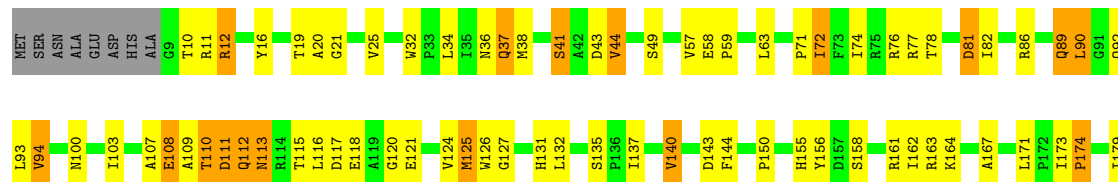
• Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit

Chain C: 61% 28% 6% 5%



• Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit

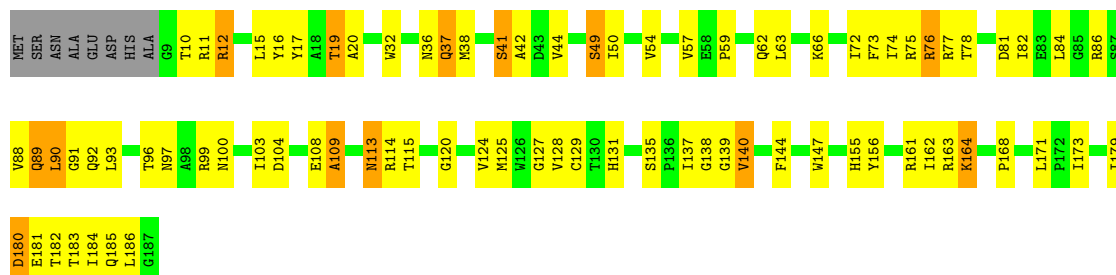
Chain F: 54% 33% 9% 4%





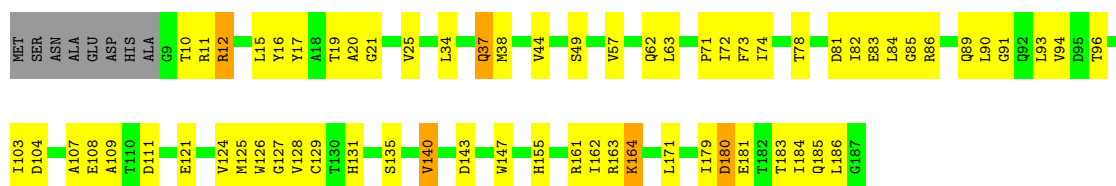
• Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit

Chain I: 52% 37% 7%



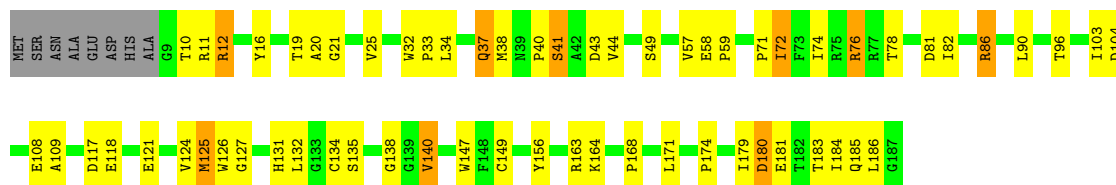
• Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit

Chain L: 60% 33%



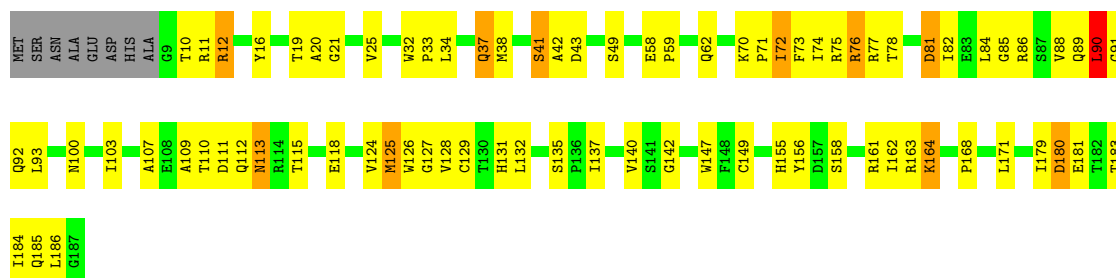
• Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit

Chain O: 62% 29% 5%



• Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit

Chain R: 53% 37% 5%



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	351.30Å 147.13Å 160.83Å 90.00° 103.94° 90.00°	Depositor
Resolution (Å)	18.00 – 3.20	Depositor
% Data completeness (in resolution range)	95.2 (18.00-3.20)	Depositor
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.224 , 0.254	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	41688	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.65	5/3570 (0.1%)	0.73	0/4897
1	D	0.63	0/3570	0.75	0/4897
1	G	0.66	0/3570	0.76	0/4897
1	J	0.65	2/3570 (0.1%)	0.74	0/4897
1	M	0.60	0/3570	0.72	0/4897
1	P	0.59	0/3570	0.73	0/4897
2	B	0.54	0/2010	0.73	0/2733
2	E	0.59	2/2010 (0.1%)	0.76	1/2733 (0.0%)
2	H	0.67	2/2010 (0.1%)	0.78	3/2733 (0.1%)
2	K	0.58	0/2010	0.74	0/2733
2	N	0.56	0/2010	0.73	0/2733
2	Q	0.57	0/2010	0.78	1/2733 (0.0%)
3	C	0.66	0/1370	0.83	1/1866 (0.1%)
3	F	0.64	0/1370	0.84	1/1866 (0.1%)
3	I	0.65	0/1370	0.89	2/1866 (0.1%)
3	L	0.66	0/1370	0.81	0/1866
3	O	0.60	0/1370	0.83	1/1866 (0.1%)
3	R	0.61	0/1370	0.83	2/1866 (0.1%)
All	All	0.62	11/41700 (0.0%)	0.76	12/56976 (0.0%)

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	M	0	1
1	P	0	2
2	E	0	1
2	N	0	1
2	Q	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	6

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	14	GLU	CG-CD	10.19	1.67	1.51
2	H	14	GLU	CB-CG	9.76	1.70	1.52
1	A	121	TYR	CE2-CZ	-7.38	1.28	1.38
1	A	121	TYR	CE1-CZ	-7.18	1.29	1.38
1	J	121	TYR	CE1-CZ	-6.93	1.29	1.38
1	J	121	TYR	CE2-CZ	-6.56	1.30	1.38
1	A	403	TYR	CE1-CZ	-6.08	1.30	1.38
2	E	14	GLU	CG-CD	6.07	1.61	1.51
1	A	403	TYR	CE2-CZ	-5.40	1.31	1.38
2	E	39	CYS	CB-SG	5.13	1.91	1.82
1	A	121	TYR	CG-CD2	-5.11	1.32	1.39

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	145	CYS	CA-CB-SG	9.36	130.84	114.00
2	H	14	GLU	OE1-CD-OE2	-7.65	114.12	123.30
2	H	145	CYS	CA-CB-SG	-5.81	103.54	114.00
2	H	183	ILE	CB-CA-C	-5.64	100.32	111.60
3	C	76	ARG	N-CA-C	-5.30	96.69	111.00
3	R	76	ARG	N-CA-C	-5.29	96.71	111.00
3	F	76	ARG	N-CA-C	-5.29	96.72	111.00
3	I	139	GLY	N-CA-C	-5.26	99.95	113.10
3	O	76	ARG	N-CA-C	-5.24	96.84	111.00
2	E	14	GLU	OE1-CD-OE2	-5.22	117.04	123.30
3	R	149	CYS	CA-CB-SG	-5.15	104.73	114.00
3	I	76	ARG	N-CA-C	-5.14	97.11	111.00

