



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 7, 2023 – 02:23 PM JST

PDB ID : 5XMJ  
Title : Crystal structure of quinol:fumarate reductase from *Desulfovibrio gigas*  
Authors : Guan, H.H.; Hsieh, Y.C.; Lin, P.R.; Chen, C.J.  
Deposited on : 2017-05-15  
Resolution : 3.60 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

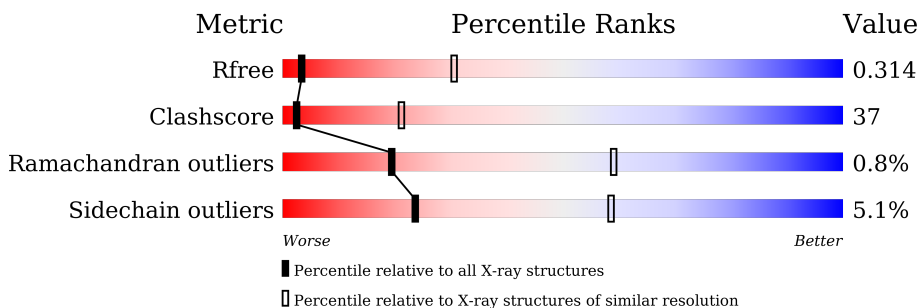
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.60 Å.

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





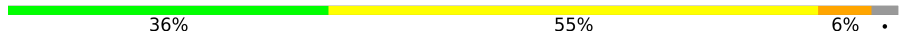
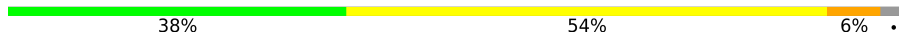
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	627	48% (green), 48% (yellow), 0% (orange), 0% (red), 0% (grey)
1	E	627	44% (green), 53% (yellow), 0% (orange), 0% (red), 0% (grey)
1	I	627	43% (green), 52% (yellow), 0% (orange), 0% (red), 0% (grey)
1	M	627	42% (green), 52% (yellow), 0% (orange), 0% (red), 5% (grey)
2	B	264	48% (green), 41% (yellow), 0% (orange), 0% (red), 9% (grey)
2	F	264	45% (green), 44% (yellow), 0% (orange), 0% (red), 9% (grey)
2	J	264	45% (green), 42% (yellow), 0% (orange), 0% (red), 9% (grey)

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Mol	Chain	Length	Quality of chain
2	N	264	
3	C	218	
3	G	218	
3	K	218	
3	O	218	

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
10	LMT	C	303	-	-	X	-
10	LMT	O	301	-	-	X	-
4	FAD	I	701	-	-	X	-
5	FUM	A	702	-	-	X	-
5	FUM	E	702	-	-	X	-
5	FUM	M	702	-	-	X	-
6	F3S	F	301	-	-	X	-

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 34118 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 fumarate reductase flavoprotein subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	622	4769	2976	854	903	36	0	0	0
1	E	622	4767	2975	853	903	36	0	0	0
1	I	622	4767	2975	853	903	36	0	0	0
1	M	622	4769	2976	854	903	36	0	0	0

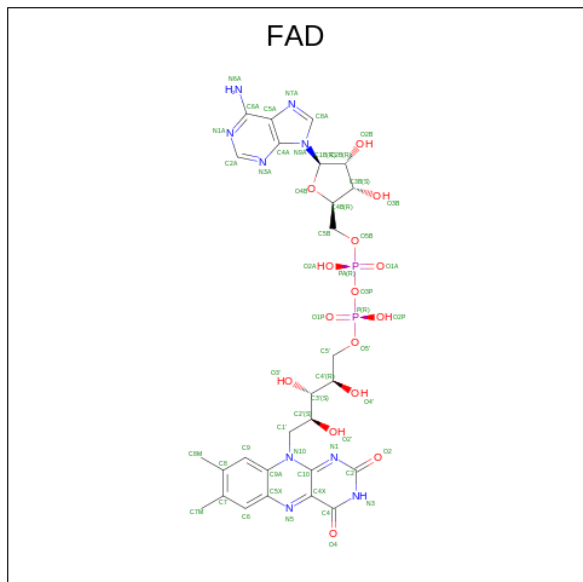
- Molecule 2 is a protein called Succinate dehydrogenase iron-sulfur subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	240	1879	1171	325	355	28	0	0	0
2	F	240	1879	1171	325	355	28	0	0	0
2	J	240	1879	1171	325	355	28	0	0	0
2	N	240	1879	1171	325	355	28	0	0	0

- Molecule 3 is a protein called fumarate reductase respiratory complex.

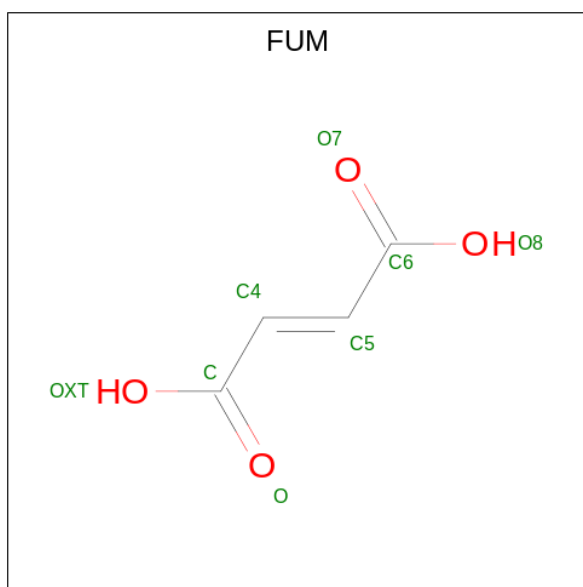
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	212	1693	1130	282	265	16	0	0	0
3	G	212	1693	1130	282	265	16	0	0	0
3	K	212	1693	1130	282	265	16	0	0	0
3	O	212	1693	1130	282	265	16	0	0	0

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).



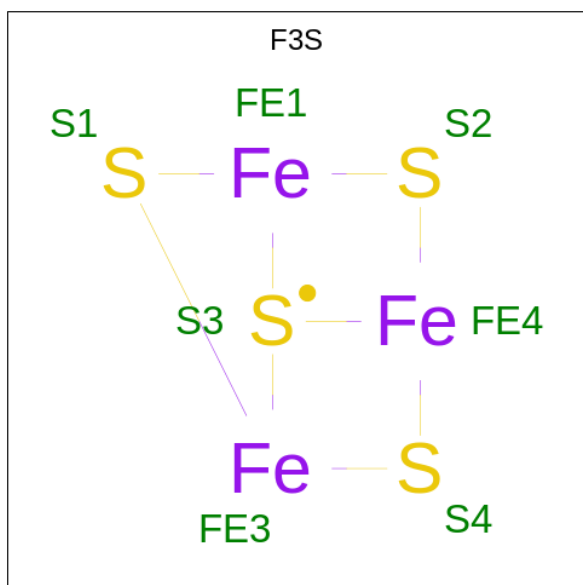
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	N	O	P			
4	A	1	Total	53	27	9	15	2	0	0
4	E	1	Total	53	27	9	15	2	0	0
4	I	1	Total	53	27	9	15	2	0	0
4	M	1	Total	53	27	9	15	2	0	0

- Molecule 5 is FUMARIC ACID (three-letter code: FUM) (formula:  $C_4H_4O_4$ ).



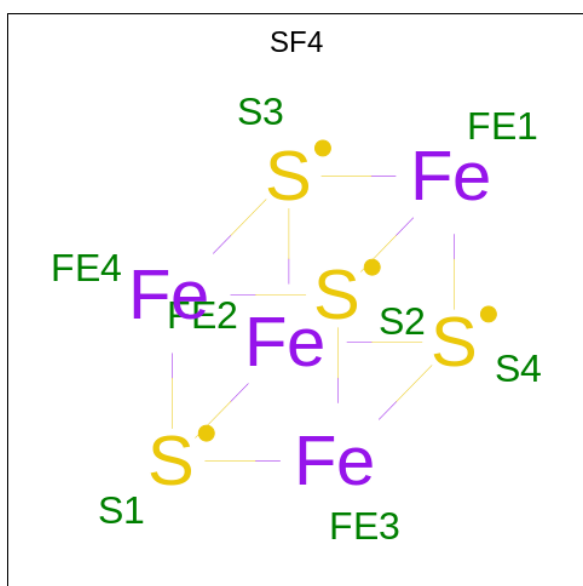
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 8 4 4	0	0
5	E	1	Total C O 8 4 4	0	0
5	I	1	Total C O 8 4 4	0	0
5	M	1	Total C O 8 4 4	0	0

- Molecule 6 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe<sub>3</sub>S<sub>4</sub>).



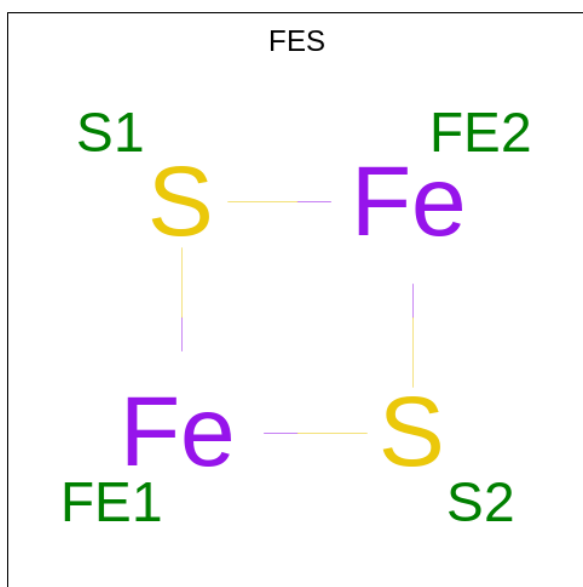
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	Fe	S	0	0
			7	3	4		
6	F	1	Total	Fe	S	0	0
			7	3	4		
6	J	1	Total	Fe	S	0	0
			7	3	4		
6	N	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 7 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



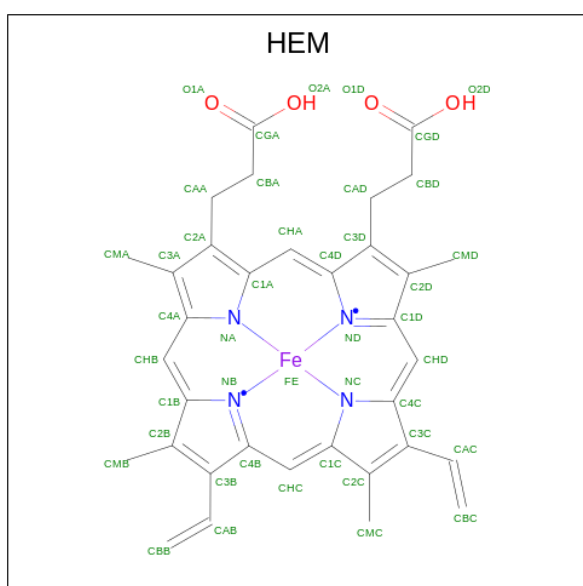
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	Fe	S	0	0
			8	4	4		
7	F	1	Total	Fe	S	0	0
			8	4	4		
7	J	1	Total	Fe	S	0	0
			8	4	4		
7	N	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 8 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total Fe S 4 2 2	0	0
8	F	1	Total Fe S 4 2 2	0	0
8	J	1	Total Fe S 4 2 2	0	0
8	N	1	Total Fe S 4 2 2	0	0

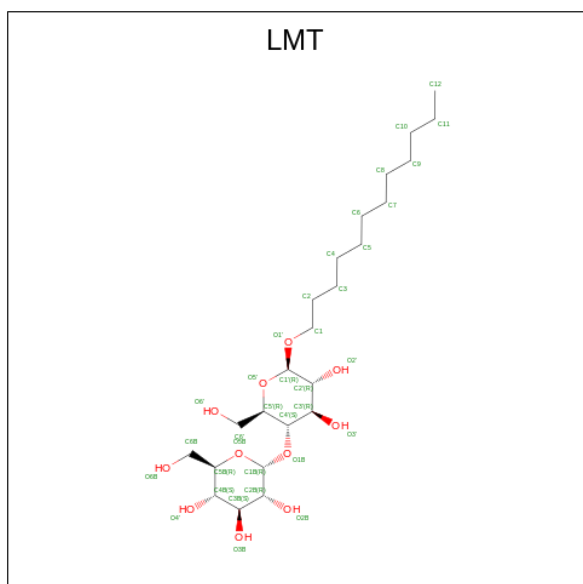
- Molecule 9 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).





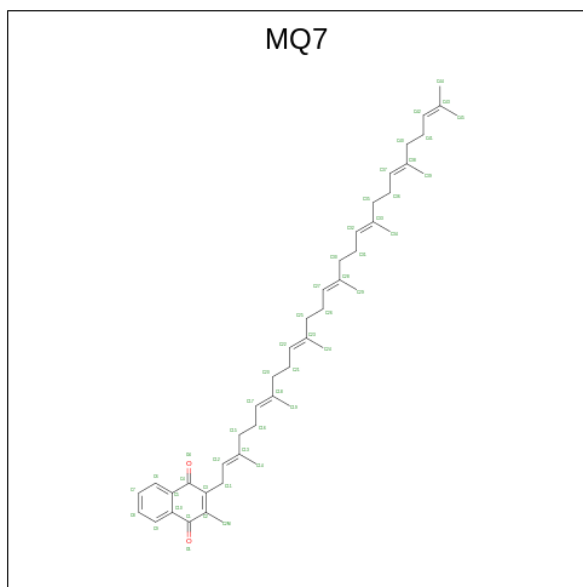
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
9	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
9	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
9	G	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
9	G	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
9	K	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
9	K	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
9	O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

- Molecule 10 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula:  $C_{24}H_{46}O_{11}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	C	1	Total	C	O	0	0
			35	24	11		
10	O	1	Total	C	O	0	0
			35	24	11		

- Molecule 11 is MENAQUINONE-7 (three-letter code: MQ7) (formula:  $C_{46}H_{64}O_2$ ).

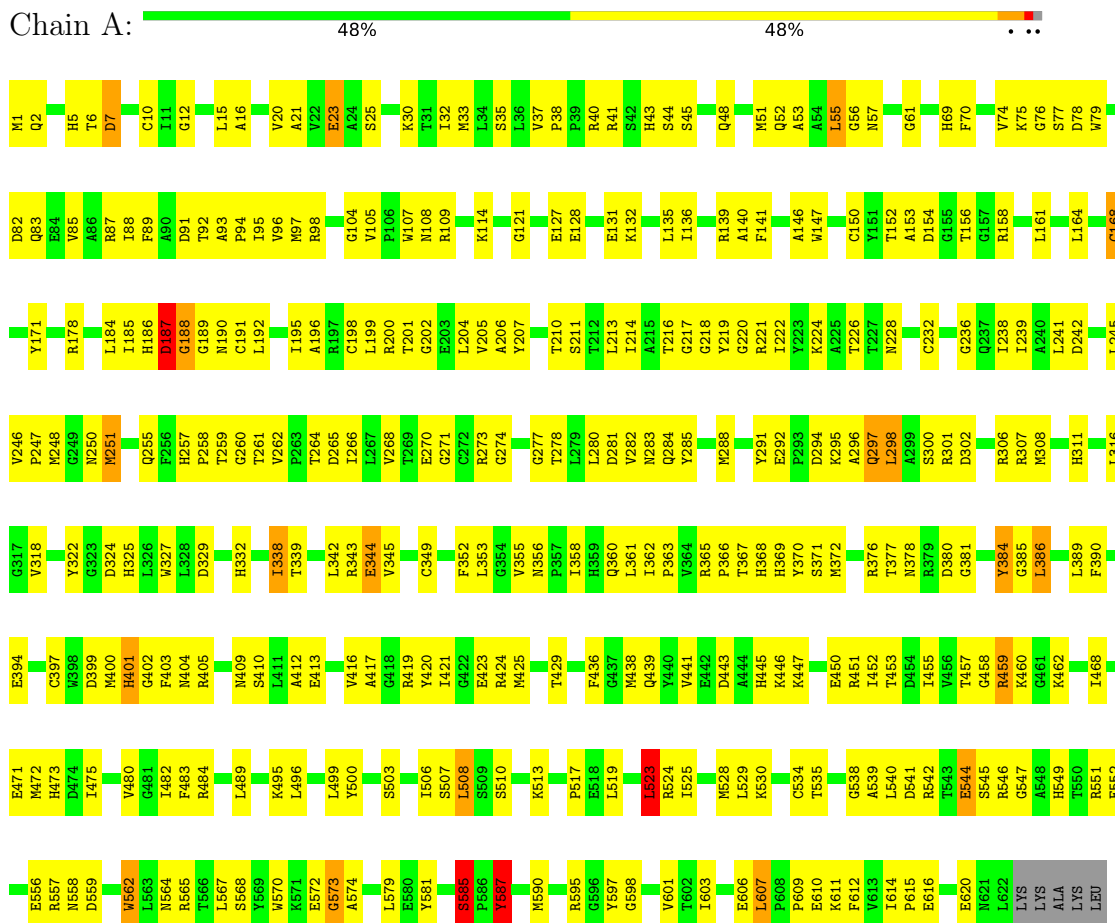


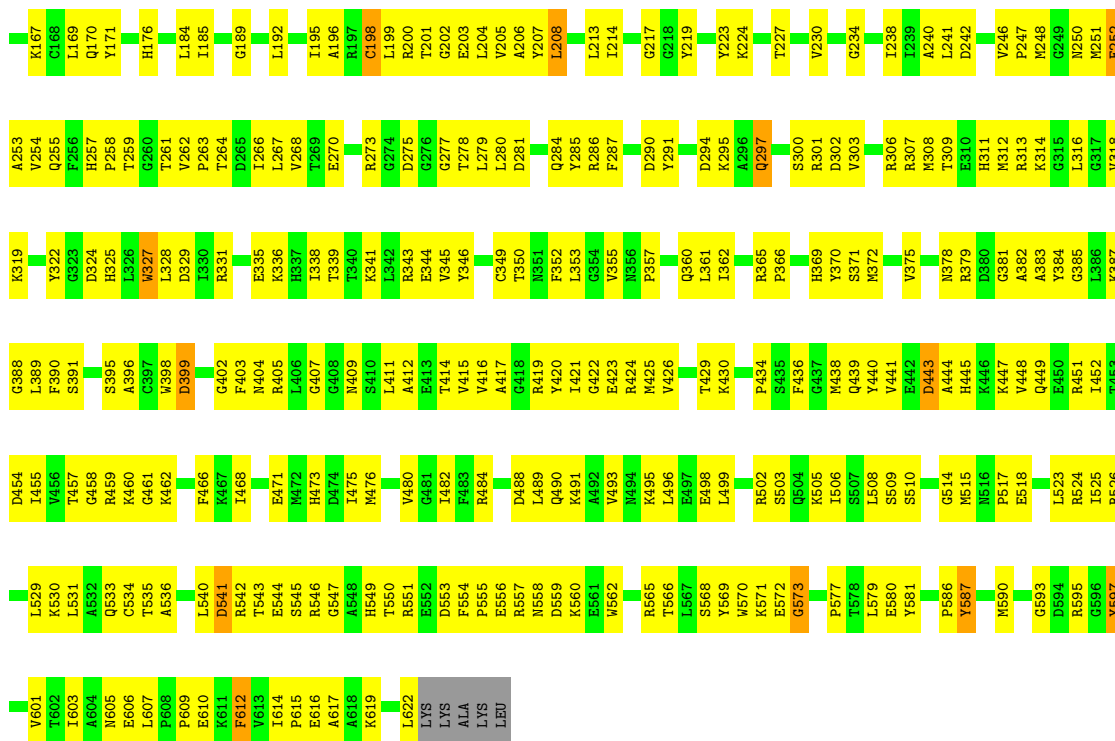
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	C	1	Total	C	O	0	0
			24	22	2		

### 3 Residue-property plots

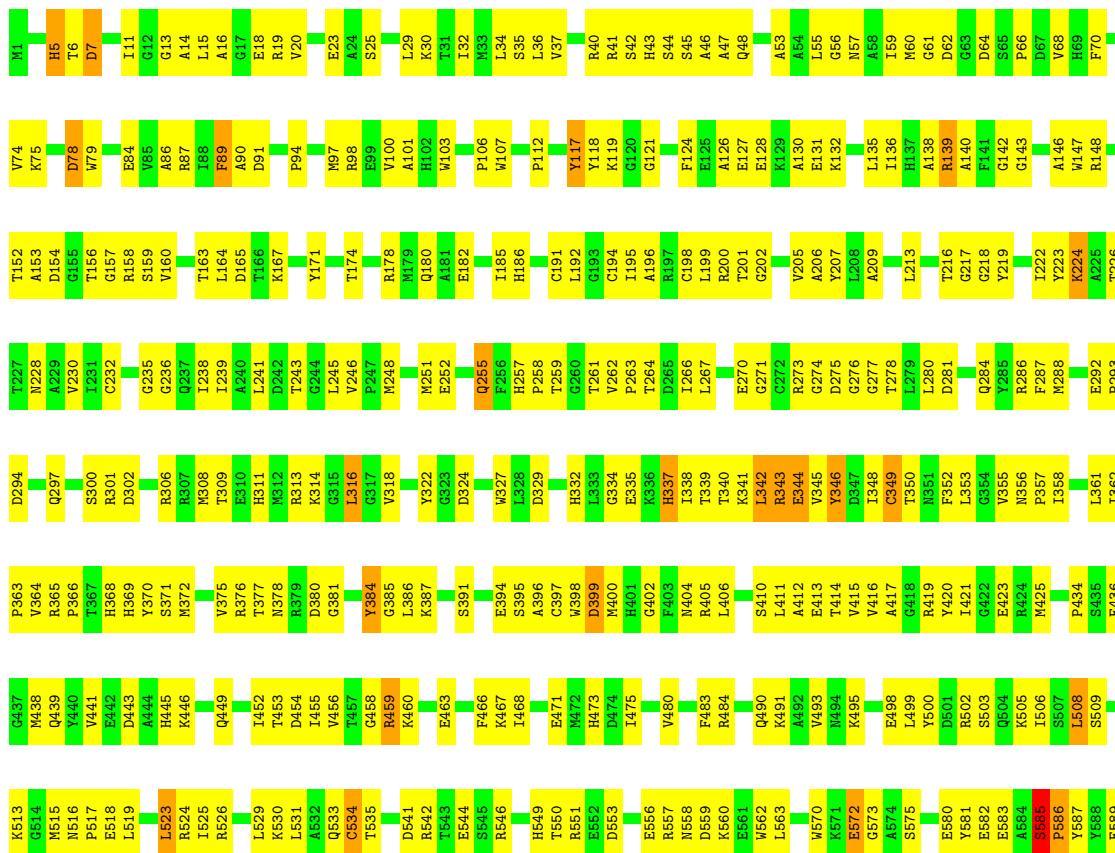
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

- Molecule 1: fumarate reductase flavoprotein subunit



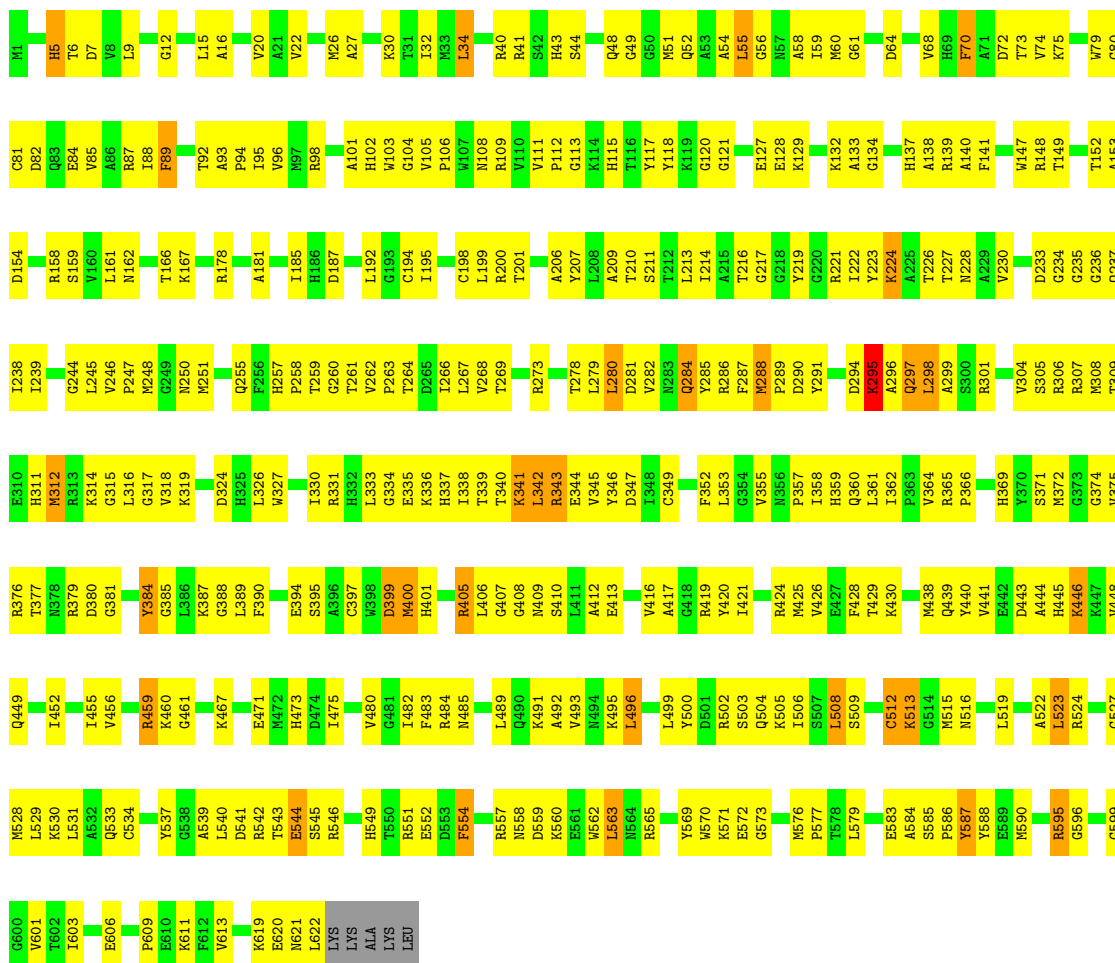


● Molecule 1: fumarate reductase flavoprotein subunit

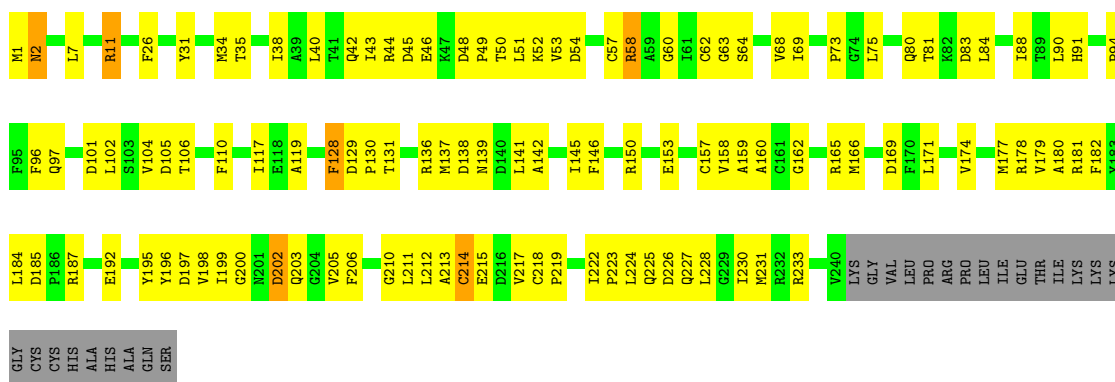




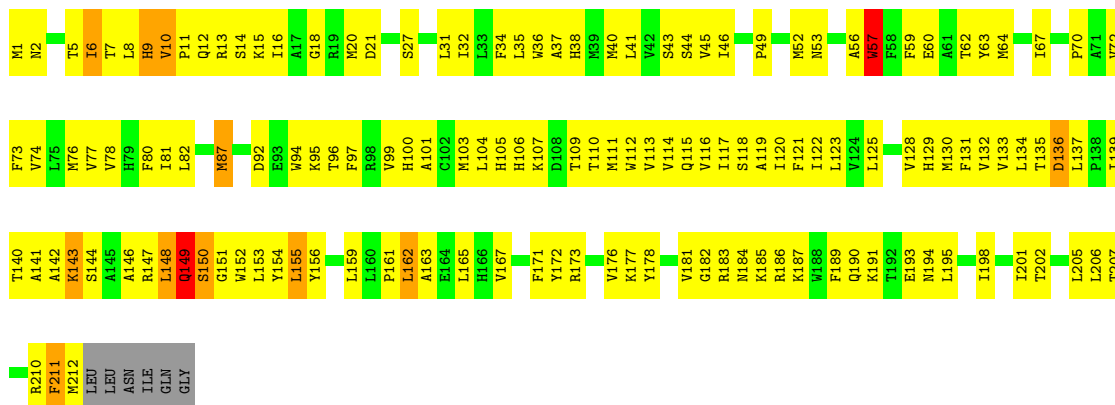
• Molecule 1: fumarate reductase flavoprotein subunit



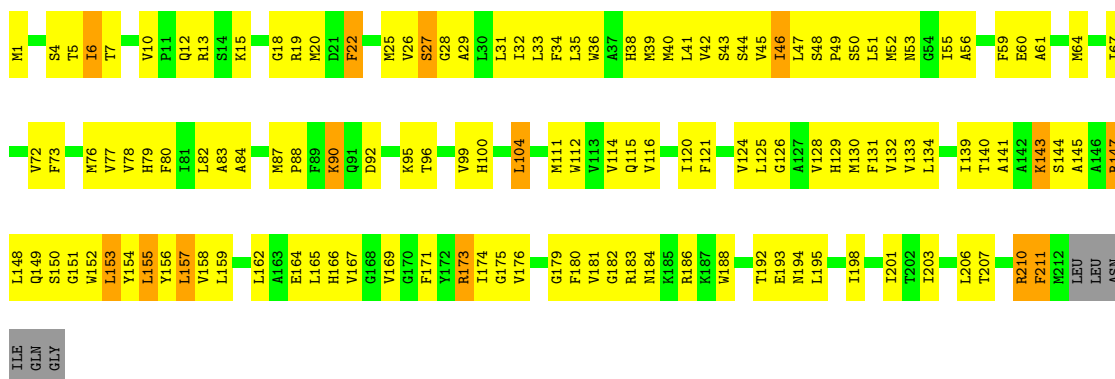
• Molecule 2: Succinate dehydrogenase iron-sulfur subunit



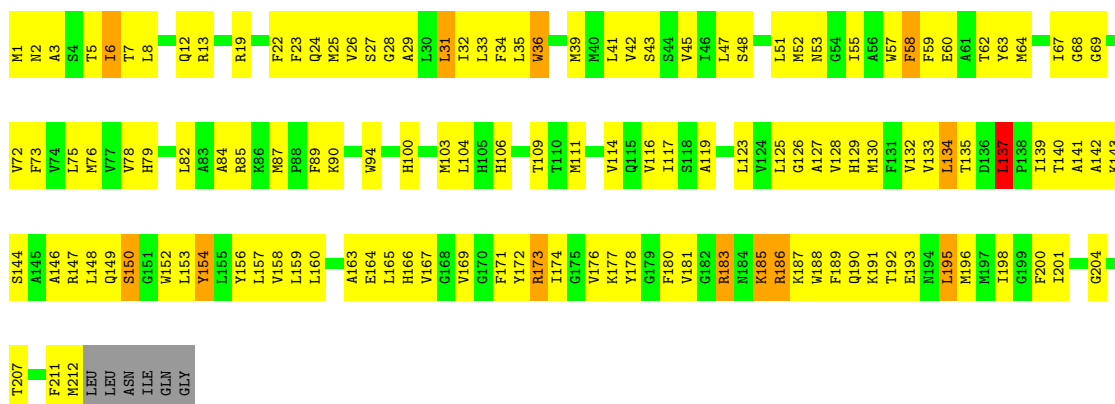
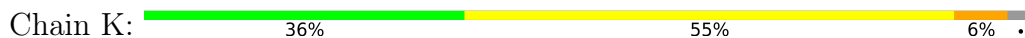




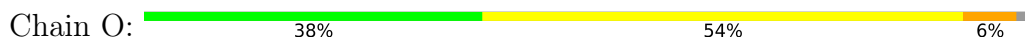
• Molecule 3: fumarate reductase respiratory complex



• Molecule 3: fumarate reductase respiratory complex



• Molecule 3: fumarate reductase respiratory complex



M1
M2
A3
S4
T5
I6
T7
L8
H9
V10
P11
Q12
R13
S14
K15
I16
A17
G18
R19
M20
F23
Q24
M25
V26
S27
G28
A29
L30
L31
I32
L35
H38
L41
V42
S43
S44
V45
I46
L51
M52
M53
G54
I55
A56
W57
F58
F59
E60
A61
T62
Y63
M64
A65
Q66
I67
G68
G69
V72
F73
W74
L75
W76
F80
I81
L82
A83
A84
R85
K86
M87
P88
F89
K90
Q91
W94
K95
T96
F97
R98
L104
H105
H106
T109
W112
V116
I122
L123
V128
H129
M130
F131
V132
V133
L134
T135
D136
L137
P138
I139
T140
A141
A142
K143
S144
A145
A146
R147
L148
Q149
S150
ASN
ILE
GLN
GLY
M152
L153
Y154
L155
Y156
L157
V158
L159
L160
P161
L162
A163
E164
L165
H166
V167
F171
Y172
R173
I174
G175
V176
K177
Y178
V181
G182
R183
N184
K185
R186
K187
W188
F189
Q190
K191
T192
E193
M194
L195
I198
G199
F200
I203
G204
L205
L206
T207
L208
V209
R210
F211
M212
LEU
LEU
ASN
ILE
GLN
GLY



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	112.14Å 131.77Å 195.43Å 90.00° 94.22° 90.00°	Depositor
Resolution (Å)	29.80 – 3.60 29.80 – 3.50	Depositor EDS
% Data completeness (in resolution range)	98.3 (29.80-3.60) 98.4 (29.80-3.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.87 (at 3.47Å)	Xtrriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, $R_{free}$	0.232 , 0.313 0.234 , 0.314	Depositor DCC
$R_{free}$ test set	3515 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	120.2	Xtrriage
Anisotropy	0.152	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.15 , 1.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	34118	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	97.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, FUM, FES, MQ7, F3S, HEM, FAD, LMT

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	0.73	3/4868 (0.1%)	0.97	14/6581 (0.2%)
1	E	0.57	2/4866 (0.0%)	0.83	3/6579 (0.0%)
1	I	0.60	1/4866 (0.0%)	0.85	5/6579 (0.1%)
1	M	0.57	2/4868 (0.0%)	0.90	12/6581 (0.2%)
2	B	0.71	1/1915 (0.1%)	0.94	4/2587 (0.2%)
2	F	0.60	1/1915 (0.1%)	0.88	3/2587 (0.1%)
2	J	0.62	4/1915 (0.2%)	0.81	0/2587
2	N	0.68	0/1915	0.97	7/2587 (0.3%)
3	C	0.65	1/1739 (0.1%)	0.94	5/2355 (0.2%)
3	G	0.53	0/1739	0.85	5/2355 (0.2%)
3	K	0.62	2/1739 (0.1%)	0.86	5/2355 (0.2%)
3	O	0.59	0/1739	0.95	6/2355 (0.3%)
All	All	0.62	17/34084 (0.0%)	0.90	69/46088 (0.1%)

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	144	GLU	CD-OE1	-7.99	1.16	1.25
3	K	183	ARG	NE-CZ	-7.30	1.23	1.33
1	A	397	CYS	CB-SG	-6.95	1.70	1.82
2	J	144	GLU	CD-OE2	-6.86	1.18	1.25
3	K	183	ARG	CZ-NH1	-6.71	1.24	1.33
1	E	327	TRP	CB-CG	-6.62	1.38	1.50
1	I	534	CYS	CB-SG	-6.29	1.71	1.82
1	A	562	TRP	CB-CG	-5.82	1.39	1.50
2	J	56	CYS	CB-SG	5.75	1.92	1.82
2	B	83	ASP	C-N	-5.64	1.21	1.34
1	E	198	CYS	CB-SG	-5.58	1.72	1.81
3	C	87	MET	C-N	5.49	1.44	1.34
1	M	595	ARG	CZ-NH2	-5.46	1.25	1.33
1	A	534	CYS	CB-SG	-5.46	1.73	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	595	ARG	NE-CZ	-5.42	1.26	1.33
2	F	161	CYS	CB-SG	-5.37	1.73	1.81
2	J	65	CYS	CB-SG	-5.11	1.73	1.81

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	496	LEU	CA-CB-CG	9.92	138.11	115.30
3	C	137	LEU	CA-CB-CG	9.55	137.26	115.30
1	M	342	LEU	CA-CB-CG	9.46	137.05	115.30
3	O	206	LEU	CA-CB-CG	8.91	135.80	115.30
1	M	563	LEU	CA-CB-CG	8.89	135.74	115.30
3	O	137	LEU	CA-CB-CG	8.15	134.04	115.30
1	I	563	LEU	CA-CB-CG	7.81	133.27	115.30
2	F	171	LEU	CA-CB-CG	7.51	132.58	115.30
3	G	153	LEU	CA-CB-CG	7.45	132.43	115.30
2	B	171	LEU	CB-CG-CD2	-7.15	98.85	111.00
2	N	75	LEU	CA-CB-CG	6.94	131.26	115.30
3	G	33	LEU	CA-CB-CG	6.84	131.04	115.30
3	O	31	LEU	CA-CB-CG	6.51	130.28	115.30
3	C	162	LEU	CA-CB-CG	-6.51	100.33	115.30
1	M	523	LEU	CA-CB-CG	6.49	130.22	115.30
1	M	280	LEU	CB-CG-CD2	-6.40	100.12	111.00
3	K	195	LEU	CA-CB-CG	6.39	130.01	115.30
1	A	496	LEU	CA-CB-CG	6.27	129.72	115.30
3	G	157	LEU	CA-CB-CG	6.19	129.54	115.30
3	O	148	LEU	N-CA-C	6.17	127.67	111.00
3	K	134	LEU	CA-CB-CG	6.14	129.42	115.30
1	I	607	LEU	CA-CB-CG	6.12	129.37	115.30
2	F	126	LYS	N-CA-C	6.11	127.51	111.00
2	B	141	LEU	CA-CB-CG	6.06	129.23	115.30
2	N	205	VAL	CG1-CB-CG2	-5.96	101.37	110.90
1	I	342	LEU	CA-CB-CG	5.85	128.75	115.30
1	A	298	LEU	CA-CB-CG	-5.85	101.85	115.30
3	K	123	LEU	CA-CB-CG	5.84	128.73	115.30
2	B	171	LEU	CA-CB-CG	5.80	128.65	115.30
1	M	298	LEU	CA-CB-CG	5.79	128.62	115.30
2	N	132	ALA	C-N-CA	5.78	136.16	121.70
3	O	155	LEU	CA-CB-CG	5.77	128.58	115.30
1	A	168	CYS	CA-CB-SG	5.76	124.37	114.00
1	A	188	GLY	N-CA-C	-5.72	98.80	113.10
1	A	607	LEU	CA-CB-CG	5.66	128.31	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	91	ASP	CB-CG-OD2	5.65	123.39	118.30
2	B	75	LEU	CB-CG-CD1	-5.64	101.41	111.00
1	A	573	GLY	N-CA-C	-5.63	99.02	113.10
1	E	573	GLY	N-CA-C	-5.62	99.06	113.10
1	E	208	LEU	CA-CB-CG	5.60	128.17	115.30
3	C	57	TRP	CA-CB-CG	5.56	124.26	113.70
1	A	523	LEU	CA-CB-CG	5.55	128.07	115.30
1	M	563	LEU	N-CA-C	-5.55	96.02	111.00
3	C	195	LEU	CA-CB-CG	5.53	128.01	115.30
1	M	295	LYS	C-N-CA	5.52	135.49	121.70
3	G	46	ILE	N-CA-C	5.51	125.87	111.00
3	K	31	LEU	CA-CB-CG	5.48	127.90	115.30
2	N	134	GLU	CA-CB-CG	5.45	125.40	113.40
1	M	34	LEU	CA-CB-CG	-5.45	102.77	115.30
1	A	91	ASP	CB-CG-OD1	-5.44	113.41	118.30
3	C	148	LEU	O-C-N	5.38	131.31	122.70
1	I	563	LEU	N-CA-C	-5.38	96.48	111.00
1	A	401	HIS	C-N-CA	-5.38	111.01	122.30
2	N	133	ASP	CB-CG-OD1	5.30	123.07	118.30
1	M	55	LEU	CB-CG-CD1	5.20	119.84	111.00
1	A	386	LEU	CB-CG-CD2	-5.20	102.16	111.00
1	I	572	GLU	C-N-CA	5.18	133.17	122.30
2	F	171	LEU	C-N-CA	-5.17	111.44	122.30
2	N	135	MET	CA-CB-CG	5.17	122.09	113.30
1	A	376	ARG	NE-CZ-NH1	5.15	122.88	120.30
2	N	184	LEU	CA-CB-CG	5.12	127.08	115.30
3	K	137	LEU	CA-CB-CG	5.11	127.04	115.30
1	M	446	LYS	CD-CE-NZ	5.08	123.40	111.70
1	M	508	LEU	CA-CB-CG	5.08	126.99	115.30
3	O	147	ARG	CA-CB-CG	5.08	124.57	113.40
3	G	104	LEU	CA-CB-CG	5.08	126.97	115.30
1	E	514	GLY	N-CA-C	-5.06	100.46	113.10
1	A	23	GLU	CA-CB-CG	-5.05	102.29	113.40
1	A	188	GLY	C-N-CA	-5.03	111.74	122.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [\(i\)](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4769	0	4681	301	0
1	E	4767	0	4674	340	0
1	I	4767	0	4674	383	1
1	M	4769	0	4681	404	1
2	B	1879	0	1821	99	0
2	F	1879	0	1823	121	1
2	J	1879	0	1821	126	0
2	N	1879	0	1821	141	0
3	C	1693	0	1775	224	0
3	G	1693	0	1775	157	0
3	K	1693	0	1775	157	1
3	O	1693	0	1775	175	0
4	A	53	0	28	2	0
4	E	53	0	29	4	0
4	I	53	0	31	21	0
4	M	53	0	31	15	0
5	A	8	0	1	7	0
5	E	8	0	1	5	0
5	I	8	0	1	3	0
5	M	8	0	1	5	0
6	B	7	0	0	0	0
6	F	7	0	0	3	0
6	J	7	0	0	0	0
6	N	7	0	0	0	0
7	B	8	0	0	1	0
7	F	8	0	0	0	0
7	J	8	0	0	0	0
7	N	8	0	0	1	0
8	B	4	0	0	1	0
8	F	4	0	0	1	0
8	J	4	0	0	0	0
8	N	4	0	0	1	0
9	C	86	0	60	22	0
9	G	86	0	60	20	0
9	K	86	0	60	25	0
9	O	86	0	60	20	0
10	C	35	0	46	30	0
10	O	35	0	46	23	0
11	C	24	0	23	19	0
All	All	34118	0	33574	2526	2

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 37.

All (2526) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:43:HIS:NE2	4:M:701:FAD:C8M	1.76	1.46
3:C:10:VAL:HG22	3:C:11:PRO:CD	1.42	1.45
1:I:43:HIS:NE2	4:I:701:FAD:HM82	1.25	1.42
1:I:43:HIS:NE2	4:I:701:FAD:C8M	1.89	1.35
1:M:43:HIS:CD2	4:M:701:FAD:HM82	1.65	1.30
3:C:130:MET:O	3:C:134:LEU:HB2	1.27	1.28
1:M:43:HIS:CD2	4:M:701:FAD:C8M	2.18	1.25
3:C:148:LEU:HB3	3:C:149:GLN:OE1	1.05	1.22
1:M:513:LYS:HE2	2:N:13:ASN:HB3	1.21	1.18
3:K:186:ARG:O	3:K:190:GLN:HB2	1.44	1.15
1:M:43:HIS:NE2	4:M:701:FAD:HM82	0.82	1.15
3:C:16:ILE:CD1	10:O:301:LMT:C6 <sup>7</sup>	2.25	1.14
3:C:16:ILE:CG1	10:O:301:LMT:H6E	1.76	1.14
3:C:144:SER:HA	3:C:146:ALA:H	1.02	1.14
3:C:16:ILE:CD1	10:O:301:LMT:H6E	1.79	1.11
3:C:10:VAL:CG2	3:C:11:PRO:HD3	1.81	1.10
3:K:84:ALA:HA	3:K:87:MET:HG3	1.18	1.10
3:C:16:ILE:HG13	10:O:301:LMT:H6E	1.29	1.09
3:C:148:LEU:CB	3:C:149:GLN:OE1	2.02	1.08
3:C:16:ILE:HD12	10:O:301:LMT:C6 <sup>7</sup>	1.85	1.07
1:A:77:SER:CB	1:A:401:HIS:O	2.03	1.07
2:N:42:GLN:O	2:N:46:GLU:HB2	1.54	1.07
3:G:49:PRO:HD3	3:G:210:ARG:HH12	1.16	1.06
1:I:224:LYS:HG2	1:I:473:HIS:HB3	1.37	1.05
1:M:513:LYS:HE2	2:N:13:ASN:CB	1.87	1.04
3:C:148:LEU:HD23	3:C:149:GLN:HE22	1.17	1.04
3:G:130:MET:O	3:G:134:LEU:HB2	1.55	1.04
3:O:143:LYS:O	3:O:146:ALA:HB3	1.56	1.03
3:C:53:ASN:HD21	3:C:140:THR:HA	1.19	1.02
1:I:43:HIS:CE1	4:I:701:FAD:HM82	1.94	1.01
1:M:79:TRP:HE1	1:M:563:LEU:HD12	1.27	1.00
3:O:133:VAL:HG23	3:O:147:ARG:HH22	1.24	1.00
1:A:413:GLU:O	1:A:417:ALA:HB3	1.61	1.00
1:A:82:ASP:HA	1:A:585:SER:HB2	1.41	0.99
1:E:273:ARG:HA	1:E:277:GLY:HA3	1.42	0.99
3:C:10:VAL:CG2	3:C:11:PRO:CD	2.38	0.99
1:A:77:SER:HB2	1:A:401:HIS:O	1.62	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:10:VAL:HG22	3:C:11:PRO:HD3	0.99	0.98
3:C:144:SER:HA	3:C:146:ALA:N	1.79	0.98
1:M:6:THR:HG22	1:M:30:LYS:HG3	1.45	0.97
1:I:558:ASN:HA	1:I:603:ILE:HB	1.46	0.96
3:O:53:ASN:HD21	3:O:141:ALA:H	1.10	0.96
1:I:608:PRO:HD2	1:I:609:PRO:HD3	1.48	0.96
1:E:480:VAL:HG23	1:E:484:ARG:HE	1.25	0.96
1:E:300:SER:OG	1:E:302:ASP:OD2	1.84	0.96
3:O:150:SER:HA	3:O:152:TRP:CD1	2.01	0.95
3:C:10:VAL:HG22	3:C:11:PRO:HD2	1.47	0.95
2:N:128:PHE:HA	2:N:129:ASP:CG	1.87	0.95
1:I:338:ILE:HG23	1:I:342:LEU:H	1.29	0.95
1:I:341:LYS:O	1:I:342:LEU:HB2	1.65	0.94
1:A:412:ALA:O	1:A:416:VAL:HB	1.68	0.93
1:A:572:GLU:HB3	1:A:573:GLY:HA3	1.47	0.93
3:C:148:LEU:O	3:C:149:GLN:O	1.86	0.93
3:K:27:SER:O	3:K:31:LEU:HB3	1.69	0.93
10:C:303:LMT:O6'	3:O:16:ILE:CG2	2.17	0.92
3:O:95:LYS:NZ	10:O:301:LMT:H5'	1.83	0.92
3:C:37:ALA:HA	11:C:304:MQ7:C2M	1.99	0.92
1:A:77:SER:HB3	1:A:401:HIS:O	1.69	0.92
10:C:303:LMT:H2O1	10:C:303:LMT:H3O2	1.11	0.91
3:G:27:SER:HG	3:G:79:HIS:HD1	1.00	0.91
3:C:16:ILE:CD1	10:O:301:LMT:H6D	2.00	0.90
1:M:79:TRP:HH2	1:M:546:ARG:HE	1.14	0.90
3:C:57:TRP:HA	3:C:62:THR:HG22	1.51	0.90
3:C:176:VAL:HA	3:C:181:VAL:HG22	1.52	0.90
3:O:188:TRP:HD1	3:O:192:THR:HG1	1.20	0.89
1:M:43:HIS:CD2	4:M:701:FAD:HM81	2.04	0.89
1:M:227:THR:HG1	1:M:369:HIS:HD1	1.07	0.89
9:K:301:HEM:HBC2	9:K:301:HEM:HHD	1.54	0.89
10:C:303:LMT:H3'	10:C:303:LMT:H3B	1.53	0.89
1:E:77:SER:HB2	1:E:402:GLY:HA3	1.54	0.89
2:J:150:ARG:NH2	2:J:220:LYS:O	2.06	0.89
2:N:128:PHE:HA	2:N:129:ASP:CB	2.03	0.89
3:G:52:MET:O	3:G:56:ALA:HB3	1.72	0.89
1:A:273:ARG:HA	1:A:277:GLY:HA3	1.54	0.88
1:I:612:PHE:O	1:I:614:ILE:HG13	1.73	0.88
1:M:79:TRP:HB2	1:M:80:GLY:HA2	1.55	0.88
1:E:22:VAL:O	1:E:26:MET:HB2	1.74	0.88
1:I:43:HIS:NE2	4:I:701:FAD:HM81	1.88	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:28:GLY:O	3:K:32:ILE:HB	1.74	0.88
3:O:139:ILE:HG13	3:O:143:LYS:HZ1	1.37	0.88
3:O:95:LYS:HZ2	10:O:301:LMT:H5'	1.36	0.88
1:I:139:ARG:NH2	1:I:271:GLY:O	2.07	0.88
3:C:16:ILE:HD11	10:O:301:LMT:H6D	1.54	0.87
3:C:148:LEU:HD23	3:C:149:GLN:NE2	1.88	0.87
2:N:128:PHE:HA	2:N:129:ASP:OD1	1.73	0.87
1:A:343:ARG:HG2	1:A:345:VAL:HG12	1.56	0.87
3:O:184:ASN:OD1	3:O:185:LYS:NZ	2.07	0.87
1:A:224:LYS:HG2	1:A:473:HIS:HB3	1.54	0.86
3:K:47:LEU:HB3	3:K:51:LEU:HD21	1.57	0.86
3:K:84:ALA:HA	3:K:87:MET:CG	2.05	0.86
1:A:262:VAL:HG22	1:A:365:ARG:HE	1.40	0.86
3:K:150:SER:HA	3:K:152:TRP:H	1.40	0.86
1:I:343:ARG:HB3	1:I:345:VAL:HG12	1.55	0.86
1:E:551:ARG:HB3	1:E:553:ASP:OD1	1.76	0.86
3:G:150:SER:HB3	3:G:151:GLY:CA	2.05	0.85
1:I:273:ARG:HA	1:I:277:GLY:HA3	1.57	0.85
3:K:8:LEU:HD13	3:K:13:ARG:HB3	1.56	0.85
1:I:413:GLU:O	1:I:417:ALA:HB3	1.77	0.85
3:K:84:ALA:CA	3:K:87:MET:HG3	2.06	0.85
1:A:178:ARG:HB3	1:A:199:LEU:HB2	1.58	0.84
1:M:40:ARG:HB3	1:M:158:ARG:HH22	1.41	0.84
2:N:62:CYS:SG	2:N:63:GLY:N	2.50	0.84
3:C:149:GLN:O	3:C:151:GLY:N	2.10	0.84
3:C:37:ALA:HA	11:C:304:MQ7:H2M1	1.59	0.84
1:M:316:LEU:HB3	1:M:317:GLY:HA3	1.58	0.84
1:E:38:PRO:HD2	1:E:41:ARG:HH12	1.43	0.84
1:E:38:PRO:HD2	1:E:41:ARG:NH1	1.93	0.84
3:K:5:THR:HG23	3:K:6:ILE:H	1.43	0.84
1:M:546:ARG:HH22	1:M:562:TRP:HB2	1.41	0.84
1:M:224:LYS:HG2	1:M:473:HIS:HB3	1.60	0.84
1:A:587:TYR:HE1	1:A:615:PRO:HA	1.42	0.84
1:E:242:ASP:OD2	1:E:530:LYS:NZ	2.11	0.83
1:E:509:SER:HB2	2:F:49:PRO:HG3	1.60	0.83
3:O:181:VAL:HG12	3:O:182:GLY:H	1.43	0.83
3:O:151:GLY:N	3:O:152:TRP:HA	1.92	0.83
3:G:148:LEU:C	3:G:150:SER:O	2.17	0.83
2:F:105:ASP:OD2	2:F:108:SER:OG	1.96	0.83
1:I:342:LEU:O	1:I:344:GLU:N	2.11	0.83
1:I:270:GLU:OE2	1:I:301:ARG:NH2	2.11	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:49:PRO:HD3	3:G:210:ARG:NH1	1.94	0.82
3:G:56:ALA:HB1	3:G:139:ILE:HG21	1.61	0.82
2:B:210:GLY:HA3	3:C:177:LYS:HD2	1.61	0.82
3:K:59:PHE:HD2	3:K:63:TYR:HA	1.43	0.82
3:C:40:MET:HB3	11:C:304:MQ7:H17	1.60	0.82
1:E:217:GLY:H	1:E:395:SER:HB3	1.46	0.81
3:K:6:ILE:HG22	3:K:7:THR:H	1.44	0.81
1:M:264:THR:HG21	1:M:352:PHE:HB3	1.61	0.81
1:M:282:VAL:HA	1:M:317:GLY:O	1.79	0.81
1:A:322:TYR:O	1:A:365:ARG:NH2	2.14	0.81
3:G:150:SER:HB3	3:G:151:GLY:HA2	1.62	0.81
3:K:64:MET:HB2	3:K:67:ILE:HG22	1.60	0.81
1:A:186:HIS:H	1:A:445:HIS:HE1	1.26	0.81
2:B:226:ASP:N	2:B:226:ASP:OD1	2.13	0.81
10:C:303:LMT:O6'	3:O:16:ILE:HG23	1.80	0.81
2:J:42:GLN:O	2:J:46:GLU:HB2	1.80	0.81
1:I:264:THR:HG21	1:I:352:PHE:HB3	1.62	0.81
1:M:316:LEU:HD22	1:M:324:ASP:HB3	1.60	0.81
2:N:130:PRO:O	2:N:131:THR:HB	1.79	0.80
1:A:270:GLU:OE2	1:A:301:ARG:NH1	2.13	0.80
1:A:558:ASN:HA	1:A:603:ILE:HB	1.60	0.80
3:K:43:SER:HA	3:K:207:THR:HG21	1.61	0.80
1:M:461:GLY:HA3	1:M:505:LYS:HB3	1.62	0.80
1:I:413:GLU:O	1:I:417:ALA:CB	2.29	0.80
1:I:518:GLU:HB2	2:J:49:PRO:HB2	1.63	0.80
1:M:316:LEU:HB3	1:M:317:GLY:CA	2.11	0.80
1:M:546:ARG:NH2	1:M:562:TRP:O	2.14	0.80
1:E:270:GLU:OE2	1:E:301:ARG:NH1	2.14	0.80
1:I:346:TYR:CE1	1:I:350:THR:HG21	2.17	0.80
3:G:188:TRP:NE1	3:G:192:THR:OG1	2.14	0.80
3:G:166:HIS:CE1	9:G:302:HEM:NB	2.51	0.79
1:A:270:GLU:H	5:A:702:FUM:C	1.93	0.79
1:E:369:HIS:NE2	5:E:702:FUM:O7	2.13	0.79
1:A:405:ARG:NE	1:A:410:SER:OG	2.11	0.79
1:I:349:CYS:HB3	1:I:353:LEU:HD22	1.64	0.79
1:A:281:ASP:OD1	1:A:285:TYR:N	2.16	0.79
3:O:123:LEU:HD13	9:O:303:HEM:HBB1	1.64	0.79
1:A:439:GLN:O	1:A:443:ASP:HB2	1.83	0.79
2:J:188:ASP:OD1	2:J:195:TYR:OH	1.99	0.79
1:M:376:ARG:NH1	1:M:397:CYS:O	2.15	0.79
1:I:112:PRO:HB3	1:I:130:ALA:HA	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:251:MET:HG3	1:I:534:CYS:HB3	1.65	0.79
1:I:612:PHE:O	1:I:614:ILE:N	2.16	0.78
1:A:413:GLU:O	1:A:417:ALA:CB	2.31	0.78
2:B:165:ARG:NH2	3:O:3:ALA:O	2.15	0.78
1:E:246:VAL:HG23	1:E:385:GLY:H	1.48	0.78
9:C:301:HEM:HMD1	9:C:301:HEM:HBD1	1.65	0.78
1:E:587:TYR:CE1	1:E:615:PRO:HB3	2.19	0.78
2:J:202:ASP:CG	2:J:203:GLN:H	1.86	0.78
1:M:55:LEU:HD12	1:M:56:GLY:H	1.48	0.78
3:O:150:SER:HA	3:O:152:TRP:NE1	1.97	0.78
3:C:143:LYS:NZ	9:C:301:HEM:HBA1	1.99	0.78
10:C:303:LMT:O6'	3:O:16:ILE:HG21	1.82	0.78
1:I:121:GLY:HA3	1:I:286:ARG:HH12	1.48	0.78
1:I:132:LYS:HG2	1:I:135:LEU:HD12	1.66	0.78
3:G:45:VAL:HA	3:G:47:LEU:H	1.46	0.78
1:M:79:TRP:HH2	1:M:546:ARG:NE	1.81	0.78
1:E:587:TYR:HD1	1:E:614:ILE:HD11	1.48	0.78
3:G:48:SER:HA	3:G:210:ARG:NH1	1.98	0.78
2:F:230:ILE:HG22	2:F:233:ARG:HH21	1.49	0.77
1:I:40:ARG:HH22	2:J:178:ARG:HH21	1.29	0.77
2:N:157:CYS:SG	2:N:174:VAL:HG23	2.24	0.77
3:C:6:ILE:HD12	3:C:7:THR:HG22	1.66	0.77
9:G:302:HEM:HHD	9:G:302:HEM:HBC2	1.67	0.77
1:E:219:TYR:CE2	1:E:371:SER:HB3	2.19	0.77
1:I:255:GLN:HB2	1:I:372:MET:SD	2.25	0.77
3:G:53:ASN:HD21	3:G:140:THR:HA	1.50	0.77
3:K:12:GLN:HG2	3:K:13:ARG:HG2	1.64	0.77
1:E:40:ARG:HA	1:E:161:LEU:HD21	1.67	0.76
1:I:55:LEU:HD12	1:I:56:GLY:H	1.48	0.76
1:A:186:HIS:H	1:A:445:HIS:CE1	2.03	0.76
3:G:64:MET:HB2	3:G:67:ILE:HG22	1.68	0.76
2:N:225:GLN:HE22	3:O:186:ARG:HD3	1.51	0.76
2:J:16:ASP:OD2	2:J:19:SER:OG	2.03	0.76
1:E:34:LEU:HD21	1:E:207:TYR:CZ	2.21	0.76
1:E:263:PRO:HB3	1:E:322:TYR:CE2	2.21	0.76
1:E:480:VAL:HG23	1:E:484:ARG:NE	2.00	0.76
2:F:157:CYS:SG	2:F:174:VAL:HG23	2.26	0.76
1:M:200:ARG:NH1	2:N:105:ASP:OD2	2.19	0.76
1:M:544:GLU:OE1	1:M:546:ARG:HD2	1.86	0.76
1:M:288:MET:SD	1:M:288:MET:N	2.59	0.76
1:M:318:VAL:HA	1:M:319:LYS:HB2	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:114:LYS:HA	1:E:127:GLU:HA	1.66	0.75
1:I:84:GLU:HA	1:I:587:TYR:HE2	1.51	0.75
3:K:55:ILE:HA	3:K:58:PHE:CD2	2.22	0.75
3:K:185:LYS:O	3:K:188:TRP:N	2.19	0.75
1:I:439:GLN:O	1:I:443:ASP:HB2	1.85	0.75
1:M:440:TYR:O	1:M:445:HIS:ND1	2.19	0.75
3:G:5:THR:OG1	3:G:6:ILE:N	2.16	0.75
1:I:610:GLU:HG3	1:I:611:LYS:NZ	2.01	0.75
2:B:97:GLN:OE1	2:B:97:GLN:N	2.17	0.75
3:G:155:LEU:HD22	3:G:158:VAL:HG23	1.69	0.75
1:M:289:PRO:HG3	1:M:296:ALA:HB2	1.68	0.75
1:M:309:THR:HG21	1:M:482:ILE:HD13	1.69	0.75
3:O:159:LEU:HD22	9:O:302:HEM:HMD1	1.67	0.75
3:G:183:ARG:HA	3:G:186:ARG:HB3	1.69	0.74
2:B:225:GLN:HE22	3:C:186:ARG:HD3	1.51	0.74
1:M:178:ARG:HB3	1:M:199:LEU:HB2	1.67	0.74
3:G:148:LEU:O	3:G:150:SER:O	2.05	0.74
1:I:405:ARG:NH1	5:I:702:FUM:O7	2.19	0.74
1:I:610:GLU:HG2	1:I:611:LYS:H	1.53	0.74
3:C:41:LEU:N	11:C:304:MQ7:H141	2.02	0.74
1:E:107:TRP:HA	1:E:152:THR:HG22	1.69	0.74
3:G:1:MET:HA	2:J:23:MET:HE3	1.70	0.74
1:A:453:THR:HG23	1:A:519:LEU:HD21	1.69	0.74
1:I:117:TYR:HD1	1:I:126:ALA:HB3	1.53	0.74
2:J:1:MET:N	2:J:30:GLU:O	2.16	0.74
3:O:53:ASN:ND2	3:O:141:ALA:H	1.85	0.74
3:C:35:LEU:HD13	3:C:167:VAL:HG11	1.69	0.74
1:I:154:ASP:HB2	1:I:343:ARG:O	1.86	0.74
1:A:542:ARG:NE	1:A:544:GLU:OE2	2.21	0.74
1:M:105:VAL:O	2:N:187:ARG:NH2	2.19	0.74
1:A:247:PRO:HD2	1:A:384:TYR:HB2	1.70	0.73
3:G:90:LYS:H	3:G:90:LYS:HD2	1.53	0.73
1:A:381:GLY:HA3	1:A:421:ILE:HD12	1.69	0.73
3:O:95:LYS:NZ	10:O:301:LMT:C5'	2.51	0.73
2:B:157:CYS:SG	2:B:174:VAL:HG23	2.28	0.73
1:I:124:PHE:CE2	1:I:126:ALA:HB2	2.23	0.73
1:I:306:ARG:NH2	1:I:550:THR:OG1	2.20	0.73
3:G:133:VAL:HG12	3:G:147:ARG:HH12	1.53	0.73
1:A:607:LEU:O	1:A:610:GLU:HG3	1.88	0.73
1:M:104:GLY:HA2	2:N:187:ARG:HD2	1.71	0.73
1:M:79:TRP:NE1	1:M:563:LEU:HD12	2.02	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:151:GLY:H	3:O:152:TRP:HD1	1.34	0.73
1:E:213:LEU:HB2	1:E:425:MET:HE1	1.69	0.73
1:A:140:ALA:HB2	1:A:147:TRP:CE2	2.23	0.72
3:C:139:ILE:HD11	3:C:143:LYS:HE2	1.71	0.72
1:I:405:ARG:NE	1:I:410:SER:OG	2.20	0.72
2:J:157:CYS:SG	2:J:174:VAL:HG23	2.29	0.72
1:M:280:LEU:HD21	1:M:327:TRP:HB2	1.71	0.72
3:O:56:ALA:HB1	3:O:62:THR:HA	1.71	0.72
1:A:105:VAL:O	2:B:187:ARG:NH2	2.22	0.72
2:B:117:ILE:HA	2:B:198:VAL:HG13	1.72	0.72
2:J:210:GLY:O	3:K:173:ARG:NH1	2.22	0.72
3:K:25:MET:HG2	3:K:174:ILE:HD11	1.71	0.72
1:M:278:THR:O	1:M:279:LEU:HG	1.90	0.72
1:A:41:ARG:HB3	2:B:62:CYS:HB2	1.70	0.72
3:C:59:PHE:O	3:C:63:TYR:N	2.21	0.72
2:J:11:ARG:NH1	2:J:24:GLN:OE1	2.23	0.72
3:K:171:PHE:HA	3:K:174:ILE:HG22	1.71	0.72
3:K:87:MET:HB2	3:K:89:PHE:CE2	2.24	0.72
3:O:143:LYS:O	3:O:146:ALA:CB	2.35	0.72
3:O:88:PRO:HD3	3:O:112:TRP:CH2	2.24	0.71
1:E:559:ASP:O	1:E:605:ASN:ND2	2.23	0.71
2:F:214:CYS:HB3	2:F:224:LEU:HD13	1.71	0.71
1:I:301:ARG:HB2	1:I:404:ASN:HD21	1.55	0.71
1:I:338:ILE:HG23	1:I:342:LEU:N	2.04	0.71
1:E:96:VAL:HG21	1:E:416:VAL:HA	1.72	0.71
2:F:150:ARG:NH2	2:F:220:LYS:O	2.23	0.71
1:I:106:PRO:HB3	2:J:145:ILE:HG22	1.72	0.71
2:J:10:PHE:HB2	2:J:91:HIS:CD2	2.26	0.71
1:I:370:TYR:CE1	1:I:394:GLU:HG3	2.26	0.71
2:N:42:GLN:O	2:N:46:GLU:CB	2.37	0.71
3:O:159:LEU:HD21	9:O:302:HEM:CBC	2.20	0.71
1:A:306:ARG:HH12	1:A:482:ILE:HG22	1.55	0.71
1:I:35:SER:OG	1:I:37:VAL:O	2.07	0.71
1:A:306:ARG:NH1	1:A:482:ILE:HG22	2.06	0.71
1:E:488:ASP:HA	1:E:491:LYS:HE2	1.73	0.71
1:M:79:TRP:HB2	1:M:80:GLY:CA	2.21	0.71
1:A:349:CYS:SG	1:A:362:ILE:HD12	2.31	0.71
3:G:6:ILE:HG13	3:G:7:THR:H	1.56	0.71
1:M:54:ALA:HB3	1:M:94:PRO:HG3	1.72	0.71
3:O:147:ARG:CB	3:O:150:SER:O	2.39	0.71
1:E:5:HIS:O	1:E:6:THR:HG23	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:139:ILE:CG1	3:O:143:LYS:HZ1	2.04	0.71
3:C:16:ILE:HG13	3:O:95:LYS:HZ1	1.56	0.70
1:I:219:TYR:CE2	1:I:371:SER:HB3	2.26	0.70
3:K:129:HIS:NE2	9:K:301:HEM:ND	2.37	0.70
1:M:108:ASN:HD21	1:M:153:ALA:H	1.39	0.70
1:A:606:GLU:O	1:A:609:PRO:HD2	1.91	0.70
1:I:200:ARG:NH1	2:J:105:ASP:OD2	2.24	0.70
3:K:150:SER:HA	3:K:152:TRP:N	2.04	0.70
1:M:73:THR:HA	1:M:406:LEU:HD12	1.73	0.70
1:I:15:LEU:HD12	1:I:44:SER:HB3	1.73	0.70
2:N:224:LEU:O	2:N:228:LEU:HB2	1.91	0.70
1:A:255:GLN:HB2	1:A:372:MET:SD	2.31	0.70
1:M:500:TYR:HD1	1:M:529:LEU:HD11	1.56	0.70
1:A:245:LEU:O	1:A:385:GLY:HA3	1.91	0.70
1:A:556:GLU:HA	1:A:601:VAL:HG23	1.71	0.70
1:A:545:SER:OG	1:A:551:ARG:N	2.22	0.70
2:F:208:CYS:O	2:F:232:ARG:NH1	2.17	0.70
3:O:161:PRO:O	3:O:165:LEU:HB2	1.92	0.70
3:O:203:ILE:HA	3:O:206:LEU:HD23	1.74	0.70
1:I:608:PRO:CD	1:I:609:PRO:HD3	2.20	0.70
2:B:202:ASP:OD1	2:B:203:GLN:N	2.23	0.70
2:F:208:CYS:HA	6:F:301:F3S:S1	2.32	0.70
1:I:513:LYS:HZ2	2:J:13:ASN:HD21	1.39	0.70
2:N:211:LEU:HD22	3:O:109:THR:HA	1.74	0.70
1:I:139:ARG:NH2	1:I:275:ASP:HB2	2.07	0.69
1:I:405:ARG:HH21	1:I:410:SER:HB2	1.57	0.69
3:K:156:TYR:CD1	9:K:301:HEM:HAD2	2.27	0.69
2:N:126:LYS:N	2:N:127:ALA:HA	2.06	0.69
1:E:104:GLY:HA2	2:F:187:ARG:HD2	1.74	0.69
2:F:110:PHE:HE1	2:F:174:VAL:HG11	1.56	0.69
1:I:97:MET:O	1:I:101:ALA:HB2	1.91	0.69
3:K:156:TYR:HD1	9:K:301:HEM:HAD2	1.57	0.69
9:O:303:HEM:HBB2	9:O:303:HEM:HMB1	1.73	0.69
1:A:57:ASN:HA	1:A:132:LYS:HD3	1.75	0.69
1:A:264:THR:HG21	1:A:352:PHE:HB3	1.75	0.69
1:A:530:LYS:HE3	1:A:570:TRP:CE2	2.27	0.69
3:C:176:VAL:HG23	3:C:177:LYS:HG3	1.75	0.69
1:E:378:ASN:OD1	1:E:382:ALA:N	2.26	0.69
3:G:48:SER:HA	3:G:210:ARG:HH12	1.57	0.69
1:M:6:THR:HG21	1:M:32:ILE:HG13	1.75	0.69
1:M:546:ARG:NH2	1:M:562:TRP:HB2	2.07	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:139:ILE:HA	3:O:143:LYS:HE3	1.74	0.69
1:A:273:ARG:NH1	1:A:297:GLN:O	2.26	0.69
3:O:129:HIS:CE1	9:O:302:HEM:ND	2.61	0.69
3:O:132:VAL:HG21	3:O:153:LEU:HD21	1.74	0.69
1:A:75:LYS:O	1:A:595:ARG:HD3	1.93	0.68
3:C:9:HIS:ND1	3:C:10:VAL:N	2.41	0.68
1:E:542:ARG:HA	1:E:562:TRP:CH2	2.28	0.68
1:I:55:LEU:HD21	1:I:138:ALA:HB2	1.73	0.68
1:I:513:LYS:NZ	2:J:13:ASN:HD21	1.91	0.68
3:K:69:GLY:HA3	3:K:134:LEU:HD13	1.75	0.68
3:C:149:GLN:OE1	3:C:149:GLN:N	2.25	0.68
1:E:261:THR:HG21	1:E:353:LEU:HD11	1.75	0.68
1:E:452:ILE:HD12	1:E:526:ARG:HH21	1.58	0.68
1:M:245:LEU:O	1:M:385:GLY:HA3	1.93	0.68
2:F:37:PHE:HA	2:F:55:PHE:CZ	2.28	0.68
3:C:53:ASN:ND2	3:C:140:THR:HA	2.02	0.68
2:F:222:ILE:HG22	2:F:223:PRO:HD2	1.75	0.68
1:M:221:ARG:NH1	1:M:228:ASN:O	2.24	0.68
2:N:151:CYS:SG	2:N:152:ILE:N	2.66	0.68
3:C:87:MET:SD	10:C:303:LMT:H123	2.34	0.68
1:A:355:VAL:HG13	1:A:360:GLN:HB2	1.75	0.68
1:A:587:TYR:CE1	1:A:615:PRO:HA	2.27	0.68
3:C:64:MET:HB3	3:C:67:ILE:HG22	1.75	0.68
1:I:107:TRP:HA	1:I:152:THR:HG22	1.75	0.68
1:M:513:LYS:CE	2:N:13:ASN:CB	2.69	0.68
2:N:211:LEU:HD23	3:O:173:ARG:HH12	1.57	0.68
2:B:212:LEU:HD22	2:B:225:GLN:HG3	1.74	0.68
1:A:85:VAL:HG12	1:A:400:MET:HB3	1.76	0.68
3:C:148:LEU:HB3	3:C:149:GLN:CD	2.06	0.68
1:E:343:ARG:HG2	1:E:345:VAL:HG12	1.74	0.68
1:I:14:ALA:HB2	4:I:701:FAD:H4B	1.74	0.68
3:K:23:PHE:HA	3:K:26:VAL:HB	1.76	0.68
3:K:163:ALA:O	3:K:167:VAL:HG13	1.94	0.68
3:C:125:LEU:HA	3:C:128:VAL:HG22	1.75	0.68
2:B:218:CYS:SG	2:B:222:ILE:HG12	2.34	0.67
3:C:94:TRP:HH2	3:C:117:ILE:HD11	1.59	0.67
1:I:610:GLU:HG3	1:I:611:LYS:HZ1	1.59	0.67
1:A:378:ASN:OD1	1:A:381:GLY:N	2.26	0.67
3:C:148:LEU:HD11	3:C:212:MET:HB2	1.74	0.67
1:E:280:LEU:HB2	1:E:327:TRP:HB2	1.77	0.67
1:M:405:ARG:NH2	1:M:407:GLY:HA2	2.08	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:128:PHE:CA	2:N:129:ASP:CB	2.72	0.67
2:N:232:ARG:O	2:N:236:ALA:CB	2.42	0.67
3:K:159:LEU:HD22	9:K:301:HEM:HMD1	1.76	0.67
1:I:195:ILE:HD13	1:I:206:ALA:HB2	1.75	0.67
1:M:185:ILE:HG22	1:M:192:LEU:HB2	1.76	0.67
2:N:136:ARG:HG3	2:N:137:MET:H	1.60	0.67
3:C:130:MET:HG2	3:C:134:LEU:HD22	1.75	0.67
1:A:484:ARG:O	1:A:552:GLU:N	2.21	0.67
3:G:52:MET:O	3:G:56:ALA:CB	2.42	0.67
1:I:185:ILE:HG22	1:I:192:LEU:HB2	1.77	0.67
1:I:186:HIS:H	1:I:445:HIS:CE1	2.12	0.67
1:M:312:MET:CG	1:M:326:LEU:HD11	2.25	0.67
3:C:34:PHE:O	3:C:37:ALA:N	2.28	0.67
1:E:109:ARG:C	1:E:137:HIS:HB2	2.15	0.67
3:K:180:PHE:HB3	3:K:181:VAL:HG23	1.75	0.67
1:M:79:TRP:CH2	1:M:546:ARG:NE	2.60	0.67
2:N:210:GLY:O	3:O:173:ARG:NH1	2.28	0.67
1:E:246:VAL:HG21	1:E:383:ALA:HB1	1.77	0.67
1:M:248:MET:HE1	1:M:375:VAL:HA	1.77	0.67
1:A:185:ILE:HA	1:A:445:HIS:CE1	2.30	0.67
3:C:97:PHE:CE1	3:C:112:TRP:HE3	2.13	0.67
1:I:513:LYS:HB2	1:I:516:ASN:HD22	1.57	0.67
1:M:342:LEU:HD12	1:M:343:ARG:HG3	1.77	0.67
1:M:500:TYR:CD1	1:M:529:LEU:HD11	2.30	0.66
2:B:7:LEU:HD23	2:B:88:ILE:HB	1.76	0.66
1:I:7:ASP:OD1	1:I:30:LYS:HB2	1.95	0.66
1:I:20:VAL:HG21	1:I:213:LEU:HD13	1.75	0.66
2:B:48:ASP:OD1	2:B:50:THR:HG22	1.94	0.66
3:G:29:ALA:O	3:G:32:ILE:HG22	1.95	0.66
1:I:41:ARG:HB3	2:J:62:CYS:HB2	1.78	0.66
3:K:59:PHE:CD2	3:K:63:TYR:HA	2.29	0.66
1:M:334:GLY:O	1:M:338:ILE:HD11	1.95	0.66
1:A:472:MET:HE1	1:A:528:MET:HB3	1.76	0.66
1:I:241:LEU:HD13	1:I:248:MET:HG2	1.77	0.66
1:A:195:ILE:HG13	1:A:445:HIS:HB3	1.77	0.66
10:C:303:LMT:H6D	10:C:303:LMT:O1'	1.95	0.66
3:K:119:ALA:HB1	9:K:302:HEM:HMB3	1.76	0.66
1:M:262:VAL:HG13	1:M:263:PRO:HD3	1.76	0.66
1:A:20:VAL:HG21	1:A:213:LEU:HD13	1.78	0.66
2:J:197:ASP:OD1	3:K:13:ARG:HG3	1.96	0.66
2:N:225:GLN:HE21	3:O:176:VAL:HG13	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:43:SER:HG	3:C:207:THR:HG1	1.38	0.66
1:M:15:LEU:HD12	1:M:44:SER:HB3	1.77	0.66
1:M:619:LYS:NZ	1:M:621:ASN:O	2.27	0.66
3:O:84:ALA:HA	3:O:87:MET:HG3	1.77	0.66
1:E:559:ASP:HB3	1:E:605:ASN:HB2	1.78	0.66
1:I:499:LEU:HG	1:I:529:LEU:HD21	1.77	0.66
1:E:263:PRO:HB3	1:E:322:TYR:HE2	1.60	0.66
3:G:150:SER:CB	3:G:151:GLY:HA2	2.24	0.66
1:M:513:LYS:HD3	2:N:13:ASN:HB2	1.77	0.66
1:E:606:GLU:O	1:E:609:PRO:HD2	1.96	0.65
2:F:197:ASP:CG	3:G:13:ARG:HG3	2.14	0.65
1:I:259:THR:CG2	1:I:273:ARG:HE	2.08	0.65
1:I:375:VAL:O	1:I:397:CYS:N	2.19	0.65
1:M:108:ASN:ND2	1:M:153:ALA:H	1.93	0.65
2:N:232:ARG:O	2:N:236:ALA:HB3	1.96	0.65
1:A:291:TYR:HB3	1:A:307:ARG:HE	1.61	0.65
2:J:146:PHE:O	2:J:150:ARG:HB2	1.96	0.65
2:N:3:ARG:O	2:N:30:GLU:HB3	1.97	0.65
2:B:94:PRO:HD2	2:B:159:ALA:HB1	1.76	0.65
1:E:278:THR:HB	1:E:329:ASP:HB3	1.78	0.65
1:E:311:HIS:CE1	1:E:316:LEU:HD13	2.30	0.65
2:B:11:ARG:HH22	2:B:50:THR:HG23	1.62	0.65
1:E:217:GLY:N	1:E:395:SER:HB3	2.12	0.65
1:E:287:PHE:H	1:E:287:PHE:HD2	1.44	0.65
1:M:380:ASP:OD1	1:M:424:ARG:NH1	2.29	0.65
9:O:302:HEM:HHD	9:O:302:HEM:HBC2	1.79	0.65
1:E:200:ARG:NH1	2:F:105:ASP:OD2	2.30	0.65
1:E:253:ALA:HB1	1:E:372:MET:HE3	1.79	0.65
1:M:185:ILE:HA	1:M:445:HIS:CE1	2.32	0.65
1:E:278:THR:HA	1:E:297:GLN:HE22	1.61	0.65
1:E:587:TYR:CD1	1:E:614:ILE:HD11	2.30	0.65
1:I:544:GLU:HG2	1:I:562:TRP:CG	2.32	0.65
3:O:140:THR:H	3:O:143:LYS:HZ2	1.45	0.65
1:A:219:TYR:CE2	1:A:371:SER:HB3	2.31	0.65
1:E:255:GLN:HB2	1:E:372:MET:SD	2.37	0.65
1:E:278:THR:HA	1:E:297:GLN:NE2	2.12	0.65
1:A:154:ASP:OD2	1:A:344:GLU:HB3	1.96	0.64
1:A:380:ASP:OD1	1:A:424:ARG:NH1	2.31	0.64
1:A:539:ALA:O	1:A:551:ARG:NH1	2.30	0.64
2:B:210:GLY:O	3:C:173:ARG:NH1	2.30	0.64
1:E:95:ILE:HG23	2:F:131:THR:HG22	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:259:THR:HG23	1:I:273:ARG:HE	1.62	0.64
3:C:14:SER:OG	3:C:16:ILE:HG12	1.97	0.64
3:C:112:TRP:HA	3:C:115:GLN:OE1	1.97	0.64
1:E:140:ALA:HB2	1:E:147:TRP:CE2	2.32	0.64
1:I:40:ARG:HH22	2:J:178:ARG:NH2	1.93	0.64
1:I:452:ILE:O	1:I:455:ILE:HG22	1.97	0.64
2:J:165:ARG:HH11	3:K:100:HIS:HD2	1.45	0.64
1:M:512:CYS:HA	1:M:516:ASN:HD22	1.62	0.64
1:M:544:GLU:CD	1:M:546:ARG:HD2	2.18	0.64
1:A:489:LEU:HD13	1:A:540:LEU:HA	1.79	0.64
1:E:41:ARG:HD3	2:F:62:CYS:O	1.98	0.64
1:I:89:PHE:CZ	1:I:400:MET:HE1	2.33	0.64
1:A:48:GLN:HB3	1:A:154:ASP:OD1	1.97	0.64
3:G:27:SER:OG	3:G:79:HIS:ND1	2.19	0.64
3:G:140:THR:H	3:G:143:LYS:HE3	1.61	0.64
1:M:376:ARG:HA	1:M:397:CYS:HB3	1.80	0.64
1:E:16:ALA:HB2	1:E:414:THR:HG22	1.79	0.64
1:I:198:CYS:SG	1:I:201:THR:HG23	2.38	0.64
1:M:141:PHE:HB2	1:M:149:THR:HG21	1.80	0.64
2:N:66:ALA:HB1	2:N:93:LEU:HD11	1.80	0.64
2:N:202:ASP:OD1	2:N:203:GLN:N	2.31	0.64
3:C:16:ILE:HG13	10:O:301:LMT:C6'	2.19	0.64
2:F:11:ARG:HB3	2:F:22:ARG:HG3	1.80	0.64
1:I:455:ILE:HD12	1:I:459:ARG:HH21	1.61	0.64
1:M:248:MET:HB3	1:M:251:MET:HG2	1.80	0.64
1:M:312:MET:HG2	1:M:326:LEU:HD11	1.78	0.64
1:A:185:ILE:HG22	1:A:192:LEU:HB2	1.80	0.64
9:C:301:HEM:HBC2	9:C:301:HEM:HHD	1.79	0.64
1:I:140:ALA:O	1:I:274:GLY:HA3	1.97	0.64
3:C:94:TRP:CH2	3:C:117:ILE:HD11	2.33	0.64
10:C:303:LMT:H3'	10:C:303:LMT:C3B	2.24	0.64
1:E:111:VAL:HG13	2:F:139:ASN:HD22	1.63	0.64
1:I:411:LEU:N	4:I:701:FAD:O2	2.23	0.64
1:A:139:ARG:HH11	1:A:271:GLY:HA3	1.63	0.63
3:G:88:PRO:HD3	3:G:112:TRP:CH2	2.32	0.63
3:K:27:SER:O	3:K:31:LEU:CB	2.45	0.63
1:M:342:LEU:O	1:M:343:ARG:NE	2.31	0.63
3:O:147:ARG:HB3	3:O:150:SER:O	1.97	0.63
2:F:13:ASN:OD1	2:F:52:LYS:NZ	2.32	0.63
10:C:303:LMT:O3'	10:C:303:LMT:O2B	2.05	0.63
1:E:329:ASP:OD1	1:E:331:ARG:NE	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:257:HIS:ND1	1:I:258:PRO:HD2	2.12	0.63
1:M:134:GLY:HA3	2:N:136:ARG:HH11	1.61	0.63
1:M:216:THR:HG21	1:M:236:GLY:H	1.62	0.63
1:M:247:PRO:HD2	1:M:384:TYR:HB3	1.80	0.63
3:O:195:LEU:HA	3:O:198:ILE:HG22	1.80	0.63
3:G:169:VAL:HG12	3:G:173:ARG:HE	1.64	0.63
1:I:263:PRO:HB3	1:I:322:TYR:CE2	2.33	0.63
1:I:434:PRO:HG2	1:I:436:PHE:CZ	2.33	0.63
1:M:210:THR:HG21	1:M:429:THR:HG23	1.81	0.63
1:A:85:VAL:HG12	1:A:400:MET:CB	2.28	0.63
1:A:188:GLY:O	1:A:189:GLY:C	2.34	0.63
10:C:303:LMT:H6'	3:O:16:ILE:CG2	2.11	0.63
2:F:225:GLN:HE22	3:G:186:ARG:HH11	1.47	0.63
3:G:80:PHE:HB2	9:G:302:HEM:CBB	2.28	0.63
3:C:183:ARG:O	3:C:186:ARG:HB3	1.98	0.63
1:E:40:ARG:HB3	1:E:158:ARG:HH22	1.64	0.63
1:E:250:ASN:HB2	1:E:565:ARG:HG3	1.79	0.63
1:E:379:ARG:NH2	1:E:619:LYS:HB2	2.14	0.63
1:M:595:ARG:H	1:M:596:GLY:HA3	1.64	0.63
10:O:301:LMT:O3'	10:O:301:LMT:H1B	1.98	0.63
3:C:140:THR:O	3:C:143:LYS:HG3	1.99	0.63
1:E:255:GLN:NE2	1:E:301:ARG:HE	1.96	0.63
1:E:262:VAL:HG13	1:E:365:ARG:HH21	1.63	0.63
3:O:44:SER:HB2	3:O:52:MET:HB3	1.81	0.63
1:A:210:THR:HG23	1:A:211:SER:H	1.64	0.62
2:F:222:ILE:CG2	2:F:223:PRO:HD2	2.29	0.62
1:I:352:PHE:HA	2:J:80:GLN:HE21	1.63	0.62
2:J:171:LEU:O	2:J:175:SER:OG	2.10	0.62
1:M:227:THR:HG21	1:M:267:LEU:HB2	1.81	0.62
2:N:128:PHE:CA	2:N:129:ASP:HB3	2.29	0.62
3:O:159:LEU:HD21	9:O:302:HEM:HBC2	1.80	0.62
9:K:302:HEM:HBC2	9:K:302:HEM:HHD	1.80	0.62
1:M:491:LYS:HG3	1:M:495:LYS:HE3	1.81	0.62
1:E:587:TYR:HD1	1:E:614:ILE:CD1	2.13	0.62
3:G:72:VAL:O	3:G:76:MET:HB2	1.98	0.62
2:F:190:ARG:HD3	2:F:195:TYR:CE1	2.34	0.62
1:I:277:GLY:O	1:I:297:GLN:NE2	2.31	0.62
1:M:449:GLN:O	1:M:452:ILE:HG22	1.99	0.62
1:A:85:VAL:CG1	1:A:400:MET:HB3	2.30	0.62
1:A:405:ARG:HH21	1:A:410:SER:HB2	1.64	0.62
1:E:246:VAL:HG23	1:E:385:GLY:N	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:42:SER:O	1:I:45:SER:OG	2.18	0.62
1:M:59:ILE:HD13	1:M:128:GLU:HG2	1.81	0.62
1:M:410:SER:HB3	4:M:701:FAD:O3'	1.99	0.62
2:N:130:PRO:O	2:N:131:THR:CB	2.46	0.62
3:O:8:LEU:HB3	3:O:14:SER:HB3	1.81	0.62
3:O:69:GLY:HA3	3:O:134:LEU:HD11	1.81	0.62
1:E:399:ASP:OD2	1:E:565:ARG:NE	2.32	0.62
3:G:53:ASN:ND2	3:G:140:THR:HA	2.15	0.62
1:I:572:GLU:CB	1:I:573:GLY:HA3	2.29	0.62
1:M:12:GLY:HA2	4:M:701:FAD:H1B	1.82	0.62
1:M:27:ALA:HB1	1:M:430:LYS:NZ	2.14	0.62
1:M:51:MET:CE	1:M:412:ALA:HA	2.30	0.62
1:M:455:ILE:O	1:M:459:ARG:HB3	1.99	0.62
2:N:222:ILE:HG22	2:N:223:PRO:HD2	1.82	0.62
3:O:9:HIS:CE1	3:O:14:SER:HA	2.34	0.62
3:O:140:THR:H	3:O:143:LYS:NZ	1.97	0.62
1:A:611:LYS:HG3	1:A:612:PHE:H	1.65	0.62
1:I:475:ILE:HD12	1:I:495:LYS:HD3	1.82	0.62
1:I:572:GLU:HB2	1:I:573:GLY:HA3	1.80	0.62
2:N:65:CYS:HB2	2:N:75:LEU:HB2	1.80	0.62
3:O:52:MET:HA	3:O:55:ILE:HG22	1.81	0.62
3:C:16:ILE:HD11	10:O:301:LMT:C6'	2.15	0.62
1:E:32:ILE:HG21	1:E:207:TYR:CE2	2.35	0.62
3:G:145:ALA:O	3:G:148:LEU:HG	2.00	0.62
3:O:10:VAL:HG22	3:O:11:PRO:CD	2.30	0.62
1:A:261:THR:HB	1:A:266:ILE:O	2.00	0.62
3:C:41:LEU:HA	11:C:304:MQ7:H161	1.82	0.62
3:C:147:ARG:HG2	3:C:148:LEU:N	2.14	0.62
3:C:167:VAL:HG12	9:C:302:HEM:CAC	2.30	0.62
2:J:56:CYS:HB3	2:J:62:CYS:SG	2.39	0.62
1:M:40:ARG:HH22	2:N:178:ARG:HH12	1.47	0.62
1:M:542:ARG:HA	1:M:562:TRP:CH2	2.35	0.62
1:E:616:GLU:HG2	1:E:617:ALA:N	2.14	0.62
1:M:227:THR:OG1	1:M:369:HIS:ND1	2.12	0.62
1:M:341:LYS:HG2	1:M:342:LEU:HB3	1.82	0.62
3:G:169:VAL:O	3:G:173:ARG:HB2	1.99	0.61
2:N:225:GLN:HE22	3:O:186:ARG:CD	2.12	0.61
1:E:314:LYS:HB2	1:E:316:LEU:HD12	1.83	0.61
3:G:53:ASN:OD1	3:G:141:ALA:N	2.29	0.61
3:G:120:ILE:HG13	3:G:121:PHE:N	2.14	0.61
9:K:301:HEM:HBB2	9:K:301:HEM:HMB2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:31:LEU:HD12	9:O:303:HEM:C3C	2.35	0.61
2:B:146:PHE:O	2:B:150:ARG:HB2	2.01	0.61
3:C:56:ALA:HB1	3:C:139:ILE:HG21	1.82	0.61
2:F:42:GLN:O	2:F:46:GLU:HB2	2.00	0.61
1:I:11:ILE:N	1:I:213:LEU:O	2.29	0.61
1:M:118:TYR:O	1:M:273:ARG:NH2	2.33	0.61
1:A:217:GLY:HA2	1:A:394:GLU:HB3	1.81	0.61
2:B:26:PHE:CE2	2:B:43:ILE:HG23	2.35	0.61
1:I:613:VAL:O	1:I:613:VAL:HG12	2.01	0.61
1:E:355:VAL:HG13	1:E:360:GLN:HB2	1.81	0.61
2:F:190:ARG:HD3	2:F:195:TYR:CZ	2.35	0.61
1:A:343:ARG:O	1:A:345:VAL:N	2.32	0.61
1:E:571:LYS:O	1:E:572:GLU:HB2	2.00	0.61
1:M:257:HIS:CE1	1:M:301:ARG:HH22	2.19	0.61
1:M:294:ASP:OD1	1:M:294:ASP:N	2.34	0.61
3:O:95:LYS:HZ2	10:O:301:LMT:C5'	2.09	0.61
1:A:93:ALA:HA	1:A:416:VAL:CG2	2.31	0.61
1:A:499:LEU:HG	1:A:529:LEU:HD21	1.82	0.61
10:C:303:LMT:O6B	3:O:9:HIS:HB2	2.01	0.61
9:G:302:HEM:HBB2	9:G:302:HEM:HMB2	1.83	0.61
1:I:377:THR:OG1	1:I:398:TRP:HA	2.01	0.61
1:A:216:THR:HG22	4:A:701:FAD:C4A	2.31	0.61
3:C:36:TRP:C	11:C:304:MQ7:H2M3	2.21	0.61
3:C:142:ALA:O	3:C:144:SER:N	2.33	0.61
3:G:38:HIS:CE1	9:G:301:HEM:C3D	2.89	0.61
1:I:40:ARG:O	1:I:158:ARG:NH1	2.34	0.61
3:C:172:TYR:HA	3:C:189:PHE:CE1	2.36	0.61
1:E:258:PRO:HD2	1:E:301:ARG:HD2	1.83	0.61
1:I:14:ALA:HB2	4:I:701:FAD:C4B	2.31	0.61
2:F:148:LEU:HD13	2:F:177:MET:HG2	1.83	0.61
3:K:5:THR:HG23	3:K:6:ILE:N	2.15	0.61
3:O:45:VAL:HG21	3:O:211:PHE:HA	1.82	0.61
2:B:185:ASP:OD2	2:B:187:ARG:NH1	2.34	0.60
3:C:60:GLU:HG3	3:C:64:MET:HB2	1.83	0.60
1:E:381:GLY:HA3	1:E:421:ILE:HG23	1.83	0.60
3:G:35:LEU:HD13	3:G:167:VAL:HG11	1.83	0.60
1:I:542:ARG:HD3	1:I:549:HIS:CD2	2.36	0.60
1:M:120:GLY:CA	1:M:297:GLN:HG2	2.31	0.60
1:A:186:HIS:O	1:A:187:ASP:HB2	2.00	0.60
1:A:250:ASN:OD1	1:A:565:ARG:HA	2.00	0.60
1:A:262:VAL:HG21	1:A:325:HIS:CB	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:245:LEU:O	1:I:385:GLY:HA3	2.00	0.60
1:M:388:GLY:HA2	1:M:428:PHE:CE2	2.36	0.60
3:G:38:HIS:HE1	9:G:301:HEM:C3D	2.18	0.60
1:M:280:LEU:CD2	1:M:327:TRP:HB2	2.30	0.60
1:A:61:GLY:HA2	1:A:146:ALA:HB1	1.82	0.60
2:J:202:ASP:C	2:J:204:GLY:H	2.04	0.60
3:K:150:SER:CA	3:K:152:TRP:H	2.12	0.60
1:M:327:TRP:HB3	1:M:361:LEU:HD13	1.84	0.60
1:M:489:LEU:HB3	1:M:540:LEU:HB2	1.83	0.60
2:N:199:ILE:CG1	2:N:205:VAL:HG23	2.32	0.60
1:A:141:PHE:CE1	1:A:270:GLU:HB3	2.36	0.60
1:E:558:ASN:HA	1:E:603:ILE:HD12	1.83	0.60
3:G:129:HIS:NE2	9:G:301:HEM:ND	2.50	0.60
1:I:530:LYS:HE3	1:I:570:TRP:CD2	2.37	0.60
3:K:196:MET:O	3:K:200:PHE:HD2	1.84	0.60
2:N:191:SER:HB3	2:N:194:ASP:OD2	2.01	0.60
3:O:154:TYR:O	3:O:156:TYR:CD2	2.54	0.60
1:I:355:VAL:HG11	1:I:362:ILE:HD13	1.83	0.60
1:I:524:ARG:CZ	1:I:524:ARG:HB3	2.30	0.60
1:I:605:ASN:CG	1:I:608:PRO:HD3	2.22	0.60
1:M:89:PHE:HB2	1:M:416:VAL:HG11	1.82	0.60
1:M:308:MET:HG2	1:M:326:LEU:HD13	1.82	0.60
3:O:55:ILE:HA	3:O:58:PHE:HB2	1.82	0.60
1:A:221:ARG:NH1	1:A:228:ASN:O	2.35	0.60
1:E:405:ARG:NH1	5:E:702:FUM:O8	2.33	0.60
2:J:190:ARG:NH2	2:J:194:ASP:OD2	2.30	0.60
1:M:439:GLN:O	1:M:443:ASP:HB2	2.02	0.60
3:O:128:VAL:O	3:O:132:VAL:HG13	2.01	0.60
1:E:557:ARG:NH2	1:E:593:GLY:O	2.33	0.60
1:I:386:LEU:HD23	1:I:387:LYS:N	2.16	0.60
2:J:5:LEU:HD12	2:J:28:VAL:HG23	1.83	0.60
1:M:331:ARG:HA	1:M:338:ILE:HD13	1.83	0.60
1:I:246:VAL:HG12	1:I:385:GLY:H	1.67	0.60
1:A:377:THR:HB	1:A:381:GLY:HA2	1.83	0.59
1:M:261:THR:CG2	1:M:263:PRO:HD2	2.32	0.59
2:N:94:PRO:C	2:N:96:PHE:H	2.03	0.59
1:A:380:ASP:HB3	1:A:424:ARG:HG3	1.85	0.59
1:E:580:GLU:HG2	1:E:581:TYR:N	2.16	0.59
2:F:208:CYS:CA	6:F:301:F3S:S1	2.90	0.59
1:M:379:ARG:O	1:M:420:TYR:HE2	1.85	0.59
1:M:489:LEU:HD23	1:M:540:LEU:HA	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:VAL:HG21	1:A:325:HIS:HB3	1.83	0.59
1:E:339:THR:HB	1:E:343:ARG:HA	1.84	0.59
1:E:449:GLN:O	1:E:452:ILE:HG22	2.01	0.59
3:K:45:VAL:HG12	3:K:207:THR:HG23	1.85	0.59
1:M:546:ARG:NH2	1:M:558:ASN:O	2.35	0.59
1:A:1:MET:HG2	1:A:2:GLN:HG3	1.84	0.59
3:C:60:GLU:OE2	3:C:64:MET:HB2	2.02	0.59
3:G:48:SER:O	3:G:50:SER:N	2.34	0.59
2:J:199:ILE:HB	2:J:205:VAL:HG23	1.84	0.59
2:J:225:GLN:OE1	3:K:186:ARG:HD3	2.02	0.59
3:K:41:LEU:HG	3:K:42:VAL:HG23	1.83	0.59
3:O:164:GLU:HG2	3:O:200:PHE:HB3	1.84	0.59
1:I:61:GLY:HA2	1:I:146:ALA:HB1	1.85	0.59
2:N:199:ILE:HG13	2:N:205:VAL:HG23	1.85	0.59
1:A:5:HIS:HE1	1:M:5:HIS:HE1	1.49	0.59
2:B:44:ARG:HG2	2:B:49:PRO:HA	1.83	0.59
3:C:163:ALA:O	3:C:167:VAL:HG13	2.02	0.59
1:E:89:PHE:HE1	1:E:412:ALA:HB1	1.68	0.59
1:E:439:GLN:O	1:E:443:ASP:HB2	2.03	0.59
1:M:530:LYS:HG2	1:M:570:TRP:CZ2	2.38	0.59
2:N:202:ASP:O	2:N:203:GLN:HB3	2.01	0.59
3:O:106:HIS:HD2	3:O:109:THR:H	1.51	0.59
1:A:210:THR:HG21	1:A:429:THR:HG23	1.85	0.59
1:E:499:LEU:HG	1:E:529:LEU:HD21	1.84	0.59
1:M:261:THR:HG21	1:M:353:LEU:HD11	1.85	0.59
1:A:140:ALA:HB3	1:A:274:GLY:O	2.02	0.59
2:B:119:ALA:HB1	2:B:182:PHE:CE2	2.37	0.59
1:E:55:LEU:HD12	1:E:57:ASN:ND2	2.17	0.59
2:N:11:ARG:HA	2:N:101:ASP:OD1	2.02	0.59
3:O:83:ALA:HB1	9:O:303:HEM:C3A	2.38	0.59
2:F:202:ASP:OD1	2:F:203:GLN:N	2.36	0.59
2:J:106:THR:HB	2:J:110:PHE:HE2	1.67	0.59
3:O:29:ALA:O	3:O:32:ILE:HG22	2.03	0.59
1:A:10:CYS:SG	1:A:21:ALA:HB2	2.43	0.59
2:B:137:MET:HG2	2:B:142:ALA:HB2	1.85	0.59
1:I:199:LEU:HD23	1:I:515:MET:HE1	1.84	0.59
3:K:48:SER:HB3	3:K:51:LEU:HG	1.85	0.59
1:A:40:ARG:O	1:A:158:ARG:NH1	2.37	0.58
1:E:277:GLY:O	1:E:297:GLN:NE2	2.36	0.58
1:I:216:THR:HG21	1:I:236:GLY:H	1.67	0.58
3:K:173:ARG:HG2	3:K:177:LYS:HE2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:247:PRO:HD2	1:M:384:TYR:CB	2.33	0.58
3:O:155:LEU:C	3:O:157:LEU:H	2.07	0.58
1:A:5:HIS:CE1	1:M:5:HIS:HE1	2.21	0.58
1:A:400:MET:CG	1:A:401:HIS:CD2	2.86	0.58
3:C:103:MET:O	3:C:105:HIS:ND1	2.34	0.58
1:E:94:PRO:O	1:E:98:ARG:HD3	2.03	0.58
1:M:572:GLU:HB3	1:M:573:GLY:CA	2.32	0.58
2:N:35:THR:H	2:N:38:ILE:HD12	1.68	0.58
3:O:46:ILE:HD13	3:O:210:ARG:HB3	1.85	0.58
3:G:6:ILE:HG13	3:G:7:THR:N	2.18	0.58
3:G:56:ALA:CB	3:G:139:ILE:HG21	2.31	0.58
1:I:91:ASP:O	1:I:94:PRO:HD2	2.02	0.58
1:I:616:GLU:HG2	1:I:617:ALA:H	1.67	0.58
3:K:64:MET:O	3:K:68:GLY:N	2.25	0.58
3:K:148:LEU:HD12	3:K:149:GLN:N	2.17	0.58
1:M:539:ALA:HB1	1:M:549:HIS:CE1	2.38	0.58
1:M:557:ARG:HD2	1:M:559:ASP:OD1	2.03	0.58
2:N:7:LEU:HD23	2:N:88:ILE:HB	1.85	0.58
1:A:52:GLN:HG2	1:A:69:HIS:NE2	2.18	0.58
1:A:152:THR:HG23	1:A:156:THR:HG23	1.84	0.58
1:A:400:MET:CE	1:A:401:HIS:CE1	2.86	0.58
1:E:346:TYR:O	1:E:350:THR:OG1	2.20	0.58
1:I:558:ASN:H	1:I:603:ILE:H	1.50	0.58
3:K:129:HIS:NE2	9:K:301:HEM:C4D	2.71	0.58
1:M:227:THR:HG1	1:M:369:HIS:CE1	2.20	0.58
1:M:258:PRO:HD2	1:M:301:ARG:NH2	2.18	0.58
1:A:178:ARG:HA	1:A:199:LEU:HD12	1.85	0.58
2:B:110:PHE:CZ	2:B:153:GLU:HG2	2.39	0.58
3:C:43:SER:OG	3:C:207:THR:OG1	2.11	0.58
3:K:129:HIS:HE1	9:K:301:HEM:HBA1	1.67	0.58
2:N:128:PHE:HA	2:N:129:ASP:HB3	1.85	0.58
3:O:139:ILE:HG13	3:O:143:LYS:NZ	2.16	0.58
3:O:154:TYR:CG	3:O:155:LEU:N	2.71	0.58
2:F:57:CYS:SG	2:F:61:ILE:O	2.62	0.58
1:I:613:VAL:C	1:I:615:PRO:HD3	2.24	0.58
3:K:186:ARG:HG3	3:K:190:GLN:NE2	2.18	0.58
1:M:546:ARG:HH12	1:M:562:TRP:HB2	1.68	0.58
1:A:195:ILE:HD13	1:A:206:ALA:HB2	1.85	0.58
1:A:369:HIS:NE2	5:A:702:FUM:O7	2.33	0.58
1:E:257:HIS:O	1:E:366:PRO:HA	2.03	0.58
1:E:459:ARG:HG2	1:E:460:LYS:N	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:318:VAL:O	1:I:324:ASP:HA	2.03	0.58
2:B:224:LEU:O	2:B:228:LEU:HB2	2.04	0.58
1:E:200:ARG:HG2	2:F:99:LEU:HD22	1.85	0.58
2:F:165:ARG:NH2	3:K:3:ALA:O	2.35	0.58
1:I:458:GLY:HA3	1:I:459:ARG:HH11	1.69	0.58
1:M:405:ARG:NH2	5:M:702:FUM:O8	2.36	0.58
2:N:185:ASP:OD2	2:N:187:ARG:NH1	2.36	0.58
3:O:35:LEU:HD13	3:O:167:VAL:HG11	1.86	0.58
1:A:452:ILE:HA	1:A:455:ILE:HG22	1.86	0.58
1:E:279:LEU:HD12	1:E:297:GLN:HB3	1.86	0.58
3:G:149:GLN:HA	3:G:150:SER:O	2.03	0.58
1:I:346:TYR:CD1	1:I:350:THR:HG21	2.38	0.58
3:O:25:MET:HG2	3:O:174:ILE:HD11	1.86	0.58
1:A:484:ARG:O	1:A:551:ARG:HA	2.04	0.58
1:A:524:ARG:CZ	1:A:524:ARG:HB3	2.34	0.58
2:B:42:GLN:O	2:B:46:GLU:HB2	2.03	0.58
1:E:20:VAL:HG23	1:E:422:GLY:HA2	1.86	0.58
1:I:25:SER:OG	1:I:171:TYR:HB3	2.04	0.58
1:I:306:ARG:HG3	1:I:483:PHE:CZ	2.38	0.58
1:I:616:GLU:N	1:I:616:GLU:OE1	2.36	0.58
1:M:278:THR:HG23	1:M:286:ARG:HG3	1.85	0.58
1:E:19:ARG:NH2	1:E:99:GLU:OE1	2.31	0.57
3:G:206:LEU:O	3:G:210:ARG:HB2	2.03	0.57
1:I:70:PHE:CZ	1:I:74:VAL:HG21	2.39	0.57
1:I:121:GLY:HA3	1:I:286:ARG:NH1	2.17	0.57
1:M:512:CYS:O	1:M:513:LYS:HG2	2.04	0.57
1:M:513:LYS:HD3	2:N:13:ASN:CB	2.33	0.57
1:E:557:ARG:HD2	1:E:559:ASP:OD1	2.05	0.57
2:J:199:ILE:HD13	2:J:205:VAL:HG21	1.86	0.57
3:O:5:THR:HG23	3:O:6:ILE:H	1.69	0.57
3:O:133:VAL:HG23	3:O:147:ARG:NH2	2.07	0.57
1:E:185:ILE:HG22	1:E:192:LEU:HB2	1.86	0.57
1:M:217:GLY:H	1:M:395:SER:HB3	1.69	0.57
1:A:35:SER:OG	1:A:37:VAL:O	2.12	0.57
1:E:97:MET:O	1:E:101:ALA:HB2	2.05	0.57
3:G:40:MET:O	3:G:44:SER:OG	2.19	0.57
1:I:459:ARG:HB2	1:I:460:LYS:HA	1.84	0.57
3:O:80:PHE:HB2	9:O:303:HEM:CBB	2.35	0.57
1:A:184:LEU:O	1:A:445:HIS:NE2	2.37	0.57
1:A:302:ASP:HB2	1:A:306:ARG:HH21	1.69	0.57
3:C:148:LEU:C	3:C:149:GLN:O	2.42	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:378:ASN:ND2	1:E:382:ALA:HB3	2.19	0.57
1:E:454:ASP:O	1:E:458:GLY:N	2.38	0.57
1:I:348:ILE:O	1:I:352:PHE:HB2	2.05	0.57
1:M:493:VAL:HA	1:M:496:LEU:HD23	1.87	0.57
2:B:215:GLU:CD	3:C:183:ARG:HD3	2.24	0.57
3:C:31:LEU:HD22	9:C:302:HEM:CAC	2.34	0.57
9:G:301:HEM:HMB2	9:G:301:HEM:HBB2	1.85	0.57
1:M:257:HIS:O	1:M:366:PRO:HA	2.03	0.57
1:M:444:ALA:HA	1:M:448:VAL:HG13	1.86	0.57
3:C:153:LEU:HD23	3:C:156:TYR:OH	2.04	0.57
3:G:121:PHE:HD2	3:G:162:LEU:HD13	1.69	0.57
1:I:40:ARG:HG2	1:I:165:ASP:OD2	2.04	0.57
1:I:278:THR:HB	1:I:329:ASP:HB3	1.85	0.57
1:I:340:THR:HG22	1:I:340:THR:O	2.03	0.57
1:M:306:ARG:HD2	1:M:482:ILE:HG22	1.87	0.57
2:N:190:ARG:HB2	2:N:195:TYR:CE2	2.40	0.57
3:O:130:MET:O	3:O:134:LEU:HB2	2.05	0.57
3:C:16:ILE:HD12	10:O:301:LMT:H6E	1.59	0.57
3:C:191:LYS:HD2	3:C:194:ASN:HB3	1.85	0.57
1:E:291:TYR:CD2	1:E:307:ARG:HD2	2.40	0.57
3:O:171:PHE:O	3:O:174:ILE:HG22	2.05	0.57
3:O:189:PHE:O	3:O:193:GLU:HB2	2.04	0.57
3:C:120:ILE:HG23	10:C:303:LMT:H121	1.87	0.57
1:E:510:SER:HB3	2:F:49:PRO:HG2	1.86	0.57
1:E:586:PRO:O	1:E:587:TYR:HB2	2.05	0.57
2:F:110:PHE:HA	2:F:113:THR:HG22	1.87	0.57
1:I:463:GLU:HB3	1:I:468:ILE:HD11	1.86	0.57
2:J:165:ARG:HH11	3:K:100:HIS:CD2	2.22	0.57
1:M:32:ILE:HD13	1:M:207:TYR:CE2	2.39	0.57
1:A:412:ALA:O	1:A:416:VAL:CB	2.49	0.57
3:G:154:TYR:CZ	3:G:155:LEU:HG	2.40	0.57
1:I:44:SER:OG	4:I:701:FAD:O5'	2.23	0.57
2:J:6:THR:O	2:J:88:ILE:N	2.22	0.57
2:N:211:LEU:HD23	3:O:173:ARG:NH1	2.19	0.57
1:A:76:GLY:O	1:A:404:ASN:HB3	2.05	0.56
10:C:303:LMT:O6B	3:O:9:HIS:CB	2.52	0.56
1:E:255:GLN:HE22	1:E:301:ARG:HE	1.52	0.56
1:E:517:PRO:HG2	2:F:49:PRO:O	2.05	0.56
2:F:65:CYS:HB3	2:F:76:ALA:H	1.70	0.56
3:G:60:GLU:H	3:G:60:GLU:CD	2.07	0.56
2:N:131:THR:HG22	2:N:132:ALA:N	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:131:THR:HG22	2:N:132:ALA:H	1.70	0.56
1:A:108:ASN:OD1	1:A:153:ALA:N	2.20	0.56
1:A:417:ALA:O	1:A:421:ILE:HG12	2.05	0.56
3:C:143:LYS:HZ2	9:C:301:HEM:HBA1	1.70	0.56
1:E:595:ARG:HD2	1:E:597:TYR:HE1	1.70	0.56
3:G:140:THR:HB	3:G:143:LYS:HG3	1.87	0.56
1:I:301:ARG:NH2	5:I:702:FUM:O	2.39	0.56
3:K:31:LEU:HD11	9:K:302:HEM:C3C	2.40	0.56
1:M:301:ARG:NH1	1:M:405:ARG:HH12	2.03	0.56
3:O:10:VAL:HG22	3:O:11:PRO:HD3	1.87	0.56
1:A:32:ILE:HD13	1:A:207:TYR:CE2	2.40	0.56
1:A:210:THR:CG2	1:A:429:THR:HG23	2.35	0.56
1:A:214:ILE:HG23	1:A:236:GLY:HA3	1.88	0.56
3:C:77:VAL:O	3:C:80:PHE:HB3	2.06	0.56
1:E:51:MET:HG3	1:E:411:LEU:HB3	1.88	0.56
1:E:306:ARG:NH2	1:E:547:GLY:O	2.38	0.56
3:G:19:ARG:O	3:G:22:PHE:HB3	2.04	0.56
1:I:235:GLY:HA3	4:I:701:FAD:N6A	2.20	0.56
3:K:174:ILE:HD13	9:K:302:HEM:HBD1	1.87	0.56
1:M:92:THR:HA	1:M:95:ILE:HD12	1.86	0.56
1:M:98:ARG:O	1:M:102:HIS:ND1	2.38	0.56
1:A:400:MET:HE3	1:A:401:HIS:CE1	2.40	0.56
3:G:38:HIS:HE1	9:G:301:HEM:CAD	2.18	0.56