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	32	TYR	Sidechain
1	M	302	TYR	Sidechain
2	N	32	TYR	Sidechain
1	P	199	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	P	302	TYR	Sidechain
2	Q	32	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	3440	0	3428	170	0
1	D	3440	0	3428	174	0
1	G	3440	0	3428	183	0
1	J	3440	0	3428	185	0
1	M	3440	0	3428	189	0
1	P	3440	0	3428	175	0
2	B	1953	0	1848	92	0
2	E	1953	0	1848	107	0
2	H	1953	0	1848	102	0
2	K	1953	0	1848	103	0
2	N	1953	0	1848	109	0
2	Q	1953	0	1848	127	0
3	C	1340	0	1303	59	0
3	F	1340	0	1303	74	0
3	I	1340	0	1303	67	0
3	L	1340	0	1303	51	0
3	O	1340	0	1303	54	0
3	R	1340	0	1303	72	0
4	A	86	0	60	7	0
4	B	43	0	30	0	0
4	D	86	0	60	12	0
4	E	43	0	30	1	0
4	G	86	0	60	10	0
4	H	43	0	30	2	0
4	J	86	0	60	17	0
4	K	43	0	30	1	0
4	M	86	0	60	13	0
4	N	43	0	30	2	0
4	P	86	0	60	11	0
4	Q	43	0	30	1	0
5	A	37	0	42	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	37	0	42	1	0
5	G	37	0	42	1	0
5	J	37	0	42	1	0
5	M	37	0	42	2	0
5	P	37	0	42	0	0
6	A	45	0	67	3	0
6	D	45	0	67	1	0
6	G	45	0	67	5	0
6	J	45	0	67	1	0
6	M	45	0	67	3	0
6	P	45	0	67	1	0
7	C	4	0	0	2	0
7	F	4	0	0	2	0
7	I	4	0	0	0	0
7	L	4	0	0	0	0
7	O	4	0	0	1	0
7	R	4	0	0	1	0
All	All	41688	0	40668	1946	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 (1946) 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)
2:Q:157:ASN:HB2	2:Q:183:ILE:HD11	1.30	1.14
2:B:183:ILE:HG23	2:B:185:MET:H	1.12	1.09
1:G:33:ILE:HD11	1:G:249:ILE:HD11	1.32	1.09
1:J:33:ILE:HD11	1:J:249:ILE:HD11	1.31	1.06
1:P:33:ILE:HD11	1:P:249:ILE:HD11	1.37	1.06
1:M:33:ILE:HD11	1:M:249:ILE:HD11	1.37	1.06
3:R:90:LEU:H	3:R:90:LEU:HD12	1.23	1.04
1:A:33:ILE:HD11	1:A:249:ILE:HD11	1.39	1.03
1:D:239:LYS:HE2	1:D:239:LYS:HA	1.42	1.00
1:M:239:LYS:HE2	1:M:239:LYS:HA	1.42	1.00
3:L:103:ILE:HG22	3:L:104:ASP:H	1.26	0.99
1:A:195:PHE:HE2	1:D:195:PHE:HE2	1.08	0.99
1:P:239:LYS:HE2	1:P:239:LYS:HA	1.40	0.99
1:P:281:ILE:HD11	2:Q:107:ARG:HH12	1.25	0.98
3:I:103:ILE:HG22	3:I:104:ASP:H	1.27	0.98
1:M:195:PHE:HE2	1:P:195:PHE:HE2	1.12	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:360:ARG:HD2	1:P:415:GLU:OE2	1.65	0.97
1:G:195:PHE:HE2	1:J:195:PHE:HE2	1.09	0.96
1:A:239:LYS:HE2	1:A:239:LYS:HA	1.47	0.96
1:G:239:LYS:HE2	1:G:239:LYS:HA	1.46	0.95
1:D:33:ILE:HD11	1:D:249:ILE:HD11	1.48	0.95
1:J:239:LYS:HE2	1:J:239:LYS:HA	1.48	0.93
3:C:83:GLU:HG2	3:L:83:GLU:HG2	1.52	0.92
1:G:319:ASN:HD22	1:G:319:ASN:C	1.72	0.92
2:B:140:GLU:CD	2:B:140:GLU:H	1.73	0.91
1:M:329:LYS:HE3	3:R:131:HIS:O	1.71	0.91
2:H:160:PHE:CD2	2:H:183:ILE:HG23	2.05	0.91
1:M:200:LEU:HD22	1:P:63:ILE:HD12	1.51	0.90
2:K:150:GLU:HG3	2:K:182:TRP:CZ3	2.07	0.90
2:E:250:ARG:HD3	3:F:12:ARG:NH2	1.89	0.88
1:A:142:THR:HG21	4:A:502:HEM:HBB2	1.56	0.88
2:Q:106:ALA:O	2:Q:107:ARG:HG2	1.73	0.88
1:G:82:HIS:CD2	1:G:86:ASN:HD22	1.93	0.86
2:H:138:PHE:CZ	2:H:183:ILE:HD11	2.10	0.86
3:R:89:GLN:O	3:R:91:GLY:N	2.08	0.86
1:A:13:THR:HG22	1:A:14:GLY:H	1.39	0.85
1:D:13:THR:HG22	1:D:14:GLY:H	1.41	0.85
2:N:250:ARG:HD3	3:O:12:ARG:NH2	1.92	0.85
1:D:142:THR:HG21	4:D:502:HEM:HBB2	1.57	0.85
1:M:13:THR:HG22	1:M:14:GLY:H	1.42	0.85
1:G:112:ILE:HG12	4:G:501:HEM:HAC	1.57	0.84
1:J:411:LEU:O	1:J:415:GLU:HG2	1.78	0.84
1:P:13:THR:HG22	1:P:14:GLY:H	1.43	0.83
1:D:376:ILE:O	1:D:380:VAL:HG23	1.79	0.83
3:C:131:HIS:O	1:D:329:LYS:HE3	1.78	0.83
1:A:200:LEU:HD22	1:D:63:ILE:HD12	1.60	0.82
1:J:142:THR:HG21	4:J:502:HEM:HBB2	1.60	0.82
2:K:150:GLU:HG3	2:K:182:TRP:HZ3	1.40	0.82
3:L:103:ILE:HG22	3:L:104:ASP:N	1.94	0.82
1:D:132:GLY:C	4:D:501:HEM:HBC2	2.00	0.82
3:I:131:HIS:O	1:J:329:LYS:HE3	1.79	0.82
3:R:74:ILE:HG12	3:R:124:VAL:HG22	1.62	0.81
1:G:13:THR:HG22	1:G:14:GLY:H	1.45	0.81
1:P:376:ILE:O	1:P:380:VAL:HG23	1.78	0.81
1:P:414:ILE:HG22	1:P:415:GLU:N	1.94	0.81
1:J:13:THR:HG22	1:J:14:GLY:H	1.45	0.81
2:Q:220:GLU:OE2	2:Q:226:ARG:NH1	2.13	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:4:ILE:HD12	1:G:4:ILE:H	1.44	0.81
2:K:250:ARG:HD3	3:L:12:ARG:NH2	1.96	0.81
1:M:142:THR:HG21	4:M:502:HEM:HBB2	1.62	0.81
1:A:193:ARG:HD3	3:F:38:MET:HE3	1.63	0.81
2:Q:47:ILE:HG13	2:Q:87:ASP:O	1.81	0.80
1:P:142:THR:HG21	4:P:502:HEM:HBB2	1.64	0.80
1:M:376:ILE:O	1:M:380:VAL:HG23	1.82	0.80
1:G:128:THR:HG21	4:G:501:HEM:HBD1	1.63	0.79
3:F:93:LEU:HD13	3:F:161:ARG:HD2	1.64	0.79
1:A:128:THR:HG21	4:A:501:HEM:HBD1	1.65	0.79
1:D:82:HIS:CD2	1:D:86:ASN:HD22	2.00	0.79
3:C:140:VAL:O	3:C:140:VAL:HG12	1.83	0.78
1:M:414:ILE:HG22	1:M:415:GLU:N	1.99	0.78
2:Q:89:PHE:HB3	2:Q:90:PRO:HD2	1.63	0.78
3:F:89:GLN:HG2	3:F:92:GLN:HG3	1.66	0.78
1:J:82:HIS:CD2	1:J:86:ASN:HD22	2.01	0.78
1:G:410:ILE:HG23	1:G:414:ILE:HD12	1.63	0.78
1:A:358:ARG:HH21	6:A:504:LOP:H21	1.45	0.77
2:Q:250:ARG:HD3	3:R:12:ARG:NH2	1.98	0.77
1:D:39:ARG:HH12	2:E:255:VAL:CG1	1.97	0.77
1:D:39:ARG:HH12	2:E:255:VAL:HG13	1.47	0.77
1:M:63:ILE:HD12	1:P:200:LEU:HD22	1.66	0.77
1:A:82:HIS:CD2	1:A:86:ASN:HD22	2.02	0.77
2:Q:103:MET:HG3	2:Q:131:ILE:HD11	1.66	0.77
1:A:370:LEU:HD22	1:A:403:TYR:CE2	2.20	0.77
2:B:183:ILE:HG23	2:B:185:MET:N	1.96	0.77
1:G:193:ARG:HD3	3:L:38:MET:HE3	1.67	0.76
1:G:213:ILE:HA	1:G:216:PHE:CE2	2.20	0.76
1:A:199:TYR:CD2	4:A:502:HEM:HBC1	2.20	0.76
2:E:47:ILE:HG13	2:E:87:ASP:O	1.86	0.76
3:I:12:ARG:HD3	3:I:16:TYR:CE1	2.20	0.76
1:M:82:HIS:CD2	1:M:86:ASN:HD22	2.03	0.76
1:P:199:TYR:CD2	4:P:502:HEM:HBC1	2.20	0.76
1:G:423:THR:HG23	1:G:426:GLU:H	1.51	0.76
2:N:47:ILE:HG13	2:N:87:ASP:O	1.86	0.76
3:I:66:LYS:HG3	1:J:286:LEU:HD21	1.67	0.76
2:Q:157:ASN:HB2	2:Q:183:ILE:CD1	2.13	0.76
3:O:185:GLN:O	3:O:185:GLN:HG3	1.86	0.75
1:J:213:ILE:HA	1:J:216:PHE:CE2	2.20	0.75
1:M:91:PHE:CE1	1:M:92:MET:HG2	2.21	0.75
2:N:105:LYS:HE3	2:N:220:GLU:HG2	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:ASP:HA	1:A:316:GLN:NE2	2.02	0.75
1:M:223:ASN:OD1	1:M:225:THR:HB	1.86	0.74
1:G:317:ILE:O	1:G:321:ILE:HG13	1.87	0.74
1:G:406:VAL:O	1:G:409:PRO:HD2	1.87	0.74
1:J:91:PHE:CE1	1:J:92:MET:HG2	2.23	0.74
2:Q:66:TYR:HE1	2:Q:70:PHE:CE2	2.04	0.74
1:A:407:ILE:O	1:A:411:LEU:HD23	1.87	0.74
3:C:185:GLN:HG3	3:C:185:GLN:O	1.87	0.74
1:P:428:PHE:CZ	2:Q:256:LYS:HB2	2.22	0.74
1:A:319:ASN:HD22	1:A:319:ASN:C	1.91	0.74
1:P:423:THR:HG23	1:P:426:GLU:H	1.53	0.74
1:A:370:LEU:HD22	1:A:403:TYR:CD2	2.22	0.74
3:F:185:GLN:HG3	3:F:185:GLN:O	1.87	0.74
1:P:82:HIS:CD2	1:P:86:ASN:HD22	2.05	0.74
1:A:195:PHE:HE2	1:D:195:PHE:CE2	2.01	0.73
2:Q:100:LEU:HD13	2:Q:215:LEU:HD11	1.69	0.73
2:N:31:VAL:HB	2:N:211:VAL:HG22	1.71	0.73
1:P:122:LYS:HE3	1:P:350:ASP:OD2	1.87	0.73
1:A:376:ILE:O	1:A:380:VAL:HG23	1.88	0.73
2:K:128:PRO:HG2	2:K:129:GLU:OE1	1.88	0.73
1:M:123:ALA:O	1:M:355:ARG:NH1	2.20	0.73
1:G:91:PHE:CE1	1:G:92:MET:HG2	2.24	0.73
1:G:39:ARG:HH12	2:H:255:VAL:CG1	2.02	0.73
1:G:312:VAL:HB	1:G:315:VAL:HG23	1.71	0.72
2:N:137:GLY:O	2:N:139:PRO:HD3	1.89	0.72
3:R:163:ARG:O	3:R:164:LYS:HB2	1.89	0.72
1:G:414:ILE:HG22	1:G:415:GLU:N	2.03	0.72
1:M:319:ASN:C	1:M:319:ASN:HD22	1.93	0.72
1:P:281:ILE:HD11	2:Q:107:ARG:NH1	2.03	0.72
2:Q:128:PRO:HG2	2:Q:129:GLU:H	1.53	0.72
1:J:312:VAL:O	1:J:316:GLN:HG2	1.90	0.72
3:R:185:GLN:HG3	3:R:185:GLN:O	1.88	0.72
1:G:142:THR:HG21	4:G:502:HEM:HBB2	1.72	0.72
1:G:319:ASN:C	1:G:319:ASN:ND2	2.43	0.72
3:F:78:THR:O	3:F:82:ILE:HG13	1.89	0.72
2:K:20:PHE:HB3	2:K:25:LEU:HD11	1.71	0.72
1:A:13:THR:HG22	1:A:14:GLY:N	2.05	0.72
2:E:220:GLU:OE2	2:E:226:ARG:NH1	2.23	0.72
2:H:125:ILE:HD13	2:H:125:ILE:N	2.04	0.72
3:I:103:ILE:HG22	3:I:104:ASP:N	2.04	0.72
1:J:121:TYR:CE2	1:J:346:VAL:HG12	2.25	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:39:ARG:HD3	1:P:428:PHE:CD2	2.25	0.71
1:A:9:TYR:HB2	1:A:30:TYR:CD2	2.26	0.71
1:A:195:PHE:CE2	1:D:195:PHE:HE2	2.00	0.71
1:D:213:ILE:HA	1:D:216:PHE:CE2	2.25	0.71
1:G:195:PHE:CE2	1:J:195:PHE:HE2	2.01	0.71
1:P:91:PHE:CE1	1:P:92:MET:HG2	2.26	0.71
1:P:223:ASN:OD1	1:P:225:THR:HB	1.89	0.71
1:G:261:LEU:HD11	2:H:234:VAL:HG13	1.72	0.71
3:R:90:LEU:H	3:R:90:LEU:CD1	2.01	0.71
3:C:41:SER:HB2	3:C:43:ASP:OD1	1.90	0.71
1:J:123:ALA:O	1:J:355:ARG:NH1	2.24	0.71
1:P:39:ARG:HH12	2:Q:255:VAL:HG13	1.54	0.71
1:G:122:LYS:HE2	1:G:350:ASP:OD2	1.91	0.70
3:L:12:ARG:HD3	3:L:16:TYR:CE1	2.25	0.70
1:G:199:TYR:CD2	4:G:502:HEM:HBC1	2.26	0.70
3:C:38:MET:HE3	1:D:193:ARG:HD3	1.73	0.70
1:D:122:LYS:HE3	1:D:350:ASP:OD2	1.91	0.70
1:M:33:ILE:HD11	1:M:249:ILE:CD1	2.19	0.70
1:M:43:TRP:CZ3	1:M:251:LYS:HE2	2.27	0.70
3:F:82:ILE:O	3:F:86:ARG:HG3	1.91	0.70
1:P:33:ILE:HD11	1:P:249:ILE:CD1	2.19	0.70
1:D:387:PHE:CE1	1:D:388:PRO:HB3	2.27	0.69
2:K:105:LYS:HE3	2:K:220:GLU:HG2	1.72	0.69
1:M:319:ASN:ND2	1:M:324:GLY:HA2	2.05	0.69
2:B:138:PHE:CG	2:B:187:PRO:HB3	2.28	0.69
2:Q:31:VAL:HB	2:Q:211:VAL:HG22	1.74	0.69
1:D:13:THR:HG22	1:D:14:GLY:N	2.06	0.69
2:H:16:PRO:HG2	2:H:17:PHE:CD1	2.28	0.69
2:H:20:PHE:HB3	2:H:25:LEU:HD11	1.75	0.69
2:H:103:MET:HE1	4:H:301:HEM:HAA2	1.73	0.69
3:I:38:MET:HE3	1:J:193:ARG:HD3	1.74	0.69
1:J:313:TRP:HA	1:J:316:GLN:HG3	1.75	0.69
2:Q:48:ARG:HG2	2:Q:48:ARG:HH11	1.58	0.69
2:N:100:LEU:HD13	2:N:215:LEU:HD11	1.74	0.69
1:A:91:PHE:CE1	1:A:92:MET:HG2	2.28	0.69
1:A:213:ILE:HA	1:A:216:PHE:CE2	2.27	0.69
1:D:287:ARG:HG2	1:D:287:ARG:HH11	1.56	0.69
1:G:63:ILE:HD13	1:J:200:LEU:HD22	1.74	0.69
1:J:199:TYR:CD2	4:J:502:HEM:HBC1	2.28	0.69
1:M:406:VAL:O	1:M:409:PRO:HD2	1.93	0.69
1:D:43:TRP:HA	1:D:43:TRP:CE3	2.27	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:108:ALA:HA	2:E:125:ILE:HG22	1.74	0.69
1:A:329:LYS:HE3	3:F:131:HIS:O	1.93	0.69
1:D:43:TRP:HA	1:D:43:TRP:HE3	1.58	0.69
1:P:291:HIS:O	1:P:293:VAL:HG23	1.93	0.69
1:D:223:ASN:HD22	1:D:223:ASN:H	1.41	0.68
1:A:223:ASN:OD1	1:A:225:THR:HB	1.93	0.68
1:J:13:THR:HG22	1:J:14:GLY:N	2.08	0.68
3:O:179:ILE:HD11	3:O:183:THR:CG2	2.22	0.68
2:H:31:VAL:HB	2:H:211:VAL:HG22	1.75	0.68
1:J:132:GLY:C	4:J:501:HEM:HBC2	2.13	0.68
1:M:43:TRP:HZ3	1:M:251:LYS:HE2	1.58	0.68
1:M:67:MET:HG2	1:P:193:ARG:HA	1.76	0.68
1:A:312:VAL:HB	1:A:315:VAL:CG2	2.24	0.68
2:N:220:GLU:OE2	2:N:226:ARG:NH1	2.27	0.68
3:C:103:ILE:HG22	3:C:104:ASP:H	1.59	0.68
1:D:223:ASN:HD22	1:D:223:ASN:N	1.91	0.68
1:M:13:THR:HG22	1:M:14:GLY:N	2.08	0.68
1:M:193:ARG:HA	1:P:67:MET:HG2	1.75	0.68
1:D:91:PHE:CE1	1:D:92:MET:HG2	2.29	0.68
1:A:144:PHE:HE2	5:A:503:SMA:H43	1.59	0.68
1:A:418:VAL:HG12	1:A:419:ALA:N	2.08	0.68
2:E:142:PRO:HG2	2:E:150:GLU:OE2	1.93	0.68
2:H:250:ARG:HD3	3:I:12:ARG:NH2	2.09	0.68
2:B:31:VAL:HB	2:B:211:VAL:HG22	1.75	0.67
1:D:133:MET:N	4:D:501:HEM:HBC2	2.09	0.67
1:G:13:THR:HG22	1:G:14:GLY:N	2.08	0.67
2:H:105:LYS:HD3	2:H:220:GLU:HG2	1.76	0.67
2:E:137:GLY:O	2:E:139:PRO:HD3	1.94	0.67
1:M:195:PHE:HE2	1:P:195:PHE:CE2	2.05	0.67
1:M:294:PRO:HA	5:M:503:SMA:H10	1.74	0.67
2:N:40:HIS:CE1	2:N:97:ALA:HB1	2.29	0.67
1:G:23:LEU:HD13	1:J:215:ALA:HA	1.76	0.67
2:B:47:ILE:HG13	2:B:87:ASP:O	1.93	0.67
3:I:12:ARG:HD3	3:I:16:TYR:HE1	1.58	0.67
1:G:360:ARG:HD2	1:G:415:GLU:OE1	1.94	0.67
1:M:314:VAL:HA	1:M:317:ILE:HD12	1.76	0.67
1:P:366:TYR:HD2	1:P:411:LEU:HD11	1.60	0.67
1:D:406:VAL:O	1:D:409:PRO:HD2	1.95	0.67
2:E:157:ASN:CB	2:E:183:ILE:HD11	2.23	0.67
1:J:3:GLY:O	1:J:231:ARG:HD2	1.95	0.67
2:K:160:PHE:CD2	2:K:183:ILE:HG23	2.30	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:41:SER:O	3:I:44:VAL:HG23	1.95	0.67
2:N:48:ARG:HG2	2:N:48:ARG:HH11	1.59	0.67
5:A:503:SMA:H39	5:A:503:SMA:H33	1.77	0.67
2:N:160:PHE:CD2	2:N:183:ILE:HG12	2.28	0.67
3:O:103:ILE:HG22	3:O:104:ASP:N	2.10	0.67
1:P:128:THR:HG21	4:P:501:HEM:HBD1	1.77	0.67
1:D:46:ILE:HD13	1:D:255:ALA:HB1	1.77	0.66
2:K:31:VAL:HB	2:K:211:VAL:HG22	1.76	0.66
1:M:39:ARG:HD3	1:M:428:PHE:CD2	2.30	0.66
1:M:281:ILE:HD11	2:N:107:ARG:HH12	1.60	0.66
1:J:33:ILE:HD11	1:J:249:ILE:CD1	2.19	0.66
2:K:40:HIS:HE1	2:K:98:PRO:HD2	1.59	0.66
2:H:220:GLU:OE2	2:H:226:ARG:NH1	2.28	0.66
1:A:193:ARG:HD3	3:F:38:MET:CE	2.25	0.66
3:L:185:GLN:O	3:L:185:GLN:HG3	1.93	0.66
3:F:110:THR:HB	3:F:112:GLN:NE2	2.10	0.66
1:J:406:VAL:O	1:J:409:PRO:HD2	1.95	0.66
1:A:360:ARG:NH1	1:A:415:GLU:OE2	2.27	0.66
3:I:74:ILE:HG12	3:I:124:VAL:HG22	1.78	0.66
2:K:125:ILE:HD12	2:K:125:ILE:N	2.11	0.66
1:G:39:ARG:HH12	2:H:255:VAL:HG13	1.61	0.65
3:O:74:ILE:HG12	3:O:124:VAL:HG22	1.77	0.65
2:Q:39:CYS:HB3	2:Q:94:LEU:HB3	1.77	0.65
1:A:312:VAL:HB	1:A:315:VAL:HG23	1.78	0.65
1:J:33:ILE:CD1	1:J:249:ILE:HD11	2.19	0.65
1:P:291:HIS:NE2	2:Q:2:GLY:HA3	2.12	0.65
3:C:82:ILE:O	3:C:86:ARG:HG3	1.96	0.65
1:M:23:LEU:HD23	1:M:25:ILE:HD11	1.79	0.65
1:P:166:PHE:O	1:P:169:ILE:HD12	1.96	0.65
1:D:23:LEU:HD23	1:D:25:ILE:HD11	1.77	0.65
4:D:502:HEM:O2D	4:D:502:HEM:O1A	2.15	0.65
2:E:100:LEU:HD13	2:E:215:LEU:HD11	1.79	0.65
3:F:41:SER:O	3:F:44:VAL:HG23	1.97	0.65
2:K:16:PRO:HG2	2:K:17:PHE:CD1	2.32	0.65
1:P:13:THR:HG22	1:P:14:GLY:N	2.09	0.65
1:P:354:VAL:HG21	1:P:417:PRO:HB3	1.77	0.65
2:Q:160:PHE:CE2	2:Q:183:ILE:HG23	2.32	0.65
3:F:90:LEU:HD11	3:F:108:GLU:HB3	1.79	0.65
2:E:31:VAL:HB	2:E:211:VAL:HG22	1.77	0.65
1:G:410:ILE:CG2	1:G:414:ILE:HD12	2.26	0.65
3:I:185:GLN:HG3	3:I:185:GLN:O	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:205:ILE:O	1:J:209:VAL:HG23	1.97	0.64
1:P:117:TYR:HB2	1:P:367:PHE:CE2	2.32	0.64
3:F:127:GLY:O	3:F:135:SER:HA	1.97	0.64
1:G:376:ILE:O	1:G:380:VAL:HG23	1.98	0.64
2:H:147:GLU:OE1	2:H:147:GLU:HA	1.97	0.64
1:P:326:ILE:HG22	1:P:326:ILE:O	1.95	0.64
3:C:78:THR:O	3:C:82:ILE:HG13	1.96	0.64
3:F:94:VAL:HG23	3:F:162:ILE:O	1.96	0.64
2:K:161:GLN:HE21	2:K:176:LYS:NZ	1.95	0.64
1:M:213:ILE:HA	1:M:216:PHE:CE2	2.32	0.64
3:R:179:ILE:HD11	3:R:183:THR:CG2	2.27	0.64
2:N:20:PHE:HB3	2:N:25:LEU:HD11	1.80	0.64
2:Q:66:TYR:CE1	2:Q:70:PHE:CE2	2.86	0.64
1:D:130:ILE:HD11	1:D:348:TRP:HH2	1.63	0.64
3:F:12:ARG:HD3	3:F:16:TYR:CE1	2.33	0.64
1:M:33:ILE:CD1	1:M:249:ILE:HD11	2.22	0.64
1:G:195:PHE:HE2	1:J:195:PHE:CE2	2.01	0.64
3:R:89:GLN:C	3:R:91:GLY:H	1.99	0.64
1:A:46:ILE:HD13	1:A:255:ALA:HB1	1.80	0.64
1:A:63:ILE:HD12	1:D:200:LEU:HD22	1.80	0.64
3:F:125:MET:SD	3:F:171:LEU:HD12	2.38	0.64
1:J:418:VAL:HG12	1:J:419:ALA:N	2.13	0.64
2:E:193:LEU:HD23	2:E:193:LEU:O	1.98	0.64
1:G:39:ARG:HD3	1:G:428:PHE:CD2	2.33	0.64
3:O:78:THR:O	3:O:82:ILE:HG13	1.98	0.64
1:P:418:VAL:HG12	1:P:419:ALA:N	2.13	0.64
1:A:23:LEU:HD23	1:A:25:ILE:HD11	1.80	0.63
1:G:281:ILE:HD11	2:H:107:ARG:HH12	1.62	0.63
1:J:425:GLU:HG3	1:J:429:ASN:HD21	1.63	0.63
1:G:43:TRP:HZ3	1:G:251:LYS:HG2	1.63	0.63
1:G:387:PHE:CD1	1:G:388:PRO:HA	2.33	0.63
2:K:48:ARG:HH11	2:K:48:ARG:HG2	1.62	0.63
2:Q:108:ALA:HA	2:Q:125:ILE:HG22	1.79	0.63
1:A:233:SER:OG	1:A:236:GLU:HG2	1.98	0.63
2:Q:127:GLY:N	2:Q:128:PRO:HD2	2.13	0.63
3:R:12:ARG:HD3	3:R:16:TYR:CE1	2.34	0.63
1:J:376:ILE:O	1:J:380:VAL:HG23	1.99	0.63
2:N:40:HIS:ND1	2:N:97:ALA:HB1	2.14	0.63
3:O:82:ILE:O	3:O:86:ARG:HG3	1.97	0.63
3:C:125:MET:SD	3:C:171:LEU:HD12	2.39	0.63
1:G:312:VAL:O	1:G:316:GLN:HG3	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:ARG:HA	1:D:67:MET:HG2	1.80	0.63
2:B:20:PHE:HB3	2:B:25:LEU:HD11	1.79	0.63
3:C:12:ARG:HD3	3:C:16:TYR:CE1	2.33	0.63
1:D:223:ASN:H	1:D:223:ASN:ND2	1.97	0.63
2:H:193:LEU:HD23	2:H:193:LEU:O	1.99	0.63
2:K:220:GLU:OE2	2:K:226:ARG:NH1	2.31	0.63
1:P:39:ARG:HH12	2:Q:255:VAL:CG1	2.11	0.63
2:B:250:ARG:HD3	3:C:12:ARG:NH2	2.14	0.63
2:E:48:ARG:HG2	2:E:48:ARG:HH11	1.62	0.63
2:H:126:GLY:HA2	2:H:129:GLU:OE1	1.99	0.63
3:O:117:ASP:OD2	3:O:121:GLU:HG2	1.99	0.63
1:D:187:ASP:CG	1:D:188:ASN:H	2.03	0.63
1:J:228:GLU:O	1:J:424:ILE:HD11	1.99	0.63
1:J:403:TYR:C	1:J:403:TYR:CD1	2.71	0.63
1:M:91:PHE:CE1	1:M:92:MET:CG	2.82	0.63
2:H:128:PRO:HD3	2:H:216:MET:CE	2.28	0.62
1:P:281:ILE:CD1	2:Q:107:ARG:HH12	2.08	0.62
3:R:78:THR:O	3:R:82:ILE:HG13	1.98	0.62
1:D:4:ILE:HD12	1:D:4:ILE:N	2.14	0.62
1:A:130:ILE:HD11	1:A:348:TRP:HH2	1.64	0.62
1:J:199:TYR:HA	4:J:502:HEM:HBC2	1.81	0.62
3:L:12:ARG:HD3	3:L:16:TYR:HE1	1.63	0.62
1:M:195:PHE:CE2	1:P:195:PHE:HE2	2.05	0.62
1:M:418:VAL:HG12	1:M:419:ALA:N	2.14	0.62
1:P:428:PHE:HZ	2:Q:256:LYS:HB2	1.64	0.62
2:Q:105:LYS:HE3	2:Q:220:GLU:HG2	1.80	0.62
3:R:82:ILE:O	3:R:86:ARG:HG3	1.99	0.62
1:A:105:PHE:HA	1:A:108:VAL:HG12	1.82	0.62
3:I:90:LEU:HD21	3:I:108:GLU:HB3	1.81	0.62
1:J:133:MET:N	4:J:501:HEM:HBC2	2.14	0.62
3:O:103:ILE:HG22	3:O:104:ASP:H	1.65	0.62
2:Q:11:PHE:HB2	2:Q:14:GLU:HG3	1.81	0.62
1:D:414:ILE:HG22	1:D:415:GLU:N	2.14	0.62
1:M:326:ILE:HG22	1:M:326:ILE:O	2.00	0.62
2:B:160:PHE:CD2	2:B:183:ILE:HG13	2.34	0.62
2:N:127:GLY:N	2:N:128:PRO:HD2	2.14	0.62
4:P:502:HEM:O1A	4:P:502:HEM:O2D	2.18	0.62
1:J:350:ASP:HB2	1:J:408:LEU:HD12	1.81	0.62
1:P:423:THR:HG22	1:P:426:GLU:HB2	1.80	0.62
2:Q:165:VAL:CG1	2:Q:169:CYS:HB3	2.30	0.62
1:G:360:ARG:NH2	1:G:363:PHE:CD2	2.68	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:425:GLU:HG2	1:M:429:ASN:HD21	1.65	0.62
3:O:179:ILE:HD11	3:O:183:THR:HG22	1.81	0.62
1:P:223:ASN:ND2	1:P:223:ASN:H	1.97	0.62
2:H:66:TYR:HE1	2:H:70:PHE:CE2	2.17	0.62
2:K:160:PHE:CE2	2:K:183:ILE:HG23	2.35	0.62
2:E:138:PHE:CG	2:E:187:PRO:HB3	2.35	0.61
2:E:157:ASN:ND2	2:E:183:ILE:HD11	2.15	0.61
1:G:33:ILE:HD11	1:G:249:ILE:CD1	2.20	0.61
2:H:66:TYR:CE1	2:H:70:PHE:HE2	2.17	0.61
2:N:40:HIS:HE1	2:N:98:PRO:HD2	1.65	0.61
2:B:100:LEU:HD13	2:B:215:LEU:HD11	1.82	0.61
1:G:358:ARG:HA	1:G:364:LYS:HE2	1.80	0.61
1:M:215:ALA:HA	1:P:23:LEU:HD13	1.82	0.61
2:N:17:PHE:CE2	2:N:231:PHE:CZ	2.88	0.61
2:N:43:LYS:HE3	2:N:44:PHE:CZ	2.35	0.61
2:H:48:ARG:HG2	2:H:48:ARG:HH11	1.66	0.61
3:I:138:GLY:HA3	3:I:147:TRP:CD1	2.36	0.61
1:A:311:ASP:HA	1:A:316:GLN:HE21	1.65	0.61
2:K:66:TYR:O	2:K:69:GLN:HG2	2.01	0.61
2:K:138:PHE:CG	2:K:187:PRO:HB3	2.36	0.61
1:G:59:ILE:O	1:G:63:ILE:HG13	2.01	0.61
1:M:193:ARG:HD3	3:R:38:MET:HE3	1.83	0.61
1:M:291:HIS:O	1:M:293:VAL:HG23	2.00	0.61
1:D:326:ILE:O	1:D:326:ILE:HG22	2.01	0.61
3:L:103:ILE:CG2	3:L:104:ASP:H	2.09	0.61
1:P:213:ILE:HA	1:P:216:PHE:CE2	2.35	0.61
3:R:125:MET:HE2	3:R:147:TRP:CH2	2.35	0.61
2:B:48:ARG:HG2	2:B:48:ARG:HH11	1.64	0.61
2:E:157:ASN:CG	2:E:183:ILE:HD11	2.21	0.61
1:D:4:ILE:HD12	1:D:4:ILE:H	1.66	0.61
1:D:39:ARG:NH1	2:E:255:VAL:CG1	2.64	0.61
1:G:23:LEU:HD23	1:G:25:ILE:HD11	1.81	0.61
3:O:12:ARG:HD3	3:O:16:TYR:CE1	2.35	0.61
1:D:366:TYR:HD2	1:D:411:LEU:HD11	1.66	0.60
3:I:103:ILE:CG2	3:I:104:ASP:H	2.08	0.60
1:A:418:VAL:CG1	1:A:419:ALA:N	2.64	0.60
2:B:220:GLU:OE2	2:B:226:ARG:NH1	2.34	0.60
2:Q:112:GLY:HA2	2:Q:119:SER:HB3	1.83	0.60
3:L:143:ASP:OD2	3:L:164:LYS:NZ	2.33	0.60
2:B:127:GLY:N	2:B:128:PRO:HD2	2.16	0.60
1:P:418:VAL:HG12	1:P:419:ALA:H	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:ASN:HD21	1:A:324:GLY:HA2	1.65	0.60
1:G:346:VAL:HG22	1:G:404:PHE:CD1	2.36	0.60
1:J:330:PHE:CE2	1:J:334:LEU:HD11	2.37	0.60
2:Q:20:PHE:HB3	2:Q:25:LEU:HD11	1.83	0.60
1:G:193:ARG:HA	1:J:67:MET:HG2	1.82	0.60
1:J:130:ILE:HD11	1:J:348:TRP:HH2	1.66	0.60
2:Q:193:LEU:O	2:Q:193:LEU:HD23	2.02	0.60
1:D:152:GLY:HA3	1:D:279:ASN:OD1	2.02	0.60
2:E:108:ALA:HA	2:E:125:ILE:CG2	2.32	0.60
1:G:205:ILE:O	1:G:209:VAL:HG23	2.02	0.60
1:G:261:LEU:CD1	2:H:234:VAL:HG13	2.31	0.60
1:G:410:ILE:HG23	1:G:414:ILE:CD1	2.31	0.60
1:J:223:ASN:OD1	1:J:225:THR:HB	2.01	0.60
1:M:81:GLU:HG3	1:M:85:ARG:HE	1.66	0.60
2:Q:66:TYR:CE1	2:Q:70:PHE:HE2	2.20	0.60
3:R:100:ASN:HB3	3:R:103:ILE:CG1	2.32	0.60
1:A:291:HIS:O	1:A:293:VAL:HG23	2.02	0.60
1:D:223:ASN:OD1	1:D:225:THR:HB	2.01	0.60
1:G:225:THR:HG22	1:G:227:VAL:H	1.66	0.60
1:J:3:GLY:C	1:J:4:ILE:HD12	2.22	0.60
1:M:46:ILE:HD13	1:M:255:ALA:HB1	1.82	0.60
2:N:39:CYS:HB3	2:N:94:LEU:HB3	1.82	0.60
1:P:223:ASN:N	1:P:223:ASN:HD22	2.00	0.60
1:A:223:ASN:HD22	1:A:223:ASN:N	2.00	0.60
1:G:360:ARG:HB3	1:G:415:GLU:OE2	2.02	0.60
2:K:193:LEU:O	2:K:193:LEU:HD23	2.02	0.60
2:N:66:TYR:HE1	2:N:70:PHE:CE2	2.20	0.60
2:Q:160:PHE:CD2	2:Q:183:ILE:HG23	2.36	0.60
1:A:226:GLY:HA2	1:A:355:ARG:HD2	1.83	0.59
1:A:319:ASN:ND2	1:A:324:GLY:HA2	2.17	0.59
3:C:127:GLY:O	3:C:135:SER:HA	2.01	0.59
1:J:346:VAL:HG22	1:J:404:PHE:CD1	2.37	0.59
3:O:71:PRO:HB3	1:P:286:LEU:HD22	1.84	0.59
2:H:9:VAL:O	2:H:14:GLU:OE1	2.19	0.59
1:D:312:VAL:O	1:D:316:GLN:HG3	2.02	0.59
2:E:128:PRO:HD3	2:E:216:MET:CE	2.33	0.59
1:G:312:VAL:HB	1:G:315:VAL:CG2	2.32	0.59
1:J:58:GLN:OE1	1:J:100:GLY:HA3	2.02	0.59
1:M:418:VAL:HG12	1:M:419:ALA:H	1.66	0.59
1:P:130:ILE:HD11	1:P:348:TRP:HH2	1.68	0.59
2:Q:114:MET:HG2	2:Q:114:MET:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:151:PRO:HD2	2:Q:182:TRP:CD1	2.37	0.59
2:Q:207:MET:O	2:Q:211:VAL:HG23	2.02	0.59
1:A:33:ILE:CD1	1:A:249:ILE:HD11	2.26	0.59
2:H:160:PHE:CG	2:H:183:ILE:HG23	2.37	0.59
1:J:425:GLU:HG3	1:J:429:ASN:ND2	2.16	0.59
2:K:129:GLU:O	2:K:132:TYR:HB3	2.02	0.59
1:G:106:ILE:HD12	6:G:504:LOP:H221	1.84	0.59
1:J:23:LEU:HD23	1:J:25:ILE:HD11	1.85	0.59
1:M:362:MET:HB2	1:M:415:GLU:HG3	1.84	0.59
1:G:330:PHE:CE2	1:G:334:LEU:HD11	2.37	0.59
3:I:72:ILE:HG21	3:I:186:LEU:HD13	1.83	0.59
1:M:130:ILE:HD11	1:M:348:TRP:HH2	1.67	0.59
1:P:83:ILE:O	1:P:90:GLY:HA3	2.03	0.59
1:G:130:ILE:HD11	1:G:348:TRP:HH2	1.66	0.59
3:I:82:ILE:O	3:I:86:ARG:HG3	2.02	0.59
1:M:118:TYR:CD1	1:M:224:PRO:HA	2.38	0.59
1:M:223:ASN:H	1:M:223:ASN:ND2	2.01	0.59
2:N:112:GLY:HA3	2:N:117:GLY:HA2	1.84	0.59
1:P:33:ILE:CD1	1:P:249:ILE:HD11	2.23	0.59
1:P:418:VAL:O	1:P:420:PRO:HD3	2.03	0.59
3:R:41:SER:HB2	3:R:43:ASP:OD1	2.02	0.59
1:D:370:LEU:HD22	1:D:403:TYR:CE2	2.37	0.59
1:J:59:ILE:O	1:J:63:ILE:HG13	2.03	0.59
1:M:366:TYR:HD2	1:M:411:LEU:HD11	1.67	0.59
2:N:138:PHE:CD2	2:N:187:PRO:HD3	2.38	0.59
3:F:140:VAL:O	3:F:140:VAL:HG12	2.02	0.59
1:G:223:ASN:OD1	1:G:225:THR:HB	2.03	0.59
1:G:113:PHE:HB3	6:G:504:LOP:H271	1.85	0.58
1:P:423:THR:CG2	1:P:426:GLU:H	2.14	0.58
2:Q:149:HIS:CD2	2:Q:168:THR:HG21	2.38	0.58
2:E:112:GLY:HA2	2:E:119:SER:HB3	1.85	0.58
2:B:160:PHE:CE2	2:B:183:ILE:HG13	2.38	0.58
2:H:39:CYS:HB3	2:H:94:LEU:HB3	1.85	0.58
1:M:117:TYR:HB2	1:M:367:PHE:CE2	2.37	0.58
2:Q:138:PHE:CZ	2:Q:183:ILE:HD13	2.38	0.58
1:A:4:ILE:H	1:A:4:ILE:HD12	1.67	0.58
1:A:205:ILE:O	1:A:209:VAL:HG23	2.03	0.58
1:A:8:HIS:H	1:A:8:HIS:CD2	2.21	0.58
2:B:141:GLU:OE1	2:B:141:GLU:O	2.22	0.58
1:G:121:TYR:CE2	1:G:346:VAL:HG12	2.38	0.58
1:J:350:ASP:CB	1:J:408:LEU:HD12	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:157:ASN:CB	2:N:183:ILE:HD11	2.34	0.58
2:N:193:LEU:O	2:N:193:LEU:HD23	2.03	0.58
3:O:131:HIS:HB3	7:O:200:FES:S2	2.44	0.58
1:P:64:VAL:O	1:P:67:MET:HB2	2.03	0.58
2:B:17:PHE:CE2	2:B:231:PHE:CZ	2.92	0.58
1:J:39:ARG:HD3	1:J:428:PHE:CD2	2.39	0.58
1:P:39:ARG:HD3	1:P:428:PHE:HD2	1.66	0.58
1:P:387:PHE:CE1	1:P:388:PRO:HB3	2.39	0.58
1:A:326:ILE:O	1:A:326:ILE:HG22	2.03	0.58
1:J:187:ASP:CG	1:J:188:ASN:H	2.06	0.58
1:M:223:ASN:N	1:M:223:ASN:HD22	2.02	0.58
2:Q:128:PRO:HG2	2:Q:129:GLU:N	2.18	0.58
1:A:67:MET:HG2	1:D:193:ARG:HA	1.85	0.58
1:D:128:THR:HG21	4:D:501:HEM:HBD1	1.86	0.58
1:G:418:VAL:CG1	1:G:419:ALA:N	2.65	0.58
3:I:19:THR:HG22	3:I:20:ALA:N	2.17	0.58
1:J:105:PHE:HA	1:J:108:VAL:HG12	1.85	0.58
1:J:291:HIS:O	1:J:293:VAL:HG23	2.03	0.58
1:J:407:ILE:O	1:J:411:LEU:HG	2.03	0.58
3:L:19:THR:HG22	3:L:20:ALA:N	2.19	0.58
1:A:91:PHE:CE1	1:A:92:MET:CG	2.87	0.58
2:B:193:LEU:HD23	2:B:193:LEU:O	2.03	0.58
2:H:149:HIS:CE1	2:H:168:THR:HG21	2.38	0.58
3:L:74:ILE:HG12	3:L:124:VAL:HG22	1.84	0.58
1:P:60:VAL:CG2	1:P:61:THR:N	2.67	0.58
1:D:223:ASN:N	1:D:223:ASN:ND2	2.52	0.58
1:D:225:THR:HG22	1:D:227:VAL:HG23	1.86	0.58
1:P:23:LEU:HD23	1:P:25:ILE:HD11	1.85	0.58
1:P:319:ASN:HD21	1:P:324:GLY:HA2	1.68	0.58
2:B:105:LYS:HE3	2:B:220:GLU:HG2	1.85	0.57
2:E:128:PRO:HG2	2:E:129:GLU:H	1.69	0.57
2:H:40:HIS:HE1	2:H:98:PRO:HD2	1.69	0.57
1:A:261:LEU:HD11	2:B:234:VAL:HG13	1.86	0.57
1:D:91:PHE:CE1	1:D:92:MET:CG	2.87	0.57
1:G:215:ALA:HA	1:J:23:LEU:HD13	1.86	0.57
3:C:19:THR:HG22	3:C:20:ALA:N	2.18	0.57
1:D:199:TYR:O	1:D:202:PRO:HD2	2.04	0.57
2:E:160:PHE:CE2	2:E:183:ILE:HG23	2.39	0.57
1:P:147:TYR:HA	4:P:502:HEM:HAA2	1.86	0.57
1:D:153:GLN:HB3	1:D:289:PRO:HG2	1.85	0.57
2:E:66:TYR:HE1	2:E:70:PHE:CE2	2.22	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:117:ASP:OD2	3:F:121:GLU:HB2	2.05	0.57
3:L:78:THR:O	3:L:82:ILE:HG13	2.04	0.57
1:M:239:LYS:HA	1:M:239:LYS:CE	2.27	0.57
2:B:164:SER:O	2:B:182:TRP:HB2	2.05	0.57
1:G:91:PHE:CD2	2:H:222:LYS:HG3	2.40	0.57
1:G:291:HIS:O	1:G:293:VAL:HG23	2.03	0.57
1:M:226:GLY:HA2	1:M:355:ARG:HG2	1.84	0.57
2:N:125:ILE:HD12	2:N:125:ILE:N	2.20	0.57
1:D:125:ARG:NH2	1:D:228:GLU:OE2	2.37	0.57
3:R:84:LEU:O	3:R:88:VAL:HG23	2.04	0.57
1:D:105:PHE:HA	1:D:108:VAL:HG12	1.85	0.57
1:D:245:TRP:HE3	1:D:249:ILE:HD12	1.70	0.57
2:H:66:TYR:HE1	2:H:70:PHE:HE2	1.48	0.57
2:H:66:TYR:CE1	2:H:70:PHE:CE2	2.93	0.57
3:I:163:ARG:O	3:I:164:LYS:HB2	2.05	0.57
2:N:155:TYR:N	2:N:155:TYR:CD1	2.71	0.57
2:Q:138:PHE:CD2	2:Q:187:PRO:HD3	2.40	0.57
2:Q:236:PHE:CE1	3:R:25:VAL:HG12	2.40	0.57
3:R:179:ILE:HD11	3:R:183:THR:HG22	1.86	0.57
1:A:223:ASN:HD22	1:A:223:ASN:H	1.52	0.57
2:K:143:PRO:HG2	2:K:178:THR:CG2	2.34	0.57
1:P:406:VAL:O	1:P:409:PRO:HD2	2.05	0.57
3:F:34:LEU:O	3:F:37:GLN:NE2	2.37	0.57
1:G:128:THR:HG21	4:G:501:HEM:CBD	2.35	0.57
1:A:223:ASN:H	1:A:223:ASN:ND2	2.03	0.57
1:D:291:HIS:O	1:D:293:VAL:HG23	2.05	0.57
2:E:127:GLY:N	2:E:128:PRO:HD2	2.20	0.57
1:J:4:ILE:HD12	1:J:4:ILE:N	2.19	0.57
1:J:8:HIS:CG	1:J:9:TYR:H	2.23	0.57
3:O:19:THR:HG22	3:O:20:ALA:N	2.20	0.57
1:A:8:HIS:CD2	1:A:8:HIS:N	2.73	0.56
2:N:112:GLY:HA3	2:N:117:GLY:CA	2.35	0.56
1:P:223:ASN:H	1:P:223:ASN:HD22	1.52	0.56
1:P:366:TYR:CD2	1:P:411:LEU:HD11	2.40	0.56
1:A:153:GLN:HB3	1:A:289:PRO:HG2	1.87	0.56
1:A:358:ARG:NH2	6:A:504:LOP:H21	2.18	0.56
1:J:360:ARG:NH2	1:J:363:PHE:CD2	2.73	0.56
1:J:387:PHE:HA	1:J:390:ASP:OD1	2.05	0.56
1:M:233:SER:OG	1:M:236:GLU:HG2	2.04	0.56
1:M:361:PRO:HD3	1:M:418:VAL:HG23	1.86	0.56
1:D:418:VAL:HG12	1:D:419:ALA:N	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:43:TRP:O	1:G:46:ILE:HG12	2.04	0.56
2:K:66:TYR:HE1	2:K:70:PHE:CE2	2.23	0.56
2:K:155:TYR:CD1	2:K:155:TYR:N	2.74	0.56
2:N:112:GLY:HA2	2:N:119:SER:HB3	1.87	0.56
2:N:138:PHE:CG	2:N:187:PRO:HB3	2.41	0.56
1:P:291:HIS:CE1	2:Q:2:GLY:HA3	2.40	0.56
2:Q:16:PRO:HG2	2:Q:17:PHE:CD1	2.41	0.56
1:A:281:ILE:HD11	2:B:107:ARG:HH12	1.71	0.56
1:A:330:PHE:CE2	1:A:334:LEU:HD11	2.40	0.56
2:B:17:PHE:CE2	2:B:231:PHE:HZ	2.23	0.56
1:G:187:ASP:CG	1:G:188:ASN:H	2.08	0.56
1:M:39:ARG:HH12	2:N:255:VAL:CG1	2.19	0.56
3:O:21:GLY:O	3:O:25:VAL:HG23	2.04	0.56
3:O:125:MET:SD	3:O:171:LEU:HD12	2.45	0.56
2:Q:154:PHE:C	2:Q:155:TYR:CD1	2.79	0.56
2:H:103:MET:CE	4:H:301:HEM:HAA2	2.36	0.56
2:H:158:ARG:HG2	2:H:158:ARG:HH11	1.69	0.56
1:J:153:GLN:HB3	1:J:289:PRO:HG2	1.88	0.56
1:A:81:GLU:HG3	1:A:85:ARG:HE	1.71	0.56
1:A:215:ALA:HA	1:D:23:LEU:HD13	1.86	0.56
1:J:414:ILE:HG22	1:J:415:GLU:N	2.21	0.56
1:A:418:VAL:CG1	1:A:419:ALA:H	2.19	0.56
1:G:4:ILE:HD12	1:G:4:ILE:N	2.19	0.56
3:L:82:ILE:O	3:L:86:ARG:HG3	2.05	0.56
2:Q:230:GLY:O	2:Q:234:VAL:HG23	2.06	0.56
2:K:39:CYS:HB3	2:K:94:LEU:HB3	1.87	0.56
2:Q:3:GLY:HA2	2:Q:111:HIS:CD2	2.41	0.56
3:C:89:GLN:HB2	3:C:92:GLN:HG3	1.88	0.56
2:E:17:PHE:CE2	2:E:231:PHE:CZ	2.94	0.56
2:E:157:ASN:HB2	2:E:183:ILE:HD11	1.86	0.56
1:G:58:GLN:OE1	1:G:100:GLY:HA3	2.05	0.56
1:G:319:ASN:ND2	1:G:319:ASN:O	2.39	0.56
1:M:153:GLN:HB3	1:M:289:PRO:HG2	1.88	0.56
2:N:125:ILE:HD12	2:N:125:ILE:H	1.71	0.56
1:P:105:PHE:HA	1:P:108:VAL:HG12	1.85	0.56
1:A:406:VAL:O	1:A:409:PRO:HD2	2.06	0.56
2:B:155:TYR:N	2:B:155:TYR:CD1	2.74	0.56
1:D:330:PHE:CE2	1:D:334:LEU:HD11	2.41	0.56
2:H:16:PRO:HG2	2:H:17:PHE:HD1	1.72	0.56
2:K:127:GLY:N	2:K:128:PRO:HD2	2.21	0.56
2:Q:110:PHE:CD1	2:Q:126:GLY:HA3	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:20:PHE:HB3	2:E:25:LEU:HD11	1.88	0.55
3:F:90:LEU:CD1	3:F:108:GLU:HB3	2.36	0.55
2:H:205:HIS:C	2:H:205:HIS:ND1	2.59	0.55
2:K:150:GLU:CG	2:K:182:TRP:HZ3	2.15	0.55
1:M:166:PHE:O	1:M:169:ILE:HD12	2.05	0.55
1:M:205:ILE:O	1:M:209:VAL:HG23	2.06	0.55
1:A:43:TRP:CZ3	1:A:251:LYS:HE3	2.42	0.55
2:E:40:HIS:HE1	2:E:98:PRO:HD2	1.70	0.55
1:J:225:THR:HG22	1:J:227:VAL:H	1.71	0.55
1:M:354:VAL:HG21	1:M:417:PRO:HB3	1.88	0.55
2:Q:155:TYR:CD1	2:Q:155:TYR:N	2.73	0.55
2:H:155:TYR:CD1	2:H:155:TYR:N	2.74	0.55
3:R:127:GLY:O	3:R:135:SER:HA	2.06	0.55
1:A:33:ILE:HD11	1:A:249:ILE:CD1	2.24	0.55
1:G:102:SER:O	1:G:106:ILE:HG13	2.07	0.55
2:H:66:TYR:O	2:H:68:THR:N	2.38	0.55
2:K:161:GLN:NE2	2:K:176:LYS:NZ	2.54	0.55
2:K:205:HIS:ND1	2:K:205:HIS:C	2.59	0.55
1:M:43:TRP:HZ3	1:M:251:LYS:CE	2.19	0.55
2:N:66:TYR:O	2:N:69:GLN:NE2	2.39	0.55
2:B:205:HIS:C	2:B:205:HIS:ND1	2.60	0.55
2:E:238:THR:O	2:E:242:VAL:HG23	2.07	0.55
1:G:63:ILE:CD1	1:J:200:LEU:HD22	2.35	0.55
1:M:346:VAL:HG22	1:M:404:PHE:CD1	2.42	0.55
1:P:223:ASN:ND2	1:P:223:ASN:N	2.54	0.55
2:Q:114:MET:HB3	2:Q:116:THR:HG23	1.89	0.55
1:D:370:LEU:HD22	1:D:403:TYR:CD2	2.42	0.55
2:E:155:TYR:N	2:E:155:TYR:CD1	2.75	0.55
1:G:13:THR:O	1:G:17:LYS:HG3	2.07	0.55
1:G:39:ARG:HD3	1:G:428:PHE:HD2	1.71	0.55
1:A:39:ARG:HH12	2:B:255:VAL:CG1	2.18	0.55
1:D:250:ILE:HG22	2:E:248:ASN:OD1	2.06	0.55
1:G:33:ILE:HG13	1:G:245:TRP:HB2	1.88	0.55
1:M:83:ILE:O	1:M:90:GLY:HA3	2.06	0.55
2:N:207:MET:O	2:N:211:VAL:HG23	2.06	0.55
2:Q:66:TYR:HE1	2:Q:70:PHE:CZ	2.24	0.55
1:A:108:VAL:CG2	4:A:501:HEM:HMC2	2.37	0.55
1:D:153:GLN:OE1	1:D:153:GLN:HA	2.06	0.55
2:K:128:PRO:HD3	2:K:216:MET:CE	2.36	0.55
1:M:53:PHE:CE2	1:M:260:LEU:HD21	2.41	0.55
1:P:81:GLU:HG3	1:P:85:ARG:HE	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:ASP:CG	1:A:188:ASN:H	2.10	0.55
1:G:317:ILE:HG22	1:G:321:ILE:HD11	1.89	0.55
2:H:207:MET:O	2:H:211:VAL:HG23	2.07	0.55
2:N:16:PRO:HG2	2:N:17:PHE:CD1	2.42	0.55
1:P:46:ILE:HD13	1:P:255:ALA:HB1	1.88	0.55
2:B:48:ARG:HH22	3:C:43:ASP:HB3	1.72	0.55
1:G:39:ARG:NH1	2:H:255:VAL:CG1	2.70	0.55
1:G:103:LEU:HD13	6:G:504:LOP:H212	1.88	0.55
2:H:48:ARG:HB3	2:H:85:PRO:O	2.07	0.55
1:J:199:TYR:CG	4:J:502:HEM:HBC1	2.40	0.55
1:J:423:THR:O	1:J:426:GLU:HG2	2.06	0.55
2:K:48:ARG:HB3	2:K:85:PRO:O	2.06	0.55
3:O:72:ILE:HG21	3:O:186:LEU:HD13	1.88	0.55
3:R:34:LEU:O	3:R:37:GLN:NE2	2.40	0.55
1:M:370:LEU:HD22	1:M:403:TYR:CD2	2.42	0.54
2:Q:165:VAL:HG12	2:Q:169:CYS:HB3	1.89	0.54
1:A:360:ARG:HD2	1:A:415:GLU:OE2	2.07	0.54
1:D:418:VAL:O	1:D:420:PRO:HD3	2.06	0.54
1:G:117:TYR:HB2	1:G:367:PHE:CZ	2.42	0.54
1:J:13:THR:O	1:J:17:LYS:HG3	2.07	0.54
1:J:123:ALA:HB2	1:J:126:GLU:CD	2.28	0.54
1:M:13:THR:O	1:M:17:LYS:HG3	2.08	0.54
1:M:112:ILE:HG12	4:M:501:HEM:HAC	1.89	0.54
1:M:239:LYS:HD3	1:M:425:GLU:OE2	2.07	0.54
2:Q:128:PRO:CG	2:Q:129:GLU:H	2.20	0.54
1:A:225:THR:HG22	1:A:227:VAL:H	1.72	0.54
2:E:128:PRO:HD3	2:E:216:MET:HE3	1.89	0.54
3:I:93:LEU:HD12	3:I:109:ALA:HB3	1.89	0.54
3:I:179:ILE:HD11	3:I:183:THR:CG2	2.38	0.54
1:J:53:PHE:CE2	1:J:260:LEU:HD21	2.43	0.54
1:P:60:VAL:HG23	1:P:61:THR:N	2.23	0.54
1:P:205:ILE:O	1:P:209:VAL:HG23	2.08	0.54
3:R:21:GLY:O	3:R:25:VAL:HG23	2.06	0.54
3:C:140:VAL:O	3:C:140:VAL:CG1	2.54	0.54
2:E:190:MET:O	2:E:190:MET:HG3	2.08	0.54
1:M:23:LEU:HD13	1:P:215:ALA:HA	1.90	0.54
1:D:263:PHE:O	1:D:267:VAL:HG23	2.08	0.54
3:F:179:ILE:HD11	3:F:183:THR:CG2	2.38	0.54
1:G:153:GLN:HB3	1:G:289:PRO:HG2	1.88	0.54
1:M:39:ARG:HH12	2:N:255:VAL:HG13	1.71	0.54
2:Q:236:PHE:HE1	3:R:25:VAL:CG1	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:117:TYR:HB2	1:D:367:PHE:CE2	2.42	0.54
3:F:12:ARG:HD3	3:F:16:TYR:HE1	1.72	0.54
1:G:362:MET:CE	1:G:415:GLU:HA	2.37	0.54
1:G:387:PHE:HA	1:G:390:ASP:OD1	2.08	0.54
1:M:358:ARG:NE	6:M:504:LOP:H21	2.23	0.54
1:M:370:LEU:HD22	1:M:403:TYR:CE2	2.42	0.54
3:R:93:LEU:HD23	3:R:163:ARG:HD3	1.90	0.54
1:A:346:VAL:HG22	1:A:404:PHE:CD1	2.43	0.54
3:C:138:GLY:HA2	3:C:147:TRP:CD1	2.43	0.54
2:E:40:HIS:HB3	2:E:100:LEU:HG	1.90	0.54
2:N:250:ARG:HD3	3:O:12:ARG:CZ	2.38	0.54
1:A:200:LEU:HD22	1:D:63:ILE:CD1	2.36	0.54
3:C:12:ARG:HD3	3:C:16:TYR:HE1	1.73	0.54
2:E:17:PHE:CE2	2:E:231:PHE:HZ	2.25	0.54
2:E:207:MET:O	2:E:211:VAL:HG23	2.07	0.54
3:I:59:PRO:HD3	3:I:76:ARG:NH1	2.23	0.54
3:R:19:THR:HG22	3:R:20:ALA:N	2.22	0.54
1:D:287:ARG:HG2	1:D:287:ARG:NH1	2.22	0.54
2:E:205:HIS:C	2:E:205:HIS:ND1	2.62	0.54
3:F:72:ILE:HG21	3:F:186:LEU:HD13	1.90	0.54
3:F:100:ASN:HB3	3:F:103:ILE:HG12	1.90	0.54
1:G:63:ILE:HG21	1:J:200:LEU:HD22	1.90	0.54
2:K:143:PRO:HG2	2:K:178:THR:HG21	1.88	0.54
1:M:223:ASN:H	1:M:223:ASN:HD22	1.56	0.54
2:N:125:ILE:O	2:N:125:ILE:HG22	2.08	0.54
1:P:73:VAL:HG23	1:P:151:TRP:NE1	2.23	0.54
2:B:183:ILE:CG2	2:B:185:MET:H	2.03	0.53
1:D:239:LYS:HA	1:D:239:LYS:CE	2.29	0.53
1:M:91:PHE:HE1	1:M:92:MET:HG2	1.70	0.53
3:O:125:MET:HE2	3:O:147:TRP:CH2	2.43	0.53
1:P:153:GLN:HB3	1:P:289:PRO:HG2	1.89	0.53
2:Q:40:HIS:HB3	2:Q:100:LEU:HG	1.90	0.53
1:G:8:HIS:CG	1:G:9:TYR:H	2.26	0.53
1:G:295:GLU:N	1:G:295:GLU:OE1	2.41	0.53
2:Q:66:TYR:HE1	2:Q:70:PHE:HE2	1.49	0.53
1:A:4:ILE:HD12	1:A:4:ILE:N	2.23	0.53
1:A:9:TYR:CD2	1:A:27:ALA:HA	2.43	0.53
2:B:104:ALA:HB1	2:B:216:MET:HE2	1.89	0.53
2:B:66:TYR:O	2:B:69:GLN:HG2	2.07	0.53
2:E:151:PRO:HD2	2:E:182:TRP:CD1	2.44	0.53
2:H:165:VAL:CG1	2:H:169:CYS:HB2	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:105:LYS:HE3	2:K:220:GLU:CG	2.37	0.53
3:L:72:ILE:HG21	3:L:186:LEU:HD13	1.90	0.53
1:M:39:ARG:HD3	1:M:428:PHE:HD2	1.71	0.53
4:M:501:HEM:HBD2	4:M:501:HEM:HHA	1.90	0.53
2:N:48:ARG:HH22	3:O:43:ASP:HB3	1.73	0.53
1:P:330:PHE:CE2	1:P:334:LEU:HD11	2.42	0.53
2:B:40:HIS:HE1	2:B:98:PRO:HD2	1.72	0.53
1:D:114:ARG:O	1:D:114:ARG:HD2	2.09	0.53
1:M:193:ARG:CA	1:P:67:MET:HG2	2.38	0.53
1:M:223:ASN:ND2	1:M:223:ASN:N	2.56	0.53
1:M:286:LEU:HD22	3:R:71:PRO:HB3	1.90	0.53
2:N:128:PRO:HG2	2:N:129:GLU:H	1.73	0.53
2:N:154:PHE:C	2:N:155:TYR:CD1	2.81	0.53
1:P:122:LYS:CE	1:P:350:ASP:OD2	2.56	0.53
2:B:251:LEU:HD12	2:B:251:LEU:O	2.08	0.53
1:D:428:PHE:CZ	2:E:256:LYS:HB2	2.44	0.53
3:F:37:GLN:O	3:F:37:GLN:HG2	2.09	0.53
1:G:403:TYR:CD1	1:G:403:TYR:C	2.82	0.53
2:K:207:MET:O	2:K:211:VAL:HG23	2.08	0.53
1:A:53:PHE:CE2	1:A:260:LEU:HD21	2.44	0.53
2:B:66:TYR:HE1	2:B:70:PHE:CE2	2.27	0.53
2:E:29:LEU:O	2:E:33:THR:OG1	2.22	0.53
3:F:131:HIS:HB3	7:F:200:FES:S2	2.49	0.53
3:I:16:TYR:O	3:I:17:TYR:HD1	1.90	0.53
2:K:251:LEU:O	2:K:251:LEU:HD12	2.07	0.53
1:M:73:VAL:HG23	1:M:151:TRP:NE1	2.24	0.53
1:M:225:THR:HG22	1:M:227:VAL:H	1.74	0.53
1:M:313:TRP:HA	1:M:316:GLN:HG3	1.89	0.53
2:N:17:PHE:CE2	2:N:231:PHE:HZ	2.25	0.53
1:A:364:LYS:O	1:A:368:TRP:HD1	1.92	0.53
1:D:239:LYS:HD3	1:D:425:GLU:OE2	2.08	0.53
1:G:247:TYR:HB3	2:H:252:TRP:CZ2	2.44	0.53
3:I:72:ILE:HG21	3:I:186:LEU:CD1	2.39	0.53
1:J:91:PHE:CE1	1:J:92:MET:CG	2.92	0.53
1:J:207:ALA:O	1:J:210:ALA:HB3	2.08	0.53
2:K:108:ALA:HA	2:K:125:ILE:HG22	1.91	0.53
1:M:105:PHE:HA	1:M:108:VAL:HG12	1.90	0.53
1:A:225:THR:HG22	1:A:227:VAL:HG23	1.91	0.53
1:D:233:SER:OG	1:D:236:GLU:HG2	2.08	0.53
1:G:326:ILE:O	1:G:326:ILE:HG22	2.09	0.53
2:H:138:PHE:HZ	2:H:183:ILE:HD11	1.69	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:319:ASN:C	1:J:319:ASN:HD22	2.12	0.53
1:M:153:GLN:OE1	1:M:153:GLN:HA	2.08	0.53
1:D:73:VAL:HG23	1:D:151:TRP:NE1	2.24	0.53
1:G:123:ALA:HB2	1:G:126:GLU:CD	2.29	0.53
1:A:117:TYR:HB2	1:A:367:PHE:CE2	2.45	0.52
2:B:207:MET:O	2:B:211:VAL:HG23	2.09	0.52
1:D:73:VAL:HG23	1:D:151:TRP:CE2	2.43	0.52
1:D:225:THR:HG22	1:D:227:VAL:H	1.74	0.52
1:D:361:PRO:HD3	1:D:418:VAL:HG23	1.90	0.52
1:J:418:VAL:CG1	1:J:419:ALA:N	2.72	0.52
3:L:125:MET:SD	3:L:171:LEU:HD12	2.49	0.52
1:M:329:LYS:CE	3:R:131:HIS:O	2.50	0.52
2:N:151:PRO:HD3	2:N:166:PRO:HG3	1.89	0.52
1:A:223:ASN:N	1:A:223:ASN:ND2	2.57	0.52
1:D:81:GLU:HG3	1:D:85:ARG:HE	1.73	0.52
2:E:185:MET:HB2	4:E:301:HEM:C1D	2.44	0.52
1:G:33:ILE:CD1	1:G:249:ILE:HD11	2.21	0.52
2:N:114:MET:HB3	2:N:116:THR:HG23	1.91	0.52
3:R:89:GLN:C	3:R:91:GLY:N	2.58	0.52
3:R:137:ILE:O	3:R:147:TRP:CD1	2.63	0.52
2:B:104:ALA:HB1	2:B:216:MET:CE	2.39	0.52
1:G:207:ALA:O	1:G:210:ALA:HB3	2.09	0.52
1:M:343:MET:O	1:M:346:VAL:HG23	2.09	0.52
2:N:157:ASN:CG	2:N:183:ILE:HD11	2.30	0.52
1:P:343:MET:O	1:P:346:VAL:HG23	2.10	0.52
2:Q:138:PHE:CG	2:Q:187:PRO:HB3	2.44	0.52
2:Q:205:HIS:C	2:Q:205:HIS:ND1	2.63	0.52
1:A:39:ARG:HH12	2:B:255:VAL:HG13	1.74	0.52
1:D:240:ASP:HB3	1:D:424:ILE:HD12	1.91	0.52
2:E:5:HIS:HD2	2:E:158:ARG:HH22	1.58	0.52
2:K:103:MET:HG3	2:K:131:ILE:HD11	1.91	0.52
1:P:33:ILE:HG13	1:P:245:TRP:HB2	1.92	0.52
1:P:91:PHE:CE1	1:P:92:MET:CG	2.91	0.52
3:R:72:ILE:HG21	3:R:186:LEU:HD13	1.91	0.52
3:C:72:ILE:HG21	3:C:186:LEU:HD13	1.90	0.52
2:H:112:GLY:HA3	2:H:117:GLY:H	1.75	0.52
2:K:89:PHE:HB3	2:K:90:PRO:HD2	1.92	0.52
1:M:301:PHE:HB3	1:M:336:MET:HG3	1.92	0.52
1:M:319:ASN:ND2	1:M:319:ASN:O	2.40	0.52
1:D:281:ILE:HD11	2:E:107:ARG:HH12	1.73	0.52
1:G:395:ILE:O	1:G:398:ALA:HB3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:100:ASN:ND2	3:I:173:ILE:HD13	2.25	0.52
1:J:354:VAL:HG21	1:J:417:PRO:HB3	1.90	0.52
1:P:245:TRP:HE3	1:P:249:ILE:HD12	1.75	0.52
2:Q:59:PRO:CG	2:Q:62:GLN:HE21	2.22	0.52
1:A:73:VAL:HG23	1:A:151:TRP:NE1	2.24	0.52
1:G:53:PHE:CE2	1:G:260:LEU:HD21	2.45	0.52
1:J:81:GLU:HG3	1:J:85:ARG:HE	1.74	0.52
1:J:133:MET:CE	4:J:501:HEM:HBC1	2.39	0.52
3:R:62:GLN:NE2	3:R:73:PHE:CD1	2.77	0.52
2:B:48:ARG:HB3	2:B:85:PRO:O	2.09	0.52
3:F:21:GLY:O	3:F:25:VAL:HG23	2.10	0.52
1:J:33:ILE:HG13	1:J:245:TRP:HB2	1.90	0.52
1:M:407:ILE:HG22	1:M:411:LEU:HD12	1.92	0.52
1:P:346:VAL:HG22	1:P:404:PHE:CD1	2.45	0.52
2:Q:189:LEU:CB	2:Q:204:VAL:HG13	2.40	0.52
1:A:199:TYR:O	1:A:202:PRO:HD2	2.09	0.52
1:G:346:VAL:HG22	1:G:404:PHE:HD1	1.75	0.52
2:H:142:PRO:CG	2:H:150:GLU:OE2	2.58	0.52
1:J:229:VAL:HG22	1:J:424:ILE:HD12	1.92	0.52
1:P:117:TYR:HB2	1:P:367:PHE:CZ	2.45	0.52
3:R:100:ASN:HB3	3:R:103:ILE:HG12	1.91	0.52
1:A:153:GLN:OE1	1:A:153:GLN:HA	2.10	0.52
1:D:318:ALA:O	1:D:322:SER:HB3	2.10	0.52
1:G:24:PRO:HB2	1:G:27:ALA:HB3	1.91	0.52
1:G:105:PHE:HA	1:G:108:VAL:HG12	1.90	0.52
1:G:239:LYS:HA	1:G:239:LYS:CE	2.31	0.52
1:J:366:TYR:HD2	1:J:411:LEU:HD11	1.75	0.52
1:M:122:LYS:NZ	1:M:350:ASP:OD2	2.39	0.52
1:M:330:PHE:CE2	1:M:334:LEU:HD11	2.45	0.52
1:A:22:ARG:HH11	1:A:22:ARG:HG3	1.75	0.51
2:B:128:PRO:HD3	2:B:216:MET:CE	2.39	0.51
2:B:140:GLU:CD	2:B:140:GLU:N	2.53	0.51
1:D:13:THR:O	1:D:17:LYS:HG3	2.10	0.51
1:D:205:ILE:O	1:D:209:VAL:HG23	2.10	0.51
2:K:66:TYR:CE1	2:K:70:PHE:CE2	2.98	0.51
3:L:155:HIS:O	3:L:162:ILE:HD12	2.10	0.51
2:N:230:GLY:O	2:N:234:VAL:HG23	2.10	0.51
2:E:138:PHE:CD2	2:E:187:PRO:HB3	2.45	0.51
1:G:8:HIS:CG	1:G:9:TYR:N	2.78	0.51
1:J:13:THR:CG2	1:J:14:GLY:H	2.21	0.51
1:J:364:LYS:O	1:J:368:TRP:HD1	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:89:GLN:C	3:L:91:GLY:N	2.62	0.51
1:M:425:GLU:O	1:M:429:ASN:ND2	2.43	0.51
1:P:53:PHE:CE1	1:P:260:LEU:HD21	2.46	0.51
1:A:73:VAL:HG23	1:A:151:TRP:CE2	2.46	0.51
1:M:261:LEU:HD11	2:N:234:VAL:HG13	1.92	0.51
1:M:319:ASN:HD21	1:M:324:GLY:HA2	1.76	0.51
1:A:118:TYR:CD1	1:A:224:PRO:HA	2.45	0.51
1:D:261:LEU:HD11	2:E:234:VAL:HG13	1.92	0.51
1:M:421:PRO:HB3	1:M:426:GLU:OE2	2.09	0.51
1:P:199:TYR:O	1:P:202:PRO:HD2	2.11	0.51
1:D:41:LEU:HD22	1:D:45:TRP:CD1	2.46	0.51
1:D:118:TYR:CD1	1:D:224:PRO:HA	2.45	0.51
2:N:128:PRO:HD3	2:N:216:MET:CE	2.40	0.51
3:R:77:ARG:NH2	3:R:115:THR:HG21	2.25	0.51
1:D:22:ARG:HH11	1:D:22:ARG:HG3	1.75	0.51
1:G:54:CYS:SG	1:G:103:LEU:HG	2.51	0.51
1:G:244:PHE:CD1	1:G:248:PHE:HB2	2.46	0.51
2:H:138:PHE:CE1	2:H:183:ILE:HD11	2.45	0.51
2:K:11:PHE:HB2	2:K:14:GLU:HG3	1.92	0.51
2:N:114:MET:HG2	2:N:114:MET:O	2.11	0.51
2:N:138:PHE:CE2	2:N:185:MET:O	2.63	0.51
2:E:114:MET:HB3	2:E:116:THR:HG23	1.93	0.51
2:E:134:VAL:O	2:E:138:PHE:HE1	1.94	0.51
1:G:248:PHE:CD1	1:G:251:LYS:HD3	2.45	0.51
3:I:88:VAL:CG1	3:I:93:LEU:HD21	2.41	0.51
1:J:39:ARG:HH12	2:K:255:VAL:HG13	1.75	0.51
2:K:40:HIS:HB3	2:K:100:LEU:HG	1.92	0.51
2:K:40:HIS:CE1	2:K:98:PRO:HD2	2.44	0.51
2:K:66:TYR:CE1	2:K:70:PHE:HE2	2.28	0.51
3:L:179:ILE:HD11	3:L:183:THR:CG2	2.41	0.51
1:M:117:TYR:HB2	1:M:367:PHE:CZ	2.46	0.51
1:M:366:TYR:CD2	1:M:411:LEU:HD11	2.43	0.51
2:N:59:PRO:CG	2:N:62:GLN:HE21	2.24	0.51
1:P:39:ARG:NH1	2:Q:255:VAL:CG1	2.73	0.51
2:E:72:VAL:HG12	2:E:73:THR:N	2.26	0.51
3:F:93:LEU:CD1	3:F:161:ARG:HD2	2.37	0.51
1:G:225:THR:HG22	1:G:227:VAL:HG23	1.92	0.51
1:G:244:PHE:HD1	1:G:248:PHE:HB2	1.76	0.51
3:I:93:LEU:CD1	3:I:109:ALA:HB3	2.41	0.51
1:J:223:ASN:HD22	1:J:223:ASN:N	2.09	0.51
2:N:40:HIS:CE1	2:N:98:PRO:HD2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:133:MET:HE1	4:G:501:HEM:HBC1	1.93	0.51
1:J:64:VAL:O	1:J:67:MET:HB2	2.11	0.51
1:J:348:TRP:O	1:J:349:LEU:HD23	2.11	0.51
1:A:166:PHE:O	1:A:169:ILE:HD12	2.11	0.51
1:A:387:PHE:HA	1:A:390:ASP:OD1	2.11	0.51
2:K:130:TYR:O	2:K:134:VAL:HG23	2.11	0.51
1:M:360:ARG:HA	1:M:415:GLU:OE2	2.11	0.51
2:B:16:PRO:HG2	2:B:17:PHE:CD1	2.45	0.50
2:E:31:VAL:CB	2:E:211:VAL:HG22	2.42	0.50
3:F:19:THR:HG22	3:F:20:ALA:N	2.25	0.50
3:F:115:THR:HG21	3:F:120:GLY:HA2	1.93	0.50
2:H:17:PHE:CE2	2:H:231:PHE:CZ	2.99	0.50
1:J:114:ARG:HD2	1:J:114:ARG:C	2.31	0.50
2:N:242:VAL:O	2:N:246:LEU:HG	2.11	0.50
2:Q:189:LEU:HB2	2:Q:204:VAL:HG13	1.93	0.50
1:A:291:HIS:HE1	2:B:2:GLY:N	2.10	0.50
1:G:136:TYR:HB2	4:G:501:HEM:HMC2	1.94	0.50
1:J:133:MET:HE1	4:J:501:HEM:HBC1	1.93	0.50
2:N:205:HIS:ND1	2:N:205:HIS:C	2.64	0.50
2:B:112:GLY:HA2	2:B:119:SER:HB3	1.92	0.50
1:D:354:VAL:HG21	1:D:417:PRO:HB3	1.92	0.50
1:G:200:LEU:HD22	1:J:63:ILE:CD1	2.41	0.50
1:G:233:SER:OG	1:G:236:GLU:HG2	2.11	0.50
3:I:127:GLY:O	3:I:135:SER:HA	2.11	0.50
2:N:155:TYR:CZ	2:N:186:PRO:HB3	2.45	0.50
1:P:48:GLY:HA3	4:P:501:HEM:O1A	2.12	0.50
1:D:147:TYR:HA	4:D:502:HEM:HAA2	1.92	0.50
2:E:13:PHE:CZ	2:E:216:MET:HG2	2.46	0.50
1:G:113:PHE:CB	6:G:504:LOP:H271	2.41	0.50
1:J:418:VAL:CG1	1:J:419:ALA:H	2.25	0.50
2:N:138:PHE:CB	2:N:187:PRO:HB3	2.42	0.50
2:Q:48:ARG:HB3	2:Q:85:PRO:O	2.12	0.50
3:C:110:THR:O	3:C:113:ASN:N	2.31	0.50
1:D:114:ARG:HD2	1:D:114:ARG:C	2.31	0.50
1:D:229:VAL:HG22	1:D:424:ILE:CD1	2.42	0.50
1:P:114:ARG:HD2	1:P:114:ARG:O	2.11	0.50
2:Q:30:GLN:HG2	2:Q:34:GLU:OE2	2.11	0.50
3:R:125:MET:SD	3:R:171:LEU:HD12	2.52	0.50
1:A:13:THR:O	1:A:17:LYS:HG3	2.12	0.50
1:A:319:ASN:C	1:A:319:ASN:ND2	2.63	0.50
1:D:49:VAL:HG21	1:D:252:ASP:HB3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:133:MET:HE1	4:M:501:HEM:HBC1	1.93	0.50
3:R:90:LEU:HD12	3:R:90:LEU:N	2.07	0.50
1:D:33:ILE:HD11	1:D:249:ILE:CD1	2.32	0.50
1:D:43:TRP:O	1:D:46:ILE:HG12	2.12	0.50
2:E:40:HIS:CE1	2:E:97:ALA:HB1	2.46	0.50
1:G:406:VAL:C	1:G:409:PRO:HD2	2.32	0.50
3:I:93:LEU:HD13	3:I:161:ARG:HD2	1.93	0.50
3:O:127:GLY:O	3:O:135:SER:HA	2.11	0.50
3:R:12:ARG:HD3	3:R:16:TYR:HE1	1.75	0.50
3:R:110:THR:OG1	3:R:113:ASN:HB2	2.12	0.50
1:A:58:GLN:OE1	1:A:100:GLY:HA3	2.12	0.50
1:D:33:ILE:CD1	1:D:249:ILE:HD11	2.32	0.50
2:E:251:LEU:HD12	2:E:251:LEU:O	2.11	0.50
1:G:418:VAL:HG12	1:G:419:ALA:N	2.26	0.50
1:J:322:SER:C	1:J:323:PHE:CD1	2.85	0.50
1:M:190:THR:O	1:M:193:ARG:HG2	2.11	0.50
3:O:90:LEU:HD22	3:O:108:GLU:OE1	2.11	0.50
1:P:153:GLN:OE1	1:P:153:GLN:HA	2.12	0.50
3:C:179:ILE:HD11	3:C:183:THR:CG2	2.42	0.50
2:E:41:GLY:N	2:E:92:SER:HA	2.26	0.50
2:E:48:ARG:HB3	2:E:85:PRO:O	2.11	0.50
2:E:138:PHE:CD2	2:E:187:PRO:HD3	2.47	0.50
2:H:47:ILE:HG21	2:H:67:ALA:HB2	1.94	0.50
1:M:425:GLU:CG	1:M:429:ASN:HD21	2.24	0.50
2:N:112:GLY:HA3	2:N:117:GLY:N	2.27	0.50
1:P:118:TYR:CD1	1:P:224:PRO:HA	2.47	0.50
1:P:406:VAL:C	1:P:409:PRO:HD2	2.33	0.50
2:E:172:ALA:HB1	3:L:90:LEU:HB2	1.93	0.49
2:E:189:LEU:CB	2:E:204:VAL:HG13	2.42	0.49
3:F:110:THR:O	3:F:113:ASN:N	2.37	0.49
2:K:20:PHE:CB	2:K:25:LEU:HD11	2.41	0.49
1:M:128:THR:HG21	4:M:501:HEM:HBD1	1.94	0.49
1:P:114:ARG:HD2	1:P:114:ARG:C	2.32	0.49
2:Q:110:PHE:HD1	2:Q:126:GLY:HA3	1.77	0.49
3:F:110:THR:HB	3:F:112:GLN:HE22	1.75	0.49
3:I:125:MET:SD	3:I:171:LEU:HD12	2.52	0.49
2:K:100:LEU:HD13	2:K:215:LEU:HD11	1.94	0.49
3:L:12:ARG:HB2	3:L:12:ARG:CZ	2.42	0.49
1:M:49:VAL:HG21	1:M:252:ASP:HB3	1.94	0.49
1:A:286:LEU:HD22	3:F:71:PRO:HB3	1.93	0.49
1:D:33:ILE:HG13	1:D:245:TRP:HB2	1.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:249:ILE:O	1:D:253:VAL:HG23	2.12	0.49
1:G:91:PHE:CE1	1:G:92:MET:CG	2.95	0.49
1:J:117:TYR:HB2	1:J:367:PHE:CZ	2.48	0.49