1:I:281:ASP:HB3	1:I:311:HIS:NE2	2.19	0.56
1:A:198:CYS:SG	1:A:201:THR:HG23	2.45	0.56
2:B:165:ARG:HD3	3:C:100:HIS:HB2	1.88	0.56
1:E:89:PHE:HA	1:E:416:VAL:HG11	1.85	0.56
1:I:607:LEU:HD12	1:I:607:LEU:N	2.20	0.56
2:J:190:ARG:HH21	2:J:194:ASP:CG	2.09	0.56
1:M:259:THR:HB	1:M:268:VAL:CG2	2.35	0.56
1:M:338:ILE:HD12	1:M:358:ILE:HA	1.88	0.56
3:O:6:ILE:HG23	3:O:7:THR:N	2.20	0.56
1:A:344:GLU:OE2	2:B:150:ARG:HD2	2.05	0.56
3:G:12:GLN:HG3	3:G:13:ARG:H	1.71	0.56
3:G:27:SER:O	3:G:31:LEU:HB2	2.06	0.56
1:M:43:HIS:HD2	4:M:701:FAD:HM81	1.66	0.56
3:O:188:TRP:O	3:O:192:THR:HB	2.06	0.56
1:A:257:HIS:CE1	5:A:702:FUM:H5	2.40	0.56
1:E:85:VAL:HG13	1:E:398:TRP:CE2	2.41	0.56
1:I:452:ILE:HD12	1:I:526:ARG:HH21	1.70	0.56
1:M:221:ARG:HD2	1:M:226:THR:HG21	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:306:ARG:HH22	1:M:483:PHE:HD1	1.53	0.56
1:A:278:THR:HB	1:A:329:ASP:HB3	1.87	0.56
1:A:510:SER:OG	2:B:49:PRO:HG2	2.06	0.56
2:B:214:CYS:HB2	2:B:224:LEU:HD13	1.86	0.56
3:G:32:ILE:HA	9:G:302:HEM:HBC1	1.88	0.56
1:I:327:TRP:CE3	1:I:361:LEU:HB2	2.40	0.56
1:A:70:PHE:O	1:A:74:VAL:HG23	2.05	0.56
1:E:468:ILE:HD12	1:E:506:ILE:HD11	1.88	0.56
1:E:556:GLU:HA	1:E:601:VAL:HB	1.88	0.56
1:I:228:ASN:HD22	4:I:701:FAD:HM81	1.71	0.56
2:J:10:PHE:HB2	2:J:91:HIS:HD2	1.70	0.56
1:M:503:SER:HA	1:M:506:ILE:HD11	1.87	0.56
3:O:139:ILE:HA	3:O:143:LYS:CE	2.36	0.56
1:A:291:TYR:HB3	1:A:307:ARG:NE	2.20	0.56
1:E:251:MET:SD	1:E:534:CYS:HB3	2.46	0.56
1:I:163:THR:O	1:I:167:LYS:HG2	2.05	0.56
1:I:376:ARG:HG3	1:I:384:TYR:CD2	2.41	0.56
2:J:44:ARG:HG2	2:J:49:PRO:HA	1.87	0.56
3:K:144:SER:HB2	9:K:301:HEM:HAA1	1.87	0.56
3:K:148:LEU:HD12	3:K:149:GLN:H	1.71	0.56
1:A:311:HIS:CE1	1:A:316:LEU:HD12	2.41	0.55
1:A:338:ILE:O	1:A:343:ARG:HB2	2.05	0.55
1:E:475:ILE:HG21	1:E:496:LEU:HG	1.88	0.55
1:E:557:ARG:HB2	1:E:601:VAL:O	2.07	0.55
2:F:7:LEU:HD23	2:F:88:ILE:HB	1.87	0.55
1:I:370:TYR:CE2	1:I:372:MET:HA	2.41	0.55
1:M:22:VAL:O	1:M:26:MET:HB2	2.07	0.55
2:B:192:GLU:HA	2:B:195:TYR:HD2	1.71	0.55
3:C:116:VAL:HG13	10:C:303:LMT:H102	1.89	0.55
1:E:113:GLY:O	1:E:128:GLU:N	2.39	0.55
1:E:230:VAL:HG22	2:F:56:CYS:O	2.06	0.55
1:E:452:ILE:HD12	1:E:526:ARG:NH2	2.20	0.55
1:I:226:THR:HG1	1:I:368:HIS:HD1	1.52	0.55
1:M:509:SER:HB2	2:N:49:PRO:HG3	1.89	0.55
3:C:172:TYR:HA	3:C:189:PHE:HE1	1.72	0.55
1:E:23:GLU:HG2	1:E:423:GLU:HG2	1.87	0.55
3:C:9:HIS:O	3:C:10:VAL:HG12	2.06	0.55
9:C:302:HEM:HBB2	9:C:302:HEM:HMB1	1.88	0.55
1:E:357:PRO:HB3	1:E:362:ILE:HD11	1.88	0.55
2:F:63:GLY:N	2:F:152:ILE:HD12	2.21	0.55
1:I:143:GLY:H	1:I:406:LEU:HD21	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:266:ILE:HG21	1:I:348:ILE:HD12	1.88	0.55
1:I:544:GLU:OE2	1:I:546:ARG:NH1	2.39	0.55
1:M:40:ARG:NH2	2:N:178:ARG:HH12	2.04	0.55
1:M:79:TRP:H	1:M:79:TRP:HE3	1.53	0.55
2:B:222:ILE:HG22	2:B:223:PRO:HD2	1.89	0.55
3:C:5:THR:OG1	3:C:6:ILE:N	2.39	0.55
3:C:21:ASP:OD2	3:C:178:TYR:OH	2.23	0.55
1:E:444:ALA:HA	1:E:448:VAL:HG23	1.89	0.55
1:I:32:ILE:HG21	1:I:207:TYR:CE2	2.41	0.55
1:M:82:ASP:HA	1:M:585:SER:OG	2.06	0.55
1:M:222:ILE:HG13	1:M:223:TYR:CD1	2.41	0.55
1:M:394:GLU:OE1	4:M:701:FAD:H3'	2.06	0.55
2:N:225:GLN:HE21	3:O:176:VAL:CG1	2.19	0.55
2:N:225:GLN:NE2	3:O:186:ARG:HD3	2.20	0.55
3:O:158:VAL:O	3:O:162:LEU:HD12	2.06	0.55
1:A:6:THR:HG22	1:A:30:LYS:HG3	1.88	0.55
1:E:241:LEU:HD13	1:E:248:MET:HG2	1.89	0.55
3:G:31:LEU:HD22	9:G:302:HEM:CAC	2.37	0.55
3:K:34:PHE:CE1	3:K:72:VAL:HG11	2.42	0.55
1:M:84:GLU:O	1:M:88:ILE:HG13	2.07	0.55
2:N:166:MET:SD	3:O:97:PHE:HB2	2.47	0.55
2:F:96:PHE:O	2:F:98:LEU:HD12	2.07	0.55
3:G:128:VAL:HG12	3:K:128:VAL:HG12	1.88	0.55
1:I:124:PHE:HE2	1:I:126:ALA:HB2	1.66	0.55
1:I:560:LYS:HG3	1:I:607:LEU:HD11	1.87	0.55
1:M:108:ASN:OD1	1:M:152:THR:HA	2.06	0.55
1:M:262:VAL:CG1	1:M:263:PRO:HD3	2.37	0.55
1:A:400:MET:HG2	1:A:401:HIS:CD2	2.42	0.55
1:E:59:ILE:HG12	1:E:128:GLU:HA	1.89	0.55
1:E:436:PHE:HE2	1:I:438:MET:HG3	1.72	0.55
3:G:181:VAL:HG12	3:G:182:GLY:N	2.22	0.55
1:I:342:LEU:HD22	1:I:346:TYR:CD2	2.42	0.55
1:I:595:ARG:HH11	1:I:597:TYR:HE1	1.55	0.55
1:M:81:CYS:HB2	1:M:399:ASP:O	2.06	0.55
1:M:304:VAL:HG12	1:M:308:MET:HE1	1.89	0.55
1:M:308:MET:O	1:M:312:MET:HB2	2.06	0.55
1:A:403:PHE:HB3	1:A:547:GLY:HA3	1.88	0.55
2:B:199:ILE:HB	2:B:205:VAL:HG23	1.88	0.55
1:E:13:GLY:O	1:E:18:GLU:HG3	2.07	0.55
1:E:34:LEU:HD23	1:E:176:HIS:HB2	1.87	0.55
1:E:40:ARG:NH1	2:F:153:GLU:OE2	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:572:GLU:HB3	1:E:573:GLY:CA	2.37	0.55
1:I:559:ASP:OD2	1:I:592:PRO:HB3	2.07	0.55
2:J:63:GLY:HA2	2:J:75:LEU:HD21	1.88	0.55
1:M:278:THR:HG22	1:M:279:LEU:H	1.71	0.55
3:C:181:VAL:HG12	3:C:182:GLY:N	2.22	0.55
1:I:186:HIS:NE2	1:I:243:THR:HB	2.22	0.55
3:O:95:LYS:HZ2	10:O:301:LMT:H1'	1.72	0.55
1:A:400:MET:HG3	1:A:401:HIS:CD2	2.41	0.54
1:I:238:ILE:HG13	1:I:239:ILE:N	2.22	0.54
1:I:620:GLU:HG3	1:I:620:GLU:O	2.07	0.54
3:K:176:VAL:O	3:K:178:TYR:N	2.36	0.54
1:M:61:GLY:O	1:M:64:ASP:HB2	2.07	0.54
2:N:180:ALA:O	2:N:183:TYR:N	2.37	0.54
1:E:499:LEU:HA	1:E:502:ARG:HB2	1.90	0.54
3:G:150:SER:HB3	3:G:151:GLY:C	2.27	0.54
2:J:110:PHE:HE1	2:J:174:VAL:HG11	1.72	0.54
9:K:302:HEM:HMB2	9:K:302:HEM:HBB2	1.87	0.54
2:N:68:VAL:HA	2:N:73:PRO:HA	1.89	0.54
1:E:6:THR:HG21	1:E:32:ILE:HG13	1.89	0.54
1:E:185:ILE:HA	1:E:445:HIS:CE1	2.41	0.54
3:G:176:VAL:CG1	3:G:181:VAL:HG21	2.37	0.54
1:I:288:MET:O	1:I:292:GLU:N	2.40	0.54
2:N:36:LEU:HB2	2:N:76:ALA:O	2.07	0.54
1:A:562:TRP:HZ3	1:A:581:TYR:CE2	2.25	0.54
3:C:41:LEU:CA	11:C:304:MQ7:H141	2.37	0.54
3:C:149:GLN:O	3:C:150:SER:C	2.46	0.54
1:E:159:SER:O	1:E:163:THR:HG23	2.08	0.54
1:E:273:ARG:HD2	1:E:297:GLN:HB2	1.88	0.54
3:G:32:ILE:CD1	3:G:167:VAL:HB	2.38	0.54
3:G:45:VAL:HA	3:G:47:LEU:N	2.18	0.54
1:I:117:TYR:OH	1:I:128:GLU:OE2	2.18	0.54
3:K:62:THR:HG23	3:K:139:ILE:HB	1.90	0.54
3:K:167:VAL:HG12	9:K:302:HEM:HAC	1.89	0.54
3:O:38:HIS:HD2	9:O:302:HEM:NB	2.02	0.54
10:C:303:LMT:H6'	3:O:16:ILE:HG21	1.72	0.54
1:I:342:LEU:HD13	1:I:346:TYR:CD2	2.42	0.54
3:K:6:ILE:HG22	3:K:7:THR:N	2.19	0.54
1:A:52:GLN:OE1	1:A:409:ASN:ND2	2.38	0.54
1:A:294:ASP:OD1	1:A:294:ASP:N	2.19	0.54
2:B:35:THR:HG22	2:B:80:GLN:HG2	1.89	0.54
1:E:248:MET:O	1:E:568:SER:N	2.32	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:257:HIS:NE2	1:E:259:THR:OG1	2.40	0.54
1:E:468:ILE:HG23	1:E:499:LEU:HD11	1.90	0.54
1:M:339:THR:O	1:M:344:GLU:HG3	2.07	0.54
1:M:563:LEU:HG	1:M:588:TYR:OH	2.07	0.54
1:A:572:GLU:HB3	1:A:573:GLY:CA	2.30	0.54
1:E:405:ARG:HH12	1:E:407:GLY:HA2	1.73	0.54
1:E:559:ASP:CB	1:E:605:ASN:HB2	2.37	0.54
1:I:500:TYR:HA	1:I:529:LEU:HD22	1.90	0.54
2:J:150:ARG:HH21	2:J:220:LYS:HB3	1.73	0.54
3:K:160:LEU:HD21	3:K:204:GLY:HA3	1.89	0.54
9:O:302:HEM:HBD1	9:O:302:HEM:CMD	2.38	0.54
1:A:213:LEU:HB2	1:A:425:MET:HE3	1.90	0.54
3:C:37:ALA:HA	11:C:304:MQ7:H111	1.89	0.54
3:C:171:PHE:HD2	3:C:193:GLU:HG2	1.72	0.54
1:I:458:GLY:C	1:I:459:ARG:HD3	2.28	0.54
3:K:32:ILE:HD12	9:K:302:HEM:CBC	2.38	0.54
1:M:15:LEU:HB2	1:M:44:SER:OG	2.08	0.54
3:O:155:LEU:CD1	3:O:156:TYR:H	2.19	0.54
2:B:117:ILE:HA	2:B:198:VAL:CG1	2.37	0.54
3:C:135:THR:OG1	3:C:136:ASP:N	2.40	0.54
1:E:547:GLY:HA2	1:E:595:ARG:HH22	1.73	0.54
3:K:185:LYS:HB2	3:K:189:PHE:HB2	1.89	0.54
1:A:6:THR:HG22	1:A:30:LYS:HE3	1.90	0.54
1:A:15:LEU:HD12	1:A:44:SER:HB3	1.90	0.54
2:B:34:MET:HA	2:B:38:ILE:HD12	1.90	0.54
2:J:7:LEU:HD23	2:J:88:ILE:HD13	1.90	0.54
1:M:198:CYS:SG	1:M:201:THR:HG23	2.48	0.54
1:M:267:LEU:HD21	5:M:702:FUM:O	2.08	0.54
1:A:38:PRO:HG2	1:A:41:ARG:NH1	2.23	0.53
1:A:292:GLU:OE1	1:A:598:GLY:N	2.30	0.53
3:C:32:ILE:HD11	3:C:167:VAL:HB	1.89	0.53
3:C:159:LEU:HD22	9:C:301:HEM:CMD	2.38	0.53
1:E:15:LEU:HD22	1:E:44:SER:HB3	1.90	0.53
1:E:572:GLU:HB3	1:E:573:GLY:HA3	1.91	0.53
2:J:124:ASP:N	2:J:124:ASP:OD1	2.38	0.53
2:J:213:ALA:O	2:J:217:VAL:HG22	2.07	0.53
3:K:132:VAL:HG21	3:K:153:LEU:HD21	1.90	0.53
1:M:257:HIS:NE2	1:M:259:THR:OG1	2.40	0.53
1:M:262:VAL:HG23	1:M:365:ARG:NH2	2.23	0.53
1:M:291:TYR:CE1	1:M:311:HIS:HB2	2.43	0.53
3:O:6:ILE:HG23	3:O:7:THR:H	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:149:GLN:HG2	3:O:212:MET:HG3	1.88	0.53
3:C:148:LEU:HD21	3:C:212:MET:HA	1.90	0.53
1:E:223:TYR:OH	1:E:254:VAL:HG11	2.08	0.53
2:F:122:HIS:N	2:F:188:ASP:OD2	2.35	0.53
3:G:95:LYS:O	3:G:99:VAL:HG23	2.07	0.53
1:I:118:TYR:HD1	1:I:332:HIS:CE1	2.25	0.53
1:I:350:THR:HG22	1:I:355:VAL:O	2.08	0.53
2:J:75:LEU:HG	2:J:219:PRO:HG3	1.90	0.53
1:M:70:PHE:O	1:M:74:VAL:HG23	2.08	0.53
1:M:237:GLN:HE22	1:M:395:SER:HA	1.72	0.53
1:M:513:LYS:O	1:M:513:LYS:HG3	2.08	0.53
1:M:572:GLU:HB3	1:M:573:GLY:HA3	1.89	0.53
1:A:77:SER:HB2	1:A:402:GLY:HA3	1.90	0.53
1:A:530:LYS:HE3	1:A:570:TRP:CD2	2.43	0.53
2:B:7:LEU:HD12	2:B:43:ILE:HD11	1.90	0.53
3:C:16:ILE:HD12	10:O:301:LMT:O6'	2.07	0.53
3:G:149:GLN:CA	3:G:150:SER:O	2.57	0.53
1:I:314:LYS:HB2	1:I:316:LEU:HD12	1.90	0.53
3:O:172:TYR:HA	3:O:189:PHE:HE2	1.72	0.53
1:E:208:LEU:HG	1:E:436:PHE:CD1	2.42	0.53
3:G:83:ALA:O	3:G:87:MET:HG3	2.09	0.53
3:K:135:THR:O	3:K:137:LEU:HD23	2.09	0.53
1:A:6:THR:HG21	1:A:32:ILE:HG13	1.90	0.53
1:A:127:GLU:HG2	1:A:128:GLU:H	1.74	0.53
1:A:260:GLY:HA3	1:A:367:THR:OG1	2.08	0.53
3:C:97:PHE:CE1	3:C:113:VAL:HG23	2.43	0.53
1:E:87:ARG:HA	1:E:87:ARG:HE	1.73	0.53
1:E:318:VAL:HG21	1:E:327:TRP:NE1	2.24	0.53
3:G:125:LEU:HA	3:G:128:VAL:HG22	1.89	0.53
1:M:139:ARG:O	1:M:149:THR:HG22	2.09	0.53
1:M:326:LEU:N	1:M:326:LEU:HD12	2.23	0.53
3:O:31:LEU:HD23	3:O:75:LEU:CD2	2.39	0.53
1:A:5:HIS:CE1	1:M:5:HIS:CE1	2.97	0.53
2:B:211:LEU:HD22	3:C:109:THR:HA	1.90	0.53
3:C:38:HIS:CE1	9:C:301:HEM:ND	2.75	0.53
1:E:518:GLU:HB2	2:F:49:PRO:HB2	1.90	0.53
2:F:225:GLN:HE22	3:G:186:ARG:HD3	1.74	0.53
1:I:32:ILE:HA	1:I:174:THR:HG23	1.90	0.53
1:I:257:HIS:CD2	1:I:259:THR:H	2.26	0.53
1:I:386:LEU:HD23	1:I:387:LYS:H	1.73	0.53
1:I:508:LEU:HB2	1:I:518:GLU:OE1	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:202:ASP:CG	2:J:203:GLN:N	2.61	0.53
2:J:211:LEU:HD22	3:K:109:THR:HA	1.91	0.53
3:K:133:VAL:HG12	3:K:147:ARG:NH2	2.24	0.53
1:M:106:PRO:HD2	1:M:159:SER:HB2	1.91	0.53
1:M:340:THR:O	1:M:341:LYS:O	2.26	0.53
3:O:41:LEU:HD13	3:O:63:TYR:CD2	2.44	0.53
3:O:181:VAL:HG12	3:O:182:GLY:N	2.18	0.53
1:E:14:ALA:HB3	4:E:701:FAD:O1P	2.09	0.53
1:E:251:MET:SD	1:E:568:SER:OG	2.62	0.53
3:G:175:GLY:HA2	3:G:180:PHE:CD2	2.43	0.53
3:K:41:LEU:HD22	3:K:63:TYR:CZ	2.44	0.53
1:M:16:ALA:O	1:M:20:VAL:HG12	2.09	0.53
1:M:27:ALA:HB1	1:M:430:LYS:HZ1	1.72	0.53
1:M:233:ASP:HB3	1:M:528:MET:HE2	1.90	0.53
3:O:151:GLY:N	3:O:152:TRP:CD1	2.73	0.53
1:E:203:GLU:HG2	1:E:204:LEU:H	1.74	0.53
1:I:64:ASP:OD2	1:I:148:ARG:HB3	2.09	0.53
1:I:556:GLU:HA	1:I:601:VAL:HG23	1.91	0.53
2:J:48:ASP:OD1	2:J:50:THR:HG22	2.09	0.53
3:K:87:MET:CB	3:K:89:PHE:CE2	2.92	0.53
2:N:36:LEU:HD12	2:N:79:THR:HB	1.91	0.53
2:N:48:ASP:OD2	2:N:50:THR:HG22	2.09	0.53
3:O:95:LYS:HZ1	10:O:301:LMT:H5 <sup>?</sup>	1.70	0.53
1:A:210:THR:HG23	1:A:211:SER:N	2.23	0.53
1:E:495:LYS:HA	1:E:498:GLU:HG2	1.91	0.53
2:F:97:GLN:OE1	2:F:97:GLN:N	2.42	0.53
1:I:463:GLU:OE1	1:I:502:ARG:NH2	2.39	0.53
3:K:119:ALA:HB1	9:K:302:HEM:CMB	2.38	0.53
1:M:471:GLU:O	1:M:475:ILE:HG13	2.08	0.53
3:C:94:TRP:HD1	10:C:303:LMT:H1 <sup>?</sup>	1.73	0.53
1:E:16:ALA:O	1:E:20:VAL:HG12	2.09	0.53
1:E:96:VAL:HG13	1:E:415:VAL:HG12	1.91	0.53
2:F:94:PRO:C	2:F:96:PHE:H	2.11	0.53
2:F:98:LEU:HD13	3:K:5:THR:HG22	1.91	0.53
3:G:31:LEU:HD22	9:G:302:HEM:HAC	1.91	0.53
1:I:194:CYS:O	1:I:206:ALA:HA	2.09	0.53
1:I:349:CYS:CB	1:I:353:LEU:HD22	2.38	0.53
2:J:150:ARG:NH2	2:J:220:LYS:HB3	2.24	0.53
1:M:587:TYR:CG	1:M:587:TYR:O	2.62	0.53
3:O:129:HIS:NE2	9:O:302:HEM:ND	2.57	0.53
1:A:542:ARG:HD3	1:A:549:HIS:CD2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:37:ALA:CA	11:C:304:MQ7:C2M	2.83	0.52
3:C:149:GLN:C	3:C:151:GLY:N	2.58	0.52
3:C:176:VAL:O	3:C:178:TYR:N	2.41	0.52
1:I:217:GLY:H	1:I:395:SER:HB3	1.74	0.52
1:I:468:ILE:HG23	1:I:499:LEU:HD11	1.91	0.52
1:M:482:ILE:H	1:M:482:ILE:HD12	1.75	0.52
2:N:227:GLN:O	2:N:230:ILE:HG13	2.08	0.52
2:B:84:LEU:HB3	2:B:88:ILE:CD1	2.38	0.52
1:E:238:ILE:HG22	1:E:531:LEU:HD23	1.90	0.52
1:E:369:HIS:HD2	1:E:405:ARG:HH21	1.57	0.52
1:I:357:PRO:HB3	1:I:362:ILE:HD11	1.92	0.52
3:G:49:PRO:CD	3:G:210:ARG:HH12	2.05	0.52
1:I:43:HIS:CD2	4:I:701:FAD:HM81	2.45	0.52
1:M:216:THR:HG21	1:M:236:GLY:N	2.24	0.52
1:M:544:GLU:HA	1:M:554:PHE:CD1	2.43	0.52
1:A:16:ALA:O	1:A:20:VAL:HG12	2.09	0.52
1:A:471:GLU:O	1:A:475:ILE:HG12	2.10	0.52
1:A:500:TYR:HE2	1:A:574:ALA:O	1.92	0.52
1:E:250:ASN:N	1:E:566:THR:O	2.42	0.52
1:E:338:ILE:O	1:E:343:ARG:HB2	2.10	0.52
1:E:459:ARG:HG2	1:E:460:LYS:H	1.75	0.52
1:I:557:ARG:N	1:I:601:VAL:O	2.41	0.52
1:M:576:MET:SD	1:M:577:PRO:HD2	2.49	0.52
1:A:15:LEU:HB2	1:A:44:SER:OG	2.10	0.52
1:A:327:TRP:HB3	1:A:361:LEU:HB3	1.91	0.52
3:C:41:LEU:H	11:C:304:MQ7:C14	2.22	0.52
3:G:84:ALA:HA	3:G:87:MET:HG3	1.92	0.52
1:I:201:THR:OG1	1:I:202:GLY:N	2.42	0.52
2:J:106:THR:O	2:J:109:TRP:N	2.42	0.52
3:C:120:ILE:HG21	3:O:81:ILE:HD11	1.91	0.52
1:E:261:THR:HB	1:E:266:ILE:O	2.09	0.52
1:I:55:LEU:HD12	1:I:56:GLY:N	2.21	0.52
2:J:181:ARG:NH1	2:J:181:ARG:O	2.42	0.52
1:M:68:VAL:HB	1:M:148:ARG:HH22	1.74	0.52
2:N:107:GLY:O	2:N:111:ARG:HG3	2.09	0.52
2:N:152:ILE:O	2:N:153:GLU:HB3	2.09	0.52
3:O:53:ASN:OD1	3:O:140:THR:HA	2.10	0.52
1:A:288:MET:HB3	1:A:296:ALA:HB1	1.92	0.52
1:A:318:VAL:O	1:A:324:ASP:HA	2.10	0.52
1:E:97:MET:O	1:E:101:ALA:CB	2.57	0.52
1:E:118:TYR:CE1	1:E:123:PRO:HB3	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:302:ASP:CG	1:E:595:ARG:HH12	2.12	0.52
1:E:609:PRO:HA	1:E:612:PHE:CE1	2.45	0.52
2:F:117:ILE:HA	2:F:198:VAL:HG13	1.91	0.52
1:I:57:ASN:HA	1:I:132:LYS:HD3	1.92	0.52
1:I:500:TYR:CE2	1:I:575:SER:HA	2.44	0.52
2:J:145:ILE:HD11	2:J:185:ASP:HA	1.91	0.52
3:K:60:GLU:HG2	3:K:64:MET:SD	2.49	0.52
1:M:217:GLY:N	1:M:395:SER:HB3	2.25	0.52
1:A:246:VAL:HA	1:A:385:GLY:H	1.73	0.52
3:C:95:LYS:O	3:C:99:VAL:HG23	2.10	0.52
1:E:273:ARG:HA	1:E:277:GLY:CA	2.29	0.52
3:G:125:LEU:HB3	3:G:159:LEU:HD12	1.91	0.52
1:I:475:ILE:CD1	1:I:495:LYS:HD3	2.40	0.52
2:J:10:PHE:CE2	2:J:12:TYR:HB3	2.44	0.52
2:N:93:LEU:HD13	2:N:155:GLY:O	2.09	0.52
1:A:83:GLN:H	1:A:585:SER:CB	2.23	0.52
1:A:281:ASP:OD2	1:A:285:TYR:HB3	2.10	0.52
1:A:503:SER:HA	1:A:506:ILE:HD11	1.92	0.52
1:E:420:TYR:HD1	1:E:622:LEU:HD13	1.72	0.52
1:E:531:LEU:HA	1:E:534:CYS:HB2	1.90	0.52
3:G:32:ILE:CA	9:G:302:HEM:HBC1	2.40	0.52
2:J:138:ASP:OD1	2:J:139:ASN:N	2.42	0.52
3:K:176:VAL:HG12	3:K:177:LYS:N	2.25	0.52
1:M:79:TRP:HE1	1:M:563:LEU:CD1	2.12	0.52
2:N:183:TYR:HA	2:N:195:TYR:CZ	2.44	0.52
1:I:152:THR:O	1:I:152:THR:OG1	2.25	0.52
1:I:509:SER:HB2	2:J:49:PRO:HG3	1.92	0.52
3:K:128:VAL:O	3:K:132:VAL:HG13	2.09	0.52
1:M:219:TYR:O	1:M:222:ILE:HG12	2.10	0.52
2:N:181:ARG:O	2:N:181:ARG:NH1	2.34	0.52
1:A:213:LEU:HB2	1:A:425:MET:CE	2.40	0.51
3:C:40:MET:HB2	11:C:304:MQ7:H142	1.91	0.51
3:C:95:LYS:NZ	10:C:303:LMT:H5B	2.25	0.51
3:C:116:VAL:HG13	10:C:303:LMT:C10	2.41	0.51
3:G:92:ASP:O	3:G:96:THR:HG23	2.09	0.51
3:G:180:PHE:N	3:G:180:PHE:CD1	2.78	0.51
1:I:252:GLU:HA	1:I:535:THR:HG23	1.93	0.51
2:J:216:ASP:OD1	3:K:186:ARG:NH2	2.43	0.51
1:M:280:LEU:HD12	1:M:284:GLN:HB2	1.92	0.51
1:M:606:GLU:O	1:M:609:PRO:HD2	2.10	0.51
2:N:96:PHE:CZ	2:N:158:VAL:HG21	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:440:TYR:O	1:E:445:HIS:ND1	2.43	0.51
2:F:121:CYS:HA	2:F:188:ASP:HB2	1.91	0.51
3:K:125:LEU:HB3	3:K:159:LEU:HD12	1.92	0.51
1:M:87:ARG:NH1	1:M:620:GLU:OE1	2.34	0.51
1:M:335:GLU:OE1	1:M:335:GLU:N	2.42	0.51
1:M:500:TYR:OH	1:M:530:LYS:NZ	2.34	0.51
1:M:544:GLU:CD	1:M:546:ARG:HH11	2.14	0.51
2:N:190:ARG:HB2	2:N:195:TYR:CZ	2.45	0.51
1:E:475:ILE:HD12	1:E:495:LYS:HD3	1.91	0.51
2:F:200:GLY:C	2:F:202:ASP:H	2.12	0.51
1:I:217:GLY:N	1:I:395:SER:HB3	2.26	0.51
1:I:553:ASP:OD1	1:I:553:ASP:N	2.30	0.51
3:K:35:LEU:HD23	3:K:35:LEU:O	2.10	0.51
3:K:192:THR:O	3:K:195:LEU:HB3	2.11	0.51
1:M:413:GLU:O	1:M:417:ALA:HB3	2.10	0.51
1:M:583:GLU:CD	1:M:586:PRO:HG3	2.31	0.51
3:O:23:PHE:HA	3:O:26:VAL:HG12	1.93	0.51
1:A:140:ALA:HB2	1:A:147:TRP:NE1	2.25	0.51
3:G:176:VAL:HG12	3:G:181:VAL:HG21	1.92	0.51
1:I:48:GLN:HB3	1:I:154:ASP:OD1	2.10	0.51
1:M:255:GLN:HB2	1:M:372:MET:SD	2.50	0.51
1:M:405:ARG:NH1	5:M:702:FUM:O7	2.44	0.51
1:E:417:ALA:O	1:E:421:ILE:HB	2.10	0.51
2:B:119:ALA:HB1	2:B:182:PHE:HE2	1.75	0.51
3:C:10:VAL:HG13	3:C:12:GLN:H	1.75	0.51
3:C:45:VAL:HG11	3:C:211:PHE:CG	2.46	0.51
1:E:524:ARG:HB3	1:E:524:ARG:CZ	2.39	0.51
3:K:198:ILE:HA	3:K:201:ILE:HG22	1.91	0.51
1:M:258:PRO:CD	1:M:301:ARG:HH21	2.24	0.51
1:E:55:LEU:HD12	1:E:57:ASN:HD21	1.74	0.51
1:E:156:THR:O	1:E:160:VAL:HG22	2.10	0.51
1:E:328:LEU:HB3	1:E:362:ILE:HB	1.91	0.51
1:E:587:TYR:HE1	1:E:615:PRO:HB3	1.72	0.51
1:I:337:HIS:O	1:I:341:LYS:N	2.44	0.51
1:I:413:GLU:O	1:I:417:ALA:HB2	2.10	0.51
1:I:544:GLU:HG2	1:I:562:TRP:CD1	2.45	0.51
1:I:589:GLU:HA	1:I:613:VAL:HG22	1.92	0.51
2:J:170:PHE:HA	2:J:203:GLN:O	2.09	0.51
3:K:1:MET:HG3	3:K:2:ASN:H	1.75	0.51
1:M:238:ILE:HG22	1:M:531:LEU:HD23	1.92	0.51
3:O:203:ILE:HA	3:O:206:LEU:CD2	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:215:GLU:OE1	3:C:183:ARG:HD3	2.10	0.51
10:C:303:LMT:H3B	10:C:303:LMT:C3'	2.33	0.51
1:E:12:GLY:HA2	4:E:701:FAD:H1B	1.93	0.51
1:I:230:VAL:HG22	2:J:56:CYS:O	2.10	0.51
1:I:313:ARG:HH21	1:I:483:PHE:HB2	1.76	0.51
3:C:5:THR:O	3:C:6:ILE:HG13	2.10	0.51
1:E:32:ILE:HG21	1:E:207:TYR:HE2	1.72	0.51
1:E:595:ARG:HD2	1:E:597:TYR:CE1	2.45	0.51
3:G:140:THR:H	3:G:143:LYS:CE	2.24	0.51
1:I:19:ARG:NH1	1:I:23:GLU:HB2	2.25	0.51
2:J:65:CYS:HB3	2:J:76:ALA:H	1.76	0.51
1:M:295:LYS:HA	1:M:296:ALA:HB3	1.92	0.51
2:N:15:LEU:HD23	2:N:15:LEU:O	2.11	0.51
2:N:179:VAL:HG11	2:N:199:ILE:HG21	1.91	0.51
2:F:199:ILE:O	2:F:199:ILE:HG12	2.11	0.51
3:G:46:ILE:HD11	3:G:203:ILE:O	2.11	0.51
1:I:119:LYS:HB3	1:I:124:PHE:HE1	1.75	0.51
2:J:211:LEU:O	3:K:106:HIS:CE1	2.64	0.51
1:M:213:LEU:HB2	1:M:425:MET:HE1	1.93	0.51
1:M:309:THR:HA	1:M:312:MET:HB2	1.93	0.51
2:B:68:VAL:HA	2:B:73:PRO:HA	1.93	0.50
2:B:69:ILE:HG12	2:B:90:LEU:HD22	1.93	0.50
2:F:197:ASP:OD1	3:G:13:ARG:HG3	2.12	0.50
1:I:246:VAL:HG12	1:I:385:GLY:N	2.26	0.50
1:M:32:ILE:HD13	1:M:207:TYR:HE2	1.76	0.50
1:M:75:LYS:NZ	1:M:590:MET:O	2.44	0.50
1:M:338:ILE:HG22	1:M:338:ILE:O	2.11	0.50
3:C:115:GLN:O	3:C:119:ALA:HB2	2.11	0.50
3:G:194:ASN:O	3:G:198:ILE:HG13	2.10	0.50
1:I:6:THR:HG21	1:I:32:ILE:HG13	1.93	0.50
1:I:257:HIS:NE2	1:I:259:THR:OG1	2.44	0.50
1:I:262:VAL:HB	1:I:263:PRO:HD3	1.92	0.50
1:I:276:GLY:HA2	1:I:332:HIS:CE1	2.46	0.50
3:K:165:LEU:O	3:K:169:VAL:HG23	2.11	0.50
1:M:259:THR:HB	1:M:268:VAL:HG22	1.93	0.50
1:M:316:LEU:HB2	1:M:319:LYS:HG3	1.93	0.50
2:N:212:LEU:HD21	3:O:176:VAL:HG11	1.93	0.50
2:B:11:ARG:HE	2:B:101:ASP:CG	2.14	0.50
1:E:480:VAL:O	1:E:480:VAL:HG13	2.11	0.50
3:G:72:VAL:O	3:G:76:MET:CB	2.58	0.50
1:M:140:ALA:HB2	1:M:147:TRP:NE1	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:PRO:HD2	1:A:384:TYR:CB	2.40	0.50
1:A:261:THR:HG21	1:A:353:LEU:HD11	1.93	0.50
2:B:94:PRO:O	2:B:96:PHE:N	2.44	0.50
1:I:449:GLN:O	1:I:452:ILE:HG22	2.11	0.50
3:K:127:ALA:HA	3:K:130:MET:HE3	1.91	0.50
3:K:186:ARG:O	3:K:190:GLN:NE2	2.40	0.50
1:M:41:ARG:NH2	2:N:153:GLU:O	2.44	0.50
1:M:82:ASP:O	1:M:85:VAL:HG22	2.11	0.50
1:M:619:LYS:NZ	1:M:622:LEU:HB3	2.26	0.50
1:A:517:PRO:HG3	2:B:52:LYS:HG2	1.93	0.50
1:A:606:GLU:HG3	1:A:607:LEU:N	2.27	0.50
1:E:308:MET:HE1	1:E:366:PRO:HD3	1.93	0.50
2:F:109:TRP:HZ3	2:F:110:PHE:CE1	2.29	0.50
2:F:190:ARG:HB2	2:F:195:TYR:CZ	2.47	0.50
2:F:209:MET:N	6:F:301:F3S:S1	2.85	0.50
1:I:84:GLU:CA	1:I:587:TYR:HE2	2.20	0.50
2:J:202:ASP:OD1	2:J:203:GLN:N	2.40	0.50
3:K:167:VAL:HG12	9:K:302:HEM:CAC	2.42	0.50
3:O:150:SER:CA	3:O:152:TRP:CD1	2.87	0.50
3:C:198:ILE:HG13	3:C:201:ILE:HD11	1.94	0.50
1:E:426:VAL:O	1:E:429:THR:N	2.43	0.50
2:F:176:ILE:HG12	2:F:199:ILE:HD11	1.94	0.50
3:G:78:VAL:O	3:G:82:LEU:HG	2.12	0.50
1:I:287:PHE:HZ	1:I:308:MET:HG2	1.76	0.50
1:M:59:ILE:HG12	1:M:129:LYS:H	1.77	0.50
1:M:258:PRO:HD2	1:M:301:ARG:HH21	1.75	0.50
1:M:261:THR:N	1:M:266:ILE:O	2.41	0.50
1:A:238:ILE:HG13	1:A:239:ILE:N	2.26	0.50
1:E:84:GLU:O	1:E:87:ARG:HB2	2.12	0.50
1:E:257:HIS:ND1	1:E:258:PRO:HD2	2.26	0.50
1:E:280:LEU:HD12	1:E:361:LEU:HD23	1.94	0.50
1:I:36:LEU:HD13	4:I:701:FAD:C6A	2.42	0.50
1:I:79:TRP:NE1	1:I:591:PRO:O	2.45	0.50
1:I:200:ARG:HG2	2:J:99:LEU:HD22	1.94	0.50
1:M:355:VAL:HG11	1:M:362:ILE:HD13	1.93	0.50
1:A:82:ASP:HA	1:A:585:SER:CB	2.29	0.50
1:A:372:MET:HE1	1:A:404:ASN:HA	1.92	0.50
2:B:110:PHE:CE2	2:B:153:GLU:HG2	2.47	0.50
1:E:78:ASP:OD2	1:E:546:ARG:HG3	2.12	0.50
1:E:262:VAL:HG22	1:E:365:ARG:HE	1.77	0.50
1:E:451:ARG:O	1:E:455:ILE:HG12	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:51:LEU:O	3:G:55:ILE:HG22	2.12	0.50
3:G:206:LEU:O	3:G:210:ARG:CB	2.60	0.50
1:I:16:ALA:HB2	1:I:414:THR:HG22	1.94	0.50
1:I:68:VAL:HG12	1:I:148:ARG:HH22	1.76	0.50
1:I:89:PHE:HA	1:I:416:VAL:HG11	1.94	0.50
1:I:191:CYS:HB2	1:I:386:LEU:HD22	1.94	0.50
1:I:222:ILE:HG13	1:I:223:TYR:CD1	2.47	0.50
1:I:582:GLU:HG2	1:I:583:GLU:N	2.27	0.50
3:K:29:ALA:O	3:K:32:ILE:HG22	2.12	0.50
3:O:147:ARG:O	3:O:147:ARG:NH1	2.39	0.50
2:F:227:GLN:O	2:F:230:ILE:HG13	2.12	0.50
1:I:140:ALA:HB2	1:I:147:TRP:NE1	2.26	0.50
1:I:381:GLY:HA3	1:I:421:ILE:HD12	1.94	0.50
2:J:211:LEU:O	3:K:106:HIS:HE1	1.94	0.50
3:K:34:PHE:CD1	3:K:72:VAL:HG11	2.47	0.50
3:K:36:TRP:CZ3	3:K:200:PHE:CZ	3.00	0.50
1:M:315:GLY:O	1:M:316:LEU:HD12	2.12	0.50
1:M:358:ILE:HG13	1:M:359:HIS:CE1	2.47	0.50
1:M:599:GLY:O	1:M:601:VAL:HG23	2.12	0.50
2:N:117:ILE:HA	2:N:198:VAL:HG13	1.94	0.50
1:A:96:VAL:HG21	1:A:416:VAL:HA	1.93	0.49
1:A:262:VAL:HB	1:A:363:PRO:HB2	1.94	0.49
3:C:8:LEU:HD22	3:C:14:SER:HB3	1.94	0.49
3:C:46:ILE:HD11	3:C:207:THR:N	2.27	0.49
1:E:135:LEU:HD22	2:F:134:GLU:HG2	1.94	0.49
1:E:378:ASN:HD21	1:E:382:ALA:HB3	1.76	0.49
1:I:180:GLN:HB2	1:I:199:LEU:HD11	1.94	0.49
1:I:257:HIS:O	1:I:366:PRO:HA	2.12	0.49
1:I:495:LYS:HA	1:I:498:GLU:HG3	1.93	0.49
1:I:557:ARG:H	1:I:602:THR:HA	1.76	0.49
2:J:1:MET:C	2:J:3:ARG:H	2.15	0.49
1:M:52:GLN:HG3	1:M:148:ARG:HG3	1.92	0.49
2:N:3:ARG:HG2	2:N:30:GLU:OE2	2.12	0.49
3:O:188:TRP:O	3:O:192:THR:CB	2.60	0.49
1:E:369:HIS:HD2	1:E:405:ARG:NH2	2.10	0.49
2:F:196:TYR:O	2:F:200:GLY:N	2.43	0.49
3:G:39:MET:O	3:G:43:SER:HB3	2.12	0.49
3:G:181:VAL:CG1	3:G:182:GLY:H	2.25	0.49
1:I:270:GLU:O	1:I:274:GLY:N	2.26	0.49
1:I:300:SER:OG	1:I:404:ASN:OD1	2.25	0.49
3:K:171:PHE:HD2	3:K:193:GLU:OE2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:492:ALA:HA	1:M:495:LYS:HG2	1.93	0.49
1:A:207:TYR:N	1:A:207:TYR:CD1	2.80	0.49
1:A:457:THR:HA	1:A:508:LEU:CD2	2.42	0.49
2:B:227:GLN:OE1	2:B:230:ILE:HD11	2.12	0.49
3:C:1:MET:HG3	3:C:2:ASN:H	1.77	0.49
1:I:267:LEU:HD13	1:I:369:HIS:CE1	2.47	0.49
1:I:306:ARG:CZ	1:I:306:ARG:HB2	2.41	0.49
1:M:559:ASP:HB2	1:M:603:ILE:O	2.12	0.49
1:M:619:LYS:HZ1	1:M:622:LEU:HB3	1.78	0.49
2:N:5:LEU:O	2:N:27:THR:HA	2.12	0.49
2:N:26:PHE:CD2	2:N:43:ILE:HD13	2.47	0.49
1:A:480:VAL:HG23	1:A:484:ARG:NE	2.28	0.49
2:B:94:PRO:C	2:B:96:PHE:H	2.15	0.49
3:C:152:TRP:CD1	3:O:136:ASP:OD2	2.66	0.49
3:C:159:LEU:HD22	9:C:301:HEM:HMD3	1.94	0.49
1:E:121:GLY:N	1:E:286:ARG:HH12	2.10	0.49
1:E:198:CYS:SG	1:E:201:THR:HG23	2.52	0.49
1:M:68:VAL:HB	1:M:148:ARG:NH2	2.27	0.49
1:M:381:GLY:HA3	1:M:421:ILE:HD12	1.93	0.49
1:M:531:LEU:HA	1:M:534:CYS:HB2	1.94	0.49
9:O:302:HEM:HBB2	9:O:302:HEM:HMB1	1.93	0.49
1:A:104:GLY:HA2	2:B:187:ARG:CZ	2.42	0.49
1:E:460:LYS:HG3	1:E:462:LYS:HE3	1.93	0.49
2:F:107:GLY:O	2:F:111:ARG:HG3	2.11	0.49
3:G:111:MET:O	3:G:115:GLN:HG3	2.12	0.49
3:G:148:LEU:HB3	3:G:153:LEU:HD22	1.94	0.49
1:I:531:LEU:HA	1:I:534:CYS:HB2	1.95	0.49
2:J:195:TYR:HB3	2:J:235:MET:HE3	1.94	0.49
3:K:140:THR:HB	3:K:143:LYS:HG2	1.94	0.49
1:M:162:ASN:O	1:M:166:THR:HG23	2.13	0.49
1:M:543:THR:O	1:M:544:GLU:HB3	2.13	0.49
2:N:26:PHE:HD2	2:N:43:ILE:HD13	1.78	0.49
3:O:116:VAL:HG13	10:O:301:LMT:H121	1.94	0.49
1:A:104:GLY:HA2	2:B:187:ARG:NH1	2.28	0.49
1:A:139:ARG:NH1	1:A:271:GLY:HA3	2.27	0.49
1:I:267:LEU:HB3	4:I:701:FAD:HM73	1.95	0.49
1:I:306:ARG:HG3	1:I:483:PHE:CE2	2.48	0.49
1:M:7:ASP:OD1	1:M:30:LYS:HB3	2.13	0.49
1:M:9:LEU:HD21	1:M:194:CYS:SG	2.53	0.49
1:M:55:LEU:HD13	1:M:58:ALA:H	1.76	0.49
1:M:111:VAL:HG23	1:M:115:HIS:NE2	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:140:ALA:HB3	1:M:273:ARG:HH11	1.77	0.49
1:M:460:LYS:C	1:M:505:LYS:HE3	2.32	0.49
2:N:54:ASP:OD2	2:N:103:SER:OG	2.18	0.49
1:E:224:LYS:HG3	1:E:473:HIS:HB3	1.95	0.49
1:E:234:GLY:O	1:E:238:ILE:HG23	2.11	0.49
2:F:63:GLY:H	2:F:152:ILE:HD12	1.77	0.49
3:K:111:MET:O	3:K:114:VAL:HG22	2.11	0.49
3:K:172:TYR:HD1	3:K:189:PHE:HE1	1.60	0.49
1:M:230:VAL:HG22	2:N:56:CYS:O	2.13	0.49
1:A:400:MET:HE2	1:A:401:HIS:CE1	2.48	0.49
2:B:84:LEU:HB3	2:B:88:ILE:HD12	1.94	0.49
3:C:6:ILE:HG13	3:C:7:THR:H	1.77	0.49
3:C:130:MET:HG3	9:C:301:HEM:HHC	1.94	0.49
1:E:434:PRO:HG2	1:E:436:PHE:CE2	2.47	0.49
1:M:222:ILE:HG13	1:M:223:TYR:HD1	1.78	0.49
1:M:587:TYR:CD1	1:M:613:VAL:HG11	2.47	0.49
1:A:459:ARG:HG2	1:A:460:LYS:H	1.78	0.49
2:B:44:ARG:HD2	2:B:45:ASP:OD1	2.13	0.49
9:C:301:HEM:HMD1	9:C:301:HEM:CBD	2.40	0.49
1:E:52:GLN:OE1	1:E:409:ASN:ND2	2.45	0.49
1:E:105:VAL:O	2:F:187:ARG:NH2	2.46	0.49
1:E:169:LEU:HD22	2:F:115:LEU:HD12	1.94	0.49
1:E:255:GLN:HE21	1:E:301:ARG:CB	2.26	0.49
1:E:370:TYR:HB2	1:E:405:ARG:HE	1.78	0.49
2:F:23:MET:N	2:F:23:MET:SD	2.86	0.49
1:I:261:THR:HG21	1:I:353:LEU:HD11	1.95	0.49
1:I:377:THR:HB	1:I:381:GLY:HA2	1.94	0.49
3:C:111:MET:O	3:C:114:VAL:HG22	2.12	0.49
1:E:196:ALA:O	1:E:204:LEU:HA	2.13	0.49
2:F:212:LEU:HD11	3:G:176:VAL:HG11	1.94	0.49
1:I:294:ASP:OD1	1:I:294:ASP:N	2.33	0.49
3:K:164:GLU:O	3:K:167:VAL:HG22	2.13	0.49
3:K:176:VAL:HG12	3:K:177:LYS:H	1.77	0.49
1:M:343:ARG:HB2	1:M:347:ASP:OD2	2.12	0.49
1:M:405:ARG:CZ	1:M:407:GLY:HA2	2.43	0.49
1:A:270:GLU:N	5:A:702:FUM:OXT	2.46	0.48
3:C:8:LEU:HD13	3:C:14:SER:H	1.76	0.48
3:C:37:ALA:HA	11:C:304:MQ7:C2	2.42	0.48
3:C:148:LEU:HD21	3:C:212:MET:CA	2.43	0.48
2:F:52:LYS:HB2	2:F:101:ASP:HB2	1.93	0.48
3:G:1:MET:N	2:J:91:HIS:CE1	2.81	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:517:PRO:HG2	2:J:49:PRO:O	2.13	0.48
2:J:125:ASP:C	2:J:127:ALA:H	2.15	0.48
1:M:52:GLN:NE2	1:M:407:GLY:O	2.46	0.48
1:M:109:ARG:NH1	2:N:136:ARG:O	2.46	0.48
1:M:298:LEU:HD23	1:M:299:ALA:N	2.28	0.48
1:M:500:TYR:HB2	1:M:529:LEU:HD11	1.94	0.48
1:M:546:ARG:NH1	1:M:562:TRP:HB2	2.27	0.48
2:N:172:GLY:O	2:N:176:ILE:HG13	2.13	0.48
3:O:25:MET:HB2	3:O:178:TYR:CZ	2.48	0.48
3:O:38:HIS:O	3:O:42:VAL:HG12	2.13	0.48
1:E:247:PRO:HB3	1:E:569:TYR:CE1	2.49	0.48
2:F:94:PRO:O	2:F:96:PHE:N	2.45	0.48
3:G:10:VAL:O	3:G:12:GLN:N	2.45	0.48
1:I:218:GLY:O	1:I:232:CYS:HB3	2.12	0.48
3:K:5:THR:CG2	3:K:6:ILE:H	2.21	0.48
3:K:186:ARG:HG3	3:K:190:GLN:HE21	1.77	0.48
1:M:280:LEU:HB2	1:M:284:GLN:HA	1.94	0.48
2:N:136:ARG:CG	2:N:137:MET:H	2.26	0.48
1:A:250:ASN:ND2	1:A:399:ASP:OD2	2.46	0.48
2:F:190:ARG:HB2	2:F:195:TYR:CE2	2.48	0.48
1:I:459:ARG:HD3	1:I:459:ARG:N	2.29	0.48
2:N:2:ASN:O	2:N:2:ASN:ND2	2.30	0.48
1:A:32:ILE:HD13	1:A:207:TYR:CD2	2.49	0.48
1:E:266:ILE:HD13	2:F:59:ALA:HA	1.94	0.48
1:E:301:ARG:NH2	5:E:702:FUM:O8	2.47	0.48
1:E:484:ARG:O	1:E:551:ARG:HA	2.14	0.48
1:I:178:ARG:HB3	1:I:199:LEU:HB2	1.94	0.48
1:M:257:HIS:HB2	1:M:369:HIS:HB2	1.95	0.48
2:N:11:ARG:HH22	2:N:50:THR:HG23	1.79	0.48
3:O:56:ALA:O	3:O:62:THR:N	2.47	0.48
3:C:31:LEU:HD22	9:C:302:HEM:CBC	2.43	0.48
1:E:482:ILE:O	1:E:550:THR:OG1	2.31	0.48
1:E:542:ARG:HA	1:E:562:TRP:CZ3	2.49	0.48
2:F:148:LEU:HD11	2:F:227:GLN:HG2	1.94	0.48
3:G:156:TYR:OH	9:G:301:HEM:C3D	2.62	0.48
3:G:164:GLU:HA	3:G:167:VAL:HG22	1.96	0.48
2:J:37:PHE:O	2:J:41:THR:OG1	2.25	0.48
1:M:113:GLY:O	1:M:128:GLU:HB3	2.11	0.48
1:M:259:THR:HG22	1:M:364:VAL:HG21	1.95	0.48
1:E:438:MET:HG3	1:I:436:PHE:HE2	1.78	0.48
1:E:587:TYR:CZ	1:E:615:PRO:HB3	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:212:LEU:HD22	2:F:225:GLN:HG3	1.93	0.48
1:I:43:HIS:CD2	4:I:701:FAD:C8M	2.88	0.48
3:K:78:VAL:O	3:K:82:LEU:HG	2.13	0.48
1:M:493:VAL:HA	1:M:496:LEU:CD2	2.43	0.48
3:O:56:ALA:C	3:O:62:THR:H	2.16	0.48
3:O:84:ALA:HA	3:O:87:MET:CG	2.42	0.48
1:A:519:LEU:O	1:A:523:LEU:HG	2.14	0.48
3:C:34:PHE:CD1	3:C:72:VAL:HG11	2.49	0.48
1:E:420:TYR:HD2	1:E:421:ILE:HD13	1.77	0.48
1:E:560:LYS:HD3	1:E:606:GLU:HG2	1.96	0.48
1:M:7:ASP:O	1:M:209:ALA:HB1	2.12	0.48
1:M:512:CYS:HA	1:M:516:ASN:HB2	1.95	0.48
2:N:42:GLN:HA	2:N:46:GLU:HG3	1.96	0.48
3:O:140:THR:HG22	3:O:142:ALA:H	1.78	0.48
1:A:282:VAL:HA	1:A:318:VAL:HG22	1.96	0.48
1:A:380:ASP:HA	1:A:420:TYR:HE2	1.79	0.48
1:A:480:VAL:HG23	1:A:484:ARG:CZ	2.44	0.48
3:C:34:PHE:CE1	3:C:72:VAL:HG11	2.48	0.48
1:E:264:THR:HG21	1:E:352:PHE:HB3	1.96	0.48
1:I:5:HIS:O	1:I:6:THR:HG23	2.14	0.48
1:M:330:ILE:O	1:M:338:ILE:HG23	2.13	0.48
1:A:79:TRP:CZ2	1:A:590:MET:HE3	2.49	0.48
3:C:70:PRO:O	3:C:74:VAL:HG22	2.14	0.48
3:C:116:VAL:O	3:C:119:ALA:HB3	2.13	0.48
1:E:303:VAL:O	1:E:307:ARG:HG2	2.14	0.48
1:E:468:ILE:HD12	1:E:506:ILE:CD1	2.43	0.48
3:G:111:MET:HA	3:G:114:VAL:HG22	1.94	0.48
1:I:377:THR:O	1:I:384:TYR:HE2	1.97	0.48
1:I:467:LYS:O	1:I:471:GLU:HG3	2.14	0.48
1:I:610:GLU:CG	1:I:611:LYS:H	2.25	0.48
3:K:53:ASN:HD21	3:K:141:ALA:N	2.11	0.48
1:M:6:THR:CG2	1:M:32:ILE:HG13	2.44	0.48
1:M:79:TRP:CB	1:M:80:GLY:HA2	2.33	0.48
1:M:247:PRO:HB3	1:M:569:TYR:CE2	2.49	0.48
1:A:141:PHE:CZ	1:A:270:GLU:HB3	2.49	0.48
1:A:557:ARG:HD2	1:A:559:ASP:OD1	2.14	0.48
1:E:252:GLU:HA	1:E:535:THR:HG23	1.96	0.48
1:E:444:ALA:O	1:E:447:LYS:N	2.41	0.48
1:E:542:ARG:NH2	1:E:544:GLU:OE2	2.47	0.48
3:G:41:LEU:HG	3:G:42:VAL:HG23	1.95	0.48
1:I:356:ASN:OD1	1:I:358:ILE:HG12	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:132:VAL:HG21	3:K:153:LEU:CD2	2.43	0.48
1:M:288:MET:HB3	1:M:307:ARG:HH22	1.77	0.48
1:M:426:VAL:O	1:M:430:LYS:HB2	2.14	0.48
3:O:155:LEU:HD12	3:O:156:TYR:H	1.78	0.48
3:C:41:LEU:CA	11:C:304:MQ7:H161	2.44	0.47
3:C:81:ILE:HD13	3:O:89:PHE:HE1	1.79	0.47
1:E:29:LEU:HD22	1:E:430:LYS:HE3	1.95	0.47
1:E:543:THR:HB	1:E:554:PHE:CD1	2.49	0.47
2:F:94:PRO:HD2	2:F:159:ALA:HB1	1.95	0.47
1:I:228:ASN:ND2	4:I:701:FAD:HM81	2.28	0.47
1:I:399:ASP:OD1	1:I:402:GLY:N	2.47	0.47
3:K:64:MET:O	3:K:67:ILE:N	2.47	0.47
1:M:259:THR:O	1:M:268:VAL:HG22	2.14	0.47
1:M:345:VAL:HG22	1:M:349:CYS:SG	2.54	0.47
1:M:545:SER:OG	1:M:551:ARG:N	2.44	0.47
1:A:40:ARG:HA	1:A:161:LEU:HD21	1.95	0.47
1:A:52:GLN:CD	1:A:409:ASN:ND2	2.68	0.47
3:C:60:GLU:CG	3:C:64:MET:HB2	2.45	0.47
3:C:116:VAL:CG1	10:C:303:LMT:H102	2.44	0.47
1:E:570:TRP:CZ3	1:E:577:PRO:HB3	2.49	0.47
3:G:84:ALA:HA	3:G:87:MET:CG	2.44	0.47
1:I:23:GLU:OE1	1:I:423:GLU:HG2	2.13	0.47
3:O:140:THR:HG22	3:O:142:ALA:N	2.29	0.47
1:A:280:LEU:HB3	1:A:284:GLN:HA	1.95	0.47
2:B:57:CYS:O	2:B:58:ARG:HG3	2.13	0.47
2:B:62:CYS:SG	2:B:63:GLY:N	2.88	0.47
2:B:233:ARG:HG3	3:C:178:TYR:O	2.14	0.47
3:C:143:LYS:HZ3	9:C:301:HEM:HBA1	1.74	0.47
1:E:100:VAL:HA	1:E:103:TRP:HB2	1.97	0.47
1:E:261:THR:CG2	1:E:353:LEU:HD11	2.44	0.47
1:E:327:TRP:CE3	1:E:361:LEU:HB2	2.49	0.47
2:F:98:LEU:HD13	3:K:5:THR:CG2	2.45	0.47
2:F:174:VAL:CG1	2:F:178:ARG:HH21	2.26	0.47
3:G:149:GLN:CA	3:G:150:SER:C	2.82	0.47
1:I:19:ARG:HB2	1:I:164:LEU:HD21	1.96	0.47
1:I:34:LEU:HD21	1:I:207:TYR:CZ	2.49	0.47
1:I:306:ARG:O	1:I:309:THR:HG22	2.14	0.47
1:M:127:GLU:HG2	1:M:128:GLU:H	1.79	0.47
2:N:84:LEU:HB3	2:N:88:ILE:HD11	1.95	0.47
3:O:164:GLU:HA	3:O:167:VAL:HG22	1.97	0.47
1:A:35:SER:O	1:A:178:ARG:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:387:LYS:HG3	1:E:388:GLY:N	2.28	0.47
2:F:233:ARG:NH1	3:G:179:GLY:HA3	2.29	0.47
1:I:15:LEU:HD22	1:I:414:THR:HB	1.96	0.47
1:I:405:ARG:HH12	5:I:702:FUM:C6	2.24	0.47
1:M:343:ARG:O	1:M:346:TYR:HB3	2.14	0.47
1:M:355:VAL:HG13	1:M:360:GLN:HB2	1.96	0.47
2:N:131:THR:CG2	2:N:132:ALA:H	2.27	0.47
1:A:32:ILE:HG21	1:A:207:TYR:CD2	2.49	0.47
2:B:40:LEU:HD13	2:B:53:VAL:HG11	1.96	0.47
3:C:107:LYS:O	3:C:110:THR:N	2.48	0.47
3:C:147:ARG:NH2	3:C:211:PHE:CG	2.82	0.47
1:E:280:LEU:HB3	1:E:284:GLN:HA	1.95	0.47
2:F:146:PHE:O	2:F:150:ARG:HB2	2.13	0.47
1:I:513:LYS:NZ	2:J:13:ASN:ND2	2.59	0.47
3:K:41:LEU:HG	3:K:42:VAL:N	2.29	0.47
1:M:111:VAL:HG23	1:M:115:HIS:CE1	2.50	0.47
1:M:211:SER:OG	1:M:429:THR:OG1	2.17	0.47
1:M:341:LYS:NZ	1:M:342:LEU:HD23	2.30	0.47
1:A:370:TYR:CE2	1:A:372:MET:HA	2.49	0.47
2:B:11:ARG:NH2	2:B:50:THR:HG23	2.29	0.47
3:C:116:VAL:HG13	10:C:303:LMT:H122	1.96	0.47
1:E:196:ALA:HB3	1:E:205:VAL:CG1	2.44	0.47
1:E:300:SER:HB2	1:E:597:TYR:CZ	2.50	0.47
2:F:48:ASP:OD1	2:F:50:THR:HG22	2.15	0.47
2:F:124:ASP:OD1	2:F:124:ASP:N	2.48	0.47
2:F:196:TYR:OH	3:G:18:GLY:N	2.41	0.47
1:I:53:ALA:CB	1:I:97:MET:HG3	2.44	0.47
1:I:257:HIS:CG	1:I:258:PRO:HD2	2.50	0.47
1:I:391:SER:OG	1:I:396:ALA:HB2	2.14	0.47
2:J:232:ARG:NH1	3:K:177:LYS:HD2	2.28	0.47
1:M:519:LEU:HA	1:M:522:ALA:HB3	1.96	0.47
3:O:57:TRP:HA	3:O:61:ALA:HA	1.96	0.47
1:A:88:ILE:HG12	1:A:620:GLU:HG2	1.97	0.47
1:A:218:GLY:O	1:A:232:CYS:HB3	2.14	0.47
1:A:530:LYS:HG2	1:A:570:TRP:CZ2	2.50	0.47
2:B:162:GLY:H	2:B:211:LEU:HD12	1.78	0.47
1:E:201:THR:OG1	1:E:202:GLY:N	2.47	0.47
2:F:110:PHE:CE1	2:F:174:VAL:HG11	2.44	0.47
2:F:180:ALA:HB2	2:F:231:MET:HE3	1.97	0.47
1:I:338:ILE:HD12	1:I:358:ILE:HG22	1.96	0.47
1:I:370:TYR:CD2	1:I:405:ARG:HD2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:370:TYR:HE2	1:I:372:MET:HA	1.78	0.47
1:I:610:GLU:HG3	1:I:611:LYS:HZ3	1.78	0.47
3:K:166:HIS:HE1	9:K:302:HEM:C1B	2.32	0.47
1:M:261:THR:HG23	1:M:263:PRO:HD2	1.96	0.47
1:M:537:TYR:HE2	1:M:579:LEU:HG	1.80	0.47
1:A:43:HIS:CE1	1:A:228:ASN:HA	2.50	0.47
2:B:128:PHE:CZ	2:B:130:PRO:HG3	2.49	0.47
3:C:198:ILE:HA	3:C:201:ILE:HG13	1.97	0.47
1:E:152:THR:O	1:E:152:THR:OG1	2.31	0.47
3:G:115:GLN:OE1	3:G:173:ARG:NE	2.48	0.47
3:G:143:LYS:HD2	3:G:144:SER:N	2.30	0.47
3:G:156:TYR:OH	9:G:301:HEM:C2D	2.68	0.47
3:G:195:LEU:HA	3:G:198:ILE:HD12	1.96	0.47
1:I:75:LYS:HG3	1:I:590:MET:CE	2.45	0.47
1:M:43:HIS:CD2	4:M:701:FAD:C8	2.94	0.47
1:M:513:LYS:CD	2:N:13:ASN:CB	2.93	0.47
3:O:155:LEU:HD12	3:O:156:TYR:N	2.30	0.47
1:A:12:GLY:HA2	4:A:701:FAD:H1B	1.96	0.47
1:A:343:ARG:HG2	1:A:345:VAL:CG1	2.37	0.47
1:A:447:LYS:O	1:A:451:ARG:HB2	2.15	0.47
1:A:525:ILE:HD13	1:A:525:ILE:HA	1.70	0.47
3:C:20:MET:SD	3:O:91:GLN:HB3	2.54	0.47
3:C:116:VAL:HG13	10:C:303:LMT:C11	2.45	0.47
1:E:349:CYS:O	1:E:353:LEU:HB2	2.14	0.47
2:F:57:CYS:O	2:F:58:ARG:NH1	2.46	0.47
2:F:61:ILE:O	8:F:303:FES:S1	2.73	0.47
3:G:181:VAL:CG1	3:G:182:GLY:N	2.78	0.47
1:I:7:ASP:N	1:I:30:LYS:O	2.43	0.47
1:I:30:LYS:HD3	1:I:30:LYS:HA	1.67	0.47
1:I:491:LYS:O	1:I:495:LYS:HG2	2.14	0.47
2:J:7:LEU:CD1	2:J:43:ILE:HD11	2.45	0.47
1:M:387:LYS:HE3	1:M:428:PHE:HE1	1.79	0.47
2:B:197:ASP:OD1	3:C:13:ARG:HD3	2.14	0.47
3:G:115:GLN:HE22	3:G:173:ARG:HD2	1.80	0.47
1:M:288:MET:HE1	1:M:289:PRO:HD3	1.97	0.47
2:N:117:ILE:HG13	2:N:119:ALA:HB2	1.97	0.47
1:A:259:THR:O	1:A:268:VAL:HG22	2.15	0.46
3:C:49:PRO:HB3	3:C:141:ALA:CB	2.45	0.46
1:E:110:VAL:HG23	1:E:135:LEU:O	2.15	0.46
3:G:4:SER:HB3	3:G:5:THR:H	1.44	0.46
1:I:455:ILE:HD12	1:I:459:ARG:NH2	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:202:ASP:C	2:J:204:GLY:N	2.65	0.46
3:K:116:VAL:O	3:K:119:ALA:HB3	2.15	0.46
3:K:127:ALA:HA	3:K:130:MET:CE	2.45	0.46
1:M:250:ASN:ND2	1:M:399:ASP:OD2	2.48	0.46
1:A:270:GLU:CD	1:A:301:ARG:NH1	2.68	0.46
3:C:95:LYS:HZ3	10:C:303:LMT:C6B	2.28	0.46
3:C:118:SER:O	3:C:122:ILE:HG23	2.16	0.46
3:C:129:HIS:O	3:C:133:VAL:HG22	2.15	0.46
1:E:258:PRO:CD	1:E:301:ARG:HD2	2.45	0.46
2:F:117:ILE:HG13	2:F:119:ALA:HB2	1.97	0.46
3:G:111:MET:HB3	3:G:169:VAL:HG11	1.96	0.46
1:I:14:ALA:CB	4:I:701:FAD:H4B	2.42	0.46
1:I:300:SER:OG	1:I:301:ARG:N	2.48	0.46
1:M:412:ALA:O	1:M:416:VAL:HB	2.15	0.46
1:M:546:ARG:HH12	1:M:562:TRP:CB	2.28	0.46
2:N:199:ILE:HG13	2:N:205:VAL:CG2	2.44	0.46
3:O:147:ARG:HB2	3:O:150:SER:O	2.12	0.46
3:C:35:LEU:HD13	3:C:167:VAL:CG1	2.44	0.46
1:E:189:GLY:O	1:E:387:LYS:N	2.38	0.46
1:E:503:SER:HB3	1:E:529:LEU:HD22	1.97	0.46
1:I:59:ILE:HG21	1:I:127:GLU:O	2.15	0.46
1:I:322:TYR:O	1:I:365:ARG:NH2	2.49	0.46
3:K:166:HIS:HE1	9:K:302:HEM:CHB	2.29	0.46
3:O:69:GLY:O	3:O:73:PHE:HB2	2.16	0.46
1:A:38:PRO:HG2	1:A:41:ARG:HH12	1.81	0.46
1:A:564:ASN:OD1	1:A:564:ASN:N	2.48	0.46
1:I:60:MET:HB2	1:I:147:TRP:CD2	2.50	0.46
3:K:185:LYS:H	3:K:185:LYS:HD3	1.79	0.46
1:M:44:SER:OG	4:M:701:FAD:O5'	2.33	0.46
1:M:195:ILE:HA	1:M:206:ALA:HA	1.98	0.46
1:M:413:GLU:O	1:M:417:ALA:CB	2.63	0.46
1:M:480:VAL:HG23	1:M:484:ARG:CZ	2.46	0.46
2:N:1:MET:HG2	2:N:30:GLU:OE2	2.14	0.46
2:N:12:TYR:HE2	2:N:14:PRO:HB3	1.81	0.46
1:A:55:LEU:HG	1:A:56:GLY:H	1.80	0.46
1:A:248:MET:HB2	1:A:568:SER:OG	2.16	0.46
2:B:54:ASP:HB3	2:B:64:SER:OG	2.15	0.46
3:C:172:TYR:HD1	3:C:189:PHE:HE1	1.61	0.46
2:F:22:ARG:NH2	2:F:24:GLN:OE1	2.48	0.46
3:K:171:PHE:O	3:K:174:ILE:HG22	2.15	0.46
1:M:96:VAL:HG21	1:M:416:VAL:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:279:LEU:HA	1:M:327:TRP:O	2.15	0.46
1:M:358:ILE:HG13	1:M:359:HIS:ND1	2.31	0.46
1:A:399:ASP:OD2	1:A:565:ARG:NE	2.48	0.46
2:B:34:MET:HG3	2:B:38:ILE:HB	1.97	0.46
1:E:378:ASN:OD1	1:E:381:GLY:N	2.48	0.46