1:M:193:ARG:CB	1:P:67:MET:HG2	2.42	0.49
1:P:43:TRP:O	1:P:46:ILE:HG12	2.13	0.49
1:P:49:VAL:CG1	1:P:256:LEU:HD22	2.42	0.49
1:A:33:ILE:HG13	1:A:245:TRP:HB2	1.94	0.49
1:A:122:LYS:CE	1:A:355:ARG:HA	2.42	0.49
1:J:83:ILE:O	1:J:90:GLY:HA3	2.12	0.49
1:P:49:VAL:HG21	1:P:252:ASP:HB3	1.93	0.49
1:P:64:VAL:HG11	1:P:93:LEU:HD13	1.94	0.49
1:P:322:SER:O	1:P:324:GLY:N	2.46	0.49
3:R:163:ARG:O	3:R:164:LYS:CB	2.58	0.49
3:I:12:ARG:HB2	3:I:12:ARG:CZ	2.41	0.49
3:I:62:GLN:NE2	3:I:73:PHE:CG	2.81	0.49
3:I:137:ILE:HD11	1:J:290:ALA:HA	1.93	0.49
1:J:24:PRO:HB2	1:J:27:ALA:HB3	1.95	0.49
1:J:244:PHE:CD1	1:J:248:PHE:HB2	2.48	0.49
1:M:425:GLU:HG2	1:M:429:ASN:ND2	2.27	0.49
2:Q:143:PRO:HG2	2:Q:178:THR:CG2	2.43	0.49
2:Q:236:PHE:HE1	3:R:25:VAL:HG12	1.77	0.49
3:C:90:LEU:CD1	3:C:108:GLU:HB3	2.42	0.49
2:H:127:GLY:N	2:H:128:PRO:HD2	2.27	0.49
2:H:138:PHE:CZ	2:H:183:ILE:CD1	2.91	0.49
1:J:302:TYR:HE2	1:J:381:GLY:O	1.96	0.49
1:J:428:PHE:CZ	2:K:256:LYS:HB2	2.47	0.49
2:K:66:TYR:O	2:K:68:THR:N	2.45	0.49
3:R:156:TYR:HA	3:R:161:ARG:O	2.12	0.49
2:B:149:HIS:CE1	2:B:167:ASP:H	2.30	0.49
3:C:34:LEU:O	3:C:37:GLN:NE2	2.45	0.49
1:J:190:THR:O	1:J:193:ARG:HG2	2.13	0.49
1:J:244:PHE:HD1	1:J:248:PHE:HB2	1.76	0.49
1:P:43:TRP:CZ3	1:P:251:LYS:HE2	2.47	0.49
2:H:171:ASP:OD2	2:H:175:VAL:HB	2.13	0.49
1:J:128:THR:HG21	4:J:501:HEM:HBD2	1.93	0.49
1:M:13:THR:CG2	1:M:14:GLY:H	2.20	0.49
1:M:133:MET:CE	4:M:501:HEM:HBC1	2.42	0.49
1:P:168:ALA:CB	1:P:333:VAL:HG21	2.42	0.49
3:R:137:ILE:O	3:R:147:TRP:HD1	1.95	0.49
2:B:39:CYS:HB3	2:B:94:LEU:HB3	1.94	0.49
1:D:133:MET:CE	4:D:501:HEM:HBC1	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:237:ALA:O	1:D:241:THR:HG23	2.11	0.49
3:F:58:GLU:HG3	3:F:59:PRO:HD2	1.94	0.49
1:G:223:ASN:HD22	1:G:223:ASN:N	2.10	0.49
1:J:403:TYR:C	1:J:403:TYR:HD1	2.15	0.49
1:M:63:ILE:N	4:M:502:HEM:HBC2	2.27	0.49
1:M:114:ARG:HD2	1:M:114:ARG:C	2.33	0.49
1:M:319:ASN:C	1:M:319:ASN:ND2	2.64	0.49
2:B:13:PHE:CZ	2:B:216:MET:HG2	2.48	0.49
3:F:124:VAL:O	3:F:124:VAL:HG12	2.13	0.49
1:G:222:ASN:ND2	1:G:223:ASN:H	2.11	0.49
1:J:237:ALA:O	1:J:241:THR:HG23	2.13	0.49
2:N:251:LEU:O	2:N:251:LEU:HD12	2.12	0.49
1:P:301:PHE:HB3	1:P:336:MET:HG3	1.94	0.49
2:Q:66:TYR:C	2:Q:68:THR:H	2.15	0.49
2:Q:251:LEU:HD12	2:Q:251:LEU:O	2.13	0.49
1:A:13:THR:CG2	1:A:14:GLY:H	2.17	0.48
1:A:39:ARG:HD3	1:A:428:PHE:CD2	2.48	0.48
1:A:239:LYS:HA	1:A:239:LYS:CE	2.31	0.48
2:B:113:PRO:HG2	2:B:116:THR:OG1	2.13	0.48
2:E:66:TYR:O	2:E:69:GLN:HG2	2.13	0.48
2:E:81:ARG:NH1	2:E:82:GLU:O	2.45	0.48
3:F:110:THR:O	3:F:112:GLN:N	2.46	0.48
2:H:8:ASP:HB2	2:H:110:PHE:HZ	1.78	0.48
3:I:15:LEU:C	3:I:17:TYR:H	2.16	0.48
4:J:502:HEM:O2D	4:J:502:HEM:HHA	2.13	0.48
3:O:12:ARG:HD3	3:O:16:TYR:HE1	1.77	0.48
2:Q:89:PHE:HB3	2:Q:90:PRO:CD	2.40	0.48
2:Q:143:PRO:HG2	2:Q:178:THR:HG22	1.95	0.48
1:A:13:THR:CG2	1:A:14:GLY:N	2.76	0.48
2:B:114:MET:O	2:B:114:MET:HG2	2.13	0.48
2:E:165:VAL:CG1	2:E:169:CYS:HB2	2.43	0.48
1:G:114:ARG:HD2	1:G:114:ARG:C	2.33	0.48
1:G:394:LEU:HD23	1:G:394:LEU:HA	1.66	0.48
1:M:193:ARG:HB2	1:P:67:MET:HG2	1.95	0.48
1:M:225:THR:HG22	1:M:227:VAL:HG23	1.94	0.48
2:N:66:TYR:O	2:N:68:THR:N	2.46	0.48
1:P:225:THR:HG22	1:P:227:VAL:HG23	1.94	0.48
1:P:367:PHE:CD1	1:P:367:PHE:C	2.87	0.48
2:Q:48:ARG:HG2	2:Q:48:ARG:NH1	2.25	0.48
3:R:77:ARG:HD2	3:R:81:ASP:HB3	1.95	0.48
3:F:108:GLU:O	3:F:110:THR:N	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:160:PHE:CE2	2:H:183:ILE:HG23	2.47	0.48
3:I:74:ILE:HD13	3:I:184:ILE:HD12	1.94	0.48
1:M:60:VAL:CG2	1:M:61:THR:N	2.76	0.48
2:N:48:ARG:HB3	2:N:85:PRO:O	2.13	0.48
2:N:138:PHE:CE1	2:N:157:ASN:ND2	2.81	0.48
2:Q:155:TYR:CZ	2:Q:186:PRO:HB3	2.48	0.48
3:F:12:ARG:HB2	3:F:12:ARG:CZ	2.44	0.48
1:G:348:TRP:O	1:G:349:LEU:HD23	2.13	0.48
3:I:155:HIS:O	3:I:162:ILE:HD12	2.13	0.48
1:J:73:VAL:HG23	1:J:151:TRP:CE2	2.47	0.48
1:M:33:ILE:HG13	1:M:245:TRP:HB2	1.94	0.48
2:N:30:GLN:HG2	2:N:34:GLU:OE2	2.13	0.48
2:K:68:THR:HG23	2:K:82:GLU:OE1	2.14	0.48
2:K:161:GLN:NE2	2:K:176:LYS:HZ3	2.11	0.48
2:K:182:TRP:CD1	2:K:182:TRP:N	2.81	0.48
1:A:117:TYR:HB2	1:A:367:PHE:CZ	2.49	0.48
1:D:346:VAL:HG22	1:D:404:PHE:CD1	2.48	0.48
2:E:66:TYR:CE1	2:E:70:PHE:CE2	3.01	0.48
3:F:143:ASP:C	3:F:144:PHE:CD1	2.87	0.48
1:M:114:ARG:HD2	1:M:114:ARG:O	2.14	0.48
2:N:98:PRO:CG	2:N:103:MET:HE1	2.43	0.48
1:P:394:LEU:HD23	1:P:394:LEU:HA	1.65	0.48
3:R:37:GLN:O	3:R:37:GLN:HG2	2.12	0.48
3:R:41:SER:O	3:R:43:ASP:N	2.46	0.48
1:A:75:LEU:HD11	1:D:75:LEU:HD11	1.96	0.48
2:B:40:HIS:HB3	2:B:100:LEU:HG	1.95	0.48
1:D:133:MET:HE1	4:D:501:HEM:HBC1	1.95	0.48
2:E:39:CYS:HB3	2:E:94:LEU:HB3	1.95	0.48
1:P:4:ILE:HD13	1:P:229:VAL:HG11	1.95	0.48
3:R:86:ARG:HG2	3:R:111:ASP:HB3	1.95	0.48
2:E:40:HIS:ND1	2:E:97:ALA:HB1	2.28	0.48
2:K:155:TYR:O	2:K:183:ILE:HD12	2.13	0.48
2:N:156:TYR:HB2	2:N:182:TRP:CE2	2.49	0.48
2:N:160:PHE:CE2	2:N:183:ILE:HG23	2.49	0.48
3:R:155:HIS:O	3:R:162:ILE:HD12	2.13	0.48
1:J:118:TYR:CD1	1:J:224:PRO:HA	2.49	0.48
1:J:290:ALA:HB1	2:K:1:ALA:H1	1.79	0.48
2:N:240:LEU:O	2:N:244:LEU:HB2	2.14	0.48
1:P:370:LEU:HD22	1:P:403:TYR:CD2	2.49	0.48
2:B:27:ARG:HD2	2:B:196:TYR:CE2	2.49	0.48
1:D:13:THR:CG2	1:D:14:GLY:H	2.19	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:31:VAL:HG11	2:E:211:VAL:CG2	2.44	0.48
3:F:72:ILE:HG13	3:F:126:TRP:CE3	2.49	0.48
1:J:326:ILE:HG22	1:J:326:ILE:O	2.12	0.48
3:L:15:LEU:C	3:L:17:TYR:H	2.17	0.48
1:M:249:ILE:O	1:M:253:VAL:HG23	2.14	0.48
2:N:13:PHE:CZ	2:N:216:MET:HG2	2.49	0.48
2:N:94:LEU:CD2	4:N:301:HEM:HAC	2.44	0.48
3:R:125:MET:CE	3:R:147:TRP:CH2	2.96	0.48
3:C:74:ILE:HG12	3:C:124:VAL:HG22	1.95	0.47
1:D:58:GLN:OE1	1:D:100:GLY:HA3	2.14	0.47
1:D:75:LEU:O	1:D:79:SER:HB3	2.14	0.47
2:E:142:PRO:CG	2:E:150:GLU:OE2	2.59	0.47
3:F:162:ILE:HG12	3:F:167:ALA:O	2.13	0.47
1:J:54:CYS:SG	1:J:103:LEU:HG	2.54	0.47
1:J:233:SER:OG	1:J:236:GLU:HG2	2.14	0.47
1:M:75:LEU:O	1:M:79:SER:HB3	2.14	0.47
1:M:245:TRP:HE3	1:M:249:ILE:HD12	1.79	0.47
1:P:153:GLN:HB2	1:P:278:ASP:O	2.14	0.47
3:C:63:LEU:HB3	3:C:74:ILE:HB	1.96	0.47
3:C:71:PRO:HB3	1:D:286:LEU:HD22	1.96	0.47
3:C:126:TRP:NE1	3:C:174:PRO:HB3	2.29	0.47
1:D:360:ARG:HD2	1:D:415:GLU:OE1	2.13	0.47
2:E:192:ASP:HA	2:E:202:ALA:CB	2.44	0.47
1:G:193:ARG:HD3	3:L:38:MET:CE	2.39	0.47
1:J:418:VAL:HG12	1:J:419:ALA:H	1.78	0.47
2:K:114:MET:O	2:K:114:MET:HG2	2.14	0.47
1:M:364:LYS:O	1:M:368:TRP:HD1	1.97	0.47
2:N:31:VAL:CB	2:N:211:VAL:HG22	2.40	0.47
2:N:175:VAL:HG12	2:N:176:LYS:O	2.14	0.47
3:O:34:LEU:O	3:O:37:GLN:NE2	2.47	0.47
3:O:96:THR:CG2	3:O:108:GLU:HG2	2.43	0.47
1:P:249:ILE:O	1:P:253:VAL:HG23	2.15	0.47
2:Q:223:LEU:HD21	2:Q:227:LYS:NZ	2.29	0.47
1:A:245:TRP:HE3	1:A:249:ILE:HD12	1.77	0.47
3:C:21:GLY:O	3:C:25:VAL:HG23	2.14	0.47
1:G:125:ARG:NH2	1:G:228:GLU:OE1	2.47	0.47
2:H:8:ASP:HB2	2:H:110:PHE:CZ	2.48	0.47
2:K:48:ARG:HG2	2:K:48:ARG:NH1	2.30	0.47
2:K:66:TYR:HE1	2:K:70:PHE:HE2	1.62	0.47
1:M:22:ARG:HH11	1:M:22:ARG:HG3	1.78	0.47
1:M:406:VAL:C	1:M:409:PRO:HD2	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:12:ARG:CZ	3:C:12:ARG:HB2	2.45	0.47
2:E:192:ASP:HA	2:E:202:ALA:HB3	1.95	0.47
1:J:117:TYR:HB2	1:J:367:PHE:CE2	2.50	0.47
1:J:136:TYR:HB2	4:J:501:HEM:HMC2	1.96	0.47
2:Q:66:TYR:O	2:Q:68:THR:N	2.48	0.47
3:C:110:THR:O	3:C:111:ASP:C	2.52	0.47
1:D:117:TYR:HB2	1:D:367:PHE:CZ	2.48	0.47
3:F:110:THR:O	3:F:111:ASP:C	2.53	0.47
2:H:113:PRO:HG2	2:H:116:THR:OG1	2.14	0.47
2:K:143:PRO:O	2:K:144:LYS:C	2.53	0.47
1:P:233:SER:OG	1:P:236:GLU:HG2	2.15	0.47
3:R:12:ARG:CZ	3:R:12:ARG:HB2	2.44	0.47
1:D:387:PHE:HA	1:D:390:ASP:OD1	2.14	0.47
1:G:200:LEU:HD22	1:J:63:ILE:HD13	1.95	0.47
1:P:263:PHE:O	1:P:267:VAL:HG23	2.15	0.47
1:P:317:ILE:O	1:P:320:PHE:HB3	2.14	0.47
1:A:8:HIS:H	1:A:8:HIS:HD2	1.61	0.47
1:A:263:PHE:O	1:A:267:VAL:HG23	2.14	0.47
1:A:414:ILE:HG22	1:A:415:GLU:N	2.29	0.47
2:B:72:VAL:HG12	2:B:73:THR:N	2.29	0.47
1:D:24:PRO:HB2	1:D:27:ALA:HB3	1.97	0.47
1:D:64:VAL:O	1:D:67:MET:HB2	2.15	0.47
2:E:21:ASP:HB3	2:E:24:GLN:HG3	1.97	0.47
2:E:240:LEU:O	2:E:244:LEU:HB2	2.15	0.47
2:E:250:ARG:HD3	3:F:12:ARG:HH21	1.75	0.47
1:G:13:THR:CG2	1:G:14:GLY:N	2.77	0.47
1:G:117:TYR:HB2	1:G:367:PHE:CE2	2.49	0.47
1:G:317:ILE:CG2	1:G:321:ILE:HD11	2.44	0.47
3:I:140:VAL:O	3:I:140:VAL:HG12	2.15	0.47
1:J:13:THR:CG2	1:J:14:GLY:N	2.77	0.47
2:K:145:CYS:SG	2:K:146:ALA:N	2.86	0.47
1:M:54:CYS:SG	1:M:103:LEU:HG	2.54	0.47
1:M:67:MET:HG2	1:P:193:ARG:CA	2.43	0.47
1:M:91:PHE:CD1	1:M:92:MET:N	2.83	0.47
1:M:281:ILE:HD11	2:N:106:ALA:HB1	1.95	0.47
2:N:43:LYS:HE3	2:N:44:PHE:CE2	2.50	0.47
2:N:157:ASN:O	2:N:180:GLY:HA3	2.15	0.47
1:P:312:VAL:O	1:P:316:GLN:HG3	2.14	0.47
2:Q:125:ILE:HG22	2:Q:125:ILE:O	2.14	0.47
3:R:74:ILE:HD13	3:R:184:ILE:HD12	1.97	0.47
1:A:49:VAL:HG21	1:A:252:ASP:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:58:GLU:HG3	3:C:59:PRO:HD2	1.97	0.47
1:D:129:TRP:HE3	4:D:501:HEM:HMD1	1.80	0.47
2:H:158:ARG:HH11	2:H:158:ARG:CG	2.27	0.47
1:J:360:ARG:HD2	1:J:415:GLU:OE1	2.15	0.47
3:L:127:GLY:O	3:L:135:SER:HA	2.14	0.47
1:M:418:VAL:O	1:M:420:PRO:HD3	2.14	0.47
1:P:22:ARG:HG3	1:P:22:ARG:HH11	1.80	0.47
1:G:122:LYS:CE	1:G:350:ASP:OD2	2.62	0.47
3:O:131:HIS:O	1:P:329:LYS:HE3	2.14	0.47
1:P:13:THR:CG2	1:P:14:GLY:H	2.21	0.47
1:P:49:VAL:HG12	1:P:256:LEU:HD22	1.96	0.47
1:P:58:GLN:OE1	1:P:100:GLY:HA3	2.13	0.47
2:Q:65:ALA:O	2:Q:68:THR:HB	2.15	0.47
2:Q:127:GLY:N	2:Q:128:PRO:CD	2.78	0.47
2:Q:242:VAL:O	2:Q:246:LEU:HG	2.14	0.47
1:A:193:ARG:HB2	1:D:67:MET:HG2	1.97	0.47
1:D:43:TRP:HZ3	1:D:251:LYS:HG2	1.80	0.47
3:F:163:ARG:HH11	3:F:163:ARG:HG3	1.80	0.47
1:G:118:TYR:CD1	1:G:224:PRO:HA	2.50	0.47
2:H:112:GLY:HA3	2:H:117:GLY:N	2.29	0.47
2:H:240:LEU:O	2:H:244:LEU:HB2	2.15	0.47
1:J:51:LEU:HB3	4:J:501:HEM:HMB1	1.96	0.47
2:Q:106:ALA:O	2:Q:107:ARG:CG	2.56	0.47
2:Q:128:PRO:HD3	2:Q:216:MET:CE	2.44	0.47
1:A:312:VAL:HB	1:A:315:VAL:HG21	1.97	0.46
2:B:40:HIS:CE1	2:B:98:PRO:HD2	2.50	0.46
2:B:108:ALA:HA	2:B:125:ILE:O	2.15	0.46
1:D:406:VAL:C	1:D:409:PRO:HD2	2.35	0.46
1:G:329:LYS:HE3	3:L:131:HIS:O	2.15	0.46
2:H:20:PHE:CB	2:H:25:LEU:HD11	2.43	0.46
1:J:27:ALA:O	1:J:30:TYR:HB3	2.14	0.46
1:J:229:VAL:HG13	1:J:240:ASP:HB2	1.96	0.46
1:J:249:ILE:O	1:J:253:VAL:HG23	2.15	0.46
1:M:43:TRP:O	1:M:46:ILE:HG12	2.15	0.46
2:N:48:ARG:HG2	2:N:48:ARG:NH1	2.26	0.46
2:B:151:PRO:HD3	2:B:166:PRO:HG3	1.98	0.46
1:D:166:PHE:O	1:D:169:ILE:HD12	2.16	0.46
2:H:103:MET:HG3	2:H:131:ILE:HD11	1.97	0.46
2:H:112:GLY:HA3	2:H:117:GLY:CA	2.45	0.46
1:J:351:THR:OG1	1:J:412:GLY:HA3	2.15	0.46
2:Q:128:PRO:CG	2:Q:129:GLU:N	2.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:59:PRO:HD3	3:R:76:ARG:NH1	2.30	0.46
1:D:122:LYS:CE	1:D:350:ASP:OD2	2.59	0.46
1:G:27:ALA:O	1:G:30:TYR:HB3	2.16	0.46
1:G:83:ILE:O	1:G:90:GLY:HA3	2.16	0.46
1:G:209:VAL:HG22	4:G:501:HEM:HBB2	1.96	0.46
2:H:154:PHE:N	2:H:154:PHE:CD1	2.83	0.46
3:I:77:ARG:NH2	3:I:115:THR:HG21	2.31	0.46
1:J:225:THR:HG22	1:J:227:VAL:HG23	1.97	0.46
1:J:358:ARG:HA	1:J:364:LYS:HE2	1.98	0.46
2:K:125:ILE:N	2:K:125:ILE:CD1	2.78	0.46
1:M:64:VAL:O	1:M:67:MET:HB2	2.15	0.46
1:M:84:MET:SD	1:M:91:PHE:HA	2.55	0.46
2:N:66:TYR:CE1	2:N:70:PHE:CE2	3.02	0.46
1:P:128:THR:HG21	4:P:501:HEM:CBD	2.44	0.46
3:R:85:GLY:C	3:R:111:ASP:HB2	2.36	0.46
1:A:193:ARG:CA	1:D:67:MET:HG2	2.44	0.46
1:D:25:ILE:H	1:D:25:ILE:HG13	1.52	0.46
3:L:72:ILE:HG13	3:L:126:TRP:CE3	2.51	0.46
1:M:229:VAL:HG13	1:M:240:ASP:HB2	1.97	0.46
1:M:342:VAL:HG12	1:M:343:MET:N	2.31	0.46
2:N:126:GLY:HA2	2:N:129:GLU:OE1	2.14	0.46
3:O:180:ASP:OD1	3:O:181:GLU:N	2.49	0.46
1:P:420:PRO:O	1:P:421:PRO:C	2.53	0.46
2:E:40:HIS:CE1	2:E:98:PRO:HD2	2.49	0.46
3:F:89:GLN:O	3:F:92:GLN:N	2.37	0.46
1:G:73:VAL:HG23	1:G:151:TRP:CE2	2.51	0.46
1:G:133:MET:CE	4:G:501:HEM:HBC1	2.46	0.46
1:G:299:LEU:HD23	1:G:299:LEU:HA	1.68	0.46
1:G:358:ARG:O	1:G:364:LYS:NZ	2.44	0.46
2:K:220:GLU:HA	2:K:220:GLU:OE1	2.15	0.46
1:M:365:ILE:HD13	1:M:365:ILE:HA	1.78	0.46
1:P:112:ILE:HG12	4:P:501:HEM:HAC	1.97	0.46
1:A:249:ILE:O	1:A:253:VAL:HG23	2.15	0.46
2:E:48:ARG:HG2	2:E:48:ARG:NH1	2.30	0.46
2:H:112:GLY:HA3	2:H:117:GLY:HA2	1.98	0.46
2:K:47:ILE:HG13	2:K:87:ASP:O	2.15	0.46
1:M:9:TYR:CD2	1:M:27:ALA:HA	2.50	0.46
3:O:90:LEU:HG	3:O:90:LEU:O	2.15	0.46
1:A:75:LEU:O	1:A:79:SER:HB3	2.16	0.46
1:D:84:MET:SD	1:D:91:PHE:HA	2.56	0.46
1:D:415:GLU:O	1:D:417:PRO:HD3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:364:LYS:O	1:G:368:TRP:HD1	1.98	0.46
2:H:128:PRO:HD3	2:H:216:MET:HE1	1.97	0.46
1:J:239:LYS:HA	1:J:239:LYS:CE	2.32	0.46
3:L:37:GLN:OE1	3:L:38:MET:HG3	2.16	0.46
1:M:263:PHE:O	1:M:267:VAL:HG23	2.15	0.46
2:N:127:GLY:N	2:N:128:PRO:CD	2.78	0.46
1:P:319:ASN:ND2	1:P:324:GLY:HA2	2.29	0.46
1:P:363:PHE:O	1:P:364:LYS:C	2.53	0.46
2:Q:66:TYR:C	2:Q:66:TYR:CD1	2.89	0.46
1:A:24:PRO:HB2	1:A:27:ALA:HB3	1.97	0.46
1:A:261:LEU:CD1	2:B:234:VAL:HG13	2.46	0.46
1:D:41:LEU:HD22	1:D:45:TRP:CG	2.51	0.46
1:P:225:THR:HG22	1:P:227:VAL:H	1.81	0.46
2:Q:13:PHE:CZ	2:Q:216:MET:HG2	2.51	0.46
2:Q:31:VAL:CB	2:Q:211:VAL:HG22	2.45	0.46
2:Q:59:PRO:HG2	2:Q:62:GLN:HG3	1.97	0.46
1:A:84:MET:SD	1:A:91:PHE:HA	2.55	0.46
3:F:113:ASN:HD22	3:F:113:ASN:HA	1.53	0.46
1:G:193:ARG:HB2	1:J:67:MET:HG2	1.98	0.46
1:G:213:ILE:HA	1:G:216:PHE:CD2	2.51	0.46
1:J:223:ASN:N	1:J:223:ASN:ND2	2.64	0.46
1:M:58:GLN:OE1	1:M:100:GLY:HA3	2.16	0.46
1:P:123:ALA:HB2	1:P:126:GLU:CD	2.36	0.46
3:R:86:ARG:NH2	3:R:112:GLN:OE1	2.49	0.46
1:A:295:GLU:OE1	1:A:295:GLU:N	2.49	0.46
1:D:394:LEU:HA	1:D:394:LEU:HD23	1.71	0.46
2:E:66:TYR:O	2:E:68:THR:N	2.49	0.46
3:F:126:TRP:NE1	3:F:174:PRO:HB3	2.30	0.46
2:H:138:PHE:HZ	2:H:183:ILE:CD1	2.28	0.46
3:I:162:ILE:HD12	3:I:163:ARG:H	1.81	0.46
1:J:169:ILE:O	1:J:173:GLY:HA3	2.16	0.46
1:J:312:VAL:O	1:J:316:GLN:CG	2.62	0.46
1:M:153:GLN:HB2	1:M:278:ASP:O	2.15	0.46
1:M:169:ILE:O	1:M:173:GLY:HA3	2.16	0.46
3:O:58:GLU:HG3	3:O:59:PRO:HD2	1.98	0.46
1:A:67:MET:HG2	1:D:193:ARG:HB2	1.98	0.45
1:D:102:SER:O	1:D:106:ILE:HG13	2.17	0.45
2:E:189:LEU:HB2	2:E:204:VAL:HG13	1.98	0.45
1:J:60:VAL:HG23	1:J:61:THR:N	2.29	0.45
1:J:395:ILE:O	1:J:398:ALA:HB3	2.15	0.45
3:L:89:GLN:O	3:L:91:GLY:N	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:72:VAL:HG12	2:N:73:THR:N	2.30	0.45
3:O:96:THR:HG22	3:O:108:GLU:HG2	1.98	0.45
1:A:237:ALA:O	1:A:241:THR:HG23	2.17	0.45
3:F:32:TRP:CZ2	3:F:36:ASN:HB2	2.52	0.45
1:G:108:VAL:CG2	4:G:501:HEM:HMC3	2.46	0.45
1:G:166:PHE:O	1:G:169:ILE:HD12	2.16	0.45
1:G:248:PHE:HD1	1:G:251:LYS:HD3	1.81	0.45
1:G:365:ILE:HD13	1:G:365:ILE:HA	1.76	0.45
5:G:503:SMA:H30	5:G:503:SMA:H11	1.76	0.45
2:H:251:LEU:HD12	2:H:251:LEU:O	2.16	0.45
1:J:306:ARG:NH2	1:J:383:GLN:O	2.42	0.45
3:L:34:LEU:O	3:L:37:GLN:NE2	2.49	0.45
1:M:358:ARG:HE	6:M:504:LOP:H21	1.80	0.45
1:M:414:ILE:HG22	1:M:415:GLU:H	1.79	0.45
1:P:302:TYR:HE2	1:P:381:GLY:O	1.99	0.45
1:P:395:ILE:O	1:P:398:ALA:HB3	2.16	0.45
2:Q:41:GLY:N	2:Q:92:SER:HA	2.31	0.45
2:Q:215:LEU:HD23	2:Q:215:LEU:HA	1.64	0.45
3:R:131:HIS:HB3	7:R:200:FES:S2	2.56	0.45
3:R:142:GLY:HA2	3:R:155:HIS:ND1	2.32	0.45
1:A:169:ILE:O	1:A:173:GLY:HA3	2.16	0.45
1:D:244:PHE:CD1	1:D:248:PHE:HB2	2.51	0.45
1:G:81:GLU:HG3	1:G:85:ARG:HE	1.80	0.45
3:I:88:VAL:HA	3:I:92:GLN:NE2	2.31	0.45
3:I:89:GLN:H	3:I:92:GLN:HE21	1.64	0.45
2:K:51:SER:OG	2:K:63:VAL:HG21	2.16	0.45
2:K:138:PHE:CD2	2:K:187:PRO:HB3	2.52	0.45
3:L:128:VAL:O	3:L:129:CYS:C	2.55	0.45
1:P:9:TYR:CD2	1:P:27:ALA:HA	2.51	0.45
1:P:348:TRP:O	1:P:349:LEU:HD23	2.16	0.45
3:R:37:GLN:HE21	3:R:37:GLN:HB3	1.62	0.45
1:A:365:ILE:HD13	1:A:365:ILE:HA	1.79	0.45
2:E:190:MET:O	2:E:190:MET:CG	2.64	0.45
3:F:41:SER:HB2	3:F:43:ASP:OD1	2.16	0.45
1:G:286:LEU:HD22	3:L:71:PRO:HB3	1.98	0.45
1:G:362:MET:HE1	1:G:415:GLU:HA	1.97	0.45
1:M:24:PRO:HB2	1:M:27:ALA:HB3	1.97	0.45
3:O:140:VAL:O	3:O:140:VAL:HG12	2.15	0.45
2:Q:141:GLU:OE1	2:Q:141:GLU:N	2.44	0.45
2:H:21:ASP:HB3	2:H:24:GLN:HG3	1.98	0.45
1:J:411:LEU:O	1:J:415:GLU:CG	2.56	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:108:VAL:CG2	4:M:501:HEM:HMC3	2.47	0.45
1:M:199:TYR:O	1:M:202:PRO:HD2	2.17	0.45
2:N:192:ASP:HA	2:N:202:ALA:HB3	1.98	0.45
2:Q:233:ALA:O	2:Q:237:LEU:HD12	2.16	0.45
1:A:133:MET:HE1	4:A:501:HEM:HBC1	1.99	0.45
2:B:147:GLU:OE1	2:B:147:GLU:HA	2.17	0.45
2:B:157:ASN:O	2:B:180:GLY:HA3	2.17	0.45
2:H:14:GLU:OE2	2:H:129:GLU:OE2	2.33	0.45
1:J:223:ASN:ND2	1:J:223:ASN:H	2.14	0.45
2:K:112:GLY:HA3	2:K:117:GLY:HA2	1.98	0.45
3:L:74:ILE:HD13	3:L:184:ILE:HD12	1.98	0.45
1:M:73:VAL:HG23	1:M:151:TRP:CE2	2.51	0.45
2:N:59:PRO:HG2	2:N:62:GLN:HG3	1.97	0.45
2:Q:191:ASP:N	2:Q:204:VAL:HG23	2.32	0.45
1:D:209:VAL:HG22	4:D:501:HEM:HBB2	1.99	0.45
1:D:387:PHE:CD1	1:D:387:PHE:C	2.90	0.45
2:E:30:GLN:HG2	2:E:34:GLU:OE2	2.17	0.45
1:G:49:VAL:HG21	1:G:252:ASP:OD2	2.16	0.45
2:H:113:PRO:HD3	2:H:119:SER:HB2	1.97	0.45
2:K:192:ASP:HA	2:K:202:ALA:HB3	1.99	0.45
2:K:236:PHE:HE1	3:L:25:VAL:HG12	1.82	0.45
3:L:37:GLN:O	3:L:37:GLN:HG2	2.15	0.45
3:L:140:VAL:O	3:L:140:VAL:HG12	2.16	0.45
2:N:66:TYR:C	2:N:68:THR:H	2.20	0.45
2:Q:113:PRO:HD3	2:Q:119:SER:HB2	1.99	0.45
1:D:343:MET:O	1:D:346:VAL:HG23	2.17	0.45
1:D:366:TYR:CD2	1:D:411:LEU:HD11	2.49	0.45
2:E:160:PHE:CD2	2:E:183:ILE:HG23	2.51	0.45
3:F:100:ASN:HA	3:F:173:ILE:HB	1.98	0.45
1:G:44:MET:O	1:G:114:ARG:HG3	2.16	0.45
2:H:48:ARG:HG2	2:H:48:ARG:NH1	2.30	0.45
2:H:187:PRO:HA	2:H:188:PRO:HD2	1.85	0.45
1:J:420:PRO:O	1:J:421:PRO:C	2.53	0.45
1:M:229:VAL:HG22	1:M:424:ILE:HD12	1.98	0.45
1:P:41:LEU:HD12	1:P:248:PHE:CZ	2.52	0.45
1:P:147:TYR:HE2	1:P:154:MET:HB3	1.81	0.45
1:P:342:VAL:HG12	1:P:343:MET:N	2.32	0.45
2:Q:106:ALA:C	2:Q:107:ARG:HG2	2.35	0.45
2:Q:192:ASP:HA	2:Q:202:ALA:HB3	1.99	0.45
3:R:75:ARG:HD3	3:R:77:ARG:HG2	1.99	0.45
1:A:39:ARG:NE	1:A:239:LYS:O	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:LEU:HB2	1:A:409:PRO:HD3	1.98	0.45
2:B:66:TYR:HE1	2:B:70:PHE:CZ	2.35	0.45
3:C:111:ASP:C	3:C:111:ASP:OD1	2.55	0.45
1:D:418:VAL:HG12	1:D:419:ALA:H	1.82	0.45
3:F:63:LEU:HB3	3:F:74:ILE:HB	1.97	0.45
3:F:89:GLN:HG2	3:F:92:GLN:CG	2.43	0.45
1:G:22:ARG:HH11	1:G:22:ARG:HG3	1.82	0.45
1:G:67:MET:HG2	1:J:193:ARG:HA	1.98	0.45
1:J:44:MET:O	1:J:114:ARG:HG3	2.17	0.45
1:J:290:ALA:HB1	2:K:1:ALA:N	2.31	0.45
3:L:63:LEU:HB3	3:L:74:ILE:HB	1.99	0.45
1:P:169:ILE:O	1:P:173:GLY:HA3	2.17	0.45
1:P:407:ILE:O	1:P:411:LEU:HG	2.16	0.45
2:Q:157:ASN:O	2:Q:180:GLY:HA3	2.17	0.45
3:R:72:ILE:HG13	3:R:126:TRP:CE3	2.52	0.45
1:A:343:MET:O	1:A:346:VAL:HG23	2.17	0.45
2:B:27:ARG:HB3	2:B:196:TYR:CZ	2.52	0.45
2:B:31:VAL:CB	2:B:211:VAL:HG22	2.44	0.45
1:G:82:HIS:CD2	1:G:86:ASN:ND2	2.74	0.45
3:I:66:LYS:CG	1:J:286:LEU:HD21	2.42	0.45
2:K:3:GLY:C	2:K:161:GLN:HG2	2.37	0.45
3:L:162:ILE:HD12	3:L:163:ARG:H	1.82	0.45
1:M:41:LEU:HD12	1:M:248:PHE:CZ	2.51	0.45
1:M:60:VAL:HG23	1:M:61:THR:N	2.32	0.45
2:N:31:VAL:HG11	2:N:211:VAL:HG21	1.99	0.45
2:N:149:HIS:CD2	2:N:168:THR:HG21	2.52	0.45
3:O:12:ARG:CZ	3:O:12:ARG:HB2	2.45	0.45
1:A:244:PHE:CD1	1:A:248:PHE:HB2	2.52	0.44
1:D:60:VAL:HG23	1:D:61:THR:N	2.32	0.44
1:D:190:THR:O	1:D:193:ARG:HG2	2.18	0.44
3:F:74:ILE:HG12	3:F:124:VAL:HG22	1.97	0.44
2:H:66:TYR:C	2:H:68:THR:N	2.70	0.44
3:I:180:ASP:C	3:I:180:ASP:OD1	2.55	0.44
1:J:112:ILE:HG12	4:J:501:HEM:HAC	1.99	0.44
1:J:114:ARG:HD2	1:J:114:ARG:O	2.16	0.44
3:O:37:GLN:O	3:O:37:GLN:HG2	2.17	0.44
1:P:156:PHE:HB2	1:P:283:ALA:HB1	1.99	0.44
1:A:83:ILE:O	1:A:90:GLY:HA3	2.17	0.44
1:A:133:MET:HG2	1:A:344:ALA:CB	2.48	0.44
1:A:410:ILE:N	1:A:410:ILE:CD1	2.80	0.44
1:D:169:ILE:O	1:D:173:GLY:HA3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:372:ALA:O	1:D:376:ILE:HG13	2.17	0.44
5:D:503:SMA:H11	5:D:503:SMA:H30	1.69	0.44
2:H:20:PHE:HB3	2:H:25:LEU:CD1	2.46	0.44
2:H:40:HIS:CE1	2:H:98:PRO:HD2	2.50	0.44
3:I:54:VAL:HG22	3:I:182:THR:O	2.17	0.44
1:J:49:VAL:HG21	1:J:252:ASP:OD2	2.17	0.44
1:J:166:PHE:O	1:J:169:ILE:HD12	2.17	0.44
1:M:360:ARG:NH2	1:M:363:PHE:CD2	2.85	0.44
2:N:94:LEU:HD23	4:N:301:HEM:HAC	1.99	0.44
1:P:261:LEU:HD11	2:Q:234:VAL:HG13	1.99	0.44
1:P:418:VAL:CG1	1:P:419:ALA:N	2.80	0.44
2:B:66:TYR:O	2:B:68:THR:N	2.50	0.44
2:B:154:PHE:C	2:B:155:TYR:CD1	2.91	0.44
3:F:155:HIS:CD2	3:F:164:LYS:HD3	2.52	0.44
3:I:180:ASP:OD1	3:I:181:GLU:N	2.51	0.44
2:N:48:ARG:NH2	3:O:43:ASP:HB3	2.32	0.44
2:Q:112:GLY:HA3	2:Q:117:GLY:HA2	2.00	0.44
1:A:229:VAL:HG13	1:A:240:ASP:HB2	2.00	0.44
1:A:321:ILE:HG13	1:A:322:SER:N	2.32	0.44
1:A:415:GLU:O	1:A:417:PRO:HD3	2.17	0.44
2:B:150:GLU:O	2:B:151:PRO:C	2.56	0.44
2:B:240:LEU:O	2:B:244:LEU:HB2	2.17	0.44
2:E:157:ASN:O	2:E:180:GLY:HA3	2.18	0.44
3:F:156:TYR:HA	3:F:161:ARG:O	2.17	0.44
1:G:33:ILE:HD12	1:G:33:ILE:HA	1.74	0.44
1:J:301:PHE:HB3	1:J:336:MET:HG3	1.99	0.44
3:O:40:PRO:O	3:O:41:SER:O	2.35	0.44
3:O:74:ILE:HD13	3:O:184:ILE:HD12	1.99	0.44
1:P:137:LEU:HD12	1:P:137:LEU:HA	1.90	0.44
1:P:199:TYR:CE2	4:P:502:HEM:HBC1	2.51	0.44
1:A:190:THR:O	1:A:193:ARG:HG2	2.17	0.44
2:E:66:TYR:HE1	2:E:70:PHE:CZ	2.35	0.44
1:G:193:ARG:CA	1:J:67:MET:HG2	2.46	0.44
2:H:27:ARG:HB3	2:H:196:TYR:CZ	2.52	0.44
1:J:46:ILE:HD13	1:J:255:ALA:HB1	2.00	0.44
1:M:91:PHE:CD1	1:M:91:PHE:C	2.91	0.44
1:P:310:ALA:HA	1:P:328:ALA:HB2	2.00	0.44
1:A:244:PHE:HD1	1:A:248:PHE:HB2	1.83	0.44
2:B:48:ARG:HG2	2:B:48:ARG:NH1	2.30	0.44
1:D:261:LEU:CD1	2:E:234:VAL:HG13	2.46	0.44
3:F:163:ARG:HG3	3:F:163:ARG:NH1	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:105:PHE:O	1:G:108:VAL:HG12	2.17	0.44
1:G:121:TYR:HB2	1:G:347:PRO:HG3	1.99	0.44
1:J:3:GLY:N	1:J:4:ILE:HD12	2.32	0.44
2:K:154:PHE:C	2:K:155:TYR:CD1	2.90	0.44
1:M:33:ILE:HD12	1:M:33:ILE:HA	1.86	0.44
1:M:420:PRO:O	1:M:421:PRO:C	2.55	0.44
3:O:126:TRP:NE1	3:O:174:PRO:HB3	2.32	0.44
2:Q:193:LEU:O	2:Q:193:LEU:CD2	2.65	0.44
1:A:108:VAL:O	1:A:112:ILE:HG13	2.18	0.44
1:A:394:LEU:HA	1:A:394:LEU:HD23	1.71	0.44
2:E:236:PHE:HE1	3:F:25:VAL:HG12	1.82	0.44
1:G:193:ARG:CB	1:J:67:MET:HG2	2.48	0.44
1:G:428:PHE:CZ	2:H:256:LYS:HB2	2.53	0.44
1:M:39:ARG:HG3	1:M:240:ASP:O	2.18	0.44
1:M:410:ILE:CG2	1:M:414:ILE:HD12	2.46	0.44
2:N:112:GLY:HA3	2:N:117:GLY:H	1.82	0.44
3:O:156:TYR:CD2	3:O:171:LEU:HG	2.53	0.44
3:O:180:ASP:OD1	3:O:180:ASP:C	2.56	0.44
1:P:239:LYS:HD3	1:P:425:GLU:OE2	2.17	0.44
2:Q:138:PHE:CD2	2:Q:187:PRO:HB3	2.52	0.44
2:B:112:GLY:HA3	2:B:117:GLY:HA2	1.98	0.44
2:B:128:PRO:HG2	2:B:129:GLU:H	1.83	0.44
1:J:299:LEU:HA	1:J:299:LEU:HD23	1.70	0.44
2:K:114:MET:HB3	2:K:116:THR:HG23	1.99	0.44
2:K:240:LEU:O	2:K:244:LEU:HB2	2.17	0.44
2:K:250:ARG:HD3	3:L:12:ARG:HH21	1.75	0.44
1:M:123:ALA:HB2	1:M:126:GLU:CD	2.38	0.44
2:N:233:ALA:O	2:N:237:LEU:HD12	2.17	0.44
3:O:90:LEU:CD2	3:O:108:GLU:OE1	2.65	0.44
2:B:112:GLY:HA3	2:B:117:GLY:CA	2.48	0.44
2:E:191:ASP:N	2:E:204:VAL:HG23	2.33	0.44
2:E:236:PHE:CE1	3:F:25:VAL:HG12	2.53	0.44
1:J:39:ARG:HH12	2:K:255:VAL:CG1	2.31	0.44
2:N:105:LYS:HE3	2:N:220:GLU:CG	2.44	0.44
2:N:160:PHE:HB2	2:N:183:ILE:HD11	2.00	0.44
3:O:59:PRO:HD3	3:O:76:ARG:NH1	2.33	0.44
1:P:209:VAL:HG22	4:P:501:HEM:HBB2	1.99	0.44
2:Q:40:HIS:CE1	2:Q:97:ALA:HB1	2.53	0.44
3:R:32:TRP:HB3	3:R:33:PRO:CD	2.48	0.44
3:R:131:HIS:CD2	3:R:132:LEU:HG	2.52	0.44
1:A:59:ILE:HA	4:A:502:HEM:HMC2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:219:ALA:C	2:E:221:PRO:HD3	2.37	0.43
3:F:137:ILE:HD13	3:F:150:PRO:HD3	1.99	0.43
2:K:112:GLY:HA3	2:K:117:GLY:H	1.82	0.43
3:L:93:LEU:HD13	3:L:161:ARG:HD2	1.99	0.43
5:M:503:SMA:H30	5:M:503:SMA:H11	1.77	0.43
2:N:189:LEU:CB	2:N:204:VAL:HG13	2.48	0.43
1:P:75:LEU:O	1:P:79:SER:HB3	2.18	0.43
2:Q:149:HIS:HB3	2:Q:166:PRO:HB3	1.99	0.43
1:A:9:TYR:HB2	1:A:30:TYR:CG	2.53	0.43
1:A:63:ILE:CD1	1:D:200:LEU:HD22	2.47	0.43
3:C:152:HIS:HB2	7:C:200:FES:S1	2.58	0.43
1:D:244:PHE:HD1	1:D:248:PHE:HB2	1.83	0.43
1:D:276:HIS:CE1	1:D:278:ASP:HB2	2.54	0.43
2:E:128:PRO:HG2	2:E:129:GLU:N	2.33	0.43
1:J:295:GLU:OE1	1:J:295:GLU:N	2.51	0.43
2:K:164:SER:O	2:K:182:TRP:CD1	2.71	0.43
1:M:418:VAL:CG1	1:M:419:ALA:H	2.30	0.43
1:P:103:LEU:HB2	6:P:504:LOP:H222	2.00	0.43
2:Q:205:HIS:ND1	2:Q:206:ALA:N	2.65	0.43
1:D:199:TYR:CZ	4:D:502:HEM:HBC1	2.53	0.43
1:J:22:ARG:HH11	1:J:22:ARG:HG3	1.84	0.43
1:J:60:VAL:CG2	1:J:61:THR:N	2.80	0.43
2:K:59:PRO:HG2	2:K:62:GLN:HG3	2.00	0.43
3:L:180:ASP:C	3:L:180:ASP:OD1	2.56	0.43
2:N:66:TYR:HE1	2:N:70:PHE:CZ	2.37	0.43
1:P:346:VAL:HG22	1:P:404:PHE:CE1	2.53	0.43
1:P:370:LEU:HD22	1:P:403:TYR:CE2	2.54	0.43
3:R:180:ASP:OD1	3:R:181:GLU:N	2.52	0.43
1:A:23:LEU:HD13	1:D:215:ALA:HA	1.99	0.43
2:B:192:ASP:HA	2:B:202:ALA:HB3	1.98	0.43
2:B:238:THR:O	2:B:242:VAL:HG23	2.17	0.43
1:D:60:VAL:CG2	1:D:61:THR:N	2.81	0.43
1:G:64:VAL:O	1:G:67:MET:HB2	2.18	0.43
1:G:91:PHE:HE1	1:G:92:MET:HG2	1.79	0.43
1:G:223:ASN:N	1:G:223:ASN:ND2	2.65	0.43
1:G:223:ASN:H	1:G:223:ASN:ND2	2.16	0.43
2:H:100:LEU:HD13	2:H:215:LEU:HD11	1.99	0.43
2:H:192:ASP:HA	2:H:202:ALA:HB3	2.00	0.43
1:M:49:VAL:CG1	1:M:256:LEU:HD22	2.48	0.43
2:N:41:GLY:N	2:N:92:SER:HA	2.34	0.43
3:O:38:MET:HE3	1:P:193:ARG:HD3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:118:GLU:CD	3:O:118:GLU:N	2.70	0.43
1:A:64:VAL:O	1:A:67:MET:HB2	2.18	0.43
2:E:130:TYR:O	2:E:134:VAL:HG23	2.18	0.43
3:F:116:LEU:HD23	3:F:116:LEU:HA	1.81	0.43
3:I:63:LEU:HB3	3:I:74:ILE:HB	2.00	0.43
3:I:115:THR:OG1	3:I:120:GLY:HA2	2.18	0.43
1:J:110:LEU:HA	1:J:110:LEU:HD23	1.78	0.43
3:L:84:LEU:N	3:L:84:LEU:HD12	2.34	0.43
1:M:209:VAL:HG22	4:M:501:HEM:HBB2	1.99	0.43
3:C:90:LEU:HD11	3:C:108:GLU:HB3	2.01	0.43
3:C:90:LEU:HB2	2:H:172:ALA:HB1	2.00	0.43
1:D:418:VAL:CG1	1:D:419:ALA:N	2.81	0.43
2:E:138:PHE:CE1	2:E:157:ASN:ND2	2.87	0.43
3:F:115:THR:HG21	3:F:120:GLY:CA	2.48	0.43
1:G:25:ILE:H	1:G:25:ILE:HG13	1.47	0.43
3:I:124:VAL:O	3:I:173:ILE:HG23	2.19	0.43
3:L:62:GLN:NE2	3:L:73:PHE:CG	2.86	0.43
3:L:125:MET:HE2	3:L:147:TRP:CH2	2.54	0.43
1:M:64:VAL:HG11	1:M:93:LEU:HD13	1.99	0.43
1:M:132:GLY:C	4:M:501:HEM:HBC2	2.39	0.43
1:M:230:ARG:HD2	1:M:236:GLU:OE1	2.18	0.43
1:M:418:VAL:CG1	1:M:419:ALA:N	2.81	0.43
1:A:60:VAL:CG2	1:A:61:THR:N	2.81	0.43
1:A:60:VAL:HG23	1:A:61:THR:N	2.33	0.43
2:B:114:MET:HB3	2:B:116:THR:HG23	2.00	0.43
2:H:66:TYR:C	2:H:68:THR:H	2.21	0.43
3:I:73:PHE:CE1	3:I:127:GLY:HA3	2.53	0.43
1:J:51:LEU:HD13	4:J:501:HEM:C3B	2.54	0.43
2:K:112:GLY:HA3	2:K:117:GLY:CA	2.49	0.43
1:M:49:VAL:HG12	1:M:256:LEU:HD22	2.00	0.43
1:M:407:ILE:HG22	1:M:411:LEU:CD1	2.49	0.43
2:N:128:PRO:HG2	2:N:129:GLU:N	2.34	0.43
1:P:190:THR:O	1:P:193:ARG:HG2	2.19	0.43
2:Q:240:LEU:O	2:Q:244:LEU:HB2	2.18	0.43
1:A:91:PHE:HE1	1:A:92:MET:HG2	1.80	0.43
1:A:287:ARG:HE	1:A:287:ARG:HB3	1.25	0.43
2:B:220:GLU:OE1	2:B:220:GLU:HA	2.18	0.43
1:D:299:LEU:HD23	1:D:299:LEU:HA	1.79	0.43
1:D:422:ALA:O	1:D:423:THR:HG23	2.19	0.43
1:G:315:VAL:O	1:G:318:ALA:HB3	2.18	0.43
2:H:113:PRO:C	2:H:115:GLY:H	2.22	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:100:ASN:HD22	3:I:173:ILE:HD13	1.82	0.43
1:J:46:ILE:CD1	1:J:255:ALA:HB1	2.49	0.43
2:K:144:LYS:O	2:K:147:GLU:HB2	2.19	0.43
1:M:126:GLU:OE1	1:P:22:ARG:NE	2.43	0.43
2:N:66:TYR:C	2:N:68:THR:N	2.72	0.43
1:P:54:CYS:SG	1:P:103:LEU:HG	2.59	0.43
3:R:62:GLN:NE2	3:R:73:PHE:CG	2.87	0.43
1:D:133:MET:HG2	1:D:344:ALA:CB	2.48	0.43
2:E:113:PRO:C	2:E:115:GLY:H	2.21	0.43
2:E:147:GLU:OE1	2:E:147:GLU:HA	2.19	0.43
3:F:115:THR:CB	3:F:120:GLY:HA2	2.49	0.43
1:G:190:THR:O	1:G:193:ARG:HG2	2.19	0.43
2:H:142:PRO:HG3	2:H:150:GLU:OE2	2.18	0.43
1:J:84:MET:SD	1:J:91:PHE:HA	2.59	0.43
1:J:223:ASN:HD22	1:J:223:ASN:H	1.67	0.43
2:N:192:ASP:HA	2:N:202:ALA:CB	2.48	0.43
2:Q:66:TYR:C	2:Q:68:THR:N	2.72	0.43
1:D:187:ASP:CG	1:D:188:ASN:N	2.69	0.43
1:D:229:VAL:HG13	1:D:240:ASP:HB2	2.01	0.43
2:E:250:ARG:HD3	3:F:12:ARG:CZ	2.48	0.43
3:F:132:LEU:N	7:F:200:FES:S2	2.86	0.43
1:G:13:THR:CG2	1:G:14:GLY:H	2.21	0.43
2:H:20:PHE:CG	2:H:25:LEU:HD11	2.54	0.43
3:I:84:LEU:HD12	3:I:84:LEU:N	2.34	0.43
1:M:108:VAL:O	1:M:112:ILE:HG13	2.19	0.43
1:M:225:THR:CG2	1:M:227:VAL:HB	2.49	0.43
1:M:233:SER:C	1:M:235:ALA:N	2.72	0.43
1:P:136:TYR:O	1:P:140:MET:HG3	2.19	0.43
2:Q:40:HIS:ND1	2:Q:97:ALA:HB1	2.34	0.43
3:R:128:VAL:O	3:R:129:CYS:C	2.57	0.43
1:A:43:TRP:O	1:A:46:ILE:HG12	2.19	0.42
1:A:91:PHE:CD1	1:A:92:MET:N	2.87	0.42
1:D:116:LEU:HA	1:D:121:TYR:HE2	1.84	0.42
3:F:144:PHE:CD1	3:F:144:PHE:N	2.87	0.42
1:G:420:PRO:O	1:G:421:PRO:C	2.57	0.42
2:H:17:PHE:CE2	2:H:231:PHE:HZ	2.36	0.42
3:I:89:GLN:O	3:I:91:GLY:N	2.51	0.42
1:J:319:ASN:ND2	1:J:324:GLY:HA2	2.34	0.42
3:L:21:GLY:O	3:L:25:VAL:HG23	2.19	0.42
3:L:85:GLY:HA3	3:L:111:ASP:OD2	2.19	0.42
2:N:22:GLN:HE21	2:N:22:GLN:HB2	1.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:406:VAL:O	1:P:410:ILE:HD13	2.19	0.42
2:B:59:PRO:CG	2:B:62:GLN:HE21	2.32	0.42
1:D:43:TRP:HZ3	1:D:251:LYS:CG	2.32	0.42
1:D:225:THR:HG22	1:D:227:VAL:CG2	2.49	0.42
1:D:229:VAL:HG22	1:D:424:ILE:HD12	2.01	0.42
2:E:59:PRO:CG	2:E:62:GLN:HE21	2.32	0.42
2:E:66:TYR:CE1	2:E:70:PHE:HE2	2.36	0.42
3:F:72:ILE:O	3:F:72:ILE:HG22	2.19	0.42
3:F:89:GLN:NE2	3:F:89:GLN:H	2.17	0.42
1:G:43:TRP:CZ3	1:G:251:LYS:HG2	2.50	0.42
1:J:394:LEU:HD23	1:J:394:LEU:HA	1.70	0.42
1:J:414:ILE:O	1:J:415:GLU:O	2.37	0.42
2:K:242:VAL:O	2:K:245:TYR:HB3	2.19	0.42
1:P:43:TRP:CE3	1:P:43:TRP:HA	2.55	0.42
1:P:410:ILE:CG2	1:P:414:ILE:HD12	2.49	0.42
1:P:418:VAL:CG1	1:P:419:ALA:H	2.30	0.42
1:A:114:ARG:HD2	1:A:114:ARG:C	2.39	0.42
2:B:155:TYR:CZ	2:B:186:PRO:HB3	2.54	0.42
2:E:215:LEU:HD23	2:E:215:LEU:HA	1.85	0.42
1:G:229:VAL:HG13	1:G:240:ASP:HB2	2.00	0.42
2:K:242:VAL:O	2:K:246:LEU:HG	2.19	0.42
3:L:37:GLN:HE21	3:L:37:GLN:HB3	1.60	0.42
1:M:216:PHE:CD1	1:M:216:PHE:C	2.93	0.42
2:Q:14:GLU:OE2	2:Q:129:GLU:OE1	2.36	0.42
1:A:314:VAL:HG23	1:A:315:VAL:N	2.34	0.42
1:G:114:ARG:HD2	1:G:114:ARG:O	2.20	0.42
1:G:280:TYR:CE1	2:H:105:LYS:HE3	2.54	0.42
2:H:155:TYR:O	2:H:182:TRP:HA	2.19	0.42
3:I:89:GLN:O	3:I:92:GLN:N	2.47	0.42
2:K:215:LEU:HD23	2:K:215:LEU:HA	1.82	0.42
1:M:358:ARG:HA	1:M:364:LYS:HE2	2.02	0.42
1:M:374:PHE:CD2	6:M:504:LOP:H321	2.55	0.42
4:M:501:HEM:HHA	4:M:501:HEM:HBA1	2.01	0.42
2:N:238:THR:O	2:N:242:VAL:HG23	2.19	0.42
3:O:103:ILE:CG2	3:O:104:ASP:N	2.79	0.42
3:O:132:LEU:HD23	3:O:132:LEU:HA	1.86	0.42
1:P:25:ILE:H	1:P:25:ILE:HG13	1.53	0.42
1:P:125:ARG:NH2	1:P:228:GLU:OE1	2.53	0.42
1:P:389:TYR:HA	1:P:392:ILE:HD12	2.02	0.42
2:Q:40:HIS:HE1	2:Q:98:PRO:HD2	1.84	0.42
1:A:123:ALA:HB2	1:A:126:GLU:CD	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:ARG:HH11	3:F:38:MET:HE2	1.84	0.42
2:B:43:LYS:HE3	2:B:44:PHE:CZ	2.54	0.42
3:C:139:GLY:O	3:C:140:VAL:C	2.57	0.42
1:G:203:PHE:CE2	1:J:203:PHE:CD2	3.08	0.42
1:G:418:VAL:HG13	1:G:419:ALA:H	1.84	0.42
2:H:40:HIS:HB3	2:H:100:LEU:HG	2.02	0.42
1:J:199:TYR:HA	4:J:502:HEM:CBC	2.49	0.42
1:J:374:PHE:HD2	6:J:504:LOP:H321	1.84	0.42
2:K:192:ASP:HA	2:K:202:ALA:CB	2.50	0.42
2:N:66:TYR:C	2:N:66:TYR:CD1	2.93	0.42
3:C:180:ASP:OD1	3:C:180:ASP:C	2.57	0.42
1:D:77:PHE:CD2	1:D:282:GLU:HG2	2.54	0.42
1:D:88:ASN:HB2	3:F:37:GLN:HA	2.02	0.42
1:D:110:LEU:HA	1:D:110:LEU:HD23	1.82	0.42
1:D:387:PHE:CD1	1:D:388:PRO:N	2.88	0.42
3:F:179:ILE:HD11	3:F:183:THR:HG22	2.01	0.42
3:I:75:ARG:HD3	3:I:77:ARG:HG2	2.00	0.42
1:J:209:VAL:HG22	4:J:501:HEM:HBB2	2.00	0.42
2:N:154:PHE:N	2:N:154:PHE:CD1	2.87	0.42
2:N:236:PHE:CE1	3:O:25:VAL:HG12	2.55	0.42
2:Q:36:CYS:O	2:Q:38:ALA:N	2.52	0.42
1:A:114:ARG:HD2	1:A:114:ARG:O	2.20	0.42
2:B:112:GLY:HA3	2:B:117:GLY:N	2.35	0.42
1:D:182:GLY:HA3	1:D:193:ARG:NH2	2.34	0.42
3:F:32:TRP:CE2	3:F:36:ASN:HB2	2.54	0.42
1:G:302:TYR:HE2	1:G:381:GLY:O	2.01	0.42
2:H:39:CYS:HB3	2:H:94:LEU:CB	2.50	0.42
2:H:183:ILE:HB	2:H:185:MET:H	1.85	0.42
3:I:156:TYR:HA	3:I:161:ARG:O	2.19	0.42
1:J:153:GLN:HA	1:J:153:GLN:OE1	2.20	0.42
2:K:22:GLN:HE21	2:K:22:GLN:HB2	1.61	0.42
1:M:133:MET:HG2	1:M:344:ALA:CB	2.50	0.42
1:M:226:GLY:CA	1:M:355:ARG:HG2	2.50	0.42
3:R:85:GLY:O	3:R:111:ASP:HB2	2.19	0.42
1:A:91:PHE:CD1	1:A:91:PHE:C	2.93	0.42
1:A:193:ARG:CB	1:D:67:MET:HG2	2.49	0.42
2:B:138:PHE:CB	2:B:187:PRO:HB3	2.50	0.42
2:B:192:ASP:HA	2:B:202:ALA:CB	2.49	0.42
1:G:126:GLU:OE1	1:J:22:ARG:NE	2.48	0.42
1:G:249:ILE:O	1:G:253:VAL:HG23	2.20	0.42
1:J:245:TRP:HE3	1:J:249:ILE:HD12	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:21:ASP:HB3	2:K:24:GLN:HG3	2.02	0.42
2:K:66:TYR:C	2:K:68:THR:N	2.73	0.42
2:K:112:GLY:HA3	2:K:117:GLY:N	2.35	0.42
2:N:66:TYR:CE1	2:N:70:PHE:HE2	2.38	0.42
2:Q:103:MET:C	2:Q:105:LYS:H	2.23	0.42
1:D:136:TYR:HB2	4:D:501:HEM:HMC2	2.01	0.42
2:E:192:ASP:OD1	2:E:202:ALA:HB3	2.20	0.42
2:H:220:GLU:HA	2:H:220:GLU:OE1	2.20	0.42
1:J:213:ILE:HA	1:J:216:PHE:CD2	2.54	0.42
2:N:31:VAL:HG11	2:N:211:VAL:CG2	2.49	0.42
1:P:133:MET:CE	4:P:501:HEM:HBC1	2.50	0.42
1:P:233:SER:C	1:P:235:ALA:N	2.73	0.42
2:Q:39:CYS:HB3	2:Q:94:LEU:CB	2.46	0.42
2:Q:59:PRO:HG3	2:Q:62:GLN:HE21	1.84	0.42
3:R:41:SER:C	3:R:43:ASP:H	2.23	0.42
1:A:122:LYS:HE2	1:A:355:ARG:HA	2.01	0.42
1:A:299:LEU:HD23	1:A:299:LEU:HA	1.77	0.42
2:B:66:TYR:CE1	2:B:70:PHE:CE2	3.07	0.42
2:B:112:GLY:HA3	2:B:117:GLY:H	1.85	0.42
2:B:236:PHE:HE1	3:C:25:VAL:HG12	1.85	0.42
3:C:72:ILE:HG21	3:C:186:LEU:CD1	2.50	0.42
3:C:124:VAL:O	3:C:124:VAL:HG12	2.19	0.42
3:C:128:VAL:O	3:C:129:CYS:C	2.58	0.42
3:C:131:HIS:HB3	7:C:200:FES:S2	2.60	0.42
1:D:53:PHE:CE2	1:D:260:LEU:HD21	2.55	0.42
1:D:250:ILE:HG21	2:E:248:ASN:HA	2.01	0.42
2:E:16:PRO:HG2	2:E:17:PHE:CD1	2.55	0.42
1:G:36:PRO:HB2	1:G:241:THR:HG21	2.02	0.42
1:G:203:PHE:CD2	1:J:203:PHE:CD2	3.07	0.42
1:G:229:VAL:HG22	1:G:424:ILE:CD1	2.50	0.42
3:I:103:ILE:HD11	3:I:113:ASN:O	2.20	0.42
2:K:108:ALA:HA	2:K:125:ILE:CG2	2.49	0.42
3:O:72:ILE:HG21	3:O:186:LEU:CD1	2.50	0.42
1:P:110:LEU:HA	1:P:110:LEU:HD23	1.79	0.42
1:P:361:PRO:HD3	1:P:418:VAL:HG23	2.02	0.42
1:P:401:PHE:HB3	1:P:405:LEU:HD12	2.02	0.42
3:R:70:LYS:HE3	3:R:70:LYS:HB2	1.87	0.42
3:C:72:ILE:HG13	3:C:126:TRP:CE3	2.55	0.41
1:D:354:VAL:HB	1:D:360:ARG:HD3	2.01	0.41
2:H:193:LEU:O	2:H:193:LEU:CD2	2.68	0.41
2:H:211:VAL:O	2:H:215:LEU:HG	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:143:PRO:C	2:K:145:CYS:N	2.73	0.41
3:L:163:ARG:HG3	3:L:163:ARG:NH1	2.34	0.41
3:O:125:MET:CE	3:O:147:TRP:CH2	3.03	0.41
2:Q:27:ARG:HD2	2:Q:196:TYR:CE2	2.54	0.41
1:A:67:MET:HG2	1:D:193:ARG:CA	2.49	0.41
2:B:48:ARG:NH2	3:C:43:ASP:HB3	2.34	0.41
2:B:113:PRO:C	2:B:115:GLY:H	2.22	0.41
2:B:243:LEU:HB3	3:C:19:THR:OG1	2.20	0.41
3:C:15:LEU:C	3:C:17:TYR:H	2.23	0.41
3:C:126:TRP:C	3:C:128:VAL:H	2.23	0.41
1:D:317:ILE:O	1:D:320:PHE:HB3	2.20	0.41
2:E:66:TYR:CD1	2:E:66:TYR:C	2.94	0.41
1:J:222:ASN:ND2	1:J:223:ASN:H	2.18	0.41
1:J:346:VAL:HG22	1:J:404:PHE:HD1	1.81	0.41
1:M:346:VAL:HG22	1:M:404:PHE:CE1	2.55	0.41
3:O:138:GLY:CA	3:O:147:TRP:CD1	3.03	0.41
1:P:108:VAL:O	1:P:112:ILE:HG13	2.20	0.41
1:P:360:ARG:NH2	1:P:363:PHE:CD2	2.88	0.41
2:Q:60:GLU:O	2:Q:64:ARG:HB2	2.20	0.41
1:D:121:TYR:HB2	1:D:347:PRO:HG3	2.03	0.41
1:D:121:TYR:CE1	1:D:346:VAL:HG12	2.55	0.41
1:D:214:TRP:CD1	1:D:214:TRP:O	2.74	0.41
2:E:31:VAL:HG11	2:E:211:VAL:HG21	2.02	0.41
2:E:143:PRO:HG2	2:E:178:THR:CG2	2.49	0.41
2:H:142:PRO:HG2	2:H:150:GLU:OE2	2.19	0.41
1:J:296:TRP:CD2	1:J:297:TYR:N	2.89	0.41
2:Q:59:PRO:CG	2:Q:62:GLN:NE2	2.83	0.41
1:D:103:LEU:HD13	6:D:504:LOP:H202	2.01	0.41
1:G:35:ILE:O	1:G:35:ILE:CG2	2.68	0.41
3:I:37:GLN:HE21	3:I:37:GLN:HB3	1.52	0.41
3:I:90:LEU:CD1	3:I:90:LEU:H	2.33	0.41
1:J:33:ILE:HD12	1:J:33:ILE:HA	1.79	0.41
1:M:40:ASN:OD1	1:M:424:ILE:CG2	2.69	0.41
1:M:367:PHE:CD1	1:M:367:PHE:C	2.93	0.41
1:P:379:TRP:NE1	2:Q:114:MET:HE2	2.34	0.41
2:Q:43:LYS:HG2	2:Q:99:ASP:OD1	2.20	0.41
2:Q:203:SER:C	2:Q:205:HIS:N	2.74	0.41
1:A:33:ILE:HD12	1:A:33:ILE:HA	1.80	0.41
1:D:225:THR:CG2	1:D:227:VAL:HG23	2.50	0.41
1:D:296:TRP:CD2	1:D:297:TYR:N	2.88	0.41
1:J:187:ASP:CG	1:J:188:ASN:N	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:133:MET:N	4:M:501:HEM:HBC2	2.35	0.41
1:M:201:LEU:HD23	1:M:201:LEU:HA	1.91	0.41
1:M:296:TRP:CD2	1:M:297:TYR:N	2.89	0.41
3:O:163:ARG:O	3:O:164:LYS:HB2	2.21	0.41
2:Q:138:PHE:CE2	2:Q:187:PRO:HD3	2.55	0.41
2:Q:250:ARG:HD3	3:R:12:ARG:CZ	2.51	0.41
3:R:58:GLU:HG3	3:R:59:PRO:HD2	2.02	0.41
3:R:73:PHE:CZ	3:R:127:GLY:HA3	2.56	0.41
1:A:11:PRO:HB2	1:A:17:LYS:HG2	2.03	0.41
2:B:250:ARG:HH11	3:C:12:ARG:HH21	1.68	0.41
2:E:154:PHE:C	2:E:155:TYR:CD1	2.94	0.41
5:J:503:SMA:H36	5:J:503:SMA:H15	1.86	0.41
2:K:9:VAL:HG13	2:K:10:PRO:HD2	2.01	0.41
2:K:138:PHE:CD2	2:K:187:PRO:HD3	2.54	0.41
1:M:322:SER:C	1:M:323:PHE:CD1	2.94	0.41
2:Q:42:MET:O	2:Q:44:PHE:N	2.54	0.41
1:A:64:VAL:HG11	1:A:93:LEU:HD13	2.02	0.41
1:A:302:TYR:HE2	1:A:381:GLY:O	2.04	0.41
1:A:372:ALA:O	1:A:376:ILE:HG13	2.21	0.41
1:A:374:PHE:CE2	6:A:504:LOP:H341	2.56	0.41
3:C:37:GLN:HE21	3:C:37:GLN:HB3	1.55	0.41
2:E:13:PHE:CE1	2:E:216:MET:HG2	2.56	0.41
3:F:77:ARG:HD2	3:F:81:ASP:HB3	2.02	0.41
2:H:154:PHE:HB3	2:H:182:TRP:HB3	2.03	0.41
2:H:186:PRO:O	2:H:187:PRO:C	2.58	0.41
3:I:78:THR:O	3:I:82:ILE:HG13	2.21	0.41
1:J:105:PHE:O	1:J:108:VAL:HG12	2.21	0.41
2:K:128:PRO:HD3	2:K:216:MET:HE3	2.03	0.41
2:K:147:GLU:OE1	2:K:147:GLU:HA	2.21	0.41
3:L:89:GLN:C	3:L:91:GLY:H	2.23	0.41
3:L:94:VAL:HG23	3:L:162:ILE:O	2.20	0.41
2:N:9:VAL:HG13	2:N:10:PRO:HD2	2.03	0.41
2:N:65:ALA:O	2:N:68:THR:HB	2.20	0.41
3:O:76:ARG:HA	3:O:121:GLU:O	2.20	0.41
1:P:73:VAL:HG23	1:P:151:TRP:CE2	2.55	0.41
1:A:122:LYS:O	1:A:123:ALA:C	2.59	0.41
1:A:133:MET:HG2	1:A:344:ALA:HB2	2.03	0.41
1:A:316:GLN:O	1:A:317:ILE:C	2.59	0.41
3:C:132:LEU:HD23	3:C:132:LEU:HA	1.80	0.41
1:G:169:ILE:HA	1:G:170:PRO:HD3	1.91	0.41
2:H:27:ARG:HD2	2:H:196:TYR:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:51:SER:OG	2:H:63:VAL:HG21	2.20	0.41
2:K:113:PRO:HG2	2:K:116:THR:OG1	2.21	0.41
3:L:72:ILE:HG21	3:L:186:LEU:CD1	2.49	0.41
1:M:67:MET:HG2	1:P:193:ARG:CB	2.50	0.41
1:M:136:TYR:HB2	4:M:501:HEM:HMC2	2.03	0.41
1:M:302:TYR:HE2	1:M:381:GLY:O	2.03	0.41
1:M:310:ALA:HA	1:M:328:ALA:HB2	2.01	0.41
1:P:239:LYS:HA	1:P:239:LYS:CE	2.29	0.41
2:B:130:TYR:O	2:B:134:VAL:HG23	2.21	0.41
3:C:37:GLN:OE1	3:C:38:MET:HG3	2.21	0.41
3:C:38:MET:CE	1:D:193:ARG:HD3	2.45	0.41
3:C:138:GLY:CA	3:C:147:TRP:CD1	3.04	0.41
3:C:163:ARG:NH1	3:C:163:ARG:HG3	2.36	0.41
3:F:137:ILE:CD1	3:F:150:PRO:HD3	2.51	0.41
1:G:113:PHE:HB3	6:G:504:LOP:C27	2.49	0.41
1:G:369:LEU:O	1:G:373:ASP:N	2.48	0.41
1:G:418:VAL:CG1	1:G:419:ALA:H	2.33	0.41
2:H:242:VAL:O	2:H:245:TYR:HB3	2.21	0.41
3:I:32:TRP:CZ2	3:I:36:ASN:HB2	2.55	0.41
3:I:97:ASN:HD22	3:I:99:ARG:HD3	1.85	0.41
1:J:42:ASN:C	1:J:44:MET:H	2.24	0.41
2:K:107:ARG:HH21	4:K:301:HEM:CGA	2.33	0.41
2:K:143:PRO:HG2	2:K:178:THR:HG22	2.02	0.41
2:K:157:ASN:O	2:K:180:GLY:HA3	2.21	0.41
1:M:4:ILE:HB	1:M:36:PRO:HG2	2.03	0.41
1:M:67:MET:HG2	1:P:193:ARG:HB2	2.02	0.41
2:N:29:LEU:HD22	2:N:50:LEU:HD22	2.03	0.41
2:N:130:TYR:O	2:N:134:VAL:HG23	2.21	0.41
1:P:27:ALA:O	1:P:30:TYR:HB3	2.21	0.41
1:P:169:ILE:HA	1:P:170:PRO:HD3	1.86	0.41
1:P:322:SER:C	1:P:324:GLY:N	2.74	0.41
2:Q:186:PRO:O	2:Q:187:PRO:C	2.59	0.41
2:Q:192:ASP:HA	2:Q:202:ALA:CB	2.50	0.41
1:A:133:MET:CE	4:A:501:HEM:HBC1	2.51	0.41
2:B:42:MET:O	2:B:44:PHE:N	2.54	0.41
2:B:154:PHE:CD1	2:B:154:PHE:N	2.87	0.41
2:B:189:LEU:CB	2:B:204:VAL:HG13	2.51	0.41
2:B:250:ARG:HD3	3:C:12:ARG:CZ	2.51	0.41
1:G:20:HIS:O	1:G:20:HIS:ND1	2.54	0.41
2:H:27:ARG:HD2	2:H:196:TYR:CD2	2.56	0.41
2:H:158:ARG:CG	2:H:158:ARG:NH1	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:49:SER:OG	3:I:50:ILE:N	2.54	0.41
3:I:90:LEU:CD1	3:I:90:LEU:N	2.84	0.41
1:J:4:ILE:HG13	1:J:231:ARG:CD	2.51	0.41
1:J:73:VAL:HG23	1:J:151:TRP:NE1	2.35	0.41
1:J:201:LEU:HD23	1:J:201:LEU:HA	1.79	0.41
1:J:422:ALA:N	1:J:426:GLU:OE2	2.52	0.41
1:M:82:HIS:CD2	1:M:86:ASN:ND2	2.82	0.41
1:M:312:VAL:O	1:M:316:GLN:HG2	2.21	0.41
3:O:32:TRP:HB3	3:O:33:PRO:CD	2.51	0.41
1:P:24:PRO:HB2	1:P:27:ALA:HB3	2.03	0.41
1:P:342:VAL:HG13	1:P:404:PHE:CG	2.56	0.41
3:R:126:TRP:C	3:R:128:VAL:H	2.22	0.41
3:R:180:ASP:OD1	3:R:180:ASP:C	2.59	0.41
2:B:127:GLY:N	2:B:128:PRO:CD	2.81	0.40
2:E:25:LEU:CD2	2:E:214:PHE:HA	2.51	0.40
2:E:66:TYR:C	2:E:68:THR:N	2.75	0.40
2:E:193:LEU:O	2:E:193:LEU:CD2	2.68	0.40
1:G:37:THR:OG1	1:G:248:PHE:CD2	2.74	0.40
1:G:346:VAL:CG2	1:G:404:PHE:CE1	3.03	0.40
1:G:414:ILE:HG22	1:G:415:GLU:H	1.82	0.40
1:G:423:THR:HG23	1:G:426:GLU:CB	2.51	0.40
2:K:66:TYR:C	2:K:68:THR:H	2.24	0.40
1:M:41:LEU:HD22	1:M:45:TRP:CD1	2.56	0.40
1:M:136:TYR:O	1:M:140:MET:HG3	2.22	0.40
1:M:394:LEU:HA	1:M:394:LEU:HD23	1.69	0.40
1:M:401:PHE:HB3	1:M:405:LEU:HD12	2.04	0.40
3:O:134:CYS:HB2	3:O:149:CYS:SG	2.61	0.40
2:Q:88:HIS:O	2:Q:89:PHE:C	2.59	0.40
2:Q:183:ILE:HG22	4:Q:301:HEM:O2D	2.21	0.40
2:B:242:VAL:O	2:B:245:TYR:HB3	2.21	0.40
3:C:103:ILE:H	3:C:103:ILE:HG13	1.59	0.40
1:D:123:ALA:HB2	1:D:126:GLU:CD	2.41	0.40
2:E:106:ALA:O	2:E:107:ARG:HD3	2.21	0.40
2:E:145:CYS:SG	2:E:146:ALA:N	2.91	0.40
2:H:25:LEU:HD23	2:H:25:LEU:HA	1.87	0.40
3:I:37:GLN:OE1	3:I:38:MET:HG3	2.21	0.40
3:I:144:PHE:CD1	3:I:144:PHE:N	2.89	0.40
1:J:199:TYR:CG	4:J:502:HEM:CBC	3.04	0.40
2:K:16:PRO:HG2	2:K:17:PHE:HD1	1.81	0.40
2:K:81:ARG:NH1	2:K:82:GLU:O	2.54	0.40
2:K:151:PRO:HD3	2:K:166:PRO:HG3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:244:PHE:HD1	1:M:248:PHE:HB2	1.87	0.40
2:N:236:PHE:HE1	3:O:25:VAL:CG1	2.34	0.40
1:P:415:GLU:O	1:P:417:PRO:HD3	2.21	0.40
2:Q:231:PHE:O	2:Q:235:MET:HG2	2.21	0.40
3:R:132:LEU:HA	3:R:132:LEU:HD23	1.86	0.40
1:A:301:PHE:HB3	1:A:336:MET:HG3	2.02	0.40
2:B:236:PHE:CE1	3:C:25:VAL:HG12	2.57	0.40
1:D:258:VAL:O	1:D:261:LEU:HB3	2.21	0.40
2:E:111:HIS:O	2:E:112:GLY:O	2.39	0.40
3:I:114:ARG:NH1	3:I:173:ILE:CD1	2.84	0.40
1:J:9:TYR:CD2	1:J:20:HIS:HD2	2.39	0.40
1:J:403:TYR:O	1:J:408:LEU:HD23	2.21	0.40
2:K:6:VAL:CG1	2:K:129:GLU:HB3	2.51	0.40
2:K:59:PRO:CG	2:K:62:GLN:HE21	2.33	0.40
1:M:342:VAL:HG13	1:M:404:PHE:CG	2.56	0.40
2:N:203:SER:C	2:N:205:HIS:N	2.75	0.40
2:Q:112:GLY:HA3	2:Q:117:GLY:CA	2.51	0.40
2:Q:143:PRO:O	2:Q:144:LYS:C	2.60	0.40
1:A:314:VAL:O	1:A:315:VAL:C	2.59	0.40
1:A:329:LYS:CE	3:F:131:HIS:O	2.64	0.40
3:C:93:LEU:HD13	3:C:109:ALA:HB3	2.04	0.40
1:D:64:VAL:HG11	1:D:93:LEU:HD13	2.03	0.40
1:D:407:ILE:O	1:D:411:LEU:HG	2.22	0.40
1:G:117:TYR:CD1	1:G:117:TYR:C	2.95	0.40
1:G:225:THR:CG2	1:G:227:VAL:HG23	2.52	0.40
2:H:114:MET:HB3	2:H:116:THR:HG23	2.03	0.40
3:I:128:VAL:O	3:I:129:CYS:C	2.59	0.40
1:J:25:ILE:H	1:J:25:ILE:HG13	1.48	0.40
1:J:75:LEU:O	1:J:79:SER:HB3	2.21	0.40
1:J:91:PHE:HE1	1:J:92:MET:HG2	1.78	0.40
1:J:322:SER:C	1:J:323:PHE:HD1	2.25	0.40
2:K:17:PHE:CE2	2:K:231:PHE:CZ	3.10	0.40
3:L:180:ASP:OD1	3:L:181:GLU:N	2.54	0.40
2:N:113:PRO:HD3	2:N:119:SER:HB2	2.04	0.40
2:N:156:TYR:HB2	2:N:182:TRP:CZ2	2.56	0.40
1:P:180:LEU:O	1:P:193:ARG:HD2	2.22	0.40
1:A:43:TRP:CE3	1:A:251:LYS:HE3	2.55	0.40
2:B:20:PHE:CB	2:B:25:LEU:HD11	2.50	0.40
1:D:27:ALA:O	1:D:30:TYR:HB3	2.22	0.40
2:H:13:PHE:CZ	2:H:216:MET:HG2	2.56	0.40
3:I:66:LYS:HB2	1:J:286:LEU:HD11	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:83:ILE:O	1:J:83:ILE:HG22	2.20	0.40
2:K:20:PHE:HB3	2:K:25:LEU:CD1	2.44	0.40
2:N:108:ALA:HA	2:N:125:ILE:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	426/445 (96%)	392 (92%)	28 (7%)	6 (1%)	11	46
1	D	426/445 (96%)	385 (90%)	37 (9%)	4 (1%)	17	56
1	G	426/445 (96%)	384 (90%)	34 (8%)	8 (2%)	8	39
1	J	426/445 (96%)	379 (89%)	37 (9%)	10 (2%)	6	34
1	M	426/445 (96%)	380 (89%)	38 (9%)	8 (2%)	8	39
1	P	426/445 (96%)	380 (89%)	39 (9%)	7 (2%)	9	43
2	B	254/269 (94%)	224 (88%)	23 (9%)	7 (3%)	5	29
2	E	254/269 (94%)	218 (86%)	28 (11%)	8 (3%)	4	26
2	H	254/269 (94%)	220 (87%)	29 (11%)	5 (2%)	7	38
2	K	254/269 (94%)	225 (89%)	21 (8%)	8 (3%)	4	26
2	N	254/269 (94%)	219 (86%)	26 (10%)	9 (4%)	3	24
2	Q	254/269 (94%)	215 (85%)	30 (12%)	9 (4%)	3	24
3	C	177/187 (95%)	153 (86%)	20 (11%)	4 (2%)	6	34
3	F	177/187 (95%)	153 (86%)	18 (10%)	6 (3%)	3	24
3	I	177/187 (95%)	151 (85%)	19 (11%)	7 (4%)	3	21
3	L	177/187 (95%)	151 (85%)	21 (12%)	5 (3%)	5	29
3	O	177/187 (95%)	154 (87%)	19 (11%)	4 (2%)	6	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	R	177/187 (95%)	149 (84%)	21 (12%)	7 (4%)	3	21
All	All	5142/5406 (95%)	4532 (88%)	488 (10%)	122 (2%)	6	34

All (122) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	415	GLU
2	B	43	LYS
3	C	109	ALA
1	D	414	ILE
1	D	415	GLU
2	E	43	LYS
3	F	109	ALA
1	G	414	ILE
1	G	415	GLU
1	J	43	TRP
1	J	414	ILE
1	J	415	GLU
1	M	415	GLU
2	N	43	LYS
3	O	41	SER
3	O	109	ALA
1	P	415	GLU
2	Q	43	LYS
3	R	140	VAL
1	A	414	ILE
2	B	112	GLY
2	B	113	PRO
2	E	112	GLY
2	E	113	PRO
3	F	111	ASP
3	F	140	VAL
2	H	112	GLY
2	H	113	PRO
3	I	57	VAL
3	I	90	LEU
3	I	109	ALA
2	K	43	LYS
2	K	112	GLY
2	K	113	PRO
3	L	107	ALA
3	L	164	LYS

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Mol	Chain	Res	Type
1	M	414	ILE
2	N	2	GLY
2	N	113	PRO
2	N	126	GLY
1	P	323	PHE
2	Q	37	ALA
2	Q	112	GLY
2	Q	113	PRO
2	Q	255	VAL
3	R	42	ALA
3	R	90	LEU
3	R	164	LYS
2	B	255	VAL
3	C	158	SER
2	E	67	ALA
2	E	95	GLU
3	F	158	SER
2	H	67	ALA
2	H	255	VAL
3	I	42	ALA
3	I	164	LYS
2	K	67	ALA
2	K	255	VAL
3	L	57	VAL
3	L	109	ALA
1	M	43	TRP
1	M	173	GLY
1	M	355	ARG
2	N	255	VAL
1	P	173	GLY
2	Q	2	GLY
2	Q	67	ALA
2	Q	191	ASP
3	R	107	ALA
3	R	109	ALA
1	A	43	TRP
1	A	173	GLY
1	A	355	ARG
2	B	67	ALA
2	B	95	GLU
3	C	111	ASP
2	E	191	ASP