2:F:154:CYS:SG	2:F:155:GLY:N	2.89	0.46
2:F:215:GLU:OE2	2:F:225:GLN:HB2	2.14	0.46
1:I:16:ALA:O	1:I:20:VAL:HG12	2.15	0.46
1:I:47:ALA:HB3	1:I:157:GLY:HA3	1.96	0.46
1:I:308:MET:HB3	1:I:308:MET:HE2	1.87	0.46
2:J:6:THR:HB	2:J:87:GLU:HA	1.98	0.46
2:J:11:ARG:HH22	2:J:50:THR:HG23	1.79	0.46
2:J:104:VAL:HG23	2:J:106:THR:HG23	1.97	0.46
2:J:190:ARG:NE	2:J:190:ARG:HA	2.30	0.46
1:M:237:GLN:NE2	1:M:395:SER:HA	2.29	0.46
1:M:500:TYR:C	1:M:500:TYR:CD2	2.89	0.46
3:O:31:LEU:HD12	9:O:303:HEM:CAC	2.46	0.46
1:A:257:HIS:HE1	1:A:301:ARG:NH1	2.11	0.46
3:C:162:LEU:HD23	3:C:162:LEU:HA	1.77	0.46
1:E:438:MET:HA	1:E:441:VAL:HG12	1.98	0.46
1:E:622:LEU:O	1:E:622:LEU:HD23	2.15	0.46
2:F:188:ASP:OD1	2:F:195:TYR:OH	2.29	0.46
1:I:152:THR:HG23	1:I:156:THR:HG23	1.98	0.46
2:J:7:LEU:HD13	2:J:43:ILE:HD11	1.96	0.46
2:J:96:PHE:CD2	2:J:106:THR:HG22	2.50	0.46
3:K:24:GLN:OE1	3:K:85:ARG:NH2	2.49	0.46
3:K:142:ALA:O	3:K:146:ALA:N	2.48	0.46
1:M:6:THR:HA	1:M:30:LYS:HG2	1.98	0.46
1:M:185:ILE:HG23	1:M:445:HIS:CE1	2.51	0.46
1:M:316:LEU:CB	1:M:319:LYS:HG3	2.46	0.46
1:M:341:LYS:CG	1:M:342:LEU:HB3	2.46	0.46
2:N:11:ARG:HE	2:N:101:ASP:CG	2.18	0.46
3:O:104:LEU:HA	3:O:104:LEU:HD12	1.68	0.46
1:A:242:ASP:OD2	1:A:530:LYS:NZ	2.44	0.46
1:A:545:SER:O	1:A:557:ARG:HA	2.16	0.46
1:A:614:ILE:N	1:A:615:PRO:HD3	2.30	0.46
3:G:28:GLY:O	3:G:32:ILE:HB	2.16	0.46
1:I:586:PRO:O	1:I:587:TYR:HB3	2.16	0.46
2:J:12:TYR:CE1	2:J:19:SER:O	2.68	0.46
2:J:137:MET:SD	2:J:142:ALA:HB2	2.56	0.46
1:M:55:LEU:CD2	1:M:138:ALA:HB2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:156:TYR:HA	3:O:159:LEU:HB3	1.98	0.46
1:A:20:VAL:HG11	1:A:213:LEU:HD13	1.97	0.46
1:A:45:SER:HB3	1:A:158:ARG:HH11	1.80	0.46
1:A:53:ALA:HB3	1:A:97:MET:HG3	1.98	0.46
1:A:152:THR:O	1:A:152:THR:OG1	2.33	0.46
2:B:2:ASN:O	2:B:2:ASN:ND2	2.28	0.46
3:C:128:VAL:O	3:C:132:VAL:HG13	2.15	0.46
3:C:184:ASN:OD1	3:C:185:LYS:N	2.41	0.46
1:E:112:PRO:HB3	1:E:130:ALA:HA	1.98	0.46
2:F:233:ARG:CZ	3:G:179:GLY:HA3	2.46	0.46
1:I:64:ASP:OD1	1:I:148:ARG:NH2	2.48	0.46
1:I:612:PHE:HB3	1:I:613:VAL:H	1.59	0.46
2:J:13:ASN:HD22	2:J:16:ASP:HB3	1.81	0.46
3:K:45:VAL:HG21	3:K:211:PHE:HA	1.98	0.46
1:M:259:THR:HA	1:M:364:VAL:HB	1.97	0.46
3:O:27:SER:O	3:O:31:LEU:HB2	2.15	0.46
1:A:10:CYS:HB2	1:A:33:MET:HG3	1.98	0.46
1:E:491:LYS:O	1:E:495:LYS:HG2	2.15	0.46
1:E:606:GLU:HG3	1:E:607:LEU:N	2.31	0.46
3:G:25:MET:CG	3:G:174:ILE:HD11	2.46	0.46
1:I:36:LEU:HD13	4:I:701:FAD:C5A	2.46	0.46
1:I:335:GLU:O	1:I:338:ILE:HG22	2.16	0.46
1:M:279:LEU:HD23	1:M:327:TRP:O	2.16	0.46
1:M:346:TYR:HA	1:M:357:PRO:HG3	1.98	0.46
3:O:12:GLN:HG2	3:O:13:ARG:HG3	1.98	0.46
1:E:255:GLN:HE21	1:E:301:ARG:CG	2.30	0.45
3:G:175:GLY:HA2	3:G:180:PHE:HD2	1.81	0.45
1:I:377:THR:HG1	1:I:398:TRP:HA	1.81	0.45
1:I:559:ASP:CB	1:I:605:ASN:HB3	2.45	0.45
1:I:580:GLU:HG2	1:I:581:TYR:H	1.81	0.45
1:M:269:THR:HA	5:M:702:FUM:O	2.15	0.45
1:M:280:LEU:CD1	1:M:284:GLN:HB2	2.46	0.45
2:N:201:ASN:O	2:N:202:ASP:O	2.33	0.45
1:A:200:ARG:NH1	2:B:105:ASP:OD2	2.49	0.45
1:A:489:LEU:HD13	1:A:540:LEU:CA	2.43	0.45
2:B:138:ASP:OD1	2:B:139:ASN:N	2.49	0.45
3:C:148:LEU:HD21	3:C:212:MET:CB	2.46	0.45
1:E:542:ARG:CG	1:E:549:HIS:CE1	2.99	0.45
2:F:102:LEU:HA	2:F:102:LEU:HD23	1.58	0.45
1:I:6:THR:HB	1:I:30:LYS:O	2.16	0.45
2:J:94:PRO:HD2	2:J:159:ALA:HB1	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:110:PHE:CE1	2:J:174:VAL:HG11	2.51	0.45
2:J:117:ILE:HA	2:J:198:VAL:HG13	1.98	0.45
2:J:211:LEU:HD23	3:K:173:ARG:HH12	1.81	0.45
3:K:8:LEU:CD1	3:K:13:ARG:HB3	2.38	0.45
3:K:51:LEU:HD12	3:K:52:MET:N	2.31	0.45
3:K:172:TYR:O	3:K:176:VAL:HG23	2.16	0.45
3:O:116:VAL:CG1	10:O:301:LMT:H121	2.45	0.45
1:A:40:ARG:HB3	1:A:158:ARG:HH22	1.82	0.45
1:A:75:LYS:HG3	1:A:590:MET:HE3	1.98	0.45
3:C:38:HIS:CE1	9:C:301:HEM:C4D	3.05	0.45
1:E:294:ASP:OD1	1:E:294:ASP:N	2.45	0.45
1:E:343:ARG:O	1:E:345:VAL:N	2.48	0.45
1:E:526:ARG:O	1:E:530:LYS:HG3	2.16	0.45
2:F:96:PHE:CZ	2:F:158:VAL:HG21	2.51	0.45
1:I:158:ARG:HE	2:J:152:ILE:HA	1.82	0.45
1:I:484:ARG:O	1:I:551:ARG:HA	2.16	0.45
1:M:51:MET:HE3	1:M:412:ALA:HA	1.96	0.45
1:M:117:TYR:OH	1:M:137:HIS:NE2	2.49	0.45
2:N:2:ASN:HD22	2:N:2:ASN:C	2.15	0.45
3:C:92:ASP:O	3:C:96:THR:OG1	2.26	0.45
1:E:259:THR:O	1:E:268:VAL:HG22	2.17	0.45
2:F:24:GLN:HE21	2:F:25:THR:N	2.15	0.45
3:G:130:MET:O	3:G:134:LEU:CB	2.46	0.45
1:I:40:ARG:C	1:I:158:ARG:HH12	2.20	0.45
1:I:216:THR:HG21	1:I:236:GLY:N	2.30	0.45
2:J:55:PHE:CD1	2:J:65:CYS:SG	3.09	0.45
1:M:380:ASP:O	1:M:421:ILE:HG23	2.17	0.45
2:N:222:ILE:CG2	2:N:223:PRO:HD2	2.47	0.45
3:O:35:LEU:O	3:O:35:LEU:HD23	2.17	0.45
3:O:72:VAL:HG23	3:O:130:MET:SD	2.57	0.45
3:O:146:ALA:O	3:O:148:LEU:O	2.35	0.45
3:C:37:ALA:N	11:C:304:MQ7:H2M3	2.31	0.45
3:C:44:SER:HB2	3:C:52:MET:HB2	1.98	0.45
1:E:199:LEU:HD23	1:E:199:LEU:HA	1.74	0.45
1:I:57:ASN:HB2	1:I:136:ILE:O	2.16	0.45
1:I:182:GLU:HB3	1:I:449:GLN:HG3	1.99	0.45
1:I:219:TYR:CD1	1:I:531:LEU:HD13	2.52	0.45
1:I:313:ARG:NH2	1:I:483:PHE:HB2	2.31	0.45
2:J:106:THR:HB	2:J:110:PHE:CE2	2.49	0.45
3:K:126:GLY:O	3:K:130:MET:CB	2.65	0.45
1:M:55:LEU:CD1	1:M:56:GLY:H	2.26	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:406:LEU:O	1:M:409:ASN:HB2	2.17	0.45
2:N:73:PRO:HG2	2:N:217:VAL:HG21	1.98	0.45
3:O:10:VAL:HG22	3:O:11:PRO:HD2	1.99	0.45
1:A:438:MET:HE3	1:A:438:MET:HB3	1.89	0.45
3:C:52:MET:O	3:C:56:ALA:HB2	2.17	0.45
3:C:76:MET:HE1	3:C:123:LEU:HA	1.99	0.45
1:E:570:TRP:HD1	1:E:572:GLU:O	1.99	0.45
2:F:118:GLU:O	2:F:122:HIS:HE1	2.00	0.45
3:G:153:LEU:O	3:G:153:LEU:HD23	2.16	0.45
1:I:449:GLN:O	1:I:453:THR:HG23	2.16	0.45
2:N:169:ASP:HB2	2:N:203:GLN:OE1	2.16	0.45
2:N:185:ASP:OD1	2:N:187:ARG:N	2.49	0.45
1:A:32:ILE:HD13	1:A:207:TYR:HE2	1.82	0.45
1:A:300:SER:HB2	1:A:597:TYR:CE1	2.52	0.45
1:A:438:MET:HA	1:A:441:VAL:HG12	1.99	0.45
3:C:143:LYS:HD2	3:C:144:SER:N	2.32	0.45
1:E:248:MET:HE1	1:E:375:VAL:HA	1.99	0.45
1:E:457:THR:HG23	1:E:508:LEU:HD21	1.98	0.45
1:I:100:VAL:HG22	1:I:103:TRP:CE3	2.51	0.45
1:I:118:TYR:CD1	1:I:332:HIS:CE1	3.05	0.45
1:I:257:HIS:CE1	1:I:258:PRO:HD2	2.51	0.45
1:I:460:LYS:HG2	1:I:505:LYS:HA	1.98	0.45
1:I:605:ASN:ND2	1:I:608:PRO:HD3	2.32	0.45
1:M:257:HIS:CD2	1:M:259:THR:HG1	2.34	0.45
1:M:258:PRO:CB	1:M:308:MET:HE1	2.47	0.45
1:M:260:GLY:HA2	1:M:267:LEU:HA	1.98	0.45
1:M:333:LEU:HB2	1:M:338:ILE:H	1.82	0.45
1:M:579:LEU:HD23	1:M:579:LEU:HA	1.82	0.45
3:O:25:MET:CG	3:O:174:ILE:HD11	2.46	0.45
3:O:183:ARG:O	3:O:186:ARG:HB3	2.16	0.45
1:A:7:ASP:N	1:A:7:ASP:OD1	2.49	0.45
10:C:303:LMT:H2O1	10:C:303:LMT:C3'	2.24	0.45
10:C:303:LMT:O5B	10:C:303:LMT:H5'	2.16	0.45
1:E:338:ILE:HG23	1:E:341:LYS:C	2.37	0.45
2:F:61:ILE:O	2:F:62:CYS:SG	2.74	0.45
1:I:19:ARG:HH12	1:I:23:GLU:HB2	1.81	0.45
2:J:8:ASN:O	2:J:90:LEU:N	2.37	0.45
2:J:113:THR:O	2:J:117:ILE:HG12	2.17	0.45
3:K:185:LYS:O	3:K:187:LYS:N	2.50	0.45
1:M:387:LYS:HE3	1:M:428:PHE:CE1	2.51	0.45
1:M:441:VAL:HA	1:M:445:HIS:ND1	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:554:PHE:CD1	1:M:554:PHE:C	2.90	0.45
2:N:51:LEU:HD12	2:N:52:LYS:H	1.81	0.45
2:N:171:LEU:HD11	2:N:204:GLY:HA3	1.98	0.45
1:A:20:VAL:HG21	1:A:213:LEU:CD1	2.46	0.45
1:A:23:GLU:OE1	1:A:423:GLU:HG2	2.17	0.45
3:C:59:PHE:HB3	3:C:63:TYR:HA	1.98	0.45
3:C:149:GLN:C	3:C:151:GLY:H	2.20	0.45
1:E:471:GLU:O	1:E:475:ILE:HG12	2.17	0.45
3:G:38:HIS:CE1	9:G:301:HEM:C2D	3.05	0.45
1:I:195:ILE:HD12	1:I:446:LYS:HB2	1.98	0.45
1:M:140:ALA:CB	1:M:273:ARG:HH11	2.30	0.45
1:M:338:ILE:HG21	1:M:357:PRO:O	2.17	0.45
1:M:405:ARG:NH2	5:M:702:FUM:C6	2.80	0.45
1:A:458:GLY:O	1:A:459:ARG:HB2	2.17	0.45
3:C:32:ILE:HD12	3:C:32:ILE:HA	1.87	0.45
3:C:119:ALA:HB1	9:C:302:HEM:HMB2	1.99	0.45
3:G:1:MET:N	2:J:91:HIS:HE1	2.15	0.45
1:I:301:ARG:HG3	1:I:405:ARG:O	2.16	0.45
2:J:55:PHE:HD1	2:J:65:CYS:SG	2.40	0.45
1:M:261:THR:HG22	1:M:263:PRO:HD2	1.99	0.45
1:M:369:HIS:HE1	4:M:701:FAD:C7	2.30	0.45
1:M:485:ASN:O	1:M:489:LEU:HD13	2.16	0.45
1:M:489:LEU:HD23	1:M:540:LEU:CA	2.46	0.45
1:M:565:ARG:NH2	1:M:584:ALA:HB1	2.32	0.45
2:N:48:ASP:OD1	2:N:50:THR:HG22	2.17	0.45
2:N:199:ILE:HD12	2:N:204:GLY:HA3	1.99	0.45
3:O:25:MET:HB2	3:O:178:TYR:OH	2.17	0.45
9:O:303:HEM:HBB2	9:O:303:HEM:CMB	2.43	0.45
1:I:106:PRO:HB3	2:J:145:ILE:CG2	2.46	0.44
1:I:513:LYS:HE3	1:I:513:LYS:HB3	1.49	0.44
3:K:147:ARG:HA	3:K:150:SER:O	2.17	0.44
1:M:406:LEU:HD23	1:M:407:GLY:N	2.32	0.44
1:A:308:MET:HB3	1:A:308:MET:HE2	1.90	0.44
1:A:365:ARG:HG3	1:A:367:THR:HG23	1.99	0.44
2:B:180:ALA:HB2	2:B:231:MET:HE3	1.97	0.44
1:E:170:GLN:NE2	1:E:171:TYR:HE2	2.16	0.44
1:E:255:GLN:HE21	1:E:301:ARG:HG2	1.82	0.44
1:I:306:ARG:CZ	1:I:550:THR:OG1	2.65	0.44
1:I:530:LYS:HE3	1:I:570:TRP:CE2	2.52	0.44
1:I:583:GLU:OE1	1:I:586:PRO:HD3	2.17	0.44
3:K:148:LEU:HD23	3:K:212:MET:HG3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:305:SER:O	1:M:309:THR:HG23	2.16	0.44
1:M:503:SER:O	1:M:504:GLN:C	2.55	0.44
2:N:62:CYS:N	8:N:303:FES:S1	2.90	0.44
2:N:211:LEU:O	3:O:106:HIS:NE2	2.42	0.44
3:O:156:TYR:O	3:O:160:LEU:HB2	2.17	0.44
1:A:188:GLY:O	1:A:190:ASN:N	2.51	0.44
1:E:262:VAL:HG12	1:E:263:PRO:N	2.32	0.44
1:E:484:ARG:HD3	1:E:489:LEU:HD21	2.00	0.44
1:E:515:MET:HA	1:E:515:MET:HE2	1.99	0.44
2:F:230:ILE:HG22	2:F:233:ARG:NH2	2.26	0.44
1:I:235:GLY:HA2	1:I:524:ARG:HH21	1.81	0.44
1:M:178:ARG:HA	1:M:199:LEU:HD12	1.99	0.44
1:M:261:THR:CG2	1:M:353:LEU:HD11	2.47	0.44
2:N:131:THR:CG2	2:N:132:ALA:N	2.80	0.44
3:O:65:ALA:O	3:O:134:LEU:HD11	2.16	0.44
3:O:98:ARG:NH1	10:O:301:LMT:O2'	2.50	0.44
1:A:462:LYS:HA	1:A:507:SER:HB2	1.99	0.44
3:C:140:THR:O	3:C:143:LYS:HE3	2.17	0.44
3:C:156:TYR:CD1	9:C:301:HEM:HAD1	2.52	0.44
1:E:184:LEU:HD12	1:E:240:ALA:HA	2.00	0.44
2:F:34:MET:O	2:F:81:THR:HG23	2.17	0.44
1:I:140:ALA:HB2	1:I:147:TRP:CE2	2.52	0.44
2:J:66:ALA:HA	2:J:74:GLY:O	2.17	0.44
3:K:29:ALA:O	3:K:33:LEU:HG	2.18	0.44
3:K:35:LEU:HD13	3:K:167:VAL:HG11	1.98	0.44
1:M:34:LEU:HD23	1:M:34:LEU:HA	1.65	0.44
1:M:40:ARG:HA	1:M:161:LEU:HD21	1.99	0.44
1:M:377:THR:HB	1:M:381:GLY:HA2	1.99	0.44
1:M:584:ALA:HA	1:M:585:SER:HA	1.55	0.44
1:A:214:ILE:CG2	1:A:236:GLY:HA3	2.46	0.44
2:B:60:GLY:HA2	8:B:303:FES:S1	2.57	0.44
2:B:179:VAL:HB	2:B:199:ILE:HD13	1.99	0.44
3:C:56:ALA:HB1	3:C:139:ILE:CG2	2.45	0.44
3:C:142:ALA:C	3:C:144:SER:H	2.21	0.44
3:G:39:MET:HA	3:G:43:SER:HB2	1.99	0.44
1:I:142:GLY:H	1:I:270:GLU:CD	2.20	0.44
1:I:530:LYS:HG2	1:I:570:TRP:CZ2	2.52	0.44
1:M:32:ILE:HG21	1:M:207:TYR:CD2	2.52	0.44
1:M:112:PRO:HG3	1:M:133:ALA:HB2	1.98	0.44
1:M:248:MET:HA	1:M:374:GLY:O	2.17	0.44
1:M:251:MET:HE2	1:M:531:LEU:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:338:ILE:CD1	1:M:358:ILE:HA	2.46	0.44
1:A:92:THR:HB	1:A:416:VAL:HG13	1.99	0.44
3:C:155:LEU:O	3:C:159:LEU:N	2.43	0.44
1:E:389:LEU:C	1:E:390:PHE:HD1	2.21	0.44
1:E:490:GLN:HB2	1:E:540:LEU:HD13	1.99	0.44
2:F:67:MET:O	2:F:73:PRO:HA	2.18	0.44
1:I:60:MET:HB2	1:I:147:TRP:CE3	2.53	0.44
1:I:136:ILE:N	2:J:134:GLU:OE2	2.43	0.44
1:I:346:TYR:HE1	1:I:350:THR:HG21	1.74	0.44
1:I:417:ALA:O	1:I:421:ILE:HG12	2.18	0.44
3:K:34:PHE:CE2	9:K:301:HEM:HMC2	2.52	0.44
3:K:137:LEU:HD13	3:K:143:LYS:NZ	2.32	0.44
1:M:389:LEU:HD12	1:M:389:LEU:HA	1.73	0.44
1:M:460:LYS:O	1:M:505:LYS:HE3	2.17	0.44
1:M:554:PHE:C	1:M:554:PHE:HD1	2.21	0.44
2:N:206:PHE:CZ	3:O:18:GLY:HA2	2.52	0.44
1:A:270:GLU:O	1:A:270:GLU:HG2	2.17	0.44
1:A:274:GLY:HA2	1:A:298:LEU:HD21	1.98	0.44
2:B:2:ASN:HD22	2:B:2:ASN:C	2.15	0.44
2:B:96:PHE:HZ	2:B:158:VAL:HG21	1.83	0.44
10:C:303:LMT:C3'	10:C:303:LMT:C2B	2.95	0.44
1:E:261:THR:OG1	1:E:268:VAL:HG13	2.17	0.44
2:F:137:MET:HG3	2:F:138:ASP:N	2.33	0.44
2:F:222:ILE:HG22	2:F:223:PRO:CD	2.46	0.44
1:I:66:PRO:HB3	1:I:91:ASP:HA	1.99	0.44
1:I:340:THR:O	1:I:341:LYS:C	2.56	0.44
1:I:343:ARG:C	1:I:345:VAL:H	2.20	0.44
3:K:192:THR:O	3:K:196:MET:HG2	2.18	0.44
1:M:60:MET:HB2	1:M:147:TRP:CE3	2.53	0.44
2:N:161:CYS:HB3	2:N:164:ALA:HB3	2.00	0.44
3:O:139:ILE:HA	3:O:143:LYS:HZ1	1.83	0.44
1:A:556:GLU:HG3	1:A:603:ILE:HG13	2.00	0.44
3:C:94:TRP:CG	10:C:303:LMT:H22	2.53	0.44
3:C:171:PHE:HB3	3:C:193:GLU:OE2	2.18	0.44
1:E:24:ALA:HA	1:E:426:VAL:CG2	2.47	0.44
1:E:587:TYR:CD2	1:E:587:TYR:O	2.71	0.44
1:I:121:GLY:O	1:I:332:HIS:NE2	2.50	0.44
1:I:139:ARG:HG3	1:I:139:ARG:NH1	2.32	0.44
1:M:103:TRP:CD1	1:M:167:LYS:HE2	2.53	0.44
1:M:304:VAL:HG12	1:M:308:MET:CE	2.46	0.44
2:N:110:PHE:HA	2:N:113:THR:HG22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:64:MET:HB2	3:O:67:ILE:HG22	2.00	0.44
1:A:97:MET:SD	1:A:107:TRP:CZ2	3.11	0.44
2:B:215:GLU:OE2	2:B:225:GLN:N	2.42	0.44
1:E:309:THR:O	1:E:313:ARG:HG3	2.18	0.44
1:E:466:PHE:CZ	2:F:45:ASP:HA	2.53	0.44
2:F:199:ILE:HD13	2:F:205:VAL:HB	2.00	0.44
3:G:34:PHE:HE2	9:G:301:HEM:HMC2	1.83	0.44
3:G:111:MET:O	3:G:114:VAL:HG22	2.16	0.44
1:I:119:LYS:HB3	1:I:124:PHE:CE1	2.51	0.44
1:I:302:ASP:O	1:I:306:ARG:HB3	2.18	0.44
1:I:467:LYS:HD2	1:I:467:LYS:HA	1.78	0.44
1:M:129:LYS:HE3	1:M:132:LYS:HG2	1.99	0.44
1:M:452:ILE:O	1:M:455:ILE:HG22	2.17	0.44
1:M:524:ARG:HG3	1:M:528:MET:CE	2.47	0.44
1:M:595:ARG:N	1:M:596:GLY:HA3	2.30	0.44
1:A:121:GLY:O	1:A:332:HIS:HE1	2.00	0.43
3:C:121:PHE:HD2	3:C:162:LEU:HD13	1.83	0.43
1:E:257:HIS:CG	1:E:258:PRO:HD2	2.53	0.43
1:E:559:ASP:HB2	1:E:603:ILE:O	2.18	0.43
2:F:151:CYS:SG	2:F:152:ILE:N	2.90	0.43
3:G:181:VAL:HG12	3:G:182:GLY:H	1.80	0.43
3:G:182:GLY:HA3	3:G:183:ARG:C	2.36	0.43
1:I:493:VAL:HG13	1:I:533:GLN:OE1	2.18	0.43
9:K:301:HEM:HAD1	9:K:301:HEM:HMD2	1.74	0.43
1:M:496:LEU:HG	1:M:533:GLN:HB2	1.98	0.43
2:N:96:PHE:HZ	2:N:158:VAL:HG21	1.82	0.43
3:O:188:TRP:HD1	3:O:192:THR:OG1	1.92	0.43
3:O:191:LYS:O	3:O:195:LEU:HD23	2.17	0.43
2:B:213:ALA:O	2:B:217:VAL:HG13	2.17	0.43
10:C:303:LMT:H3'	10:C:303:LMT:C2B	2.48	0.43
1:E:587:TYR:HD1	1:E:614:ILE:CG1	2.29	0.43
2:F:11:ARG:HA	2:F:101:ASP:OD1	2.17	0.43
2:F:226:ASP:OD1	2:F:226:ASP:N	2.46	0.43
3:G:22:PHE:O	3:G:26:VAL:HG23	2.19	0.43
3:G:87:MET:HG2	9:G:302:HEM:HMA3	1.99	0.43
1:I:546:ARG:NH2	1:I:562:TRP:O	2.50	0.43
3:K:154:TYR:CD2	3:K:154:TYR:O	2.70	0.43
1:M:40:ARG:HH22	2:N:178:ARG:NH1	2.14	0.43
1:M:365:ARG:HG2	1:M:366:PRO:N	2.32	0.43
2:N:57:CYS:O	2:N:58:ARG:HG3	2.18	0.43
3:O:45:VAL:HB	3:O:211:PHE:CZ	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:153:LEU:O	3:O:155:LEU:HG	2.18	0.43
2:B:11:ARG:NH2	2:B:51:LEU:HA	2.34	0.43
3:C:5:THR:HG23	3:C:6:ILE:H	1.83	0.43
3:C:159:LEU:HD23	3:C:163:ALA:HB2	1.99	0.43
1:E:158:ARG:HD2	1:E:158:ARG:HA	1.65	0.43
1:E:339:THR:HB	1:E:343:ARG:HG3	2.00	0.43
2:F:202:ASP:C	2:F:204:GLY:H	2.21	0.43
2:F:226:ASP:O	2:F:230:ILE:HG23	2.18	0.43
1:I:78:ASP:HB3	1:I:546:ARG:HG3	1.99	0.43
1:I:261:THR:CG2	1:I:353:LEU:HD11	2.48	0.43
2:J:52:LYS:HB2	2:J:101:ASP:HB2	2.00	0.43
2:J:110:PHE:HA	2:J:113:THR:HG22	1.99	0.43
3:K:47:LEU:HB2	3:K:51:LEU:HD11	1.98	0.43
1:M:214:ILE:HG23	1:M:236:GLY:HA3	2.00	0.43
1:M:619:LYS:O	1:M:621:ASN:N	2.51	0.43
2:N:63:GLY:N	2:N:152:ILE:HD12	2.33	0.43
3:O:60:GLU:OE1	3:O:64:MET:HB3	2.18	0.43
1:A:301:ARG:NH2	5:A:702:FUM:O8	2.50	0.43
3:C:181:VAL:HG12	3:C:182:GLY:H	1.83	0.43
1:E:238:ILE:HG22	1:E:531:LEU:CD2	2.48	0.43
1:E:614:ILE:N	1:E:615:PRO:HD2	2.34	0.43
2:F:177:MET:SD	2:F:222:ILE:HG21	2.59	0.43
1:I:14:ALA:HB2	4:I:701:FAD:C3B	2.48	0.43
1:I:153:ALA:HB3	2:J:146:PHE:CZ	2.53	0.43
1:I:318:VAL:HG21	1:I:327:TRP:NE1	2.33	0.43
1:M:75:LYS:HB3	1:M:595:ARG:HB3	1.99	0.43
1:M:109:ARG:HG3	2:N:137:MET:O	2.18	0.43
1:M:267:LEU:HD13	1:M:369:HIS:CE1	2.54	0.43
3:O:41:LEU:HD22	3:O:63:TYR:CE2	2.53	0.43
1:A:32:ILE:HG21	1:A:207:TYR:CE2	2.54	0.43
1:A:248:MET:O	1:A:567:LEU:HA	2.19	0.43
1:A:372:MET:CE	1:A:404:ASN:HA	2.49	0.43
2:B:219:PRO:HD2	7:B:302:SF4:S3	2.58	0.43
2:B:225:GLN:NE2	3:C:186:ARG:HD3	2.24	0.43
3:C:5:THR:CG2	3:C:6:ILE:H	2.30	0.43
3:C:37:ALA:O	11:C:304:MQ7:H142	2.18	0.43
2:F:22:ARG:H	2:F:22:ARG:HG2	1.62	0.43
2:F:96:PHE:HZ	2:F:158:VAL:HG21	1.84	0.43
1:I:456:VAL:HG11	1:I:519:LEU:HD13	2.00	0.43
1:M:247:PRO:HB3	1:M:569:TYR:CZ	2.54	0.43
1:M:484:ARG:O	1:M:551:ARG:HA	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:122:ILE:HG21	3:O:122:ILE:HD13	1.76	0.43
1:A:109:ARG:HB3	1:A:135:LEU:O	2.19	0.43
1:A:196:ALA:HB3	1:A:205:VAL:CG1	2.49	0.43
1:A:370:TYR:HE2	1:A:372:MET:HA	1.83	0.43
1:A:609:PRO:HA	1:A:612:PHE:CD1	2.53	0.43
2:B:225:GLN:HE22	3:C:186:ARG:CD	2.27	0.43
3:C:41:LEU:HB2	11:C:304:MQ7:C14	2.49	0.43
3:C:72:VAL:HG21	9:C:301:HEM:HAB	2.01	0.43
3:C:149:GLN:N	3:C:149:GLN:CD	2.72	0.43
9:G:302:HEM:HBB2	9:G:302:HEM:CMB	2.46	0.43
1:I:59:ILE:HA	1:I:62:ASP:HB2	2.01	0.43
1:I:378:ASN:OD1	1:I:381:GLY:N	2.51	0.43
2:J:163:THR:HG21	2:J:207:GLY:O	2.19	0.43
1:M:318:VAL:HA	1:M:319:LYS:CB	2.39	0.43
2:N:94:PRO:O	2:N:96:PHE:N	2.52	0.43
2:N:158:VAL:HG23	2:N:159:ALA:H	1.81	0.43
1:A:192:LEU:HD13	1:A:436:PHE:HA	2.00	0.43
3:C:41:LEU:CB	11:C:304:MQ7:H141	2.49	0.43
3:C:97:PHE:O	3:C:101:ALA:CB	2.66	0.43
1:I:380:ASP:HA	1:I:420:TYR:HE2	1.84	0.43
1:I:562:TRP:CD1	1:I:562:TRP:N	2.86	0.43
1:I:607:LEU:N	1:I:608:PRO:CD	2.82	0.43
2:J:57:CYS:O	2:J:58:ARG:NH1	2.51	0.43
3:K:47:LEU:CB	3:K:51:LEU:HD11	2.48	0.43
3:K:140:THR:O	3:K:144:SER:OG	2.33	0.43
1:M:235:GLY:CA	1:M:524:ARG:HH21	2.31	0.43
1:M:390:PHE:CE2	1:M:425:MET:HG3	2.54	0.43
2:N:117:ILE:HA	2:N:198:VAL:CG1	2.49	0.43
3:O:172:TYR:O	3:O:176:VAL:HG23	2.19	0.43
3:O:205:LEU:O	3:O:208:LEU:HB3	2.18	0.43
1:A:595:ARG:HD2	1:A:597:TYR:CE1	2.53	0.43
3:C:10:VAL:HG13	3:C:11:PRO:N	2.33	0.43
3:C:97:PHE:O	3:C:101:ALA:HB2	2.19	0.43
1:E:312:MET:HB3	1:E:312:MET:HE2	1.77	0.43
1:E:489:LEU:O	1:E:493:VAL:HG23	2.19	0.43
1:E:525:ILE:HD13	1:E:525:ILE:HA	1.87	0.43
1:E:616:GLU:HG2	1:E:617:ALA:H	1.81	0.43
2:F:215:GLU:OE1	3:G:183:ARG:CZ	2.67	0.43
1:I:7:ASP:O	1:I:209:ALA:HB1	2.18	0.43
1:I:13:GLY:O	1:I:18:GLU:HG3	2.19	0.43
1:M:492:ALA:HA	1:M:495:LYS:CG	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:151:CYS:CB	7:N:302:SF4:S1	3.04	0.43
1:A:306:ARG:HG3	1:A:483:PHE:CZ	2.53	0.43
1:A:339:THR:HG1	1:A:343:ARG:HA	1.83	0.43
1:A:587:TYR:OH	1:A:615:PRO:HB3	2.18	0.43
2:B:196:TYR:O	2:B:200:GLY:N	2.50	0.43
3:C:74:VAL:O	3:C:78:VAL:HG23	2.18	0.43
3:C:201:ILE:HD12	3:C:202:THR:N	2.32	0.43
1:E:5:HIS:O	1:E:6:THR:CG2	2.64	0.43
1:E:118:TYR:O	1:E:275:ASP:HA	2.19	0.43
1:E:223:TYR:CZ	1:E:254:VAL:HG11	2.54	0.43
1:E:370:TYR:CB	1:E:405:ARG:HE	2.32	0.43
1:E:531:LEU:O	1:E:534:CYS:HB2	2.18	0.43
1:I:258:PRO:HG2	1:I:273:ARG:NH2	2.34	0.43
1:I:559:ASP:HB3	1:I:605:ASN:HB3	2.00	0.43
2:J:11:ARG:O	2:J:22:ARG:HG2	2.19	0.43
3:K:104:LEU:HG	3:K:106:HIS:HB2	2.00	0.43
1:M:441:VAL:O	1:M:445:HIS:HB2	2.19	0.43
1:M:541:ASP:O	1:M:562:TRP:HH2	2.01	0.43
2:N:51:LEU:HD12	2:N:52:LYS:N	2.34	0.43
2:N:94:PRO:C	2:N:96:PHE:N	2.72	0.43
3:O:157:LEU:O	3:O:161:PRO:HD2	2.19	0.43
1:A:51:MET:N	1:A:150:CYS:O	2.40	0.43
1:A:542:ARG:HA	1:A:562:TRP:CH2	2.53	0.43
3:C:45:VAL:HG21	3:C:211:PHE:CD1	2.53	0.43
3:C:146:ALA:O	3:C:153:LEU:HB2	2.19	0.43
1:E:424:ARG:HD3	1:E:424:ARG:HA	1.65	0.43
1:E:560:LYS:HA	1:E:605:ASN:OD1	2.18	0.43
3:G:73:PHE:O	3:G:77:VAL:HG23	2.19	0.43
1:I:570:TRP:HD1	1:I:572:GLU:O	2.02	0.43
2:J:200:GLY:C	2:J:202:ASP:H	2.21	0.43
3:K:47:LEU:HB3	3:K:51:LEU:CD2	2.39	0.43
3:K:103:MET:HE2	3:K:103:MET:HB3	1.93	0.43
1:M:346:TYR:HD1	1:M:357:PRO:HG2	1.84	0.43
3:O:44:SER:HB3	3:O:51:LEU:HD22	2.00	0.43
3:O:91:GLN:OE1	3:O:91:GLN:N	2.49	0.43
3:C:167:VAL:HG12	9:C:302:HEM:CBC	2.49	0.42
1:E:163:THR:O	1:E:167:LYS:HG2	2.19	0.42
2:F:52:LYS:HG3	2:F:101:ASP:OD2	2.19	0.42
2:J:42:GLN:O	2:J:46:GLU:CB	2.61	0.42
2:J:43:ILE:HD13	2:J:43:ILE:HG21	1.80	0.42
3:K:180:PHE:HA	3:K:181:VAL:HA	1.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:559:ASP:H	1:M:603:ILE:HG23	1.83	0.42
1:A:257:HIS:ND1	1:A:301:ARG:HD2	2.34	0.42
1:A:283:ASN:O	1:A:284:GLN:HB2	2.18	0.42
1:A:318:VAL:HG21	1:A:327:TRP:CE2	2.54	0.42
1:A:499:LEU:CG	1:A:529:LEU:HD21	2.46	0.42
3:C:172:TYR:HD1	3:C:189:PHE:CE1	2.37	0.42
1:E:76:GLY:O	1:E:404:ASN:HB3	2.19	0.42
1:E:140:ALA:HB2	1:E:147:TRP:CZ2	2.54	0.42
1:I:70:PHE:CB	1:I:87:ARG:HH11	2.33	0.42
1:I:441:VAL:O	1:I:446:LYS:HB3	2.19	0.42
1:I:607:LEU:HD12	1:I:607:LEU:H	1.84	0.42
2:J:12:TYR:CG	2:J:13:ASN:N	2.87	0.42
2:J:34:MET:O	2:J:81:THR:HG23	2.18	0.42
3:O:143:LYS:HG2	3:O:144:SER:N	2.34	0.42
1:A:262:VAL:HG13	1:A:365:ARG:HH21	1.83	0.42
2:B:11:ARG:NE	2:B:101:ASP:OD1	2.49	0.42
1:E:251:MET:O	1:E:535:THR:HG23	2.19	0.42
1:E:300:SER:OG	1:E:301:ARG:N	2.51	0.42
1:E:318:VAL:HG21	1:E:327:TRP:CE2	2.54	0.42
1:E:343:ARG:C	1:E:345:VAL:H	2.22	0.42
3:G:45:VAL:O	3:G:207:THR:HG23	2.19	0.42
3:G:149:GLN:N	3:G:150:SER:O	2.53	0.42
1:I:235:GLY:HA3	4:I:701:FAD:H61A	1.85	0.42
1:M:49:GLY:HA3	1:M:141:PHE:CZ	2.54	0.42
1:M:379:ARG:NH2	1:M:424:ARG:HH12	2.17	0.42
3:O:163:ALA:O	3:O:167:VAL:HG13	2.19	0.42
1:A:104:GLY:HA2	2:B:187:ARG:HD2	2.02	0.42
2:B:104:VAL:HG23	2:B:106:THR:HG23	2.01	0.42
3:C:80:PHE:HB2	9:C:302:HEM:CBB	2.49	0.42
3:C:94:TRP:CD1	10:C:303:LMT:H1'	2.52	0.42
3:C:206:LEU:O	3:C:210:ARG:HB2	2.18	0.42
9:C:301:HEM:HBB2	9:C:301:HEM:HMB1	2.00	0.42
1:E:214:ILE:O	1:E:391:SER:OG	2.35	0.42
1:E:227:THR:CG2	1:E:267:LEU:HB2	2.50	0.42
2:F:128:PHE:CG	2:F:129:ASP:N	2.86	0.42
3:G:126:GLY:O	3:G:130:MET:CB	2.67	0.42
1:I:196:ALA:HB3	1:I:205:VAL:CG1	2.49	0.42
1:I:264:THR:HB	1:I:266:ILE:HG13	2.01	0.42
1:I:412:ALA:O	1:I:416:VAL:HB	2.20	0.42
1:M:452:ILE:O	1:M:456:VAL:HG23	2.20	0.42
1:A:468:ILE:HG22	1:A:529:LEU:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:541:ASP:O	1:A:562:TRP:HH2	2.01	0.42
3:C:16:ILE:HG13	3:O:95:LYS:NZ	2.28	0.42
3:C:97:PHE:HE1	3:C:113:VAL:HG23	1.85	0.42
3:C:149:GLN:CD	3:C:149:GLN:H	2.23	0.42
1:E:240:ALA:HB1	1:E:246:VAL:CG1	2.50	0.42
1:E:247:PRO:HB3	1:E:569:TYR:CD1	2.54	0.42
2:F:199:ILE:CD1	2:F:205:VAL:HB	2.50	0.42
3:G:124:VAL:O	3:G:128:VAL:HG13	2.20	0.42
1:I:127:GLU:HG2	1:I:128:GLU:H	1.84	0.42
1:I:198:CYS:HB3	1:I:201:THR:OG1	2.19	0.42
1:I:251:MET:CG	1:I:534:CYS:HB3	2.44	0.42
1:I:525:ILE:HA	1:I:525:ILE:HD13	1.78	0.42
2:J:52:LYS:HG3	2:J:101:ASP:OD2	2.20	0.42
2:J:171:LEU:HD13	2:J:175:SER:HB2	2.01	0.42
1:M:5:HIS:O	1:M:6:THR:HG23	2.19	0.42
1:M:216:THR:HG21	1:M:236:GLY:HA3	2.01	0.42
1:M:287:PHE:O	1:M:290:ASP:HB2	2.19	0.42
1:M:308:MET:HE2	1:M:308:MET:HB2	1.64	0.42
2:N:117:ILE:HD11	2:N:178:ARG:HG2	2.01	0.42
3:O:54:GLY:O	3:O:58:PHE:N	2.53	0.42
3:C:87:MET:HE3	10:C:303:LMT:H112	2.01	0.42
3:C:187:LYS:HB2	3:C:187:LYS:HE2	1.69	0.42
1:E:26:MET:SD	1:E:171:TYR:CZ	3.13	0.42
1:E:127:GLU:HG2	1:E:128:GLU:H	1.83	0.42
1:E:484:ARG:NH1	1:E:549:HIS:HA	2.33	0.42
3:G:34:PHE:CE2	9:G:301:HEM:HMC2	2.55	0.42
1:I:224:LYS:CG	1:I:473:HIS:HB3	2.27	0.42
1:I:280:LEU:HB3	1:I:284:GLN:HA	2.01	0.42
1:I:334:GLY:O	1:I:338:ILE:HB	2.19	0.42
2:J:67:MET:O	2:J:73:PRO:HA	2.18	0.42
3:K:79:HIS:HE1	9:K:302:HEM:C1D	2.37	0.42
9:K:302:HEM:HBB2	9:K:302:HEM:CMB	2.49	0.42
1:M:244:GLY:O	1:M:571:LYS:HE3	2.19	0.42
1:M:273:ARG:CZ	1:M:273:ARG:HB3	2.50	0.42
1:M:544:GLU:OE1	1:M:545:SER:N	2.52	0.42
3:O:80:PHE:CD1	9:O:303:HEM:HBB2	2.55	0.42
3:O:167:VAL:HG12	9:O:303:HEM:CAC	2.49	0.42
1:A:55:LEU:HD12	1:A:57:ASN:HB2	2.02	0.42
1:A:356:ASN:OD1	1:A:358:ILE:HG12	2.19	0.42
1:A:389:LEU:C	1:A:390:PHE:HD1	2.23	0.42
3:C:104:LEU:HG	3:C:106:HIS:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:36:LEU:N	4:E:701:FAD:O2B	2.47	0.42
1:E:189:GLY:O	1:E:387:LYS:HB3	2.20	0.42
1:E:262:VAL:HG21	1:E:325:HIS:CB	2.50	0.42
1:E:480:VAL:CG2	1:E:484:ARG:HH21	2.33	0.42
3:G:1:MET:HA	2:J:23:MET:CE	2.45	0.42
1:I:7:ASP:OD2	1:I:29:LEU:HB3	2.20	0.42
1:I:454:ASP:O	1:I:459:ARG:NH1	2.52	0.42
1:I:608:PRO:N	1:I:609:PRO:CD	2.83	0.42
2:J:20:GLN:N	2:J:20:GLN:OE1	2.53	0.42
1:M:121:GLY:N	1:M:297:GLN:HG2	2.35	0.42
1:M:537:TYR:CE2	1:M:579:LEU:HG	2.54	0.42
1:A:187:ASP:OD1	1:A:188:GLY:N	2.52	0.42
1:A:191:CYS:HB2	1:A:386:LEU:HD22	2.00	0.42
3:C:182:GLY:HA3	3:C:186:ARG:HB2	2.02	0.42
1:E:420:TYR:O	1:E:424:ARG:HG2	2.20	0.42
2:F:7:LEU:O	2:F:25:THR:HA	2.19	0.42
2:F:137:MET:HG3	2:F:138:ASP:H	1.84	0.42
3:G:61:ALA:HA	3:G:64:MET:HG3	2.01	0.42
1:I:156:THR:O	1:I:160:VAL:HG22	2.20	0.42
2:J:11:ARG:HH21	2:J:51:LEU:HA	1.85	0.42
3:K:62:THR:CG2	3:K:139:ILE:HB	2.50	0.42
1:M:236:GLY:O	1:M:239:ILE:HG12	2.19	0.42
1:M:262:VAL:HG23	1:M:365:ARG:CZ	2.49	0.42
1:A:220:GLY:HA3	1:A:228:ASN:OD1	2.19	0.42
2:B:213:ALA:O	2:B:217:VAL:HG22	2.20	0.42
3:C:147:ARG:CG	3:C:148:LEU:N	2.81	0.42
1:E:369:HIS:CD2	1:E:405:ARG:NH2	2.88	0.42
1:E:391:SER:OG	1:E:396:ALA:HB2	2.20	0.42
1:E:444:ALA:O	1:E:445:HIS:C	2.56	0.42
1:E:555:PRO:O	1:E:601:VAL:HG21	2.20	0.42
1:E:570:TRP:HZ3	1:E:577:PRO:HB3	1.85	0.42
2:F:199:ILE:O	2:F:205:VAL:HG12	2.19	0.42
3:G:111:MET:HE3	3:G:169:VAL:HG21	2.00	0.42
2:J:6:THR:O	2:J:88:ILE:HD12	2.20	0.42
1:M:235:GLY:HA2	1:M:524:ARG:HH21	1.84	0.42
1:M:316:LEU:HD23	1:M:319:LYS:H	1.85	0.42
3:O:172:TYR:HA	3:O:189:PHE:CE2	2.54	0.42
1:A:95:ILE:H	1:A:95:ILE:HG13	1.61	0.42
1:A:164:LEU:HD12	1:A:164:LEU:HA	1.69	0.42
1:A:261:THR:O	1:A:265:ASP:HA	2.20	0.42
1:A:282:VAL:HB	1:A:316:LEU:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:445:HIS:O	1:A:446:LYS:C	2.58	0.42
3:C:20:MET:HE2	3:C:82:LEU:HD22	2.02	0.42
3:C:172:TYR:CD1	3:C:189:PHE:HE1	2.38	0.42
1:E:70:PHE:O	1:E:74:VAL:HG23	2.19	0.42
2:F:148:LEU:HD21	2:F:223:PRO:HG2	2.02	0.42
1:I:64:ASP:OD1	1:I:146:ALA:HB3	2.19	0.42
1:I:259:THR:HG21	1:I:273:ARG:HE	1.82	0.42
1:I:343:ARG:O	1:I:345:VAL:N	2.50	0.42
2:J:1:MET:HG2	2:J:30:GLU:OE2	2.19	0.42
2:J:201:ASN:OD1	2:J:201:ASN:N	2.52	0.42
3:K:12:GLN:HG2	3:K:13:ARG:CG	2.43	0.42
3:K:34:PHE:HZ	9:K:301:HEM:CHC	2.33	0.42
1:M:262:VAL:HG13	1:M:263:PRO:CD	2.48	0.42
2:N:191:SER:HB3	2:N:194:ASP:CG	2.40	0.42
3:O:156:TYR:O	3:O:160:LEU:N	2.38	0.42
1:A:20:VAL:HG11	1:A:213:LEU:CD1	2.51	0.41
1:A:222:ILE:HG21	1:A:222:ILE:HD13	1.81	0.41
1:A:270:GLU:N	5:A:702:FUM:C	2.72	0.41
1:A:339:THR:OG1	1:A:343:ARG:HA	2.20	0.41
1:A:342:LEU:HA	1:A:342:LEU:HD12	1.74	0.41
2:B:34:MET:O	2:B:81:THR:HG23	2.21	0.41
1:E:405:ARG:NH1	1:E:407:GLY:HA2	2.34	0.41
1:E:476:MET:CE	1:E:480:VAL:HG11	2.50	0.41
2:F:34:MET:HA	2:F:38:ILE:HD12	2.01	0.41
3:G:48:SER:HA	3:G:210:ARG:CZ	2.49	0.41
1:I:264:THR:C	1:I:266:ILE:H	2.24	0.41
4:I:701:FAD:H8A	4:I:701:FAD:H2B	1.68	0.41
3:K:19:ARG:O	3:K:22:PHE:HB3	2.20	0.41
1:M:405:ARG:HH21	1:M:408:GLY:H	1.67	0.41
2:N:200:GLY:O	2:N:206:PHE:CE2	2.73	0.41
3:O:151:GLY:N	3:O:152:TRP:CA	2.73	0.41
2:B:227:GLN:O	2:B:230:ILE:HG13	2.20	0.41
3:C:60:GLU:CD	3:C:64:MET:HB2	2.40	0.41
1:E:114:LYS:O	1:E:114:LYS:HG3	2.18	0.41
3:G:139:ILE:HD12	3:G:143:LYS:HZ1	1.85	0.41
1:I:503:SER:HA	1:I:506:ILE:HD11	2.02	0.41
1:I:523:LEU:HD12	1:I:524:ARG:N	2.35	0.41
1:I:560:LYS:HE3	1:I:603:ILE:HG22	2.02	0.41
2:J:11:ARG:HB3	2:J:22:ARG:HG3	2.02	0.41
3:K:35:LEU:HD23	3:K:39:MET:HG2	2.02	0.41
1:M:181:ALA:H	4:M:701:FAD:C2A	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:238:ILE:HD13	1:M:527:GLY:HA3	2.02	0.41
1:M:512:CYS:HA	1:M:516:ASN:ND2	2.33	0.41
1:A:226:THR:HA	1:A:368:HIS:HB3	2.02	0.41
1:A:361:LEU:HD12	1:A:361:LEU:N	2.35	0.41
3:C:40:MET:HB3	11:C:304:MQ7:C17	2.42	0.41
3:C:97:PHE:CE1	3:C:112:TRP:CE3	3.01	0.41
1:E:68:VAL:HB	1:E:148:ARG:NH2	2.35	0.41
1:E:338:ILE:C	1:E:343:ARG:HB2	2.40	0.41
1:E:355:VAL:HG11	1:E:362:ILE:HD13	2.01	0.41
1:E:461:GLY:CA	1:E:505:LYS:HB3	2.50	0.41
3:G:145:ALA:HB2	3:G:211:PHE:HD1	1.85	0.41
1:I:376:ARG:HG3	1:I:384:TYR:CE2	2.55	0.41
2:J:107:GLY:O	2:J:111:ARG:HG3	2.19	0.41
3:K:94:TRP:HH2	3:K:117:ILE:HD11	1.85	0.41
1:M:247:PRO:HG3	1:M:569:TYR:CZ	2.55	0.41
1:M:400:MET:HE2	1:M:401:HIS:CE1	2.56	0.41
1:M:500:TYR:HB2	1:M:529:LEU:CD1	2.50	0.41
9:O:302:HEM:HBD1	9:O:302:HEM:HMD2	2.01	0.41
1:A:5:HIS:HE1	1:M:5:HIS:CE1	2.33	0.41
1:A:97:MET:HE3	1:A:136:ILE:HD13	2.02	0.41
1:A:270:GLU:N	5:A:702:FUM:O	2.32	0.41
2:B:177:MET:SD	2:B:222:ILE:HG21	2.61	0.41
1:E:281:ASP:HB3	1:E:311:HIS:HE2	1.86	0.41
1:E:515:MET:HA	1:E:515:MET:CE	2.50	0.41
1:E:579:LEU:HD23	1:E:579:LEU:HA	1.94	0.41
3:G:129:HIS:HA	3:G:132:VAL:HG12	2.01	0.41
1:I:87:ARG:HD2	1:I:87:ARG:HA	1.82	0.41
1:I:139:ARG:HG3	1:I:139:ARG:HH11	1.85	0.41
1:I:342:LEU:C	1:I:344:GLU:H	2.14	0.41
3:K:53:ASN:OD1	3:K:139:ILE:HG23	2.20	0.41
1:M:48:GLN:HB3	1:M:154:ASP:OD1	2.20	0.41
1:A:258:PRO:HA	1:A:366:PRO:HA	2.02	0.41
2:B:177:MET:O	2:B:180:ALA:HB3	2.20	0.41
3:C:176:VAL:O	3:C:177:LYS:HB2	2.21	0.41
3:C:187:LYS:O	3:C:190:GLN:N	2.53	0.41
3:G:171:PHE:HA	3:G:174:ILE:HG22	2.03	0.41
1:I:362:ILE:O	1:I:364:VAL:HG13	2.21	0.41
2:J:96:PHE:CZ	2:J:158:VAL:HG21	2.56	0.41
1:M:6:THR:HA	1:M:30:LYS:CG	2.50	0.41
1:M:216:THR:HG21	1:M:236:GLY:CA	2.50	0.41
1:M:308:MET:HG2	1:M:326:LEU:CD1	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:333:LEU:HD22	1:M:337:HIS:HB2	2.02	0.41
1:M:440:TYR:C	1:M:445:HIS:ND1	2.73	0.41
2:N:129:ASP:OD2	2:N:130:PRO:HD2	2.21	0.41
1:A:94:PRO:HB3	1:A:98:ARG:NH1	2.36	0.41
1:A:546:ARG:NH2	1:A:559:ASP:OD1	2.53	0.41
1:A:614:ILE:O	1:A:616:GLU:N	2.54	0.41
3:C:143:LYS:O	3:C:146:ALA:N	2.52	0.41
1:E:541:ASP:O	1:E:562:TRP:HH2	2.03	0.41
1:E:566:THR:HG22	1:E:579:LEU:HD22	2.03	0.41
3:G:32:ILE:HD12	3:G:167:VAL:HB	2.01	0.41
3:G:87:MET:HE3	3:G:116:VAL:HG13	2.02	0.41
3:G:100:HIS:NE2	3:G:104:LEU:HD22	2.36	0.41
1:I:55:LEU:HD11	1:I:138:ALA:HB2	2.03	0.41
1:I:213:LEU:HB2	1:I:425:MET:CE	2.49	0.41
2:J:110:PHE:CD1	2:J:153:GLU:HG3	2.55	0.41
2:N:129:ASP:CG	2:N:130:PRO:HD2	2.40	0.41
1:A:264:THR:O	1:A:265:ASP:HB2	2.19	0.41
1:A:446:LYS:O	1:A:450:GLU:HB3	2.21	0.41
1:A:541:ASP:O	1:A:562:TRP:CH2	2.73	0.41
2:B:40:LEU:HD11	2:B:90:LEU:CD1	2.50	0.41
1:E:100:VAL:HG22	1:E:103:TRP:HE3	1.86	0.41
1:E:261:THR:CG2	1:E:263:PRO:HD2	2.51	0.41
1:E:270:GLU:H	5:E:702:FUM:C	2.30	0.41
1:E:403:PHE:HZ	1:E:542:ARG:NH1	2.19	0.41
2:F:68:VAL:HG23	2:F:91:HIS:O	2.21	0.41
3:G:60:GLU:HA	3:G:61:ALA:HA	1.81	0.41
3:G:88:PRO:HD2	3:G:116:VAL:HG21	2.02	0.41
3:G:131:PHE:HE2	3:K:153:LEU:HD12	1.85	0.41
1:I:159:SER:O	1:I:163:THR:HG23	2.21	0.41
1:I:292:GLU:HA	1:I:293:PRO:HD3	1.94	0.41
1:I:480:VAL:HG23	1:I:484:ARG:NE	2.35	0.41
2:J:157:CYS:O	2:J:161:CYS:HB2	2.21	0.41
3:K:154:TYR:O	3:K:154:TYR:CG	2.73	0.41
1:M:93:ALA:HA	1:M:416:VAL:CG2	2.50	0.41
1:M:306:ARG:HD2	1:M:482:ILE:CG2	2.50	0.41
1:M:485:ASN:HB3	1:M:552:GLU:OE2	2.21	0.41
1:M:530:LYS:HZ2	1:M:570:TRP:HE1	1.64	0.41
3:O:46:ILE:HD11	3:O:210:ARG:CZ	2.50	0.41
1:E:195:ILE:HA	1:E:206:ALA:HA	2.03	0.41
1:E:306:ARG:NE	1:E:550:THR:HG21	2.36	0.41
1:E:533:GLN:HA	1:E:536:ALA:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:2:ASN:O	2:F:2:ASN:ND2	2.33	0.41
3:G:39:MET:SD	3:G:43:SER:HB2	2.60	0.41
3:G:207:THR:O	3:G:211:PHE:CD2	2.73	0.41
1:I:86:ALA:O	1:I:90:ALA:HB2	2.21	0.41
1:I:335:GLU:O	1:I:337:HIS:N	2.54	0.41
3:K:41:LEU:HD22	3:K:63:TYR:CE1	2.55	0.41
1:A:191:CYS:HB2	1:A:386:LEU:CD2	2.51	0.41
1:A:257:HIS:CE1	1:A:301:ARG:NH1	2.89	0.41
1:A:500:TYR:HA	1:A:503:SER:OG	2.21	0.41
2:B:53:VAL:HG12	2:B:102:LEU:HD12	2.02	0.41
2:B:84:LEU:HD23	2:B:88:ILE:HD12	2.03	0.41
2:B:117:ILE:HD11	2:B:178:ARG:NH1	2.36	0.41
2:B:145:ILE:HG12	2:B:184:LEU:HD12	2.03	0.41
2:B:223:PRO:O	2:B:227:GLN:HB2	2.21	0.41
3:C:60:GLU:HG3	3:C:64:MET:N	2.36	0.41
3:C:95:LYS:HE2	3:O:9:HIS:HB3	2.02	0.41
3:C:205:LEU:O	3:C:205:LEU:HD23	2.21	0.41
1:E:15:LEU:HA	1:E:15:LEU:HD12	1.69	0.41
1:E:74:VAL:HB	1:E:590:MET:HE1	2.02	0.41
1:E:154:ASP:CG	1:E:344:GLU:HB3	2.42	0.41
4:E:701:FAD:O2'	4:E:701:FAD:H9	2.21	0.41
2:F:5:LEU:HB2	2:F:28:VAL:O	2.20	0.41
3:G:154:TYR:CG	3:G:155:LEU:N	2.89	0.41
1:I:46:ALA:O	1:I:48:GLN:HG3	2.21	0.41
1:I:261:THR:HB	1:I:266:ILE:O	2.21	0.41
1:I:559:ASP:C	1:I:605:ASN:HB3	2.42	0.41
1:I:560:LYS:HE3	1:I:560:LYS:HB2	1.92	0.41
1:I:585:SER:O	1:I:586:PRO:O	2.39	0.41
1:I:611:LYS:HA	1:I:614:ILE:HD11	2.02	0.41
2:J:141:LEU:HA	2:J:144:GLU:HB2	2.03	0.41
2:J:172:GLY:O	2:J:176:ILE:HG13	2.21	0.41
3:K:55:ILE:HA	3:K:58:PHE:CE2	2.55	0.41
3:K:126:GLY:O	3:K:130:MET:HB2	2.21	0.41
1:M:41:ARG:HB3	2:N:62:CYS:HB2	2.03	0.41
1:M:98:ARG:O	1:M:101:ALA:HB3	2.21	0.41
1:M:228:ASN:HD22	4:M:701:FAD:HM81	1.86	0.41
1:M:513:LYS:HD3	2:N:13:ASN:CG	2.41	0.41
1:M:513:LYS:HB2	1:M:513:LYS:HE3	1.69	0.41
1:M:546:ARG:CZ	1:M:562:TRP:HB2	2.49	0.41
2:N:35:THR:HG22	2:N:80:GLN:HG2	2.02	0.41
3:O:129:HIS:HE1	9:O:302:HEM:C1A	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:ARG:C	1:A:158:ARG:HH12	2.22	0.41
1:A:192:LEU:HA	1:A:192:LEU:HD23	1.83	0.41
1:A:216:THR:HG21	1:A:236:GLY:H	1.85	0.41
1:A:460:LYS:O	1:A:462:LYS:N	2.54	0.41
1:A:538:GLY:HA2	1:A:579:LEU:HD11	2.02	0.41
3:C:41:LEU:N	11:C:304:MQ7:C14	2.74	0.41
3:C:161:PRO:O	3:C:165:LEU:HB2	2.21	0.41
1:E:405:ARG:NH2	5:E:702:FUM:O7	2.54	0.41
1:E:509:SER:N	1:E:518:GLU:OE1	2.54	0.41
1:E:544:GLU:OE1	1:E:557:ARG:O	2.38	0.41
1:I:228:ASN:HD22	4:I:701:FAD:C8M	2.33	0.41
1:I:262:VAL:CG2	1:I:363:PRO:HB2	2.51	0.41
1:I:278:THR:HB	1:I:329:ASP:CB	2.49	0.41
1:I:459:ARG:CB	1:I:460:LYS:HA	2.50	0.41
3:K:33:LEU:O	3:K:36:TRP:HB2	2.21	0.41
1:M:235:GLY:O	1:M:238:ILE:N	2.54	0.41
1:M:467:LYS:O	1:M:471:GLU:HG3	2.21	0.41
4:M:701:FAD:H8A	4:M:701:FAD:H2B	1.62	0.41
2:N:128:PHE:N	2:N:129:ASP:HB3	2.36	0.41
2:N:129:ASP:CG	2:N:130:PRO:CD	2.89	0.41
3:O:72:VAL:O	3:O:76:MET:HB3	2.20	0.41
3:O:155:LEU:C	3:O:157:LEU:N	2.73	0.41
3:O:164:GLU:HG2	3:O:200:PHE:CB	2.48	0.41
10:O:301:LMT:H122	10:O:301:LMT:H92	1.80	0.41
1:A:114:LYS:HA	1:A:127:GLU:HA	2.03	0.40
1:A:201:THR:OG1	1:A:202:GLY:N	2.54	0.40
1:A:241:LEU:HD13	1:A:248:MET:HG2	2.03	0.40
1:E:34:LEU:CD2	1:E:176:HIS:HB2	2.50	0.40
1:E:279:LEU:O	1:E:286:ARG:HA	2.21	0.40
2:F:7:LEU:HD12	2:F:43:ILE:HD11	2.02	0.40
3:G:1:MET:H1	2:J:91:HIS:HE1	1.68	0.40
3:G:165:LEU:O	3:G:169:VAL:HG23	2.21	0.40
1:I:117:TYR:CD1	1:I:126:ALA:HB3	2.43	0.40
1:I:278:THR:CB	1:I:329:ASP:HB3	2.50	0.40
1:I:281:ASP:O	1:I:327:TRP:HD1	2.05	0.40
1:I:452:ILE:O	1:I:456:VAL:HG23	2.21	0.40
3:K:153:LEU:O	3:K:156:TYR:HE2	2.04	0.40
2:N:84:LEU:HA	2:N:84:LEU:HD13	1.77	0.40
2:N:110:PHE:CD2	2:N:153:GLU:HG2	2.56	0.40
2:N:232:ARG:O	2:N:236:ALA:HB2	2.18	0.40
1:A:204:LEU:H	1:A:204:LEU:HG	1.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:68:VAL:HB	2:B:91:HIS:HB2	2.02	0.40
3:C:156:TYR:HB3	9:C:301:HEM:HAD1	2.02	0.40
1:E:461:GLY:HA3	1:E:505:LYS:HB3	2.02	0.40
1:E:545:SER:OG	1:E:551:ARG:N	2.46	0.40
3:G:15:LYS:HA	3:G:15:LYS:HD3	1.92	0.40
3:G:201:ILE:HD13	3:G:201:ILE:HG21	1.88	0.40
1:I:339:THR:O	1:I:343:ARG:HA	2.22	0.40
1:I:411:LEU:O	1:I:415:VAL:HG23	2.21	0.40
3:K:157:LEU:CD2	3:K:158:VAL:HG23	2.52	0.40
3:K:160:LEU:HD12	3:K:160:LEU:HA	1.83	0.40
1:M:413:GLU:O	1:M:413:GLU:HG2	2.21	0.40
1:M:417:ALA:O	1:M:421:ILE:HG12	2.20	0.40
1:M:424:ARG:HA	1:M:424:ARG:HD3	1.77	0.40
1:M:438:MET:HA	1:M:441:VAL:HG12	2.02	0.40
1:M:444:ALA:O	1:M:445:HIS:C	2.60	0.40
1:M:499:LEU:HA	1:M:502:ARG:HB2	2.03	0.40
2:N:48:ASP:CG	2:N:50:THR:HG22	2.40	0.40
2:N:93:LEU:O	2:N:104:VAL:HG11	2.21	0.40
2:N:150:ARG:HE	2:N:150:ARG:HB2	1.78	0.40
3:O:94:TRP:CD1	10:O:301:LMT:H21	2.56	0.40
3:O:139:ILE:HA	3:O:143:LYS:NZ	2.36	0.40
1:A:25:SER:OG	1:A:171:TYR:HB3	2.22	0.40
1:A:251:MET:O	1:A:535:THR:HG23	2.20	0.40
1:A:475:ILE:CD1	1:A:495:LYS:HD3	2.52	0.40
2:B:73:PRO:HG3	2:B:160:ALA:HB2	2.04	0.40
2:B:206:PHE:CE2	3:C:18:GLY:HA2	2.56	0.40
3:C:131:PHE:CD2	3:O:128:VAL:HB	2.57	0.40
3:C:187:LYS:HA	3:C:190:GLN:HB2	2.03	0.40
1:E:324:ASP:OD1	1:E:324:ASP:N	2.52	0.40
1:E:490:GLN:HG2	1:E:540:LEU:HD22	2.03	0.40
1:E:508:LEU:H	1:E:508:LEU:HD23	1.87	0.40
3:G:155:LEU:HA	3:G:155:LEU:HD23	1.81	0.40
1:I:98:ARG:O	1:I:101:ALA:HB3	2.21	0.40
1:I:466:PHE:CZ	2:J:45:ASP:HA	2.57	0.40
2:J:118:GLU:OE1	2:J:122:HIS:NE2	2.55	0.40
3:K:171:PHE:CA	3:K:174:ILE:HG22	2.46	0.40
1:M:40:ARG:HH12	2:N:178:ARG:HH12	1.69	0.40
1:M:246:VAL:HG23	1:M:384:TYR:CB	2.51	0.40
1:M:503:SER:OG	1:M:504:GLN:N	2.54	0.40
3:O:20:MET:HE3	3:O:85:ARG:HD3	2.03	0.40
2:B:162:GLY:O	2:B:166:MET:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:6:ILE:CD1	3:C:7:THR:HG22	2.45	0.40
3:C:59:PHE:CD2	3:C:60:GLU:HG2	2.55	0.40
1:E:251:MET:H	1:E:251:MET:HG3	1.76	0.40
1:E:319:LYS:HA	1:E:319:LYS:HD3	1.90	0.40
2:F:225:GLN:NE2	3:G:186:ARG:HH11	2.14	0.40
3:G:198:ILE:HG13	3:G:198:ILE:H	1.73	0.40
1:I:517:PRO:HG2	2:J:50:THR:HA	2.02	0.40
1:I:542:ARG:HA	1:I:562:TRP:CH2	2.55	0.40
3:K:5:THR:CG2	3:K:6:ILE:N	2.84	0.40
3:K:6:ILE:CG2	3:K:7:THR:H	2.18	0.40
3:K:31:LEU:HB2	3:K:75:LEU:HD21	2.03	0.40
3:K:164:GLU:HA	3:K:167:VAL:HG22	2.04	0.40
1:M:219:TYR:CE2	1:M:371:SER:HB3	2.57	0.40
2:N:147:GLU:O	2:N:150:ARG:HG2	2.22	0.40
3:O:206:LEU:O	3:O:210:ARG:HG2	2.21	0.40
1:A:281:ASP:HB3	1:A:311:HIS:NE2	2.36	0.40
2:B:26:PHE:CD2	2:B:43:ILE:HG23	2.56	0.40
2:B:129:ASP:HB3	2:B:131:THR:HG22	2.03	0.40
3:C:103:MET:O	3:C:103:MET:HG2	2.20	0.40
3:C:149:GLN:O	3:C:151:GLY:O	2.40	0.40
1:E:185:ILE:HD13	1:E:441:VAL:HG23	2.03	0.40
1:E:285:TYR:OH	1:E:290:ASP:OD1	2.26	0.40
1:E:287:PHE:HZ	1:E:308:MET:HG2	1.86	0.40
1:E:349:CYS:HA	1:E:353:LEU:HD22	2.03	0.40
1:I:121:GLY:CA	1:I:286:ARG:HH12	2.26	0.40
3:K:171:PHE:CD2	3:K:193:GLU:OE2	2.72	0.40
1:M:6:THR:HG21	1:M:32:ILE:CG1	2.49	0.40
1:M:234:GLY:O	1:M:237:GLN:HB2	2.21	0.40
2:N:158:VAL:H	2:N:158:VAL:HG22	1.51	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:187:LYS:NZ	1:M:285:TYR:OH[1_454]	1.97	0.23
2:F:27:THR:OG1	1:I:575:SER:OG[2_545]	2.19	0.01

## 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	620/627 (99%)	556 (90%)	59 (10%)	5 (1%)	19	59
1	E	620/627 (99%)	558 (90%)	61 (10%)	1 (0%)	47	79
1	I	620/627 (99%)	552 (89%)	63 (10%)	5 (1%)	19	59
1	M	620/627 (99%)	550 (89%)	65 (10%)	5 (1%)	19	59
2	B	238/264 (90%)	216 (91%)	21 (9%)	1 (0%)	34	71
2	F	238/264 (90%)	209 (88%)	28 (12%)	1 (0%)	34	71
2	J	238/264 (90%)	215 (90%)	21 (9%)	2 (1%)	19	59
2	N	238/264 (90%)	207 (87%)	25 (10%)	6 (2%)	5	36
3	C	210/218 (96%)	180 (86%)	25 (12%)	5 (2%)	6	37
3	G	210/218 (96%)	181 (86%)	27 (13%)	2 (1%)	15	55
3	K	210/218 (96%)	180 (86%)	29 (14%)	1 (0%)	29	68
3	O	210/218 (96%)	181 (86%)	28 (13%)	1 (0%)	29	68
All	All	4272/4436 (96%)	3785 (89%)	452 (11%)	35 (1%)	19	59

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	149	GLN
3	C	150	SER
1	E	587	TYR
1	I	343	ARG
1	I	613	VAL
1	M	341	LYS
2	N	129	ASP
1	A	585	SER
1	A	587	TYR
3	C	10	VAL
3	C	136	ASP
2	F	203	GLN