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Mol	Chain	Res	Type
2	E	255	VAL
3	F	107	ALA
1	G	417	PRO
2	H	95	GLU
1	J	173	GLY
2	K	95	GLU
2	K	145	CYS
2	K	146	ALA
2	N	37	ALA
2	N	67	ALA
1	P	414	ILE
3	R	158	SER
1	A	123	ALA
2	B	144	LYS
1	D	173	GLY
1	G	73	VAL
1	G	173	GLY
1	J	73	VAL
1	J	123	ALA
2	N	95	GLU
1	P	125	ARG
2	Q	95	GLU
2	E	2	GLY
1	J	11	PRO
3	L	140	VAL
2	N	112	GLY
1	P	421	PRO
3	C	57	VAL
3	F	57	VAL
1	G	325	ILE
3	I	140	VAL
1	J	421	PRO
1	M	123	ALA
3	O	140	VAL
1	D	73	VAL
1	J	5	PRO
1	G	38	PRO
1	G	123	ALA
1	M	321	ILE
3	O	57	VAL
3	I	168	PRO
1	J	321	ILE

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Mol	Chain	Res	Type
1	M	421	PRO
1	P	123	ALA

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	353/366 (96%)	332 (94%)	21 (6%)	19	54
1	D	353/366 (96%)	331 (94%)	22 (6%)	18	53
1	G	353/366 (96%)	332 (94%)	21 (6%)	19	54
1	J	353/366 (96%)	329 (93%)	24 (7%)	16	49
1	M	353/366 (96%)	330 (94%)	23 (6%)	17	51
1	P	353/366 (96%)	330 (94%)	23 (6%)	17	51
2	B	203/215 (94%)	191 (94%)	12 (6%)	19	54
2	E	203/215 (94%)	187 (92%)	16 (8%)	12	43
2	H	203/215 (94%)	192 (95%)	11 (5%)	22	58
2	K	203/215 (94%)	190 (94%)	13 (6%)	17	52
2	N	203/215 (94%)	189 (93%)	14 (7%)	15	49
2	Q	203/215 (94%)	190 (94%)	13 (6%)	17	52
3	C	138/144 (96%)	122 (88%)	16 (12%)	5	24
3	F	138/144 (96%)	118 (86%)	20 (14%)	3	15
3	I	138/144 (96%)	126 (91%)	12 (9%)	10	37
3	L	138/144 (96%)	127 (92%)	11 (8%)	12	42
3	O	138/144 (96%)	126 (91%)	12 (9%)	10	37
3	R	138/144 (96%)	123 (89%)	15 (11%)	6	26
All	All	4164/4350 (96%)	3865 (93%)	299 (7%)	14	47

All (299) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	25	ILE
1	A	63	ILE
1	A	79	SER
1	A	94	ARG
1	A	104	PHE
1	A	192	ASN
1	A	199	TYR
1	A	217	HIS
1	A	219	THR
1	A	223	ASN
1	A	242	VAL
1	A	246	PRO
1	A	311	ASP
1	A	316	GLN
1	A	319	ASN
1	A	342	VAL
1	A	362	MET
1	A	384	GLN
1	A	385	THR
1	A	410	ILE
2	B	26	GLN
2	B	48	ARG
2	B	61	ASP
2	B	66	TYR
2	B	80	ASP
2	B	95	GLU
2	B	140	GLU
2	B	141	GLU
2	B	155	TYR
2	B	183	ILE
2	B	205	HIS
2	B	220	GLU
3	C	10	THR
3	C	11	ARG
3	C	12	ARG
3	C	37	GLN
3	C	41	SER
3	C	44	VAL
3	C	49	SER
3	C	72	ILE
3	C	81	ASP
3	C	103	ILE

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Mol	Chain	Res	Type
3	C	111	ASP
3	C	113	ASN
3	C	125	MET
3	C	174	PRO
3	C	180	ASP
3	C	185	GLN
1	D	6	HIS
1	D	10	GLU
1	D	25	ILE
1	D	43	TRP
1	D	63	ILE
1	D	79	SER
1	D	94	ARG
1	D	104	PHE
1	D	192	ASN
1	D	199	TYR
1	D	217	HIS
1	D	219	THR
1	D	223	ASN
1	D	242	VAL
1	D	246	PRO
1	D	287	ARG
1	D	311	ASP
1	D	314	VAL
1	D	342	VAL
1	D	384	GLN
1	D	385	THR
1	D	421	PRO
2	E	26	GLN
2	E	48	ARG
2	E	61	ASP
2	E	66	TYR
2	E	80	ASP
2	E	82	GLU
2	E	95	GLU
2	E	129	GLU
2	E	141	GLU
2	E	145	CYS
2	E	155	TYR
2	E	158	ARG
2	E	183	ILE
2	E	188	PRO

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Mol	Chain	Res	Type
2	E	205	HIS
2	E	220	GLU
3	F	10	THR
3	F	11	ARG
3	F	12	ARG
3	F	37	GLN
3	F	41	SER
3	F	44	VAL
3	F	49	SER
3	F	72	ILE
3	F	81	ASP
3	F	89	GLN
3	F	90	LEU
3	F	94	VAL
3	F	108	GLU
3	F	110	THR
3	F	112	GLN
3	F	113	ASN
3	F	118	GLU
3	F	125	MET
3	F	174	PRO
3	F	180	ASP
1	G	4	ILE
1	G	6	HIS
1	G	10	GLU
1	G	25	ILE
1	G	73	VAL
1	G	79	SER
1	G	94	ARG
1	G	104	PHE
1	G	192	ASN
1	G	199	TYR
1	G	201	LEU
1	G	217	HIS
1	G	219	THR
1	G	223	ASN
1	G	242	VAL
1	G	246	PRO
1	G	311	ASP
1	G	319	ASN
1	G	342	VAL
1	G	385	THR

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Mol	Chain	Res	Type
1	G	421	PRO
2	H	26	GLN
2	H	48	ARG
2	H	61	ASP
2	H	80	ASP
2	H	95	GLU
2	H	141	GLU
2	H	145	CYS
2	H	181	SER
2	H	183	ILE
2	H	205	HIS
2	H	220	GLU
3	I	10	THR
3	I	11	ARG
3	I	12	ARG
3	I	19	THR
3	I	37	GLN
3	I	41	SER
3	I	49	SER
3	I	81	ASP
3	I	89	GLN
3	I	96	THR
3	I	113	ASN
3	I	180	ASP
1	J	10	GLU
1	J	25	ILE
1	J	79	SER
1	J	94	ARG
1	J	104	PHE
1	J	174	HIS
1	J	192	ASN
1	J	199	TYR
1	J	217	HIS
1	J	219	THR
1	J	223	ASN
1	J	242	VAL
1	J	246	PRO
1	J	311	ASP
1	J	316	GLN
1	J	319	ASN
1	J	321	ILE
1	J	342	VAL

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Mol	Chain	Res	Type
1	J	362	MET
1	J	385	THR
1	J	403	TYR
1	J	415	GLU
1	J	421	PRO
1	J	424	ILE
2	K	26	GLN
2	K	48	ARG
2	K	61	ASP
2	K	80	ASP
2	K	95	GLU
2	K	102	LEU
2	K	129	GLU
2	K	140	GLU
2	K	155	TYR
2	K	178	THR
2	K	183	ILE
2	K	205	HIS
2	K	220	GLU
3	L	10	THR
3	L	11	ARG
3	L	12	ARG
3	L	37	GLN
3	L	44	VAL
3	L	49	SER
3	L	81	ASP
3	L	96	THR
3	L	108	GLU
3	L	121	GLU
3	L	180	ASP
1	M	6	HIS
1	M	7	ASP
1	M	10	GLU
1	M	25	ILE
1	M	43	TRP
1	M	63	ILE
1	M	79	SER
1	M	94	ARG
1	M	104	PHE
1	M	178	THR
1	M	192	ASN
1	M	199	TYR

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Mol	Chain	Res	Type
1	M	217	HIS
1	M	219	THR
1	M	223	ASN
1	M	242	VAL
1	M	246	PRO
1	M	311	ASP
1	M	314	VAL
1	M	316	GLN
1	M	319	ASN
1	M	342	VAL
1	M	385	THR
2	N	26	GLN
2	N	48	ARG
2	N	61	ASP
2	N	66	TYR
2	N	69	GLN
2	N	80	ASP
2	N	95	GLU
2	N	140	GLU
2	N	149	HIS
2	N	152	ASP
2	N	155	TYR
2	N	183	ILE
2	N	205	HIS
2	N	220	GLU
3	O	10	THR
3	O	11	ARG
3	O	12	ARG
3	O	37	GLN
3	O	44	VAL
3	O	49	SER
3	O	72	ILE
3	O	81	ASP
3	O	86	ARG
3	O	125	MET
3	O	168	PRO
3	O	180	ASP
1	P	6	HIS
1	P	7	ASP
1	P	25	ILE
1	P	63	ILE
1	P	79	SER

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Mol	Chain	Res	Type
1	P	94	ARG
1	P	104	PHE
1	P	178	THR
1	P	192	ASN
1	P	199	TYR
1	P	217	HIS
1	P	219	THR
1	P	223	ASN
1	P	242	VAL
1	P	246	PRO
1	P	277	PRO
1	P	311	ASP
1	P	319	ASN
1	P	342	VAL
1	P	362	MET
1	P	384	GLN
1	P	385	THR
1	P	421	PRO
2	Q	8	ASP
2	Q	26	GLN
2	Q	48	ARG
2	Q	61	ASP
2	Q	66	TYR
2	Q	80	ASP
2	Q	95	GLU
2	Q	129	GLU
2	Q	155	TYR
2	Q	169	CYS
2	Q	183	ILE
2	Q	205	HIS
2	Q	220	GLU
3	R	10	THR
3	R	11	ARG
3	R	12	ARG
3	R	37	GLN
3	R	41	SER
3	R	49	SER
3	R	72	ILE
3	R	81	ASP
3	R	90	LEU
3	R	92	GLN
3	R	113	ASN

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Mol	Chain	Res	Type
3	R	118	GLU
3	R	125	MET
3	R	168	PRO
3	R	180	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (84) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	82	HIS
1	A	99	ASN
1	A	177	GLN
1	A	192	ASN
1	A	222	ASN
1	A	291	HIS
1	A	316	GLN
1	A	319	ASN
2	B	5	HIS
2	B	22	GLN
2	B	62	GLN
2	B	69	GLN
2	B	120	GLN
2	B	149	HIS
2	B	161	GLN
3	C	37	GLN
3	C	113	ASN
1	D	82	HIS
1	D	177	GLN
1	D	192	ASN
1	D	222	ASN
2	E	5	HIS
2	E	22	GLN
2	E	62	GLN
2	E	96	ASN
2	E	149	HIS
3	F	37	GLN
3	F	89	GLN
3	F	92	GLN
3	F	112	GLN
3	F	113	ASN
1	G	82	HIS
1	G	177	GLN

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Mol	Chain	Res	Type
1	G	222	ASN
1	G	319	ASN
1	G	429	ASN
2	H	22	GLN
2	H	24	GLN
2	H	62	GLN
3	I	37	GLN
3	I	89	GLN
3	I	97	ASN
3	I	112	GLN
3	I	113	ASN
1	J	20	HIS
1	J	82	HIS
1	J	177	GLN
1	J	222	ASN
1	J	319	ASN
1	J	429	ASN
2	K	22	GLN
2	K	62	GLN
2	K	149	HIS
2	K	161	GLN
3	L	113	ASN
1	M	82	HIS
1	M	177	GLN
1	M	192	ASN
1	M	222	ASN
1	M	238	GLN
1	M	291	HIS
1	M	319	ASN
1	M	429	ASN
2	N	22	GLN
2	N	62	GLN
2	N	69	GLN
2	N	96	ASN
2	N	149	HIS
2	N	161	GLN
3	O	37	GLN
3	O	113	ASN
1	P	82	HIS
1	P	177	GLN
1	P	192	ASN
1	P	222	ASN

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Mol	Chain	Res	Type
1	P	223	ASN
1	P	238	GLN
1	P	319	ASN
2	Q	22	GLN
2	Q	62	GLN
2	Q	149	HIS
2	Q	161	GLN
3	R	113	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

36 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	HEM	G	502	1	27,50,50	2.13	8 (29%)	17,82,82	1.04	1 (5%)
4	HEM	D	501	1	27,50,50	1.74	5 (18%)	17,82,82	0.79	1 (5%)
7	FES	I	200	3	0,4,4	-	-	-	-	-
5	SMA	M	503	-	35,38,38	2.05	7 (20%)	46,52,52	2.21	12 (26%)
7	FES	C	200	3	0,4,4	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	FES	R	200	3	0,4,4	-	-	-		
4	HEM	G	501	1	27,50,50	1.77	7 (25%)	17,82,82	0.96	0
5	SMA	P	503	-	35,38,38	2.10	7 (20%)	46,52,52	1.93	12 (26%)
4	HEM	K	301	2	27,50,50	1.76	5 (18%)	17,82,82	1.27	2 (11%)
6	LOP	P	504	-	44,44,44	0.65	1 (2%)	47,49,49	1.34	6 (12%)
5	SMA	G	503	-	35,38,38	1.79	7 (20%)	46,52,52	2.27	12 (26%)
7	FES	L	200	3	0,4,4	-	-	-		
6	LOP	G	504	-	44,44,44	0.77	1 (2%)	47,49,49	1.42	6 (12%)
4	HEM	D	502	1	27,50,50	1.82	6 (22%)	17,82,82	1.09	1 (5%)
4	HEM	N	301	2	27,50,50	1.66	4 (14%)	17,82,82	1.26	2 (11%)
4	HEM	P	502	1	27,50,50	2.13	8 (29%)	17,82,82	1.00	1 (5%)
5	SMA	D	503	-	35,38,38	2.39	9 (25%)	46,52,52	1.94	11 (23%)
5	SMA	A	503	-	35,38,38	1.87	7 (20%)	46,52,52	2.27	13 (28%)
4	HEM	B	301	2	27,50,50	1.71	6 (22%)	17,82,82	1.23	1 (5%)
7	FES	F	200	3	0,4,4	-	-	-		
4	HEM	P	501	1	27,50,50	2.06	9 (33%)	17,82,82	0.73	0
6	LOP	D	504	-	44,44,44	0.71	0	47,49,49	1.38	5 (10%)
6	LOP	J	504	-	44,44,44	0.65	0	47,49,49	1.31	4 (8%)
4	HEM	J	502	1	27,50,50	2.33	9 (33%)	17,82,82	1.01	1 (5%)
4	HEM	M	502	1	27,50,50	2.18	6 (22%)	17,82,82	1.13	2 (11%)
4	HEM	E	301	2	27,50,50	1.83	6 (22%)	17,82,82	0.93	0
6	LOP	A	504	-	44,44,44	0.64	0	47,49,49	1.33	7 (14%)
6	LOP	M	504	-	44,44,44	0.71	0	47,49,49	1.38	7 (14%)
7	FES	O	200	3	0,4,4	-	-	-		
4	HEM	H	301	2	27,50,50	1.79	5 (18%)	17,82,82	1.19	0
4	HEM	M	501	1	27,50,50	1.67	6 (22%)	17,82,82	0.96	0
4	HEM	J	501	1	27,50,50	1.86	7 (25%)	17,82,82	0.89	0
4	HEM	Q	301	2	27,50,50	1.77	6 (22%)	17,82,82	0.97	0
5	SMA	J	503	-	35,38,38	1.85	5 (14%)	46,52,52	2.19	11 (23%)
4	HEM	A	501	1	27,50,50	1.83	7 (25%)	17,82,82	1.14	1 (5%)
4	HEM	A	502	1	27,50,50	2.29	9 (33%)	17,82,82	1.26	2 (11%)

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
4	HEM	G	502	1	-	1/6/54/54	-
4	HEM	D	501	1	-	0/6/54/54	-
7	FES	I	200	3	-	-	0/1/1/1
5	SMA	M	503	-	-	11/33/34/34	0/2/2/2
7	FES	C	200	3	-	-	0/1/1/1
7	FES	R	200	3	-	-	0/1/1/1
4	HEM	G	501	1	-	0/6/54/54	-
5	SMA	P	503	-	-	7/33/34/34	0/2/2/2
4	HEM	K	301	2	-	0/6/54/54	-
6	LOP	P	504	-	-	4/48/48/48	-
5	SMA	G	503	-	-	7/33/34/34	0/2/2/2
7	FES	L	200	3	-	-	0/1/1/1
6	LOP	G	504	-	-	10/48/48/48	-
4	HEM	D	502	1	-	1/6/54/54	-
4	HEM	N	301	2	-	5/6/54/54	-
4	HEM	P	502	1	-	1/6/54/54	-
5	SMA	D	503	-	-	6/33/34/34	0/2/2/2
5	SMA	A	503	-	-	7/33/34/34	0/2/2/2
4	HEM	B	301	2	-	0/6/54/54	-
7	FES	F	200	3	-	-	0/1/1/1
4	HEM	P	501	1	-	3/6/54/54	-
6	LOP	D	504	-	-	6/48/48/48	-
6	LOP	J	504	-	-	12/48/48/48	-
4	HEM	J	502	1	-	0/6/54/54	-
4	HEM	M	502	1	-	0/6/54/54	-
4	HEM	E	301	2	-	0/6/54/54	-
6	LOP	A	504	-	-	12/48/48/48	-
6	LOP	M	504	-	-	8/48/48/48	-
7	FES	O	200	3	-	-	0/1/1/1
4	HEM	H	301	2	-	0/6/54/54	-
4	HEM	M	501	1	-	4/6/54/54	-
4	HEM	J	501	1	-	0/6/54/54	-
4	HEM	Q	301	2	-	2/6/54/54	-
5	SMA	J	503	-	-	8/33/34/34	0/2/2/2
4	HEM	A	501	1	-	0/6/54/54	-
4	HEM	A	502	1	-	0/6/54/54	-

All (163) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	503	SMA	O5-C5	7.58	1.50	1.36
5	M	503	SMA	O5-C5	6.78	1.48	1.36
5	P	503	SMA	O5-C5	6.47	1.48	1.36
5	J	503	SMA	O5-C5	6.47	1.48	1.36
5	P	503	SMA	O7-C7	6.46	1.47	1.37
5	A	503	SMA	O7-C7	6.26	1.47	1.37
4	J	502	HEM	C3C-CAC	-6.02	1.35	1.47
4	A	502	HEM	C3C-CAC	-5.67	1.36	1.47
5	D	503	SMA	O7-C7	5.65	1.46	1.37
5	D	503	SMA	O1-C2	5.57	1.43	1.35
5	M	503	SMA	O7-C7	5.53	1.46	1.37
4	M	502	HEM	C3B-C2B	-5.39	1.32	1.40
4	J	502	HEM	C3C-C2C	-5.24	1.33	1.40
4	P	501	HEM	C3C-C2C	-5.16	1.33	1.40
5	G	503	SMA	O1-C2	5.08	1.42	1.35
5	A	503	SMA	O5-C5	5.07	1.45	1.36
5	J	503	SMA	O7-C7	4.90	1.45	1.37
4	A	502	HEM	C3B-CAB	-4.89	1.38	1.47
4	J	501	HEM	C3B-CAB	-4.89	1.38	1.47
4	M	502	HEM	C3B-CAB	-4.86	1.38	1.47
4	H	301	HEM	C3C-CAC	-4.80	1.38	1.47
4	E	301	HEM	C3C-CAC	-4.76	1.38	1.47
4	G	502	HEM	C3B-CAB	-4.70	1.38	1.47
4	P	502	HEM	C3C-CAC	-4.68	1.38	1.47
4	Q	301	HEM	C3C-CAC	-4.52	1.38	1.47
4	G	502	HEM	C3C-C2C	-4.51	1.34	1.40
4	P	501	HEM	C3C-CAC	-4.47	1.38	1.47
5	G	503	SMA	O5-C5	4.37	1.44	1.36
4	D	501	HEM	C3C-CAC	-4.32	1.39	1.47
4	J	502	HEM	C3B-CAB	-4.31	1.39	1.47
5	G	503	SMA	O7-C7	4.30	1.44	1.37
4	A	501	HEM	C3B-CAB	-4.29	1.39	1.47
4	P	502	HEM	C3C-C2C	-4.28	1.34	1.40
4	M	502	HEM	C3C-CAC	-4.14	1.39	1.47
4	B	301	HEM	C3C-CAC	-4.14	1.39	1.47
4	A	502	HEM	C3C-C2C	-4.11	1.34	1.40
5	M	503	SMA	O1-C2	4.06	1.41	1.35
4	K	301	HEM	C3C-CAC	-4.04	1.39	1.47
4	G	502	HEM	C3C-CAC	-4.02	1.39	1.47
4	N	301	HEM	CBC-CAC	3.88	1.55	1.29
4	D	502	HEM	C3B-CAB	-3.88	1.40	1.47
5	D	503	SMA	C7-C8	-3.87	1.35	1.40
4	A	502	HEM	C3B-C2B	-3.85	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	K	301	HEM	CBB-CAB	3.79	1.54	1.29
4	A	501	HEM	C3B-C2B	-3.78	1.35	1.40
4	E	301	HEM	CBB-CAB	3.76	1.54	1.29
4	P	502	HEM	C3B-C2B	-3.74	1.35	1.40
4	B	301	HEM	CBC-CAC	3.74	1.54	1.29
4	G	502	HEM	CBB-CAB	3.73	1.54	1.29
4	Q	301	HEM	CBB-CAB	3.72	1.54	1.29
4	K	301	HEM	CBC-CAC	3.69	1.53	1.29
4	B	301	HEM	CBB-CAB	3.68	1.53	1.29
4	G	502	HEM	C3B-C2B	-3.68	1.35	1.40
4	H	301	HEM	CBB-CAB	3.68	1.53	1.29
4	P	502	HEM	C3B-CAB	-3.67	1.40	1.47
4	H	301	HEM	CBC-CAC	3.67	1.53	1.29
4	P	502	HEM	CBB-CAB	3.63	1.53	1.29
4	N	301	HEM	CBB-CAB	3.62	1.53	1.29
4	M	502	HEM	CBB-CAB	3.62	1.53	1.29
4	G	501	HEM	C3C-CAC	-3.60	1.40	1.47
4	Q	301	HEM	CBC-CAC	3.59	1.53	1.29
5	A	503	SMA	O1-C2	3.57	1.40	1.35
4	M	501	HEM	CBC-CAC	3.56	1.52	1.29
4	P	501	HEM	CBB-CAB	3.56	1.52	1.29
4	D	502	HEM	CBC-CAC	3.55	1.52	1.29
4	D	501	HEM	CBB-CAB	3.53	1.52	1.29
4	G	501	HEM	CBB-CAB	3.51	1.52	1.29
5	P	503	SMA	C20-C19	3.50	1.36	1.33
4	J	501	HEM	CBB-CAB	3.48	1.52	1.29
4	A	501	HEM	CBC-CAC	3.46	1.52	1.29
4	M	501	HEM	C3B-CAB	-3.45	1.40	1.47
4	G	502	HEM	CBC-CAC	3.44	1.52	1.29
4	A	502	HEM	CBB-CAB	3.44	1.52	1.29
4	M	501	HEM	CBB-CAB	3.43	1.52	1.29
4	E	301	HEM	CBC-CAC	3.43	1.52	1.29
4	D	502	HEM	CBB-CAB	3.40	1.51	1.29
5	P	503	SMA	O1-C2	3.39	1.40	1.35
4	P	501	HEM	CBC-CAC	3.38	1.51	1.29
4	G	501	HEM	C3B-CAB	-3.38	1.41	1.47
4	J	502	HEM	CBB-CAB	3.38	1.51	1.29
4	M	502	HEM	C3C-C2C	-3.36	1.35	1.40
4	M	502	HEM	CBC-CAC	3.33	1.51	1.29
4	A	501	HEM	CBB-CAB	3.33	1.51	1.29
4	P	501	HEM	C3B-CAB	-3.31	1.41	1.47
4	A	502	HEM	CBC-CAC	3.31	1.51	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	N	301	HEM	C3C-CAC	-3.31	1.41	1.47
5	P	503	SMA	O1-C8A	3.31	1.41	1.36
4	P	502	HEM	CBC-CAC	3.31	1.51	1.29
4	J	501	HEM	CBC-CAC	3.27	1.51	1.29
4	G	501	HEM	CBC-CAC	3.24	1.50	1.29
5	D	503	SMA	O1-C8A	3.22	1.41	1.36
4	D	501	HEM	C3B-CAB	-3.20	1.41	1.47
4	E	301	HEM	C3B-CAB	-3.19	1.41	1.47
4	G	501	HEM	C3C-C2C	-3.16	1.36	1.40
4	D	501	HEM	C3C-C2C	-3.14	1.36	1.40
4	J	502	HEM	C3B-C2B	-3.13	1.36	1.40
4	D	501	HEM	CBC-CAC	3.11	1.49	1.29
4	J	502	HEM	CBC-CAC	3.11	1.49	1.29
4	D	502	HEM	C3C-C2C	-3.09	1.36	1.40
4	A	501	HEM	C3C-CAC	-3.07	1.41	1.47
5	D	503	SMA	O8-C8	3.07	1.45	1.35
4	J	501	HEM	C3B-C2B	-3.05	1.36	1.40
4	J	501	HEM	C3C-CAC	-3.03	1.41	1.47
5	P	503	SMA	O8-C8	2.94	1.45	1.35
4	K	301	HEM	C3B-CAB	-2.93	1.42	1.47
4	D	502	HEM	C3B-C2B	-2.90	1.36	1.40
5	D	503	SMA	O12-C12	2.87	1.50	1.42
5	P	503	SMA	C7-C8	-2.80	1.36	1.40
4	D	502	HEM	C3C-CAC	-2.80	1.42	1.47
5	J	503	SMA	O1-C8A	2.79	1.41	1.36
4	B	301	HEM	C3B-CAB	-2.77	1.42	1.47
4	M	501	HEM	C3C-C2C	-2.77	1.36	1.40
4	M	501	HEM	C3C-CAC	-2.75	1.42	1.47
5	J	503	SMA	O8-C8	2.75	1.44	1.35
5	J	503	SMA	O1-C2	2.70	1.39	1.35
4	E	301	HEM	C3B-C2B	-2.63	1.36	1.40
4	H	301	HEM	C3B-CAB	-2.62	1.42	1.47
4	B	301	HEM	C3C-C2C	-2.62	1.36	1.40
5	G	503	SMA	O1-C8A	2.57	1.40	1.36
4	Q	301	HEM	C3B-CAB	-2.53	1.42	1.47
4	G	501	HEM	C1D-ND	2.52	1.41	1.36
4	E	301	HEM	C3C-C2C	-2.52	1.36	1.40
4	Q	301	HEM	C3C-C2C	-2.51	1.36	1.40
5	M	503	SMA	C7-C8	-2.47	1.37	1.40
4	G	501	HEM	C3B-C2B	-2.40	1.37	1.40
5	M	503	SMA	O1-C8A	2.39	1.40	1.36
4	J	502	HEM	C1B-C2B	2.38	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	Q	301	HEM	C3B-C2B	-2.38	1.37	1.40
4	P	501	HEM	C3B-C2B	-2.36	1.37	1.40
5	M	503	SMA	O8-C8	2.34	1.43	1.35
5	G	503	SMA	O8-C8	2.34	1.43	1.35
5	A	503	SMA	C20-C19	2.34	1.35	1.33
4	P	501	HEM	C1B-C2B	2.31	1.47	1.42
5	D	503	SMA	C3-C2	2.31	1.42	1.39
5	A	503	SMA	O1-C8A	2.29	1.40	1.36
4	P	501	HEM	C4A-NA	2.26	1.40	1.36
5	M	503	SMA	C13-C12	2.24	1.59	1.54
4	A	501	HEM	C4A-NA	2.24	1.40	1.36
4	J	501	HEM	C3C-C2C	-2.23	1.37	1.40
5	A	503	SMA	O8-C8	2.22	1.43	1.35
4	P	502	HEM	CAA-C2A	-2.21	1.48	1.52
5	G	503	SMA	C22-C11	2.19	1.58	1.53
4	A	502	HEM	C4B-CHC	-2.17	1.35	1.41
4	A	502	HEM	C1B-C2B	2.17	1.47	1.42
4	J	502	HEM	C1D-ND	2.15	1.40	1.36
4	G	502	HEM	C1B-C2B	2.15	1.47	1.42
5	G	503	SMA	C11-C12	2.15	1.57	1.53
4	M	501	HEM	C3B-C2B	-2.14	1.37	1.40
4	N	301	HEM	C3C-C2C	-2.13	1.37	1.40
5	D	503	SMA	C13-C12	2.12	1.59	1.54
6	P	504	LOP	O5-C4	-2.10	1.41	1.46
4	J	501	HEM	C1D-ND	2.08	1.40	1.36
5	A	503	SMA	O12-C12	2.08	1.48	1.42
4	B	301	HEM	C3B-C2B	-2.07	1.37	1.40
4	J	502	HEM	C4A-NA	2.07	1.40	1.36
4	A	501	HEM	C1D-ND	2.06	1.40	1.36
6	G	504	LOP	O5-C6	2.06	1.40	1.34
4	G	502	HEM	C4B-CHC	-2.05	1.35	1.41
4	P	501	HEM	C4B-NB	2.05	1.40	1.36
4	P	502	HEM	C4D-C3D	2.05	1.47	1.42
4	A	502	HEM	C4A-NA	2.04	1.40	1.36
4	H	301	HEM	C1A-CHA	-2.01	1.35	1.41
4	K	301	HEM	CAA-C2A	-2.00	1.49	1.52

All (121) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	503	SMA	O1-C2-C9	7.46	120.75	111.91
5	A	503	SMA	C5M-O5-C5	-7.23	107.63	117.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	503	SMA	O7-C7-C8	6.91	121.51	114.54
5	D	503	SMA	O1-C2-C9	6.29	119.37	111.91
5	A	503	SMA	O7-C7-C8	6.13	120.72	114.54
5	G	503	SMA	O1-C2-C9	6.03	119.06	111.91
5	P	503	SMA	O1-C2-C9	5.79	118.77	111.91
5	M	503	SMA	O7-C7-C8	5.78	120.37	114.54
5	G	503	SMA	C5M-O5-C5	-5.73	109.73	117.75
5	M	503	SMA	O1-C2-C9	5.60	118.55	111.91
5	M	503	SMA	C5M-O5-C5	-5.59	109.92	117.75
5	A	503	SMA	C9-C10-C11	-5.51	107.30	114.72
5	J	503	SMA	C5M-O5-C5	-5.02	110.72	117.75
5	A	503	SMA	O1-C2-C9	5.01	117.86	111.91
6	D	504	LOP	C19-C18-C17	-5.01	88.99	114.42
5	M	503	SMA	O5-C5-C4A	4.98	123.22	115.89
5	J	503	SMA	O7-C7-C8	4.96	119.54	114.54
6	P	504	LOP	C19-C18-C17	-4.53	91.43	114.42
5	P	503	SMA	C5M-O5-C5	-4.41	111.58	117.75
6	J	504	LOP	O5-C6-C7	4.40	120.99	111.50
5	M	503	SMA	C7M-O7-C7	-4.17	111.24	117.53
5	G	503	SMA	O5-C5-C4A	4.09	121.91	115.89
6	G	504	LOP	C30-C29-C28	-4.02	94.00	114.42
5	D	503	SMA	C17-C18-C19	-3.99	115.20	126.42
6	M	504	LOP	C12-C11-C10	-3.95	94.39	114.42
6	G	504	LOP	O5-C6-C7	3.94	120.00	111.50
5	J	503	SMA	O5-C5-C4A	3.93	121.66	115.89
5	J	503	SMA	C7M-O7-C7	-3.88	111.68	117.53
6	A	504	LOP	C19-C18-C17	-3.74	95.44	114.42
5	J	503	SMA	O1-C8A-C8	3.74	120.81	116.12
5	A	503	SMA	O5-C5-C4A	3.73	121.38	115.89
5	P	503	SMA	O7-C7-C8	3.70	118.27	114.54
5	G	503	SMA	C17-C18-C19	-3.66	116.14	126.42
5	P	503	SMA	O5-C5-C4A	3.64	121.24	115.89
6	M	504	LOP	C10-C9-C8	-3.62	96.05	114.42
5	P	503	SMA	C16-C17-C18	-3.56	115.77	124.67
5	G	503	SMA	O7-C7-C6	-3.53	118.05	124.12
6	A	504	LOP	C21-C20-C19	-3.49	96.69	114.42
5	G	503	SMA	C7M-O7-C7	-3.48	112.28	117.53
5	P	503	SMA	O1-C8A-C8	3.39	120.39	116.12
5	G	503	SMA	O1-C8A-C8	3.31	120.28	116.12
5	D	503	SMA	O5-C5-C4A	3.29	120.73	115.89
5	D	503	SMA	O7-C7-C8	3.29	117.86	114.54
6	D	504	LOP	O6-C24-C25	3.21	121.99	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	503	SMA	C7M-O7-C7	-3.20	112.70	117.53
5	D	503	SMA	C9-C10-C11	-3.17	110.45	114.72
6	D	504	LOP	C21-C20-C19	-3.16	98.40	114.42
6	M	504	LOP	O5-C6-C7	3.15	118.28	111.50
6	J	504	LOP	C19-C18-C17	-3.06	98.89	114.42
5	J	503	SMA	C17-C18-C19	-3.04	117.86	126.42
4	A	502	HEM	CBA-CAA-C2A	-3.01	106.93	112.49
5	D	503	SMA	O1-C8A-C8	2.95	119.83	116.12
5	G	503	SMA	O5-C5-C6	-2.94	118.10	123.34
5	M	503	SMA	C17-C18-C19	-2.92	118.21	126.42
5	P	503	SMA	C7M-O7-C7	-2.88	113.18	117.53
5	M	503	SMA	O7-C7-C6	-2.86	119.20	124.12
5	M	503	SMA	O5-C5-C6	-2.82	118.31	123.34
5	A	503	SMA	O1-C8A-C8	2.81	119.65	116.12
5	D	503	SMA	C5M-O5-C5	-2.79	113.84	117.75
6	G	504	LOP	C32-C31-C30	-2.73	100.55	114.42
6	J	504	LOP	C21-C20-C19	-2.69	100.76	114.42
5	D	503	SMA	C4-C4A-C5	-2.66	121.00	124.96
6	A	504	LOP	O5-C6-C7	2.65	117.22	111.50
5	M	503	SMA	O1-C8A-C8	2.64	119.44	116.12
5	D	503	SMA	C14-C15-C16	2.64	130.78	125.61
6	A	504	LOP	C31-C30-C29	-2.63	101.09	114.42
6	J	504	LOP	O6-C24-C25	2.59	120.05	111.91
5	A	503	SMA	C16-C17-C18	-2.59	118.20	124.67
5	A	503	SMA	O7-C7-C6	-2.59	119.66	124.12
6	G	504	LOP	C20-C19-C18	-2.59	101.30	114.42
5	P	503	SMA	C9-C10-C11	-2.58	111.25	114.72
6	A	504	LOP	C20-C19-C18	2.56	127.42	114.42
6	P	504	LOP	C21-C20-C19	-2.55	101.46	114.42
5	J	503	SMA	C4-C3-C2	2.54	119.42	116.63
6	M	504	LOP	C11-C10-C9	2.54	127.30	114.42
5	P	503	SMA	C4-C3-C2	2.52	119.39	116.63
6	P	504	LOP	O6-C24-C25	2.44	119.57	111.91
5	M	503	SMA	C4-C3-C2	2.43	119.29	116.63
4	A	502	HEM	C3B-C4B-NB	2.39	112.30	109.21
5	A	503	SMA	C25-O14-C14	-2.38	107.28	113.01
6	G	504	LOP	O6-C24-C25	2.38	119.38	111.91
6	A	504	LOP	C29-C28-C27	-2.38	102.34	114.42
5	D	503	SMA	C4-C3-C2	2.38	119.23	116.63
5	G	503	SMA	C9-C10-C11	-2.37	111.53	114.72
6	P	504	LOP	C18-C17-C16	2.36	124.08	113.79
5	A	503	SMA	O5-C5-C6	-2.36	119.13	123.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	502	HEM	C3B-C4B-NB	2.36	112.26	109.21
5	A	503	SMA	C26-C19-C18	2.34	121.76	118.08
5	G	503	SMA	C4-C3-C2	2.32	119.17	116.63
5	J	503	SMA	O7-C7-C6	-2.31	120.14	124.12
4	J	502	HEM	C3B-C4B-NB	2.31	112.19	109.21
4	K	301	HEM	CMB-C2B-C3B	2.29	128.97	124.68
4	B	301	HEM	CAA-CBA-CGA	-2.28	108.85	112.67
4	A	501	HEM	CMC-C2C-C3C	2.27	128.93	124.68
5	P	503	SMA	C22-C11-C10	2.27	113.92	110.36
5	J	503	SMA	C4-C4A-C5	-2.27	121.58	124.96
6	M	504	LOP	C31-C30-C29	-2.24	103.05	114.42
5	P	503	SMA	C14-C15-C16	-2.23	121.24	125.61
6	P	504	LOP	O5-C6-C7	2.23	116.30	111.50
5	A	503	SMA	C4-C3-C2	2.21	119.05	116.63
5	P	503	SMA	C4-C4A-C5	-2.20	121.68	124.96
6	A	504	LOP	C18-C17-C16	2.19	123.34	113.79
4	M	502	HEM	C3B-C4B-NB	2.18	112.03	109.21
4	N	301	HEM	CBA-CAA-C2A	2.17	116.48	112.49
5	G	503	SMA	C4-C4A-C5	-2.16	121.75	124.96
6	G	504	LOP	O5-C4-C3	2.16	116.21	108.40
5	J	503	SMA	O5-C5-C6	-2.15	119.50	123.34
4	N	301	HEM	C3B-C4B-NB	2.15	111.99	109.21
4	P	502	HEM	C3B-C4B-NB	2.10	111.92	109.21
4	D	502	HEM	C3B-C4B-NB	2.07	111.89	109.21
5	M	503	SMA	C9-C10-C11	-2.07	111.93	114.72
4	K	301	HEM	CAA-CBA-CGA	-2.06	109.21	112.67
6	D	504	LOP	O5-C6-C7	2.06	115.94	111.50
6	P	504	LOP	C27-C26-C25	-2.05	105.81	113.19
6	M	504	LOP	C21-C20-C19	-2.04	104.06	114.42
4	M	502	HEM	C1D-C2D-C3D	-2.02	105.59	107.00
5	A	503	SMA	C7M-O7-C7	-2.02	114.48	117.53
6	D	504	LOP	P1-O1-C2	-2.02	111.67	121.59
5	M	503	SMA	C23-O12-C12	-2.01	109.25	114.52
6	M	504	LOP	O6-C24-C25	2.01	118.21	111.91
4	D	501	HEM	C3B-C4B-NB	2.00	111.80	109.21

There are no chirality outliers.

All (115) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	M	501	HEM	C1A-C2A-CAA-CBA
4	M	501	HEM	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
4	N	301	HEM	C1A-C2A-CAA-CBA
4	N	301	HEM	C3A-C2A-CAA-CBA
4	N	301	HEM	C2A-CAA-CBA-CGA
4	N	301	HEM	C2D-C3D-CAD-CBD
4	N	301	HEM	C4D-C3D-CAD-CBD
4	P	501	HEM	C1A-C2A-CAA-CBA
4	P	502	HEM	C2A-CAA-CBA-CGA
4	Q	301	HEM	C4D-C3D-CAD-CBD
5	G	503	SMA	C4A-C5-O5-C5M
5	G	503	SMA	C6-C5-O5-C5M
5	J	503	SMA	C6-C5-O5-C5M
5	P	503	SMA	C4A-C5-O5-C5M
5	P	503	SMA	C6-C5-O5-C5M
5	P	503	SMA	C13-C14-O14-C25
5	P	503	SMA	C15-C14-O14-C25
6	D	504	LOP	C2-O1-P1-O4
6	G	504	LOP	C2-O1-P1-O3
6	G	504	LOP	C3-O2-P1-O3
6	J	504	LOP	C2-O1-P1-O2
6	J	504	LOP	C2-O1-P1-O3
6	J	504	LOP	C2-O1-P1-O4
6	P	504	LOP	C2-O1-P1-O3
5	A	503	SMA	C6-C5-O5-C5M
5	M	503	SMA	C6-C5-O5-C5M
5	J	503	SMA	C9-C10-C11-C22
5	P	503	SMA	C9-C10-C11-C22
5	A	503	SMA	C4A-C5-O5-C5M
5	J	503	SMA	C4A-C5-O5-C5M
5	M	503	SMA	C4A-C5-O5-C5M
5	A	503	SMA	C8-C7-O7-C7M
5	M	503	SMA	C8-C7-O7-C7M
5	M	503	SMA	C6-C7-O7-C7M
5	D	503	SMA	C9-C10-C11-C22
5	G	503	SMA	C9-C10-C11-C22
5	J	503	SMA	C11-C10-C9-C2
5	M	503	SMA	C11-C10-C9-C2
5	A	503	SMA	C6-C7-O7-C7M
5	M	503	SMA	C9-C10-C11-C22
5	G	503	SMA	C8-C7-O7-C7M
5	G	503	SMA	C11-C10-C9-C2
6	A	504	LOP	C2-O1-P1-O2
6	P	504	LOP	C2-O1-P1-O2

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Mol	Chain	Res	Type	Atoms
5	G	503	SMA	C6-C7-O7-C7M
6	M	504	LOP	O2-C3-C4-O5
5	M	503	SMA	C24-C13-C14-C15
5	M	503	SMA	C24-C13-C14-O14
5	M	503	SMA	C12-C13-C14-O14
5	D	503	SMA	C11-C10-C9-C2
5	J	503	SMA	C8-C7-O7-C7M
6	J	504	LOP	C3-C4-C5-O6
6	J	504	LOP	O2-C3-C4-O5
6	J	504	LOP	O5-C4-C5-O6
6	G	504	LOP	O2-C3-C4-C5
6	M	504	LOP	O2-C3-C4-C5
6	A	504	LOP	O5-C4-C5-O6
6	A	504	LOP	C3-C4-C5-O6
6	A	504	LOP	O2-C3-C4-O5
6	G	504	LOP	O2-C3-C4-O5
5	D	503	SMA	O14-C14-C15-C16
6	G	504	LOP	C3-O2-P1-O1
6	M	504	LOP	C2-O1-P1-O2
4	D	502	HEM	C2A-CAA-CBA-CGA
6	A	504	LOP	C2-O1-P1-O4
6	A	504	LOP	O2-C3-C4-C5
5	A	503	SMA	C15-C14-O14-C25
4	M	501	HEM	C2D-C3D-CAD-CBD
4	M	501	HEM	C4D-C3D-CAD-CBD
4	P	501	HEM	C3A-C2A-CAA-CBA
4	Q	301	HEM	C2D-C3D-CAD-CBD
5	J	503	SMA	C6-C7-O7-C7M
6	J	504	LOP	C3-C4-O5-C6
6	D	504	LOP	C2-O1-P1-O2
6	G	504	LOP	C2-O1-P1-O2
6	M	504	LOP	C3-O2-P1-O1
5	M	503	SMA	C13-C14-C15-C16
5	D	503	SMA	C6-C5-O5-C5M
5	D	503	SMA	C4A-C5-O5-C5M
4	G	502	HEM	C3D-CAD-CBD-CGD
6	A	504	LOP	C14-C15-C16-C17
5	A	503	SMA	C9-C10-C11-C22
5	J	503	SMA	O14-C14-C15-C16
5	M	503	SMA	O14-C14-C15-C16
6	G	504	LOP	C14-C15-C16-C17
5	A	503	SMA	C13-C14-O14-C25

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Mol	Chain	Res	Type	Atoms
6	G	504	LOP	C12-C13-C14-C15
6	M	504	LOP	C12-C13-C14-C15
6	M	504	LOP	C14-C15-C16-C17
4	P	501	HEM	C2A-CAA-CBA-CGA
5	D	503	SMA	C13-C14-C15-C16
5	J	503	SMA	C13-C14-C15-C16
6	J	504	LOP	O2-C3-C4-C5
6	A	504	LOP	O5-C6-C7-C8
6	D	504	LOP	C14-C15-C16-C17
6	J	504	LOP	C14-C15-C16-C17
6	P	504	LOP	C14-C15-C16-C17
6	D	504	LOP	O5-C6-C7-C8
5	P	503	SMA	C24-C13-C14-O14
6	A	504	LOP	O6-C24-C25-C26
5	P	503	SMA	C12-C13-C14-O14
6	A	504	LOP	C12-C13-C14-C15
6	J	504	LOP	C12-C13-C14-C15
6	P	504	LOP	C12-C13-C14-C15
6	M	504	LOP	O6-C24-C25-C26
6	J	504	LOP	O5-C6-C7-C8
5	G	503	SMA	O14-C14-C15-C16
6	D	504	LOP	C12-C13-C14-C15
6	M	504	LOP	O8-C24-C25-C26
6	G	504	LOP	C2-O1-P1-O4
6	G	504	LOP	C3-O2-P1-O4
6	A	504	LOP	O8-C24-C25-C26
6	A	504	LOP	O7-C6-C7-C8
6	D	504	LOP	O7-C6-C7-C8
6	J	504	LOP	O7-C6-C7-C8

There are no ring outliers.

32 monomers are involved in 104 short contacts:

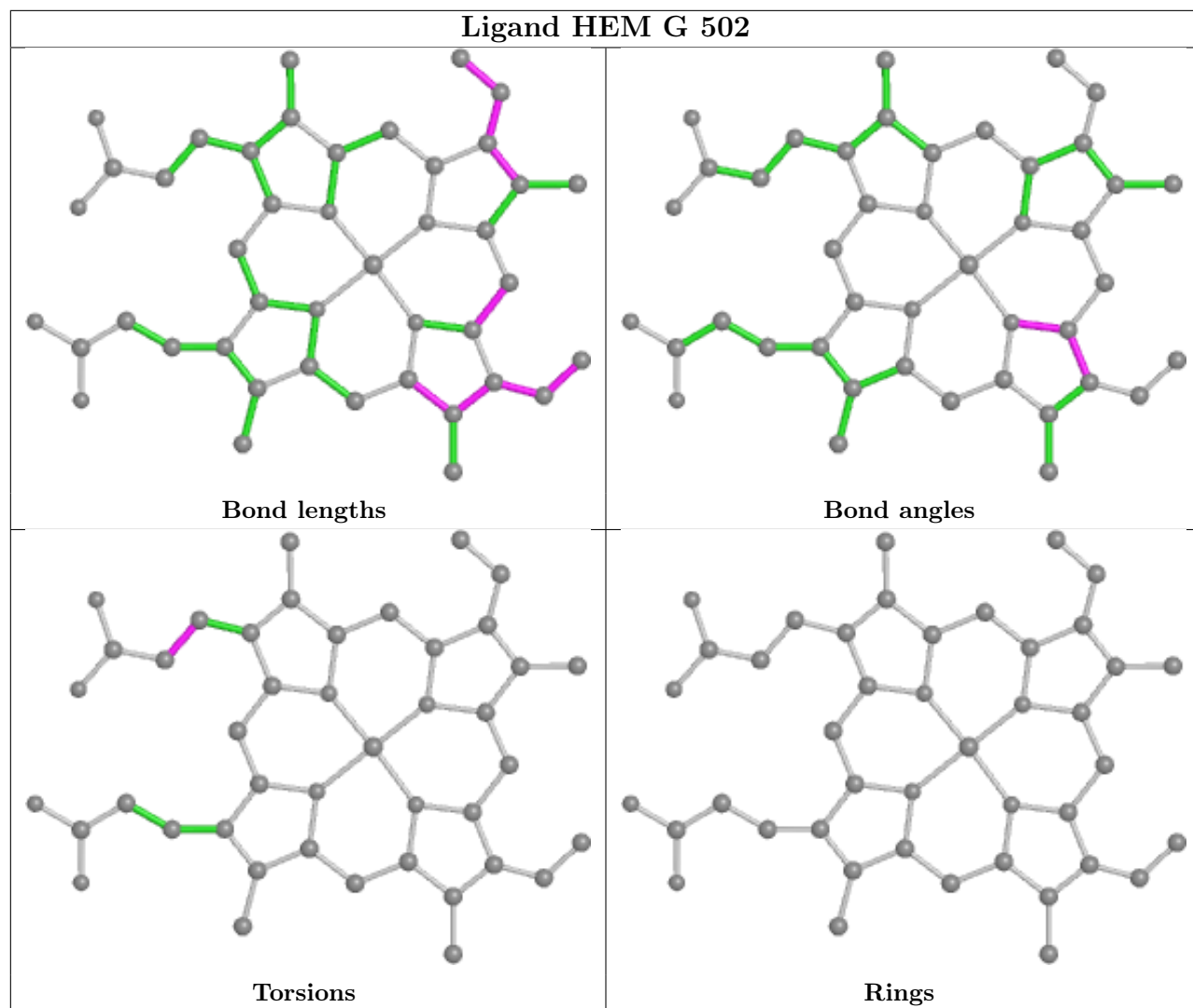
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	502	HEM	2	0
4	D	501	HEM	8	0
5	M	503	SMA	2	0
7	C	200	FES	2	0
7	R	200	FES	1	0
4	G	501	HEM	8	0
4	K	301	HEM	1	0
6	P	504	LOP	1	0

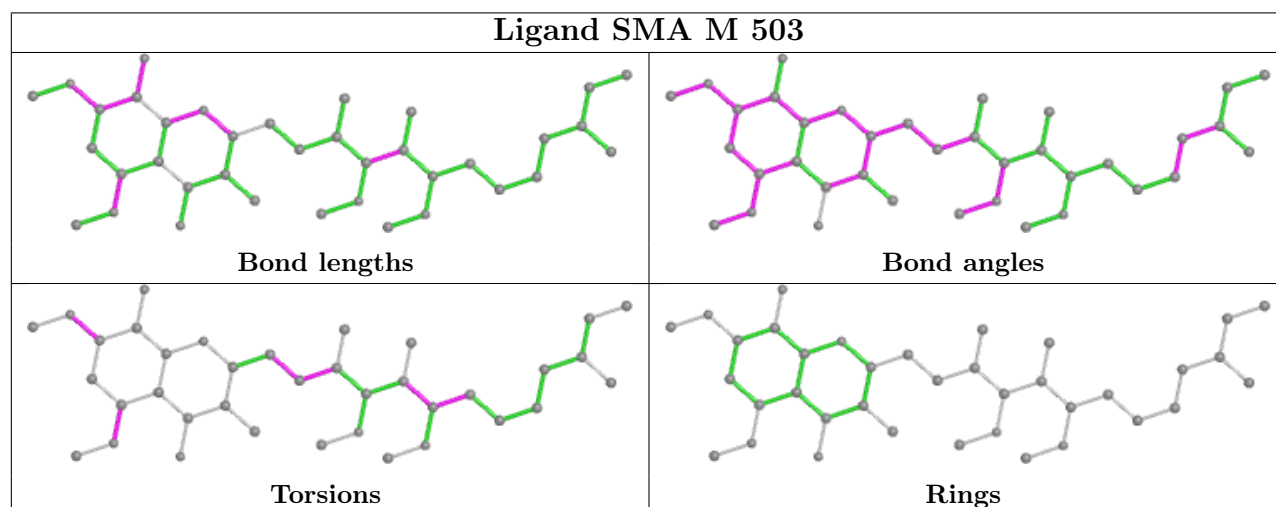
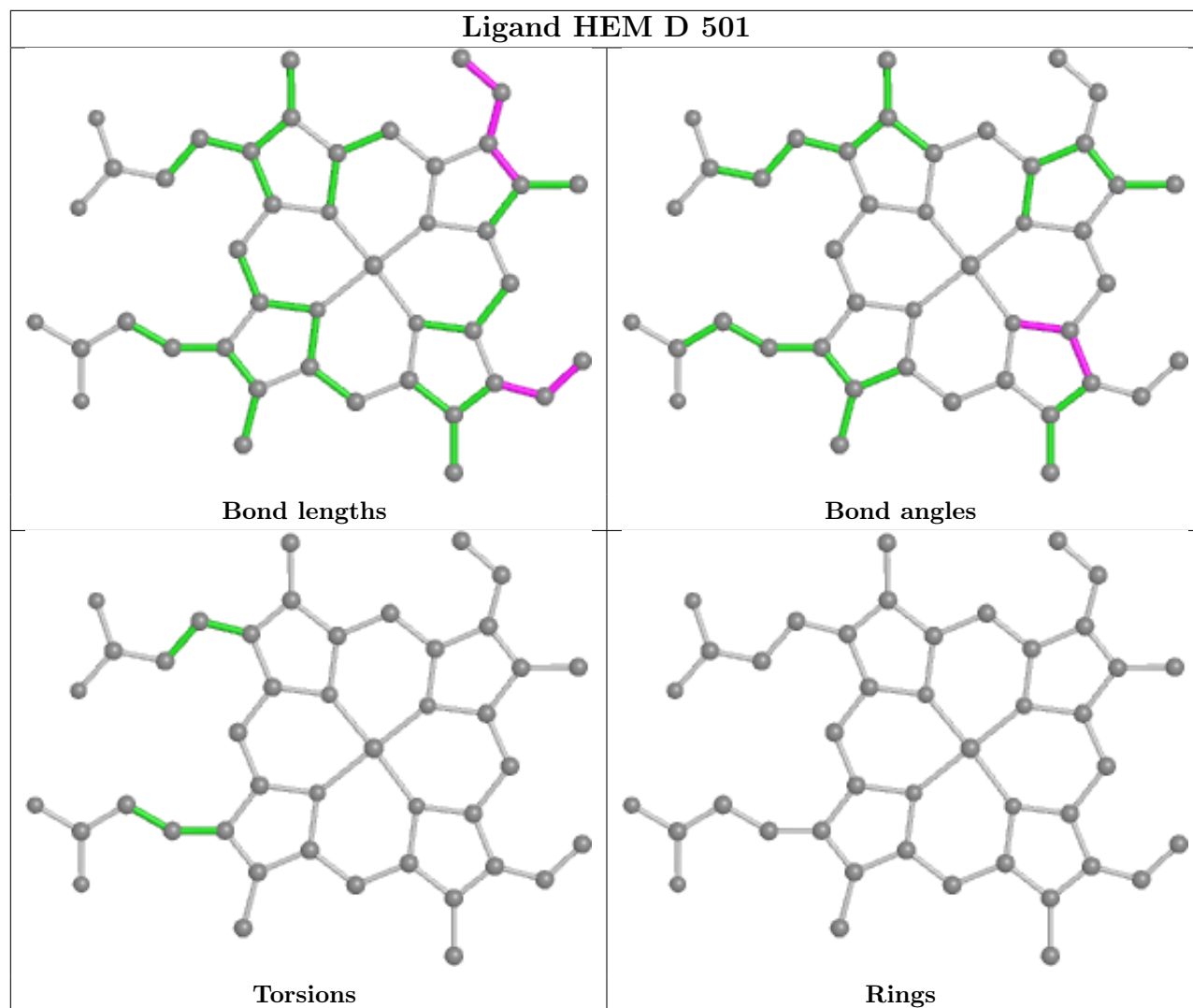
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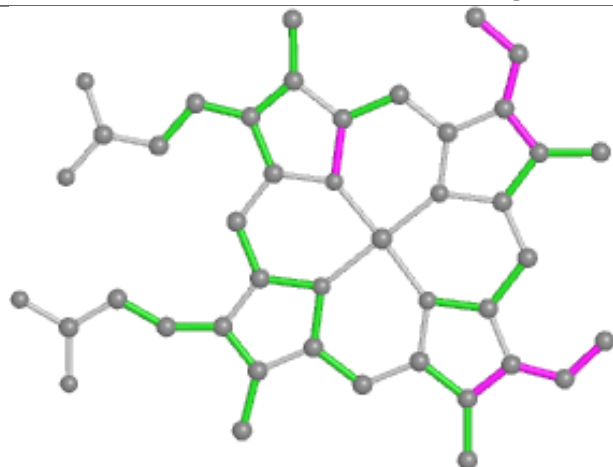
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	503	SMA	1	0
6	G	504	LOP	5	0
4	D	502	HEM	4	0
4	N	301	HEM	2	0
4	P	502	HEM	5	0
5	D	503	SMA	1	0
5	A	503	SMA	2	0
7	F	200	FES	2	0
4	P	501	HEM	6	0
6	D	504	LOP	1	0
6	J	504	LOP	1	0
4	J	502	HEM	7	0
4	M	502	HEM	2	0
4	E	301	HEM	1	0
6	A	504	LOP	3	0
6	M	504	LOP	3	0
7	O	200	FES	1	0
4	H	301	HEM	2	0
4	M	501	HEM	11	0
4	J	501	HEM	10	0
4	Q	301	HEM	1	0
5	J	503	SMA	1	0
4	A	501	HEM	4	0
4	A	502	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.