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Mol	Chain	Res	Type
2	J	203	GLN
3	K	6	ILE
1	M	343	ARG
2	N	131	THR
1	A	187	ASP
2	B	202	ASP
3	G	6	ILE
1	I	585	SER
1	A	344	GLU
1	I	586	PRO
1	M	512	CYS
1	M	544	GLU
2	N	136	ARG
3	O	6	ILE
3	G	184	ASN
2	J	58	ARG
1	M	314	LYS
1	I	344	GLU
2	N	202	ASP
1	A	338	ILE
3	C	6	ILE
2	N	85	PRO
2	N	130	PRO

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	495/500 (99%)	475 (96%)	20 (4%)	31 65
1	E	494/500 (99%)	473 (96%)	21 (4%)	29 63
1	I	494/500 (99%)	468 (95%)	26 (5%)	22 58
1	M	495/500 (99%)	467 (94%)	28 (6%)	20 55
2	B	208/228 (91%)	198 (95%)	10 (5%)	25 60
2	F	208/228 (91%)	197 (95%)	11 (5%)	22 58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	J	208/228 (91%)	201 (97%)	7 (3%)	37	69
2	N	208/228 (91%)	197 (95%)	11 (5%)	22	58
3	C	180/185 (97%)	170 (94%)	10 (6%)	21	56
3	G	180/185 (97%)	165 (92%)	15 (8%)	11	42
3	K	180/185 (97%)	166 (92%)	14 (8%)	12	44
3	O	180/185 (97%)	172 (96%)	8 (4%)	28	63
All	All	3530/3652 (97%)	3349 (95%)	181 (5%)	24	58

All (181) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ASP
1	A	55	LEU
1	A	78	ASP
1	A	87	ARG
1	A	89	PHE
1	A	131	GLU
1	A	168	CYS
1	A	187	ASP
1	A	251	MET
1	A	295	LYS
1	A	297	GLN
1	A	384	TYR
1	A	419	ARG
1	A	459	ARG
1	A	508	LEU
1	A	513	LYS
1	A	523	LEU
1	A	544	GLU
1	A	585	SER
1	A	587	TYR
2	B	1	MET
2	B	2	ASN
2	B	11	ARG
2	B	31	TYR
2	B	58	ARG
2	B	128	PHE
2	B	136	ARG
2	B	169	ASP
2	B	181	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	B	214	CYS
3	C	9	HIS
3	C	15	LYS
3	C	27	SER
3	C	57	TRP
3	C	73	PHE
3	C	143	LYS
3	C	149	GLN
3	C	154	TYR
3	C	155	LEU
3	C	211	PHE
1	E	78	ASP
1	E	87	ARG
1	E	89	PHE
1	E	117	TYR
1	E	124	PHE
1	E	131	GLU
1	E	139	ARG
1	E	252	GLU
1	E	295	LYS
1	E	297	GLN
1	E	335	GLU
1	E	336	LYS
1	E	384	TYR
1	E	399	ASP
1	E	419	ARG
1	E	443	ASP
1	E	523	LEU
1	E	541	ASP
1	E	597	TYR
1	E	610	GLU
1	E	612	PHE
2	F	1	MET
2	F	2	ASN
2	F	4	MET
2	F	11	ARG
2	F	23	MET
2	F	58	ARG
2	F	87	GLU
2	F	178	ARG
2	F	181	ARG
2	F	237	MET

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	F	238	HIS
3	G	20	MET
3	G	22	PHE
3	G	27	SER
3	G	36	TRP
3	G	59	PHE
3	G	90	LYS
3	G	143	LYS
3	G	147	ARG
3	G	152	TRP
3	G	155	LEU
3	G	157	LEU
3	G	173	ARG
3	G	193	GLU
3	G	210	ARG
3	G	211	PHE
1	I	5	HIS
1	I	7	ASP
1	I	78	ASP
1	I	89	PHE
1	I	117	TYR
1	I	131	GLU
1	I	139	ARG
1	I	224	LYS
1	I	255	GLN
1	I	316	LEU
1	I	337	HIS
1	I	346	TYR
1	I	349	CYS
1	I	384	TYR
1	I	399	ASP
1	I	419	ARG
1	I	459	ARG
1	I	490	GLN
1	I	508	LEU
1	I	523	LEU
1	I	541	ASP
1	I	585	SER
1	I	595	ARG
1	I	597	TYR
1	I	607	LEU
1	I	611	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	J	1	MET
2	J	2	ASN
2	J	4	MET
2	J	11	ARG
2	J	42	GLN
2	J	58	ARG
2	J	181	ARG
3	K	36	TRP
3	K	57	TRP
3	K	58	PHE
3	K	73	PHE
3	K	76	MET
3	K	90	LYS
3	K	137	LEU
3	K	150	SER
3	K	154	TYR
3	K	173	ARG
3	K	183	ARG
3	K	185	LYS
3	K	186	ARG
3	K	191	LYS
1	M	5	HIS
1	M	70	PHE
1	M	72	ASP
1	M	89	PHE
1	M	187	ASP
1	M	224	LYS
1	M	281	ASP
1	M	284	GLN
1	M	288	MET
1	M	295	LYS
1	M	297	GLN
1	M	312	MET
1	M	336	LYS
1	M	384	TYR
1	M	399	ASP
1	M	400	MET
1	M	405	ARG
1	M	419	ARG
1	M	446	LYS
1	M	459	ARG
1	M	508	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	M	513	LYS
1	M	515	MET
1	M	523	LEU
1	M	554	PHE
1	M	560	LYS
1	M	587	TYR
1	M	611	LYS
2	N	2	ASN
2	N	11	ARG
2	N	42	GLN
2	N	58	ARG
2	N	126	LYS
2	N	129	ASP
2	N	133	ASP
2	N	178	ARG
2	N	181	ARG
2	N	192	GLU
2	N	193	ASP
3	O	5	THR
3	O	23	PHE
3	O	73	PHE
3	O	76	MET
3	O	147	ARG
3	O	150	SER
3	O	152	TRP
3	O	211	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	43	HIS
1	A	186	HIS
1	A	332	HIS
1	A	401	HIS
1	A	445	HIS
1	A	449	GLN
2	B	225	GLN
1	E	43	HIS
1	E	57	ASN
1	E	228	ASN
1	E	255	GLN
1	E	409	ASN

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Mol	Chain	Res	Type
2	F	225	GLN
3	G	38	HIS
1	I	228	ASN
1	I	409	ASN
1	I	445	HIS
1	I	516	ASN
2	J	13	ASN
2	J	80	GLN
2	J	91	HIS
3	K	190	GLN
1	M	5	HIS
1	M	311	HIS
1	M	332	HIS
1	M	401	HIS
2	N	225	GLN
3	O	53	ASN
3	O	129	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

31 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
9	HEM	C	301	3	41,50,50	1.76	8 (19%)	45,82,82	1.45	5 (11%)
4	FAD	M	701	-	53,58,58	3.66	15 (28%)	68,89,89	2.35	19 (27%)
7	SF4	J	302	2	0,12,12	-	-	-	-	-
9	HEM	C	302	3	41,50,50	1.76	7 (17%)	45,82,82	1.51	8 (17%)
9	HEM	O	303	3	41,50,50	1.74	7 (17%)	45,82,82	1.92	12 (26%)
8	FES	B	303	2	0,4,4	-	-	-	-	-
5	FUM	E	702	-	7,7,7	1.62	1 (14%)	8,8,8	0.92	0
7	SF4	B	302	2	0,12,12	-	-	-	-	-
8	FES	N	303	2	0,4,4	-	-	-	-	-
9	HEM	K	301	3	41,50,50	1.77	8 (19%)	45,82,82	2.63	12 (26%)
7	SF4	N	302	2	0,12,12	-	-	-	-	-
10	LMT	C	303	-	36,36,36	0.46	0	47,47,47	0.83	1 (2%)
9	HEM	G	302	3	41,50,50	1.72	7 (17%)	45,82,82	1.57	8 (17%)
9	HEM	K	302	3	41,50,50	1.68	6 (14%)	45,82,82	1.23	4 (8%)
10	LMT	O	301	-	36,36,36	0.40	0	47,47,47	0.69	1 (2%)
11	MQ7	C	304	-	25,25,49	2.99	11 (44%)	31,34,63	1.60	4 (12%)
5	FUM	I	702	-	7,7,7	1.20	0	8,8,8	1.65	2 (25%)
5	FUM	A	702	-	7,7,7	1.53	1 (14%)	8,8,8	1.23	2 (25%)
5	FUM	M	702	-	7,7,7	1.37	0	8,8,8	1.19	1 (12%)
4	FAD	E	701	1	53,58,58	3.62	15 (28%)	68,89,89	2.27	15 (22%)
8	FES	J	303	2	0,4,4	-	-	-	-	-
4	FAD	I	701	-	53,58,58	3.77	18 (33%)	68,89,89	2.19	21 (30%)
8	FES	F	303	2	0,4,4	-	-	-	-	-
9	HEM	O	302	3	41,50,50	1.54	5 (12%)	45,82,82	1.46	7 (15%)
6	F3S	F	301	2	0,9,9	-	-	-	-	-
9	HEM	G	301	3	41,50,50	1.68	7 (17%)	45,82,82	1.67	9 (20%)
6	F3S	J	301	2	0,9,9	-	-	-	-	-
6	F3S	B	301	2	0,9,9	-	-	-	-	-
4	FAD	A	701	1	53,58,58	3.60	18 (33%)	68,89,89	2.38	21 (30%)
6	F3S	N	301	2	0,9,9	-	-	-	-	-
7	SF4	F	302	2	0,12,12	-	-	-	-	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	HEM	C	301	3	-	6/12/54/54	-
4	FAD	M	701	-	-	12/30/50/50	0/6/6/6
9	HEM	C	302	3	-	1/12/54/54	-
7	SF4	J	302	2	-	-	0/6/5/5
9	HEM	O	303	3	-	1/12/54/54	-
8	FES	B	303	2	-	-	0/1/1/1
5	FUM	E	702	-	-	4/5/5/5	-
7	SF4	B	302	2	-	-	0/6/5/5
8	FES	N	303	2	-	-	0/1/1/1
9	HEM	K	301	3	-	5/12/54/54	-
7	SF4	N	302	2	-	-	0/6/5/5
10	LMT	C	303	-	-	13/21/61/61	0/2/2/2
9	HEM	G	302	3	-	1/12/54/54	-
9	HEM	K	302	3	-	1/12/54/54	-
10	LMT	O	301	-	-	10/21/61/61	0/2/2/2
11	MQ7	C	304	-	-	5/13/33/61	0/2/2/2
5	FUM	I	702	-	-	2/5/5/5	-
5	FUM	A	702	-	-	4/5/5/5	-
7	SF4	F	302	2	-	-	0/6/5/5
5	FUM	M	702	-	-	4/5/5/5	-
4	FAD	E	701	1	-	13/30/50/50	0/6/6/6
8	FES	J	303	2	-	-	0/1/1/1
4	FAD	I	701	-	-	16/30/50/50	0/6/6/6
8	FES	F	303	2	-	-	0/1/1/1
6	F3S	F	301	2	-	-	0/3/3/3
9	HEM	G	301	3	-	1/12/54/54	-
6	F3S	J	301	2	-	-	0/3/3/3
6	F3S	B	301	2	-	-	0/3/3/3
4	FAD	A	701	1	-	15/30/50/50	0/6/6/6
6	F3S	N	301	2	-	-	0/3/3/3
9	HEM	O	302	3	-	10/12/54/54	-

All (134) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	701	FAD	C2B-C1B	-16.32	1.29	1.53
4	E	701	FAD	O4B-C1B	15.44	1.62	1.41
4	I	701	FAD	C2B-C1B	-15.36	1.30	1.53
4	A	701	FAD	C2B-C1B	-15.34	1.30	1.53
4	I	701	FAD	O4B-C1B	15.20	1.62	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	701	FAD	C2B-C1B	-14.88	1.31	1.53
4	A	701	FAD	O4B-C1B	14.39	1.61	1.41
4	M	701	FAD	O4B-C1B	14.32	1.61	1.41
11	C	304	MQ7	C3-C2	8.56	1.50	1.35
4	I	701	FAD	C4X-N5	6.98	1.44	1.30
4	E	701	FAD	C4X-N5	6.69	1.43	1.30
4	A	701	FAD	O4B-C4B	-6.48	1.30	1.45
4	I	701	FAD	O4B-C4B	-6.12	1.31	1.45
4	A	701	FAD	C4X-N5	5.98	1.42	1.30
4	M	701	FAD	C4X-N5	5.82	1.42	1.30
4	E	701	FAD	O4B-C4B	-5.77	1.32	1.45
9	K	301	HEM	FE-NB	5.69	2.25	1.96
9	C	301	HEM	C3C-C2C	-5.55	1.32	1.40
4	M	701	FAD	O4B-C4B	-5.49	1.32	1.45
9	C	302	HEM	C3C-C2C	-5.44	1.32	1.40
11	C	304	MQ7	C5-C4	5.38	1.58	1.48
9	K	302	HEM	C3C-C2C	-5.37	1.32	1.40
11	C	304	MQ7	C10-C1	5.19	1.58	1.48
4	I	701	FAD	C10-N1	4.87	1.43	1.33
9	G	302	HEM	FE-ND	4.87	2.21	1.96
4	M	701	FAD	C10-N1	4.75	1.43	1.33
9	O	303	HEM	C3C-CAC	4.48	1.57	1.47
4	M	701	FAD	C9A-N10	4.39	1.48	1.41
11	C	304	MQ7	C11-C12	4.36	1.57	1.50
4	M	701	FAD	C2-N1	4.35	1.47	1.36
4	A	701	FAD	C10-N1	4.28	1.42	1.33
11	C	304	MQ7	C11-C3	4.23	1.58	1.51
9	G	301	HEM	C3C-C2C	-4.22	1.34	1.40
4	I	701	FAD	C2-N1	4.17	1.46	1.36
9	O	303	HEM	FE-ND	4.17	2.17	1.96
9	K	301	HEM	C3C-C2C	-4.14	1.34	1.40
4	A	701	FAD	O4-C4	-4.12	1.15	1.23
9	G	301	HEM	FE-ND	4.07	2.17	1.96
4	I	701	FAD	C9A-N10	4.07	1.48	1.41
9	G	302	HEM	C3C-C2C	-4.06	1.34	1.40
9	O	302	HEM	C3C-CAC	4.04	1.56	1.47
9	K	302	HEM	C3C-CAC	4.02	1.56	1.47
4	A	701	FAD	C2A-N3A	3.98	1.38	1.32
9	O	302	HEM	C3C-C2C	-3.88	1.35	1.40
9	C	301	HEM	FE-ND	3.87	2.16	1.96
9	O	303	HEM	C3C-C2C	-3.78	1.35	1.40
4	E	701	FAD	C10-N1	3.75	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	701	FAD	O4-C4	-3.75	1.16	1.23
9	G	301	HEM	C3C-CAC	3.74	1.55	1.47
9	C	302	HEM	C3C-CAC	3.71	1.55	1.47
4	E	701	FAD	C2A-N3A	3.69	1.38	1.32
9	K	302	HEM	FE-ND	3.65	2.14	1.96
9	K	301	HEM	C3C-CAC	3.65	1.55	1.47
4	E	701	FAD	C5X-N5	3.64	1.46	1.39
4	E	701	FAD	C2-N1	3.64	1.45	1.36
4	I	701	FAD	C2A-N3A	3.59	1.37	1.32
4	A	701	FAD	C6A-N6A	3.59	1.47	1.34
9	G	302	HEM	C3C-CAC	3.58	1.55	1.47
4	A	701	FAD	C2-N1	3.52	1.45	1.36
4	E	701	FAD	O4-C4	-3.48	1.17	1.23
4	M	701	FAD	C6A-N6A	3.45	1.46	1.34
4	I	701	FAD	C6A-N6A	3.45	1.46	1.34
4	I	701	FAD	O2B-C2B	3.41	1.51	1.43
4	E	701	FAD	C9A-N10	3.39	1.47	1.41
4	E	701	FAD	C2-N3	3.38	1.46	1.39
9	O	302	HEM	FE-ND	3.33	2.13	1.96
4	A	701	FAD	O2-C2	-3.31	1.18	1.24
4	M	701	FAD	C2A-N3A	3.31	1.37	1.32
4	M	701	FAD	O4-C4	-3.31	1.17	1.23
9	G	301	HEM	FE-NB	3.29	2.13	1.96
4	E	701	FAD	C6A-N6A	3.27	1.46	1.34
4	E	701	FAD	O2B-C2B	3.26	1.50	1.43
4	I	701	FAD	C5X-N5	3.25	1.45	1.39
4	M	701	FAD	C2-N3	3.16	1.46	1.39
9	C	301	HEM	C3C-CAC	3.07	1.54	1.47
11	C	304	MQ7	C15-C13	3.03	1.57	1.51
9	C	302	HEM	CAA-C2A	2.98	1.56	1.52
9	O	302	HEM	CAB-C3B	2.98	1.55	1.47
9	C	302	HEM	CAB-C3B	2.98	1.55	1.47
4	M	701	FAD	C10-N10	2.98	1.43	1.37
9	G	301	HEM	CAB-C3B	2.97	1.55	1.47
9	C	301	HEM	CAB-C3B	2.91	1.55	1.47
4	A	701	FAD	O3B-C3B	-2.90	1.36	1.43
4	A	701	FAD	O2B-C2B	2.89	1.49	1.43
9	K	301	HEM	CAB-C3B	2.88	1.55	1.47
4	I	701	FAD	C5A-C4A	-2.84	1.33	1.40
4	M	701	FAD	O2B-C2B	2.83	1.49	1.43
9	C	301	HEM	CAA-C2A	2.83	1.56	1.52
11	C	304	MQ7	C16-C17	2.81	1.59	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	O	303	HEM	CAB-C3B	2.81	1.55	1.47
4	M	701	FAD	C5X-N5	2.78	1.44	1.39
4	I	701	FAD	C2-N3	2.76	1.45	1.39
4	A	701	FAD	C5X-N5	2.74	1.44	1.39
11	C	304	MQ7	C20-C18	2.71	1.59	1.51
4	A	701	FAD	C9A-N10	2.70	1.45	1.41
9	O	303	HEM	CAA-C2A	2.64	1.55	1.52
4	E	701	FAD	C5A-C4A	-2.62	1.34	1.40
9	G	302	HEM	CAB-C3B	2.61	1.54	1.47
5	E	702	FUM	C4-C	2.61	1.54	1.48
4	A	701	FAD	C9A-C5X	-2.49	1.37	1.41
4	M	701	FAD	O3B-C3B	-2.48	1.37	1.43
9	K	302	HEM	CAB-C3B	2.41	1.54	1.47
9	G	302	HEM	CMB-C2B	2.37	1.55	1.50
11	C	304	MQ7	O1-C1	-2.37	1.18	1.23
4	A	701	FAD	C2-N3	2.36	1.44	1.39
4	A	701	FAD	C2A-N1A	2.36	1.38	1.33
4	I	701	FAD	C4'-C3'	-2.32	1.49	1.53
9	G	301	HEM	CMB-C2B	2.30	1.55	1.50
9	C	302	HEM	CAD-C3D	2.29	1.57	1.51
9	O	303	HEM	CMB-C2B	2.26	1.55	1.50
9	K	302	HEM	CAA-C2A	2.25	1.55	1.52
9	G	302	HEM	CAA-C2A	2.25	1.55	1.52
9	K	301	HEM	C3D-C2D	-2.25	1.31	1.36
4	E	701	FAD	O3B-C3B	-2.25	1.37	1.43
11	C	304	MQ7	C17-C18	2.23	1.38	1.33
4	I	701	FAD	C9-C9A	2.23	1.43	1.39
9	C	301	HEM	C1B-NB	-2.22	1.36	1.40
9	K	301	HEM	C4A-NA	2.22	1.40	1.36
9	K	301	HEM	CMB-C2B	2.21	1.55	1.50
4	I	701	FAD	O3B-C3B	-2.20	1.37	1.43
4	A	701	FAD	C10-N10	2.19	1.42	1.37
9	G	301	HEM	CAA-C2A	2.18	1.55	1.52
5	A	702	FUM	C4-C	2.18	1.53	1.48
9	C	301	HEM	CMD-C2D	2.17	1.55	1.50
9	O	303	HEM	C1A-NA	2.15	1.40	1.36
11	C	304	MQ7	O4-C4	-2.12	1.18	1.23
9	K	302	HEM	CMB-C2B	2.11	1.55	1.50
9	C	301	HEM	CMB-C2B	2.10	1.55	1.50
4	I	701	FAD	C6-C5X	2.09	1.43	1.40
9	C	302	HEM	CMB-C2B	2.09	1.55	1.50
9	O	302	HEM	CMB-C2B	2.07	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	K	301	HEM	C1A-NA	2.06	1.40	1.36
9	C	302	HEM	C3B-C2B	-2.06	1.33	1.37
9	G	302	HEM	C1A-NA	2.02	1.40	1.36

All (152) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	701	FAD	C7M-C7-C6	-8.74	103.33	119.49
4	M	701	FAD	C7M-C7-C6	-8.13	104.46	119.49
4	A	701	FAD	C7M-C7-C6	-8.11	104.50	119.49
4	E	701	FAD	C7M-C7-C8	7.69	136.50	120.74
4	A	701	FAD	C7M-C7-C8	7.33	135.76	120.74
9	K	301	HEM	CAD-C3D-C2D	-7.04	114.77	127.88
4	M	701	FAD	C7M-C7-C8	6.94	134.96	120.74
9	K	301	HEM	CAD-C3D-C4D	6.84	136.62	124.66
4	I	701	FAD	C7M-C7-C6	-6.46	107.55	119.49
4	A	701	FAD	N3A-C2A-N1A	-6.39	118.70	128.68
4	E	701	FAD	N3A-C2A-N1A	-6.35	118.75	128.68
9	K	301	HEM	C4C-CHD-C1D	6.17	130.71	122.56
4	I	701	FAD	C7M-C7-C8	6.15	133.33	120.74
11	C	304	MQ7	C11-C12-C13	-6.14	116.56	126.79
4	I	701	FAD	N3A-C2A-N1A	-6.10	119.15	128.68
9	K	301	HEM	CBA-CAA-C2A	-5.75	102.81	112.62
4	M	701	FAD	N3A-C2A-N1A	-5.68	119.80	128.68
4	M	701	FAD	O4B-C1B-C2B	-5.64	98.68	106.93
9	O	303	HEM	CBA-CAA-C2A	5.63	122.22	112.62
9	K	301	HEM	CHD-C1D-ND	5.40	130.30	124.43
4	A	701	FAD	C5A-C6A-N6A	5.39	128.54	120.35
4	A	701	FAD	C4-N3-C2	-5.31	115.84	125.64
9	G	302	HEM	CBA-CAA-C2A	-5.11	103.91	112.62
9	C	301	HEM	CBA-CAA-C2A	4.97	121.10	112.62
9	O	303	HEM	C4C-CHD-C1D	4.81	128.91	122.56
4	E	701	FAD	C5A-C6A-N6A	4.80	127.65	120.35
4	I	701	FAD	O4B-C1B-C2B	-4.64	100.14	106.93
4	M	701	FAD	C4'-C3'-C2'	-4.44	104.13	113.36
9	G	301	HEM	C4C-CHD-C1D	-4.39	116.76	122.56
4	M	701	FAD	C5A-C6A-N6A	4.28	126.86	120.35
9	K	301	HEM	CAD-CBD-CGD	-4.23	104.50	113.60
4	E	701	FAD	C3B-C2B-C1B	4.04	107.06	100.98
9	K	301	HEM	C3D-C4D-ND	-4.02	105.69	110.17
9	K	301	HEM	C4D-ND-C1D	3.99	109.19	105.07
9	G	301	HEM	CAD-CBD-CGD	-3.98	105.04	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	701	FAD	N6A-C6A-N1A	-3.94	110.39	118.57
4	I	701	FAD	C1B-N9A-C4A	3.92	133.54	126.64
4	E	701	FAD	C4X-C10-N10	3.91	122.20	116.48
4	I	701	FAD	C5A-C6A-N6A	3.90	126.27	120.35
4	E	701	FAD	N6A-C6A-N1A	-3.88	110.53	118.57
4	M	701	FAD	C4-N3-C2	-3.86	118.51	125.64
9	C	302	HEM	C4C-CHD-C1D	3.81	127.59	122.56
4	E	701	FAD	C4-N3-C2	-3.81	118.61	125.64
9	O	303	HEM	CAA-CBA-CGA	-3.81	103.08	113.76
4	I	701	FAD	C4X-C4-N3	3.61	122.35	113.19
4	I	701	FAD	C4-N3-C2	-3.59	119.01	125.64
4	M	701	FAD	C4-C4X-C10	3.54	122.74	116.79
9	O	302	HEM	C4C-CHD-C1D	3.50	127.17	122.56
4	M	701	FAD	O4-C4-C4X	-3.47	117.39	126.60
4	A	701	FAD	O4-C4-C4X	-3.46	117.42	126.60
9	C	301	HEM	C4C-CHD-C1D	3.44	127.10	122.56
9	G	301	HEM	CAD-C3D-C4D	3.37	130.54	124.66
4	M	701	FAD	C2B-C3B-C4B	-3.34	96.15	102.64
11	C	304	MQ7	C19-C18-C20	3.32	119.78	115.98
9	K	301	HEM	CHA-C4D-C3D	3.30	131.51	125.33
4	I	701	FAD	P-O3P-PA	-3.30	121.52	132.83
9	G	301	HEM	CAD-C3D-C2D	-3.27	121.79	127.88
4	A	701	FAD	C4X-C4-N3	3.26	121.48	113.19
5	I	702	FUM	C5-C4-C	-3.26	110.51	127.26
9	O	303	HEM	CMA-C3A-C4A	-3.24	123.48	128.46
4	A	701	FAD	C3B-C2B-C1B	3.24	105.85	100.98
9	O	303	HEM	C2C-C3C-C4C	3.20	109.14	106.90
4	I	701	FAD	O4'-C4'-C5'	3.20	117.12	109.92
9	G	301	HEM	CBA-CAA-C2A	-3.19	107.18	112.62
9	G	302	HEM	C4B-CHC-C1C	3.11	126.67	122.56
9	C	301	HEM	CMA-C3A-C4A	-3.09	123.72	128.46
4	A	701	FAD	O2-C2-N1	-3.08	116.72	121.83
4	A	701	FAD	C4X-C10-N1	-3.08	117.58	124.73
4	M	701	FAD	C4X-C10-N1	-3.08	117.59	124.73
9	K	302	HEM	CBA-CAA-C2A	-3.08	107.37	112.62
4	E	701	FAD	C4X-C4-N3	3.06	120.95	113.19
9	G	302	HEM	CHA-C4D-ND	3.00	128.09	124.38
4	A	701	FAD	C4-C4X-C10	3.00	121.83	116.79
11	C	304	MQ7	C14-C13-C12	-2.99	116.01	123.68
4	E	701	FAD	O4-C4-C4X	-2.98	118.71	126.60
9	G	302	HEM	C2C-C3C-C4C	2.97	108.97	106.90
4	I	701	FAD	C4-C4X-N5	2.95	122.42	118.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	701	FAD	C4X-C10-N10	2.91	120.73	116.48
4	I	701	FAD	C4X-C10-N10	2.83	120.62	116.48
4	A	701	FAD	C4'-C3'-C2'	-2.83	107.48	113.36
9	C	302	HEM	C2C-C3C-C4C	2.83	108.87	106.90
9	G	301	HEM	C4D-ND-C1D	2.79	107.95	105.07
9	O	303	HEM	CHD-C1D-C2D	2.77	129.31	124.98
9	O	302	HEM	CAA-CBA-CGA	-2.76	106.02	113.76
4	A	701	FAD	O2'-C2'-C3'	-2.75	102.40	109.10
9	C	302	HEM	CHD-C1D-C2D	2.74	129.26	124.98
9	O	302	HEM	C1B-NB-C4B	2.67	107.83	105.07
9	C	302	HEM	CHB-C1B-NB	-2.66	121.10	124.38
4	I	701	FAD	N6A-C6A-N1A	-2.65	113.08	118.57
4	I	701	FAD	O2'-C2'-C1'	-2.64	103.40	109.80
9	O	302	HEM	CMD-C2D-C1D	-2.61	121.06	125.04
4	I	701	FAD	C10-N1-C2	2.61	122.13	116.90
4	I	701	FAD	C3B-C2B-C1B	2.61	104.90	100.98
4	M	701	FAD	C4X-C4-N3	2.60	119.78	113.19
9	G	301	HEM	CMA-C3A-C4A	-2.60	124.47	128.46
9	O	303	HEM	CMD-C2D-C1D	2.59	128.99	125.04
9	O	303	HEM	C3C-C4C-NC	-2.55	106.13	110.94
4	A	701	FAD	C5X-C9A-N10	2.52	120.56	117.95
9	C	302	HEM	C4B-CHC-C1C	2.51	125.87	122.56
4	M	701	FAD	N6A-C6A-N1A	-2.50	113.39	118.57
4	M	701	FAD	C3B-C2B-C1B	2.49	104.73	100.98
10	O	301	LMT	C1B-O1B-C4'	-2.49	111.80	117.96
4	M	701	FAD	O3'-C3'-C4'	2.48	114.80	108.81
11	C	304	MQ7	C15-C13-C12	2.47	126.12	121.12
4	E	701	FAD	C1'-N10-C9A	2.46	124.61	120.51
9	C	302	HEM	CMA-C3A-C4A	-2.45	124.70	128.46
4	I	701	FAD	C10-C4X-N5	-2.43	119.69	124.86
4	A	701	FAD	C5B-C4B-C3B	-2.41	106.14	115.18
5	M	702	FUM	C5-C4-C	-2.39	114.96	127.26
4	I	701	FAD	C4'-C3'-C2'	-2.39	108.40	113.36
9	O	303	HEM	C1D-C2D-C3D	2.38	109.45	106.96
4	I	701	FAD	C9A-C5X-N5	-2.36	119.86	122.43
4	M	701	FAD	C5'-C4'-C3'	-2.36	107.65	112.20
4	A	701	FAD	C10-C4X-N5	-2.35	119.86	124.86
9	O	302	HEM	C4A-C3A-C2A	2.34	108.62	107.00
9	C	302	HEM	CAA-CBA-CGA	-2.32	107.26	113.76
9	K	301	HEM	CAA-CBA-CGA	-2.31	107.28	113.76
9	C	301	HEM	CHA-C4D-ND	-2.31	121.53	124.38
4	E	701	FAD	O2-C2-N1	-2.30	118.02	121.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	O	303	HEM	CHC-C4B-C3B	2.30	128.09	124.57
9	K	302	HEM	C4C-CHD-C1D	2.30	125.59	122.56
9	O	302	HEM	C3B-C2B-C1B	2.27	108.17	106.49
9	O	303	HEM	C4A-C3A-C2A	2.26	108.57	107.00
9	G	302	HEM	CAD-CBD-CGD	-2.26	108.75	113.60
5	A	702	FUM	OXT-C-O	-2.25	117.99	122.67
4	E	701	FAD	O2'-C2'-C1'	-2.25	104.36	109.80
4	I	701	FAD	C2B-C3B-C4B	-2.25	98.27	102.64
4	I	701	FAD	O4-C4-C4X	-2.25	120.64	126.60
9	O	303	HEM	C2D-C1D-ND	-2.24	107.19	109.88
4	M	701	FAD	O3'-C3'-C2'	2.20	114.12	108.81
9	G	302	HEM	C4A-C3A-C2A	2.19	108.52	107.00
9	C	301	HEM	C2C-C3C-C4C	2.16	108.41	106.90
4	A	701	FAD	C5'-C4'-C3'	-2.15	108.05	112.20
9	K	301	HEM	C2D-C1D-ND	-2.14	107.31	109.88
5	I	702	FUM	C4-C5-C6	-2.14	116.29	127.26
9	K	301	HEM	C1D-C2D-C3D	2.13	109.20	106.96
9	G	302	HEM	C3C-C4C-NC	-2.13	106.92	110.94
4	A	701	FAD	N3-C2-N1	2.12	123.55	119.38
9	K	302	HEM	O1A-CGA-CBA	-2.12	116.28	123.08
9	G	302	HEM	CMA-C3A-C4A	-2.11	125.22	128.46
5	A	702	FUM	C4-C5-C6	-2.09	116.50	127.26
9	C	302	HEM	CHD-C1D-ND	-2.09	122.16	124.43
9	G	301	HEM	C3C-C4C-NC	-2.09	107.00	110.94
4	M	701	FAD	C4X-C10-N10	2.08	119.52	116.48
4	M	701	FAD	C5X-C9A-N10	2.08	120.10	117.95
9	K	302	HEM	C4B-CHC-C1C	-2.07	119.83	122.56
4	E	701	FAD	C10-C4X-N5	-2.07	120.47	124.86
4	A	701	FAD	O3'-C3'-C2'	2.05	113.77	108.81
10	C	303	LMT	C3B-C4B-C5B	2.04	113.87	110.24
4	E	701	FAD	C5X-C9A-N10	2.03	120.05	117.95
9	G	301	HEM	C3D-C4D-ND	-2.03	107.91	110.17
9	O	302	HEM	O1A-CGA-CBA	-2.01	116.64	123.08

There are no chirality outliers.