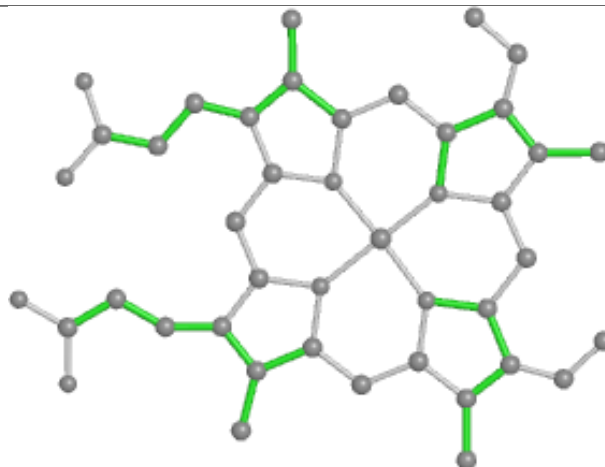




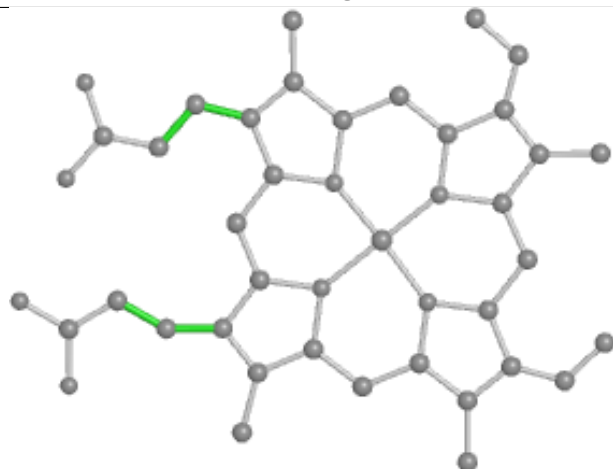
Ligand HEM G 501



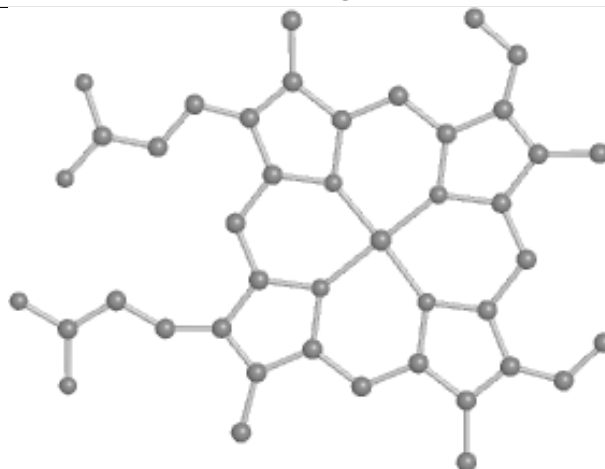
Bond lengths



Bond angles

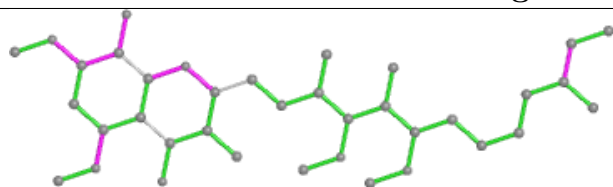


Torsions

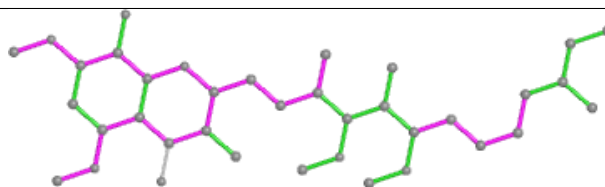


Rings

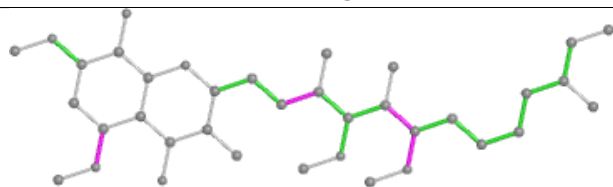
Ligand SMA P 503



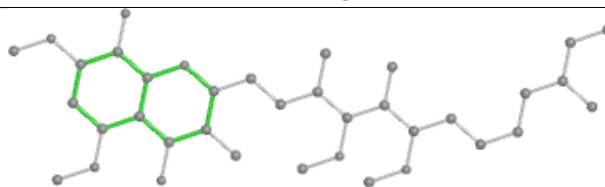
Bond lengths



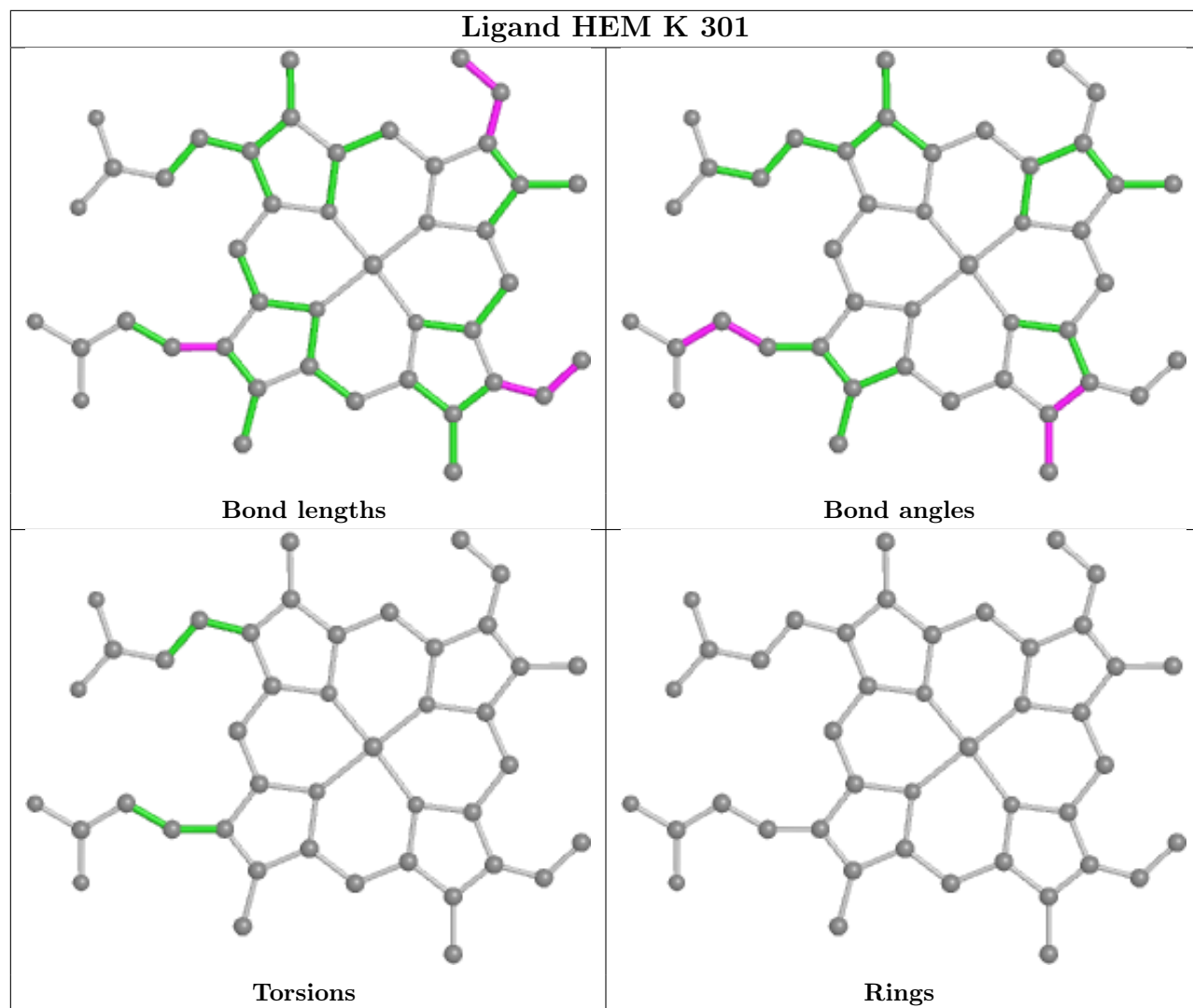
Bond angles



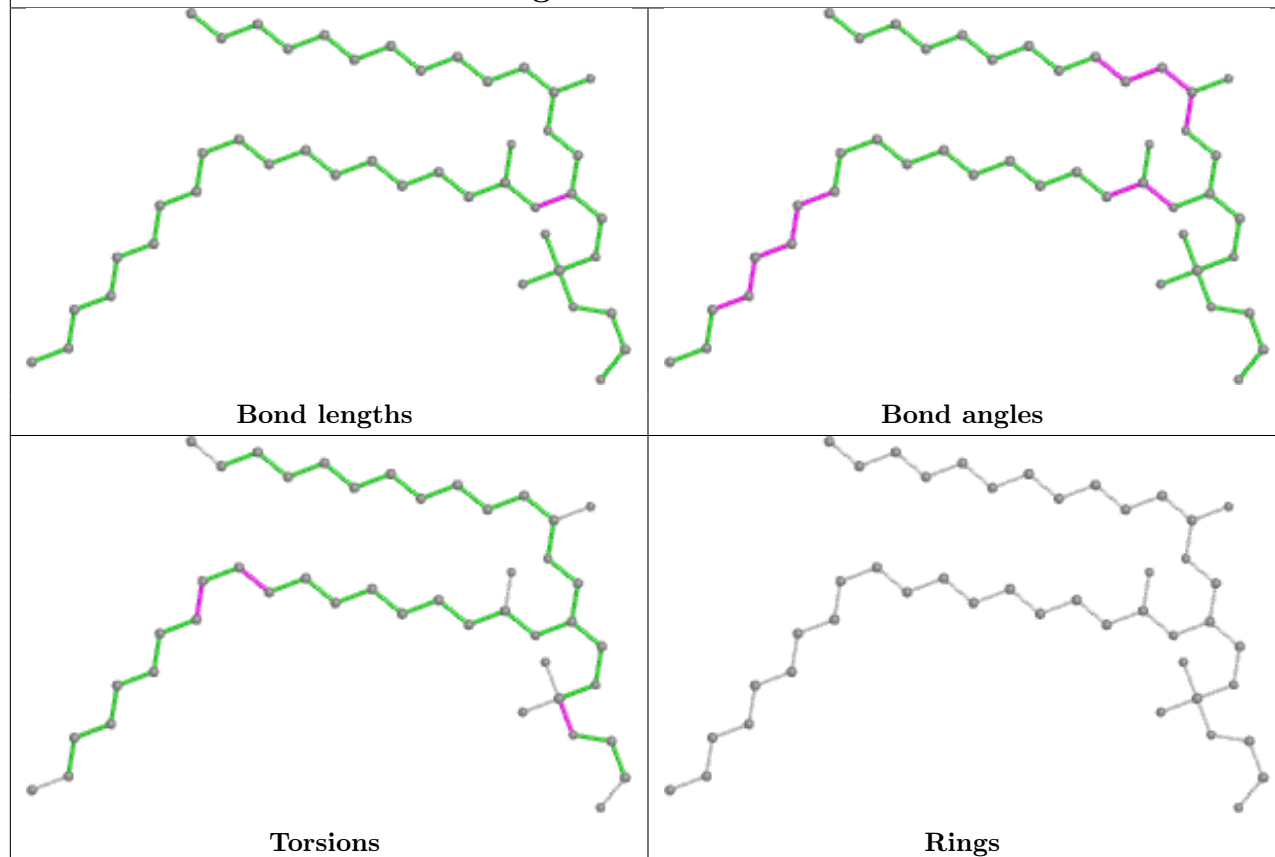
Torsions



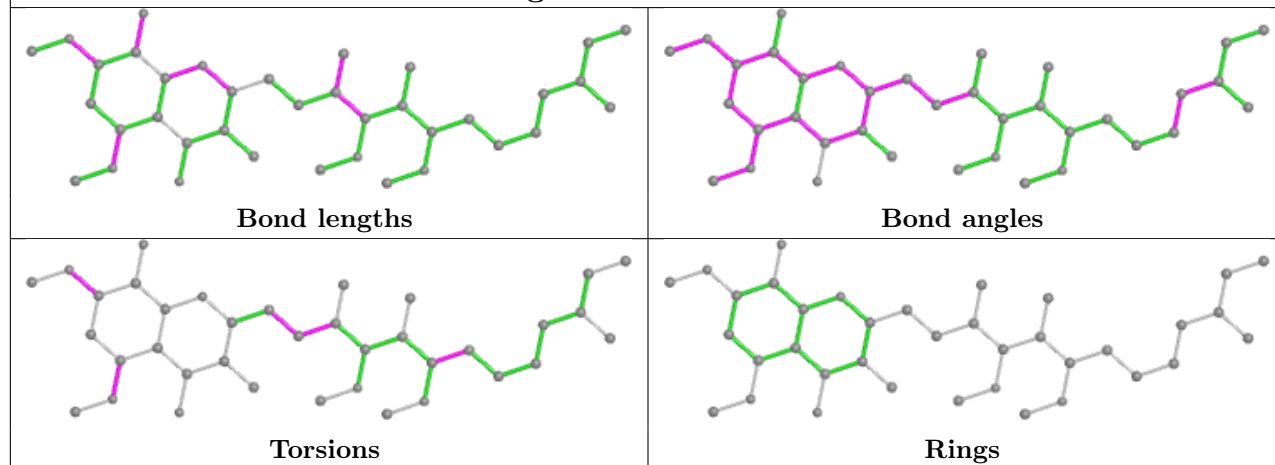
Rings

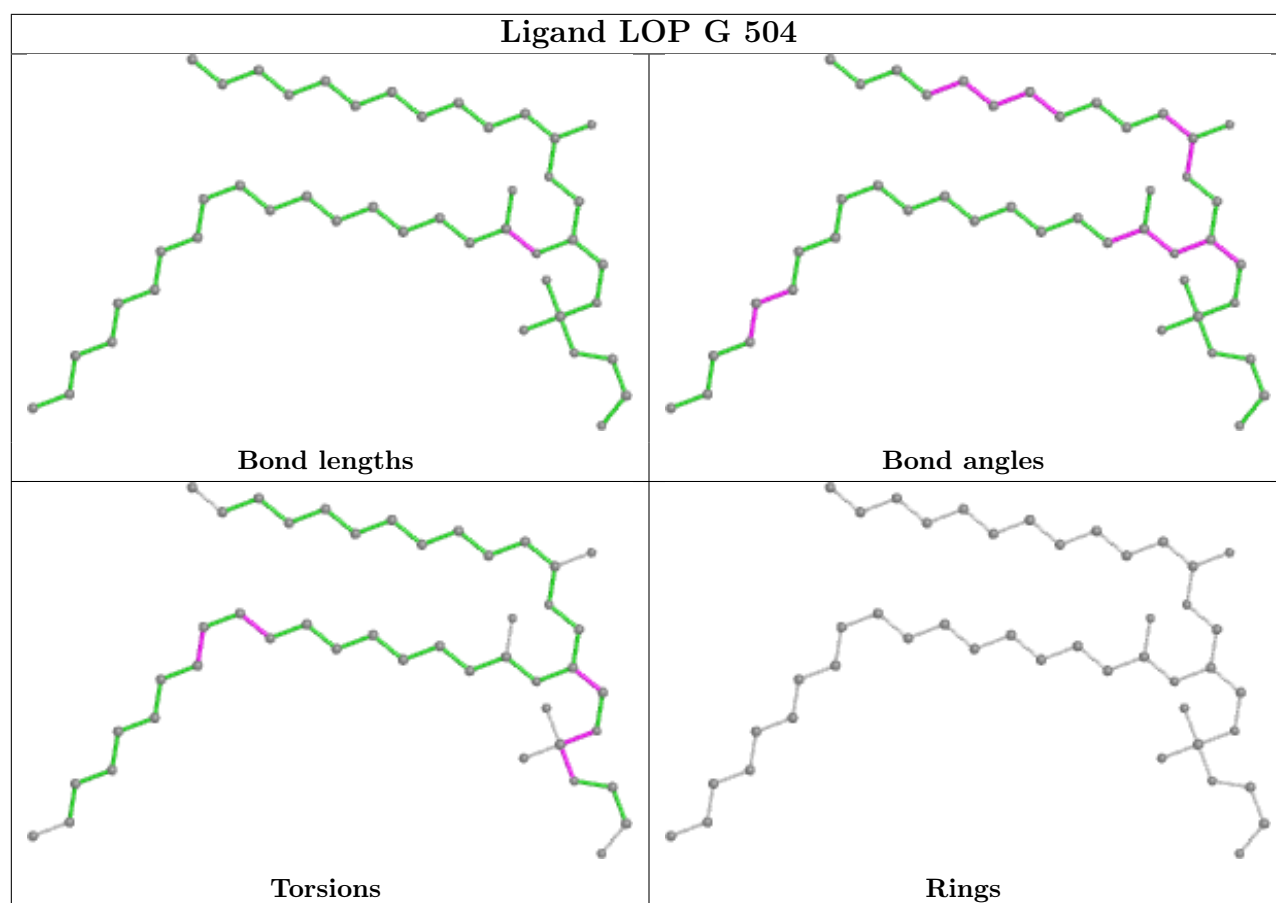


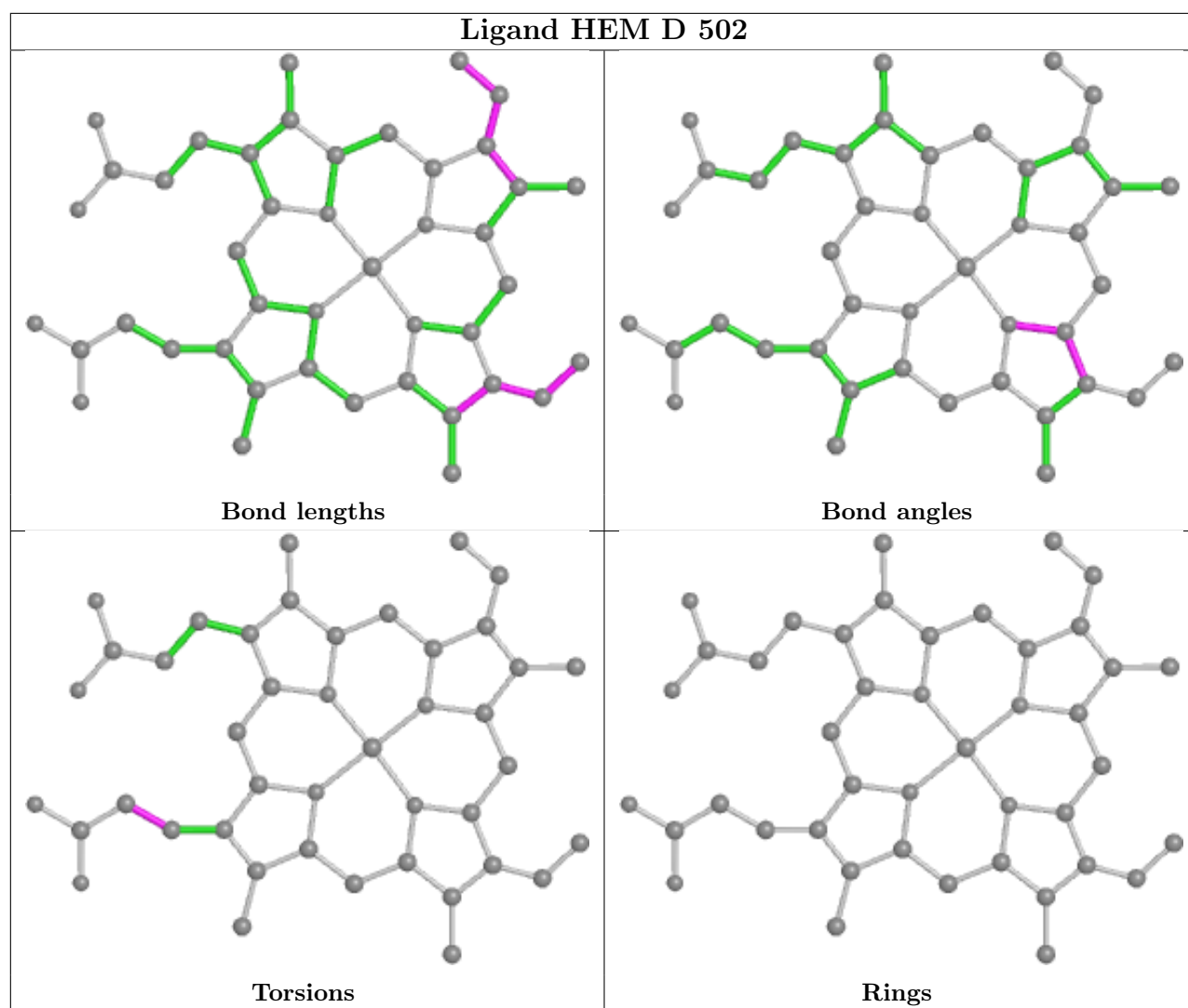
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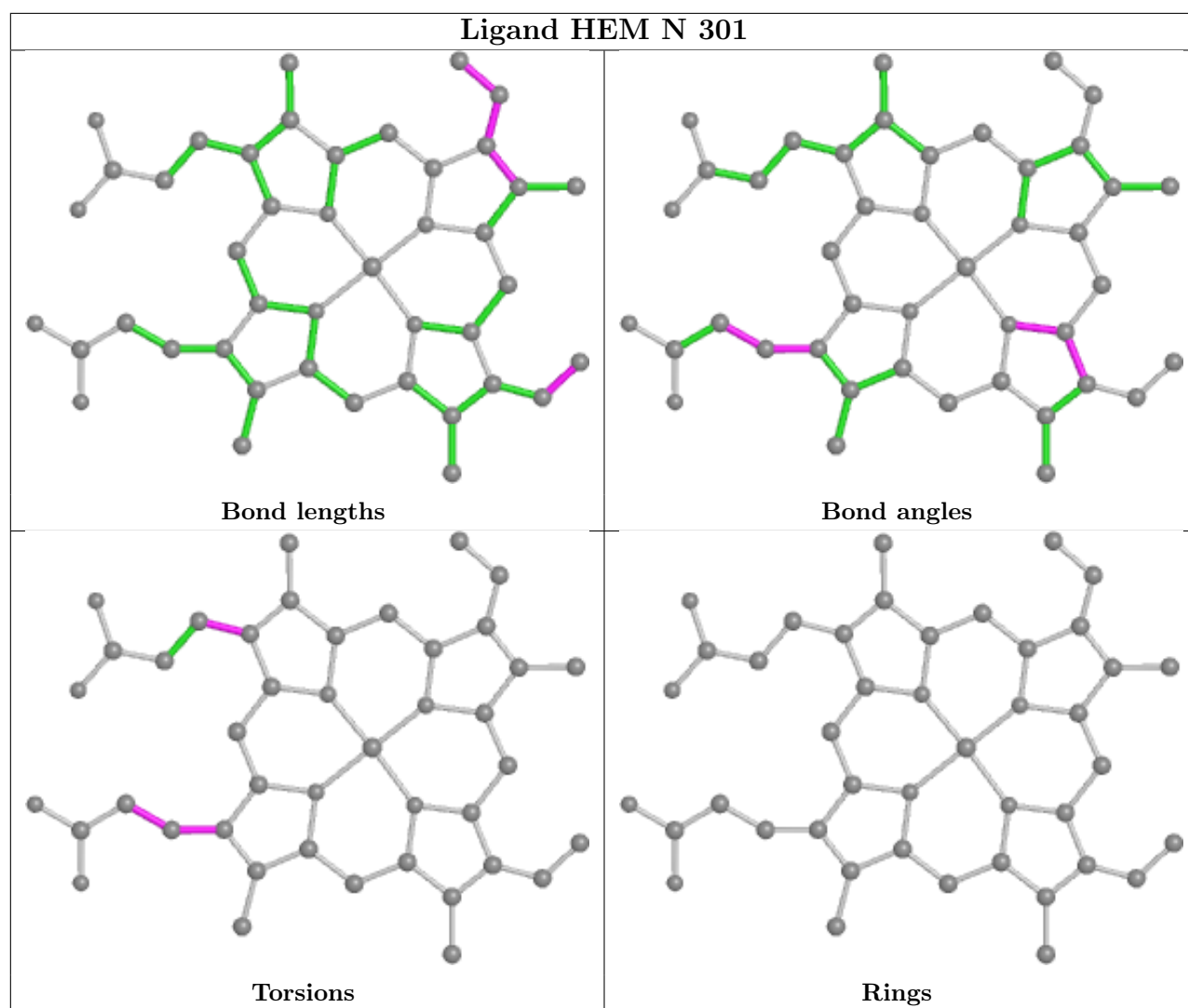


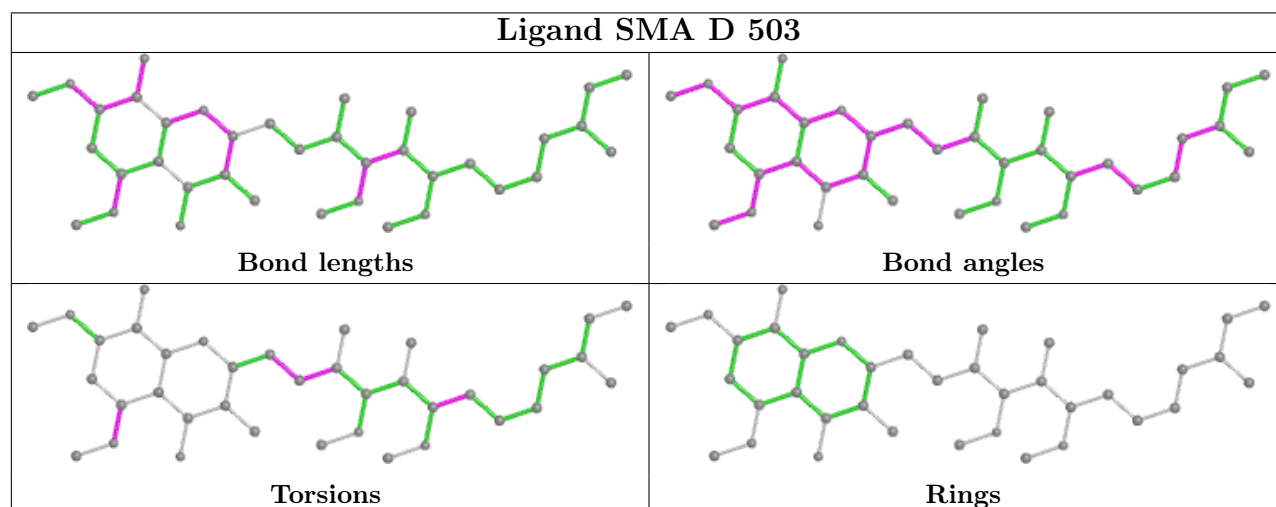
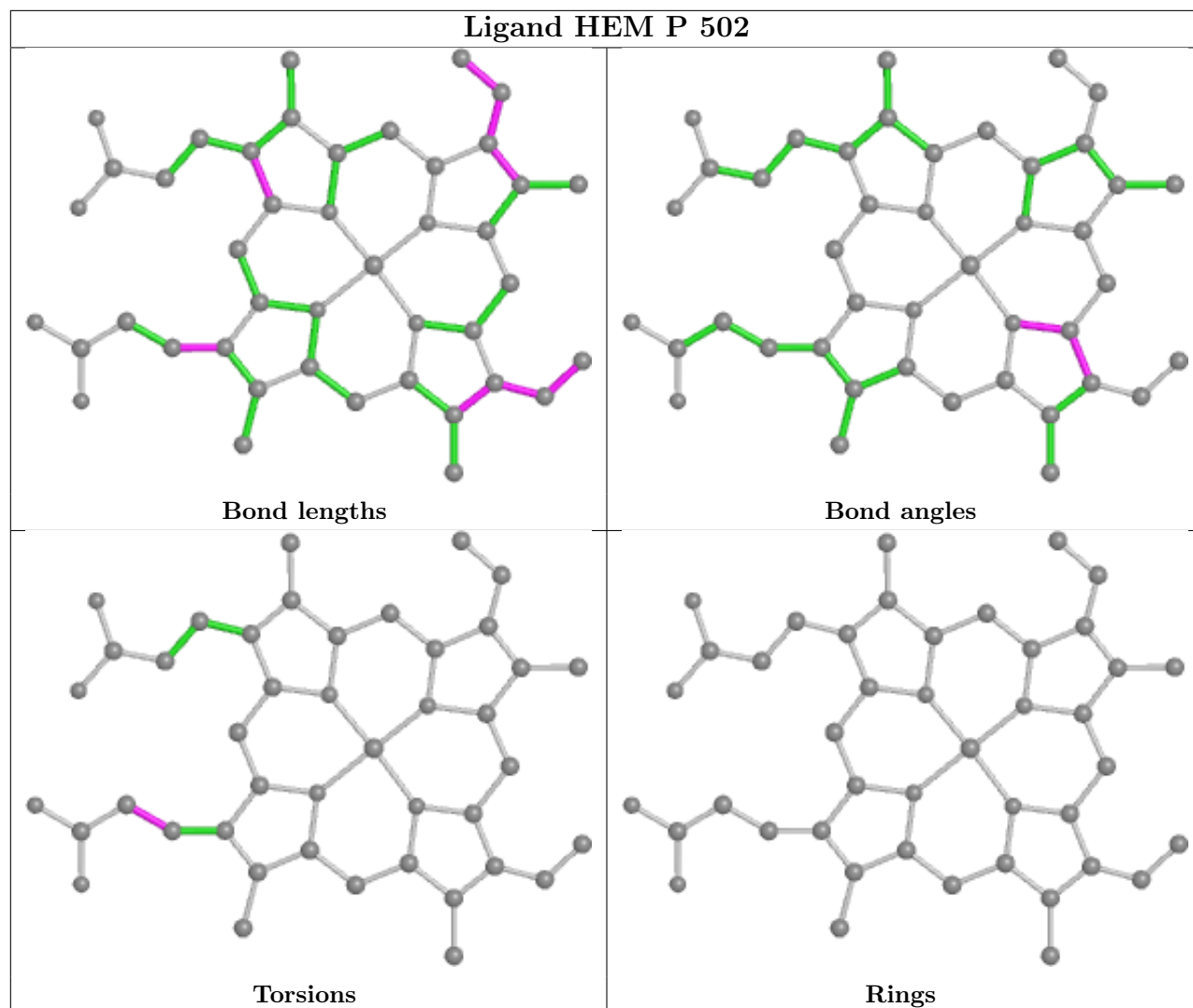
Ligand SMA G 503

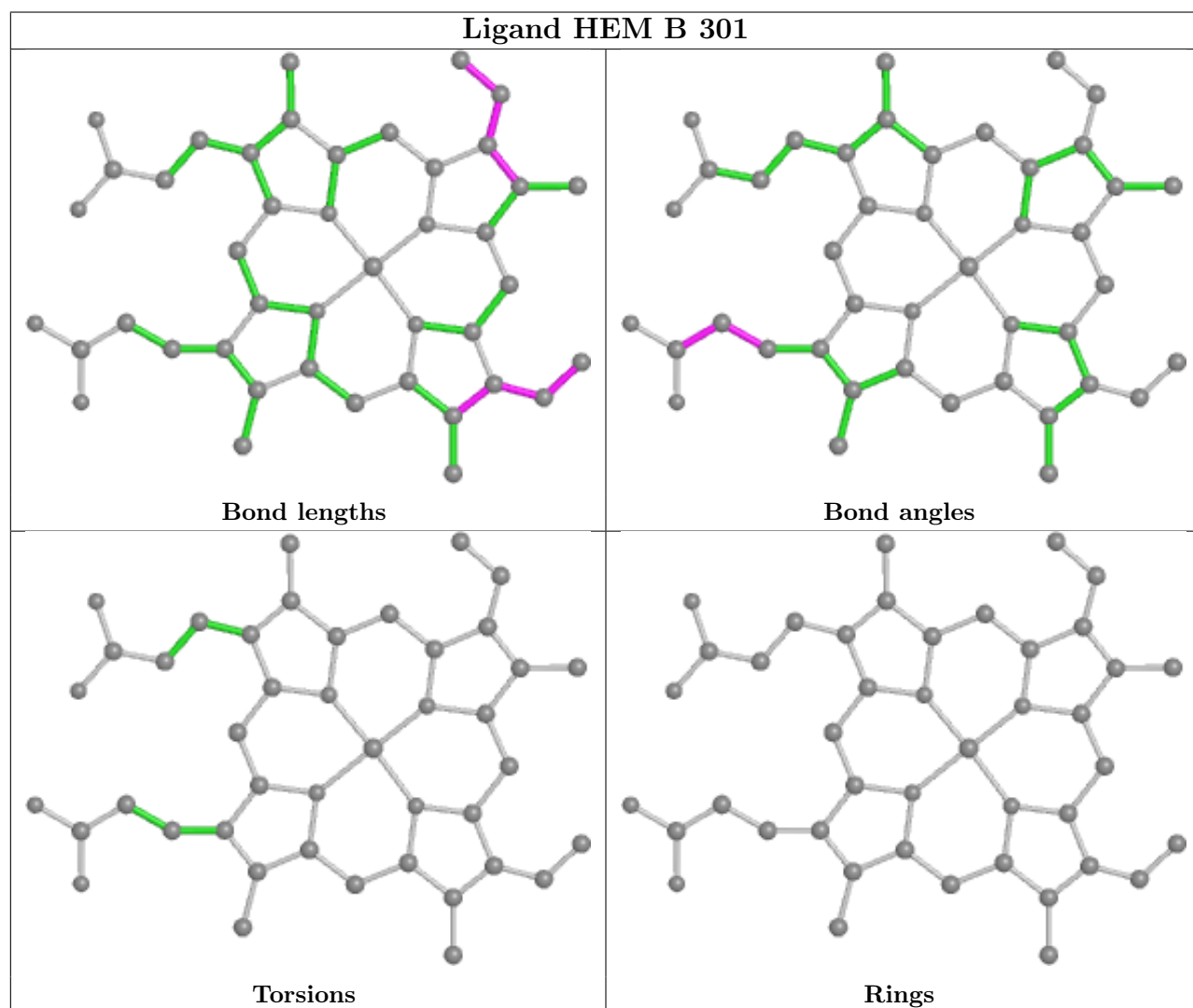
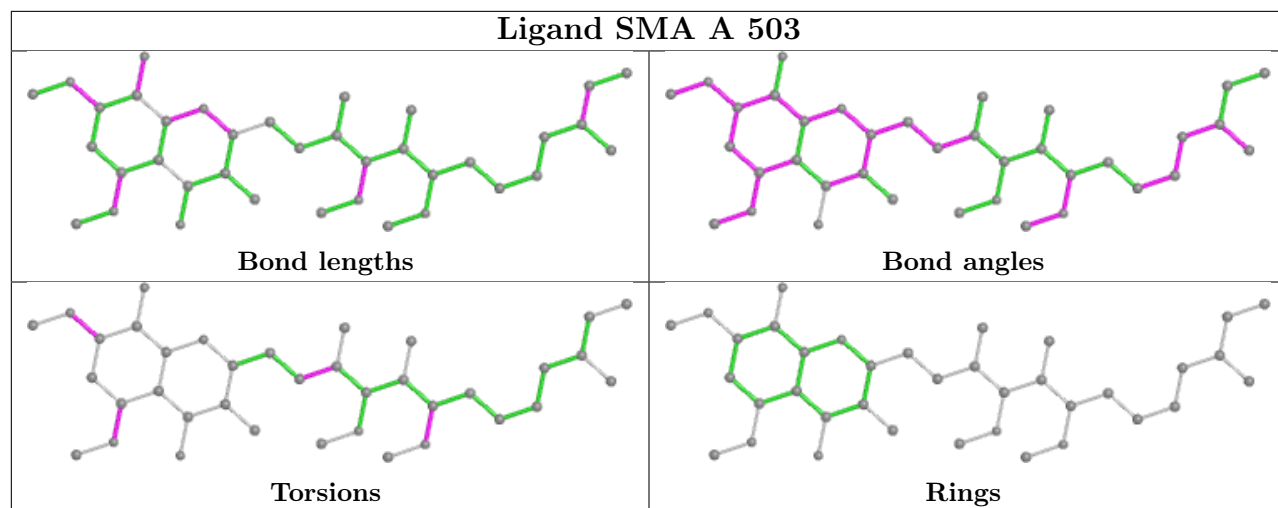