All (124) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	701	FAD	C5B-O5B-PA-O3P
4	A	701	FAD	C2'-C3'-C4'-C5'
4	A	701	FAD	O3'-C3'-C4'-C5'
4	E	701	FAD	C5B-O5B-PA-O1A

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Mol	Chain	Res	Type	Atoms
4	E	701	FAD	N10-C1'-C2'-O2'
4	E	701	FAD	N10-C1'-C2'-C3'
4	E	701	FAD	C1'-C2'-C3'-C4'
4	E	701	FAD	O2'-C2'-C3'-C4'
4	E	701	FAD	C2'-C3'-C4'-O4'
4	E	701	FAD	C2'-C3'-C4'-C5'
4	I	701	FAD	C5B-O5B-PA-O3P
4	I	701	FAD	N10-C1'-C2'-O2'
4	I	701	FAD	N10-C1'-C2'-C3'
4	I	701	FAD	C1'-C2'-C3'-O3'
4	I	701	FAD	C1'-C2'-C3'-C4'
4	I	701	FAD	O2'-C2'-C3'-O3'
4	I	701	FAD	O2'-C2'-C3'-C4'
4	I	701	FAD	C2'-C3'-C4'-C5'
4	M	701	FAD	C1'-C2'-C3'-O3'
4	M	701	FAD	C1'-C2'-C3'-C4'
4	M	701	FAD	C2'-C3'-C4'-O4'
4	M	701	FAD	C2'-C3'-C4'-C5'
4	M	701	FAD	O3'-C3'-C4'-O4'
4	M	701	FAD	O3'-C3'-C4'-C5'
5	A	702	FUM	O-C-C4-C5
9	C	301	HEM	C2A-CAA-CBA-CGA
9	C	301	HEM	C2D-C3D-CAD-CBD
9	C	301	HEM	C4D-C3D-CAD-CBD
9	G	301	HEM	C3D-CAD-CBD-CGD
9	O	302	HEM	C1A-C2A-CAA-CBA
9	O	302	HEM	C2D-C3D-CAD-CBD
10	C	303	LMT	C2-C1-O1'-C1'
11	C	304	MQ7	C17-C18-C20-C21
11	C	304	MQ7	C19-C18-C20-C21
10	C	303	LMT	O5B-C1B-O1B-C4'
5	A	702	FUM	OXT-C-C4-C5
5	E	702	FUM	OXT-C-C4-C5
9	O	302	HEM	C4D-C3D-CAD-CBD
10	C	303	LMT	C3'-C4'-O1B-C1B
10	C	303	LMT	C4B-C5B-C6B-O6B
10	C	303	LMT	O5B-C5B-C6B-O6B
4	A	701	FAD	O3'-C3'-C4'-O4'
4	E	701	FAD	O2'-C2'-C3'-O3'
4	M	701	FAD	O2'-C2'-C3'-O3'
5	E	702	FUM	O-C-C4-C5
5	E	702	FUM	C4-C5-C6-O8

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Mol	Chain	Res	Type	Atoms
5	M	702	FUM	C4-C5-C6-O8
4	A	701	FAD	C2'-C3'-C4'-O4'
4	I	701	FAD	C2'-C3'-C4'-O4'
4	M	701	FAD	O2'-C2'-C3'-C4'
9	K	301	HEM	C3D-CAD-CBD-CGD
11	C	304	MQ7	C14-C13-C15-C16
11	C	304	MQ7	C12-C13-C15-C16
4	E	701	FAD	O3'-C3'-C4'-C5'
4	I	701	FAD	O3'-C3'-C4'-C5'
5	A	702	FUM	C4-C5-C6-O7
5	E	702	FUM	C4-C5-C6-O7
5	M	702	FUM	C4-C5-C6-O7
10	C	303	LMT	C2B-C1B-O1B-C4'
5	A	702	FUM	C4-C5-C6-O8
5	I	702	FUM	C4-C5-C6-O7
5	I	702	FUM	C4-C5-C6-O8
9	K	301	HEM	C2A-CAA-CBA-CGA
10	C	303	LMT	C4'-C5'-C6'-O6'
11	C	304	MQ7	C13-C15-C16-C17
5	M	702	FUM	OXT-C-C4-C5
4	E	701	FAD	O3'-C3'-C4'-O4'
4	I	701	FAD	O3'-C3'-C4'-O4'
10	C	303	LMT	C11-C10-C9-C8
9	C	301	HEM	C3D-CAD-CBD-CGD
5	M	702	FUM	O-C-C4-C5
10	O	301	LMT	C5-C6-C7-C8
10	O	301	LMT	C11-C10-C9-C8
10	O	301	LMT	C2'-C1'-O1'-C1
9	K	301	HEM	C4D-C3D-CAD-CBD
9	O	302	HEM	C2A-CAA-CBA-CGA
4	A	701	FAD	O2'-C2'-C3'-O3'
10	O	301	LMT	C4-C5-C6-C7
9	O	302	HEM	C3D-CAD-CBD-CGD
10	O	301	LMT	C1-C2-C3-C4
9	K	301	HEM	C2D-C3D-CAD-CBD
4	M	701	FAD	P-O3P-PA-O1A
10	C	303	LMT	C3-C4-C5-C6
4	A	701	FAD	PA-O3P-P-O5'
4	E	701	FAD	PA-O3P-P-O5'
4	I	701	FAD	PA-O3P-P-O5'
4	M	701	FAD	PA-O3P-P-O5'
10	C	303	LMT	O1'-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
10	O	301	LMT	C3'-C4'-O1B-C1B
10	C	303	LMT	O5'-C5'-C6'-O6'
10	C	303	LMT	C5'-C4'-O1B-C1B
10	O	301	LMT	C5'-C4'-O1B-C1B
10	O	301	LMT	C3-C4-C5-C6
4	M	701	FAD	C5'-O5'-P-O3P
4	A	701	FAD	P-O3P-PA-O2A
10	C	303	LMT	C5-C6-C7-C8
4	A	701	FAD	O2'-C2'-C3'-C4'
4	A	701	FAD	C5B-O5B-PA-O1A
4	I	701	FAD	C5B-O5B-PA-O1A
4	I	701	FAD	C5B-O5B-PA-O2A
4	E	701	FAD	C1'-C2'-C3'-O3'
9	O	302	HEM	C3A-C2A-CAA-CBA
10	O	301	LMT	C7-C8-C9-C10
9	G	302	HEM	C3D-CAD-CBD-CGD
4	A	701	FAD	O4B-C4B-C5B-O5B
9	C	302	HEM	C3D-CAD-CBD-CGD
9	K	302	HEM	C3D-CAD-CBD-CGD
9	O	303	HEM	C3D-CAD-CBD-CGD
4	I	701	FAD	P-O3P-PA-O2A
9	C	301	HEM	CAA-CBA-CGA-O2A
9	O	302	HEM	CAA-CBA-CGA-O2A
9	C	301	HEM	CAA-CBA-CGA-O1A
9	O	302	HEM	CAD-CBD-CGD-O2D
9	O	302	HEM	CAA-CBA-CGA-O1A
4	E	701	FAD	O4B-C4B-C5B-O5B
4	A	701	FAD	P-O3P-PA-O1A
4	A	701	FAD	C5B-O5B-PA-O2A
4	I	701	FAD	O4B-C4B-C5B-O5B
4	M	701	FAD	O4B-C4B-C5B-O5B
4	A	701	FAD	C1'-C2'-C3'-O3'
9	K	301	HEM	CAD-CBD-CGD-O1D
9	O	302	HEM	CAD-CBD-CGD-O1D
4	A	701	FAD	N10-C1'-C2'-O2'
10	O	301	LMT	C9-C10-C11-C12

There are no ring outliers.

25 monomers are involved in 229 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	C	301	HEM	15	0

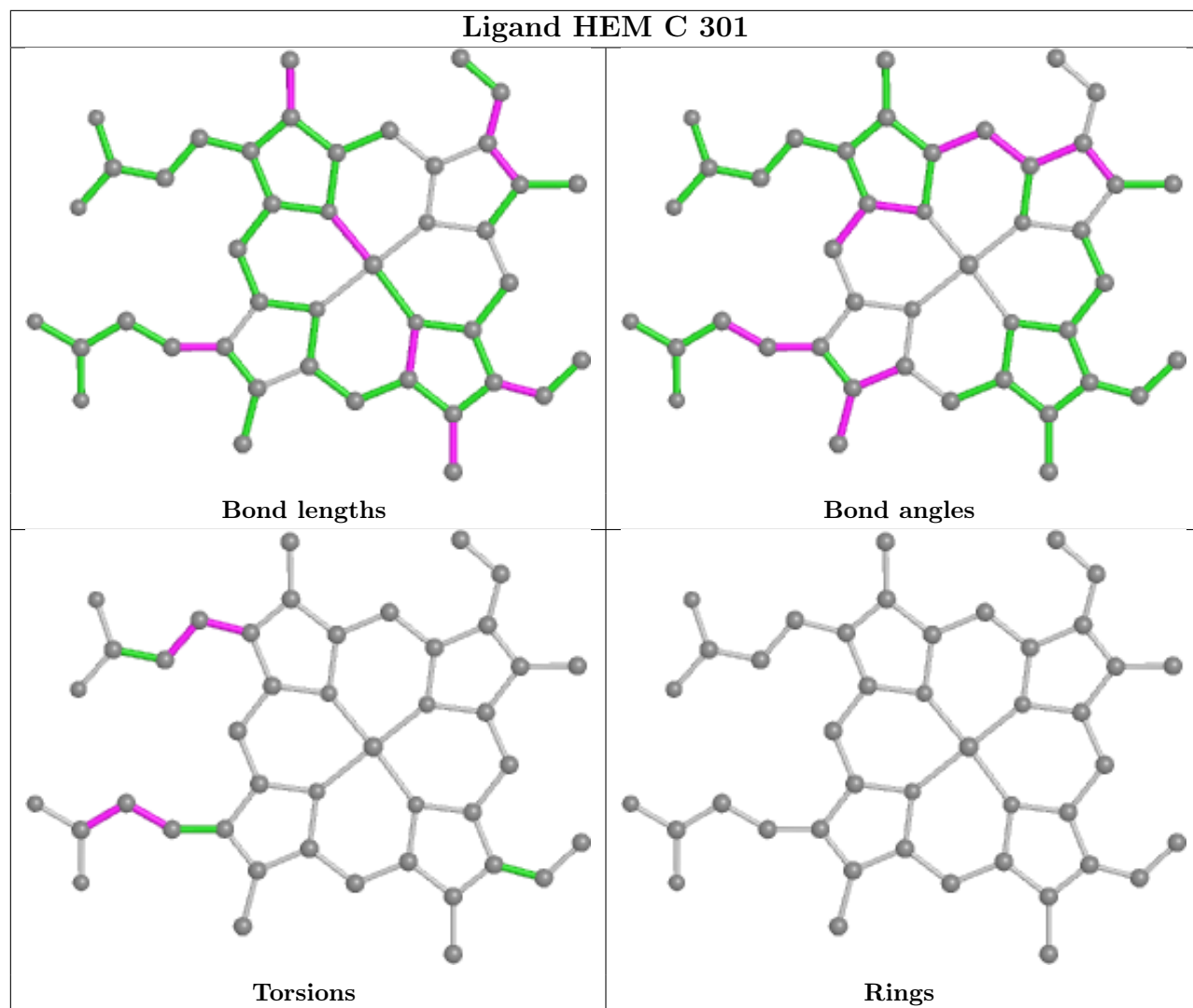
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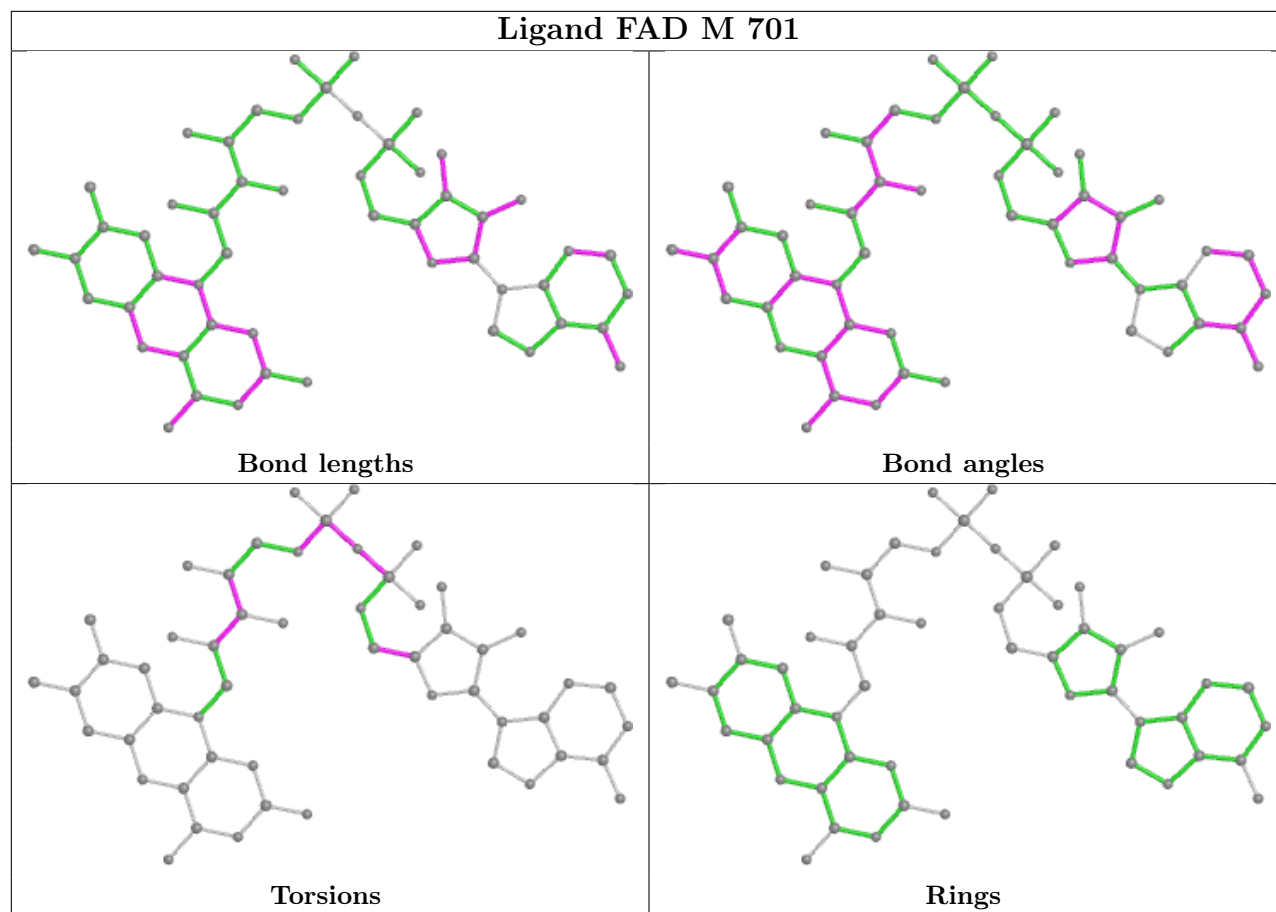
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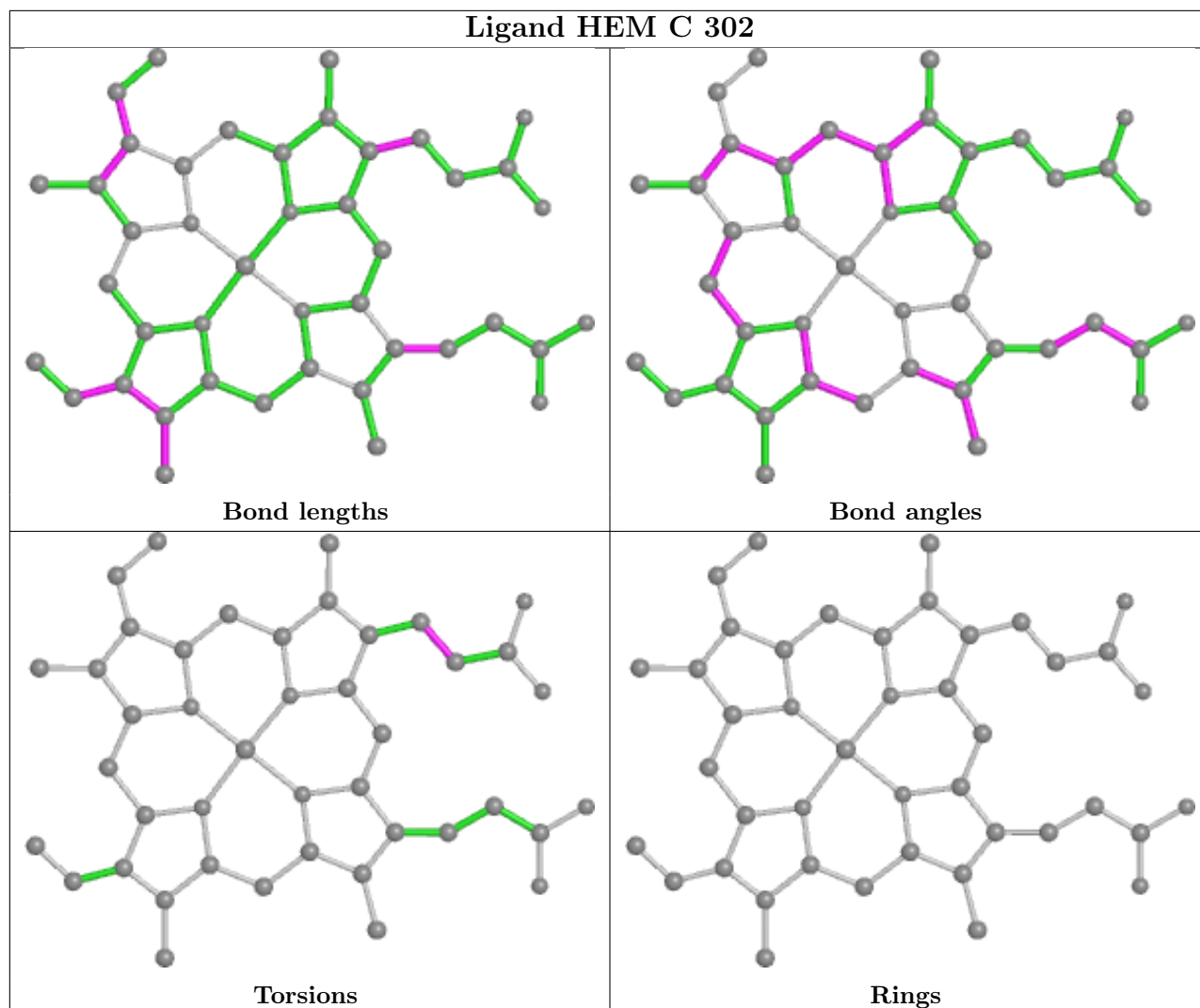
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	M	701	FAD	15	0
9	C	302	HEM	7	0
9	O	303	HEM	9	0
8	B	303	FES	1	0
5	E	702	FUM	5	0
7	B	302	SF4	1	0
8	N	303	FES	1	0
9	K	301	HEM	12	0
7	N	302	SF4	1	0
10	C	303	LMT	30	0
9	G	302	HEM	10	0
9	K	302	HEM	13	0
10	O	301	LMT	23	0
11	C	304	MQ7	19	0
5	I	702	FUM	3	0
5	A	702	FUM	7	0
5	M	702	FUM	5	0
4	E	701	FAD	4	0
4	I	701	FAD	21	0
8	F	303	FES	1	0
9	O	302	HEM	11	0
6	F	301	F3S	3	0
9	G	301	HEM	10	0
4	A	701	FAD	2	0

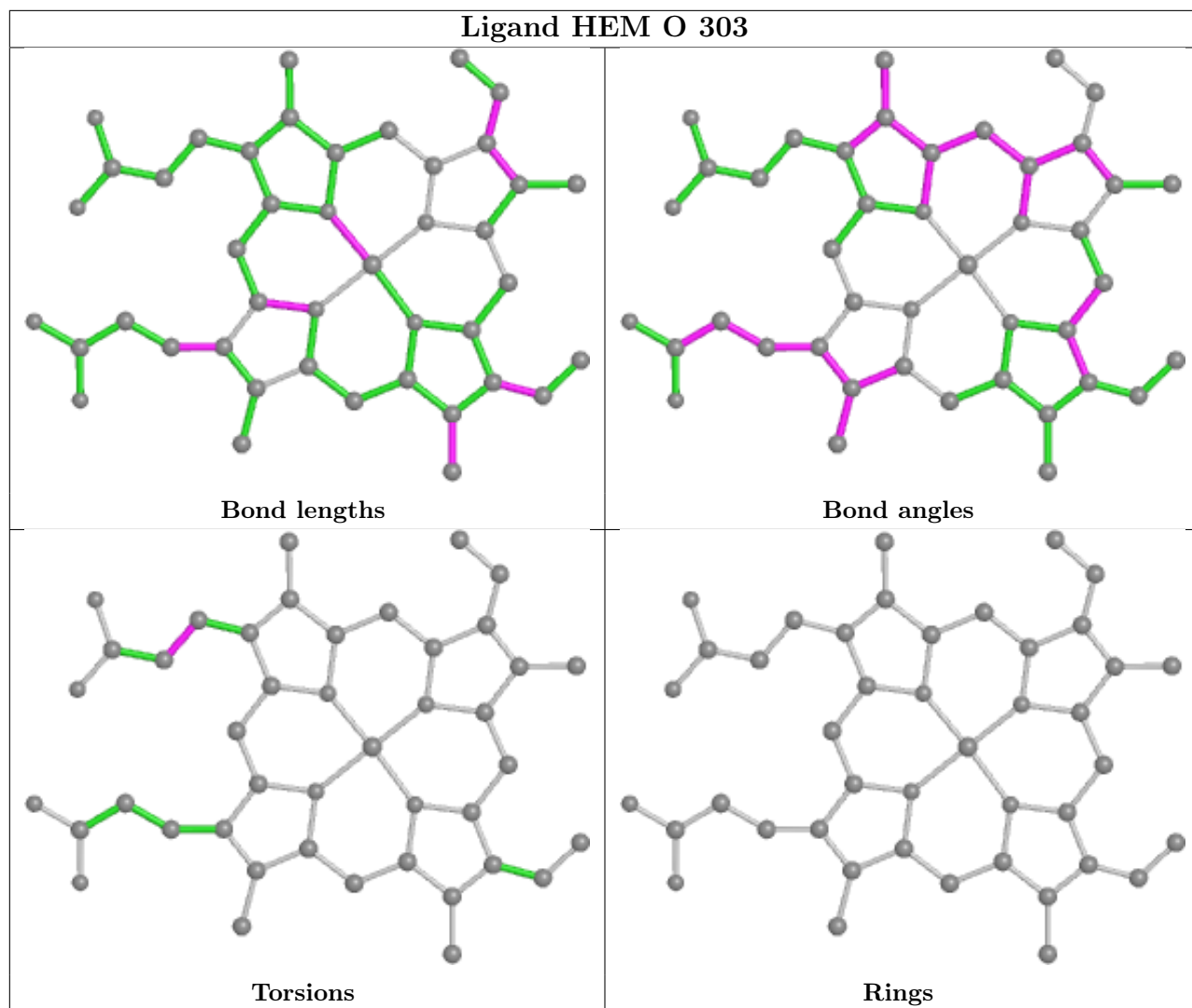
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

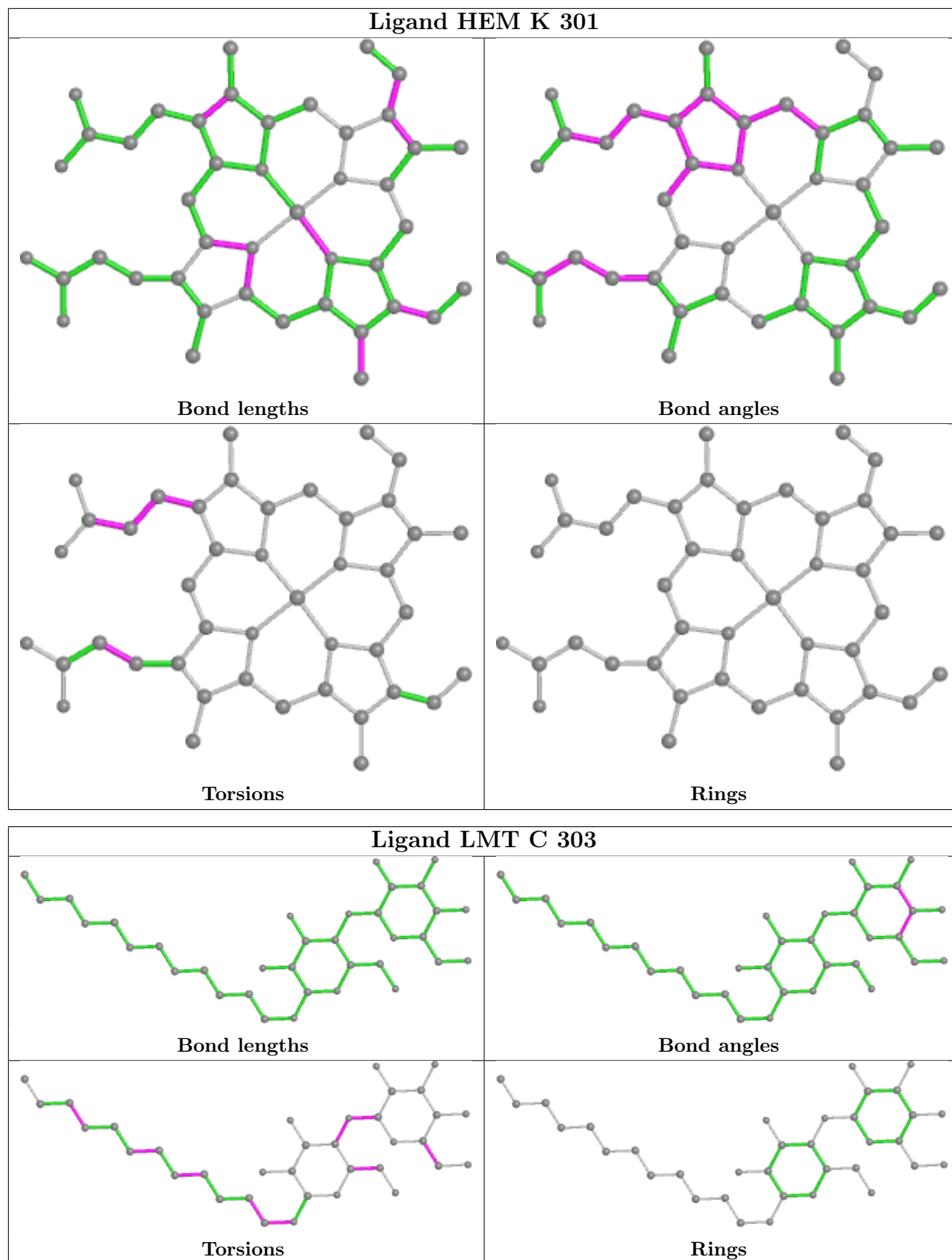


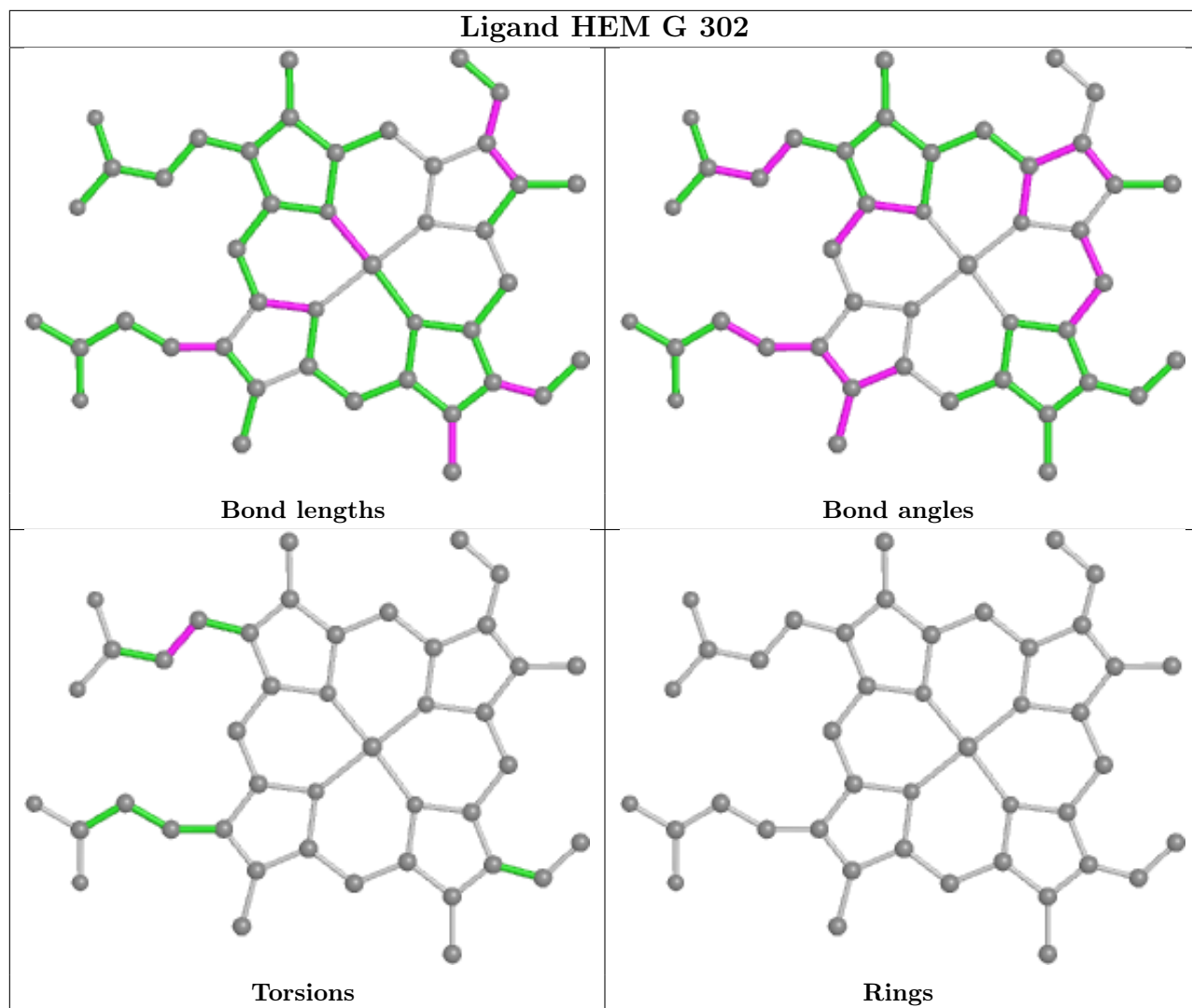


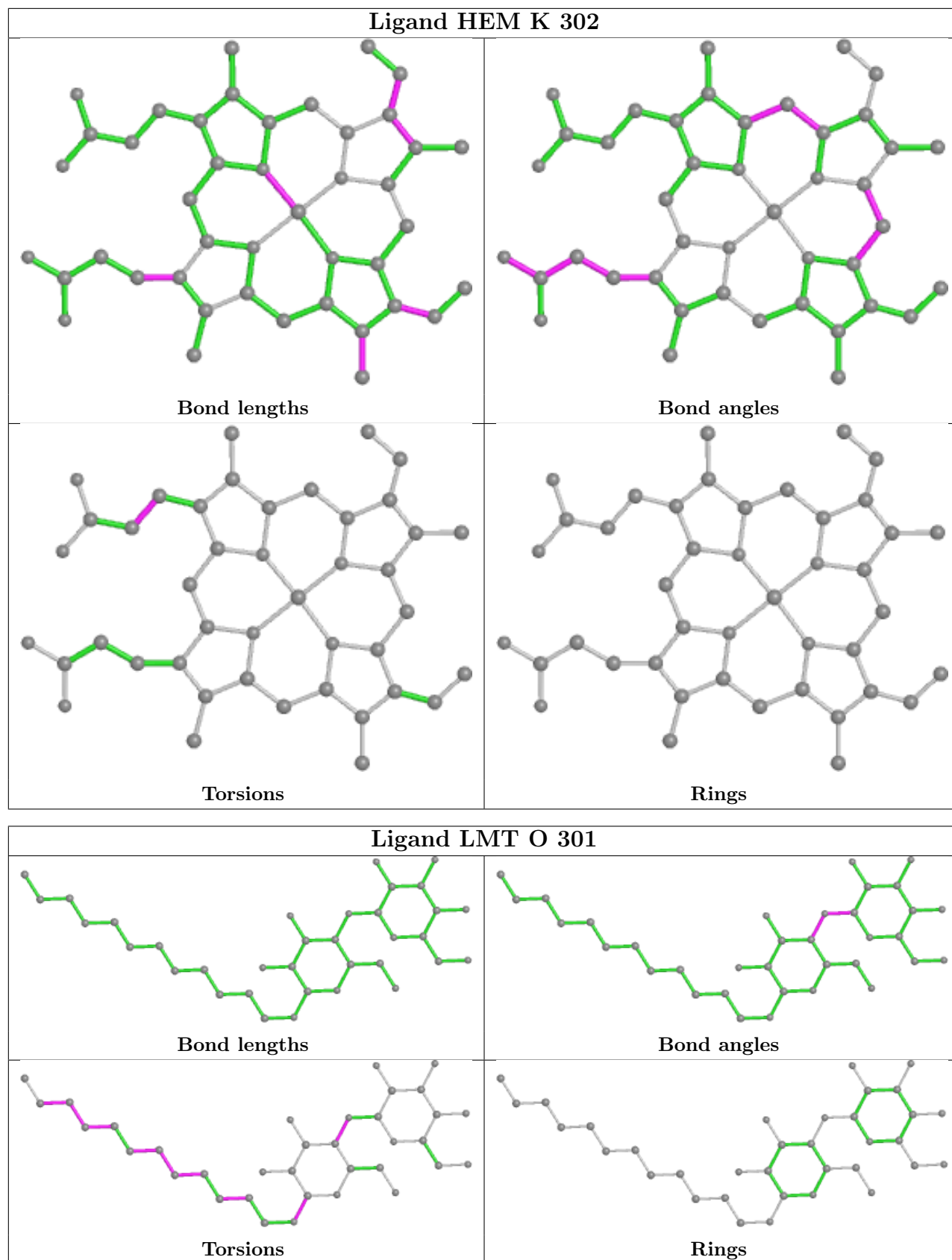


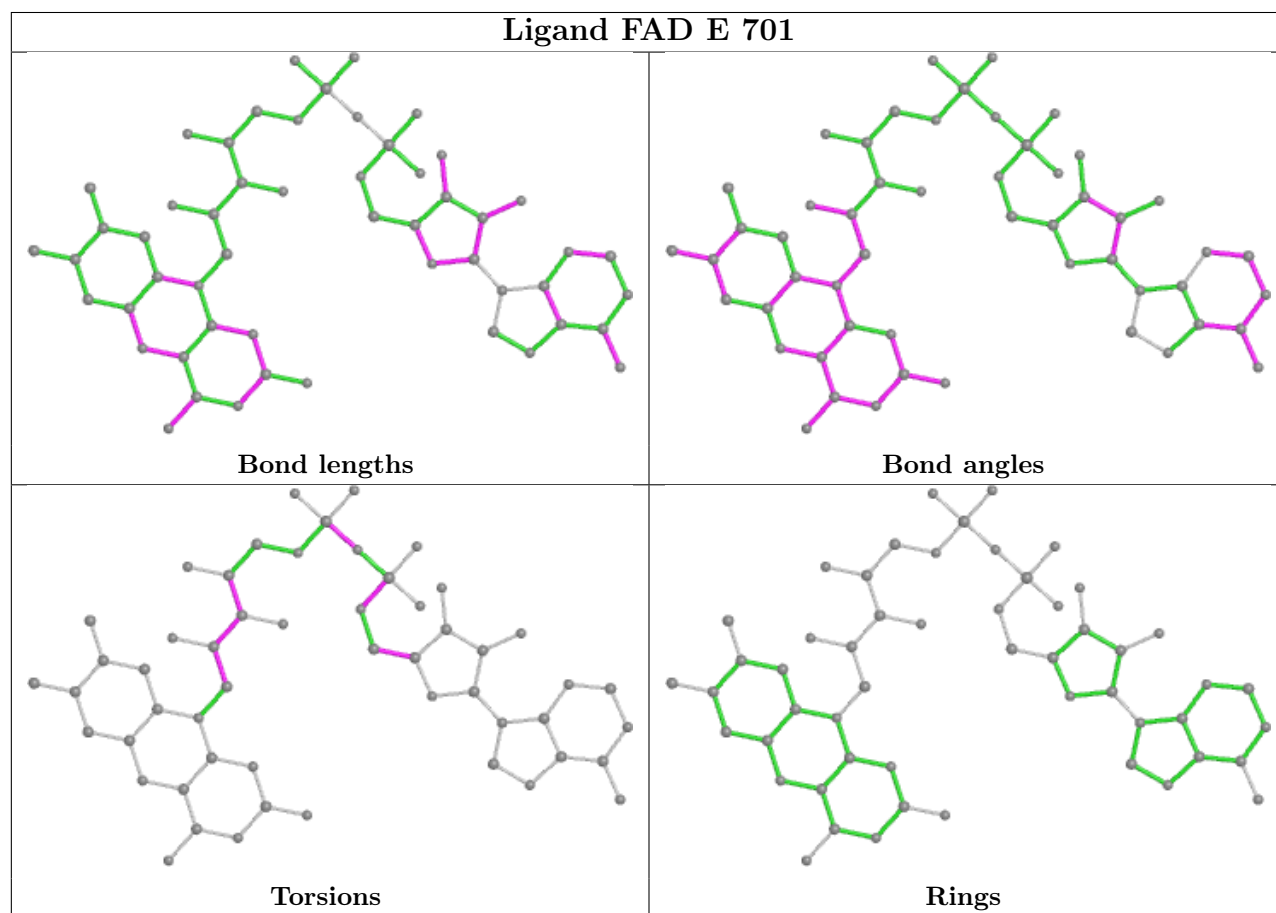
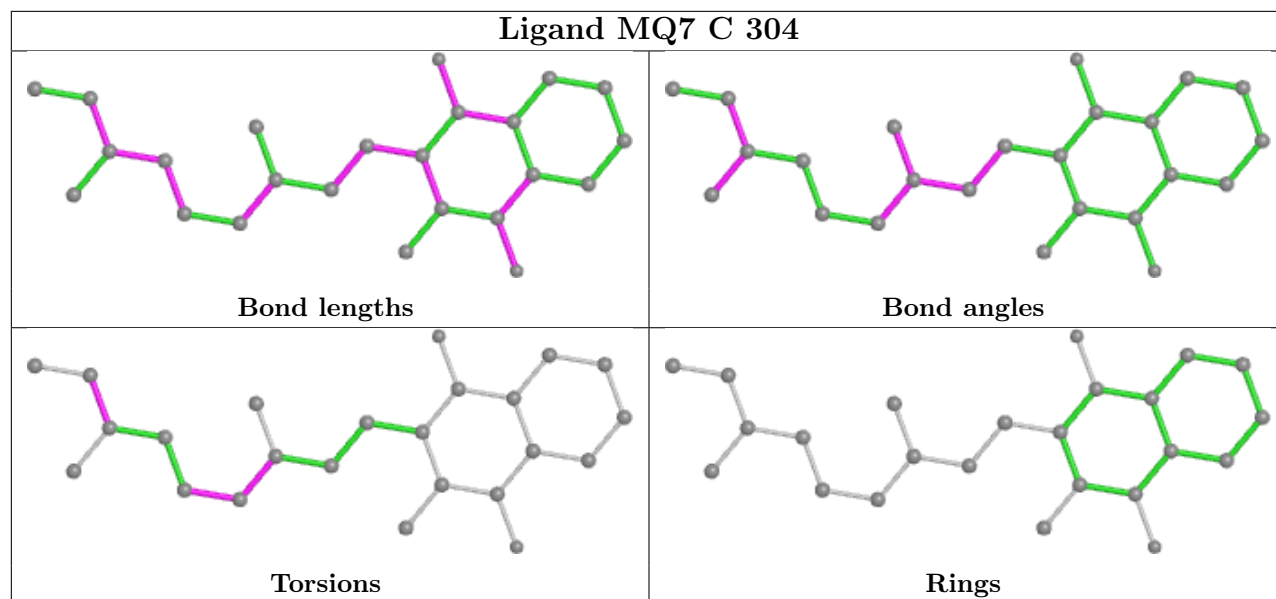




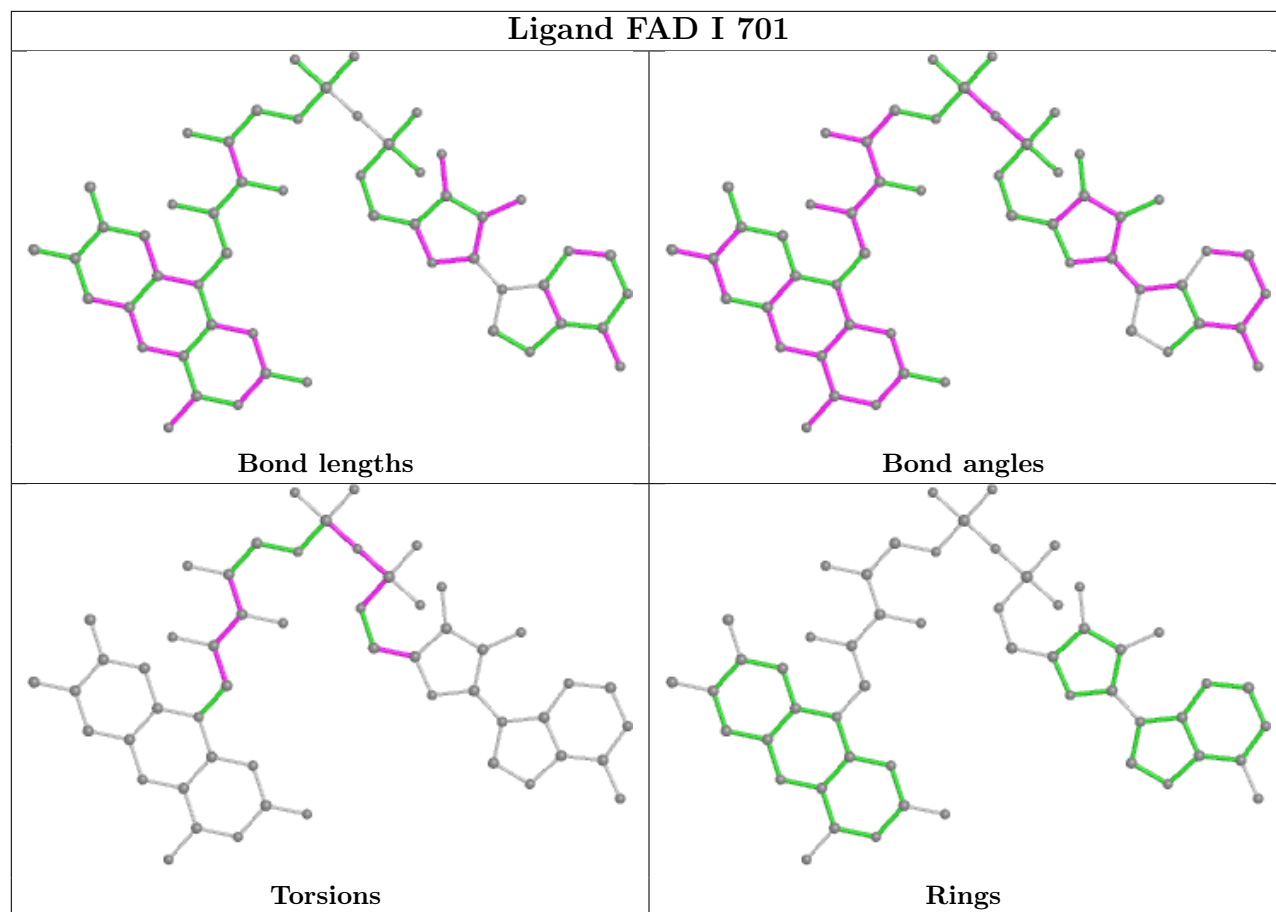


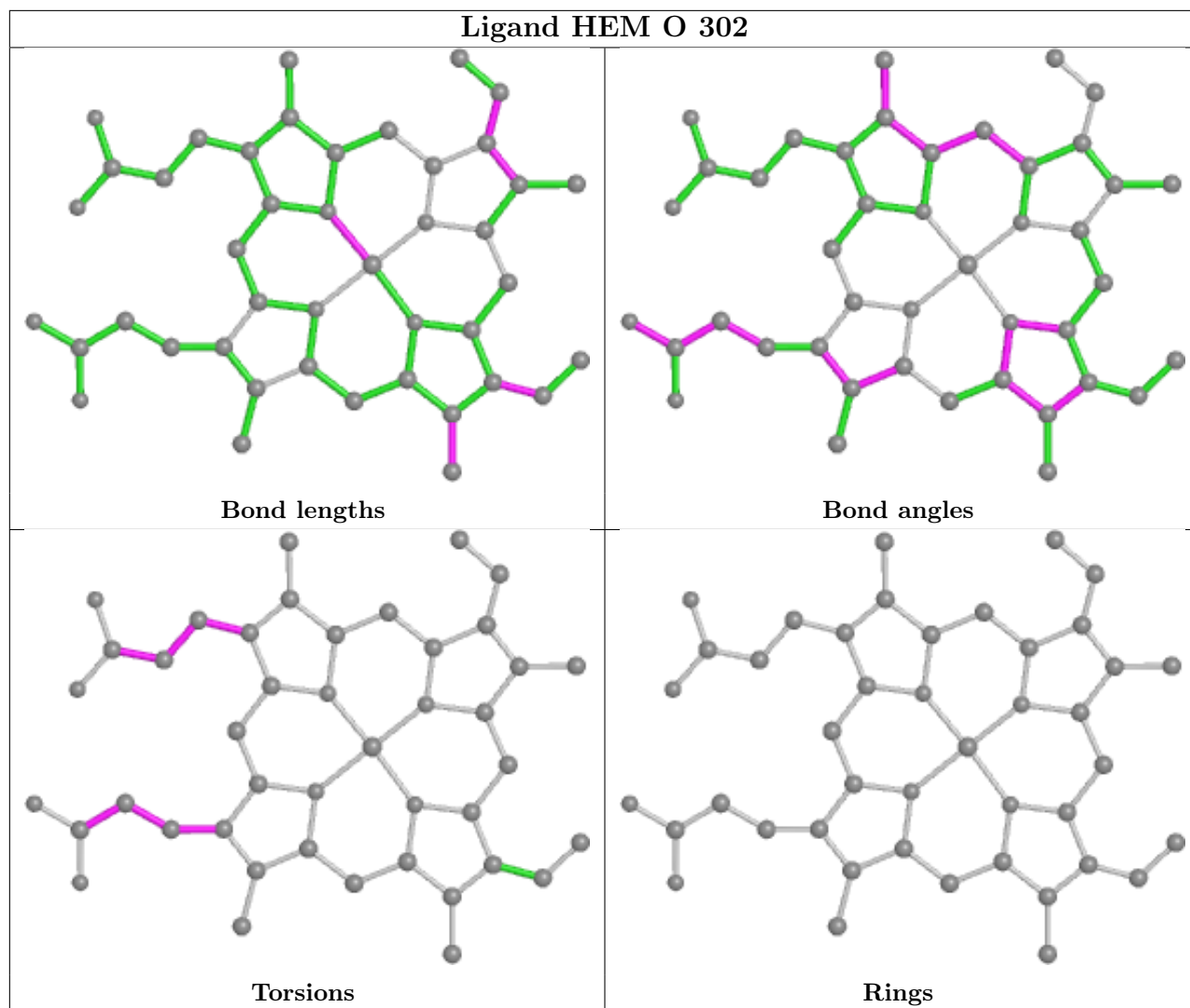


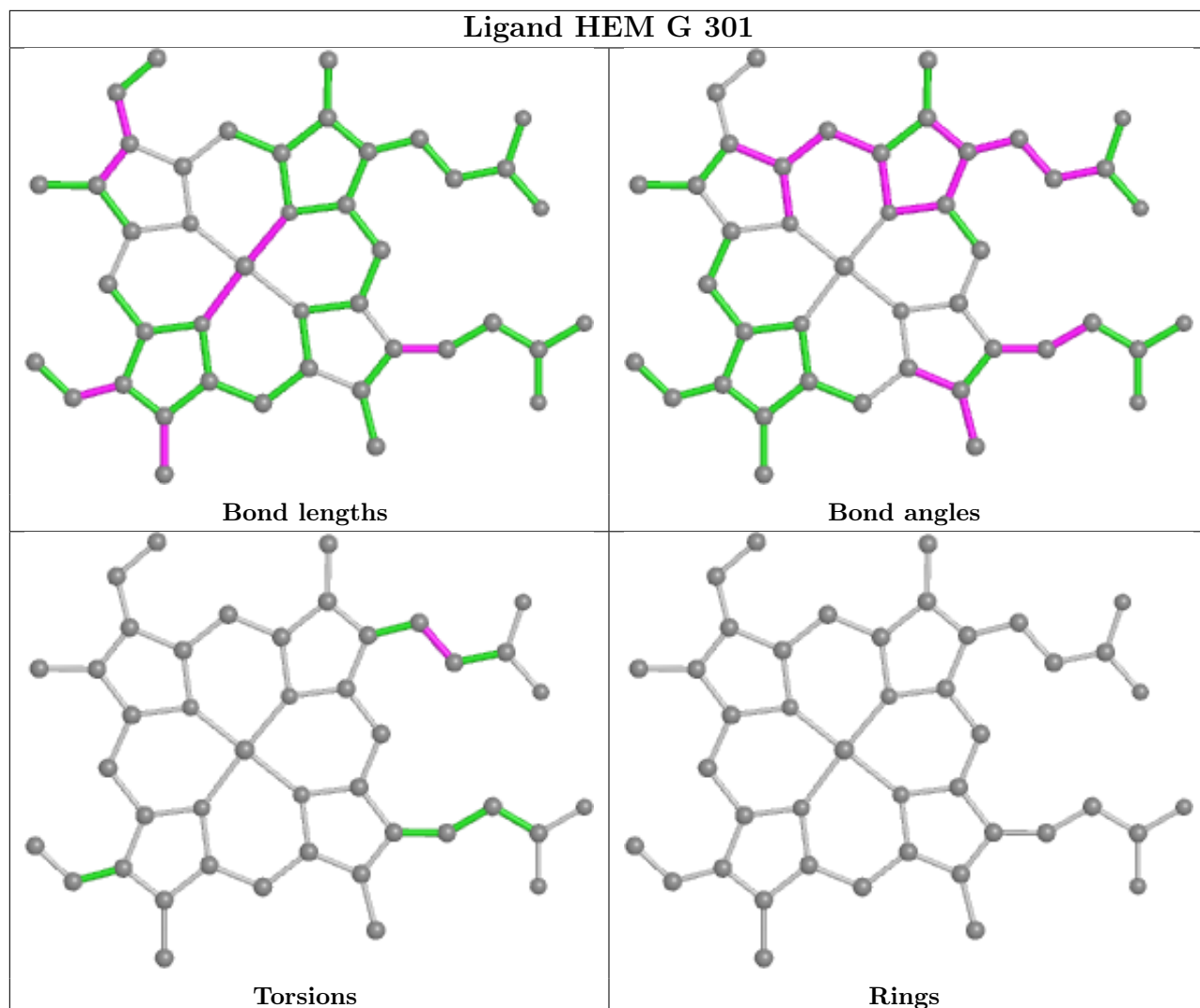


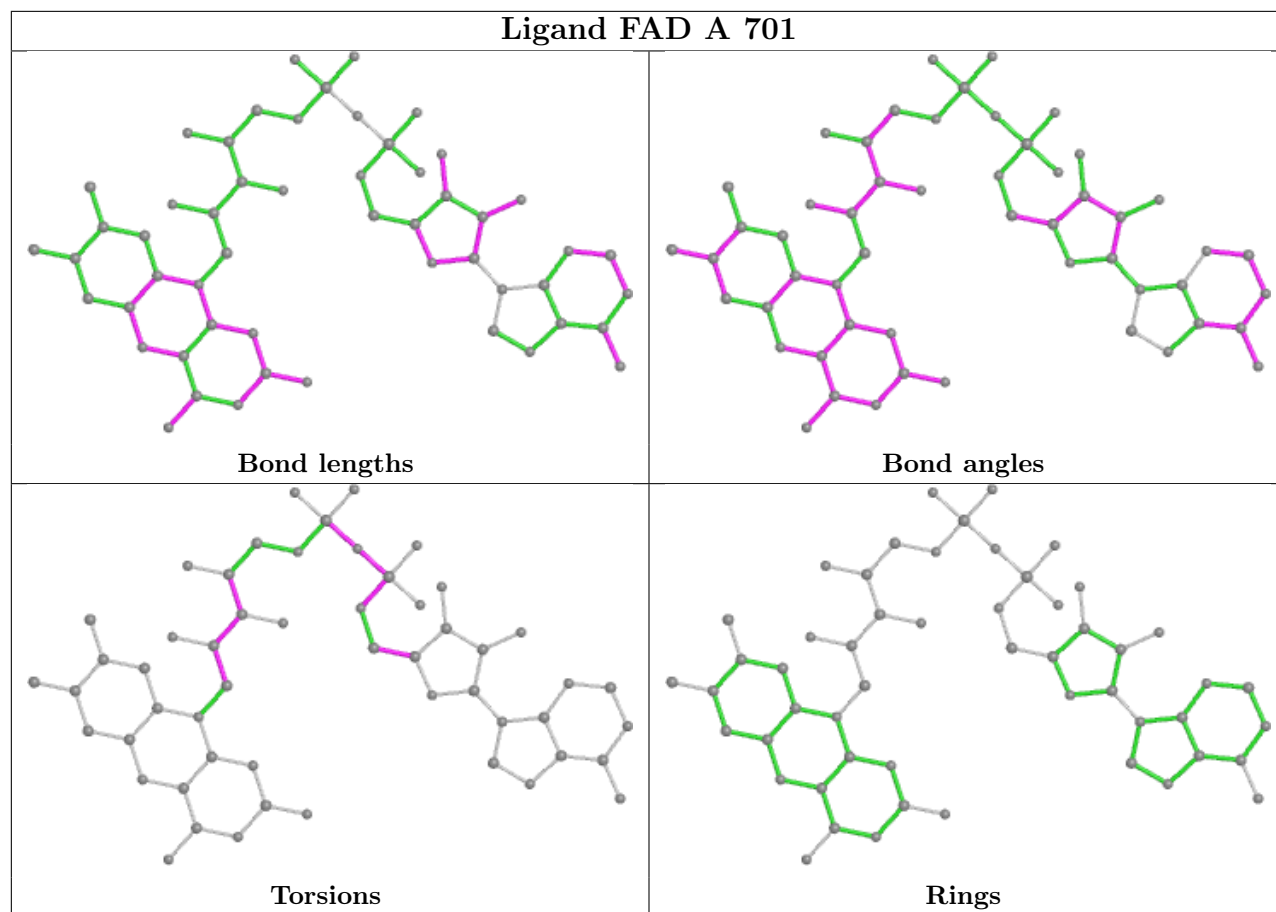












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

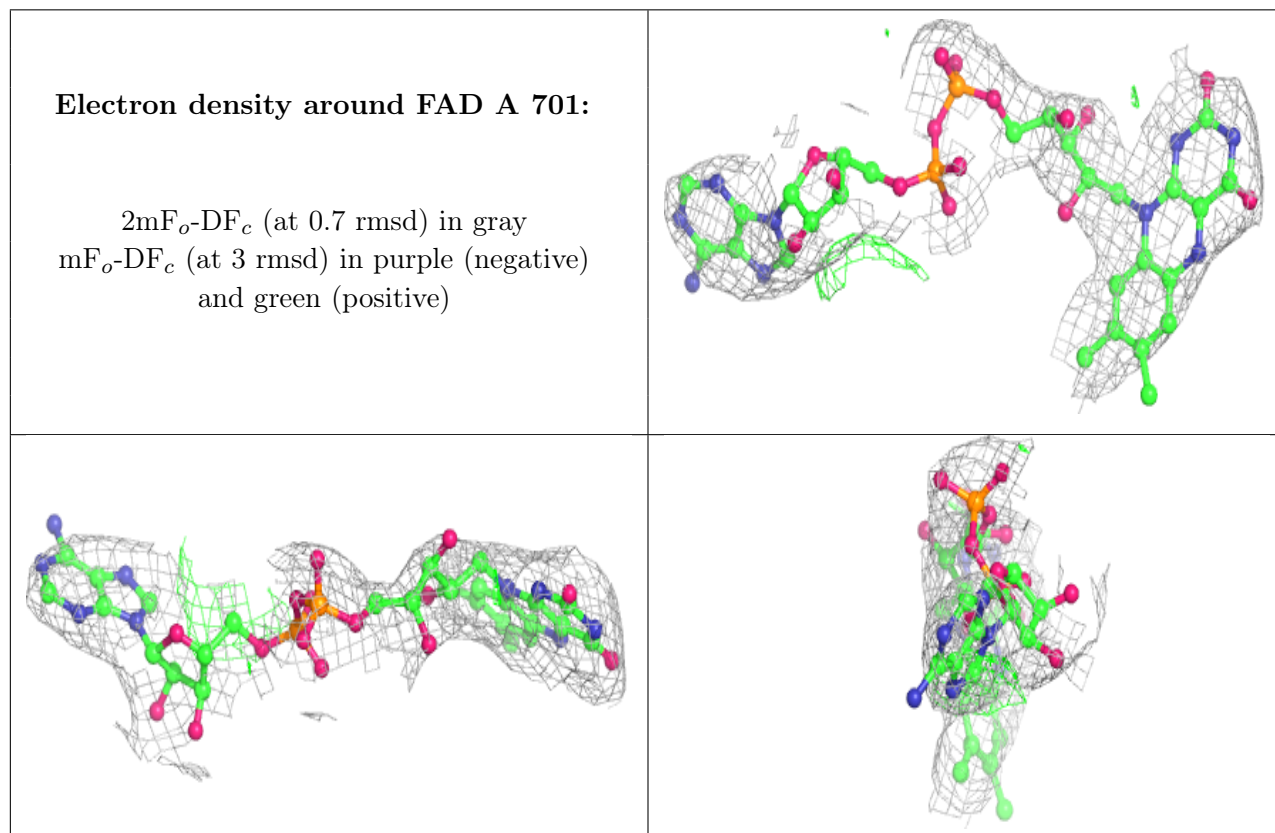
### 6.3 Carbohydrates [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands [i](#)

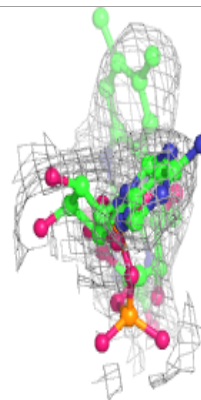
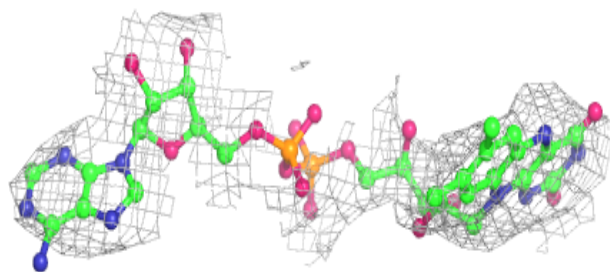
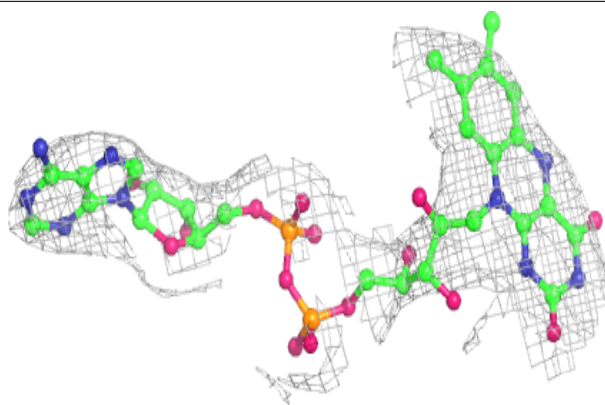
Unable to reproduce the depositors R factor - this section is therefore empty.

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

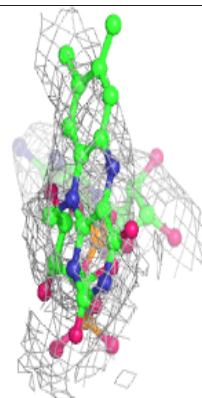
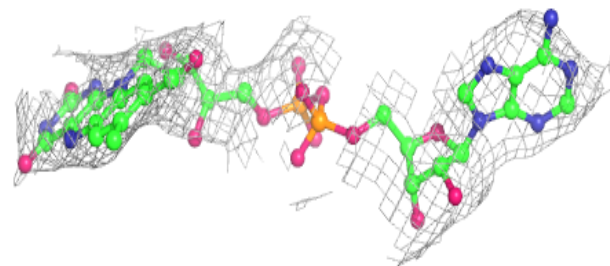
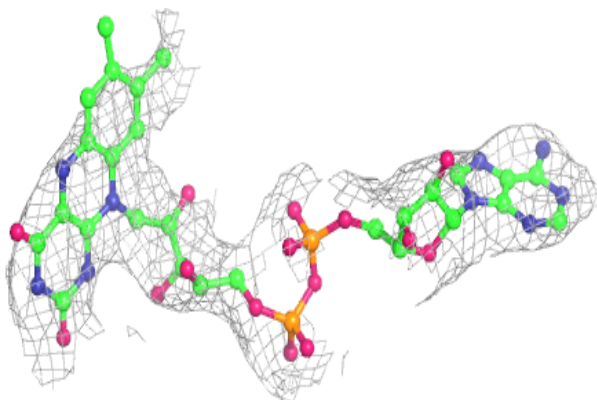


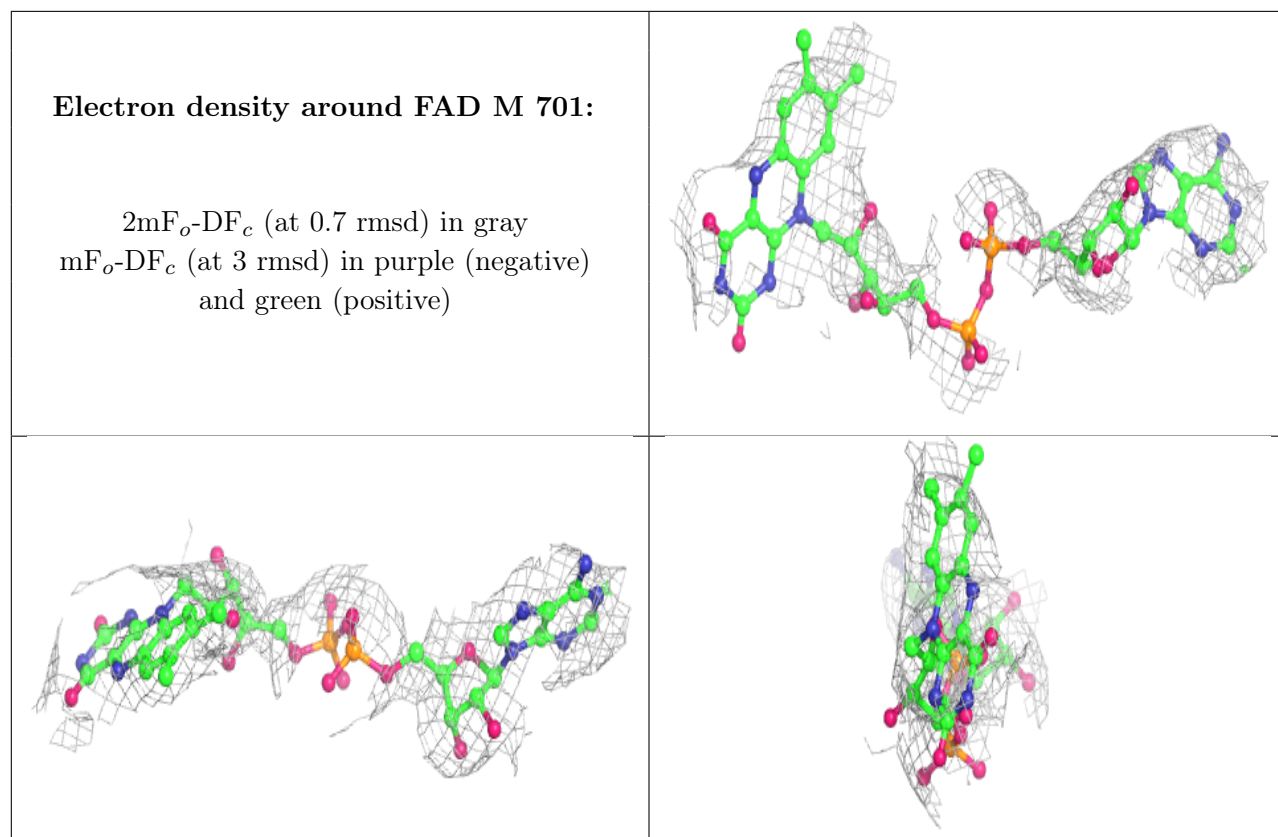
**Electron density around FAD E 701:**

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

**Electron density around FAD I 701:**

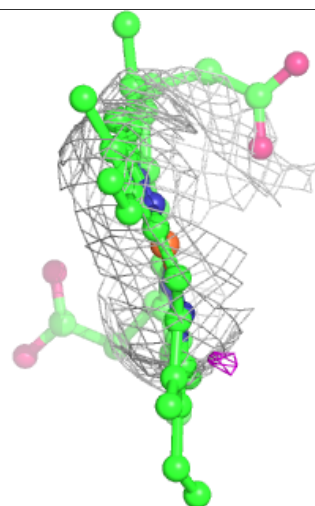
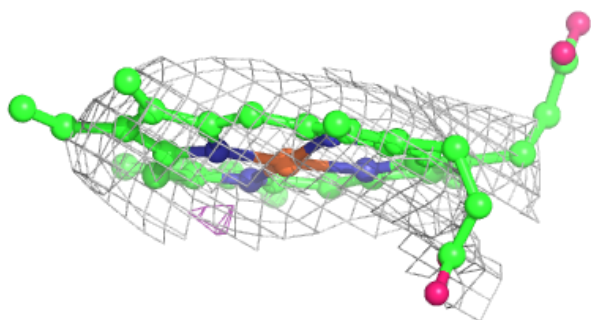
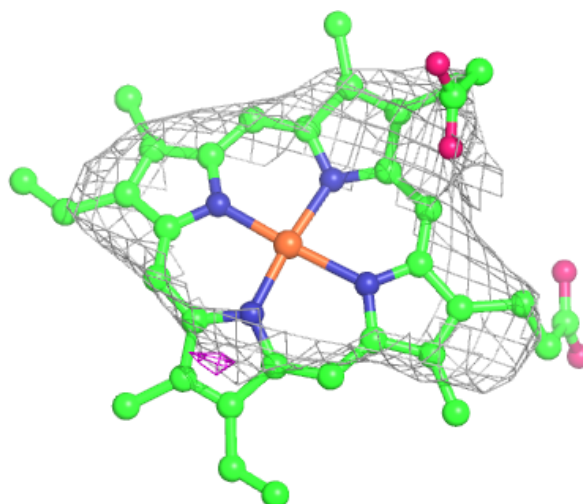
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around HEM C 301:**

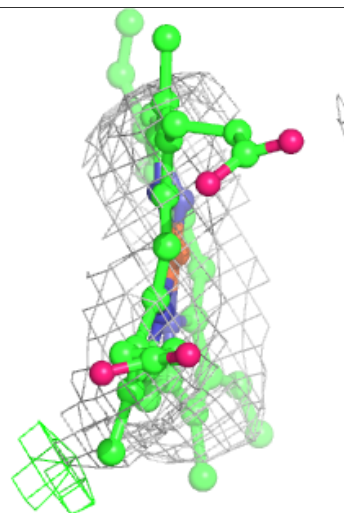
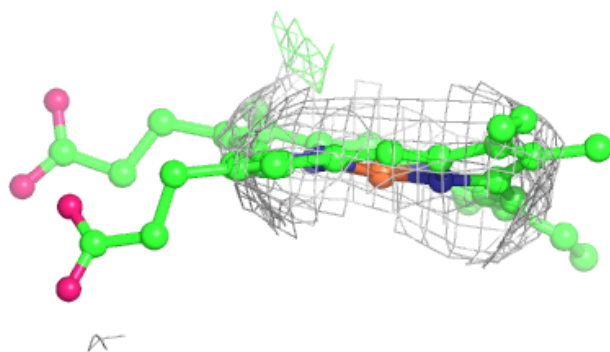
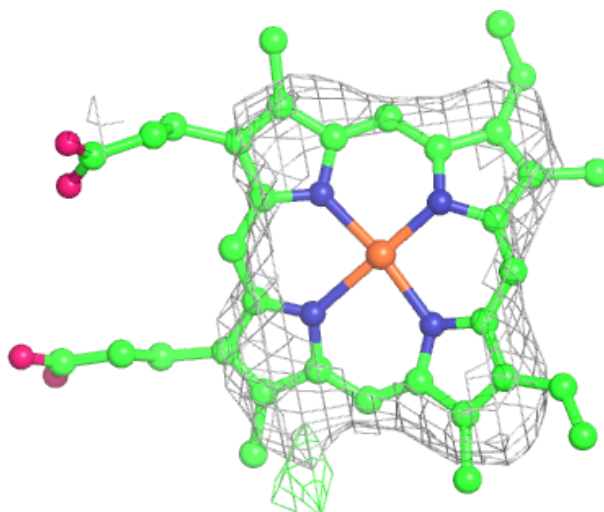
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





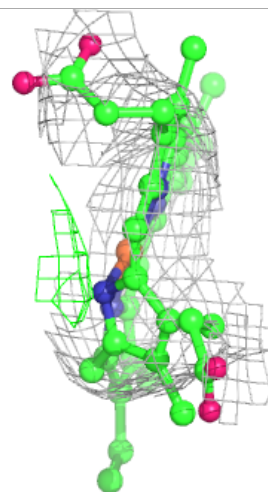
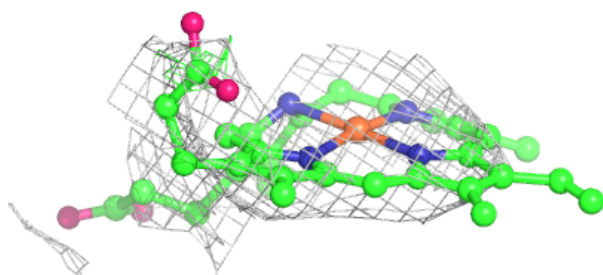
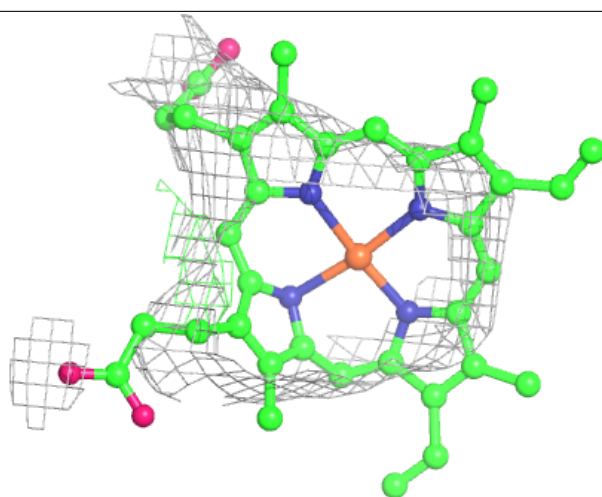
**Electron density around HEM C 302:**

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



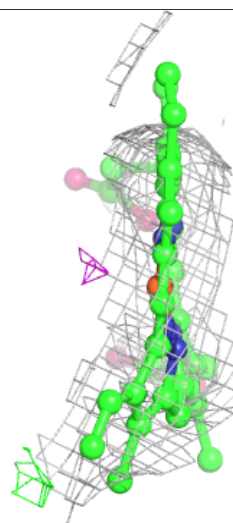
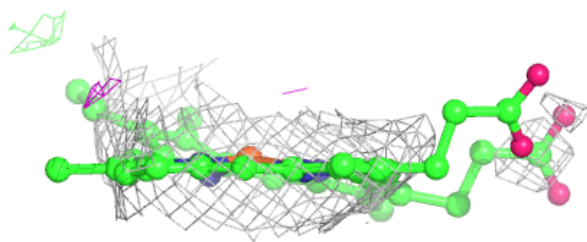
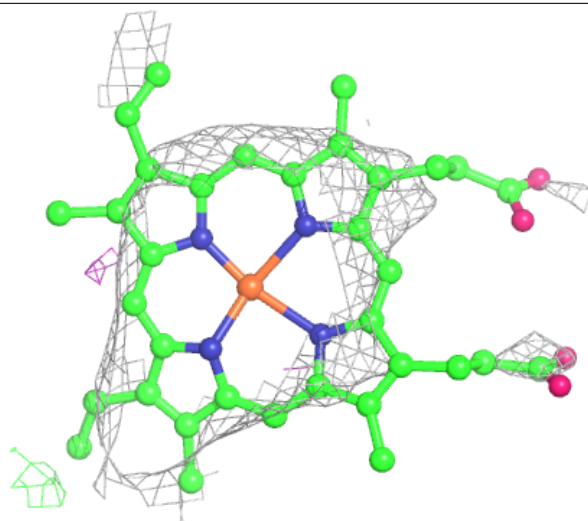
**Electron density around HEM G 301:**

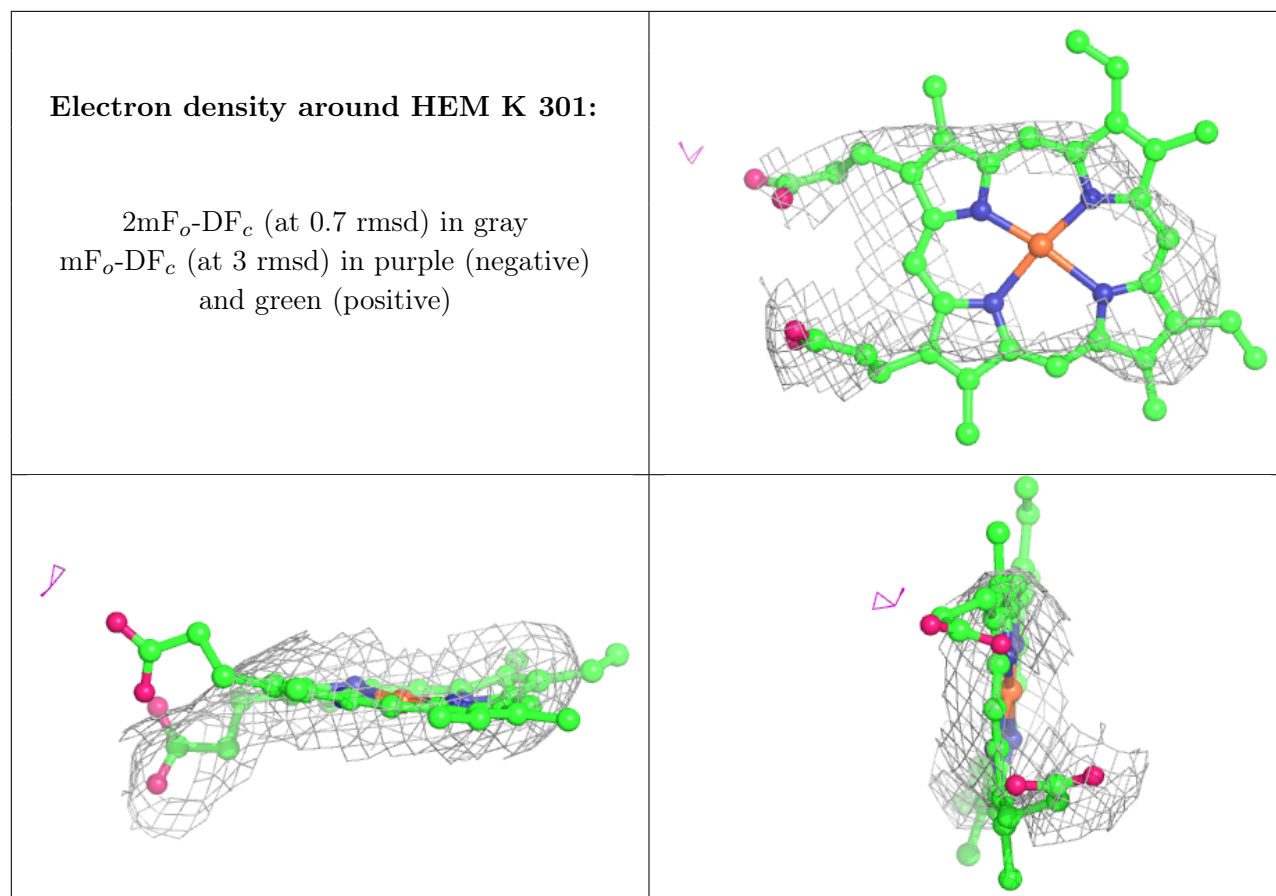
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEM G 302:**

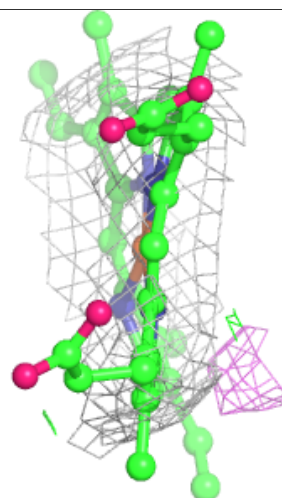
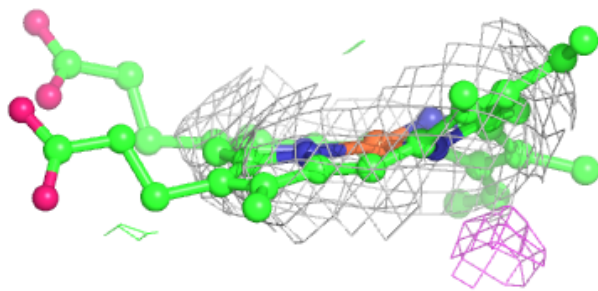
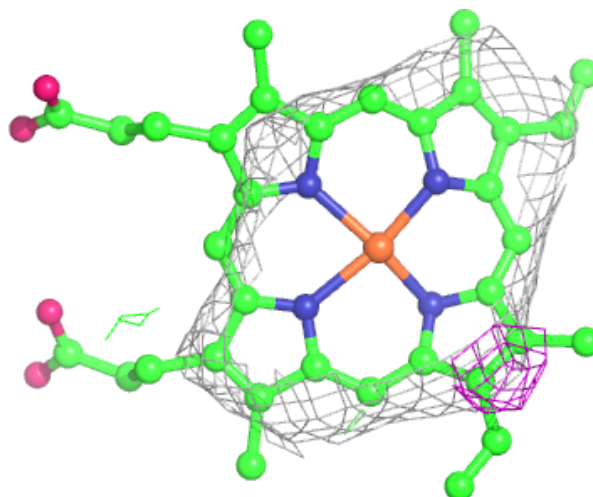
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





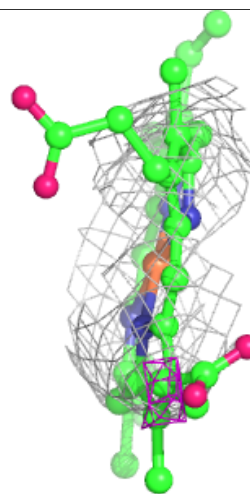
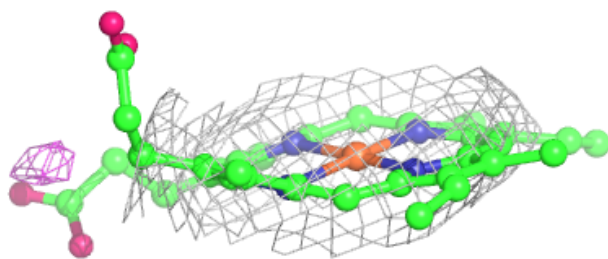
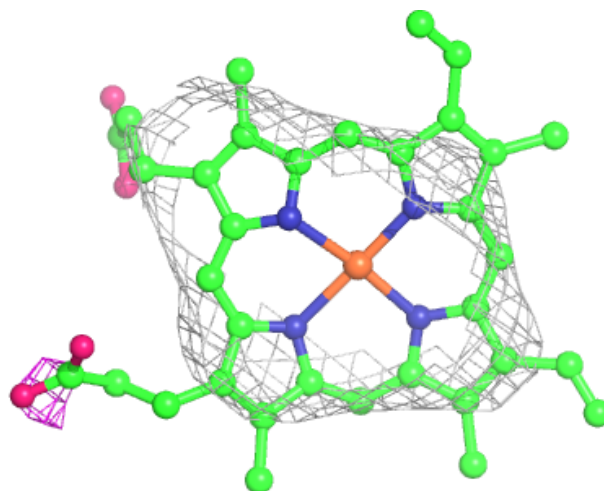
**Electron density around HEM K 302:**

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



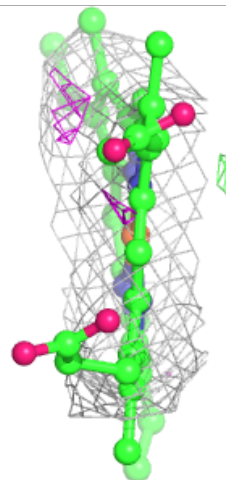
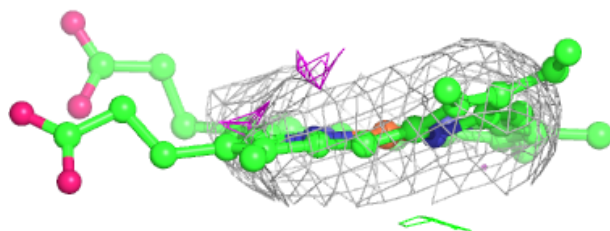
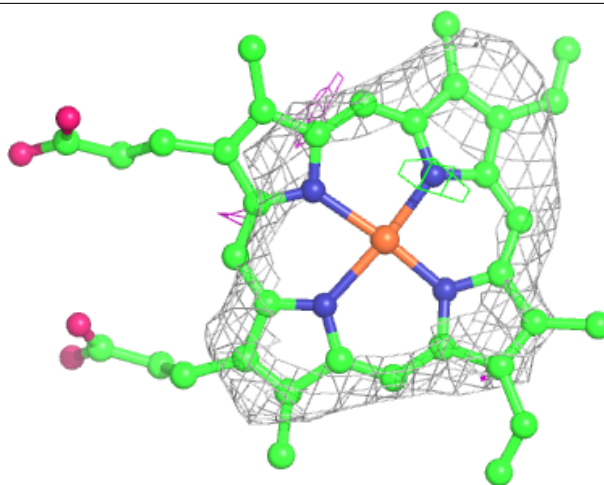
**Electron density around HEM O 302:**

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



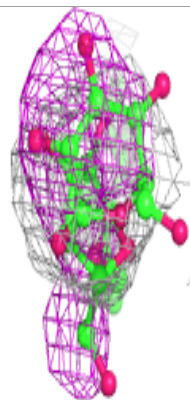
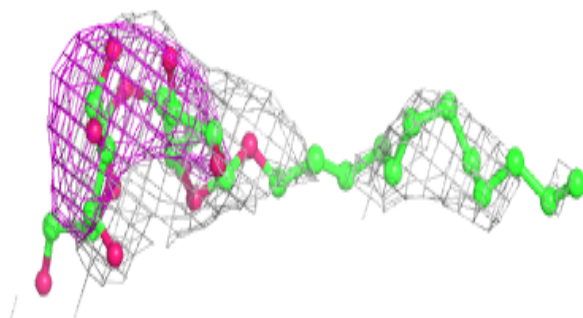
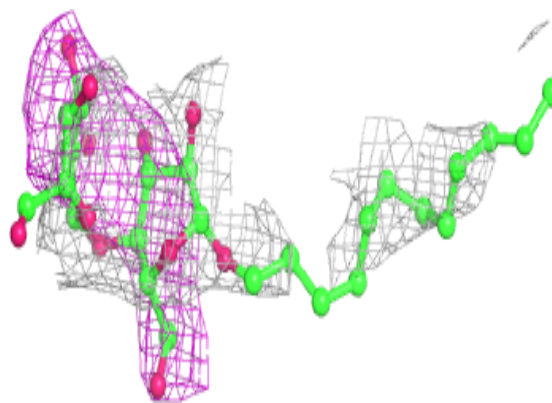
**Electron density around HEM O 303:**

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

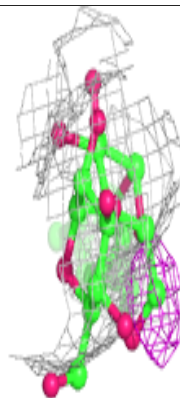
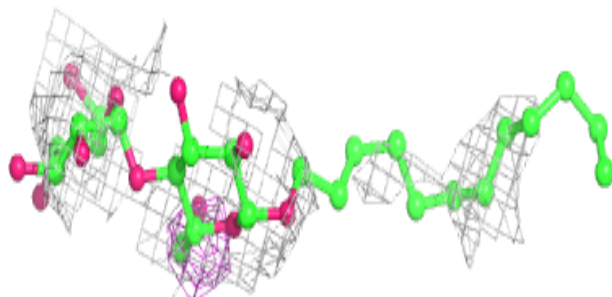
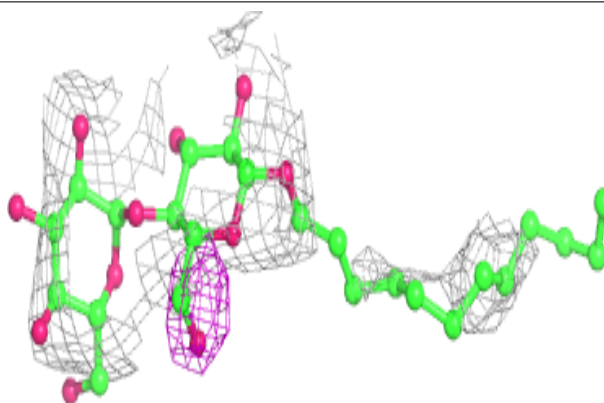


**Electron density around LMT C 303:**

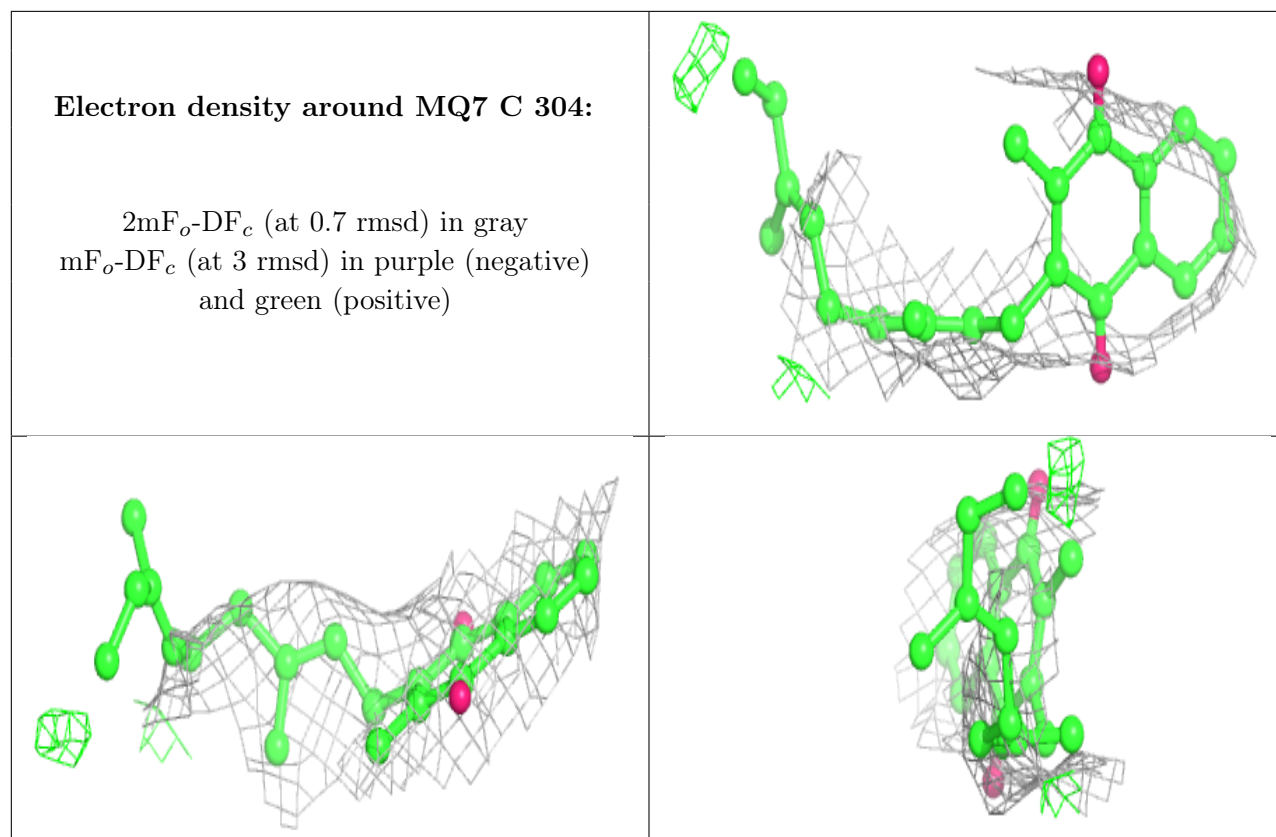
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around LMT O 301:**

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







## 6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.