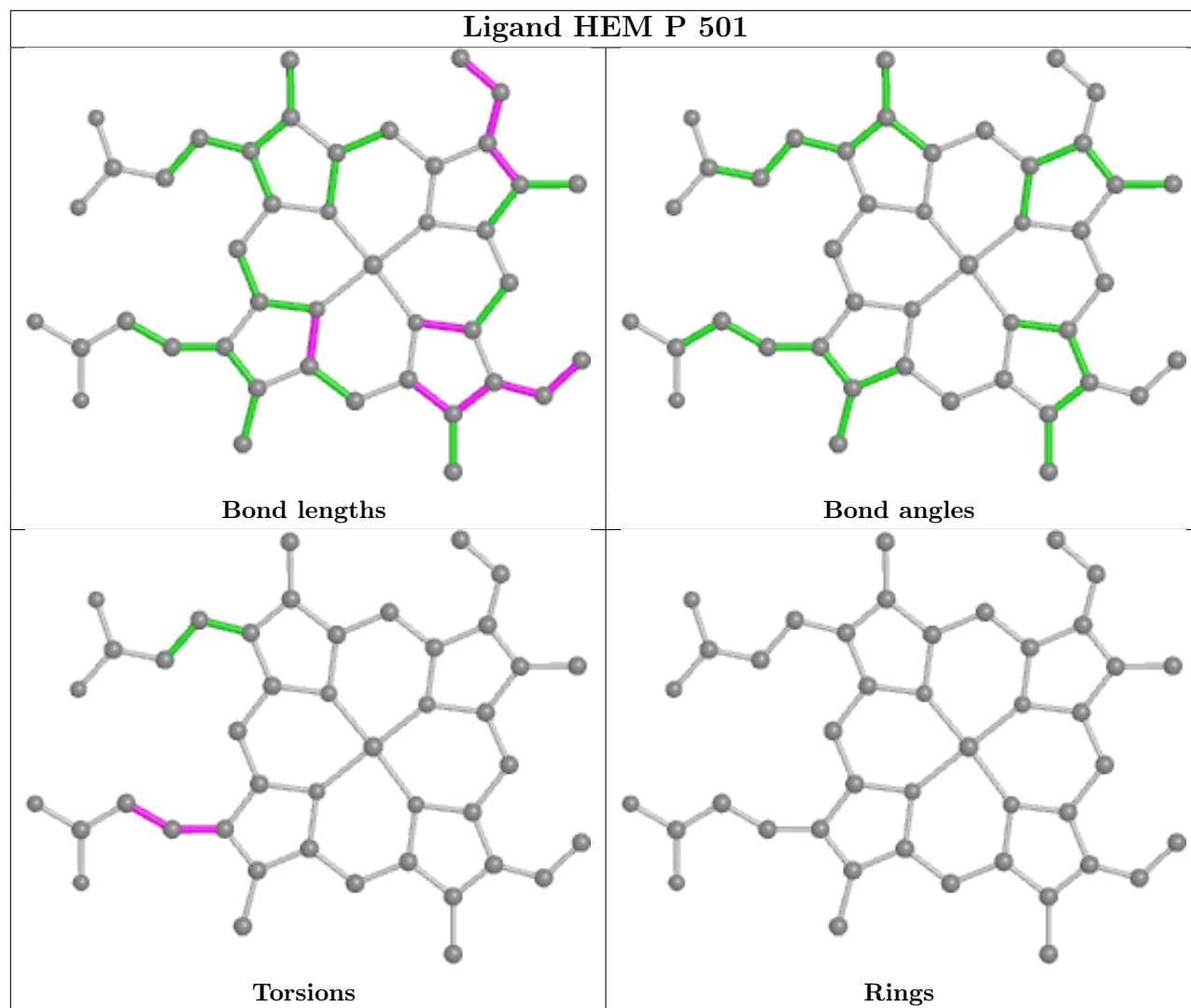




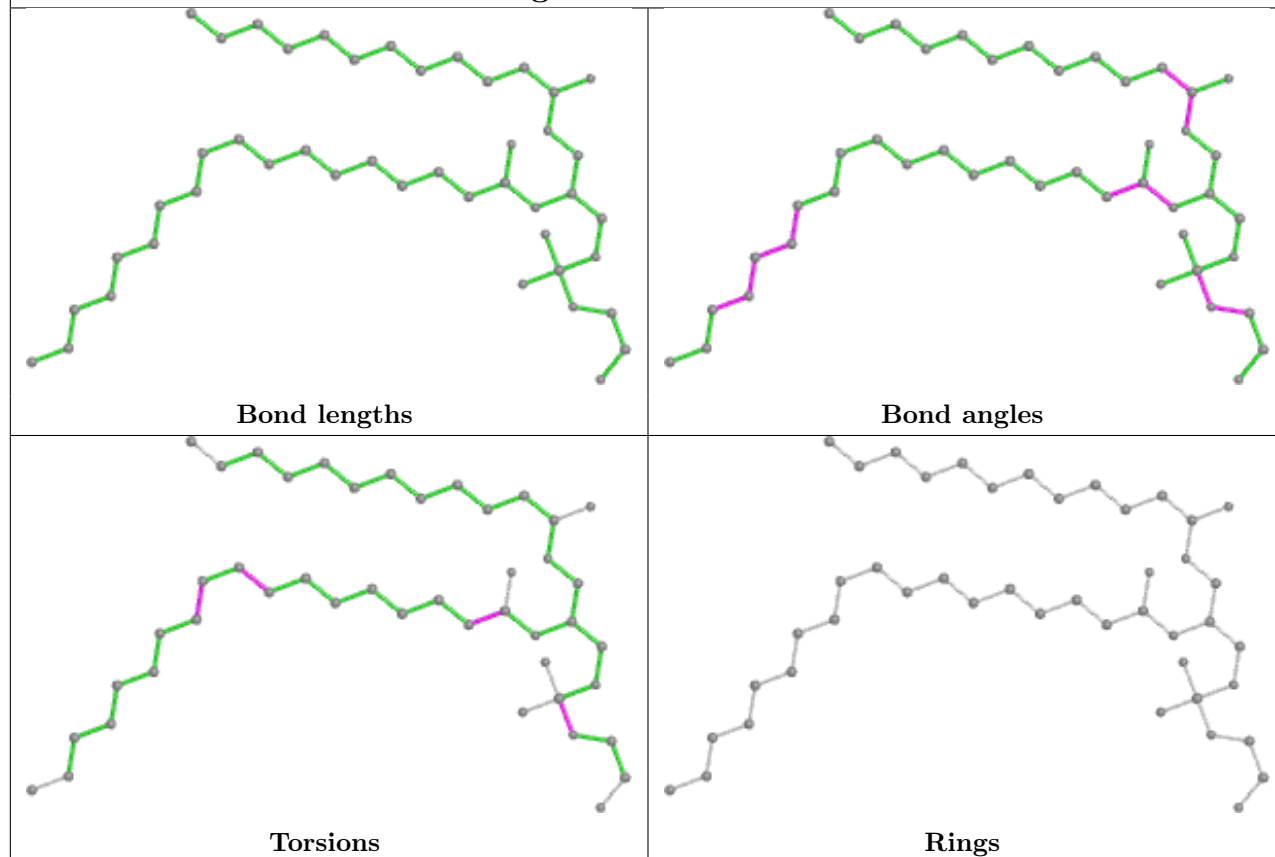




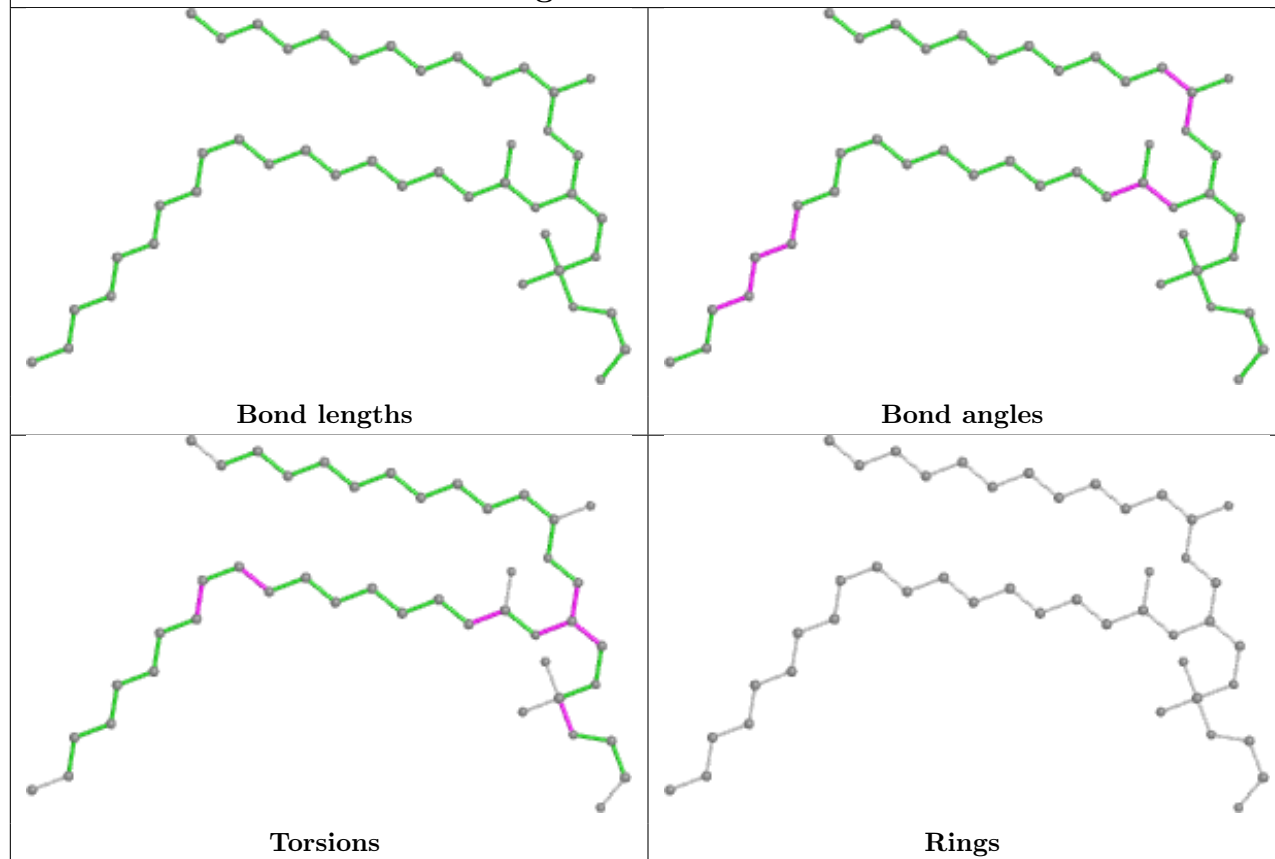


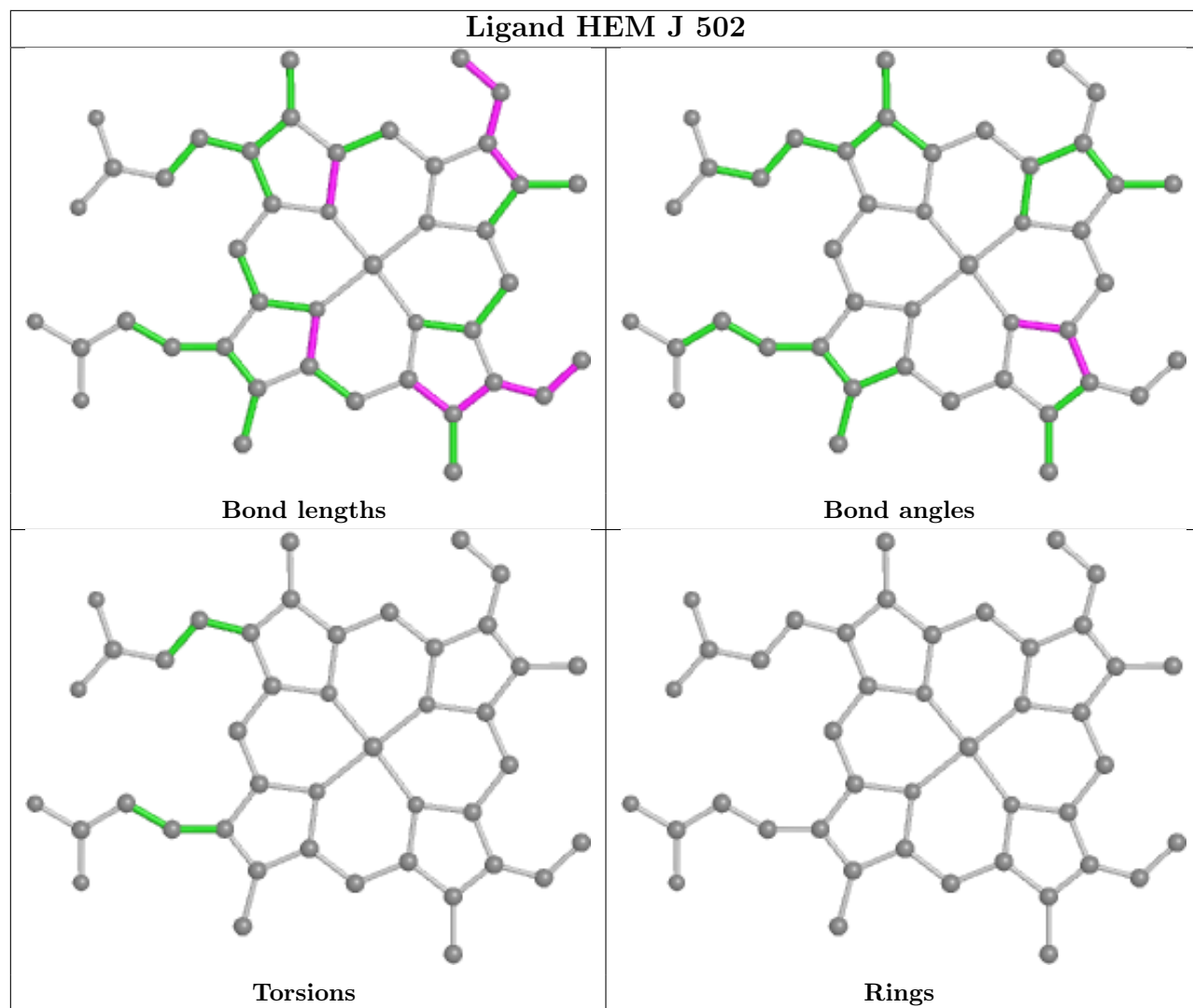


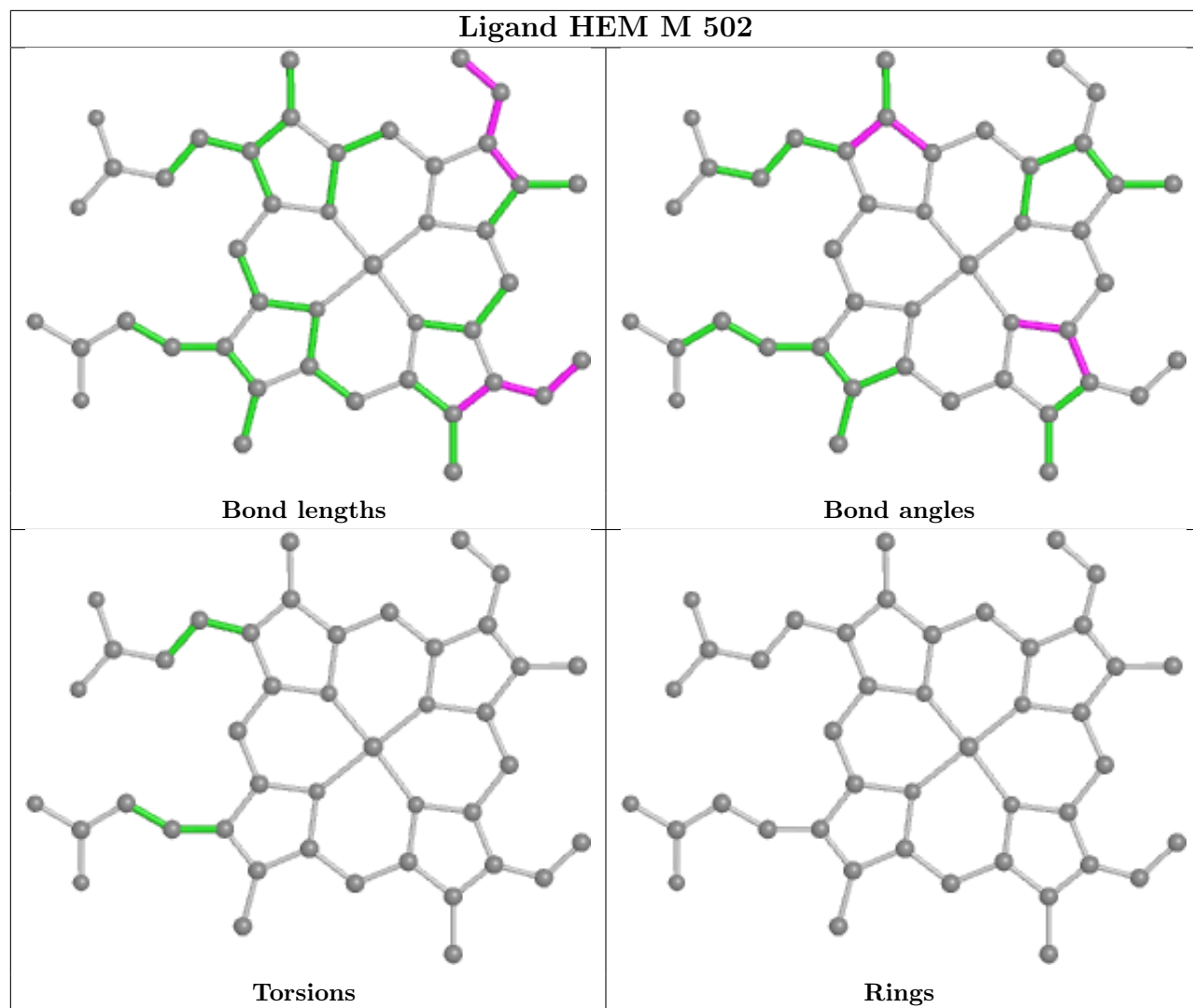
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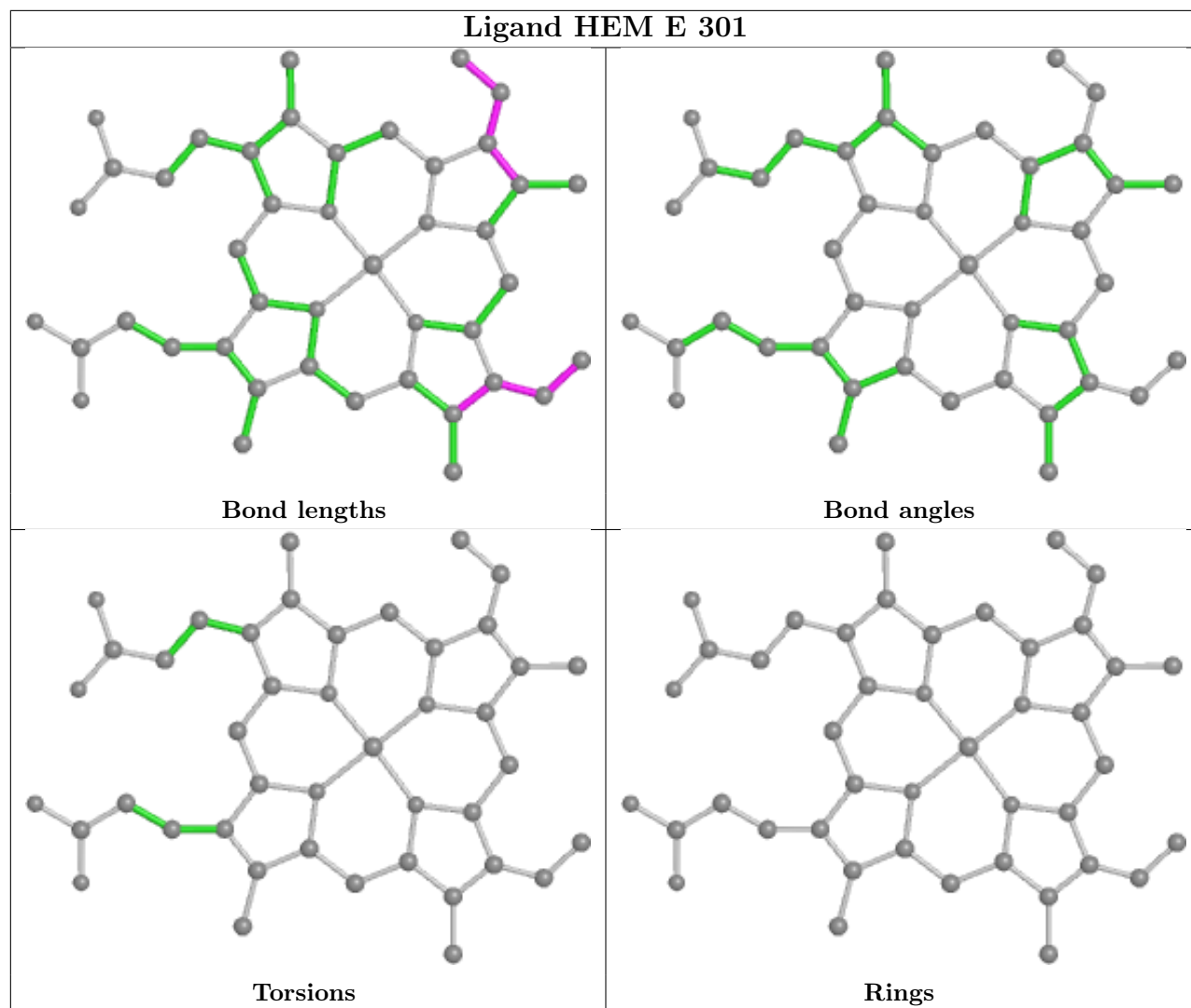


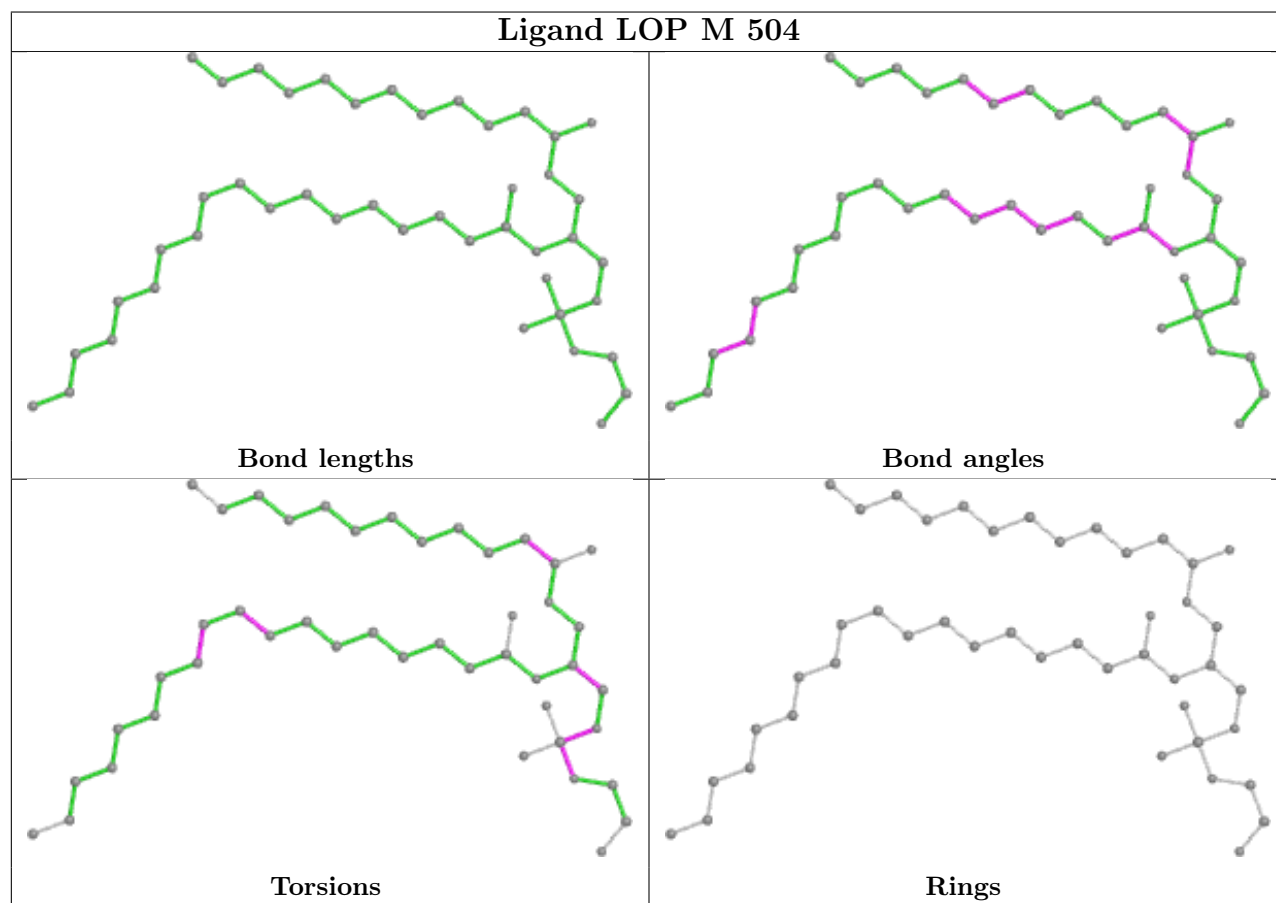
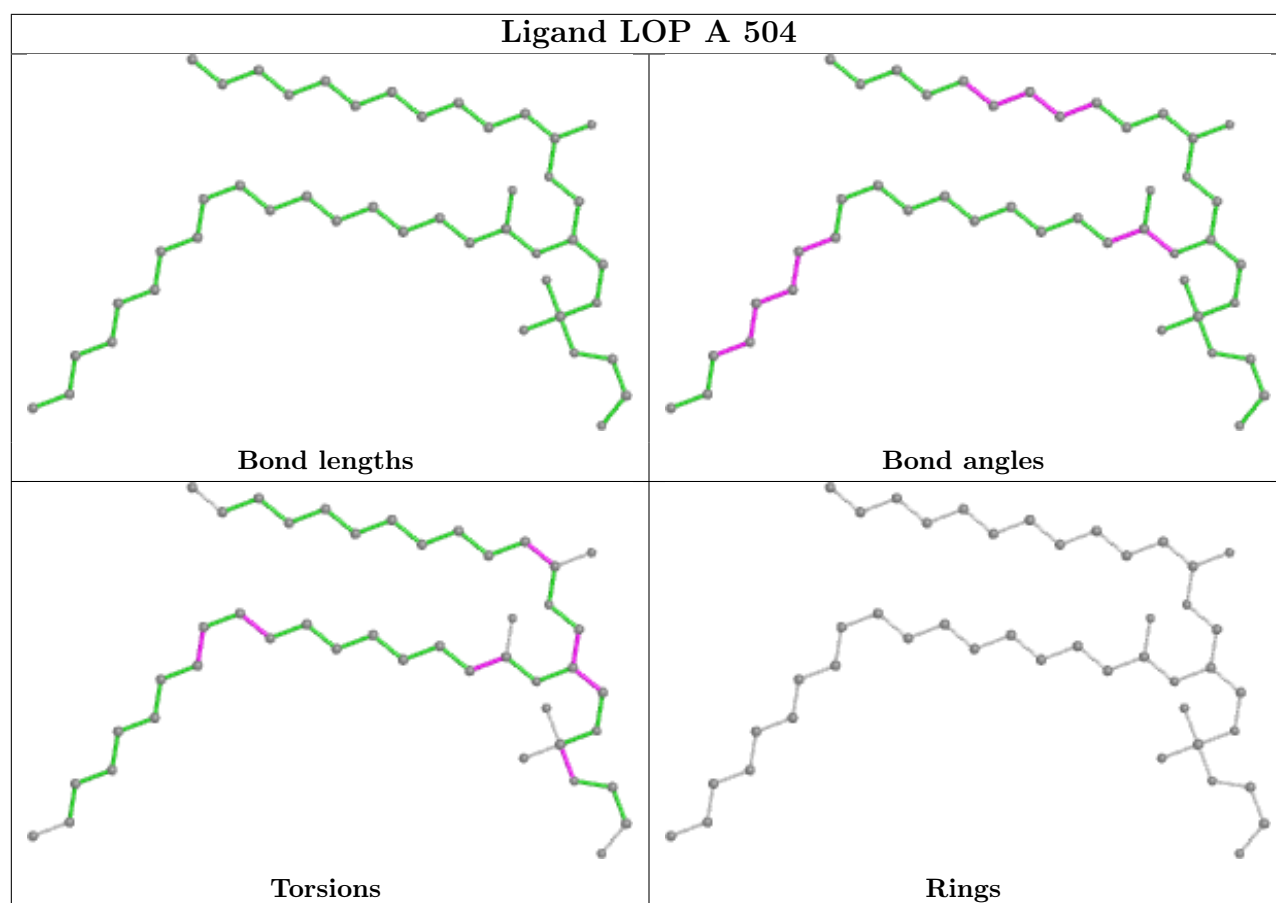
Ligand LOP J 504

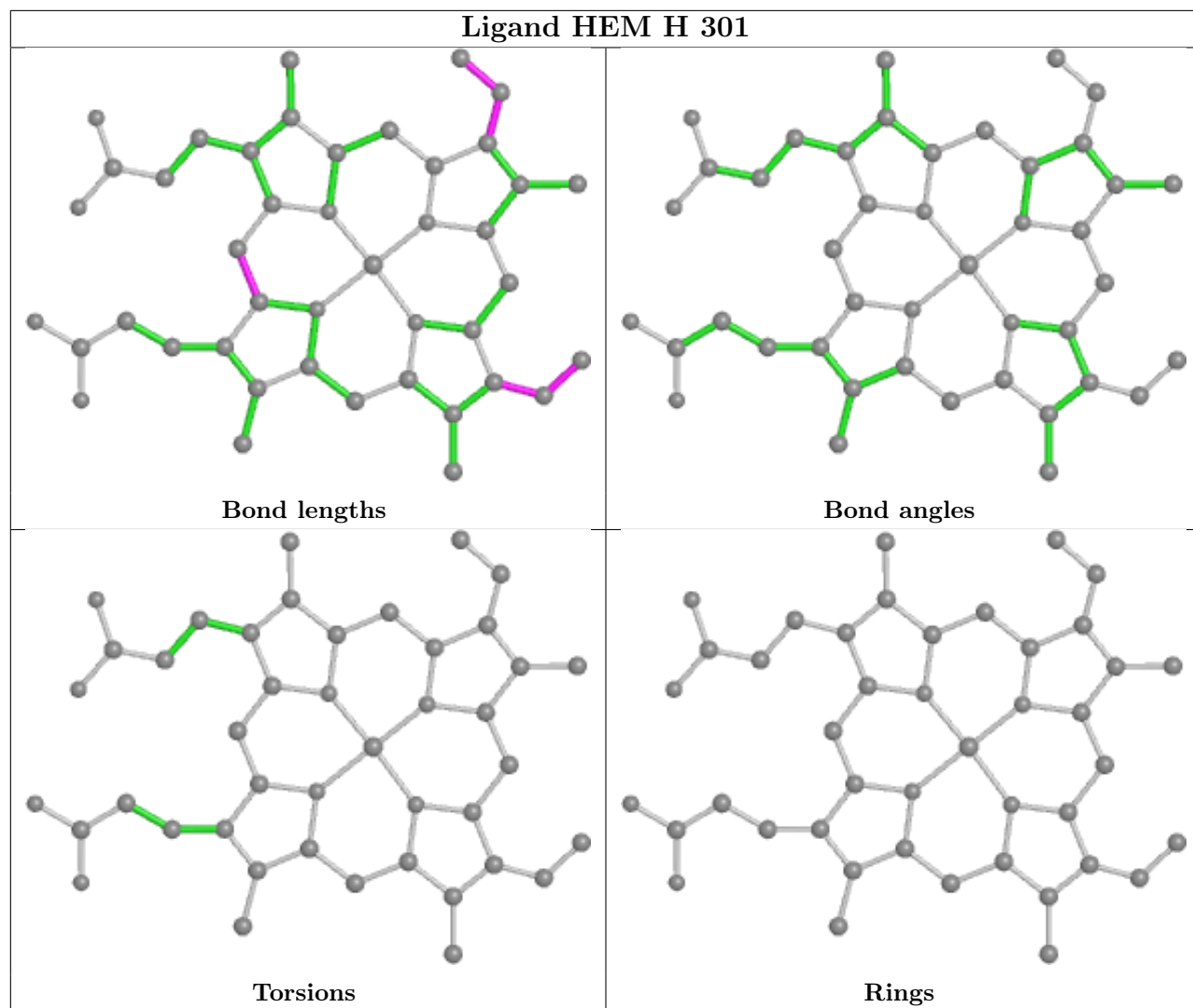


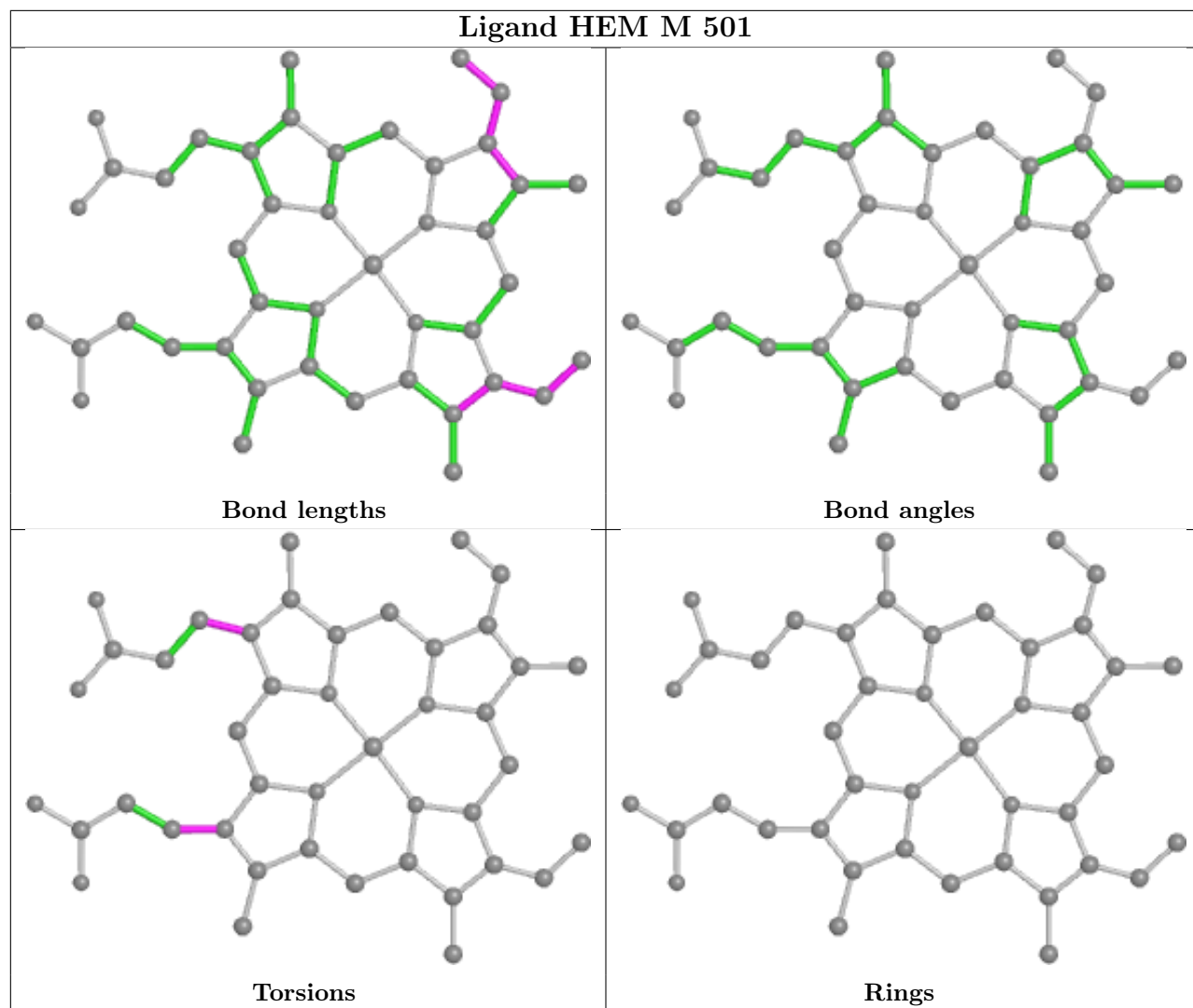


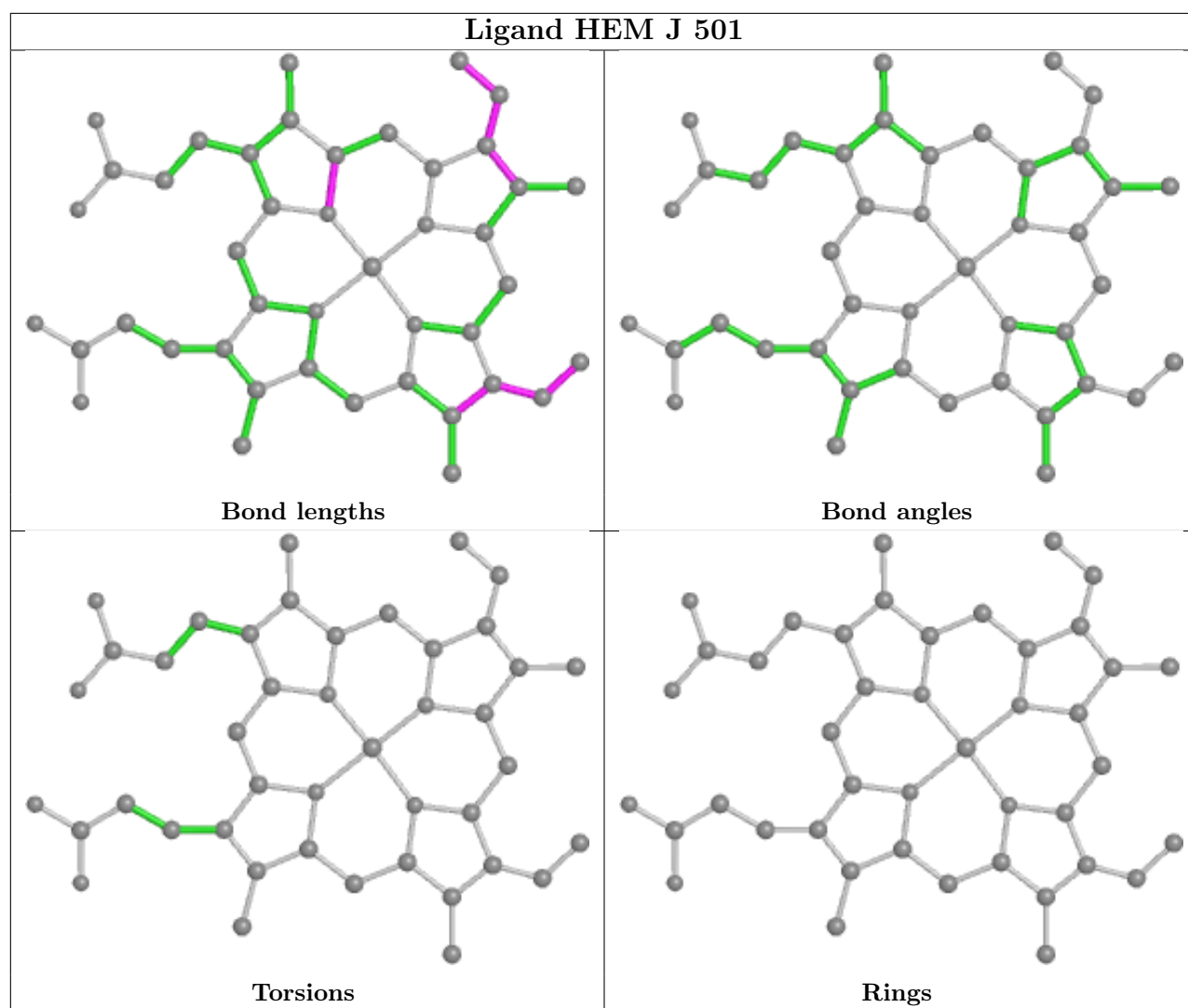


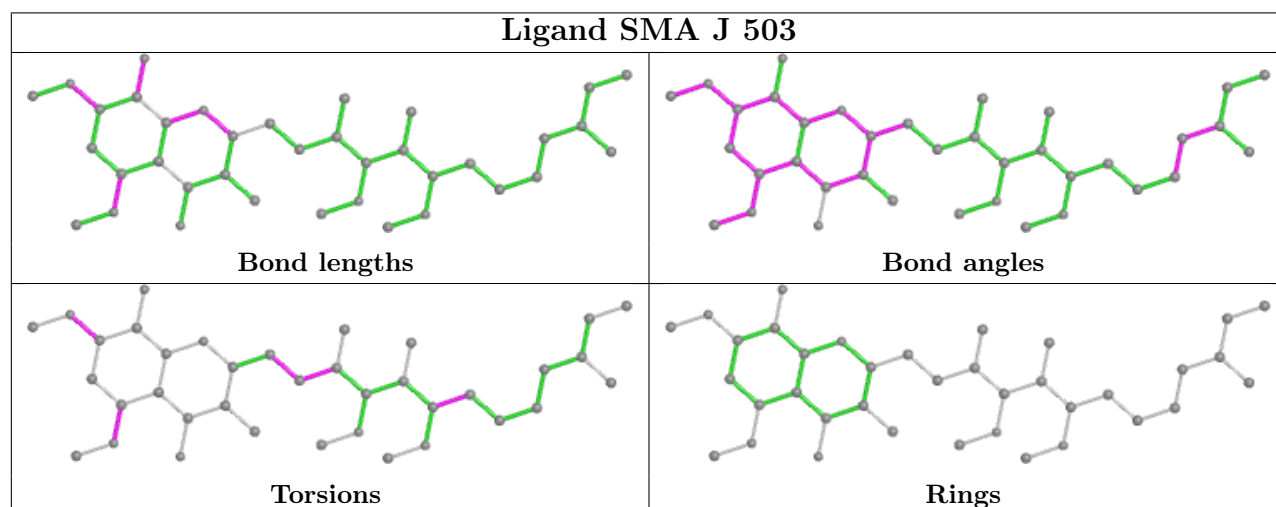
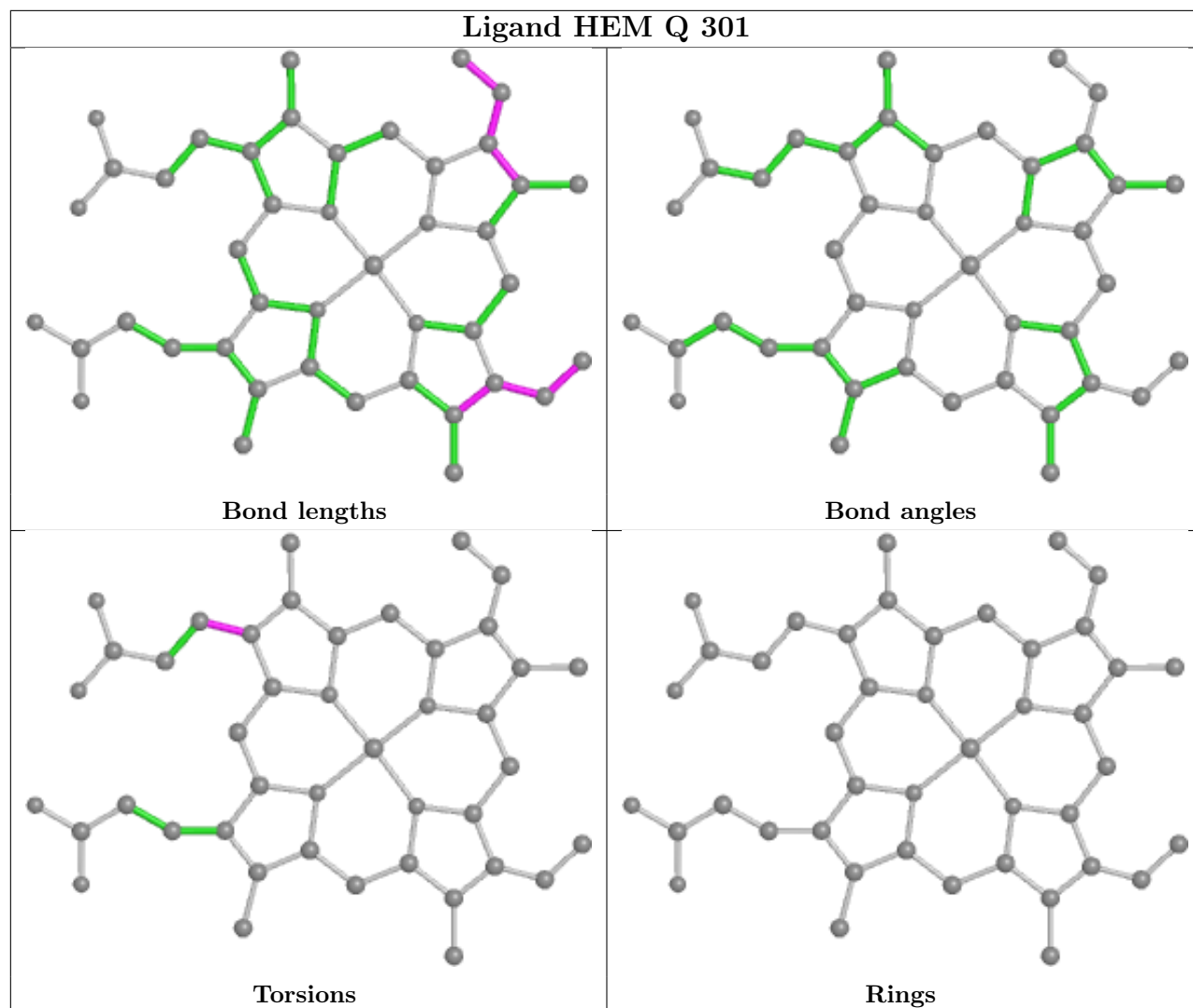


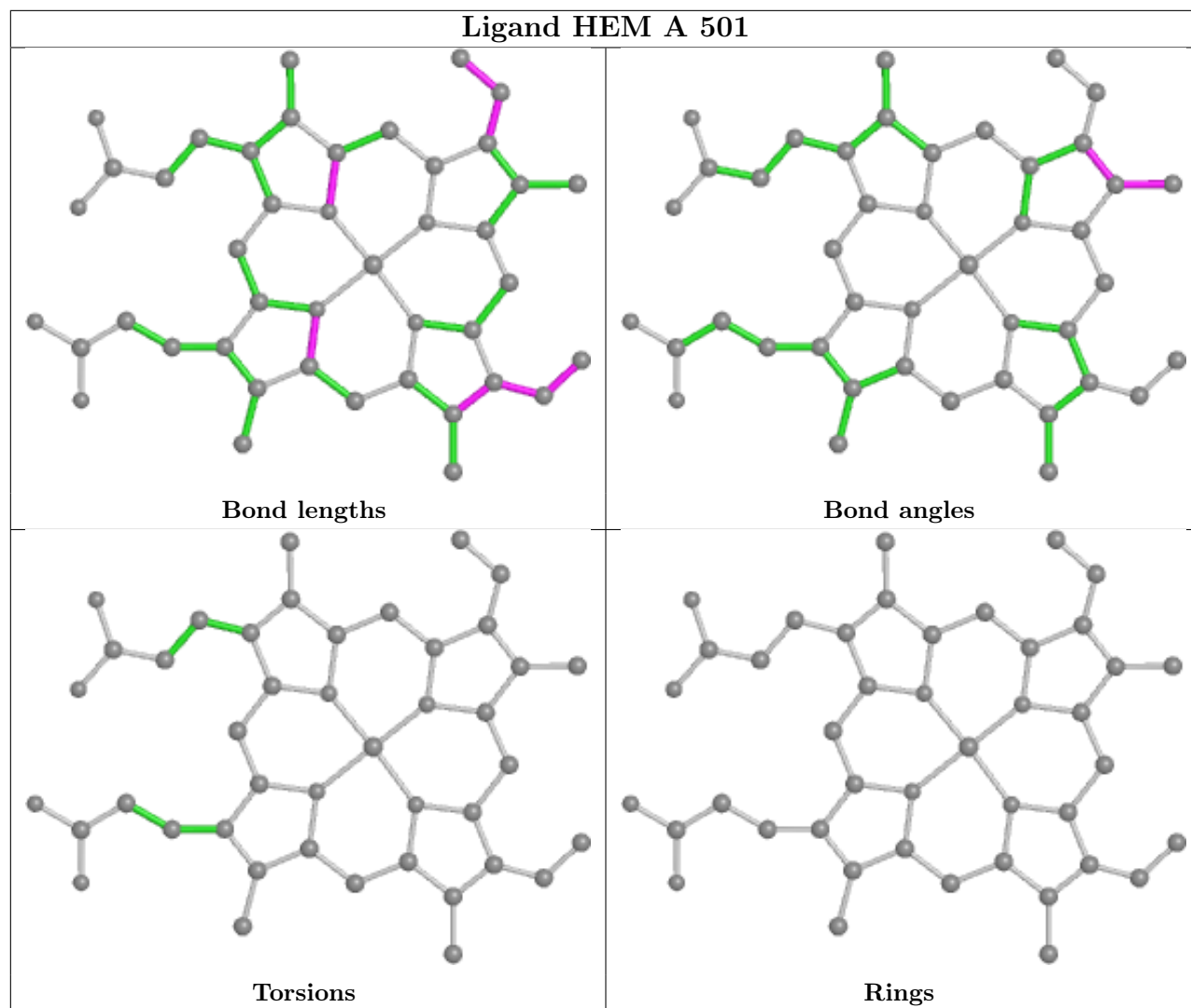


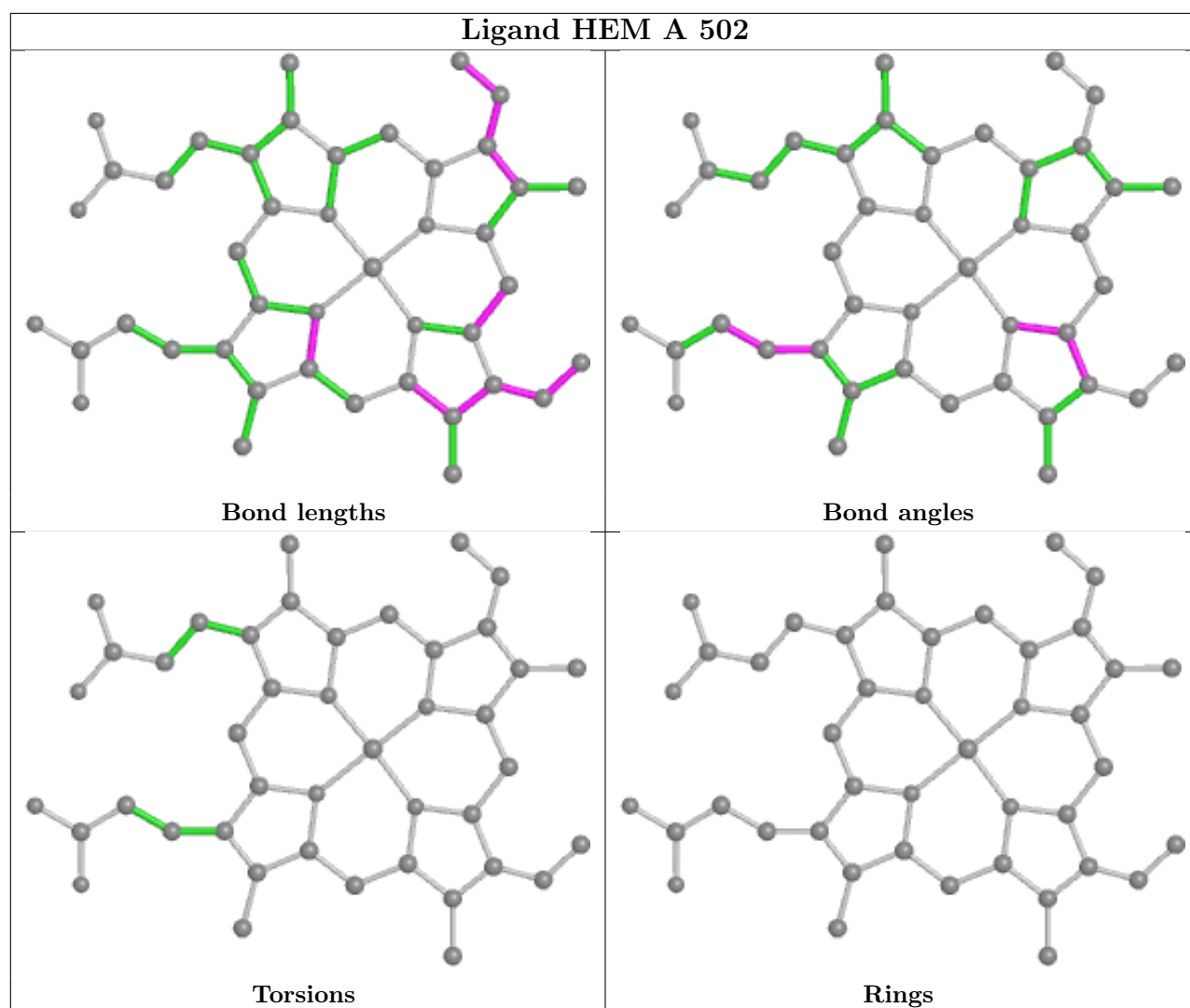












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.